Studying the role of selective gene set in Mycobacterium Tuberculosis metabolic pathway using flux balance analysis

A thesis submitted in partial fulfillment of the requirements
for the award of the degree of

Master of Technology
In
Computational and Systems Biology

Submitted By:
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CERTIFICATE

This is to certify that the thesis entitled "**Studying the role of selective gene set in Mycobacterium Tuberculosis metabolic pathway using flux balance analysis** " is an authentic record of the dissertation carried out by **Ashish Kumar Singh** at **School of Computational and Integrative Sciences** under my guidance and supervision. The contents of this project work, in full or in parts, have not been submitted elsewhere for award of any degree or diploma. The work fulfills the requirement for the award of the Master of Technology degree in Computational and Systems Biology.

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26 July 2012

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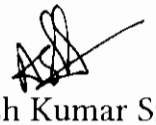
Declaration

*I hereby declare that the thesis titled "**Studying the role of selective gene set in Mycobacterium Tuberculosis metabolic pathway using flux balance analysis**" submitted by me for the partial fulfillment of the requirements for the degree of **Master of Technology** in **Computational & Systems Biology** in the **Center for Computational Biology & Bioinformatics, School of Computational & Integrative Sciences, Jawaharlal Nehru University**, is record of work carried out by me under the guidance of **Prof. Indira Ghosh**, and has not formed the basis for the award of any degree, diploma or fellowship in any other institution.*

I further declare that the research done under this dissertation is entirely original and the material obtained from other sources has been acknowledged in the thesis.

27 July 2012
Dated



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I would like to dedicate this thesis to my Guru, who's teachings always motivated me to keep going.....

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Chapter 1

Literature Survey on Systems Biology

1.1 Introduction:

Literature survey is the key to the works associated to any upcoming area. Literature survey is making list of documents available and then selection of them to serve the starting materials to do research in the area, papers on the selected topic which contains information, ideas, data and evidence written related to that particular topic. The available literature associated to the concerned topic explains the importance and the popularity of the of the topic, more the work done in that particular area explains more the urgency is related to the topic among researchers. How the literature survey evaluated for the effective investigation in relation to that topic provides researcher stepping stone to design future related work (*chris hart, 1998*). As Systems Biology is an emerging field and gained more popularity in the last decade, hence the trends in systems biology are needed for the further studies. Over the next 10 to 20 years, medicine will move toward predictive and preventive modes. New technologies will allow individuals to have the relevant portions of their genomes sequenced, and multi-parameter informative molecular diagnostics via blood analysis will become a routine procedure for assessing health and disease status (Leroy Hood, James R. Heath, Michael E. Phelps, Biaoyang Lin,2004). This study and analysis of literature associated to the areas of systems biology addresses previous works and the trends in this area. Here, in this work, main objective was searching the literature associated with systems biology through different (selective) searching methodologies for particular topics and analyze the results for the most worked topics in systems biology area. Here in the present work, three methodologies used for searching different topics. The different topics considered here are well known topics of systems biology and three different queries were based on year wise development of the field, application to disease and research tools/ methods developed in the area.

This literature survey consists of almost 29000 references from different topics of systems biology, hence it was difficult to manage large data (selection, searching and categorizing), and for making it easy to access, so an Intranet based website is developed as part of this study for content management of this enormous data. This will enable the updating and query required for sustaining of such literature survey.

1.2 Why Literature Survey?

Literature survey is the study and analysis of a topics associated literature to understand the development and direction for the initiation of the research in the topics and for the help of topic selection for future research. This literature survey done to understand the global view of trends in the systems biology and to come up with the popular and mostly worked out areas. Also this literature survey is one way to find out the areas which are ignored or less explored, hence expresses the need of more study and more work in that area. Another feature of this kind of study is to find the proper guidance and enough material to direct towards the further research work, hence the information produced and the conclusions drawn from the study provides suitable and better tuned and fine research work, more over this provides a good guidance to the new comer in the field.

Results form this survey indicates that a major area developed recently is Flux Balance Analysis as methodology , tools and scripts to use it, however the field has not been exploited enough in context to different disease to study, so required further work. Flux Balance Analysis (detailed in Chapter-2, chapter-3) chosen for research area as applied to pathogen *Mycobacterium tuberculosis*, a dreaded disease has not been eradicated since the human society begins , ancient mummies from Peru and Egypt are found to be infected by tuberculosis and the reason of death.

(http://ancienthistory.about.com/od/mummies/qt/TBinMummies.htm)

1.3 Objective:

The goal of this chapter is to collect and analyze the data accumulated, associated with literature, the different searching methodologies, what are the statistics and the growth in this field, as well as to gather information regarding the application of systems biology methods in context of understanding of disease.

1.4 Methodologies used for study:

In this study three types of queries used for collecting data, first was by year, in which last 21 year's references (1990-2010) are collected for the areas of systems biology and analysis is done on the literature growth rate in the field. Second query was set to collect the data on methods used, broadly seven systems biology related methods were initially focused for study ,like Flux Balance Analysis(FBA), Metabolic Control Analysis(MCA), Gene Networks, Phylogeny Method, Gene Silencing, Micro-array Data Analysis, Single Nucleotide Polymorphism (SNP). References by literature survey were collected for each of these methods. Third query was set to collect data on disease to which these methods are applied , eight major diseases were focused like Bacterial Disease, Viral Disease, Fungal Disease, Genetic Disease, Cancerous Disease, Cardiovascular Disease, Parasitic Disease, Respiratory Disease, and the references were collected from published literature on the application of systems biology method for understanding of each disease. Reason for choosing three different approaches is to find the differential perspective of literature data and its growth.

Collection by Year wise search:

Year wise searching methodology goes through published literature since year 1990 to year 2010. Here the queries done through each individual year. Data collection is done form NCBI-PUBMED (http://www.ncbi.nlm.nih.gov/pubmed)a comprehensive literature database. Here out of approximately 11700000 papers (since year1990-2010), only 21000 papers **(%)**found which were associated with systems biology. As expected, results from the search shows that, in 90's decade, there was less work been done comparable to next decade in this field (2670 systems biology papers found, between 1990-2000). From year 2000 on-words, there has been an exponential growth of work in this field (17704 systems biology papers found, between 2001-2010), which shows the growing importance of this field of research in Biology (appendix:Table1). Although databases of nucleic acid and amino-acid sequences are still the largest, most utilized, and best maintained databases,

there has been a demand and generation of databases to store other types of molecular data like interactions, patterns, reactions in pathways, enzyme cataloging, metabolic pathway networks etc. Such interest is primarily in response to demands placed by functional genomics and other emerging systems approaches (Trey Ideker, Timothy Galitski, Leroy Hood; 2001), availability of high throughput experiments generating large, better and diverse information are one of the basic reasons of growing popularity of this field.

Collection by Method wise search:

This searching methodology takes different approach for the survey, firstly seven methods (FBA, MCA, Gene Networks, Phylogeny Method, Gene Silencing, Micro-array Data Analysis, SNP,) related to systems biology were selected for searching and surveying. The selection of method was done on the basis of popularity of methods, judged by manual study and frequent use of it. The results for each individual method collected were compared with other method. Here in this methodology, queries done were syntactically based on the terms associated with each individual method. All data collection is done from the NCBI-PUBMED database (http://www.ncbi.nlm.nih.gov/pubmed). Here, size of method-wised data collection of all methods is 8850, which is lesser then the data-size of year-wise data collection.

Collection by Disease wise search:

A set of eight diseases (Bacterial, Viral, Fungal, Respiratory, Cardiovascular, Genetic, Cancerous and Parasitic Diseases) were focused and selected to search for Systems Biological application. Syntactic queries are done for each of these individual diseases. Results generated show the present scenario for all these eight disease in context of application of methods and reveals the more commonly used disease for application of systems biology approach among researchers. Database used for the data collection was the results of Year wise search (number of references are 21000). Total numbers of papers

found in this categorical search are 6548, which is very small part of the main year wise database.

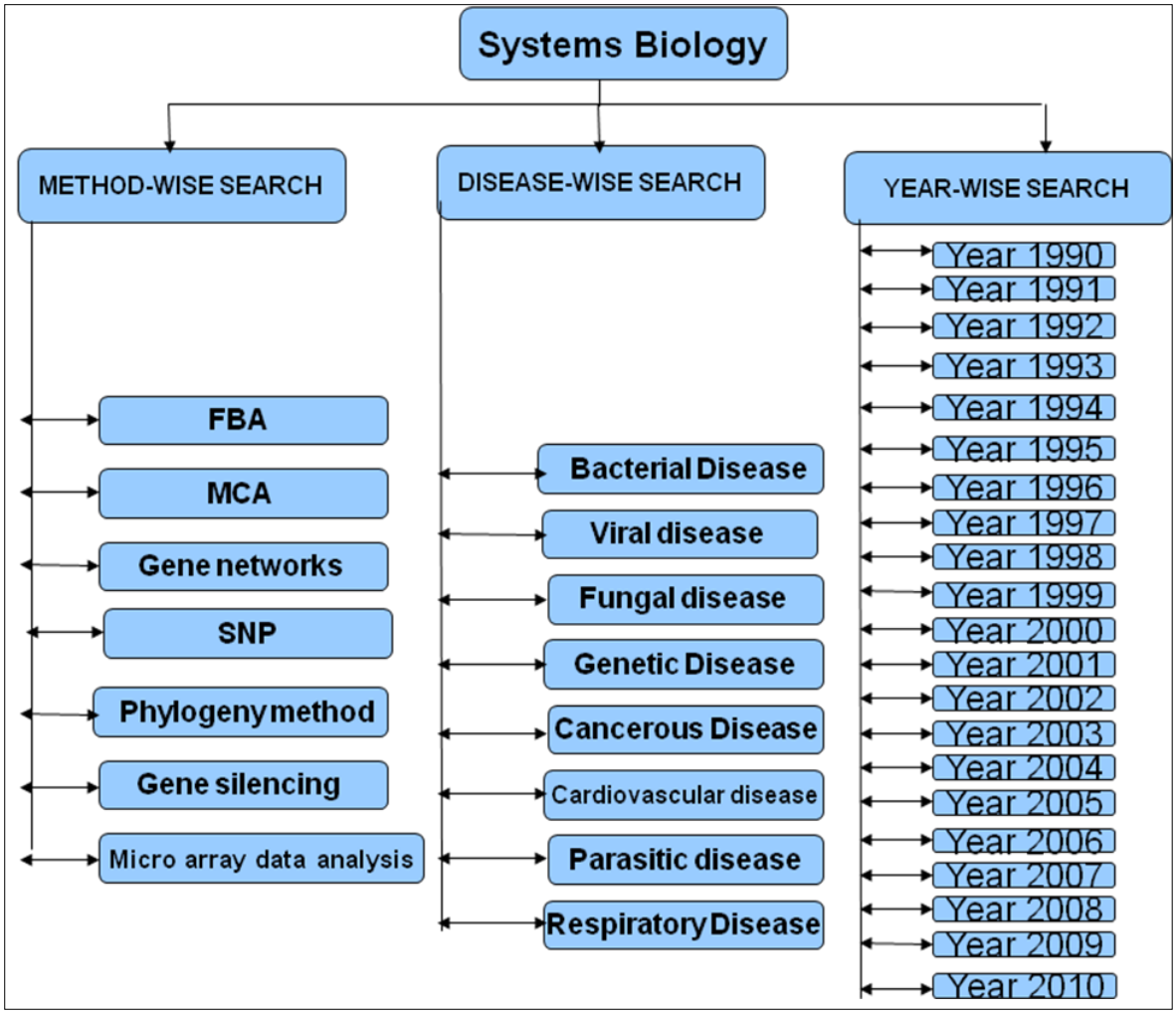


Fig-1 : Workflow of the literature survey.

Database Used for Collection:

Literature search refers to the process in which people use tools relevant to their individual needs (Zhiyong Lu , 2010). Though the literature is limited towards systems biology only, the data associated with it, is so enormous (approximately 20 millions bio-medical literature)that, searching for publications pertinent to a specific topic (e.g. a method or a disease) , or searching for the bibliographic information about a specific article need dedicated tools. For this purpose there are so many web based tools available (study of these tools is done by Zhiyoung Lu in 2010, *"PubMed and beyond: a survey of web tools for searching biomedical literature"*). List of these tools is available as table (Table 1) below.

In our study, NCBI-PUBMED database was the only one used for the searching. PubMed is a free Web literature search service developed and maintained by the National Center for Biotechnology Information (NCBI). Pubmed is service of the National Library of Medicine (http://www.nlm.nih.gov/) that provides access to over 17 million citations from MEDLINE and additional life sciences journals. PubMed includes links to many sites providing full text articles and other related resources.
Following facts supports its selection as database for searching.

- In PubMed, the size of the bibliome has grown exponentially over the past few years, as of 2010; there are over 20-million citations. So one of the biggest databases for biological data.
- PubMed is as part of NCBI's Entrez retrieval system that provides access to a diverse set of 38 databases.
- Currently, PubMed includes citations and abstracts from over 5000 life science journals for bio-medical articles back to 1948.
- Over one-third of PubMed queries result in 100 or more citations. So larger result generation is possible for each query.
- Availability of more filtering tool (date tuning, database tuning, type of article

tuning, species tuning etc.) makes search more precise and result more accurate while searching literature.

Table 1: There are many web tools available for searching bio-medical literature. Here 37 most popular among them are described in tabular format.

(Information source: **http://www.ncbi.nlm.nih.gov/CBBresearch/Lu/search/**)

Systems	Last Update (assessed on 08/23/10)	Service Provider Profile	Basic Information
RefMed	2010	Academic	Enabling multi-level relevance feedback for PubMed searches
iPubMed	Current	Academic	Supports fuzzy type-ahead searches
Quertle	2010		Relationship-driven search and supports searches with categorical concepts
MiSearch	Current	Academic	Ranks citations based on implicit user feedback
MedlineRanker	Current	Academic	Flexible ranking of biomedical literature
MScanner	2007	Academic	A classfier for retrieving Medline citations
Anne O'Tate	Current	Academic	Clustering by important words, topics, journals, authors, etc.
Medline.Cognition	8/6/2010	Private	Powered by Cognition's proprietary search technology
hakia	2010	Private	Part of the semantic search engine hakia.com
MedEvi	2010	Government	Providing textual evidence of semantic relations in output
EBIMed	2010	Government	Offers associations between protein/genes, GO annotations, drugs and species.
McSyBi	Current	Academic	Biomedical knowledge navigation by literature clustering
PICO	Current	Government	Using Patient, Intervention, Comparison, Outcome (PICO) framework for clinical questions

eTBLAST	2010	Academic	Finding documents similar to input text
PubGet	Current	Private	Retrieving results in PDFs
HubMed	Current	Private	Incorporating external web services for improving search efficiency
PubFocus	Current	Private	Semantic analytics through integration of controlled bio-dictionaries and ranking algorithm
BabelMeSH	2010	Government	a cross-language tool for MEDLINE/PubMed
MEDIE	12/10/2009	Academic	Extracting text fragments matching queried semantics
CiteXplore	Current	Government	EBI's tool for integrating biomedical literature and data
Twease	Current	Academic	Expands search queries and automatically discovers common abbreviations
PubNet	Current	Academic	A flexible system for visualizing literature derived networks
GoPubMed	Current	Private	Exploring PubMed with the Gene Ontology
askMEDLINE	2010	Government	This tool would translate a question into an efficient search
SLIM	Current	Government	Features interactive slider bars in the search form
ClusterMedTM	Current	Private	A demo service by Vivisimo
XplorMed	Current	Academic	Summarizing the subjects contained in the search results
PubCrawler	Current	Academic	Alerting users with new articles based on saved searches
MEDPILOT	2010	Government	A service provided by the Geman National Library of Medicine (ZB MED)
LigerCat	Current	Academic	Generating "MeSH Clouds" for exploring search results
BioMedLib	2010	Private	Does both keyword-based and meaning-based search
CISMeF	2006	Academic	Providing access to MEDLINE/PubMed

			using queries in French
Semantic MEDLINE	Current	Government	Summarizing and visualizing semantic relations extracted from literature
MARTINI	Current	Government	Searches literature and uses keywords to compare gene sets.
CAIPIRINI	Current	Academic	Uses gene sets and SVM to rank literature search results
BibliMed	Current	Private	Providing contextual help like MeSH terms organized by qualifiers
MEDSUM	Current	Academic	The MEDLINE summary tool

Query Selection:

Literature survey done here is based on syntactic searching of the literature, and hence queries are needed to search the appropriate literature. Queries done here only on titles and abstracts to achieve the accuracy of searches. Here queries are the words, phrases and statement, which are more frequently used in the literature, so that while doing queries we find the desired results. Though the possibilities of false positives are high, optimum query and combination query will help to minimize that, however the data needs to be verified after the validation process. This tuning of the queries made the results more accurate. For validation of the data accumulated, a random subset of data was repeatedly picked up and manually verified for each database (Detailed formulas for accuracy calculation is discussed later in this chapter). Average accuracy of results is around 85-90% percent, which itself explains the successful searches.

Queries for Year wise Search:

Here query done at NCBI-PUBMED for year-wise searching was *"(((systems biology methods) OR computational biology methods)) OR Bioinformatics"*, which get tuned by selecting the threshold publishing time for each individual year by putting the boundaries for each individual year. The query code generated at NCBI-

PUBMED website is as follows:

Table 2: List of query fields while searching year wise.

Year	Query
1990	((Systems[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract]) OR (Computational[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract]) OR (Bioinformatics[Title/Abstract]))AND ((Introductory Journal Article[ptyp] OR Journal Article[ptyp]) AND ("1990/01/01"[PDAT] : "1990/12/31"[PDAT]))
1991	((Systems[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract]) OR (Computational[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract])OR (Bioinformatics[Title/Abstract]))AND ((Introductory Journal Article[ptyp] OR Journal Article[ptyp]) AND ("1991/01/01"[PDAT] : "1991/12/31"[PDAT]))
1992	((Systems[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract]) OR (Computational[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract])OR (Bioinformatics[Title/Abstract]))AND ((Introductory Journal Article[ptyp] OR Journal Article[ptyp]) AND ("1992/01/01"[PDAT] : "1992/12/31"[PDAT]))
1993	((Systems[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract]) OR (Computational[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract]) OR (Bioinformatics[Title/Abstract]))AND ((Introductory Journal Article[ptyp] OR Journal Article[ptyp]) AND ("1993/01/01"[PDAT] : "1993/12/31"[PDAT]))
1994	((Systems[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract]) OR (Computational[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract]) OR (Bioinformatics[Title/Abstract]))AND ((Introductory Journal Article[ptyp] OR Journal Article[ptyp]) AND ("1994/01/01"[PDAT] : "1994/12/31"[PDAT]))
1995	((Systems[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract]) OR (Computational[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract]) OR (Bioinformatics[Title/Abstract]))AND ((Introductory Journal Article[ptyp] OR Journal Article[ptyp]) AND ("1995/01/01"[PDAT] : "1995/12/31"[PDAT]))
1996	((Systems[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract]) OR (Computational[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract]) OR

Year	Query
	(Bioinformatics[Title/Abstract]))AND ((Introductory Journal Article[ptyp] OR Journal Article[ptyp]) AND ("1996/01/01"[PDAT] : "1996/12/31"[PDAT]))
1997	((Systems[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract]) OR (Computational[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract]) OR (Bioinformatics[Title/Abstract]))AND ((Introductory Journal Article[ptyp] OR Journal Article[ptyp]) AND ("1997/01/01"[PDAT] : "1997/12/31"[PDAT]))
1998	((Systems[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract]) OR (Computational[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract]) OR (Bioinformatics[Title/Abstract]))AND ((Introductory Journal Article[ptyp] OR Journal Article[ptyp]) AND ("1998/01/01"[PDAT] : "1998/12/31"[PDAT]))
1999	((Systems[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract]) OR (Computational[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract]) OR (Bioinformatics[Title/Abstract]))AND ((Introductory Journal Article[ptyp] OR Journal Article[ptyp]) AND ("1999/01/01"[PDAT] : "1999/12/31"[PDAT]))
2000	((Systems[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract]) OR (Computational[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract]) OR (Bioinformatics[Title/Abstract]))AND ((Introductory Journal Article[ptyp] OR Journal Article[ptyp]) AND ("2000/01/01"[PDAT] : "2000/12/31"[PDAT]))
2001	((Systems[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract]) OR (Computational[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract])OR (Bioinformatics[Title/Abstract]))AND ((Introductory Journal Article[ptyp] OR Journal Article[ptyp]) AND ("2001/01/01"[PDAT] : "2001/12/31"[PDAT]))
2002	((Systems[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract]) OR (Computational[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract])OR (Bioinformatics[Title/Abstract]))AND ((Introductory Journal Article[ptyp] OR Journal Article[ptyp]) AND ("2002/01/01"[PDAT] : "2002/12/31"[PDAT]))
2003	((Systems[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract]) OR (Computational[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract])OR (Bioinformatics[Title/Abstract]))AND ((Introductory Journal Article[ptyp] OR Journal Article[ptyp]) AND ("2003/01/01"[PDAT] : "2003/12/31"[PDAT]))

Year	Query
2004	((Systems[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract]) OR (Computational[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract]) OR (Bioinformatics[Title/Abstract]))AND ((Introductory Journal Article[ptyp] OR Journal Article[ptyp]) AND ("2004/01/01"[PDAT] : "2004/12/31"[PDAT]))
2005	((Systems[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract]) OR (Computational[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract]) OR (Bioinformatics[Title/Abstract]))AND ((Introductory Journal Article[ptyp] OR Journal Article[ptyp]) AND ("2005/01/01"[PDAT] : "2005/12/31"[PDAT]))
2006	((Systems[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract]) OR (Computational[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract]) OR (Bioinformatics[Title/Abstract]))AND ((Introductory Journal Article[ptyp] OR Journal Article[ptyp]) AND ("2006/01/01"[PDAT] : "2006/12/31"[PDAT]))
2007	((Systems[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract]) OR (Computational[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract])OR (Bioinformatics[Title/Abstract]))AND ((Introductory Journal Article[ptyp] OR Journal Article[ptyp]) AND ("2007/01/01"[PDAT] : "2007/12/31"[PDAT]))
2008	((Systems[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract]) OR (Computational[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract])OR (Bioinformatics[Title/Abstract]))AND ((Introductory Journal Article[ptyp] OR Journal Article[ptyp]) AND ("2008/01/01"[PDAT] : "2008/12/31"[PDAT]))
2009	((Systems[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract]) OR (Computational[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract])OR (Bioinformatics[Title/Abstract]))AND ((Introductory Journal Article[ptyp] OR Journal Article[ptyp]) AND ("2009/01/01"[PDAT] : "2009/12/31"[PDAT]))
2010	((Systems[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract]) OR (Computational[Title/Abstract] AND Biology[Title/Abstract] AND method[Title/Abstract]) OR (Bioinformatics[Title/Abstract]))AND ((Introductory Journal Article[ptyp] OR Journal Article[ptyp]) AND ("2010/01/01"[PDAT] : "2010/12/31"[PDAT]))

Queries for Method wise Search:

In this method wise search, again the search is done on the database PUBMED,the results generated is further validated by sensitivity calculation (% Sensitivity = [True Positive / (True Positive + False negative)]* 100) of randomly selected samples sets of size 20. Method wise queries done on the basis of key words , which frequently occurs in the method which searched (again it is a syntactic searching). These key words itself can match to the full name of the method, or it's short form like for example, Flux Balance Analysis, key word can be FBA or Flux Balance Analysis itself.

Here in the table 3, query generated at PUBMED at time of searching is also included as follows:

Table 3 : List of query & keywords used while disease wise search

Method	**Key words**	**Query generated at PUBMED**
Flux balance analysis	*Flux balance Analysis, FBA*	(flux[Title/Abstract] AND balance[Title/Abstract] AND analysis[Title/Abstract]) AND ((Introductory Journal Article[ptyp] OR Journal Article[ptyp]) AND ("1990/01/01"[PDAT] : "2010/12/31"[PDAT]))
Metabolic control analysis	*Metabolic control analysis, MCA*	(Metabolic[Title] AND control[Title] AND analysis[Title]) AND ((Introductory Journal Article[ptyp] OR Journal Article[ptyp]) AND ("1990/01/01"[PDAT] : "2010/12/31"[PDAT]))
Gene networks	*Gene Network*	(gene[Title] AND networks[Title]) AND ((Introductory Journal Article[ptyp] OR Journal Article[ptyp]) AND English[lang] AND medline[sb] AND ("1990/01/01"[PDAT] : "2010/12/31"[PDAT]))
Phylogeny method	*Phylogeny*	phylogeny[Title] AND ((Introductory Journal Article[ptyp] OR Journal Article[ptyp]) AND ("1990/01/01"[PDAT] :

		"2010/12/31"[PDAT]))
Gene silencing	*Gene silencing*	(Gene[Title] AND silencing[Title]) AND ((Introductory Journal Article[ptyp] OR Journal Article[ptyp]) AND ("1990/01/01"[PDAT] : "2010/12/31"[PDAT]))
Microarray data analysis	*microarray*	microarray[Title] AND ((Introductory Journal Article[ptyp] OR Journal Article[ptyp]) AND ("1990/01/01"[PDAT] : "2010/12/31"[PDAT]))
SNP	*SNP, Single nucleotide polymorphism*	(single[Title] AND nucleotide[Title] AND polymorphism[Title]) OR SNP[Title] AND ((Introductory Journal Article[ptyp] OR Journal Article[ptyp]) AND ("1990/01/01"[PDAT] : "2010/12/31"[PDAT]))

Queries for Disease wise Search:

In Disease wise searching, different approach was taken, here query done locally on the results generated after year wise searching instead of using the main Database. Using PERL programming for pattern match (see appendix for the PERL code), queries generated were mainly the terms and words which were associated to the disease for which the search done. For example, in parasitic disease, terms used are typhus, giardia, roundworm, toxoplasmosis, scabies etc., which are common diseases comes under this parasitic disease category. It is to be noted that a full context based /ontology based query formation (medical ontology: Semantic spaces that can be defined from the semantic information that is provided by existing terminologies, knowledge bases, expert systems, or extracted from the medical literature) would have provided us a comprehensive result, as we have used a limited database (database of Year-wise search, of size around 21000 papers) so a manual verification was possible.

Table 4 shows the Keywords for the query generation in disease wise search is as follows:

Disease	**Keywords**
Bacterial disease	*Bactria, Mycobacterium, tuberculosis*
Viral disease	*Virus, viral, HIV*
Fungal disease	*Fungus, fungal*
Genetic diseases	*Genetic disease, Cystic fibrosis, Down syndrome, Duchene muscular dystrophy, neurofibromatosis, sickle-cell disease, Polycystic kidney disease.*
Cancerous disease	*Cancer*
Cardiovascular disease	*Cardiac, hypertension*
Parasitic disease	*Parasitic, typhus, giardia ,roundworm, toxoplasmosis, scabies*
Respiratory disease	*Asthma, respiratory, lung disease*

All the data generated using **NCBI-PUBMED database** using proper keywords, Pubmed itself generated the queries for searching. **PERL Programming** language was used for querying, searching and counting locally the Database created by the results. For the statistical analysis and validation work **R-Programming** was used in addition to **Matlab**, **Microsoft-office-excel** and a web based statistical tool **ReaderFit** (Online Curve Fitting Tool, http://www.readerfit.com/) for plotting results.

Three basic steps followed for this literature survey, *first*: Data collection (by searching in Pubmed database), *Second*: Result Validation, *Third*: Result analysis.

Steps followed by each of the three methodologies for searching are as follows:

Year wise search

All data collected from the website NCBI-PUBMED. Following steps are done:

1. Go to the website http://www.ncbi.nlm.nih.gov/pubmed.
2. Put the year wise limit on the publication date on the search(e.g. For year 2010, Limits Activated will be: Publication Date from "2010/01/01 to 2010/12/31")
3. Do the query:
4. **"**(((systems biology methods) OR computational biology methods)) OR Bioinformatics**"**
5. Send the search result to file (i.e. collection of abstracts, summery, PMIDs)
6. Repeat the step 3 and 4 for all years since 1990 to year 2010, to find the individual year results.

Method wise search

All data collected from the website NCBI-PUBMED. Following steps are done:

1. Browsed the website http://www.ncbi.nlm.nih.gov/pubmed.

2. Advance search, by selecting search option "***Advanced***", by putting the following limits and followed the steps :

- Put time limit on the publication date on the search. Publication Date from "**1990/01/01 to 2010/12/31**")
- Put the database limit only to **MEDLINE.**
- Select language as "**English".**
- Limit the search area only to "**Title"**.

3. Has done the following query :

"(((**METHOD_KEYWORD1**) OR **METHOD_KEYWORD2**)) OR **METHOD_KEYWORD3"** *(Note: keword2 and keyword3 are optional)*

4. Sent the search result to file (i.e. of abstracts, summery, PMIDs)

5. Repeated the step 3 and 4 for all for all methods to find the individual year results

Disease wise search

Steps to search by Disease:

1. Merged all individual year's hit list of abstracts (since1990 to 2010) to create the complete database of abstracts since 1990 to 2010.
2. Did disease wise search by checking **Keywords** in the database.
3. (all the search done using PERL Programming)
4. After search, extracted the PMIDs from the abstract of papers in hit list.

1.5 Web-Development for literature survey

A website is a set of related web pages containing content including text, video, image, graphs, audio, which are created for the purpose of sharing the information in well organized and easy manner. As well as a web-interface provides the easy ways to remote access of all the data web-developer want to share.

1.5.1 Objective:

Results generated after the literature search is so enormous (29000 papers aprox.), that to search for a particular paper or finding literature according to need, or managing all this big data set required proper content management tool. For the purpose there are software available like Mendeley (http://www.mendeley.com/). But as these software are not freely available so an intra-net based website has been developed as a part of fulfillment of this survey. However it is worth to use Mendlay in future to organize the database and access the PDF /abstract files wherever available.

1.5.2 Methods & Software for website development:

Here LAMP technology was used for the web development, in which all the component

included are open sources.

What is an "Open Source"?:

1. Open-Source refers to software that is not only free, but includes the source codes as well .
2. Users are free to make whatever modifications they like to make the software work better for them.
3. Users are generally encouraged to submit improvements for inclusion in the master distribution.

LAMP Technology:

L.A.M.P.= LINUX + APACHE + MYSQL + PHP

(1)Linux:

Fedora operating system on Linux platform to work on. It is an Open source, freely available Linux is a UNIX-like operating system that is designed to provide personal computer users a free or very low-cost operating system comparable to traditional and usually more expensive Unix systems. Linux has a reputation as a very efficient and fast-performing system.

(2)Apache:

Apache is a public domain Web server developed by a loosely knit group of programmers. Public domain refers to any program that is not copyrighted. Public-domain software is free and can be used without restrictions. As a result of its sophisticated features, excellent performance, and low price- free, Apache has become the world's most popular Web server. The Apache httpd server is a powerful, flexible, HTTP/2.2.21 compliant web server. It implements the latest protocols, including HTTP/2.2.21 (RFC2616) and is highly configurable and extensible with third-party modules. It can be customized by writing 'modules' using the Apache module API provides full source code and comes with an unrestricted license runs on Windows NT/9x, Netware 5.x and above, OS/2, and most versions of Unix, as well as several other operating systems.

(3)Mysql:

A database is a structured collection of data. It may be anything from a simple shopping list to a picture gallery or the vast amounts of information in a corporate network. To add, access, and process data stored in a computer database, a database management system is needed. So for the purpose MYSQL is used. MySQL is a open-source relational database management system (RDBMS) that runs as a server providing multi-user access to a number of databases.

1. MySQL is released under an open-source license. So it is freely available.
2. MySQL is a very powerful program in its own right. It handles a large subset of the functionality of the most expensive and powerful database packages.
3. MySQL uses a standard form of the well-known SQL data language.
4. MySQL works on many operating systems and with many languages including PHP, PERL, C, C++, JAVA etc.
5. MySQL works very quickly and works well even with large data sets.
6. MySQL is very friendly to PHP, the most appreciated language for web development.
7. MySQL supports large databases, up to 50 million rows or more in a table. The default file size limit for a table is 4GB, but it can be increased up to (if your operating system can handle it) a theoretical limit of 8 million terabytes (TB).
8. MySQL is customizable. The open source GPL license allows programmers to modify the MySQL software to fit their own specific environments.

(4)PHP:

PHP stands for **H**ypertext **P**reprocessor. PHP is a general-purpose server-side scripting language originally designed for web development to produce dynamic web pages. It is among one of the first developed server-side scripting languages that is embedded into a HTML source document, rather than calling an external file to process data. Ultimately, the code is interpreted by a web server with a PHP processor module which generates the

resulting web page. It also has evolved to include a command-line interface capability and can be used in standalone graphical applications. PHP can be deployed on most web servers and also as a standalone shell on almost every operating system and platform free of charge.

Outlines of PHP:

1. PHP is a server-side scripting language, like ASP.
2. PHP scripts are executed on the server.
3. PHP supports many databases (MySQL, Informix, Oracle, Sybase, Solid, PostgreSQL, Generic ODBC, etc.)
4. PHP is open source software.
5. PHP is free to download and use.

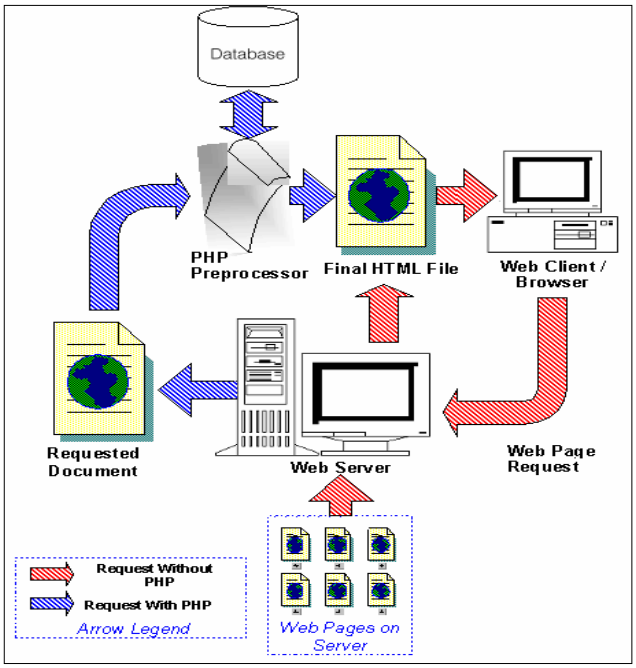


Fig 2: Work flow of PHP

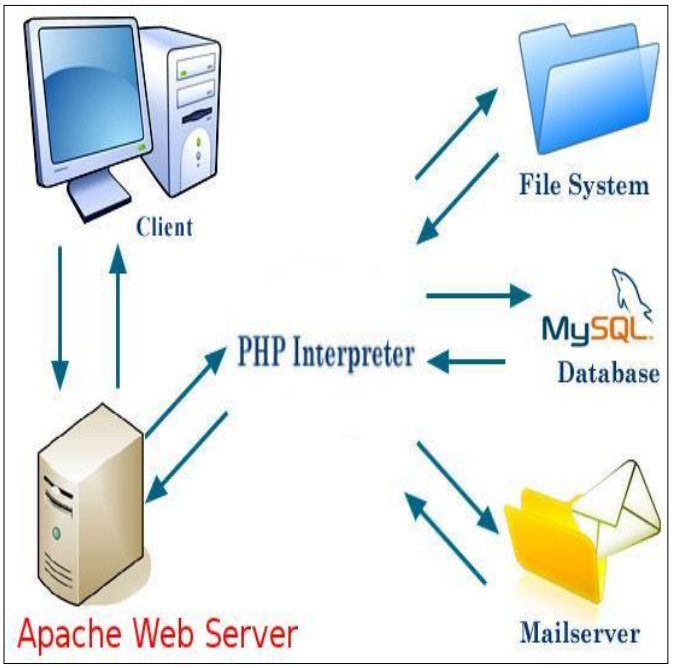


Fig-3: LAMP Architecture

1.5.3 Website properties:

Following are the properties of this website.

Home page (http://172.16.4.140/litrature_survey.html)

Home page contains the basic definitions of systems biology as well as it explains the objective of literature survey done here. Also it explains the work flow of this literature survey through a data flow diagram. After this basic information, this home page has three hyperlinks for three methodologies, Year-wise Search, Method-wise Search Disease-wise search.

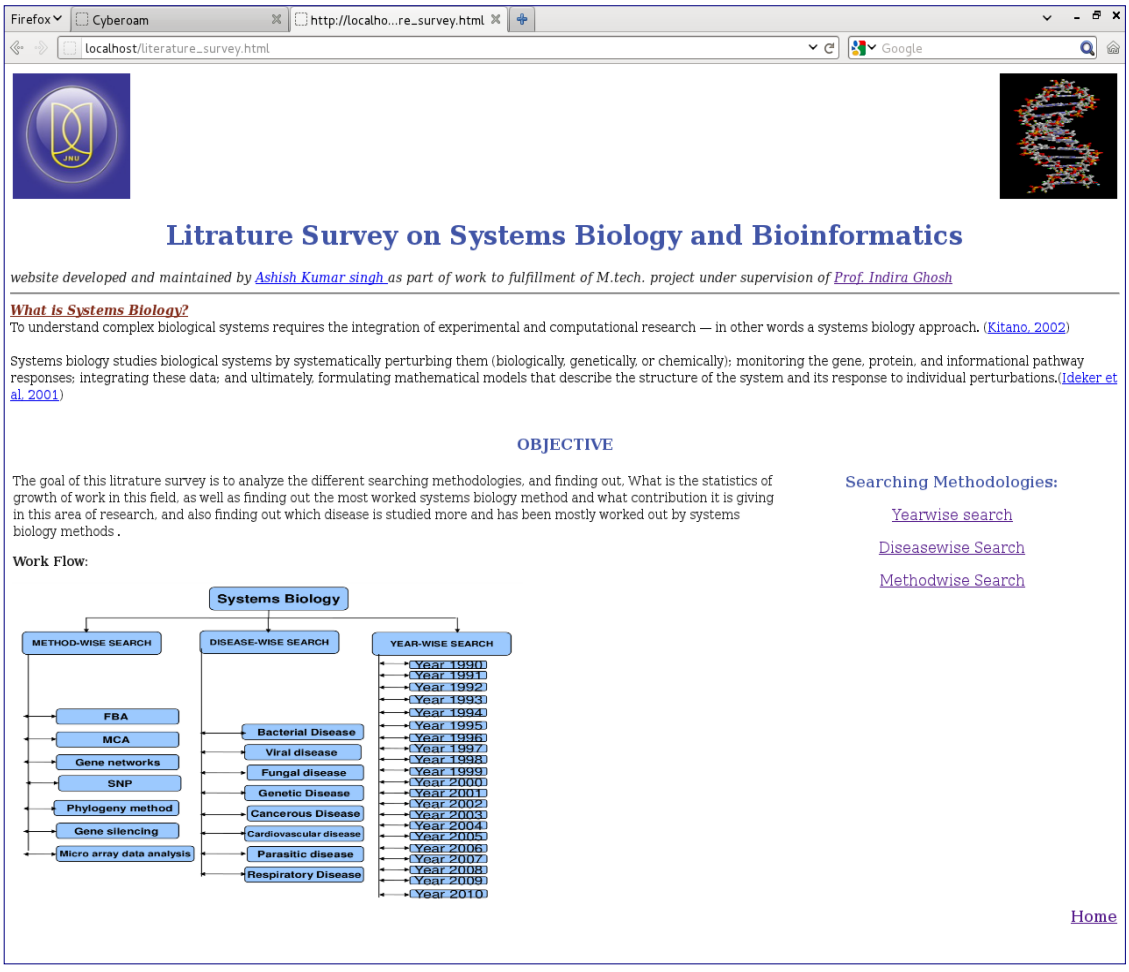


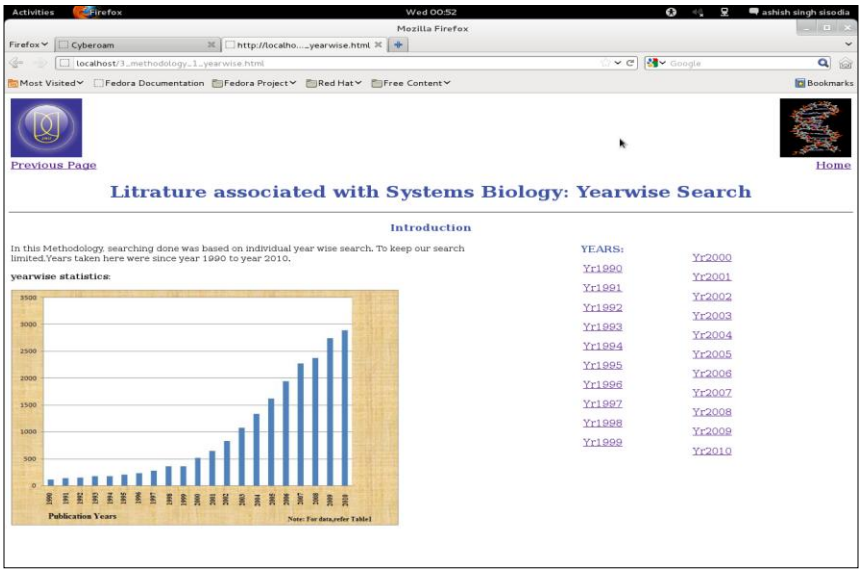
Fig-4 Webpage: Home

Searching Methodology's Pages for each Database:

(a) Year-wise search page:(http://172.16.4.140/3_methodology_1_yearwise.html)

This page contains the results and statistics generated after year-wise search. In this page a graphical representation of year wise contribution of literature can be seen, which displays the literature growth rate in work in the area of systems biology. This page contains 21 hyperlinks for each individual year from year 1990 to year 2010, these hyperlinks will leads towards the search result for each individual year.

Fig-5 Web page for Individual Years



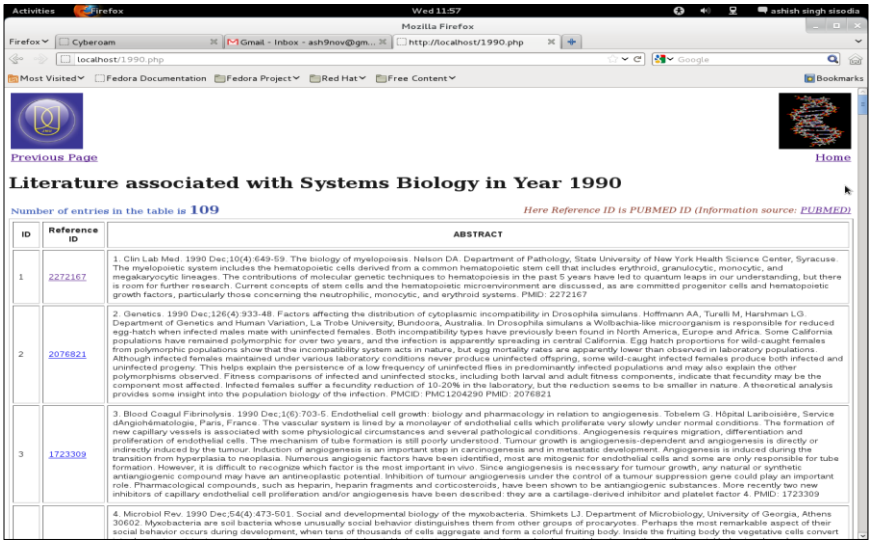


Fig-6 Literature page for Year 1990: (http://172.16.4.140/1990.php)

This web page (Figure-6) illustrates each individual hit in year 1990 in a tabular form. In the table first column is for PMIDs, which are hyperlink to the pubmed web page for that paper, second column contains the abstract with respect to that PMID. Here PMIDs are the unique IDs, as well as this web page tell about the number of hits in this selected year.

(b) Method-wise Search page: (http://172.16.4.140/3_methodology_2_methodwise.html)
This page contains the statistics of contribution of each method as a pie-chart,as well as it contains the 7 hyperlink for each method, these hyperlinks will leads towards the search result for each individual method.

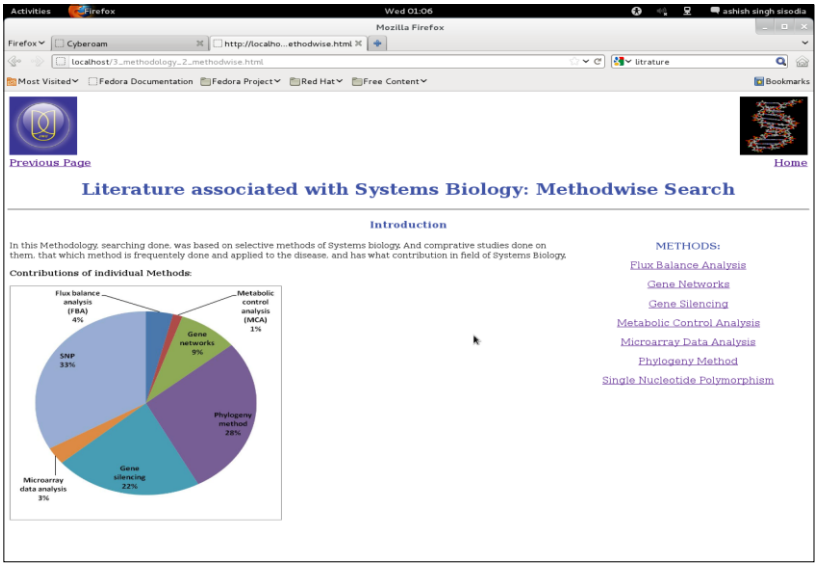


Figure-7
Method-wise search

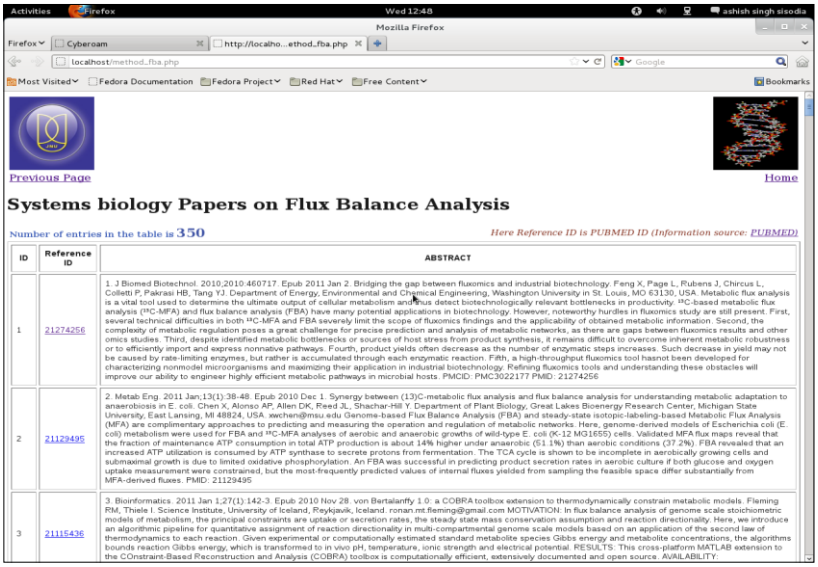


Fig-8
Web page for Flux Balance Analysis

Web page for Individual method: (http://172.16.4.140/method_fba.php/)

This web page (figure 8) illustrates each individual hit in this method in a tabular form. In the table first column is for PMIDs, which are hyperlink to the pubmed web page for that paper, second column contains the abstract with respect to that PMID. Here PMIDs are the unique IDs, this web page tells about the number of hits obtained by selected method.

(C) Disease-wise Search page: http://172.16.4.140/3_methodology_3_diseasewise.html

This page contains the statistics of contribution of each disease as a pie-chart same like in method page, it contains the 8 hyperlink for each disease, and these hyperlinks will leads towards the search result for each individual disease.

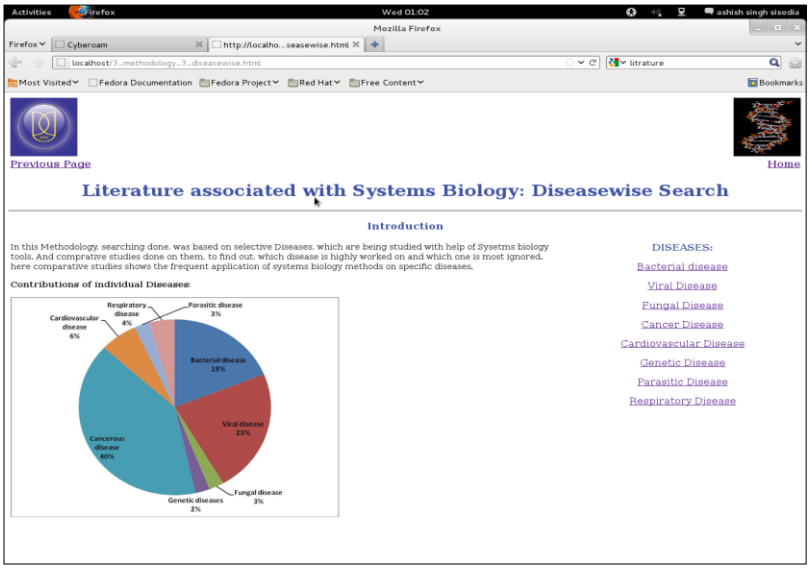


Figure 9

Disease-wise search

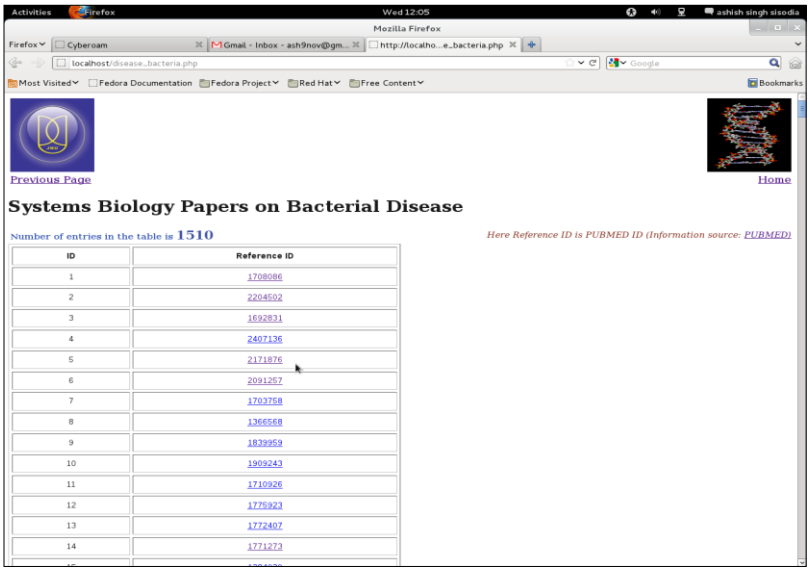


Fig10

Web page for Bacterial Disease

Web page for Individual Disease (http://172.16.4.140/disease_bacteria.php/)

This web page illustrates each individual hit in the selected disease in a tabular form. In the table first column is for serial number and second column contains the PMIDs, which are hyperlink to the pubmed web page for that paper, this web page tell about the number of hits occurs related to the selected disease.

1.6 Results & Discussions:

(A) Results for Year-wise Search:

After following the steps described earlier for year-wise search, results generated are as follows:

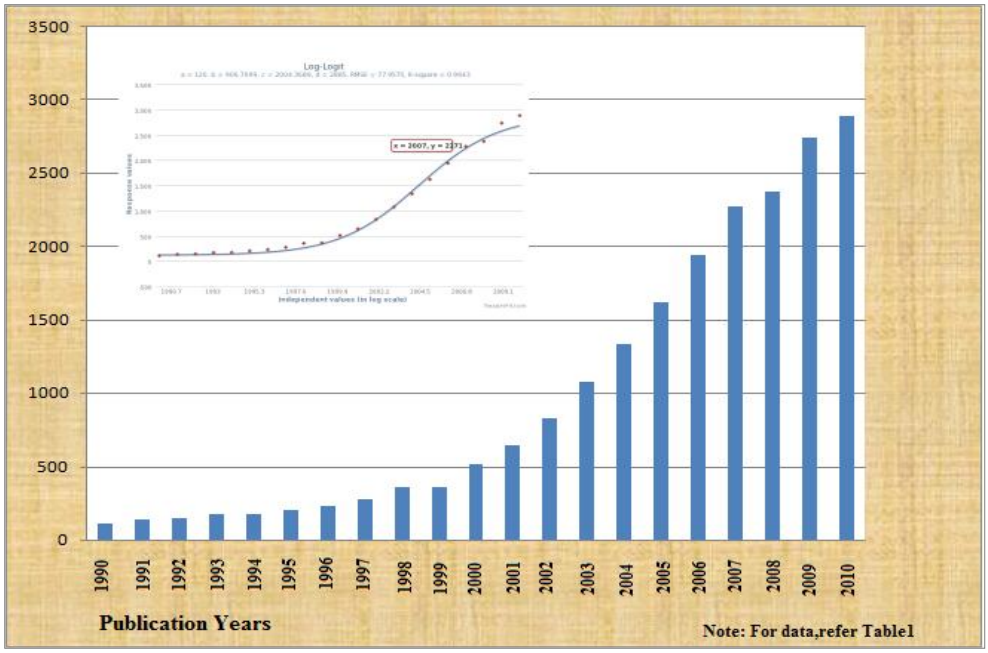


Fig-11: This plot indicates a steady growth of publications in the field of systems biology and it grows exponentially after year 2000.

Discussions:

Systems biology approach most likely first was used in 1952 by Nobel laureates, Alan Lloyd Hodgkin and Andrew Fielding Huxley to build mathematical model to explain

action potential propagating through axon of a neuron cell. However not much progress happened till 1970 when quantitative methods flourished in Biochemistry and enzyme kinetics started 1900 explored in1990. The other group related to this field was working on mathematical modeling of population growth, control systems etc. However the efflux of biologically relevant literature came out due to the advent of the progress in molecular biology, genomics and functional proteomics during 1990. Hence here we have considered the literature survey since 1990 onward.

This searching result shows that, in 90's decade, there was less work published as comparable to next decade in field of application of Systems Biology to disease. From year 2000 and on-words, there has been an exponential growth (verified by curve-fitting) in this field.

(B) Results for Method-wise Search:

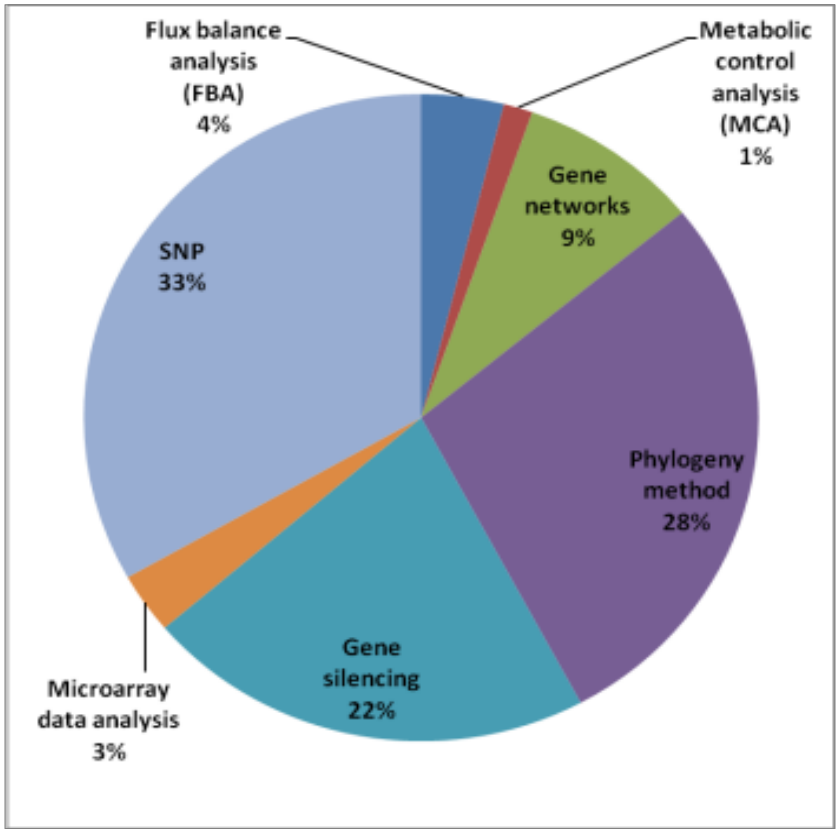
After following the steps described earlier for method-wise search, results generated are shown in the table 5 & figure-12 as follows:

This data consist of literature belong to only eight diseases.

Table 5:

Method	**Number of hits**
Flux balance analysis (FBA)	**350**
Metabolic control analysis (MCA)	**123**
Gene networks	**773**
Phylogeny method	**2485**
Gene silencing	**1911**
Microarray data analysis	**269**
SNP	**2939**
TOTAL	***8850***

Figure- 12



Discussions:

Here total number of hits are only 8850, that is only 43.5% approximately of the total search space (i.e. All papers since 1990 to 2010 found in year wise search). This is due to the fact that here only selected seven methods are taken in to consideration out of so many other methods(e.g. Sequence alignment, genome assembly, genome-wide association studies, structure prediction, pattern recognition, High-throughput image analysis, kinetic Modeling, Transcriptomics, Metabolomics, Proteomics, genomics etc.). In addition to this here only analytical/theoretical methods involved or developed are included, but literature search space contains many experimental methods(e.g. mass spectrometry, DNA sequencing NMR, Structure prediction, Protein purification, Gel electrophoresis, Microscopy and imaging, Flow cytometry, Metagenomic RNA profiling, X-ray crystallography, etc.) .

(C) Results for Disease-wise Search:

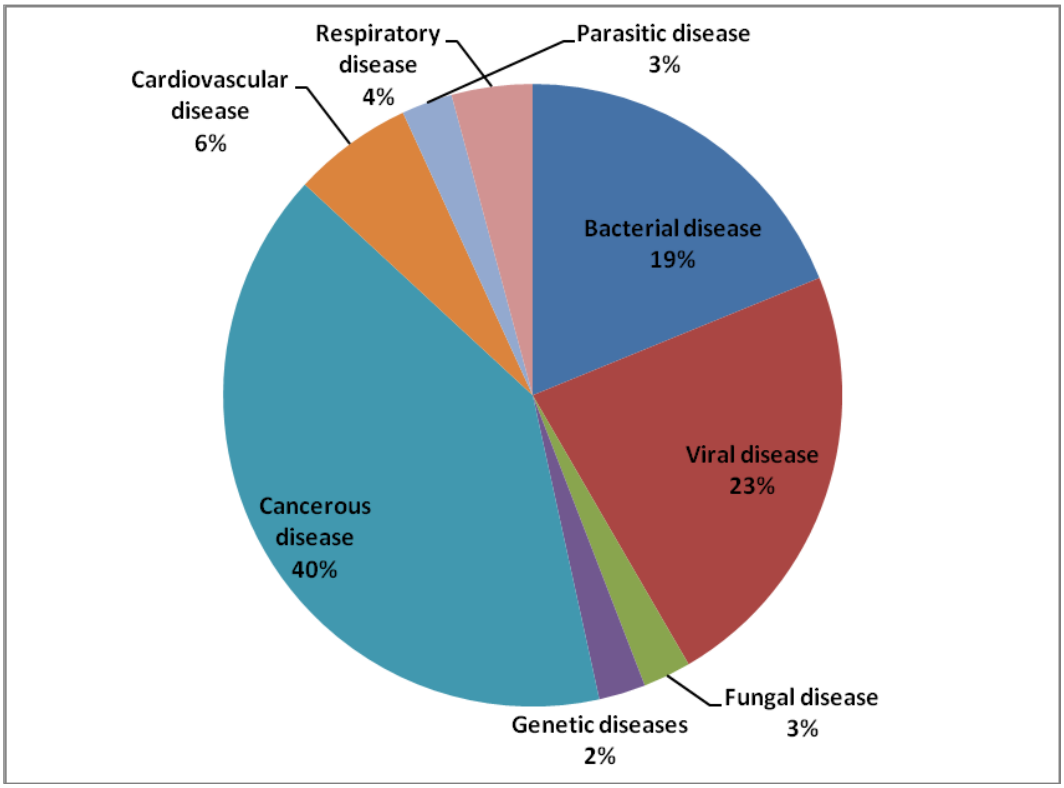
This method yielded limited hits as the query search was done on the literature collected by year wise method mentioned above. Each cases systems biology approach has been verified by using abstract search/ title survey.

Table 6 & Fig-13 shows the list of disease wise data available in literature.

Table-6:

Disease	**No. of hits**
Bacterial disease	**1234**
Viral disease	**1490**
Fungal disease	**164**
Genetic diseases	**160**
Cancerous disease	**2638**
Cardiovascular disease	**411**
Parasitic disease	**174**
Respiratory disease	**277**
TOTAL	**6548**

Figure-13



Discussion:

Search has been done here locally in the result set of Year-wise searching methodology; understanding of disease have been pursued using reductionist approach earlier, whereas these references contain the holistic approach to build model of disease or providing clues to identify the target genes or causative reason for disease while considering the whole system. When it is searched globally (on PUBMED website), many additional hits that does not belong to field of systems biology appeared (e.g. Traditional methods, wet lab methods etc) that will contribute to more false positive and reduce the impact of searching result, hence only the database developed using Year-wise was used. Here total numbers of hits are only 6548 out of complete data set (Year-wise search results 20374), only 32% approximately of the total search space from year-wise searches. Reasons behind this result are, first here only diseases are taken in to consideration for search, other topics (e.g. aquatic research, ecological research, earth science, agricultural research, plant research

etc.) are not considered, second reason is that out of so many diseases, only eight diseases are taken in to account for the present study. If we do more narrow searches (like, application to cures of disease), then this figure (32%) will become more limited. However, the study provides a good starting point and comprehensive approach to continue and focus our research area. In addition one can learn many techniques as applied to other related diseases, which provides a scope of horizontal study in this area.

Validation of Results:

Validation of result is done by using the binary classification. Binary classification is the task of classifying the members of a given set of objects into two groups on the basis of whether they have some property or not. In this binary classification, sensitivity calculation performed. Sensitivity is the statistical measures of the performance of a binary classification test. Sensitivity measures the proportion of actual positives which are correctly identified as such (e.g. the percentage of FBA abstracts who are correctly identified in the FBA method result set). Formula for sensitivity calculation is as follows:

% Sensitivity = [True Positive / (True Positive + False negative)]* 100

Where,

True positive: FBA abstracts correctly identified in FBA result set. (FBA example taken)

False negative: Abstracts which are not associated to FBA, incorrectly identified in FBA result set. (FBA example taken)

Steps:

1. Randomly pick 20 abstracts form the particular class (e.g. from any disease or from any method).(Here random selection done with help of R-programming, and input parameters are the unique Pubmed IDs).
2. Check manually each of the 20 abstracts from this randomly chosen set of abstracts, whether these belong to that particular class or not.
3. Calculate the percentage sensitivity for each sample by applying the formula

4. % Sensitivity = [True Positive / (True Positive + False negative)]* 100
5. Repeat the step**1-3** for at least 6 samples.

6. Calculate the final average %Sensitivity by taking average of %sensitivity of each sample.

Validation of method-wise Search results:

In method-wise searching, Sensitivity calculation done for the % correctness of results.

% Sensitivity = [True Positive / (True Positive + False negative)]* 100

Table 7 shows correctness using sample size taken for each trial was 20.

Method name	**Average % sensitivity**
Flux balance analysis (FBA)	74.4%
Metabolic control analysis (MCA)	94%
Gene Networks	81%
Phylogeny method	81%
Gene silencing	100%
Microarray data analysis	100%
SNP	90%

Discussion:

Here in most of the methods, the percentage sensitivity is less than %100 , which is because the search done by text search (no semantics has been used), so many times hits contains the paper those publishing topics emphasizing on some other topic but the "query" text is cited as an example hence such papers are not directly relevant to our query.(e.g. flux balance analysis search space gets hit from paper which talks about the metabolic control analysis, and is taking example of methods working on SBML data, so gets repeated hit for FBA. etc.) As it is observed from the table that such repeated hit do not occur in Gene silencing & microarray data analysis as mostly these papers based on experimental results and distantly related to biochemical pathways also are not cross-

refereed. As well as some of the errors generated due to right query, but different meanings of query generating different result. As example in FBA set an abstract hit is “Glycolytic and non-glycolytic functions of Mycobacterium tuberculosis fructose-1,6-bisphosphate aldolase, an essential enzyme produced by replicating and non-replicating bacilli”
(de la Paz Santangelo M, Gest PM, Guerin ME, Coinçon M, Pham H, Ryan G, Puckett SE, Spencer JS, Gonzalez-Juarrero M, Daher R, Lenaerts AJ, Schnappinger D, Therisod M, Ehrt S, Sygusch J, Jackson M). here fructose-1,6-bisphosphate aldolase is called as FBA in short form, and while doing queries for Flux Balance Analysis, the query “*FBA”* wrongly hit by this paper, which is a false hit.

Validation of Disease-wise Search results:

In disease-wise searching, Sensitivity calculation done for the % correctness of results.
% Sensitivity = [True Positive / (True Positive + False negative)]* 100
Here sample size taken for each trial was 20.
Table 8 shows correctness using sample size taken for each trial was 20.

Disease name	**Average % sensitivity**
Bacterial disease	83%
Viral disease	85%
Fungal disease	75%
Genetic diseases	80%
Cancerous disease	77%
Cardiovascular disease	78%
Parasitic disease	79%
Respiratory disease	76%

Discussions:

Here in diseases also percentage sensitivity is not 100% for any disease, because the true negatives is the false hit of diseases in papers which are not talking about that diseases, but their emphasis is some other disease (e.g. Fungal disease gets hits in the papers which talks about the plant growth, and the living organisms that lives in their roots, so these papers is contributing to the false hit).

1.7 Limitation:

There are many limitations in this present work, which are listed as follows:

- Searching should be more like Ontology based searching, include context of the topics.
- More regression method should be included for better validation of the results
- Data size should be larger(may be included more reference library data) for more accuracy to achieve.
- Data can be expanded including more years (searching years can go backward earlier to year 1990), more methods and disease may be included in future.
- More analytical methods can be used for training and directing the searching work in data for achieving accuracy.

However the methods and scripts developed are generalized type ,so can be used to search other databases and with different text, hence has expansion capabilities.

1.8 Conclusions:

The year-wise search result analysis on systems biology shows that in earlier years (decade of 1990) there has not been significant published work in field **titled as** systems biology, most likely due to the lack of appropriate theoretical and experimental methods and lack of reliable data. The field systems biology has also been synonymous with “SYSTEM BIOLOGY”, which also may be the reason for loosing some data in early 90 or before. Repeating the same query using “system biology” (without the s)the following graph was obtained (Fig-14) which shows that our data includes both “SYSTEM” & “SYSTEMS” .

Fig 14a) .Query is “SYSTEM BIOLOGY” july2012

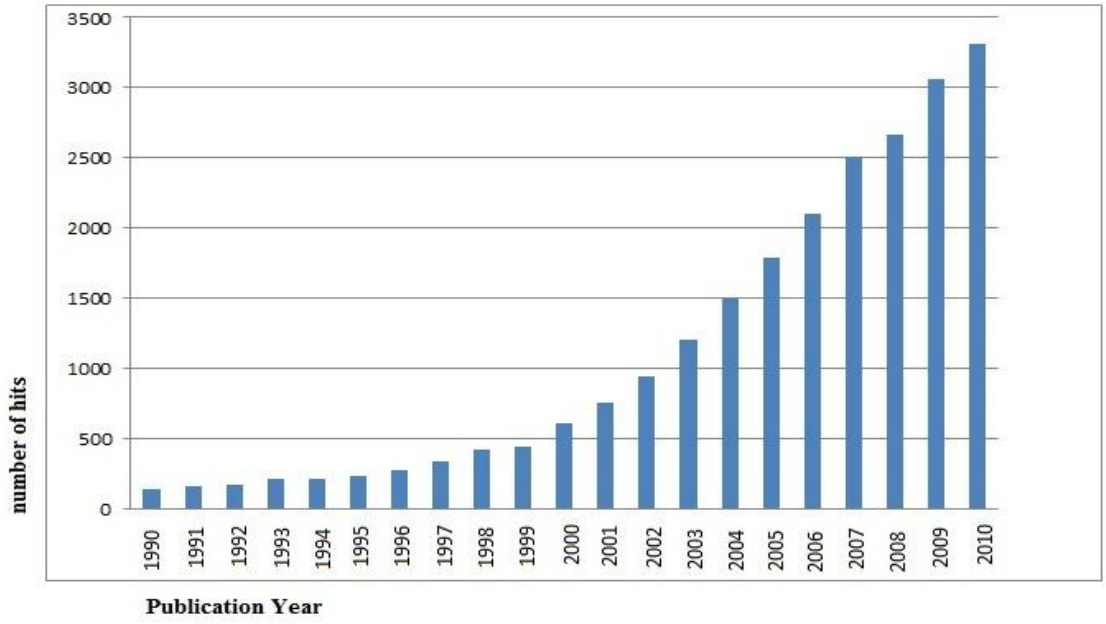
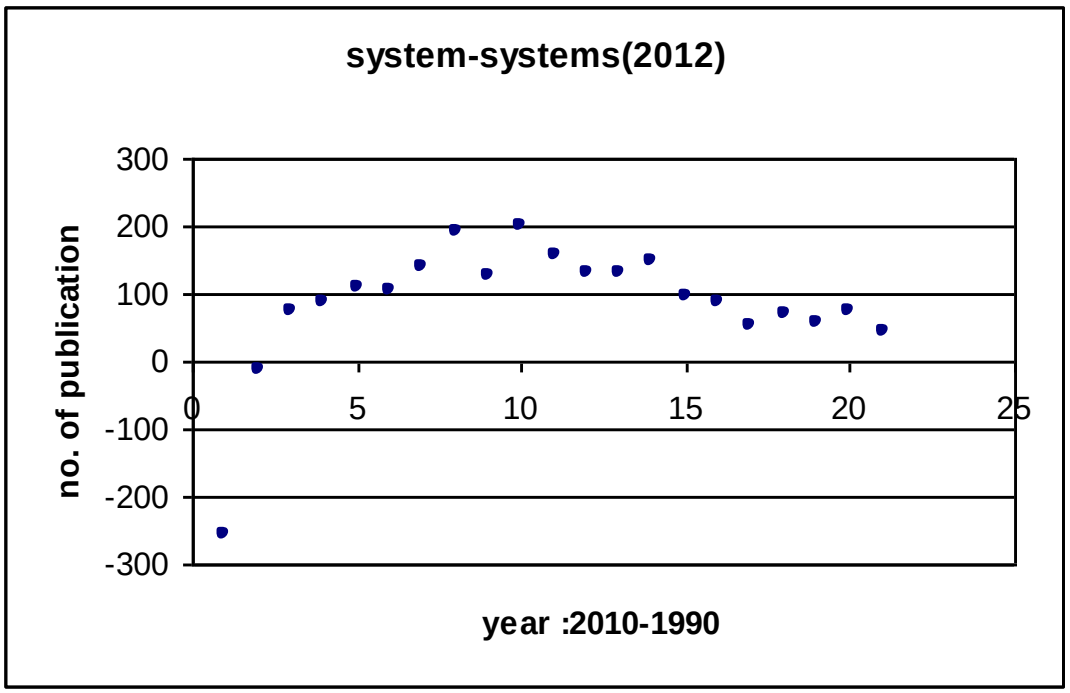


Fig. 14 b) Differential plot between two recent queries.



The difference as seen is fluctuating between the two queries “system biology” & “systems biology” with year of search till 2009, this is due to fact that Pubmed queries are done not using “Exact match”. However 2009 and 2010 searches highlight the disappearance of System Biology and conversion into Systems Biology, shown by negative values.

However in early years of the decade 2000, due to discovery of genomics and proteomics data and many computational techniques to analyze reliable data has emerged which are the major source for surge in publication in this field almost exponentially.

The analysis of method wise search results indicates that SNP is the most frequently used method among above mentioned methods. Phylogeny method and Gene silencing are the next of the most frequently used methods. Reason behind this high contribution, is the availability of data, due to new and better sequencing methods (e.g. high throughput sequencing, next generation sequencing etc.) reliable and large data is getting produced and so the higher in number analytical work is achieved in this field. In addition the SW requirement in such fields are almost saturated and available very easily through websites (Table 1) Other methods like micro-array data analysis, Flux balance analysis, and metabolic control analysis are less publicized methods among these seven methods (included in our study) FBA and MCA methods are more calculation intensive *in-silico* methods which occasionally produce different result from experimental results, the methods and computational tools are not fully standardized, our results indicate that more development work are required in such fields.

The analysis of disease-wise search results shows that the research in Cancer Disease are the most published over the last two decades, which is expected, as total number of publication in Biology is dominated in this field , also it shows the impact of the funding. It is clear that availability of large quantity of experimental data from genomics and proteomics influences strongly the theoretical research and mathematical modeling. Bacterial and Viral diseases are the next among most published research fields. Same reason holds well here too, the high availability of data supporting the more publication in these fields. Publication of the systems biology approach in Genetic diseases represent

less contributing component, as this disease category is recently worked upon and require more medical input.

The disease area like cardiovascular, respiratory, parasitic and fungal diseases have less contribution in publication (though belongs to very old disease categories) it reflects that there are ample opportunities to work in the systems biology and bioinformatics approach in such complex diseases.

More study and analysis in the created reference /literature database may reveal many interesting ideas related to this upcoming field in Biology like, collaboration work instigate more publication in this field? Has the use of web (virtual collaboration!) contributed significant research development in this field? How much more the medical science involvement is required to give impetus in this field?

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4. Zhiyoung Lu. **PubMed and beyond: a survey of web tools for searching biomedical literature.** *Database, Vol. 2011, Article ID baq036, doi:10.1093/database/baq036*

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6. Maria de la Paz Santangelo, Petra M. Gest, Marcelo E. Guerin, Mathieu Coinçon, Ha Pham, Gavin Ryan, Susan E. Puckett, John S. Spencer, Mercedes Gonzalez-Juarrero, Racha Daher, Anne J. Lenaerts, Dirk Schnappinger, Michel Therisod, Sabine Ehrt, Jurgen Sygusch, Mary Jackson. **Glycolytic and Non-glycolytic Functions of Mycobacterium tuberculosis Fructose-1,6-bisphosphate Aldolase, an Essential Enzyme Produced by Replicating and Non-replicating Bacilli.** *Journal of biological chemistry VOL. 286, NO. 46, pp. 40219 –40231, November 18, 2011*.

Chapter-1: Appendix

Code for Literature Survey

Code to extract PMIDs:

```
open(file,$ARGV[0]);
open(out,">$ARGV[2]");
           $a='';
         while($b=<file>){
         $a=$a.$b;
                         }
        close(file);
         @a=split(/\n\n\n\d/,$a);
         for($i=0;$i<scalar @a;$i++){
             $pos=index($a[$i],'PMID:');
               $pmid[$i]=substr($a[$i],$pos+5,10);
                 $a[$i]=lc $a[$i];
                                    }
             $key=lc $ARGV[1];
         for($i=0;$i<scalar @a;$i++){
                   if($a[$i]=~/$key/){
                   print out"$pmid[$i]\n";
                                       }
                                    }
```

Result generated after data-collection from year-wise search:

Table1:

Publishing Year	Number of published papers
2010	2885
2009	2736
2008	2374
2007	2271
2006	1942
2005	1620
2004	1335
2003	1074
2002	828
2001	639
2000	510
1999	362
1998	355
1997	276
1996	231
1995	204
1994	172
1993	170
1992	145
1991	136
1990	109
TOTAL	**20374**

Codes for website Development:

Codes for Individual Pages:

Homepage: (literature_survey.html)

```
--------------------------------------------------------------------------------------------------------------------------
--
<HTML>
       <TABLE width="100%">
   <TR>
        <TD align="left">        <img src="jnu_logo.jpg" width="150" height="150">     </TD>
        <TD align="right">              <img src="DNA_animation.gif" width="150"
height="150"></TD>

   </TR>

</TABLE>
<font color="4054A6">
<H1 align="center">Litrature Survey on Systems Biology and Bioinformatics</h1>
</font>
<i> website developed and maintained by <a href="mailto:ash9nov@gmail.com">Ashish Kumar
singh </a> under supervision of <a href="http://www.jnu.ac.in/Faculty/Indira/">Prof. Indira
Ghosh</a></i>

<hr>
<font color="4054A6">
<center><h3>OBJECTIVE</h3></center>
</font>
<TABLE width="100%">
<TR valign="top"><TD width="70%">
<p> The goal of this work is to analyze the different searching methodologies, What are
the statistics of growth of work in this field, as well as to come to the conclusion that
which
systems biology method, and which disease has what contribution in this area of research.


<p><b> Work Flow: </b>
<p> <img src="pc.png" width="650" height="380">
</TD><TD align="center"> <b><font size="4.5" color="4054A6">Searching Methodologies:</b>
<p><a href="2_methodologies.html" > Yearwise search</a>
<p><a href="3_methodology_3_diseasewise.html" >Diseasewise Search</a>
<p><a href="3_methodology_2_methodwise.html" >Methodwise Search</a>

</TD></TR></TABLE>
</HTML>
--------------------------------------------------------------------------------------------------------------------------
--
```

Methodology's Pages:

Year wise search page: (3_methodology_1_yearwise.html)

```
<HTML>
       <TABLE width="100%">
   <TR>
        <TD align="left">        <img src="jnu_logo.jpg" width="120" height="120">     </TD>
        <TD align="right">       <img src="DNA_animation.gif" width="120" height="120">
       </TD>

   </TR>
   <TR>
             <TD align="left"> <b><font size="4.5" color="4054A6"> <a
href="litrature_survey.html" > Previous Page</a></b> </TD>
             <TD align="right"> <b><font size="4.5" color="4054A6"> <a
href="litrature_survey.html" > Home</a></b> </TD>
       </TR>

</TABLE>
<font color="4054A6">
<H1 align="center">Literature associated with Systems Biology: Yearwise Search</h1>
</font>

<hr>
<font color="4054A6">
<center><h3>Introduction</h3></center>
</font>
<TABLE width="100%">

<TR valign="top">

<TD width="60%">
<p> In this Methodology, searching done was based on individual year wise search. To keep
our search limited,Years taken here were since year 1990 to year 2010.
<p><b> yearwise statistics: </b>
<p> <img src="year_wise_statistics.jpg" width="650" height="480">
</TD>

<TD align="center"> <b><font size="4.5" color="4054A6">YEARS:</b>
<p><a href="1990.php" >Yr1990</a>
<p><a href="1991.php" >Yr1991</a>
<p><a href="1992.php" >Yr1992</a>
<p><a href="1993.php" >Yr1993</a>
<p><a href="1994.php" >Yr1994</a>
<p><a href="1995.php" >Yr1995</a>
<p><a href="1996.php" >Yr1996</a>
<p><a href="1997.php" >Yr1997</a>
<p><a href="1998.php" >Yr1998</a>
<p><a href="1999.php" >Yr1999</a>
</TD>
<TD><font size="4.5" color="4054A6">
<p> </p>
<p> </p>
<p> </p>
<p><a href="2000.php" >Yr2000</a>
<p><a href="2001.php" >Yr2001</a>
<p><a href="2002.php" >Yr2002</a>
<p><a href="2003.php" >Yr2003</a>
<p><a href="2004.php" >Yr2004</a>
<p><a href="2005.php" >Yr2005</a>
<p><a href="2006.php" >Yr2006</a>
<p><a href="2007.php" >Yr2007</a>
```

```
<p><a href="2008.php" >Yr2008</a>
<p><a href="2009.php" >Yr2009</a>
<p><a href="2010.php" >Yr2010</a>
</TD>

</TR>

</TABLE>


</HTML>
```

Disease wise search page: (3_methodology_2_diseasewise.html)

```
<HTML>
       <TABLE width="100%">
   <TR>
        <TD align="left">        <img src="jnu_logo.jpg" width="120" height="120">     </TD>
        <TD align="right">       <img src="DNA_animation.gif" width="120" height="120">
       </TD>

   </TR>
   <TR>
             <TD align="left"> <b><font size="4.5" color="4054A6"> <a
href="litrature_survey.html" > Previous Page</a></b> </TD>
             <TD align="right"> <b><font size="4.5" color="4054A6"> <a
href="litrature_survey.html" > Home</a></b> </TD>
       </TR>

</TABLE>


<font color="4054A6">
<H1 align="center">Literature associated with Systems Biology: Diseasewise Search</h1>
</font>

<hr>
<font color="4054A6">
<center><h3>Introduction</h3></center>
</font>
<TABLE width="100%">

<TR valign="top">

<TD width="70%">
<p> In this Methodology, searching done, was based on selective Diseases, which are being
studied with help of Sysetms biology tools. And comprative studies done
on them, to find out, which disease is highly worked on and which one is most ignored.  here
comparative studies shows the
frequent application of systems biology methods on specific diseases.
<p><b>Contributions of individual Diseases: </b>
<p> <img src="contribution_of_individual_diseases.jpg" width="585" height="450">
</TD>

<TD align="center"> <b><font size="4.5" color="4054A6">DISEASES:</b>
<p><a href="disease_bacteria.php" > Bacterial disease </a>
<p><a href="disease_viral.php" > Viral Disease</a>
<p><a href="disease_fungal.php" > Fungal Disease</a>
<p><a href="disease_cancer.php" > Cancer Disease</a>
```

```
<p><a href="disease_cardiovascular.php" > Cardiovascular Disease</a>
<p><a href="disease_genetic.php" > Genetic Disease</a>
<p><a href="disease_parasitic.php" > Parasitic Disease </a>
<p><a href="disease_respiratory.php" > Respiratory Disease</a>

</TD>


</TR>

</TABLE>


</HTML>
```

Method wise Search Page: (3_methodology_3_methodwise.html)

```
<HTML>
       <TABLE width="100%">
   <TR>
        <TD align="left">        <img src="jnu_logo.jpg" width="120" height="120">     </TD>
        <TD align="right">       <img src="DNA_animation.gif" width="120" height="120">
       </TD>

   </TR>
   <TR>
             <TD align="left"> <b><font size="4.5" color="4054A6"> <a
href="litrature_survey.html" > Previous Page</a></b> </TD>
             <TD align="right"> <b><font size="4.5" color="4054A6"> <a
href="litrature_survey.html" > Home</a></b> </TD>
       </TR>

</TABLE>
<font color="4054A6">
<H1 align="center">Literature associated with Systems Biology: Methodwise Search</h1>
</font>

<hr>
<font color="4054A6">
<center><h3>Introduction</h3></center>
</font>
<TABLE width="100%">

<TR valign="top">

<TD width="70%">
<p> In this Methodology, searching done, was based on selective methods of Systems biology.
And comprative studies done on them, that which method is frequentely done and applied to
the disease,
and has what contribution in field of Systems Biology.
<p><b>Contributions of individual Methods: </b>
<p> <img src="contribution_of_individual_methods.jpg" width="480" height="480">
</TD>

<TD align="center"> <b><font size="4.5" color="4054A6">METHODS:</b>
<p><a href="method_fba.php" >Flux Balance Analysis</a>
<p><a href="method_gene_networks.php" >Gene Networks</a>
<p><a href="method_gene_silencing.php" >Gene Silencing</a>
<p><a href="method_mca.php" > Metabolic Control Analysis</a>
<p><a href="method_microarray_technology.php" > Microarray Data Analysis</a>
<p><a href="method_phylogenetic_analysis.php" > Phylogeny Method</a>
```

```
<p><a href="method_snp.php" > Single Nucleotide Polymorphism</a>

</TD>


</TR>

</TABLE>

</HTML>
```

PHP output pages for Individual Year wise Results:

1990.php:

```
<html>
<body>
       <TABLE width="100%">
   <TR>
        <TD align="left">        <img src="jnu_logo.jpg" width="120" height="120">   </TD>
        <TD align="right">       <img src="DNA_animation.gif" width="120" height="120">
       </TD>

   </TR>

<TABLE width="100%">
       <TR>
              <TD align="left"> <b><font size="4.5" color="4054A6"> <a
href="3_methodology_1_yearwise.html" > Previous Page</a></b> </TD>
              <TD align="right"> <b><font size="4.5" color="4054A6"> <a
href="litrature_survey.html" > Home</a></b> </TD>
       </TR>

</TABLE>

       <h1>Literature associated with Systems Biology in Year 1990</h1>
<TABLE width="100%">
              <TD align="left"><b><font size="3.5" color="4060B9"> Number of entries in the
table is <font size="5" color="4054A6">109</font> </b></TD>
              <TD align="right"> <I> <font color="#812A18"> Here Reference ID is PUBMED ID
(Information source: <a href="http://www.ncbi.nlm.nih.gov/pubmed/"> PUBMED)</I>   </TD>
</TABLE>

<?php
$username="ashish";
$password="ashish";
$database="year";

mysql_connect(localhost,$username,$password);
@mysql_select_db($database) or die( "Unable to select database");
$query="SELECT * FROM yr_1990";
$result=mysql_query($query);

$num=mysql_numrows($result);

mysql_close();
?>
<table border="2" cellspacing="5" cellpadding="8" class="db-table">
<tr>
<th><font face="Arial, Helvetica, sans-serif">ID</font></th>
<th><font face="Arial, Helvetica, sans-serif">Reference ID</font></th>
```

```
<th><font face="Arial, Helvetica, sans-serif">ABSTRACT</font></th>
</tr>

<?php
$i=0;
while ($i < $num) {

$f1=mysql_result($result,$i,"id");
$f2=mysql_result($result,$i,"PMID");
$f3=mysql_result($result,$i,"abstract");

?>

<tr>
<td><font face="Arial, Helvetica, sans-serif"><?php echo $f1; ?></font></td>
<td><font face="Arial, Helvetica, sans-serif"> <?php echo "<A
HREF='http://www.ncbi.nlm.nih.gov/pubmed?term=$f2'>$f2</A>"; ?></font></td>
<td><font face="Arial, Helvetica, sans-serif"><?php echo $f3; ?></font></td>

</tr>

<?php
$i++;
}
?>
</body>
</html>
```

2010.php:

```
<html>
<body>

       <TABLE width="100%">
              <TR>
        <TD align="left">        <img src="jnu_logo.jpg" width="120" height="120">   </TD>
        <TD align="right">       <img src="DNA_animation.gif" width="120" height="120">
       </TD>

   </TR>
       <TR>
              <TD align="left"> <b><font size="4.5" color="4054A6"> <a
href="3_methodology_1_yearwise.html" > Previous Page</a></b> </TD>
              <TD align="right"> <b><font size="4.5" color="4054A6"> <a
href="litrature_survey.html" > Home</a></b> </TD>
       </TR>

</TABLE>

       <h1>Literature associated with Systems Biology in Year 2010</h1>
<TABLE width="100%">
              <TD align="left"><b><font size="3.5" color="4060B9"> Number of entries in the
table is <font size="5" color="4054A6">2885</font> </b></TD>
              <TD align="right"> <I> <font color="#812A18"> Here Reference ID is PUBMED ID
(Information source: <a href="http://www.ncbi.nlm.nih.gov/pubmed/"> PUBMED)</I>   </TD>
</TABLE>

<?php
$username="ashish";
$password="ashish";
$database="year";
```

```
mysql_connect(localhost,$username,$password);
@mysql_select_db($database) or die( "Unable to select database");
$query="SELECT * FROM yr_2010";
$result=mysql_query($query);

$num=mysql_numrows($result);

mysql_close();
?>
<table border="2" cellspacing="5" cellpadding="8" class="db-table">
<tr>
<th><font face="Arial, Helvetica, sans-serif">ID</font></th>
<th><font face="Arial, Helvetica, sans-serif">Reference ID</font></th>
<th><font face="Arial, Helvetica, sans-serif">ABSTRACT</font></th>
</tr>

<?php
$i=0;
while ($i < $num) {

$f1=mysql_result($result,$i,"id");
$f2=mysql_result($result,$i,"PMID");
$f3=mysql_result($result,$i,"abstract");

?>

<tr>
<td><font face="Arial, Helvetica, sans-serif"><?php echo $f1; ?></font></td>
<td><font face="Arial, Helvetica, sans-serif"> <?php echo "<A
HREF='http://www.ncbi.nlm.nih.gov/pubmed?term=$f2'>$f2</A>"; ?></font></td>
<td><font face="Arial, Helvetica, sans-serif"><?php echo $f3; ?></font></td>

</tr>

<?php
$i++;
}
?>
</body>
</html>
```

PHP output pages for Individual Disease wise Results:

disease_bacteria.php:

```
<html>
<body>

      <TABLE width="100%">
               <TR>
       <TD align="left">        <img src="jnu_logo.jpg" width="150" height="150">     </TD>
       <TD align="right">              <img src="DNA_animation.gif" width="150"
height="150"></TD>

   </TR>
      <TR>
            <TD align="left"> <b><font size="4.5" color="4054A6"> <a
href="3_methodology_3_diseasewise.html" > Previous Page</a></b> </TD>
            <TD align="right"> <b><font size="4.5" color="4054A6"> <a
```

```
href="litrature_survey.html" > Home</a></b> </TD>
	</TR>

	</TABLE>

	<h1> Systems Biology Papers on Bacterial Disease</h1>
		<TABLE width="100%">
		<TD align="left"><b><font size="3.5" color="4060B9"> Number of entries in the
table is <font size="5" color="4054A6">1510</font> </b></TD>
		<TD align="right"> <I> <font color="#812A18"> Here Reference ID is PUBMED ID
(Information source: <a href="http://www.ncbi.nlm.nih.gov/pubmed/"> PUBMED)</I>   </TD>
	</TABLE>

<?php
$username="ashish";
$password="ashish";
$database="disease";

mysql_connect(localhost,$username,$password);
@mysql_select_db($database) or die( "Unable to select database");
$query="SELECT * FROM disease_bacteria";
$result=mysql_query($query);

$num=mysql_numrows($result);

mysql_close();
?>
<table border="2" cellspacing="5" cellpadding="8" class="db-table" width="50%">
<tr>
<th><font face="Arial, Helvetica, sans-serif">ID</font></th>
<th><font face="Arial, Helvetica, sans-serif">Reference ID</font></th>
</tr>

<?php
$i=0;
while ($i < $num) {

$f1=mysql_result($result,$i,"id");
$f2=mysql_result($result,$i,"PMID");


?>

<tr>
<td align="center"><font face="Arial, Helvetica, sans-serif"><?php echo $f1; ?></font></td>
<td align="center"><font face="Arial, Helvetica, sans-serif"> <?php echo "<A
HREF='http://www.ncbi.nlm.nih.gov/pubmed?term=$f2'>$f2</A>"; ?></font></td>

</tr>

<?php
$i++;
}
?>
</body>
</html>
```

PHP output pages for Individual Method wise Results:

method_fba.php:

```
<html>
<body>

       <TABLE width="100%">
                 <TR>
        <TD align="left">        <img src="jnu_logo.jpg" width="150" height="150">     </TD>
        <TD align="right">              <img src="DNA_animation.gif" width="150"
height="150"></TD>

   </TR>
       <TR>
             <TD align="left"> <b><font size="4.5" color="4054A6"> <a
href="3_methodology_2_methodwise.html" > Previous Page</a></b> </TD>
             <TD align="right"> <b><font size="4.5" color="4054A6"> <a
href="litrature_survey.html" > Home</a></b> </TD>
       </TR>

       </TABLE>

       <h1> Systems biology Papers on Flux Balance Analysis</h1>
       <TABLE width="100%">
             <TD align="left"><b><font size="3.5" color="4060B9"> Number of entries in the
table is <font size="5" color="4054A6">350</font> </b></TD>
             <TD align="right"> <I> <font color="#812A18"> Here Reference ID is PUBMED ID
(Information source: <a href="http://www.ncbi.nlm.nih.gov/pubmed/"> PUBMED)</I>   </TD>
       </TABLE>

<?php
$username="ashish";
$password="ashish";
$database="method";

mysql_connect(localhost,$username,$password);
@mysql_select_db($database) or die( "Unable to select database");
$query="SELECT * FROM method_fba";
$result=mysql_query($query);

$num=mysql_numrows($result);

mysql_close();
?>
<table border="2" cellspacing="5" cellpadding="8" class="db-table">
<tr>
<th><font face="Arial, Helvetica, sans-serif">ID</font></th>
<th><font face="Arial, Helvetica, sans-serif">Reference ID</font></th>
<th><font face="Arial, Helvetica, sans-serif">ABSTRACT</font></th>
</tr>

<?php
$i=0;
while ($i < $num) {

$f1=mysql_result($result,$i,"id");
$f2=mysql_result($result,$i,"PMID");
$f3=mysql_result($result,$i,"abstract");

?>

<tr>
```

```
<td><font face="Arial, Helvetica, sans-serif"><?php echo $f1; ?></font></td>
<td><font face="Arial, Helvetica, sans-serif"> <?php echo "<A
HREF='http://www.ncbi.nlm.nih.gov/pubmed?term=$f2'>$f2</A>"; ?></font></td>
<td><font face="Arial, Helvetica, sans-serif"><?php echo $f3; ?></font></td>

</tr>

<?php
$i++;
}
?>
</body>
</html>
```

PHP code to create data tables and inserting data in to MySQL database:

```
<html>
<head>
	<title>ashishsingh</title>
	<meta http-equiv="Content-Type" content="text/html; charset=ISO-8859-1">
</head>
<body>
	<h1>ashish</h1>
	<p>
	<b>hi! all</b><br />
		<?php echo "The Current Date and Time in my system is: <br>";
			echo date("g:i A l, F j Y.");?>

	<p>
		  <b>
			<?php


		    // Making a MySQL Connection
			mysql_connect("localhost", "ashish", "ashish") or
die(mysql_error());
			mysql_select_db("method") or die(mysql_error());


$file = "method_SNP_text.txt"; //giving the file name.
echo  "Data for the DATABASE: METHOD has been inserted:".
$file."\n-------------------------------------------------------------------------------
-------------\n\n\n";
$fp = fopen($file, "r");
$output = fread($fp, filesize($file));
fclose($fp);
//str_replace( "[PubMed - indexed for MEDLINE]", "[PubMed - indexed for MEDLINE]\n\n\n",
$output,$Count) ;
//echo $output;
$output1 = explode("[PubMed - indexed for MEDLINE]", $output);
$count=0;
foreach($output1 as $var)
{
$count= $count +1;
echo $count. "- " ;

//mysql_query("INSERT INTO method_snp (abstract) VALUES('$var')") or die("Insert failed: " .
mysql_error());
```

```
}
echo $count;
echo "data inserted sucessfully! he he he :)";



?>
            </b>
        </p>



</body>
</html>
```

Chapter 2

Study of Systems Biology methods: FBA & web based GSMN

2.1 Background:

Imbalance in Metabolism has been implicated in major human diseases including obesity, diabetes, cancer, and heart disease (Hsu PP, Sabatini DM). Metabolism has been an important field of study and research for many branches of medicine. Particularly in obesity, a disease due to over weight, leading to the cause of the heart disease and diabetes occurs often. The recent abundance of complete genome sequences has enabled the generation of genome-scale metabolic reconstructions for various microorganisms (Covert et al. 2001; Price et al. 2003; Reed and Palsson 2003). These models are complete skeleton of the metabolic reactions present in the organism. To express and illustrate the organizational principles of metabolic interactions inside the cell network, the structural and topological properties of metabolic networks needs to be studied and examined at practical level, as well as at conceptual level, this practice provides more effective consistency of the metabolic reconstructions. Genome-scale metabolic reconstructions provide a biologically meaningful mechanistic basis for the genotype-phenotype relationship(Edwards & Palsson,2000). In support to this, identification of stopped or blocked reactions (i.e., reactions incapable of carrying flux due to the stoichiometric ratios of the metabolites in the network under steady-state conditions) and enzyme subsets (i.e., groups of reactions that operate together in fixed flux proportions under steady-state conditions) in metabolic models has attracted considerable interest in recent years (Kholodenko et al. 1995; Rohwer et al. 1996; Pfeiffer et al. 1999; Klamt et al. 2003). Analysis and simulations of this metabolic network provides the results which convey biologically significant insight. The reactions which are missing or which are under coordinated regulation, hints to the organization's mechanism for the regular and continuous refinement of metabolic reconstructions by a model-building interactive process. As to the exemplify the above, Flux Balance Analysis has been performed on the stoichiometric models of *Escherichia coli* metabolism and the objectives are as follows (1) qualitatively predicting the outcomes of gene knockout experiments (Edwards and Palsson 2000; Badarinarayana et al. 2001); (2) identifying the correct sequence of byproduct secretion under increasingly anaerobic conditions (Varma et al. 1993); (3) quantitatively predicting cellular growth rates (Edwards et al. 2001; Ibarra et al. 2002); (4) assessing the

performance limits of metabolic networks in response to gene additions or deletions (Burgard and Maranas 2001); and (5) suggesting gene knockout strategies for enhancing biochemical production (Burgard et al. 2003; Pharkya et al. 2004) and many other.

2.2 Introduction:

Any organism's biochemical systems can be represented in form of metabolic reaction network, where each node is a reaction. This reaction network model-building is based on SBML platform. Presently there are 233 methods listed which are based on SBML platform and takes SBML model for creating network, simulating results, and other workouts on the SBML model. For example, ABC-SysBio *(*http://abc-sysbio.sourceforge.net/*)* ,BioMet Toolbox (http://www.sysbio.se/) , CADLIVE (http://www.cadlive.jp), COBRA (http://gcrg.ucsd.edu/Downloads/Cobra_Toolbox), COPASI (http://copasi.org), FASIMU (http://www.bioinformatics.org/fasimu), SurreyFBA (http://sysbio3.fhms.surrey.ac.uk/), etc. Like this many other weblinks are available for metabolic network simulation and analysis. The reconstruction of metabolic network is done for use in Flux balance Analysis to calculate the flux flow of metabolites in the pathway network at the steady state conditions, for the purpose. Flux Balance Analysis can be used as tool to identify the organism's biochemical behavior computationally. Here in present work (chapter 3), *Mycobacterium tuberculosis* is chosen as the organism to work on. The GSMN (Genome Scaled Metabolic Network) model of Mycobacterium tuberculosis is focused for study which has been build up already as the web-based model GSMN-Tb by Johnjoe McFadden group(Dany JV Beste, Tracy Hooper, Graham Stewart, Bhushan Bonde, Claudio Avignone-Rossa, Michael E Bushell, Paul Wheeler, Steffen Klamt, Andrzej M Kierzek and Johnjoe McFadden). The GSMN-Tb tool itself handles the FBA calculations, so no other setups needed for the following work mentioned in the next chapter. We shall be discussing on some of the popularly used Markup languages here.

2.3 SBML:

SBML is the Systems Biology Markup Language; it is a free, open, XML-based format for representing biochemical reaction networks. SBML is a software-independent language for describing models common to research in many areas of computational biology, including cell signaling pathways, metabolic pathways, gene regulation, and others. Broken down into its constituents, this model contains a number of components: reactant species, product species, reactions, reaction rates, and parameters in the rate expressions. To analyze or simulate this network, additional components must be made explicit, including compartments where the species are located, and units on the various quantities.

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1. beginning of model definition
2. list of function definitions (optional)
3. list of unit definitions (optional)
4. list of compartments (optional)
5. list of species (optional)
6. list of parameters (optional)
7. list of rules (optional)
8. list of reactions (optional)
9. list of events (optional)
10. end of model definition

The meaning of each component is as follows:

- **Function definition:** A named mathematical function that may be used throughout the rest of a model.

- **Unit definition:** A name for a unit used in the expression of quantities in a model.

- **Compartment:** A container of finite size for substances.

- **Species:** A substance or entity that takes part in a reaction. Some examples are like molecules such as glucose or ATP and species are ions such as Ca.

- **Parameter:** A quantity with a symbolic name. SBML Level 2 provides the ability to define parameters that are global to a model as well as parameters that are local to a single reaction.

- **Rule:** A mathematical expression used in combination with the differential equations constructed based on the set of reactions in a model; it can be used to establish constraints between variables, define how a variable can be calculated from other variables, or used to define the rate of change of a variable.

- **Reaction:** A statement describing some transformation, transport or binding process that can change the amount of one or more species. For example, a reaction may describe how certain entities (reactants) are transformed into certain other entities (products). Reactions have associated kinetic rate expressions describing how quickly they take place.

- **Event:** A statement describing an instantaneous, discontinuous change in a set of variables of any type (species concentration, compartment size or parameter value) when a triggering condition is satisfied.

A software package can read an SBML model description and translate it into its own internal format for model analysis. For example, a package might provide the ability to simulate the model by constructing differential equations representing the network and then perform numerical time integration on the equations to explore the model's dynamic

behavior. There are many software packages which read SBML models for simulating and analyzing the metabolic network. Detailed list of SBML software is as follows:

SBML based Systems Biology software are categorized in 10 categories, which are as follows:

1. Analysis software
2. Annotation software
3. Creation/development software
4. Data integration and management software
5. Framework or library
6. Repository or database
7. Scripting module
8. Simulation software
9. Utility software
10. Visualization software

2.3.1SBML based Systems Biology software

1. **Analysis software (58 software available)**

    1. **ABC-SysBio:** *(*http://abc-sysbio.sourceforge.net/ *)*
    2. **AutoSBW:** *(*http://frank-fbergmann.blogspot.com/2009/02/simplifying-bifurcation-analysis.html*)*
    3. **Bifurcation Discovery Tool:** (http://sys-bio.org/sbwWiki/sbw/biftool)
    4. **BioBayes:** (http://www.dcs.gla.ac.uk/BioBayes/)
    5. **BioMet Toolbox** :(http://www.sysbio.se/)
    6. **ByoDyn** :(http://byodyn.imim.es)
    7. **CADLIVE:** (http://www.cadlive.jp)
    8. **CellNetAnalyzer:** (http://www.mpi-magdeburg.mpg.de/projects/cna/cna.html)
    9. **COBRA:** (http://gcrg.ucsd.edu/Downloads/Cobra_Toolbox)
    10. **COPASI:** (http://copasi.org)

11. **Crdata:** (http://crdata.org/)
12. **DBSolve:** (http://insysbio.ru/en/soft/dbsolveoptimum.html)
13. **DOTcvpSB:** (http://www.iim.csic.es/~dotcvpsb/)
14. **Facile:** (http://facile.sourceforge.net)
15. **FASIMU** (http://www.bioinformatics.org/fasimu)
16. **FBASBW** (http://frank-fbergmann.blogspot.com/2009/03/fluxbalance-analysis-with-sbw.html)
17. **Fluxor** (http://arep.med.harvard.edu/moma/FluxorPipeline.tar.gz)
18. **Genetic Network Analyzer** (http://www-helix.inrialpes.fr/gna)
19. **GNU MCSim** (http://www.gnu.org/software/mcsim/)
20. **iBioSim** (http://www.async.ece.utah.edu/iBioSim/)
21. **Jacobian Viewer** (http://jdesigner.sourceforge.net/Site/Jacobian_Viewer.html)
22. **Jarnac** (http://jdesigner.sourceforge.net/Site/Jarnac.html)
23. **JigCell** (http://jigcell.cs.vt.edu/)
24. **JSim** (http://www.physiome.org/jsim/)
25. **KEGGconverter** (http://www.grissom.gr/keggconverter/index.html)
26. **MatCont** (http://sourceforge.net/projects/matcont/)
27. **MesoRD** (http://mesord.sourceforge.net)
28. **Metaboflux** (http://www.cbib.u-bordeaux2.fr/metaboflux/)
29. **MetaFluxNet** (http://metafluxnet.kaist.ac.kr)
30. **MetExplore** (http://metexplore.toulouse.inra.fr)
31. **MMT2** (http://www.simtec.mb.uni-siegen.de/software_mmt2.0.html)
32. **MOOSE** (http://moose.ncbs.res.in/)
33. **Odefy** (http://www.helmholtz-muenchen.de/cmb/odefy)
34. **ONDEX:**(http://www.ondex.org/)
35. **OptFlux** (http://www.optflux.org/)
36. **Pathway Analyser** (http://sourceforge.net/projects/pathwayanalyser)
37. **PET** (http://mpf.biol.vt.edu/pet)
38. **PK-Sim / MoBi** (http://www.systems-biology.com)
39. **PRISM** (http://www.prismmodelchecker.org/)

40. **ProcessDB** (http://www.integrativebioinformatics.com/processdb.html)
41. **PySCeS** (http://pysces.sourceforge.net)
42. **SBML Harvester** (http://code.google.com/p/sbmlharvester/)
43. **SBMLSim** (http://www.dim.uchile.cl/~dremenik/SBMLSim/)
44. **SBSI** (http://www.sbsi.ed.ac.uk)
45. **SBToolbox2** (http://www.sbtoolbox2.org/)
46. **SBW** (http://sys-bio.org/)
47. **SensSB** (http://www.iim.csic.es/~gingproc/SensSB.html)
48. **SimBiology** (http://www.mathworks.com/products/simbiology/)
49. **SloppyCell** (http://sloppycell.sourceforge.net/)
50. **SOSlib** (http://www.tbi.univie.ac.at/~raim/odeSolver/)
51. **SurreyFBA** (http://sysbio3.fhms.surrey.ac.uk/)
52. **SYCAMORE** (http://sycamore.eml.org)
53. **Systrip** (http://tulip.labri.fr/TulipDrupal/?q=systrip)
54. **Tide** (http://sysbio.molgen.mpg.de/tide/)
55. **TinkerCell** (http://www.tinkercell.com/)
56. **VANTED** (http://vanted.ipk-gatersleben.de/)
57. **WebCell** (http://webcell.kaist.ac.kr/)
58. **WinSCAMP** (http://www.sys-bio.org/software/winscamp.htm)

2. **Annotation software (10 software available):**

1. **CellDesigner** (http://celldesigner.org)
2. **COPASI** (http://copasi.org)
3. **KEGGtranslator** (http://www.ra.cs.uni-tuebingen.de/software/KEGGtranslator/)
4. **Metannogen** (http://www.bioinformatics.org/strap/metannogen/)
5. **PAYAO** (http://www.payaologue.org)
6. **Saint** (http://saint.ncl.ac.uk/)

7. **SBMLEditor** (http://www.ebi.ac.uk/compneur-srv/SBMLeditor.html)
8. **SBMLsqueezer** (http://www.cogsys.cs.uni-tuebingen.de/software/SBMLsqueezer/)
9. **SBW** (http://sys-bio.org/)
10. **semanticSBML** (http://semanticsbml.org)

3. **Creation/development software (50 software available):**

1. **ALC** (http://layer.mpi-magdeburg.mpg.de/)
2. **Antimony** (http://antimony.sourceforge.net/)
3. **Asmparts** (http://soft.synth-bio.org/asmparts.html)
4. **Athena** (http://athena.codeplex.com/)
5. **BALSA** (http://depts.washington.edu/ventures/UW_Technology/Emerging_Technologies/CSI.php)
6. **Bio Sketch Pad**
7. **BioCharon** (http://www.cis.upenn.edu/biocomp)
8. **BioNetGen** (http://bionetgen.org/)
9. **BioSpreadsheet** (http://biocomp.ece.utk.edu/tools.html)
10. **BioTapestry** (http://www.biotapestry.org/)
11. **BioUML** (http://www.biouml.org/)
12. **Cell Illustrator** (http://www.fqs.pl/life_science/cell_illustrator)
13. **CellDesigner** (http://celldesigner.org)
14. **Cellerator** (http://www.cellerator.net/)
15. **COPASI** (http://copasi.org)
16. **DBSolve** (http://insysbio.ru/en/soft/dbsolveoptimum.html)
17. **Facile** (http://facile.sourceforge.net)
18. **Genetic Network Analyzer** (http://www-helix.inrialpes.fr/gna)
19. **GNU MCSim** (http://www.gnu.org/software/mcsim/)
20. **HSMB**
21. **HybridSBML** (http://biocomp.cis.upenn.edu/software.php3)

22. **iBioSim** (http://www.async.ece.utah.edu/iBioSim/)
23. **insilicoIDE** (http://www.physiome.jp/)
24. **JACOBIAN** (http://numericatech.com/jacobian.htm)
25. **Jarnac** (http://jdesigner.sourceforge.net/Site/Jarnac.html)
26. **JarnacLite** (http://www.sys-bio.org/sbwWiki/sbw/jarnaclite)
27. **JDesigner** (http://sbw.kgi.edu/software/jdesigner.htm)
28. **JigCell** (http://jigcell.cs.vt.edu/)
29. **JSim** (http://www.physiome.org/jsim/)
30. **Karyote** (http://biodynamics.indiana.edu/CellModeling/)
31. **KEGGtranslator** (http://www.ra.cs.uni-tuebingen.de/software/KEGGtranslator/)
32. **MetaFluxNet** (http://metafluxnet.kaist.ac.kr)
33. **MetNetMaker** (http://www.metnetmaker.com)
34. **Monod** (http://monod.molsci.org/)
35. **NetBuilder**' (http://strc.herts.ac.uk/bio/maria/Apostrophe/)
36. **Pathway Builder** (http://biospice.sourceforge.net/)
37. **PathwayLab** (http://innetics.com/)
38. **PK-Sim / MoBi** (http://www.systems-biology.com)
39. **ProcessDB** (http://www.integrativebioinformatics.com/processdb.html)
40. **ProMoT** (http://www.mpi-magdeburg.mpg.de/projects/promot)
41. **Saint** (http://saint.ncl.ac.uk/)
42. **SBML2NEURON** (http://www.neuroml.org/neuron_tools.php)
43. **SBMLEditor** (http://www.ebi.ac.uk/compneur-srv/SBMLeditor.html)
44. **SBML-shorthand** (http://www.staff.ncl.ac.uk/d.j.wilkinson/software/sbml-sh/)
45. **SBMLsqueezer** (http://www.cogsys.cs.uni-tuebingen.de/software/SBMLsqueezer/)
46. **SBMLToolbox** (http://sbml.org/Software/SBMLToolbox)
47. **SBW** (http://sys-bio.org/)
48. **semanticSBML** (http://semanticsbml.org)
49. **SigTran**

(http://www.cellsystems.org/teams/modeling/projects/sigtran/overview.html)

50. **SimBiology** (http://www.mathworks.com/products/simbiology/)

4. **Data integration and management software (33 software available):**

1. **BioPathwise** (http://www.bioanalyticsgroup.com/index_files/Page465.htm)
2. **CADLIVE** (http://www.cadlive.jp)
3. **CARMEN** (http://carmen.cebitec.uni-bielefeld.de/cgi-bin/index.cgi)
4. **Insilico Discovery** (http://www.insilico-biotechnology.com/insilico_discovery)
5. **JSim** (http://www.physiome.org/jsim/)
6. **KEGGconverter** (http://www.grissom.gr/keggconverter/index.html)
7. **KEGGtranslator** (http://www.ra.cs.uni-tuebingen.de/software/KEGGtranslator/)
8. **Medicel** (http://www.euformatics.com)
9. **MetaCrop** (http://metacrop.ipk-gatersleben.de/)
10. **Metannogen** (http://www.bioinformatics.org/strap/metannogen/)
11. **MIRIAM** Resources (http://www.ebi.ac.uk/miriam)
12. **ONDEX** (http://www.ondex.org/)
13. **Pathway Access** (http://vrac.iastate.edu/~jlv/pathwayaccess/)
14. **Pathway Tools** (http://bioinformatics.ai.sri.com/ptools/)
15. **PATIKAweb** (http://www.patika.org/)
16. **PK-Sim / MoBi** (http://www.systems-biology.com)
17. **ProcessDB** (http://www.integrativebioinformatics.com/processdb.html)
18. **PROTON** (http://tunicata.techfak.uni-bielefeld.de/proton/web/main.jsp)
19. **ReMatch** (http://www.cs.helsinki.fi/group/sysfys/software/rematch/)
20. **SABIO-RK** (http://sabiork.h-its.org/)
21. **Saint** (http://saint.ncl.ac.uk/)
22. **SBML Harvester** (http://code.google.com/p/sbmlharvester/)
23. **SBMM assistant** (http://cath.gisum.uma.es:8080/sbmm/)
24. **SBO** (http://www.ebi.ac.uk/sbo/)

25. **SCIpath**
26. **semanticSBML** (http://semanticsbml.org)
27. **SIGNALIGN** (http://agbi.techfak.uni-bielefeld.de/signalign/index.jsp)
28. **SigPath** (http://www.sigpath.org/)
29. **SimBiology** (http://www.mathworks.com/products/simbiology/)
30. **SRS** (http://www.biowisdom.com/2009/12/srs/)
31. **SYCAMORE** (http://sycamore.eml.org)
32. **VANTED** (http://vanted.ipk-gatersleben.de/)
33. **BioSPICE Dashboard** (http://www.biospice.org/)

5. **Framework or library (18 software available):**

1. **BioSPICE** Dashboard (http://www.biospice.org/)
2. **CLEML** (http://bioinfo.ustc.edu.cn/softwares/CLEML/)
3. **CL-SBML** (http://common-lisp.net/project/cl-sbml)
4. **COPASI** (http://copasi.org)
5. **JSBML** (http://sourceforge.net/projects/jsbml/)
6. **JSim** (http://www.physiome.org/jsim/)
7. **libAnnotationSBML** (http://sbml.org/Community/Programs/libAnnotationSBML)
8. **libSBML** (http://www.sbml.org/software/libsbml)
9. **libStruct** (http://sourceforge.net/apps/mediawiki/libstruct/index.php?title=Main_Page
10. **Metannogen** (http://www.bioinformatics.org/strap/metannogen/)
11. **Odefy** (http://www.helmholtz-muenchen.de/cmb/odefy)
12. **PySCeS** (http://pysces.sourceforge.net)
13. **SBML Layout** (http://sbmllayout.sf.net/)
14. **SBW** (http://sys-bio.org/)
15. **semanticSBML** (http://semanticsbml.org)
16. **SimBiology** (http://www.mathworks.com/products/simbiology/)
17. **SOSlib** (http://www.tbi.univie.ac.at/~raim/odeSolver/)

18. **TERANODE Suite** (http://teranode.com/products/index.php)

6. **Repository or database (32 software available):**

1. **BASIS** (http://www.basis.ncl.ac.uk/)
2. **BiGG** (http://bigg.ucsd.edu/)
3. **BioCyc** (http://www.biocyc.org/)
4. **BioGRID** (http://thebiogrid.org/)
5. **BioModels Database** (http://www.ebi.ac.uk/biomodels/)
6. **BioModels Importer** (http://jdesigner.sourceforge.net/Site/Biomodels_Importer.html)
7. **BRENDA** (http://brenda-enzymes.org/)
8. **ByoDyn** (http://byodyn.imim.es)
9. **CADLIVE** (http://www.cadlive.jp)
10. **ConsensusPathDB** (http://cpdb.molgen.mpg.de/)
11. **CRdata** (http://crdata.org/)
12. **CycSim** (http://www.genoscope.cns.fr/cycsim/)
13. **insilicoIDE** (http://www.physiome.jp/)
14. **JSim** (http://www.physiome.org/jsim/)
15. **JWS Online** (http://jjj.biochem.sun.ac.za/index.html)
16. **Meta-All** (http://bic-gh.de/meta-all)
17. **MetaCrop** (http://metacrop.ipk-gatersleben.de/)
18. **MetExplore** (http://metexplore.toulouse.inra.fr)
19. **NetPath** (http://www.netpath.org/)
20. **NetPro** (http://www.molecularconnections.com/products.html)
21. **PANTHER Pathway** (http://https://panther.appliedbiosystems.com/pathway/)
22. **PathArt** (http://jubilantbiosys.com/ppa.htm)
23. **PAYAO** (http://www.payaologue.org)
24. **PK-Sim / MoBi** (http://www.systems-biology.com)
25. **ProcessDB** (http://www.integrativebioinformatics.com/processdb.html)
26. **Reactome** (http://www.reactome.org/)

27. **SABIO-RK** (http://sabiork.h-its.org/)
28. **SBMLEditor** (http://www.ebi.ac.uk/compneur-srv/SBMLeditor.html)
29. **SGMP** (http://www.signaling-gateway.org/molecule/)
30. **Sigmoid** (http://sigmoid.sf.net/)
31. **SPDBS** (http://www.springerlink.com/content/c883514423513036/)
32. **SYCAMORE** (http://sycamore.eml.org)

7. **Scripting module (32 software available):**

1. **acslXtreme** (http://acslx.com/)
2. **BioSens** (http://www.chemengr.ucsb.edu/~ceweb/faculty/doyle/biosens/BioSens.htm)
3. **BSTLab**
4. **CADLIVE** (http://www.cadlive.jp)
5. **CellNetAnalyzer** (http://www.mpimagdeburg.mpg.de/projects/cna/cna.html)
6. **COBRA** (http://gcrg.ucsd.edu/Downloads/Cobra_Toolbox)
7. **COPASI** (http://copasi.org)
8. **DOTcvpSB** (http://www.iim.csic.es/~dotcvpsb/)
9. **JSim** (http://www.physiome.org/jsim/)
10. **MatCont** (http://sourceforge.net/projects/matcont/)
11. **MathSBML** (http://www.sbml.org/mathsbml.html)
12. **Metatool** (http://pinguin.biologie.unijena.de/bioinformatik/networks/metatool/metatool5.1/metatool5.1.html)
13. **modelMaGe** (http://modelmage.org/)
14. **Odefy** (http://www.helmholtz-muenchen.de/cmb/odefy)
15. **PathwayLab** (http://innetics.com/)
16. **PK-Sim / MoBi** (http://www.systems-biology.com)
17. **PottersWheel** (http://www.potterswheel.de/)
18. **PySCeS** (http://pysces.sourceforge.net)

19. **RANGE** (http://range.sourceforge.net/)
20. **RMBNToolbox** (http://sourceforge.net/projects/rmbntoolbox)
21. **RSBML** (http://cran.r-project.org/)
22. **SBMLR** (http://www.bioconductor.org/packages/release/bioc/html/SBMLR.html)
23. **SBMLToolbox** (http://sbml.org/Software/SBMLToolbox)
24. **SBToolbox2** (http://www.sbtoolbox2.org/)
25. **SBW** (http://sys-bio.org/)
26. **SimBiology** (http://www.mathworks.com/products/simbiology/)
27. **Simpathica** (http://bioinformatics.nyu.edu/Projects/Simpathica/)
28. **SloppyCell** (http://sloppycell.sourceforge.net/)
29. **SYCAMORE** (http://sycamore.eml.org)
30. **Tide** (http://sysbio.molgen.mpg.de/tide/)
31. **TinkerCell** (http://www.tinkercell.com/)
32. **xCellerator** (http://xlr8r.info/)

8. **Simulation software (87 software available):**

1. **BetaWB** (http://www.cosbi.eu/index.php?option=com_content&view=article&catid=41&id=67&Itemid=156)
2. **BIOCHAM** (http://contraintes.inria.fr/BIOCHAM/)
3. **BioNessie** (http://www.bionessie.org/)
4. **BioNetGen** (http://bionetgen.org/)
5. **BioRica** (http://biorica.gforge.inria.fr/)
6. **BioSyS** (http://applications.eu-eela.eu/application_details.php?l=20&ID=68
7. **BioTapestry** (http://www.biotapestry.org/)
8. **braincirc** (http://braincirc.sourceforge.net/)
9. **ByoDyn** (http://byodyn.imim.es)
10. **CADLIVE** (http://www.cadlive.jp)
11. **Cain** (http://cain.sourceforge.net/)

12. **Cell Illustrator** (http://www.fqs.pl/life_science/cell_illustrator)
13. **CellDesigner** (http://celldesigner.org)
14. **CellNetAnalyzer** (http://www.mpi-magdeburg.mpg.de/projects/cna/cna.html)
15. **Cellware** (http://www.bii.a-star.edu.sg/achievements/applications/cellware/)
16. **CompuCell3D** (http://www.compucell3d.org/)
17. **COPASI** (http://copasi.org)
18. **CRdata** (http://crdata.org/)
19. **Cyto-Sim** (http://www.cosbi.eu/Rpty_Soft_CytoSim.php)
20. **DBSolve** (http://insysbio.ru/en/soft/dbsolveoptimum.html)
21. **Dizzy** (http://magnet.systemsbiology.net/software/Dizzy)
22. **E-CELL** (http://ecell.sourceforge.net/)
23. **ESS** (http://biocomp.ece.utk.edu/)
24. **Facile** (http://facile.sourceforge.net)
25. **FASIMU** (http://www.bioinformatics.org/fasimu)
26. **FERN** (http://www.bio.ifi.lmu.de/FERN)
27. **Genetdes** (http://synth-bio.yi.org/genetdes.html)
28. **Genetic Network Analyzer** (http://www-helix.inrialpes.fr/gna)
29. **Gepasi** (http://www.gepasi.org/)
30. **Gillespie2** (http://www.basis.ncl.ac.uk/software.html)
31. **GNU MCSim** (http://www.gnu.org/software/mcsim/)
32. **iBioSim** (http://www.async.ece.utah.edu/iBioSim/)
33. **insilicoIDE** (http://www.physiome.jp/)
34. **Jarnac** (http://jdesigner.sourceforge.net/Site/Jarnac.html)
35. **JigCell** (http://jigcell.cs.vt.edu/)
36. **JSim** (http://www.physiome.org/jsim/)
37. **Kinsolver** (http://www.cs.uga.edu/~thiab/kinsolver.html)
38. **MatCont** (http://sourceforge.net/projects/matcont/)
39. **MesoRD** (http://mesord.sourceforge.net)
40. **Metaboflux** (http://www.cbib.u-bordeaux2.fr/metaboflux/)
41. **MetaFluxNet** (http://metafluxnet.kaist.ac.kr)

42. **Modesto** (http://bioinformatics.oxfordjournals.org/cgi/content/abstract/20/3/316)
43. **Moleculizer** (http://www.molsci.org/~lok/moleculizer/)
44. **MOOSE** (http://moose.ncbs.res.in/)
45. **Narrator** (http://narrator-tool.org/)
46. **nemo** (http://range.sf.net)
47. **NetBuilder**' (http://strc.herts.ac.uk/bio/maria/Apostrophe/)
48. **Odefy** (http://www.helmholtz-muenchen.de/cmb/odefy)
49. **Oscill8** (http://oscill8.sf.net/)
50. **Pathway Solver** (http://ariadnegenomics.com/technology-research/dynamic-modeling/)
51. **PathwayLab** (http://innetics.com/)
52. **PET** (http://mpf.biol.vt.edu/pet)
53. **PhysioLab** Modeler (http://www.entelos.com/physiolabModeler.php)
54. **PK-Sim** / MoBi (http://www.systems-biology.com)
55. **PNK** (http://page.mi.fu-berlin.de/~trieglaf/PNK2e/index.html)
56. **ProcessDB** (http://www.integrativebioinformatics.com/processdb.html)
57. **PySCeS** (http://pysces.sourceforge.net)
58. **roadRunner** (http://roadrunner.sf.net)
59. **SBML2NEURON** (http://www.neuroml.org/neuron_tools.php)
60. **SBML-PET-MPI** (http://www.bioss.uni-freiburg.de/cms/sbml-pet-mpi.html)
61. **SBMLR** (http://www.bioconductor.org/packages/release/bioc/html/SBMLR.html)
62. **SBML-SAT** (http://sysbio.molgen.mpg.de/SBML-SAT/)
63. **SBMLToolbox** (http://sbml.org/Software/SBMLToolbox)
64. **SBToolbox2** (http://www.sbtoolbox2.org/)
65. **SBW** (http://sys-bio.org/)
66. **sbw**: **javasim** (http://sys-bio.org/sbwWiki/sbw/javasim)
67. **sbw: stochastic simulator** (http://jdesigner.sourceforge.net/Site/Stochastic_Simulation.html)

68. **SIMBA** (http://www.ifak-system.com/services/dynamic-simulation.html)
69. **SimBiology** (http://www.mathworks.com/products/simbiology/)
70. **SloppyCell** (http://sloppycell.sourceforge.net/)
71. **SmartCell** (http://smartcell.embl.de/)
72. **Snoopy** (http://www-dssz.informatik.tu-cottbus.de/DSSZ/Software/Snoopy)
73. **SOSlib** (http://www.tbi.univie.ac.at/~raim/odeSolver/)
74. **STEPS** (http://steps.sourceforge.net/STEPS/)
75. **StochKit** (http://www.engineering.ucsb.edu/~cse/StochKit/)
76. **StochSim** (http://www.pdn.cam.ac.uk/comp-cell/StochSim.html)
77. **STOCKS** (http://www.sysbio.pl/stocks/)
78. **SYCAMORE** (http://sycamore.eml.org)
79. **SynBioSS** (http://synbioss.sourceforge.net/)
80. **TinkerCell** (http://www.tinkercell.com/)
81. **Trelis** (http://www.sourceforge.net/projects/trelis)
82. **VANTED** (http://vanted.ipk-gatersleben.de/)
83. **Vcell** (http://www.vcell.org/)
84. **WebCell** (http://webcell.kaist.ac.kr/)
85. **xCellerator** (http://xlr8r.info/)
86. **Xholon** (http://primordion.com/Xholon)
87. **XPPAUT** (http://www.math.pitt.edu/~bard/xpp/xpp.html)

9. **Utility software (37 software available):**

1. **Antimony** (http://antimony.sourceforge.net/)
2. **BiNoM** (http://bioinfo.curie.fr/projects/binom/)
3. **ByoDyn** (http://byodyn.imim.es)
4. **CADLIVE** (http://www.cadlive.jp)
5. **CellMC** (http://www.cellmc.org/)
6. **CellML2SBML** (http://bioinformatics.oxfordjournals.org/cgi/content/abstract/btl047v1)
7. **CL-SBML** (http://common-lisp.net/project/cl-sbml)

8. **COPASI** (http://copasi.org)
9. **ecellJ** (http://www.jweimar.de/ecellJ)
10. **Facile** (http://facile.sourceforge.net)
11. **GRENDEL** (http://mblab.wustl.edu/software/grendel/)
12. **JSim** (http://www.physiome.org/jsim/)
13. **KEGG2SBML** (http://www.sbml.org/kegg2sbml.html)
14. **KEGGconverter** (http://www.grissom.gr/keggconverter/index.html)
15. **KEGGtranslator** (http://www.ra.cs.uni-tuebingen.de/software/KEGGtranslator/)
16. **MetaFluxNet** (http://metafluxnet.kaist.ac.kr)
17. **MetExplore** (http://metexplore.toulouse.inra.fr)
18. **Odefy** (http://www.helmholtz-muenchen.de/cmb/odefy)
19. **PINT** (http://csb2.ym.edu.tw/cgi-bin/pint/index.cgi)
20. **PK-Sim** / MoBi (http://www.systems-biology.com)
21. **SBFC** (http://sbfc.sourceforge.net/)
22. **SBML Harvester** (http://code.google.com/p/sbmlharvester/)
23. **SBML Translators** (http://www.sys-bio.org/sbwWiki/doku.php?id=sysbio:downloads).
24. **SBML2Antimony** (http://antimony.sourceforge.net/)
25. **SBML2BioPax** (http://www.ebi.ac.uk/compneur-srv/sbml/converters/SBMLtoBioPax.html)
26. **SBML2LaTeX** (http://www.cogsys.cs.uni-tuebingen.de/software/SBML2LaTeX/)
27. **SBML2NEURON** (http://www.neuroml.org/neuron_tools.php)
28. **SBML2Octave** (http://www.ebi.ac.uk/compneur-srv/sbml/converters/SBMLtoOctave.html)
29. **SBML2SMW** (http://code.google.com/p/sbml2smw/)
30. **SBML2XPP** (http://www.ebi.ac.uk/compneur-srv/sbml/converters/SBMLtoXPP-Aut.html)
31. **SBML-SAT** (http://sysbio.molgen.mpg.de/SBML-SAT/)
32. **SBML-shorthand** (http://www.staff.ncl.ac.uk/d.j.wilkinson/software/sbml-

sh/)

33. **SBMLsqueezer** (http://www.cogsys.cs.uni-tuebingen.de/software/SBMLsqueezer/)
34. **sbmltidy** (http://sbml.org/Community/Programs/sbmltidy)
35. **SBW** (http://sys-bio.org/)
36. **semanticSBML** (http://semanticsbml.org)
37. **UTKornTools** (http://biospice.sourceforge.net/)

10. Visualization software (39 software available):

1. **Arcadia** (http://arcadiapathways.sourceforge.net/)
2. **AVIS** (http://actin.pharm.mssm.edu/AVIS2/)
3. **BiNoM Cytoscape Plugin** (http://bioinfo.curie.fr/projects/binom/)
4. **CADLIVE** (http://www.cadlive.jp)
5. **CellDesigner** (http://celldesigner.org)
6. **CellNetAnalyzer** (http://www.mpi-magdeburg.mpg.de/projects/cna/cna.html)
7. **COPASI** (http://copasi.org)
8. **Cytoscape** (http://www.cytoscape.org/)
9. **DBSolve** (http://insysbio.ru/en/soft/dbsolveoptimum.html)
10. **EPE** (http://www.bioinformatics.ed.ac.uk/epe)
11. **Genetic Network Analyzer** (http://www-helix.inrialpes.fr/gna)
12. **iBioSim** (http://www.async.ece.utah.edu/iBioSim/)
13. **iPathways** (http://www.ipathways.org)
14. **JigCell** (http://jigcell.cs.vt.edu/)
15. **JSim** (http://www.physiome.org/jsim/)
16. **KEGGtranslator** (http://www.ra.cs.uni-tuebingen.de/software/KEGGtranslator/)
17. **MesoRD** (http://mesord.sourceforge.net)
18. **MetaFluxNet** (http://metafluxnet.kaist.ac.kr)
19. **MetExplore** (http://metexplore.toulouse.inra.fr)

20. **MOOSE** (http://moose.ncbs.res.in/)
21. **NetBuilder**' (http://strc.herts.ac.uk/bio/maria/Apostrophe/)
22. **Omix** (http://www.13cflux.net/omix)
23. **PaVESy** (http://pavesy.mpimp-golm.mpg.de/)
24. **PET** (http://mpf.biol.vt.edu/pet)
25. **PK-Sim** / MoBi (http://www.systems-biology.com)
26. **ProcessDB** (http://www.integrativebioinformatics.com/processdb.html)
27. **ProMoT** (http://www.mpi-magdeburg.mpg.de/projects/promot)
28. **PySCeS** (http://pysces.sourceforge.net)
29. **SBML Layout** (http://sbmllayout.sf.net/)
30. **SBW** (http://sys-bio.org/)
31. **SBW: Auto Layout** (http://jdesigner.sourceforge.net/Site/Auto_Layout.html)
32. **semanticSBML** (http://semanticsbml.org)
33. **SimBiology** (http://www.mathworks.com/products/simbiology/)
34. **Simulate3D** (http://sys-bio.org/fbergman/Simulate3D.htm)
35. **SimWiz** (http://projects.villa-bosch.de/bcb/software/software/Ulla/SimWiz/)
36. **Snoopy** (http://www-dssz.informatik.tu-cottbus.de/DSSZ/Software/Snoopy)
37. **SYCAMORE** (http://sycamore.eml.org)
38. **Systrip** (http://tulip.labri.fr/TulipDrupal/?q=systrip)
39. **VANTED** (http://vanted.ipk-gatersleben.de/)

2.3.2 Discussion on the Software available for systems Biology:

There are many developments since late nineties in order to help different application in this research area (systems biology) of Biology. Some of them aid to the Metabolic Control Analysis, Flux Balance Analysis, gene network studies, metabolic network analysis, metabolic network reconstruction etc. The most popular software used in the community of systems biology developer (classified by applicability in different fields) are described here along with some interesting and recent tools, which work in the field of systems biology

with new approaches.

1: Analysis software

(a) COBRA: (http://gcrg.ucsd.edu/Downloads/Cobra_Toolbox)

("*Quantitative prediction of cellular metabolism with constraint-based models: the COBRA Toolbox.*

", Becker SA, Feist AM, Mo ML, Hannum G, Palsson BØ, Herrgard MJ, 2007)

COBRA is one of the most popular SBML based analysis software among systems biology software.

COBRA stands for Constraint-Based Reconstruction and Analysis. This software package is based on Matlab platform. It uses the constraint based approach for the quantitative prediction of cell behavior. It includes implementations of many of the commonly used forms of constraint-based analysis such as FBA, gene deletions, flux variability analysis, sampling, and batch simulations together with tools to read in and manipulate constraint-based models.

(b) COPASI: (http://copasi.org)

("*COPASI—a COmplex PAthway Simulator*", Stefan Hoops, Christine Lee, Mudita Singhal, Liang Xu, Pedro Mendes. 2006). COPASI is a software application for simulation and analysis of biochemical networks and their dynamics. COPASI is a stand-alone program that supports models in the SBML standard and can simulate their behavior using ODEs or Gillespie's stochastic simulation algorithm; arbitrary discrete events can be included in such simulations. COPASI provides a C++ API with language bindings for Perl, python, R, Java, and Octave and is able to communicate with the Systems Biology Workbench COPASI carries out several analyses of the network and its dynamics and has extensive support for parameter estimation and optimization. COPASI provides means to visualize data in customizable plots, histograms and animations of network diagrams.

COPASI: feature list

- *Model:*
  - Chemical reaction network.
  - Arbitrary kinetic functions.

- ODEs for compartments, species, and global quantities.
- Assignments for compartments, species, and global quantities.
- Initial assignments for compartments, species, and global quantities.
- SBML import (L1V1-2, L2V1-4, L3V1) and export (L1V2, L2V1-4).

- Analysis:
  - Stochastic and deterministic time course simulation
  - Steady state analysis (including stability).
  - Metabolic control analysis/sensitivity analysis.
  - Elementary mode analysis .
  - Mass conservation analysis.
  - Time scale separation analysis
  - Calculation of Lyapunov exponents.
  - Parameter scans.
  - Optimization of arbitrary objective functions.
  - Parameter estimation using data from time course and/or steady state experiments simultaneously.
- *Graphical User Interface (CopasiUI)*
  - Sliders for interactive parameter changes.
  - Color-coded tables
  - 3D bar charts
  - Plots and Histograms.
  - Network diagram visualization of results.
- Command Line (CopasiSE) for batch processing.
- Versions for MS Windows, Linux, Mac OS X, and Solaris SPARC.
- Loading of legacy Gepasi files.
- Export to Berkeley Madonna, XPPAUT, and C source code of the ODE system generated from the model.
- Saving of mathematical formulas and ODEs in MathML or LaTeX

(c) TinkerCell: (http://www.tinkercell.com/)

(“ *TinkerCell: modular CAD tool for synthetic biology* ”, Chandran D, Bergmann FT, Sauro HM, 2009)

TinkerCell is a Computer-Aided Design software tool for Synthetic Biology. It combines visual interface with programming API (Python, Octave, C, and Ruby) and allows users to share their code with each other via a central repository. TinkerCell is designed with the anticipation that the future of synthetic biology will be an intricate interplay between a variety of experimental techniques, databases that store results from experiments, and mathematical models explaining different aspects of the experiments. At present, the functionalities include deterministic and stochastic simulation (C libraries), steady state analysis, flux balance analysis using LPsolve C library, graph analysis through the NetworkX python module, and all the functionalities of PySCeS python module, including sensitivity and structural analysis. TinkerCell can build models by connecting modules. TinkerCell models contain meta-data for supporting a parts database. The visual display format is flexible.

The analysis step can potentially include:

1. mathematical analysis of non-linear systems.
2. stochastic simulations, structural analysis, and other methods from systems biology.
3. prediction of evolutionary trajectories for directed evolution.
4. analysis and optimization of the DNA sequence.
5. database look-up to find suitable components.
6. generate different versions of the same design.
7. load experimental data from database(s) and relate them to the diagram.

2: Annotation software

(a) **CellDesigner (http://celldesigner.org)**

(“*CellDesigner: a modeling tool for biochemical networks* ”, Akira Funahashi , Yukiko Matsuoka, Akiya Jouraku, Hiroaki Kitano, 2008)

CellDesigner is a structured diagram editor for drawing gene-regulatory and biochemical networks. Networks are drawn based on the process diagram, with graphical notation

system, proposed by Kitano, and are stored using the Systems Biology Markup Language (SBML), a standard for representing models of biochemical and gene-regulatory networks. CellDesigner supports simulation and parameter scan by integration with SBML ODE Solver and Copasi. By using CellDesigner, users can browse and modify existing SBML models with references to existing databases (MIRIAM supported), simulate and view the dynamics through an intuitive graphical interface.

CellDesigner has following features.

- Representation of biochemical semantics;
- Detailed description of state transition of proteins;
- SBML compliant (SBML Level-1 and Level-2);
- Integration with SBW-enabled simulation/analysis modules;
- Integration with native simulation library (SBML ODE Solver);
- Capability of database connections;
- Extreme portability as a Java application .

(b) PAYAO (http://www.payaologue.org **)**

(“*Payao: Web 2.0 community tagging system to SBML models* ”, Norihiro Kikuchi, Yukiko Matsuoka, Haruka Sugimura, Hiroaki Kitano, 2008)

PAYAO is a community collaborative web service platform for gene-regulatory and biochemical pathway model curation. PK-Sim / MoBi, Systems biology software platform for multiscale physiological modeling and simulation with a focus on physiologically-based pharmacokinetics and -dynamics (PBPK/PD) including interfaces to MATLAB and R. Available to academic researchers via a free non-commercial license.

Major features of “Payao” alpha version are as follows;

- User access control
- Register SBML models to the system
- View the list of all the registered models
- Manage MyModels, and FavoriteModels
- View SBML models in CellDesigner 3.5 notation.
- View “Notes” added by CellDesigner 3.5

- Add Tags which contain keywords, links, pubmed IDs and free text to the target Species/Reactions, as well as user-defined components and areas.
- Add comments to the tags

System Requirement:

Tomcat 5.5.x as servlet container, JRE 5.0 and above, Seaser 2 (S2Flex2) as framework.

RDBMS: MySQL 5.0 and above, and CellDesigner 3.5 API

3:Creation/development software

(a) SBML2NEURON: (http://www.neuroml.org/neuron_tools.php)

("*NeuroML: A Language for Describing Data Driven Models of Neurons and Networks with a High Degree of Biological Detail"*, P Gleeson, S Crook, RC Cannon, ML Hines, GO Billings, M Farinella, TM Morse, AP Davison, S Ray, US Bhalla, SR Barnes, YD Dimitrova, RA Silver, 2010)

SBML2NEURON is a provisional implementation of an SBML to NEURON converter. This uses the Python bindings of libSBML to generate an NMODL file containing the model represented in a basic SBML file, which can then be inserted onto a section in NEURON for simulation. It can be used to simulate some of the models in BioModels Database. This is a software allows closer integration between NeuroML and SBML in realistic neuronal models. Here,The NeuroML project focuses on the development of an XML based description language that provides a common data format for defining and exchanging descriptions of neuronal cell and network models. Approach in the project uses XML schemas to define the model specifications. The current scope of NeuroML focuses on models which are based on the biophysical and anatomical properties of real neurons, i.e. which include details of the detailed neuronal morphologies, the membrane conductance which underlay action potential generation (conductance based models), and which are based on known anatomical connectivity.

(b) SigTran: (http://www.cellsystems.org/teams/modeling/projects/sigtran/overview.html)

SigTran is a modeling environment especially designed to enable biological researchers to carry out large scale simulations and analysis of complex signal transduction networks.

SigTran has incorporated some of the latest developments in the field of stochastic simulation of biological networks. Some of these major developments include the Firth-Bray algorithm with molecular complexes treated as software objects with multistate functionality, spatial organization of cell signaling pathways and the algorithmic enhancements to the Gillespie algorithm.

SigTran is built around a powerful and flexible stochastic engine, written entirely in Fortran 90/95. SigTran offers biological researchers a choice of four major stochastic algorithms including (a) the Firth-Bray algorithm of StochSim (b) Gillespie (c) Gillespie-Gibson and (d) a novel uniform time stepping algorithm. In addition to running simulations of biological network models in a stochastic mode, SigTran can be switched into a deterministic mode. SigTran provides full simulation support for systems of ordinary differential and algebraic equations.

SigTran currently supports

- Complete elementary reaction capability up to and including ternary reactions
- Michaelis-Menton kinetics
- Clamping of species copy numbers
- Multistate specification and simulation
- Tagged molecule or reaction tracking
- DAE based kinetic simulations for comparison with stochastic simulations and model debugging
- Ensemble simulation with run time and post run time statistical processing
- Graphical display and plotting of simulation output.

(c) Athena: (http://athena.codeplex.com/)

("Athena: Modular CAM/CAD Software for Synthetic Biology", Deepak Chandran, Frank T. Bergmann, Herbert M. Sauro, 2009)

Athena allows biological models to be constructed as modules. Modules can be connected to one another without altering the modules themselves. In addition, Athena houses various tools useful for designing synthetic networks including tools to perform simulations, automatically derive transcription rate expressions, and view and edit synthetic DNA sequences. New tools can be incorporated into Athena without modifying existing program via a plug-in interface, IronPython scripts, Systems Biology Workbench interfacing and the R statistical language.

4:Data integration and management software

(a)**CADLIVE: (http://www.cadlive.jp) C**omputer-**A**ided **D**esign of **LIV**ing syst**E**ms)

(*"CADLIVE dynamic simulator: Direct link of biochemical networks to dynamic models"*, Kentaro Inoue, Sayaka Tomeda, Shinpei Tonami, Yuki Shimokawa, Masayo Ono, Hiroyuki Kurata, 2005)

CADLIVE is a comprehensive computational tool that analyzes and rationally designs large-scale biochemical networks at the molecular interaction level. It provided a rule-based automatic way to convert biochemical network maps into dynamic models, which enables simulating their dynamics without going through all of the reactions down to the details of exact kinetic parameters. It consists of a GUI network constructor, database, a pathway search module for knockout mutants, a network layout module, and the dynamic simulator that automatically converts biochemical network maps into mathematical models. Once a biochemical map is provided, CADLIVE automatically builds a mathematical model, thereby facilitating one to simulate and analyze it.

(b) JSim (http://www.physiome.org/jsim/ **)**

("A Java-based Simulation and Animation Environment: JSIM's Foundation Library (1997)", Zhiwei Zhang , Zhiwei Zhang , Zhiwei Zhang)

JSim is a Java-based simulation system for building quantitative numeric models and analyzing them with respect to experimental reference data. JSim's primary focus is in physiology and biomedicine, however its computational engine is quite general and

applicable to a wide range of scientific domains. JSim models may intermix ODEs, PDEs, implicit equations, integrals, summations, discrete events and procedural code as appropriate. JSim's model compiler can automatically insert conversion factors for compatible physical units as well as detect and reject unit unbalanced equations. JSim also supports model archive formats SBML (import and export) and CellML (import only).

(c) ONDEX (http://www.ondex.org/ **)**

("Graph-based analysis and visualization of experimental results with ONDEX", Jacob Köhler, Jan Baumbach, Jan Taubert, Michael Specht, Andre Skusa , Alexander Rüegg, Chris Rawlings, Paul Verrier Stephan Philippi, 2006).

The Ondex data integration platform enables data from diverse biological data sets to be linked, integrated and visualized through graph analysis techniques. The central idea behind data integration in ONDEX is to overcome technical and semantic heterogeneities between different data sources., this means converting different heterogeneous data sources into a common graph-based data structure in two fully automatic steps

1. Import of databases and ontology.
2. Alignment of data from different sources.

Ondex uses a rich and flexible core data structure, which has the ability to bring together information from structured databases and unstructured sources such as biological sequence data and free text. Ondex also allows users to visualize and analyze the integrated data. Ondex is free and open-source software.

5:Framework or library

(a)**Metannogen** (http://www.bioinformatics.org/strap/metannogen/)

"Metannogen: annotation of biological reaction networks" ,Christoph Gille, Katrin Hübner, Andreas Hoppe, Hermann−Georg Holzhütter, 2011).

Metannogen can do following things.

(I) browse and annotate existing biological networks

(II)reconstruct biological networks.

I) Annotating existing networks:

Metannogen is a JAVA program with which we can browse and annotate existing biological networks given in SBML. It is optimized for compartmentalized metabolic networks. Metannogen provides advance features to facilitate manual attachment of annotation texts and cross-references.

Types of annotations added by curators:

1. Free text
    - Source of information (Database or literature cross-references)
    - Private notes, remarks, to-do's
    - Questions to colleagues
    - Database searches: Google, Pubmed, Blast
    - Predictions: Sub-cellular localizations
2. Controlled vocabulary. Syntax like string variable declaration in programming language BASIC. Customizable input masks may be defined.
    - Simple XML Attributes
    - Rdf Annotations
    - Highlighting rules
    - Evidence level

II) Reconstruction of metabolic networks:

Metannogen can also be used as the primary tool for network reconstruction. This is particular useful for large metabolic networks. It had been the basic tool for the reconstruction of HepatoNet, a compartmentalized metabolic network of the hepatocyte. However, smaller networks are easier reconstructed using a graphical network constructor. In this case Metannogen may serve as an interactive annotation tool.

Features of Metannogen are as follows:

i)Text views:

- Pubmed based literature management
    - Association of full text PDF files

- Automated download of Uniprot and Pubmed documents
- Sharing PDF full text files

- Spell-check
- Multi keyword highlighting
- Customizable crosslinks
- Auto word completion
- Balloon help.
- Context menu
  - Customizable cross-links
  - Customizable shell commands

ii) Data Management/Export:

- Search&Replace
- Customizable export as SBML, SQL and CSV.
- Interface to libSBML.
- Backup for each session with time stamp. Logging all dataset uploads on the server.
- Tools for topological network analysis

iii) Kegg Pathway maps:

- Click-able reactions and metabolites
- Context menu
- Highlighting by marching ants
- Visualization of numeric data like mRNA expression levels

(b) Odefy (http://www.helmholtz-muenchen.de/cmb/odefy)

("Odefy - From discrete to continuous models", Jan Krumsiek, Sebastian Pölster, Dominik M Wittmann , Fabian J Theis, 2010).

Odefy, is a MATLAB- and Octave-compatible toolbox for the automated transformation of Boolean models into systems of ordinary differential equations. Models can be created

from sets of Boolean equations or graph representations of Boolean networks. Alternatively, the user can import Boolean models from the CellNetAnalyzer toolbox, GINSim and the PBN toolbox. The Boolean models are transformed to systems of ordinary differential equations by multivariate polynomial interpolation and optional application of sigmoidal Hill functions. This toolbox contains basic simulation and visualization functionalities for both, the Boolean as well as the continuous models. For further analyses, models can be exported to SQUAD, GNA, MATLAB script files, the SB toolbox, SBML and R script files. Odefy contains a user-friendly graphical user interface for convenient access to the simulation and exporting functionalities.

(c) PySCeS (http://pysces.sourceforge.net)

("PySCeS -Python Simulator for Cellular Systems ", Johann Rohwer, Brett Olivier, Jannie Hofmeyr).

PySCeS the Python Simulator for Cellular Systems is an extendable toolkit for the analysis and investigation of cellular systems. PySCeS is developed in Python and has been designed to be used both interactively and as a library. It utilizes a human readable, model description language for describing models as well as being SBML compatible. PySCeS includes stoichiometric, simulation, steady state and Eigen analysis using direct non-linear root finders. It also includes full support for Metabolic Control Analysis (MCA), the characterization of static bifurcations, multidimensional parameter scanning and 2/3D graph capabilities. Currently an extension PySCeS-CBM is being developed that allows for the interactive manipulation, modeling and optimization of genome scale, constraint based models (e.g. flux balance analysis)

6:Repository or database

(a) BioCyc: (http://www.biocyc.org/ **)**

BioCyc is a collection of 1763 Pathway/Genome Databases (PGDBs). Each BioCyc PGDB describes the genome and metabolic pathways of a single organism. The BioCyc Web site contains tools for navigating, visualizing, and analyzing these databases, and for analyzing

omics data:

- Genome browser
- Display of individual metabolic pathways, and of full metabolic maps
- Visual analysis of user-supplied omics datasets by painting onto metabolic maps, regulatory maps, and genome maps
- Enrichment analysis of omics datasets
- Store groups of genes and pathways in your account; share, analyze, transform those groups
- Comparative analysis tools

The BioCyc databases are divided into three tiers, based on their quality. Tier 1 databases have received person-decades of literature-based curation, and are the most accurate. Tier 2 and Tier 3 databases contain computationally predicted metabolic pathways, predictions as to which genes code for missing enzymes in metabolic pathways, and predicted operons.

(b) BRENDA: (http://brenda-enzymes.org/ **)**

("BRENDA, enzyme data and metabolic information",Ida Schomburg, Antje Chang, Dietmar Schomburg , 2002)

the BRaunschweig ENzyme Database is a comprehensive information system covering enzymes and their activities. The majority of the data are manually extracted from the primary literature. The content covers information on function, structure, occurrence, preparation and application of enzymes as well as properties of mutants and engineered variants. In 2011, BRENDA introduced the ability to output data in SBML format.

(c) Reactome: (http://www.reactome.org/ **)**

("Reactome: a knowledgebase of biological pathways", G. Joshi-Tope1, M. Gillespie1, I. Vastrik, P. D' Eustachio, E. Schmidt, B. de Bono, B. Jassal, G.R. Gopinath, G.R. Wu, L. Matthews, E. Birney, L. Stein)

REACTOME is an open-source, open access, manually curated and peer-reviewed pathway database. Pathway annotations are authored by expert biologists, in collaboration with Reactome editorial staff and cross-referenced to many bioinformatics databases.

These include NCBI Entrez Gene, Ensembl and UniProt databases, the UCSC and HapMap Genome Browsers, the KEGG Compound and ChEBI small molecule databases,PubMed, andGene Ontology. Reactome provides an intuitive website to navigate pathway knowledge and a suite of data analysis tools to support the pathway-based analysis of complex experimental and computational data sets. Visualization of Reactome data is facilitated by the Pathway Browser, a Systems Biology Graphical Notation (SBGN)-based interface that supports zooming, scrolling and event highlighting. It exploits the PSIQUIC web services to overlay molecular interaction data from the Reactome Functional Interaction Network and external interaction databases such as IntAct, ChEMBL, BioGRID and iRefIndex. Reactome is an all-inclusive resource of human pathways for basic research, genome analysis, pathway modeling, systems biology and education.

7:Scripting module

(a) **SYCAMORE: (**http://sycamore.eml.org **)**

(“SYCAMORE--a systems biology computational analysis and modeling research environment”, Weidemann A, Richter S, Stein M, Sahle S, Gauges R, Gabdoulline R, Surovtsova I, Semmelrock N, Besson B, Rojas I, Wade R, Kummer U, 2008).

SYCAMORE is a system that provides you with a facilitated access to a number of tools and methods in order to build models of biochemical systems, view, analyze and refine them, as well as perform quick simulations. SYCAMORE is not intended to substitute for expert simulation and modeling software packages, but might interact with those. It is rather intended to support and guide system biologists when doing computational research.

One important function of SYCAMORE is to allows us to build a draft model of your system of interest in such a way that kinetic expressions and parameters are as close to reality as possible. We want to emphasize that the resulting model still has a draft character and should not be taken as "the final model". However, setting up your model in such a way that parameters etc. are as close to reality as possible on the basis of literature data and computational parameter estimation methods should facilitate any parameter fitting methods that you want to employ later on.

SYCAMORE allows to build, view and edit models, to analyze and refine them, to perform

simulations, sensitivity analysis and parameter estimations. To do so, one of these following options can be selected:

- Build a new model starting from scratch by defining reactions, metabolites, kinetic equations and parameters.(build new model)
- Build a new model with the support of SABIORK, a database that stores reactions and their corresponding kinetic parameters. (build SABIORK model)
- Load a SBML model from your hard disk.(load model from disk)
- Load a SBML model from projects. SYCAMORE offers the possibility to store complete and incomplete models in an internal database as your personal 'projects'.(load model from projects)
- Load an example model for testing of SYCAMORE. (load example model)
- Additionally, you may perform parameter estimations in order to determine unknown parameter values. (parameter estimation)

(b) acslXtreme (http://acslx.com/)

(“An implementation of the Expectation-Maximisation (EM) algorithm for population pharmacokinetic–pharmacodynamic modeling in ACSLXTREME”, James W.T. Yates, 2009)

acslX is a modeling, execution, and analysis environment for continuous dynamic systems and processes. acslXtreme provides an intuitive environment for users at all levels and is versatile and powerful enough to address the most challenging simulation problems. acslXtreme allows to model the full nonlinear behavior of the system or process. When modeling systems that involve both controls and physical systems, for example, there is no need to linearize the physical system model to be able to design and apply the controller. With acslXtreme, nonlinear system attributes can be fully represented. There is no limitation on program size, number of equations, states or variables. So, large real-life systems with all of the complexities can be represented. The acslXtreme graphical modeling environment utilizes the concept of PowerBlocks and Libraries to manage

reusable modeling assets. PowerBlocks represent reusable models with functionality ranging form the simple (e.g., math function to sum two numbers) to the very complex (e.g., a complete engine model.) Libraries are encapsulated block sets organized by function, application domain, or any other paradigm the user chooses to incorporate. Several Libraries are provided free with acslXtreme to accomplish common modeling functions such as math, linear operations, and plotting. acslXtreme provides more than 300 advanced mathematical, statistical, scientific, and engineering functions including general math, linear algebra, and matrix manipulation for the analysis of simulation results.

8: Simulation software

(a) FASIMU: (http://www.bioinformatics.org/fasimu)

("FASIMU: flexible software for flux-balance computation series in large metabolic networks". Andreas Hoppe, Sabrina Hoffmann, Andreas Gerasch, Christoph Gille, Hermann-Georg Holzhütter, 2011)

FASIMU is a command line oriented software for the computation of flux distributions using a variety of the most common FBA algorithms, it implement the following also

(i) weighted flux minimization

(ii) fitness maximization for partially inhibited enzymes,

(iii)the concentration-based thermodynamic feasibility constraint.

It allows heterogeneous computation series suited for network pruning, leak analysis, FVA, and systematic probing of metabolic objectives for network curation controlled by an intuitive description file. The metabolic network can be supplied in SBML, CellNetAnalyzer, and plain text format. The platform-independent program is an open-source project, freely available under GNU public license.

(b) CellNetAnalyzer: (http://www.mpi-magdeburg.mpg.de/projects/cna/cna.html **)**

("Structural and functional analysis of cellular networks with *CellNetAnalyzer"*, Steffen Klamt, Julio Saez-Rodriguez Ernst D Gilles, 2007 **)**

CellNetAnalyzer is a toolbox for MATLAB facilitating, it is an interactive and visual software, and for the comprehensive structural analysis of metabolic, signaling and regulatory networks. CNA facilitates the analysis of metabolic (stoichiometric) as well as signaling and regulatory networks solely on their network topology, i.e. independent of kinetic mechanisms and parameters. CNA provides a powerful collection of tools and algorithms for structural network analysis which can be started in a menu-controlled manner within interactive network maps.
CellNetAnalyzer consists of:

(i) user-defined network projects and

(ii) a toolbox with various functions for structural network analysis:

(i) Network projects that are created and designed by the user. A network project is of type *Mass-flow* (modeling material flows as in metabolic or other stoichiometric reaction networks) or of type *Signal-flow* (modeling information or signal flows as in signal transduction networks or regulatory networks). Each network project comprises an abstract (symbolic) network representation as well as one or several network graphics visualizing the network under investigation. The abstract network model is composed by declaring network elements such as reactions or compounds, whereas the network graphics have to be imported and thus created by other programs

(ii) The toolbox of *CellNetAnalyzer* provides functions and procedures which, depending on the network type, facilitate stoichiometric (metabolic) network analysis or the analysis of signal-flow networks.

Here is a list of functions for network analysis provided in *CellNetAnalyzer*:

Mass-flow (stoichiometric, metabolic) networks:

i) Metabolic flux analysis

- Classification of flux scenarios (determinacy and redundancy) and rates (balance-ability and calculation-ability)
- Calculation of flux distributions (for all types of flux scenarios)

- Consistency checks in redundant systems
- Flux optimization subject to an arbitrary linear objective function (flux balance analysis, FBA)
- Sensitivity analysis of calculated rates
- Feasibility check of a given scenario

ii) Analysis of basic topological/structural properties

- Graphical display of the stoichiometric matrix
- Computation of graph-theoretical path lengths in an directed and undirected graph representation of the reaction network; determination of network diameter
- Detection of (elementary) conservation relations, enzyme subsets, isoenzymes, blocked and parallel reactions
- Connectivity histogram

iii) Metabolic pathway analysis

- Large-scale calculation of elementary (flux) modes, extreme pathways and convex bases with new algorithms (optionally, METATOOL or EFMTOOL can be used (on the fly) for calculations)
- New: inhomogeneous constraints can be considered
- Display of computed pathways in the interactive maps
- Selection of pathways with respect to certain criteria
- Statistical analysis of pathways:
    - Yield histogram; detection of optimal and sub-optimal pathways
    - Reaction participation; prediction of mutant phenotype
    - Quantitative estimating the importance of reactions: control-effective fluxes (CEF)
    - Pathway lengths histogram
    - Export of computed elementary modes for external analysis

iv) Minimal cut sets

- Finding targets in and analyzing the fragility of biochemical reaction networks
- Efficient calculation of minimal cut sets (with respect to a specified set of (target) elementary modes)
- New: constrained minimal cut sets can be computed (by specifying a set of target modes and a set of desired modes)
- Display of minimal cut sets within the interactive maps
- Statistical analysis and assessment of minimal cut sets

Signal-flow (signaling, regulatory) networks:

i)Analysis of interaction graphs

- Basic topological properties
- Large-scale computation of all positive and negative signaling paths connecting inputs with outputs or of all signaling paths between given sets of start and end nodes; statistical analysis of these paths
- Large-scale computation of all positive and negative feedback loops; statistical analysis of these loops
    - Computation of minimal cut sets (removing reactions or species) for a given set of paths or/and loops
    - Computation of distance (shortest paths) matrices; separately for positive and negative paths
    - Large-scale dependency analysis (which species has (positive/negative) influence on which species; identification of activators and inhibitors of a given species enabling predictions on perturbation experiments)
    - Detection of inconsistencies between experimental (high-throughput) data and dependency matrix

ii)Analysis of logical (Boolean) interaction networks

- Arbitrary logical models (constructed with AND,OR and NOT operators) with

multiple discrete levels can be set-up

- Logical steady state analysis for a given set of inputs/fixed states: useful for studying input-output behavior and signal processing
- Odefy plug-in (developed by Fabian Theis' group: Jan Krumsiek, Dominik Wittmann): simulate and export ODE models created from Boolean models
- Computation of (logical) minimal intervention sets (sets of knock-outs/knock-ins) repressing or provoking a certain behavior or function of the network
- Computation of species equivalence classes
- Automated conversion of the logical model into an interaction graph

General features (for mass-flow and signal-flow networks):

- API: The API (Application Programming Interface) of CNA allows interested users and developers
  - To read/write or import/export the network structure of a project
  - To read values from text boxes (GUIs), then to perform own calculations and finally to display the results in the interactive network maps
  - To call selected functions of CNA (such as the computation of elementary modes or signaling paths) independently of the CNA GUI
  - To integrate own functions as a new menu-entry in CNA's menu - you can thus construct and integrate plugging for CNA
  - To change network/project attributes directly from MATLAB's command line (only for advanced users; not recommended for beginners)
- Clipboard function: for saving (temporarily) intermediate results; allows also to combine different scenarios arithmetically (+, -, \, *) - useful for comparing different scenarios (e.g. two different flux distributions)
- Network composer (Fig. 1): editing the network structure (with the help of masks as in Fig. 2)
- Element selector: search for species and reactions/interactions using diverse filters and specifications
- Scenarios (e.g. different flux distributions) can be saved and then loaded later again
- Export of the network in ASCII format

- SBML export and import (mass-flow networks only)
- Zoom tool (for zooming in and out in large maps)
- API functionalities: exchange of data/variables/models between CellNetAnalyzer and external functions or applications
- Toolbar for frequently used actions (e.g. loading or saving a scenario)

(c) E-CELL: (http://ecell.sourceforge.net/)

("E-CELL: software environment for whole-cell simulation", M Tomita, K Hashimoto, K Takahashi, T S Shimizu, Y Matsuzaki, F Miyoshi, K Saito, S Tanida, K Yugi, J C Venter, C A Hutchison 3rd, 1999)

E-Cell System is an object-oriented software suite for modeling, simulation, and analysis of large scale complex systems such as biological cells. The E-CELL system allows a user to define functions of proteins, protein–protein interactions, protein–DNA interactions, regulation of gene expression and other features of cellular metabolism, as a set of reaction rules. E-CELL simulates cell behavior by numerically integrating the differential equations described implicitly in these reaction rules. The user can observe, through a computer display, dynamic changes in concentrations of proteins, protein complexes and other chemical compounds in the cell.

E-Cell System consists of the following three major parts:

- E-Cell Simulation Environment (or E-Cell SE)
- E-Cell Modeling Environment (or E-Cell ME)
- E-Cell Analysis Toolkit

9: Utility software

(a) CellMC: (http://www.cellmc.org/)

("CellMC—a multiplatform model compiler for the Cell Broadband Engine and ×86", Department of Information Technology, Uppsala University, 2009)

CellMC is an open source program generator that compiles a mesoscopic model of a biochemical reaction network, expressed as SBML, into an executable program that realizes stochastic simulation algorithm (Gillespie algorithm) for that model. *CellMC* generates a program that implements SSA for a model expressed as SBML Level 2, Version 3. *CellMC* uses a vectorized version of ODM (the optimized direct method) and has command-line arguments for tuning certain features of the vectorized algorithm. *CellMC* works by transforming a model expressed as SBML into performance-optimized C (including inline assembly and/or SSE2 intrinsic), then calling gcc — and whatever utilities must be used to produce an executable for the host platform to compile the model-specific code and link with model-invariant supporting libraries. *CellMC* was developed in the Computational Systems Biology Group of the Division of Scientific Computing in the Department of Information Technology at Uppsala University.

(b) PINT: (http://csb2.ym.edu.tw/cgi-bin/pint/index.cgi)

("PINT: **P**athways **IN**tegration **T**ool", Y.T. Wang, Y.H. Huang, Y.C. Chen, C.L. Hsu, U.C. Yang, 2010)

The Pathways integration tool (PINT) is designed to assist users to conduct biological pathway integration (BPI), and to explore the possible phenotypic outcomes under a particular physiological or pathological condition. Pathways integration Tool (PINT) may integrate the standard SBML files. Since these files may be obtained from different sources, any inconsistency in component names can be revised by using an annotation editor upon uploading a pathway model. This integration function greatly simplifies the building of a complex model from small models. Relevant models can be selected and sent to the workbench by using a user-friendly query interface, which also accepts a gene list derived from high-throughput experiments. The models on the workbench, from either a public or a private source, can be integrated and painted. The painting function is useful for highlighting important genes or even their expression level on a merged pathway diagram, so that the biological significance can be revealed.

10: Visualization software

(a) **Snoopy:** (http://www-dssz.informatik.tu-cottbus.de/DSSZ/Software/Snoopy)

("Snoopy- a unifying Petri net framework to investigate biomolecular networks", Christian Rohr, Wolfgang Marwan, Monika Heiner,2010)

Snoopy is a software tool to design and animate hierarchical graphs, among others Petri nets. The tool is in use for the verification of technical systems, especially software-based systems, as well as for the validation of natural systems, i.e. biochemical networks as metabolic, signal transduction, gene regulatory networks

Basic Properties

- extensible
- generic design facilitates add on of new graph types
- adaptive
- simultaneous use of several graph types
- GUI adopts dynamically to graph type in active window
- platform independent
- implementation: C++, wxWidgets, Xerces
- supported for Windows, Mac OS X and Linux

(b) **Omix:** (http://www.13cflux.net/omix)

(Visualizing multi-omics data in metabolic networks with the software Omix: a case study", Droste P, Miebach S, Niedenführ S, Wiechert W, Nöh K)

Omix is software for the visualization of any data in biochemical networks. The unique feature of Omix is: the software is programmable by a scripting language called Omix Visualization Language (OVL). In Omix, the visualization of data coming from experiment or simulation is completely performed by the software user realized in concise OVL scripts. By this, visualization becomes most flexible and adaptable to the requirements of the user and can be adapted to new application fields.

Features

Omix' unique features include:

- Drawing stylish network diagrams with extensive annotation potential.
- Interactive visualization of data from experiment as well as simulation in metabolic networks.
- Different levels of detail to decrease complexity and flexibly highlight different aspects of the network structure.
- Support of the drawing process by semi-automatic drawing features.
- Extensible by plug-ins.
- Visual analysis of time-dependent data by animations.
- Visualization of chemical structures.
- 3D visualization of data and network topologies.
- Network analysis: elementary flux modes, network dependencies, flux balances.

Programmability:

One outstanding feature of Omix is *OVL*, an object-oriented scripting engine that allows programming of network diagrams. Here, programming networks means for example definition of event-driven user interaction and dynamic modification of all individual attributes of graphical elements in a drawing. This way, time-dependent numerical data are animated in the context of network diagrams with ease.

Usability:

Although Omix has been developed having primarily drawings of biochemical networks in mind, the software is actually a fairly general vector-based network drawing program: nodes may be arbitrary polygons or image maps and the line type and stroke of edges can be chosen freely.

2.4 Flux Balance Analysis:

Flux balance analysis is on of the most popular approach to study biological networks. FBA is very helpful in studying the Genome-scaled metabolic networks. The study is done

by biological network reconstruction. Calculation of metabolic flux flows through network can be calculated by FBA. As so it can predict the growth rate of an organism as well as growth rate of metabolite which is biologically important for the survival of organism. The metabolic models 35 organisms already available (http://systemsbiology.ucsd.edu/In_Silico_Organisms/Other_Organisms) and the availability of high-throughput technologies which are enabling the construction of many more models each year , so FBA is becoming an important tool for solving the unanswered questions related to these models.

Steps of FBA calculation: (example calculation)

1: Reaction network creation

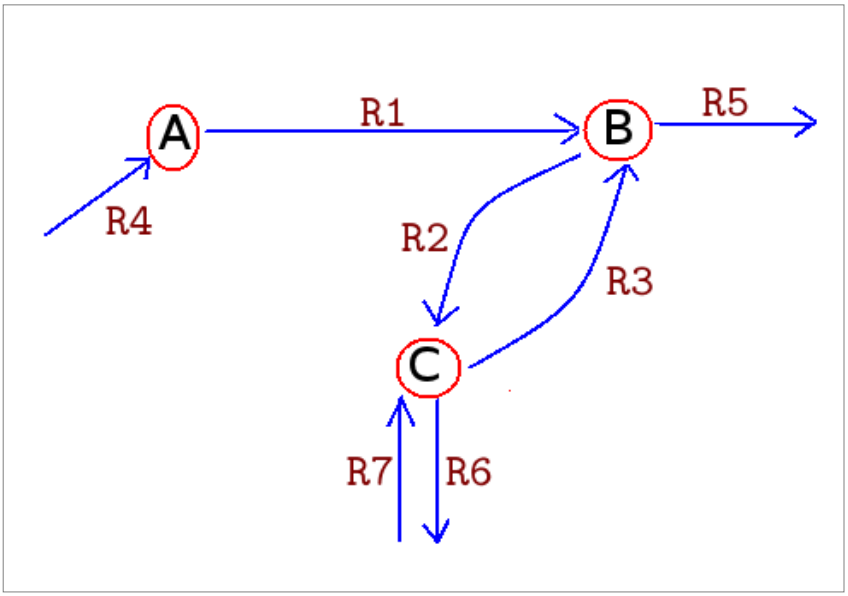


Fig-1 example of a chemical reaction

Chemical reaction associated to this network:

Internal reactions:

R1: -1A---> 1B

R2: -1B---> 1C

R3: -1C---> 1B

Exchange Reactions:

R4: 1A

R5: -1B

R6: -1C

R7: 1C

Stoichiometric matrix: S=

	R1	R2	R3	R4	R5	R6	R7
A	**-1**	**0**	**0**	**1**	**0**	**0**	**0**
B	**1**	**-1**	**1**	**0**	**-1**	**0**	**0**
C	**0**	**1**	**-1**	**0**	**0**	**-1**	**1**

2: FBA formulation

Dynamic mass balance:

$$\mathbf{d}C/\mathbf{d}t = \mathbf{S}v$$

Where: **C**: Concentration

***t*:** Time

S: Stoichiometric matrix

***v*:** Flux Vector

Steady State Assumption:

$$\mathbf{S}v=0$$

Liner Programming Formulation:

(Here objective is to maximize the **B** production hence maximize the **R5.)**

So, **Objective Z max R5**

(Assumption here is the **max value of R5=1**)

Constrains:

	R1	R2	R3	R4	R5	R6	R7
A	-1	0	0	1	0	0	0
B	1	-1	1	0	-1	0	0
C	0	1	-1	0	0	-1	1

$$\begin{bmatrix} V1 \\ \vdots \\ V7 \end{bmatrix} = 0$$

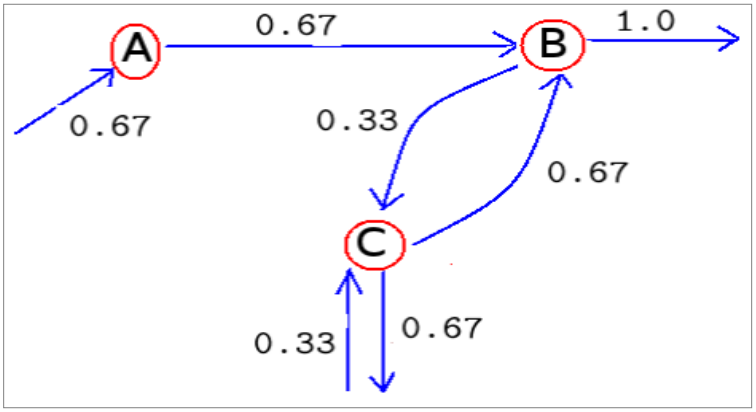
0<=V1.....V7<=1;

3: Relative Flux distribution at steady state

Z=1

V= [**0.67 0.33 0.67 0.67 1.0 0.33 0.67**]T

Fig-2: Flux through the example reaction pathway



So here is the flux distribution for each reaction of the network.

Table 1 : Questions that can be addressed using Flux Balance Analysis:

Question	***Objective***	***References***
What are the biochemical production capabilities?	Maximize metabolic product	Verma, Boesch & Palsson, 1993
What is the maximum growth rate and biomass yield?	Maximize growth rate	Verma & Palsson, 1993; Verma & Palsson, 1994b
How efficiently can metabolism channel metabolites through network?	Minimize the Euclidean Norm	Bonarius et al.,1996
How energetically efficient can metabolism operate?	Minimize ATP production or minimize nutrient uptake	Majewski & Domach, 1990; Savinell & Palsson, 1992; Fell & Small, 1986
What is the trade off between biomass production and metabolite overproduction?	Maximize biomass production for a given metabolite production	Verma et.al.

Advantages and disadvantages of FBA:

Advantages:

- It relies solely on stoichiometric characteristics (can be used on any fully sequenced/characterized organism)
- Does not need kinetic parameters (that are difficult to obtain)

Disadvantages:

- It does not uniquely specify the fluxes (the particular flux distribution

chosen by the cell is a function of regulatory mechanisms that determine the kinetic characteristics of enzymes/enzyme expression)

- Sometimes disagrees with experimental data (discrepancies can often be accounted for when regulatory loops are considered)
- Cannot be used for modeling dynamic behavior (but might be integrated with modal analysis etc.)

2.4.1 Requirements for setting up FBA:

Flux balance analysis works on metabolic networks, so for establishing the FBA setup a metabolic network model is the basic requirement, as well as to simulate this network model, a liner programming calculation setup is required. So this LP setup will use the metabolic network model to simulate different aspects of organism, by using different constraints.

So following steps can be followed for FBA:

1. Setting up a metabolic pathway network for analysis
2. Setting up a liner programming calculation setup for flux calculations.
3. Analyzing the metabolic pathway.
4. Determining the optimal genetic manipulations using different constraints.
5. Validating the results by comparing with experimental results.

2.4.2 Software available for FBA:

There are many developments since early nineties in order to help different application in this research area of Biology. Some of them aid to the Metabolic control analysis, FBA , gene network, metabolic network reconstruction etc. Many software are available which work only on Flux Balance Analysis. Lists of popular software used in the community of systems biology developer is here:

Available Software for FBA:

1. **BioMet Toolbox** :(http://www.sysbio.se/)
2. **COBRA:** (http://gcrg.ucsd.edu/Downloads/Cobra_Toolbox)
3. **CellNetAnalyzer:** (http://www.mpi-magdeburg.mpg.de/projects/cna/cna.html)
4. **COPASI:** (http://copasi.org)
5. **FASIMU** (http://www.bioinformatics.org/fasimu)
6. **FBASBW** (http://frank-fbergmann.blogspot.com/2009/03/fluxbalance-analysis-with-sbw.html)
7. **Fluxor** (http://arep.med.harvard.edu/moma/FluxorPipeline.tar.gz)
8. **Metaboflux** (http://www.cbib.u-bordeaux2.fr/metaboflux/)
9. **MetaFluxNet** (http://metafluxnet.kaist.ac.kr)
10. **OptFlux** (http://www.optflux.org/)
11. **Pathway Analyser** (http://sourceforge.net/projects/pathwayanalyser)
12. **SurreyFBA** (http://sysbio3.fhms.surrey.ac.uk/)
13. **TinkerCell** (http://www.tinkercell.com/)
14. **VANTED** (http://vanted.ipk-gatersleben.de/)
15. **PySCeS** (http://pysces.sourceforge.net)
16. **libStruct** (http://sourceforge.net/apps/mediawiki/libstruct/index.php?title=Main_Page)

2.5 Genome-scaled Metabolic Network Model:

The availability of fully sequenced genomes has enabled the assembly of high-quality, genome-scale metabolic reconstructions(Oberhardt *et al., 2009*). The Genome scale model always better and have an upper edge on the predictive accuracy of the dynamical behavior of a system. So many techniques have been developed to predict the steady-state flux distribution through a metabolic network after various environmental and genetic

perturbations. One of them is Flux balance analysis. Flux Balance Analysis (FBA) (Schilling, Edwards et al. 1999), (Varma and Palsson 1994) is a methodology that can be employed to compute the metabolic capabilities of an organism (Edwards and Palsson 2000a), and it has been put into use for computing the effects of gene knockouts on the phenotype of the organisms such as *Escherichia coli* (Edwards and Palsson 2000) and Helicobacter pylori (Schilling, Covert et al. 2002). FBA was also applied to the identification of anti-tuberculous drug targets, but, the analysis was limited to mycolic acid pathway (Raman, Rajagopalan et al. 2005). The constraints-based framework, with flux balance analysis (FBA), has successfully predicted the time course of growth and by-product secretion, effects of mutation and knock-outs, and gene expression profiles. However, some times in situations where regulatory effects are more dominant influence on the organism's behavior, FBA leads towards wrong predictions. Even though flux balance analysis has so many limitations, the unavailability of enough kinetic details of mostly enzymes made FBA to be used in place of kinetic modeling, for such a large scale model. Expectation of the improved kinetic details is possible in for coming future. Till then FBA is the method of choice for work. A biochemical network is the per-requisite to perform the *in-silico* knockout study in an organism. The whole-genome network reconstruction is imperative if objective of study is global genome-scale effect of gene knockout. The genome-scale metabolic network model of M.tb was constructed by two groups at almost the same time (Beste, Hooper et al. 2007), (Jamshidi and Palsson 2007), and these models, can essentially be employed for predicting the global effects of in-silico gene knockouts for therapeutic applications.

2.5.1 Existing Genome-Scale Network models:

Genome-scale constraints-based models of metabolism have been built for several organisms, few of which are discussed as follows:

Escherichia coli:

(a) "*The Escherichia coli MG1655 in silico metabolic genotype: its definition,*

characteristics, and capabilities", J.S Edwards, B.O Palsson, 1999.

Here in this work the information of annotated sequence, biochemical information, and other information were used from complete genome sequence of *Escherichia coli* MG1655, to reconstruct the *E.coli* metabolic map. The stoichiometric coefficients for each metabolic enzyme in the *E. coli* metabolic map were assembled to construct a genome-specific stoichiometric matrix. The *E. coli* stoichiometric matrix was used to define the system's characteristics and the capabilities of *E. coli* metabolism.

(b)"*Stoichiometric model of Escherichia coli metabolism: incorporation of growth-rate dependent biomass composition and mechanistic energy requirements*", J Pramanik, J.D Keasling. 1997

In this work, development of a stoichiometric model was done, taking the growth-rate at steady state of E. Coli on glucose and mineral salts. In this model, there are 300 reactions in which 153 reactions are reversible and 147 reactions are irreversible. As well as it has 289 metabolites.

Haemophilus influenzae:

"Systems properties of the Haemophilus influenzae Rd metabolic genotype", J.S Edwards, B.O Palsson. 1999

Haemophilus influenzae Rd was the first free-living organism for which the complete genomic sequence was established. Here in this work, this annotated sequence and biological information was used to define the metabolic genotype of *Haemophilus influenzae,* this model contains 488 metabolic reactions operating on 343 metabolites, and the stoichiometric matrix was created on the basis of this information, which uses to determine the systems characteristics of the metabolic genotype and metabolic capabilities of H. Influenzae.

Helicobacter pylori:

"*Genome-scale metabolic model of Helicobacter pylori 26695*", C.H Schilling *et al.2002.*

As like previous mentioned works, here in this work, information from genome sequence annotation, biochemical, and physiological data was taken to construct a genome-scale metabolic model of *Helicobacter pylori* 26695. in this model, there is substantially less biochemical information available relative to previously modeled organisms such as *Escherichia coli*. In this metabolic model, 388 enzymatic and transport reactions and accounts for 291 open reading frames. Flux balance analysis were used to explore the metabolic capabilities of this In-silico model

Saccharomyces cerevisiae:

"*Genome-scale reconstruction of the Saccharomyces cerevisiae metabolic network*", J Forster *et al.* 2003

In this work the metabolic network in the yeast *Saccharomyces cerevisiae*was reconstructed using currently available genomic, biochemical, and physiological information. Compartmentalization of metabolic reaction was done between cytosol and the mitochondria, and the transport steps between the compartments and the environment were included. For the reconstruction of network , a total of 708 structural open reading frames were taken corresponding to 1035 metabolic reactions. Further, 140 reactions were included on the basis of biochemical evidence resulting in a genome-scale reconstructed metabolic network containing 1175 metabolic reactions and 584 metabolites.

Bacillus subtilis:

"*Genome-scale Reconstruction of Metabolic Network in Bacillus subtilis Based on High-throughput Phenotyping and Gene Essentiality Data*", You-Kwan Oh, Rernhard O. Palsson, Sung M. Park, Christophe H. Schilling, Radhakrishnan Mahadevan. 2007

This model development is done on information which is based on combination of genomic, biochemical, and physiological information and high-throughput phenotyping experiments. The initial re-construction was converted into an in-silico model. The final reconstruction accounted for 844 open reading frames and consisted of 1020 metabolic reactions and 988 metabolites.

Pseudomonas aeruginosa:

*("*Genome-Scale Metabolic Network Analysis of the Opportunistic Pathogen Pseudomonas aeruginosa PAO1*",* Matthew A, Oberhardt, Kimberly E. Fryer, Jason A. Papin, 2008.

In this work, a genome-scale metabolic network of *Pseudomonas aeruginosa* PAO1 created. And this reconstruction was based on 1,056 genes (19% of the genome), 1,030 proteins, and 883 reactions. As well as to identify the key features (e.g. Growth rate) of this organism, flux balance analysis was used as tool.

Pseudomonas putida:

"*Genome-Scale Reconstruction and Analysis of the Pseudomonas putida KT2440 Metabolic Network Facilitates Applications in Biotechnology*", Jacek Puchałka, Miguel Godinho, Agata Bielecka, Vítor A. P. Martins dos Santos. 2008

This work includes the development of a genome-scale constraint-based model of the metabolism of *P. putida* KT2440. Here network reconstruction and flux balance analysis were used to define the structure of metabolic network of this organism. FBA and flux variability analysis were used to analyze the properties, potential, and limits of the model. The model accounts for the function of 877 reactions that connect 886 metabolites and

builds upon a constraint-based modeling framework.

Mycobacterium Tuberculosis:

Here we describe two distinct methods for M.tb.

(a) *"GSMN-TB: a web-based genome-scale network model of Mycobacterium tuberculosis metabolism "*, Dany JV Beste, Tracy Hooper, Graham Stewart, Bhushan Bonde, Claudio Avignone-Rossa , Michael E Bushell, Paul Wheeler, Steffen Klamt, Andrzej M Kierzek and Johnjoe McFadden, 2007.

GSMN-TB, a genome-scale metabolic model of M. tuberculosis, was constructed, consisting of 849 unique reactions and 739 metabolites, and involving 726 genes. Flux balance analysis was used as tool to calculate substrate consumption rate. A web based interface if this model is created to interactively utilize this model for knock out studies, for and for gene essentiality.

(b) *"Investigating the metabolic capabilities of Mycobacterium tuberculosis H37Rv using the in silico strain INJ661 and proposing alternative drug targets"*, Neema Jamshidi and Bernohard o Palsson. 2007

This genome scaled metabolic network model has 661 genes and 939 intra-system reactions. a bottom up reconstruction of the metabolic network of *Mycobacterium tuberculosis* H37Rv is done (In-Silico) here to find the capabilities of the system.

GSMN models for Plants are described here :

Arbidopsis thaliana:

(a) "*A Genome-Scale Metabolic Model of Arabidopsis and Some of Its Properties*", Mark G. Poolman, Laurent Miguet, Lee J. Sweetlove, David A. Fell. 2009

Here construction of the genome-scale metabolic model of Arabidopsis (Arabidopsis thaliana) was done on the basis of annotations in the Aracyc database. Liner progamming was used to demonstrate the following; (1) capability of model for the production of biomass components (amino acids, nucleotides, lipid, starch, and cellulose) in the proportions observed experimentally in a heterotrophic suspension culture; (2) minimal size of organism is achieved, an only 15% of the total reactions are needed for this purpose. (3) reactions may be grouped according to the changes in flux resulting from a hypothetical stimulus (4) total ATP demand for growth and maintenance can be inferred form this model.

(b) "AraGEM, a Genome-Scale Reconstruction of the Primary Metabolic Network in Arabidopsis", Cristiana Gomes de Oliveira Dal'Molin, Lake-Ee Quek, Robin William Palfreyman, Stevens Michael Brumbley, Lars Keld Nielsen. 2010

AeaGEM is a literature-based genome-scale metabolic reconstruction that accounts for the functions of 1,419 unique open reading frames, 1,748 metabolites, 5,253 gene-enzyme reaction-association entries, and 1,567 unique reactions compartmentalized into the cytoplasm, mitochondrion, plastid, peroxisome, and vacuole.

Zea Maize:

"*Zea mays i*RS1563: A Comprehensive Genome-Scale Metabolic Reconstruction of Maize Metabolism", Rajib Saha, Patrick F. Suthers, Costas D. Maranas, 2011.

This metabolic network contains 1,563 genes and 1,825 metabolites involved in 1,985 reactions from primary and secondary maize metabolism.

2.5.2 GSMN-TB: a web-based genome-scale network model

(*"GSMN-TB: a web-based genome-scale network model of Mycobacterium tuberculosis metabolism "*, Dany JV Beste, Tracy Hooper, Graham Stewart, Bhushan Bonde , Claudio Avignone-Rossa, Michael E Bushell, Paul Wheeler, Steffen Klamt, Andrzej M Kierzek, Johnjoe McFadden , 2007.)

GSMN-TB is a genome-scaled metabolic network model of *Mycobactrium Tuberculosis.* Based on 849 unique reactions and 739 metabolites, this model involves 726 genes. Flux balance analysis was used as technique to calculate substrate consumption rates, and to calculate gene essentiality prediction. This FBA calculation includes the stoichiometric coefficients for each metabolic enzyme in the *Mycobactrium Tuberculosis* metabolic map, which were assembled to construct a genome-specific stoichiometric matrix. The *Mycobactrium Tuberculosis* stoichiometric matrix was used to define the system's characteristics and the capabilities of *Mycobactrium Tuberculosis* metabolism.

Table 2: Statistics of the GSMN-TB model

Reaction Class	Number
Enzymatic conversions	723
Transport reactions	126
Total number of reactions	849
Orphan reactions	210
Genes	726
Internal metabolites	638
External metabolites	101
Total number of metabolites	739

Models available at GSMN-TB:

Following models are available at GSMN-TB server.

Genome Scale Metabolic Reaction Networks:

1. Mycobacterium tuberculosis (Beste et al. 2007), original in-vitro model.
2. Mycobacterium tuberculoisis (Beste et al. 2007), original in vivo model.
3. Mycobacterium tuberculosis (Beste et al., 2007) slow growth rate
4. Streptomyces coelicolor (Borodina et al, 2005)
5. Streptomyces lividans (according to CGH with S. coelicolor)
6. Neisseria meningiatis Nmb_iTM560

Out of these six network models, first model, Mycobacterium tuberculosis (Beste et al. 2007), original in-vitro model, was taken as base model for our study (chapter 3).

Networks available at GSMN-TB, are based on SBML. Properties of this SBML model is as follows:

(a) SBML Version here used is Version-2, Level-1.

<sbml xmlns="http://www.sbml.org/sbml/level2" level="2" version="1" xmlns:html="http://www.w3.org/1999/xhtml">

(b) Here two compartment were taken in to consideration, first is Cytosol, and out side of it , the second one is Extra_organism.

<listOfCompartments>

<compartment id="Extra_organism"/>

<compartment id="Cytosol" outside="Extra_organism"/>

</listOfCompartments>

(c) total 739 metabolites (638 as internal,101as external) were coded as individual species. An example of it is as follows:

<listOfSpecies>

<species id="M_DHLIPOYLPROTEIN_c"

name="DHLIPOYLPROTEIN" compartment="Cytosol" charge="0" boundaryCondition="false" />

<species id="M_PTC_c" name="PTC" compartment="Cytosol" charge="0" boundaryCondition="false" />

<species id="M_NACxt_b" name="NACxt" compartment="Extra_organism" charge="0" boundaryCondition="true" />

</listOfSpecies>

in some species, boundary condition is true, means they are at the boundary of it's compartment, and participating in the exchange flux, as well as for some species, boundary condition is false, means it is not involved in exchanging flux. Here in example, DHLIPOYLPROTEIN is not at boundary, but PTC & NACxt are at boundary of cytosol.

(d) This model involves total of 1185 reactions in which 126 transport reactions, 849 internal reactions (inside cytosol compartment), and 210 are the orphan reactions (which don't provide any information of gene, or don't code for any gene). Example of a reaction is as follows:

GL + ATP ------> ADP + GL3P

here two reactants GL & ATP and two products ADP & GL3P are involved in the reaction, and reaction is irreversible. Gene associated to this reaction is Rv3696c. In this reaction, unit of FLUX-value is mili-mole per gram per hour, and the lower limit of it is 0.0, and upper bound is 100000.0

SBML code for this reaction is as follows:

<reaction id="R1" name="R1" reversible="false">

<notes>

<html:p>GENE_ASSOCIATION: Rv3696c </html:p>

<html:p>PROTEIN_ASSOCIATION: </html:p>

<html:p>SUBSYSTEM: </html:p>

```
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_GL_c" stoichiometry="1.0"/>
            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
            <speciesReference species="M_GL3P_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0"
units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0"
                                    units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000"
                                    units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
```

</kineticLaw>

</reaction>

Simulations available in GSMN-TB model:

Simulations are based on the principle of Flux Balance Analysis. All intracellular metabolites are assumed to be at steady state, where their concentration is constant. Extracellular metabolites are not required to be balanced. In all models available on the system the names of extracellular metabolites end with "xt" string. The variables of the model are reaction fluxes. The media conditions for a particular simulation are defined as bounds on extracellular metabolite transport reactions. If particular metabolite is absent from the medium the transport reaction for this metabolite is bound to (0, 0) otherwise it is allowed to assume positive (transport) or negative (secretion) flux. Nutritional conditions are defined within model interface by typing reaction name, lower flux bound, upper flux bound (white-space separated) into "Edit media conditions field" form. This form may be used not only to specify active transport reactions, but also to constraint any reaction in the model.

Following are the four simulations available at GSMN-TB.

1. Computation of maximum growth rate (Flux Balance analysis)
2. Flux variability analysis
3. Reactions essentiality Scan
4. Gene essentiality prediction

1. Computation of Maximum Growth Rate (Flux Balance Analysis)

Flux Balance Analysis simulation results in the maximal value of the selected flux under given media conditions. The optimization target may be specified as a reaction or metabolite name. If optimization target is a reaction, maximal value of the reaction flux is calculated. If the metabolite name is given the system calculates maximal production rate of the metabolite. The usual optimization target is a BIOMASS metabolite. Biomass synthesis rate models growth rate. The linear programming algorithm guarantees that the

unique, maximal value of the optimized flux is found. However, the flux distribution is not unique. System reports one of many possible distributions sustaining maximal flux towards optimization target.

Steps:

- Go to website http://sysbio3.fhms.surrey.ac.uk/ , and select any GSMN model. (here first model Mycobacterium tuberculosis (Beste et al. 2007), original in-vitro model selected as example). And clict the link for run simulation (http://sysbio3.fhms.surrey.ac.uk/cgi-bin/fba/fbapy?model=GSMN_TB-Viv&cmd=methods).
- Select *Flux balance analysis* option out of four available options. (http://sysbio3.fhms.surrey.ac.uk/cgi-bin/fba/fbapy?model=GSMN_TB-Viv&cmd=fba).
- Put the optimization target to BIOMASS (by default it is BIOMASS), and edit media conditions according to media model created(constrains applied to organism).
- Now click the RUN button, to start the simulation.
- Now the web-page displayed, will show the results of flux balance ability.

Fig 3: Webpage for FBA

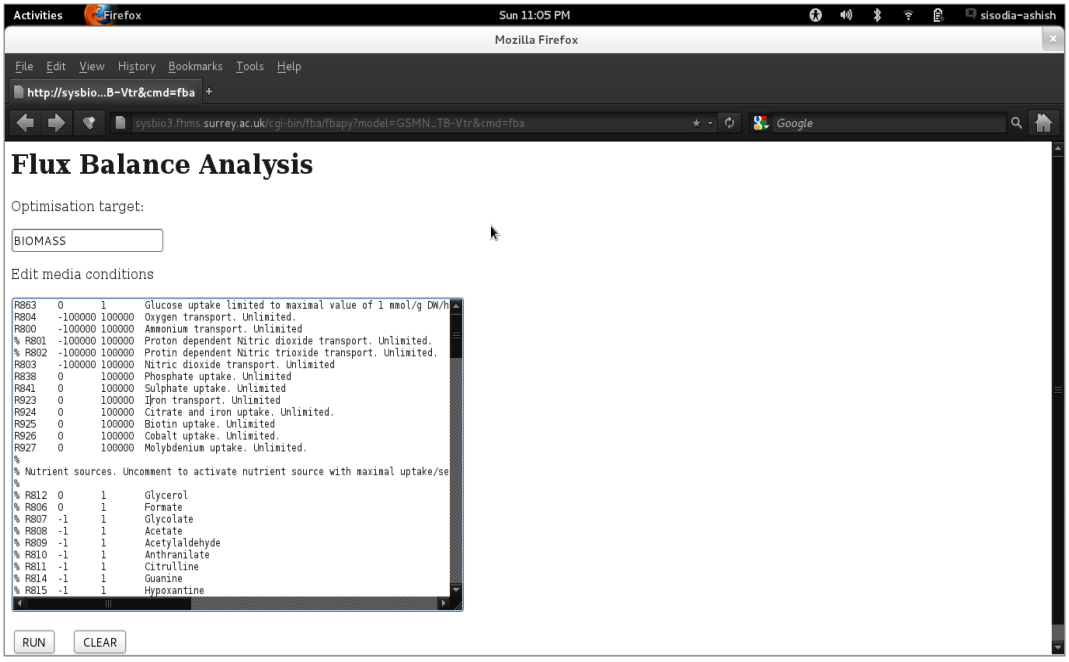
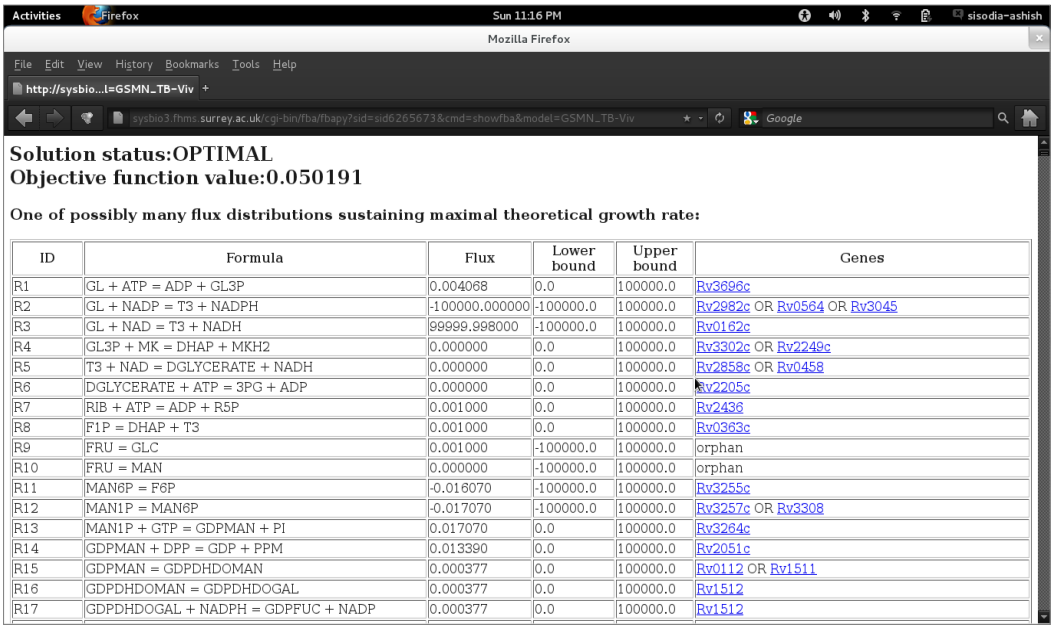


Fig 4: Webpage, Optimal condition the objective function.



Solution status:OPTIMAL
Objective function value:0.050191

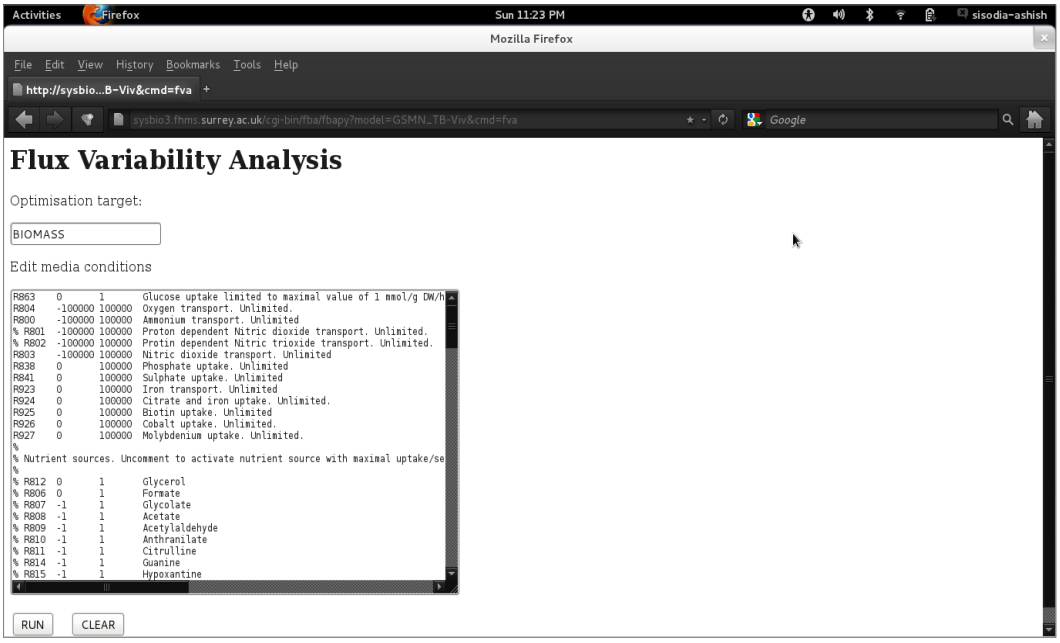
One of possibly many flux distributions sustaining maximal theoretical growth rate:

ID	Formula	Flux	Lower bound	Upper bound	Genes
R1	GL + ATP = ADP + GL3P	0.004068	0.0	100000.0	Rv3696c
R2	GL + NADP = T3 + NADPH	-100000.000000	-100000.0	100000.0	Rv2982c OR Rv0564 OR Rv3045
R3	GL + NAD = T3 + NADH	99999.998000	-100000.0	100000.0	Rv0162c
R4	GL3P + MK = DHAP + MKH2	0.000000	0.0	100000.0	Rv3302c OR Rv2249c
R5	T3 + NAD = DGLYCERATE + NADH	0.000000	0.0	100000.0	Rv2858c OR Rv0458
R6	DGLYCERATE + ATP = 3PG + ADP	0.000000	0.0	100000.0	Rv2205c
R7	RIB + ATP = ADP + R5P	0.001000	0.0	100000.0	Rv2436
R8	F1P = DHAP + T3	0.001000	0.0	100000.0	Rv0363c
R9	FRU = GLC	0.001000	-100000.0	100000.0	orphan
R10	FRU = MAN	0.000000	-100000.0	100000.0	orphan
R11	MAN6P = F6P	-0.016070	-100000.0	100000.0	Rv3255c
R12	MAN1P = MAN6P	-0.017070	-100000.0	100000.0	Rv3257c OR Rv3308
R13	MAN1P + GTP = GDPMAN + PI	0.017070	0.0	100000.0	Rv3264c
R14	GDPMAN + DPP = GDP + PPM	0.013390	0.0	100000.0	Rv2051c
R15	GDPMAN = GDPDHDOMAN	0.000377	0.0	100000.0	Rv0112 OR Rv1511
R16	GDPDHDOMAN = GDPDHDOGAL	0.000377	0.0	100000.0	Rv1512
R17	GDPDHDOGAL + NADPH = GDPFUC + NADP	0.000377	0.0	100000.0	Rv1512

2. Flux Variability Analysis:

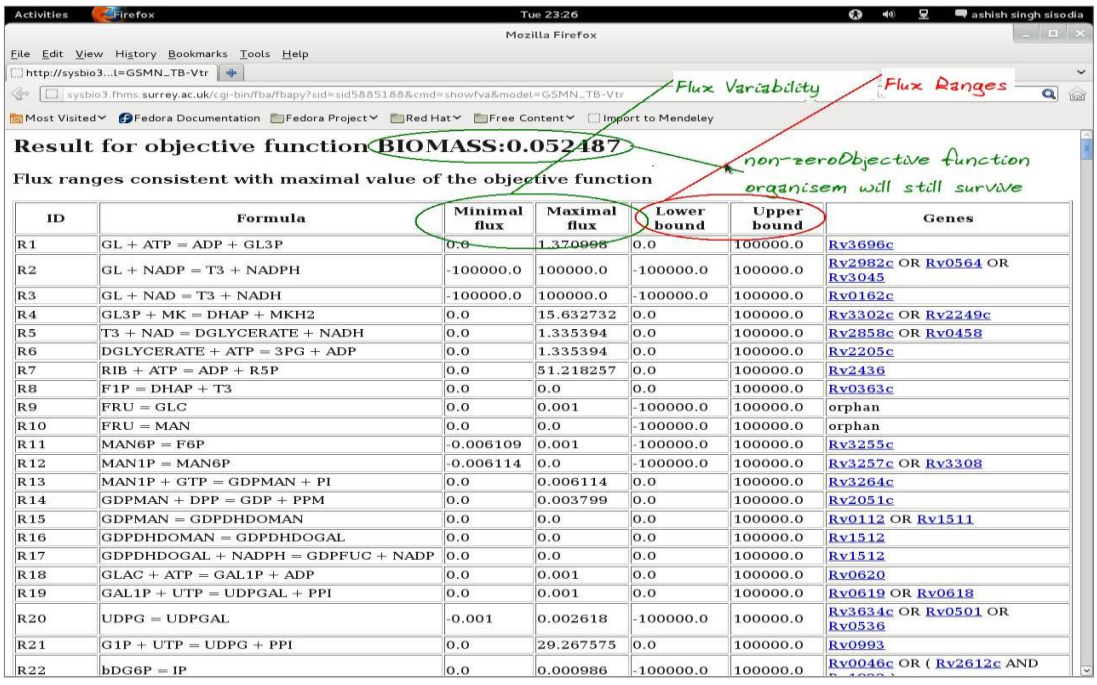
Flux Variability analysis allows exploration of the flux ranges consistent with the maximal flux towards optimization target. The Flux Balance Analysis is performed first and the target flux is constrained to the maximal value. Subsequently, each reaction becomes an optimization target and the minimal and maximal flux through this reaction is calculated.

Fig 5: Webpage for FVA



Steps for FVA calculation:

- Go to website http://sysbio3.fhms.surrey.ac.uk/ , and select any GSMN model. (here first model Mycobacterium tuberculosis (Beste et al. 2007), original in-vitro model selected as example). And clict the link for run simulation (http://sysbio3.fhms.surrey.ac.uk/cgi-bin/fba/fbapy?model=GSMN_TB-Viv&cmd=methods).
- Select *Flux Variability analysis* option out of four available options. (http://sysbio3.fhms.surrey.ac.uk/cgi-bin/fba/fbapy?model=GSMN_TB-Viv&cmd=fva).
- Put the optimization target to BIOMASS (by default it is BIOMASS), and edit media conditions according to media model created(constrains applied to organism).
- Now click the RUN button, to start the simulation.
- Now the web-page displayed, will show the results of flux variability ability.



ID	Formula	Minimal flux	Maximal flux	Lower bound	Upper bound	Genes
R1	GL + ATP = ADP + GL3P	0.0	1.370998	0.0	100000.0	Rv3696c
R2	GL + NADP = T3 + NADPH	-100000.0	100000.0	-100000.0	100000.0	Rv2982c OR Rv0564 OR Rv3045
R3	GL + NAD = T3 + NADH	-100000.0	100000.0	-100000.0	100000.0	Rv0162c
R4	GL3P + MK = DHAP + MKH2	0.0	15.632732	0.0	100000.0	Rv3302c OR Rv2249c
R5	T3 + NAD = DGLYCERATE + NADH	0.0	1.335394	0.0	100000.0	Rv2858c OR Rv0458
R6	DGLYCERATE + ATP = 3PG + ADP	0.0	1.335394	0.0	100000.0	Rv2205c
R7	RIB + ATP = ADP + R5P	0.0	51.218257	0.0	100000.0	Rv2436
R8	F1P = DHAP + T3	0.0	0.0	0.0	100000.0	Rv0363c
R9	FRU = GLC	0.0	0.001	-100000.0	100000.0	orphan
R10	FRU = MAN	0.0	0.0	-100000.0	100000.0	orphan
R11	MAN6P = F6P	-0.006109	0.001	-100000.0	100000.0	Rv3255c
R12	MAN1P = MAN6P	-0.006114	0.0	-100000.0	100000.0	Rv3257c OR Rv3308
R13	MAN1P + GTP = GDPMAN + PI	0.0	0.006114	0.0	100000.0	Rv3264c
R14	GDPMAN + DPP = GDP + PPM	0.0	0.003799	0.0	100000.0	Rv2051c
R15	GDPMAN = GDPDHDOMAN	0.0	0.0	0.0	100000.0	Rv0112 OR Rv1511
R16	GDPDHDOMAN = GDPDHDOGAL	0.0	0.0	0.0	100000.0	Rv1512
R17	GDPDHDOGAL + NADPH = GDPFUC + NADP	0.0	0.0	0.0	100000.0	Rv1512
R18	GLAC + ATP = GAL1P + ADP	0.0	0.001	0.0	100000.0	Rv0620
R19	GAL1P + UTP = UDPGAL + PPI	0.0	0.001	0.0	100000.0	Rv0619 OR Rv0618
R20	UDPG = UDPGAL	-0.001	0.002618	-100000.0	100000.0	Rv3634c OR Rv0501 OR Rv0536
R21	G1P + UTP = UDPG + PPI	0.0	29.267575	0.0	100000.0	Rv0993
R22	bDG6P = IP	0.0	0.000986	-100000.0	100000.0	Rv0046c OR (Rv2612c AND

Fig 6 : Webpage Optimal condition the objective function.

3. Reactions essentiality Scan:

The Reaction Essentiality Scan is an iterative simulation protocol. Each reaction in the model is removed and the maximal flux towards optimization target is re-calculated. This allows identification of reactions essential for the particular metabolic function.

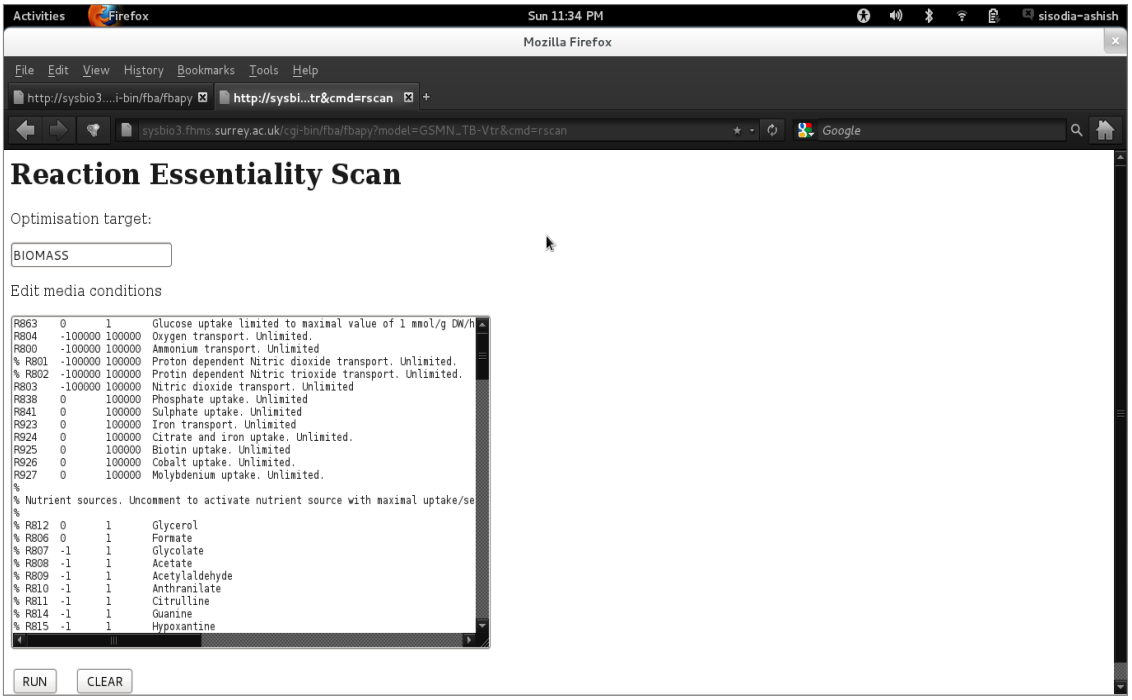


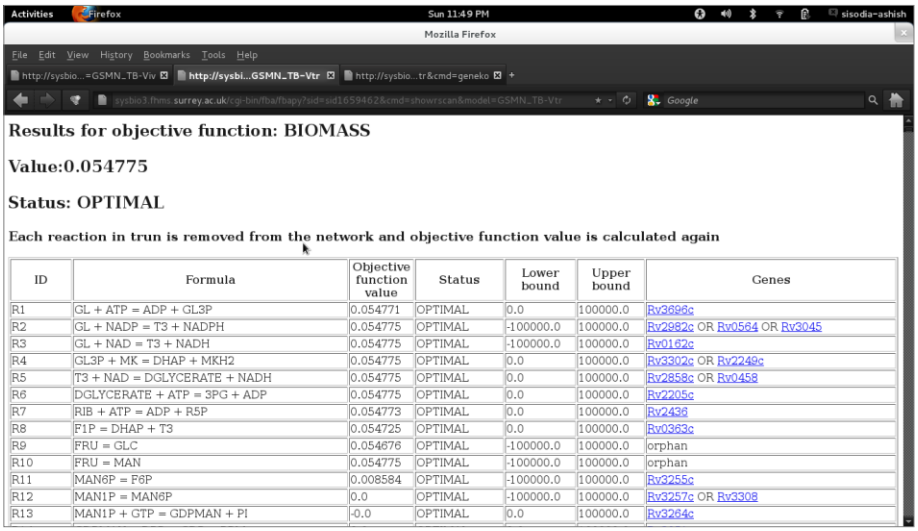
Fig 7 : Webpage showing reaction essentiality .

Steps:

- Go to website http://sysbio3.fhms.surrey.ac.uk/ , and select any GSMN model. (here first model Mycobacterium tuberculosis (Beste et al. 2007), original in-vitro model selected as example). And clict the link for run simulation (http://sysbio3.fhms.surrey.ac.uk/cgi-bin/fba/fbapy?model=GSMN_TB-Viv&cmd=methods).
- Select *Reaction Essentiality Scan* option out of four available options. (http://sysbio3.fhms.surrey.ac.uk/cgi-bin/fba/fbapy?model=GSMN_TB-Vtr&cmd=rscan).
- Put the optimization target to BIOMASS (by default it is BIOMASS), and edit media conditions according to media model created(constrains applied to

organism).

- Now click the RUN button, to start the simulation.
- Now the web-page displayed, will show the results of Reaction Essentiality Scan.



Results for objective function: BIOMASS

Value:0.054775

Status: OPTIMAL

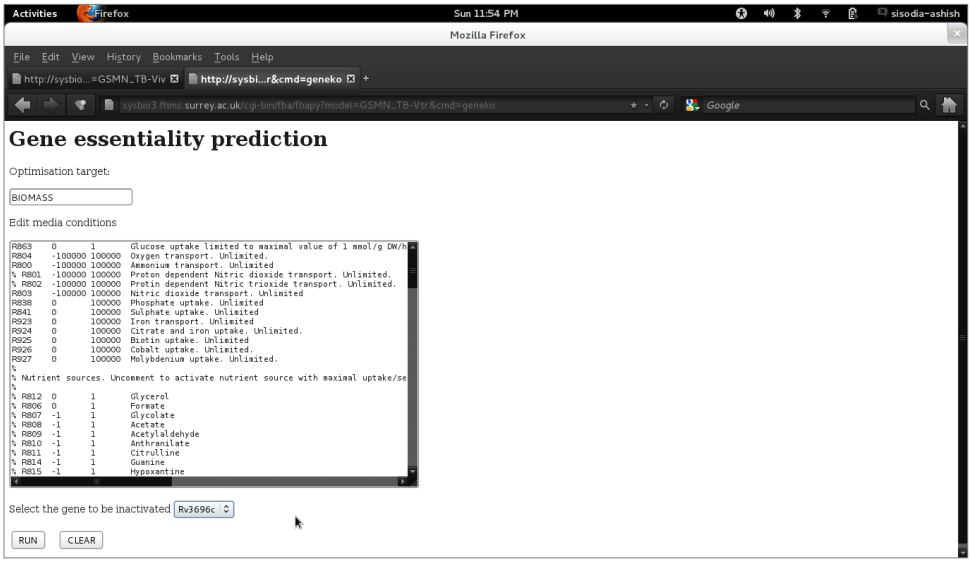
Each reaction in trun is removed from the network and objective function value is calculated again

ID	Formula	Objective function value	Status	Lower bound	Upper bound	Genes
R1	GL + ATP = ADP + GL3P	0.054771	OPTIMAL	0.0	100000.0	Rv3696c
R2	GL + NADP = T3 + NADPH	0.054775	OPTIMAL	-100000.0	100000.0	Rv2982c OR Rv0584 OR Rv3045
R3	GL + NAD = T3 + NADH	0.054775	OPTIMAL	-100000.0	100000.0	Rv0162c
R4	GL3P + MK = DHAP + MKH2	0.054775	OPTIMAL	0.0	100000.0	Rv3302c OR Rv2249c
R5	T3 + NAD = DGLYCERATE + NADH	0.054775	OPTIMAL	0.0	100000.0	Rv2858c OR Rv0458
R6	DGLYCERATE + ATP = 3PG + ADP	0.054775	OPTIMAL	0.0	100000.0	Rv2205c
R7	RIB + ATP = ADP + R5P	0.054773	OPTIMAL	0.0	100000.0	Rv2436
R8	F1P = DHAP + T3	0.054725	OPTIMAL	0.0	100000.0	Rv0363c
R9	FRU = GLC	0.054676	OPTIMAL	-100000.0	100000.0	orphan
R10	FRU = MAN	0.054775	OPTIMAL	-100000.0	100000.0	orphan
R11	MAN6P = F6P	0.008584	OPTIMAL	-100000.0	100000.0	Rv3255c
R12	MAN1P = MAN6P	0.0	OPTIMAL	-100000.0	100000.0	Rv3257c OR Rv3308
R13	MAN1P + GTP = GDPMAN + PI	-0.0	OPTIMAL	0.0	100000.0	Rv3264c

Fig 8 : Webpage Optimal condition showing the objective function.

4. Gene essentiality prediction:

this program allows single Gene Essentiality Prediction. All reactions that require selected gene are constrained to (0, 0) and the maximal flux towards optimization target is calculated. Therefore, the method predicts essentiality of a particular gene, for metabolic function of interest, under specified media conditions.



Gene essentiality prediction

Optimisation target:

BIOMASS

Edit media conditions

```
R863    0       1       Glucose uptake limited to maximal value of 1 mmol/g DW/h
R804    -100000 100000  Oxygen transport. Unlimited.
R800    -100000 100000  Ammonium transport. Unlimited
% R801  -100000 100000  Proton dependent Nitric dioxide transport. Unlimited.
% R802  -100000 100000  Protin dependent Nitric trioxide transport. Unlimited.
R803    -100000 100000  Nitric dioxide transport. Unlimited
R838    0       100000  Phosphate uptake. Unlimited
R841    0       100000  Sulphate uptake. Unlimited
R923    0       100000  Iron transport. Unlimited
R924    0       100000  Citrate and iron uptake. Unlimited.
R925    0       100000  Biotin uptake. Unlimited
R926    0       100000  Cobalt uptake. Unlimited.
R927    0       100000  Molybdenium uptake. Unlimited.
%
% Nutrient sources. Uncomment to activate nutrient source with maximal uptake/se
%
% R812  0       1       Glycerol
% R806  0       1       Formate
% R807  -1      1       Glycolate
% R808  -1      1       Acetate
% R809  -1      1       Acetylaldehyde
% R810  -1      1       Anthranilate
% R811  -1      1       Citrulline
% R814  -1      1       Guanine
% R815  -1      1       Hypoxantine
```

Select the gene to be inactivated Rv3696c

RUN CLEAR

Fig 9: Webpage Gene Essentiality

Steps:

- Go to website http://sysbio3.fhms.surrey.ac.uk/ , and select any GSMN model. (here first model Mycobacterium tuberculosis (Beste et al. 2007), original in-vitro model selected as example). And clict the link for run simulation (http://sysbio3.fhms.surrey.ac.uk/cgi-bin/fba/fbapy?model=GSMN_TB-Viv&cmd=methods).
- Select *Gene Essentiality Prediction* option out of four available options. (http://sysbio3.fhms.surrey.ac.uk/cgi-bin/fba/fbapy?model=GSMN_TB-Vtr&cmd=geneko).
- Put the optimization target to BIOMASS (by default it is BIOMASS), and edit media conditions according to media model created(constrains applied to organism).
- Select the gene to be inactivated, from drop-down button. (here in example Rv3696c selected for Knockout), to check its essentiality.
- Now click the RUN button, to start the simulation.
- Now the web-page displayed, will show the results of Gene Essentiality Prediction. (here in example, biomass value in non-zero, and hence, gene Rv3696c found as Non-Essential)

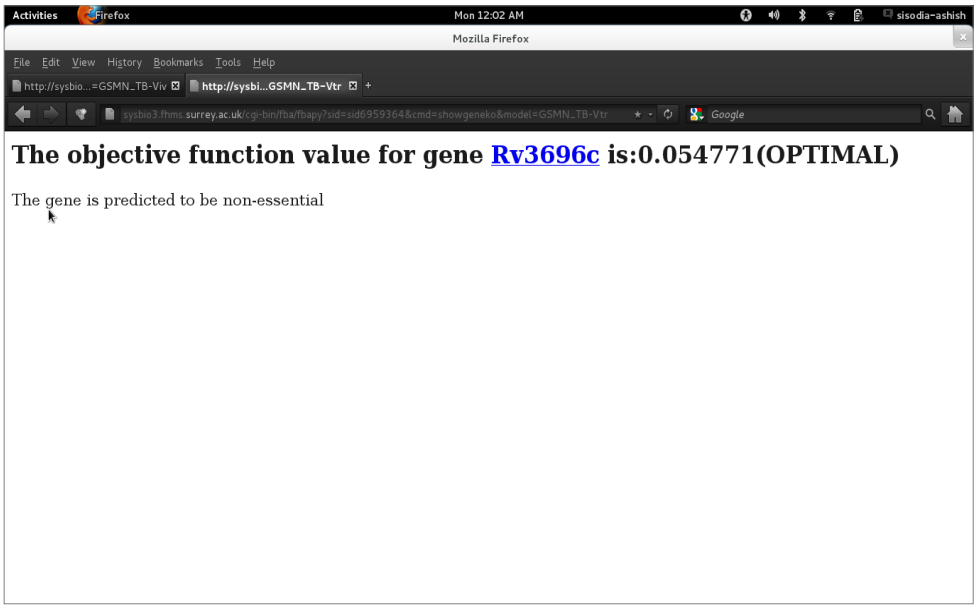


Fig 10 : Webpage showing the objective function value of selected gene

References:

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SBML Software summery

Contents:

1. Analysis Software

1. **ABC-SysBio:** *(http://abc-sysbio.sourceforge.net/)* — ABC-SysBio implements likelihood free parameter inference and model selection in dynamical systems. It is designed to work with both stochastic and deterministic models written in Systems Biology Markup Language (SBML). ABC-SysBio is a Python package that combines three algorithms: ABC rejection sampler, ABC SMC for parameter inference and ABC SMC for model selection.

2. **AutoSBW:** *(http://frank-fbergmann.blogspot.com/2009/02/simplifying-bifurcation-analysis.html)* — A frontend around AUTO to simplify bifurcation analysis.

3. **Bifurcation Discovery Tool:** (http://sys-bio.org/sbwWiki/sbw/biftool) — The Bifurcation Discovery Tool uses a genetic algorithm to search for Hopf bifurcations, turning points, and bistable switches. The user can select parameters to be searched, admissible parameter ranges, and the nature of the bifurcation to be sought. The tool returns parameter values for the model for which the particular behavior is observed.

4. **BioBayes:** (http://www.dcs.gla.ac.uk/BioBayes/) — software package for applying the Bayesian inferential methodology to problems in systems biology.

5. **BioMet Toolbox** :(http://www.sysbio.se/) — The BioMet ToolBox is a web-based resource for analysis of high-throughput data, together with methods for flux analysis (fluxomics) and integration of transcriptome data exploiting the capabilites of metabolic networks described in genome scale models.
6. **ByoDyn** :(http://byodyn.imim.es) — ByoDyn includes a set of tools to 1) integrate ordinary differential equations (ODEs), including systems with events, rules (differential algebraic equations, DAE) and delays built from a given biological model; 2) stochastic simulators: SSA and tau-leap; 3) globally optimize the parameters that fit the provided experimental information and evaluate the sensitivity of the model with respect to the different parameters; 4) include the sensitivity of the parameters in an optimal experimental design pipeline based on the Fisher information matrix; and 5) Monte Carlo sampling coupled with cluster analysis and PCA to determine the global shape of the parameter landscape. The program makes use of external software, providing a Python binding schema that allows the user to easily implement new software in the desired calculation protocol. Furtermore, a webserver has been

developed to manage the models, calculations and results easily.

7. **CADLIVE:** (http://www.cadlive.jp) — CADLIVE (Computer-Aided Design of LIVing systEms) is a comprehensive computational tool for constructing large-scale biological network maps, analyzing the topological features of them, and simulating their dynamics. Using CADLIVE, we rationally design a biological system at the molecular interaction level for an engineering purpose.

8. **CellNetAnalyzer:** (http://www.mpi-magdeburg.mpg.de/projects/cna/cna.html) — CellNetAnalyzer (CNA) is a package for MATLAB and provides a comprehensive and user-friendly environment for structural and functional analysis of biochemical networks. CNA facilitates the analysis of metabolic (stoichiometric) as well as signaling and regulatory networks solely on their network topology, i.e. independent of kinetic mechanisms and parameters. CNA provides a powerful collection of tools and algorithms for structural network analysis which can be started in a menu-controlled manner within interactive network maps. Recently, API functionalities have been added to enable interested users to call algorithms of CNA from external programs. Applications of CNA can be found in systems biology, biotechnology, metabolic engineering, pharmacology, microbiology, chemical engineering.

9. **COBRA:** (http://gcrg.ucsd.edu/Downloads/Cobra_Toolbox) — The COnstraint-Based Reconstruction and Analysis Toolbox for Matlab includes implementations of many of the commonly used forms of constraint-based analysis such as FBA, gene deletions, flux variability analysis, sampling, and batch simulations together with tools to read in and manipulate constraint-based models.

10. **COPASI:** (http://copasi.org) — COPASI is a software application for simulation and analysis of biochemical networks and their dynamics. COPASI is a stand-alone program that supports models in the SBML standard and can simulate their behavior using ODEs or Gillespie's stochastic simulation algorithm; arbitrary discrete events can be included in such simulations. COPASI provides an C++ API with language bindings for Perl, python, R, Java, and Octave and is able to communicate with the Systems Biology Workbench COPASI carries out several analyses of the network and its dynamics and has extensive support for parameter estimation and optimization. COPASI provides means to visualize data in customizable plots, histograms and animations of network diagrams. For a complete list of feature please see: http://www.copasi.org/tiki- index.php?page=FeatureList (http://www.copasi.org/tiki-index.php?page=FeatureList)

11. **Crdata:** (http://crdata.org/) — CRdata.org offers menu-driven access to the Amazon Elastic Computing Cloud (EC2) and related resources for bioinformatic computing with R and Bioconductor. Users can launch their own processing nodes, and share nodes, scripts, and data with others if they wish.

12. **DBSolve:** (http://insysbio.ru/en/soft/dbsolveoptimum.html) — DBSolveOptimum is a free software for kinetic modeling of metabolic pathways, analysis, and fitting parameters to experimental data. The program has text-based user interface for model description and graphical interface for data analysis. In addition to standart algorithms of simulation (ODE

solver, explicit solver, steady-state analysis) the software include also automated local sencetivity analysis, parameters optimization procedures and bifurcaion analysis. The last version of DBSolveOptimum includes advanced tool for data visualization.

13. **DOTcvpSB:** (http://www.iim.csic.es/~dotcvpsb/) — MatLab toolbox for optimization of models.

14. **Facile:** (http://facile.sourceforge.net) — Facile / EasyStoch. A command-line network compiler for systems biology. Facile reads models given in a simple and human-readable textual input format and exports the model in a format for readable by Matlab, Mathematica, Maple, XPP/AUTO. Other tools are supported via SBML export. For stochastic simulations, Facile uses the EasyStoch stochastic simulator. An important feature of EasyStoch that distinguishes it from other Gillespie-algorithm implementations is that it is capable of simulating dynamically changing or noisy biochemical parameters (i.e. extrinsic noise).

15. **FASIMU** (http://www.bioinformatics.org/fasimu) — FASIMU is a command line oriented software implementing the most frequently applied FBA algorithms. It offers the first freely available implementation of (i) weighted flux minimization, (ii) fitness maximization for partially inhibited enzymes, and (iii) the concentration-based thermodynamic feasibility constraint. It allows heterogenous computation series suited for network pruning, leak analysis, FVA, and systematic probing of metabolic objectives for network curation controlled by an intuitive description file. The metabolic network can be supplied in SBML, CellNetAnalyzer, and plain text format. FASIMU uses the optimization capabilities of free (lp solve and GLPK) and commercial solvers (CPLEX, LINDO). The results can be visualized in Cytoscape or BiNA using newly developed plugins. The platform- independent program is an open-source project, freely available under GNU public license, including manual, tutorial, BiNA and Cytoscape plugin and respective manuals.

16. **FBASBW** (http://frank-fbergmann.blogspot.com/2009/03/fluxbalance-analysis-with-sbw.html) — A program allowing to define flux constraints using SBML annotations.

17. **Fluxor** (http://arep.med.harvard.edu/moma/FluxorPipeline.tar.gz) — Flux analysis. Free, part of BioSpice tool set. Linux.

18. **Genetic Network Analyzer** (http://www-helix.inrialpes.fr/gna) — Genetic Network Analyzer (GNA) is a computer tool for the modeling, simulation, analysis and verification of genetic regulatory networks. The aim of GNA is to assist biologists and bioinformaticians in constructing a qualitative model of a genetic regulatory network from knowledge about regulatory interactions and gene expression data. GNA provides a variety of functions to analyze the steady-state and transient dynamics of the network, among other things by exploiting state- of-the-art model-checking tools

19. **GNU MCSim** (http://www.gnu.org/software/mcsim/) — GNU MCSim is a free standalone simulation package that allows you to design your own statistical or simulation models. It efficiently performs Bayesian inference through Markov Chain Monte Carlo simulations. Standard Monte Carlo and experimental design optimization are also available. GNU MCSim can import and simulate levels 1 and 2 SBML models

20. **iBioSim** (http://www.async.ece.utah.edu/iBioSim/) — The iBioSim tool supports the modeling,

analysis, and design of genetic circuits with applications in both systems and synthetic biology. It includes editors to construct genetic circuit models (GCM), Systems Biology Markup Language (SBML) models (L2V4 and L3V1 supported), and labeled Petri net (LPN) models. Models can be constructed by hand, imported from model databases, or learned from experimental data. These models can be analyzed using a variety of ODE and stochastic simulators as well as Markov chain analysis. The efficiency of these analysis methods is enhanced using a variety of automatic reaction-based and logical abstractions. The analysis results can be plotted as graphs or visualized upon the genetic circuit schematic.

21. **Jacobian Viewer** (http://jdesigner.sourceforge.net/Site/Jacobian_Viewer.html) — The Jacobian matrix is of central importance in the analysis of a computational model. The Jacobian specifies the local dynamics of the model. The entries in the matrix indicate the influence of model variables on the rates of change.The Jacobian Viewer will dynamically show these changes. In order to do so we generate a dependency graph for a computational model, with nodes denoting all species in the model and arcs denoting the influence of one species on the rates of change of another species. This provides insight of how those changes occur. The researcher is of course able to change the time-steps taken by the simulator as well as the starting point of the simulation.

22. **Jarnac** (http://jdesigner.sourceforge.net/Site/Jarnac.html) — SBW tool for metabolic analysis, includes dynamic simulation. Simulation engine for JDesigner. BSD License.

23. **JigCell** (http://jigcell.cs.vt.edu/) — JigCell is a set of computational tools with user-friendly interfaces developed for studying complex biochemical regulatory systems in general and the cell cycle control system in particular. For example, The JigCell Model Builder (JCMB) aides the modeler in defining a system to be modeled using SBML with a novel spreadsheet interface, allowing a large amount of data to be displayed in an organized manner. The JigCell Run Manager (JCRM) allows a user to specify a set of specifications for simulation runs using a spreadsheet interface. JigCell Aggregation Connector has been designed to define models in terms of components, for the purpose of being combined in a larger model. JigCell also aims in parameter estimation. A parameter estimator (PET, Parameter Estimation Toolkit) takes a biological model, experimental data, and the relationship between the model and data. Using this information the parameter estimator uses numerical tools to vary the parameters to the model looking for the parameters that best fit the experimental data.

24. **JSim** (http://www.physiome.org/jsim/) — JSim is a Java-based simulation system for building quantitative numeric models and analyzing them with respect to experimental reference data. JSim's primary focus is in physiology and biomedicine, however its computational engine is quite general and applicable to a wide range of scientific domains. JSim models may intermix ODEs, PDEs, implicit equations, integrals, summations, discrete events and procedural code as appropriate. JSim's model compiler can automatically insert conversion factors for compatible physical units as well as detect and reject unit unbalanced equations. JSim also supports model archive formats SBML (import and export) and CellML (import only).

25. **KEGGconverter** (http://www.grissom.gr/keggconverter/index.html) — KEGGconverter automatically produces merged and converted to SBML fully functional pathway models, enhanced with default kinetics, by inputting only KGML files.The final derived models do not enclose trivial metabolites -reproducing inconsistencies of the KGML visualization-oriented, simplified information pattern- but at the same time they contain all the available information

regarding the number of the included reactions in each pathway. Furthermore, additional reactions to neighbouring pathways are constructed which indicate the direction of the metabolic flows in the network and thus providing better stability in the boundary conditions of the models.

26. **MatCont** (http://sourceforge.net/projects/matcont/) — MatCont is a Matlab software package for the numerical study of parameterized continuous and discrete dynamical systems.

27. **MesoRD** (http://mesord.sourceforge.net) — MesoRD is a stochastic and deterministic simulator of coupled chemical reactions and diffusions in space.

28. **Metaboflux** (http://www.cbib.u-bordeaux2.fr/metaboflux/) — Metaboflux is a computational tool for predicting flux distribution in metabolic networks under multiple and various constraints deducted from the experiments. It aims to increase the biological relevance of models by integrating experimental data. The tool is available in two versions : a command line tool optimized for running on HPC servers and a user-friendly interface designed to define model parameters and run simple computations. Metaboflux embedded a stochastic simulator of metabolic networks coupled with a non linear solver (GSL). It solves constraints defined as proportions (for example, metabolite proportions) or as equations. Results can be visualized directly in Metaboflux or within specific tools like Systrip.

29. **MetaFluxNet** (http://metafluxnet.kaist.ac.kr) — MetaFluxNet is a program package for managing information on the metabolic reaction network and for quantitatively analyzing metabolic fluxes in an interactive and customized way, which allows users to interpret and examine metabolic behavior in response to genetic and/or environmental modifications. As a result, quantitative in silico simulations of metabolic pathways can be carried out to understand the metabolic status and to design the metabolic engineering strategies.

30. **MetExplore** (http://metexplore.toulouse.inra.fr) — A web server to link metabolic experiments and genome-scale metabolic networks. MetExplore contains original network filters, allows to export in SBML and visualise filtered metabolic networks, and map masses from metabolic experiments onto complete metabolic networks. It also contains some graph-based methods to enrich the analyses.

31. **MMT2** (http://www.simtec.mb.uni-siegen.de/software_mmt2.0.html) — Metabolic modeling, model fitting, automated high-performance code generation. (Linux only).

32. **MOOSE** (http://moose.ncbs.res.in/) — MOOSE is the base and numerical core for large, detailed simulations including Computational Neuroscience and Systems Biology. MOOSE spans the range from single molecules to subcellular networks, from single cells to neuronal networks, and to still larger systems. it is backwards- compatible with GENESIS, and forward compatible with Python and XML-based model definition standards like SBML and NeuroML.

33. **Odefy** (http://www.helmholtz-muenchen.de/cmb/odefy) — Odefy is a MATLAB and Octave compatible toolbox which a modeling technique called HillCube, a canonical method to convert boolean models into continuous ordinary differential equation (ODE) systems. HillCubes are based on multivariate polynomial interpolation and incorporate Hill kinetics which are known to provide a good approximation of the synergistic dynamics of gene regulation.

34. **ONDEX:**(http://www.ondex.org/) — The Ondex data integration platform enables data from diverse biological data sets to be linked, integrated and visualised through graph analysis techniques. Ondex uses a rich and flexible core data structure, which has the ability to bring together information from structured databases and unstructured sources such as biological sequence data and free text. Ondex also allows users to visualise and analyse the integrated data.
35. **OptFlux** (http://www.optflux.org/) — The OptFlux application includes a number of tools to support in silico metabolic engineering .

36. **Pathway Analyser** (http://sourceforge.net/projects/pathwayanalyser) — Flux analysis. Free download, open source (Linux).

37. **PET** (http://mpf.biol.vt.edu/pet) — Parameter optimization and exploration is the primary feature of PET. Some of the other tasks PET can perform are simulations, setting up multiple experiments for a model, comparing parameter sets, and exporting plots for presentations.

38. **PK-Sim / MoBi** (http://www.systems-biology.com) — Systems biology software platform for multiscale physiological modeling and simulation with a focus on physiologically-based pharmokinetics and -dynamics (PBPK/PD) including interfaces to MATLAB and R. Available to academic researchers via a free non-commercial license.

39. **PRISM** (http://www.prismmodelchecker.org/) — PRISM is a probabilistic model checker, a tool for formal verification of systems that exhibit stochastic behaviour. It supports construction and analysis of, amongst others, continuous-time Markov chains (CTMCs) and offers direct input from SBML models. PRISM performs exhaustive model analysis and computes exact values for a range of quantitative queries such as "what is the probability that ligand A eventually binds to protein B?" or "what is the expected amount of protein C at time T?".

40. **ProcessDB** (http://www.integrativebioinformatics.com/processdb.html) — ProcessDB helps molecular cell biologists manage and test their increasingly complex mechanistic hypotheses. ProcessDB does this with a bio-savvy graphical user interface that helps users formulate, visualize, compare, modify, manage and test their own mechanistic theories of cellular function. All models in ProcessDB can be automatically combined with user-specified experimental protocols and exported to the Berkeley Madonna solver for testing against experimental data. ProcessDB allows investigators to know with precision what their theories predict, and speeds discovery of mechanisms that account for all of the available data.

41. **PySCeS** (http://pysces.sourceforge.net) — PySCeS: the Python Simulator for Cellular Systems is an extendable toolkit for the analysis and investigation of cellular systems. PySCeS is developed in Python and has been designed to be used both interactively or as a library. It utilises a human readable, model description language for describing models as well as being SBML compatible. PySCeS includes stoichiometric, simulation, steady state and Eigen analysis using direct non-linear root finders. It also includes full support for Metabolic Control Analysis (MCA), the characterisation of static bifurcations, multidimensional parameter scanning and 2/3D graph capabilities. Currently an extension PySCeS-CBM is being developed that allows for the interactive manipulation, modelling and optimization of genome scale, constraint based models (e.g. flux balance analysis)

42. **SBML Harvester** (http://code.google.com/p/sbmlharvester/) — The SBML Harvester creates a complex ontology-based representation of SBML models, utilizing both the structure of the SBML model and the models' MIRIAM annotations. This representation can then be used for the consistency verification of SBML models as well as complex queries across both models and biomedical ontologies.
43. **SBMLSim** (http://www.dim.uchile.cl/~dremenik/SBMLSim/) — Matlab GUI that allows the user to import a SBML model, simulate it, and visualize the simulations.

44. **SBSI** (http://www.sbsi.ed.ac.uk) — SBSI provides high performance fitting of model parameters to experimental data, with especial focus on models with oscillatory components. Additionally SBSI provides a modelling environment for the Bio-PEPA and Kappa languages, as well as standard model editing and simulation capabilities

45. **SBToolbox2** (http://www.sbtoolbox2.org/) — MCA: Steady state control coefficients and elasticities; Structural analaysis: conservation relation analysis; model development; simulation; SBML Import/Export; parameter estimation; analysis tools. Requires MatLab(Linux/Win/Mac).

46. **SBW** (http://sys-bio.org/) — Systems Biology Workbench. A framework for connecting and running various applications written in different languages or on different systems, and a collection of available modules for model development, analysis, and simulation. Free/Open Source. (BSD)

47. **SensSB** (http://www.iim.csic.es/~gingproc/SensSB.html) — A software toolbox for the development and sensitivity analysis of systems biology models

48. **SimBiology** (http://www.mathworks.com/products/simbiology/) — SimBiology ® is a MATLAB ® product from MathWorks that provides graphical and programmatic tools for computational systems biology and pharmacokinetics. It contains functionality for creating, simulating, and analyzing biological models. The SimBiology desktop lets you build a model using a block diagram editor, a model wizard, or a tabular interface. You can also create a model at the command line or directly from SBML files. SimBiology lets you simulate a model using stochastic or deterministic solvers. The product supports parameter estimation, sensitivity analysis, parameter scans, and other model analysis methods. All SimBiology features can be used together with the MATLAB programming language, letting you customize models, create or modify analysis tasks, and automate your workflow.

49. **SloppyCell** (http://sloppycell.sourceforge.net/) — SloppyCell is focused on parameter estimation and sensitivity analysis for ODE models. In particular, SloppyCell includes semi-analytic sensitivity integration, along with capability for building Bayesian ensembles of parameters sets consistent with given data.

50. **SOSlib** (http://www.tbi.univie.ac.at/~raim/odeSolver/) — SOSlib is both a programming library and a command-line application for symbolic and numerical analysis of a system of ordinary differential equations (ODEs) derived from a chemical reaction network encoded in the Systems Biology Markup Language (SBML). It is written in ANSI/ISO C and distributed under the terms of the GNU Lesser General Public License (LGPL). The package employs libSBML's AST (Abstract Syntax Tree) for formula representation to construct ODE systems, their Jacobian matrix and other derivatives. CVODES, the sensitivity-enabled ODE solver in the

SUNDIALS package is used for numerical integration and sensitivity analysis of stiff and non-stiff ODE systems. The native API provides fine-grained interfaces to all internal data structures, symbolic operations and numerical routines, enabling the construction of powerful and efficient analytic applications, hybrid solvers or multi-scale models with interfaces to non SBML data sources. Optional modules based on Graphviz and XMGrace allow a quick inspection of a model's structure and dynamics.

51. **SurreyFBA** (http://sysbio3.fhms.surrey.ac.uk/) — provides constraint-based simulations of genome scale metabolic networks and network map visualization in a free, stand-alone software. In addition to basic simulation protocols the tool also implements the analysis of minimal substrate and product sets, which is useful for metabolic engineering and prediction of nutritional requirements in complex in vivo environments. The SurreyFBA is based on a command line interface to the GLPK solver distributed as binary and source code for the three major operating systems. The command line tool, implemented in C++, is easily executed within scripting languages used in the bioinformatics community and provides efficient implementation of tasks requiring iterative calls to the linear programming solver. SurreyFBA includes JyMet, a graphics user interface allowing spreadsheet based model presentation, visualization of numerical results on metabolic networks represented in the Petri net convention, as well as in charts and plots.

52. **SYCAMORE** (http://sycamore.eml.org) — SYCAMORE is a system that provides you with a faciliated access to a number of tools and methods in order to build models of biochemical systems, view, analyse and refine them, as well as perform quick simulations.

53. **Systrip** (http://tulip.labri.fr/TulipDrupal/?q=systrip) — Systrip is a visual environment for the analysis of time-series data in the context of biological networks. This software gathers bioinformatics and graph theoretical algorithms that can be assembled in different ways to help biologists in their visual mining process. Main features : 1. SBML file import and export. 2. Multiple kind of metabolic network representations (3D, force directed, biological convention preserving, hierachical ...). 3. Both graph theoritical measures and metabolic network analysis algorithms (choke points, scope, centrality...). 4. Time-series data import and visualization (table view, parallel coordinates, scatter plot). 5. Visualization of time-series in the context of the metabolic network. 6. 3D molecular visualization. 7. Database querry tools (Kegg, PublicHouse).

54. **Tide** (http://sysbio.molgen.mpg.de/tide/) — Tide is a tool for the automatic identification of optimal drug targets in kinetic models based on ordinary differential equations. Give a model in the popular SBML format it will identify promising drug targets for different effective modifier concentrations.

55. **TinkerCell** (http://www.tinkercell.com/) — TinkerCell is a visual application for constructing genetic, signaling, or metabolic networks with an extensive C and Python API. At present, the functionalities include deterministic and stochastic simulation (C libraries), steady state analysis, flux balance analysis using LPsolve C library, graph analysis through the NetworkX python module, and all the functionalities of PySCeS python module, including sensitivity and structural analysis. TinkerCell can build models by connecting modules. TinkerCell models contain meta-data for supporting a parts database. The visual display format is flexible.

56. **VANTED** (http://vanted.ipk-gatersleben.de/) — This system makes it possible to load and edit graphs, which may represent biological pathways or functional hierarchies. It is possible to map experimental datasets onto the graph elements and visualize time series data or data of different genotypes or environmental conditions in the context of a the underlying biological processes. Built-in statistic functions allow a fast evaluation of the data (e.g. t-Test or correlation analysis). Vanted can be extended for various functionalities, e.g. Flux simulation, database access and 3D visualisation.

57. **WebCell** (http://webcell.kaist.ac.kr/) — Online simulator, model builder, metabolic controal analysis. Includes database of bimodels and JWS models. Registration required.

58. **WinSCAMP** (http://www.sys-bio.org/software/winscamp.htm) — Windows Binary for SCAMP. Metabolic analysis, ODE solver. Binary download only. Source code on request.

2. Annotation software

1. **CellDesigner** (http://celldesigner.org) — CellDesigner is a structured diagram editor for drawing gene-regulatory and biochemical networks. Networks are drawn based on the process diagram, with graphical notation system. CellDesigner supports simulation and parameter scan by an integration with SBML ODE Solver and Copasi. By using CellDesigner, users can browse and modify existing SBML models with references to existing databases (MIRIAM supported), simulate and view the dynamics through an intuitive graphical interface.

2. **COPASI** (http://copasi.org) — COPASI is a software application for simulation and analysis of biochemical networks and their dynamics. COPASI is a stand-alone program that supports models in the SBML standard and can simulate their behavior using ODEs or Gillespie's stochastic simulation algorithm; arbitrary discrete events can be included in such simulations. COPASI provides an C++ API with language bindings for Perl, python, R, Java, and Octave and is able to communicate with the Systems Biology Workbench COPASI carries out several analyses of the network and its dynamics and has extensive support for parameter estimation and optimization. COPASI provides means to visualize data in customizable plots, histograms and animations of network diagrams. For a complete list of feature please see: http://www.copasi.org/tiki- index.php?page=FeatureList (http://www.copasi.org/tiki-index.php?page=FeatureList)

3. **KEGGtranslator** (http://www.ra.cs.uni-tuebingen.de/software/KEGGtranslator/) — Nowadays, the KEGG PATHWAY database provides a widely used service for pathway-based information. It contains manually drawn pathway maps with information about the genes, reactions and relations contained therein. To store these pathways, KEGG uses an own XML-format (called “KGML Parsers and translators are needed to process the pathway maps for usage ”). in other applications and algorithms. We have developed KEGGtranslator, which is an easy-to-use stand-alone application that can visualize and convert KGML formatted XML-files into multiple output formats. Unlike other translators, KEGGtranslator supports a plethora of output formats, is able to augment the information in translated documents (e.g., MIRIAM annotations) beyond the scope of the KGML document, and amends missing components to fragmentary reactions within the pathway to allow simulations on those. KEGGtranslator converts KEGG files (KGML formatted XML-files) to SBML, GML, GraphML,

JPG, GIF, LaTeX, etc. KEGG pathways can be obtained from ftp://ftp.genome.jp/pub/kegg/xml/kgml

4. **Metannogen** (http://www.bioinformatics.org/strap/metannogen/) — Metannogen is used to browse and annotate existing biological networks given in SBML. It can work together with any network editor that creates SBML files. Its capability of communication with other programs via network sockets allows embedding as a module within other software. It can also be used for network reconstruction to create a network from scratch.

5. **PAYAO** (http://www.payaologue.org) — PAYAO is a community collaborative web service platform for gene-regulatory and biochemical pathway model curation. PK-Sim / MoBi (http://www.systems-biology.com) — Systems biology software platform for multiscale physiological modeling and simulation with a focus on physiologically-based pharmokinetics and -dynamics (PBPK/PD) including interfaces to MATLAB and R. Available to academic researchers via a free non-commercial license.

6. **Saint** (http://saint.ncl.ac.uk/) — The creation of accurate quantitative Systems Biology Markup Language (SBML) models is a time-intensive manual process. Modelers need to know and understand both the systems they are modeling and the intricacies of SBML. However, the amount of relevant data for even a relatively small and well-scoped model is overwhelming. Saint, an automated SBML annotation integration environment, aims to aid the modeler and reduce development time by providing extra information about any given SBML model in an easy-to-use interface. Saint accepts SBML-formatted files and integrates information from multiple databases automatically. Any new information that the user agrees with is then automatically added to the SBML model. The purpose of Saint is to aid the researcher in the difficult task of information discovery by seamlessly querying multiple databases and providing the results of that query within the SBML model itself. By providing a modeling interface to existing data integration resources, modelers are able to add information to models quickly and simply.

7. **SBMLEditor** (http://www.ebi.ac.uk/compneur-srv/SBMLeditor.html) — SBMLeditor a very simple, low level editor of SBML files. Users can create and remove all the necessary bits and pieces of SBML in a controlled way, that maintains the validity and consistency of the final SBML file .

8. **SBMLsqueezer** (http://www.cogsys.cs.uni-tuebingen.de/software/SBMLsqueezer/) — SBMLsqueezer generates kinetic equations for biochemical networks according to context of each reaction. When used as a plug-in for CellDesigner it uses the information from the SBGN representation of all network components. In the stand-alone mode, SBMLsqueezer evaluates the Systems Biology Ontology (SBO) annotations to extract this information. An online version of SBMLsqueezer is available that runs without instally any software on the local machine. The rate laws that can be produced by SBMLsqueezer include several types of generalized mass action; detailed and generalized enzyme kinetics, various types of Hill equations, S- and H-systems, and additive models for gene regulation. User defined settings specify which equation to apply for any type of reaction and how to ensure unit consistency of the model. Equations can be created using contextual menus. All newly created parameters are equipped with the derived unit and annotated with SBO terms if available and meaningful textual names. MathML is inserted directly into the SBML file. LaTeX or text export of ordinary differential equations is provided.

9. **SBW** (http://sys-bio.org/) — Systems Biology Workbench. A framework for connecting and running various applications written in different languages or on different systems, and a collection of available modules for model development, analysis, and simulation. Free/Open Source. (BSD)

10. **semanticSBML** (http://semanticsbml.org) — Create, check, visualize, retrieve, cluster, annotate, merge SBML models. The program includes a web based graphical user interface. For tool developers a programming interface (Python) and RESTful web-services are provided. It features advanced functions to edit MIRIAM and SBO terms. The latest version of semanticSBML is fully web based and can be accessed under http://semanticsbml.org /semanticSBML/simple/index (http://semanticsbml.org/semanticSBML/simple/index)

3.Creation/development software

1. **ALC** (http://layer.mpi-magdeburg.mpg.de/) — ALC (Automated Layer Construction) (Koschorreck et al., BMC Systems Biology 2008, 2:91) is a computer program that highly simplifies the building of reduced modular models, according to the layer-based approach. The model is defined using a simple but powerful rule-based syntax that supports the concepts of modularity and macrostates. ALC performs consistency checks on the model definition and provides the model output in different formats (C MEX, MATLAB, Mathematica and SBML) as ready-to-run simulation files. ALC also provides additional documentation files that simplify the publication or presentation of the models. The tool can be used offline (which requires Perl) or via a form on the ALC website. ALC can bedownloaded from the ALC website or from SourceForge.

2. **Antimony** (http://antimony.sourceforge.net/) — libAntimony is a C/C++ library that can parse Antimony-formatted models, convert them to SBML, and provides an API to allow other tools access to model elements. Antimony models are modular, text-based, human readable and writable, largely compatible with SBML, and have a special syntax for creating genetic networks.

3. **Asmparts** (http://soft.synth-bio.org/asmparts.html) — Produces models of biological systems by assembling models from biological parts.

4. **Athena** (http://athena.codeplex.com/) — Athena is a graphical modeling tool experimenting with modular systems. Athena is integrated with SBW and allows the analysis of models through a multitude of plugins. It is available for windows only, and released under the BSD license.

5. **BALSA** (http://depts.washington.edu/ventures/UW_Technology/Emerging_Technologies/CSI.php) — Front end for Sigtran (inactive?)

6. **Bio Sketch Pad** (http://sbml.org/SBML_Software_Guide/We_Don %27t_Have_A_Link_For_This_Tool) — graphical model design tool, front
7. end for BioCharon

8. **BioCharon** (http://www.cis.upenn.edu/biocomp) — BioCharon includes a suite of tools for

developing models for use with CHARON. It includes the graphical BioSketchPad for desigining models, a hybrid SBML/C++ language model builder, and a metabolic analyzer. Biological Networks (http://www.biologicalnetworks.org/) — Pathway model development supports SBML Import/Export (only supports simple mass action kinetics); visualization; data management; network/metabolic analysis; clustering. No simulation engine. Free academic download (Java web start, Windows/Linux/Mac).

9. **BioNetGen** (http://bionetgen.org/) — BioNetGen is a software system for the specification and simulation of rule-based models of biochemical systems. In rule-based models, molecules and molecular complexes are represented using graphs, and molecular interactions and their consequences are represented using graph-rewriting rules. Open source. Download requires email based registration. Requires Perl. Optional GUI uses JRE. (Linux/Mac/Win)

10. **BioSpreadsheet** (http://biocomp.ece.utk.edu/tools.html) — SBML model editor. Part of the UTK/ORNL Bio-SPICE tool set which includes the Exact Stochastic Simulator (ESS). Requires BioSpice Dashboard. Free download. Includes Source code.

11. **BioTapestry** (http://www.biotapestry.org/) — Graphical model development and simulation tool for genetic regulatory networks based on JRE. Uses Java Web Start. Free download. SBML export.

12. **BioUML** (http://www.biouml.org/) — platform for building virtual cell and virtual physiological human .

13. **Cell Illustrator** (http://www.fqs.pl/life_science/cell_illustrator) — Graphical model editor; Petri-net based simulation algorithm; SBML Import. Commercial. (Linux/Mac/Win).

14. **CellDesigner** (http://celldesigner.org) — CellDesigner is a structured diagram editor for drawing gene-regulatory and biochemical networks. Networks are drawn based on the process diagram, with graphical notation system. CellDesigner supports simulation and parameter scan by an integration with SBML ODE Solver and Copasi. By using CellDesigner, users can browse and modify existing SBML models with references to existing databases (MIRIAM supported), simulate and view the dynamics through an intuitive graphical interface.

15. **Cellerator** (http://www.cellerator.net/) — Cellerator describes single and multi-cellular signal transduction networks (STN) with a compact, optionally palette-driven, arrow-based notation to represent biochemical reactions and transcriptional activation. Multi-compartment systems are represented as graphs with STNs embedded in each node. Interactions include mass-action, enzymatic, allosteric and connectionist models. Reactions are translated into differential equations and can be solved numerically to generate predictive time courses or output as systems of equations that can be read by other programs. Cellerator simulations are fully extensible and portable to any operating system that supports Mathematica, and can be indefinitely nested within larger data structures to produce highly scaleable models.. Cellerator is superseeded by xCellerator.

16. **COPASI** (http://copasi.org) — COPASI is a software application for simulation and analysis of biochemical networks and their dynamics. COPASI is a stand-alone program that supports models in the SBML standard and can simulate their behavior using ODEs or Gillespie's

stochastic simulation algorithm; arbitrary discrete events can be included in such simulations. COPASI provides an C++ API with language bindings for Perl, python, R, Java, and Octave and is able to communicate with the Systems Biology Workbench COPASI carries out several analyses of the network and its dynamics and has extensive support for parameter estimation and optimization. COPASI provides means to visualize data in customizable plots, histograms and animations of network diagrams. For a complete list of feature please see: http://www.copasi.org/tiki- index.php?page=FeatureList (http://www.copasi.org/tiki-index.php?page=FeatureList)

17. **DBSolve** (http://insysbio.ru/en/soft/dbsolveoptimum.html) — DBSolveOptimum is a free software for kinetic modeling of metabolic pathways, analysis, and fitting parameters to experimental data. The program has text-based user interface for model description and graphical interface for data analysis. In addition to standart algorithms of simulation (ODE solver, explicit solver, steady-state analysis) the software include also automated local sencetivity analysis, parameters optimization procedures and bifurcaion analysis. The last version of DBSolveOptimum includes advanced tool for data visualization.

18. **Facile** (http://facile.sourceforge.net) — Facile / EasyStoch. A command-line network compiler for systems biology. Facile reads models given in a simple and human-readable textual input format and exports the model in a format for readable by Matlab, Mathematica, Maple, XPP/AUTO. Other tools are supported via SBML export. For stochastic simulations, Facile uses the EasyStoch stochastic simulator. An important feature of EasyStoch that distinguishes it from other Gillespie-algorithm implementations is that it is capable of simulating dynamically changing or noisy biochemical parameters (i.e. extrinsic noise).

19. **Genetic Network Analyzer** (http://www-helix.inrialpes.fr/gna) — Genetic Network Analyzer (GNA) is a computer tool for the modeling, simulation, analysis and verification of genetic regulatory networks. The aim of GNA is to assist biologists and bio-informaticians in constructing a qualitative model of a genetic regulatory network from knowledge about regulatory interactions and gene expression data. GNA provides a variety of functions to analyze the steady-state and transient dynamics of the network, among other things by exploiting state- of-the-art model-checking tools.

20. **GNU MCSim** (http://www.gnu.org/software/mcsim/) — GNU MCSim is a free standalone simulation package that allows you to design your own statistical or simulation models. It efficiently performs Bayesian inference through Markov Chain Monte Carlo simulations. Standard Monte Carlo and experimental design optimization are also available. GNU MCSim can import and simulate levels 1 and 2 SBML models .

21. **HSMB** (http://sbml.org/SBML_Software_Guide/We_Don%27t_Have_A_Link_For_This_Tool) — Hybrid SBML Model Builder for BioCharon.

22. **HybridSBML** (http://biocomp.cis.upenn.edu/software.php3) — Hybrid SBML Model Builder for BioCharon

23. **iBioSim** (http://www.async.ece.utah.edu/iBioSim/) — The iBioSim tool supports the modeling, analysis, and design of genetic circuits with applications in both systems and synthetic biology. It includes editors to construct genetic circuit models (GCM), Systems Biology Markup Language (SBML) models (L2V4 and L3V1 supported), and labeled Petri net (LPN)

models. Models can be constructed by hand, imported from model databases, or learned from experimental data. These models can be analyzed using a variety of ODE and stochastic simulators as well as Markov chain analysis. The efficiency of these analysis methods is enhanced using a variety of automatic reaction-based and logical abstractions. The analysis results can be plotted as graphs or visualized upon the genetic circuit schematic.

24. **insilicoIDE** (http://www.physiome.jp/) — insilicoIDE (ISIDE) assists users to build models of physiological functions with multilevel hierarchical structure and to run simulations. A model is built as a functional network of "modules" which represent physiological entities. In each module, equations such as ODEs and PDEs, parameters and morphological information can be defined. Besides, a module can include a model written in SBML. The SBML model is functionally embedded in the module network. There is an open model database at www.physiome.jp. Users can use models in the database freely as parts to build their own model. The modularity of the model representation in ISIDE makes reuse and integration of multiple models easier. The simulator included in ISIDE supports parallel computing.

25. **JACOBIAN** (http://numericatech.com/jacobian.htm) — numerical engine underlying OpenBio

26. **Jarnac** (http://jdesigner.sourceforge.net/Site/Jarnac.html) — SBW tool for metabolic analysis, includes dynamic simulation. Simulation engine for JDesigner. BSD License.

27. **JarnacLite** (http://www.sys-bio.org/sbwWiki/sbw/jarnaclite) — JarnacLite allows to edit SBML through a simple script based format. It is integrated with SBW, so that a model created with JarnacLite can be quickly simulated and analyzed with a variety of tools. JarnacLite is available on all platforms, and as translator also online. It is released under the BSD license.

28. **JDesigner** (http://sbw.kgi.edu/software/jdesigner.htm) — Graphical model design tool. Typically uses RoadRunner as a simulation engine via SBW. Free/Open Source (BSD).

29. **JigCell** (http://jigcell.cs.vt.edu/) — JigCell is a set of computational tools with user-friendly interfaces developed for studying complex biochemical regulatory systems in general and the cell cycle control system in particular. For example, The JigCell Model Builder (JCMB) aides the modeler in defining a system to be modeled using SBML with a novel spreadsheet interface, allowing a large amount of data to be displayed in an organized manner. The JigCell Run Manager (JCRM) allows a user to specify a set of specifications for simulation runs using a spreadsheet interface. JigCell Aggregation Connector has been designed to define models in terms of components, for the purpose of being combined in a larger model. JigCell also aims in parameter estimation. A parameter estimator (PET, Parameter Estimation Toolkit) takes a biological model, experimental data, and the relationship between the model and data. Using this information the parameter estimator uses numerical tools to vary the parameters to the model looking for the parameters that best fit the experimental data.

30. **JSim** (http://www.physiome.org/jsim/) — JSim is a Java-based simulation system for building quantitative numeric models and analyzing them with respect to experimental reference data. JSim's primary focus is in physiology and biomedicine, however its computational engine is quite general and applicable to a wide range of scientific domains. JSim models may intermix ODEs, PDEs, implicit equations, integrals, summations, discrete events and procedural code as appropriate. JSim's model compiler can automatically insert conversion factors for compatible physical units as well as detect and reject unit unbalanced equations. JSim also supports model

archive formats SBML (import and export) and CellML (import only).

31. **Karyote** (http://biodynamics.indiana.edu/CellModeling/) — Online model development tool based on online database of parts. Claims to have some sort of simulator and SBML support. Level unclear. Documentation absent.

32. **KEGGtranslator** (http://www.ra.cs.uni-tuebingen.de/software/KEGGtranslator/) — Nowadays, the KEGG PATHWAY database provides a widely used service for pathway-based information. It contains manually drawn pathway maps with information about the genes, reactions and relations contained therein. To store these pathways, KEGG uses an own XML-format (called "KGML Parsers and translators are needed to process the pathway maps for usage "). in other applications and algorithms. We have developed KEGGtranslator, which is an easy-to-use stand-alone application that can visualize and convert KGML formatted XML-files into multiple output formats. Unlike other translators, KEGGtranslator supports a plethora of output formats, is able to augment the information in translated documents (e.g., MIRIAM annotations) beyond the scope of the KGML document, and amends missing components to fragmentary reactions within the pathway to allow simulations on those. KEGGtranslator converts KEGG files (KGML formatted XML-files) to SBML, GML, GraphML, JPG, GIF, LaTeX, etc. KEGG pathways can be obtained from ftp://ftp.genome.jp/pub/kegg/xml/kgml

33. **MetaFluxNet** (http://metafluxnet.kaist.ac.kr) — MetaFluxNet is a program package for managing information on the metabolic reaction network and for quantitatively analyzing metabolic fluxes in an interactive and customized way, which allows users to interpret and examine metabolic behavior in response to genetic and/or environmental modifications. As a result, quantitative in silico simulations of metabolic pathways can be carried out to understand the metabolic status and to design the metabolic engineering strategies.

34. **MetNetMaker** (http://www.metnetmaker.com) — MetNetMaker is the simplest way to create SBML-format metabolic models based on the KEGG LIGAND ontology. Models can be visualised in Cytoscape and are ready for FBA using the COBRA toolbox.

35. **Monod** (http://monod.molsci.org/) — "Modeler's Notebook and Data Store" model annotation manager. (Linux/Mac OS) Open Source, Must build from source (LGPL).

36. **NetBuilder**' (http://strc.herts.ac.uk/bio/maria/Apostrophe/) — NetBuilder' is a software tool that is intended to help experimentalists creating and manipulating the mathematical representations they need to predict the behaviour of their systems. NetBuilder' has a graphical user interface, which allows its users to create a picture of the (known) components and interactions in the system, and enter quantitative information, such as know or estimated quantities and rates. A (hidden) translator converts the picture and the other data into a mathematical description, whereupon NetBuilder's "simulation engine" may be used to find out how the modelled system responds to changing input.

37. **Pathway Builder** (http://biospice.sourceforge.net/) — Graphical model design. Part of Bio-Spice. (BioSpice BSD License)

38. **PathwayLab** (http://innetics.com/) — Deterministic simulation; Visualization; MCA; Mathematica and Matlab integration; model creation. (Windows) (Commercial).

39. **PK-Sim / MoBi** (http://www.systems-biology.com) — Systems biology software platform for multiscale physiological modeling and simulation with a focus on physiologically-based pharmokinetics and -dynamics (PBPK/PD) including interfaces to MATLAB and R. Available to academic researchers via a free non-commercial license.

40. **ProcessDB** (http://www.integrativebioinformatics.com/processdb.html) — ProcessDB helps molecular cell biologists manage and test their increasingly complex mechanistic hypotheses. ProcessDB does this with a bio-savvy graphical user interface that helps users formulate, visualize, compare, modify, manage and test their own mechanistic theories of cellular function. All models in ProcessDB can be automatically combined with user-specified experimental protocols and exported to the Berkeley Madonna solver for testing against experimental data. ProcessDB allows investigators to know with precision what their theories predict, and speeds discovery of mechanisms that account for all of the available data.

41. **ProMoT** (http://www.mpi-magdeburg.mpg.de/projects/promot) — The process modeling tool ProMoT is a software for the set-up and manipulation of models of complex technical or biological systems. Key features are the support of modular models, modeling libraries for different application areas, efficient and robust numerical algorithms, a own modeling language MDL and advanced graphical support. Dynamic models can contain DAE and discrete events for simulation in DIVA, Diana or MATLAB. Logical (Boolean) models are exported to CellNetAnalyzer.

42. **Saint** (http://saint.ncl.ac.uk/) — The creation of accurate quantitative Systems Biology Markup Language (SBML) models is a time-intensive manual process. Modelers need to know and understand both the systems they are modeling and the intricacies of SBML. However, the amount of relevant data for even a relatively small and well-scoped model is overwhelming. Saint, an automated SBML annotation integration environment, aims to aid the modeler and reduce development time by providing extra information about any given SBML model in an easy-to-use interface. Saint accepts SBML-formatted files and integrates information from multiple databases automatically. Any new information that the user agrees with is then automatically added to the SBML model. The purpose of Saint is to aid the researcher in the difficult task of information discovery by seamlessly querying multiple databases and providing the results of that query within the SBML model itself. By providing a modeling interface to existing data integration resources, modelers are able to add information to models quickly and simply.

43. **SBML2NEURON** (http://www.neuroml.org/neuron_tools.php) — SBML2NEURON is a provisional implementation of an SBML to NEURON converter. This uses the Python bindings of libSBML to generate an NMODL file containing the model represented in a basic SBML file, which can then be inserted onto a section in NEURON for simulation. Note that only a restricted set of SBML elements are supported (see the notes), but it can be used to simulate some of the models in BioModels Database. This is a work in progress and will be developed further to allow closer integration between NeuroML and SBML in realistic neuronal models.

44. **SBMLEditor** (http://www.ebi.ac.uk/compneur-srv/SBMLeditor.html) — SBMLeditor a very simple, low level editor of SBML files. Users can create and remove all the necessary bits and pieces of SBML in a controlled way, that maintains the validity and consistency of the final SBML file

45. **SBML-shorthand** (http://www.staff.ncl.ac.uk/d.j.wilkinson/software/sbml-sh/) — Specification and conversion tools for a simple human-readable shorthand notation for a subset of SBML. Used for rapid building of SBML models without using a sophisticated GUI tool.

46. **SBMLsqueezer** (http://www.cogsys.cs.uni-tuebingen.de/software/SBMLsqueezer/) — SBMLsqueezer generates kinetic equations for biochemical networks according to context of each reaction. When used as a plug-in for CellDesigner it uses the information from the SBGN representation of all network components. In the stand-alone mode, SBMLsqueezer evaluates the Systems Biology Ontology (SBO) annotations to extract this information. An online version of SBMLsqueezer is available that runs without instally any software on the local machine. The rate laws that can be produced by SBMLsqueezer include several types of generalized mass action; detailed and generalized enzyme kinetics, various types of Hill equations, S- and H-systems, and additive models for gene regulation. User defined settings specify which equation to apply for any type of reaction and how to ensure unit consistency of the model. Equations can be created using contextual menus. All newly created parameters are equipped with the derived unit and annotated with SBO terms if available and meaningful textual names. MathML is inserted directly into the SBML file. LaTeX or text export of ordinary differential equations is provided.

47. **SBMLToolbox** (http://sbml.org/Software/SBMLToolbox) — Manipulation of SBML in both the MATLAB and Octave environments. Some simulation support but the main focus is on allowing users to adapt SBML to their existing MATLAB/Octave functions.

48. **SBW** (http://sys-bio.org/) — Systems Biology Workbench. A framework for connecting and running various applications written in different languages or on different systems, and a collection of available modules for model development, analysis, and simulation. Free/Open Source. (BSD)

49. **semanticSBML** (http://semanticsbml.org) — Create, check, visualize, retrieve, cluster, annotate, merge SBML models. The program includes a web based graphical user interface. For tool developers a programming interface (Python) and RESTful web-services are provided. It features advanced functions to edit MIRIAM and SBO terms. The latest version of semanticSBML is fully web based and can be accessed under http://semanticsbml.org /semanticSBML/simple/index (http://semanticsbml.org/semanticSBML/simple/index)

50. **SigTran** (http://www.cellsystems.org/teams/modeling/projects/sigtran/overview.html) — SigTran is a modeling environment especially designed to enable biological researchers to carry out large scale simulations and analysis of complex signal transduction networks.

51. **SimBiology** (http://www.mathworks.com/products/simbiology/) — SimBiology ® is a MATLAB ® product from MathWorks that provides graphical and programmatic tools for computational systems biology and pharmacokinetics. It contains functionality for creating, simulating, and analyzing biological models. The SimBiology desktop lets you build a model using a block diagram editor, a model wizard, or a tabular interface. You can also create a model at the command line or directly from SBML files. SimBiology lets you simulate a model using stochastic or deterministic solvers. The product supports parameter estimation, sensitivity analysis, parameter scans, and other model analysis methods. All SimBiology features can be used together with the MATLAB programming language, letting you

customize models, create or modify analysis tasks, and automate your work-flow.

4.Data integration and management software

1. **BioPathwise** (http://www.bioanalyticsgroup.com/index_files/Page465.htm) — BioPathwise is a pathway-centric environment for interdisciplinary collaborative research. The main interface is a pathway whiteboard that allows graphic representation of pathways, visualization of experimental data, pathway simulation, statistical analysis and regression. Extensible via an open API.

2. **CADLIVE** (http://www.cadlive.jp) — CADLIVE (Computer-Aided Design of LIVing systEms) is a comprehensive computational tool for constructing large-scale biological network maps, analyzing the topological features of them, and simulating their dynamics. Using CADLIVE, we rationally design a biological system at the molecular interaction level for an engineering purpose.

3. **CARMEN** (http://carmen.cebitec.uni-bielefeld.de/cgi-bin/index.cgi) — The software CARMEN was developed to support functional and comparative genome analysis. CARMEN provides the visualization of automatically obtained metabolic networks based on KEGG database information and stores the generated data in standardized SBML format. SBML is an open source XML-based format that facilitates the description of models and their exchange between various simulation and analysis tools (Hucka, 2003).

4. **Insilico Discovery** (http://www.insilico-biotechnology.com/insilico_discovery) — modeling and simulation platform for graphically oriented setup, management and engineering of cellular networks insilicoIDE (http://www.physiome.jp/) — insilicoIDE (ISIDE) assists users to build models of physiological functions with multilevel hierarchical structure and to run simulations. A model is built as a functional network of "modules" which represent physiological entities. In each module, equations such as ODEs and PDEs, parameters and morphological information can be defined. Besides, a module can include a model written in SBML. The SBML model is functionally embedded in the module network. There is an open model database at www.physiome.jp. Users can use models in the database freely as parts to build their own model. The modularity of the model representation in ISIDE makes reuse and integration of multiple models easier. The simulator included in ISIDE supports parallel computing.

5. **JSim** (http://www.physiome.org/jsim/) — JSim is a Java-based simulation system for building quantitative numeric models and analyzing them with respect to experimental reference data. JSim's primary focus is in physiology and biomedicine, however its computational engine is quite general and applicable to a wide range of scientific domains. JSim models may intermix ODEs, PDEs, implicit equations, integrals, summations, discrete events and procedural code as appropriate. JSim's model compiler can automatically insert conversion factors for compatible physical units as well as detect and reject unit unbalanced equations. JSim also supports model archive formats SBML (import and export) and CellML (import only).

6. **KEGGconverter** (http://www.grissom.gr/keggconverter/index.html) — KEGGconverter automatically produces merged and converted to SBML fully functional pathway models, enhanced with default kinetics, by inputting only KGML files.The final derived models do not

enclose trivial metabolites -reproducing inconsistencies of the KGML visualization-oriented, simplified information pattern- but at the same time they contain all the available information regarding the number of the included reactions in each pathway. Furthermore, additional reactions to neighbouring pathways are constructed which indicate the direction of the metabolic flows in the network and thus providing better stability in the boundary conditions of the models.

7. **KEGGtranslator** (http://www.ra.cs.uni-tuebingen.de/software/KEGGtranslator/) — Nowadays, the KEGG PATHWAY database provides a widely used service for pathway-based information. It contains manually drawn pathway maps with information about the genes, reactions and relations contained therein. To store these pathways, KEGG uses an own XML-format (called "KGML Parsers and translators are needed to process the pathway maps for usage "). in other applications and algorithms. We have developed KEGGtranslator, which is an easy-to-use stand-alone application that can visualize and convert KGML formatted XML-files into multiple output formats. Unlike other translators, KEGGtranslator supports a plethora of output formats, is able to augment the information in translated documents (e.g., MIRIAM annotations) beyond the scope of the KGML document, and amends missing components to fragmentary reactions within the pathway to allow simulations on those. KEGGtranslator converts KEGG files (KGML formatted XML-files) to SBML, GML, GraphML, JPG, GIF, LaTeX, etc. KEGG pathways can be obtained from ftp://ftp.genome.jp/pub/kegg/xml/kgml

8. **Medicel** (http://www.euformatics.com) — commercial data integration framework. (now euformatics)

9. **MetaCrop** (http://metacrop.ipk-gatersleben.de/) — MetaCrop is a database that contains manually curated, highly detailed information about metabolic pathways in crop plants, including location information, transport processes, and reaction kinetics. The web interface supports an easy exploration of the information from overview pathways to single reactions and therefore helps users understanding the metabolism of crop plants. It also allows automatic data export for the creation of detailed models of metabolic pathways to support simulation approaches.

10. **Metannogen** (http://www.bioinformatics.org/strap/metannogen/) — Metannogen is used to browse and annotate existing biological networks given in SBML. It can work together with any network editor that creates SBML files. Its capability of communication with other programs via network sockets allows embedding as a module within other software. It can also be used for network reconstruction to create a network from scratch.

11. **MIRIAM** Resources (http://www.ebi.ac.uk/miriam) — a set of online services created in support of MIRIAM, a set of guidelines for the annotation and curation of computational models.

12. **ONDEX** (http://www.ondex.org/) — The Ondex data integration platform enables data from diverse biological data sets to be linked, integrated and visualized through graph analysis techniques. Ondex uses a rich and flexible core data structure, which has the ability to bring together information from structured databases and unstructured sources such as biological sequence data and free text. Ondex also allows users to visualise and analyse the integrated data.

13. **Pathway Access** (http://vrac.iastate.edu/~jlv/pathwayaccess/) — PathwayAccess is a suite of CellDesigner plugins which directly interact with pathway datasources

14. **Pathway Tools** (http://bioinformatics.ai.sri.com/ptools/) — Extracts and integrates information from pathway/genome databases (see BioCyc); metabolic analysis; gene code prediction; operon prediction; gene expression analysis. Optional support: Oracle or MySQL, Browser, BLAST, Marvin Msketch, JME/OpenBabel. SBML support via BioCyc. Free academic; fee for commercial. License application must be reviewed by SRIC before download. SRI unique license. (Linux/Windows/Solaris/Mac).

15. **PATIKAweb** (http://www.patika.org/) — Pathway database integration; pathway visualization and analysis. Online tool only. (Acad/NP)

16. **PK-Sim / MoBi** (http://www.systems-biology.com) — Systems biology software platform for multiscale physiological modeling and simulation with a focus on physiologically-based pharmokinetics and -dynamics (PBPK/PD) including interfaces to MATLAB and R. Available to academic researchers via a free non-commercial license.

17. **ProcessDB** (http://www.integrativebioinformatics.com/processdb.html) — ProcessDB helps molecular cell biologists manage and test their increasingly complex mechanistic hypotheses. ProcessDB does this with a bio-savvy graphical user interface that helps users formulate, visualize, compare, modify, manage and test their own mechanistic theories of cellular function. All models in ProcessDB can be automatically combined with user-specified experimental protocols and exported to the Berkeley Madonna solver for testing against experimental data. ProcessDB allows investigators to know with precision what their theories predict, and speeds discovery of mechanisms that account for all of the available data.

18. **PROTON** (http://tunicata.techfak.uni-bielefeld.de/proton/web/main.jsp) — Integrated modeling environment. Reconstructs biochemical systems from molecular databases in an automated and user-centric way. Fuses information from distributed databases and the reconstruction of systems is interactively controlled by the user. The approach is based on different layers which allow the integrative modelling of biochemical systems at multiple levels. ODE based modeling and simulation. (Free Download. Optional Server, Windows; Client: Linus/Windows/Mac).

19. **ReMatch** (http://www.cs.helsinki.fi/group/sysfys/software/rematch/) — ReMatch is a web-based tool for integration of user-given stoichiometric metabolic models into a database collected from public data sources such as KEGG, MetaCyc, CheBI and ARM. ReMatch is geared particularly towards 13C metabolic flux analysis: it is possible to augment the model with carbon mappings and export the model to analysis in 13C flux analysis software

20. **SABIO-RK** (http://sabiork.h-its.org/) — SABIO-RK is a curated database for biochemical reaction kinetics data. The data is drawn from different sources: by extraction from published literature or direct submission by experimenters, and is supplemented with additional data from other databases. The system offers standardized data by the use of controlled vocabularies and annotations pointing to other resources and biological ontologies. It can be accessed either manually via a web-based search interface or automatically via web services that allow direct data access by other tools. Both interfaces support the export of the data

together with its annotations in SBML. SABIO-RK facilitates the exchange of kinetic data between experimentalists and modellers, and thereby supports the setup of quantitative computer models.

21. **Saint** (http://saint.ncl.ac.uk/) — The creation of accurate quantitative Systems Biology Markup Language (SBML) models is a time-intensive manual process. Modelers need to know and understand both the systems they are modeling and the intricacies of SBML. However, the amount of relevant data for even a relatively small and well-scoped model is overwhelming. Saint, an automated SBML annotation integration environment, aims to aid the modeler and reduce development time by providing extra information about any given SBML model in an easy-to-use interface. Saint accepts SBML-formatted files and integrates information from multiple databases automatically. Any new information that the user agrees with is then automatically added to the SBML model. The purpose of Saint is to aid the researcher in the difficult task of information discovery by seamlessly querying multiple databases and providing the results of that query within the SBML model itself. By providing a modeling interface to existing data integration resources, modelers are able to add information to models quickly and simply.

22. **SBML Harvester** (http://code.google.com/p/sbmlharvester/) — The SBML Harvester creates a complex ontology-based representation of SBML models, utilizing both the structure of the SBML model and the models' MIRIAM annotations. This representation can then be used for the consistency verification of SBML models as well as complex queries across both models and biomedical ontologies.

23. **SBMM assistant** (http://cath.gisum.uma.es:8080/sbmm/) — Systems Biology Metabolic Modeling assistant (SBMM assistant) is a web application to consult basic metabolic information, to build metabolic models, and to annotate them in SBML files with external resource annotations suggested by MIRIAM

24. **SBO** (http://www.ebi.ac.uk/sbo/) — The Systems Biology Ontology is a set of controlled, relational vocabularies of terms commonly used in Systems Biology, and in particular in computational modeling.

25. **SCIpath** (http://sbml.org/SBML_Software_Guide/We_Don%27t_Have_A_Link_For_This_Tool) — microarray data management. (Linux/Windows).

26. **semanticSBML** (http://semanticsbml.org) — Create, check, visualize, retrieve, cluster, annotate, merge SBML models. The program includes a web based graphical user interface. For tool developers a programming interface (Python) and RESTful web-services are provided. It features advanced functions to edit MIRIAM and SBO terms. The latest version of semanticSBML is fully web based and can be accessed under http://semanticsbml.org /semanticSBML/simple/index (http://semanticsbml.org/semanticSBML/simple/index)

27. **SIGNALIGN** (http://agbi.techfak.uni-bielefeld.de/signalign/index.jsp) — online pathway alignment service.

28. **SigPath** (http://www.sigpath.org/) — Bioinformatic database and pathway management (GPL).

29. **SimBiology** (http://www.mathworks.com/products/simbiology/) — SimBiology ® is a MATLAB ® product from MathWorks that provides graphical and programmatic tools for computational systems biology and pharmacokinetics. It contains functionality for creating, simulating, and analyzing biological models. The SimBiology desktop lets you build a model using a block diagram editor, a model wizard, or a tabular interface. You can also create a model at the command line or directly from SBML files. SimBiology lets you simulate a model using stochastic or deterministic solvers. The product supports parameter estimation, sensitivity analysis, parameter scans, and other model analysis methods. All SimBiology features can be used together with the MATLAB programming language, letting you customize models, create or modify analysis tasks, and automate your workflow.

30. **SRS** (http://www.biowisdom.com/2009/12/srs/) — Data integration for bioinformatics. Commercial.

31. **SYCAMORE** (http://sycamore.eml.org) — SYCAMORE is a system that provides you with a faciliated access to a number of tools and methods in order to build models of biochemical systems, view, analyse and refine them, as well as perform quick simulations.

32. **VANTED** (http://vanted.ipk-gatersleben.de/) — This system makes it possible to load and edit graphs, which may represent biological pathways or functional hierarchies. It is possible to map experimental datasets onto the graph elements and visualize time series data or data of different genotypes or environmental conditions in the context of a the underlying biological processes. Built-in statistic functions allow a fast evaluation of the data (e.g. t-Test or correlation analysis). Vanted can be extended for various functionalities, e.g. Flux simulation, database access and 3D visualisation. Framework or library

33. **BioSPICE** Dashboard (http://www.biospice.org/) — Large collection of tools

5.Framework or library

1. **BioSPICE** Dashboard (http://www.biospice.org/) — Large collection of tools, integrated via a "Dashboard." Free download (BSD), various platforms.

2. **CLEML** (http://bioinfo.ustc.edu.cn/softwares/CLEML/) — Carbon Labeling Experiment Markup Language. The libCLEML is freely downloadable (GPL). (Linux/Win).

3. **CL-SBML** (http://common-lisp.net/project/cl-sbml) — Common Lisp implementation of the SBML Standard (Level 2). I/O library for SBML in Common Lisp.

4. **COPASI** (http://copasi.org) — COPASI is a software application for simulation and analysis of biochemical networks and their dynamics. COPASI is a stand-alone program that supports models in the SBML standard and can simulate their behavior using ODEs or Gillespie's stochastic simulation algorithm; arbitrary discrete events can be included in such simulations. COPASI provides an C++ API with language bindings for Perl, python, R, Java, and Octave and is able to communicate with the Systems Biology Workbench COPASI carries out several analyses of the network and its dynamics and has extensive support for parameter estimation and optimization. COPASI provides means to visualize data in customizable plots, histograms and animations of network diagrams. For a complete list of feature please see: http://www.copasi.org/tiki- index.php?page=FeatureList (http://www.copasi.org/tiki-

index.php?page=FeatureList)

5. **JSBML** (http://sourceforge.net/projects/jsbml/) — open-source, Java library for reading, writing, and manipulating SBML files

6. **JSim** (http://www.physiome.org/jsim/) — JSim is a Java-based simulation system for building quantitative numeric models and analyzing them with respect to experimental reference data. JSim's primary focus is in physiology and biomedicine, however its computational engine is quite general and applicable to a wide range of scientific domains. JSim models may intermix ODEs, PDEs, implicit equations, integrals, summations, discrete events and procedural code as appropriate. JSim's model compiler can automatically insert conversion factors for compatible physical units as well as detect and reject unit unbalanced equations. JSim also supports model archive formats SBML (import and export) and CellML (import only).

7. **libAnnotationSBML** (http://sbml.org/Community/Programs/libAnnotationSBML) — Java library for reading and writing MIRIAM- compliant SBML annotations

8. **libSBML** (http://www.sbml.org/software/libsbml) — Library for C, C++, .NET, Java, Lisp, Python, Perl, Matlab, Octave, and Ruby. Free Download (LGPL). (Linux/Mac/Win).

9. **libStruct** (http://sourceforge.net/apps/mediawiki/libstruct/index.php?title=Main_Page) — The structural analysis library is a C/C++ portable software library for analyzing the structural properties of stoichiometric networks. The library supports the analysis of both flux balance and moiety conservation. The library will accept models in the form of either standard SBML or raw stoichiometry matrices. The software is distributed under the BSD license and was developed through funding from NIH grant 1R01GM081070-01.

10. **Metannogen** (http://www.bioinformatics.org/strap/metannogen/) — Metannogen is used to browse and annotate existing biological networks given in SBML. It can work together with any network editor that creates SBML files. Its capability of communication with other programs via network sockets allows embedding as a module within other software. It can also be used for network reconstruction to create a network from scratch.

11. **Odefy** (http://www.helmholtz-muenchen.de/cmb/odefy) — Odefy is a MATLAB and Octave compatible toolbox which a modeling technique called HillCube, a canonical method to convert boolean models into continuous ordinary differential equation (ODE) systems. HillCubes are based on multivariate polynomial interpolation and incorporate Hill kinetics which are known to provide a good approximation of the synergistic dynamics of gene regulation.

12. **PySCeS** (http://pysces.sourceforge.net) — PySCeS: the Python Simulator for Cellular Systems is an extendable toolkit for the analysis and investigation of cellular systems. PySCeS is developed in Python and has been designed to be used both interactively or as a library. It utilises a human readable, model description language for describing models as well as being SBML compatible. PySCeS includes stoichiometric, simulation, steady state and Eigen analysis using direct non-linear root finders. It also includes full support for Metabolic Control Analysis (MCA), the characterisation of static bifurcations, multidimensional parameter scanning and 2/3D graph capabilities. Currently an extension PySCeS-CBM is being developed that allows for the interactive manipulation, modelling and optimization of genome scale,

constraint based models (e.g. flux balance analysis)

13. **SBML Layout** (http://sbmllayout.sf.net/) — SBML Layout encompasses: 1. a online application (http://sys-bio.org/Layout) for layouting / rendering an SBML file , 2. a library for reading / writing SBML Layout and Rendering information as well as SBGN-ML and 3. a standalone application for displaying files with the SBML Layout or Rendering information. It is written in .net and available under the BSD for all platforms.

14. **SBW** (http://sys-bio.org/) — Systems Biology Workbench. A framework for connecting and running various applications written in different languages or on different systems, and a collection of available modules for model development, analysis, and simulation. Free/Open Source. (BSD)

15. **semanticSBML** (http://semanticsbml.org) — Create, check, visualize, retrieve, cluster, annotate, merge SBML models. The program includes a web based graphical user interface. For tool developers a programming interface (Python) and RESTful web-services are provided. It features advanced functions to edit MIRIAM and SBO terms. The latest version of semanticSBML is fully web based and can be accessed under http://semanticsbml.org /semanticSBML/simple/index (http://semanticsbml.org/semanticSBML/simple/index)

16. **SimBiology** (http://www.mathworks.com/products/simbiology/) — SimBiology ® is a MATLAB ® product from MathWorks that provides graphical and programmatic tools for computational systems biology and pharmacokinetics. It contains functionality for creating, simulating, and analyzing biological models. The SimBiology desktop lets you build a model using a block diagram editor, a model wizard, or a tabular interface. You can also create a model at the command line or directly from SBML files. SimBiology lets you simulate a model using stochastic or deterministic solvers. The product supports parameter estimation, sensitivity analysis, parameter scans, and other model analysis methods. All SimBiology features can be used together with the MATLAB programming language, letting you customize models, create or modify analysis tasks, and automate your workflow.

17. **SOSlib** (http://www.tbi.univie.ac.at/~raim/odeSolver/) — SOSlib is both a programming library and a command-line application for symbolic and numerical analysis of a system of ordinary differential equations (ODEs) derived from a chemical reaction network encoded in the Systems Biology Markup Language (SBML). It is written in ANSI/ISO C and distributed under the terms of the GNU Lesser General Public License (LGPL). The package employs libSBML's AST (Abstract Syntax Tree) for formula representation to construct ODE systems, their Jacobian matrix and other derivatives. CVODES, the sensitivity-enabled ODE solver in the SUNDIALS package is used for numerical integration and sensitivity analysis of stiff and non-stiff ODE systems. The native API provides fine-grained interfaces to all internal data structures, symbolic operations and numerical routines, enabling the construction of powerful and efficient analytic applications, hybrid solvers or multi-scale models with interfaces to non SBML data sources. Optional modules based on Graphviz and XMGrace allow a quick inspection of a model's structure and dynamics.

18. **TERANODE Suite** (http://teranode.com/products/index.php) — Suite of tools for model management, design, and simulation. (Linux/Mac/Windows) Commercial (30-day trial available).

6.Repository or database

1. **BASIS** (http://www.basis.ncl.ac.uk/) — BASIS is a project developing web-based services for quantitative study of the biology of ageing. The project also hosts the Stochastic Test Suite.

2. **BiGG** (http://bigg.ucsd.edu/) — Database of human, yeast and bacterial metabolites, pathways and reactions as well as SBML reconstructions for metabolic modeling.

3. **BioCyc** (http://www.biocyc.org/) — Collection of pathway/genome databases. May be downloaded in SBML, BioPAX, or flat format. Free limited academic license (detailed). May be explored with Pathway Tools

4. **BioGRID** (http://thebiogrid.org/) — BioGRID is an online interaction repository with data compiled through comprehensive curation efforts.

5. **BioModels Database** (http://www.ebi.ac.uk/biomodels/) — BioModels Database is a repository of peer-reviewed, published, computational models. These mathematical models are primarily from the field of systems biology, but more generally are those of biological interest. This resource allows biologists to store, search and retrieve published mathematical models. In addition, models in the database can be used to generate sub-models, can be simulated online, and can be converted between different representational formats. This resource also features programmatic access via Web Services.

6. **BioModels Importer** (http://jdesigner.sourceforge.net/Site/Biomodels_Importer.html) — The database component of BioModels.net is especially designed for working with annotated computational models: each model is carefully reviewed and augmented by human annotators on the BioModels.net team to add metadata linking the model elements to other biological databases and resources. The BioModels Database at the EBI system goes far beyond other collections of models by being a true database, featuring browsing, cross-referencing, searching, and facilities for visualization, exporting models in different formats, and remote API access. The BioModels Importer is such a tool, allowing to search for a specific model (or to quickly access them all). Integrated with SBW the Importer sends a model to JDesigner, Jarnac or any other tool in a snap.

7. **BRENDA** (http://brenda-enzymes.org/) — the BRaunschweig ENzyme Database is a comprehensive information system covering enzymes and their activities. The majority of the data are manually extracted from the primary literature. The content covers information on function, structure, occurrence, preparation and application of enzymes as well as properties of mutants and engineered variants. In 2011, BRENDA introduced the ability to output data in SBML format.

8. **ByoDyn** (http://byodyn.imim.es) — ByoDyn includes a set of tools to 1) integrate ordinary differential equations (ODEs), including systems with events, rules (differential algebraic equations, DAE) and delays built from a given biological model; 2) stochastic simulators: SSA and tau-leap; 3) globally optimize the parameters that fit the provided experimental information and evaluate the sensitivity of the model with respect to the different parameters; 4) include the sensitivity of the parameters in an optimal experimental design pipeline based on the Fisher information matrix; and 5) Monte Carlo sampling coupled with cluster analysis

and PCA to determine the global shape of the parameter landscape. The program makes use of external software, providing a Python binding schema that allows the user to easily implement new software in the desired calculation protocol. Furtermore, a webserver has been developed to manage the models, calculations and results easily.

9. **CADLIVE** (http://www.cadlive.jp) — CADLIVE (Computer-Aided Design of LIVing systEms) is a comprehensive computational tool for constructing large-scale biological network maps, analyzing the topological features of them, and simulating their dynamics. Using CADLIVE, we rationally design a biological system at the molecular interaction level for an engineering purpose.

10. **ConsensusPathDB** (http://cpdb.molgen.mpg.de/) — integrates functional interaction networks including complex protein- protein, metabolic, signaling and gene regulatory interaction networks

11. **CRdata** (http://crdata.org/) — CRdata.org offers menu-driven access to the Amazon Elastic Computing Cloud (EC2) and related resources for bioinformatic computing with R and Bioconductor. Users can launch their own processing nodes, and share nodes, scripts, and data with others if they wish.

12. **CycSim** (http://www.genoscope.cns.fr/cycsim/) — CycSim is a web application dedicated to in silico experiments with genome-scale metabolic models coupled to the exploration of knowledge from BioCyc and KEGG. it supports the design of knockout experiments: simulation of growth phenotypes of single or multiple gene deletions mutants on specified media, comparison of these predictions with experimental phenotypes and direct visualization of both on metabolic maps. CycSim also functions as an online repository of genome-scale metabolic models.

13. **insilicoIDE** (http://www.physiome.jp/) — insilicoIDE (ISIDE) assists users to build models of physiological functions with multilevel hierarchical structure and to run simulations. A model is built as a functional network of "modules" which represent physiological entities. In each module, equations such as ODEs and PDEs, parameters and morphological information can be defined. Besides, a module can include a model written in SBML. The SBML model is functionally embedded in the module network. There is an open model database at www.physiome.jp. Users can use models in the database freely as parts to build their own model. The modularity of the model representation in ISIDE makes reuse and integration of multiple models easier. The simulator included in ISIDE supports parallel computing.

14. **JSim** (http://www.physiome.org/jsim/) — JSim is a Java-based simulation system for building quantitative numeric models and analyzing them with respect to experimental reference data. JSim's primary focus is in physiology and biomedicine, however its computational engine is quite general and applicable to a wide range of scientific domains. JSim models may intermix ODEs, PDEs, implicit equations, integrals, summations, discrete events and procedural code as appropriate. JSim's model compiler can automatically insert conversion factors for compatible physical units as well as detect and reject unit unbalanced equations. JSim also supports model archive formats SBML (import and export) and CellML (import only).

15. **JWS Online** (http://jjj.biochem.sun.ac.za/index.html) — Online database and simulator. Kineticon (http://sbml.org/SBML_Software_Guide/We_Don

%27t_Have_A_Link_For_This_Tool) — Online resource for kinetic data, reactions, enzymes, pathways. SBML L2V1 Export.

16. **Meta-All** (http://bic-gh.de/meta-all) — Pathway database manager.

17. **MetaCrop** (http://metacrop.ipk-gatersleben.de/) — MetaCrop is a database that contains manually curated, highly detailed information about metabolic pathways in crop plants, including location information, transport processes, and reaction kinetics. The web interface supports an easy exploration of the information from overview pathways to single reactions and therefore helps users understanding the metabolism of crop plants. It also allows automatic data export for the creation of detailed models of metabolic pathways to support simulation approaches.

18. **MetExplore** (http://metexplore.toulouse.inra.fr) — A web server to link metabolic experiments and genome-scale metabolic networks. MetExplore contains original network filters, allows to export in SBML and visualize filtered metabolic networks, and map masses from metabolic experiments onto complete metabolic networks. It also contains some graph-based methods to enrich the analyses.

19. **NetPath** (http://www.netpath.org/) — 'NetPath' is a curated resource of signal transduction pathways in humans. All pathways are freely available in BioPAX, PSI-MI and SBML formats. The pathways are freely available under an adaptive Creative Commons License which stipulates that the pathways may be used if adequate credit is given to the authors. Feedback on the NetPath website and its contents can be sent to info@netpath.org.

20. **NetPro** (http://www.molecularconnections.com/products.html) — Molecular interaction database (commercial).

21. **PANTHER Pathway** (http://https://panther.appliedbiosystems.com/pathway/) — Pathway database (online resource).

22. **PathArt** (http://jubilantbiosys.com/ppa.htm) — Pathway database collection. (Commercial)

23. **PAYAO** (http://www.payaologue.org) — PAYAO is a community collaborative web service platform for gene-regulatory and biochemical pathway model curation.

24. **PK-Sim / MoBi** (http://www.systems-biology.com) — Systems biology software platform for multiscale physiological modeling and simulation with a focus on physiologically-based pharmokinetics and -dynamics (PBPK/PD) including interfaces to MATLAB and R. Available to academic researchers via a free non-commercial license.

25. **ProcessDB** (http://www.integrativebioinformatics.com/processdb.html) — ProcessDB helps molecular cell biologists manage and test their increasingly complex mechanistic hypotheses. ProcessDB does this with a bio-savvy graphical user interface that helps users formulate, visualize, compare, modify, manage and test their own mechanistic theories of cellular function. All models in ProcessDB can be automatically combined with user-specified experimental protocols and exported to the Berkeley Madonna solver for testing against experimental data. ProcessDB allows investigators to know with precision what their theories predict, and speeds discovery of mechanisms that account for all of the available data.

26. **Reactome** (http://www.reactome.org/) — Pathway database (online resource).

27. **SABIO-RK** (http://sabiork.h-its.org/) — SABIO-RK is a curated database for biochemical reaction kinetics data. The data is drawn from different sources: by extraction from published literature or direct submission by experimenters, and is supplemented with additional data from other databases. The system offers standardized data by the use of controlled vocabularies and annotations pointing to other resources and biological ontologies. It can be accessed either manually via a web-based search interface or automatically via web services that allow direct data access by other tools. Both interfaces support the export of the data together with its annotations in SBML. SABIO-RK facilitates the exchange of kinetic data between experimentalists and modellers, and thereby supports the setup of quantitative computer models.

28. **SBMLEditor** (http://www.ebi.ac.uk/compneur-srv/SBMLeditor.html) — SBMLeditor a very simple, low level editor of SBML files. Users can create and remove all the necessary bits and pieces of SBML in a controlled way, that maintains the validity and consistency of the final SBML file

29. **SGMP** (http://www.signaling-gateway.org/molecule/) — The UCSD Signaling Gateway Molecule Pages provide essential information on over 4000 proteins involved in cellular signaling. Each Molecule Page contains regularly updated information derived from public data sources as well as sequence analysis, references and links to other databases. Published Molecule Pages contain an expert-authored review article that describes the biological activity, regulation and localization of the protein. This review is supplemented by highly structured data that illustrate protein-protein interactions, post-translational modifications, sub-cellular localization and biological function. Prior to publication, there is rigorous peer and editorial review of each Molecule Page. The published pages are citable by digital object identifiers (DOIs). All data in the Molecule Pages are freely available to the public.

30. **Sigmoid** (http://sigmoid.sf.net/) — Model database, explorer, visualization, Cellerator-based simulations as a web service.

31. **SPDBS** (http://www.springerlink.com/content/c883514423513036/) — SBML-Based Biochemical Pathway Database System

32. **SYCAMORE** (http://sycamore.eml.org) — SYCAMORE is a system that provides you with a faciliated access to a number of tools and methods in order to build models of biochemical systems, view, analyse and refine them, as well as perform quick simulations.

7.Scripting module

1. **acslXtreme** (http://acslx.com/) — commercial modeling environment that uses a script language called CSL. Has SBML import. Windows only.

2. **BioSens** (http://www.chemengr.ucsb.edu/~ceweb/faculty/doyle/biosens/BioSens.htm) — ODE Simulation & Sensitivity analysis for BioSpice Dashboard Dashboard. Requires dashboard, Matlab, XPP, Cygwin, libSBML, DASPK, Tapenade. Requires Biospice dashboard, Matlab, XPP,

Cygwin, libSBML, DASPK, Tapenade. Free download (License unspecified). (Windows)

3. **BSTLab** — GMA and S-Systems based toolbox for Biochemical Systems Theory.

4. **CADLIVE** (http://www.cadlive.jp) — CADLIVE (Computer-Aided Design of LIVing systEms) is a comprehensive computational tool for constructing large-scale biological network maps, analyzing the topological features of them, and simulating their dynamics. Using CADLIVE, we rationally design a biological system at the molecular interaction level for an engineering purpose.

5. **CellNetAnalyzer** (http://www.mpi-magdeburg.mpg.de/projects/cna/cna.html) — CellNetAnalyzer (CNA) is a package for MATLAB and provides a comprehensive and user-friendly environment for structural and functional analysis of biochemical networks. CNA facilitates the analysis of metabolic (stoichiometric) as well as signaling and regulatory networks solely on their network topology, i.e. independent of kinetic mechanisms and parameters. CNA provides a powerful collection of tools and algorithms for structural network analysis which can be started in a menu-controlled manner within interactive network maps. Recently, API functionalities have been added to enable interested users to call algorithms of CNA from external programs. Applications of CNA can be found in systems biology, biotechnology, metabolic engineering, pharmacology, microbiology, chemical engineering.

6. **COBRA** (http://gcrg.ucsd.edu/Downloads/Cobra_Toolbox) — The COnstraint-Based Reconstruction and Analysis Toolbox for Matlab includes implementations of many of the commonly used forms of constraint-based analysis such as FBA, gene deletions, flux variability analysis, sampling, and batch simulations together with tools to read in and manipulate constraint-based models.

7. **COPASI** (http://copasi.org) — COPASI is a software application for simulation and analysis of biochemical networks and their dynamics. COPASI is a stand-alone program that supports models in the SBML standard and can simulate their behavior using ODEs or Gillespie's stochastic simulation algorithm; arbitrary discrete events can be included in such simulations. COPASI provides an C++ API with language bindings for Perl, python, R, Java, and Octave and is able to communicate with the Systems Biology Workbench COPASI carries out several analyses of the network and its dynamics and has extensive support for parameter estimation and optimization. COPASI provides means to visualize data in customizable plots, histograms and animations of network diagrams. For a complete list of feature please see: http://www.copasi.org/tiki- index.php?page=FeatureList (http://www.copasi.org/tiki-index.php?page=FeatureList)

8. **DOTcvpSB** (http://www.iim.csic.es/~dotcvpsb/) — MatLab toolbox for optimization of models.

9. **JSim** (http://www.physiome.org/jsim/) — JSim is a Java-based simulation system for building quantitative numeric models and analyzing them with respect to experimental reference data. JSim's primary focus is in physiology and biomedicine, however its computational engine is quite general and applicable to a wide range of scientific domains. JSim models may intermix ODEs, PDEs, implicit equations, integrals, summations, discrete events and procedural code as appropriate. JSim's model compiler can automatically insert conversion factors for compatible physical units as well as detect and reject unit unbalanced equations. JSim also supports model

archive formats SBML (import and export) and CellML (import only).

10. **MatCont** (http://sourceforge.net/projects/matcont/) — MatCont is a Matlab software package for the numerical study of parameterized continuous and discrete dynamical systems.

11. **MathSBML** (http://www.sbml.org/mathsbml.html) — SBML import/export and simulation within Mathematica.

12. **Metatool** (http://pinguin.biologie.uni-jena.de/bioinformatik/networks/metatool/metatool5.1/metatool5.1.html) — A tool for metabolic pathway analysis with the main focus in elementary modes calculation. Enzyme subsets and conservation relations are also determined.

13. **modelMaGe** (http://modelmage.org/) — generates SBML or Copasi candidate models by removing specified model components from a given master model. modelMaGe automatically documents candidate models, automatically fits candidate models to data using CopasiSE, and finally provides a ranking of candidate models fits based on the AIC.

14. **Odefy** (http://www.helmholtz-muenchen.de/cmb/odefy) — Odefy is a MATLAB and Octave compatible toolbox which a modeling technique called HillCube, a canonical method to convert boolean models into continuous ordinary differential equation (ODE) systems. HillCubes are based on multivariate polynomial interpolation and incorporate Hill kinetics which are known to provide a good approximation of the synergistic dynamics of gene regulation.

15. **PathwayLab** (http://innetics.com/) — Deterministic simulation; Visualization; MCA; Mathematica and Matlab integration; model creation. (Windows) (Commercial).

16. **PK-Sim / MoBi** (http://www.systems-biology.com) — Systems biology software platform for multiscale physiological modeling and simulation with a focus on physiologically-based pharmokinetics and -dynamics (PBPK/PD) including interfaces to MATLAB and R. Available to academic researchers via a free non-commercial license.

17. **PottersWheel** (http://www.potterswheel.de/) — ODE based Simulation, model fitting, visualization, clustering, model design. (Free download; Optimization toolbox recommended).

18. **PySCeS** (http://pysces.sourceforge.net) — PySCeS: the Python Simulator for Cellular Systems is an extendable toolkit for the analysis and investigation of cellular systems. PySCeS is developed in Python and has been designed to be used both interactively or as a library. It utilises a human readable, model description language for describing models as well as being SBML compatible. PySCeS includes stoichiometric, simulation, steady state and Eigen analysis using direct non-linear root finders. It also includes full support for Metabolic Control Analysis (MCA), the characterisation of static bifurcations, multidimensional parameter scanning and 2/3D graph capabilities. Currently an extension PySCeS-CBM is being developed that allows for the interactive manipulation, modelling and optimization of genome scale, constraint based models (e.g. flux balance analysis)

19. **RANGE** (http://range.sourceforge.net/) — Random network generator. Noise added by R-script. Source code in C, yacc, lex. (GPL).

20. **RMBNToolbox** (http://sourceforge.net/projects/rmbntoolbox) — Toolbox for generating random notebooks (GPL).

21. **RSBML** (http://cran.r-project.org/) — SBML interface library for R (GPL). (available from CRAN).

22. **SBMLR** (http://www.bioconductor.org/packages/release/bioc/html/SBMLR.html) — This package uses the R package XML to bring SBML models into and out of R.

23. SBMLToolbox (http://sbml.org/Software/SBMLToolbox) — Manipulation of SBML in both the MATLAB and Octave environments. Some simulation support but the main focus is on allowing users to adapt SBML to their existing MATLAB/Octave functions.

24. SBToolbox2 (http://www.sbtoolbox2.org/) — MCA: Steady state control coefficients and elasticities; Structural analaysis: conservation relation analysis; model development; simulation; SBML Import/Export; parameter estimation; analysis tools. Requires MatLab (Linux/Win/Mac).

25. SBW (http://sys-bio.org/) — Systems Biology Workbench. A framework for connecting and running various applications written in different languages or on different systems, and a collection of available modules for model development, analysis, and simulation. Free/Open Source. (BSD)

26. SimBiology (http://www.mathworks.com/products/simbiology/) — SimBiology ® is a MATLAB ® product from MathWorks that provides graphical and programmatic tools for computational systems biology and pharmacokinetics. It contains functionality for creating, simulating, and analyzing biological models. The SimBiology desktop lets you build a model using a block diagram editor, a model wizard, or a tabular interface. You can also create a model at the command line or directly from SBML files. SimBiology lets you simulate a model using stochastic or deterministic solvers. The product supports parameter estimation, sensitivity analysis, parameter scans, and other model analysis methods. All SimBiology features can be used together with the MATLAB programming language, letting you customize models, create or modify analysis tasks, and automate your work-flow.

27. Simpathica (http://bioinformatics.nyu.edu/Projects/Simpathica/) — ODE based simulation. Part of BioSpice.

28. SloppyCell (http://sloppycell.sourceforge.net/) — SloppyCell is focused on parameter estimation and sensitivity analysis for ODE models. In particular, SloppyCell includes semi-analytic sensitivity integration, along with capability for building Bayesian ensembles of parameters sets consistent with given data.

29. SYCAMORE (http://sycamore.eml.org) — SYCAMORE is a system that provides you with a faciliated access to a number of tools and methods in order to build models of biochemical systems, view, analyze and refine them, as well as perform quick simulations.

30. Tide (http://sysbio.molgen.mpg.de/tide/) — Tide is a tool for the automatic identification of optimal drug targets in kinetic models based on ordinary differential equations. Give a model

in the popular SBML format it will identify promising drug targets for different effective modifier concentrations.

31. TinkerCell (http://www.tinkercell.com/) — TinkerCell is a visual application for constructing genetic, signaling, or metabolic networks with an extensive C and Python API. At present, the functionalities include deterministic and stochastic simulation (C libraries), steady state analysis, flux balance analysis using LPsolve C library, graph analysis through the NetworkX python module, and all the functionalities of PySCeS python module, including sensitivity and structural analysis. TinkerCell can build models by connecting modules. TinkerCell models contain meta-data for supporting a parts database. The visual display format is flexible.

32. xCellerator (http://xlr8r.info/) — Mathematica based ODE simulator. SBML inport/export uses MathSBML. Requires Mathematica. Free download (LGPL). (Linux/Mac/Win).

8.Simulation software

1. BetaWB (http://www.cosbi.eu/index.php?option=com_content&view=article&catid=41&id=67&Itemid=156) — BetaWB is a collection of tools based on the programming language BlenX, explicitly designed to represent biological entities and their interactions. The BetaWB includes the BetaWB simulator, a stochastic simulator based on an efficient variant of the Gillespie Stochastic Simulation Algorithm (SSA), the BetaWB designer, a graphical editor for developing models and the BetaWB plotter, a tool to analyze the results of a stochastic simulation run.

2. BIOCHAM (http://contraintes.inria.fr/BIOCHAM/) — Programming environment with GUI, simulator, and rule-based modeling language. SBML import & export.

3. BioNessie (http://www.bionessie.org/) — BioNessie is a free, state-of-the-art platform-independent biochemical networks simulation and analysis software environment software. It is developed using Java technology and can run on many platforms that support JRE (Java Runtime Environment 1.5 or higher). It provides a full user-friendly Graphical User Interface (GUI) which allows the user to import, create, edit and export the biochemical models with the SBML (Systems Biology Markup Language) standard.

4. BioNetGen (http://bionetgen.org/) — BioNetGen is a software system for the specification and simulation of rule-based models of biochemical systems. In rule-based models, molecules and molecular complexes are represented using graphs, and molecular interactions and their consequences are represented using graph-rewriting rules. Open source. Download requires email based registration. Requires Perl. Optional GUI uses JRE. (Linux/Mac/Win)

5. BioRica (http://biorica.gforge.inria.fr/) — BioRica is a high-level hierarchical modeling framework integrating discrete and continuous multi-scale dynamics. The co-existence of continuous and discrete dynamics is assured by flux connections with the continuous parts of the model. Once connected, these parts of the model act as components that can be queried for the function value, but also modified, therefore accounting for any trajectory modification induced by discrete parts of the model. BioRica is available upon request.

6. BioSyS (http://applications.eu-eela.eu/application_details.php?l=20&ID=68) — a system that

facilitates the study of biological systems that are described by Ordinary Differential Equations (ODEs). This software is designed to be capable of performing distributed simulations using Grid computing, stores the results in a database and allow further studies, incorporating various types of analysis such as charts, population dynamics, algorithms of clustering, classification, user-defined rules, stability and bifurcations, using data mining techniques. BioSyS 1.0 makes it
easier for researchers with a number of tools and algorithms that allow them to carry out investigations in an easier way.

7. BioTapestry (http://www.biotapestry.org/) — Graphical model development and simulation tool for genetic regulatory networks based on JRE. Uses Java Web Start. Free download. SBML export.

8. braincirc (http://braincirc.sourceforge.net/) — Braincirc is an open source model development and simulation environment developed primarily for linux platforms, originally developed to simulate brain circulation (Linux).

9. ByoDyn (http://byodyn.imim.es) — ByoDyn includes a set of tools to 1) integrate ordinary differential equations (ODEs), including systems with events, rules (differential algebraic equations, DAE) and delays built from a given biological model; 2) stochastic simulators: SSA and tau-leap; 3) globally optimize the parameters that fit the provided experimental information and evaluate the sensitivity of the model with respect to the different parameters; 4) include the sensitivity of the parameters in an optimal experimental design pipeline based on the Fisher information matrix; and 5) Monte Carlo sampling coupled with cluster analysis and PCA to determine the global shape of the parameter landscape. The program makes use of external software, providing a Python binding schema that allows the user to easily implement new software in the desired calculation protocol. Furthermore, a web-server has been developed to manage the models, calculations and results easily.

10. CADLIVE (http://www.cadlive.jp) — CADLIVE (Computer-Aided Design of LIVing systEms) is a comprehensive computational tool for constructing large-scale biological network maps, analyzing the topological features of them, and simulating their dynamics. Using CADLIVE, we rationally design a biological system at the molecular interaction level for an engineering purpose.

11. Cain (http://cain.sourceforge.net/) — Cain is an application that performs stochastic and deterministic simulations of chemical reactions. It stores models, simulation parameters, and simulation results in an XML format. The models and simulation parameters can be read from input files or edited within the program. Cain offers a variety of solvers including: Gillespie's direct method, Gillespie's first reaction method, Gibson and Bruck's next reaction method, tau-leaping, hybrid direct/tau-leaping, and ODE integration.

12. Cell Illustrator (http://www.fqs.pl/life_science/cell_illustrator) — Graphical model editor; Petri-net based simulation algorithm; SBML Import. Commercial. (Linux/Mac/Win).

13. CellDesigner (http://celldesigner.org) — CellDesigner is a structured diagram editor for drawing gene-regulatory and biochemical networks. Networks are drawn based on the process diagram, with graphical notation system. CellDesigner supports simulation and parameter scan by an integration with SBML ODE Solver and Copasi. By using CellDesigner,

users can browse and modify existing SBML models with references to existing databases (MIRIAM supported), simulate and view the dynamics through an intuitive graphical interface.

14. **CellNetAnalyzer** (http://www.mpi-magdeburg.mpg.de/projects/cna/cna.html) — CellNetAnalyzer (CNA) is a package for MATLAB and provides a comprehensive and user-friendly environment for structural and functional analysis of biochemical networks. CNA facilitates the analysis of metabolic (stoichiometric) as well as signaling and regulatory networks solely on their network topology, i.e. independent of kinetic mechanisms and parameters. CNA provides a powerful collection of tools and algorithms for structural network analysis which can be started in a menu-controlled manner within interactive network maps. Recently, API functionalities have been added to enable interested users to call algorithms of CNA from external programs. Applications of CNA can be found in systems biology, biotechnology, metabolic engineering, pharmacology, microbiology, chemical engineering.

15. Cellware (http://www.bii.a-star.edu.sg/achievements/applications/cellware/) — Block diagram model editor & simulator. SBML import. Free download (Academic/Non-Profit) (Linux/Mac/Win).

16. CompuCell3D (http://www.compucell3d.org/) — CompuCell3D (CC3D) is an open-source environment for building and running multi-cell, multi-scale simulations based on the GGH model, utilizing the Systems Biology Workbench (SBW) suite. Scripting use the CC3DML Model Description Language and Python. Can simulate at more than 5 x 10^5 cells / processor; provides PDE support; utilizes SOSLIB/Jarnac/JDesigner.

17. COPASI (http://copasi.org) — COPASI is a software application for simulation and analysis of biochemical networks and their dynamics. COPASI is a stand-alone program that supports models in the SBML standard and can simulate their behavior using ODEs or Gillespie's stochastic simulation algorithm; arbitrary discrete events can be included in such simulations. COPASI provides an C++ API with language bindings for Perl, python, R, Java, and Octave and is able to communicate with the Systems Biology Workbench COPASI carries out several analyses of the network and its dynamics and has extensive support for parameter estimation and optimization. COPASI provides means to visualize data in customizable plots, histograms and animations of network diagrams.complete list and features are available at (http://www.copasi.org/tiki-index.php?page=FeatureList)

18. CRdata (http://crdata.org/) — CRdata.org offers menu-driven access to the Amazon Elastic Computing Cloud (EC2) and related resources for bioinformatic computing with R and Bioconductor. Users can launch their own processing nodes, and share nodes, scripts, and data with others if they wish.

19. Cyto-Sim (http://www.cosbi.eu/Rpty_Soft_CytoSim.php) — Stochastic simulator based on automata theory (P system). Free download. JVM Based.

20. DBSolve (http://insysbio.ru/en/soft/dbsolveoptimum.html) — DBSolveOptimum is a free software for kinetic modeling of metabolic pathways, analysis, and fitting parameters to experimental data. The program has text-based user interface for model description and graphical interface for data analysis. In addition to standart algorithms of simulation (ODE

solver, explicit solver, steady-state analysis) the software include also automated local sencetivity analysis, parameters optimization procedures and bifurcaion analysis. The last version of DBSolveOptimum includes advanced tool for data visualization.

21. Dizzy (http://magnet.systemsbiology.net/software/Dizzy) — Chemical kinetics simulator. SBML Import/Export (L1 Subset). Includes Gillespie, Gibson-Bruck and Tau Leap stochastic and ODE/RK5 deterministic methods. LGPL, open source, Free download. (Linux/Mac/Windows).
22. E-CELL (http://ecell.sourceforge.net/) — (Linux RPM/Win). Requires Python, Numpy, GSL, Boost. Command line, scripting, and GUI. Supports ODE/DAE and Gibson-Bruck SSA models. GUI requires Gnome, gnome-python2, and pygtk. GPL with exceptions. SBML import via SBML2EML converter. Limited SBML export via ecellj converter.

23. ESS (http://biocomp.ece.utk.edu/) — Exact Stochastic Simulator. Part of the UTK/ORNL Bio-SPICE tool set which includes the BioSpreadsheet SBML model editor. Requires BioSpice Dashboard. Free download. Includes Source code.

24. Facile (http://facile.sourceforge.net) — Facile / EasyStoch. A command-line network compiler for systems biology. Facile reads models given in a simple and human-readable textual input format and exports the model in a format for readable by Matlab, Mathematica, Maple, XPP/AUTO. Other tools are supported via SBML export. For stochastic simulations, Facile uses the EasyStoch stochastic simulator. An important feature of EasyStoch that distinguishes it from other Gillespie-algorithm implementations is that it is capable of simulating dynamically changing or noisy biochemical parameters (i.e. extrinsic noise).

25. FASIMU (http://www.bioinformatics.org/fasimu) — FASIMU is a command line oriented software implementing the most frequently applied FBA algorithms. It offers the first freely available implementation of (i) weighted flux minimization, (ii) fitness maximization for partially inhibited enzymes, and (iii) the concentration-based thermodynamic feasibility constraint. It allows heterogenous computation series suited for network pruning, leak analysis, FVA, and systematic probing of metabolic objectives for network curation controlled by an intuitive description file. The metabolic network can be supplied in SBML, CellNetAnalyzer, and plain text format. FASIMU uses the optimization capabilities of free (lp solve and GLPK) and commercial solvers (CPLEX, LINDO). The results can be visualized in Cytoscape or BiNA using newly developed plugins. The platform- independent program is an open-source project, freely available under GNU public license, including manual, tutorial, BiNA and Cytoscape plugin and respective manuals.

26. FERN (http://www.bio.ifi.lmu.de/FERN) — FERN is a Java framework for the efficient simulation of chemical reaction networks. It provides a broad range of efficient and accurate algorithms both for exact and approximate stochastic simulation and a simple interface for extending to new algorithms. Furthermore, it can be used in a straightforward way both as a stand-alone program and within new systems biology applications. Finally, complex scenarios requiring intervention during the simulation progress can be modeled easily with FERN.

27. Genetdes (http://synth-bio.yi.org/genetdes.html) — Network optimization using Simulated Annealing. SBML Import/Export. Free download, requires email license (CCL- AN). (Linux)

28. Genetic Network Analyzer (http://www-helix.inrialpes.fr/gna) — Genetic Network Analyzer

(GNA) is a computer tool for the modeling, simulation, analysis and verification of genetic regulatory networks. The aim of GNA is to assist biologists and bioinformaticians in constructing a qualitative model of a genetic regulatory network from knowledge about regulatory interactions and gene expression data. GNA provides a variety of functions to analyze the steady-state and transient dynamics of the network, among other things by exploiting state- of-the-art model-checking tools.

29. Gepasi (http://www.gepasi.org/) — Forerunner of COPASI. ODE simulations, metabolic analysis. SBML L1 Inport/Export. (Windows or Linux under Wine). Limited license.

30. Gillespie2 (http://www.basis.ncl.ac.uk/software.html) — from the BASIS Project. Source code.

31. GNU MCSim (http://www.gnu.org/software/mcsim/) — GNU MCSim is a free standalone simulation package that allows you to design your own statistical or simulation models. It efficiently performs Bayesian inference through Markov Chain Monte Carlo simulations. Standard Monte Carlo and experimental design optimization are also available. GNU MCSim can import and simulate levels 1 and 2 SBML models

32. iBioSim (http://www.async.ece.utah.edu/iBioSim/) — The iBioSim tool supports the modeling, analysis, and design of genetic circuits with applications in both systems and synthetic biology. It includes editors to construct genetic circuit models (GCM), Systems Biology Markup Language (SBML) models (L2V4 and L3V1 supported), and labeled Petri net (LPN) models. Models can be constructed by hand, imported from model databases, or learned from experimental data. These models can be analyzed using a variety of ODE and stochastic simulators as well as Markov chain analysis. The efficiency of these analysis methods is enhanced using a variety of automatic reaction-based and logical abstractions. The analysis results can be plotted as graphs or visualized upon the genetic circuit schematic.

33. **insilicoIDE** (http://www.physiome.jp/) — insilicoIDE (ISIDE) assists users to build models of physiological functions with multilevel hierarchical structure and to run simulations. A model is built as a functional network of "modules" which represent physiological entities. In each module, equations such as ODEs and PDEs, parameters and morphological information can be defined. Besides, a module can include a model written in SBML. The SBML model is functionally embedded in the module network. There is an open model database at www.physiome.jp. Users can use models in the database freely as parts to build their own model. The modularity of the model representation in ISIDE makes reuse and integration of multiple models easier. The simulator included in ISIDE supports parallel computing.

34. Jarnac (http://jdesigner.sourceforge.net/Site/Jarnac.html) — SBW tool for metabolic analysis, includes dynamic simulation. Simulation engine for JDesigner. BSD License.

35. JigCell (http://jigcell.cs.vt.edu/) — JigCell is a set of computational tools with user-friendly interfaces developed for studying complex biochemical regulatory systems in general and the cell cycle control system in particular. For example, The JigCell Model Builder (JCMB) aides the modeler in defining a system to be modeled using SBML with a novel spreadsheet interface, allowing a large amount of data to be displayed in an organized manner. The JigCell Run Manager (JCRM) allows a user to specify a set of specifications for simulation runs using a spreadsheet interface. JigCell Aggregation Connector has been designed to define models in terms of components, for the purpose of being combined in a larger model. JigCell also aims in

parameter estimation. A parameter estimator (PET, Parameter Estimation Toolkit) takes a biological model, experimental data, and the relationship between the model and data. Using this information the parameter estimator uses numerical tools to vary the parameters to the model looking for the parameters that best fit the experimental data.

36. JSim (http://www.physiome.org/jsim/) — JSim is a Java-based simulation system for building quantitative numeric models and analyzing them with respect to experimental reference data. JSim's primary focus is in physiology and biomedicine, however its computational engine is quite general and applicable to a wide range of scientific domains. JSim models may intermix ODEs, PDEs, implicit equations, integrals, summations, discrete events and procedural code as appropriate. JSim's model compiler can automatically insert conversion factors for compatible physical units as well as detect and reject unit unbalanced equations. JSim also supports model archive formats SBML (import and export) and CellML (import only).

37. Kinsolver (http://www.cs.uga.edu/~thiab/kinsolver.html) — A simulator for biochemical and gene regulatory networks

38. MatCont (http://sourceforge.net/projects/matcont/) — MatCont is a Matlab software package for the numerical study of parameterized continuous and discrete dynamical systems.

39. MesoRD (http://mesord.sourceforge.net) — MesoRD is a stochastic and deterministic simulator of coupled chemical reactions and diffusions in space.

40. Metaboflux (http://www.cbib.u-bordeaux2.fr/metaboflux/) — Metaboflux is a computational tool for predicting flux distribution in metabolic networks under multiple and various constraints deducted from the experiments. It aims to increase the biological relevance of models by integrating experimental data. The tool is available in two versions : a command line tool optimized for running on HPC servers and a user-friendly interface designed to define model parameters and run simple computations. Metaboflux embedded a stochastic simulator of metabolic networks coupled with a non linear solver (GSL). It solves constraints defined as proportions (for example, metabolite proportions) or as equations. Results can be visualized directly in Metaboflux or within specific tools like Systrip.

41. MetaFluxNet (http://metafluxnet.kaist.ac.kr) — MetaFluxNet is a program package for managing information on the metabolic reaction network and for quantitatively analyzing metabolic fluxes in an interactive and customized way, which allows users to interpret and examine metabolic behavior in response to genetic and/or environmental modifications. As a result, quantitative in silico simulations of metabolic pathways can be carried out to understand the metabolic status and to design the metabolic engineering strategies.

42. Modesto (http://bioinformatics.oxfordjournals.org/cgi/content/abstract/20/3/316) — Merged ODE and Stochastic Simulator. Source code only. Linux. (MPL 1.1)

43. Moleculizer (http://www.molsci.org/~lok/moleculizer/) — Command line stochastic simulator. Open source. (Linux) (GPL)

44. MOOSE (http://moose.ncbs.res.in/) — MOOSE is the base and numerical core for large, detailed simulations including Computational Neuroscience and Systems Biology. MOOSE spans the range from single molecules to subcellular networks, from single cells to neuronal

networks, and to still larger systems. it is backwards- compatible with GENESIS, and forward compatible with Python and XML-based model definition standards like SBML and NeuroML.

45. Narrator (http://narrator-tool.org/) — Graphical model design and simulation. Java-based, platform independent. Open source/free download (LGPL).

46. nemo (http://range.sf.net) — RANGE will generate large random transcription networks, with up to 16,000 genes, in the NEMO language. NEMO's compiler (nemo2sbml) uses lex and yacc to output a Systems Biology Markup Language (SBML) model for either user-specified and/or randomized gene input functions. The SBML model of the known network may be input to a biochemical simulator (i.e. COPASI), allowing the generation of synthetic microarray data for algorithm development purposes. Alternately, NEMO may be used by itself to simply describe and SBML-ize your existing biochemical network.

47. NetBuilder' (http://strc.herts.ac.uk/bio/maria/Apostrophe/) — NetBuilder' is a software tool that is intended to help experimentalists creating and manipulating the mathematical representations they need to predict the behaviour of their systems. NetBuilder' has a graphical user interface, which allows its users to create a picture of the (known) components and interactions in the system, and enter quantitative information, such as know or estimated quantities and rates. A (hidden) translator converts the picture and the other data into a mathematical description, whereupon NetBuilder's "simulation engine" may be used to find out how the modelled system responds to changing input.

48. Odefy (http://www.helmholtz-muenchen.de/cmb/odefy) — Odefy is a MATLAB and Octave compatible toolbox which a modeling technique called HillCube, a canonical method to convert boolean models into continuous ordinary differential equation (ODE) systems. HillCubes are based on multivariate polynomial interpolation and incorporate Hill kinetics which are known to provide a good approximation of the synergistic dynamics of gene regulation.
49. Oscill8 (http://oscill8.sf.net/) — Bifurcation and Simulation. Windows Binary. (BSD).

50. Pathway Solver (http://ariadnegenomics.com/technology-research/dynamic-modeling/) — ODE based simulation. Commercial. (formerly runSMBL)

51. PathwayLab (http://innetics.com/) — Deterministic simulation; Visualization; MCA; Mathematica and Matlab integration; model creation. (Windows) (Commercial).

52. PET (http://mpf.biol.vt.edu/pet) — Parameter optimization and exploration is the primary feature of PET. Some of the other tasks PET can perform are simulations, setting up multiple experiments for a model, comparing parameter sets, and exporting plots for presentations.

53. PhysioLab Modeler (http://www.entelos.com/physiolabModeler.php) — Whole organism modeling environment. Commercial.
54.
55. PK-Sim / MoBi (http://www.systems-biology.com) — Systems biology software platform for multiscale physiological modeling and simulation with a focus on physiologically-based pharmokinetics and -dynamics (PBPK/PD) including interfaces to MATLAB and R. Available to academic researchers via a free non-commercial license.

56. PNK (http://page.mi.fu-berlin.de/~trieglaf/PNK2e/index.html) — Petri Net Simulator (JRE/SBW required) (GPL).

57. ProcessDB (http://www.integrativebioinformatics.com/processdb.html) — ProcessDB helps molecular cell biologists manage and test their increasingly complex mechanistic hypotheses. ProcessDB does this with a bio-savvy graphical user interface that helps users formulate, visualize, compare, modify, manage and test their own mechanistic theories of cellular function. All models in ProcessDB can be automatically combined with user-specified experimental protocols and exported to the Berkeley Madonna solver for testing against experimental data. ProcessDB allows investigators to know with precision what their theories predict, and speeds discovery of mechanisms that account for all of the available data.

58. PySCeS (http://pysces.sourceforge.net) — PySCeS: the Python Simulator for Cellular Systems is an extendable toolkit for the analysis and investigation of cellular systems. PySCeS is developed in Python and has been designed to be used both interactively or as a library. It utilises a human readable, model description language for describing models as well as being SBML compatible. PySCeS includes stoichiometric, simulation, steady state and Eigen analysis using direct non-linear root finders. It also includes full support for Metabolic Control Analysis (MCA), the characterisation of static bifurcations, multidimensional parameter scanning and 2/3D graph capabilities. Currently an extension PySCeS-CBM is being developed that allows for the interactive manipulation, modelling and optimization of genome scale, constraint based models (e.g. flux balance analysis)

59. roadRunner (http://roadrunner.sf.net) — roadRunner is a high performance cellular network simulation. RoadRunner accepts standard SBML Level 2 and generates the necessary ordinary differential equations that are solved either by CVODE to generate time course data or NLEQ to compute the steady state. roadRunner supports many functions, including: 1.ODE simulation and steady state analysis; 2.Conservation analysis to ensure a non-singular Jacobian; 3.Steady state metabolic control analysis; 4.Frequency domain metabolic control analysis; 5.Simple continuation of steady states .

60. SBML2NEURON (http://www.neuroml.org/neuron_tools.php) — SBML2NEURON is a provisional implementation of an SBML to NEURON converter. This uses the Python bindings of libSBML to generate an NMODL file containing the model represented in a basic SBML file, which can then be inserted onto a section in NEURON for simulation. Note that only a restricted set of SBML elements are supported (see the notes), but it can be used to simulate some of the models in BioModels Database. This is a work in progress and will be developed further to allow closer integration between NeuroML and SBML in realistic neuronal models.

61. SBML-PET-MPI (http://www.bioss.uni-freiburg.de/cms/sbml-pet-mpi.html) — SBML-PET-MPI is a parallel parameter estimation tool for Systems Biology Markup Language (SBML) based models. The tool allows the user to perform parameter estimation, parameter uncertainty and identifiability analysis by collectively fitting multiple experimental data sets. SBML-PET-MPI can run on Windows, Linux and Mac OS X systems.

62. SBMLR (http://www.bioconductor.org/packages/release/bioc/html/SBMLR.html) — This package uses the R package XML to bring SBML models into and out of R.

63. SBML-SAT (http://sysbio.molgen.mpg.de/SBML-SAT/) — SBML-SAT implements algorithms

for simulation, steady state analysis, robustness analysis and local and global sensitivity analysis for SBML models. This software tool extends current capabilities through its execution of global sensitivity analyses using multi-parametric sensitivity analysis, partial rank correlation coefficient, SOBOL's method, and weighted average of local sensitivity analyses in addition to its ability to handle systems with discontinuous events and intuitive graphical user interface.

64. SBMLToolbox (http://sbml.org/Software/SBMLToolbox) — Manipulation of SBML in both the MATLAB and Octave environments. Some simulation support but the main focus is on allowing users to adapt SBML to their existing MATLAB/Octave functions.

65. SBToolbox2 (http://www.sbtoolbox2.org/) — MCA: Steady state control coefficients and elasticities; Structural analaysis: conservation relation analysis; model development; simulation; SBML Import/Export; parameter estimation; analysis tools. Requires MatLab (Linux/Win/Mac).

66. SBW (http://sys-bio.org/) — Systems Biology Workbench. A framework for connecting and running various applications written in different languages or on different systems, and a collection of available modules for model development, analysis, and simulation. Free/Open Source. (BSD)

67. sbw: javasim (http://sys-bio.org/sbwWiki/sbw/javasim) — Set of Java simulators implementing; Chemical Langevin, CVODE, Gibson NRM, Gillespie DM, Gillespie FRM, and LSODA.

68. sbw: stochastic simulator (http://jdesigner.sourceforge.net/Site/Stochastic_Simulation.html) — GillespieGUI is a new user interface for biochemical networks that has been designed to integrate both tasks of interest to biologists – namely, simulating a model and analyzing the data. The data simulation is carried out by a stochastic simulator, whose parameters such as simulation start and end times, as well as data or time sampling options can be set prior to starting the simulation. This being a tool designed for statistical analysis, users can specify the number of runs of the model that the simulation should generate. Once the data for the specified number of runs has been generated, the tool then computes correlations between various species, along with their power spectral densities and transfer functions. In particular the following capabilities are supported:

69. SIMBA (http://www.ifak-system.com/services/dynamic-simulation.html) — Wastewater simulation. SBML Support unspecified. Commercial(?).

70. SimBiology (http://www.mathworks.com/products/simbiology/) — SimBiology ® is a MATLAB ® product from MathWorks that provides graphical and programmatic tools for computational systems biology and pharmacokinetics. It contains functionality for creating, simulating, and analyzing biological models. The SimBiology desktop lets you build a model using a block diagram editor, a model wizard, or a tabular interface. You can also create a model at the command line or directly from SBML files. SimBiology lets you simulate a model using stochastic or deterministic solvers. The product supports parameter estimation, sensitivity analysis, parameter scans, and other model analysis methods. All SimBiology features can be used together with the MATLAB programming language, letting you customize models, create or modify analysis tasks, and automate your workflow.

71. SloppyCell (http://sloppycell.sourceforge.net/) — SloppyCell is focused on parameter estimation and sensitivity analysis for ODE models. In particular, SloppyCell includes semi-analytic sensitivity integration, along with capability for building Bayesian ensembles of parameters sets consistent with given data.

72. SmartCell (http://smartcell.embl.de/) — Stochastic Reaction/Diffusion Simulator (Linux/Mac/Win) (Acad/NP).

73. Snoopy (http://www-dssz.informatik.tu-cottbus.de/DSSZ/Software/Snoopy) — a software tool to design and animate hierarchical graphs, among others Petri nets. To investigate biomolecular networks, Snoopy provides a unifying Petri net framework comprising a family of related Petri net classes. Models can be hierarchically structured, allowing for the mastering of larger networks. To move easily between the qualitative, stochastic and continuous modelling paradigms, models can be converted into each other. We get models sharing structure, but being specialized by their kinetic information. The analysis and iterative reverse engineering of biomolecular networks is supported by the simultaneous use of several Petri net classes, while the GUI adapts dynamically to the active one. Built-in animation and simulation are complemented by exports to various analysis tools.

74. SOSlib (http://www.tbi.univie.ac.at/~raim/odeSolver/) — SOSlib is both a programming library and a command-line application for symbolic and numerical analysis of a system of ordinary differential equations (ODEs) derived from a chemical reaction network encoded in the Systems Biology Markup Language (SBML). It is written in ANSI/ISO C and distributed under the terms of the GNU Lesser General Public License (LGPL). The package employs libSBML's AST (Abstract Syntax Tree) for formula representation to construct ODE systems, their Jacobian matrix and other derivatives. CVODES, the sensitivity-enabled ODE solver in the SUNDIALS package is used for numerical integration and sensitivity analysis of stiff and non-stiff ODE systems. The native API provides fine-grained interfaces to all internal data structures, symbolic operations and numerical routines, enabling the construction of powerful and efficient analytic applications, hybrid solvers or multi-scale models with interfaces to non SBML data sources. Optional modules based on Graphviz and XMGrace allow a quick inspection of a model's structure and dynamics.

75. STEPS (http://steps.sourceforge.net/STEPS/) — STEPS is a package for exact stochastic simulation of reaction-diffusion systems in arbitrarily complex 3D geometries. Our core simulation algorithm is an implementation of Gillespie's SSA, extended to deal with diffusion of molecules over the elements of a 3D tetrahedral mesh. Tetrahedral meshes offer much better morphological resolution than the cubic voxels used in other SSA based software and so STEPS is the first spatial SSA software to allow realistic boundary representation. While STEPS was mainly developed for simulating detailed models of neuronal signaling pathways in dendrites and around synapses, it is a general tool and can be used for studying any biochemical pathway in which spatial gradients and morphology are thought to play a role. We have implemented STEPS as a set of Python modules, which means STEPS users can use Python scripts to control all aspects of setting up the model, generating a mesh, controlling the simulation and generating and analyzing output. The core computational routines are still implemented as C/C++ extension modules for maximal speed of execution.

76. StochKit (http://www.engineering.ucsb.edu/~cse/StochKit/) — C++ library that provides

various SSA, tau-leaping and adaptive step size algorithms. Source code only. (Linux) (Acad/NP).

77. StochSim (http://www.pdn.cam.ac.uk/comp-cell/StochSim.html) — STOCHSIM is a stochastic simulator for (bio)chemical reactions. The particles are represented as individual software objects which react according to probabilities derived from concentrations and rate constants. In the version 1.4 of STOCHSIM simple two-dimensional spatial structures have been implemented, in which nearest-neighbour interactions of molecules can be simulated.

78. STOCKS (http://www.sysbio.pl/stocks/) — SSA, Gibson-Bruck, and Tau-Leaping algorithms. Command line based tool. (source code, Linux/Windows) (GPL).

79. SYCAMORE (http://sycamore.eml.org) — SYCAMORE is a system that provides you with a faciliated access to a number of tools and methods in order to build models of biochemical systems, view, analyse and refine them, as well as perform quick simulations.

80. SynBioSS (http://synbioss.sourceforge.net/) — a suite of software tools for the modeling and simulation of synthetic gene constructs. SynBioSS utilizes the registry of standard biological parts, a database of kinetic parameters, and both graphical and command-line interfaces to multiscale (stochastic-discrete, stochastic-continuous and continuous-deterministic simulation) algorithms. A user can enter a sequence of BioBricks to synthesize a new gene network, obtain a set of biochemical reactions and model the dynamic behavior.

81. TinkerCell (http://www.tinkercell.com/) — TinkerCell is a visual application for constructing genetic, signaling, or metabolic networks with an extensive C and Python API. At present, the functionalities include deterministic and stochastic simulation (C libraries), steady state analysis, flux balance analysis using LPsolve C library, graph analysis through the NetworkX python module, and all the functionalities of PySCeS python module, including sensitivity and structural analysis. TinkerCell can build models by connecting modules. TinkerCell models contain meta-data for supporting a parts database. The visual display format is flexible.

82. Trelis (http://www.sourceforge.net/projects/trelis) — Monte Carlo Simulator.

83. VANTED (http://vanted.ipk-gatersleben.de/) — This system makes it possible to load and edit graphs, which may represent biological pathways or functional hierarchies. It is possible to map experimental datasets onto the graph elements and visualize time series data or data of different genotypes or environmental conditions in the context of a the underlying biological processes. Built-in statistic functions allow a fast evaluation of the data (e.g. t-Test or correlation analysis). Vanted can be extended for various functionalities, e.g. Flux simulation, database access and 3D visualisation.

84. Vcell (http://www.vcell.org/) — VCell is a complete model building, editing and simulation environment. Includes spatial modeling capabilites, deterministic, stochastic, and hybrid algorithms. Parameter sensitivity analysis and parameter optimization. Desktop application and web-based environment. Bio- and math-based interfaces. Database and model sharing/publishing. Free, registration required. Open source, source code available upon request. (Linux/Mac/Win/Web).

85. WebCell (http://webcell.kaist.ac.kr/) — Online simulator, model builder, metabolic controal

analysis. Includes database of bimodels and JWS models. Registration required.

86. xCellerator (http://xlr8r.info/) — Mathematica based ODE simulator. SBML inport/export uses MathSBML. Requires Mathematica. Free download (LGPL). (Linux/Mac/Win).

87. Xholon (http://primordion.com/Xholon) — Model development environment, tool set, simulation. (Linux/Win) Open Source (LGPL).

88. XPPAUT (http://www.math.pitt.edu/~bard/xpp/xpp.html) — ODE solver, analysis tool. Open Source. Free download. (Linux/Mac/Win)

9.Utility software

1. Antimony (http://antimony.sourceforge.net/) — libAntimony is a C/C++ library that can parse Antimony-formatted models, convert them to SBML, and provides an API to allow other tools access to model elements. Antimony models are modular, text-based, human readable and writable, largely compatible with SBML, and have a special syntax for creating genetic networks.

2. BiNoM (http://bioinfo.curie.fr/projects/binom/) — Biological Network Manager. Network design and manipulation. Visualization. Model conversion (CellDesigner, BioPAX); Structural Analysis; BioPAX Queries. Available as an independent library or Cytoscape plugin.

3. ByoDyn (http://byodyn.imim.es) — ByoDyn includes a set of tools to 1) integrate ordinary differential equations (ODEs), including systems with events, rules (differential algebraic equations, DAE) and delays built from a given biological model; 2) stochastic simulators: SSA and tau-leap; 3) globally optimize the parameters that fit the provided experimental information and evaluate the sensitivity of the model with respect to the different parameters; 4) include the sensitivity of the parameters in an optimal experimental design pipeline based on the Fisher information matrix; and 5) Monte Carlo sampling coupled with cluster analysis and PCA to determine the global shape of the parameter landscape. The program makes use of external software, providing a Python binding schema that allows the user to easily implement new software in the desired calculation protocol. Furtermore, a webserver has been developed to manage the models, calculations and results easily.

4. CADLIVE (http://www.cadlive.jp) — CADLIVE (Computer-Aided Design of LIVing systEms) is a comprehensive computational tool for constructing large-scale biological network maps, analyzing the topological features of them, and simulating their dynamics. Using CADLIVE, we rationally design a biological system at the molecular interaction level for an engineering purpose.

5. CellMC (http://www.cellmc.org/) — CellMC is a program generator that emits highly optimized executables realizing the stochastic simulation algorithm (SSA) given a model expressed as SBML (Level 2). It works on Intel/AMD based PCs and Cell/BE platforms (e.g. Sony PS3, IBM QS22).

6. CellML2SBML (http://bioinformatics.oxfordjournals.org/cgi/content/abstract/btl047v1) —

Converts CELLML to SBML

7. CL-SBML (http://common-lisp.net/project/cl-sbml) — Common Lisp implementation of the SBML Standard (Level 2). I/O library for SBML in Common Lisp.

8. COPASI (http://copasi.org) — COPASI is a software application for simulation and analysis of biochemical networks and their dynamics. COPASI is a stand-alone program that supports models in the SBML standard and can simulate their behavior using ODEs or Gillespie's stochastic simulation algorithm; arbitrary discrete events can be included in such simulations. COPASI provides an C++ API with language bindings for Perl, python, R, Java, and Octave and is able to communicate with the Systems Biology Workbench COPASI carries out several analyses of the network and its dynamics and has extensive support for parameter estimation and optimization. COPASI provides means to visualize data in customizable plots, histograms and animations of network diagrams. For a complete list of feature please see: http://www.copasi.org/tiki- index.php?page=FeatureList (http://www.copasi.org/tiki-index.php?page=FeatureList)

9. ecellJ (http://www.jweimar.de/ecellJ) — Converts between Ecell models and various other formats including SBML and open office spreadsheets.

10. Facile (http://facile.sourceforge.net) — Facile / EasyStoch. A command-line network compiler for systems biology. Facile reads models given in a simple and human-readable textual input format and exports the model in a format for readable by Matlab, Mathematica, Maple, XPP/AUTO. Other tools are supported via SBML export. For stochastic simulations, Facile uses the EasyStoch stochastic simulator. An important feature of EasyStoch that distinguishes it from other Gillespie-algorithm implementations is that it is capable of simulating dynamically changing or noisy biochemical parameters (i.e. extrinsic noise).

11. GRENDEL (http://mblab.wustl.edu/software/grendel/) — GRENDEL (Gene Regulatory Network Decoding Evaluations tooL), generates random gene regulatory networks according to user specified constraints on the network topology and kinetics (in addition to generating random topologies, it can also take a predefined topology as input). It then outputs SBML to define the state of each regulatory network under various user specified experimental designs, which can be integrated to produce simulated gene expression data.

12. JSim (http://www.physiome.org/jsim/) — JSim is a Java-based simulation system for building quantitative numeric models and analyzing them with respect to experimental reference data. JSim's primary focus is in physiology and biomedicine, however its computational engine is quite general and applicable to a wide range of scientific domains. JSim models may intermix ODEs, PDEs, implicit equations, integrals, summations, discrete events and procedural code as appropriate. JSim's model compiler can automatically insert conversion factors for compatible physical units as well as detect and reject unit unbalanced equations. JSim also supports model archive formats SBML (import and export) and CellML (import only).

13. KEGG2SBML (http://www.sbml.org/kegg2sbml.html) — Converts KEGG models to SBML.

14. KEGGconverter (http://www.grissom.gr/keggconverter/index.html) — KEGGconverter automatically produces merged and converted to SBML fully functional pathway models, enhanced with default kinetics, by inputting only KGML files.The final derived models do not

enclose trivial metabolites -reproducing inconsistencies of the KGML visualization-oriented, simplified information pattern- but at the same time they contain all the available information regarding the number of the included reactions in each pathway. Furthermore, additional reactions to neighbouring pathways are constructed which indicate the direction of the metabolic flows in the network and thus providing better stability in the boundary conditions of the models.

15. KEGGtranslator (http://www.ra.cs.uni-tuebingen.de/software/KEGGtranslator/) — Nowadays, the KEGG PATHWAY database provides a widely used service for pathway-based information. It contains manually drawn pathway maps with information about the genes, reactions and relations contained therein. To store these pathways, KEGG uses an own XML-format (called "KGML Parsers and translators are needed to process the pathway maps for usage "). in other applications and algorithms. We have developed KEGGtranslator, which is an easy-to-use stand-alone application that can visualize and convert KGML formatted XML-files into multiple output formats. Unlike other translators, KEGGtranslator supports a plethora of output formats, is able to augment the information in translated documents (e.g., MIRIAM annotations) beyond the scope of the KGML document, and amends missing components to fragmentary reactions within the pathway to allow simulations on those. KEGGtranslator converts KEGG files (KGML formatted XML-files) to SBML, GML, GraphML, JPG, GIF, LaTeX, etc. KEGG pathways can be obtained from ftp://ftp.genome.jp/pub/kegg/xml/kgml

16. MetaFluxNet (http://metafluxnet.kaist.ac.kr) — MetaFluxNet is a program package for managing information on the metabolic reaction network and for quantitatively analyzing metabolic fluxes in an interactive and customized way, which allows users to interpret and examine metabolic behavior in response to genetic and/or environmental modifications. As a result, quantitative in silico simulations of metabolic pathways can be carried out to understand the metabolic status and to design the metabolic engineering strategies.

17. MetExplore (http://metexplore.toulouse.inra.fr) — A web server to link metabolic experiments and genome-scale metabolic networks. MetExplore contains original network filters, allows to export in SBML and visualise filtered metabolic networks, and map masses from metabolic experiments onto complete metabolic networks. It also contains some graph-based methods to enrich the analyses.

18. Odefy (http://www.helmholtz-muenchen.de/cmb/odefy) — Odefy is a MATLAB and Octave compatible toolbox which a modeling technique called HillCube, a canonical method to convert boolean models into continuous ordinary differential equation (ODE) systems. HillCubes are based on multivariate polynomial interpolation and incorporate Hill kinetics which are known to provide a good approximation of the synergistic dynamics of gene regulation.

19. PINT (http://csb2.ym.edu.tw/cgi-bin/pint/index.cgi) — New pathway databases generally display pathways by retrieving information from a database dynamically. Some of them even provide their pathways in SBML or other exchangeable formats. Integrating these models is a challenging work, because these models were not built in the same way. Pathways integration Tool (PINT) may integrate the standard SBML files. Since these files may be obtained from different sources, any inconsistency in component names can be revised by using an annotation editor upon uploading a pathway model. This integration function greatly

simplifies the building of a complex model from small models. To get new users started, about 190 curated public models of human pathways were collected by PINT. Relevant models can be selected and sent to the workbench by using a user-friendly query interface, which also accepts a gene list derived from high-throughput experiments. The models on the workbench, from either a public or a private source, can be integrated and painted. The painting function is useful for highlighting important genes or even their expression level on a merged pathway diagram, so that the biological significance can be revealed. This tool is freely available.

20. PK-Sim / MoBi (http://www.systems-biology.com) — Systems biology software platform for multiscale physiological modeling and simulation with a focus on physiologically-based pharmokinetics and -dynamics (PBPK/PD) including interfaces to MATLAB and R. Available to academic researchers via a free non-commercial license.

21. SBFC (http://sbfc.sourceforge.net/) — The System Biology Format Converter (SBFC) aims is to provide a generic framework that potentially allows any conversion between two formats. Inter operability between formats is a recurring issue in Systems Biology. Although there are various tools available to convert models from one format to another, most of them have been independently developed and cannot easily be combined, specially to provide support for more formats. The framework is written in Java and can be used as a standalone executable. This is a collaborative project and we hope that developers will provide support for more formats by creating new modules.SBFC allows anyone to easily add new converters and to integrate existing converters with a minimum of changes.

22. SBML Harvester (http://code.google.com/p/sbmlharvester/) — The SBML Harvester creates a complex ontology-based representation of SBML models, utilizing both the structure of the SBML model and the models' MIRIAM annotations. This representation can then be used for the consistency verification of SBML models as well as complex queries across both models and biomedical ontologies.

23. SBML Translators (http://www.sys-bio.org/sbwWiki/doku.php?id=sysbio:downloads) — translators from SBML to a wide variety of other formats such as: •C / C++ / C# •Jarnac •Java •Matlab / Mathematica •XPP To name but a few. All translators are available from one UI.

24. **SBML2Antimony** (http://antimony.sourceforge.net/) — Antimony2sbml and sbml2antimony convert models between the SBML and Antimony formats. See separate listing above for Antimony.

25. **SBML2BioPax** (http://www.ebi.ac.uk/compneur-srv/sbml/converters/SBMLtoBioPax.html) — SBML2BioPax is a tool to convert any SBML files into BioPax. It can create BioPax level 2 or BioPax level 3. It uses the MIRIAM annotations as well as the SBO terms present in the SBML model to improve the BioPAX file generated. The tool is developed inside the SBFC (http://sbfc.sourceforge.net/) (http://sbfc.sourceforge.net/)) framework.

26. SBML2LaTeX (http://www.cogsys.cs.uni-tuebingen.de/software/SBML2LaTeX/) — SBML2LATEX is a tool to convert files in the System Biology Markup Language SBML) format into LATEX files. A convenient online version is available, which allows the user to directly generate various file types from SBML including PDF, TeX, DVI, PS, EPS, GIF, JPG or PNG. SBML2LATEX can also be downloaded and used locally in batch mode or interactively with its Graphical User Interface or several command line options. The purpose of SBML2LATEX is to

provide a way to read the contents of XML-based SBML files. This is helpful and important for, e.g., error detection, proofreading and model communication.

27. SBML2NEURON (http://www.neuroml.org/neuron_tools.php) — SBML2NEURON is a provisional implementation of an SBML to NEURON converter. This uses the Python bindings of libSBML to generate an NMODL file containing the model represented in a basic SBML file, which can then be inserted onto a section in NEURON for simulation. Note that only a restricted set of SBML elements are supported (see the notes), but it can be used to simulate some of the models in BioModels Database. This is a work in progress and will be developed further to allow closer integration between NeuroML and SBML in realistic neuronal models.

28. SBML2Octave (http://www.ebi.ac.uk/compneur-srv/sbml/converters/SBMLtoOctave.html) — SBML2Octave is a tool to convert any SBML files into Octave. It will create a .m file that should be usable inside MATLAB as well. It support all the
29. SBML elements until SBML level 3 core 1 apart for delay. The tool is developed inside the SBFC (http://sbfc.sourceforge.net/) (http://sbfc.sourceforge.net/)) framework.

30. SBML2SMW (http://code.google.com/p/sbml2smw/) — CellDesigner plugin for extracting Celldesigner model information, storing this information to a Semantic Mediawiki server and context-sensitive restoring and integration of this information in a Celldesigner model.

31. SBML2XPP (http://www.ebi.ac.uk/compneur-srv/sbml/converters/SBMLtoXPP-Aut.html) — Converter between SBML and XPPAut or Oscill8.

32. SBML-SAT (http://sysbio.molgen.mpg.de/SBML-SAT/) — SBML-SAT implements algorithms for simulation, steady state analysis, robustness analysis and local and global sensitivity analysis for SBML models. This software tool extends current capabilities through its execution of global sensitivity analyses using multi-parametric sensitivity analysis, partial rank correlation coefficient, SOBOL's method, and weighted average of local sensitivity analyses in addition to its ability to handle systems with discontinuous events and intuitive graphical user interface.

33. SBML-shorthand (http://www.staff.ncl.ac.uk/d.j.wilkinson/software/sbml-sh/) — Specification and conversion tools for a simple human-readable shorthand notation for a subset of SBML. Used for rapid building of SBML models without using a sophisticated GUI tool.

34. SBMLsqueezer (http://www.cogsys.cs.uni-tuebingen.de/software/SBMLsqueezer/) — SBMLsqueezer generates kinetic equations for biochemical networks according to context of each reaction. When used as a plug-in for CellDesigner it uses the information from the SBGN representation of all network components. In the stand-alone mode, SBMLsqueezer evaluates the Systems Biology Ontology (SBO) annotations to extract this information. An online version of SBMLsqueezer is available that runs without instally any software on the local machine. The rate laws that can be produced by SBMLsqueezer include several types of generalized mass action; detailed and generalized enzyme kinetics, various types of Hill equations, S- and H-systems, and additive models for gene regulation. User defined settings specify which equation to apply for any type of reaction and how to ensure unit consistency of the model. Equations can be created using contextual menus. All newly created parameters are equipped with the derived unit and annotated with SBO terms if available and meaningful textual names. MathML is inserted directly into the SBML file. LaTeX or text export of

ordinary differential equations is provided.

35. sbmltidy (http://sbml.org/Community/Programs/sbmltidy) — A wrapper around the tidy command-line utility that will reformat ("pretty-print") an SBML file.

36. SBW (http://sys-bio.org/) — Systems Biology Workbench. A framework for connecting and running various applications written in different languages or on different systems, and a collection of available modules for model development, analysis, and simulation. Free/Open Source. (BSD)

37. semanticSBML (http://semanticsbml.org) — Create, check, visualize, retrieve, cluster, annotate, merge SBML models. The program includes a web based graphical user interface. For tool developers a programming interface (Python) and RESTful web-services are provided. It features advanced functions to edit MIRIAM and SBO terms. The latest version of semanticSBML is fully web based and can be accessed under http://semanticsbml.org /semanticSBML/simple/index (http://semanticsbml.org/semanticSBML/simple/index)

38. UTKornTools (http://biospice.sourceforge.net/) — UTK/ORNL Bio-SPICE tool set (inactive)

10.Visualization software

1. Arcadia (http://arcadiapathways.sourceforge.net/) — Arcadia is an open-source, light-weight, cross-platform, C++ desktop application designed for visualizing biological networks such as metabolic pathways. It automatically translates SBML files into SBGN maps (using additional semantic information such as SBO terms when available). The default layout can be improved semi-automatically, e.g. by "cloning" (duplicating) highly connected species, or focusing on the neighborhood around a given species or reaction. The resulting map can be saved in the SBML file itself (using the layout extension) or exported as a vector image (PDF or SVG)

2. AVIS (http://actin.pharm.mssm.edu/AVIS2/) — AVIS is a Google gadget compatible web-based viewer of interactive cell signaling networks. AVIS is an implementation of AJAX (Asynchronous JavaScript with XML) with the usage of the libraries GraphViz, ImageMagic (PerlMagic) and overLib. AVIS provides web-based visualization of text-based signaling networks with dynamical zooming, panning and linking capabilities. AVIS is a cross- platform web-based tool that can be used to visualize network maps as embedded objects in any web page. AVIS was implemented for visualization of PathwayGenerator, a tool that displays over 4000 automatically generated mammalian cell signaling maps; NodeNeighborhood a tool to visualize first and second interacting neighbors of yeast and mammalian proteins; and for Genes2Networks, a tool to connect lists of genes and protein using background protein interaction networks.

3. BiNoM Cytoscape Plugin (http://bioinfo.curie.fr/projects/binom/) — BiNoM is a Cytoscape plugin, developed to facilitate the manipulation of biological networks represented in standard systems biology formats (SBML, SBGN, BioPAX) and to carry out studies on the network structure. BiNoM provides the user with a complete interface for the analysis of biological networks in Cytoscape environment.

4. CADLIVE (http://www.cadlive.jp) — CADLIVE (Computer-Aided Design of LIVing systEms) is

a comprehensive computational tool for constructing large-scale biological network maps, analyzing the topological features of them, and simulating their dynamics. Using CADLIVE, we rationally design a biological system at the molecular interaction level for an engineering purpose.

5. CellDesigner (http://celldesigner.org) — CellDesigner is a structured diagram editor for drawing gene-regulatory and biochemical networks. Networks are drawn based on the process diagram, with graphical notation system. CellDesigner supports simulation and parameter scan by an integration with SBML ODE Solver and Copasi. By using CellDesigner, users can browse and modify existing SBML models with references to existing databases (MIRIAM supported), simulate and view the dynamics through an intuitive graphical interface.

6. CellNetAnalyzer (http://www.mpi-magdeburg.mpg.de/projects/cna/cna.html) — CellNetAnalyzer (CNA) is a package for MATLAB and provides a comprehensive and user-friendly environment for structural and functional analysis of biochemical networks. CNA facilitates the analysis of metabolic (stoichiometric) as well as signaling and regulatory networks solely on their network topology, i.e. independent of kinetic mechanisms and parameters. CNA provides a powerful collection of tools and algorithms for structural network analysis which can be started in a menu-controlled manner within interactive network maps. Recently, API functionalities have been added to enable interested users to call algorithms of CNA from external programs. Applications of CNA can be found in systems biology, biotechnology, metabolic engineering, pharmacology, microbiology, chemical engineering.

7. COPASI (http://copasi.org) — COPASI is a software application for simulation and analysis of biochemical networks and their dynamics. COPASI is a stand-alone program that supports models in the SBML standard and can simulate their behavior using ODEs or Gillespie's stochastic simulation algorithm; arbitrary discrete events can be included in such simulations. COPASI provides an C++ API with language bindings for Perl, python, R, Java, and Octave and is able to communicate with the Systems Biology Workbench COPASI carries out several analyses of the network and its dynamics and has extensive support for parameter estimation and optimization. COPASI provides means to visualize data in customizable plots, histograms and animations of network diagrams. For a complete list of feature please see: http://www.copasi.org/tiki-index.php?page=FeatureList (http://www.copasi.org/tiki-index.php?page=FeatureList)

8. Cytoscape (http://www.cytoscape.org/) — open source software platform for visualizing complex-networks and integrating these with any type of attribute data

9. DBSolve (http://insysbio.ru/en/soft/dbsolveoptimum.html) — DBSolveOptimum is a free software for kinetic modeling of metabolic pathways, analysis, and fitting parameters to experimental data. The program has text-based user interface for model description and graphical interface for data analysis. In addition to standart algorithms of simulation (ODE solver, explicit solver, steady-state analysis) the software include also automated local sensetivity analysis, parameters optimization procedures and bifurcaion analysis. The last version of DBSolveOptimum includes advanced tool for data visualization.
10.
11. EPE (http://www.bioinformatics.ed.ac.uk/epe) — Edinburgh Pathway Editor is a biological

pathway drawing/editing application. Currently it can draw diagrams using SBGN PD Level 1, Cytoscape and Metabolic notations. It can export SBML Level 2 v3 and BioPAX Level 3 from the metabolic notation and BioPAX export for SBGN will be coming soon. It is completely customisable and can be configured to support a wide variety of graphical notations. In addition it has an extensible architecture that allows addition exporters to be added. The ability to import SBML models will come soon.

12. Genetic Network Analyzer (http://www-helix.inrialpes.fr/gna) — Genetic Network Analyzer (GNA) is a computer tool for the modeling, simulation, analysis and verification of genetic regulatory networks. The aim of GNA is to assist biologists and bioinformaticians in constructing a qualitative model of a genetic regulatory network from knowledge about regulatory interactions and gene expression data. GNA provides a variety of functions to analyze the steady-state and transient dynamics of the network, among other things by exploiting state- of-the-art model-checking tools.

13. iBioSim (http://www.async.ece.utah.edu/iBioSim/) — The iBioSim tool supports the modeling, analysis, and design of genetic circuits with applications in both systems and synthetic biology. It includes editors to construct genetic circuit models (GCM), Systems Biology Markup Language (SBML) models (L2V4 and L3V1 supported), and labeled Petri net (LPN) models. Models can be constructed by hand, imported from model databases, or learned from experimental data. These models can be analyzed using a variety of ODE and stochastic simulators as well as Markov chain analysis. The efficiency of these analysis methods is enhanced using a variety of automatic reaction-based and logical abstractions. The analysis results can be plotted as graphs or visualized upon the genetic circuit schematic.

14. **iPathways** (http://www.ipathways.org) — Explore biological pathways on your palm!! In comprehending the biological complexity of living systems in disease and healthy states, molecular pathway maps form an integral part of a researcher's arsenal. iPathways, developed by The Systems Biology Institute, Tokyo, brings your pathways from the desktop to the device for the first time!! iPathways provides access to molecular maps constructed in CellDesignerTM , compatible with SBML (Systems Biology Markup Language) and SBGN(Systems Biology Graphical Notation) standards. Browse pathways from your account and explore publications and genes of interest. Features (1.1): - Register Free! or use a guest login - Navigate pathway information by tapping on a gene or protein molecule or a reaction box - View publications associated with a reaction by tapping the PUBMED id on a reaction - Explore genes of interest on IHOP or Entrez directly from your pathways

15. JigCell (http://jigcell.cs.vt.edu/) — JigCell is a set of computational tools with user-friendly interfaces developed for studying complex biochemical regulatory systems in general and the cell cycle control system in particular. For example, The JigCell Model Builder (JCMB) aides the modeler in defining a system to be modeled using SBML with a novel spreadsheet interface, allowing a large amount of data to be displayed in an organized manner. The JigCell Run Manager (JCRM) allows a user to specify a set of specifications for simulation runs using a spreadsheet interface. JigCell Aggregation Connector has been designed to define models in terms of components, for the purpose of being combined in a larger model. JigCell also aims in parameter estimation. A parameter estimator (PET, Parameter Estimation Toolkit) takes a biological model, experimental data, and the relationship between the model and data. Using this information the parameter estimator uses numerical tools to vary the parameters to the model looking for the parameters that best fit the experimental data.

16. JSim (http://www.physiome.org/jsim/) — JSim is a Java-based simulation system for building quantitative numeric models and analyzing them with respect to experimental reference data. JSim's primary focus is in physiology and biomedicine, however its computational engine is quite general and applicable to a wide range of scientific domains. JSim models may intermix ODEs, PDEs, implicit equations, integrals, summations, discrete events and procedural code as appropriate. JSim's model compiler can automatically insert conversion factors for compatible physical units as well as detect and reject unit unbalanced equations. JSim also supports model
17. archive formats SBML (import and export) and CellML (import only).

18. KEGGtranslator (http://www.ra.cs.uni-tuebingen.de/software/KEGGtranslator/) — Nowadays, the KEGG PATHWAY database provides a widely used service for pathway-based information. It contains manually drawn pathway maps with information about the genes, reactions and relations contained therein. To store these pathways, KEGG uses an own XML-format (called "KGML Parsers and translators are needed to process the pathway maps for usage "). in other applications and algorithms. We have developed KEGGtranslator, which is an easy-to-use stand-alone application that can visualize and convert KGML formatted XML-files into multiple output formats. Unlike other translators, KEGGtranslator supports a plethora of output formats, is able to augment the information in translated documents (e.g., MIRIAM annotations) beyond the scope of the KGML document, and amends missing components to fragmentary reactions within the pathway to allow simulations on those. KEGGtranslator converts KEGG files (KGML formatted XML-files) to SBML, GML, GraphML, JPG, GIF, LaTeX, etc. KEGG pathways can be obtained from ftp://ftp.genome.jp/pub/kegg/xml/kgml

19. MesoRD (http://mesord.sourceforge.net) — MesoRD is a stochastic and deterministic simulator of coupled chemical reactions and diffusions in space.

20. MetaFluxNet (http://metafluxnet.kaist.ac.kr) — MetaFluxNet is a program package for managing information on the metabolic reaction network and for quantitatively analyzing metabolic fluxes in an interactive and customized way, which allows users to interpret and examine metabolic behavior in response to genetic and/or environmental modifications. As a result, quantitative in silico simulations of metabolic pathways can be carried out to understand the metabolic status and to design the metabolic engineering strategies.

21. MetExplore (http://metexplore.toulouse.inra.fr) — A web server to link metabolic experiments and genome-scale metabolic networks. MetExplore contains original network filters, allows to export in SBML and visualise filtered metabolic networks, and map masses from metabolic experiments onto complete metabolic networks. It also contains some graph-based methods to enrich the analyses.

22. MOOSE (http://moose.ncbs.res.in/) — MOOSE is the base and numerical core for large, detailed simulations including Computational Neuroscience and Systems Biology. MOOSE spans the range from single molecules to sub-cellular networks, from single cells to neuronal networks, and to still larger systems. it is backwards- compatible with GENESIS, and forward compatible with Python and XML-based model definition standards like SBML and NeuroML.

23. NetBuilder' (http://strc.herts.ac.uk/bio/maria/Apostrophe/) — NetBuilder' is a software tool that is intended to help experimentalists creating and manipulating the mathematical

representations they need to predict the behaviour of their systems. NetBuilder' has a graphical user interface, which allows its users to create a picture of the (known) components and interactions in the system, and enter quantitative information, such as know or estimated quantities and rates. A (hidden) translator converts the picture and the other data into a mathematical description, whereupon NetBuilder's "simulation engine" may be used to find out how the modelled system responds to changing input.

24. Omix (http://www.13cflux.net/omix) — an editor for metabolic network diagrams and a customizable visualization framework. With Omix, high quality diagrams can be created, suitable for publication and presentation. For this, Omix is designed towards the standards in user-guidance as known from the most important graphics software tools. Thus, a fast access to the functionalities of the software is warranted even for newcomers. Omix allows the design of metabolic network diagrams according the established network layout standards. For this, semi-automatic network drawing techniques support and accelerate the manual drawing process. Furthermore, Omix comes up with extensive visualization features. Any kind of data coming from experiment and simulation can be visualized with Omix. The way, data is visualized in Omix can completely be defined by the user because Visualization takes place in a scripting language called OVL (Omix Visualization Language). OVL allows changing the visual properties of network components. In this way, multi-omics data can be visualized by being mapped on the appearance of network components and their connections. Furthermore, user-interaction can be defined in OVL. Another visualization technique realized in Omix is Visualization on Demand, allowing the network-integrated visualization of multiple, hierarchical organized information in an interactive manner. Omix is equipped with a plug-in interface. Thus, the functionality of the software is extensible. Many plug-ins have been developed in recent years allowing network import from KEGG, im- and export of GML and SBML files as well as Modelica and Matlab code, network analysis tools such as elementary flux modes, flux balances and free fluxes, export of flash animations, data import from excel spreadsheets and much more.

25. PaVESy (http://pavesy.mpimp-golm.mpg.de/) — Pathway Visualization Editing System. Java based. (Linux/Mac/Win). Free download.

26. PET (http://mpf.biol.vt.edu/pet) — Parameter optimization and exploration is the primary feature of PET. Some of the other tasks PET can perform are simulations, setting up multiple experiments for a model, comparing parameter sets, and exporting plots for presentations.

27. PK-Sim / MoBi (http://www.systems-biology.com) — Systems biology software platform for multiscale physiological modeling and simulation with a focus on physiologically-based pharmokinetics and -dynamics (PBPK/PD) including interfaces to MATLAB and R. Available to academic researchers via a free non-commercial license.

28. ProcessDB (http://www.integrativebioinformatics.com/processdb.html) — ProcessDB helps molecular cell biologists manage and test their increasingly complex mechanistic hypotheses. ProcessDB does this with a bio-savvy graphical user interface that helps users formulate, visualize, compare, modify, manage and test their own mechanistic theories of cellular function. All models in ProcessDB can be automatically combined with user-specified experimental protocols and exported to the Berkeley Madonna solver for testing against experimental data. ProcessDB allows investigators to know with precision what their theories predict, and speeds discovery of mechanisms that account for all of the available data.

29. ProMoT (http://www.mpi-magdeburg.mpg.de/projects/promot) — The process modeling tool ProMoT is a software for the set-up and manipulation of models of complex technical or biological systems. Key features are the support of modular models, modeling libraries for different application areas, efficient and robust numerical algorithms, a own modeling language MDL and advanced graphical support. Dynamic models can contain DAE and discrete events for simulation in DIVA, Diana or MATLAB. Logical (Boolean) models are exported to CellNetAnalyzer.

30. PySCeS (http://pysces.sourceforge.net) — PySCeS: the Python Simulator for Cellular Systems is an extendable toolkit for the analysis and investigation of cellular systems. PySCeS is developed in Python and has been designed to be used both interactively or as a library. It utilises a human readable, model description language for describing models as well as being SBML compatible. PySCeS includes stoichiometric, simulation, steady state and Eigen analysis using direct non-linear root finders. It also includes full support for Metabolic Control Analysis (MCA), the characterisation of static bifurcations, multidimensional parameter scanning and 2/3D graph capabilities. Currently an extension PySCeS-CBM is being developed that allows for the interactive manipulation, modelling and optimization of genome scale, constraint based models (e.g. flux balance analysis)

31. **SBML Layout** (http://sbmllayout.sf.net/) — SBML Layout encompasses: 1. a online application (http://sys-bio.org/Layout) for layouting / rendering an SBML file , 2. a library for reading / writing SBML Layout and Rendering information as well as SBGN-ML and 3. a standalone application for displaying files with the SBML Layout or Rendering information. It is written in .net and available under the BSD for all platforms.
32. **SBML2TikZ** (http://sbml2tikz.org/default.aspx) — SBML2TikZ provides automatic generation of TeX Macros to illustrate Systems Biology Markup Language (SBML) graphs. The rendering is dependent on the SBML Render Extension proposed by Gauges et al. and the rendering library is built on the existing SBML Layout Library.

33. **SBW** (http://sys-bio.org/) — Systems Biology Workbench. A framework for connecting and running various applications written in different languages or on different systems, and a collection of available modules for model development, analysis, and simulation. Free/Open Source. (BSD)

34. **SBW: Auto Layout** (http://jdesigner.sourceforge.net/Site/Auto_Layout.html) — The SBW AutoLayout module automatically creates lucid layouts of biochemical models. The SBW AutoLayout module has a graphical user interface (GUI) and an application programming interface (API). The GUI provides a typical window application for using AutoLayout's functionality, while the API allows programmers to incorporate AutoLayout's functionality into their own programs

35. **semanticSBML** (http://semanticsbml.org) — Create, check, visualize, retrieve, cluster, annotate, merge SBML models. The program includes a web based graphical user interface. For tool developers a programming interface (Python) and RESTful web-services are provided. It features advanced functions to edit MIRIAM and SBO terms. The latest version of semanticSBML is fully web based and can be accessed under http://semanticsbml.org /semanticSBML/simple/index (http://semanticsbml.org/semanticSBML/simple/index)

36. **SimBiology** (http://www.mathworks.com/products/simbiology/) — SimBiology ® is a MATLAB ® product from MathWorks that provides graphical and programmatic tools for computational systems biology and pharmacokinetics. It contains functionality for creating, simulating, and analyzing biological models. The SimBiology desktop lets you build a model using a block diagram editor, a model wizard, or a tabular interface. You can also create a model at the command line or directly from SBML files. SimBiology lets you simulate a model using stochastic or deterministic solvers. The product supports parameter estimation, sensitivity analysis, parameter scans, and other model analysis methods. All SimBiology features can be used together with the MATLAB programming language, letting you customize models, create or modify analysis tasks, and automate your workflow.

37. **Simulate3D** (http://sys-bio.org/fbergman/Simulate3D.htm) — Traditionally simulation results are available as either data tables or X-Y plots. Data tables are helpful for further processing by other computational tools. X-Y plots, on the other hand, tend to get complex even for a limited number of species. In creating a new visualization tool, we had two goals in mind. A first goal was to tie simulation results strongly to the model. A next goal was to be able to view the simulation in real time to refine or broaden it where necessary. These goals have been realized in form of a 3D Time-course Visualization module.

38. **SimWiz** (http://projects.villa-bosch.de/bcb/software/software/Ulla/SimWiz/) — Visualizes simulation outputs from tools such as Copasi and STODE. (Linux/Win) (European Media License)

39. **Snoopy** (http://www-dssz.informatik.tu-cottbus.de/DSSZ/Software/Snoopy) — a software tool to design and animate hierarchical graphs, among others Petri nets. To investigate biomolecular networks, Snoopy provides a unifying Petri net framework comprising a family of related Petri net classes. Models can be hierarchically structured, allowing for the mastering of larger networks. To move easily between the qualitative, stochastic and continuous modelling paradigms, models can be converted into each other. We get models sharing structure, but being specialized by their kinetic information. The analysis and iterative reverse engineering of biomolecular networks is supported by the simultaneous use of several Petri net classes, while the GUI adapts dynamically to the active one. Built-in animation and simulation are complemented by exports to various analysis tools.

40. **SYCAMORE** (http://sycamore.eml.org) — SYCAMORE is a system that provides you with a faciliated access to a number of tools and methods in order to build models of biochemical systems, view, analyse and refine them, as well as perform quick simulations.

41. **Systrip** (http://tulip.labri.fr/TulipDrupal/?q=systrip) — Systrip is a visual environment for the analysis of time-series data in the context of biological networks. This software gathers bioinformatics and graph theoretical algorithms that can be assembled in different ways to help biologists in their visual mining process. Main features : 1. SBML file import and export. 2. Multiple kind of metabolic network representations (3D, force directed, biological convention preserving, hierachical ...). 3. Both graph theoritical measures and metabolic network analysis algorithms (choke points, scope, centrality...). 4. Time-series data import and visualization (table view, parallel coordinates, scatter plot). 5. Visualization of time-series in the context of the metabolic network. 6. 3D molecular visualization. 7. Database querry tools (Kegg, PublicHouse).

42. **VANTED** (http://vanted.ipk-gatersleben.de/) — This system makes it possible to load and edit graphs, which may represent biological pathways or functional hierarchies. It is possible to map experimental datasets onto the graph elements and visualize time series data or data of different genotypes or environmental conditions in the context of a the underlying biological processes. Built-in statistic functions allow a fast evaluation of the data (e.g. t-Test or correlation analysis). Vanted can be extended for various functionalities, e.g. Flux simulation, database access and 3D visualisation.

GSMN-TB

List of Metabolites

ID	Name
13PDG	1,3-diphosphateglycerate
1-AMINO-PROPAN-2-OL	1-amino-propan-2-ol
2A3KB	2-amino-3-oxobutanoate
2MBECOA	2-methylbut-2-enoyl-CoA
2MBUTCOA	S-2-methyl-butyryl-CoA
2MBUTLIPO	enzyme_N6-(S-[2-methylpropanoyl]dihydrolipoyl)lysine
2METHYLCISACONITATE	2-methyl-cis-aconitate
2METHYLCITRATE	2-methylcitrate
2PCDPMDE	2-phospho-4-(cytidine_5'-diphospho)-2-C-methyl-D-erythritol
2PG	2-phosphoglycerate
2-PHOSPHO-L-LACTATE	2-phospho-L-lactate
3DDAH7P	3-deoxy-D-arabino-heptulosonate-7-phosphate
3MBECOA	3-methylbut-2-enoyl-CoA
3MBUTCOA	S-3-methyl-butyryl-CoA
3MBUTLIPO	enzyme_N6-(S-[3-methylbutanoyl]dihydrolipoyl)lysine
3PG	3-phosphoglycerate
3PSER	3-phospho-serine
3PSME	5-enolpyruvyl-shikimate-3-phosphate
4HPP	p-hydroxyphenylpyruvate
4PPNCYS	R-4'-phosphopantothenoyl-L-cysteine
4PPNTE	pantetheine_4'-phosphate
4PPNTO	D-4'-phosphopantothenate
5-AMINO-LEVULINATE	5-amino-levulinate
5MTA	5'-methylthioadenosine
5PARAPP	5'-phosphoarabinose-pyrophosphate
7-8-DIAMINONONANOATE	7,8-Diaminononanoate
8-AMINO7-OXONONANOATE	8-amino-7-oxononanoate
9-HEXADECENOATE	9-hexadecenoate
9-HEXADECENOYL-ACP	9-hexadecenoyl-ACP
9-HEXADECENOYL-COA	9-hexadecenoyl-CoA
9-OCTADECENOATE	9-octadecenoate
9-OCTADECENOYL-ACP	9-octadecenoyl-ACP

9-OCTADECENOYL-COA	9-octadecenoyl-CoA
A160GL3P	A160GL3P
A6RP	5-amino-6-(5'-phosphoribosylamino)uracil
A6RP5P	5-amino-6-(5'-phosphoribitylamino)uracil
A6RP5P2	5-amino-6-(5'-phosphoribosylamino)uracil
AACCOA	acetoacetyl-CoA
ABUT	2-aceto-2-hydroxy-butyrate
AC	acetate
AC1PIM1	AC1PIM1
AC1PIM2	AC1PIM2
AC1PIM3	AC1PIM3
AC2PIM1	AC2PIM1
AC2PIM2	AC2PIM2
AC2PIM3	AC2PIM3
AC3PIM1	AC3PIM1
AC3PIM2	AC3PIM2
AC3PIM3	AC3PIM3
AC3PIM4	AC3PIM4
AC3PIM5	AC3PIM5
AC4PIM1	AC4PIM1
AC4PIM2	AC4PIM2
AC4PIM3	AC4PIM3
AC4PIM5	AC4PIM5
AC4PIM6	AC4PIM6
AC4PIM7	AC4PIM7
ACACP	acetyl-ACP
ACAL	acetaldehyde
ACCOA	acetyl-CoA
ACETYLP	acetylphosphate
ACLAC	2-acetolactate
ACP	acyl-carrier-protein
ACRCOA	acrylyl-CoA
ACTAC	acetoacetate
ACYL-MAS	ACYL-MAS
ACYL-TRE-S-COA	ACYL-TRE-S-COA
AD	adenine
ADCHOR	4-amino-4-deoxychorismate
ADENOSYLCOBINAMIDE	adenosylcobinamide

ADENOSYLCOBINAMIDE-GDP	adenosylcobinamide-GDP
ADENOSYLCOBINIMIDE-P	adenosylcobinamide-P
ADENOSYL-COBRATE	adenosyl-cobyrate
ADENOSYL-COBRINICACID-A-C-DIAMI	adenosyl-cobyrinic
ADLIPO	enzyme_N6-(S-acetyldihydrolipoyl)lysine
ADN	adenosine
ADP	adenosine-diphosphate
AGL3P	1-acyl-sn-glycerol-3P
AHHMD	2-amino-4-hydroxy-6-hydroxymethyl-7,8-dihydropteridine_diphosphate
AHHMP	6-hydroxymethyl-dihydropterin
AHMMP	hydroxymethylpyrimidine
AHTD	7,8-dihydroneopterin_3'-triphosphate
AICAR	amino-4-imidazolecarboxamide_ribotide
AIR	5-aminoimidazole_ribonucleotide
AKG	Œ±-ketoglutarate
AKP	2-dehydropantoate
ALA	D-alanine
ALAALA	D-alanyl-D-alanine
AMINOACETONE	aminoacetone
AMP	adenosine-monophosphate
AMPMP	hydroxymethylpyrimidine_phosphate
AN	anthranilate
APS	adenylyl-sulfate
ARABINOGALACTAN_PEPTIDOGLYCA	arabinogalactan_peptidoglycan
ARABINOGALACTANDPP	arabinogalactan-decaprenylphosphate
ARAbr1brGALACTANDPP	ARA[1]GALACTANDPP
ARAFDPP	arabinofuranose-decaprenylphosphate
ARG	L-arginine
ARGSUCC	L-arginino-succinate
ASER	O-acetyl-L-serine
ASN	L-asparagine
ASP	L-aspartate
ASP4P	L-aspartyl-4-phosphate
ASPSA	L-aspartate-semialdehyde
ASUC	adenylo-succinate
ATP	adenosine-triphosphate
bALA	Œ≤-alanine

bDG1P	Œ≤-D-Glucose_1-phosphate
bDG6P	Œ≤-D-glucose-6-phosphate
bDGLC	Œ≤-D-glucose
BETA-KETO-C22-ACYL-ACP	BETA-KETO-C22-ACYL-ACP
BIOMASS	biomass
BIOTIN	biotin
BIOTIN-BCCP	biotin-BCCP
BIOTIN-CO2	BCCP-biotin-CO2
brn-1brPOLYP	(polyphosphate)(n-1)
brnbrPOLYP	(polyphosphate)(n)
BUTANOYL-COA	butanoyl-CoA
C78-3-OXY-MYCOLATE-ENZ	3-oxo-C78-Œ±-mycolate-ENZ
C78MYCOLATE-ENZ	C78-Œ±-mycolate-ENZ
C78MYCOLATE-PP	C78-Œ±-mycolate-PP
CAASP	carbamoyl-L-aspartate
CADA	cadaverine
CAIR	4-carboxyaminoimidazole_ribonucleotide
cAMP	cyclic-AMP
CAP	carbamoyl-phosphate
CATECHOL	catechol
CBHCAP	3-carboxy-2-hydroxy-4-methylpentanoate
CDP	cytidine-diphosphate
CDPDAG-TBA	CDP-diacylglycerol-TBA
CDPDG	CDP-diacylglycerol
CDPMDE	4-(cytidine_5'-diphospho)-2-C-methyl-D-erythritol
CELB	cellobiose
cGMP	cyclic-GMP
CHOR	chorismate
CIS-DELTA-13-ENOYL-C32-ACYL-ACP	CIS-DELTA-13-ENOYL-C32-ACYL-ACP
CIS-DELTA-19-ENOYL-C38-ACYL-ACP	CIS-DELTA-19-ENOYL-C38-ACYL-ACP
CIS-DELTA-2-19,31-ENOYL-C50-ACYL-	CIS-DELTA-2-19,31-ENOYL-C50-ACYL-ACP
CIS-DELTA-2-19,37-ENOYL-C56-ACYL-	CIS-DELTA-2-19,37-ENOYL-C56-ACYL-ACP
CIS-DELTA-2-3,15-ENOYL-C34-ACYL-A	CIS-DELTA-2-3,15-ENOYL-C34-ACYL-ACP
CIS-DELTA-2-3,21-ENOYL-C40-ACYL-A	CIS-DELTA-2-3,21-ENOYL-C40-ACYL-ACP
CIS-DELTA-37-ENOYL-DIMETHY-HYDR	CIS-DELTA-37-ENOYL-DIMETHY-HYDROXY-C56-ACYL-ACP
CIS-DELTA-37-ENOYL-METHY-HYDRO	CIS-DELTA-37-ENOYL-METHY-HYDROXY-C56-ACYL-ACP

CIS-DELTA-3-DODECANOYL-COA	CIS-DELTA-3-DODECANOYL-COA
CIS-DELTA-3-ENOYL-C22-ACYL-ACP	CIS-DELTA-3-ENOYL-C22-ACYL-ACP
CIS-DELTA-5-TETRADECANOYL-COA	CIS-DELTA-5-TETRADECANOYL-COA
CIS-KETO-MEROACYL-ACP	CIS-KETO-MEROACYL-ACP
CIS-METHOXY-MEROACYL-ACP	CIS-METHOXY-MEROACYL-ACP
CIT	citrate
CITR	citrulline
CITxt	external_citrate
CL	cardiolipin
CMP	cytidine-monophosphate
CO2	carbon_dioxide
CO2xt	external_carbon_dioxide
COA	coenzyme_A
COB-I	coenzyme
COB-II	COB-II
COB-III	COB-III
COB-II-RINICACID-A-C-DIAMIDE	cob(II)yrinic
COB-I-RINICACID-A-C-DIAMIDE	cob(I)yrinic
CO-II	Co2+
CO-IIxt	external
COPROPORPHYRINOGEN-III	coproporphyrinogen_III
CPAD5P	1-(o-carboxyphenylamino)-1'-deoxyribulose-5'-phosphate
CROTONOYLCOA	crotonoyl-CoA
CTP	cytidine-5'-triphosphate
CYCLOPROPYL-MEROACYL-ACP	CYCLOPROPYL-MEROACYL-ACP
CYS	L-cysteine
CYS-NG-INS	desacetylmycothiol_(1-D-myo-inosityl-2-(L-cysteinyl)amido-2-deoxy-Œ±-D-glucopyranoside)
D-3-HYDROXY-C22-ACYL-ACP	D-3-HYDROXY-C22-ACYL-ACP
D6PGC	6-phospho-D-gluconate
D6PGL	D-glucono-Œ¥-lactone-6-phosphate
D6RP5P	2,5-diamino-6-(ribosylamino)-4-(3H)-pyrimidinone_5'-phosphate
D8RL	6,7-dimethyl-8-(1-D-ribityl)lumazine
DA	deoxyadenosine
DADP	deoxyadenosine-diphosphate
DAG	1,2-diacylglycerol
DALA	D-alanine

DAPIM	L,L-diaminopimelate
DATP	deoxyadenosine-triphosphate
DB4P	2,5-diamino-6-(ribosylamino)-4-(3H)-pyrimidinone_5'-phosphate
DCDP	deoxycytidine-diphosphate
DCMP	deoxycytidine_monophosphate
DCTP	deoxycytidine-triphosphate
DECANOATE	decanoate
DECANOYL-COA	decanoyl-CoA
DETHIOBIOTIN	dethiobiotin
DG	DG
DGDP	deoxyguanosine-diphosphate
DGLN	D-glutamine
DGLU	D-glutamate
DGLYCERATE	D-glycerate
DGMP	deoxyguanosine-monophosphate
DGTP	deoxyguanosine-triphosphate
DHAP	dihydroxyacetone-phosphate
DHF	7,8-dihydrofolate
DHLIPOYLPROTEIN	enzyme_N6-(dihydrolipoyl)lysine
DHMVA	2,3-dihydroxy-3-methylvalerate
DHN	1,4-dihydroxy-2-naphthoate
DHP	dihydro-neo-pterin
DHPT	7,8-dihydropteroate
DHSK	3-dehydro-shikimate
DIACYLTREHALOSE	diacyltrehalose.
DIHYDRODIPICOLINATE	L-2,3-dihydrodipicolinate
DIHYDROXYMETHYLPENTANOATE	Dihydroxy-methylpentanoate
DIM	dimycocerosate
DIM-CYTO	cytoplasmic_dimycocerosate
DIMGP	D-erythro-imidazole-glycerol-phosphate
DIN	deoxyinosine
DLIPO	DLIPO
DMK	3-demethylubiquinone-8
DMPP	dimethylallyl-pyrophosphate
DNA	deoxyribonucleic
DOCOSANOATE	docosanoate
DOCOSANOYL-ACP	docosanoyl-ACP

DOCOSANOYL-COA	docosanoyl-CoA
DODECANOATE	dodecanoate
DODECANOYL-COA	dodecanoyl-CoA
DOROA	dihydroorotate
DPCOA	dephospho-CoA
DPP	dimethylallyl-pyrophosphate
DPPARA	decaprenylphosphate-arabinose
DPPPR	DPPPR
DPPR	DPPR
DQT	3-dehydroquinate
DR1P	deoxyribose-1-phosphate
DR5P	deoxyribose-5-phosphate
DT	DT
DTDP	deoxythymidine-5'-diphosphate
DTDP4DH6DGLC	dTDP-4-dehydro-6-deoxy-D-glucose
DTDP4DH6DMAN	dTDP-4-dehydro-6-deoxy-L-mannose
DTDPGLC	dTDP-glucose
DTDPRHAM	dTDP-Œ±-L-rhamnose
DTMP	deoxythymidine
DTTP	deoxythymidine
DUDP	deoxyuridine-diphosphate
DUMP	deoxyuridine-phosphate
DUTP	deoxyuridine-triphosphate
DX5P	1-deoxy-D-xylulose
E4P	D-erythrose-4-phosphate
EICOSANOATE	eicosanoate
EICOSANOYL-ACP	eicosanoyl-ACP
EICOSANOYL-COA	eicosanoyl-CoA
ETH	ethanol
F1P	fructose-1-phosphate
F420	coenzyme
F420-0	F420-0
F6P	D-fructose-6-phosphate
FAD	flavin
FADH2	flavin
FDP	fructose-1,6-bisphosphate
FE2	ferrous
FE3	ferric

FE3xt	external
FERI	oxidized
FERO	reduced
FGAM	5-phosphoribosyl-N-formylglycineamidine
FGAR	5'-phosphoribosyl-N-formylglycineamide
FMN	flavin_mononucleotide
FO	FO
FOR	formate
FPP	trans,
FRU	fructose
FTHF	N10-formyl-THF
FUACAC	4-fumaryl-acetoacetate
FUC1P	Œ≤-L-fucose_1-phosphate
FUM	fumarate
G1P	Œ±-D-glucose_1-phosphate
G3P	D-glyceraldehyde-3-phosphate
G6P	Œ≤-D-glucose-6-phosphate
GA1P	D-glucosamine-1-phosphate
GA6P	D-glucosamine-6-phosphate
GABA	4-aminobutyrate_(GABA)
GAL1P	Œ±-D-galactose_1-phosphate
GALACTANDPP	galactan-decaprenylphosphate
GAR	5-phospho-ribosyl-glycineamide
GDP	guanosine_diphosphate
GDPDHDOGAL	GDP-4-dehydro-6-L-deoxygalactose
GDPDHDOMAN	GDP-4-dehydro-6-deoxy-D-mannose
GDPFUC	GDP-L-fucose
GDPMAN	guanosine_diphosphate_mannose
GGPP	geranylgeranyl_diphosphate
GL	Glycerol
GL3P	glycerol-3-phosphate
GLAC	D-galactose
GLAL	glycolaldehyde
GLC	Œ≤-D-glucose
GLCxt	external_Œ≤-D-glucose
GLN	glutamine
GLU	glutamate
GLU1SEMIALD	glutamate-1-semialdehyde

GLUGSAL	L-glutamate_Œ≥-semialdehyde
GLUP	L-glutamate-5-phosphate
GLUT	GLUT
GLUTCOA	GLUTCOA
GLX	glyoxylate
GLY	glycine
GLYCOLATE	glycolate
GMP	guanosine-monophosphate
GN	guanine
GPP	geranyl-PP
GSN	guanosine
GTP	guanosine-triphosphate
GUAIACOL	guaiacol
H	proton
H2O2	hydrogen_peroxide
H2S	hydrogen_sulfide
H2SO3	sulfurous_acid_
HBA	salicylate_(o-hydroxybenzoic_acid)
HCO3	bicarbonate
HCYS	L-homocysteine
HEME-FE2	HEME-FE2
HEME-FE3	HEME-FE3
HEMT	4-methyl-5-(Œ≤-hydroxyethyl)thiazole
HEPPP	HEPPP
HEPTADECANOATE	heptadecanoate
HEPTADECANOYL-ACP	heptadecanoyl-ACP
HEPTADECANOYL-COA	heptadecanoyl-CoA
HEPTANOYL-COA	heptanoyl-CoA
HEXACOSANOATE	hexacosanoate
HEXACOSANOYL-ACP	hexacosanoyl-ACP
HEXACOSANOYL-COA	hexacosanoyl-CoA
HEXACOSANOYL-COA-CO2	hexacosanoyl-CoA-CO2
HEXADECANOATE	hexadecanoate
HEXADECANOYL-ACP	hexadecanoyl-ACP
HEXADECANOYL-COA	hexadecanoyl-COA
HEXADECANOYL-MAS	hexadecanoyl-MAS
HEXANOATE	hexanoate
HEXANOYL-ACP	hexanoyl-ACP

HEXANOYL-COA	hexanoyl-CoA
HIBUT	3-hydroxy-isobutyrate
HIBUTCOA	3-hydroxy-isobutyryl-CoA
HIS	L-histidine
HISOL	histidinol
HISOLP	L-histidinol-phosphate
HMB4PP	1-hydroxy-2-methyl-2-(E)-butenyl_4-diphosphate
HMBUTCOA	3-hydroxybutyryl-CoA
HMGLUTCOA	3-hydroxy-3-methyl-glutaryl-CoA
HOMOGEN	homogentisate
HPCOA	HPCOA
HPPP	HPPP
HSER	homoserine
HYDROGENOBYRINATE	hydrogenobyrinate
HYDROGENOBYRINATE-A-C-DIAMIDE	hydrogenobyrinate_a,c_diamide
HYDROXYAKG	D-4-hydroxy-2-keto-glutarate
HYDROXYMETHYLBILANE	hydroxymethylbilane
HYDROXYPHTHIOCERANOYL-COA	hydroxyphthioceranoyl-CoA
HYXN	hypoxanthine
IBUTCOA	IBUTCOA
IBUTLIPO	IBUTLIPO
ICHOR	isochorismate
ICIT	isocitrate
IDP	inosine_diphosphate
IGP	indole-3-glycerol-phosphate
ILE	L-isoleucine
IMACP	imidazole_acetol-phosphate
IMP	inosine-5'-phosphate
INS	inosine
IP	inositol_phosphate
IPP	Œî3-isopentenyl-PP
IPPMAL	2-isopropylmalate
ISUCC	iminoaspartate_(Œ±-iminosuccinate)
ITP	inosine_triphosphate
LAC	D-lactate
LACTAL	lactaldehyde
LAM	lipoarabinomannan
LEU	L-leucine

LIPID1	LIPID1
LIPID2	LIPID2
LIPID2-AMIDATED	LIPID2-AMIDATED
LIPO	enzyme
LIPOYLPROTEIN	H-protein-(lipoyl)lysine
LLAC	lactate
LLCT	cystathionine
LM	ipomannan
LPPG	?
LYS	L-lysine
MAACCOA	MAACCOA
MACAC	4-maleyl-acetoacetate
MACRCOA	methylacrylyl-CoA
MAG	monoacylglycerol
MAHMPPP	4-amino-5-hydroxymethyl-2-methylpyrimidine-pyrophosphate
MAL	malate
MALACP	malonyl-ACP
MALCOA	malonyl-CoA
MAN	mannose
MAN1P	Œ±-D-mannose_1-phosphate
MAN6P	mannose-6-phosphate
MAPC	mycolic_acid,Äìarabinogalactan-peptidoglycan_complex
MAS	MAS
MBT	mycobactin
MBTA-HOLO	mycobactinA-HOLO
MBTA-SAL	mycobactinA-SAL
MBTB-HOLO	mycobactinB-HOLO
MBTB-SER	mycobactinB-SER
MBTCD-HBA	mycobactinCD-HBA
MBTCD-HOLO	mycobactinCD-HOLO
MBTE-HOLO	mycobactinE-HOLO
MBTE-LYS	mycobactinE-LYS
MBTF-HOLO	mycobactinF-HOLO
MBTF-LYS	mycobactinF-LYS
MBTSEC	mycobactinSEC
MBTWALL	mycobactinWALL
MDAPIM	meso-diaminopimelate

MDE4P	2-C-methyl-D-erythritol-4-phosphate
MDECPP	2-C-methyl-D-erythritol-2,4-cyclodiphosphate
MEROACYL-AMP	meroacyl-AMP
MET	methionine
METHF	5,10-methenyl-THF
METHYMALONATE	methylmalonate
METTHF	5,10-methylene-THF
MGLUTCOA	3-methylglutaconyl-CoA
MI	myo-inositol
MK	ubiquinone-8
MKH2	ubiquinol-8
MLT	maltose
MO2	molybdenum_ion
MO2xt	external_molybdenum_ion
MOAD-COOH	MOAD-COOH
MOAD-COSH	MOAD-COSH
MOLYBDENUM	molybdenum
MOLYBDOPTERIN	molybdopterin
MOLYBDOPTERIN-GDP	molybdopterin_guanine_dinucleotide
MOP	4-methyl-2-oxopentanoate
MPD	mannosyl-√ü-1-phosphodolichol
MPET	4-methyl-5-(Œ≤-hydroxyethyl)thiazole_phosphate
MTHF	5-methyl-THF
MTHPTGLU	MTHPTGLU
MTR1P	5-methylthioribose-1-phosphate
MYCOCEROSOYL-MAS	MYCOCEROSOYL-MAS
MYCOLIPANOIC-ACP	mycolipanoic-ACP
MYCOLIPDIENOYL-ACP	MYCOLIPDIENOYL-ACP
MYCOLIPENOYL-ACP	MYCOLIPENOYL-ACP
MYCOSIDE_B	mycoside_B
MYCOTHIOL	mycothiol
MYCOTHIONE	mycothione
NAAD	deamido-NAD
NAC	nicotinate
NACD	nicotinate_ribonucleoside
NACN	nicotinate_nucleotide
NAD	nicotinamide_adenine_dinucleotide
NADH	nicotinamide_adenine_dinucleotide_-_reduced

NADP	nicotinamide_adenine_dinucleotide_phosphate
NADPH	Nicotinamide_adenine_dinucleotide_phosphate_-_reduced
NAGA1P	N-acetyl-glucosamine-1-phosphate
NAGDPP	N-acetyl-glucosamine-DPP
NAG-INS	1-D-myo-inosityl-2-acetamido-2-deoxy-Œ±-D-glucopyranoside
NAGLU	N-acetyl-L-glutamate
NAGLUP	N-acetylglutamyl-phosphate
NAGLUS	N-acetyl-L-glutamate_5-semialdehyde
NAM	nicotinamide
NAMD	nicotinamide_riboside
NAMN	nicotinamide_mononucleotide
NAORN	N-acetyl-L-ornithine
NG-INS	glucosaminyl-inositol
NH3	ammonia
NH3xt	external_ammonia
NO2	nitrite
NO2xt	external_nitrite
NO3	nitrate_
NONADECANOATE	nonadecanoate
NONADECANOYL-ACP	nonadecanoyl-ACP
NONADECANOYL-COA	nonadecanoyl-COA
NONANOYL-COA	nonanoyl-COA
NPP	nerylpyrophosphate
NPRAN	N-(5'-phosphoribosyl)-anthranilate
O2	oxygen
O2xt	external_oxygen
OA	oxaloacetate
OAHSER	O-acetyl-L-homoserine
OBUT	2-oxobutanoate
OCTACOSANOYL-ACP	octacosanoyl-ACP
OCTACOSANOYL-COA	octacosanoyl-COA
OCTADECANOATE	octadecanoate
OCTADECANOYL-ACP	octadecanoyl-ACP
OCTADECANOYL-COA	octadecanoyl-CoA
OCTANOYL-COA	octanoyl-CoA
OICAP	OICAP

OMP	orotidine-5'-phosphate
OMVAL	2-keto-3-methyl-valerate
OPP	octaprenyl_diphosphate
ORN	ornithine
OROA	orotate
OSB	O-succinylbenzoate
OSBCOA	O-succinylbenzoyl-CoA
OSLHSER	O-succinyl-L-homoserine
OTHIO	thioredoxin_disulfide
OXOMETHYLPENTANOATE	2-oxo-3-methylpentanoate
P5C	pyrroline_5-carboxylate
PA	L-phosphatidate
PABA	para-aminobenzoic_acid
PANT	L-pantoate
PAP	adenosine_3',5'-bisphosphate
PAPS	3'-phosphoadenylyl-sulfate
PA-TBA	PA-tuberculostearic_acid
PE	L-1-phosphatidyl-ethanolamine
PENTADECANOATE	pentadecanoate
PENTADECANOYL-ACP	pentadecanoyl-ACP
PENTADECANOYL-COA	pentadecanoyl-CoA
PENTA-METHYL-TRICONTANOYL	PENTA-METHYL-TRICONTANOYL
PENTA-METHYL-TRICONTANOYL-COA	PENTA-METHYL-TRICONTANOYL-COA
PENTANOYL-COA	pentanoyl-CoA
PEP	phosphoenolpyruvate
PEPTIDOGLYCAN	peptidoglycan
PG	L-1-phosphatidyl-glycero
PGL-TB	phenolglycolipid_antigen_(PLG-Tb_1)
PGP	L-1-phosphatidylglycerol-phosphate
PHDIM	phthiocerol
PHDIM-CYTO	cytoplasmic_phthiocerol_dimycocerosate
PHDIMRHAM1	PHDIMRHAM1
PHDIMRHAM2	PHDIMRHAM2
PHE	phenylalanine
PHEN	prephenate
PHENOLPHTHIODIOLONE-A	phenolphthiodiolone
PHOSPHATIDYLCHOLINE	phosphatidylcholine
PHOSPHO-PENTA-METHYL-TRICONTA	PHOSPHO-PENTA-METHYL-TRICONTANOYL-COA

PHP	3-phospho-hydroxypyruvate
PHPAA-COA	PHPAA-COA
PHPYR	phenylpyruvate
PHSER	O-phospho-L-homoserine
PHTHIODIOLONE-A	phthiodiolone_A
PI	phosphate
PIMELOYL-COA	pimeloyl-CoA
PIMS	phosphatidyl_myo-inositol_mannosides
PI-TBA	PI-tuberculostearic_acid
PIxt	external_phosphate
P-L-GLX	poly-L-glutamate/glutamine
PNTO	pantothenate
POLYACYLTREHALOSE	polyacyltrehalose
PORPHOBILILOGIN	porphobilinogen
ppGpp	ppGpp
PPI	pyrophosphate
PPM	polyprenolmannose
PPPI	Inorganic_triphosphate
PPPP	PPPP
PPTC	phenolphthiocerol
PPTT	PPTT
PRAM	5-phosphoribosylamine
PRBAMP	phosphoribosylformiminoAICAR-phosphate
PRBATP	5-phosphoribosyl_1-pyrophosphate
PRECORIN-2	precorrin-2
PRECORIN-3A	precorrin-3A
PRECORIN-3B	precorrin-3B
PRECORIN-4B	precorrin-4B
PRECORIN-5	precorrin-5
PRECORIN-6X	precorrin-6x
PRECORIN-6Y	precorrin-6y
PRECORIN-8X	precorrin-8x
PRECURSOR-Z	precursor-Z
PRFICA	phosphoribosyl-formamido-carboxamide
PRFP	phosphoribosylformiminoAICAR-phosphate
PRLP	phosphoribulosylformimino-AICAR-P
PRO	proline
PROPANOATE	propanoate

PROPIONYLACP	propionyl-ACP
PROPIONYLCOA	propionyl-CoA
PROPIONYLP	propionyl-P
PROTEIN	average_mycobacterial_protein
PROTOHEME-FE2	protoheme
PROTOPORPHYRIN-IX	protoporphyrin_IX
PROTOPORPHYRINOGEN	protoporphyrinogen_IX
PRPP	5-phosphoribosyl_1-pyrophosphate
PS	phosphatidylserine
PTC	phthiocerol
PTHIOCERANOYL-COA	phthioceranoyl-COA
PTRSC	putrescine
PTT	PTT
PURI5P	pseudouridine_5'-phosphate
PYR	pyruvate
QA	quinolinate
R1P	ribose-1-phosphate
R5P	D-ribose-5-phosphate
RHAMNAGDPP	Rha-GlcNAc-DPP
RHYDROXYBUTANOYL	(R)-3-Hydroxybutanoyl
RIB	Ribose
RIBFLAV	riboflavin
RL5P	D-ribulose-5-phosphate
RMMALONYLACP	(R)-methylmalonyl-ACP
RMMALONYLCOA	(R)-methylmalonyl-CoA
RNA	ribonucleic_acid
RTHIO	reduced_thioredoxin
S7P	D-sedoheptulose-7-phosphate
SAH	S-adenosyl-L-homocysteine
SAICAR	5'-phosphoribosyl-4-(N-succinocarboxamide)-5-aminoimidazole
SAL	salicylate
SAM	S-adenosyl-L-methionine
SAM-2-OXOBUTANOATE	S-adenosyl-4-methylthio-2-oxobutanoate
SAOPIM	N-succinyl-2-amino-6-ketopimelate
SAP	H-protein-S-(aminomethyldihydrolipoyl)lysine
SDAPIM	N-succinyl-L,L-2,6-diaminopimelate
SER	serine

SHCHC	2-succinyl-6-hydroxy-2,4-cyclohexadiene-1-carboxylate
SHYDROXYBUTANOYL	SHYDROXYBUTANOYL
SL-1	sulfolipid-1
SL1278-CYTO	cyptoplasmic_SL1278_(SL-1_precursor)
SL1278-WALL	wallbound_SL1278_(SL-1_precursor)
SLF	sulfate
SLFxt	external_sulfate
SMALLMOLECULES	small_molecules
SME	shikimate
SME3P	shikimate-3-phosphate
SMMALONYLCOA	(S)-methyl-malonyl-CoA
SPRMD	spermidine
SUC	sucrose
SUCC	succinate
SUCCOA	succinyl-CoA
SUCCSAL	succinate_semialdehyde_(succinic_semialdehyde)
SUGARS	sugars
T3	D-glyceraldehyde-3-phosphate
TAG	triacylglycerol
TETRACOSANOATE	tetracosanoate
TETRACOSANOYL-ACP	tetracosanoyl-ACP
TETRACOSANOYL-COA	tetracosanoyl-CoA
TETRADECANOATE	tetradecanoate_
TETRADECANOYL-ACP	tetradecanoyl-ACP
TETRADECANOYL-COA	tetradecanoyl-CoA
TETRAHYDRODIPICOLINATE	tetrahydrodipicolinate
THF	tetrahydrofolate
THFG	THF-L-glutamate
THI	thiamine
THIP	thiamine-phosphate
THPTGLU	tetrahydropteroyltri-L-glutamate
THR	threonine
THY	THY
TRANS-DELTA-2-DODECANOYL-COA	TRANS-DELTA-2-DODECANOYL-COA
TRANS-DELTA-2-ENOYL-C22-ACYL-AC	TRANS-DELTA-2-ENOYL-C22-ACYL-ACP
TRANS-DELTA-2-HYDROXY-DODECAN	TRANS-DELTA-2-HYDROXY-DODECANOYL-COA
TRANS-KETO-MEROACYL-ACP	TRANS-KETO-MEROACYL-ACP
TRANS-METHOXY-MEROACYL-ACP	TRANS-METHOXY-MEROACYL-ACP

TRE	trehalose
TRE6P	trehalose_6-phosphate
TREHALOSEDIMYCOLATE	trehalosedimycolate_(TDM)
TREHALOSEMONOMYCOLATE	trehalosemonomycolate_(TMM)
TREHALOSEMONOMYCOLATEbrCYbr	cytoplasmic_trehalosemonomycolate_(TMM)
TREHALOSEMONOMYCOLATE-P	cytoplasmic_trehalosemonomycolate-P
TRE-S	sulfated_trehalose
TRIDECANOYL-COA	tridecanoyl-CoA
TRNA-GLU	tRNAGlu
TRP	tryptophan
TS-COSH-TYR	L-tyrosine/ThiS-COSH_complex
TS-PROTEIN	ThiS_protein/C1of_Tyrosine,_4hydroxybenzyl_alcohol_complex
TUBERCULOSTEROYL-ACP	Tuberculostearic
TYR	tyrosine
UDP	uridine-diphosphate
UDPbrNAM:NGMbrAGMDAPIM	UDP[NAM:NGM]AGMDAPIM
UDPbrNAM:NGMbrAGMDAPIMAA	UDP[NAM:NGM]AGMDAPIMAA
UDPbrNAM:NGMbrALA	UDP[NAM:NGM]ALA
UDPbrNAM:NGMbrALAGLU	UDP[NAM:NGM]ALAGLU
UDPDGLUC	UDPDGLUC
UDPG	UDP-D-glucose
UDPGAL	UDP-galactose
UDPGALF	UDP-D-galacto-1,4-furanose
UDPNACVG	UDP-N-acetyl-3-O-(1-carboxyvinyl)-D-glucosamine)
UDPNAG	UDP-N-acetyl-D-glucosamine
UDPNAGPEE	UDP-GlcNAc-pyruvate_enol_ether
UDPNAM	UDP-N-acetylmuramate
UDPNGM	UDPNGM
UMP	uridine-monophosphate
UNDECANOYL-COA	undecanoyl-CoA
URA	uracil
UREA	urea
UROPORPHYRINOGEN-III	uroporphyrinogen-III
UTP	uridine-triphosphate
VAL	valine
X5P	D-xylulose-5-phosphate
XAN	xanthine

XMP	xanthosine-5-phosphate
XTSINE	xanthosine

List of Reactions

ID	Formula	Lower bound	Upper bound	Genes
R1	GL + ATP = ADP + GL3P	0.0	100000.0	Rv3696c
R2	GL + NADP = T3 + NADPH	-100000.0	100000.0	Rv2982c OR Rv0564 OR Rv3045
R3	GL + NAD = T3 + NADH	-100000.0	100000.0	Rv0162c
R4	GL3P + MK = DHAP + MKH2	0.0	100000.0	Rv3302c OR Rv2249c
R5	T3 + NAD = DGLYCERATE + NADH	0.0	100000.0	Rv2858c OR Rv0458
R6	DGLYCERATE + ATP = 3PG + ADP	0.0	100000.0	Rv2205c
R7	RIB + ATP = ADP + R5P	0.0	100000.0	Rv2436
R8	F1P = DHAP + T3	0.0	100000.0	Rv0363c
R9	FRU = GLC	-100000.0	100000.0	orphan
R10	FRU = MAN	-100000.0	100000.0	orphan
R11	MAN6P = F6P	-100000.0	100000.0	Rv3255c
R12	MAN1P = MAN6P	-100000.0	100000.0	Rv3257c OR Rv3308
R13	MAN1P + GTP = GDPMAN + PI	0.0	100000.0	Rv3264c
R14	GDPMAN + DPP = GDP + PPM	0.0	100000.0	Rv2051c
R15	GDPMAN = GDPDHDOMAN	0.0	100000.0	Rv0112 OR Rv1511
R16	GDPDHDOMAN = GDPDHDOGAL	0.0	100000.0	Rv1512
R17	GDPDHDOGAL + NADPH = GDPFUC + NADP	0.0	100000.0	Rv1512
R18	GLAC + ATP = GAL1P + ADP	0.0	100000.0	Rv0620
R19	GAL1P + UTP = UDPGAL + PPI	0.0	100000.0	Rv0619 OR Rv0618
R20	UDPG = UDPGAL	-100000.0	100000.0	Rv3634c OR Rv0501 OR Rv0536
R21	G1P + UTP = UDPG + PPI	0.0	100000.0	Rv0993
R22	bDG6P = IP	-100000.0	100000.0	Rv0046c OR (Rv2612c AND Rv1822)
R23	IP = PI + MI	0.0	100000.0	Rv2701c
R24	MLT = GLC	0.0	100000.0	Rv2471
R25	SUC = GLC + FRU	0.0	100000.0	Rv2471
R26	CELB = bDGLC	0.0	100000.0	Rv0186
R27	G6P + UDPG = TRE6P +	0.0	100000.0	Rv3490

	UDP			
R28	MLT + PI = bDG1P + bDGLC	0.0	100000.0	Rv3401
R29	bDG1P = bDG6P	-100000.0	100000.0	Rv3400
R30	MLT = TRE	-100000.0	100000.0	orphan
R31	TRE6P = PI + TRE	0.0	100000.0	Rv3372
R32	FOR + NAD = NADH + CO2	0.0	100000.0	Rv2900c
R33	GLC + ATP = G6P + ADP	0.0	100000.0	Rv0650
R34	bDGLC + ATP = bDG6P + ADP	0.0	100000.0	Rv0650
R35	GLC + (n)POLYP = G6P + (n-1)POLYP	0.0	100000.0	Rv2702
R36	bDGLC + (n)POLYP = bDG6P + (n-1)POLYP	0.0	100000.0	Rv2702
R37	G6P = bDG6P	-100000.0	100000.0	Rv0946c
R38	G6P = G1P	-100000.0	100000.0	Rv3068c
R39	bDG6P = F6P	-100000.0	100000.0	Rv0946c
R40	G6P = F6P	-100000.0	100000.0	Rv0946c
R41	F6P + ATP = FDP + ADP	0.0	100000.0	Rv3010c OR Rv2029c
R42	F6P + ATP = FDP + ADP	0.0	100000.0	Rv2029c
R43	FDP = F6P + PI	0.0	100000.0	Rv1099c
R44	FDP = DHAP + G3P	-100000.0	100000.0	Rv0363c
R45	DHAP = G3P	-100000.0	100000.0	Rv1438
R46	G3P + NAD + PI = 13PDG + NADH	-100000.0	100000.0	Rv1436
R48	13PDG + ADP = 3PG + ATP	-100000.0	100000.0	Rv1437
R49	3PG = 2PG	-100000.0	100000.0	Rv3214 OR Rv0489
R50	2PG = PEP	-100000.0	100000.0	Rv1023
R51	PEP + ADP = ATP + PYR	0.0	100000.0	Rv1617
R52	LIPO + PYR + THI = ADLIPO + CO2	0.0	100000.0	Rv2241
R53	ADLIPO + COA = ACCOA + DLIPO	-100000.0	100000.0	Rv2215
R54	NAD + DLIPO = LIPO + NADH	-100000.0	100000.0	Rv0462
R55	OA + ACCOA = CIT + COA	0.0	100000.0	Rv0896 OR Rv0889c OR Rv1131
R56	CIT = CISACONITATE	-100000.0	100000.0	Rv1475c
R57	CISACONITATE = ICIT	-100000.0	100000.0	Rv1475c
R58	ICIT + NADP = AKG + NADPH + CO2	0.0	100000.0	Rv3339c OR Rv0066c

R61	AKG = SUCCSAL + CO2	0.0	100000.0	Rv1248c OR Rv0555
R63	SUCCOA + ADP + PI = SUCC + COA + ATP	-100000.0	100000.0	Rv0952 AND Rv0951
R64	FUM = MAL	-100000.0	100000.0	Rv1098c
R65	MAL + NAD = OA + NADH	-100000.0	100000.0	Rv1240
R66	CIT = OA + AC	0.0	100000.0	Rv3075c
R67	AC + COA + ATP = ACCOA + AMP + PPI	0.0	100000.0	Rv3667
R68	ACAL + NAD = AC + NADH	0.0	100000.0	Rv0458
R69	PYR + ATP + PI = PEP + AMP + PPI	0.0	100000.0	Rv1127c
R70	LAC + NAD = PYR + NADH	-100000.0	100000.0	Rv0728c
R71	LLAC + NAD = PYR + NADH	-100000.0	100000.0	Rv1872c OR Rv0694
R72	MAL + NAD = PYR + NADH + CO2	0.0	100000.0	Rv2332
R73	ACAL + NADH = ETH + NAD	-100000.0	100000.0	Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c
R74	ACAL + NADPH = ETH + NADP	-100000.0	100000.0	Rv3045
R75	AC + ATP = ACETYLP + ADP	0.0	100000.0	Rv0409
R76	COA + ACETYLP = ACCOA + PI	-100000.0	100000.0	Rv0408
R77	ACETYLP = AC + PI	0.0	100000.0	Rv2922A
R78	PROPIONYLP + COA = PROPIONYLCOA + PI	-100000.0	100000.0	Rv0408
R79	PROPANOATE + ATP = PROPIONYLP + ADP	0.0	100000.0	Rv0409
R80	SMMALONYLCOA = PROPIONYLCOA + CO2	0.0	100000.0	Rv0974c OR Rv3280
R81	PROPANOATE + COA + ATP = PROPIONYLCOA + AMP + PPI	0.0	100000.0	Rv3667
R82	PROPIONYLCOA + OA = 2METHYLCITRATE + COA	0.0	100000.0	Rv1131
R83	2METHYLCITRATE = 2METHYLCISACONITATE	0.0	100000.0	Rv1130
R84	2METHYLCISACONITATE = METHYLISOCITRATE	0.0	100000.0	Rv1475c
R85	METHYLISOCITRATE =	0.0	100000.0	Rv0467 OR (Rv1915 AND Rv1916)

	SUCC + PYR			
R86	PROPIONYLCOA + MK = ACRCOA + MKH2	0.0	100000.0	Rv3140
R87	G6P + NADP + F420 = D6PGL + NADPH	0.0	100000.0	Rv1447c OR Rv1121
R88	D6PGL = D6PGC	0.0	100000.0	Rv1445c
R89	D6PGC + NADP = RL5P + NADPH + CO2	0.0	100000.0	Rv1122 OR Rv1844c
R90	RL5P = X5P	-100000.0	100000.0	Rv1408
R91	RL5P = R5P	-100000.0	100000.0	Rv2465c
R92	R1P = R5P	-100000.0	100000.0	Rv3068c
R93	X5P + R5P + THI = G3P + S7P	0.0	100000.0	Rv1449c
R94	G3P + S7P + THI = X5P + R5P	0.0	100000.0	Rv1449c
R95	X5P + E4P + THI = G3P + F6P	0.0	100000.0	Rv1449c
R96	G3P + F6P + THI = X5P + E4P	0.0	100000.0	Rv1449c
R97	G3P + S7P = E4P + F6P	-100000.0	100000.0	Rv1448c
R98	RIB + ATP = DR5P + ADP	0.0	100000.0	Rv2436
R99	DR5P = ACAL + G3P	0.0	100000.0	Rv0478
R100	PYR + BIOTIN-CO2 = OA + BIOTIN	0.0	100000.0	Rv2967c
R101	GDP + PEP + CO2 = OA + GTP	-100000.0	100000.0	Rv0211
R102	ICIT = GLX + SUCC	0.0	100000.0	Rv0467 OR (Rv1915 AND Rv1916)
R103	GLX + ACCOA = MAL + COA	0.0	100000.0	Rv1837c
R104	GLAL + NAD = GLYCOLATE + NADH	0.0	100000.0	orphan
R105	GLYCOLATE + O2 = GLX + H2O2	0.0	100000.0	Rv1257c
R106	NADP + METTHF = METHF + NADPH	-100000.0	100000.0	Rv3356c
R107	METHF = FTHF	-100000.0	100000.0	Rv3356c
R108	FADH2 + METTHF = MTHF + FAD	0.0	100000.0	orphan
R109	SLF + ATP = APS + PPI	0.0	100000.0	Rv1285
R110	APS + ATP = PAPS + ADP	0.0	100000.0	Rv1286
R111	APS + RTHIO = AMP +	0.0	100000.0	Rv2392

	H2SO3 + OTHIO			
R112	H2SO3 + FERO = FERI + H2S	-100000.0	100000.0	Rv2391
R113	PAP = AMP + PI	0.0	100000.0	orphan
R114	MKH2 + NO3 + MOLYBDENUM = MK + NO2 + H	0.0	100000.0	(Rv1161 AND Rv1162 AND Rv1164 AND Rv1163) OR Rv1736c
R119	MK + NADH = MKH2 + NAD + H	0.0	100000.0	Rv3145 AND Rv3146 AND Rv3147 AND Rv3148 AND Rv3149 AND Rv3150 AND Rv3151 AND Rv3152 AND Rv3153 AND Rv3154 AND Rv3155 AND Rv3156 AND Rv3157 AND Rv3158
R120	MK + NADH = MKH2 + NAD	0.0	100000.0	Rv1854c OR Rv0392c
R121	MK + NADPH = MKH2 + NADP	0.0	100000.0	Rv3303c
R122	MK + SUCC = MKH2 + FUM	-100000.0	100000.0	Rv3318 AND Rv3319 AND Rv3316 AND Rv3317
R123	FAD + SUCC = FADH2 + FUM	-100000.0	100000.0	(Rv3318 AND Rv3319 AND Rv3316 AND Rv3317) OR (Rv1552 AND Rv1553 AND Rv1554 AND Rv1555)
R124	FE3 + NADPH = FE2 + NADP	-100000.0	100000.0	Rv3106
R125	MKH2 + HEME-FE3 = MK + HEME-FE2	-100000.0	100000.0	(Rv2194 AND Rv2195 AND Rv2196 AND Rv2196 AND Rv1451 AND Rv1456c AND Rv3029c AND Rv3028c AND Rv2200c AND Rv3043c AND Rv2193 AND Rv3043c AND Rv1623c AND Rv1622c) OR (Rv1623c AND Rv1622c)
R126	HEME-FE2 + O2 = HEME-FE3 + H	0.0	100000.0	(Rv2194 AND Rv2195 AND Rv2196 AND Rv2196 AND Rv1451 AND Rv1456c AND Rv3029c AND Rv3028c AND Rv2200c AND Rv3043c AND Rv2193 AND Rv3043c) AND (Rv1623c AND Rv1622c)
R127	HEME-FE2 + O2 = HEME-FE3 + H	0.0	100000.0	Rv1623c AND Rv1622c
R128	ADP + PI + H = ATP	-10000000.0	10000000.0	Rv1308 AND Rv1304 AND Rv1311 AND Rv1310 AND Rv1305 AND Rv1306 AND Rv1309 AND Rv1307
R129	ATP = ADP + PI	1.0	1.0001	Rv1811
R130	PPI = PI	0.0	100000.0	Rv3628
R131	PPI = PI + H	0.0	100000.0	Rv3628
R132	(n-1)POLYP + ATP = (n)POLYP + ADP	-100000.0	100000.0	Rv2984
R133	NADP + FERO = FERI + NADPH	-100000.0	100000.0	Rv3106 OR Rv0886

R134	H2O2 = O2	0.0	100000.0	Rv1908c
R135	GLU = GABA + CO2	0.0	100000.0	Rv3432c
R136	GABA + AKG = SUCCSAL + GLU	-100000.0	100000.0	Rv2589
R137	SUCCSAL + NADP = SUCC + NADPH	0.0	100000.0	Rv0234c OR Rv1731
R138	PRO + FAD = P5C + FADH2	0.0	100000.0	Rv1188
R139	P5C + NAD = HYDROXYGLU + NADH	0.0	100000.0	Rv1187
R140	HYDROXYGLU + AKG = HYDROXYAKG + GLU	0.0	100000.0	orphan
R141	HYDROXYAKG = GLX + PYR	-100000.0	100000.0	Rv1223
R142	P5C + NAD = GLU + NADH	0.0	100000.0	Rv1187
R143	ARG = NH3 + CITR	0.0	100000.0	Rv1001
R144	ORN + AKG = GLUGSAL + GLU	0.0	100000.0	Rv2321c OR Rv2322c
R145	CAP + ORN = PI + CITR	0.0	100000.0	Rv1656
R146	ORN = PTRSC + CO2	0.0	100000.0	Rv2531c
R147	SAM + PTRSC = 5MTA + SPRMD	0.0	100000.0	Rv2601
R148	UREA = NH3 + CO2	0.0	100000.0	Rv1850 AND Rv1849 AND Rv1848 AND Rv1853 AND Rv1851 AND Rv1852
R149	ILE + AKG = GLU + OMVAL	-100000.0	100000.0	Rv2210c
R150	LIPO + OXOMETHYLPENTANOATE = 2MBUTLIPO + CO2	0.0	100000.0	Rv2497c AND Rv2496c
R151	2MBUTLIPO + COA = 2MBUTCOA + DLIPO	-100000.0	100000.0	Rv2495c
R152	MK + 2MBUTCOA = MKH2 + 2MBECOA	0.0	100000.0	Rv3140
R153	2MBECOA = HMBUTCOA	0.0	100000.0	Rv1070c OR Rv0905 OR Rv2486 OR Rv1472
R154	HMBUTCOA + NAD = MAACCOA + NADH	0.0	100000.0	Rv3774 OR Rv1144
R155	COA + MAACCOA = PROPIONYLCOA + ACCOA	-100000.0	100000.0	Rv1074c
R156	PROPIONYLCOA + BIOTIN-CO2 = SMMALONYLCOA + BIOTIN	0.0	100000.0	Rv0904c OR Rv2502c OR Rv0974c OR Rv0904c OR Rv3799c OR Rv3280 OR Rv2247
R157	SMMALONYLCOA =	-100000.0	100000.0	orphan

	RMMALONYLCOA			
R158	RMMALONYLCOA + COB-III = SUCCOA	0.0	100000.0	Rv1492 AND Rv1493
R159	SUCCOA + COB-III = RMMALONYLCOA	0.0	100000.0	Rv1492 AND Rv1493
R160	MOP + LIPO = 3MBUTLIPO + CO2	0.0	100000.0	Rv2496c AND Rv2497c
R161	3MBUTLIPO + COA = 3MBUTCOA + DLIPO	-100000.0	100000.0	Rv2495c
R162	MK + 3MBUTCOA = MKH2 + 3MBECOA	0.0	100000.0	Rv3140
R163	3MBECOA + BIOTIN-CO2 = MGLUTCOA + BIOTIN	0.0	100000.0	Rv0904c OR Rv2502c OR Rv0974c OR Rv0904c OR Rv3799c OR Rv3280 OR Rv2247
R164	MGLUTCOA = HMGLUTCOA	0.0	100000.0	orphan
R165	HMGLUTCOA = ACCOA + ACTAC	0.0	100000.0	orphan
R166	ACTAC + COA + ATP = AMP + AACCOA + PPI	0.0	100000.0	orphan
R167	SUCCOA + ACTAC = SUCC + AACCOA	-100000.0	100000.0	Rv2504c AND Rv2503c
R168	LIPO + OMVAL = IBUTLIPO + CO2	0.0	100000.0	Rv2497c AND Rv2496c
R169	IBUTLIPO + COA = DLIPO + IBUTCOA	-100000.0	100000.0	Rv2495c
R170	MK + IBUTCOA = MKH2 + MACRCOA	0.0	100000.0	Rv3140
R171	MACRCOA = HIBUTCOA	0.0	100000.0	Rv1070c OR Rv0905 OR Rv2486 OR Rv1472
R172	HIBUTCOA = HIBUT + COA	0.0	100000.0	orphan
R173	HIBUT + NAD = METHYMALONATE + NADH	0.0	100000.0	Rv1144 OR Rv0751c
R174	METHYMALONATE + NAD + COA = PROPIONYLCOA + NADH + CO2	0.0	100000.0	Rv0753c
R175	ISUCC = OA + NH3	0.0	100000.0	orphan
R176	ASP = bALA + CO2	0.0	100000.0	Rv3601c
R177	ASN = ASP + NH3	0.0	100000.0	Rv1538c
R178	THR + NAD = 2A3KB + NADH	0.0	100000.0	Rv2259

R179	2A3KB = AMINOACETONE + CO2	0.0	100000.0	orphan
R180	AMINOACETONE + NADH = 1-AMINO-PROPAN-2-OL + NAD	0.0	100000.0	orphan
R181	OBUT + NH3 + CYS = LLCT	0.0	100000.0	Rv1079
R182	LYS = CADA + CO2	0.0	100000.0	Rv2531c
R183	PI + OBUT + O2 = PROPIONYLP + CO2	0.0	100000.0	orphan
R184	SAP + THF = NH3 + METTHF + DHLIPOYLPROTEIN	0.0	100000.0	Rv2211c
R185	SER + THF = METTHF + GLY	-100000.0	100000.0	Rv1093 OR Rv0070c
R186	GLY + LIPOYLPROTEIN = SAP + CO2	0.0	100000.0	Rv1832
R187	NAD + DHLIPOYLPROTEIN = NADH + LIPOYLPROTEIN	-100000.0	100000.0	Rv0462 OR Rv3303c
R188	SER = NH3 + PYR	0.0	100000.0	Rv0069c
R189	CYS = NH3 + PYR + H2S	0.0	100000.0	Rv1464
R190	TYR + AKG = 4HPP + GLU	-100000.0	100000.0	Rv3565 OR Rv0337c
R191	4HPP + O2 = HOMOGEN + CO2	0.0	100000.0	MT1364
R192	HOMOGEN + O2 = MACAC	0.0	100000.0	orphan
R193	MACAC = FUACAC	-100000.0	100000.0	orphan
R194	FUACAC = FUM + ACTAC	0.0	100000.0	orphan
R195	AKG + PHE = PHPYR + GLU	-100000.0	100000.0	Rv3565 OR Rv0337c
R196	GLU + NH3 + ATP = GLN + ADP + PI	0.0	100000.0	Rv2220 OR Rv1878 OR Rv2860c
R197	GLN + AKG + NADH = GLU + NAD	-100000.0	100000.0	Rv3859c AND Rv3858c
R198	NH3 + AKG + NADPH = GLU + NADP	-100000.0	100000.0	Rv2476c
R199	GLU + ATP = GLUP + ADP	0.0	100000.0	Rv2439c
R200	NADPH + GLUP = GLUGSAL + NADP + PI	0.0	100000.0	Rv2427c
R201	GLUGSAL = P5C	-100000.0	100000.0	orphan
R202	P5C + NADPH + NADH = PRO + NADP + NAD	-100000.0	100000.0	Rv0500
R203	GLU + ACCOA = NAGLU +	-100000.0	100000.0	Rv2747

	COA			
R204	NAGLU + ATP = NAGLUP + ADP	0.0	100000.0	Rv1654
R205	NADPH + NAGLUP = NAGLUS + NADP + PI	0.0	100000.0	Rv1652
R206	NAGLUS + GLU = NAORN + AKG	0.0	100000.0	Rv1655
R207	NAORN + GLU = NAGLU + ORN	-100000.0	100000.0	Rv1653
R208	GLN + ATP + CO2 = CAP + GLU + ADP + PI	0.0	100000.0	Rv1383 AND Rv1384
R209	ASP + CITR + ATP = AMP + ARGSUCC + PPI	0.0	100000.0	Rv1658
R210	ARGSUCC = ARG + FUM	0.0	100000.0	Rv1659
R211	PYR + THI = ACLAC + CO2	0.0	100000.0	Rv3002c AND Rv3003c
R212	ACLAC + NADPH = DHMVA + NADP	0.0	100000.0	Rv3001c
R213	DHMVA = OMVAL	0.0	100000.0	Rv0189c
R214	GLU + OMVAL = VAL + AKG	-100000.0	100000.0	Rv2210c
R215	THR = OBUT + NH3	0.0	100000.0	Rv1559
R216	PYR + OBUT = ABUT + CO2	0.0	100000.0	Rv3509c OR Rv1820 OR Rv3003c OR (Rv3470c AND Rv3002c)
R217	ABUT + NADPH = DIHYDROXYMETHYLPENTANOATE + NADP	0.0	100000.0	Rv3001c
R218	DIHYDROXYMETHYLPENTANOATE = OXOMETHYLPENTANOATE	0.0	100000.0	Rv0189c
R219	GLU + OXOMETHYLPENTANOATE = ILE + AKG	-100000.0	100000.0	Rv2210c
R220	OMVAL + ACCOA = IPPMAL + COA	0.0	100000.0	Rv3710
R221	IPPMAL = CBHCAP	-100000.0	100000.0	Rv2988c AND Rv2987c
R222	CBHCAP + NAD = OICAP + NADH	0.0	100000.0	Rv2995c
R223	OICAP = MOP + CO2	0.0	100000.0	orphan
R224	MOP + GLU = LEU + AKG	-100000.0	100000.0	Rv2210c
R225	OA + GLU = ASP + AKG	-100000.0	100000.0	Rv3565 OR Rv0337c
R226	ASP + GLN + ATP = GLU +	0.0	100000.0	Rv2201

	ASN + AMP + PPI			
R227	ASP + ATP = ASP4P + ADP	0.0	100000.0	Rv3709c
R228	ASP4P + NADPH = ASPSA + NADP + PI	0.0	100000.0	Rv3708c
R229	ASPSA + NADPH = HSER + NADP	0.0	100000.0	Rv1294
R230	HSER + ATP = PHSER + ADP	0.0	100000.0	Rv1296
R231	PHSER = THR + PI	0.0	100000.0	Rv1295
R232	PYR + ASPSA = DIHYDRODIPICOLINATE	0.0	100000.0	Rv2753c
R233	DIHYDRODIPICOLINATE + NADPH + NADH = TETRAHYDRODIPICOLINATE + NADP + NAD	0.0	100000.0	Rv2773c
R234	TETRAHYDRODIPICOLINATE + SUCCOA = SAOPIM + COA	0.0	100000.0	Rv1201c
R235	SAOPIM + GLU = SDAPIM + AKG	-100000.0	100000.0	Rv1655 OR Rv0858c
R236	SDAPIM = SUCC + DAPIM	0.0	100000.0	Rv1202
R237	DAPIM = MDAPIM	-100000.0	100000.0	Rv2726c
R238	MDAPIM = LYS + CO2	0.0	100000.0	Rv1293
R239	SUCCOA + HSER = OSLHSER + COA	-100000.0	100000.0	orphan
R240	CYS + OSLHSER = SUCC + LLCT	0.0	100000.0	Rv1079
R241	LLCT = HCYS + PYR + NH3	0.0	100000.0	MT3443
R242	SAM + HCYS = SAH + MET	0.0	100000.0	Rv2458
R243	MTHF + HCYS + COB-I = MET + THF + COB-II	0.0	100000.0	Rv2124c
R244	MET + THF + COB-I = MTHF + HCYS + COB-II	0.0	100000.0	Rv2124c
R245	MTHF + HCYS = MET + THF	-100000.0	100000.0	Rv1133c
R246	PYR + NADH + NH3 = ALA + NAD	-100000.0	100000.0	Rv2780
R247	3PG + NAD = PHP + NADH	0.0	100000.0	Rv2996c
R248	GLU + PHP = 3PSER + AKG	-100000.0	100000.0	Rv0884c
R249	3PSER = SER + PI	0.0	100000.0	Rv3042c
R250	SER + ACCOA = ASER + COA	-100000.0	100000.0	Rv2335

R251	H2S + ASER = CYS + AC	0.0	100000.0	Rv2334 OR Rv1336
R252	ACCOA + HSER = OAHSER + COA	-100000.0	100000.0	Rv3341
R253	OAHSER + CYS = AC + LLCT	0.0	100000.0	Rv1079
R254	OAHSER + H2S = AC + HCYS	0.0	100000.0	Rv1079
R255	OSLHSER + H2S = SUCC + HCYS	0.0	100000.0	Rv1079
R256	OSLHSER = SUCC + OBUT + NH3	0.0	100000.0	Rv1079
R257	SER + HCYS = LLCT	0.0	100000.0	Rv1077
R258	LLCT = OBUT + NH3 + CYS	0.0	100000.0	Rv1079
R259	MET + ATP = SAM + PPI + PI	0.0	100000.0	Rv1392
R260	SAH = ADN + HCYS	0.0	100000.0	Rv3248c
R261	PRPP + ATP = PRBATP + PPI	0.0	100000.0	Rv2121c
R262	PRBATP = PRBAMP + PPI	0.0	100000.0	Rv2122c
R263	PRBAMP = PRFP	0.0	100000.0	Rv1606
R264	PRFP = PRLP	0.0	100000.0	Rv1603
R265	GLN + PRLP = GLU + DIMGP + AICAR	0.0	100000.0	Rv1602
R266	DIMGP = IMACP	0.0	100000.0	Rv1601
R267	IMACP + GLU = HISOLP + AKG	-100000.0	100000.0	Rv3772 OR Rv1600
R268	HISOLP = HISOL + PI	0.0	100000.0	Rv1601
R269	HISOL + NAD = HIS + NADH	0.0	100000.0	Rv1599
R270	PEP + E4P = 3DDAH7P + PI	0.0	100000.0	Rv2178c
R271	3DDAH7P = DQT + PI	0.0	100000.0	Rv2538c
R272	DQT = DHSK	0.0	100000.0	Rv2537c
R273	NADPH + DHSK = SME + NADP	0.0	100000.0	Rv2552c
R274	SME + ATP = SME3P + ADP	0.0	100000.0	Rv2539c
R275	PEP + SME3P = 3PSME + PI	0.0	100000.0	Rv3227
R276	3PSME = CHOR + PI	0.0	100000.0	Rv2540c
R277	CHOR + GLN = AN + GLU + PYR	0.0	100000.0	Rv1609
R278	AN + PRPP = NPRAN + PPI	0.0	100000.0	Rv2192c
R279	NPRAN = CPAD5P	0.0	100000.0	Rv1603

R280	CPAD5P = IGP + CO2	0.0	100000.0	Rv1611
R281	SER + IGP = TRP + G3P	0.0	100000.0	Rv1613 AND Rv1612
R282	CHOR = PHEN	-100000.0	100000.0	Rv1885c OR Rv0948c
R283	PHEN = PHPYR + CO2	0.0	100000.0	Rv3838c
R284	PHPYR + GLU = AKG + PHE	-100000.0	100000.0	Rv3565 OR Rv0337c
R285	PHEN + NAD = 4HPP + NADH + CO2	0.0	100000.0	Rv3754
R286	4HPP + GLU = TYR + AKG	-100000.0	100000.0	Rv3565 OR Rv0337c
R287	R5P + ATP = PRPP + AMP	-100000.0	100000.0	Rv1017c
R288	ASP + CAP = CAASP + PI	0.0	100000.0	Rv1380
R289	CAASP = DOROA	-100000.0	100000.0	Rv1381
R290	O2 + DOROA = OROA + H2O2	0.0	100000.0	Rv2139
R291	OROA + PRPP = OMP + PPI	0.0	100000.0	Rv0382c
R292	OMP = UMP + CO2	0.0	100000.0	Rv1385
R293	UMP + ATP = UDP + ADP	-100000.0	100000.0	Rv1712
R294	UDP + ATP = ADP + UTP	-100000.0	100000.0	Rv2445c
R295	GLN + UTP + ATP = GLU + ADP + CTP + PI	0.0	100000.0	Rv1699
R296	NH3 + UTP + ATP = CTP + ADP + PI	0.0	100000.0	Rv1699
R297	RTHIO + CDP + O2 = OTHIO + DCDP	0.0	100000.0	Rv3051c AND Rv3048c
R299	DCDP + ATP = DCTP + ADP	0.0	100000.0	Rv2445c
R300	DCTP = DUTP + NH3	0.0	100000.0	Rv0321
R301	DUTP = DUMP + PPI	0.0	100000.0	Rv2697c
R302	DUMP + FADH2 + METTHF = DTMP + THF + FAD	-100000.0	100000.0	Rv2754c
R303	DUMP + METTHF = DTMP + DHF	-100000.0	100000.0	Rv2764c
R304	DTMP + ATP = DTDP + ADP	-100000.0	100000.0	Rv3247c
R305	DTDP + ATP = DTTP + ADP	-100000.0	100000.0	Rv2445c
R306	CDP + ATP = CTP + ADP	-100000.0	100000.0	Rv2445c
R307	CMP + ATP = ADP + CDP	-100000.0	100000.0	Rv1712
R308	DCTP = DCMP + PPI	0.0	100000.0	orphan
R309	DCMP + ATP = DCDP + ADP	-100000.0	100000.0	Rv1712

R310	OTHIO + NADPH = RTHIO + NAD	0.0	100000.0	Rv3913
R311	UMP + PPI = URA + PRPP	0.0	100000.0	Rv3309c
R312	URA + PRPP = UMP + PPI	0.0	100000.0	Rv3309c
R313	GLN + PRPP = GLU + PRAM + PPI	0.0	100000.0	Rv0808
R314	ATP + GLY + PRAM = GAR + ADP + PI	0.0	100000.0	Rv0772
R315	FTHF + GAR = FGAR + THF	0.0	100000.0	Rv0956
R316	FGAR + GLN + ATP = GLU + FGAM + ADP + PI	0.0	100000.0	Rv0803
R317	FGAM + ATP = AIR + ADP + PI	0.0	100000.0	Rv0809
R318	AIR + HCO3 + ATP = CAIR + ADP + PI	0.0	100000.0	Rv3276c
R319	CAIR + ASP + ATP = SAICAR + ADP + PI	0.0	100000.0	Rv0780
R320	SAICAR = FUM + AICAR	-100000.0	100000.0	Rv0777
R321	FTHF + AICAR = PRFICA + THF	-100000.0	100000.0	Rv0957
R322	PRFICA = IMP	-100000.0	100000.0	Rv0957
R323	ATP = cAMP + PPI	0.0	100000.0	Rv1625c
R324	GTP = cGMP + PPI	0.0	100000.0	Rv2435c
R325	cAMP = AMP	0.0	100000.0	orphan
R326	cGMP = GMP	0.0	100000.0	orphan
R327	DGMP + ATP = ADP + DGDP	-100000.0	100000.0	Rv1389
R328	GMP + DATP = GDP + DADP	-100000.0	100000.0	Rv1389
R329	DUDP + ATP = ADP + DUTP	-100000.0	100000.0	Rv2445c
R330	RTHIO + UDP + O2 = DUDP + OTHIO	0.0	100000.0	Rv3051c AND Rv3048c
R332	5MTA + PI = AD + MTR1P	0.0	100000.0	Rv0535
R333	AD + PRPP = AMP + PPI	0.0	100000.0	Rv2584c
R334	GN + PRPP = GMP + PPI	0.0	100000.0	Rv3624c
R335	HYXN + PRPP = IMP + PPI	0.0	100000.0	Rv3624c
R336	XAN + PRPP = XMP + PPI	0.0	100000.0	orphan
R337	DIN + PI = HYXN + DR1P	-100000.0	100000.0	Rv3307
R338	DA + PI = AD + DR1P	-100000.0	100000.0	Rv3307
R338	DR1P = R5P	-100000.0	100000.0	Rv3068c

b				
R339	HYXN + R1P = INS + PI	-100000.0	100000.0	Rv3307
R340	AD + R1P = ADN + PI	-100000.0	100000.0	Rv3307
R341	GN + R1P = GSN + PI	-100000.0	100000.0	Rv3307
R342	XAN + R1P = XTSINE + PI	-100000.0	100000.0	Rv3307
R343	XTSINE = XAN + RIB	0.0	100000.0	orphan
R344	ADN = INS + NH3	0.0	100000.0	Rv3313c
R345	DA = DIN + NH3	0.0	100000.0	Rv3313c
R346	DGTP = DGMP + PPI	0.0	100000.0	orphan
R347	ATP + GTP = ppGpp + AMP	0.0	100000.0	Rv2583c
R348	ppGpp = GDP + PPI	0.0	100000.0	Rv2583c
R349	ASP + IMP + GTP = GDP + ASUC + PI	0.0	100000.0	Rv0357c
R350	ASUC = FUM + AMP	-100000.0	100000.0	Rv0777
R351	AMP + ATP = ADP	-100000.0	100000.0	Rv0733
R351b	ADN + ATP = AMP + ADP	-100000.0	100000.0	Rv2202c
R352	RTHIO + ADP + O2 = DADP + OTHIO	0.0	100000.0	Rv3051c AND Rv3048c
R354	DADP + ATP = ADP + DATP	-100000.0	100000.0	Rv2445c
R355	IMP + NAD = XMP + NADH	0.0	100000.0	Rv3411c AND Rv3410c AND Rv1843c
R356	XMP + GLN + ATP = GLU + GMP + AMP + PPI	0.0	100000.0	Rv3396c
R357	GMP + ATP = GDP + ADP	-100000.0	100000.0	Rv1389
R358	GDP + ATP = ADP + GTP	-100000.0	100000.0	Rv2445c
R359	GDP + RTHIO + O2 = OTHIO + DGDP	0.0	100000.0	Rv3051c AND Rv3048c
R361	ATP + DGDP = DGTP + ADP	-100000.0	100000.0	Rv2445c
R362	ASP + FUM = SUCC + ISUCC	0.0	100000.0	Rv1595
R363	ASP + O2 = ISUCC + H2O2	0.0	100000.0	Rv1595
R364	DHAP + ISUCC = QA + PI	0.0	100000.0	Rv1594
R365	QA + PRPP = NACN + PPI + CO2	0.0	100000.0	Rv1596
R366	NAM = NAC + NH3	-100000.0	100000.0	Rv2043c
R367	NAC + PRPP = NACN + PPI	0.0	100000.0	Rv0573c
R368	NACN + ATP = NAAD +	0.0	100000.0	Rv2421c

	PPI			
R369	NH3 + NAAD + ATP = AMP + NAD + PPI	0.0	100000.0	Rv2438c
R370	GLN + NAAD + ATP = AMP + GLU + NAD + PPI	0.0	100000.0	Rv2438c
R371	R1P + NAC = NACD + PI	0.0	100000.0	Rv3307
R372	R1P + NAM = NAMD + PI	0.0	100000.0	Rv3307
R373	NACD + ATP = NACN + ADP	0.0	100000.0	Rv0410c
R374	NAMD + ATP = NAMN + ADP	0.0	100000.0	orphan
R375	NAMN + ATP = NAD + PPI	0.0	100000.0	Rv2421c
R376	NAD + NADPH = NADP + NADH	-100000.0	100000.0	Rv0155 AND Rv0157 AND Rv0156
R377	NAD + ATP = NADP + ADP	0.0	100000.0	Rv1695
R378	NADP = NAD + PI	0.0	100000.0	orphan
R379	NADPH + NAD = NADP + NADH	0.0	100000.0	Rv2713 OR Rv3303c
R380	NAD = AMP + NAMN	0.0	100000.0	Rv3199c
R381	GTP = D6RP5P + FOR + PPI	0.0	100000.0	Rv1415 OR Rv1940
R382	D6RP5P = A6RP5P + NH3	0.0	100000.0	Rv2671 OR Rv1409
R383	A6RP5P + NADPH = A6RP5P2 + NADP	0.0	100000.0	Rv2671 OR Rv1409
R384	A6RP5P2 = A6RP + PI	0.0	100000.0	orphan
R385	RL5P = DB4P + FOR	0.0	100000.0	Rv1940
R386	DB4P + A6RP = D8RL + PI	0.0	100000.0	Rv1416
R387	D8RL = RIBFLAV + A6RP	0.0	100000.0	Rv1412
R388	RIBFLAV + ATP = ADP + FMN	0.0	100000.0	Rv2786c
R389	ATP + FMN = FAD + PPI	0.0	100000.0	Rv2786c
R390	OMVAL + METTHF = AKP + THF	0.0	100000.0	Rv2225
R391	AKP + NADPH = PANT + NADP	0.0	100000.0	Rv2573
R392	PANT + bALA + ATP = PNTO + AMP + PPI	0.0	100000.0	Rv3602c
R393	PNTO + ATP = 4PPNTO + ADP	0.0	100000.0	Rv1092c
R394	4PPNTO + CYS + CTP = 4PPNCYS + CMP + PPI	0.0	100000.0	Rv1391
R395	4PPNCYS = 4PPNTE + CO2	0.0	100000.0	Rv1391

R396	4PPNTE + ATP = DPCOA + PPI	0.0	100000.0	Rv2965c
R397	DPCOA + ATP = ADP + COA	0.0	100000.0	Rv1631
R398	COA = ACP	0.0	100000.0	Rv2523c OR Rv2794c
R399	GTP = FOR + AHTD	0.0	100000.0	Rv3609c
R400	AHTD = DHP + PI	0.0	100000.0	Rv0757 AND Rv0758
R401	DHP = AHHMP + GLAL	0.0	100000.0	Rv3607c
R402	AHHMP + ATP = AHHMD + AMP	0.0	100000.0	Rv3606c
R403	CHOR + GLN = GLU + ADCHOR	0.0	100000.0	Rv0013
R404	ADCHOR = PABA + PYR	0.0	100000.0	Rv0812
R405	PABA + AHHMD = DHPT + PPI	0.0	100000.0	Rv3608c OR Rv1207
R406	AHHMP + PABA = DHPT	0.0	100000.0	Rv3608c OR Rv1207
R407	DHPT + GLU + ATP = DHF + ADP + PI	0.0	100000.0	Rv2447c
R408	DHF + NADPH = THF + NADP	0.0	100000.0	Rv2763c
R409	GLU + THF + ATP = THFG + ADP + PI	0.0	100000.0	Rv2447c
R410	THFG = THF + GLU	0.0	100000.0	orphan
R411	CYS + FE2 = FERO + ALA	0.0	100000.0	Rv3025c OR Rv1464
R412	CHOR = ICHOR	-100000.0	100000.0	Rv3215 OR Rv2386c
R413	AKG + ICHOR = PYR + SHCHC + CO2	0.0	100000.0	Rv0555
R414	SHCHC = OSB	0.0	100000.0	orphan
R415	OSB + COA + ATP = OSBCOA + AMP + PPI	0.0	100000.0	Rv0542c AND Rv0553
R416	OSBCOA = DHN + COA	0.0	100000.0	Rv0548c
R417	NPP + DHN = DMK + PPI + CO2	0.0	100000.0	Rv0534c
R418	SAM + DMK = MKH2 + SAH	0.0	100000.0	orphan
R419	ACCOA = PIMELOYL-COA + COA	0.0	100000.0	orphan
R420	PIMELOYL-COA + ALA = 8-AMINO7-OXONONANOATE + COA + CO2	0.0	100000.0	Rv1569 AND Rv0032
R421	8-AMINO7-	0.0	100000.0	Rv1568

	OXONONANOATE + SAM = 7-8-DIAMINONONANOATE + SAM-2-OXOBUTANOATE			
R422	SAM-2-OXOBUTANOATE = SAM	0.0	100000.0	orphan
R423	7-8-DIAMINONONANOATE + ATP + CO2 = DETHIOBIOTIN + ADP	0.0	100000.0	Rv1570
R424	DETHIOBIOTIN + H2S + SAM = BIOTIN + DA	0.0	100000.0	Rv1589
R425	CO2 = HCO3	0.0	100000.0	Rv3588c OR Rv1284
R426	BIOTIN + ATP = BIOTIN-BCCP + AMP + PPI	0.0	100000.0	Rv3279c
R427	BIOTIN-BCCP + HCO3 + ATP = BIOTIN-CO2 + ADP + PI	0.0	100000.0	Rv2501c OR Rv0973c OR Rv3285
R427b	OCTANOYL-ACP = APO-LIPO + ACP	0.0	100000.0	Rv2217
R427c	APO-LIPO + SAM + H2S = LIPO + DA + MET	0.0	100000.0	Rv2218
R428	ATP + GLU = TRNA-GLU + AMP + PPI	0.0	100000.0	Rv2992c
R429	TRNA-GLU + NADPH = GLU1SEMIALD + NADP	0.0	100000.0	Rv0509
R430	GLU1SEMIALD = 5-AMINO-LEVULINATE	0.0	100000.0	Rv0524
R431	5-AMINO-LEVULINATE = PORPHOBILILOGIN	0.0	100000.0	Rv0512
R432	PORPHOBILILOGIN = HYDROXYMETHYLBILANE + NH3	0.0	100000.0	Rv0510
R433	HYDROXYMETHYLBILANE = UROPORPHYRINOGEN-III	0.0	100000.0	Rv0511
R434	UROPORPHYRINOGEN-III = COPROPORPHYRINOGEN-III + CO2	0.0	100000.0	Rv2678c
R435	COPROPORPHYRINOGEN-III + O2 = PROTOPORPHYRINOGEN + H2O2 + CO2	0.0	100000.0	orphan

R436	COPROPORPHYRINOGEN-III + SAM = PROTOPORPHYRINOGEN + MET + CO2	0.0	100000.0	Rv2388C
R437	PROTOPORPHYRINOGEN + O2 = PROTOPORPHYRIN-IX	0.0	100000.0	Rv2677 OR Rv1300
R438	PROTOPORPHYRIN-IX + FE2 = PROTOHEME-FE2	0.0	100000.0	Rv1485
R439	PROTOHEME-FE2 + FPP = HEME-FE2 + PPI	0.0	100000.0	orphan
R440	UROPORPHYRINOGEN-III + SAM = PRECORIN-2 + SAH	0.0	100000.0	Rv2847c OR Rv0511
R441	PRECORIN-2 + SAM = PRECORIN-3A + SAH	0.0	100000.0	Rv2066
R442	PRECORIN-3A + O2 = PRECORIN-3B	0.0	100000.0	Rv2064
R443	PRECORIN-3B + SAM = PRECORIN-4B + SAH	0.0	100000.0	Rv2066
R444	PRECORIN-4B + SAM = PRECORIN-5 + SAH	0.0	100000.0	Rv2071c
R445	PRECORIN-5 + SAM = PRECORIN-6X + SAH + AC	0.0	100000.0	orphan
R446	PRECORIN-6X + NADPH = PRECORIN-6Y + NADP	0.0	100000.0	Rv2070c
R447	PRECORIN-6Y + SAM = PRECORIN-8X + SAH + CO2	0.0	100000.0	Rv2072c
R448	PRECORIN-8X = HYDROGENOBYRINATE	0.0	100000.0	Rv2065
R449	HYDROGENOBYRINATE + ATP + GLN = HYDROGENOBYRINATE-A-C-DIAMIDE + PI + ADP + GLU	0.0	100000.0	Rv2848c
R450	HYDROGENOBYRINATE-A-C-DIAMIDE + ATP + CO-II = COB-II-RINICACID-A-C-DIAMIDE + ADP + PI	0.0	100000.0	orphan
R451	COB-II-RINICACID-A-C-DIAMIDE + NADH = COB-I-RINICACID-A-C-DIAMIDE + NAD	0.0	100000.0	orphan

R452	COB-I-RINICACID-A-C-DIAMIDE + ATP = ADENOSYL-COBRINICACID-A-C-DIAMIDE + PPI	0.0	100000.0	Rv2849c
R453	ADENOSYL-COBRINICACID-A-C-DIAMIDE + ATP + GLN = ADENOSYL-COBRATE + ADP + PI + GLU	0.0	100000.0	Rv0255c
R454	ADENOSYL-COBRATE + 1-AMINO-PROPAN-2-OL = ADENOSYLCOBINAMIDE	0.0	100000.0	Rv2231c
R455	ADENOSYLCOBINAMIDE + ATP = ADENOSYLCOBINIMIDE-P + ADP	0.0	100000.0	Rv0254c
R456	ADENOSYLCOBINIMIDE-P + GTP = ADENOSYLCOBINAMIDE-GDP + PPI	0.0	100000.0	orphan
R457	ADENOSYLCOBINAMIDE-GDP = COB-I + GMP	0.0	100000.0	Rv2208
R458	COB-II + NADH = COB-I + NAD	-100000.0	100000.0	orphan
R459	COB-III + NADH = COB-II + NAD	-100000.0	100000.0	orphan
R460	MOAD-COOH + CYS + ATP = MOAD-COSH + AMP + SER + PPI	0.0	100000.0	Rv3206c AND Rv3025c
R461	GTP = PRECURSOR-Z + PPI	0.0	100000.0	Rv3109 AND Rv3116 AND Rv3111
R462	MOAD-COSH + PRECURSOR-Z = MOLYBDOPTERIN + MOAD-COOH	0.0	100000.0	(Rv3119 OR Rv0866) AND Rv3322c
R463	MOLYBDOPTERIN + MO2 = MOLYBDENUM	0.0	100000.0	Rv0994 OR Rv0438
R464	MOLYBDENUM + GTP = MOLYBDOPTERIN-GDP + PPI	0.0	100000.0	Rv2453c
R465	TYR = TS-COSH-TYR	0.0	100000.0	orphan
R466	TS-PROTEIN = TS-COSH-TYR	0.0	100000.0	orphan
R467	AIR = AHMMP	0.0	100000.0	Rv0423c

R468	AHMMP + ATP = AMPMP + ADP	0.0	100000.0	Rv0422c
R469	AMPMP + ATP = MAHMPPP + ADP	0.0	100000.0	Rv0422c
R470	DX5P + TS-COSH-TYR = HEMT + TS-PROTEIN	0.0	100000.0	Rv0417
R471	HEMT + ATP = MPET + ADP	0.0	100000.0	orphan
R472	MAHMPPP + MPET = THIP + PPI	0.0	100000.0	Rv0414c
R473	THIP = THI + PI	0.0	100000.0	orphan
R474	THI = AHMMP + HEMT	0.0	100000.0	orphan
R475	LLAC + GTP = 2-PHOSPHO-L-LACTATE + GDP	0.0	100000.0	orphan
R476	2-PHOSPHO-L-LACTATE + GTP = LPPG + PPI	0.0	100000.0	orphan
R477	A6RP + 4HPP = FO + NH3	0.0	100000.0	Rv1173
R478	FO + LPPG = F420-0 + GMP	0.0	100000.0	Rv3261 AND Rv3262
R479	F420-0 + ATP + GLU = F420	0.0	100000.0	Rv3261 AND Rv3263
R480	UDPNAG + IP = NAG-INS + UDP + PI	0.0	100000.0	Rv0486
R481	NAG-INS = NG-INS + AC	0.0	100000.0	Rv1170
R482	NG-INS + CYS + ATP = CYS-NG-INS + AMP + PPI	0.0	100000.0	Rv2130
R483	CYS-NG-INS + ACCOA = MYCOTHIOL + COA	0.0	100000.0	Rv0819
R484	MYCOTHIOL + ELECTROPHILE-X = MYCOTHIOL-S-CONJUGATE + H2X	0.0	100000.0	orphan
R484b	MYCOTHIOL-S-CONJUGATE = N-ACETYL-S-CONJUGATE + NG-INS	0.0	100000.0	Rv1082
R485	ICHOR = SAL + PYR	0.0	100000.0	orphan
R486	COA = MBT-HOLO	0.0	100000.0	Rv2523c
R487	MBT-HOLO + SAL + ATP = MBTA-SAL + AMP + PPI	0.0	100000.0	Rv2384
R488	MBT-HOLO + SER + ATP = MBTB-SER + AMP + PPI	0.0	100000.0	Rv2383c
R489	MBT-HOLO + LYS + ATP = MBTE-LYS + AMP + PPI	0.0	100000.0	Rv2380c

R490	MBT-HOLO + LYS + ATP = MBTF-LYS + AMP + PPI	0.0	100000.0	Rv2380c
R491	MBT-HOLO + ACCOA + MALCOA = MBTCD-HBA + COA	0.0	100000.0	Rv2382c AND Rv2381c
R492	MBTA-SAL + MBTB-SER + MBTE-LYS + MBTF-LYS + MBTCD-HBA = MBT + MBT-HOLO	0.0	100000.0	orphan
R493	MBT + ACCOA + NADPH = MBTSEC + COA + NADP	0.0	100000.0	orphan
R494	MBT + ACCOA + NADPH = MBTWALL + COA + NADP	0.0	100000.0	orphan
R495	ACCOA + BIOTIN-CO2 = MALCOA + BIOTIN	0.0	100000.0	Rv0904c OR Rv2502c OR Rv0974c OR Rv0904c OR Rv3799c OR Rv3280 OR Rv2247
R496	ACCOA + ACP = COA + ACACP	-100000.0	100000.0	(Rv2243 OR Rv0649) AND Rv2244
R497	MALACP + NADPH + ACACP = NADP + HEXANOYL-ACP + ACP + CO2	0.0	100000.0	Rv2524c
R497 b	MALACP + NADPH + ACACP = NADP + OCTANOYL-ACP + ACP + CO2	0.0	100000.0	Rv2524c
R498	MALACP + NADPH + ACACP = NADP + TETRADECANOYL-ACP + ACP + CO2	0.0	100000.0	Rv2524c
R499	MALACP + NADPH + ACACP = HEXADECANOYL-ACP + NADP + ACP + CO2	0.0	100000.0	Rv2524c
R500	MALACP + NADPH + ACACP = 9-HEXADECENOYL-ACP + NADP + ACP + CO2	0.0	100000.0	Rv2524c
R501	MALACP + NADPH + ACACP = OCTADECANOYL-ACP + NADP + ACP + CO2	0.0	100000.0	Rv2524c
R502	MALACP + NADPH + ACACP = 9-OCTADECENOYL-ACP + NADP + ACP + CO2	0.0	100000.0	Rv2524c

R503	ACACP + MALACP + NADPH = EICOSANOYL-ACP + NADP + ACP + CO2	0.0	100000.0	Rv2524c
R504	ACACP + MALACP + NADPH = DOCOSANOYL-ACP + NADP + ACP + CO2	0.0	100000.0	Rv2524c
R505	ACACP + MALACP + NADPH = TETRACOSANOYL-ACP + NADP + ACP + CO2	0.0	100000.0	Rv2524c
R506	ACACP + MALACP + NADPH = HEXACOSANOYL-ACP + NADP + ACP + CO2	0.0	100000.0	Rv2524c
R507	ACACP + MALACP + NADPH = OCTACOSANOYL-ACP + NADP + ACP + CO2	0.0	100000.0	Rv2524c
R508	HEXACOSANOYL-COA + BIOTIN-CO2 = HEXACOSANOYL-COA-CO2 + BIOTIN	0.0	100000.0	Rv3280 AND Rv3799c AND Rv3285
R509	HEXANOYL-ACP + COA = HEXANOYL-COA + ACP	-100000.0	100000.0	(Rv2243 OR Rv0649) AND Rv2244
R510	TETRADECANOYL-ACP + COA = TETRADECANOYL-COA + ACP	-100000.0	100000.0	(Rv2243 OR Rv0649) AND Rv2244
R511	HEXADECANOYL-ACP + COA = HEXADECANOYL-COA + ACP	-100000.0	100000.0	(Rv2243 OR Rv0649) AND Rv2244
R512	9-HEXADECENOYL-ACP + COA = 9-HEXADECENOYL-COA + ACP	-100000.0	100000.0	(Rv2243 OR Rv0649) AND Rv2244
R513	OCTADECANOYL-ACP + COA = OCTADECANOYL-COA + ACP	-100000.0	100000.0	(Rv2243 OR Rv0649) AND Rv2244
R514	9-OCTADECENOYL-ACP + COA = 9-OCTADECENOYL-COA + ACP	-100000.0	100000.0	(Rv2243 OR Rv0649) AND Rv2244
R515	EICOSANOYL-ACP + COA = EICOSANOYL-COA + ACP	-100000.0	100000.0	(Rv2243 OR Rv0649) AND Rv2244
R516	DOCOSANOYL-ACP +	-100000.0	100000.0	(Rv2243 OR Rv0649) AND Rv2244

	COA = DOCOSANOYL-COA + ACP			
R517	TETRACOSANOYL-ACP + COA = TETRACOSANOYL-COA + ACP	-100000.0	100000.0	(Rv2243 OR Rv0649) AND Rv2244
R518	HEXACOSANOYL-ACP + COA = HEXACOSANOYL-COA + ACP	-100000.0	100000.0	(Rv2243 OR Rv0649) AND Rv2244
R519	OCTACOSANOYL-ACP + COA = OCTACOSANOYL-COA + ACP	-100000.0	100000.0	(Rv2243 OR Rv0649) AND Rv2244
R520	NONADECANOYL-ACP + COA = NONADECANOYL-COA + ACP	-100000.0	100000.0	(Rv2243 OR Rv0649) AND Rv2244
R521	HEPTADECANOYL-ACP + COA = HEPTADECANOYL-COA + ACP	-100000.0	100000.0	(Rv2243 OR Rv0649) AND Rv2244
R522	PENTADECANOYL-ACP + COA = PENTADECANOYL-COA + ACP	-100000.0	100000.0	(Rv2243 OR Rv0649) AND Rv2244
R533	PROPIONYLCOA + ACP = PROPIONYLACP + COA	0.0	100000.0	(Rv2243 OR Rv0649) AND Rv2244
R534	MALACP + NADPH + PROPIONYLACP = NADP + ACP + PENTADECANOYL-ACP + CO2	0.0	100000.0	Rv2524c
R535	MALACP + NADPH + PENTADECANOYL-ACP = NADP + ACP + HEPTADECANOYL-ACP + CO2	0.0	100000.0	Rv2524c
R536	MALACP + NADPH + HEPTADECANOYL-ACP = NADP + ACP + NONADECANOYL-ACP + CO2	0.0	100000.0	Rv2524c
R537	HEXANOATE + COA + ATP = HEXANOYL-COA + AMP + PPI	0.0	100000.0	Rv0035 OR Rv0099 OR Rv0119 OR Rv0166 OR Rv0214 OR Rv0270 OR Rv0275c OR Rv0404 OR Rv0551c OR Rv0852 OR Rv1058 OR Rv1185c OR Rv1193 OR Rv1206 OR Rv1345 OR Rv1427c OR Rv1521 OR Rv1529 OR Rv1750c OR Rv1925 OR Rv2187 OR Rv2505c OR Rv2590 OR Rv2930 OR Rv2941 OR Rv2948c OR Rv2950c OR Rv3089 OR Rv3506 OR Rv3513c OR Rv3515c OR Rv3561 OR Rv3801c OR Rv3826

R538	DECANOATE + COA + ATP = DECANOYL-COA + AMP + PPI	0.0	100000.0	Rv0035 OR Rv0099 OR Rv0119 OR Rv0166 OR Rv0214 OR Rv0270 OR Rv0275c OR Rv0404 OR Rv0551c OR Rv0852 OR Rv1058 OR Rv1185c OR Rv1193 OR Rv1206 OR Rv1345 OR Rv1427c OR Rv1521 OR Rv1529 OR Rv1750c OR Rv1925 OR Rv2187 OR Rv2505c OR Rv2590 OR Rv2930 OR Rv2941 OR Rv2948c OR Rv2950c OR Rv3089 OR Rv3506 OR Rv3513c OR Rv3515c OR Rv3561 OR Rv3801c OR Rv3826
R539	DODECANOATE + COA + ATP = DODECANOYL-COA + AMP + PPI	0.0	100000.0	Rv0035 OR Rv0099 OR Rv0119 OR Rv0166 OR Rv0214 OR Rv0270 OR Rv0275c OR Rv0404 OR Rv0551c OR Rv0852 OR Rv1058 OR Rv1185c OR Rv1193 OR Rv1206 OR Rv1345 OR Rv1427c OR Rv1521 OR Rv1529 OR Rv1750c OR Rv1925 OR Rv2187 OR Rv2505c OR Rv2590 OR Rv2930 OR Rv2941 OR Rv2948c OR Rv2950c OR Rv3089 OR Rv3506 OR Rv3513c OR Rv3515c OR Rv3561 OR Rv3801c OR Rv3826
R540	TETRADECANOATE + COA + ATP = TETRADECANOYL-COA + AMP + PPI	0.0	100000.0	Rv0035 OR Rv0099 OR Rv0119 OR Rv0166 OR Rv0214 OR Rv0270 OR Rv0275c OR Rv0404 OR Rv0551c OR Rv0852 OR Rv1058 OR Rv1185c OR Rv1193 OR Rv1206 OR Rv1345 OR Rv1427c OR Rv1521 OR Rv1529 OR Rv1750c OR Rv1925 OR Rv2187 OR Rv2505c OR Rv2590 OR Rv2930 OR Rv2941 OR Rv2948c OR Rv2950c OR Rv3089 OR Rv3506 OR Rv3513c OR Rv3515c OR Rv3561 OR Rv3801c OR Rv3826
R541	HEXADECANOATE + COA + ATP = HEXADECANOYL-COA + AMP + PPI	0.0	100000.0	Rv0035 OR Rv0099 OR Rv0119 OR Rv0166 OR Rv0214 OR Rv0270 OR Rv0275c OR Rv0404 OR Rv0551c OR Rv0852 OR Rv1058 OR Rv1185c OR Rv1193 OR Rv1206 OR Rv1345 OR Rv1427c OR Rv1521 OR Rv1529 OR Rv1750c OR Rv1925 OR Rv2187 OR Rv2505c OR Rv2590 OR Rv2930 OR Rv2941 OR Rv2948c OR Rv2950c OR Rv3089 OR Rv3506 OR Rv3513c OR Rv3515c OR Rv3561 OR Rv3801c OR Rv3826
R542	9-HEXADECENOATE + COA + ATP = 9-HEXADECENOYL-COA + AMP + PPI	0.0	100000.0	Rv0035 OR Rv0099 OR Rv0119 OR Rv0166 OR Rv0214 OR Rv0270 OR Rv0275c OR Rv0404 OR Rv0551c OR Rv0852 OR Rv1058 OR Rv1185c OR Rv1193 OR Rv1206 OR Rv1345 OR Rv1427c OR Rv1521 OR Rv1529 OR Rv1750c OR Rv1925 OR Rv2187 OR Rv2505c OR Rv2590 OR Rv2930 OR Rv2941 OR Rv2948c OR Rv2950c OR Rv3089 OR Rv3506 OR Rv3513c OR Rv3515c OR Rv3561 OR Rv3801c OR Rv3826
R543	OCTADECANOATE + COA + ATP = OCTADECANOYL-	0.0	100000.0	Rv0035 OR Rv0099 OR Rv0119 OR Rv0166 OR Rv0214 OR Rv0270 OR Rv0275c OR Rv0404 OR

	COA + AMP + PPI			Rv0551c OR Rv0852 OR Rv1058 OR Rv1185c OR Rv1193 OR Rv1206 OR Rv1345 OR Rv1427c OR Rv1521 OR Rv1529 OR Rv1750c OR Rv1925 OR Rv2187 OR Rv2505c OR Rv2590 OR Rv2930 OR Rv2941 OR Rv2948c OR Rv2950c OR Rv3089 OR Rv3506 OR Rv3513c OR Rv3515c OR Rv3561 OR Rv3801c OR Rv3826
R544	9-OCTADECENOATE + COA + ATP = 9-OCTADECENOYL-COA + AMP + PPI	0.0	100000.0	Rv0035 OR Rv0099 OR Rv0119 OR Rv0166 OR Rv0214 OR Rv0270 OR Rv0275c OR Rv0404 OR Rv0551c OR Rv0852 OR Rv1058 OR Rv1185c OR Rv1193 OR Rv1206 OR Rv1345 OR Rv1427c OR Rv1521 OR Rv1529 OR Rv1750c OR Rv1925 OR Rv2187 OR Rv2505c OR Rv2590 OR Rv2930 OR Rv2941 OR Rv2948c OR Rv2950c OR Rv3089 OR Rv3506 OR Rv3513c OR Rv3515c OR Rv3561 OR Rv3801c OR Rv3826
R545	EICOSANOATE + COA + ATP = EICOSANOYL-COA + AMP + PPI	0.0	100000.0	Rv0035 OR Rv0099 OR Rv0119 OR Rv0166 OR Rv0214 OR Rv0270 OR Rv0275c OR Rv0404 OR Rv0551c OR Rv0852 OR Rv1058 OR Rv1185c OR Rv1193 OR Rv1206 OR Rv1345 OR Rv1427c OR Rv1521 OR Rv1529 OR Rv1750c OR Rv1925 OR Rv2187 OR Rv2505c OR Rv2590 OR Rv2930 OR Rv2941 OR Rv2948c OR Rv2950c OR Rv3089 OR Rv3506 OR Rv3513c OR Rv3515c OR Rv3561 OR Rv3801c OR Rv3826
R546	DOCOSANOATE + COA + ATP = DOCOSANOYL-COA + AMP + PPI	0.0	100000.0	Rv0035 OR Rv0099 OR Rv0119 OR Rv0166 OR Rv0214 OR Rv0270 OR Rv0275c OR Rv0404 OR Rv0551c OR Rv0852 OR Rv1058 OR Rv1185c OR Rv1193 OR Rv1206 OR Rv1345 OR Rv1427c OR Rv1521 OR Rv1529 OR Rv1750c OR Rv1925 OR Rv2187 OR Rv2505c OR Rv2590 OR Rv2930 OR Rv2941 OR Rv2948c OR Rv2950c OR Rv3089 OR Rv3506 OR Rv3513c OR Rv3515c OR Rv3561 OR Rv3801c OR Rv3826
R547	TETRACOSANOATE + COA + ATP = TETRACOSANOYL-COA + AMP + PPI	0.0	100000.0	Rv0035 OR Rv0099 OR Rv0119 OR Rv0166 OR Rv0214 OR Rv0270 OR Rv0275c OR Rv0404 OR Rv0551c OR Rv0852 OR Rv1058 OR Rv1185c OR Rv1193 OR Rv1206 OR Rv1345 OR Rv1427c OR Rv1521 OR Rv1529 OR Rv1750c OR Rv1925 OR Rv2187 OR Rv2505c OR Rv2590 OR Rv2930 OR Rv2941 OR Rv2948c OR Rv2950c OR Rv3089 OR Rv3506 OR Rv3513c OR Rv3515c OR Rv3561 OR Rv3801c OR Rv3826
R548	HEXACOSANOATE + COA + ATP = HEXACOSANOYL-COA + AMP + PPI	0.0	100000.0	Rv0035 OR Rv0099 OR Rv0119 OR Rv0166 OR Rv0214 OR Rv0270 OR Rv0275c OR Rv0404 OR Rv0551c OR Rv0852 OR Rv1058 OR Rv1185c OR Rv1193 OR Rv1206 OR Rv1345 OR Rv1427c OR

				Rv1521 OR Rv1529 OR Rv1750c OR Rv1925 OR Rv2187 OR Rv2505c OR Rv2590 OR Rv2930 OR Rv2941 OR Rv2948c OR Rv2950c OR Rv3089 OR Rv3506 OR Rv3513c OR Rv3515c OR Rv3561 OR Rv3801c OR Rv3826
R549	PENTADECANOATE + COA + ATP = PENTADECANOYL-COA + AMP + PPI	0.0	100000.0	Rv0035 OR Rv0099 OR Rv0119 OR Rv0166 OR Rv0214 OR Rv0270 OR Rv0275c OR Rv0404 OR Rv0551c OR Rv0852 OR Rv1058 OR Rv1185c OR Rv1193 OR Rv1206 OR Rv1345 OR Rv1427c OR Rv1521 OR Rv1529 OR Rv1750c OR Rv1925 OR Rv2187 OR Rv2505c OR Rv2590 OR Rv2930 OR Rv2941 OR Rv2948c OR Rv2950c OR Rv3089 OR Rv3506 OR Rv3513c OR Rv3515c OR Rv3561 OR Rv3801c OR Rv3826
R550	HEPTADECANOATE + COA + ATP = HEPTADECANOYL-COA + AMP + PPI	0.0	100000.0	Rv0035 OR Rv0099 OR Rv0119 OR Rv0166 OR Rv0214 OR Rv0270 OR Rv0275c OR Rv0404 OR Rv0551c OR Rv0852 OR Rv1058 OR Rv1185c OR Rv1193 OR Rv1206 OR Rv1345 OR Rv1427c OR Rv1521 OR Rv1529 OR Rv1750c OR Rv1925 OR Rv2187 OR Rv2505c OR Rv2590 OR Rv2930 OR Rv2941 OR Rv2948c OR Rv2950c OR Rv3089 OR Rv3506 OR Rv3513c OR Rv3515c OR Rv3561 OR Rv3801c OR Rv3826
R551	NONADECANOATE + COA + ATP = NONADECANOYL-COA + AMP + PPI	0.0	100000.0	Rv0035 OR Rv0099 OR Rv0119 OR Rv0166 OR Rv0214 OR Rv0270 OR Rv0275c OR Rv0404 OR Rv0551c OR Rv0852 OR Rv1058 OR Rv1185c OR Rv1193 OR Rv1206 OR Rv1345 OR Rv1427c OR Rv1521 OR Rv1529 OR Rv1750c OR Rv1925 OR Rv2187 OR Rv2505c OR Rv2590 OR Rv2930 OR Rv2941 OR Rv2948c OR Rv2950c OR Rv3089 OR Rv3506 OR Rv3513c OR Rv3515c OR Rv3561 OR Rv3801c OR Rv3826
R552	OCTACOSANOYL-COA + FAD + NAD + COA = HEXACOSANOYL-COA + FADH2 + NADH + ACCOA	0.0	100000.0	(Rv0131c OR Rv0154c OR Rv0215c OR Rv0231 OR Rv0244c OR Rv0271c OR Rv0400c OR Rv0752c OR Rv0873 OR Rv0972c OR Rv0975c OR Rv1346 OR Rv1467c OR Rv1679 OR Rv1933c OR Rv1934c OR Rv2724c OR Rv2789c OR Rv3061c OR Rv3139 OR Rv3140 OR Rv3274c OR Rv3504 OR Rv3505 OR Rv3543c OR Rv3544c OR Rv3560c OR Rv3562 OR Rv3563 OR Rv3564 OR Rv3573c OR Rv3761c OR Rv3797 OR Rv0672 OR Rv2500c) AND (Rv0222 OR Rv0456c OR Rv0632c OR Rv0673 OR Rv0675 OR Rv0971c OR Rv1070c OR Rv1071c OR Rv1141c OR Rv1142c OR Rv1472 OR Rv1935c OR Rv2486 OR Rv2679 OR Rv2831 OR Rv3039c OR Rv3516 OR Rv3550 OR Rv3774 OR Rv0905 OR Rv3374 OR Rv3373) AND (Rv0468 OR Rv1715 OR Rv1912c OR

				Rv3141) AND (Rv0243 OR Rv1074c OR Rv3546 OR Rv3556c OR Rv1323 OR Rv0859)
R553	HEXACOSANOYL-COA + FAD + NAD + COA = TETRACOSANOYL-COA + FADH2 + NADH + ACCOA	0.0	100000.0	(Rv0131c OR Rv0154c OR Rv0215c OR Rv0231 OR Rv0244c OR Rv0271c OR Rv0400c OR Rv0752c OR Rv0873 OR Rv0972c OR Rv0975c OR Rv1346 OR Rv1467c OR Rv1679 OR Rv1933c OR Rv1934c OR Rv2724c OR Rv2789c OR Rv3061c OR Rv3139 OR Rv3140 OR Rv3274c OR Rv3504 OR Rv3505 OR Rv3543c OR Rv3544c OR Rv3560c OR Rv3562 OR Rv3563 OR Rv3564 OR Rv3573c OR Rv3761c OR Rv3797 OR Rv0672 OR Rv2500c) AND (Rv0222 OR Rv0456c OR Rv0632c OR Rv0673 OR Rv0675 OR Rv0971c OR Rv1070c OR Rv1071c OR Rv1141c OR Rv1142c OR Rv1472 OR Rv1935c OR Rv2486 OR Rv2679 OR Rv2831 OR Rv3039c OR Rv3516 OR Rv3550 OR Rv3774 OR Rv0905 OR Rv3374 OR Rv3373) AND (Rv0468 OR Rv1715 OR Rv1912c OR Rv3141) AND (Rv0243 OR Rv1074c OR Rv3546 OR Rv3556c OR Rv1323 OR Rv0859)
R554	TETRACOSANOYL-COA + FAD + NAD + COA = DOCOSANOYL-COA + FADH2 + NADH + ACCOA	0.0	100000.0	(Rv0131c OR Rv0154c OR Rv0215c OR Rv0231 OR Rv0244c OR Rv0271c OR Rv0400c OR Rv0752c OR Rv0873 OR Rv0972c OR Rv0975c OR Rv1346 OR Rv1467c OR Rv1679 OR Rv1933c OR Rv1934c OR Rv2724c OR Rv2789c OR Rv3061c OR Rv3139 OR Rv3140 OR Rv3274c OR Rv3504 OR Rv3505 OR Rv3543c OR Rv3544c OR Rv3560c OR Rv3562 OR Rv3563 OR Rv3564 OR Rv3573c OR Rv3761c OR Rv3797 OR Rv0672 OR Rv2500c) AND (Rv0222 OR Rv0456c OR Rv0632c OR Rv0673 OR Rv0675 OR Rv0971c OR Rv1070c OR Rv1071c OR Rv1141c OR Rv1142c OR Rv1472 OR Rv1935c OR Rv2486 OR Rv2679 OR Rv2831 OR Rv3039c OR Rv3516 OR Rv3550 OR Rv3774 OR Rv0905 OR Rv3374 OR Rv3373) AND (Rv0468 OR Rv1715 OR Rv1912c OR Rv3141) AND (Rv0243 OR Rv1074c OR Rv3546 OR Rv3556c OR Rv1323 OR Rv0859)
R555	DOCOSANOYL-COA + FAD + NAD + COA = EICOSANOYL-COA + FADH2 + NADH + ACCOA	0.0	100000.0	(Rv0131c OR Rv0154c OR Rv0215c OR Rv0231 OR Rv0244c OR Rv0271c OR Rv0400c OR Rv0752c OR Rv0873 OR Rv0972c OR Rv0975c OR Rv1346 OR Rv1467c OR Rv1679 OR Rv1933c OR Rv1934c OR Rv2724c OR Rv2789c OR Rv3061c OR Rv3139 OR Rv3140 OR Rv3274c OR Rv3504 OR Rv3505 OR Rv3543c OR Rv3544c OR Rv3560c OR Rv3562 OR Rv3563 OR Rv3564 OR Rv3573c OR Rv3761c OR Rv3797 OR Rv0672 OR Rv2500c) AND (Rv0222 OR Rv0456c OR

				Rv0632c OR Rv0673 OR Rv0675 OR Rv0971c OR Rv1070c OR Rv1071c OR Rv1141c OR Rv1142c OR Rv1472 OR Rv1935c OR Rv2486 OR Rv2679 OR Rv2831 OR Rv3039c OR Rv3516 OR Rv3550 OR Rv3774 OR Rv0905 OR Rv3374 OR Rv3373) AND (Rv0468 OR Rv1715 OR Rv1912c OR Rv3141) AND (Rv0243 OR Rv1074c OR Rv3546 OR Rv3556c OR Rv1323 OR Rv0859)
R556	EICOSANOYL-COA + FAD + NAD + COA = OCTADECANOYL-COA + FADH2 + NADH + ACCOA	0.0	100000.0	(Rv0131c OR Rv0154c OR Rv0215c OR Rv0231 OR Rv0244c OR Rv0271c OR Rv0400c OR Rv0752c OR Rv0873 OR Rv0972c OR Rv0975c OR Rv1346 OR Rv1467c OR Rv1679 OR Rv1933c OR Rv1934c OR Rv2724c OR Rv2789c OR Rv3061c OR Rv3139 OR Rv3140 OR Rv3274c OR Rv3504 OR Rv3505 OR Rv3543c OR Rv3544c OR Rv3560c OR Rv3562 OR Rv3563 OR Rv3564 OR Rv3573c OR Rv3761c OR Rv3797 OR Rv0672 OR Rv2500c) AND (Rv0222 OR Rv0456c OR Rv0632c OR Rv0673 OR Rv0675 OR Rv0971c OR Rv1070c OR Rv1071c OR Rv1141c OR Rv1142c OR Rv1472 OR Rv1935c OR Rv2486 OR Rv2679 OR Rv2831 OR Rv3039c OR Rv3516 OR Rv3550 OR Rv3774 OR Rv0905 OR Rv3374 OR Rv3373) AND (Rv0468 OR Rv1715 OR Rv1912c OR Rv3141) AND (Rv0243 OR Rv1074c OR Rv3546 OR Rv3556c OR Rv1323 OR Rv0859)
R557	OCTADECANOYL-COA + FAD + NAD + COA = HEXADECANOYL-COA + FADH2 + NADH + ACCOA	0.0	100000.0	(Rv0131c OR Rv0154c OR Rv0215c OR Rv0231 OR Rv0244c OR Rv0271c OR Rv0400c OR Rv0752c OR Rv0873 OR Rv0972c OR Rv0975c OR Rv1346 OR Rv1467c OR Rv1679 OR Rv1933c OR Rv1934c OR Rv2724c OR Rv2789c OR Rv3061c OR Rv3139 OR Rv3140 OR Rv3274c OR Rv3504 OR Rv3505 OR Rv3543c OR Rv3544c OR Rv3560c OR Rv3562 OR Rv3563 OR Rv3564 OR Rv3573c OR Rv3761c OR Rv3797 OR Rv0672 OR Rv2500c) AND (Rv0222 OR Rv0456c OR Rv0632c OR Rv0673 OR Rv0675 OR Rv0971c OR Rv1070c OR Rv1071c OR Rv1141c OR Rv1142c OR Rv1472 OR Rv1935c OR Rv2486 OR Rv2679 OR Rv2831 OR Rv3039c OR Rv3516 OR Rv3550 OR Rv3774 OR Rv0905 OR Rv3374 OR Rv3373) AND (Rv0468 OR Rv1715 OR Rv1912c OR Rv3141) AND (Rv0243 OR Rv1074c OR Rv3546 OR Rv3556c OR Rv1323 OR Rv0859)
R558	HEXADECANOYL-COA + FAD + NAD + COA = TETRADECANOYL-COA + FADH2 + NADH + ACCOA	0.0	100000.0	(Rv0131c OR Rv0154c OR Rv0215c OR Rv0231 OR Rv0244c OR Rv0271c OR Rv0400c OR Rv0752c OR Rv0873 OR Rv0972c OR Rv0975c OR Rv1346 OR Rv1467c OR Rv1679 OR Rv1933c

				OR Rv1934c OR Rv2724c OR Rv2789c OR Rv3061c OR Rv3139 OR Rv3140 OR Rv3274c OR Rv3504 OR Rv3505 OR Rv3543c OR Rv3544c OR Rv3560c OR Rv3562 OR Rv3563 OR Rv3564 OR Rv3573c OR Rv3761c OR Rv3797 OR Rv0672 OR Rv2500c) AND (Rv0222 OR Rv0456c OR Rv0632c OR Rv0673 OR Rv0675 OR Rv0971c OR Rv1070c OR Rv1071c OR Rv1141c OR Rv1142c OR Rv1472 OR Rv1935c OR Rv2486 OR Rv2679 OR Rv2831 OR Rv3039c OR Rv3516 OR Rv3550 OR Rv3774 OR Rv0905 OR Rv3374 OR Rv3373) AND (Rv0468 OR Rv1715 OR Rv1912c OR Rv3141) AND (Rv0243 OR Rv1074c OR Rv3546 OR Rv3556c OR Rv1323 OR Rv0859)
R559	TETRADECANOYL-COA + FAD + NAD + COA = DODECANOYL-COA + FADH2 + NADH + ACCOA	0.0	100000.0	(Rv0131c OR Rv0154c OR Rv0215c OR Rv0231 OR Rv0244c OR Rv0271c OR Rv0400c OR Rv0752c OR Rv0873 OR Rv0972c OR Rv0975c OR Rv1346 OR Rv1467c OR Rv1679 OR Rv1933c OR Rv1934c OR Rv2724c OR Rv2789c OR Rv3061c OR Rv3139 OR Rv3140 OR Rv3274c OR Rv3504 OR Rv3505 OR Rv3543c OR Rv3544c OR Rv3560c OR Rv3562 OR Rv3563 OR Rv3564 OR Rv3573c OR Rv3761c OR Rv3797 OR Rv0672 OR Rv2500c) AND (Rv0222 OR Rv0456c OR Rv0632c OR Rv0673 OR Rv0675 OR Rv0971c OR Rv1070c OR Rv1071c OR Rv1141c OR Rv1142c OR Rv1472 OR Rv1935c OR Rv2486 OR Rv2679 OR Rv2831 OR Rv3039c OR Rv3516 OR Rv3550 OR Rv3774 OR Rv0905 OR Rv3374 OR Rv3373) AND (Rv0468 OR Rv1715 OR Rv1912c OR Rv3141) AND (Rv0243 OR Rv1074c OR Rv3546 OR Rv3556c OR Rv1323 OR Rv0859)
R560	DODECANOYL-COA + FAD + NAD + COA = DECANOYL-COA + FADH2 + NADH + ACCOA	0.0	100000.0	(Rv0131c OR Rv0154c OR Rv0215c OR Rv0231 OR Rv0244c OR Rv0271c OR Rv0400c OR Rv0752c OR Rv0873 OR Rv0972c OR Rv0975c OR Rv1346 OR Rv1467c OR Rv1679 OR Rv1933c OR Rv1934c OR Rv2724c OR Rv2789c OR Rv3061c OR Rv3139 OR Rv3140 OR Rv3274c OR Rv3504 OR Rv3505 OR Rv3543c OR Rv3544c OR Rv3560c OR Rv3562 OR Rv3563 OR Rv3564 OR Rv3573c OR Rv3761c OR Rv3797 OR Rv0672 OR Rv2500c) AND (Rv0222 OR Rv0456c OR Rv0632c OR Rv0673 OR Rv0675 OR Rv0971c OR Rv1070c OR Rv1071c OR Rv1141c OR Rv1142c OR Rv1472 OR Rv1935c OR Rv2486 OR Rv2679 OR Rv2831 OR Rv3039c OR Rv3516 OR Rv3550 OR Rv3774 OR Rv0905 OR Rv3374 OR Rv3373) AND (Rv0468 OR Rv1715 OR Rv1912c OR

				Rv3141) AND (Rv0243 OR Rv1074c OR Rv3546 OR Rv3556c OR Rv1323 OR Rv0859)
R561	DECANOYL-COA + FAD + NAD + COA = OCTANOYL-COA + FADH2 + NADH + ACCOA	0.0	100000.0	(Rv0131c OR Rv0154c OR Rv0215c OR Rv0231 OR Rv0244c OR Rv0271c OR Rv0400c OR Rv0752c OR Rv0873 OR Rv0972c OR Rv0975c OR Rv1346 OR Rv1467c OR Rv1679 OR Rv1933c OR Rv1934c OR Rv2724c OR Rv2789c OR Rv3061c OR Rv3139 OR Rv3140 OR Rv3274c OR Rv3504 OR Rv3505 OR Rv3543c OR Rv3544c OR Rv3560c OR Rv3562 OR Rv3563 OR Rv3564 OR Rv3573c OR Rv3761c OR Rv3797 OR Rv0672 OR Rv2500c) AND (Rv0222 OR Rv0456c OR Rv0632c OR Rv0673 OR Rv0675 OR Rv0971c OR Rv1070c OR Rv1071c OR Rv1141c OR Rv1142c OR Rv1472 OR Rv1935c OR Rv2486 OR Rv2679 OR Rv2831 OR Rv3039c OR Rv3516 OR Rv3550 OR Rv3774 OR Rv0905 OR Rv3374 OR Rv3373) AND (Rv0468 OR Rv1715 OR Rv1912c OR Rv3141) AND (Rv0243 OR Rv1074c OR Rv3546 OR Rv3556c OR Rv1323 OR Rv0859)
R562	OCTANOYL-COA + FAD + NAD + COA = HEXANOYL-COA + FADH2 + NADH + ACCOA	0.0	100000.0	(Rv0131c OR Rv0154c OR Rv0215c OR Rv0231 OR Rv0244c OR Rv0271c OR Rv0400c OR Rv0752c OR Rv0873 OR Rv0972c OR Rv0975c OR Rv1346 OR Rv1467c OR Rv1679 OR Rv1933c OR Rv1934c OR Rv2724c OR Rv2789c OR Rv3061c OR Rv3139 OR Rv3140 OR Rv3274c OR Rv3504 OR Rv3505 OR Rv3543c OR Rv3544c OR Rv3560c OR Rv3562 OR Rv3563 OR Rv3564 OR Rv3573c OR Rv3761c OR Rv3797 OR Rv0672 OR Rv2500c) AND (Rv0222 OR Rv0456c OR Rv0632c OR Rv0673 OR Rv0675 OR Rv0971c OR Rv1070c OR Rv1071c OR Rv1141c OR Rv1142c OR Rv1472 OR Rv1935c OR Rv2486 OR Rv2679 OR Rv2831 OR Rv3039c OR Rv3516 OR Rv3550 OR Rv3774 OR Rv0905 OR Rv3374 OR Rv3373) AND (Rv0468 OR Rv1715 OR Rv1912c OR Rv3141) AND (Rv0243 OR Rv1074c OR Rv3546 OR Rv3556c OR Rv1323 OR Rv0859)
R563	HEXANOYL-COA + FAD + NAD + COA = BUTANOYL-COA + FADH2 + NADH + ACCOA	0.0	100000.0	(Rv0131c OR Rv0154c OR Rv0215c OR Rv0231 OR Rv0244c OR Rv0271c OR Rv0400c OR Rv0752c OR Rv0873 OR Rv0972c OR Rv0975c OR Rv1346 OR Rv1467c OR Rv1679 OR Rv1933c OR Rv1934c OR Rv2724c OR Rv2789c OR Rv3061c OR Rv3139 OR Rv3140 OR Rv3274c OR Rv3504 OR Rv3505 OR Rv3543c OR Rv3544c OR Rv3560c OR Rv3562 OR Rv3563 OR Rv3564 OR Rv3573c OR Rv3761c OR Rv3797 OR Rv0672 OR Rv2500c) AND (Rv0222 OR Rv0456c OR

				Rv0632c OR Rv0673 OR Rv0675 OR Rv0971c OR Rv1070c OR Rv1071c OR Rv1141c OR Rv1142c OR Rv1472 OR Rv1935c OR Rv2486 OR Rv2679 OR Rv2831 OR Rv3039c OR Rv3516 OR Rv3550 OR Rv3774 OR Rv0905 OR Rv3374 OR Rv3373) AND (Rv0468 OR Rv1715 OR Rv1912c OR Rv3141) AND (Rv0243 OR Rv1074c OR Rv3546 OR Rv3556c OR Rv1323 OR Rv0859)
R564	BUTANOYL-COA + FAD + NAD + COA = FADH2 + NADH + ACCOA	0.0	100000.0	(Rv0131c OR Rv0154c OR Rv0215c OR Rv0231 OR Rv0244c OR Rv0271c OR Rv0400c OR Rv0752c OR Rv0873 OR Rv0972c OR Rv0975c OR Rv1346 OR Rv1467c OR Rv1679 OR Rv1933c OR Rv1934c OR Rv2724c OR Rv2789c OR Rv3061c OR Rv3139 OR Rv3140 OR Rv3274c OR Rv3504 OR Rv3505 OR Rv3543c OR Rv3544c OR Rv3560c OR Rv3562 OR Rv3563 OR Rv3564 OR Rv3573c OR Rv3761c OR Rv3797 OR Rv0672 OR Rv2500c) AND (Rv0222 OR Rv0456c OR Rv0632c OR Rv0673 OR Rv0675 OR Rv0971c OR Rv1070c OR Rv1071c OR Rv1141c OR Rv1142c OR Rv1472 OR Rv1935c OR Rv2486 OR Rv2679 OR Rv2831 OR Rv3039c OR Rv3516 OR Rv3550 OR Rv3774 OR Rv0905 OR Rv3374 OR Rv3373) AND (Rv0468 OR Rv1715 OR Rv1912c OR Rv3141) AND (Rv0243 OR Rv1074c OR Rv3546 OR Rv3556c OR Rv1323 OR Rv0859)
R565	9-OCTADECENOYL-COA + FAD + NAD + COA = 9-HEXADECENOYL-COA + FADH2 + NADH + ACCOA	0.0	100000.0	(Rv0131c OR Rv0154c OR Rv0215c OR Rv0231 OR Rv0244c OR Rv0271c OR Rv0400c OR Rv0752c OR Rv0873 OR Rv0972c OR Rv0975c OR Rv1346 OR Rv1467c OR Rv1679 OR Rv1933c OR Rv1934c OR Rv2724c OR Rv2789c OR Rv3061c OR Rv3139 OR Rv3140 OR Rv3274c OR Rv3504 OR Rv3505 OR Rv3543c OR Rv3544c OR Rv3560c OR Rv3562 OR Rv3563 OR Rv3564 OR Rv3573c OR Rv3761c OR Rv3797 OR Rv0672 OR Rv2500c) AND (Rv0222 OR Rv0456c OR Rv0632c OR Rv0673 OR Rv0675 OR Rv0971c OR Rv1070c OR Rv1071c OR Rv1141c OR Rv1142c OR Rv1472 OR Rv1935c OR Rv2486 OR Rv2679 OR Rv2831 OR Rv3039c OR Rv3516 OR Rv3550 OR Rv3774 OR Rv0905 OR Rv3374 OR Rv3373) AND (Rv0468 OR Rv1715 OR Rv1912c OR Rv3141) AND (Rv0243 OR Rv1074c OR Rv3546 OR Rv3556c OR Rv1323 OR Rv0859)
R566	9-HEXADECENOYL-COA + FAD + NAD + COA = CIS-DELTA-5-TETRADECANOYL-COA +	0.0	100000.0	(Rv0131c OR Rv0154c OR Rv0215c OR Rv0231 OR Rv0244c OR Rv0271c OR Rv0400c OR Rv0752c OR Rv0873 OR Rv0972c OR Rv0975c OR Rv1346 OR Rv1467c OR Rv1679 OR Rv1933c

	FADH2 + NADH + ACCOA			OR Rv1934c OR Rv2724c OR Rv2789c OR Rv3061c OR Rv3139 OR Rv3140 OR Rv3274c OR Rv3504 OR Rv3505 OR Rv3543c OR Rv3544c OR Rv3560c OR Rv3562 OR Rv3563 OR Rv3564 OR Rv3573c OR Rv3761c OR Rv3797 OR Rv0672 OR Rv2500c) AND (Rv0222 OR Rv0456c OR Rv0632c OR Rv0673 OR Rv0675 OR Rv0971c OR Rv1070c OR Rv1071c OR Rv1141c OR Rv1142c OR Rv1472 OR Rv1935c OR Rv2486 OR Rv2679 OR Rv2831 OR Rv3039c OR Rv3516 OR Rv3550 OR Rv3774 OR Rv0905 OR Rv3374 OR Rv3373) AND (Rv0468 OR Rv1715 OR Rv1912c OR Rv3141) AND (Rv0243 OR Rv1074c OR Rv3546 OR Rv3556c OR Rv1323 OR Rv0859)
R567	CIS-DELTA-5-TETRADECANOYL-COA + FAD + NAD + COA = CIS-DELTA-3-DODECANOYL-COA + FADH2 + NADH + ACCOA	0.0	100000.0	(Rv0131c OR Rv0154c OR Rv0215c OR Rv0231 OR Rv0244c OR Rv0271c OR Rv0400c OR Rv0752c OR Rv0873 OR Rv0972c OR Rv0975c OR Rv1346 OR Rv1467c OR Rv1679 OR Rv1933c OR Rv1934c OR Rv2724c OR Rv2789c OR Rv3061c OR Rv3139 OR Rv3140 OR Rv3274c OR Rv3504 OR Rv3505 OR Rv3543c OR Rv3544c OR Rv3560c OR Rv3562 OR Rv3563 OR Rv3564 OR Rv3573c OR Rv3761c OR Rv3797 OR Rv0672 OR Rv2500c) AND (Rv0222 OR Rv0456c OR Rv0632c OR Rv0673 OR Rv0675 OR Rv0971c OR Rv1070c OR Rv1071c OR Rv1141c OR Rv1142c OR Rv1472 OR Rv1935c OR Rv2486 OR Rv2679 OR Rv2831 OR Rv3039c OR Rv3516 OR Rv3550 OR Rv3774 OR Rv0905 OR Rv3374 OR Rv3373) AND (Rv0468 OR Rv1715 OR Rv1912c OR Rv3141) AND (Rv0243 OR Rv1074c OR Rv3546 OR Rv3556c OR Rv1323 OR Rv0859)
R568	CIS-DELTA-3-DODECANOYL-COA = TRANS-DELTA-2-DODECANOYL-COA	0.0	100000.0	(Rv0131c OR Rv0154c OR Rv0215c OR Rv0231 OR Rv0244c OR Rv0271c OR Rv0400c OR Rv0752c OR Rv0873 OR Rv0972c OR Rv0975c OR Rv1346 OR Rv1467c OR Rv1679 OR Rv1933c OR Rv1934c OR Rv2724c OR Rv2789c OR Rv3061c OR Rv3139 OR Rv3140 OR Rv3274c OR Rv3504 OR Rv3505 OR Rv3543c OR Rv3544c OR Rv3560c OR Rv3562 OR Rv3563 OR Rv3564 OR Rv3573c OR Rv3761c OR Rv3797 OR Rv0672 OR Rv2500c) AND (Rv0222 OR Rv0456c OR Rv0632c OR Rv0673 OR Rv0675 OR Rv0971c OR Rv1070c OR Rv1071c OR Rv1141c OR Rv1142c OR Rv1472 OR Rv1935c OR Rv2486 OR Rv2679 OR Rv2831 OR Rv3039c OR Rv3516 OR Rv3550 OR Rv3774 OR Rv0905 OR Rv3374 OR Rv3373) AND (Rv0468 OR Rv1715 OR Rv1912c OR

				Rv3141) AND (Rv0243 OR Rv1074c OR Rv3546 OR Rv3556c OR Rv1323 OR Rv0859)
R569	TRANS-DELTA-2-DODECANOYL-COA = TRANS-DELTA-2-HYDROXY-DODECANOYL-COA	0.0	100000.0	(Rv0131c OR Rv0154c OR Rv0215c OR Rv0231 OR Rv0244c OR Rv0271c OR Rv0400c OR Rv0752c OR Rv0873 OR Rv0972c OR Rv0975c OR Rv1346 OR Rv1467c OR Rv1679 OR Rv1933c OR Rv1934c OR Rv2724c OR Rv2789c OR Rv3061c OR Rv3139 OR Rv3140 OR Rv3274c OR Rv3504 OR Rv3505 OR Rv3543c OR Rv3544c OR Rv3560c OR Rv3562 OR Rv3563 OR Rv3564 OR Rv3573c OR Rv3761c OR Rv3797 OR Rv0672 OR Rv2500c) AND (Rv0222 OR Rv0456c OR Rv0632c OR Rv0673 OR Rv0675 OR Rv0971c OR Rv1070c OR Rv1071c OR Rv1141c OR Rv1142c OR Rv1472 OR Rv1935c OR Rv2486 OR Rv2679 OR Rv2831 OR Rv3039c OR Rv3516 OR Rv3550 OR Rv3774 OR Rv0905 OR Rv3374 OR Rv3373) AND (Rv0468 OR Rv1715 OR Rv1912c OR Rv3141) AND (Rv0243 OR Rv1074c OR Rv3546 OR Rv3556c OR Rv1323 OR Rv0859)
R570	TRANS-DELTA-2-HYDROXY-DODECANOYL-COA + NAD = DODECANOYL-COA + NADH	0.0	100000.0	(Rv0131c OR Rv0154c OR Rv0215c OR Rv0231 OR Rv0244c OR Rv0271c OR Rv0400c OR Rv0752c OR Rv0873 OR Rv0972c OR Rv0975c OR Rv1346 OR Rv1467c OR Rv1679 OR Rv1933c OR Rv1934c OR Rv2724c OR Rv2789c OR Rv3061c OR Rv3139 OR Rv3140 OR Rv3274c OR Rv3504 OR Rv3505 OR Rv3543c OR Rv3544c OR Rv3560c OR Rv3562 OR Rv3563 OR Rv3564 OR Rv3573c OR Rv3761c OR Rv3797 OR Rv0672 OR Rv2500c) AND (Rv0222 OR Rv0456c OR Rv0632c OR Rv0673 OR Rv0675 OR Rv0971c OR Rv1070c OR Rv1071c OR Rv1141c OR Rv1142c OR Rv1472 OR Rv1935c OR Rv2486 OR Rv2679 OR Rv2831 OR Rv3039c OR Rv3516 OR Rv3550 OR Rv3774 OR Rv0905 OR Rv3374 OR Rv3373) AND (Rv0468 OR Rv1715 OR Rv1912c OR Rv3141) AND (Rv0243 OR Rv1074c OR Rv3546 OR Rv3556c OR Rv1323 OR Rv0859)
R571	PA = DAG + PI	0.0	100000.0	orphan
R571 b	TAGcat = TAGbio	-100000.0	100000.0	orphan
R572	TAGcat = DAG + HEXADECANOATE + OCTADECANOATE + 9-OCTADECENOATE + EICOSANOATE + TETRACOSANOATE +	0.0	100000.0	Rv3097c

	HEXACOSANOATE + PENTADECANOATE + NONADECANOATE			
R573	DAG = MAG + HEXADECANOATE + OCTADECANOATE + 9-OCTADECENOATE + EICOSANOATE + TETRACOSANOATE + HEXACOSANOATE + PENTADECANOATE + NONADECANOATE	0.0	100000.0	orphan
R574	MAG = GL + HEXADECANOATE + OCTADECANOATE + 9-OCTADECENOATE + EICOSANOATE + TETRACOSANOATE + HEXACOSANOATE + PENTADECANOATE + NONADECANOATE	0.0	100000.0	Rv0183 OR Rv2854
R575	NONADECANOYL-COA + FAD + NAD + COA = HEPTADECANOYL-COA + FADH2 + NADH + ACCOA	0.0	100000.0	(Rv0131c OR Rv0154c OR Rv0215c OR Rv0231 OR Rv0244c OR Rv0271c OR Rv0400c OR Rv0752c OR Rv0873 OR Rv0972c OR Rv0975c OR Rv1346 OR Rv1467c OR Rv1679 OR Rv1933c OR Rv1934c OR Rv2724c OR Rv2789c OR Rv3061c OR Rv3139 OR Rv3140 OR Rv3274c OR Rv3504 OR Rv3505 OR Rv3543c OR Rv3544c OR Rv3560c OR Rv3562 OR Rv3563 OR Rv3564 OR Rv3573c OR Rv3761c OR Rv3797 OR Rv0672 OR Rv2500c) AND (Rv0222 OR Rv0456c OR Rv0632c OR Rv0673 OR Rv0675 OR Rv0971c OR Rv1070c OR Rv1071c OR Rv1141c OR Rv1142c OR Rv1472 OR Rv1935c OR Rv2486 OR Rv2679 OR Rv2831 OR Rv3039c OR Rv3516 OR Rv3550 OR Rv3774 OR Rv0905 OR Rv3374 OR Rv3373) AND (Rv0468 OR Rv1715 OR Rv1912c OR Rv3141) AND (Rv0243 OR Rv1074c OR Rv3546 OR Rv3556c OR Rv1323 OR Rv0859)
R576	HEPTADECANOYL-COA + FAD + NAD + COA = PENTADECANOYL-COA + FADH2 + NADH + ACCOA	0.0	100000.0	(Rv0131c OR Rv0154c OR Rv0215c OR Rv0231 OR Rv0244c OR Rv0271c OR Rv0400c OR Rv0752c OR Rv0873 OR Rv0972c OR Rv0975c OR Rv1346 OR Rv1467c OR Rv1679 OR Rv1933c OR Rv1934c OR Rv2724c OR Rv2789c OR Rv3061c OR Rv3139 OR Rv3140 OR Rv3274c OR Rv3504 OR Rv3505 OR Rv3543c OR Rv3544c OR Rv3560c OR Rv3562 OR Rv3563 OR Rv3564 OR Rv3573c OR Rv3761c OR Rv3797 OR Rv0672 OR

				Rv2500c) AND (Rv0222 OR Rv0456c OR Rv0632c OR Rv0673 OR Rv0675 OR Rv0971c OR Rv1070c OR Rv1071c OR Rv1141c OR Rv1142c OR Rv1472 OR Rv1935c OR Rv2486 OR Rv2679 OR Rv2831 OR Rv3039c OR Rv3516 OR Rv3550 OR Rv3774 OR Rv0905 OR Rv3374 OR Rv3373) AND (Rv0468 OR Rv1715 OR Rv1912c OR Rv3141) AND (Rv0243 OR Rv1074c OR Rv3546 OR Rv3556c OR Rv1323 OR Rv0859)
R577	PENTADECANOYL-COA + FAD + NAD + COA = TRIDECANOYL-COA + FADH2 + NADH + ACCOA	0.0	100000.0	(Rv0131c OR Rv0154c OR Rv0215c OR Rv0231 OR Rv0244c OR Rv0271c OR Rv0400c OR Rv0752c OR Rv0873 OR Rv0972c OR Rv0975c OR Rv1346 OR Rv1467c OR Rv1679 OR Rv1933c OR Rv1934c OR Rv2724c OR Rv2789c OR Rv3061c OR Rv3139 OR Rv3140 OR Rv3274c OR Rv3504 OR Rv3505 OR Rv3543c OR Rv3544c OR Rv3560c OR Rv3562 OR Rv3563 OR Rv3564 OR Rv3573c OR Rv3761c OR Rv3797 OR Rv0672 OR Rv2500c) AND (Rv0222 OR Rv0456c OR Rv0632c OR Rv0673 OR Rv0675 OR Rv0971c OR Rv1070c OR Rv1071c OR Rv1141c OR Rv1142c OR Rv1472 OR Rv1935c OR Rv2486 OR Rv2679 OR Rv2831 OR Rv3039c OR Rv3516 OR Rv3550 OR Rv3774 OR Rv0905 OR Rv3374 OR Rv3373) AND (Rv0468 OR Rv1715 OR Rv1912c OR Rv3141) AND (Rv0243 OR Rv1074c OR Rv3546 OR Rv3556c OR Rv1323 OR Rv0859)
R578	TRIDECANOYL-COA + FAD + NAD + COA = UNDECANOYL-COA + FADH2 + NADH + ACCOA	0.0	100000.0	(Rv0131c OR Rv0154c OR Rv0215c OR Rv0231 OR Rv0244c OR Rv0271c OR Rv0400c OR Rv0752c OR Rv0873 OR Rv0972c OR Rv0975c OR Rv1346 OR Rv1467c OR Rv1679 OR Rv1933c OR Rv1934c OR Rv2724c OR Rv2789c OR Rv3061c OR Rv3139 OR Rv3140 OR Rv3274c OR Rv3504 OR Rv3505 OR Rv3543c OR Rv3544c OR Rv3560c OR Rv3562 OR Rv3563 OR Rv3564 OR Rv3573c OR Rv3761c OR Rv3797 OR Rv0672 OR Rv2500c) AND (Rv0222 OR Rv0456c OR Rv0632c OR Rv0673 OR Rv0675 OR Rv0971c OR Rv1070c OR Rv1071c OR Rv1141c OR Rv1142c OR Rv1472 OR Rv1935c OR Rv2486 OR Rv2679 OR Rv2831 OR Rv3039c OR Rv3516 OR Rv3550 OR Rv3774 OR Rv0905 OR Rv3374 OR Rv3373) AND (Rv0468 OR Rv1715 OR Rv1912c OR Rv3141) AND (Rv0243 OR Rv1074c OR Rv3546 OR Rv3556c OR Rv1323 OR Rv0859)
R579	UNDECANOYL-COA + FAD + NAD + COA = NONANOYL-COA +	0.0	100000.0	(Rv0131c OR Rv0154c OR Rv0215c OR Rv0231 OR Rv0244c OR Rv0271c OR Rv0400c OR Rv0752c OR Rv0873 OR Rv0972c OR Rv0975c

	FADH2 + NADH + ACCOA			OR Rv1346 OR Rv1467c OR Rv1679 OR Rv1933c OR Rv1934c OR Rv2724c OR Rv2789c OR Rv3061c OR Rv3139 OR Rv3140 OR Rv3274c OR Rv3504 OR Rv3505 OR Rv3543c OR Rv3544c OR Rv3560c OR Rv3562 OR Rv3563 OR Rv3564 OR Rv3573c OR Rv3761c OR Rv3797 OR Rv0672 OR Rv2500c) AND (Rv0222 OR Rv0456c OR Rv0632c OR Rv0673 OR Rv0675 OR Rv0971c OR Rv1070c OR Rv1071c OR Rv1141c OR Rv1142c OR Rv1472 OR Rv1935c OR Rv2486 OR Rv2679 OR Rv2831 OR Rv3039c OR Rv3516 OR Rv3550 OR Rv3774 OR Rv0905 OR Rv3374 OR Rv3373) AND (Rv0468 OR Rv1715 OR Rv1912c OR Rv3141) AND (Rv0243 OR Rv1074c OR Rv3546 OR Rv3556c OR Rv1323 OR Rv0859)
R580	NONANOYL-COA + FAD + NAD + COA = HEPTANOYL-COA + FADH2 + NADH + ACCOA	0.0	100000.0	(Rv0131c OR Rv0154c OR Rv0215c OR Rv0231 OR Rv0244c OR Rv0271c OR Rv0400c OR Rv0752c OR Rv0873 OR Rv0972c OR Rv0975c OR Rv1346 OR Rv1467c OR Rv1679 OR Rv1933c OR Rv1934c OR Rv2724c OR Rv2789c OR Rv3061c OR Rv3139 OR Rv3140 OR Rv3274c OR Rv3504 OR Rv3505 OR Rv3543c OR Rv3544c OR Rv3560c OR Rv3562 OR Rv3563 OR Rv3564 OR Rv3573c OR Rv3761c OR Rv3797 OR Rv0672 OR Rv2500c) AND (Rv0222 OR Rv0456c OR Rv0632c OR Rv0673 OR Rv0675 OR Rv0971c OR Rv1070c OR Rv1071c OR Rv1141c OR Rv1142c OR Rv1472 OR Rv1935c OR Rv2486 OR Rv2679 OR Rv2831 OR Rv3039c OR Rv3516 OR Rv3550 OR Rv3774 OR Rv0905 OR Rv3374 OR Rv3373) AND (Rv0468 OR Rv1715 OR Rv1912c OR Rv3141) AND (Rv0243 OR Rv1074c OR Rv3546 OR Rv3556c OR Rv1323 OR Rv0859)
R581	HEPTANOYL-COA + FAD + NAD + COA = PENTANOYL-COA + FADH2 + NADH + ACCOA	0.0	100000.0	(Rv0131c OR Rv0154c OR Rv0215c OR Rv0231 OR Rv0244c OR Rv0271c OR Rv0400c OR Rv0752c OR Rv0873 OR Rv0972c OR Rv0975c OR Rv1346 OR Rv1467c OR Rv1679 OR Rv1933c OR Rv1934c OR Rv2724c OR Rv2789c OR Rv3061c OR Rv3139 OR Rv3140 OR Rv3274c OR Rv3504 OR Rv3505 OR Rv3543c OR Rv3544c OR Rv3560c OR Rv3562 OR Rv3563 OR Rv3564 OR Rv3573c OR Rv3761c OR Rv3797 OR Rv0672 OR Rv2500c) AND (Rv0222 OR Rv0456c OR Rv0632c OR Rv0673 OR Rv0675 OR Rv0971c OR Rv1070c OR Rv1071c OR Rv1141c OR Rv1142c OR Rv1472 OR Rv1935c OR Rv2486 OR Rv2679 OR Rv2831 OR Rv3039c OR Rv3516 OR Rv3550 OR Rv3774 OR Rv0905 OR Rv3374 OR Rv3373)

				AND (Rv0468 OR Rv1715 OR Rv1912c OR Rv3141) AND (Rv0243 OR Rv1074c OR Rv3546 OR Rv3556c OR Rv1323 OR Rv0859)
R582	PENTANOYL-COA + FAD + NAD + COA = PROPIONYLCOA + FADH2 + NADH + ACCOA	0.0	100000.0	(Rv0131c OR Rv0154c OR Rv0215c OR Rv0231 OR Rv0244c OR Rv0271c OR Rv0400c OR Rv0752c OR Rv0873 OR Rv0972c OR Rv0975c OR Rv1346 OR Rv1467c OR Rv1679 OR Rv1933c OR Rv1934c OR Rv2724c OR Rv2789c OR Rv3061c OR Rv3139 OR Rv3140 OR Rv3274c OR Rv3504 OR Rv3505 OR Rv3543c OR Rv3544c OR Rv3560c OR Rv3562 OR Rv3563 OR Rv3564 OR Rv3573c OR Rv3761c OR Rv3797 OR Rv0672 OR Rv2500c) AND (Rv0222 OR Rv0456c OR Rv0632c OR Rv0673 OR Rv0675 OR Rv0971c OR Rv1070c OR Rv1071c OR Rv1141c OR Rv1142c OR Rv1472 OR Rv1935c OR Rv2486 OR Rv2679 OR Rv2831 OR Rv3039c OR Rv3516 OR Rv3550 OR Rv3774 OR Rv0905 OR Rv3374 OR Rv3373) AND (Rv0468 OR Rv1715 OR Rv1912c OR Rv3141) AND (Rv0243 OR Rv1074c OR Rv3546 OR Rv3556c OR Rv1323 OR Rv0859)
R583	HEXADECANOYL-COA + 9-HEXADECENOYL-COA + OCTADECANOYL-COA + 9-OCTADECENOYL-COA + EICOSANOYL-COA + TETRACOSANOYL-COA + HEXACOSANOYL-COA + NONADECANOYL-COA + PENTADECANOYL-COA + GL3P = AGL3P + COA	0.0	100000.0	Rv2482c OR Rv1551
R587	AGL3P + HEXADECANOYL-COA + 9-HEXADECENOYL-COA + OCTADECANOYL-COA + 9-OCTADECENOYL-COA + EICOSANOYL-COA + TETRACOSANOYL-COA + HEXACOSANOYL-COA + NONADECANOYL-COA + PENTADECANOYL-COA = PA + COA	0.0	100000.0	Rv2483c OR Rv2182c
R588	PA + CTP = CDPDG + PPI	-100000.0	100000.0	Rv2881c
R589	CDPDG + SER = CMP + PS	-100000.0	100000.0	Rv0436c
R590	PHOSPHATIDYLCHOLINE = DAG	0.0	100000.0	Rv0217c OR Rv0220 OR Rv0646c OR Rv1076 OR Rv1104 OR Rv1105 OR Rv1399c OR Rv1400c OR Rv1426c OR Rv1497 OR Rv1755c OR Rv1900c

				OR Rv1923 OR Rv2045c OR Rv2284 OR Rv2349c OR Rv2350c OR Rv2351c OR Rv2385 OR Rv2463 OR Rv2485c OR Rv2970c OR Rv3084 OR Rv3176c OR Rv3203 OR Rv3487c OR Rv3775
R591	DHAP + NADH = NAD + GL3P	-100000.0	100000.0	Rv2982c OR Rv0564
R592	CDPDG + GL3P = PGP + CMP	-100000.0	100000.0	Rv2746c
R593	PGP = PI + PG	0.0	100000.0	orphan
R594	HEXADECANOYL-ACP + GL3P = ACP + A160GL3P	0.0	100000.0	Rv2482c
R595	A160GL3P + TUBERCULOSTEROYL-ACP = PA-TBA + ACP	0.0	100000.0	Rv2483c OR Rv2182c
R596	CTP + PA-TBA = PPI + CDPDAG-TBA	0.0	100000.0	Rv2881c
R597	MI + CDPDAG-TBA = CMP + PI-TBA	0.0	100000.0	Rv2612c
R598	GDPMAN + PI-TBA = GDP + AC1PIM1	0.0	100000.0	Rv2610c
R599	HEXADECANOYL-ACP + AC1PIM1 = ACP + AC2PIM1	-100000.0	100000.0	Rv2611c
R600	HEXADECANOYL-ACP + AC2PIM1 = ACP + AC3PIM1	-100000.0	100000.0	Rv2611c
R601	HEXADECANOYL-ACP + AC3PIM1 = ACP + AC4PIM1	-100000.0	100000.0	Rv2611c
R602	GDPMAN + AC1PIM1 = GDP + AC1PIM2	0.0	100000.0	Rv0557
R603	HEXADECANOYL-ACP + AC1PIM2 = ACP + AC2PIM2	-100000.0	100000.0	Rv2611c
R604	HEXADECANOYL-ACP + AC2PIM2 = ACP + AC3PIM2	-100000.0	100000.0	Rv2611c
R605	HEXADECANOYL-ACP + AC3PIM2 = ACP + AC4PIM2	-100000.0	100000.0	Rv2611c
R606	GDPMAN + AC1PIM2 = GDP + AC1PIM3	0.0	100000.0	orphan
R607	HEXADECANOYL-ACP + AC1PIM3 = ACP +	-100000.0	100000.0	Rv2611c

	AC2PIM3			
R608	HEXADECANOYL-ACP + AC2PIM3 = ACP + AC3PIM3	-100000.0	100000.0	Rv2611c
R609	HEXADECANOYL-ACP + AC3PIM3 = ACP + AC4PIM3	-100000.0	100000.0	Rv2611c
R610	PPM + AC3PIM3 = DPP + AC3PIM4	0.0	100000.0	orphan
R611	PPM + AC3PIM4 = DPP + AC3PIM5	0.0	100000.0	orphan
R612	HEXADECANOYL-ACP + AC3PIM5 = ACP + AC4PIM5	-100000.0	100000.0	Rv2611c
R613	PPM + AC4PIM5 = DPP + AC4PIM6	0.0	100000.0	Rv1500
R614	PPM + AC4PIM6 = DPP + AC4PIM7	0.0	100000.0	orphan
R615	HEXANOYL-COA + MALCOA + SMMALONYLCOA + NADPH = PENTA-METHYL-TRICONTANOYL + CO2 + NADP + COA	0.0	100000.0	Rv2048c
R616	PENTA-METHYL-TRICONTANOYL + COA = PENTA-METHYL-TRICONTANOYL-COA	0.0	100000.0	Rv2048c
R617	PENTA-METHYL-TRICONTANOYL-COA + ATP = PHOSPHO-PENTA-METHYL-TRICONTANOYL-COA + ADP	0.0	100000.0	orphan
R618	MALCOA + ACP = MALACP + COA	0.0	100000.0	(Rv2243 OR Rv0649) AND Rv2244
R619	SMMALONYLCOA + ACP = RMMALONYLACP + COA	0.0	100000.0	(Rv2243 OR Rv0649) AND Rv2244
R620	EICOSANOYL-COA + MALACP = BETA-KETO-C22-ACYL-ACP + CO2 + COA	0.0	100000.0	Rv0533c
R621	BETA-KETO-C22-ACYL-ACP + NADPH = D-3-HYDROXY-C22-ACYL-ACP	0.0	100000.0	Rv1483 OR Rv1350 OR Rv2002 OR Rv0242c OR Rv2766c

	+ NADP			
R622	D-3-HYDROXY-C22-ACYL-ACP = TRANS-DELTA-2-ENOYL-C22-ACYL-ACP	0.0	100000.0	Rv0098 OR Rv0130
R623	TRANS-DELTA-2-ENOYL-C22-ACYL-ACP = CIS-DELTA-3-ENOYL-C22-ACYL-ACP	0.0	100000.0	Rv1142 OR Rv1141c
R624	CIS-DELTA-3-ENOYL-C22-ACYL-ACP + MALACP + NADPH = CIS-DELTA-13-ENOYL-C32-ACYL-ACP + CO2 + NADP + ACP	0.0	100000.0	(Rv2245 OR Rv2246) AND (Rv1483 OR Rv1350 OR Rv2002 OR Rv0242c OR Rv2766c) AND (Rv0098 OR Rv0130) AND Rv1484
R625	CIS-DELTA-13-ENOYL-C32-ACYL-ACP + MALACP + NADPH = CIS-DELTA-2-3,15-ENOYL-C34-ACYL-ACP + NADP + CO2 + ACP	0.0	100000.0	(Rv2245 OR Rv2246) AND (Rv1483 OR Rv1350 OR Rv2002 OR Rv0242c OR Rv2766c) AND (Rv0098 OR Rv0130) AND (Rv1142c OR Rv1141c)
R626	CIS-DELTA-2-3,15-ENOYL-C34-ACYL-ACP + MALACP + NADPH = CIS-DELTA-2-19,31-ENOYL-C50-ACYL-ACP + CO2 + NADP + ACP	0.0	100000.0	(Rv2245 OR Rv2246) AND (Rv1483 OR Rv1350 OR Rv2002 OR Rv0242c OR Rv2766c) AND (Rv0098 OR Rv0130) AND Rv1484
R627	CIS-DELTA-2-19,31-ENOYL-C50-ACYL-ACP + SAM + NADP = CYCLOPROPYL-MEROACYL-ACP + SAH + NADPH	0.0	100000.0	Rv0643c AND Rv0503c
R628	CIS-DELTA-3-ENOYL-C22-ACYL-ACP + MALACP + NADPH = CIS-DELTA-19-ENOYL-C38-ACYL-ACP + CO2 + NADP + ACP	0.0	100000.0	(Rv2245 OR Rv2246) AND (Rv1483 OR Rv1350 OR Rv2002 OR Rv0242c OR Rv2766c) AND (Rv0098 OR Rv0130) AND Rv1484
R629	CIS-DELTA-19-ENOYL-C38-ACYL-ACP + MALACP + NADPH = CIS-DELTA-2-3,21-ENOYL-C40-ACYL-ACP + CO2 + NADP + ACP	0.0	100000.0	(Rv2245 OR Rv2246) AND (Rv1483 OR Rv1350 OR Rv2002 OR Rv0242c OR Rv2766c) AND (Rv0098 OR Rv0130) AND (Rv1142c OR Rv1141c)
R630	CIS-DELTA-2-3,21-ENOYL-C40-ACYL-ACP + MALACP + NADPH = CIS-DELTA-2-19,37-ENOYL-C56-ACYL-ACP + CO2 + NADP + ACP	0.0	100000.0	(Rv2245 OR Rv2246) AND (Rv1483 OR Rv1350 OR Rv2002 OR Rv0242c OR Rv2766c) AND (Rv0098 OR Rv0130) AND Rv1484
R631	CIS-DELTA-2-19,37-ENOYL-C56-ACYL-ACP + SAM = CIS-DELTA-37-ENOYL-	0.0	100000.0	Rv0642c

	METHY-HYDROXY-C56-ACYL-ACP + SAH			
R632	CIS-DELTA-37-ENOYL-METHY-HYDROXY-C56-ACYL-ACP + SAM + NADP = CIS-METHOXY-MEROACYL-ACP + SAH + NADPH	0.0	100000.0	Rv0643c AND Rv0644c
R633	CIS-DELTA-37-ENOYL-METHY-HYDROXY-C56-ACYL-ACP + SAM + NADP = CIS-KETO-MEROACYL-ACP + SAH + NADPH	0.0	100000.0	Rv0644c
R634	CIS-DELTA-37-ENOYL-METHY-HYDROXY-C56-ACYL-ACP + SAM + NADP = CIS-DELTA-37-ENOYL-DIMETHY-HYDROXY-C56-ACYL-ACP + SAH + NADPH	0.0	100000.0	Rv0645c
R635	CIS-DELTA-37-ENOYL-DIMETHY-HYDROXY-C56-ACYL-ACP + SAM + NADP = TRANS-METHOXY-MEROACYL-ACP + SAH + NADPH	0.0	100000.0	Rv0643c AND Rv0503c
R636	CIS-DELTA-37-ENOYL-DIMETHY-HYDROXY-C56-ACYL-ACP + SAM + NADP = TRANS-KETO-MEROACYL-ACP + SAH + NADPH	0.0	100000.0	Rv0503c
R637	CYCLOPROPYL-MEROACYL-ACP + CIS-METHOXY-MEROACYL-ACP + TRANS-METHOXY-MEROACYL-ACP + CIS-KETO-MEROACYL-ACP + TRANS-KETO-MEROACYL-ACP + ATP = MEROACYL-AMP + ACP + PI	0.0	100000.0	Rv3801c
R638	MEROACYL-AMP + HEXACOSANOYL-COA-CO2 = C78-3-OXY-MYCOLATE-ENZ + CO2 + AMP + COA	0.0	100000.0	Rv3800c

R639	C78-3-OXY-MYCOLATE-ENZ + NADPH = C78MYCOLATE-ENZ	0.0	100000.0	orphan
R640	C78MYCOLATE-ENZ + PPM = C78MYCOLATE-PP	0.0	100000.0	Rv3802c
R641	C78MYCOLATE-PP + TRE6P = TREHALOSEMONOMYCOLATE-P + PPM	0.0	100000.0	Rv1288 OR Rv0519c OR Rv0774c
R642	TREHALOSEMONOMYCOLATE-P = TREHALOSEMONOMYCOLATE(CY) + PI	0.0	100000.0	Rv3400 OR Rv2006
R643	COA = MAS	0.0	100000.0	orphan
R644	EICOSANOYL-ACP + DOCOSANOYL-ACP + TETRACOSANOYL-ACP + OCTACOSANOYL-ACP + MAS = ACYL-MAS + ACP	0.0	100000.0	Rv2941
R645	ACYL-MAS + SMMALONYLCOA + NADPH = MYCOCEROSOYL-MAS + NADP + CO2 + COA	0.0	100000.0	Rv2940c
R646	HEXADECANOYL-COA + MAS = HEXADECANOYL-MAS + COA	0.0	100000.0	Rv2940c
R647	HEXADECANOYL-MAS + SMMALONYLCOA + NADPH = PTHIOCERANOYL-COA + NADP + CO2 + COA + MAS	0.0	100000.0	Rv3825c
R648	HEXADECANOYL-MAS + SMMALONYLCOA + NADPH = HYDROXYPHTHIOCERANOYL-COA + NADP + CO2 + COA + MAS	0.0	100000.0	Rv3825c
R649	SMMALONYLCOA + HEXADECANOYL-ACP + NADPH = NADP + COA + CO2 + TUBERCULOSTEROYL-ACP	0.0	100000.0	Rv2940c
R650	CHOR = HBA + PYR	0.0	100000.0	Rv2949c

R651	DOCOSANOYL-COA + ATP + MALCOA + SMMALONYLCOA + NADPH = PHTHIODIOLONE-A + CO2 + NADP + AMP + PPI	0.0	100000.0	Rv2931 AND Rv2932 AND Rv2933 AND Rv2934 AND Rv2935
R652	PHTHIODIOLONE-A + NADPH = PTT + NADP	0.0	100000.0	Rv2951c
R653	PTT + SAM = PTC + SAH	0.0	100000.0	Rv2952
R654	PTC + MYCOCEROSOYL-MAS = DIM-CYTO + MAS	0.0	100000.0	Rv2939
R655	HBA + MALCOA + NADPH + ATP = PHPAA-COA + COA + CO2 + AMP + PPI	0.0	100000.0	Rv2947c AND Rv2946c
R656	PHPAA-COA + MALCOA + SMMALONYLCOA = PHENOLPHTHIODIOLONE-A + CO2 + COA	0.0	100000.0	Rv2931 AND Rv2932 AND Rv2933 AND Rv2934 AND Rv2935 AND Rv2930 AND Rv2941 AND Rv1661
R657	PHENOLPHTHIODIOLONE-A + NADPH = PPTT + NADP	0.0	100000.0	Rv2951c
R658	PPTT + SAM = PPTC + SAH	0.0	100000.0	Rv2952
R659	PPTC + MYCOCEROSOYL-MAS = PHDIM-CYTO + MAS	0.0	100000.0	Rv2939
R660	PHDIM-CYTO = PHDIM	0.0	100000.0	Rv2942 AND Rv2936 AND Rv2937 AND Rv2938
R661	PHDIM + DTDPRHAM = PHDIMRHAM1 + DTDP	0.0	100000.0	Rv2962c
R662	PHDIMRHAM1 + DTDPRHAM = PHDIMRHAM2 + DTDP	0.0	100000.0	Rv2958c
R663	PHDIMRHAM2 + SAM = MYCOSIDE_B + SAH	0.0	100000.0	Rv2959c
R668	TRE + PAPS = TRE-S + PAP	0.0	100000.0	Rv3529c OR Rv1373 OR Rv2267c
R669	TRE-S + HEXADECANOYL-COA + OCTADECANOYL-COA + EICOSANOYL-COA = ACYL-TRE-S-COA	0.0	100000.0	orphan
R670	ACYL-TRE-S-COA + HYDROXYPHTHIOCERANOYL-COA = SL1278-CYTO + COA	0.0	100000.0	orphan
R671	SL1278-CYTO = SL1278-WALL	0.0	100000.0	Rv3823c

R672	OCTADECANOYL-COA + RMMALONYLACP + NADPH = MYCOLIPANOIC-ACP + CO2 + NADP + COA + ACP	0.0	100000.0	Rv1180 AND Rv1181
R673	OCTADECANOYL-COA + RMMALONYLACP + NADPH = MYCOLIPENOYL-ACP + CO2 + NADP + COA + ACP	0.0	100000.0	Rv1180 AND Rv1182
R674	OCTADECANOYL-COA + RMMALONYLACP + NADPH = MYCOLIPDIENOYL-ACP + CO2 + NADP + COA + ACP	0.0	100000.0	Rv1180 AND Rv1183
R678	G3P + PYR = DX5P + CO2	0.0	100000.0	Rv3379c OR Rv2682c
R679	DX5P + NADPH = MDE4P + NADP	0.0	100000.0	Rv2870c
R680	MDE4P + CTP = CDPMDE + PPI	0.0	100000.0	Rv3582c
R681	CDPMDE + ATP = 2PCDPMDE + ADP	0.0	100000.0	Rv1011
R682	2PCDPMDE = MDECPP + CMP	0.0	100000.0	Rv3581c
R683	MDECPP + NADH = HMB4PP + NAD	0.0	100000.0	Rv2868c
R684	HMB4PP + NADH = IPP + NAD	0.0	100000.0	Rv3382c OR Rv1110
R685	IPP = DMPP	-100000.0	100000.0	Rv1745c
R686	IPP + DMPP = GPP + PPI	0.0	100000.0	Rv3398c OR Rv3383c OR Rv2173
R687	IPP + GPP = FPP + PPI	0.0	100000.0	Rv1086
R688	IPP + FPP = GGPP + PPI	0.0	100000.0	Rv3398c
R689	IPP + GGPP = PPPP + PPI	0.0	100000.0	Rv3398c
R690	IPP + PPPP = HPPP + PPI	0.0	100000.0	orphan
R691	IPP + HPPP = HEPPP + PPI	0.0	100000.0	Rv0562
R692	IPP + HEPPP = OPP + PPI	0.0	100000.0	orphan
R693	IPP + OPP = NPP + PPI	0.0	100000.0	orphan
R694	FPP + IPP = DPP	0.0	100000.0	Rv2361c
R695	PRPP + DPP = PPI + DPPPR	0.0	100000.0	Rv3806c
R696	DPPPR = PI + DPPR	0.0	100000.0	orphan
R697	DPPR = ARAFDPP	0.0	100000.0	Rv3790 AND Rv3791
R698	ALA = DALA	-100000.0	100000.0	Rv3423c

R699	DALA + ATP = ALAALA + PI + ADP	0.0	100000.0	Rv2981c
R700	DPP + UDPNAG = NAGDPP + UMP	0.0	100000.0	orphan
R701	NAGDPP + DTDPRHAM = RHAMNAGDPP + DTDP	0.0	100000.0	Rv3265c OR Rv1525
R702	RHAMNAGDPP + UDPGALF = GALACTANDPP + UDP	-100000.0	100000.0	Rv3808c
R705	GALACTANDPP + ARAFDPP = ARA[1]GALACTANDPP + DPP	-100000.0	100000.0	Rv3792
R706	ARA[1]GALACTANDPP + ARAFDPP = ARABINOGALACTANDPP + DPP	-100000.0	100000.0	Rv3794 OR Rv3795
R707	G1P + DTTP = DTDPGLC + PPI	0.0	100000.0	Rv0334
R708	DTDPGLC = DTDP4DH6DGLC	-100000.0	100000.0	Rv3464 OR Rv3634c OR Rv3468 OR Rv3784
R709	DTDP4DH6DGLC = DTDP4DH6DMAN	0.0	100000.0	Rv3465
R710	DTDP4DH6DMAN + NADPH = DTDPRHAM + NADP	0.0	100000.0	Rv3260c
R711	UDPGAL = UDPGALF	0.0	100000.0	Rv3809c
R712	GLN + F6P = GLU + GA6P	-100000.0	100000.0	Rv3436c
R713	GLU = DGLU	0.0	100000.0	Rv1338
R714	GA6P = F6P + NH3	-100000.0	100000.0	orphan
R715	GA1P = GA6P	-100000.0	100000.0	Rv3068c
R716	ACCOA + GA1P = COA + NAGA1P	-100000.0	100000.0	orphan
R717	NAGA1P + UTP = UDPNAG + PPI	0.0	100000.0	Rv1018c
R718	UDPNAG + PEP = UDPNAGPEE	-100000.0	100000.0	Rv1315
R719	UDPNAGPEE + NADPH = UDPNAM + NADP	0.0	100000.0	Rv0482
R722	UDPNAM + NADPH = UDPNGM + NADP	0.0	100000.0	Rv3818
R723	UDPNGM + UDPNAM + ATP + ALA =	-100000.0	100000.0	Rv2152c

	UDP[NAM:NGM]ALA + ADP + PI			
R724	UDP[NAM:NGM]ALA + ATP + DGLU = UDP[NAM:NGM]ALAGLU + ADP + PI	0.0	100000.0	Rv2155c
R725	UDP[NAM:NGM]ALAGLU + ATP + MDAPIM = UDP[NAM:NGM]AGMDAPIM + ADP + PI	0.0	100000.0	Rv2158c
R726	UDP[NAM:NGM]AGMDAPIM + ALAALA + ATP = UDP[NAM:NGM]AGMDAPIMAA + ADP + PI	0.0	100000.0	Rv2157c
R727	UDP[NAM:NGM]AGMDAPIMAA + DPP = LIPID1 + UMP	-100000.0	100000.0	Rv2156c
R728	LIPID1 + UDPNAG = LIPID2 + UDP	0.0	100000.0	Rv2153c
R729	LIPID2 + NH3 + ATP = LIPID2-AMIDATED + ADP + PI	0.0	100000.0	orphan
R730	LIPID2-AMIDATED = PEPTIDOGLYCAN + DPP	0.0	100000.0	orphan
R731	PEPTIDOGLYCAN + ARABINOGALACTANDPP = ARABINOGALACTAN_PEPTIDOGLYCAN + DPP	0.0	100000.0	orphan
PROT	ILE + VAL + MET + ALA + HIS + LYS + LEU + ARG + ASP + SER + GLU + GLN + THR + TRP + TYR + CYS + ASN + ATP + GLY + PRO + PHE = PROTEIN	0.0	100000.0	orphan
RNA	UTP + CTP + ATP + GTP = RNA + ADP + PI + PPI	0.0	100000.0	orphan
DNA	DTTP + DGTP + DCTP + ATP + DATP = DNA + ADP + PI + PPI	0.0	100000.0	orphan
SM_MOL	NAD + NADP + COA + ACP + LIPO + MBT-HOLO + MK + FMN + FAD + MAS + HEME-FE2 + HEME-FE3 + FE2 + FE3 + FERO + FERI +	0.0	100000.0	orphan

	SPRMD + MTR1P = SMALLMOLECULES			
PE	PS = PE + CO2	0.0	100000.0	Rv0437c
TAG	HEXADECANOYL-COA + 9-HEXADECENOYL-COA + OCTADECANOYL-COA + 9-OCTADECENOYL-COA + EICOSANOYL-COA + TETRACOSANOYL-COA + HEXACOSANOYL-COA + NONADECANOYL-COA + PENTADECANOYL-COA + DAG = PI + TAGbio + COA	0.0	100000.0	orphan
PIMS	AC2PIM1 + AC2PIM2 + AC3PIM5 + AC4PIM6 + AC4PIM7 = PIMS	0.0	100000.0	orphan
LAM	LM + ARAFDPP = DPP + LAM	0.0	100000.0	Rv3793
MAPC	ARABINOGALACTAN_PEPTIDOGLYCAN + TREHALOSEMONOMYCOLATE = MAPC + TRE	0.0	100000.0	Rv3804c AND Rv1886c AND Rv0129c
P-L-GLX	GLU + GLN = P-L-GLX	0.0	100000.0	Rv2220
CL	CDPDG + PG = CMP + CL	0.0	100000.0	Rv1822
LM	PPM + AC3PIM2 = DPP + LM	0.0	100000.0	orphan
TDM	TREHALOSEMONOMYCOLATE(CY) = TREHALOSEDIMYCOLATE + TRE	0.0	100000.0	Rv3804c AND Rv1886c AND Rv0129c
TMM	TREHALOSEMONOMYCOLATE(CY) + ATP = TREHALOSEMONOMYCOLATE + ADP + PI	0.0	100000.0	(Rv1273c AND Rv1272c) OR (Rv1348 AND Rv1349) OR Rv0194 OR Rv1819c OR Rv1747 OR (Rv1687c AND Rv1686c)
DAT	MYCOLIPENOYL-ACP + TRE6P = DIACYLTREHALOSE + ACP	0.0	100000.0	orphan
PAT	MYCOLIPANOIC-ACP + MYCOLIPENOYL-ACP + MYCOLIPDIENOYL-ACP + TRE6P = POLYACYLTREHALOSE + ACP	0.0	100000.0	orphan

MPD	PHOSPHO-PENTA-METHYL-TRICONTANOYL-COA + GDPMAN = MPD + GDP + COA	0.0	100000.0	orphan
DIM	DIM-CYTO = DIM	0.0	100000.0	Rv2942 AND Rv2936 AND Rv2937 AND Rv2938
PGL	MYCOSIDE_B + GDPFUC + DTDP + SAM = PGL-TB + SAH	0.0	100000.0	Rv2957
SL-1	SL1278-WALL + HYDROXYPHTHIOCERANOYL-COA + PTHIOCERANOYL-COA = SL-1 + COA	0.0	100000.0	orphan
GLUCAN	GLC = GLUCAN	0.0	100000.0	orphan
BIOMASSe	PROTEIN + RNA + DNA + SMALLMOLECULES + PE + TAGbio + PIMS + LAM + MAPC + P-L-GLX + ATP = BIOMASS + ADP + PI	0.0	100000.0	orphan
BXT	BIOMASS = BIOMASSxt	0.0	100000.0	orphan
R800	NH3xt = NH3	0.0	1.0	orphan
R801	NO3xt + H = NO3	0.0	1.0	Rv1737c
R802	NO2xt + H = NO2	0.0	1.0	Rv1737c
R803	NO2xt = NO2	0.0	1.0	orphan
R804	O2xt = O2	0.0	1.0	orphan
R805	CO2xt = CO2	-100000.0	100000.0	orphan
R806	FORxt = FOR	0.0	1.0	orphan
R807	GLYCOLATExt = GLYCOLATE	0.0	1.0	orphan
R808	ACxt = AC	0.0	1.0	orphan
R809	ACALxt = ACAL	0.0	1.0	orphan
R810	ANxt = AN	0.0	1.0	orphan
R811	CITRxt = CITR	0.0	1.0	orphan
R812	GLxt = GL	0.0	1.0	orphan
R814	GNxt = GN	0.0	1.0	orphan
R815	HYXNxt = HYXN	0.0	1.0	orphan
R816	NACxt = NAC	0.0	1.0	orphan
R817	T3xt = T3	0.0	1.0	orphan
R818	UREAxt = UREA	0.0	1.0	orphan
R819	XANxt = XAN	0.0	1.0	orphan

R820	ALAxt + ATP = ALA + ADP	0.0	1.0	orphan
R821	ARGxt + ATP = ARG + ADP + PI	0.0	1.0	orphan
R822	ASNxt + ATP = ASN + ADP + PI	0.0	1.0	orphan
R823	ASPxt + ATP = ASP + ADP + PI	0.0	1.0	Rv2127
R824	SUCxt + ATP = SUC + ADP + PI	0.0	1.0	orphan
R825	CELBxt + ATP = CELB + ADP + PI	0.0	1.0	orphan
R826	CYSxt + ATP = CYS + ADP + PI	0.0	1.0	Rv2834c
R827	DAPIMxt + ATP = DAPIM + ADP + PI	0.0	1.0	orphan
R828	DGLUxt + ATP = DGLU + ADP + PI	0.0	1.0	orphan
R829	GLNxt + ATP = GLN + ADP + PI	0.0	1.0	Rv0411c AND Rv2565
R830	GLUxt + ATP = GLU + ADP + PI	0.0	1.0	orphan
R831	HISxt + ATP = HIS + ADP + PI	0.0	1.0	Rv0411c
R832	ILExt + ATP = ILE + ADP + PI	0.0	1.0	orphan
R833	LEUxt + ATP = LEU + ADP + PI	0.0	1.0	orphan
R834	LYSxt + ATP = LYS + ADP + PI	0.0	1.0	orphan
R835	METxt + ATP = MET + ADP + PI	0.0	1.0	orphan
R836	MLTxt + ATP = MLT + ADP + PI	0.0	1.0	orphan
R837	ORNxt + ATP = ORN + ADP + PI	0.0	1.0	Rv2833c AND Rv2835c AND Rv2834c AND Rv2832c
R838	PIxt + ATP = PI + ADP	0.0	1.0	(Rv0934 AND Rv0936 AND Rv0935 AND Rv0933) OR (Rv0932c AND Rv0930 AND Rv0929 AND Rv0933) OR (Rv0928 AND Rv0930 AND Rv0928 AND Rv0933)
R839	PROxt + ATP = PRO + ADP + PI	0.0	1.0	Rv0934 AND Rv0935 AND Rv0936 AND Rv0933
R840	RIBxt + ATP = RIB + ADP + PI	0.0	1.0	orphan

R841	SLFxt + ATP = SLF + ADP + PI	0.0	1.0	Rv2397c AND Rv2398c AND Rv2399c AND Rv2400c
R842	THRxt + ATP = THR + ADP + PI	0.0	1.0	orphan
R843	VALxt + ATP = VAL + ADP + PI	0.0	1.0	orphan
R844	ACxt + H = AC	0.0	1.0	orphan
R845	ADxt + H = AD	0.0	1.0	orphan
R846	ADNxt + H = ADN	0.0	1.0	orphan
R847	AKGxt + H = AKG	0.0	1.0	orphan
R848	ASPxt + H = ASP	0.0	1.0	orphan
R849	ASPxt + H = ASP	0.0	1.0	orphan
R850	ASPxt + H = ASP	0.0	1.0	orphan
R851	CITxt + H = CIT	0.0	1.0	orphan
R852	DAxt + H = DA	0.0	1.0	orphan
R853	DALAxt + H = DALA	0.0	1.0	orphan
R854	DCxt + H = DC	0.0	1.0	orphan
R855	DINxt + H = DIN	0.0	1.0	orphan
R856	DTxt + H = DT	0.0	1.0	orphan
R857	DUxt + H = DU	0.0	1.0	orphan
R858	ETHxt + H = ETH	0.0	1.0	orphan
R859	FUMxt + H = FUM	0.0	1.0	orphan
R860	FUMxt + H = FUM	0.0	1.0	orphan
R861	GABAxt + H = GABA	0.0	1.0	orphan
R862	GLACxt + H = GLAC	0.0	1.0	orphan
R863	GLCxt + H = GLC	0.0	1.0	orphan
R864	GLUxt + H = GLU	0.0	1.0	orphan
R865	GLUCxt + H = GLUC	0.0	1.0	orphan
R866	GLYxt + H = GLY	0.0	1.0	orphan
R867	GSNxt + H = GSN	0.0	1.0	orphan
R868	HISxt + H = HIS	0.0	1.0	orphan
R869	HIS = HISxt + H	0.0	1.0	orphan
R870	ILExt + H = ILE	0.0	1.0	orphan
R871	ILE = ILExt + H	0.0	1.0	orphan
R872	INSxt + H = INS	0.0	1.0	orphan
R873	LACxt + H = LAC	0.0	1.0	orphan
R874	LEUxt + H = LEU	0.0	1.0	orphan
R875	LEU = H + LEUxt	0.0	1.0	orphan
R876	LLACxt + H = LLAC	0.0	1.0	orphan

R877	LYSxt + H = LYS	0.0	1.0	orphan
R878	LYS = LYSxt + H	0.0	1.0	orphan
R879	MALxt + H = MAL	0.0	1.0	orphan
R880	MALxt + H = MAL	0.0	1.0	orphan
R881	PHExt + H = PHE	0.0	1.0	orphan
R882	PIxt + H = PI	0.0	1.0	orphan
R883	PROxt + H = PRO	0.0	1.0	Rv2281
R884	PRO = PROxt + H	0.0	1.0	orphan
R885	PYRxt + H = PYR	0.0	1.0	orphan
R886	SERxt + H = SER	0.0	1.0	orphan
R887	SER = SERxt + H	0.0	1.0	orphan
R888	SUCCxt + H = SUCC	0.0	1.0	orphan
R889	SUCCxt + H = SUCC	0.0	1.0	orphan
R890	SUCC = SUCCxt + H	0.0	1.0	orphan
R891	THRxt + H = THR	0.0	1.0	orphan
R892	THR = THRxt + H	0.0	1.0	orphan
R893	TRPxt + H = TRP	0.0	1.0	orphan
R894	TYRxt + H = TYR	0.0	1.0	orphan
R895	URAxt + H = URA	0.0	1.0	orphan
R896	URIxt + H = URI	0.0	1.0	orphan
R897	VALxt + H = VAL	0.0	1.0	orphan
R898	VAL = VALxt + H	0.0	1.0	orphan
R899	FRUxt + PEP = PYR + F6P	0.0	1.0	orphan
R900	FRUxt + PEP = F1P + PYR	0.0	1.0	orphan
R901	MANxt + PEP = MAN6P + PYR	0.0	1.0	orphan
R902	TRExt + PEP = TRE6P + PYR	0.0	1.0	orphan
R903	CADA + LYSxt + H = LYS + CADAxt	0.0	1.0	orphan
R904	SUCC + CITxt = SUCCxt + CIT	0.0	1.0	orphan
R905	SUCC + FUMxt = SUCCxt + FUM	0.0	1.0	orphan
R906	GL3Pxt + PI = PIxt + GL3P	0.0	1.0	orphan
R907	PROPANOATExt = PROPANOATE	0.0	1.0	orphan
R908	HEXANOATExt = HEXANOATE	0.0	1.0	orphan
R909	HEXACOSANOATExt = HEXACOSANOATE	0.0	1.0	orphan

R910	TETRACOSANOATExt = TETRACOSANOATE	0.0	1.0	orphan
R911	TETRADECANOATExt = TETRADECANOATE	0.0	1.0	orphan
R912	EICOSANOATExt = EICOSANOATE	0.0	1.0	orphan
R913	PENTADECANOATExt = PENTADECANOATE	0.0	1.0	orphan
R914	HEPTADECANOATExt = HEPTADECANOATE	0.0	1.0	orphan
R915	NONADECANOATExt = NONADECANOATE	0.0	1.0	orphan
R916	HEXADECANOATExt = HEXADECANOATE	0.0	1.0	orphan
R917	9-HEXADECENOATExt = 9-HEXADECENOATE	0.0	1.0	orphan
R918	9-OCTADECENOATExt = 9-OCTADECENOATE	0.0	1.0	orphan
R919	PENTADECANOATExt = PENTADECANOATE	0.0	1.0	orphan
R920	DODECANOATExt = DODECANOATE	0.0	1.0	orphan
R921	TAGxt = TAGcat	0.0	1.0	orphan
R922	PHOSPHATIDYLCHOLINExt = PHOSPHATIDYLCHOLINE	0.0	1.0	orphan
R923	MBTSEC + MBTWALL + ATP + FE3xt = FE3 + ADP + PI	0.0	1.0	orphan
R924	CITxt + FE3xt = CIT + FE3	0.0	1.0	orphan
R925	BIOTINxt = BIOTIN	0.0	1.0	orphan
R926	CO-IIxt = CO-II	0.0	1.0	orphan
R927	MO2xt = MO2	0.0	1.0	orphan
R928	BSA = ILExt + VALxt + METxt + ALAxt + HISxt + LYSxt + LEUxt + ARGxt + ASPxt + SERxt + GLUxt + GLNxt + THRxt + TRPxt + TYRxt + CYSxt + ASNxt + GLYxt + PROxt + PHExt	0.0	1.0	orphan
R929	ELECTROPHILE-Xxt = ELECTROPHILE-X	0.0	1.0	orphan
R930	H2Xxt = H2X	0.0	1.0	orphan

R931	N-ACETYL-S-CONJUGATExt = N-ACETYL-S-CONJUGATE	0.0	1.0	orphan

SBML code for GSMN-TB Model

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<species id="M_TAGxt_b" name="TAGxt" compartment="Extra_organism" charge="0" boundaryCondition="true" />
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      </listOfProducts>
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            <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
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            <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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</reaction>
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          <html:p>SUBSYSTEM: </html:p>
          <html:p>PROTEIN_CLASS: </html:p>
      </notes>
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      <listOfProducts>
          <speciesReference species="M_GLC_c" stoichiometry="1.0"/>
      </listOfProducts>
      <kineticLaw>
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              <ci> FLUX_VALUE </ci>
          </math>
          <listOfParameters>
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                <parameter id="LOWER_BOUND" value="-100000.0"
units="mmol_per_gDW_per_hr"/>
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            <html:p>PROTEIN_CLASS: </html:p>
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            <speciesReference species="M_MAN_c" stoichiometry="1.0"/>
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units="mmol_per_gDW_per_hr"/>
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    <reaction id="R11" name="R11" reversible="true">
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                <html:p>SUBSYSTEM: </html:p>
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            <listOfReactants>
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units="mmol_per_gDW_per_hr"/>
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                <html:p>SUBSYSTEM: </html:p>
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            </math>
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            <html:p>SUBSYSTEM: </html:p>
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        <listOfProducts>
            <speciesReference species="M_GDP_c" stoichiometry="1.0"/>
            <speciesReference species="M_PPM_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
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            </math>
            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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        </kineticLaw>
    </reaction>
    <reaction id="R15" name="R15" reversible="false">
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        <notes>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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        <listOfProducts>
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        </listOfProducts>
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            </math>
            <listOfParameters>
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              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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        </kineticLaw>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
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        <listOfReactants>
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        <listOfProducts>
            <speciesReference species="M_GDPDHDOGAL_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
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            </math>
            <listOfParameters>
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              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
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        </kineticLaw>
    </reaction>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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            <speciesReference species="M_NADPH_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_GDPFUC_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
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            </math>
            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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    <reaction id="R18" name="R18" reversible="false">
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_GAL1P_c" stoichiometry="1.0"/>
            <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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                <ci> FLUX_VALUE </ci>
            </math>
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            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
      </notes>
      <listOfReactants>
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            <speciesReference species="M_UTP_c" stoichiometry="1.0"/>
      </listOfReactants>
      <listOfProducts>
            <speciesReference species="M_UDPGAL_c" stoichiometry="1.0"/>
            <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
      </listOfProducts>
      <kineticLaw>
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            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
      </kineticLaw>
</reaction>
<reaction id="R20" name="R20" reversible="true">
      <notes>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
      </notes>
      <listOfReactants>
            <speciesReference species="M_UDPG_c" stoichiometry="1.0"/>
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      <listOfProducts>
            <speciesReference species="M_UDPGAL_c" stoichiometry="1.0"/>
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            </listOfProducts>
            <kineticLaw>
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                </math>
                <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
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                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
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                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
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            </notes>
            <listOfReactants>
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                <speciesReference species="M_UTP_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_UDPG_c" stoichiometry="1.0"/>
                <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
            </listOfProducts>
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                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
                  <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
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                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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                  <parameter id="REDUCED_COST" value="0.000000"/>
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            </kineticLaw>
        </reaction>
        <reaction id="R22" name="R22" reversible="true">
            <notes>
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                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
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            </notes>
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            </listOfProducts>
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                </math>
                <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
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                <html:p>SUBSYSTEM: </html:p>
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            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_PI_c" stoichiometry="1.0"/>
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            </listOfProducts>
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                </math>
                <listOfParameters>
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            </kineticLaw>
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        <notes>
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            <html:p>SUBSYSTEM: </html:p>
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            <speciesReference species="M_GLC_c" stoichiometry="2.0"/>
        </listOfProducts>
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            <math xmlns="http://www.w3.org/1998/Math/MathML">
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            </math>
            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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            </listOfParameters>
        </kineticLaw>
    </reaction>
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            <html:p>SUBSYSTEM: </html:p>
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        </notes>
        <listOfReactants>
            <speciesReference species="M_SUC_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_GLC_c" stoichiometry="1.0"/>
            <speciesReference species="M_FRU_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
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            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R26" name="R26" reversible="false">
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            <html:p>SUBSYSTEM: </html:p>
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        </notes>
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        <listOfProducts>
            <speciesReference species="M_bDGLC_c" stoichiometry="2.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
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            </math>
            <listOfParameters>
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        </kineticLaw>
    </reaction>
    <reaction id="R27" name="R27" reversible="false">
        <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
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        </notes>
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            <speciesReference species="M_UDPG_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_TRE6P_c" stoichiometry="1.0"/>
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        </listOfProducts>
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            </math>
            <listOfParameters>
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</reaction>
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      </notes>
      <listOfReactants>
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          <speciesReference species="M_PI_c" stoichiometry="1.0"/>
      </listOfReactants>
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          <speciesReference species="M_bDG1P_c" stoichiometry="1.0"/>
          <speciesReference species="M_bDGLC_c" stoichiometry="1.0"/>
      </listOfProducts>
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          </math>
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</reaction>
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      </notes>
      <listOfReactants>
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      </listOfReactants>
      <listOfProducts>
          <speciesReference species="M_bDG6P_c" stoichiometry="1.0"/>
      </listOfProducts>
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        <kineticLaw>
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            </math>
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units="mmol_per_gDW_per_hr"/>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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        <listOfProducts>
            <speciesReference species="M_TRE_c" stoichiometry="1.0"/>
        </listOfProducts>
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            </math>
            <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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        <listOfProducts>
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            <speciesReference species="M_TRE_c" stoichiometry="1.0"/>
        </listOfProducts>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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            <speciesReference species="M_NAD_c" stoichiometry="1.0"/>
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            <speciesReference species="M_CO2_c" stoichiometry="1.0"/>
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            </math>
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              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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    </reaction>
    <reaction id="R33" name="R33" reversible="false">
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            <html:p>PROTEIN_CLASS: </html:p>
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        <listOfReactants>
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            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_G6P_c" stoichiometry="1.0"/>
            <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
        </listOfProducts>
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            </math>
            <listOfParameters>
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              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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        </kineticLaw>
    </reaction>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_bDG6P_c" stoichiometry="1.0"/>
            <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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            <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
            <parameter id="REDUCED_COST" value="0.000000"/>
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      </kineticLaw>
</reaction>
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          <html:p>SUBSYSTEM: </html:p>
          <html:p>PROTEIN_CLASS: </html:p>
      </notes>
      <listOfReactants>
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          <speciesReference species="M_(n)POLYP_c" stoichiometry="1.0"/>
      </listOfReactants>
      <listOfProducts>
          <speciesReference species="M_G6P_c" stoichiometry="1.0"/>
          <speciesReference species="M_(n-1)POLYP_c" stoichiometry="1.0"/>
      </listOfProducts>
      <kineticLaw>
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          </math>
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            <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
            <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
            <parameter id="REDUCED_COST" value="0.000000"/>
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</reaction>
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          <html:p>SUBSYSTEM: </html:p>
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      </notes>
      <listOfReactants>
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          <speciesReference species="M_(n)POLYP_c" stoichiometry="1.0"/>
      </listOfReactants>
      <listOfProducts>
          <speciesReference species="M_bDG6P_c" stoichiometry="1.0"/>
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      </listOfProducts>
      <kineticLaw>
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                </math>
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                  <parameter id="REDUCED_COST" value="0.000000"/>
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            </kineticLaw>
        </reaction>
        <reaction id="R37" name="R37" reversible="true">
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                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
                <speciesReference species="M_G6P_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_bDG6P_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
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                </math>
                <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
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            </kineticLaw>
        </reaction>
        <reaction id="R38" name="R38" reversible="true">
            <notes>
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                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
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            </listOfReactants>
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            <listOfProducts>
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                </math>
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units="mmol_per_gDW_per_hr"/>
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                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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        </reaction>
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                <html:p>SUBSYSTEM: </html:p>
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            </notes>
            <listOfReactants>
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            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_F6P_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
                <math xmlns="http://www.w3.org/1998/Math/MathML">
                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
                  <parameter id="LOWER_BOUND" value="-100000.0"
units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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        </reaction>
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            <notes>
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                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
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            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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        <listOfProducts>
            <speciesReference species="M_F6P_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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            <html:p>SUBSYSTEM: </html:p>
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        </notes>
        <listOfReactants>
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            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_FDP_c" stoichiometry="1.0"/>
            <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
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</reaction>
<reaction id="R42" name="R42" reversible="false">
    <notes>
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        <html:p>SUBSYSTEM: </html:p>
        <html:p>PROTEIN_CLASS: </html:p>
    </notes>
    <listOfReactants>
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        <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
    </listOfReactants>
    <listOfProducts>
        <speciesReference species="M_FDP_c" stoichiometry="1.0"/>
        <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
    </listOfProducts>
    <kineticLaw>
        <math xmlns="http://www.w3.org/1998/Math/MathML">
            <ci> FLUX_VALUE </ci>
        </math>
        <listOfParameters>
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          <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
          <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
          <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
          <parameter id="REDUCED_COST" value="0.000000"/>
        </listOfParameters>
    </kineticLaw>
</reaction>
<reaction id="R43" name="R43" reversible="false">
    <notes>
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        <html:p>SUBSYSTEM: </html:p>
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    </notes>
    <listOfReactants>
        <speciesReference species="M_FDP_c" stoichiometry="1.0"/>
    </listOfReactants>
    <listOfProducts>
        <speciesReference species="M_F6P_c" stoichiometry="1.0"/>
        <speciesReference species="M_PI_c" stoichiometry="1.0"/>
    </listOfProducts>
    <kineticLaw>
        <math xmlns="http://www.w3.org/1998/Math/MathML">
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        </math>
        <listOfParameters>
          <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
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<parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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<html:p>SUBSYSTEM: </html:p>
<html:p>PROTEIN_CLASS: </html:p>
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</listOfReactants>
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<kineticLaw>
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</math>
<listOfParameters>
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<parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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<kineticLaw>

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                </math>
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units="mmol_per_gDW_per_hr"/>
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        <reaction id="R46" name="R46" reversible="true">
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                <html:p>SUBSYSTEM: </html:p>
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            </notes>
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                <speciesReference species="M_PI_c" stoichiometry="1.0"/>
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            <listOfProducts>
                <speciesReference species="M_13PDG_c" stoichiometry="1.0"/>
                <speciesReference species="M_NADH_c" stoichiometry="1.0"/>
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units="mmol_per_gDW_per_hr"/>
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                <html:p>PROTEIN_CLASS: </html:p>
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            </notes>
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            </listOfReactants>
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                </math>
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                <html:p>SUBSYSTEM: </html:p>
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                <speciesReference species="M_2PG_c" stoichiometry="1.0"/>
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            <speciesReference species="M_PEP_c" stoichiometry="1.0"/>
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            </math>
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units="mmol_per_gDW_per_hr"/>
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    </reaction>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
            <speciesReference species="M_PYR_c" stoichiometry="1.0"/>
        </listOfProducts>
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<parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
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<parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
<parameter id="REDUCED_COST" value="0.000000"/>
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<html:p>SUBSYSTEM: </html:p>
<html:p>PROTEIN_CLASS: </html:p>
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<speciesReference species="M_PYR_c" stoichiometry="1.0"/>
<speciesReference species="M_THI_c" stoichiometry="0.001"/>
</listOfReactants>
<listOfProducts>
<speciesReference species="M_ADLIPO_c" stoichiometry="1.0"/>
<speciesReference species="M_CO2_c" stoichiometry="1.0"/>
</listOfProducts>
<kineticLaw>
<math xmlns="http://www.w3.org/1998/Math/MathML">
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</math>
<listOfParameters>
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<parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
<parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
<parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
<parameter id="REDUCED_COST" value="0.000000"/>
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<reaction id="R53" name="R53" reversible="true">
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<html:p>SUBSYSTEM: </html:p>
<html:p>PROTEIN_CLASS: </html:p>
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<speciesReference species="M_COA_c" stoichiometry="1.0"/>
</listOfReactants>
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<speciesReference species="M_ACCOA_c" stoichiometry="1.0"/>

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                <speciesReference species="M_DLIPO_c" stoichiometry="1.0"/>
            </listOfProducts>
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                </math>
                <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
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                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R54" name="R54" reversible="true">
            <notes>
                <html:p>GENE_ASSOCIATION: Rv0462 </html:p>
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                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
                <speciesReference species="M_NAD_c" stoichiometry="1.0"/>
                <speciesReference species="M_DLIPO_c" stoichiometry="1.0"/>
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            <listOfProducts>
                <speciesReference species="M_LIPO_c" stoichiometry="1.0"/>
                <speciesReference species="M_NADH_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
                <math xmlns="http://www.w3.org/1998/Math/MathML">
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                </math>
                <listOfParameters>
                  <parameter id="LOWER_BOUND" value="-100000.0"
units="mmol_per_gDW_per_hr"/>
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                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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        </reaction>
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            <notes>
                <html:p>GENE_ASSOCIATION: Rv0896 or Rv0889c or Rv1131 </html:p>
                <html:p>PROTEIN_ASSOCIATION: </html:p>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_ACCOA_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_CIT_c" stoichiometry="1.0"/>
            <speciesReference species="M_COA_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R56" name="R56" reversible="true">
        <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_CIT_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_CISACONITATE_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
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            </kineticLaw>
        </reaction>
        <reaction id="R57" name="R57" reversible="true">
            <notes>
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                <html:p>PROTEIN_ASSOCIATION: </html:p>
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                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
                <speciesReference species="M_CISACONITATE_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_ICIT_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
                <math xmlns="http://www.w3.org/1998/Math/MathML">
                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
                  <parameter id="LOWER_BOUND" value="-100000.0"
units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R58" name="R58" reversible="false">
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                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
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            <listOfReactants>
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                <speciesReference species="M_NADP_c" stoichiometry="1.0"/>
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                <speciesReference species="M_AKG_c" stoichiometry="1.0"/>
                <speciesReference species="M_NADPH_c" stoichiometry="1.0"/>
                <speciesReference species="M_CO2_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
                <math xmlns="http://www.w3.org/1998/Math/MathML">
                    <ci> FLUX_VALUE </ci>
                </math>
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            <listOfParameters>
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              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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        </kineticLaw>
    </reaction>
    <reaction id="R61" name="R61" reversible="false">
        <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_AKG_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_SUCCSAL_c" stoichiometry="1.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
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            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
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              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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        </kineticLaw>
    </reaction>
    <reaction id="R63" name="R63" reversible="true">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv0952 and Rv0951 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
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        <listOfReactants>
            <speciesReference species="M_SUCCOA_c" stoichiometry="1.0"/>
            <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
            <speciesReference species="M_PI_c" stoichiometry="1.0"/>
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        <listOfProducts>
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                <speciesReference species="M_COA_c" stoichiometry="1.0"/>
                <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
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                </math>
                <listOfParameters>
                  <parameter id="LOWER_BOUND" value="-100000.0"
units="mmol_per_gDW_per_hr"/>
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                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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                </listOfParameters>
            </kineticLaw>
        </reaction>
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                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
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            </notes>
            <listOfReactants>
                <speciesReference species="M_FUM_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_MAL_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
                <math xmlns="http://www.w3.org/1998/Math/MathML">
                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
                  <parameter id="LOWER_BOUND" value="-100000.0"
units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R65" name="R65" reversible="true">
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                <html:p>PROTEIN_ASSOCIATION: </html:p>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_NAD_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_OA_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADH_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="-100000.0"
units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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        </kineticLaw>
    </reaction>
    <reaction id="R66" name="R66" reversible="false">
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_CIT_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_OA_c" stoichiometry="1.0"/>
            <speciesReference species="M_AC_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
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            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R67" name="R67" reversible="false">
        <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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            <speciesReference species="M_COA_c" stoichiometry="1.0"/>
            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_ACCOA_c" stoichiometry="1.0"/>
            <speciesReference species="M_AMP_c" stoichiometry="1.0"/>
            <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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        </kineticLaw>
    </reaction>
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        <notes>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_NAD_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_AC_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADH_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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<math xmlns="http://www.w3.org/1998/Math/MathML">
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</math>
<listOfParameters>
<parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
<parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
<parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
<parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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</listOfParameters>
</kineticLaw>
</reaction>
<reaction id="R69" name="R69" reversible="false">
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<html:p>GENE_ASSOCIATION: Rv1127c </html:p>
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<html:p>SUBSYSTEM: </html:p>
<html:p>PROTEIN_CLASS: </html:p>
</notes>
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<speciesReference species="M_ATP_c" stoichiometry="1.0"/>
<speciesReference species="M_PI_c" stoichiometry="1.0"/>
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<speciesReference species="M_PEP_c" stoichiometry="1.0"/>
<speciesReference species="M_AMP_c" stoichiometry="1.0"/>
<speciesReference species="M_PPI_c" stoichiometry="1.0"/>
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</math>
<listOfParameters>
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<parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
<parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
<parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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</reaction>
<reaction id="R70" name="R70" reversible="true">
<notes>
<html:p>GENE_ASSOCIATION: Rv0728c </html:p>
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<html:p>SUBSYSTEM: </html:p>
<html:p>PROTEIN_CLASS: </html:p>
</notes>

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                <speciesReference species="M_NAD_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_PYR_c" stoichiometry="1.0"/>
                <speciesReference species="M_NADH_c" stoichiometry="1.0"/>
            </listOfProducts>
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                </math>
                <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
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            </kineticLaw>
        </reaction>
        <reaction id="R71" name="R71" reversible="true">
            <notes>
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                <html:p>SUBSYSTEM: </html:p>
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                <speciesReference species="M_NAD_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_PYR_c" stoichiometry="1.0"/>
                <speciesReference species="M_NADH_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
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                </math>
                <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
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                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
                </listOfParameters>
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        </kineticLaw>
    </reaction>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
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            <speciesReference species="M_PYR_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADH_c" stoichiometry="1.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R73" name="R73" reversible="true">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv1862 or Rv1530 or Rv0162c or Rv0761c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_NADH_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_ETH_c" stoichiometry="1.0"/>
            <speciesReference species="M_NAD_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
```

```
                </math>
                <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
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                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
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        <reaction id="R74" name="R74" reversible="true">
            <notes>
                <html:p>GENE_ASSOCIATION: Rv3045 </html:p>
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                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
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                <speciesReference species="M_NADPH_c" stoichiometry="1.0"/>
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            <listOfProducts>
                <speciesReference species="M_ETH_c" stoichiometry="1.0"/>
                <speciesReference species="M_NADP_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
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                </math>
                <listOfParameters>
                  <parameter id="LOWER_BOUND" value="-100000.0"
units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
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        </reaction>
        <reaction id="R75" name="R75" reversible="false">
            <notes>
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                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
                <speciesReference species="M_AC_c" stoichiometry="1.0"/>
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<speciesReference species="M_ATP_c" stoichiometry="1.0"/>
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<speciesReference species="M_ACETYLP_c" stoichiometry="1.0"/>
<speciesReference species="M_ADP_c" stoichiometry="1.0"/>
</listOfProducts>
<kineticLaw>
<math xmlns="http://www.w3.org/1998/Math/MathML">
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</math>
<listOfParameters>
<parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
<parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
<parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
<parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
<parameter id="REDUCED_COST" value="0.000000"/>
</listOfParameters>
</kineticLaw>
</reaction>
<reaction id="R76" name="R76" reversible="true">
<notes>
<html:p>GENE_ASSOCIATION: Rv0408 </html:p>
<html:p>PROTEIN_ASSOCIATION: </html:p>
<html:p>SUBSYSTEM: </html:p>
<html:p>PROTEIN_CLASS: </html:p>
</notes>
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<speciesReference species="M_ACETYLP_c" stoichiometry="1.0"/>
</listOfReactants>
<listOfProducts>
<speciesReference species="M_ACCOA_c" stoichiometry="1.0"/>
<speciesReference species="M_PI_c" stoichiometry="1.0"/>
</listOfProducts>
<kineticLaw>
<math xmlns="http://www.w3.org/1998/Math/MathML">
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</math>
<listOfParameters>
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units="mmol_per_gDW_per_hr"/>
<parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
<parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
<parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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</reaction>
<reaction id="R77" name="R77" reversible="false">

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        <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_ACETYLP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_AC_c" stoichiometry="1.0"/>
            <speciesReference species="M_PI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
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            </math>
            <listOfParameters>
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              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R78" name="R78" reversible="true">
        <notes>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_PROPIONYLP_c" stoichiometry="1.0"/>
            <speciesReference species="M_COA_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_PROPIONYLCOA_c" stoichiometry="1.0"/>
            <speciesReference species="M_PI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="-100000.0"
units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
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<parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
<parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
<parameter id="REDUCED_COST" value="0.000000"/>
</listOfParameters>
</kineticLaw>
</reaction>
<reaction id="R79" name="R79" reversible="false">
<notes>
<html:p>GENE_ASSOCIATION: Rv0409 </html:p>
<html:p>PROTEIN_ASSOCIATION: </html:p>
<html:p>SUBSYSTEM: </html:p>
<html:p>PROTEIN_CLASS: </html:p>
</notes>
<listOfReactants>
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<speciesReference species="M_ATP_c" stoichiometry="1.0"/>
</listOfReactants>
<listOfProducts>
<speciesReference species="M_PROPIONYLP_c" stoichiometry="1.0"/>
<speciesReference species="M_ADP_c" stoichiometry="1.0"/>
</listOfProducts>
<kineticLaw>
<math xmlns="http://www.w3.org/1998/Math/MathML">
<ci> FLUX_VALUE </ci>
</math>
<listOfParameters>
<parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
<parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
<parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
<parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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</listOfParameters>
</kineticLaw>
</reaction>
<reaction id="R80" name="R80" reversible="false">
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<html:p>PROTEIN_ASSOCIATION: </html:p>
<html:p>SUBSYSTEM: </html:p>
<html:p>PROTEIN_CLASS: </html:p>
</notes>
<listOfReactants>
<speciesReference species="M_SMMALONYLCOA_c" stoichiometry="1.0"/>
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<listOfProducts>
<speciesReference species="M_PROPIONYLCOA_c" stoichiometry="1.0"/>
<speciesReference species="M_CO2_c" stoichiometry="1.0"/>
</listOfProducts>
<kineticLaw>

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            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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        </kineticLaw>
    </reaction>
    <reaction id="R81" name="R81" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv3667 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_PROPANOATE_c" stoichiometry="1.0"/>
            <speciesReference species="M_COA_c" stoichiometry="1.0"/>
            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_PROPIONYLCOA_c" stoichiometry="1.0"/>
            <speciesReference species="M_AMP_c" stoichiometry="1.0"/>
            <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R82" name="R82" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv1131 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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            <speciesReference species="M_OA_c" stoichiometry="1.0"/>
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        <listOfProducts>
            <speciesReference species="M_2METHYLCITRATE_c" stoichiometry="1.0"/>
            <speciesReference species="M_COA_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R83" name="R83" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv1130 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_2METHYLCITRATE_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_2METHYLCISACONITATE_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R84" name="R84" reversible="false">
        <notes>
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            <html:p>GENE_ASSOCIATION: Rv1475c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_2METHYLCISACONITATE_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_METHYLISOCITRATE_c" stoichiometry="1.0"/>
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        <kineticLaw>
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            </math>
            <listOfParameters>
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              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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        </kineticLaw>
    </reaction>
    <reaction id="R85" name="R85" reversible="false">
        <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
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            </math>
            <listOfParameters>
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        </kineticLaw>
    </reaction>
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            <html:p>SUBSYSTEM: </html:p>
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        </notes>
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            <speciesReference species="M_MK_c" stoichiometry="1.0"/>
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            <speciesReference species="M_MKH2_c" stoichiometry="1.0"/>
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            </math>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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        <notes>
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            <html:p>SUBSYSTEM: </html:p>
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        </notes>
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            <speciesReference species="M_NADP_c" stoichiometry="1.0"/>
            <speciesReference species="M_F420_c" stoichiometry="0.001"/>
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        <kineticLaw>
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                <ci> FLUX_VALUE </ci>
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            </math>
            <listOfParameters>
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        <listOfProducts>
            <speciesReference species="M_D6PGC_c" stoichiometry="1.0"/>
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            </math>
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    </reaction>
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        <notes>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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            <speciesReference species="M_NADP_c" stoichiometry="1.0"/>
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        <listOfProducts>
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                </math>
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                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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                <html:p>SUBSYSTEM: </html:p>
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            </notes>
            <listOfReactants>
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            <listOfProducts>
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            </listOfProducts>
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                </math>
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units="mmol_per_gDW_per_hr"/>
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                <html:p>SUBSYSTEM: </html:p>
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units="mmol_per_gDW_per_hr"/>
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            </kineticLaw>
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            <notes>
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                <html:p>SUBSYSTEM: </html:p>
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            <listOfReactants>
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            <listOfProducts>
                <speciesReference species="M_R5P_c" stoichiometry="1.0"/>
            </listOfProducts>
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units="mmol_per_gDW_per_hr"/>
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                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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            </kineticLaw>
        </reaction>
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        <notes>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_THI_c" stoichiometry="0.001"/>
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        <listOfProducts>
            <speciesReference species="M_G3P_c" stoichiometry="1.0"/>
            <speciesReference species="M_S7P_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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        </kineticLaw>
    </reaction>
    <reaction id="R94" name="R94" reversible="false">
        <notes>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_S7P_c" stoichiometry="1.0"/>
            <speciesReference species="M_THI_c" stoichiometry="0.001"/>
        </listOfReactants>
        <listOfProducts>
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            <speciesReference species="M_R5P_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
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            </math>
            <listOfParameters>
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            <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
            <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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</reaction>
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          <html:p>SUBSYSTEM: </html:p>
          <html:p>PROTEIN_CLASS: </html:p>
      </notes>
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      </listOfReactants>
      <listOfProducts>
          <speciesReference species="M_G3P_c" stoichiometry="1.0"/>
          <speciesReference species="M_F6P_c" stoichiometry="1.0"/>
      </listOfProducts>
      <kineticLaw>
          <math xmlns="http://www.w3.org/1998/Math/MathML">
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          </math>
          <listOfParameters>
            <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
            <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
            <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
            <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
            <parameter id="REDUCED_COST" value="0.000000"/>
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      </notes>
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          <speciesReference species="M_THI_c" stoichiometry="0.001"/>
      </listOfReactants>
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            <speciesReference species="M_E4P_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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    </reaction>
    <reaction id="R97" name="R97" reversible="true">
        <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
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        </notes>
        <listOfReactants>
            <speciesReference species="M_G3P_c" stoichiometry="1.0"/>
            <speciesReference species="M_S7P_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_E4P_c" stoichiometry="1.0"/>
            <speciesReference species="M_F6P_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
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            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="-100000.0"
units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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            </listOfParameters>
        </kineticLaw>
    </reaction>
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        <notes>
            <html:p>GENE_ASSOCIATION: Rv2436 </html:p>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
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        </notes>
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            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
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        <listOfProducts>
            <speciesReference species="M_DR5P_c" stoichiometry="1.0"/>
            <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
        </listOfProducts>
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            </math>
            <listOfParameters>
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              <parameter id="REDUCED_COST" value="0.000000"/>
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        </kineticLaw>
    </reaction>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_DR5P_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_ACAL_c" stoichiometry="1.0"/>
            <speciesReference species="M_G3P_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R100" name="R100" reversible="false">
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
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        </notes>
        <listOfReactants>
            <speciesReference species="M_PYR_c" stoichiometry="1.0"/>
            <speciesReference species="M_BIOTIN-CO2_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_OA_c" stoichiometry="1.0"/>
            <speciesReference species="M_BIOTIN_c" stoichiometry="0.999"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R101" name="R101" reversible="true">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv0211 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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            <speciesReference species="M_CO2_c" stoichiometry="1.0"/>
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        <listOfProducts>
            <speciesReference species="M_OA_c" stoichiometry="1.0"/>
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        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
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                </math>
                <listOfParameters>
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                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R102" name="R102" reversible="false">
            <notes>
                <html:p>GENE_ASSOCIATION: Rv0467 or ( Rv1915 and Rv1916 ) </html:p>
                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
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            <listOfProducts>
                <speciesReference species="M_GLX_c" stoichiometry="1.0"/>
                <speciesReference species="M_SUCC_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
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                    <ci> FLUX_VALUE </ci>
                </math>
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                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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        </reaction>
        <reaction id="R103" name="R103" reversible="false">
            <notes>
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                <html:p>SUBSYSTEM: </html:p>
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            </notes>
            <listOfReactants>
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                <speciesReference species="M_ACCOA_c" stoichiometry="1.0"/>
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        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_MAL_c" stoichiometry="1.0"/>
            <speciesReference species="M_COA_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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        </kineticLaw>
    </reaction>
    <reaction id="R104" name="R104" reversible="false">
        <notes>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_GLAL_c" stoichiometry="1.0"/>
            <speciesReference species="M_NAD_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_GLYCOLATE_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADH_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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    </reaction>
    <reaction id="R105" name="R105" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv1257c </html:p>
```

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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_GLYCOLATE_c" stoichiometry="1.0"/>
            <speciesReference species="M_O2_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_GLX_c" stoichiometry="1.0"/>
            <speciesReference species="M_H2O2_c" stoichiometry="1.0"/>
        </listOfProducts>
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            </math>
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              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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        </kineticLaw>
    </reaction>
    <reaction id="R106" name="R106" reversible="true">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv3356c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_METTHF_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_METHF_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADPH_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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                <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                <parameter id="REDUCED_COST" value="0.000000"/>
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        </kineticLaw>
    </reaction>
    <reaction id="R107" name="R107" reversible="true">
        <notes>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_FTHF_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
                <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                <parameter id="REDUCED_COST" value="0.000000"/>
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    </reaction>
    <reaction id="R108" name="R108" reversible="false">
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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            <speciesReference species="M_METTHF_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_MTHF_c" stoichiometry="1.0"/>
            <speciesReference species="M_FAD_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
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```
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
</reaction>
<reaction id="R109" name="R109" reversible="false">
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_SLF_c" stoichiometry="1.0"/>
            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_APS_c" stoichiometry="1.0"/>
            <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
</reaction>
<reaction id="R110" name="R110" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv1286 </html:p>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
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        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_PAPS_c" stoichiometry="1.0"/>
            <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
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            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R111" name="R111" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2392 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_RTHIO_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_AMP_c" stoichiometry="1.0"/>
            <speciesReference species="M_H2SO3_c" stoichiometry="1.0"/>
            <speciesReference species="M_OTHIO_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R112" name="R112" reversible="true">
        <notes>
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            <html:p>GENE_ASSOCIATION: Rv2391 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_H2SO3_c" stoichiometry="1.0"/>
            <speciesReference species="M_FERO_c" stoichiometry="6.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_FERI_c" stoichiometry="6.0"/>
            <speciesReference species="M_H2S_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="-100000.0"
units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R113" name="R113" reversible="false">
        <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_PAP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_AMP_c" stoichiometry="1.0"/>
            <speciesReference species="M_PI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
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            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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                <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                <parameter id="REDUCED_COST" value="0.000000"/>
              </listOfParameters>
          </kineticLaw>
      </reaction>
      <reaction id="R114" name="R114" reversible="false">
          <notes>
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Rv1736c </html:p>
              <html:p>PROTEIN_ASSOCIATION: </html:p>
              <html:p>SUBSYSTEM: </html:p>
              <html:p>PROTEIN_CLASS: </html:p>
          </notes>
          <listOfReactants>
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              <speciesReference species="M_NO3_c" stoichiometry="1.0"/>
              <speciesReference species="M_MOLYBDENUM_c" stoichiometry="0.001"/>
          </listOfReactants>
          <listOfProducts>
              <speciesReference species="M_MK_c" stoichiometry="1.0"/>
              <speciesReference species="M_NO2_c" stoichiometry="1.0"/>
              <speciesReference species="M_H_c" stoichiometry="2.0"/>
          </listOfProducts>
          <kineticLaw>
              <math xmlns="http://www.w3.org/1998/Math/MathML">
                  <ci> FLUX_VALUE </ci>
              </math>
              <listOfParameters>
                <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
                <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                <parameter id="REDUCED_COST" value="0.000000"/>
              </listOfParameters>
          </kineticLaw>
      </reaction>
      <reaction id="R119" name="R119" reversible="false">
          <notes>
              <html:p>GENE_ASSOCIATION: Rv3145 and Rv3146 and Rv3147 and Rv3148 and
Rv3149 and Rv3150 and Rv3151 and Rv3152 and Rv3153 and Rv3154 and Rv3155 and Rv3156 and
Rv3157 and Rv3158 </html:p>
              <html:p>PROTEIN_ASSOCIATION: </html:p>
              <html:p>SUBSYSTEM: </html:p>
              <html:p>PROTEIN_CLASS: </html:p>
          </notes>
          <listOfReactants>
              <speciesReference species="M_MK_c" stoichiometry="1.0"/>
              <speciesReference species="M_NADH_c" stoichiometry="1.0"/>
          </listOfReactants>
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        <listOfProducts>
            <speciesReference species="M_MKH2_c" stoichiometry="1.0"/>
            <speciesReference species="M_NAD_c" stoichiometry="1.0"/>
            <speciesReference species="M_H_c" stoichiometry="4.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R120" name="R120" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv1854c or Rv0392c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_MK_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADH_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_MKH2_c" stoichiometry="1.0"/>
            <speciesReference species="M_NAD_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R121" name="R121" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv3303c </html:p>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_MK_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADPH_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_MKH2_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R122" name="R122" reversible="true">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv3318 and Rv3319 and Rv3316 and Rv3317 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_MK_c" stoichiometry="1.0"/>
            <speciesReference species="M_SUCC_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_MKH2_c" stoichiometry="1.0"/>
            <speciesReference species="M_FUM_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="-100000.0"
units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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                <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                <parameter id="REDUCED_COST" value="0.000000"/>
              </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R123" name="R123" reversible="true">
        <notes>
            <html:p>GENE_ASSOCIATION: ( Rv3318 and Rv3319 and Rv3316 and Rv3317 ) or
( Rv1552 and Rv1553 and Rv1554 and Rv1555 ) </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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            <speciesReference species="M_SUCC_c" stoichiometry="1.0"/>
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        <listOfProducts>
            <speciesReference species="M_FADH2_c" stoichiometry="1.0"/>
            <speciesReference species="M_FUM_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
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units="mmol_per_gDW_per_hr"/>
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        </notes>
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            <speciesReference species="M_NADPH_c" stoichiometry="1.0"/>
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            </listOfProducts>
            <kineticLaw>
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Rv1451 and Rv1456c and Rv3029c and Rv3028c and Rv2200c and Rv3043c and Rv2193 and Rv3043c and
Rv1623c and Rv1622c ) or ( Rv1623c and Rv1622c ) </html:p>
                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
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            <listOfProducts>
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Rv1451 and Rv1456c and Rv3029c and Rv3028c and Rv2200c and Rv3043c and Rv2193 and Rv3043c) and (Rv1623c and Rv1622c) </html:p>
<html:p>PROTEIN_ASSOCIATION: </html:p>
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<html:p>PROTEIN_CLASS: </html:p>
</notes>
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<speciesReference species="M_HEME-FE3_c" stoichiometry="2.0"/>
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<reaction id="R127" name="R127" reversible="false">
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<html:p>SUBSYSTEM: </html:p>
<html:p>PROTEIN_CLASS: </html:p>
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<listOfProducts>
<speciesReference species="M_HEME-FE3_c" stoichiometry="2.0"/>
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</kineticLaw>
</reaction>
<reaction id="R128" name="R128" reversible="true">
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<html:p>SUBSYSTEM: </html:p>
<html:p>PROTEIN_CLASS: </html:p>
</notes>
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<listOfProducts>
<speciesReference species="M_ADP_c" stoichiometry="1.0"/>

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            <speciesReference species="M_PI_c" stoichiometry="1.0"/>
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    <reaction id="R130" name="R130" reversible="false">
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            <html:p>SUBSYSTEM: </html:p>
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        </notes>
        <listOfReactants>
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        <listOfProducts>
            <speciesReference species="M_PI_c" stoichiometry="2.0"/>
        </listOfProducts>
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        </kineticLaw>
    </reaction>
    <reaction id="R131" name="R131" reversible="false">
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
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        <listOfProducts>
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            <speciesReference species="M_H_c" stoichiometry="1.0"/>
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            </math>
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              <parameter id="REDUCED_COST" value="0.000000"/>
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    </reaction>
    <reaction id="R132" name="R132" reversible="true">
        <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
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        <listOfProducts>
            <speciesReference species="M_(n)POLYP_c" stoichiometry="1.0"/>
            <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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            <notes>
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                <html:p>SUBSYSTEM: </html:p>
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            </notes>
            <listOfReactants>
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                <speciesReference species="M_FERO_c" stoichiometry="2.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_FERI_c" stoichiometry="2.0"/>
                <speciesReference species="M_NADPH_c" stoichiometry="1.0"/>
            </listOfProducts>
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                  <parameter id="REDUCED_COST" value="0.000000"/>
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        </reaction>
        <reaction id="R134" name="R134" reversible="false">
            <notes>
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                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
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            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_O2_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
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                </math>
                <listOfParameters>
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            <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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</reaction>
<reaction id="R135" name="R135" reversible="false">
      <notes>
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          <html:p>SUBSYSTEM: </html:p>
          <html:p>PROTEIN_CLASS: </html:p>
      </notes>
      <listOfReactants>
          <speciesReference species="M_GLU_c" stoichiometry="1.0"/>
      </listOfReactants>
      <listOfProducts>
          <speciesReference species="M_GABA_c" stoichiometry="1.0"/>
          <speciesReference species="M_CO2_c" stoichiometry="1.0"/>
      </listOfProducts>
      <kineticLaw>
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          </math>
          <listOfParameters>
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            <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
            <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
            <parameter id="REDUCED_COST" value="0.000000"/>
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      </kineticLaw>
</reaction>
<reaction id="R136" name="R136" reversible="true">
      <notes>
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          <html:p>SUBSYSTEM: </html:p>
          <html:p>PROTEIN_CLASS: </html:p>
      </notes>
      <listOfReactants>
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          <speciesReference species="M_AKG_c" stoichiometry="1.0"/>
      </listOfReactants>
      <listOfProducts>
          <speciesReference species="M_SUCCSAL_c" stoichiometry="1.0"/>
          <speciesReference species="M_GLU_c" stoichiometry="1.0"/>
      </listOfProducts>
      <kineticLaw>
          <math xmlns="http://www.w3.org/1998/Math/MathML">
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                </math>
                <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
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                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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            </kineticLaw>
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                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
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                <speciesReference species="M_NADP_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_SUCC_c" stoichiometry="1.0"/>
                <speciesReference species="M_NADPH_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
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                </math>
                <listOfParameters>
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                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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            </kineticLaw>
        </reaction>
        <reaction id="R138" name="R138" reversible="false">
            <notes>
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                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
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        </listOfReactants>
        <listOfProducts>
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            <speciesReference species="M_FADH2_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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        <notes>
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            <html:p>SUBSYSTEM: </html:p>
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        </notes>
        <listOfReactants>
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            <speciesReference species="M_NAD_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
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            <speciesReference species="M_NADH_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
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            </math>
            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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        </kineticLaw>
    </reaction>
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        <notes>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_AKG_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_HYDROXYAKG_c" stoichiometry="1.0"/>
            <speciesReference species="M_GLU_c" stoichiometry="1.0"/>
        </listOfProducts>
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            </math>
            <listOfParameters>
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              <parameter id="REDUCED_COST" value="0.000000"/>
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        </kineticLaw>
    </reaction>
    <reaction id="R141" name="R141" reversible="true">
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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        <listOfProducts>
            <speciesReference species="M_GLX_c" stoichiometry="1.0"/>
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        </listOfProducts>
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            </math>
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units="mmol_per_gDW_per_hr"/>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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<parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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<html:p>SUBSYSTEM: </html:p>
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<speciesReference species="M_NAD_c" stoichiometry="1.0"/>
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<listOfProducts>
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</listOfProducts>
<kineticLaw>
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</math>
<listOfParameters>
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<parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
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<html:p>SUBSYSTEM: </html:p>
<html:p>PROTEIN_CLASS: </html:p>
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<listOfProducts>
<speciesReference species="M_NH3_c" stoichiometry="1.0"/>
<speciesReference species="M_CITR_c" stoichiometry="1.0"/>
</listOfProducts>
<kineticLaw>
<math xmlns="http://www.w3.org/1998/Math/MathML">

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                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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        </kineticLaw>
</reaction>
<reaction id="R144" name="R144" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2321c or Rv2322c </html:p>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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            <speciesReference species="M_AKG_c" stoichiometry="1.0"/>
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            <speciesReference species="M_GLUGSAL_c" stoichiometry="1.0"/>
            <speciesReference species="M_GLU_c" stoichiometry="1.0"/>
        </listOfProducts>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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</reaction>
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        <notes>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_ORN_c" stoichiometry="1.0"/>
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        <listOfProducts>
            <speciesReference species="M_PI_c" stoichiometry="1.0"/>
            <speciesReference species="M_CITR_c" stoichiometry="1.0"/>
        </listOfProducts>
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            </math>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R146" name="R146" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2531c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_ORN_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_PTRSC_c" stoichiometry="1.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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        </kineticLaw>
    </reaction>
    <reaction id="R147" name="R147" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2601 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_PTRSC_c" stoichiometry="1.0"/>
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        <listOfProducts>
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            <speciesReference species="M_SPRMD_c" stoichiometry="1.0"/>
        </listOfProducts>
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            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R148" name="R148" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv1850 and Rv1849 and Rv1848 and Rv1853 and
Rv1851 and Rv1852 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_UREA_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_NH3_c" stoichiometry="1.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R149" name="R149" reversible="true">
            <notes>
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                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
                <speciesReference species="M_ILE_c" stoichiometry="1.0"/>
                <speciesReference species="M_AKG_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_GLU_c" stoichiometry="1.0"/>
                <speciesReference species="M_OMVAL_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
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                </math>
                <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
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                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
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            </kineticLaw>
        </reaction>
        <reaction id="R150" name="R150" reversible="false">
            <notes>
                <html:p>GENE_ASSOCIATION: Rv2497c and Rv2496c </html:p>
                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
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                <speciesReference species="M_OXOMETHYLPENTANOATE_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_2MBUTLIPO_c" stoichiometry="1.0"/>
                <speciesReference species="M_CO2_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
                <math xmlns="http://www.w3.org/1998/Math/MathML">
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                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
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                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R151" name="R151" reversible="true">
            <notes>
                <html:p>GENE_ASSOCIATION: Rv2495c </html:p>
                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
                <speciesReference species="M_2MBUTLIPO_c" stoichiometry="1.0"/>
                <speciesReference species="M_COA_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_2MBUTCOA_c" stoichiometry="1.0"/>
                <speciesReference species="M_DLIPO_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
                <math xmlns="http://www.w3.org/1998/Math/MathML">
                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R152" name="R152" reversible="false">
            <notes>
                <html:p>GENE_ASSOCIATION: Rv3140 </html:p>
                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
                <speciesReference species="M_MK_c" stoichiometry="1.0"/>
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<speciesReference species="M_2MBUTCOA_c" stoichiometry="1.0"/>
</listOfReactants>
<listOfProducts>
<speciesReference species="M_MKH2_c" stoichiometry="1.0"/>
<speciesReference species="M_2MBECOA_c" stoichiometry="1.0"/>
</listOfProducts>
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<math xmlns="http://www.w3.org/1998/Math/MathML">
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</math>
<listOfParameters>
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<parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
<parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
<parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
<parameter id="REDUCED_COST" value="0.000000"/>
</listOfParameters>
</kineticLaw>
</reaction>
<reaction id="R153" name="R153" reversible="false">
<notes>
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<html:p>PROTEIN_ASSOCIATION: </html:p>
<html:p>SUBSYSTEM: </html:p>
<html:p>PROTEIN_CLASS: </html:p>
</notes>
<listOfReactants>
<speciesReference species="M_2MBECOA_c" stoichiometry="1.0"/>
</listOfReactants>
<listOfProducts>
<speciesReference species="M_HMBUTCOA_c" stoichiometry="1.0"/>
</listOfProducts>
<kineticLaw>
<math xmlns="http://www.w3.org/1998/Math/MathML">
<ci> FLUX_VALUE </ci>
</math>
<listOfParameters>
<parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
<parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
<parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
<parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
<parameter id="REDUCED_COST" value="0.000000"/>
</listOfParameters>
</kineticLaw>
</reaction>
<reaction id="R154" name="R154" reversible="false">
<notes>
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<html:p>PROTEIN_ASSOCIATION: </html:p>

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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_HMBUTCOA_c" stoichiometry="1.0"/>
            <speciesReference species="M_NAD_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_MAACCOA_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADH_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R155" name="R155" reversible="true">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv1074c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_MAACCOA_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_PROPIONYLCOA_c" stoichiometry="1.0"/>
            <speciesReference species="M_ACCOA_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="-100000.0"
units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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                <parameter id="REDUCED_COST" value="0.000000"/>
              </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R156" name="R156" reversible="false">
            <notes>
                <html:p>GENE_ASSOCIATION: Rv0904c or Rv2502c or Rv0974c or Rv0904c or Rv3799c
or Rv3280 or Rv2247 </html:p>
                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
                <speciesReference species="M_PROPIONYLCOA_c" stoichiometry="1.0"/>
                <speciesReference species="M_BIOTIN-CO2_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_SMMALONYLCOA_c" stoichiometry="1.0"/>
                <speciesReference species="M_BIOTIN_c" stoichiometry="0.999"/>
            </listOfProducts>
            <kineticLaw>
                <math xmlns="http://www.w3.org/1998/Math/MathML">
                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
                  <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R157" name="R157" reversible="true">
            <notes>
                <html:p>GENE_ASSOCIATION: orphan </html:p>
                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
                <speciesReference species="M_SMMALONYLCOA_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_RMMALONYLCOA_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
                <math xmlns="http://www.w3.org/1998/Math/MathML">
                    <ci> FLUX_VALUE </ci>
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                </math>
                <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
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                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R158" name="R158" reversible="false">
            <notes>
                <html:p>GENE_ASSOCIATION: Rv1492 and Rv1493 </html:p>
                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
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                <speciesReference species="M_COB-III_c" stoichiometry="0.001"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_SUCCOA_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
                <math xmlns="http://www.w3.org/1998/Math/MathML">
                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
                  <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R159" name="R159" reversible="false">
            <notes>
                <html:p>GENE_ASSOCIATION: Rv1492 and Rv1493 </html:p>
                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
                <speciesReference species="M_SUCCOA_c" stoichiometry="1.0"/>
                <speciesReference species="M_COB-III_c" stoichiometry="0.001"/>
            </listOfReactants>
```

```
        <listOfProducts>
            <speciesReference species="M_RMMALONYLCOA_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R160" name="R160" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2496c and Rv2497c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_MOP_c" stoichiometry="1.0"/>
            <speciesReference species="M_LIPO_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_3MBUTLIPO_c" stoichiometry="1.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R161" name="R161" reversible="true">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2495c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
```

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            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_3MBUTLIPO_c" stoichiometry="1.0"/>
            <speciesReference species="M_COA_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_3MBUTCOA_c" stoichiometry="1.0"/>
            <speciesReference species="M_DLIPO_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="-100000.0"
units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R162" name="R162" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv3140 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_MK_c" stoichiometry="1.0"/>
            <speciesReference species="M_3MBUTCOA_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_MKH2_c" stoichiometry="1.0"/>
            <speciesReference species="M_3MBECOA_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R163" name="R163" reversible="false">
            <notes>
                <html:p>GENE_ASSOCIATION: Rv0904c or Rv2502c or Rv0974c or Rv0904c or Rv3799c
or Rv3280 or Rv2247 </html:p>
                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
                <speciesReference species="M_3MBECOA_c" stoichiometry="1.0"/>
                <speciesReference species="M_BIOTIN-CO2_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_MGLUTCOA_c" stoichiometry="1.0"/>
                <speciesReference species="M_BIOTIN_c" stoichiometry="0.999"/>
            </listOfProducts>
            <kineticLaw>
                <math xmlns="http://www.w3.org/1998/Math/MathML">
                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
                  <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R164" name="R164" reversible="false">
            <notes>
                <html:p>GENE_ASSOCIATION: orphan </html:p>
                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
                <speciesReference species="M_MGLUTCOA_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_HMGLUTCOA_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
                <math xmlns="http://www.w3.org/1998/Math/MathML">
                    <ci> FLUX_VALUE </ci>
                </math>
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            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R165" name="R165" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: orphan </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_HMGLUTCOA_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_ACCOA_c" stoichiometry="1.0"/>
            <speciesReference species="M_ACTAC_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R166" name="R166" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: orphan </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_ACTAC_c" stoichiometry="1.0"/>
            <speciesReference species="M_COA_c" stoichiometry="1.0"/>
            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
```

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            <speciesReference species="M_AMP_c" stoichiometry="1.0"/>
            <speciesReference species="M_AACCOA_c" stoichiometry="1.0"/>
            <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R167" name="R167" reversible="true">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2504c and Rv2503c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_SUCCOA_c" stoichiometry="1.0"/>
            <speciesReference species="M_ACTAC_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_SUCC_c" stoichiometry="1.0"/>
            <speciesReference species="M_AACCOA_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="-100000.0"
units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R168" name="R168" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2497c and Rv2496c </html:p>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_LIPO_c" stoichiometry="1.0"/>
            <speciesReference species="M_OMVAL_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_IBUTLIPO_c" stoichiometry="1.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R169" name="R169" reversible="true">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2495c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_IBUTLIPO_c" stoichiometry="1.0"/>
            <speciesReference species="M_COA_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_DLIPO_c" stoichiometry="1.0"/>
            <speciesReference species="M_IBUTCOA_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="-100000.0"
units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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            <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
            <parameter id="REDUCED_COST" value="0.000000"/>
          </listOfParameters>
      </kineticLaw>
</reaction>
<reaction id="R170" name="R170" reversible="false">
      <notes>
          <html:p>GENE_ASSOCIATION: Rv3140 </html:p>
          <html:p>PROTEIN_ASSOCIATION: </html:p>
          <html:p>SUBSYSTEM: </html:p>
          <html:p>PROTEIN_CLASS: </html:p>
      </notes>
      <listOfReactants>
          <speciesReference species="M_MK_c" stoichiometry="1.0"/>
          <speciesReference species="M_IBUTCOA_c" stoichiometry="1.0"/>
      </listOfReactants>
      <listOfProducts>
          <speciesReference species="M_MKH2_c" stoichiometry="1.0"/>
          <speciesReference species="M_MACRCOA_c" stoichiometry="1.0"/>
      </listOfProducts>
      <kineticLaw>
          <math xmlns="http://www.w3.org/1998/Math/MathML">
              <ci> FLUX_VALUE </ci>
          </math>
          <listOfParameters>
            <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
            <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
            <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
            <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
            <parameter id="REDUCED_COST" value="0.000000"/>
          </listOfParameters>
      </kineticLaw>
</reaction>
<reaction id="R171" name="R171" reversible="false">
      <notes>
          <html:p>GENE_ASSOCIATION: Rv1070c or Rv0905 or Rv2486 or Rv1472 </html:p>
          <html:p>PROTEIN_ASSOCIATION: </html:p>
          <html:p>SUBSYSTEM: </html:p>
          <html:p>PROTEIN_CLASS: </html:p>
      </notes>
      <listOfReactants>
          <speciesReference species="M_MACRCOA_c" stoichiometry="1.0"/>
      </listOfReactants>
      <listOfProducts>
          <speciesReference species="M_HIBUTCOA_c" stoichiometry="1.0"/>
      </listOfProducts>
      <kineticLaw>
          <math xmlns="http://www.w3.org/1998/Math/MathML">
              <ci> FLUX_VALUE </ci>
```

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            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R172" name="R172" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: orphan </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_HIBUTCOA_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_HIBUT_c" stoichiometry="1.0"/>
            <speciesReference species="M_COA_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R173" name="R173" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv1144 or Rv0751c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_HIBUT_c" stoichiometry="1.0"/>
            <speciesReference species="M_NAD_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
```

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            <speciesReference species="M_METHYMALONATE_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADH_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R174" name="R174" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv0753c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_METHYMALONATE_c" stoichiometry="1.0"/>
            <speciesReference species="M_NAD_c" stoichiometry="1.0"/>
            <speciesReference species="M_COA_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_PROPIONYLCOA_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADH_c" stoichiometry="1.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R175" name="R175" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: orphan </html:p>
```

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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_ISUCC_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_OA_c" stoichiometry="1.0"/>
            <speciesReference species="M_NH3_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
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        </notes>
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            <speciesReference species="M_bALA_c" stoichiometry="1.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="1.0"/>
        </listOfProducts>
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            </math>
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        </kineticLaw>
    </reaction>
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        </notes>
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            </math>
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            <speciesReference species="M_NAD_c" stoichiometry="1.0"/>
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            <speciesReference species="M_NADH_c" stoichiometry="1.0"/>
        </listOfProducts>
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            </math>
            <listOfParameters>
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<html:p>PROTEIN_CLASS: </html:p>
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</notes>
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<speciesReference species="M_NADH_c" stoichiometry="1.0"/>
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<speciesReference species="M_NAD_c" stoichiometry="1"/>

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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_CYS_c" stoichiometry="1.0"/>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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            <speciesReference species="M_CO2_c" stoichiometry="1.0"/>
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            </math>
            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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        </kineticLaw>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
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            <speciesReference species="M_OBUT_c" stoichiometry="1.0"/>
            <speciesReference species="M_O2_c" stoichiometry="1.0"/>
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        <listOfProducts>
            <speciesReference species="M_PROPIONYLP_c" stoichiometry="1.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="1.0"/>
        </listOfProducts>
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            </math>
            <listOfParameters>
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        </kineticLaw>
    </reaction>
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            <speciesReference species="M_THF_c" stoichiometry="1.0"/>
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      <listOfProducts>
            <speciesReference species="M_NH3_c" stoichiometry="1.0"/>
            <speciesReference species="M_METTHF_c" stoichiometry="1.0"/>
            <speciesReference species="M_DHLIPOYLPROTEIN_c" stoichiometry="1.0"/>
      </listOfProducts>
      <kineticLaw>
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            </math>
            <listOfParameters>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
      </notes>
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            <speciesReference species="M_THF_c" stoichiometry="1.0"/>
      </listOfReactants>
      <listOfProducts>
            <speciesReference species="M_METTHF_c" stoichiometry="1.0"/>
            <speciesReference species="M_GLY_c" stoichiometry="1.0"/>
      </listOfProducts>
      <kineticLaw>
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            </math>
            <listOfParameters>
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                    <parameter id="LOWER_BOUND" value="-100000.0"
units="mmol_per_gDW_per_hr"/>
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                    <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                    <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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      <reaction id="R186" name="R186" reversible="false">
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                  <html:p>SUBSYSTEM: </html:p>
                  <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
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            <listOfProducts>
                  <speciesReference species="M_SAP_c" stoichiometry="1.0"/>
                  <speciesReference species="M_CO2_c" stoichiometry="1.0"/>
            </listOfProducts>
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            </notes>
            <listOfReactants>
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            <listOfProducts>
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            </notes>
            <listOfReactants>
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            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_NH3_c" stoichiometry="1.0"/>
                <speciesReference species="M_PYR_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
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                </math>
                <listOfParameters>
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            <html:p>PROTEIN_CLASS: </html:p>
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        <listOfProducts>
            <speciesReference species="M_NH3_c" stoichiometry="1.0"/>
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            </math>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
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            <speciesReference species="M_AKG_c" stoichiometry="1.0"/>
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        <listOfProducts>
            <speciesReference species="M_4HPP_c" stoichiometry="1.0"/>
            <speciesReference species="M_GLU_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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            </listOfParameters>
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            <html:p>SUBSYSTEM: </html:p>
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        </notes>
        <listOfReactants>
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            <speciesReference species="M_O2_c" stoichiometry="1.0"/>
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        <listOfProducts>
            <speciesReference species="M_HOMOGEN_c" stoichiometry="1.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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        </kineticLaw>
    </reaction>
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            <html:p>SUBSYSTEM: </html:p>
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        </notes>
        <listOfReactants>
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            <speciesReference species="M_O2_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_MACAC_c" stoichiometry="1.0"/>
        </listOfProducts>
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                <ci> FLUX_VALUE </ci>
            </math>
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                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
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            <listOfReactants>
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            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_FUACAC_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
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                </math>
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units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R194" name="R194" reversible="false">
            <notes>
                <html:p>GENE_ASSOCIATION: orphan </html:p>
                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
                <speciesReference species="M_FUACAC_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_FUM_c" stoichiometry="1.0"/>
                <speciesReference species="M_ACTAC_c" stoichiometry="1.0"/>
```

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        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R195" name="R195" reversible="true">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv3565 or Rv0337c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_AKG_c" stoichiometry="1.0"/>
            <speciesReference species="M_PHE_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_PHPYR_c" stoichiometry="1.0"/>
            <speciesReference species="M_GLU_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="-100000.0"
units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R196" name="R196" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2220 or Rv1878 or Rv2860c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
```

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            </notes>
            <listOfReactants>
                <speciesReference species="M_GLU_c" stoichiometry="1.0"/>
                <speciesReference species="M_NH3_c" stoichiometry="1.0"/>
                <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_GLN_c" stoichiometry="1.0"/>
                <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
                <speciesReference species="M_PI_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
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                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
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                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R197" name="R197" reversible="true">
            <notes>
                <html:p>GENE_ASSOCIATION: Rv3859c and Rv3858c </html:p>
                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
                <speciesReference species="M_GLN_c" stoichiometry="1.0"/>
                <speciesReference species="M_AKG_c" stoichiometry="1.0"/>
                <speciesReference species="M_NADH_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_GLU_c" stoichiometry="2.0"/>
                <speciesReference species="M_NAD_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
                <math xmlns="http://www.w3.org/1998/Math/MathML">
                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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                <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                <parameter id="REDUCED_COST" value="0.000000"/>
              </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R198" name="R198" reversible="true">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2476c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_NH3_c" stoichiometry="1.0"/>
            <speciesReference species="M_AKG_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADPH_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_GLU_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="-100000.0"
units="mmol_per_gDW_per_hr"/>
                <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                <parameter id="REDUCED_COST" value="0.000000"/>
              </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R199" name="R199" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2439c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_GLU_c" stoichiometry="1.0"/>
            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_GLUP_c" stoichiometry="1.0"/>
            <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
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        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
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              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R200" name="R200" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2427c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_NADPH_c" stoichiometry="1.0"/>
            <speciesReference species="M_GLUP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_GLUGSAL_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADP_c" stoichiometry="1.0"/>
            <speciesReference species="M_PI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R201" name="R201" reversible="true">
        <notes>
            <html:p>GENE_ASSOCIATION: orphan </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
```

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            </notes>
            <listOfReactants>
                <speciesReference species="M_GLUGSAL_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_P5C_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
                <math xmlns="http://www.w3.org/1998/Math/MathML">
                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
                  <parameter id="LOWER_BOUND" value="-100000.0"
units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R202" name="R202" reversible="true">
            <notes>
                <html:p>GENE_ASSOCIATION: Rv0500 </html:p>
                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
                <speciesReference species="M_P5C_c" stoichiometry="2.0"/>
                <speciesReference species="M_NADPH_c" stoichiometry="1.0"/>
                <speciesReference species="M_NADH_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_PRO_c" stoichiometry="2.0"/>
                <speciesReference species="M_NADP_c" stoichiometry="1.0"/>
                <speciesReference species="M_NAD_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
                <math xmlns="http://www.w3.org/1998/Math/MathML">
                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
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                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R203" name="R203" reversible="true">
            <notes>
                <html:p>GENE_ASSOCIATION: Rv2747 </html:p>
                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
                <speciesReference species="M_GLU_c" stoichiometry="1.0"/>
                <speciesReference species="M_ACCOA_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_NAGLU_c" stoichiometry="1.0"/>
                <speciesReference species="M_COA_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
                <math xmlns="http://www.w3.org/1998/Math/MathML">
                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
                  <parameter id="LOWER_BOUND" value="-100000.0"
units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R204" name="R204" reversible="false">
            <notes>
                <html:p>GENE_ASSOCIATION: Rv1654 </html:p>
                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
                <speciesReference species="M_NAGLU_c" stoichiometry="1.0"/>
                <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_NAGLUP_c" stoichiometry="1.0"/>
                <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
                <math xmlns="http://www.w3.org/1998/Math/MathML">
```

```
                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
                  <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
                </listOfParameters>
        </kineticLaw>
</reaction>
<reaction id="R205" name="R205" reversible="false">
        <notes>
                <html:p>GENE_ASSOCIATION: Rv1652 </html:p>
                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
                <speciesReference species="M_NADPH_c" stoichiometry="1.0"/>
                <speciesReference species="M_NAGLUP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
                <speciesReference species="M_NAGLUS_c" stoichiometry="1.0"/>
                <speciesReference species="M_NADP_c" stoichiometry="1.0"/>
                <speciesReference species="M_PI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
                <math xmlns="http://www.w3.org/1998/Math/MathML">
                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
                  <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
                </listOfParameters>
        </kineticLaw>
</reaction>
<reaction id="R206" name="R206" reversible="false">
        <notes>
                <html:p>GENE_ASSOCIATION: Rv1655 </html:p>
                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
                <speciesReference species="M_NAGLUS_c" stoichiometry="1.0"/>
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                <speciesReference species="M_GLU_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_NAORN_c" stoichiometry="1.0"/>
                <speciesReference species="M_AKG_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
                <math xmlns="http://www.w3.org/1998/Math/MathML">
                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
                  <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R207" name="R207" reversible="true">
            <notes>
                <html:p>GENE_ASSOCIATION: Rv1653 </html:p>
                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
                <speciesReference species="M_NAORN_c" stoichiometry="1.0"/>
                <speciesReference species="M_GLU_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_NAGLU_c" stoichiometry="1.0"/>
                <speciesReference species="M_ORN_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
                <math xmlns="http://www.w3.org/1998/Math/MathML">
                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
                  <parameter id="LOWER_BOUND" value="-100000.0"
units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R208" name="R208" reversible="false">
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        <notes>
            <html:p>GENE_ASSOCIATION: Rv1383 and Rv1384 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_GLN_c" stoichiometry="1.0"/>
            <speciesReference species="M_ATP_c" stoichiometry="2.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_CAP_c" stoichiometry="1.0"/>
            <speciesReference species="M_GLU_c" stoichiometry="1.0"/>
            <speciesReference species="M_ADP_c" stoichiometry="2.0"/>
            <speciesReference species="M_PI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R209" name="R209" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv1658 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_CITR_c" stoichiometry="1.0"/>
            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_AMP_c" stoichiometry="1.0"/>
            <speciesReference species="M_ARGSUCC_c" stoichiometry="1.0"/>
            <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
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                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
</reaction>
<reaction id="R210" name="R210" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv1659 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_ARGSUCC_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_ARG_c" stoichiometry="1.0"/>
            <speciesReference species="M_FUM_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
</reaction>
<reaction id="R211" name="R211" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv3002c and Rv3003c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_PYR_c" stoichiometry="2.0"/>
            <speciesReference species="M_THI_c" stoichiometry="0.001"/>
        </listOfReactants>
```

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        <listOfProducts>
            <speciesReference species="M_ACLAC_c" stoichiometry="1.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R212" name="R212" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv3001c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_ACLAC_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADPH_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_DHMVA_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R213" name="R213" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv0189c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
```

```
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_DHMVA_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_OMVAL_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R214" name="R214" reversible="true">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2210c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_GLU_c" stoichiometry="1.0"/>
            <speciesReference species="M_OMVAL_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_VAL_c" stoichiometry="1.0"/>
            <speciesReference species="M_AKG_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="-100000.0"
units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
```

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        </kineticLaw>
    </reaction>
    <reaction id="R215" name="R215" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv1559 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_THR_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_OBUT_c" stoichiometry="1.0"/>
            <speciesReference species="M_NH3_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R216" name="R216" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv3509c or Rv1820 or Rv3003c or ( Rv3470c and
Rv3002c ) </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_PYR_c" stoichiometry="1.0"/>
            <speciesReference species="M_OBUT_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_ABUT_c" stoichiometry="1.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
```

```
                <listOfParameters>
                  <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R217" name="R217" reversible="false">
            <notes>
                <html:p>GENE_ASSOCIATION: Rv3001c </html:p>
                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
                <speciesReference species="M_ABUT_c" stoichiometry="1.0"/>
                <speciesReference species="M_NADPH_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_DIHYDROXYMETHYLPENTANOATE_c"
stoichiometry="1.0"/>
                <speciesReference species="M_NADP_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
                <math xmlns="http://www.w3.org/1998/Math/MathML">
                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
                  <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R218" name="R218" reversible="false">
            <notes>
                <html:p>GENE_ASSOCIATION: Rv0189c </html:p>
                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
                <speciesReference species="M_DIHYDROXYMETHYLPENTANOATE_c"
stoichiometry="1.0"/>
            </listOfReactants>
```

```
        <listOfProducts>
            <speciesReference species="M_OXOMETHYLPENTANOATE_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R219" name="R219" reversible="true">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2210c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_GLU_c" stoichiometry="1.0"/>
            <speciesReference species="M_OXOMETHYLPENTANOATE_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_ILE_c" stoichiometry="1.0"/>
            <speciesReference species="M_AKG_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="-100000.0"
units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R220" name="R220" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv3710 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
```

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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_OMVAL_c" stoichiometry="1.0"/>
            <speciesReference species="M_ACCOA_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_IPPMAL_c" stoichiometry="1.0"/>
            <speciesReference species="M_COA_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R221" name="R221" reversible="true">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2988c and Rv2987c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_IPPMAL_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_CBHCAP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="-100000.0"
units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
```

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        </kineticLaw>
    </reaction>
    <reaction id="R222" name="R222" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2995c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_CBHCAP_c" stoichiometry="1.0"/>
            <speciesReference species="M_NAD_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_OICAP_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADH_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R223" name="R223" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: orphan </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_OICAP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_MOP_c" stoichiometry="1.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
```

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                <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
                <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                <parameter id="REDUCED_COST" value="0.000000"/>
              </listOfParameters>
          </kineticLaw>
      </reaction>
      <reaction id="R224" name="R224" reversible="true">
          <notes>
              <html:p>GENE_ASSOCIATION: Rv2210c </html:p>
              <html:p>PROTEIN_ASSOCIATION: </html:p>
              <html:p>SUBSYSTEM: </html:p>
              <html:p>PROTEIN_CLASS: </html:p>
          </notes>
          <listOfReactants>
              <speciesReference species="M_MOP_c" stoichiometry="1.0"/>
              <speciesReference species="M_GLU_c" stoichiometry="1.0"/>
          </listOfReactants>
          <listOfProducts>
              <speciesReference species="M_LEU_c" stoichiometry="1.0"/>
              <speciesReference species="M_AKG_c" stoichiometry="1.0"/>
          </listOfProducts>
          <kineticLaw>
              <math xmlns="http://www.w3.org/1998/Math/MathML">
                  <ci> FLUX_VALUE </ci>
              </math>
              <listOfParameters>
                <parameter id="LOWER_BOUND" value="-100000.0"
units="mmol_per_gDW_per_hr"/>
                <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                <parameter id="REDUCED_COST" value="0.000000"/>
              </listOfParameters>
          </kineticLaw>
      </reaction>
      <reaction id="R225" name="R225" reversible="true">
          <notes>
              <html:p>GENE_ASSOCIATION: Rv3565 or Rv0337c </html:p>
              <html:p>PROTEIN_ASSOCIATION: </html:p>
              <html:p>SUBSYSTEM: </html:p>
              <html:p>PROTEIN_CLASS: </html:p>
          </notes>
          <listOfReactants>
              <speciesReference species="M_OA_c" stoichiometry="1.0"/>
              <speciesReference species="M_GLU_c" stoichiometry="1.0"/>
          </listOfReactants>
          <listOfProducts>
```

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                <speciesReference species="M_ASP_c" stoichiometry="1.0"/>
                <speciesReference species="M_AKG_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
                <math xmlns="http://www.w3.org/1998/Math/MathML">
                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
                  <parameter id="LOWER_BOUND" value="-100000.0"
units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R226" name="R226" reversible="false">
            <notes>
                <html:p>GENE_ASSOCIATION: Rv2201 </html:p>
                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
                <speciesReference species="M_ASP_c" stoichiometry="1.0"/>
                <speciesReference species="M_GLN_c" stoichiometry="1.0"/>
                <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_GLU_c" stoichiometry="1.0"/>
                <speciesReference species="M_ASN_c" stoichiometry="1.0"/>
                <speciesReference species="M_AMP_c" stoichiometry="1.0"/>
                <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
                <math xmlns="http://www.w3.org/1998/Math/MathML">
                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
                  <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R227" name="R227" reversible="false">
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        <notes>
            <html:p>GENE_ASSOCIATION: Rv3709c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_ASP_c" stoichiometry="1.0"/>
            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_ASP4P_c" stoichiometry="1.0"/>
            <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R228" name="R228" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv3708c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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<html:p>SUBSYSTEM: </html:p>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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stoichiometry="1.0"/>
            <speciesReference species="M_SUCCOA_c" stoichiometry="1.0"/>
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        <listOfProducts>
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            <speciesReference species="M_COA_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
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        </notes>
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            <speciesReference species="M_GLU_c" stoichiometry="1.0"/>
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            <speciesReference species="M_AKG_c" stoichiometry="1.0"/>
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            </math>
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            </notes>
            <listOfReactants>
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            <listOfProducts>
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                <html:p>SUBSYSTEM: </html:p>
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                </math>
                <listOfParameters>
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            </kineticLaw>
        </reaction>
        <reaction id="R239" name="R239" reversible="true">
            <notes>
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                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
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                <speciesReference species="M_COA_c" stoichiometry="1.0"/>
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                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
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            <listOfProducts>
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                <speciesReference species="M_LLCT_c" stoichiometry="1.0"/>
            </listOfProducts>
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                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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</reaction>
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        <html:p>SUBSYSTEM: </html:p>
        <html:p>PROTEIN_CLASS: </html:p>
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    <listOfReactants>
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    <listOfProducts>
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        <speciesReference species="M_NH3_c" stoichiometry="1.0"/>
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        </math>
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        <html:p>SUBSYSTEM: </html:p>
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    </notes>
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    <listOfProducts>
        <speciesReference species="M_SAH_c" stoichiometry="1.0"/>
        <speciesReference species="M_MET_c" stoichiometry="1.0"/>
    </listOfProducts>
    <kineticLaw>
        <math xmlns="http://www.w3.org/1998/Math/MathML">
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        </math>
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          <html:p>SUBSYSTEM: </html:p>
          <html:p>PROTEIN_CLASS: </html:p>
      </notes>
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      </listOfReactants>
      <listOfProducts>
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          <speciesReference species="M_THF_c" stoichiometry="1.0"/>
          <speciesReference species="M_COB-II_c" stoichiometry="0.001"/>
      </listOfProducts>
      <kineticLaw>
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          </math>
          <listOfParameters>
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            <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
            <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
            <parameter id="REDUCED_COST" value="0.000000"/>
          </listOfParameters>
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</reaction>
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      </notes>
      <listOfReactants>
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                <speciesReference species="M_COB-II_c" stoichiometry="0.001"/>
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            </notes>
            <listOfReactants>
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            </listOfReactants>
            <listOfProducts>
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                <speciesReference species="M_THF_c" stoichiometry="1.0"/>
            </listOfProducts>
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                </math>
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                <speciesReference species="M_NH3_c" stoichiometry="1.0"/>
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            <listOfProducts>
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                <speciesReference species="M_NAD_c" stoichiometry="1.0"/>
            </listOfProducts>
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                </math>
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units="mmol_per_gDW_per_hr"/>
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                <speciesReference species="M_NADH_c" stoichiometry="1.0"/>
            </listOfProducts>
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                </math>
                <listOfParameters>
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</math>
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</listOfReactants>
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            </math>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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        </kineticLaw>
    </reaction>
    <reaction id="R250" name="R250" reversible="true">
        <notes>
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            <speciesReference species="M_ACCOA_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
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            <speciesReference species="M_COA_c" stoichiometry="1.0"/>
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units="mmol_per_gDW_per_hr"/>
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            <html:p>PROTEIN_CLASS: </html:p>
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            <speciesReference species="M_AC_c" stoichiometry="1.0"/>
        </listOfProducts>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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        </notes>
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        <listOfProducts>
            <speciesReference species="M_OAHSER_c" stoichiometry="1.0"/>
            <speciesReference species="M_COA_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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            </listOfParameters>
        </kineticLaw>
    </reaction>
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            <html:p>SUBSYSTEM: </html:p>
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        </notes>
        <listOfReactants>
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            <speciesReference species="M_CYS_c" stoichiometry="1.0"/>
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        <listOfProducts>
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            <speciesReference species="M_LLCT_c" stoichiometry="1.0"/>
        </listOfProducts>
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            </math>
            <listOfParameters>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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            <speciesReference species="M_H2S_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_AC_c" stoichiometry="1.0"/>
            <speciesReference species="M_HCYS_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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                <ci> FLUX_VALUE </ci>
```

```
            </math>
            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_H2S_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_SUCC_c" stoichiometry="1.0"/>
            <speciesReference species="M_HCYS_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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        </kineticLaw>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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        </listOfReactants>
        <listOfProducts>
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            <speciesReference species="M_OBUT_c" stoichiometry="1.0"/>
            <speciesReference species="M_NH3_c" stoichiometry="1.0"/>
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        <kineticLaw>
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            </math>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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        </kineticLaw>
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        </notes>
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            <speciesReference species="M_HCYS_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_LLCT_c" stoichiometry="1.0"/>
        </listOfProducts>
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            </math>
            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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        </kineticLaw>
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            <html:p>PROTEIN_CLASS: </html:p>
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        <listOfProducts>
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            <speciesReference species="M_CYS_c" stoichiometry="1.0"/>
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        </notes>
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            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_SAM_c" stoichiometry="1.0"/>
            <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
            <speciesReference species="M_PI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
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            </math>
            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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            </listOfParameters>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_ADN_c" stoichiometry="1.0"/>
            <speciesReference species="M_HCYS_c" stoichiometry="1.0"/>
        </listOfProducts>
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            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
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        </kineticLaw>
    </reaction>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_PRBATP_c" stoichiometry="1.0"/>
            <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
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            <listOfParameters>
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    <reaction id="R262" name="R262" reversible="false">
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            <html:p>SUBSYSTEM: </html:p>
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        </notes>
        <listOfReactants>
            <speciesReference species="M_PRBATP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_PRBAMP_c" stoichiometry="1.0"/>
            <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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    </reaction>
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        </notes>
        <listOfReactants>
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        </listOfReactants>
        <listOfProducts>
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        </listOfProducts>
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        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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        </kineticLaw>
    </reaction>
    <reaction id="R264" name="R264" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv1603 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_PRFP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_PRLP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R265" name="R265" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv1602 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_GLN_c" stoichiometry="1.0"/>
            <speciesReference species="M_PRLP_c" stoichiometry="1.0"/>
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        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_GLU_c" stoichiometry="1.0"/>
            <speciesReference species="M_DIMGP_c" stoichiometry="1.0"/>
            <speciesReference species="M_AICAR_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R266" name="R266" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv1601 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_DIMGP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_IMACP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R267" name="R267" reversible="true">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv3772 or Rv1600 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_IMACP_c" stoichiometry="1.0"/>
            <speciesReference species="M_GLU_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_HISOLP_c" stoichiometry="1.0"/>
            <speciesReference species="M_AKG_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="-100000.0"
units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R268" name="R268" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv1601 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_HISOLP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_HISOL_c" stoichiometry="1.0"/>
            <speciesReference species="M_PI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R269" name="R269" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv1599 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_HISOL_c" stoichiometry="1.0"/>
            <speciesReference species="M_NAD_c" stoichiometry="2.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_HIS_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADH_c" stoichiometry="2.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R270" name="R270" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2178c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_PEP_c" stoichiometry="1.0"/>
            <speciesReference species="M_E4P_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_3DDAH7P_c" stoichiometry="1.0"/>
            <speciesReference species="M_PI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
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            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R271" name="R271" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2538c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_3DDAH7P_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_DQT_c" stoichiometry="1.0"/>
            <speciesReference species="M_PI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R272" name="R272" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2537c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_DQT_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_DHSK_c" stoichiometry="1.0"/>
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        </listOfProducts>
        <kineticLaw>
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                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R273" name="R273" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2552c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_NADPH_c" stoichiometry="1.0"/>
            <speciesReference species="M_DHSK_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_SME_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R274" name="R274" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2539c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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        <listOfReactants>
            <speciesReference species="M_SME_c" stoichiometry="1.0"/>
            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_SME3P_c" stoichiometry="1.0"/>
            <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R275" name="R275" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv3227 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_PEP_c" stoichiometry="1.0"/>
            <speciesReference species="M_SME3P_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_3PSME_c" stoichiometry="1.0"/>
            <speciesReference species="M_PI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
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<reaction id="R276" name="R276" reversible="false">
	<notes>
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		<html:p>PROTEIN_ASSOCIATION: </html:p>
		<html:p>SUBSYSTEM: </html:p>
		<html:p>PROTEIN_CLASS: </html:p>
	</notes>
	<listOfReactants>
		<speciesReference species="M_3PSME_c" stoichiometry="1.0"/>
	</listOfReactants>
	<listOfProducts>
		<speciesReference species="M_CHOR_c" stoichiometry="1.0"/>
		<speciesReference species="M_PI_c" stoichiometry="1.0"/>
	</listOfProducts>
	<kineticLaw>
		<math xmlns="http://www.w3.org/1998/Math/MathML">
			<ci> FLUX_VALUE </ci>
		</math>
		<listOfParameters>
		  <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
		  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
		  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
		  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
		  <parameter id="REDUCED_COST" value="0.000000"/>
		</listOfParameters>
	</kineticLaw>
</reaction>
<reaction id="R277" name="R277" reversible="false">
	<notes>
		<html:p>GENE_ASSOCIATION: Rv1609 </html:p>
		<html:p>PROTEIN_ASSOCIATION: </html:p>
		<html:p>SUBSYSTEM: </html:p>
		<html:p>PROTEIN_CLASS: </html:p>
	</notes>
	<listOfReactants>
		<speciesReference species="M_CHOR_c" stoichiometry="1.0"/>
		<speciesReference species="M_GLN_c" stoichiometry="1.0"/>
	</listOfReactants>
	<listOfProducts>
		<speciesReference species="M_AN_c" stoichiometry="1.0"/>
		<speciesReference species="M_GLU_c" stoichiometry="1.0"/>
		<speciesReference species="M_PYR_c" stoichiometry="1.0"/>
	</listOfProducts>
	<kineticLaw>
		<math xmlns="http://www.w3.org/1998/Math/MathML">
			<ci> FLUX_VALUE </ci>
		</math>
		<listOfParameters>
		  <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
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            <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
            <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
            <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
            <parameter id="REDUCED_COST" value="0.000000"/>
          </listOfParameters>
      </kineticLaw>
</reaction>
<reaction id="R278" name="R278" reversible="false">
      <notes>
          <html:p>GENE_ASSOCIATION: Rv2192c </html:p>
          <html:p>PROTEIN_ASSOCIATION: </html:p>
          <html:p>SUBSYSTEM: </html:p>
          <html:p>PROTEIN_CLASS: </html:p>
      </notes>
      <listOfReactants>
          <speciesReference species="M_AN_c" stoichiometry="1.0"/>
          <speciesReference species="M_PRPP_c" stoichiometry="1.0"/>
      </listOfReactants>
      <listOfProducts>
          <speciesReference species="M_NPRAN_c" stoichiometry="1.0"/>
          <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
      </listOfProducts>
      <kineticLaw>
          <math xmlns="http://www.w3.org/1998/Math/MathML">
              <ci> FLUX_VALUE </ci>
          </math>
          <listOfParameters>
            <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
            <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
            <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
            <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
            <parameter id="REDUCED_COST" value="0.000000"/>
          </listOfParameters>
      </kineticLaw>
</reaction>
<reaction id="R279" name="R279" reversible="false">
      <notes>
          <html:p>GENE_ASSOCIATION: Rv1603 </html:p>
          <html:p>PROTEIN_ASSOCIATION: </html:p>
          <html:p>SUBSYSTEM: </html:p>
          <html:p>PROTEIN_CLASS: </html:p>
      </notes>
      <listOfReactants>
          <speciesReference species="M_NPRAN_c" stoichiometry="1.0"/>
      </listOfReactants>
      <listOfProducts>
          <speciesReference species="M_CPAD5P_c" stoichiometry="1.0"/>
      </listOfProducts>
      <kineticLaw>
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            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R280" name="R280" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv1611 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_CPAD5P_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_IGP_c" stoichiometry="1.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R281" name="R281" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv1613 and Rv1612 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_SER_c" stoichiometry="1.0"/>
            <speciesReference species="M_IGP_c" stoichiometry="1.0"/>
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            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_TRP_c" stoichiometry="1.0"/>
                <speciesReference species="M_G3P_c" stoichiometry="1.0"/>
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                </math>
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                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
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            </kineticLaw>
        </reaction>
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            <notes>
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                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
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                <speciesReference species="M_PHEN_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
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                </math>
                <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
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                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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        </listOfReactants>
        <listOfProducts>
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            <speciesReference species="M_CO2_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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        </kineticLaw>
    </reaction>
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        <notes>
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            <html:p>SUBSYSTEM: </html:p>
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        </notes>
        <listOfReactants>
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            <speciesReference species="M_GLU_c" stoichiometry="1.0"/>
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        <listOfProducts>
            <speciesReference species="M_AKG_c" stoichiometry="1.0"/>
            <speciesReference species="M_PHE_c" stoichiometry="1.0"/>
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            </math>
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units="mmol_per_gDW_per_hr"/>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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            </listOfParameters>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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            <speciesReference species="M_NAD_c" stoichiometry="1.0"/>
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        <listOfProducts>
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            <speciesReference species="M_NADH_c" stoichiometry="1.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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            <speciesReference species="M_GLU_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_TYR_c" stoichiometry="1.0"/>
            <speciesReference species="M_AKG_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
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                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
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                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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        <reaction id="R287" name="R287" reversible="true">
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                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
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                <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
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            <listOfProducts>
                <speciesReference species="M_PRPP_c" stoichiometry="1.0"/>
                <speciesReference species="M_AMP_c" stoichiometry="1.0"/>
            </listOfProducts>
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units="mmol_per_gDW_per_hr"/>
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                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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        </reaction>
        <reaction id="R288" name="R288" reversible="false">
            <notes>
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                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
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                <speciesReference species="M_CAP_c" stoichiometry="1.0"/>
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            <listOfProducts>
                <speciesReference species="M_CAASP_c" stoichiometry="1.0"/>
                <speciesReference species="M_PI_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
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                </math>
                <listOfParameters>
                  <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R289" name="R289" reversible="true">
            <notes>
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                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
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            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_DOROA_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
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                </math>
                <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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            </kineticLaw>
        </reaction>
        <reaction id="R290" name="R290" reversible="false">
            <notes>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_DOROA_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_OROA_c" stoichiometry="1.0"/>
            <speciesReference species="M_H2O2_c" stoichiometry="1.0"/>
        </listOfProducts>
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            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
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        <notes>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_OROA_c" stoichiometry="1.0"/>
            <speciesReference species="M_PRPP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_OMP_c" stoichiometry="1.0"/>
            <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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            <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
            <parameter id="REDUCED_COST" value="0.000000"/>
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      </kineticLaw>
</reaction>
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          <html:p>SUBSYSTEM: </html:p>
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      </notes>
      <listOfReactants>
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      </listOfReactants>
      <listOfProducts>
          <speciesReference species="M_UMP_c" stoichiometry="1.0"/>
          <speciesReference species="M_CO2_c" stoichiometry="1.0"/>
      </listOfProducts>
      <kineticLaw>
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          </math>
          <listOfParameters>
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            <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
            <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
            <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
            <parameter id="REDUCED_COST" value="0.000000"/>
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      </kineticLaw>
</reaction>
<reaction id="R293" name="R293" reversible="true">
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          <html:p>SUBSYSTEM: </html:p>
          <html:p>PROTEIN_CLASS: </html:p>
      </notes>
      <listOfReactants>
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          <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
      </listOfReactants>
      <listOfProducts>
          <speciesReference species="M_UDP_c" stoichiometry="1.0"/>
          <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
      </listOfProducts>
      <kineticLaw>
          <math xmlns="http://www.w3.org/1998/Math/MathML">
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                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
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                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
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            </kineticLaw>
        </reaction>
        <reaction id="R294" name="R294" reversible="true">
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                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
                <speciesReference species="M_UDP_c" stoichiometry="1.0"/>
                <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
                <speciesReference species="M_UTP_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
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                </math>
                <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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            </kineticLaw>
        </reaction>
        <reaction id="R295" name="R295" reversible="false">
            <notes>
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            </notes>
            <listOfReactants>
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            <speciesReference species="M_UTP_c" stoichiometry="1.0"/>
            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
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        <listOfProducts>
            <speciesReference species="M_GLU_c" stoichiometry="1.0"/>
            <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
            <speciesReference species="M_CTP_c" stoichiometry="1.0"/>
            <speciesReference species="M_PI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R296" name="R296" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv1699 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
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        </notes>
        <listOfReactants>
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            <speciesReference species="M_UTP_c" stoichiometry="1.0"/>
            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_CTP_c" stoichiometry="1.0"/>
            <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
            <speciesReference species="M_PI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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<parameter id="REDUCED_COST" value="0.000000"/>
</listOfParameters>
</kineticLaw>
</reaction>
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<notes>
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<html:p>SUBSYSTEM: </html:p>
<html:p>PROTEIN_CLASS: </html:p>
</notes>
<listOfReactants>
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<speciesReference species="M_CDP_c" stoichiometry="1.0"/>
<speciesReference species="M_O2_c" stoichiometry="1"/>
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<listOfProducts>
<speciesReference species="M_OTHIO_c" stoichiometry="1.0"/>
<speciesReference species="M_DCDP_c" stoichiometry="1.0"/>
</listOfProducts>
<kineticLaw>
<math xmlns="http://www.w3.org/1998/Math/MathML">
<ci> FLUX_VALUE </ci>
</math>
<listOfParameters>
<parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
<parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
<parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
<parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
<parameter id="REDUCED_COST" value="0.000000"/>
</listOfParameters>
</kineticLaw>
</reaction>
<reaction id="R299" name="R299" reversible="false">
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<html:p>PROTEIN_ASSOCIATION: </html:p>
<html:p>SUBSYSTEM: </html:p>
<html:p>PROTEIN_CLASS: </html:p>
</notes>
<listOfReactants>
<speciesReference species="M_DCDP_c" stoichiometry="1.0"/>
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</listOfReactants>
<listOfProducts>
<speciesReference species="M_DCTP_c" stoichiometry="1.0"/>
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</listOfProducts>
<kineticLaw>

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                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
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              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
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            </listOfReactants>
            <listOfProducts>
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                <html:p>SUBSYSTEM: </html:p>
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            <listOfProducts>
                <speciesReference species="M_DCDP_c" stoichiometry="1.0"/>
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                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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            <parameter id="REDUCED_COST" value="0.000000"/>
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      </kineticLaw>
</reaction>
<reaction id="R311" name="R311" reversible="false">
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      </notes>
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          <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
      </listOfReactants>
      <listOfProducts>
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          <speciesReference species="M_PRPP_c" stoichiometry="1.0"/>
      </listOfProducts>
      <kineticLaw>
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            </math>
            <listOfParameters>
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        <listOfProducts>
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        </listOfProducts>
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            </math>
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            <speciesReference species="M_PRAM_c" stoichiometry="1.0"/>
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        <listOfProducts>
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            <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
            <speciesReference species="M_PI_c" stoichiometry="1.0"/>
        </listOfProducts>
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            </math>
            <listOfParameters>
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        </kineticLaw>
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        <speciesReference species="M_GAR_c" stoichiometry="1.0"/>
    </listOfReactants>
    <listOfProducts>
        <speciesReference species="M_FGAR_c" stoichiometry="1.0"/>
        <speciesReference species="M_THF_c" stoichiometry="1.0"/>
    </listOfProducts>
    <kineticLaw>
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        </math>
        <listOfParameters>
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</reaction>
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        <html:p>SUBSYSTEM: </html:p>
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    </notes>
    <listOfReactants>
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    <listOfProducts>
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        <speciesReference species="M_FGAM_c" stoichiometry="1.0"/>
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        <speciesReference species="M_PI_c" stoichiometry="1.0"/>
    </listOfProducts>
    <kineticLaw>
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            <ci> FLUX_VALUE </ci>
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            </math>
            <listOfParameters>
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            <html:p>SUBSYSTEM: </html:p>
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        </notes>
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            <speciesReference species="M_PI_c" stoichiometry="1.0"/>
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        </notes>
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            <speciesReference species="M_PI_c" stoichiometry="1.0"/>
        </listOfProducts>
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            </math>
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    </reaction>
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            <speciesReference species="M_AICAR_c" stoichiometry="1.0"/>
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            <html:p>SUBSYSTEM: </html:p>
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        <listOfProducts>
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            <speciesReference species="M_THF_c" stoichiometry="1.0"/>
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            </math>
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</listOfReactants>
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<speciesReference species="M_PPI_c" stoichiometry="1.0"/>

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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
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            <html:p>SUBSYSTEM: </html:p>
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            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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            <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
            <speciesReference species="M_DGDP_c" stoichiometry="1.0"/>
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            <html:p>SUBSYSTEM: </html:p>
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            <speciesReference species="M_PI_c" stoichiometry="1.0"/>
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        <listOfProducts>
            <speciesReference species="M_AMP_c" stoichiometry="1.0"/>
            <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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            <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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        </listOfReactants>
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            </math>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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            <speciesReference species="M_XAN_c" stoichiometry="1.0"/>
            <speciesReference species="M_PRPP_c" stoichiometry="1.0"/>
        </listOfReactants>
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            <speciesReference species="M_XMP_c" stoichiometry="1.0"/>
            <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
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                <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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    </reaction>
    <reaction id="R337" name="R337" reversible="true">
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            <html:p>SUBSYSTEM: </html:p>
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        </notes>
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            <speciesReference species="M_PI_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_HYXN_c" stoichiometry="1.0"/>
            <speciesReference species="M_DR1P_c" stoichiometry="1.0"/>
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        <kineticLaw>
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            </math>
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units="mmol_per_gDW_per_hr"/>
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                <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                <parameter id="REDUCED_COST" value="0.000000"/>
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    </reaction>
    <reaction id="R338" name="R338" reversible="true">
        <notes>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_PI_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_AD_c" stoichiometry="1.0"/>
            <speciesReference species="M_DR1P_c" stoichiometry="1.0"/>
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            </listOfProducts>
            <kineticLaw>
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                </math>
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units="mmol_per_gDW_per_hr"/>
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                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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            </notes>
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                <speciesReference species="M_R5P_c" stoichiometry="1"/>
            </listOfProducts>
            <kineticLaw>
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                </math>
                <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
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                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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            </kineticLaw>
        </reaction>
        <reaction id="R339" name="R339" reversible="true">
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                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
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            </listOfProducts>
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units="mmol_per_gDW_per_hr"/>
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                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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            </kineticLaw>
        </reaction>
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            </notes>
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            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_ADN_c" stoichiometry="1.0"/>
                <speciesReference species="M_PI_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
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                </math>
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units="mmol_per_gDW_per_hr"/>
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                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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            </kineticLaw>
        </reaction>
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                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
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                <speciesReference species="M_R1P_c" stoichiometry="1.0"/>
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            <listOfProducts>
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                <speciesReference species="M_PI_c" stoichiometry="1.0"/>
            </listOfProducts>
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                </math>
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units="mmol_per_gDW_per_hr"/>
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                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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        </reaction>
        <reaction id="R342" name="R342" reversible="true">
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                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
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                <speciesReference species="M_R1P_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
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                <speciesReference species="M_PI_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
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                    <ci> FLUX_VALUE </ci>
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                </math>
                <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
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                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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        </reaction>
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                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
                <speciesReference species="M_XTSINE_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
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                <speciesReference species="M_RIB_c" stoichiometry="1"/>
            </listOfProducts>
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                </math>
                <listOfParameters>
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                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
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            </kineticLaw>
        </reaction>
        <reaction id="R344" name="R344" reversible="false">
            <notes>
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                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
                <speciesReference species="M_ADN_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
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            <speciesReference species="M_INS_c" stoichiometry="1.0"/>
            <speciesReference species="M_NH3_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R345" name="R345" reversible="false">
        <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_DA_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_DIN_c" stoichiometry="1.0"/>
            <speciesReference species="M_NH3_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R346" name="R346" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: orphan </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
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        </notes>
        <listOfReactants>
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        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_DGMP_c" stoichiometry="1.0"/>
            <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
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            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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        </kineticLaw>
    </reaction>
    <reaction id="R347" name="R347" reversible="false">
        <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_GTP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_ppGpp_c" stoichiometry="1.0"/>
            <speciesReference species="M_AMP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
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<reaction id="R348" name="R348" reversible="false">
      <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
      </notes>
      <listOfReactants>
            <speciesReference species="M_ppGpp_c" stoichiometry="1.0"/>
      </listOfReactants>
      <listOfProducts>
            <speciesReference species="M_GDP_c" stoichiometry="1.0"/>
            <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
      </listOfProducts>
      <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                  <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
      </kineticLaw>
</reaction>
<reaction id="R349" name="R349" reversible="false">
      <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
      </notes>
      <listOfReactants>
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            <speciesReference species="M_IMP_c" stoichiometry="1.0"/>
            <speciesReference species="M_GTP_c" stoichiometry="1.0"/>
      </listOfReactants>
      <listOfProducts>
            <speciesReference species="M_GDP_c" stoichiometry="1.0"/>
            <speciesReference species="M_ASUC_c" stoichiometry="1.0"/>
            <speciesReference species="M_PI_c" stoichiometry="1.0"/>
      </listOfProducts>
      <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                  <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
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                <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
                <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                <parameter id="REDUCED_COST" value="0.000000"/>
              </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R350" name="R350" reversible="true">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv0777 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_ASUC_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_FUM_c" stoichiometry="1.0"/>
            <speciesReference species="M_AMP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="-100000.0"
units="mmol_per_gDW_per_hr"/>
                <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                <parameter id="REDUCED_COST" value="0.000000"/>
              </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R351" name="R351" reversible="true">
        <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
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        </notes>
        <listOfReactants>
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            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_ADP_c" stoichiometry="2.0"/>
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            </listOfProducts>
            <kineticLaw>
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                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
                  <parameter id="LOWER_BOUND" value="-100000.0"
units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R351b" name="R351b" reversible="true">
            <notes>
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                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
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            </notes>
            <listOfReactants>
                <speciesReference species="M_ADN_c" stoichiometry="1.0"/>
                <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_AMP_c" stoichiometry="1.0"/>
                <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
                <math xmlns="http://www.w3.org/1998/Math/MathML">
                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
                  <parameter id="LOWER_BOUND" value="-100000.0"
units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R352" name="R352" reversible="false">
            <notes>
                <html:p>GENE_ASSOCIATION: Rv3051c and Rv3048c </html:p>
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            <speciesReference species="M_O2_c" stoichiometry="1"/>
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            <speciesReference species="M_OTHIO_c" stoichiometry="1.0"/>
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            </math>
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            <speciesReference species="M_DATP_c" stoichiometry="1.0"/>
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            <speciesReference species="M_OTHIO_c" stoichiometry="1.0"/>
            <speciesReference species="M_DGDP_c" stoichiometry="1.0"/>
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            <kineticLaw>
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                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
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                <speciesReference species="M_FUM_c" stoichiometry="1.0"/>
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            <listOfProducts>
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                <speciesReference species="M_ISUCC_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
                <math xmlns="http://www.w3.org/1998/Math/MathML">
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                </math>
                <listOfParameters>
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        </notes>
        <listOfReactants>
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        <listOfProducts>
                <speciesReference species="M_ISUCC_c" stoichiometry="1.0"/>
                <speciesReference species="M_H2O2_c" stoichiometry="1.0"/>
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                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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                <html:p>SUBSYSTEM: </html:p>
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              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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            <speciesReference species="M_PRPP_c" stoichiometry="1.0"/>
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            <speciesReference species="M_CO2_c" stoichiometry="1.0"/>
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        <kineticLaw>
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            </math>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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            <speciesReference species="M_NH3_c" stoichiometry="1.0"/>
        </listOfProducts>
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            </math>
            <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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        </notes>
        <listOfReactants>
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            <speciesReference species="M_PRPP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_NACN_c" stoichiometry="1.0"/>
            <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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          <html:p>SUBSYSTEM: </html:p>
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      </notes>
      <listOfReactants>
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          <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
      </listOfReactants>
      <listOfProducts>
          <speciesReference species="M_NAAD_c" stoichiometry="1.0"/>
          <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
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      <kineticLaw>
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          </math>
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      </kineticLaw>
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          <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
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      <listOfProducts>
          <speciesReference species="M_AMP_c" stoichiometry="1.0"/>
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        </listOfProducts>
        <kineticLaw>
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            </math>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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        </kineticLaw>
    </reaction>
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            <html:p>SUBSYSTEM: </html:p>
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            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
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        <listOfProducts>
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            <speciesReference species="M_GLU_c" stoichiometry="1.0"/>
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        <kineticLaw>
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            </math>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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    </reaction>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_R1P_c" stoichiometry="1.0"/>
            <speciesReference species="M_NAC_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_NACD_c" stoichiometry="1.0"/>
            <speciesReference species="M_PI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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        </kineticLaw>
    </reaction>
    <reaction id="R372" name="R372" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv3307 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_R1P_c" stoichiometry="1.0"/>
            <speciesReference species="M_NAM_c" stoichiometry="1.0"/>
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        <listOfProducts>
            <speciesReference species="M_NAMD_c" stoichiometry="1.0"/>
            <speciesReference species="M_PI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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            </listOfParameters>
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    </reaction>
    <reaction id="R373" name="R373" reversible="false">
        <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_NACN_c" stoichiometry="1.0"/>
            <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R374" name="R374" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: orphan </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
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        </notes>
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            <speciesReference species="M_NAMD_c" stoichiometry="1.0"/>
            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
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        <listOfProducts>
            <speciesReference species="M_NAMN_c" stoichiometry="1.0"/>
            <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
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            </math>
            <listOfParameters>
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              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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    </reaction>
    <reaction id="R375" name="R375" reversible="false">
        <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
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        </notes>
        <listOfReactants>
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            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_NAD_c" stoichiometry="1.0"/>
            <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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        </kineticLaw>
    </reaction>
    <reaction id="R376" name="R376" reversible="true">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv0155 and Rv0157 and Rv0156 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_NADPH_c" stoichiometry="1.0"/>
        </listOfReactants>
```

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            <listOfProducts>
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                <speciesReference species="M_NADH_c" stoichiometry="1.0"/>
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                </math>
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units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R377" name="R377" reversible="false">
            <notes>
                <html:p>GENE_ASSOCIATION: Rv1695 </html:p>
                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
                <speciesReference species="M_NAD_c" stoichiometry="1.0"/>
                <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_NADP_c" stoichiometry="1.0"/>
                <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
                <math xmlns="http://www.w3.org/1998/Math/MathML">
                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
                  <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R378" name="R378" reversible="false">
            <notes>
                <html:p>GENE_ASSOCIATION: orphan </html:p>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_NAD_c" stoichiometry="1.0"/>
            <speciesReference species="M_PI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R379" name="R379" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2713 or Rv3303c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_NADPH_c" stoichiometry="1.0"/>
            <speciesReference species="M_NAD_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_NADP_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADH_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R380" name="R380" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv3199c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_NAD_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_AMP_c" stoichiometry="1.0"/>
            <speciesReference species="M_NAMN_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R381" name="R381" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv1415 or Rv1940 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_GTP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_D6RP5P_c" stoichiometry="1.0"/>
            <speciesReference species="M_FOR_c" stoichiometry="1.0"/>
            <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
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            <listOfParameters>
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              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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        </kineticLaw>
    </reaction>
    <reaction id="R382" name="R382" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2671 or Rv1409 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_D6RP5P_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_A6RP5P_c" stoichiometry="1.0"/>
            <speciesReference species="M_NH3_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R383" name="R383" reversible="false">
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_NADPH_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_A6RP5P2_c" stoichiometry="1.0"/>
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            <speciesReference species="M_NADP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
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              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
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        <notes>
            <html:p>GENE_ASSOCIATION: orphan </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_A6RP5P2_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_A6RP_c" stoichiometry="1.0"/>
            <speciesReference species="M_PI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
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            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
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        <notes>
            <html:p>GENE_ASSOCIATION: Rv1940 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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        <listOfProducts>
            <speciesReference species="M_DB4P_c" stoichiometry="1.0"/>
            <speciesReference species="M_FOR_c" stoichiometry="1.0"/>
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        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
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            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R386" name="R386" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv1416 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_DB4P_c" stoichiometry="1.0"/>
            <speciesReference species="M_A6RP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_D8RL_c" stoichiometry="1.0"/>
            <speciesReference species="M_PI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R387" name="R387" reversible="false">
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        <notes>
            <html:p>GENE_ASSOCIATION: Rv1412 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_D8RL_c" stoichiometry="2.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_RIBFLAV_c" stoichiometry="1.0"/>
            <speciesReference species="M_A6RP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R388" name="R388" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2786c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_RIBFLAV_c" stoichiometry="1.0"/>
            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
            <speciesReference species="M_FMN_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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            <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
            <parameter id="REDUCED_COST" value="0.000000"/>
          </listOfParameters>
      </kineticLaw>
</reaction>
<reaction id="R389" name="R389" reversible="false">
      <notes>
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          <html:p>PROTEIN_ASSOCIATION: </html:p>
          <html:p>SUBSYSTEM: </html:p>
          <html:p>PROTEIN_CLASS: </html:p>
      </notes>
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          <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
          <speciesReference species="M_FMN_c" stoichiometry="1.0"/>
      </listOfReactants>
      <listOfProducts>
          <speciesReference species="M_FAD_c" stoichiometry="1.0"/>
          <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
      </listOfProducts>
      <kineticLaw>
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              <ci> FLUX_VALUE </ci>
          </math>
          <listOfParameters>
            <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
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            <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
            <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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</reaction>
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      </notes>
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          <speciesReference species="M_METTHF_c" stoichiometry="1.0"/>
      </listOfReactants>
      <listOfProducts>
          <speciesReference species="M_AKP_c" stoichiometry="1.0"/>
          <speciesReference species="M_THF_c" stoichiometry="1.0"/>
      </listOfProducts>
      <kineticLaw>
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            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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        </kineticLaw>
    </reaction>
    <reaction id="R391" name="R391" reversible="false">
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_NADPH_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_PANT_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R392" name="R392" reversible="false">
        <notes>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_PANT_c" stoichiometry="1.0"/>
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            <speciesReference species="M_bALA_c" stoichiometry="1.0"/>
            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_PNTO_c" stoichiometry="1.0"/>
            <speciesReference species="M_AMP_c" stoichiometry="1.0"/>
            <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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        </kineticLaw>
    </reaction>
    <reaction id="R393" name="R393" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv1092c </html:p>
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            <html:p>SUBSYSTEM: </html:p>
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        </notes>
        <listOfReactants>
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            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_4PPNTO_c" stoichiometry="1.0"/>
            <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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        </kineticLaw>
    </reaction>
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<reaction id="R394" name="R394" reversible="false">
    <notes>
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        <html:p>SUBSYSTEM: </html:p>
        <html:p>PROTEIN_CLASS: </html:p>
    </notes>
    <listOfReactants>
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        <speciesReference species="M_CYS_c" stoichiometry="1.0"/>
        <speciesReference species="M_CTP_c" stoichiometry="1.0"/>
    </listOfReactants>
    <listOfProducts>
        <speciesReference species="M_4PPNCYS_c" stoichiometry="1.0"/>
        <speciesReference species="M_CMP_c" stoichiometry="1.0"/>
        <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
    </listOfProducts>
    <kineticLaw>
        <math xmlns="http://www.w3.org/1998/Math/MathML">
            <ci> FLUX_VALUE </ci>
        </math>
        <listOfParameters>
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          <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
          <parameter id="REDUCED_COST" value="0.000000"/>
        </listOfParameters>
    </kineticLaw>
</reaction>
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        <html:p>SUBSYSTEM: </html:p>
        <html:p>PROTEIN_CLASS: </html:p>
    </notes>
    <listOfReactants>
        <speciesReference species="M_4PPNCYS_c" stoichiometry="1.0"/>
    </listOfReactants>
    <listOfProducts>
        <speciesReference species="M_4PPNTE_c" stoichiometry="1.0"/>
        <speciesReference species="M_CO2_c" stoichiometry="1.0"/>
    </listOfProducts>
    <kineticLaw>
        <math xmlns="http://www.w3.org/1998/Math/MathML">
            <ci> FLUX_VALUE </ci>
        </math>
        <listOfParameters>
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            <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
            <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
            <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
            <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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      </kineticLaw>
</reaction>
<reaction id="R396" name="R396" reversible="false">
      <notes>
          <html:p>GENE_ASSOCIATION: Rv2965c </html:p>
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          <html:p>SUBSYSTEM: </html:p>
          <html:p>PROTEIN_CLASS: </html:p>
      </notes>
      <listOfReactants>
          <speciesReference species="M_4PPNTE_c" stoichiometry="1.0"/>
          <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
      </listOfReactants>
      <listOfProducts>
          <speciesReference species="M_DPCOA_c" stoichiometry="1.0"/>
          <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
      </listOfProducts>
      <kineticLaw>
          <math xmlns="http://www.w3.org/1998/Math/MathML">
              <ci> FLUX_VALUE </ci>
          </math>
          <listOfParameters>
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            <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
            <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
            <parameter id="REDUCED_COST" value="0.000000"/>
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      </kineticLaw>
</reaction>
<reaction id="R397" name="R397" reversible="false">
      <notes>
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          <html:p>SUBSYSTEM: </html:p>
          <html:p>PROTEIN_CLASS: </html:p>
      </notes>
      <listOfReactants>
          <speciesReference species="M_DPCOA_c" stoichiometry="1.0"/>
          <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
      </listOfReactants>
      <listOfProducts>
          <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
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            <speciesReference species="M_COA_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R398" name="R398" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2523c or Rv2794c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_COA_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_ACP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
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            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R399" name="R399" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv3609c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_GTP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_FOR_c" stoichiometry="1.0"/>
            <speciesReference species="M_AHTD_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R400" name="R400" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv0757 and Rv0758 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_AHTD_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_DHP_c" stoichiometry="1.0"/>
            <speciesReference species="M_PI_c" stoichiometry="3.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R401" name="R401" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv3607c </html:p>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_DHP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_AHHMP_c" stoichiometry="1.0"/>
            <speciesReference species="M_GLAL_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R402" name="R402" reversible="false">
        <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_AHHMP_c" stoichiometry="1.0"/>
            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_AHHMD_c" stoichiometry="1.0"/>
            <speciesReference species="M_AMP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R403" name="R403" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv0013 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_CHOR_c" stoichiometry="1.0"/>
            <speciesReference species="M_GLN_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_GLU_c" stoichiometry="1.0"/>
            <speciesReference species="M_ADCHOR_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R404" name="R404" reversible="false">
        <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_ADCHOR_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_PABA_c" stoichiometry="1.0"/>
            <speciesReference species="M_PYR_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
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            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R405" name="R405" reversible="false">
        <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_PABA_c" stoichiometry="1.0"/>
            <speciesReference species="M_AHHMD_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_DHPT_c" stoichiometry="1.0"/>
            <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R406" name="R406" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv3608c or Rv1207 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_AHHMP_c" stoichiometry="1.0"/>
            <speciesReference species="M_PABA_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
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            <speciesReference species="M_DHPT_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
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        </kineticLaw>
    </reaction>
    <reaction id="R407" name="R407" reversible="false">
        <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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            <speciesReference species="M_GLU_c" stoichiometry="1.0"/>
            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_DHF_c" stoichiometry="1.0"/>
            <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
            <speciesReference species="M_PI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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    </reaction>
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        <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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        <listOfProducts>
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            <speciesReference species="M_NADP_c" stoichiometry="1.0"/>
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            </math>
            <listOfParameters>
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        </kineticLaw>
    </reaction>
    <reaction id="R409" name="R409" reversible="false">
        <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_THF_c" stoichiometry="1.0"/>
            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
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        <listOfProducts>
            <speciesReference species="M_THFG_c" stoichiometry="1.0"/>
            <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
            <speciesReference species="M_PI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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            <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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</reaction>
<reaction id="R410" name="R410" reversible="false">
      <notes>
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          <html:p>PROTEIN_CLASS: </html:p>
      </notes>
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      <listOfProducts>
          <speciesReference species="M_THF_c" stoichiometry="1.0"/>
          <speciesReference species="M_GLU_c" stoichiometry="1.0"/>
      </listOfProducts>
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            <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
            <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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</reaction>
<reaction id="R411" name="R411" reversible="false">
      <notes>
          <html:p>GENE_ASSOCIATION: Rv3025c or Rv1464 </html:p>
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          <html:p>SUBSYSTEM: </html:p>
          <html:p>PROTEIN_CLASS: </html:p>
      </notes>
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          <speciesReference species="M_FE2_c" stoichiometry="1.0"/>
      </listOfReactants>
      <listOfProducts>
          <speciesReference species="M_FERO_c" stoichiometry="1.0"/>
          <speciesReference species="M_ALA_c" stoichiometry="1.0"/>
      </listOfProducts>
      <kineticLaw>
          <math xmlns="http://www.w3.org/1998/Math/MathML">
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                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
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                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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        </reaction>
        <reaction id="R412" name="R412" reversible="true">
            <notes>
                <html:p>GENE_ASSOCIATION: Rv3215 or Rv2386c </html:p>
                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
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            <listOfProducts>
                <speciesReference species="M_ICHOR_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
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                </math>
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units="mmol_per_gDW_per_hr"/>
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                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R413" name="R413" reversible="false">
            <notes>
                <html:p>GENE_ASSOCIATION: Rv0555 </html:p>
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                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
                <speciesReference species="M_AKG_c" stoichiometry="1.0"/>
                <speciesReference species="M_ICHOR_c" stoichiometry="1.0"/>
            </listOfReactants>
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        <listOfProducts>
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            <speciesReference species="M_SHCHC_c" stoichiometry="1.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R414" name="R414" reversible="false">
        <notes>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_OSB_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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        </kineticLaw>
    </reaction>
    <reaction id="R415" name="R415" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv0542c and Rv0553 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
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            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_OSB_c" stoichiometry="1.0"/>
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            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_OSBCOA_c" stoichiometry="1.0"/>
            <speciesReference species="M_AMP_c" stoichiometry="1.0"/>
            <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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        </kineticLaw>
    </reaction>
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        <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_OSBCOA_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_DHN_c" stoichiometry="1.0"/>
            <speciesReference species="M_COA_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R417" name="R417" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv0534c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_DHN_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_DMK_c" stoichiometry="1.0"/>
            <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
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        <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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            <speciesReference species="M_DMK_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_MKH2_c" stoichiometry="1.0"/>
            <speciesReference species="M_SAH_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
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                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
</reaction>
<reaction id="R419" name="R419" reversible="false">
        <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_ACCOA_c" stoichiometry="4.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_PIMELOYL-COA_c" stoichiometry="1.0"/>
            <speciesReference species="M_COA_c" stoichiometry="3.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
</reaction>
<reaction id="R420" name="R420" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv1569 and Rv0032 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_PIMELOYL-COA_c" stoichiometry="1.0"/>
            <speciesReference species="M_ALA_c" stoichiometry="1.0"/>
        </listOfReactants>
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            <listOfProducts>
                <speciesReference species="M_8-AMINO7-OXONONANOATE_c"
stoichiometry="1.0"/>
                <speciesReference species="M_COA_c" stoichiometry="1.0"/>
                <speciesReference species="M_CO2_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
                <math xmlns="http://www.w3.org/1998/Math/MathML">
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                </math>
                <listOfParameters>
                  <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R421" name="R421" reversible="false">
            <notes>
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                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
                <speciesReference species="M_8-AMINO7-OXONONANOATE_c"
stoichiometry="1.0"/>
                <speciesReference species="M_SAM_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_7-8-DIAMINONONANOATE_c" stoichiometry="1.0"/>
                <speciesReference species="M_SAM-2-OXOBUTANOATE_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
                <math xmlns="http://www.w3.org/1998/Math/MathML">
                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
                  <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
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            </kineticLaw>
        </reaction>
        <reaction id="R422" name="R422" reversible="false">
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        <notes>
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            <html:p>SUBSYSTEM: </html:p>
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        </notes>
        <listOfReactants>
            <speciesReference species="M_SAM-2-OXOBUTANOATE_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_SAM_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R423" name="R423" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv1570 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_7-8-DIAMINONONANOATE_c" stoichiometry="1.0"/>
            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_DETHIOBIOTIN_c" stoichiometry="1.0"/>
            <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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<parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
<parameter id="REDUCED_COST" value="0.000000"/>
</listOfParameters>
</kineticLaw>
</reaction>
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        </notes>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_BIOTIN-BCCP_c" stoichiometry="1.0"/>
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<speciesReference species="M_ATP_c" stoichiometry="1.0"/>
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<speciesReference species="M_APO-LIPO_c" stoichiometry="1.0"/>
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</listOfProducts>
<kineticLaw>
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</math>
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            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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        <listOfProducts>
            <speciesReference species="M_LIPO_c" stoichiometry="1.0"/>
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        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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            <html:p>SUBSYSTEM: </html:p>
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            <speciesReference species="M_GLU_c" stoichiometry="1.0"/>
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        <listOfProducts>
            <speciesReference species="M_TRNA-GLU_c" stoichiometry="1.0"/>
            <speciesReference species="M_AMP_c" stoichiometry="1.0"/>
            <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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                <ci> FLUX_VALUE </ci>
            </math>
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            <listOfParameters>
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            <html:p>SUBSYSTEM: </html:p>
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        </notes>
        <listOfReactants>
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            <speciesReference species="M_NADPH_c" stoichiometry="1.0"/>
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            <speciesReference species="M_NADP_c" stoichiometry="1.0"/>
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            </math>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_GLU1SEMIALD_c" stoichiometry="1.0"/>
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        <listOfProducts>
            <speciesReference species="M_5-AMINO-LEVULINATE_c" stoichiometry="1.0"/>
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        </listOfProducts>
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            <html:p>SUBSYSTEM: </html:p>
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        </notes>
        <listOfReactants>
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        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_PORPHOBILILOGIN_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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            <html:p>SUBSYSTEM: </html:p>
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            <speciesReference species="M_NH3_c" stoichiometry="4.0"/>
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            </math>
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        <listOfProducts>
            <speciesReference species="M_UROPORPHYRINOGEN-III_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
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    </reaction>
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            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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        </listOfReactants>
        <listOfProducts>
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            <speciesReference species="M_CO2_c" stoichiometry="4.0"/>
        </listOfProducts>
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        <notes>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
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        <listOfProducts>
            <speciesReference species="M_PROTOPORPHYRINOGEN_c" stoichiometry="1.0"/>
            <speciesReference species="M_H2O2_c" stoichiometry="2.0"/>
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            </math>
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        </kineticLaw>
    </reaction>
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        <notes>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_COPROPORPHYRINOGEN-III_c" stoichiometry="1.0"/>
            <speciesReference species="M_SAM_c" stoichiometry="2.0"/>
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        <listOfProducts>
            <speciesReference species="M_PROTOPORPHYRINOGEN_c" stoichiometry="1.0"/>
            <speciesReference species="M_MET_c" stoichiometry="2.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="2.0"/>
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            </math>
            <listOfParameters>
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            <html:p>SUBSYSTEM: </html:p>
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        </notes>
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        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_PROTOPORPHYRIN-IX_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
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            </math>
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        <notes>
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            <html:p>SUBSYSTEM: </html:p>
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        </notes>
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        <listOfProducts>
            <speciesReference species="M_PROTOHEME-FE2_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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    </reaction>
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        <notes>
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            <html:p>SUBSYSTEM: </html:p>
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            <speciesReference species="M_HEME-FE2_c" stoichiometry="1.0"/>
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            <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
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        <kineticLaw>
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            </math>
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            <html:p>SUBSYSTEM: </html:p>
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        </notes>
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        <listOfProducts>
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            <speciesReference species="M_SAH_c" stoichiometry="2.0"/>
        </listOfProducts>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
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        </notes>
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            <speciesReference species="M_SAH_c" stoichiometry="1.0"/>
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            </math>
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            <html:p>SUBSYSTEM: </html:p>
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            <speciesReference species="M_O2_c" stoichiometry="1"/>
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        </kineticLaw>
    </reaction>
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		<html:p>SUBSYSTEM: </html:p>
		<html:p>PROTEIN_CLASS: </html:p>
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	<listOfProducts>
		<speciesReference species="M_PRECORIN-4B_c" stoichiometry="1.0"/>
		<speciesReference species="M_SAH_c" stoichiometry="1.0"/>
	</listOfProducts>
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		  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
		  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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	<listOfProducts>
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		<speciesReference species="M_SAH_c" stoichiometry="1.0"/>
	</listOfProducts>
	<kineticLaw>
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		</math>
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        <speciesReference species="M_NADPH_c" stoichiometry="1.0"/>
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            <html:p>SUBSYSTEM: </html:p>
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        </notes>
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            <speciesReference species="M_SAM_c" stoichiometry="2.0"/>
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              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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            <html:p>SUBSYSTEM: </html:p>
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            <html:p>PROTEIN_CLASS: </html:p>
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            </math>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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            <speciesReference species="M_GLN_c" stoichiometry="2.0"/>
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        <listOfProducts>
            <speciesReference species="M_HYDROGENOBYRINATE-A-C-DIAMIDE_c"
stoichiometry="1.0"/>
            <speciesReference species="M_PI_c" stoichiometry="2.0"/>
            <speciesReference species="M_ADP_c" stoichiometry="2.0"/>
            <speciesReference species="M_GLU_c" stoichiometry="2.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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                <parameter id="REDUCED_COST" value="0.000000"/>
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              <html:p>SUBSYSTEM: </html:p>
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          </notes>
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stoichiometry="1.0"/>
              <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
              <speciesReference species="M_CO-II_c" stoichiometry="1.0"/>
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          <listOfProducts>
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stoichiometry="1.0"/>
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              <speciesReference species="M_PI_c" stoichiometry="1.0"/>
          </listOfProducts>
          <kineticLaw>
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              </math>
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          </notes>
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stoichiometry="1.0"/>
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<listOfProducts>
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</listOfProducts>
<kineticLaw>
<math xmlns="http://www.w3.org/1998/Math/MathML">
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</math>
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<notes>

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                <html:p>SUBSYSTEM: </html:p>
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            </notes>
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stoichiometry="1.0"/>
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                <speciesReference species="M_ADENOSYL-COBRATE_c" stoichiometry="1.0"/>
                <speciesReference species="M_ADP_c" stoichiometry="4.0"/>
                <speciesReference species="M_PI_c" stoichiometry="4.0"/>
                <speciesReference species="M_GLU_c" stoichiometry="4.0"/>
            </listOfProducts>
            <kineticLaw>
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                </math>
                <listOfParameters>
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            </kineticLaw>
        </reaction>
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                <html:p>SUBSYSTEM: </html:p>
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            </notes>
            <listOfReactants>
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            <listOfProducts>
                <speciesReference species="M_ADENOSYLCOBINAMIDE_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
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                </math>
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</listOfProducts>
<kineticLaw>
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</math>
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<listOfProducts>
<speciesReference species="M_ADENOSYLCOBINAMIDE-GDP_c"

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stoichiometry="1.0"/>
                <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
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                </math>
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                <html:p>SUBSYSTEM: </html:p>
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            </notes>
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            <listOfProducts>
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                <speciesReference species="M_GMP_c" stoichiometry="1.0"/>
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                </math>
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                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
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            </notes>
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<parameter id="REDUCED_COST" value="0.000000"/>
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</reaction>
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<notes>
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<speciesReference species="M_AMP_c" stoichiometry="1.0"/>
<speciesReference species="M_SER_c" stoichiometry="1.0"/>
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</reaction>
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<html:p>SUBSYSTEM: </html:p>
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</notes>
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<speciesReference species="M_PRECURSOR-Z_c" stoichiometry="1.0"/>
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    </reaction>
    <reaction id="R462" name="R462" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: ( Rv3119 or Rv0866 ) and Rv3322c </html:p>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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        <notes>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_MO2_c" stoichiometry="1.0"/>
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              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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            <html:p>SUBSYSTEM: </html:p>
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        </notes>
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            <speciesReference species="M_PPI_c" stoichiometry="1"/>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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        </kineticLaw>
    </reaction>
    <reaction id="R465" name="R465" reversible="false">
        <notes>
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            <html:p>SUBSYSTEM: </html:p>
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            <speciesReference species="M_TS-COSH-TYR_c" stoichiometry="1.0"/>
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            </math>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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        <listOfProducts>
            <speciesReference species="M_TS-COSH-TYR_c" stoichiometry="1.0"/>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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        </kineticLaw>
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</reaction>
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        <html:p>SUBSYSTEM: </html:p>
        <html:p>PROTEIN_CLASS: </html:p>
    </notes>
    <listOfReactants>
        <speciesReference species="M_AIR_c" stoichiometry="1.0"/>
    </listOfReactants>
    <listOfProducts>
        <speciesReference species="M_AHMMP_c" stoichiometry="1"/>
    </listOfProducts>
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        </math>
        <listOfParameters>
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          <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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    </kineticLaw>
</reaction>
<reaction id="R468" name="R468" reversible="false">
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        <html:p>SUBSYSTEM: </html:p>
        <html:p>PROTEIN_CLASS: </html:p>
    </notes>
    <listOfReactants>
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        <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
    </listOfReactants>
    <listOfProducts>
        <speciesReference species="M_AMPMP_c" stoichiometry="1.0"/>
        <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
    </listOfProducts>
    <kineticLaw>
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        </math>
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<parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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<html:p>PROTEIN_CLASS: </html:p>
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</listOfReactants>
<listOfProducts>
<speciesReference species="M_MAHMPPP_c" stoichiometry="1.0"/>
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</listOfProducts>
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<speciesReference species="M_TS-PROTEIN_c" stoichiometry="1.0"/>
</listOfProducts>

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            </math>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_HEMT_c" stoichiometry="1.0"/>
            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_MPET_c" stoichiometry="1.0"/>
            <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
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            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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    </reaction>
    <reaction id="R472" name="R472" reversible="false">
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            <html:p>GENE_ASSOCIATION: Rv0414c </html:p>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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<speciesReference species="M_THIP_c" stoichiometry="1.0"/>
<speciesReference species="M_PPI_c" stoichiometry="1.0"/>
</listOfProducts>
<kineticLaw>
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</math>
<listOfParameters>
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<parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
<parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
<parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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</reaction>
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</notes>
<listOfReactants>
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</listOfReactants>
<listOfProducts>
<speciesReference species="M_THI_c" stoichiometry="1.0"/>
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</listOfProducts>
<kineticLaw>
<math xmlns="http://www.w3.org/1998/Math/MathML">
<ci> FLUX_VALUE </ci>
</math>
<listOfParameters>
<parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
<parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
<parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
<parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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</listOfParameters>
</kineticLaw>
</reaction>
<reaction id="R474" name="R474" reversible="false">
<notes>

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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_AHMMP_c" stoichiometry="1.0"/>
            <speciesReference species="M_HEMT_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
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            </math>
            <listOfParameters>
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        </notes>
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            <speciesReference species="M_GTP_c" stoichiometry="1.0"/>
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        <listOfProducts>
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            <speciesReference species="M_GDP_c" stoichiometry="1.0"/>
        </listOfProducts>
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            </math>
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</reaction>
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          <html:p>SUBSYSTEM: </html:p>
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      </notes>
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          <speciesReference species="M_LPPG_c" stoichiometry="1.0"/>
          <speciesReference species="M_PPI_c" stoichiometry="1"/>
      </listOfProducts>
      <kineticLaw>
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          </math>
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</reaction>
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            </math>
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            <html:p>SUBSYSTEM: </html:p>
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            <speciesReference species="M_GMP_c" stoichiometry="1.0"/>
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            </math>
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            <speciesReference species="M_ATP_c" stoichiometry="5.0"/>
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            <speciesReference species="M_GLU_c" stoichiometry="5.0"/>
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            </math>
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            <html:p>SUBSYSTEM: </html:p>
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        </notes>
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            <speciesReference species="M_IP_c" stoichiometry="1.0"/>
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            <speciesReference species="M_UDP_c" stoichiometry="1.0"/>
            <speciesReference species="M_PI_c" stoichiometry="1.0"/>
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        </listOfReactants>
        <listOfProducts>
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            <speciesReference species="M_AC_c" stoichiometry="1.0"/>
        </listOfProducts>
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            </math>
            <listOfParameters>
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        </kineticLaw>
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            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
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        <listOfProducts>
            <speciesReference species="M_CYS-NG-INS_c" stoichiometry="1.0"/>
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            <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
        </listOfProducts>
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            </math>
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      </notes>
      <listOfReactants>
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          <speciesReference species="M_ACCOA_c" stoichiometry="1.0"/>
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          <speciesReference species="M_COA_c" stoichiometry="1.0"/>
      </listOfProducts>
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          </math>
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</reaction>
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      <listOfProducts>
          <speciesReference species="M_MYCOTHIOL-S-CONJUGATE_c" stoichiometry="1.0"/>
          <speciesReference species="M_H2X_c" stoichiometry="1.0"/>
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        <kineticLaw>
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            </math>
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            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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            <speciesReference species="M_NG-INS_c" stoichiometry="0.999"/>
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            </math>
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        </notes>
        <listOfReactants>
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        <listOfProducts>
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        </listOfProducts>
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            </math>
            <listOfParameters>
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    </reaction>
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            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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        <listOfProducts>
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            <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
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            </math>
            <listOfParameters>
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            <html:p>SUBSYSTEM: </html:p>
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        <listOfProducts>
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        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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<parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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</reaction>
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<listOfProducts>
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<speciesReference species="M_AMP_c" stoichiometry="1.0"/>
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<kineticLaw>
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<listOfProducts>

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              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R491" name="R491" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2382c and Rv2381c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_ACCOA_c" stoichiometry="1.0"/>
            <speciesReference species="M_MALCOA_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_MBTCD-HBA_c" stoichiometry="1.0"/>
            <speciesReference species="M_COA_c" stoichiometry="2.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R492" name="R492" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: orphan </html:p>
```

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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_MBTB-SER_c" stoichiometry="1.0"/>
            <speciesReference species="M_MBTE-LYS_c" stoichiometry="1.0"/>
            <speciesReference species="M_MBTF-LYS_c" stoichiometry="1.0"/>
            <speciesReference species="M_MBTCD-HBA_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_MBT_c" stoichiometry="1.0"/>
            <speciesReference species="M_MBT-HOLO_c" stoichiometry="5.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R493" name="R493" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: orphan </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_MBT_c" stoichiometry="1.0"/>
            <speciesReference species="M_ACCOA_c" stoichiometry="2.0"/>
            <speciesReference species="M_NADPH_c" stoichiometry="2.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_MBTSEC_c" stoichiometry="1.0"/>
            <speciesReference species="M_COA_c" stoichiometry="2.0"/>
            <speciesReference species="M_NADP_c" stoichiometry="2.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
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```
                <listOfParameters>
                  <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R494" name="R494" reversible="false">
            <notes>
                <html:p>GENE_ASSOCIATION: orphan </html:p>
                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
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                <speciesReference species="M_ACCOA_c" stoichiometry="9.0"/>
                <speciesReference species="M_NADPH_c" stoichiometry="18.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_MBTWALL_c" stoichiometry="1.0"/>
                <speciesReference species="M_COA_c" stoichiometry="9.0"/>
                <speciesReference species="M_NADP_c" stoichiometry="18.0"/>
            </listOfProducts>
            <kineticLaw>
                <math xmlns="http://www.w3.org/1998/Math/MathML">
                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
                  <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
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            </kineticLaw>
        </reaction>
        <reaction id="R495" name="R495" reversible="false">
            <notes>
                <html:p>GENE_ASSOCIATION: Rv0904c or Rv2502c or Rv0974c or Rv0904c or Rv3799c
or Rv3280 or Rv2247 </html:p>
                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
                <speciesReference species="M_ACCOA_c" stoichiometry="1.0"/>
```

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                <speciesReference species="M_BIOTIN-CO2_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_MALCOA_c" stoichiometry="1.0"/>
                <speciesReference species="M_BIOTIN_c" stoichiometry="0.999"/>
            </listOfProducts>
            <kineticLaw>
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                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
                  <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R496" name="R496" reversible="true">
            <notes>
                <html:p>GENE_ASSOCIATION: ( Rv2243 or Rv0649 ) and Rv2244 </html:p>
                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
                <speciesReference species="M_ACCOA_c" stoichiometry="1.0"/>
                <speciesReference species="M_ACP_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_COA_c" stoichiometry="1.0"/>
                <speciesReference species="M_ACACP_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
                <math xmlns="http://www.w3.org/1998/Math/MathML">
                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
                  <parameter id="LOWER_BOUND" value="-100000.0"
units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R497" name="R497" reversible="false">
```

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        <notes>
            <html:p>GENE_ASSOCIATION: Rv2524c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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            <speciesReference species="M_NADPH_c" stoichiometry="4.0"/>
            <speciesReference species="M_ACACP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_NADP_c" stoichiometry="4.0"/>
            <speciesReference species="M_HEXANOYL-ACP_c" stoichiometry="1.0"/>
            <speciesReference species="M_ACP_c" stoichiometry="2.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="2.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R497b" name="R497b" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2524c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_MALACP_c" stoichiometry="4.0"/>
            <speciesReference species="M_NADPH_c" stoichiometry="8.0"/>
            <speciesReference species="M_ACACP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_NADP_c" stoichiometry="8.0"/>
            <speciesReference species="M_OCTANOYL-ACP_c" stoichiometry="1.0"/>
            <speciesReference species="M_ACP_c" stoichiometry="4.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="4.0"/>
        </listOfProducts>
        <kineticLaw>
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            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R498" name="R498" reversible="false">
        <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_NADPH_c" stoichiometry="12.0"/>
            <speciesReference species="M_ACACP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_NADP_c" stoichiometry="12.0"/>
            <speciesReference species="M_TETRADECANOYL-ACP_c" stoichiometry="1.0"/>
            <speciesReference species="M_ACP_c" stoichiometry="6.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="6.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R499" name="R499" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2524c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
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        </notes>
        <listOfReactants>
            <speciesReference species="M_MALACP_c" stoichiometry="7.0"/>
            <speciesReference species="M_NADPH_c" stoichiometry="14.0"/>
            <speciesReference species="M_ACACP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_HEXADECANOYL-ACP_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADP_c" stoichiometry="14.0"/>
            <speciesReference species="M_ACP_c" stoichiometry="7.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="7.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R500" name="R500" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2524c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_MALACP_c" stoichiometry="7.0"/>
            <speciesReference species="M_NADPH_c" stoichiometry="13.0"/>
            <speciesReference species="M_ACACP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_9-HEXADECENOYL-ACP_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADP_c" stoichiometry="13.0"/>
            <speciesReference species="M_ACP_c" stoichiometry="7.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="7.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
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            <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
            <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
            <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
            <parameter id="REDUCED_COST" value="0.000000"/>
          </listOfParameters>
    </kineticLaw>
</reaction>
<reaction id="R501" name="R501" reversible="false">
    <notes>
        <html:p>GENE_ASSOCIATION: Rv2524c </html:p>
        <html:p>PROTEIN_ASSOCIATION: </html:p>
        <html:p>SUBSYSTEM: </html:p>
        <html:p>PROTEIN_CLASS: </html:p>
    </notes>
    <listOfReactants>
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        <speciesReference species="M_NADPH_c" stoichiometry="16.0"/>
        <speciesReference species="M_ACACP_c" stoichiometry="1.0"/>
    </listOfReactants>
    <listOfProducts>
        <speciesReference species="M_OCTADECANOYL-ACP_c" stoichiometry="1.0"/>
        <speciesReference species="M_NADP_c" stoichiometry="16.0"/>
        <speciesReference species="M_ACP_c" stoichiometry="8.0"/>
        <speciesReference species="M_CO2_c" stoichiometry="8.0"/>
    </listOfProducts>
    <kineticLaw>
        <math xmlns="http://www.w3.org/1998/Math/MathML">
            <ci> FLUX_VALUE </ci>
        </math>
        <listOfParameters>
          <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
          <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
          <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
          <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
          <parameter id="REDUCED_COST" value="0.000000"/>
        </listOfParameters>
    </kineticLaw>
</reaction>
<reaction id="R502" name="R502" reversible="false">
    <notes>
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        <html:p>PROTEIN_ASSOCIATION: </html:p>
        <html:p>SUBSYSTEM: </html:p>
        <html:p>PROTEIN_CLASS: </html:p>
    </notes>
    <listOfReactants>
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        <speciesReference species="M_NADPH_c" stoichiometry="15.0"/>
        <speciesReference species="M_ACACP_c" stoichiometry="1.0"/>
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        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_9-OCTADECENOYL-ACP_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADP_c" stoichiometry="15.0"/>
            <speciesReference species="M_ACP_c" stoichiometry="8.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="8.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R503" name="R503" reversible="false">
        <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_ACACP_c" stoichiometry="1.0"/>
            <speciesReference species="M_MALACP_c" stoichiometry="9.0"/>
            <speciesReference species="M_NADPH_c" stoichiometry="18.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_EICOSANOYL-ACP_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADP_c" stoichiometry="18.0"/>
            <speciesReference species="M_ACP_c" stoichiometry="9.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="9.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
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        </kineticLaw>
    </reaction>
    <reaction id="R504" name="R504" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2524c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_MALACP_c" stoichiometry="10.0"/>
            <speciesReference species="M_NADPH_c" stoichiometry="20.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_DOCOSANOYL-ACP_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADP_c" stoichiometry="20.0"/>
            <speciesReference species="M_ACP_c" stoichiometry="10.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="10.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R505" name="R505" reversible="false">
        <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
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            </listOfProducts>
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Rv1345 or Rv1427c or Rv1521 or Rv1529 or Rv1750c or Rv1925 or Rv2187 or Rv2505c or Rv2590 or
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Rv1345 or Rv1427c or Rv1521 or Rv1529 or Rv1750c or Rv1925 or Rv2187 or Rv2505c or Rv2590 or
Rv2930 or Rv2941 or Rv2948c or Rv2950c or Rv3089 or Rv3506 or Rv3513c or Rv3515c or Rv3561 or
Rv3801c or Rv3826 </html:p>
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            <html:p>SUBSYSTEM: </html:p>
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Rv1345 or Rv1427c or Rv1521 or Rv1529 or Rv1750c or Rv1925 or Rv2187 or Rv2505c or Rv2590 or
Rv2930 or Rv2941 or Rv2948c or Rv2950c or Rv3089 or Rv3506 or Rv3513c or Rv3515c or Rv3561 or
Rv3801c or Rv3826 </html:p>
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Rv1345 or Rv1427c or Rv1521 or Rv1529 or Rv1750c or Rv1925 or Rv2187 or Rv2505c or Rv2590 or
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Rv1345 or Rv1427c or Rv1521 or Rv1529 or Rv1750c or Rv1925 or Rv2187 or Rv2505c or Rv2590 or
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Rv1345 or Rv1427c or Rv1521 or Rv1529 or Rv1750c or Rv1925 or Rv2187 or Rv2505c or Rv2590 or
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Rv1345 or Rv1427c or Rv1521 or Rv1529 or Rv1750c or Rv1925 or Rv2187 or Rv2505c or Rv2590 or
Rv2930 or Rv2941 or Rv2948c or Rv2950c or Rv3089 or Rv3506 or Rv3513c or Rv3515c or Rv3561 or
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Rv1345 or Rv1427c or Rv1521 or Rv1529 or Rv1750c or Rv1925 or Rv2187 or Rv2505c or Rv2590 or
Rv2930 or Rv2941 or Rv2948c or Rv2950c or Rv3089 or Rv3506 or Rv3513c or Rv3515c or Rv3561 or
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Rv1345 or Rv1427c or Rv1521 or Rv1529 or Rv1750c or Rv1925 or Rv2187 or Rv2505c or Rv2590 or
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Rv1345 or Rv1427c or Rv1521 or Rv1529 or Rv1750c or Rv1925 or Rv2187 or Rv2505c or Rv2590 or
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Rv1345 or Rv1427c or Rv1521 or Rv1529 or Rv1750c or Rv1925 or Rv2187 or Rv2505c or Rv2590 or Rv2930 or Rv2941 or Rv2948c or Rv2950c or Rv3089 or Rv3506 or Rv3513c or Rv3515c or Rv3561 or Rv3801c or Rv3826 </html:p>
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Rv1933c or Rv1934c or Rv2724c or Rv2789c or Rv3061c or Rv3139 or Rv3140 or Rv3274c or Rv3504 or
Rv3505 or Rv3543c or Rv3544c or Rv3560c or Rv3562 or Rv3563 or Rv3564 or Rv3573c or Rv3761c or
Rv3797 or Rv0672 or Rv2500c ) and ( Rv0222 or Rv0456c or Rv0632c or Rv0673 or Rv0675 or Rv0971c or
Rv1070c or Rv1071c or Rv1141c or Rv1142c or Rv1472 or Rv1935c or Rv2486 or Rv2679 or Rv2831 or
Rv3039c or Rv3516 or Rv3550 or Rv3774 or Rv0905 or Rv3374 or Rv3373 ) and ( Rv0468 or Rv1715 or
Rv1912c or Rv3141 ) and ( Rv0243 or Rv1074c or Rv3546 or Rv3556c or Rv1323 or Rv0859 ) </html:p>
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Rv3505 or Rv3543c or Rv3544c or Rv3560c or Rv3562 or Rv3563 or Rv3564 or Rv3573c or Rv3761c or Rv3797 or Rv0672 or Rv2500c) and (Rv0222 or Rv0456c or Rv0632c or Rv0673 or Rv0675 or Rv0971c or Rv1070c or Rv1071c or Rv1141c or Rv1142c or Rv1472 or Rv1935c or Rv2486 or Rv2679 or Rv2831 or Rv3039c or Rv3516 or Rv3550 or Rv3774 or Rv0905 or Rv3374 or Rv3373) and (Rv0468 or Rv1715 or Rv1912c or Rv3141) and (Rv0243 or Rv1074c or Rv3546 or Rv3556c or Rv1323 or Rv0859) </html:p>
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Rv3505 or Rv3543c or Rv3544c or Rv3560c or Rv3562 or Rv3563 or Rv3564 or Rv3573c or Rv3761c or
Rv3797 or Rv0672 or Rv2500c ) and ( Rv0222 or Rv0456c or Rv0632c or Rv0673 or Rv0675 or Rv0971c or
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Rv3039c or Rv3516 or Rv3550 or Rv3774 or Rv0905 or Rv3374 or Rv3373 ) and ( Rv0468 or Rv1715 or
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Rv3797 or Rv0672 or Rv2500c) and (Rv0222 or Rv0456c or Rv0632c or Rv0673 or Rv0675 or Rv0971c or Rv1070c or Rv1071c or Rv1141c or Rv1142c or Rv1472 or Rv1935c or Rv2486 or Rv2679 or Rv2831 or Rv3039c or Rv3516 or Rv3550 or Rv3774 or Rv0905 or Rv3374 or Rv3373) and (Rv0468 or Rv1715 or Rv1912c or Rv3141) and (Rv0243 or Rv1074c or Rv3546 or Rv3556c or Rv1323 or Rv0859) </html:p>
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Rv3505 or Rv3543c or Rv3544c or Rv3560c or Rv3562 or Rv3563 or Rv3564 or Rv3573c or Rv3761c or
Rv3797 or Rv0672 or Rv2500c ) and ( Rv0222 or Rv0456c or Rv0632c or Rv0673 or Rv0675 or Rv0971c or
Rv1070c or Rv1071c or Rv1141c or Rv1142c or Rv1472 or Rv1935c or Rv2486 or Rv2679 or Rv2831 or
Rv3039c or Rv3516 or Rv3550 or Rv3774 or Rv0905 or Rv3374 or Rv3373 ) and ( Rv0468 or Rv1715 or
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Rv3505 or Rv3543c or Rv3544c or Rv3560c or Rv3562 or Rv3563 or Rv3564 or Rv3573c or Rv3761c or
Rv3797 or Rv0672 or Rv2500c ) and ( Rv0222 or Rv0456c or Rv0632c or Rv0673 or Rv0675 or Rv0971c or
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Rv1070c or Rv1071c or Rv1141c or Rv1142c or Rv1472 or Rv1935c or Rv2486 or Rv2679 or Rv2831 or Rv3039c or Rv3516 or Rv3550 or Rv3774 or Rv0905 or Rv3374 or Rv3373) and (Rv0468 or Rv1715 or Rv1912c or Rv3141) and (Rv0243 or Rv1074c or Rv3546 or Rv3556c or Rv1323 or Rv0859) </html:p>
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Rv1933c or Rv1934c or Rv2724c or Rv2789c or Rv3061c or Rv3139 or Rv3140 or Rv3274c or Rv3504 or
Rv3505 or Rv3543c or Rv3544c or Rv3560c or Rv3562 or Rv3563 or Rv3564 or Rv3573c or Rv3761c or
Rv3797 or Rv0672 or Rv2500c ) and ( Rv0222 or Rv0456c or Rv0632c or Rv0673 or Rv0675 or Rv0971c or
Rv1070c or Rv1071c or Rv1141c or Rv1142c or Rv1472 or Rv1935c or Rv2486 or Rv2679 or Rv2831 or
Rv3039c or Rv3516 or Rv3550 or Rv3774 or Rv0905 or Rv3374 or Rv3373 ) and ( Rv0468 or Rv1715 or
Rv1912c or Rv3141 ) and ( Rv0243 or Rv1074c or Rv3546 or Rv3556c or Rv1323 or Rv0859 ) </html:p>
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Rv1933c or Rv1934c or Rv2724c or Rv2789c or Rv3061c or Rv3139 or Rv3140 or Rv3274c or Rv3504 or
Rv3505 or Rv3543c or Rv3544c or Rv3560c or Rv3562 or Rv3563 or Rv3564 or Rv3573c or Rv3761c or
Rv3797 or Rv0672 or Rv2500c ) and ( Rv0222 or Rv0456c or Rv0632c or Rv0673 or Rv0675 or Rv0971c or
Rv1070c or Rv1071c or Rv1141c or Rv1142c or Rv1472 or Rv1935c or Rv2486 or Rv2679 or Rv2831 or
Rv3039c or Rv3516 or Rv3550 or Rv3774 or Rv0905 or Rv3374 or Rv3373 ) and ( Rv0468 or Rv1715 or
Rv1912c or Rv3141 ) and ( Rv0243 or Rv1074c or Rv3546 or Rv3556c or Rv1323 or Rv0859 ) </html:p>
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Rv1933c or Rv1934c or Rv2724c or Rv2789c or Rv3061c or Rv3139 or Rv3140 or Rv3274c or Rv3504 or
Rv3505 or Rv3543c or Rv3544c or Rv3560c or Rv3562 or Rv3563 or Rv3564 or Rv3573c or Rv3761c or
Rv3797 or Rv0672 or Rv2500c ) and ( Rv0222 or Rv0456c or Rv0632c or Rv0673 or Rv0675 or Rv0971c or
Rv1070c or Rv1071c or Rv1141c or Rv1142c or Rv1472 or Rv1935c or Rv2486 or Rv2679 or Rv2831 or
Rv3039c or Rv3516 or Rv3550 or Rv3774 or Rv0905 or Rv3374 or Rv3373 ) and ( Rv0468 or Rv1715 or
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            <html:p>SUBSYSTEM: </html:p>
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Rv1933c or Rv1934c or Rv2724c or Rv2789c or Rv3061c or Rv3139 or Rv3140 or Rv3274c or Rv3504 or
Rv3505 or Rv3543c or Rv3544c or Rv3560c or Rv3562 or Rv3563 or Rv3564 or Rv3573c or Rv3761c or
Rv3797 or Rv0672 or Rv2500c ) and ( Rv0222 or Rv0456c or Rv0632c or Rv0673 or Rv0675 or Rv0971c or
Rv1070c or Rv1071c or Rv1141c or Rv1142c or Rv1472 or Rv1935c or Rv2486 or Rv2679 or Rv2831 or
Rv3039c or Rv3516 or Rv3550 or Rv3774 or Rv0905 or Rv3374 or Rv3373 ) and ( Rv0468 or Rv1715 or
Rv1912c or Rv3141 ) and ( Rv0243 or Rv1074c or Rv3546 or Rv3556c or Rv1323 or Rv0859 ) </html:p>
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            <html:p>SUBSYSTEM: </html:p>
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            <speciesReference species="M_COA_c" stoichiometry="1.0"/>
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Rv1933c or Rv1934c or Rv2724c or Rv2789c or Rv3061c or Rv3139 or Rv3140 or Rv3274c or Rv3504 or
Rv3505 or Rv3543c or Rv3544c or Rv3560c or Rv3562 or Rv3563 or Rv3564 or Rv3573c or Rv3761c or
Rv3797 or Rv0672 or Rv2500c ) and ( Rv0222 or Rv0456c or Rv0632c or Rv0673 or Rv0675 or Rv0971c or
Rv1070c or Rv1071c or Rv1141c or Rv1142c or Rv1472 or Rv1935c or Rv2486 or Rv2679 or Rv2831 or
Rv3039c or Rv3516 or Rv3550 or Rv3774 or Rv0905 or Rv3374 or Rv3373 ) and ( Rv0468 or Rv1715 or
Rv1912c or Rv3141 ) and ( Rv0243 or Rv1074c or Rv3546 or Rv3556c or Rv1323 or Rv0859 ) </html:p>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
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Rv1912c or Rv3141) and (Rv0243 or Rv1074c or Rv3546 or Rv3556c or Rv1323 or Rv0859) </html:p>
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<html:p>PROTEIN_ASSOCIATION: </html:p>
<html:p>SUBSYSTEM: </html:p>
<html:p>PROTEIN_CLASS: </html:p>
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Rv1933c or Rv1934c or Rv2724c or Rv2789c or Rv3061c or Rv3139 or Rv3140 or Rv3274c or Rv3504 or
Rv3505 or Rv3543c or Rv3544c or Rv3560c or Rv3562 or Rv3563 or Rv3564 or Rv3573c or Rv3761c or
Rv3797 or Rv0672 or Rv2500c ) and ( Rv0222 or Rv0456c or Rv0632c or Rv0673 or Rv0675 or Rv0971c or
Rv1070c or Rv1071c or Rv1141c or Rv1142c or Rv1472 or Rv1935c or Rv2486 or Rv2679 or Rv2831 or
Rv3039c or Rv3516 or Rv3550 or Rv3774 or Rv0905 or Rv3374 or Rv3373 ) and ( Rv0468 or Rv1715 or
Rv1912c or Rv3141 ) and ( Rv0243 or Rv1074c or Rv3546 or Rv3556c or Rv1323 or Rv0859 ) </html:p>
                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
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Rv1933c or Rv1934c or Rv2724c or Rv2789c or Rv3061c or Rv3139 or Rv3140 or Rv3274c or Rv3504 or
Rv3505 or Rv3543c or Rv3544c or Rv3560c or Rv3562 or Rv3563 or Rv3564 or Rv3573c or Rv3761c or
Rv3797 or Rv0672 or Rv2500c ) and ( Rv0222 or Rv0456c or Rv0632c or Rv0673 or Rv0675 or Rv0971c or
Rv1070c or Rv1071c or Rv1141c or Rv1142c or Rv1472 or Rv1935c or Rv2486 or Rv2679 or Rv2831 or
Rv3039c or Rv3516 or Rv3550 or Rv3774 or Rv0905 or Rv3374 or Rv3373 ) and ( Rv0468 or Rv1715 or
Rv1912c or Rv3141 ) and ( Rv0243 or Rv1074c or Rv3546 or Rv3556c or Rv1323 or Rv0859 ) </html:p>
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            <listOfProducts>
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                <speciesReference species="M_FADH2_c" stoichiometry="1.0"/>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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            <speciesReference species="M_COA_c" stoichiometry="1.0"/>
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            <speciesReference species="M_PROPIONYLCOA_c" stoichiometry="1.0"/>
            <speciesReference species="M_FADH2_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADH_c" stoichiometry="1.0"/>
            <speciesReference species="M_ACCOA_c" stoichiometry="1.0"/>
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            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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        </kineticLaw>
    </reaction>
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        <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_9-HEXADECENOYL-COA_c" stoichiometry="0.1"/>
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            <speciesReference species="M_OCTADECANOYL-COA_c" stoichiometry="0.1"/>
            <speciesReference species="M_9-OCTADECENOYL-COA_c" stoichiometry="0.1"/>
            <speciesReference species="M_EICOSANOYL-COA_c" stoichiometry="0.1"/>
            <speciesReference species="M_TETRACOSANOYL-COA_c" stoichiometry="0.1"/>
            <speciesReference species="M_HEXACOSANOYL-COA_c" stoichiometry="0.1"/>
            <speciesReference species="M_NONADECANOYL-COA_c" stoichiometry="0.1"/>
            <speciesReference species="M_PENTADECANOYL-COA_c" stoichiometry="0.1"/>
            <speciesReference species="M_GL3P_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_AGL3P_c" stoichiometry="1.0"/>
            <speciesReference species="M_COA_c" stoichiometry="1.0"/>
        </listOfProducts>
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            </math>
            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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        </kineticLaw>
    </reaction>
    <reaction id="R587" name="R587" reversible="false">
        <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_9-HEXADECENOYL-COA_c" stoichiometry="0.1"/>
            <speciesReference species="M_OCTADECANOYL-COA_c" stoichiometry="0.1"/>
            <speciesReference species="M_9-OCTADECENOYL-COA_c" stoichiometry="0.1"/>
            <speciesReference species="M_EICOSANOYL-COA_c" stoichiometry="0.1"/>
            <speciesReference species="M_TETRACOSANOYL-COA_c" stoichiometry="0.1"/>
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            <speciesReference species="M_NONADECANOYL-COA_c" stoichiometry="0.1"/>
            <speciesReference species="M_PENTADECANOYL-COA_c" stoichiometry="0.1"/>
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            <speciesReference species="M_COA_c" stoichiometry="1.0"/>
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        <kineticLaw>
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            </math>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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        </kineticLaw>
    </reaction>
    <reaction id="R588" name="R588" reversible="true">
        <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_CTP_c" stoichiometry="1.0"/>
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        <listOfProducts>
            <speciesReference species="M_CDPDG_c" stoichiometry="1.0"/>
            <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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        </kineticLaw>
    </reaction>
    <reaction id="R589" name="R589" reversible="true">
        <notes>
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            <html:p>SUBSYSTEM: </html:p>
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        </notes>
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            <listOfReactants>
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                <speciesReference species="M_SER_c" stoichiometry="1.0"/>
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            <listOfProducts>
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                <speciesReference species="M_PS_c" stoichiometry="1.0"/>
            </listOfProducts>
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                </math>
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units="mmol_per_gDW_per_hr"/>
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                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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            </kineticLaw>
        </reaction>
        <reaction id="R590" name="R590" reversible="false">
            <notes>
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Rv1105 or Rv1399c or Rv1400c or Rv1426c or Rv1497 or Rv1755c or Rv1900c or Rv1923 or Rv2045c or
Rv2284 or Rv2349c or Rv2350c or Rv2351c or Rv2385 or Rv2463 or Rv2485c or Rv2970c or Rv3084 or
Rv3176c or Rv3203 or Rv3487c or Rv3775 </html:p>
                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
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            <listOfProducts>
                <speciesReference species="M_DAG_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
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                </math>
                <listOfParameters>
                  <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
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                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
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            </kineticLaw>
        </reaction>
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            <notes>
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                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
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                <speciesReference species="M_NADH_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_NAD_c" stoichiometry="1.0"/>
                <speciesReference species="M_GL3P_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
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                </math>
                <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
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            </kineticLaw>
        </reaction>
        <reaction id="R592" name="R592" reversible="true">
            <notes>
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                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
                <speciesReference species="M_CDPDG_c" stoichiometry="1.0"/>
                <speciesReference species="M_GL3P_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_PGP_c" stoichiometry="1.0"/>
                <speciesReference species="M_CMP_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
                <math xmlns="http://www.w3.org/1998/Math/MathML">
                    <ci> FLUX_VALUE </ci>
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                </math>
                <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
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                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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            </kineticLaw>
        </reaction>
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                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
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            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_PI_c" stoichiometry="1.0"/>
                <speciesReference species="M_PG_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
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                </math>
                <listOfParameters>
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                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
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            </kineticLaw>
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                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
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                <speciesReference species="M_GL3P_c" stoichiometry="1.0"/>
            </listOfReactants>
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        <listOfProducts>
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            <speciesReference species="M_A160GL3P_c" stoichiometry="1.0"/>
        </listOfProducts>
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            </math>
            <listOfParameters>
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              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R595" name="R595" reversible="false">
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_TUBERCULOSTEROYL-ACP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_PA-TBA_c" stoichiometry="1.0"/>
            <speciesReference species="M_ACP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R596" name="R596" reversible="false">
        <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
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            <speciesReference species="M_CTP_c" stoichiometry="1.0"/>
            <speciesReference species="M_PA-TBA_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
            <speciesReference species="M_CDPDAG-TBA_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R597" name="R597" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2612c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_CDPDAG-TBA_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_CMP_c" stoichiometry="1.0"/>
            <speciesReference species="M_PI-TBA_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R598" name="R598" reversible="false">
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
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        </notes>
        <listOfReactants>
            <speciesReference species="M_GDPMAN_c" stoichiometry="1.0"/>
            <speciesReference species="M_PI-TBA_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_GDP_c" stoichiometry="1.0"/>
            <speciesReference species="M_AC1PIM1_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R599" name="R599" reversible="true">
        <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
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        </notes>
        <listOfReactants>
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            <speciesReference species="M_AC1PIM1_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_ACP_c" stoichiometry="1.0"/>
            <speciesReference species="M_AC2PIM1_c" stoichiometry="1.0"/>
        </listOfProducts>
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                </math>
                <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
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                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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                </listOfParameters>
            </kineticLaw>
        </reaction>
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                <html:p>SUBSYSTEM: </html:p>
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            </notes>
            <listOfReactants>
                <speciesReference species="M_HEXADECANOYL-ACP_c" stoichiometry="1.0"/>
                <speciesReference species="M_AC2PIM1_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_ACP_c" stoichiometry="1.0"/>
                <speciesReference species="M_AC3PIM1_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
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units="mmol_per_gDW_per_hr"/>
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                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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        </listOfReactants>
        <listOfProducts>
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        </listOfProducts>
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      <kineticLaw>
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            <listOfProducts>
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            </listOfProducts>
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        <listOfProducts>
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            <listOfProducts>
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        </reaction>
        <reaction id="R618" name="R618" reversible="false">
            <notes>
                <html:p>GENE_ASSOCIATION: ( Rv2243 or Rv0649 ) and Rv2244 </html:p>
                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
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            <speciesReference species="M_ACP_c" stoichiometry="1.0"/>
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            <speciesReference species="M_COA_c" stoichiometry="1.0"/>
        </listOfProducts>
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            <html:p>SUBSYSTEM: </html:p>
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        </notes>
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        <listOfProducts>
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            <speciesReference species="M_CO2_c" stoichiometry="1.0"/>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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            <speciesReference species="M_NADPH_c" stoichiometry="1.0"/>
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        <listOfProducts>
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stoichiometry="1.0"/>
            <speciesReference species="M_NADP_c" stoichiometry="1.0"/>
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                </math>
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                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
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stoichiometry="1.0"/>
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                </math>
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                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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        <listOfProducts>
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or Rv0242c or Rv2766c ) and ( Rv0098 or Rv0130 ) and ( Rv1142c or Rv1141c ) </html:p>
                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
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            <listOfProducts>
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                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
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                <speciesReference species="M_NADP_c" stoichiometry="16.0"/>
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                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
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                <speciesReference species="M_NADP_c" stoichiometry="2.0"/>
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            <listOfProducts>
                <speciesReference species="M_CYCLOPROPYL-MEROACYL-ACP_c"
stoichiometry="1.0"/>
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              <html:p>SUBSYSTEM: </html:p>
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          <listOfProducts>
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stoichiometry="1.0"/>
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or Rv0242c or Rv2766c ) and ( Rv0098 or Rv0130 ) and ( Rv1142c or Rv1141c ) </html:p>
              <html:p>PROTEIN_ASSOCIATION: </html:p>
              <html:p>SUBSYSTEM: </html:p>
              <html:p>PROTEIN_CLASS: </html:p>
          </notes>
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stoichiometry="1.0"/>
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<html:p>PROTEIN_ASSOCIATION: </html:p>
<html:p>SUBSYSTEM: </html:p>
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</reaction>
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<html:p>SUBSYSTEM: </html:p>
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</notes>
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<listOfProducts>
<speciesReference species="M_CIS-DELTA-37-ENOYL-METHY-HYDROXY-C56-ACYL-ACP_c" stoichiometry="1.0"/>
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</listOfProducts>
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</math>
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                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
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ACYL-ACP_c" stoichiometry="1.0"/>
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                <speciesReference species="M_NADP_c" stoichiometry="2.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_CIS-KETO-MEROACYL-ACP_c" stoichiometry="1.0"/>
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                <speciesReference species="M_NADPH_c" stoichiometry="2.0"/>
            </listOfProducts>
            <kineticLaw>
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                </math>
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            </notes>
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            </listOfReactants>
            <listOfProducts>
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ACYL-ACP_c" stoichiometry="1.0"/>
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                <speciesReference species="M_NADPH_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
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                </math>
                <listOfParameters>
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        <reaction id="R636" name="R636" reversible="false">
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ACYL-ACP_c" stoichiometry="1.0"/>
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            <listOfProducts>
                <speciesReference species="M_TRANS-KETO-MEROACYL-ACP_c"
stoichiometry="1.0"/>
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                <speciesReference species="M_NADPH_c" stoichiometry="2.0"/>
            </listOfProducts>
            <kineticLaw>
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                </math>
                <listOfParameters>
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    </reaction>
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            <html:p>SUBSYSTEM: </html:p>
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stoichiometry="0.05"/>
            <speciesReference species="M_TRANS-METHOXY-MEROACYL-ACP_c"
stoichiometry="0.05"/>
            <speciesReference species="M_CIS-KETO-MEROACYL-ACP_c" stoichiometry="0.05"/>
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stoichiometry="0.05"/>
            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
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            <speciesReference species="M_ACP_c" stoichiometry="1.0"/>
            <speciesReference species="M_PI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_CO2_c" stoichiometry="1.0"/>
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            <speciesReference species="M_COA_c" stoichiometry="1.0"/>
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              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_NADPH_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_C78MYCOLATE-ENZ_c" stoichiometry="1.0"/>
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        <kineticLaw>
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            </math>
            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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        </kineticLaw>
    </reaction>
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        <notes>
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                </math>
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            </kineticLaw>
        </reaction>
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            <notes>
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                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
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            <listOfProducts>
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stoichiometry="1.0"/>
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            </listOfProducts>
            <kineticLaw>
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                </math>
                <listOfParameters>
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          </kineticLaw>
      </reaction>
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              <html:p>PROTEIN_ASSOCIATION: </html:p>
              <html:p>SUBSYSTEM: </html:p>
              <html:p>PROTEIN_CLASS: </html:p>
          </notes>
          <listOfReactants>
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stoichiometry="1.0"/>
          </listOfReactants>
          <listOfProducts>
              <speciesReference species="M_TREHALOSEMONOMYCOLATE(CY)_c"
stoichiometry="1.0"/>
              <speciesReference species="M_PI_c" stoichiometry="1.0"/>
          </listOfProducts>
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              </math>
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      </reaction>
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          <notes>
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              <html:p>SUBSYSTEM: </html:p>
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          </notes>
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          <listOfProducts>
              <speciesReference species="M_MAS_c" stoichiometry="1.0"/>
          </listOfProducts>
          <kineticLaw>
              <math xmlns="http://www.w3.org/1998/Math/MathML">
                  <ci> FLUX_VALUE </ci>
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            </math>
            <listOfParameters>
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    </reaction>
    <reaction id="R644" name="R644" reversible="false">
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            <html:p>SUBSYSTEM: </html:p>
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        </notes>
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            <speciesReference species="M_TETRACOSANOYL-ACP_c" stoichiometry="0.25"/>
            <speciesReference species="M_OCTACOSANOYL-ACP_c" stoichiometry="0.25"/>
            <speciesReference species="M_MAS_c" stoichiometry="1"/>
        </listOfReactants>
        <listOfProducts>
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            <speciesReference species="M_ACP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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        </kineticLaw>
    </reaction>
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            <html:p>SUBSYSTEM: </html:p>
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        </notes>
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            <speciesReference species="M_NADPH_c" stoichiometry="8.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_MYCOCEROSOYL-MAS_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADP_c" stoichiometry="8.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="4.0"/>
            <speciesReference species="M_COA_c" stoichiometry="4.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
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            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R646" name="R646" reversible="false">
        <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
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        </notes>
        <listOfReactants>
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            <speciesReference species="M_MAS_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_HEXADECANOYL-MAS_c" stoichiometry="1.0"/>
            <speciesReference species="M_COA_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
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            </kineticLaw>
        </reaction>
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                <html:p>SUBSYSTEM: </html:p>
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            </notes>
            <listOfReactants>
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                <speciesReference species="M_NADPH_c" stoichiometry="12.0"/>
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            <listOfProducts>
                <speciesReference species="M_PTHIOCERANOYL-COA_c" stoichiometry="1.0"/>
                <speciesReference species="M_NADP_c" stoichiometry="12.0"/>
                <speciesReference species="M_CO2_c" stoichiometry="6.0"/>
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            </listOfProducts>
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                </math>
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            <listOfReactants>
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                <speciesReference species="M_SMMALONYLCOA_c" stoichiometry="8.0"/>
                <speciesReference species="M_NADPH_c" stoichiometry="15.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_HYDROXYPHTHIOCERANOYL-COA_c"
stoichiometry="1.0"/>
```

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            <speciesReference species="M_NADP_c" stoichiometry="15.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="8.0"/>
            <speciesReference species="M_COA_c" stoichiometry="7.0"/>
            <speciesReference species="M_MAS_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R649" name="R649" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2940c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_SMMALONYLCOA_c" stoichiometry="1.0"/>
            <speciesReference species="M_HEXADECANOYL-ACP_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADPH_c" stoichiometry="2.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_NADP_c" stoichiometry="2.0"/>
            <speciesReference species="M_COA_c" stoichiometry="1.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="1.0"/>
            <speciesReference species="M_TUBERCULOSTEROYL-ACP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
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    <reaction id="R650" name="R650" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2949c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_CHOR_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_HBA_c" stoichiometry="1.0"/>
            <speciesReference species="M_PYR_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R651" name="R651" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2931 and Rv2932 and Rv2933 and Rv2934 and
Rv2935 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_DOCOSANOYL-COA_c" stoichiometry="1.0"/>
            <speciesReference species="M_ATP_c" stoichiometry="1"/>
            <speciesReference species="M_MALCOA_c" stoichiometry="3.0"/>
            <speciesReference species="M_SMMALONYLCOA_c" stoichiometry="2.0"/>
            <speciesReference species="M_NADPH_c" stoichiometry="5.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_PHTHIODIOLONE-A_c" stoichiometry="1.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="5.0"/>
            <speciesReference species="M_NADP_c" stoichiometry="5.0"/>
            <speciesReference species="M_AMP_c" stoichiometry="1"/>
            <speciesReference species="M_PPI_c" stoichiometry="1"/>
        </listOfProducts>
```

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        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R652" name="R652" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2951c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_PHTHIODIOLONE-A_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADPH_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_PTT_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R653" name="R653" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2952 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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<speciesReference species="M_PTT_c" stoichiometry="1.0"/>
<speciesReference species="M_SAM_c" stoichiometry="1.0"/>
</listOfReactants>
<listOfProducts>
<speciesReference species="M_PTC_c" stoichiometry="1.0"/>
<speciesReference species="M_SAH_c" stoichiometry="1.0"/>
</listOfProducts>
<kineticLaw>
<math xmlns="http://www.w3.org/1998/Math/MathML">
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</math>
<listOfParameters>
<parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
<parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
<parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
<parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
<parameter id="REDUCED_COST" value="0.000000"/>
</listOfParameters>
</kineticLaw>
</reaction>
<reaction id="R654" name="R654" reversible="false">
<notes>
<html:p>GENE_ASSOCIATION: Rv2939 </html:p>
<html:p>PROTEIN_ASSOCIATION: </html:p>
<html:p>SUBSYSTEM: </html:p>
<html:p>PROTEIN_CLASS: </html:p>
</notes>
<listOfReactants>
<speciesReference species="M_PTC_c" stoichiometry="1.0"/>
<speciesReference species="M_MYCOCEROSOYL-MAS_c" stoichiometry="2.0"/>
</listOfReactants>
<listOfProducts>
<speciesReference species="M_DIM-CYTO_c" stoichiometry="1.0"/>
<speciesReference species="M_MAS_c" stoichiometry="2.0"/>
</listOfProducts>
<kineticLaw>
<math xmlns="http://www.w3.org/1998/Math/MathML">
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</math>
<listOfParameters>
<parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
<parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
<parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
<parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
<parameter id="REDUCED_COST" value="0.000000"/>
</listOfParameters>
</kineticLaw>
</reaction>
<reaction id="R655" name="R655" reversible="false">

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        <notes>
            <html:p>GENE_ASSOCIATION: Rv2947c and Rv2946c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_HBA_c" stoichiometry="1.0"/>
            <speciesReference species="M_MALCOA_c" stoichiometry="8.0"/>
            <speciesReference species="M_NADPH_c" stoichiometry="16.0"/>
            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_PHPAA-COA_c" stoichiometry="1.0"/>
            <speciesReference species="M_COA_c" stoichiometry="7.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="9.0"/>
            <speciesReference species="M_AMP_c" stoichiometry="1.0"/>
            <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R656" name="R656" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2931 and Rv2932 and Rv2933 and Rv2934 and
Rv2935 and Rv2930 and Rv2941 and Rv1661 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_PHPAA-COA_c" stoichiometry="1.0"/>
            <speciesReference species="M_MALCOA_c" stoichiometry="3.0"/>
            <speciesReference species="M_SMMALONYLCOA_c" stoichiometry="2.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_PHENOLPHTHIODIOLONE-A_c" stoichiometry="1.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="5.0"/>
            <speciesReference species="M_COA_c" stoichiometry="5.0"/>
```

```
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R657" name="R657" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2951c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_PHENOLPHTHIODIOLONE-A_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADPH_c" stoichiometry="1"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_PPTT_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADP_c" stoichiometry="1"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R658" name="R658" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2952 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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        <listOfReactants>
            <speciesReference species="M_PPTT_c" stoichiometry="1.0"/>
            <speciesReference species="M_SAM_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_PPTC_c" stoichiometry="1.0"/>
            <speciesReference species="M_SAH_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R659" name="R659" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2939 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_PPTC_c" stoichiometry="1.0"/>
            <speciesReference species="M_MYCOCEROSOYL-MAS_c" stoichiometry="2.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_PHDIM-CYTO_c" stoichiometry="1.0"/>
            <speciesReference species="M_MAS_c" stoichiometry="2.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
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<reaction id="R660" name="R660" reversible="false">
	<notes>
		<html:p>GENE_ASSOCIATION: Rv2942 and Rv2936 and Rv2937 and Rv2938 </html:p>
		<html:p>PROTEIN_ASSOCIATION: </html:p>
		<html:p>SUBSYSTEM: </html:p>
		<html:p>PROTEIN_CLASS: </html:p>
	</notes>
	<listOfReactants>
		<speciesReference species="M_PHDIM-CYTO_c" stoichiometry="1.0"/>
	</listOfReactants>
	<listOfProducts>
		<speciesReference species="M_PHDIM_c" stoichiometry="1.0"/>
	</listOfProducts>
	<kineticLaw>
		<math xmlns="http://www.w3.org/1998/Math/MathML">
			<ci> FLUX_VALUE </ci>
		</math>
		<listOfParameters>
		 <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
		 <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
		 <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
		 <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
		 <parameter id="REDUCED_COST" value="0.000000"/>
		</listOfParameters>
	</kineticLaw>
</reaction>
<reaction id="R661" name="R661" reversible="false">
	<notes>
		<html:p>GENE_ASSOCIATION: Rv2962c </html:p>
		<html:p>PROTEIN_ASSOCIATION: </html:p>
		<html:p>SUBSYSTEM: </html:p>
		<html:p>PROTEIN_CLASS: </html:p>
	</notes>
	<listOfReactants>
		<speciesReference species="M_PHDIM_c" stoichiometry="1.0"/>
		<speciesReference species="M_DTDPRHAM_c" stoichiometry="1.0"/>
	</listOfReactants>
	<listOfProducts>
		<speciesReference species="M_PHDIMRHAM1_c" stoichiometry="1.0"/>
		<speciesReference species="M_DTDP_c" stoichiometry="1.0"/>
	</listOfProducts>
	<kineticLaw>
		<math xmlns="http://www.w3.org/1998/Math/MathML">
			<ci> FLUX_VALUE </ci>
		</math>
		<listOfParameters>
		 <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
		 <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
		 <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
```

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            <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
            <parameter id="REDUCED_COST" value="0.000000"/>
          </listOfParameters>
      </kineticLaw>
</reaction>
<reaction id="R662" name="R662" reversible="false">
      <notes>
          <html:p>GENE_ASSOCIATION: Rv2958c </html:p>
          <html:p>PROTEIN_ASSOCIATION: </html:p>
          <html:p>SUBSYSTEM: </html:p>
          <html:p>PROTEIN_CLASS: </html:p>
      </notes>
      <listOfReactants>
          <speciesReference species="M_PHDIMRHAM1_c" stoichiometry="1.0"/>
          <speciesReference species="M_DTDPRHAM_c" stoichiometry="1.0"/>
      </listOfReactants>
      <listOfProducts>
          <speciesReference species="M_PHDIMRHAM2_c" stoichiometry="1.0"/>
          <speciesReference species="M_DTDP_c" stoichiometry="1.0"/>
      </listOfProducts>
      <kineticLaw>
          <math xmlns="http://www.w3.org/1998/Math/MathML">
              <ci> FLUX_VALUE </ci>
          </math>
          <listOfParameters>
            <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
            <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
            <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
            <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
            <parameter id="REDUCED_COST" value="0.000000"/>
          </listOfParameters>
      </kineticLaw>
</reaction>
<reaction id="R663" name="R663" reversible="false">
      <notes>
          <html:p>GENE_ASSOCIATION: Rv2959c </html:p>
          <html:p>PROTEIN_ASSOCIATION: </html:p>
          <html:p>SUBSYSTEM: </html:p>
          <html:p>PROTEIN_CLASS: </html:p>
      </notes>
      <listOfReactants>
          <speciesReference species="M_PHDIMRHAM2_c" stoichiometry="1.0"/>
          <speciesReference species="M_SAM_c" stoichiometry="1.0"/>
      </listOfReactants>
      <listOfProducts>
          <speciesReference species="M_MYCOSIDE_B_c" stoichiometry="1.0"/>
          <speciesReference species="M_SAH_c" stoichiometry="1.0"/>
      </listOfProducts>
      <kineticLaw>
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            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R668" name="R668" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv3529c or Rv1373 or Rv2267c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_TRE_c" stoichiometry="1.0"/>
            <speciesReference species="M_PAPS_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_TRE-S_c" stoichiometry="1.0"/>
            <speciesReference species="M_PAP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R669" name="R669" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: orphan </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_TRE-S_c" stoichiometry="1.0"/>
```

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                <speciesReference species="M_HEXADECANOYL-COA_c" stoichiometry="0.333"/>
                <speciesReference species="M_OCTADECANOYL-COA_c" stoichiometry="0.333"/>
                <speciesReference species="M_EICOSANOYL-COA_c" stoichiometry="0.333"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_ACYL-TRE-S-COA_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
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                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
                  <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R670" name="R670" reversible="false">
            <notes>
                <html:p>GENE_ASSOCIATION: orphan </html:p>
                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
                <speciesReference species="M_ACYL-TRE-S-COA_c" stoichiometry="1.0"/>
                <speciesReference species="M_HYDROXYPHTHIOCERANOYL-COA_c"
stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_SL1278-CYTO_c" stoichiometry="1.0"/>
                <speciesReference species="M_COA_c" stoichiometry="2.0"/>
            </listOfProducts>
            <kineticLaw>
                <math xmlns="http://www.w3.org/1998/Math/MathML">
                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
                  <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
                </listOfParameters>
            </kineticLaw>
        </reaction>
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<reaction id="R671" name="R671" reversible="false">
      <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
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      </notes>
      <listOfReactants>
            <speciesReference species="M_SL1278-CYTO_c" stoichiometry="1.0"/>
      </listOfReactants>
      <listOfProducts>
            <speciesReference species="M_SL1278-WALL_c" stoichiometry="1.0"/>
      </listOfProducts>
      <kineticLaw>
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            </math>
            <listOfParameters>
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              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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      </kineticLaw>
</reaction>
<reaction id="R672" name="R672" reversible="false">
      <notes>
            <html:p>GENE_ASSOCIATION: Rv1180 and Rv1181 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
      </notes>
      <listOfReactants>
            <speciesReference species="M_OCTADECANOYL-COA_c" stoichiometry="1.0"/>
            <speciesReference species="M_RMMALONYLACP_c" stoichiometry="3.0"/>
            <speciesReference species="M_NADPH_c" stoichiometry="6.0"/>
      </listOfReactants>
      <listOfProducts>
            <speciesReference species="M_MYCOLIPANOIC-ACP_c" stoichiometry="1.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="3.0"/>
            <speciesReference species="M_NADP_c" stoichiometry="6.0"/>
            <speciesReference species="M_COA_c" stoichiometry="1.0"/>
            <speciesReference species="M_ACP_c" stoichiometry="2.0"/>
      </listOfProducts>
      <kineticLaw>
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                  <ci> FLUX_VALUE </ci>
            </math>
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            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
      </kineticLaw>
</reaction>
<reaction id="R673" name="R673" reversible="false">
      <notes>
            <html:p>GENE_ASSOCIATION: Rv1180 and Rv1182 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
      </notes>
      <listOfReactants>
            <speciesReference species="M_OCTADECANOYL-COA_c" stoichiometry="1.0"/>
            <speciesReference species="M_RMMALONYLACP_c" stoichiometry="3.0"/>
            <speciesReference species="M_NADPH_c" stoichiometry="5.0"/>
      </listOfReactants>
      <listOfProducts>
            <speciesReference species="M_MYCOLIPENOYL-ACP_c" stoichiometry="1.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="3.0"/>
            <speciesReference species="M_NADP_c" stoichiometry="5.0"/>
            <speciesReference species="M_COA_c" stoichiometry="1.0"/>
            <speciesReference species="M_ACP_c" stoichiometry="2.0"/>
      </listOfProducts>
      <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                  <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
      </kineticLaw>
</reaction>
<reaction id="R674" name="R674" reversible="false">
      <notes>
            <html:p>GENE_ASSOCIATION: Rv1180 and Rv1183 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
      </notes>
      <listOfReactants>
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            <speciesReference species="M_OCTADECANOYL-COA_c" stoichiometry="1.0"/>
            <speciesReference species="M_RMMALONYLACP_c" stoichiometry="3.0"/>
            <speciesReference species="M_NADPH_c" stoichiometry="4.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_MYCOLIPDIENOYL-ACP_c" stoichiometry="1.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="3.0"/>
            <speciesReference species="M_NADP_c" stoichiometry="4.0"/>
            <speciesReference species="M_COA_c" stoichiometry="1.0"/>
            <speciesReference species="M_ACP_c" stoichiometry="2.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R678" name="R678" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv3379c or Rv2682c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_G3P_c" stoichiometry="1.0"/>
            <speciesReference species="M_PYR_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_DX5P_c" stoichiometry="1.0"/>
            <speciesReference species="M_CO2_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R679" name="R679" reversible="false">
        <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_DX5P_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADPH_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_MDE4P_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R680" name="R680" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv3582c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_MDE4P_c" stoichiometry="1.0"/>
            <speciesReference species="M_CTP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_CDPMDE_c" stoichiometry="1.0"/>
            <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
```

```
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R681" name="R681" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv1011 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_CDPMDE_c" stoichiometry="1.0"/>
            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_2PCDPMDE_c" stoichiometry="1.0"/>
            <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R682" name="R682" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv3581c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_2PCDPMDE_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
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            <speciesReference species="M_MDECPP_c" stoichiometry="1.0"/>
            <speciesReference species="M_CMP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R683" name="R683" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv2868c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_MDECPP_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADH_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_HMB4PP_c" stoichiometry="1.0"/>
            <speciesReference species="M_NAD_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R684" name="R684" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv3382c or Rv1110 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
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            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_HMB4PP_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADH_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_IPP_c" stoichiometry="1.0"/>
            <speciesReference species="M_NAD_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R685" name="R685" reversible="true">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv1745c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_IPP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_DMPP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="-100000.0"
units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
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</reaction>
<reaction id="R686" name="R686" reversible="false">
      <notes>
            <html:p>GENE_ASSOCIATION: Rv3398c or Rv3383c or Rv2173 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
      </notes>
      <listOfReactants>
            <speciesReference species="M_IPP_c" stoichiometry="1.0"/>
            <speciesReference species="M_DMPP_c" stoichiometry="1.0"/>
      </listOfReactants>
      <listOfProducts>
            <speciesReference species="M_GPP_c" stoichiometry="1.0"/>
            <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
      </listOfProducts>
      <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                  <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
      </kineticLaw>
</reaction>
<reaction id="R687" name="R687" reversible="false">
      <notes>
            <html:p>GENE_ASSOCIATION: Rv1086 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
      </notes>
      <listOfReactants>
            <speciesReference species="M_IPP_c" stoichiometry="1.0"/>
            <speciesReference species="M_GPP_c" stoichiometry="1.0"/>
      </listOfReactants>
      <listOfProducts>
            <speciesReference species="M_FPP_c" stoichiometry="1.0"/>
            <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
      </listOfProducts>
      <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                  <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
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            <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
            <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
            <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
            <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
            <parameter id="REDUCED_COST" value="0.000000"/>
          </listOfParameters>
      </kineticLaw>
</reaction>
<reaction id="R688" name="R688" reversible="false">
      <notes>
          <html:p>GENE_ASSOCIATION: Rv3398c </html:p>
          <html:p>PROTEIN_ASSOCIATION: </html:p>
          <html:p>SUBSYSTEM: </html:p>
          <html:p>PROTEIN_CLASS: </html:p>
      </notes>
      <listOfReactants>
          <speciesReference species="M_IPP_c" stoichiometry="1.0"/>
          <speciesReference species="M_FPP_c" stoichiometry="1.0"/>
      </listOfReactants>
      <listOfProducts>
          <speciesReference species="M_GGPP_c" stoichiometry="1.0"/>
          <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
      </listOfProducts>
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          </math>
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            <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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</reaction>
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      </notes>
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      <listOfProducts>
          <speciesReference species="M_PPPP_c" stoichiometry="1.0"/>
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            <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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            <speciesReference species="M_PPPP_c" stoichiometry="1.0"/>
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        <listOfProducts>
            <speciesReference species="M_HPPP_c" stoichiometry="1.0"/>
            <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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        <notes>
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        </notes>
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        </listOfProducts>
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        <notes>
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        </notes>
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        <listOfProducts>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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</reaction>
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            <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
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            </math>
            <listOfParameters>
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</reaction>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
      </notes>
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            <speciesReference species="M_IPP_c" stoichiometry="7.0"/>
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            <speciesReference species="M_DPP_c" stoichiometry="1.0"/>
      </listOfProducts>
      <kineticLaw>
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            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
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            <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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      </listOfReactants>
      <listOfProducts>
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          <speciesReference species="M_DPPPR_c" stoichiometry="1.0"/>
      </listOfProducts>
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          </math>
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            <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
            <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
            <parameter id="REDUCED_COST" value="0.000000"/>
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</reaction>
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          <html:p>SUBSYSTEM: </html:p>
          <html:p>PROTEIN_CLASS: </html:p>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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            </math>
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              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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        <notes>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            </listOfProducts>
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                </math>
                <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
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            </kineticLaw>
        </reaction>
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            <notes>
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                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
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            <listOfProducts>
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                <speciesReference species="M_PI_c" stoichiometry="1.0"/>
                <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
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                <math xmlns="http://www.w3.org/1998/Math/MathML">
                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
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                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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            <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_UDPNAG_c" stoichiometry="1.0"/>
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        <listOfProducts>
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            <speciesReference species="M_UMP_c" stoichiometry="1.0"/>
        </listOfProducts>
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            </math>
            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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        </kineticLaw>
    </reaction>
    <reaction id="R701" name="R701" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv3265c or Rv1525 </html:p>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_DTDPRHAM_c" stoichiometry="1.0"/>
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        <listOfProducts>
            <speciesReference species="M_RHAMNAGDPP_c" stoichiometry="1.0"/>
            <speciesReference species="M_DTDP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
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              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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                <parameter id="REDUCED_COST" value="0.000000"/>
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            </kineticLaw>
        </reaction>
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            <notes>
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                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
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                <speciesReference species="M_UDPGALF_c" stoichiometry="30.0"/>
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            <listOfProducts>
                <speciesReference species="M_GALACTANDPP_c" stoichiometry="1.0"/>
                <speciesReference species="M_UDP_c" stoichiometry="30.0"/>
            </listOfProducts>
            <kineticLaw>
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                </math>
                <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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                </listOfParameters>
            </kineticLaw>
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        <reaction id="R705" name="R705" reversible="true">
            <notes>
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                <html:p>SUBSYSTEM: </html:p>
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            </notes>
            <listOfReactants>
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                <speciesReference species="M_ARAFDPP_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
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            </listOfProducts>
            <kineticLaw>
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                </math>
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units="mmol_per_gDW_per_hr"/>
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                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
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            </notes>
            <listOfReactants>
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            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_ARABINOGALACTANDPP_c" stoichiometry="1.0"/>
                <speciesReference species="M_DPP_c" stoichiometry="70.0"/>
            </listOfProducts>
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                </math>
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units="mmol_per_gDW_per_hr"/>
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                <speciesReference species="M_DTDPGLC_c" stoichiometry="1.0"/>
                <speciesReference species="M_PPI_c" stoichiometry="1.0"/>
            </listOfProducts>
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                </math>
                <listOfParameters>
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                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R708" name="R708" reversible="true">
            <notes>
                <html:p>GENE_ASSOCIATION: Rv3464 or Rv3634c or Rv3468 or Rv3784 </html:p>
                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
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                <speciesReference species="M_DTDP4DH6DGLC_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
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                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R709" name="R709" reversible="false">
```

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        <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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        <listOfProducts>
            <speciesReference species="M_DTDP4DH6DMAN_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
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            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R710" name="R710" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv3260c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
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        </notes>
        <listOfReactants>
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            <speciesReference species="M_NADPH_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_DTDPRHAM_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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            <parameter id="REDUCED_COST" value="0.000000"/>
          </listOfParameters>
      </kineticLaw>
</reaction>
<reaction id="R711" name="R711" reversible="false">
      <notes>
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          <html:p>PROTEIN_ASSOCIATION: </html:p>
          <html:p>SUBSYSTEM: </html:p>
          <html:p>PROTEIN_CLASS: </html:p>
      </notes>
      <listOfReactants>
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      <listOfProducts>
          <speciesReference species="M_UDPGALF_c" stoichiometry="1.0"/>
      </listOfProducts>
      <kineticLaw>
          <math xmlns="http://www.w3.org/1998/Math/MathML">
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          </math>
          <listOfParameters>
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            <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
            <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
            <parameter id="REDUCED_COST" value="0.000000"/>
          </listOfParameters>
      </kineticLaw>
</reaction>
<reaction id="R712" name="R712" reversible="true">
      <notes>
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          <html:p>PROTEIN_ASSOCIATION: </html:p>
          <html:p>SUBSYSTEM: </html:p>
          <html:p>PROTEIN_CLASS: </html:p>
      </notes>
      <listOfReactants>
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          <speciesReference species="M_F6P_c" stoichiometry="1.0"/>
      </listOfReactants>
      <listOfProducts>
          <speciesReference species="M_GLU_c" stoichiometry="1.0"/>
          <speciesReference species="M_GA6P_c" stoichiometry="1.0"/>
      </listOfProducts>
      <kineticLaw>
          <math xmlns="http://www.w3.org/1998/Math/MathML">
              <ci> FLUX_VALUE </ci>
          </math>
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                <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
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                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R713" name="R713" reversible="false">
            <notes>
                <html:p>GENE_ASSOCIATION: Rv1338 </html:p>
                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
                <speciesReference species="M_GLU_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_DGLU_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
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                </math>
                <listOfParameters>
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                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R714" name="R714" reversible="true">
            <notes>
                <html:p>GENE_ASSOCIATION: orphan </html:p>
                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
                <speciesReference species="M_GA6P_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_F6P_c" stoichiometry="1.0"/>
                <speciesReference species="M_NH3_c" stoichiometry="1.0"/>
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            </listOfProducts>
            <kineticLaw>
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                </math>
                <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R715" name="R715" reversible="true">
            <notes>
                <html:p>GENE_ASSOCIATION: Rv3068c </html:p>
                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
                <speciesReference species="M_GA1P_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_GA6P_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
                <math xmlns="http://www.w3.org/1998/Math/MathML">
                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
                  <parameter id="LOWER_BOUND" value="-100000.0"
units="mmol_per_gDW_per_hr"/>
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                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R716" name="R716" reversible="true">
            <notes>
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                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
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        <listOfReactants>
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            <speciesReference species="M_GA1P_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_COA_c" stoichiometry="1.0"/>
            <speciesReference species="M_NAGA1P_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="-100000.0"
units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R717" name="R717" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv1018c </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_NAGA1P_c" stoichiometry="1.0"/>
            <speciesReference species="M_UTP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_UDPNAG_c" stoichiometry="1.0"/>
            <speciesReference species="M_PPI_c" stoichiometry="1"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
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    </reaction>
    <reaction id="R718" name="R718" reversible="true">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv1315 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_PEP_c" stoichiometry="1.0"/>
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        <listOfProducts>
            <speciesReference species="M_UDPNAGPEE_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="-100000.0"
units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R719" name="R719" reversible="false">
        <notes>
            <html:p>GENE_ASSOCIATION: Rv0482 </html:p>
            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_UDPNAGPEE_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADPH_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_UDPNAM_c" stoichiometry="1.0"/>
            <speciesReference species="M_NADP_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
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            <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
            <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
            <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
            <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
            <parameter id="REDUCED_COST" value="0.000000"/>
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      </kineticLaw>
</reaction>
<reaction id="R722" name="R722" reversible="false">
      <notes>
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          <html:p>PROTEIN_ASSOCIATION: </html:p>
          <html:p>SUBSYSTEM: </html:p>
          <html:p>PROTEIN_CLASS: </html:p>
      </notes>
      <listOfReactants>
          <speciesReference species="M_UDPNAM_c" stoichiometry="1.0"/>
          <speciesReference species="M_NADPH_c" stoichiometry="1.0"/>
      </listOfReactants>
      <listOfProducts>
          <speciesReference species="M_UDPNGM_c" stoichiometry="1.0"/>
          <speciesReference species="M_NADP_c" stoichiometry="1.0"/>
      </listOfProducts>
      <kineticLaw>
          <math xmlns="http://www.w3.org/1998/Math/MathML">
              <ci> FLUX_VALUE </ci>
          </math>
          <listOfParameters>
            <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
            <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
            <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
            <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
            <parameter id="REDUCED_COST" value="0.000000"/>
          </listOfParameters>
      </kineticLaw>
</reaction>
<reaction id="R723" name="R723" reversible="true">
      <notes>
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          <html:p>PROTEIN_ASSOCIATION: </html:p>
          <html:p>SUBSYSTEM: </html:p>
          <html:p>PROTEIN_CLASS: </html:p>
      </notes>
      <listOfReactants>
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          <speciesReference species="M_UDPNAM_c" stoichiometry="0.3"/>
          <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
          <speciesReference species="M_ALA_c" stoichiometry="1.0"/>
      </listOfReactants>
```

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            <listOfProducts>
                <speciesReference species="M_UDP[NAM:NGM]ALA_c" stoichiometry="1.0"/>
                <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
                <speciesReference species="M_PI_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
                <math xmlns="http://www.w3.org/1998/Math/MathML">
                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R724" name="R724" reversible="false">
            <notes>
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                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
                <speciesReference species="M_UDP[NAM:NGM]ALA_c" stoichiometry="1.0"/>
                <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
                <speciesReference species="M_DGLU_c" stoichiometry="1.0"/>
            </listOfReactants>
            <listOfProducts>
                <speciesReference species="M_UDP[NAM:NGM]ALAGLU_c" stoichiometry="1.0"/>
                <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
                <speciesReference species="M_PI_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
                <math xmlns="http://www.w3.org/1998/Math/MathML">
                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
                  <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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                </listOfParameters>
            </kineticLaw>
        </reaction>
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    <reaction id="R725" name="R725" reversible="false">
        <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
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            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
            <speciesReference species="M_MDAPIM_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_UDP[NAM:NGM]AGMDAPIM_c" stoichiometry="1.0"/>
            <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
            <speciesReference species="M_PI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
            </math>
            <listOfParameters>
              <parameter id="LOWER_BOUND" value="0.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
    <reaction id="R726" name="R726" reversible="false">
        <notes>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
        <listOfReactants>
            <speciesReference species="M_UDP[NAM:NGM]AGMDAPIM_c" stoichiometry="1.0"/>
            <speciesReference species="M_ALAALA_c" stoichiometry="1.0"/>
            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_UDP[NAM:NGM]AGMDAPIMAA_c"
stoichiometry="1.0"/>
            <speciesReference species="M_ADP_c" stoichiometry="1.0"/>
            <speciesReference species="M_PI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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                <math xmlns="http://www.w3.org/1998/Math/MathML">
                    <ci> FLUX_VALUE </ci>
                </math>
                <listOfParameters>
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                  <parameter id="UPPER_BOUND" value="100000.0" units="mmol_per_gDW_per_hr"/>
                  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
                  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
                  <parameter id="REDUCED_COST" value="0.000000"/>
                </listOfParameters>
            </kineticLaw>
        </reaction>
        <reaction id="R727" name="R727" reversible="true">
            <notes>
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                <html:p>PROTEIN_ASSOCIATION: </html:p>
                <html:p>SUBSYSTEM: </html:p>
                <html:p>PROTEIN_CLASS: </html:p>
            </notes>
            <listOfReactants>
                <speciesReference species="M_UDP[NAM:NGM]AGMDAPIMAA_c"
stoichiometry="1.0"/>
                <speciesReference species="M_DPP_c" stoichiometry="1.0"/>
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            </listOfProducts>
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                </math>
                <listOfParameters>
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units="mmol_per_gDW_per_hr"/>
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            </notes>
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            </math>
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        </notes>
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            <speciesReference species="M_ATP_c" stoichiometry="1.0"/>
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        <listOfProducts>
            <speciesReference species="M_LIPID2-AMIDATED_c" stoichiometry="1.0"/>
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            <speciesReference species="M_PI_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
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            </notes>
            <listOfReactants>
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            <listOfProducts>
                <speciesReference species="M_PEPTIDOGLYCAN_c" stoichiometry="1.0"/>
                <speciesReference species="M_DPP_c" stoichiometry="1.0"/>
            </listOfProducts>
            <kineticLaw>
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                </math>
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            </notes>
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            <listOfProducts>
                <speciesReference species="M_ARABINOGALACTAN_PEPTIDOGLYCAN_c"
stoichiometry="1.0"/>
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            <kineticLaw>
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                </math>
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            <speciesReference species="M_TYR_c" stoichiometry="0.187"/>
            <speciesReference species="M_CYS_c" stoichiometry="0.094"/>
            <speciesReference species="M_ASN_c" stoichiometry="0.213"/>
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            </math>
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          <speciesReference species="M_ATP_c" stoichiometry="1.98"/>
          <speciesReference species="M_GTP_c" stoichiometry="1.13"/>
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      <listOfProducts>
          <speciesReference species="M_RNA_c" stoichiometry="1"/>
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      <kineticLaw>
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      </notes>
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              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
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        </kineticLaw>
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            <speciesReference species="M_HEME-FE2_c" stoichiometry="0.01"/>
            <speciesReference species="M_HEME-FE3_c" stoichiometry="0.01"/>
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            <speciesReference species="M_FERO_c" stoichiometry="0.001"/>
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        </notes>
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            <speciesReference species="M_TETRACOSANOYL-COA_c" stoichiometry="0.11"/>
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            </math>
            <listOfParameters>
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        </kineticLaw>
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        <notes>
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            <speciesReference species="M_AC3PIM5_c" stoichiometry="0.082"/>
            <speciesReference species="M_AC4PIM6_c" stoichiometry="0.082"/>
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        <listOfProducts>
            <speciesReference species="M_PIMS_c" stoichiometry="1.0"/>
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        <kineticLaw>
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            </math>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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            <speciesReference species="M_ARAFDPP_c" stoichiometry="4.5"/>
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        <listOfProducts>
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            <speciesReference species="M_LAM_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
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            </math>
            <listOfParameters>
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              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
              <parameter id="REDUCED_COST" value="0.000000"/>
            </listOfParameters>
        </kineticLaw>
    </reaction>
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            <html:p>PROTEIN_ASSOCIATION: </html:p>
            <html:p>SUBSYSTEM: </html:p>
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stoichiometry="0.008"/>
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stoichiometry="0.238"/>
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        </reaction>
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            </notes>
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            <listOfProducts>
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            </listOfProducts>
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                </listOfParameters>
            </kineticLaw>
        </reaction>
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stoichiometry="0.522"/>
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        <listOfProducts>
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Rv0194 or Rv1819c or Rv1747 or ( Rv1687c and Rv1686c ) </html:p>
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            <html:p>SUBSYSTEM: </html:p>
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            <speciesReference species="M_TREHALOSEMONOMYCOLATE_c"
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stoichiometry="1.0"/>
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                <speciesReference species="M_DIACYLTREHALOSE_c" stoichiometry="1.0"/>
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COA_c" stoichiometry="1.01"/>
            <speciesReference species="M_GDPMAN_c" stoichiometry="1.01"/>
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        <speciesReference species="M_DTDP_c" stoichiometry="0.259"/>
        <speciesReference species="M_SAM_c" stoichiometry="0.778"/>
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                <speciesReference species="M_HYDROXYPHTHIOCERANOYL-COA_c"
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                <speciesReference species="M_COA_c" stoichiometry="0.65"/>
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            <speciesReference species="M_SMALLMOLECULES_c" stoichiometry="0.05"/>
            <speciesReference species="M_PE_c" stoichiometry="0.006"/>
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            <speciesReference species="M_P-L-GLX_c" stoichiometry="0.035"/>
            <speciesReference species="M_ATP_c" stoichiometry="47.0"/>
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        </listOfProducts>
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            </math>
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        <listOfProducts>
            <speciesReference species="M_NH3_c" stoichiometry="1.0"/>
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        <listOfProducts>
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        </notes>
        <listOfReactants>
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            <speciesReference species="M_H_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_NO2_c" stoichiometry="1.0"/>
        </listOfProducts>
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            </math>
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            </math>
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            <html:p>SUBSYSTEM: </html:p>
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            <speciesReference species="M_PI_c" stoichiometry="1.0"/>
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            </math>
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            <speciesReference species="M_PI_c" stoichiometry="1.0"/>
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        <kineticLaw>
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        </math>
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            </math>
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        <listOfProducts>
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            <speciesReference species="M_PI_c" stoichiometry="1.0"/>
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            </math>
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( Rv0932c and Rv0930 and Rv0929 and Rv0933 ) or ( Rv0928 and Rv0930 and Rv0928 and Rv0933 )
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        </listOfProducts>
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            <speciesReference species="M_FUM_c" stoichiometry="1.0"/>
        </listOfProducts>
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            </math>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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        </notes>
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            <speciesReference species="M_H_c" stoichiometry="1.0"/>
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            </math>
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        </kineticLaw>
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            <speciesReference species="M_H_c" stoichiometry="1.0"/>
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        <listOfProducts>
            <speciesReference species="M_GLAC_c" stoichiometry="1.0"/>
        </listOfProducts>
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              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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      </listOfReactants>
      <listOfProducts>
          <speciesReference species="M_GLU_c" stoichiometry="1.0"/>
      </listOfProducts>
      <kineticLaw>
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          </math>
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</reaction>
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          <speciesReference species="M_H_c" stoichiometry="1.0"/>
      </listOfReactants>
      <listOfProducts>
          <speciesReference species="M_GLUC_c" stoichiometry="1.0"/>
      </listOfProducts>
      <kineticLaw>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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            <speciesReference species="M_GLY_c" stoichiometry="1.0"/>
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              <parameter id="REDUCED_COST" value="0.000000"/>
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        </kineticLaw>
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            <html:p>SUBSYSTEM: </html:p>
            <html:p>PROTEIN_CLASS: </html:p>
        </notes>
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            <speciesReference species="M_H_c" stoichiometry="1.0"/>
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        </kineticLaw>
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        </notes>
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            <speciesReference species="M_H_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_HIS_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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        </kineticLaw>
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        <notes>
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            <html:p>PROTEIN_CLASS: </html:p>
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        <listOfProducts>
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            <speciesReference species="M_H_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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            <html:p>SUBSYSTEM: </html:p>
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        </notes>
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            <speciesReference species="M_H_c" stoichiometry="1.0"/>
        </listOfReactants>
        <listOfProducts>
            <speciesReference species="M_ILE_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
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            </math>
            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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        </kineticLaw>
    </reaction>
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	</listOfReactants>
	<listOfProducts>
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		<speciesReference species="M_H_c" stoichiometry="1.0"/>
	</listOfProducts>
	<kineticLaw>
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		</math>
		<listOfParameters>
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		  <parameter id="UPPER_BOUND" value="1.0" units="mmol_per_gDW_per_hr"/>
		  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
		  <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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	</kineticLaw>
</reaction>
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		<html:p>SUBSYSTEM: </html:p>
		<html:p>PROTEIN_CLASS: </html:p>
	</notes>
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		<speciesReference species="M_H_c" stoichiometry="1.0"/>
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	<listOfProducts>
		<speciesReference species="M_INS_c" stoichiometry="1.0"/>
	</listOfProducts>
	<kineticLaw>
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		</math>
		<listOfParameters>
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		  <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
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          <html:p>PROTEIN_CLASS: </html:p>
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          <speciesReference species="M_H_c" stoichiometry="1.0"/>
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      </listOfProducts>
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            <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
            <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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          <speciesReference species="M_H_c" stoichiometry="1.0"/>
      </listOfReactants>
      <listOfProducts>
          <speciesReference species="M_LEU_c" stoichiometry="1.0"/>
      </listOfProducts>
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            </math>
            <listOfParameters>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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            </math>
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              <parameter id="OBJECTIVE_COEFFICIENT" value="0.000000"/>
              <parameter id="FLUX_VALUE" value="0.000000" units="mmol_per_gDW_per_hr"/>
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            <speciesReference species="M_H_c" stoichiometry="1.0"/>
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        </listOfProducts>
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        <listOfProducts>
            <speciesReference species="M_LYS_c" stoichiometry="1.0"/>
        </listOfProducts>
        <kineticLaw>
            <math xmlns="http://www.w3.org/1998/Math/MathML">
                <ci> FLUX_VALUE </ci>
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Chapter3

Studying the role of selective gene set in *Mycobacterium Tuberculosis* metabolic pathway using Flux Balance Analysis

3.1 Introduction:

The disease Tuberculosis (TB), which is caused by *Mycobacterium tuberculosis*, is one of the most common and fatal diseases in the world now a days. It is a disease of poverty, affecting mostly young adults in their most productive years. It is responsible for more than 8 million cases of disease per-year and approximately 3 million deaths (W.H.O). 95% of deaths caused by it, are occurring in developing countries. The bacteria involved is a member of Mycobacterium family which has over 60 species with only a few like Mycobacterium leprae, Mycobacterium tuberculosis, Mycobacterium africanum and Mycobacterium avium that causes human diseases (Susmita Sarkar et.al. 2011) . Control of the human TB relies on vaccination, case finding, and chemotherapy. In present time scenario, drugs to cure TB are not very effective against the persistent bacteria and this is why long treatment time of 8-12 months and combination of many drugs is required to eliminate the infection and cure this fatal disease. There are so many obstacles and constraints in the drug development against the TB, especially in the industrially and economically under-developed countries. In these countries, TB is more prevalent. Financial lacks and logistic needs, as well as, a further complication in the development of drugs against TB are main constraints (W.H.O.). There are new emerging multi-drug-resistant strains of TB (both *M. tuberculosis* and M. bovis) in many parts of the world also, which remain resistant to the drugs developed to cure *tuberculosis*. In 2010, there was an estimated prevalence of 650,000 cases of multidrug-resistant TB (MDR-TB), and in 2008 it was estimated that there were 150,000 MDR-TB deaths annually due to TB (W.H.O) . Globally, it is estimated that around 10% of MDR-TB cases have extensively drug-resistant TB (XDR-TB). 77 countries reported at least one case of XDR- TB by end of the year 2011 (W.H.O.). The current recommended standard TB chemotherapy is called DOTS (Directly Observed Treatment, Short-course), which is a six month duration therapy consisting of an initial two-month phase of treatment with four drugs, isoniazid (INH), rifampin (RIF), pyrazinamide (PZA), and ethambutol (EMB), followed by a continuation phase of treatment with INH and RIF for another four months (Zhang et.al. 2002). As the duration is long, so there is a scope for defaulting and getting resistance the bacteria. There are very few new classes of antibiotics which have been approved for clinical use in the past few years. For instance, the oxazolidinones and daptomycin are not applicable explicitly for TB

infections (Beste et al. 2007). New anti-TB drugs are urgently required so that it will shorten the duration of treatment in addition to the drugs , will act against drug-resistant strains and specifically target persistent cells (Beste et al. 2007).

3.2 Objectives:

The availability of complete genome sequence of *M. tuberculosis* has opened up the blueprint of the bacterium to mankind (Cole et.al. 1998). This available data can be exploited and used for the identification of the important parts and components of the *Mycobacterium,* tampering and destroying those components would be fatal for the survival of the *Mycobacterium*. Here, genes are the components, which put in the context of genome, those genes govern the phenotype (properties) of the chosen organism. Thus the availability of the complete genome sequence of *M. tuberculosis* provide the platform to identification of important drug targets against the new evolving multi-drug-resistant strains of *M. tuberculosis* and against the persistent *M. Tuberculosis*. Ability of the bacteria to persist in the form of a long-term asymptomatic infection, referred to as latent (or persistent) TB, is centre of the biology of the disease (Graham et.al. 2003).

Using metabolic pathway and known gene functions ,if we remove(theoretically stop/delete the reaction) any gene from the complete metabolic system of *M. tuberculosis* model(build using FBA) and still organism is surviving means this gene is not essential for survival of the pathogen in normal condition. But if organism dies or does not produce output, then the specific gene product is marked as essential and can be an important target as it is playing a major role is the survival of the organism. The same theoretical experiments can be done by varying the media system to make it equivalent to dormancy conditions. Previous work("metabolic control analysis of biochemical pathways as an approach to in silico identification and validation of anti- tuberculous, anti-malarial and anti-diabetic drug targets", chapter- 3.4 Constraint-based genome-scale metabolic network model of persistent *M. tuberculosis*, Vivek kumar singh, 2009) have studied a set of selective genes for their essentially. The set of genes used to test were selected from the differential expression of the *M. tuberculosis* genes (microarray data) under different stress conditions vs. the normal one. Here, in present work, few other genes are also included in the knockout studies and

out of this set of genes; few selective non essential genes are further studied for double knockout.

3.3 Materials used :

The model described by Beste (Beste et al. 2007) is called as Genome Scaled Metabolic Network Model. It is used as start point in this study, to construct the metabolic model for persistent *M. tuberculosis* and to study the in-silico knock outs of selected genes in the normal(wildtype) as well as persistent *M. Tuberculosis.* This knock-out study provides information of essential and non-essential genes of the organism and henceforth the protein products of these identified essential genes could then serve as potential anti-tuberculous drug targets as well as the second most important work is to study the non-essential genes for double knockout and to identify the pair of non-essential genes, which makes the organism die on their double knock-outs . It can be Validated by comply in-vivo and in-vitro studies. The availability of an interactive web-interface (GSMN-TB) and the flexibility to change media conditions through this interface, made it more suitable for the present study .

3.4 Genes selection for in-silico knockout study:

Genes selected for this study were the genes which were found differently expressed under stress conditions (Hypoxia condition here), and assumption was taken is that they would be important for the survival of normal growing as well as persistent *M. Tuberculosis.* All of the differently expressed genes may or may not form products which can be taken into account in metabolic network model. Genes forming regulatory proteins or structural proteins, may cause fatal effect to the organism when knocked out, so these genes are very important for the organism as well as for this study but in metabolic network models these may go unnoticed. Due to this limitation, the effect of in-silico knockout of the genes that are differently expressed in persistent *M. tuberculosis* can be categorize into following four categories:

1. ***Essential in normal growing and persistent M. tuberculosis***– affects the

metabolism of the bacilli directly.

2. ***Essential only in normal growing bacilli***– has direct effect in normal growing bacilli, but may have indirect effect (for example, through regulatory networks) in persistent
3. ***Essential only in persistent bacilli***– has direct effect in persistent but may have indirect Effect in normal growing bacilli
4. ***Non-essential in both, normal growing and persistent bacilli***– may have indirect effect in both.

Selection criteria of genes:

The genes which were differently expressed during the persistence (in Hypoxia condition) were chosen for the knockout study. Information regarding differentially expressed genes was taken from database MTBreg. This database contains the list of differentially expressed genes of *M. tuberculosis* in a variety of experimental conditions (Kaufmann et.al. 2004). On the basis of environmental condition, encountered by persistent *M. tuberculosis*, the gene which are differentially expressed under following conditions:

1. ***Hypoxia condition****:* - Hypoxia is a pathological condition in which the organism is deprived of adequate oxygen supply. Hypoxic conditions are generally believed to be the environment encountered by the pathogen in the central part of the granuloma (an organized collection of macrophages). Genes from all the literature sources, which are reporting in microarray experiments under hypoxic condition(as provided in MTBreg database) were selected (Voskuil et al. 2008), (James et al. 2004), (Visconti et al. 2004), (Muttucumaru et al. 2004), (Slayden et al. 2002), (Kallenius et al. 2004). The resultant list of genes includes some genes, like ribosome binding proteins, unwell characterized proteins, hypothetical proteins, transposases, etc. These genes were not directly related to the metabolic reactions, so these were excluded from the final list.

2. ***Nutrient starvation and source dependent condition:*** – This condition includes carbon, nitrogen, and phosphate starvation, as well as many more stress conditions.

Here, genes were selected from the work of Schoolnik and co-workers (Ehrt et al. 2003), fulfilling the above criteria of stress.

Resultant gene list was further reduced by removing those who had no corresponding biochemical reaction in GSMN model. Absence of a reaction for a gene may indicate that it does not catalyze any reaction but could be a transcription factor or a regulator. Thus, the final gene list reduced to 100 of which, 58 genes from the previous work (Vivek et.al.,2009), and rest 42 are the newly found gene (due to database updates and newly found genes there are additional genes in hit list).

3.5 Construction of constraint-based models of persistent *M. Tb.*

Persistent *M. tuberculosis* models were derived from GSMN in-vivo model (normal wild-type model). As mentioned in the earlier work done by the group (Vivek et.al., 2009) all the four models constructed by altering the media conditions of normal model so that it simulates the environment similar to that encountered by persistent. Validation of these models has also been done in the previous work. These models used for performing in-silico gene knockout study.

Details of models are as follows:

Model-1: the basic model:

Synthesis of biomass is defined as the objective function of GSMN model, which is needed to be maximized in Flux Balance Analysis simulation (Beste et al. 2007). A pseudo-reaction added to the model, actually accounted for biomass synthesis, and the flux through this reaction was assumed equal to the growth rate of the bulk cell culture. Here for the purpose of biomass synthesis reaction, two different reactions were taken; In order to make the model applicable to *M. tuberculosis (*grown both *in vitro* and *in vivo),* we therefore defined two biomass components based on published experimentally derived values for macromolecular composition of *M. Tuberculosis,* the first (BIOMASS1) represents the actual macro-molecular composition of *M. tuberculosis*. and second (BIOMASSe) was a minimal macro-molecular composition of *M. tuberculosis* that includes only those components (DNA, RNA, proteins, essential co-factors and cell wall skeleton) which are thought to be essential for in vitro growth (Beste et al. 2007). Since, GSMN in vivo model

had BIOMASS1 (a relatively realistic in vivo objective function) as the objective function, means it is more near to the original organism; so it was used as the basic model (Wild type) for persistent *M. tuberculosis*.

Media conditions for model-1:

Reaction	***Flux Intake limits (mili-mole per gram per hour)***
Glucose uptake **(R863)** (GLCxt + H = GLC) external Glucose +hydrogen= glucose	0–1
Oxygen transport **(R804)** (O2xt = O2) External Oxygen = Oxygen	-100000 – 100000
Citrate and iron uptake **(R924)** (CITxt + FE3xt = CIT + FE3) External Citrate+ferrous ascorbate= Citrate+ Ferrous	0 – 100000
R141 (HYDROXYAKG = GLX + PYR) D-4-Hydroxy-2-oxoglutarate =Glyoxylate + Pyruvate	-100000 – 100000
R157 (methylmalonyl-CoA epimerase) (SMMALONYLCOA = RMMALONYLCOA)	-100000 – 100000

Here, unit of FLUX- value is mili-mole per gram per hour , and the flux intake limits includes the lowest to highest value for each reaction. The threshold limit of flux value for all reaction is 10000000.0 in all the models.

Model-2:

Bacterial growth requires the presence of environmental factors. For example, if a bacterium uses organic carbon for energy and structure (chemoheterotrophic bacteria) then sources of carbon are needed. Such sources include simple sugars (glucose and fructose are two examples). Nitrogen is needed to make amino acids, proteins, lipids and other components. Sulphur and phosphorus are also needed to manufacture the bacterial

components. Other elements, such as potassium, calcium, magnesium, iron, manganese, cobalt and zinc are necessary for functioning of the enzymes and other processes. Persistent *M. tuberculosis* is known to encounter low oxygen tension, reactive nitrogen intermediates (RNI) such as NO-, NO2-, NO3- etc. This RNI can kill bacteria by forming intrabacterial peroxynitrite (St John et al., 2001). In addition, persistent are also known to survive on fatty acids taken in from the host tissue (or macrophages), or derived from host phagosomal membrane (for example, triacylglycerols and phosphotidylcholine) (Munoz-Elias at.al. 2006). One interesting feature of the *M. tuberculosis*. genome is that approximately 8% of the genome consists of genes that encode proteins involved in lipid metabolism (Cole et. al. 1998). *M. tuberculosis* is composed of an impressive array of lipids, glycolipids, lipoglycans, and polyketides (Daffe et.al. 1998), Since, lipids are abundantly available in host tissues, it has been assumed that Mycobacterium acquires lipids by transporting them rather than synthesizing them (Bloom et.al. 1994). Host niche is also known to be low in iron, phosphate, and many other essential small molecules (Munoz-Elias et.al. 2006) which are necessary for the functioning of enzymes and other processes, but, *M. tuberculosis* produces molecules such as siderophores, and transporters such as transferrin and sulphotransferases (De Voss et. al. 1999), (Lefevre et. al. 1997), (Peirs et. al. 2005), (Wooff et. al. 2002) to scavenge these molecules. *M. tuberculosis* relies on 2-hydroxyphenyloxazoline-containing siderophore molecules called mycobactins for the acquisition of iron in the restrictive environment of the mammalian macrophage (De Voss et.al. 1999) . Thus, while glucose uptake was set to zero, supply of these molecules was kept as was there in the normal growing model. Mg2+ uptake was not explicitly mentioned in the media condition of the GSMN model, and therefore, was not dealt with in the variant models. Model-2 was constructed to represent these conditions.

Media conditions for model-2:

Reaction	***Flux Intake limits* (mili-mole per gram per hour)**
Proton dependent nitric trioxide transport **(R801)** (NO3xt + H = NO3) external nitrate hydrogen= nitrate	-100000 – 100000
Oxygen transport **(R804)**	-100000 – 100000

Reaction	***Flux Intake limits* (mili-mole per gram per hour*)***
(O2xt = O2) External Oxygen = Oxygen	
Acetate **(R808)** (ACxt = AC) external Acetate = Acetate	-1 - 1
R141 (HYDROXYAKG = GLX + PYR) D-4-Hydroxy-2-oxoglutarate =Glyoxylate + Pyruvate	-100000 – 100000
R157 (methylmalonyl-CoA epimerase) (SMMALONYLCOA = RMMALONYLCOA)	-100000 – 100000
Phosphotidylcholine **(R922)** (PHOSPHATIDYLCHOLINExt = PHOSPHATIDYLCHOLINE) external Phosphatidylcholine= Phosphatidylcholine	0 – 1
Fatty acid transport reactions **(R907- R920)**	0 – 1
Triacylglycerol **(R921)** (TAGxt = TAGcat) external Triacylglycerol= Triacylglycerol	0 – 1

Model-3:

M. tuberculosis requires Isocitrate lyase (ICL) for its survival during nutrient starvation and has a role during steady state growth in a glycerol limited chemostat indicates a function for this enzyme which extends beyond fat metabolism (Munoz-Elias et.al. 2005). ICL is needed for fixation of carbon when *M. tuberculosis* is grown on carbon source or on fatty acids (Munoz-Elias et.al. 2005). ICL fixes carbon using glyoxylate shunt where it catalyzes the conversion of isocitrate to glyoxylate and succinate, together with malate synthase, it bypasses the two decarboxylation steps of the tricarboxylic acid cycle (TCA cycle). This reaction produces a molecule of succinate without losing the carbon in the form of CO2 as occurs in the subsequent steps of TCA cycle (Bishai et.al. 2000). Tracing for reactions (in GSMN model) other than that catalyzed by ICL which can fix carbon, reaction R141 (HYDROXYAKG = GLX + PYR) that converts hydroxy-α-ketoglutarate to glyoxylate and pyruvate, was identified. This reaction was predicted by Green et al. (Green et.al. 2004), and thus, was included in GSMN model, but, no experimental evidence is available for the

reaction. Gene corresponding to the enzyme (hydroxyketoglutarate aldolase EC: 4.1.3.16) that catalyze R141, was found in E.coli but was absent in *M. tuberculosis* entry of KEGG. Sequence alignment using amino acid sequence of this enzyme from E.coli against *M. tuberculosis* showed no significant hit. Thus, a variant of model-2, named model-3, was constructed where flux through R141 was set to zero.

Media conditions for model-3:

Reaction	***Flux Intake limits* (mili-mole per gram per hour)**
Proton dependent nitric trioxide transport (**R801)** (NO3xt + H = NO3) external nitrate hydrogen= nitrate	-100000 – 100000
Oxygen transport **(R804)** (O2xt = O2) External Oxygen = Oxygen	-100000 – 100000
Acetate **(R808)** (ACxt = AC) External Acetate= Acetate	-1 - 1
R157 (methylmalonyl-CoA epimerase) (SMMALONYLCOA = RMMALONYLCOA)	-100000 – 100000
Phosphotidylcholine **(R922)** (PHOSPHATIDYLCHOLINExt = PHOSPHATIDYLCHOLINE) External phosphatidylcholine= phosphatidylcholine	0 – 1
Fatty acid transport reactions **(R907- R920)**	0 – 1
Triacylglycerol **(R921)** (TAGxt = TAGcat) external Triacylglycerol= Triacylglycerol	0 – 1

Model-4:

Model-3 could reproduce the essentiality of ICL but only in the condition when even chain fatty acids were used as the sole carbon source . In the presence of any odd chain fatty acid, ICL became dispensable. Stopping the fixation of carbon from propionyl- CoA (which is

the end product of beta-oxidation of odd chain fatty acids) by stopping the reaction R157 (SMMALONYLCOA = RMMALONYLCOA) reproduced the essentiality of ICL. Carbon is actually fixed in reaction R156 (PROPIONYLCOA + BIOTIN-CO2 = SMMALONYLCOA + BIOTIN), where propionyl-CoA is converted to S-methylmalonyl-CoA. S- methylmalonyl-CoA in turn, is a substrate for many biosynthetic reactions. In R157, there is reversible conversion of S-methylmalonyl-CoA to R-methylmalonyl-CoA, and R-methylmalonyl-CoA gets converted to succinyl-CoA by reaction R158 (RMMALONYLCOA + COB-III = SUCCOA). Thus, the reaction set R156-R158 fixes the carbon from propionyl-CoA, and stopping any one of them could stop the fixation of carbon. R157 was chosen to be stopped because there was no genomic evidence for the enzyme (methylmalonyl-CoA epimerase EC: 5.1.99.1) catalyzing this reaction in *M. tuberculosis* as well as in E.coli. This led to model-4 which was built from model-3 by constraining the flux through the reaction R157 to zero. These models differed from the well known in vitro Wayne's model for persistent *M. tuberculosis* (Wayne et.al. 1996) majorly with respect to the carbon source. In Wayne's model, oleic acid was used as the carbon source, while in these persistent *M. tuberculosis* models, various saturated and unsaturated fatty acids were the carbon source.

Media conditions for model-4:

Reaction	***Flux Intake limits* (mili-mole per gram per hour)**
Proton dependent nitric trioxide transport **(R801)** (NO3xt + H = NO3) external nitrate hydrogen= nitrate	-100000 – 100000
Oxygen transport **(R804)** (O2xt = O2) External Oxygen = Oxygen	-100000 – 100000
Acetate **(R808)** (ACxt = AC) External Acetate= Acetate	-1 - 1
Phosphotidylcholine **(R922)** (PHOSPHATIDYLCHOLINExt = PHOSPHATIDYLCHOLINE)	0 – 1

Reaction	***Flux Intake limits*** ***(*mili-mole per gram per hour*)***
External phosphatidylcholine= phosphatidylcholine	
Fatty acid transport reactions **(R907- R920)**	0 – 1
Triacylglycerol **(R921)** (TAGxt = TAGcat) external Triacylglycerol= Triacylglycerol	0 – 1

3.6 Methods and Tools used :

To study the essentiality of selected genes, a web based tool GSMN-tb was used. This GSMN-TB tool provides the platform on which metabolic flexibility of bacteria can be checked as well as the prediction of phenotype of mutants can be done. As well as this tool can be used to highlight the unexplored features of *M. tuberculosis*. metabolism.

GSMN-TB: (http://sysbio3.fhms.surrey.ac.uk/**)**

[Dany JV Beste, Tracy Hooper, Graham Stewart, Bhushan Bonde, Claudio Avignone-Rossa, Michael E Bushell, Paul Wheeler, Steffen Klamt, Andrzej M Kierzek and Johnjoe McFadden, **GSMN-TB: a web-based genome-scale network model of Mycobacterium tuberculosis metabolism**, *Genome Biology 2007, 8:R89 (doi:10.1186/gb-2007-8-5-r89)*]

This GSMN-TB, a genome-scale metabolic model of *M. Tuberculosis* consists of 849 unique reactions and 739 metabolites, and involves 726 genes. The model was calibrated by growing *Mycobacterium bovis bacille Calmette Guérin* in continuous culture and steady-state growth parameters were measured(Beste *et. al. 2007*). This model was created by using SBML (Systems Biology Markup Language) platform, and the tool used for the calculation of flux rates and substrate consumption rate, was Flux Balance Analysis, its results show the close correspondence to experimentally determined values(Beste *et. al. 2007*). This model achieves the prediction accuracy up to 78% and this is validated by the known drug targets, these known drug targets were predicted by this model correctly. An web-based version of this model is used for interactive simulation.

3.7 Gene Essentiality Calculations:

The selected genes (which were differently expressed in stress condition) were simulated for their essentiality for the *Mycobactrium*. Simulation was done with the help of GSMN-TB. In which the Basic model (model 1) was chosen as the media condition.

Following steps were followed for simulation.

Working Steps

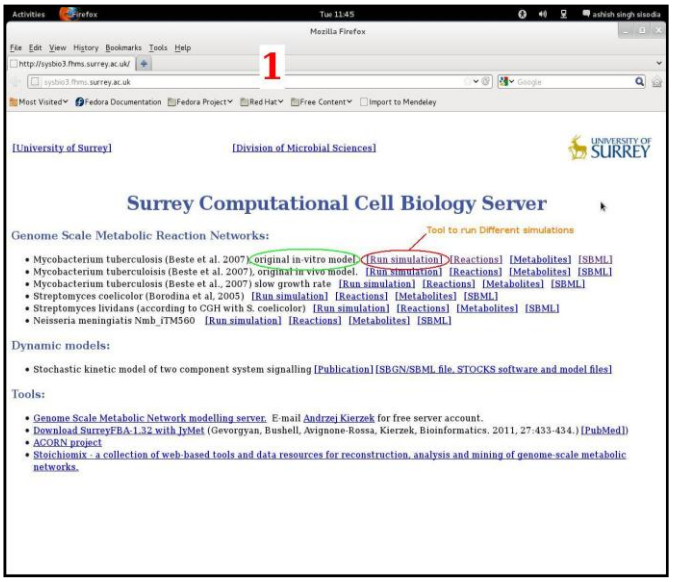


Figure-1

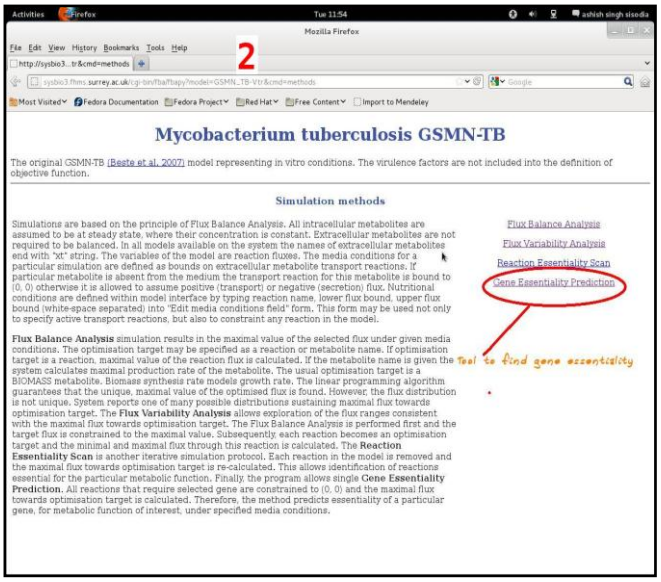


Figure-2

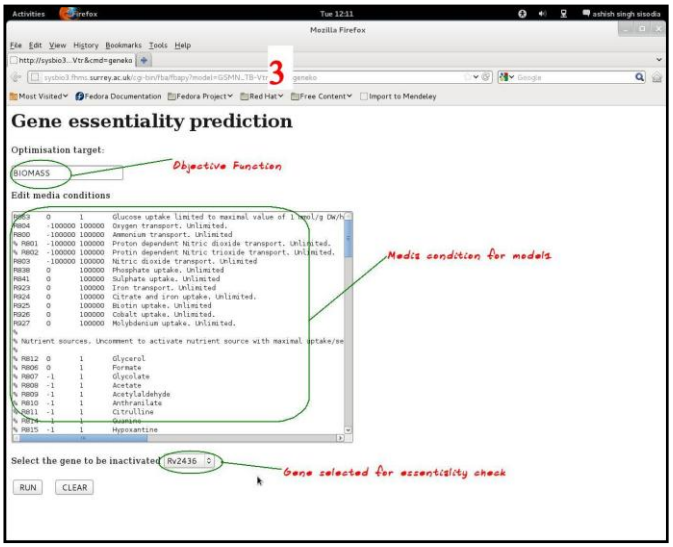


Figure-3.

Figure-4.

Steps:

1. Go to the website of GSMN-tb (http://sysbio3.fhms.surrey.ac.uk/) (Fig.1)
2. Select the Run simulation option for in-vitro model of *M. tuberculosis* (Fig.1).
3. In the Next coming web page (http://sysbio3.fhms.surrey.ac.uk/cgi-bin/fba/fbapy?model=GSMN_TB-Vtr&cmd=methods)(fig.2) out of the listed options, select Gene Essentiality Prediction option(fig.2)
4. In the next coming web page (http://sysbio3.fhms.surrey.ac.uk/cgi-bin/fba/fbapy?model=GSMN_TB-Vtr&cmd=geneko) , (Fig.3) put the media condition values of respective models then select the gene, which is to be knocked out from the drop-down button then run simulation (Fig.3).
5. The next coming web page (http://sysbio3.fhms.surrey.ac.uk/cgi-bin/fba/fbapy) is the result page, which gives the information about the gene's essentiality and the biomass produced, after the knock out of the gene (Fig.4).

Results:

Results generated after simulating all 100 genes of 4 models for essentiality produces following results.

Table 1. Numbers of essential and non-essential genes for different models are shown as follows.

Model	Number of essential genes	Number of non-essential genes
Model-1	21	79
Model-2	24	76
Model-3	25	75
Model-4	25	75

This different numbers of essential and non-essential genes for different models are due to different constraints in different models. Here, in result, four genes showed different essentiality in different models. Which are Rv1736c, Rv3206c, Rv1737c and Rv3322c.

Table 2. The different essentiality emerges in four models of the four genes are shown here:

Gene	***Model-1***	***Model-2***	***Model-3***	***Model-4***
Rv1736c	Non-essential	Essential	Essential(non-fesible)	Essential(non-fesible)
Rv3206c	Non-essential	Essential	Essential(non-fesible)	Essential(non-fesible)
Rv1737c	Non-essential	Essential	Essential	Essential
Rv3322c	Non-essential	Essential	Essential	Essential

Discussions :

Gene Rv1736c and Rv3206c are non-essential in model-1, and essential in model-2, for model-3 & model-4, knock-out study is not possible, due to calculation limitations (probably due to the zero eigen values generation while performing liner programming), as well as gene Rv1737c and Rv33322c are non-essential in model-1 but essential in model-2,3 & 4. Gene Rv1736c is a nitrate reductase and its function involves the nitrate reduction, and in the persistence in the host [catalytic activity: nitrite + acceptor = nitrate + reduced acceptor]. it serves as an immunogenic antigen, inducing the gamma-interferon responses in whole-blood cultures from *M. Tuberculosis.*

Gene Rv3206c is a adenylyltransferase/sulfurtransferase MoeZ and its function involves the Catalyzing conversion of the sulfur carrier protein CysO to CysO-thiocarboxylate (reaction is thought to proceed in two steps: first, ATP-dependent activation of CysO as acyl-adenylate (CysO-COOAMP), followed by sulfur transfer to give CysO-thiocarboxylate (CysO-COSH) Probable), this gene works in sulfur relay system and belongs to sulfur relay pathway, and catalyzes the 2-thiouridine biosynthesis and Moco biosynthesis (source: KEGG database).

Gene Rv1737c is a nitrate/nitrite transporter (NarK2). It is involved in excretion of nitrite, produced by the dissimilatory reduction of nitrate, across the membrane, responsible for the translocation of the substrate across the membrane.

Gene Rv3322c is a methyl transferase. Its function involves methylation and it is involved in Histidine metabolism, Tyrosine metabolism, Polycyclic aromatic hydrocarbon degradation, Microbial metabolism (in diverse environments). In Histidine Metabolism, it

catalyzes the the conversion of L-Histidine to 1-Methyl-L-Histidine. In Tyrosine metabolism, it catalyzes the the conversion of N-Methyl-Tyramine to Hordenine. In Polycyclic aromatic hydrocarbon degradation, it catalyzes three reactions, conversion of 1-Phenanthrol to 1-Methoxy-Phenanthrene, conversion of 1-Hydroxy-6-Methoxypyrene to 1,6-Dimethoxypyrene, and conversion of 1-Hydroxypyrene to 1-Methoxypyrene (source: KEGG database).

Persistent *M. tuberculosis* is known to encounter low reactive nitrogen intermediates (RNI) such as NO-, NO2-, NO3-. In model-2, RNI are lowered. As these two genes Rv1737c & Rv1736c are working as nitrate/nitrite transporters, so knock-outs of these two genes may possibly affect the growth rate of the organism. Similarity model-3 & model-4 are more constrained then model 2. So, these genes are essential in model-3, and model-4 also. *M. tuberculosis* produces molecules such as siderophores and transporters such as transferrin and sulphotransferases (De Voss et. al. 1999), (Lefevre et. al. 1997), (Peirs et. al. 2005), (Wooff et. al. 2002) to scavenge the molecules like iron, phosphate, sulphates and many other essential small molecules. Thus, while glucose uptake was set to zero, supply of these molecules was kept as was there in the normal growing model. Gene Rv3206c is sulfur transferase, and its function is to catalyze the conversion of the sulfur carrier protein CysO to CysO-thiocarboxylate. So may be the possible supply of these small molecules (iron, phosphate, sulphates and many other essential small molecules) supported by gene Rv3206c**.** So there is possibility of decrements in growth rate of organism by knocking out this gene. That is validated by the gene knock-out studies in further models (model-2,3& 4).

3.8 Knockout of selective non-essential genes: Double Knockout

Genes, whose deletion does not kills organism or does not make the biomass production to zero, are non-essential to the organism. Even if non essential genes are involved in important reactions then also its knock out does not affect organism, reason: as it is the rerouting of metabolic fluxes through other pathways (Edwards et.al. 1999). The new rerouting of metabolic fluxes through alternate pathways can be discovered by flux

variability analysis of organism after the knock out of that gene. Even If new alternate pathway stops, then there are two possible consequences. First, another rerouting of metabolic fluxes through other alternate pathway and Second, organism will die. Second case is of interest, because it kills the organism.

Goal of this task is to identify genes which are correlated (belong to bypass pathway, after deleting the main gene) to the selective non-essential genes (found non-essential in gene essentiality studies), and knocking out these correlated gene along with the non-essential genes, so that this double knock-out may provide a pair of non-essential genes which can be further projected as potential drug target to cure TB.

Selection criteria of non-essential genes:

After checking the essentiality of all genes in complete gene set (100 gene's set), 79 genes were found as non essential (in model-1). As this number is large to study the double knockout, so out of these 79 non-essentials, genes which were found as non-essential in previous knockout studies also (for wild type, model-1) (Vivek et.at. 2009) were selected for double knock-out studies, and henceforth 26 genes get selected for knockout study. Out of these 26 genes, GSMN-TB software failed to solve flux variability analysis (FVA) of knock-out of 3 genes, and successfully simulated for knockout of 23 genes. So, finally the double knock-out study was done only on 23 genes. Out of these 23 genes, only 21 gene were simulated by GSMN-TB for double knock-outs studies successfully.

Table-3: shows the Properties of 21 selected non-essential genes

Information sources:
http://www.geneontology.org/
http://www.uniprot.org
http://tuberculist.epfl.ch/
http://genome.tbdb.org

Gene	*Full Name*	*Synonyms*	*Database*	*Function*	*Catalytic Activity*	*Pathway & Miscellaneous*
Rv0211	**Phosphoenolpyruvate carboxykinase [GTP]**	**MT0221 MTCY08D5.06 P96393 pck1 pckA pckG PCKG_MYCTU**	UniProtKB: P65686	Catalyzes the conversion of oxaloacetate (OAA) to phosphoenolpyruvate (PEP), the rate-limiting step in the metabolic pathway that produces glucose from lactate and other	**GTP + oxaloacetate = GDP + phosphoenolpyruvate + CO_2.** HAMAP_MF_00452	**Pathway=** Carbohydrate biosynthesis; gluconeogenesis

Gene	*Full Name*	*Synonyms*	*Database*	*Function*	*Catalytic Activity*	*Pathway & Miscellaneous*
				precursors derived from the citric acid cycle		
Rv0244c	**PROBABLE ACYL-CoA DEHYDROGENASE FADE5**	**fadE5, MT0258, O53666_MYCTU, Q7DA67**	UniProtKB: O53666	acyl-CoA dehydrogenase activity flavin adenine dinucleotide binding		**Belongs to the** acyl-CoA dehydrogenase family
Rv0363c	**Fructose-bisphosphate aldolase**	**ALF_MYCTU, fba, MT0379, MTCY13E10.25c, O06313**	UniProtKB: P67475	Catalyzes the aldol condensation of dihydroxyacetone phosphate (DHAP or glycerone-phosphate) with glyceraldehyde 3-phosphate (G3P) to form fructose 1,6-bisphosphate (FBP) in gluconeogenesis and the reverse reaction in glycolysis	**D-fructose 1,6-bisphosphate = glycerone phosphate + D-glyceraldehyde 3-phosphate.**	**Was identified as a high-confidence drug target.** **Pathway=** Carbohydrate degradation; glycolysis; D-glyceraldehyde 3-phosphate and glycerone phosphate from D-glucose: step 4/4.
Rv0467	**Isocitrate lyase**	**ACEA_MYCTU icl MT0483 MTV038.11 O53752**	UniProtKB: P0A5H3	Catalyzes the formation of succinate and glyoxylate from isocitrate, a key step of the glyoxylate cycle. May be involved in the assimilation of one-carbon compounds via the isocitrate lyase-positive serine pathway	**Isocitrate = succinate + glyoxylate.**	**Pathway** Carbohydrate metabolism; glyoxylate cycle; (S)-malate from isocitrate: step 1/2. **Was identified as a natural substrate of the M.tuberculosis proteasome.**
Rv0619		**galTb**		INVOLVED IN GALACTOSE METABOLISM (LELOIR PATHWAY	**UTP + ALPHA-D-GALACTOSE 1-PHOSPHATE = DIPHOSPHATE + UDP-GALACTOSE**	
Rv0951	**Succinyl-CoA ligase [ADP-forming] subunit beta**	**MT0978 , MTCY10D7.23c, sucC , SUCC_MYCTU**	UniProtKB: P71559	Ligase	**ATP + succinate + CoA = ADP + phosphate + succinyl-CoA.** HAMAP MF_0055	**Pathway** Carbohydrate metabolism; tricarboxylic acid cycle; succinate from succinyl-CoA (ligase route): step 1/1. HAMAP MF_00558

Gene	*Full Name*	*Synonyms*	*Database*	*Function*	*Catalytic Activity*	*Pathway & Miscellaneous*
					8	
Rv1553		**frdB**		INVOLVED IN INTERCONVERSION OF FUMARATE AND SUCCINATE (ANAEROBIC RESPIRATION)	**SUCCINATE + ACCEPTOR = FUMARATE + REDUCED ACCEPTOR**	**Pathway:** mtu00020 **Citrate cycle (TCA cycle)** mtu00190 **Oxidative phosphorylation** mtu00623 **Toluene degradation** mtu00650 **Butanoate metabolism** mtu01100 **Metabolic pathways** mtu01110 **Biosynthesis of secondary metabolites** mtu01120 **Microbial metabolism in diverse environments** mtu02020 **Two-component system**
Rv1736c	**Nitrate reductase-like protein narX**	**MT1778, narX, NARX_MYCTU, Q7D821**	UniProtKB: P71994	Does not seem to have nitrate reductase activity.	**Nitrite + acceptor = nitrate + reduced acceptor.**	***Pathways::*** nitrate reduction III (dissimilatory) ***Biotechnological use:*** **This protein serves as an immunogenic antigen, inducing gamma-interferon responses in whole-blood cultures from M.tuberculosis-exposed adults in Uganda and South Africa, indicating this might be a good vaccine candidate.**
Rv1811	**POSSIBLE Mg2+ TRANSPORT P-TYPE ATPASE C MGTC**	**MgtC, MT1859 , O07221_MYCTU, Q7D7X2**	UniProtKB: O07221	Hydrolase	**catalyzes hydrolysis reaction,**	
Rv1854c	**NADH dehydrogenase**	**MT1902 , ndh, ndh-2, P95160_MYCTU, Q7D7W7**	UniProtKB: P95160	Oxidoreductase	**NADH dehydrogenase activity**	**Pathway:** mtu00190 **Oxidative phosphorylation**
Rv2029c		**pfkB**	**Tuberculist** http://t	INVOLVED IN GLYCOLYSIS: CONVERTS SUGAR-1-P TO	ATP + D-fructose-6-	**Pathways:** mtu00010 **Glycolysis / Gluconeogenesis** mtu00030 **Pentose**

Gene	Full Name	Synonyms	Database	Function	Catalytic Activity	Pathway & Miscellaneous
			ubercu list.epf l.ch/qu icksea rch.ph p?gen e+nam e=Rv2 029c& submit =Sear ch	SUGAR-1,6-P [CATALYTIC ACTIVITY: ATP + D-FRUCTOSE 6-PHOSPHATE = ADP + D-FRUCTOSE 1,6-BISPHOSPHATE].	phosphate → ADP + fructose-1,6-bisphosphate + H+	**phosphate pathway** mtu00051 **Fructose and mannose metabolism** mtu00052 **Galactose metabolism** mtu00680 **Methane metabolism** mtu01100 **Metabolic pathways** mtu01110 **Biosynthesis of secondary metabolites** mtu01120 **Microbial metabolism in diverse environments** homolactic fermentation glycolysis III glycolysis I glycolysis II
Rv2380c	**PEPTIDE SYNTHETASE MBTE (PEPTIDE SYNTHASE)**	**mbtE, O86329_MYCTU**	UniProtKB: O86329	INVOLVED IN THE BIOGENESIS OF THE HYDROXYPHENYLOXAZOLINE-CONTAINING SIDEROPHORE MYCOBACTINS. PROBABLY ACTIVATES THE TWO LYSINE RESIDUES THAT ARE INCORPORATED INTO MYCOBACTIN (LYSINE LIGATION).	**lipid metabolism**	**Pathways:** mtu01053 **Biosynthesis of siderophore group nonribosomal peptides**
Rv2381c	**POLYKETIDE SYNTHETASE MBTD (POLYKETIDE SYNTHASE)**	**mbtD, P71719_MYCTU**	UniProtKB: P71719	INVOLVED IN THE BIOGENESIS OF THE HYDROXYPHENYLOXAZOLINE-CONTAINING SIDEROPHORE MYCOBACTINS.	a holo-[acp] + malonyl-CoA + H+ → a malonyl-[acp] + coenzyme A	**Pathways:** mtu01053 **Biosynthesis of siderophore group nonribosomal peptides** fatty acid biosynthesis initiation I superpathway of mycolate biosynthesis FAS-I and FAS-II
Rv2383c	**Phenyloxazoline synthase MbtB**	**mbtB, MBTB_MYCTU, MT2451, Q7D788**	UniProtKB: P71717	Involved in the initial steps of the mycobactin biosynthetic pathway. Putatively couples activated salicylic acid with serine or threonine and cyclizes this	ATP + o-succinylbenzoate + coenzyme A → 4-(2'-	**Pathway:** mtu01053 **Biosynthesis of siderophore group nonribosomal peptides** Siderophore biosynthesis; mycobactin biosynthesis. 1,4-dihydroxy-2-naphthoate biosynthesis I

Gene	Full Name	Synonyms	Database	Function	Catalytic Activity	Pathway & Miscellaneous
				precursor to the hydroxyphenyloxazoline ring system present in this class of siderophores. Essential for growth in macrophages. Ref.3 Ref.4	carboxyphenyl)-4-oxobutyryl-CoA + AMP + diphosphate ATP + o-succinylbenzoate + coenzyme A = 4-(2'-carboxyphenyl)-4-oxobutyryl-CoA + ADP + phosphate	
Rv2385	**PUTATIVE ACETYL HYDROLASE MBTJ**	**mbtJ, Q79FE8_MYCTU**	UniProtKB: Q79FE8	INVOLVED IN THE BIOGENESIS OF THE HYDROXYPHENYLOXAZOLINE-CONTAINING SIDEROPHORE MYCOBACTINS. POSSIBLY REQUIRED FOR N-HYDROXYLATION OF THE TWO LYSINE RESIDUES AT SOME STAGE DURING MYCOBACTIN ASSEMBLY.	**acetyl hydrolase**	**Pathway:** mtu00363 **Bisphenol degradation** mtu00627 **Aminobenzoate degradation** mtu01120 **Microbial metabolism in diverse environments**
Rv2503c	**Probable succinyl-CoA:3-ketoacid-coenzyme A transferase subunit B**	**MT2578 , MTCY07A7.09c, O06166, Rv2503c, scoB, SCOB_MYCTU**	UniProtKB: P63650	INVOLVED IN VARIOUS DEGRADATION AND SYNTHESIS	**Succinyl-CoA + a 3-oxo acid = succinate + a 3-oxoacyl-CoA.**	**Pathway:** mtu00072 **Synthesis and degradation of ketone bodies** mtu00280 **Valine, leucine and isoleucine degradation** mtu00650 **Butanoate metabolism**
Rv2713	**Probable soluble pyridine nucleotide**	**MT2786, MTCY05A6.34, O07212, sthA,**	UniProtKB: P66006	Conversion of NADPH, generated by peripheral catabolic pathways, to NADH, which can	**NADPH + NAD^+ = $NADP^+$ + NADH.**	**Pathway:** mtu00760 **Nicotinate and nicotinamide metabolism** mtu01100 **Metabolic pathways**

Gene	*Full Name*	*Synonyms*	*Database*	*Function*	*Catalytic Activity*	*Pathway & Miscellaneous*
	transhydrogenase	**STHA_MYCTU**		enter the respiratory chain for energy generation	HAMAP_MF_00247	
Rv2764c	**Thymidylate synthase**	**TYSY_MYCTU, thyA, Rv2764c , MTV002.29c , MT2834, O33306**	UniProtKB: P67044	Provides the sole de novo source of dTMP for DNA biosynthesis HAMAP MF_00008	**5,10-methylenetetrahydrofolate + dUMP = dihydrofolate + dTMP.** HAMAP_MF_00008	**Pathway** Pyrimidine metabolism; dTTP biosynthesis. HAMAP MF_00008
Rv2930	**Long-chain-fatty-acid--AMP ligase FadD26**	**FAA26_MYCTU, fadD26, MT2999, MTCY338.19,**	UniProtKB: Q10976	Catalyzes the activation of long-chain fatty acids (C22-24 fatty acids) as acyl-adenylates (acyl-AMP), which are then transferred to the multifunctional polyketide synthase PpsA for further chain extension. Involved in the biosynthesis of phthiocerol dimycocerosate (DIM A) and phthiodiolone dimycocerosate (DIM B). Ref.3 Ref.4		**Pathway** Lipid metabolism; fatty acid biosynthesis.
Rv3206c	**Probable adenylyltransferase/sulfurtransferase MoeZ**	**moeB1, moeZ, MOEZ_MYCTU, MT3301 , Q6MWZ9**	UniProtKB: Q7D5X9	Catalyzes the conversion of the sulfur carrier protein CysO to CysO-thiocarboxylate. The reaction is thought to proceed in two steps: first, ATP-dependent activation of CysO as acyl-adenylate (CysO-COOAMP), followed by sulfur transfer to give CysO-thiocarboxylate (CysO-COSH) Probable. The sulfur source is unknown. Ref.4	thiosulfate + hydrogen cyanide → sulfite + thiocyanate + 2 H+	**Pathway:** mtu04122 **Sulfur relay system**

Gene	*Full Name*	*Synonyms*	*Database*	*Function*	*Catalytic Activity*	*Pathway & Miscellaneous*
Rv3774	**Enoyl-CoA hydratase/isomerase family protein**	**ech , echA21, MT3883, P75019_MYCTU, Q79C03, Q7D4W1**	UniProtKB: P75019	COULD POSSIBLY OXIDIZE FATTY ACIDS USING SPECIFIC COMPONENTS	**(3S)-3-HYDROXYACYL-CoA = TRANS-2(OR 3)-ENOYL-CoA + H(2)O**	**Pathway** mtu00071 **Fatty acid metabolism** mtu00280 **Valine, leucine and isoleucine degradation** mtu00281 **Geraniol degradation** mtu00310 **Lysine degradation** mtu00360 **Phenylalanine metabolism** mtu00362 **Benzoate degradation** mtu00380 **Tryptophan metabolism** mtu00410 **beta-Alanine metabolism** mtu00627 **Aminobenzoate degradation** mtu00640 **Propanoate metabolism** mtu00650 **Butanoate metabolism** mtu00903 **Limonene and pinene degradation** mtu00930 **Caprolactam degradation** mtu01100 **Metabolic pathways** mtu01110 **Biosynthesis of secondary metabolites** mtu01120 **Microbial metabolism in diverse environments**

The task of double knockout was done in two steps which are as follows:

1. Finding association of Non-essential genes with other genes, finding correlated genes.
2. Study of double knock out of correlated genes.

(i) Finding association of Non-essential genes with its correlated genes

Steps to find the Correlated genes:

This work can be done in two parts first part is calculation of Flux variability analysis, and second part is extracting the correlated genes from the result set of Flux variability analysis.

Following are the steps of this task.

Flux Variability Analysis calculation (after knocking out selective non-essential genes): Here GSMN-TB was used as a tool to calculate the Flux Variability Analysis again. The working steps are described below in detail:

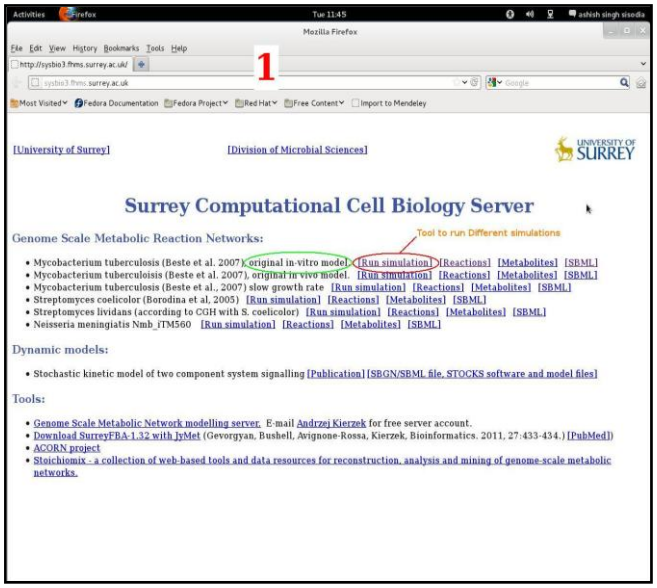


Figure-5

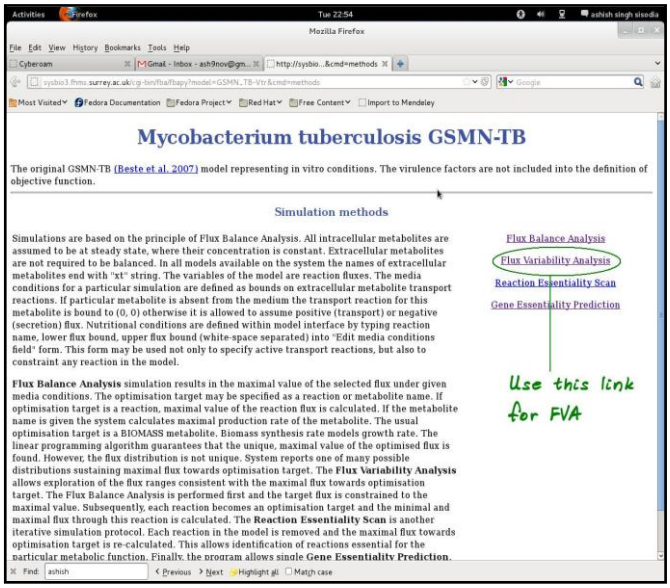


Figure-6

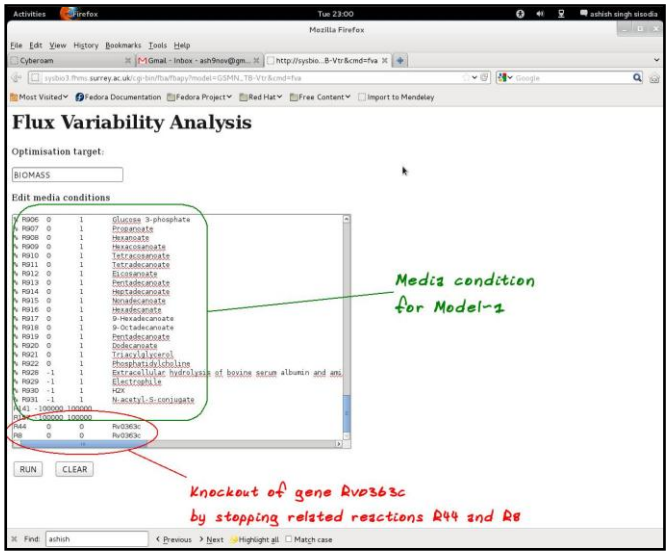


Figure-7

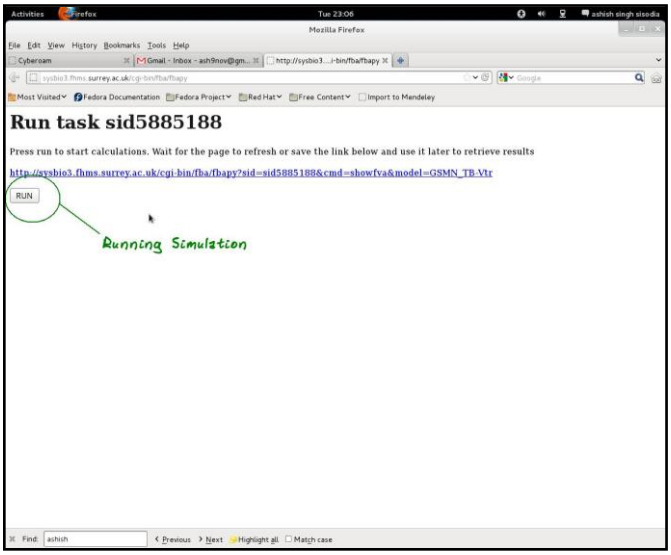
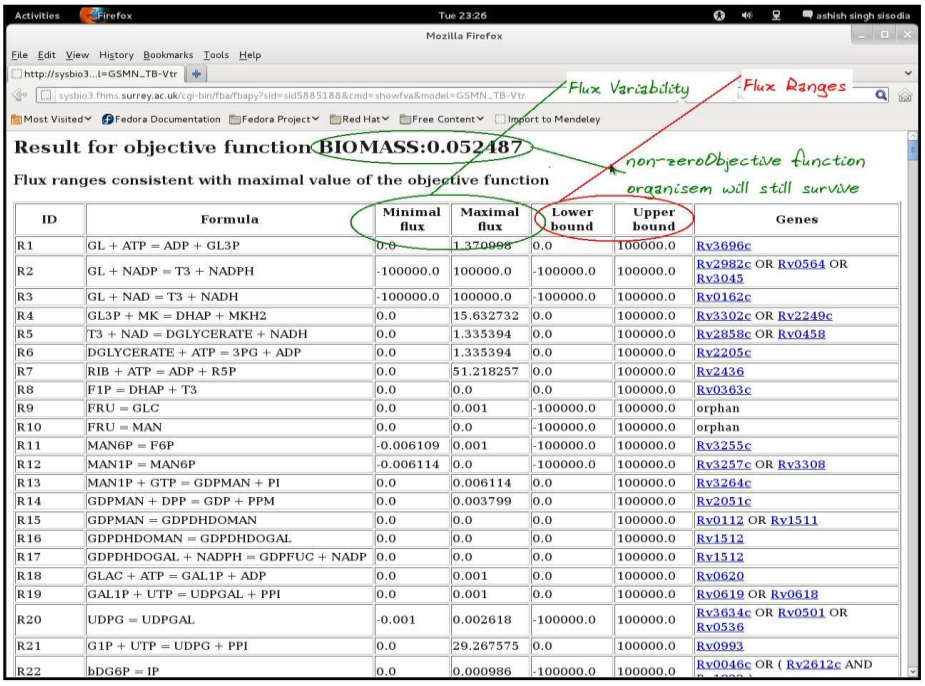


Figure-8

Figure-9



Result for objective function BIOMASS:0.052487

Flux ranges consistent with maximal value of the objective function

ID	Formula	Minimal flux	Maximal flux	Lower bound	Upper bound	Genes
R1	GL + ATP = ADP + GL3P	0.0	1.370998	0.0	100000.0	Rv3696c
R2	GL + NADP = T3 + NADPH	-100000.0	100000.0	-100000.0	100000.0	Rv2982c OR Rv0564 OR Rv3045
R3	GL + NAD = T3 + NADH	-100000.0	100000.0	-100000.0	100000.0	Rv0162c
R4	GL3P + MK = DHAP + MKH2	0.0	15.632732	0.0	100000.0	Rv3302c OR Rv2249c
R5	T3 + NAD = DGLYCERATE + NADH	0.0	1.335394	0.0	100000.0	Rv2858c OR Rv0458
R6	DGLYCERATE + ATP = 3PG + ADP	0.0	1.335394	0.0	100000.0	Rv2205c
R7	RIB + ATP = ADP + R5P	0.0	51.218257	0.0	100000.0	Rv2436
R8	F1P = DHAP + T3	0.0	0.0	0.0	100000.0	Rv0363c
R9	FRU = GLC	0.0	0.001	-100000.0	100000.0	orphan
R10	FRU = MAN	0.0	0.0	-100000.0	100000.0	orphan
R11	MAN6P = F6P	-0.006109	0.001	-100000.0	100000.0	Rv3255c
R12	MAN1P = MAN6P	-0.006114	0.0	-100000.0	100000.0	Rv3257c OR Rv3308
R13	MAN1P + GTP = GDPMAN + PI	0.0	0.006114	0.0	100000.0	Rv3264c
R14	GDPMAN + DPP = GDP + PPM	0.0	0.003799	0.0	100000.0	Rv2051c
R15	GDPMAN = GDPDHDOMAN	0.0	0.0	0.0	100000.0	Rv0112 OR Rv1511
R16	GDPDHDOMAN = GDPDHDOGAL	0.0	0.0	0.0	100000.0	Rv1512
R17	GDPDHDOGAL + NADPH = GDPFUC + NADP	0.0	0.0	0.0	100000.0	Rv1512
R18	GLAC + ATP = GAL1P + ADP	0.0	0.001	0.0	100000.0	Rv0620
R19	GAL1P + UTP = UDPGAL + PPI	0.0	0.001	0.0	100000.0	Rv0619 OR Rv0618
R20	UDPG = UDPGAL	-0.001	0.002618	-100000.0	100000.0	Rv3634c OR Rv0501 OR Rv0536
R21	G1P + UTP = UDPG + PPI	0.0	29.267575	0.0	100000.0	Rv0993
R22	bDG6P = IP	0.0	0.000986	-100000.0	100000.0	Rv0046c OR (Rv2612c AND

Steps:

1. Go to the website of GSMN-tb (http://sysbio3.fhms.surrey.ac.uk/) (Fig-5)
2. Select the Run simulation option for in-vitro model of *M. tuberculosis* (Fig-5).
3. In the Next coming web page (http://sysbio3.fhms.surrey.ac.uk/cgi-bin/fba/fbapy?model=GSMN_TB-Vtr&cmd=methods) (Fig-6) out of the listed options select Flux Variability Analysis option ((Fig-6).
4. In the next coming web page (http://sysbio3.fhms.surrey.ac.uk/cgi-bin/fba/fbapy?model=GSMN_TB-Vtr&cmd=fva) , (Figure-7) put the media condition value of model-1(for media condition values of model-1 see above text), then Put the Maximum and Minimum fluxes to Zero of reactions associated to the gene which is needed to be knocked out and run the simulation (Fig-7).
5. In the next coming web page click run button to run the simulation.(Fig-8)
6. The next page is the result page which shows the biomass value and Flux ranges of reactions after knocking off the gene.(Fig-9)

After finding the results generated by flux variability analysis (FVA) after the knockout non essential genes, the steps are followed to find the correlate genes and associated reactions to those genes are listed here.

Steps:

1. Select the Genes column (7^{th} column, Fig-9) and remove all the rows from the result set where this column has **orphan** genes.
2. Now make clusters of the result set on the basis of maximum flux.
3. Take two clusters with the highest and second highest value for the maximum flux (here highest value taken was 100000, and second highest value taken was 222).
4. Select corresponding genes which are coming in these two highest clusters.
5. Make table of Non essential genes with it's corresponding genes found this way.

Plots of Genes Vs Maximum flux (in FVA study):

Here in these plots Y-axes represents all the genes corresponding to all reactions, and the X-axes represents the values of maximum flux corresponding to those reactions , data taken for this plot is from results of flux variability analysis after knocking out the genes Rv0183, Rv0186, Rv0211, Rv0244c, Rv0363c and Rv0467 (Figure-10: a, b, c, d, e, and f).

Figure-10a: gene Rv0183 knockout

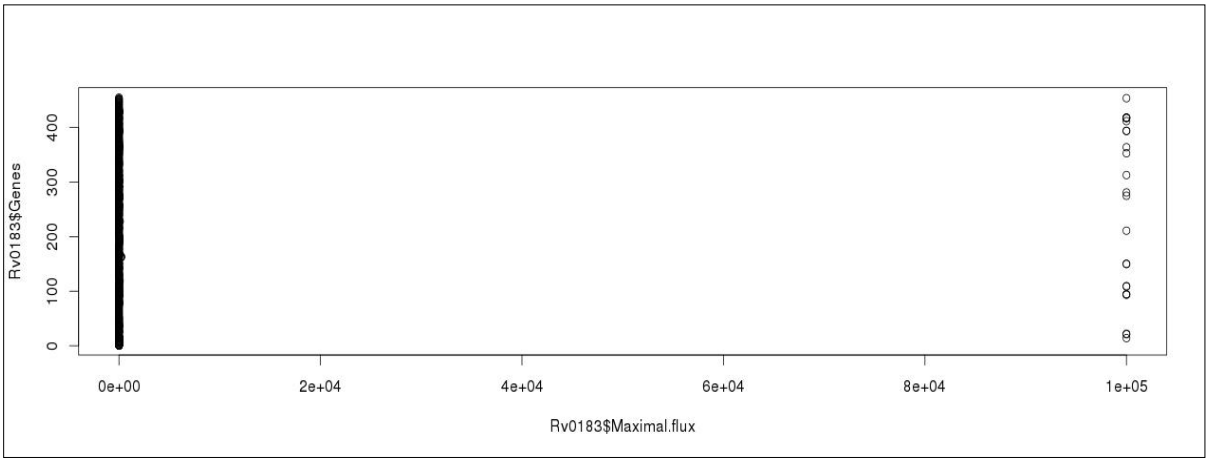


Figure-10b: gene Rv0186 knockout

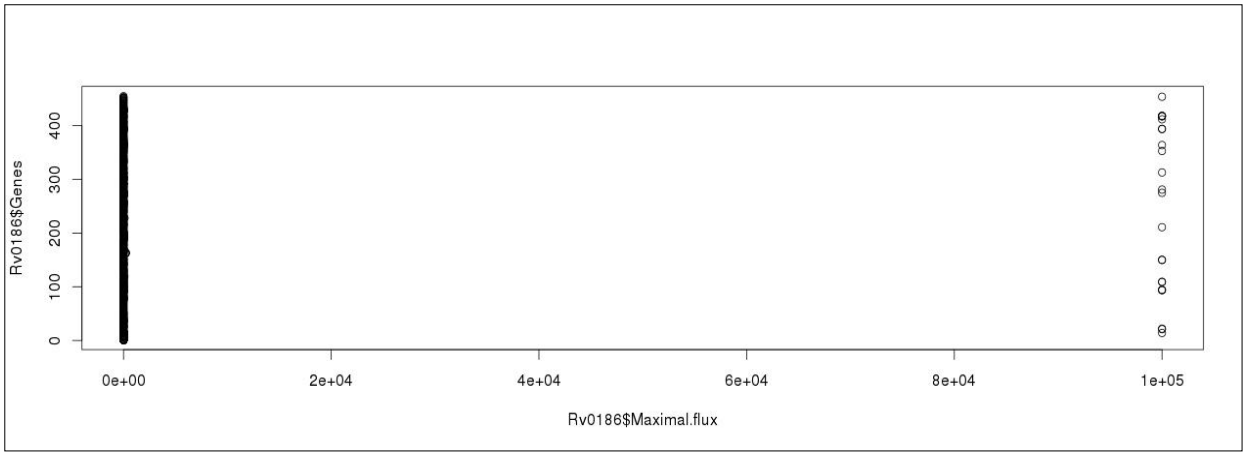


Figure-10c: gene Rv0211 knockout

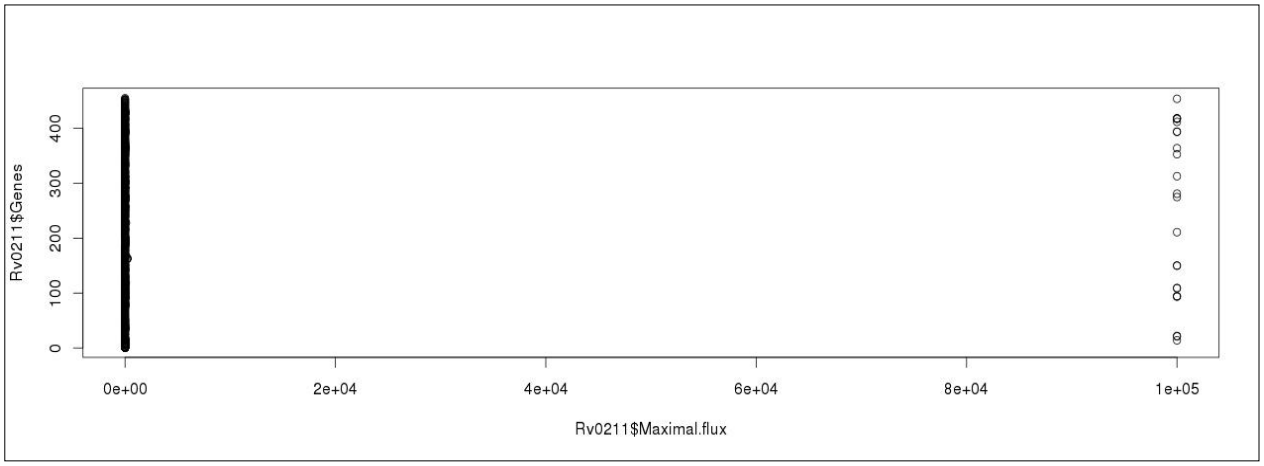


Figure-10d: gene Rv0244c knockout

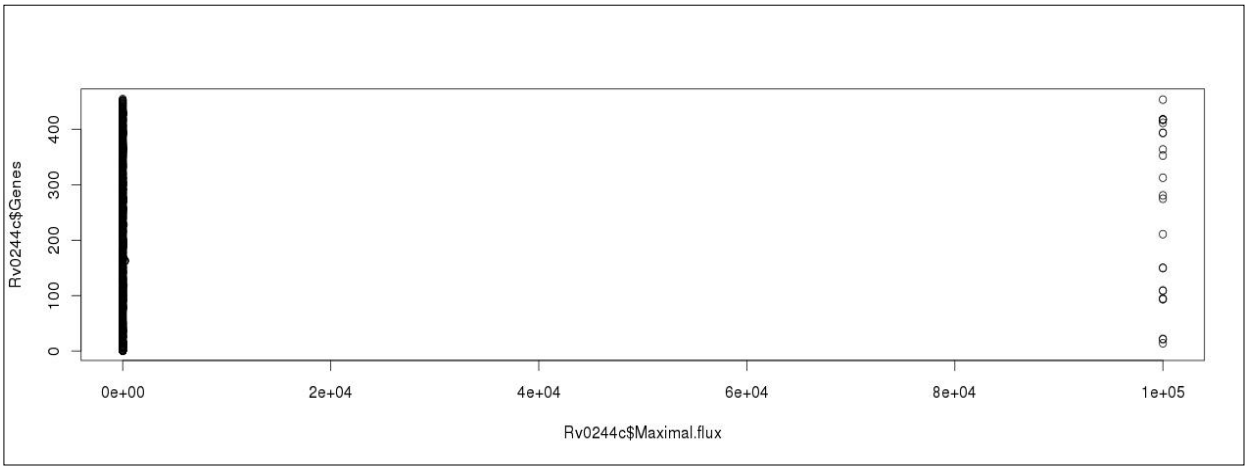


Figure-10e: gene Rv0363c knockout

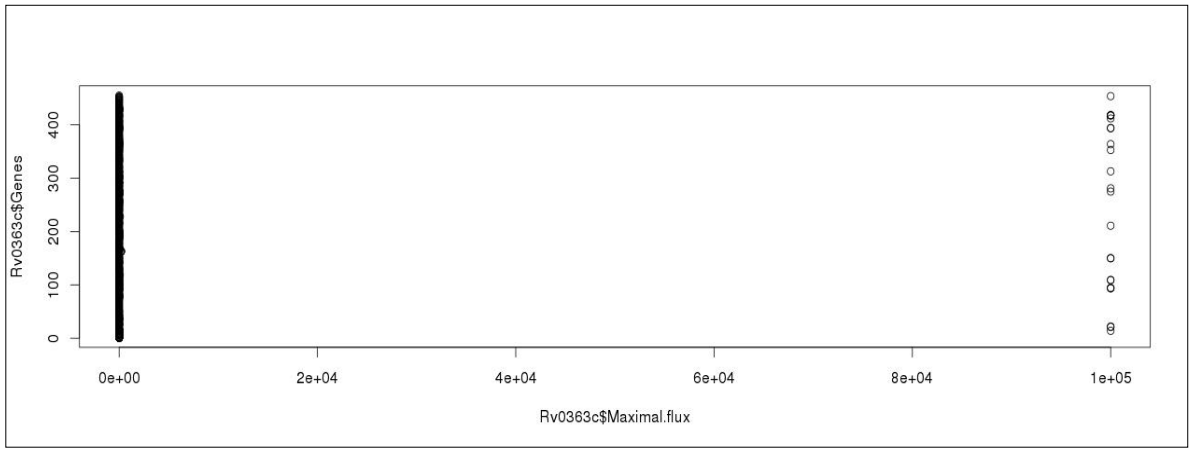
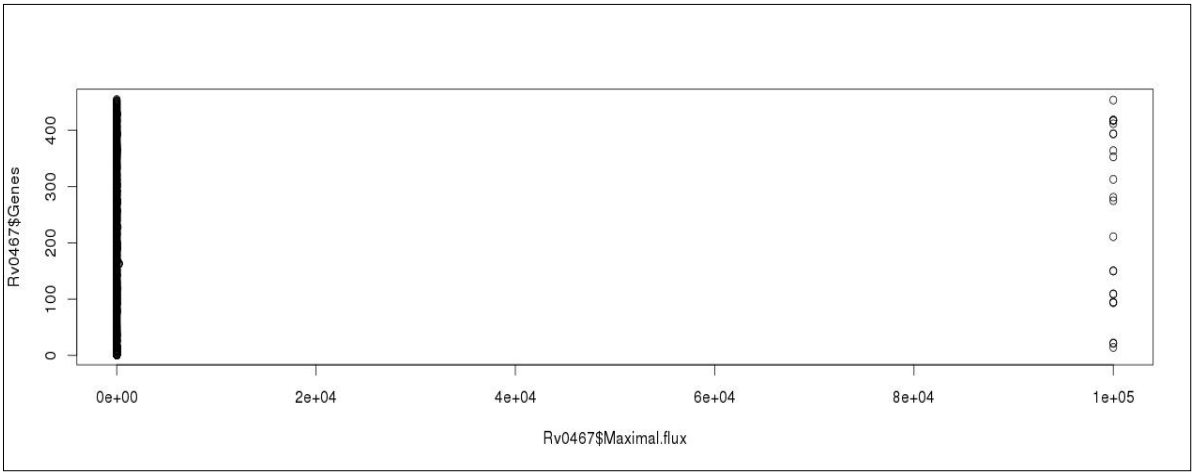


Figure-10f: gene Rv0467 knockout



After clustering genes on basis of maximum flux values, the clusters having highest maximum flux value (right hand side circles) were selected and in these clusters 16 correlated genes for Rv0183, 15 correlated genes for Rv0186, 20 correlated genes for Rv0211, 16 correlated genes for Rv0244c, 17 correlated genes for Rv0363 and 16 correlated genes for Rv0467 were found, which are associated with the reactions having highest maximum flux value (100000.0). This process was repeated for all 23 selected non-essential genes. Collectively 22 different correlated genes were found for all 23 selected non-essential genes. Study of these correlated genes was done and the properties of these genes are as follows:

Essentiality of correlated genes (Model-1):

Essentiality study was done using only model-1, normal bacterial growth medium, for correlated genes as shown in table.

Table 4: The list of 22 genes arrived by correlation, are shown here , as 3 genes are essential and 19 genes are non-essential:

Essential	Non-essential
Rv1389, Rv2445c, Rv1449c	*Rv1079, Rv2713, Rv3303c, Rv0155, Rv0156, Rv0157, Rv1862, Rv1530, Rv0162c, Rv0761c, Rv2476c, Rv2982c, Rv0564, Rv3045, Rv3436c, Rv3565, Rv0337c, Rv3859c, Rv3858c*

Pathway information of Correlated genes:

For each correlated genes pathways were identified, and the data source for pathway information collection were KEGG database (http://www.genome.jp/kegg/) & TB database(http://www.tbdb.org/). All of these genes belong to many different pathways. Metabolic pathway (mtu01100) is used for finding the pathway for all of these correlated genes. Majority of them are involved in Biosynthesis of secondary metabolites, alanine, aspartate and glutamate metabolism and degrading valine, leucine & isoleucine in addition to purine & pyrimidine metabolism

Table 5 : Here we enlists the pathways corresponding to the 22 correlated genes as follows:

Gene	***Pathways***
Rv1079	1. Sulfur metabolism mtu00920 (KEGG pathway ID) 2. Cysteine and methionine metabolism Mtu00270 3. Selenocompound metabolism mtu00450 *4.* Biosynthesis of secondary metabolites mtu01110
Rv2713	1. Nicotinate and nicotinamide metabolism Mtu00760
Rv3303c	1. Glycolysis / Gluconeogenesis Mtu00010

Gene	***Pathways***
	2. Citrate cycle (TCA cycle) mtu00020 3. Glycine, serine and threonine metabolism mtu00260 4. Valine, leucine and isoleucine degradation mtu00280 5. Pyruvate metabolism mtu00620 6. Biosynthesis of secondary metabolites mtu01110 *7.* Microbial metabolism in diverse environments mtu01120
Rv0155, Rv0156, Rv0157	1. Nicotinate and nicotinamide metabolism Mtu00760
Rv1389	1. Purine metabolism Mtu00230
Rv1862, Rv1530, Rv0162c, Rv0761c	1. Glycolysis / Gluconeogenesis Mtu00010 2. Fatty acid metabolism mtu00071 3. Tyrosine metabolism mtu00350 4. Chloroalkane and chloroalkene degradation mtu00625 5. Naphthalene degradation mtu00626 6. Biosynthesis of secondary metabolites mtu01110 *7.* Microbial metabolism in diverse environments mtu01120
Rv2445c	1. Purine metabolism Mtu00230 2. Pyrimidine metabolism mtu00240 *3.* Biosynthesis of secondary metabolites mtu01110
Rv2476c	1. Alanine, aspartate and glutamate metabolism Mtu00250 2. Arginine and proline metabolism mtu00330 3. Taurine and hypotaurine metabolism mtu00430 4. Nitrogen metabolism mtu00910
Rv2982c	*1.* Glycerophospholipid metabolism Mtu00564
Rv0564	1. phospholipid biosynthesis I 2. CDP-diacylglycerol biosynthesis I 3. CDP-diacylglycerol biosynthesis II

Gene	*Pathways*
	4. phosphatidylglycerol biosynthesis I (plastidic) 5. phosphatidylglycerol biosynthesis II (non-plastidic)
Rv3436c, *Rv0337c*	1. Alanine, aspartate and glutamate metabolism Mtu00250 2. Amino sugar and nucleotide sugar metabolism mtu00520 *3.* Biosynthesis of secondary metabolites mtu01110
Rv3565	1. alanine degradation III 2. alanine biosynthesis II *3.* superpathway of alanine biosynthesis
Rv3858c, *Rv3859c*	1. Alanine, aspartate and glutamate metabolism Mtu00250 2. Nitrogen metabolism mtu00910 3. Biosynthesis of secondary metabolites mtu01110 *4.* Microbial metabolism in diverse environments mtu01120
Rv1449c	1. Pentose phosphate pathway Mtu00030 2. Biosynthesis of secondary metabolites mtu01110 **3.** Microbial metabolism in diverse environments mtu01120

Results of double knock out of genes under normal growth (Model-1)

After identification of correlated genes to the selected non-essential genes, paired combination of non-essential genes was made with its correlated genes, and knock-out of this pair was done to identify the pair which is essential for the survival of the organism.
Steps involved in double knock-out study are as follows:

1. Select the Genes column (7^{th} column) and remove all the rows from the the result set where this column has **orphan** genes.
2. Now make clusters of the result set on the basis of maximum flux.
3. Take two clusters with the highest and second highest value for the maximum flux

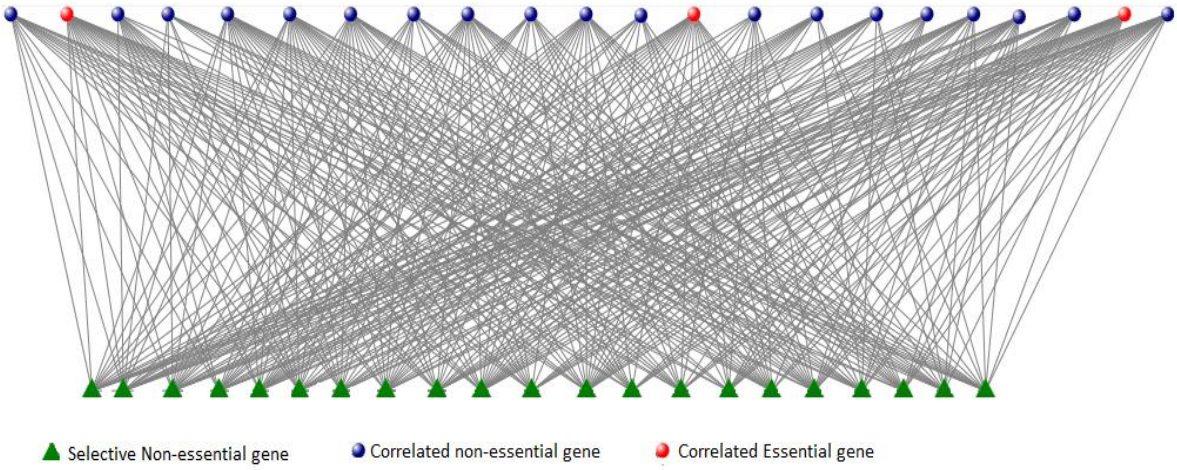
(here highest value taken was 100000, and second highest value taken was 222).

4. Select corresponding genes which are coming in these two highest clusters.
5. Find the reactions corresponding to those genes (at http://sysbio3.fhms.surrey.ac.uk/cgi-bin/fba/fbapy?model=GSMN_TB-Vtr&cmd=showmodel).
6. To knock out both non essential and correlated gene, set the lower and upper bound of the corresponding reaction to Zero(example: R45 0 0).
7. Append these parameters with the media conditions of model 1.
8. Then Run the FVA simulation for this new media condition(check figure 1-5 for FVA steps).
9. Check the biomass value of result, whether it is Zero or Non Zero.
10. If the biomass value is Zero, then it tells that this combination of genes is essential for organism. Pick the genes corresponding to this result.

3.9 Results and Discussion:

The double knockout study was done on 23 remaining genes. Out of these 23 genes, only 21 genes were successfully simulated for the FVA of double knock out of these non-essential genes with its correlated genes. Each of these 21 non-essential genes paired up with all of its identified correlated genes for double knockout (after removals of redundancy only 22 genes were identified). Here out of all 22 correlated genes, 3 genes (all are essential genes), Rv1389 (Purine metabolism pathways), Rv2445c (Purine metabolism pathways, Pyrimidine metabolism pathways, pathways of Biosynthesis of secondary metabolites) and Rv1449c (Pentose phosphate pathway, pathways for Biosynthesis of secondary metabolites, Microbial metabolism in diverse environments) were correlated to all the 21 selected non-essential genes. The double knock-outs of the selected non-essential genes with each of these three genes were producing zero bio-mass because all these three genes were found to be essential for the organism's survival. So, knocking out these genes, alone or with any essential or non-essential genes will kill the organism. This is vindicated from our simulation results.

Fig-11 Shows the network of the 21 non-essential genes(green triangle) and 22 correlated genes sets (three essential genes are connected to all the 21 genes displayed by edges)



From the data (appendix) shows that maximum connectivity is for the gene *Rv2383c(edge =20)* and minimum is 15 for *Rv2381c, Rv0363c, Rv0467.* Hence our finding signifies that the non –essential genes are highly connected among themselves and with the essential genes , hence not to be ignored as drug target identification.

3.10 Conclusions:

Here it is illustrated how to find correlated gene set driven by Flux Variability analysis. A set of 21 non-essential genes were studied using this method and identified three essential genes and 19 non essential correlated(by maximum flux) genes. Further study revels that two of these correlated non-essential genes, Rv3565 (alanine bio-synthesis and degradation pathways) and Rv0337c (Alanine, aspartate and glutamate metabolism, Valine, leucine and isoleucine biosynthesis, Biosynthesis of secondary metabolites) are found to be correlated with 20 out of 21 already identified as non-essential genes (Table 5), when knockout synchronously are also producing zero biomass(fig-12). Here we show that three non-essential genes while in combination with one another develop new properties(**the reasons yet to be identified**) behave like an essential gene for organism to survive because deletion of all the three will kill the organism as shown here by *in silico* study. This finding may be validated by future experiments.

3.11 Future Work:

As mentioned above finding combination like the list furnished in table 2 will open up many new ways of combating the bacteria under normal growth. Repeating the same using other three models will highlight more pathway and their interactions in combination of gene deletion. It will be very informative to find the real connectivity between the three combination genes which requires detail study of the reactants and the pathways.

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Gene Properties

The properties of genes which were differently expressed during the persistence (in Hypoxia condition) are illustrated here in tabular form. The information regarding differently expressed genes were taken from database **MTBreg**. This database contains the list of differently expressed genes of M.tb in a variety of experimental conditions (Kaufmann 2004). On the basis of environmental condition, encountered by persistent M.tb, the gene which are differently expressed under following conditions:

(1) *Hypoxia condition:* - All the genes from all the literature sources reporting microarray experiments under hypoxic condition, as provided in MTBreg database were selected (Sherman, Voskuil et al. 2001), (Bacon, James et al. 2004), (Voskuil, Visconti et al. 2004), (Muttucumaru, Roberts et al. 2004), (Rosenkrands, Slayden et al. 2002), (Starck, Kallenius et al. 2004). the resultant list of genes included some genes,which were like ribosome binding proteins, unwell characterized proteins, hypothetical proteins, transposases, etc. These genes were not directly related to the metabolic reactions, so these were excluded form the final list.

(2) *Nutrient starvation and source dependent condition:* – Genes were selected from the work of Schoolnik and co-workers (Schnappinger, Ehrt et al. 2003), fulfilling the above criteria.

Resultant gene list was further reduced by removing those that had no corresponding biochemical reaction in GSMN model. Absence of a reaction for a gene may indicate that it does not catalyze any reaction but could be a transcription factor or a regulator, for example. Thus, the final gene list reduced to 100 of which, 58 genes from the privious work (“metabolic control analysis of biochemical pathways as an approach to in silico identification and validation of anti- tuberculous, anti-malarial and anti-diabetic drug targets”, chapter- 3.4-”Constraint-based genome-scale metabolic network model of persistent M.tb ” , Vivek kumar singh, 2009), and rest 42 are the newly found gene (due to database updates and newly found genes more genes in to the hit list). Detailed table is illustrated below.

information sources:
http://www.geneontology.org/
http://www.uniprot.org
http://tuberculist.epfl.ch/

Table-1: Properties of 100 selected genes.

Gene	*Full Name*	*Synonyms*	*Database*	*Function*	*Catalytic Activity*	*Pathway & Miscellaneous*
Rv0046c	**Inositol-3-phosphate synthase**	**ino1 , INO1_MYCTU, MT0052 , MTCY21D4.09c**	UniProtKB:P71703	**Catalyzes the conversion of glucose 6-phosphate to 1D-myo-inositol 3-phosphate**	**D-glucose 6-phosphate = 1D-myo-inositol 3-phosphate**	**Was identified as a natural substrate of the *M.tuberculosis* proteasome.**
Rv0070c	**Pyridoxal-phosphate-dependent serine hydroxymethyltransferase 2**	**glyA2 , GLYA2_MYCTU , MT0076 , MTV030.13c**	UniProtKB:O53615	**Catalyzes the reversible interconversion of serine and glycine with tetrahydrofolate serving as the one-carbon carrier**	**5,10-methylenetetrahydrofolate + glycine + H_2O = tetrahydrofolate + L-serine.** HAMAP MF_00051	
Rv0112	**GDP-D-mannose dehydratase, putative**	**gca, MT0121, O53634_MYCTU,**	UniProtKB:O53634	GDP-mannose 4,6-dehydratase activity		

Gene	Full Name	Synonyms	Database	Function	Catalytic Activity	Pathway & Miscellaneous
		Q7DAG5		coenzyme binding nucleotide binding oxidoreductase activity		
Rv0183	**POSSIBLE LYSOPHOSPHOLIPASE**	**O07427_MYCTU**	UniProtKB:O07427	acylglycerol lipase activity		
Rv0186	**PROBABLE BETA-GLUCOSIDASE BGLS (GENTIOBIASE) (CELLOBIASE) (BETA-D-GLUCOSIDE GLUCOHYDROLASE)**	**bglS , MT0195 , O07430_MYCTU , Q7DAB2**	UniProtKB:O07430	Glycosidase		
Rv0211	**Phosphoenolpyruvate carboxykinase [GTP]**	**MT0221 MTCY08D5.06 P96393 pck1 pckA pckG PCKG_MYCTU**	UniProtKB:P65686	**Catalyzes the conversion of oxaloacetate (OAA) to phosphoenolpyruvate (PEP), the rate-limiting step in the metabolic pathway that produces glucose from lactate and other precursors derived from the citric acid cycle**	**GTP + oxaloacetate = GDP + phosphoenolpyruvate + CO_2.** HAMAP MF_00452	**Pathway=** Carbohydrate biosynthesis; gluconeogenesis
Rv0244c	**PROBABLE ACYL-CoA DEHYDROGENASE FADE5**	**fadE5, MT0258, O53666_MYCTU, Q7DA67**	UniProtKB:O53666	acyl-CoA dehydrogenase activity flavin adenine dinucleotide binding		**Belongs to the** acyl-CoA dehydrogenase family
Rv0363c	**Fructose-bisphosphate aldolase**	**ALF_MYCTU, fba, MT0379, MTCY13E10.25c, O06313**	UniProtKB:P67475	**Catalyzes the aldol condensation of dihydroxyacetone phosphate (DHAP or glycerone-phosphate) with glyceraldehyde 3-phosphate (G3P) to form fructose 1,6-bisphosphate (FBP) in gluconeogenesis and the reverse reaction in glycolysis**	**D-fructose 1,6-bisphosphate = glycerone phosphate + D-glyceraldehyde 3-phosphate.**	**Was identified as a high-confidence drug target.** **Pathway=** Carbohydrate degradation; glycolysis; D-glyceraldehyde 3-phosphate and glycerone phosphate from D-glucose: step 4/4.
Rv0404	**Long-chain-fatty-acid--AMP ligase**	**FAA30_MYCTU, fadD30,**	UniProtKB:P9	**Catalyzes the activation of long-chain fatty acids as acyl-adenylates (acyl-AMP), which are**		**Pathway=** Lipid

Gene	Full Name	Synonyms	Database	Function	Catalytic Activity	Pathway & Miscellaneous
	FadD30	**MT0417, Q7D9V7**	5213	**then transferred to the multifunctional polyketide synthase (PKS) for further chain extension**		metabolism; fatty acid biosynthesis.
Rv0467	**Isocitrate lyase**	**ACEA_MYCTU icl MT0483 MTV038.11 O53752**	UniProtKB:P0A5H3	**Catalyzes the formation of succinate and glyoxylate from isocitrate, a key step of the glyoxylate cycle. May be involved in the assimilation of one-carbon compounds via the isocitrate lyase-positive serine pathway**	**Isocitrate = succinate + glyoxylate.**	**Pathway** Carbohydrate metabolism; glyoxylate cycle; (S)-malate from isocitrate: step 1/2. **Was identified as a natural substrate of the M.tuberculosis proteasome.**
Rv0503c	**Cyclopropane mycolic acid synthase 2**	**cma2 cmaA2 CMAS-2 CMAS2_MYCTU MT0524 MTCY20G9.30c Q11196**	UniProtKB:P0A5P0	**Catalyzes the formation of trans cyclopropanated ketomycolate or methoxymycolate through the conversion of a double bond to a cyclopropane ring at the proximal position of an oxygenated mycolic acid via the transfer of a methylene group from S-adenosyl-L-methionine. In the absence of MmaA2, CmaA2 has a non-specific cis-cyclopropanating activity and is able to catalyze the conversion of a double bond to a cis cyclopropane ring at the distal position of an alpha mycolic acid. Cyclopropanated mycolic acids are key factors participating in cell envelope permeability, host immunomodulation and persistence.**	**S-adenosyl-L-methionine + phospholipid olefinic fatty acid = S-adenosyl-L-homocysteine + phospholipid cyclopropane fatty acid.**	**Pathway** Lipid metabolism; mycolic acid biosynthesis. **Was identified as a high-confidence drug target.**
Rv0619		**galTb**		**INVOLVED IN GALACTOSE METABOLISM (LELOIR PATHWAY**	**UTP + ALPHA-D-GALACTOSE 1-PHOSPHATE = DIPHOSPHATE + UDP-GALACTOSE**	
Rv0753c	**PROBABLE METHYLMALONATE-SEMIALDEHYDE DEHYDROGENASE MMSA (METHYLMALONIC ACID SEMIALDE**	**mmsA** **O53816_MYCTU**	UniProtKB:O53816	methylmalonate-semialdehyde dehydrogenase (acylating) activity		

Gene	Full Name	Synonyms	Database	Function	Catalytic Activity	Pathway & Miscellaneous
	HYDE DEHYDROGENASE) (MMSDH)					
Rv0780	**Phosphoribosylaminoimidazole-succinocarboxamide synthase**	**MT0804, MTCY369.24, P77904, PUR7_MYCTU, purC, Q59566**	UniProtKB:P0A5T4	Ligase ATP binding phosphoribosylaminoimidazolesuccinocarboxamide synthase activity	**ATP + 5-amino-1-(5-phospho-D-ribosyl)imidazole-4-carboxylate + L-aspartate = ADP + phosphate + (S)-2-(5-amino-1-(5-phospho-D-ribosyl)imidazole-4-carboxamido)succinate.** HAMAP MF_00137	
Rv0809	**Phosphoribosylformylglycinamidine cyclo-ligase**	**MT0830 O53823_MYCTU purM Q7D990**	UniProtKB:O53823		**ATP + 2-(formamido)-N(1)-(5-phospho-D-ribosyl)acetamidine = ADP + phosphate + 5-amino-1-(5-phospho-D-ribosyl)imidazole.** SAAS SAAS004733 RuleBase RU004370	**Pathway** Purine metabolism; IMP biosynthesis via de novo pathway; 5-amino-1-(5-phospho-D-ribosyl)imidazole from N(2)-formyl-N(1)-(5-phospho-D-ribosyl)glycinamide: step 2/2. SAAS SAAS004733 RuleBase RU004371
Rv0886	**Probable ferredoxin/ferredoxin--NADP reductase**	**fprB , FPRB_MYCTU, MT0909 , MTCY31.14, Q10547**	UniProtKB:P65528	Oxidoreductase	**2 reduced ferredoxin + $NADP^+$ + H^+ = 2 oxidized ferredoxin + NADPH.**	**Cofactor= Binds 1 or 2 4Fe-4S clusters.** **FAD.**
Rv0951	**Succinyl-CoA ligase [ADP-forming] subunit beta**	**MT0978 , MTCY10D7.23c, sucC , SUCC_MYCTU**	UniProtKB:P71559	Ligase	**ATP + succinate + CoA = ADP + phosphate + succinyl-CoA.** HAMAP MF_00558	**Pathway** Carbohydrate metabolism; tricarboxylic acid cycle;

Gene	Full Name	Synonyms	Database	Function	Catalytic Activity	Pathway & Miscellaneous
						succinate from succinyl-CoA (ligase route): step 1/1. HAMAP MF_00558
Rv0973c	**PROBABLE ACETYL-/PROPIONYL-COENZYME A CARBOXYLASE ALPHA CHAIN (ALPHA SUBUNIT) ACCA2: BIOTIN CARBOXYLASE + BIOTIN CARBOXYL CARRIER PROTEIN (BCCP)**	**AccA2, bccA-1, MT1001, P71538_MYCTU, Q7D917**	UniProtKB:P71538	Ligase		
Rv0974c	**PROBABLE ACETYL-/PROPIONYL-CoA CARBOXYLASE (BETA SUBUNIT) ACCD2**	**AccD2, O86318_MYCTU**	UniProtKB:O86318	Ligase		
Rv1144	**Oxidoreductase, short-chain dehydrogenase/reductase family**	**MT1177 , O06544_MYCTU, Q7D8R8**	UniProtKB:O06544	Oxidoreductase		
Rv1285	**Sulfate adenylyltransferase subunit 2**	**cysD CYSD_MYCTU MT1323 MTCY373.04 Q10599**	UniProtKB:P65670	Nucleotidyltransferase Transferase	**ATP + sulfate = diphosphate + adenylyl sulfate.** HAMAP MF_00064	**Pathway** Sulfur metabolism; hydrogen sulfide biosynthesis; sulfite from sulfate: step 1/3. HAMAP MF_00064

Gene	Full Name	Synonyms	Database	Function	Catalytic Activity	Pathway & Miscellaneous
						Was identified as a high-confidence drug target. HAMAP MF_00064
Rv1348	**Iron import ATP-binding/permease protein IrtA**	**IrtA, IRTA_MYCTU, MT1390, MTCY02B10.12, Q11018**	UniProtKB:P63391	**Part of the ABC transporter complex IrtAB involved in iron import. Transmembrane domains (TMD) form a pore in the membrane and the ATP-binding domain (NBD) is responsible for energy generation. Required for replication in human macrophages and in mouse lungs.** Ref.4 Ref.6		**Caution:** Ref.5 **reports that IrtA is a siderophore exporter, however this activity could be due to functional differences of IrtA in the molecular context of M.smegmatis and M.tuberculosis.**
Rv1464	**Probable cysteine desulfurase**	**CSD_MYCTU, csd, MTV007.11, MT1511, O53155**	UniProtKB:P63516	**Catalyzes the removal of elemental sulfur and selenium atoms from L-cysteine, L-cystine, L-selenocysteine, and L-selenocystine to produce L-alanine**	**L-cysteine + acceptor = L-alanine + S-sulfanyl-acceptor.**	**Was identified as a high-confidence drug target.**
Rv1475c	**Aconitate hydratase**	**acn, acnA, MT1522, O53166_MYCTU, Q7D8D8**	UniProtKB:O53166	Lyase		
Rv1500						
Rv1525		**wbbL2**		**POSSIBLY INVOLVED IN CELL WALL ARABINOGALACTAN LINKER FORMATION: USES DTDP-L-RHAMNOSE AS SUBSTRATE TO INSERT THE RHAMNOSYL RESIDUE INTO THE CELL WALL.**		
Rv1553		**frdB**		**INVOLVED IN INTERCONVERSION OF FUMARATE AND SUCCINATE (ANAEROBIC RESPIRATION)**	**SUCCINATE + ACCEPTOR = FUMARATE + REDUCED ACCEPTOR**	
Rv1623c		**cydA**		**INVOLVED IN THE RESPIRATORY CHAIN (AT THE TERMINAL STEP): AEROBIC RESPIRATION. CYTOCHROME D TERMINAL OXIDASE COMPLEX IS THE COMPONENT OF THE**	**UBIQUINOL-8 + O(2) = UBIQUINONE-8 + H(2)O**	

Gene	Full Name	Synonyms	Database	Function	Catalytic Activity	Pathway & Miscellaneous
				AEROBIC RESPIRATORY CHAIN THAT IS SUPPOSEDLY PREDOMINANT WHEN CELLS ARE GROWN AT LOW AERATION .		
Rv1736c	**Nitrate reductase-like protein narX**	**MT1778, narX, NARX_MYCTU, Q7D821**	UniProtKB:P71994	**Does not seem to have nitrate reductase activity.**	**Nitrite + acceptor = nitrate + reduced acceptor.**	***Biotechnological use:*** **This protein serves as an immunogenic antigen, inducing gamma-interferon responses in whole-blood cultures from M.tuberculosis-exposed adults in Uganda and South Africa, indicating this might be a good vaccine candidate.**
Rv1811	**POSSIBLE Mg2+ TRANSPORT P-TYPE ATPASE C MGTC**	**MgtC, MT1859 , O07221_MYCTU, Q7D7X2**	UniProtKB:O07221	Hydrolase		
Rv1832	**Probable glycine dehydrogenase [decarboxylating]**	**GCSP_MYCTU, gcvB, gcvP, MT1880, MTCY1A11.11c**	UniProtKB:Q50601	**The glycine cleavage system catalyzes the degradation of glycine. The P protein binds the alpha-amino group of glycine through its pyridoxal phosphate cofactor; CO_2 is released and the remaining methylamine moiety is then transferred to the lipoamide cofactor of the H protein**	**Glycine + H-protein-lipoyllysine = H-protein-S-aminomethyldihydrolipoyllysine + CO_2.** HAMAP MF_00711	
Rv1854c	**NADH dehydrogenase**	**MT1902 , ndh, ndh-2, P95160_MYCTU, Q7D7W7**	UniProtKB:P95160	Oxidoreductase		
Rv2006	**Uncharacterized glycosyl hydrolase Rv2006/MT2062**	**MT2062 , MTCY39.11c, Y2006_MYCTU**	UniProtKB:Q10850	**A member of the dormancy regulon. Induced in response to reduced oxygen tension (hypoxia), low levels of nitric oxide (NO) and carbon monoxide (CO). It is hoped that this regulon will give insight into the latent, or dormant phase of infection.** Ref.4 Ref.5 Ref.6		***Biotechnological use:*** **This protein serves as an immunogenic antigen, inducing gamma-interferon responses in whole-blood cultures from M.tuberculosis-exposed adults in Uganda, The Gambia and South Africa, indicating this might be a good vaccine candidate.** ***Caution:*** **Despite its similarity with the trehalose-phosphate phosphatase enzymes, it does not display trehalose-phosphate phosphatase activity.**

Gene	Full Name	Synonyms	Database	Function	Catalytic Activity	Pathway & Miscellaneous
Rv2029c		**pfkB**	**Tuberculist** http://tuberculist.epfl.ch/quicksearch.php?gene+name=Rv2029c&submit=Search	**INVOLVED IN GLYCOLYSIS: CONVERTS SUGAR-1-P TO SUGAR-1,6-P [CATALYTIC ACTIVITY: ATP + D-FRUCTOSE 6-PHOSPHATE = ADP + D-FRUCTOSE 1,6-BISPHOSPHATE].**		
Rv2121c	**ATP phosphoribosyltransferase**	**HIS1_MYCTU hisG, MT2181, MTCY261.17c, O33256**	UniProtKB:P60759	**Catalyzes the condensation of ATP and 5-phosphoribose 1-diphosphate to form N'-(5'-phosphoribosyl)-ATP (PR-ATP). Has a crucial role in the pathway because the rate of histidine biosynthesis seems to be controlled primarily by regulation of HisG enzymatic activity**	**1-(5-phospho-D-ribosyl)-ATP + diphosphate = ATP + 5-phospho-alpha-D-ribose 1-diphosphate.** HAMAP MF_00079	**Pathway:** Amino-acid biosynthesis; L-histidine biosynthesis; L-histidine from 5-phospho-alpha-D-ribose 1-diphosphate: step 1/9. HAMAP MF_00079
Rv2225	**3-methyl-2-oxobutanoate hydroxymethyltransferase**	**PANB_MYCTU panB MTCY427.06 MT2284 Q10505**	UniProtKB:P0A5Q8	**Catalyzes the reversible reaction in which hydroxymethyl group from 5,10-methylenetetrahydrofolate is tranferred onto alpha-ketoisovalerate to form ketopantoate.** Ref.3	**5,10-methylenetetrahydrofolate + 3-methyl-2-oxobutanoate + H_2O = tetrahydrofolate + 2-dehydropantoate.** Ref.3	**Was identified as a natural substrate of the M.tuberculosis proteasome.** **Pathway:** Cofactor biosynthesis; (R)-pantothenate biosynthesis; (R)-pantoate from 3-methyl-2-oxobutanoate: step 1/2. HAMAP MF_00156
Rv2246	**3-oxoacyl-[acyl-carrier-**	**FAB2_MYCTU,**	UniPro	**Catalyzes the condensation reaction of fatty acid synthesis by**	**Acyl-[acyl-carrier-protein] + malonyl-**	**Pathway:** Lipid

Gene	Full Name	Synonyms	Database	Function	Catalytic Activity	Pathway & Miscellaneous
	protein] synthase 2	kasB, MT2306, MTCY427.27, Q10525	tKB:P63456	the addition to an acyl acceptor of two carbons from malonyl-ACP	[acyl-carrier-protein] = 3-oxoacyl-[acyl-carrier-protein] + CO_2 + [acyl-carrier-protein].	metabolism; fatty acid biosynthesis.
Rv2380c	PEPTIDE SYNTHETASE MBTE (PEPTIDE SYNTHASE)	mbtE, O86329_MYCTU	UniProtKB:O86329	INVOLVED IN THE BIOGENESIS OF THE HYDROXYPHENYLOXAZOLINE-CONTAINING SIDEROPHORE MYCOBACTINS. PROBABLY ACTIVATES THE TWO LYSINE RESIDUES THAT ARE INCORPORATED INTO MYCOBACTIN (LYSINE LIGATION).		
Rv2381c	POLYKETIDE SYNTHETASE MBTD (POLYKETIDE SYNTHASE)	mbtD, P71719_MYCTU	UniProtKB:P71719	INVOLVED IN THE BIOGENESIS OF THE HYDROXYPHENYLOXAZOLINE-CONTAINING SIDEROPHORE MYCOBACTINS.		
Rv2383c	Phenyloxazoline synthase MbtB	mbtB, MBTB_MYCTU, MT2451, Q7D788	UniProtKB:P71717	Involved in the initial steps of the mycobactin biosynthetic pathway. Putatively couples activated salicylic acid with serine or threonine and cyclizes this precursor to the hydroxyphenyloxazoline ring system present in this class of siderophores. Essential for growth in macrophages. Ref.3 Ref.4		**Pathway:** Siderophore biosynthesis; mycobactin biosynthesis.
Rv2385	PUTATIVE ACETYL HYDROLASE MBTJ	mbtJ, Q79FE8_MYCTU	UniProtKB:Q79FE8	INVOLVED IN THE BIOGENESIS OF THE HYDROXYPHENYLOXAZOLINE-CONTAINING SIDEROPHORE MYCOBACTINS. POSSIBLY REQUIRED FOR N-HYDROXYLATION OF THE TWO LYSINE RESIDUES AT SOME STAGE DURING MYCOBACTIN ASSEMBLY.		
Rv2386c	Isochorismate synthase/isochorismate-pyruvate lyase mbtI	mbtI, MBTI_MYCTU, MT2454, Q79FE7, trpE2	UniProtKB:Q7D785	Mediates the production of salicylate from chorismate via an isochorismate intermediate. Presents both isochorismate synthase and isochorismate-pyruvate lyase activities. Salycilate is the starter unit in the production of the virulence-conferring salicylate-based siderophore mycobactin. Ref.5	Chorismate = isochorismate. Ref.5	**Pathway:** Siderophore biosynthesis; mycobactin biosynthesis.

Gene	*Full Name*	*Synonyms*	*Database*	*Function*	*Catalytic Activity*	*Pathway & Miscellaneous*
Rv2482c	**Glycerol-3-phosphate acyltransferase**	**MT2555, MTV008.38c, plsB, plsB2, PLSB_MYCTU**	UniProtKB:O53207	**INVOLVED IN PHOSPHOLIPID BIOSYNTHESIS (AT THE FIRST STEP). MAY ALSO FUNCTION IN THE REGULATION OF MEMBRANE BIOGENESIS**	**Acyl-CoA + sn-glycerol 3-phosphate = CoA + 1-acyl-sn-glycerol 3-phosphate.** HAMAP MF_00393	**Pathway** Phospholipid metabolism; CDP-diacylglycerol biosynthesis; CDP-diacylglycerol from sn-glycerol 3-phosphate: step 1/3. HAMAP MF_00393
Rv2503c	**Probable succinyl-CoA:3-ketoacid-coenzyme A transferase subunit B**	**MT2578 , MTCY07A7.09c, O06166, Rv2503c, scoB, SCOB_MYCTU**	UniProtKB:P63650	**INVOLVED IN VARIOUS DEGRADATION AND SYNTHESIS**	**Succinyl-CoA + a 3-oxo acid = succinate + a 3-oxoacyl-CoA.**	
Rv2713	**Probable soluble pyridine nucleotide transhydrogenase**	**MT2786, MTCY05A6.34, O07212, sthA, STHA_MYCTU**	UniProtKB:P66006	**Conversion of NADPH, generated by peripheral catabolic pathways, to NADH, which can enter the respiratory chain for energy generation**	**NADPH + NAD^+ = $NADP^+$ + NADH.** HAMAP MF_00247	
Rv2764c	**Thymidylate synthase**	**TYSY_MYCTU, thyA, Rv2764c , MTV002.29c, MT2834, O33306**	UniProtKB:P67044	**Provides the sole de novo source of dTMP for DNA biosynthesis** HAMAP MF_00008	**5,10-methylenetetrahydrofolate + dUMP = dihydrofolate + dTMP.** HAMAP MF_00008	**Pathway** Pyrimidine metabolism; dTTP biosynthesis. HAMAP MF_00008
Rv2780	**Alanine dehydrogenase**	**Ald, DHA_MYCTU, MT2850, MTV002.45, O33322**	UniProtKB:P30234	**May play a role in cell wall synthesis as L-alanine is an important constituent of the peptidoglycan layer.**	**L-alanine + H_2O + NAD^+ = pyruvate + NH_3 + NADH.**	**Pathway** Amino-acid degradation; L-alanine degradation via dehydrogenase pathway; NH(3) and pyruvate from L-alanine: step 1/1.

Gene	Full Name	Synonyms	Database	Function	Catalytic Activity	Pathway & Miscellaneous
Rv2930	**Long-chain-fatty-acid--AMP ligase FadD26**	**FAA26_MYCTU, fadD26, MT2999, MTCY338.19,**	UniProtKB:Q10976	**Catalyzes the activation of long-chain fatty acids (C22-24 fatty acids) as acyl-adenylates (acyl-AMP), which are then transferred to the multifunctional polyketide synthase PpsA for further chain extension. Involved in the biosynthesis of phthiocerol dimycocerosate (DIM A) and phthiodiolone dimycocerosate (DIM B).** Ref.3 Ref.4		**Pathway** Lipid metabolism; fatty acid biosynthesis.
Rv2931	**Phthiocerol synthesis polyketide synthase type I PpsA**	**PPSA_MYCTU, MTCY338.20, ppsA, MT3000**	UniProtKB:Q10977	**Involved in the elongation of either C22-24 fatty acids by the addition of malonyl-CoA and methylmalonyl-CoA extender units to yield phthiocerol derivatives**	**Acyl-[acyl-carrier-protein] + malonyl-[acyl-carrier-protein] = 3-oxoacyl- [acyl-carrier-protein] + CO_2 + [acyl-carrier-protein].**	**Pathway** Lipid metabolism; fatty acid biosynthesis.
Rv2940c	**Mycocerosic acid synthase**	**mas, mas-2, MT3010, P96291_MYCTU, Q7D6E5**	UniProtKB:P96291	**CATALYZES THE ELONGATION OF N-FATTY ACYL-CoA WITH METHYLAMALONYL-CoA (NOT MALONYL-CoA) AS THE ELONGATING AGENT TO FORM MYCOCEROSYL LIPIDS.**		
Rv2959c	**Rhamnosyl O-methyltransferase**	**RNMT_MYCTU, Rv2959c, MT3035, O08024, Q798M6, Q7D6D0**	UniProtKB:Q50457	**Catalyzes the O-methylation of the hydroxyl group located on C-2 of the first rhamnosyl residue linked to the phenolic group of glycosylated phenolphthiocerol dimycocerosates (PGL) and p-hydroxybenzoic acid derivatives (p-HBAD).** Ref.4		**Was identified as a high-confidence drug target.**
Rv3001c	**Ketol-acid reductoisomerase**	**ilvC, ILVC_MYCTU, MT3081, MTV012.15c, O53248**	UniProtKB:P65149	**INVOLVED IN VALINE AND ISOLEUCINE BIOSYNTHESIS**	**(R)-2,3-dihydroxy-3-methylbutanoate + $NADP^+$ = (S)-2-hydroxy-2-methyl-3-oxobutanoate + NADPH.** HAMAP MF_00435 **(2R,3R)-2,3-dihydroxy-3-methylpentanoate + $NADP^+$ = (S)-2-hydroxy-2-ethyl-3-oxobutanoate + NADPH.** HAMAP MF_00435	**Pathway:** Amino-acid biosynthesis; L-isoleucine biosynthesis; L-isoleucine from 2-oxobutanoate: step 2/4. HAMAP MF_00435 Amino-acid biosynthesis; L-valine

Gene	Full Name	Synonyms	Database	Function	Catalytic Activity	Pathway & Miscellaneous
						biosynthesis; L-valine from pyruvate: step 2/4. HAMAP MF_00435
Rv3002c	**Acetolactate synthase small subunit**	**IlvH, ILVH_MYCTU, ilvN, MT3082, MTV012.16c, O53249**	UniProtKB:P65161	**INVOLVED IN VALINE AND ISOLEUCINE BIOSYNTHESIS**	**2 pyruvate = 2-acetolactate + CO_2.**	**Pathway** Amino-acid biosynthesis; L-isoleucine biosynthesis; L-isoleucine from 2-oxobutanoate: step 1/4. Amino-acid biosynthesis; L-valine biosynthesis; L-valine from pyruvate: step 1/4.
Rv3048c	**Ribonucleoside-diphosphate reductase subunit beta nrdF2**	**MT3133, nrdF2, Q6MX16, Q7D680, RIR2B_MYCTU**	UniProtKB:Q50549	**Provides the precursors necessary for DNA synthesis. Catalyzes the biosynthesis of deoxyribonucleotides from the corresponding ribonucleotides. Two genes for this protein are present in M.tuberculosis; this is the active form. When coexpressed in E.coli with nrdE the 2 proteins complement a temperature-sensitive E.coli mutant.** Ref.1	**2'-deoxyribonucleoside diphosphate + thioredoxin disulfide + H_2O = ribonucleoside diphosphate + thioredoxin.** Ref.1	**Pathway** Genetic information processing; DNA replication.
Rv3206c	**Probable adenylyltransferase/sulfurtransferase MoeZ**	**moeB1, moeZ, MOEZ_MYCTU, MT3301 , Q6MWZ9**	UniProtKB:Q7D5X9	**Catalyzes the conversion of the sulfur carrier protein CysO to CysO-thiocarboxylate. The reaction is thought to proceed in two steps: first, ATP-dependent activation of CysO as acyl-adenylate (CysO-COOAMP), followed by sulfur transfer to give CysO-thiocarboxylate (CysO-COSH) Probable. The sulfur source is unknown.** Ref.4		
Rv3601	**Aspartate 1-decarboxylase**	**PAND_MYCTU, panD,**	UniProtKB:P6	**Catalyzes the pyruvoyl-dependent decarboxylation of aspartate to produce beta-alanine**	**L-aspartate = beta-alanine + CO_2.**	**Pathway** Cofactor

Gene	Full Name	Synonyms	Database	Function	Catalytic Activity	Pathway & Miscellaneous
c		**Rv3601c, MTCY07H7B.21, MT3706.1, O06281**	5660	HAMAP MF_00446	HAMAP MF_00446	biosynthesis; (R)-pantothenate biosynthesis; beta-alanine from L-aspartate: step 1/1. HAMAP MF_00446
Rv3774	**Enoyl-CoA hydratase/isomerase family protein**	**ech , echA21, MT3883, P75019_MYCTU, Q79C03, Q7D4W1**	UniProtKB:P75019	**COULD POSSIBLY OXIDIZE FATTY ACIDS USING SPECIFIC COMPONENTS**	**(3S)-3-HYDROXYACYL-CoA = TRANS-2(OR 3)-ENOYL-CoA + H(2)O**	
Rv3913	**Thioredoxin reductase**	**MT4032, MTV028.04, O53592, trxB, TRXB_MYCTU**	UniProtKB:P52214	**ENZYME THAT CATALYSE THE REDUCTION OF DISULPHIDES BY PYRIDINE NUCLEOTIDES THROUGH AN ENZYME DISULPHIDE AND A FLAVIN. SEEMS REGULATED BY SIGH (Rv3223c PRODUCT).**	**Thioredoxin + $NADP^+$ = thioredoxin disulfide + NADPH.**	**The active site is a redox-active disulfide bond.Was identified as a high-confidence drug target.**
Rv0859	**Putative acyltransferase**	**fadA,** Y0859_MYCTU	UniProtKB:O53871	**FUNCTION UNKNOWN, BUT INVOLVEMENT IN LIPID DEGRADATION.**		
Rv1467c	**Acyl-CoA dehydrogenase, putative**	**O53158_MYCTU,** MT1514, fadE15, Q7D8E4	UniProtKB:O53158	**FUNCTION UNKNOWN, BUT INVOLVEMENT IN LIPID DEGRADATION.**		
Rv1737c	**Probable nitrate/nitrite transporter narK2**	**MT1779,** narK-3, narK2, NARK2_MYCTU, Q7D820	UniProtKB:P71995	**Permits nitrate and nitrate transport into E.coli.** Ref.4		**One of the activities induced in M.tuberculosis by hypoxia is the dissimilatory reduction of nitrate to nitrite, which serves to provide energy as the bacteria adapt to anaerobiosis.**
Rv2497c	**2-oxoisovalerate dehydrogenase E1 component, alpha**	**MT2572 ,** O06161_MYCTU , pdhA ,	UniProtKB:O06161	**INVOLVED IN ENERGY METABOLISM. THE BRANCHED-CHAIN ALPHA-KETO ACID DEHYDROGENASE COMPLEX CATALYZES THE OVERALL CONVERSION OF BRANCHED CHAIN ALPHA-KETO ACIDS TO**		

Gene	Full Name	Synonyms	Database	Function	Catalytic Activity	Pathway & Miscellaneous
	subunit, putative	Q7D714		**ACYL-CoA AND CO2. IT CONTAINS MULTIPLE COPIES OF THREE ENZYMATIC COMPONENTS: BRANCHED-CHAIN ALPHA-KETO ACID DECARBOXYLASE (E1), LIPOAMIDE ACYLTRANSFERASE (E2) AND LIPOAMIDE DEHYDROGENASE (E3)**		
Rv2933	**Phthiocerol synthesis polyketide synthase type I PpsC**	**PPSC_MYCTU, ppsC**	UniProtKB:P96202	**Involved in the elongation of either C22-24 fatty acids by the addition of malonyl-CoA and methylmalonyl-CoA extender units to yield phthiocerol derivatives**	**Acyl-[acyl-carrier-protein] + malonyl-[acyl-carrier-protein] = 3-oxoacyl- [acyl-carrier-protein] + CO_2 + [acyl-carrier-protein].**	**Was identified as a high-confidence drug target.** **Pathway:** Lipid metabolism; fatty acid biosynthesis.
Rv2950c	**Long-chain-fatty-acid--AMP ligase FadD29**	**FAA29_MYCTU,** fadD29	UniProtKB:P95141	**Catalyzes the activation of the long-chain fatty acids (C22-24 fatty acids) as acyl-adenylates (acyl-AMP), which are then transferred to the multifunctional polyketide synthase PpsA for further chain extension. Involved in the biosynthesis of phenolphthioceroL, which is an important intermedaite in the biosynthesis of phenolic glycolipid (mycosid B).** Ref.2 Ref.3		**Pathway:** Lipid metabolism; fatty acid biosynthesis.
Rv2332	**Putative malate oxidoreductase [NAD]**	**MAOX_MYCTU,** mez, MT2394 , MTCY3G12.02c, MTCY98.01	UniProtKB:P71880	**CATALIZES THE OXIDATIVE DECARBOXYLATION OF MALATE INTO PYRUVATE, IMPORTANT FOR A WIDE RANGE OF METABOLIC PATHWAYS**	**(S)-malate + NAD^+ = pyruvate + CO_2 + NADH.**	
Rv3515c	**Long-chain-fatty-acid--CoA ligase FadD19**	**FAC19_MYCTU,** fadD19, MT3616, Q6MWW5	UniProtKB:Q7D5D8	**Catalyzes the activation of long-chain fatty acids as acyl-coenzyme A (acyl-CoA), which are then transferred to the multifunctional polyketide synthase (PKS) type III for further chain extension.** Ref.3	**ATP + a long-chain carboxylic acid + CoA = AMP + diphosphate + an acyl-CoA.**	**Pathway** Lipid metabolism; fatty acid biosynthesis.
Rv0468	**3-hydroxybutyryl-CoA dehydrogena**	**FadB2,** FADB2_MYC	UniProtKB:O53753	**Catalyzes the NAD-dependent dehydration of beta-hydroxybutyryl-CoA to acetoacetyl-CoA in vitro at pH 10.**	**(S)-3-hydroxybutanoyl-CoA + $NADP^+$ = 3-**	**Pathway:** Lipid metabolism;

Gene	Full Name	Synonyms	Database	Function	Catalytic Activity	Pathway & Miscellaneous
	se	TU, MT0484, Q7D9R6		**Also catalyzes the reverse reaction albeit in a lower pH range of 5.5-6.5. The reverse reaction is able to use NADPH as well as NADH.** Ref.5	**acetoacetyl-CoA + NADPH.** Ref.5	butanoate metabolism. **Enzyme regulation: Activated by magnesium and calcium, and inhibited by zinc, nickel and cobalt.** Ref.5
Rv0551c	**Substrate--CoA ligase**	**fadD8 ,** MT0577 , O06417_MYCTU , Q7D9N4	UniProtKB:O06417	**FUNCTION UNKNOWN, BUT INVOLVED IN LIPID DEGRADATION.**		
Rv0952	**Succinyl-CoA ligase [ADP-forming] subunit alpha**	**MT0979,** MTCY10D7.22c , Rv0952 , sucD , SUCD_MYCTU	UniProtKB:P71558	**INVOLVED IN TRICARBOXYLIC ACID CYCLE**	**ATP + succinate + CoA = ADP + phosphate + succinyl-CoA.**	
Rv1345	**Long-chain-fatty-acid--[acyl-carrier-protein] ligase MbtM**	**fadD33,** mbtM, MBTM_MYCTU, MT1387, MTCY02B10.09, Q11015	UniProtKB:P0A4X8	**Activates lipidic moieties required for mycobactin biosynthesis. Converts medium- to long-chain aliphatic fatty acids into acyl adenylate, which is further transferred on to the phosphopantetheine arm of the carrier protein MbtL.** Ref.4 Ref.5	**ATP + an acid + [acyl-carrier-protein] = AMP + diphosphate + acyl-[acyl-carrier-protein].**	**Pathway:** Siderophore biosynthesis; mycobactin biosynthesis.
Rv2724c		**fadE20**		**FUNCTION UNKNOWN, BUT INVOLVED IN LIPID DEGRADATION.**		
Rv2932	**Phthiocerol synthesis polyketide synthase type I PpsB**	**PPSB_MYCTU,** MTCY338.21, ppsB,	UniProtKB:Q10978	**Involved in the elongation of either C22-24 fatty acids by the addition of malonyl-CoA and methylmalonyl-CoA extender units to yield phthiocerol derivatives**	**Acyl-[acyl-carrier-protein] + malonyl-[acyl-carrier-protein] = 3-oxoacyl- [acyl-carrier-protein] +**	**Pathway** Lipid metabolism; fatty acid

Gene	Full Name	Synonyms	Database	Function	Catalytic Activity	Pathway & Miscellaneous
		Rv2932, MTV011.01, MT3002, O53234			**CO_2 + [acyl-carrier-protein].**	biosynthesis.
Rv2935	**Phthiocerol synthesis polyketide synthase type I PpsE**	**MT3005,** ppsE , PPSE_MYCTU , Q7D6E9	UniProtKB:P96204	**Involved in the elongation of either C22-24 fatty acids by the addition of malonyl-CoA and methylmalonyl-CoA extender units to yield phthiocerol derivatives.** Ref.4	**Acyl-[acyl-carrier-protein] + malonyl-[acyl-carrier-protein] = 3-oxoacyl- [acyl-carrier-protein] + CO_2 + [acyl-carrier-protein].**	**Pathway** Lipid metabolism; fatty acid biosynthesis.
Rv3003c	**Acetolactate synthase large subunit IlvB1**	**ilvB1 ,** ILVB1_MYCTU, MT3083 , MTV012.17c, O53250	UniProtKB:P0A622	**Catalyzes the conversion of 2 pyruvate molecules into acetolactate in the first common step of the biosynthetic pathway of the branched-amino acids such as leucine, isoleucine, and valine. Also involved in condensing pyruvate and 2-ketobutyrate to form 2-aceto-2-hydroxybutyrate.** Ref.3	**2 pyruvate = 2-acetolactate + CO_2.**	**Pathways:** Amino-acid biosynthesis; L-isoleucine biosynthesis; L-isoleucine from 2-oxobutanoate: step 1/4. Amino-acid biosynthesis; L-valine biosynthesis; L-valine from pyruvate: step 1/4.
Rv3061c	**PROBABLE ACYL-CoA DEHYDROGENASE FADE22**	**fadE22 ,** MT3147 , P95097_MYCTU , Q7D672	UniProtKB:P95097	**FUNCTION UNKNOWN, BUT INVOLVED IN LIPID DEGRADATION.**		
Rv3516	**POSSIBLE ENOYL-CoA HYDRATASE ECHA19 (ENOYL HYDRASE)**	**echA19 , O53561_MYCTU**	UniProtKB:O53561	**COULD POSSIBLY OXIDIZE FATTY ACIDS USING SPECIFIC COMPONENTS**	**(3S)-3-HYDROXYACYL-CoA = TRANS-2(OR 3)-ENOYL-CoA + H(2)O**	

Gene	*Full Name*	*Synonyms*	*Database*	*Function*	*Catalytic Activity*	*Pathway & Miscellaneous*
	(UNSATURATED ACYL-CoA HYDRATASE) (CROTONASE)					
Rv3546	**PROBABLE ACETYL-CoA ACETYLTRANSFERASE FADA5 (ACETOACETYL-CoA THIOLASE)**	**fadA5,** MT3650, P71855_MYCTU, Q7D5B3	UniProtKB:P71855	**FUNCTION UNKNOWN, BUT INVOLVED IN LIPID DEGRADATION**	**2 ACETYL-CoA = CoA + ACETOACETYL-CoA**	
Rv3804c	**Antigen 85-A**	**A85A_MYCTU,** fbpA, mpt44, MT3911, MTV026.09c, P17944, P17996	UniProtKB:P0A4V2	**Proteins of the antigen 85 complex are responsible for the high affinity of mycobacteria to fibronectin. Possesses a mycolyltransferase activity required for the biogenesis of trehalose dimycolate (cord factor), a dominant structure necessary for maintaining cell wall integrity.**		**Was identified as a high-confidence drug target.**
Rv0166		**fadD5**	**Tuberculist** http://tuberculist.epfl.ch/quicksearch.php?gene+name=Rv0166&submit=Search	**FUNCTION UNKNOWN, BUT INVOLVED IN LIPID DEGRADATION**		
Rv0408	**Phosphate acetyltransferase**	**MT0421,** MTCY22G10.04, pta, PTA_MYCTU	UniProtKB:P96254	**Involved in acetate metabolism**	**Acetyl-CoA + phosphate = CoA + acetyl phosphate.**	**Pathway** Metabolic intermediate biosynthesis; acetyl-CoA biosynthesis; acetyl-CoA from

Gene	Full Name	Synonyms	Database	Function	Catalytic Activity	Pathway & Miscellaneous
						acetate: step 2/2.
Rv0694	**Putative mycofactocin biosynthesis dehydrogenase MftD**	**lldD1 ,** mftD , MFTD_MYCTU , MT0721, Q8VKG1	UniProtKB:P95040	**May play a role in the maturation of mycofactocin, a conserved polypeptide that might serve as an electron carrier. The genes for mycofactocin and other proteins proposed to function in its maturation are found in a conserved gene cluster.** Ref.3	**(S)-LACTATE + 2 FERRICYTOCHROME C = PYRUVATE + 2 FERROCYTOCHROME C**	
Rv1497	**PROBABLE ESTERASE LIPL**	**lipL, P71778_MYCTU**	UniProtKB:P71778	**FUNCTION UNKNOWN, BUT SUPPOSED INVOLVEMENT IN LIPID METABOLISM**		
Rv1613	**Tryptophan synthase alpha chain**	**MT1648 ,** MTCY01B2.05, O06130 , trpA , TRPA_MYCTU	UniProtKB:P66980	**The alpha subunit is responsible for the aldol cleavage of indoleglycerol phosphate to indole and glyceraldehyde 3-phosphate.** HAMAP MF_00131	**L-serine + 1-C-(indol-3-yl)glycerol 3-phosphate = L-tryptophan + glyceraldehyde 3-phosphate + H_2O.** HAMAP MF_00131	**Was identified as a high-confidence drug target.** **Pathway:** Amino-acid biosynthesis; L-tryptophan biosynthesis; L-tryptophan from chorismate: step 5/5. HAMAP MF_00131
Rv3084	**PROBABLE ACETYL-HYDROLASE/ESTERASE LIPR**	**bah,** lipR , MT3169, O53301_MYCTU, Q7D657	UniProtKB:O53301	**FUNCTION UNKNOWN; LIPOLYTIC ENZYME INVOLVED IN CELLULAR METABOLISM.**		
Rv3145		**nuoA**	**Tuberculist** http://tuberculist.epfl.ch/quicksearch.php?gene+name=Rv	**INVOLVED IN AEROBIC|ANAEROBIC RESPIRATION**	**NADH + UBIQUINONE = NAD(+) + UBIQUINOL**	

Gene	*Full Name*	*Synonyms*	*Database*	*Function*	*Catalytic Activity*	*Pathway & Miscellaneous*
			0166&submit=Search			
Rv3146		**nuoB**	**Tuberculist** http://tuberculist.epfl.ch/quicksearch.php?gene+name=Rv0166&submit=Search	**INVOLVED IN AEROBIC|ANAEROBIC RESPIRATION**	**NADH + UBIQUINONE = NAD(+) + UBIQUINOL**	
Rv3147		**nuoC**	**Tuberculist** http://tuberculist.epfl.ch/quicksearch.php?gene+name=Rv0166&submit=Search	**INVOLVED IN AEROBIC|ANAEROBIC RESPIRATION**	**NADH + UBIQUINONE = NAD(+) + UBIQUINOL**	
Rv3148		**nuoD**	**Tuberculist** http://tuberculist.epfl.ch/quicksearch.php?gene+name=Rv	**INVOLVED IN AEROBIC|ANAEROBIC RESPIRATION**	**NADH + UBIQUINONE = NAD(+) + UBIQUINOL**	

Gene	Full Name	Synonyms	Database	Function	Catalytic Activity	Pathway & Miscellaneous
			0166&submit=Search			
Rv3149		**nuoE**	**Tuberculist** http://tuberculist.epfl.ch/quicksearch.php?gene+name=Rv0166&submit=Search	**INVOLVED IN AEROBIC|ANAEROBIC RESPIRATION**	**NADH + UBIQUINONE = NAD(+) + UBIQUINOL**	
Rv3150		**nuoF**	**Tuberculist** http://tuberculist.epfl.ch/quicksearch.php?gene+name=Rv0166&submit=Search	**INVOLVED IN AEROBIC|ANAEROBIC RESPIRATION**	**NADH + UBIQUINONE = NAD(+) + UBIQUINOL**	
Rv3152		**nuoH**	**Tuberculist** http://tuberculist.epfl.ch/quicksearch.php?gene+name=Rv	**INVOLVED IN AEROBIC|ANAEROBIC RESPIRATION**	**NADH + UBIQUINONE = NAD(+) + UBIQUINOL**	

Gene	Full Name	Synonyms	Database	Function	Catalytic Activity	Pathway & Miscellaneous
			0166&submit=Search			
Rv3153		**nuoI**	**Tuberculist** http://tuberculist.epfl.ch/quicksearch.php?gene+name=Rv0166&submit=Search	**INVOLVED IN AEROBIC|ANAEROBIC RESPIRATION**	**NADH + UBIQUINONE = NAD(+) + UBIQUINOL**	
Rv3154		**nuoJ**	**Tuberculist** http://tuberculist.epfl.ch/quicksearch.php?gene+name=Rv0166&submit=Search	**INVOLVED IN AEROBIC|ANAEROBIC RESPIRATION**	**NADH + UBIQUINONE = NAD(+) + UBIQUINOL**	
Rv3155		**nuoK**	**Tuberculist** http://tuberculist.epfl.ch/quicksearch.php?gene+name=Rv	**INVOLVED IN AEROBIC|ANAEROBIC RESPIRATION**	**NADH + UBIQUINONE = NAD(+) + UBIQUINOL**	

Gene	Full Name	Synonyms	Database	Function	Catalytic Activity	Pathway & Miscellaneous
			0166&submit=Search			
Rv3156		**nuoL**	**Tuberculist** http://tuberculist.epfl.ch/quicksearch.php?gene+name=Rv0166&submit=Search	**INVOLVED IN AEROBIC|ANAEROBIC RESPIRATION**	**NADH + UBIQUINONE = NAD(+) + UBIQUINOL**	
Rv3157		**nuoM**	**Tuberculist** http://tuberculist.epfl.ch/quicksearch.php?gene+name=Rv0166&submit=Search	**INVOLVED IN AEROBIC|ANAEROBIC RESPIRATION**	**NADH + UBIQUINONE = NAD(+) + UBIQUINOL**	
Rv3158		**nuoN**	**Tuberculist** http://tuberculist.epfl.ch/quicksearch.php?gene+name=Rv	**INVOLVED IN AEROBIC|ANAEROBIC RESPIRATION**	**NADH + UBIQUINONE = NAD(+) + UBIQUINOL**	

Gene	*Full Name*	*Synonyms*	*Database*	*Function*	*Catalytic Activity*	*Pathway & Miscellaneous*
			0166&submit=Search			
Rv3322c				**COULD CAUSE METHYLATION.**		
Rv1349	**Iron import ATP-binding/permease protein IrtB**	irtB , IRTB_MYCTU, MT1392, MTCY02B10.13, Q11019	UniProtKB:P63393	**Part of the ABC transporter complex IrtAB involved in iron import. Transmembrane domains (TMD) form a pore in the membrane and the ATP-binding domain (NBD) is responsible for energy generation. Required for replication in human macrophages and in mouse lungs.** Ref.4 Ref.6		**Caution** Ref.5 **reports that IrtB forms a siderophore importer with Rv2895c, however this activity could be due to functional differences of IrtB in the molecular context of M.smegmatis and M.tuberculosis.**

Gene Essentiality Study

Table-2: Result generated after knockout studies of all 100 genes, in four models.

Genes	*Model(1)*	*Model(2)*	*Model(3)*	*Model(4)*
Rv0046c	Essential	Essential	Essential	Essential
Rv0070c	Non-essential	Non-essential	Non-essential	Non-essential
Rv0112	Non-essential	Non-essential	Non-essential	Non-essential
Rv0183	Non-essential	Non-essential	Non-essential	Non-essential
Rv0186	Non-essential	Non-essential	Non-essential	Non-essential
Rv0211	Non-essential	Non-essential	Non-essential	Non-essential
Rv0244c	Non-essential	Non-essential	Non-essential	Non-essential
Rv0363c	Non-essential	Non-essential	Non-essential	Non-essential
Rv0404	Non-essential	Non-essential	Non-essential	Non-essential
Rv0467	Non-essential	Non-essential	Non-essential	Non-essential
Rv0503c	Essential	Essential	Essential	Essential
Rv0619	Non-essential	Non-essential	Non-essential	Non-essential
Rv0753c	Non-essential	Non-essential	Non-essential	Non-essential
Rv0780	Non-essential	Non-essential	Non-essential	Non-essential
Rv0809	Essential	Essential	Essential	Essential
Rv0886	Non-essential	Non-essential	Non-essential	Non-essential
Rv0951	Non-essential	Non-essential	Non-essential	Non-essential

Genes	*Model(1)*	*Model(2)*	*Model(3)*	*Model(4)*
Rv0973c	Essential	Essential	Essential	Essential
Rv0974c	Essential	Essential	Essential	Essential
Rv1144	Non-essential	Non-essential	Non-essential	Non-essential
Rv1285	Non-essential	Non-essential	Non-essential	Non-essential
Rv1348	Essential	Essential	Essential	Essential
Rv1464	Essential	Essential	Essential	Essential
Rv1475c	Non-essential	Non-essential	Non-essential	Non-essential
Rv1500	Essential	Essential	Essential	Essential
Rv1525	Essential	Essential	Essential	Essential
Rv1553	Non-essential	Non-essential	Non-essential	Non-essential
Rv1623c	Essential	Essential	Essential	Essential
Rv1736c	Non-essential	Essential	Essential(non-feasible)	Essential(non-feasible)
Rv1811	Non-essential	Non-essential	Non-essential	Non-essential
Rv1832	Non-essential	Non-essential	Non-essential	Non-essential
Rv1854c	Non-essential	Non-essential	Non-essential	Non-essential
Rv2006	Essential	Essential	Essential	Essential
Rv2029c	Non-essential	Non-essential	Non-essential	Non-essential
Rv2121c	Non-essential	Non-essential	Non-essential	Non-essential
Rv2225	Essential	Essential	Essential	Essential
Rv2246	Essential	Essential	Essential	Essential
Rv2380c	Non-essential	Non-essential	Non-essential	Non-essential
Rv2381c	Non-essential	Non-essential	Non-essential	Non-essential
Rv2383c	Non-essential	Non-essential	Non-essential	Non-essential
Rv2385	Non-essential	Non-essential	Non-essential	Non-essential

Genes	*Model(1)*	*Model(2)*	*Model(3)*	*Model(4)*
Rv2386c	Essential	Essential	Essential	Essential
Rv2482c	Essential	Essential	Essential	Essential
Rv2503c	Non-essential	Non-essential	Non-essential	Non-essential
Rv2713	Non-essential	Non-essential	Non-essential	Non-essential
Rv2764c	Non-essential	Non-essential	Non-essential	Non-essential
Rv2780	Non-essential	Non-essential	Non-essential	Non-essential
Rv2930	Non-essential	Non-essential	Non-essential	Non-essential
Rv2931	Non-essential	Non-essential	Non-essential	Non-essential
Rv2940c	Essential	Essential	Essential	Essential
Rv2959c	Non-essential	Non-essential	Non-essential	Non-essential
Rv3001c	Non-essential	Non-essential	Non-essential	Non-essential
Rv3002c	Non-essential	Non-essential	Non-essential	Non-essential
Rv3048c	Essential	Essential	Essential	Essential
Rv3206c	Non-essential	Essential	Essential(non-feasible)	Essential(non-feasible)
Rv3601c	Essential	Essential	Essential	Essential
Rv3774	Non-essential	Non-essential	Non-essential	Non-essential
Rv3913	Essential	Essential	Essential	Essential
Rv0752c	Non-essential	Non-essential	Non-essential	Non-essential
Rv0859	Non-essential	Non-essential	Non-essential	Non-essential
Rv1467c	Non-essential	Non-essential	Non-essential	Non-essential
Rv1737c	Non-essential	Essential	Essential	Essential
Rv2497c	Non-essential	Non-essential	Non-essential	Non-essential
Rv2933	Non-essential	Non-essential	Non-essential	Non-essential
Rv2950c	Non-essential	Non-essential	Non-essential	Non-essential

Genes	*Model(1)*	*Model(2)*	*Model(3)*	*Model(4)*
Rv2332	Non-essential	Non-essential	Non-essential	Non-essential
Rv3515c	Non-essential	Non-essential	Non-essential	Non-essential
Rv0468	Non-essential	Non-essential	Non-essential	Non-essential
Rv0551c	Non-essential	Non-essential	Non-essential	Non-essential
Rv0952	Non-essential	Non-essential	Non-essential	Non-essential
Rv1345	Non-essential	Non-essential	Non-essential	Non-essential
Rv2724c	Non-essential	Non-essential	Non-essential	Non-essential
Rv2932	Non-essential	Non-essential	Non-essential	Non-essential
Rv2935	Non-essential	Non-essential	Non-essential	Non-essential
Rv3003c	Non-essential	Non-essential	Non-essential	Non-essential
Rv3061c	Non-essential	Non-essential	Non-essential	Non-essential
Rv3516	Non-essential	Non-essential	Non-essential	Non-essential
Rv3546	Non-essential	Non-essential	Non-essential	Non-essential
Rv3804c	Essential	Essential	Essential	Essential
Rv0166	Non-essential	Non-essential	Non-essential	Non-essential
Rv0408	Non-essential	Non-essential	Non-essential	Non-essential
Rv0694	Non-essential	Non-essential	Non-essential	Non-essential
Rv1497	Non-essential	Non-essential	Non-essential	Non-essential
Rv1613	Non-essential	Non-essential	Non-essential	Non-essential
Rv3084	Non-essential	Non-essential	Non-essential	Non-essential
Rv3145	Non-essential	Non-essential	Non-essential	Non-essential
Rv3146	Non-essential	Non-essential	Non-essential	Non-essential
Rv3147	Non-essential	Non-essential	Non-essential	Non-essential
Rv3148	Non-essential	Non-essential	Non-essential	Non-essential

Genes	*Model(1)*	*Model(2)*	*Model(3)*	*Model(4)*
Rv3149	Non-essential	Non-essential	Non-essential	Non-essential
Rv3150	Non-essential	Non-essential	Non-essential	Non-essential
Rv3152	Non-essential	Non-essential	Non-essential	Non-essential
Rv3153	Non-essential	Non-essential	Non-essential	Non-essential
Rv3154	Non-essential	Non-essential	Non-essential	Non-essential
Rv3155	Non-essential	Non-essential	Non-essential	Non-essential
Rv3156	Non-essential	Non-essential	Non-essential	Non-essential
Rv3157	Non-essential	Non-essential	Non-essential	Non-essential
Rv3158	Non-essential	Non-essential	Non-essential	Non-essential
Rv3322c	Non-essential	Essential	Essential	Essential
Rv1349	Essential	Essential	Essential	Essential

Table-3: Growth rate (Biomass production) of organism after gene knock outs:

Genes	*Model-1*	*Model-2*	*Model-3*	*Model-4*
Rv0046c	0.000000	0.000000	0.000000	0.000000
Rv0070c	0.000711	0.000711	0.000711	0.000711
Rv0112	0.054775	0.013069	0.013069	0.013069
Rv0183	0.054419	0.013069	0.013069	0.013069
Rv0186	0.054676	0.013069	0.013069	0.013069
Rv0211	0.054775	0.013069	0.013069	0.013069
Rv0244c	0.05319	0.013069	0.013069	0.013069
Rv0363c	0.052487	0.002163	0.002163	0.002163
Rv0404	0.052379	0.013069	0.013069	0.013069
Rv0467	0.052752	0.013069	0.013069	0.013069
Rv0503c	0.000000	0.000000	0.000000	0.000000
Rv0619	0.054725	0.013069	0.013069	0.013069
Rv0753c	0.054775	0.013069	0.013069	0.013069
Rv0780	0.000680	0.000680	0.000680	0.000680

Genes	*Model-1*	*Model-2*	*Model-3*	*Model-4*
Rv0809	0.000000	0.000000	0.000000	0.000000
Rv0886	0.025964	0.003161	0.003161	0.003161
Rv0951	0.054772	0.013069	0.013069	0.013069
Rv0973c	0.000000	0.000000	0.000000	0.000000
Rv0974c	0.000000	0.000000	0.000000	0.000000
Rv1144	0.050816	0.013069	0.013069	0.013069
Rv1285	0.025961	0.003161	0.003161	0.003161
Rv1348	0.000000	0.000000	0.000000	0.000000
Rv1464	0.000000	0.000000	0.000000	0.000000
Rv1475c	0.010905	0.004630	0.004630	0.004630
Rv1500	0.000000	0.000000	0.000000	0.000000
Rv1525	0.000000	0.000000	0.000000	0.000000
Rv1553	0.053562	0.013069	0.013069	0.013069
Rv1623c	0.000000	0.000000	0.000000	0.000000
Rv1736c	0.054775	0.000000	0.000000	0.000000
Rv1811	0.055743	0.013069	0.013069	0.013069
Rv1832	0.000694	0.000694	0.000694	0.000694
Rv1854c	0.054775	0.013069	0.013069	0.013069
Rv2006	0.000000	0.000000	0.000000	0.000000
Rv2029c	0.052538	0.013069	0.013069	0.013069
Rv2121c	0.044932	0.013069	0.013069	0.013069
Rv2225	0.000000	0.000000	0.000000	0.000000
Rv2246	0.000000	0.000000	0.000000	0.000000
Rv2380c	0.054775	0.013069	0.013069	0.013069
Rv2381c	0.054775	0.013069	0.013069	0.013069

Genes	*Model-1*	*Model-2*	*Model-3*	*Model-4*
Rv2383c	0.054775	0.013069	0.013069	0.013069
Rv2385	0.054415	0.013069	0.013069	0.013069
Rv2386c	0.000000	0.000000	0.000000	0.000000
Rv2482c	0.000000	0.000000	0.000000	0.000000
Rv2503c	0.054775	0.013069	0.013069	0.013069
Rv2713	0.054775	0.013069	0.013069	0.013069
Rv2764c	0.054775	0.054775	0.013069	0.013069
Rv2780	0.004619	0.004619	0.004619	0.004619
Rv2930	0.052379	0.013069	0.013069	0.013069
Rv2931	0.025961	0.013069	0.013069	0.013069
Rv2940c	0.000000	0.000000	0.000000	0.000000
Rv2959c	0.054775	0.013069	0.013069	0.013069
Rv3001c	0.012718	0.012718	0.012718	0.012718
Rv3002c	0.012718	0.012718	0.012718	0.012718
Rv3048c	0.000000	0.000000	0.000000	0.000000
Rv3206c	0.054775	0.000000	0.000000	0.000000
Rv3601c	0.000000	0.000000	0.000000	0.000000
Rv3774	0.048973	0.013069	0.013069	0.013069
Rv3913	0.000000	0.000000	0.000000	0.000000
Rv0752c	0.05319	0.013069	0.013069	0.013069
Rv0859	0.05319	0.013069	0.013069	0.013069
Rv1467c	0.05319	0.013069	0.013069	0.013069
Rv1737c	0.054775	0.000000	0	0
Rv2497c	0.050816	0.013069	0.013069	0.013069
Rv2933	0.054775	0.013069	0.013069	0.013069

Genes	*Model-1*	*Model-2*	*Model-3*	*Model-4*
Rv2950c	0.052379	0.013069	0.013069	0.013069
Rv2332	0.054775	0.013069	0.013069	0.013069
Rv3515c	0.052379	0.013069	0.013069	0.013069
Rv0468	0.05319	0.013069	0.013069	0.013069
Rv0551c	0.052379	0.013069	0.013069	0.013069
Rv0952	0.054772	0.013069	0.013069	0.013069
Rv1345	0.052379	0.013069	0.013069	0.013069
Rv2724c	0.05319	0.013069	0.013069	0.013069
Rv2932	0.054775	0.013069	0.013069	0.013069
Rv2935	0.054775	0.013069	0.013069	0.013069
Rv3003c	0.012718	0.012718	0.012718	0.012718
Rv3061c	0.05319	0.013069	0.013069	0.013069
Rv3516	0.05319	0.013069	0.013069	0.013069
Rv3546	0.05319	0.013069	0.013069	0.013069
Rv3804c	0	0.000000	0	0
Rv0166	0.052379	0.013069	0.013069	0.013069
Rv0408	0.05477	0.013069	0.013069	0.013069
Rv0694	0.054751	0.013069	0.013069	0.013069
Rv1497	0.054415	0.013069	0.013069	0.013069
Rv1613	0.035401	0.013069	0.013069	0.013069
Rv3084	0.054415	0.013069	0.013069	0.013069
Rv3145	0.050417	0.013069	0.013069	0.013069
Rv3146	0.050417	0.013069	0.013069	0.013069
Rv3147	0.050417	0.013069	0.013069	0.013069
Rv3148	0.050417	0.013069	0.013069	0.013069

Genes	*Model-1*	*Model-2*	*Model-3*	*Model-4*
Rv3149	0.050417	0.013069	0.013069	0.013069
Rv3150	0.050417	0.013069	0.013069	0.013069
Rv3152	0.050417	0.013069	0.013069	0.013069
Rv3153	0.050417	0.013069	0.013069	0.013069
Rv3154	0.050417	0.013069	0.013069	0.013069
Rv3155	0.050417	0.013069	0.013069	0.013069
Rv3156	0.050417	0.013069	0.013069	0.013069
Rv3157	0.050417	0.013069	0.013069	0.013069
Rv3158	0.050417	0.013069	0.013069	0.013069
Rv3322c	0.054775	0.000000	0	0
Rv1349	0	0.000000	0	0

Table-4: Non-essential Genes and it's correlated Genes:

Gene	*Correlated genes*
Rv0183	**Rv1079 ,Rv2713 OR Rv3303c, Rv3309c ,Rv0155 AND Rv0157 AND Rv0156, Rv0162c, Rv0946c, Rv1389, Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c, Rv2445c, Rv2476c, Rv2982c OR Rv0564 OR Rv3045, Rv1449c, Rv3045, Rv3436c, Rv3565 OR Rv0337c, Rv3859c AND Rv3858c**
Rv0186	**Rv3859c AND Rv3858c , Rv3565 OR Rv0337c, Rv3436c, Rv3309c , Rv3045, Rv2982c OR Rv0564 OR Rv3045, Rv2713 OR Rv3303c, Rv2476c, Rv2445c, Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c, Rv1389 , Rv1079, Rv0946c, Rv0162c , v0155 AND Rv0157 AND Rv0156,** **Rv1449c**
Rv0211	**Rv0155 AND Rv0157 AND Rv0156 , Rv0162c , R v0946c , Rv1079 ,** **Rv1389 , Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c, Rv2445c , Rv2476c, Rv2713 OR Rv3303c , Rv2982c OR Rv0564 OR Rv3045,** **Rv3045 , Rv3309c , Rv3436c , Rv3565 OR Rv0337c ,** **Rv3859c AND Rv3858c, Rv1449c**

Gene	*Correlated genes*
Rv0244c	**Rv3859c AND Rv3858c , Rv3565 OR Rv0337c, Rv3436c, Rv3309c, Rv3045, Rv2982c OR Rv0564 OR Rv3045, Rv2713 OR Rv3303c , Rv2476c, Rv2445c, Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c , Rv1389, Rv1079, Rv0946c, Rv0162c, Rv0155 AND Rv0157 AND Rv0156, Rv1449c**
Rv0363c	**Rv3859c AND Rv3858c, Rv3565 OR Rv0337c, Rv3436c, Rv3309c, Rv3045, Rv2982c OR Rv0564 OR Rv3045 , Rv2713 OR Rv3303c, Rv2476c, Rv2445c, Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c ,Rv1389, Rv1079, Rv0946c, Rv0162c , Rv0155 AND Rv0157 AND Rv0156 , Rv1449c**
Rv0467	**Rv0155 AND Rv0157 AND Rv0156 ,Rv0162c,Rv0946c,Rv1079,Rv1389,Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c ,Rv2445c,Rv2476c,Rv2713 OR Rv3303c, Rv2982c OR Rv0564 OR Rv3045 ,Rv3045,Rv3309c,Rv3436c, Rv3565 OR Rv0337c, Rv3859c AND Rv3858c, Rv1449c**
Rv0619	**Rv2982c OR Rv0564 OR Rv3045,Rv0162c, Rv0946c ,Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c ,Rv3045, Rv1079, Rv3565 OR Rv0337c ,Rv3859c AND Rv3858c ,Rv2476c, Rv1449c,Rv3436c,Rv3309c,Rv1389, Rv2445c, Rv1389, Rv0155 AND Rv0157 AND Rv0156, Rv2713 OR Rv3303c**
Rv0951	**Rv2982c OR Rv0564 OR Rv3045, Rv0162c, Rv0946c, Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c , Rv3045, Rv1079, Rv3859c AND Rv3858c, Rv2476c, Rv3565 OR Rv0337c, Rv3309c, Rv1389, Rv2445c, Rv0155 AND Rv0157 AND Rv0156, Rv2713 OR Rv3303c, Rv3436c , Rv1449c**
Rv1553	**Rv0155 AND Rv0157 AND Rv0156 , Rv0162c, Rv0946c, Rv1079, Rv1389, Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c , Rv2445c , Rv2476c , Rv2713 OR Rv3303c , Rv2982c OR Rv0564 OR Rv3045, Rv3045, Rv3309c, Rv3436c , Rv3565 OR Rv0337c, Rv3859c AND Rv3858c, Rv1449c**
Rv1736c	**Rv0155 AND Rv0157 AND Rv0156, Rv0162c, Rv0946c, Rv1079, Rv1389, Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c , Rv2445c, Rv2476c , Rv2713 OR Rv3303c , Rv2982c OR Rv0564 OR Rv3045, Rv3045, Rv3309c , Rv3436c, Rv3565 OR Rv0337c , Rv3859c AND Rv3858c, Rv1449c**

Gene	*Correlated genes*
Rv1811	**Rv2982c OR Rv0564 OR Rv3045, Rv0162c, Rv0946c, Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c , Rv3045, Rv1079, Rv3565 OR Rv0337c,Rv3859c AND Rv3858c ,Rv2476c, Rv3309c, Rv2445c , Rv1389, Rv0155 AND Rv0157 AND Rv0156, Rv2713 OR Rv3303c, Rv3436c, Rv1449c**
Rv1854c	**Rv3859c AND Rv3858c, Rv3565 OR Rv0337c, Rv3436c, Rv3309c, Rv3045, Rv2982c OR Rv0564 OR Rv3045, Rv2713 OR Rv3303c, Rv2476c, Rv2445c, Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c, Rv1389, Rv1079, Rv0946c, Rv0162c, Rv0155 AND Rv0157 AND Rv0156, Rv1449c**
Rv2029c	**Rv3859c AND Rv3858c, Rv3565 OR Rv0337c, Rv3436c ,Rv3309c , Rv3045 ,Rv2982c OR Rv0564 OR Rv3045, Rv2713 OR Rv3303c, Rv2476c , Rv2445c , Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c, Rv1389 , Rv1079 , Rv0946c , Rv0162c , Rv0155 AND Rv0157 AND Rv0156, Rv1449c**
Rv2380c	**Rv0155 AND Rv0157 AND Rv0156 , Rv0162c , Rv0946c, Rv1079,Rv1389, Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c, Rv2445c, Rv2476c,Rv2713 OR Rv3303c, Rv2982c OR Rv0564 OR Rv3045, Rv3045, Rv3309c, Rv3436c, Rv3565 OR Rv0337c, Rv3859c AND Rv3858c, Rv1449c**
Rv2381c	**Rv0155 AND Rv0157 AND Rv0156,Rv0162c, Rv0946c, Rv1079, Rv1389,Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c,Rv2445c, Rv2476c, Rv2713 OR Rv3303c, Rv2982c OR Rv0564 OR Rv3045, Rv3045, Rv3309c, Rv3436c, Rv3565 OR Rv0337c, Rv3859c AND Rv3858c, Rv1449c**
Rv2383c	**Rv2982c OR Rv0564 OR Rv3045, Rv0162c, Rv0946c, Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c, Rv3045, Rv1079, Rv3565 OR Rv0337c, Rv3859c AND Rv3858c, Rv2476c, Rv1079, Rv3565 OR Rv0337c, Rv3309c, Rv2445c, Rv1389, Rv0155 AND Rv0157 AND Rv0156, Rv2713 OR Rv3303c, Rv3436c, Rv1449c**
Rv2385	**Rv2982c OR Rv0564 OR Rv3045, Rv0162c, Rv0946c, Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c, Rv3045, Rv1079, Rv3565 OR Rv0337c, Rv3859c AND Rv3858c, Rv2476c, Rv1079, Rv3565 OR Rv0337c , Rv3309c, Rv2445c, Rv1389, Rv0155 AND Rv0157 AND Rv0156 , Rv2713 OR Rv3303c, Rv3436c , Rv1449c**

Gene	*Correlated genes*
Rv2503c	**Rv2982c OR Rv0564 OR Rv3045 , Rv0162c, Rv0946c, Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c , Rv3045, Rv1079, Rv3859c AND Rv3858c , Rv2476c, Rv1079 , Rv3565 OR Rv0337c, Rv3309c, Rv1389 , Rv2445c, Rv0155 AND Rv0157 AND Rv0156, Rv2713 OR Rv3303c, Rv3436c, Rv1449c**
Rv2713	**Rv2982c OR Rv0564 OR Rv3045, Rv0162c , Rv0946c , Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c , Rv3045, Rv1079, Rv3565 OR Rv0337c, Rv3859c AND Rv3858c, Rv2476c, Rv1079, Rv3309c, Rv1389, Rv2445c, Rv0155 AND Rv0157 AND Rv0156, Rv3436c, Rv1449c**
Rv2764c	**Rv2982c OR Rv0564 OR Rv3045 ,Rv0162c, Rv0946c, Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c , Rv3045, Rv1079, Rv3859c AND Rv3858c, Rv2476c, Rv1079 , Rv3565 OR Rv0337c, Rv3309c, Rv1389, Rv2445c , Rv1389, Rv0155 AND Rv0157 AND Rv0156 , Rv2713 OR Rv3303c, Rv3436c, Rv1449c**
Rv2930	**Rv2982c OR Rv0564 OR Rv3045, Rv0162c , Rv0946c , Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c , Rv3045 , Rv1079 ,Rv3859c AND Rv3858c, Rv2476c , Rv3565 OR Rv0337c , Rv3309c , Rv1389 ,Rv2445c ,Rv0155 AND Rv0157 AND Rv0156 ,Rv2713 OR Rv3303c, Rv3436c , Rv1449c**
Rv3206c	**Rv2982c OR Rv0564 OR Rv3045, Rv0162c, Rv0946c, Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c , Rv3045, Rv1079, Rv3859c AND Rv3858c, Rv2476c , Rv1079, Rv3565 OR Rv0337c, Rv3309c, Rv1389, Rv2445c ,Rv0155 AND Rv0157 AND Rv0156 , Rv2713 OR Rv3303c, Rv3436c, Rv1449c**
Rv3774	**Rv2982c OR Rv0564 OR Rv3045 ,Rv0162c, Rv0946c, Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c ,Rv3045, Rv1079, Rv3565 OR Rv0337c, Rv3859c AND Rv3858c , Rv2476c, Rv1079, Rv3309c, Rv1389 , Rv2445c, Rv0155 AND Rv0157 AND Rv0156 , Rv2713 OR Rv3303c , Rv3436c, Rv1449c**

Table-5: Properties of correlated genes:

Gene	*Full Name*	*Synonyms*	*Database*	Function	Catalytic Activity	Pathway & Miscellaneous
Rv1079	**Cystathionine gamma-synthase**	**METB_MYCTU,** MTV017.32, metB, MT1110	UniProtKB:P66875	**INVOLVED IN METHIONINE BIOSYNTHESIS: CONVERTS O-SUCCINYL-L-HOMOSERINE TO CYSTATHIONINE**	**O-SUCCINYL-L-HOMOSERINE + L-CYSTEINE = CYSTATHIONINE + SUCCINATE (CAN ALSO USE HYDROGEN SULFIDE AND METHANETHIOL AS SUBSTRATES)**	**Product:** **PROBABLE CYSTATHIONINE GAMMA-SYNTHASE METB (CGS) (O-SUCCINYLHOMOSERINE [THIOL]-LYASE)** **KEGG GENES** mtu:Rv1079
Rv2713	**Probable soluble pyridine nucleotide transhydrogenase**	**SthA MT2786** MTCY05A6.34 STHA_MYCTU	UniProtKB:P66006	**CONVERSION OF NADPH, GENERATED BY PERIPHERAL CATABOLIC PATHWAYS, TO NADH, WHICH CAN ENTER THE RESPIRATORY CHAIN FOR ENERGY GENERATION**	**NADPH + NAD(+) = NADP(+) + NADH**	**Product:** **PROBABLE SOLUBLE PYRIDINE NUCLEOTIDE TRANSHYDROGENASE STHA (STH) (NAD(P)(+) TRANSHYDROGENASE [B-SPECIFIC]) (NICOTINAMIDE NUCLEOTIDE TRANSHYDROGENASE)** **KEGG GENES** mtu:Rv2713
Rv3303c	**NAD(P)H dehydrogenase (quinone)**	**lpdA ,** lpdA-2, LPDA_MYCTU , MT3402	UniProtKB:O53355	**INVOLVED IN ENERGY METABOLISM. CAN CATALYZE THE REDUCTION OF ELECTRON ACCEPTORS SUCH AS 2,6-DIMETHYL-1,4-BENZOQUINONE (DMBQ) AND 5-HYDROXY-1,4-NAPTHAQUINONE (5-HNQ)**	**CATALYTIC ACTIVITY: NAD(P)H + A QUINONE + H+ -> A QUINOL + NAD(P)+**	**Product:** **NAD(P)H QUINONE REDUCTASE LPDA** **KEGG GENES** mtu:Rv3303c
Rv0155	**PROBABLE NAD(P) TRANSHYDROGENASE (SUBUNIT ALPHA) PNTAA [FIRST PART; CATALYTIC PART] (PYRIDINE NUCLEOTIDE TRANSHYDROGENASE SUBUNIT ALPHA) (NICOTINAMIDE**	**P96832_MYCTU,** pntAa	UniProtKB:P96832	**THE TRANSHYDROGENATION BETWEEN NADH AND NADP IS COUPLED TO RESPIRATION AND ATP HYDROLYSIS AND FUNCTIONS AS A PROTON PUMP ACROSS THE MEMBRANE**	**NADPH + NAD+ = NADP+ + NADH**	**Product:** **PROBABLE NAD(P) TRANSHYDROGENASE (SUBUNIT ALPHA) PNTAA [FIRST PART; CATALYTIC PART] (PYRIDINE NUCLEOTIDE TRANSHYDROGENASE SUBUNIT ALPHA) (NICOTINAMIDE NUCLEOTIDE TRANSHYDROGENASE SUBUNIT ALPHA)** **KEGG GENES** mtu:Rv0155

Gene	*Full Name*	*Synonyms*	*Database*	Function	Catalytic Activity	Pathway & Miscellaneous
	NUCLEOTIDE TRANSHYDROGENASE SUBUNIT ALPHA)					
Rv0156	**PROBABLE NAD(P) TRANSHYDROGENASE (SUBUNIT ALPHA) PNTAB [SECOND PART; INTEGRAL MEMBRANE PROTEIN] (PYRIDINE NUCLEOTIDE TRANSHYDROGENASE SUBUNIT ALPHA) (NICOTINAMIDE NUCLEOTIDE TRANSHYDROGENASE SUBUNIT ALPHA)**	**P96833_MYCTU,** pntAb	UniProtKB:P96833	**THE TRANSHYDROGENATION BETWEEN NADH AND NADP IS COUPLED TO RESPIRATION AND ATP HYDROLYSIS AND FUNCTIONS AS A PROTON PUMP ACROSS THE MEMBRANE**	**NADPH + NAD+ = NADP+ + NADH**	**Product:** **PROBABLE NAD(P) TRANSHYDROGENASE (SUBUNIT ALPHA) PNTAB [SECOND PART; INTEGRAL MEMBRANE PROTEIN] (PYRIDINE NUCLEOTIDE TRANSHYDROGENASE SUBUNIT ALPHA) (NICOTINAMIDE NUCLEOTIDE TRANSHYDROGENASE SUBUNIT ALPHA)** **KEGG GENES** mtu:Rv0156
Rv0157	**NAD(P) transhydrogenase subunit beta**	**MT0165 ,** P96834_MYCTU , pntB	UniProtKB:P96834	**THE TRANSHYDROGENATION BETWEEN NADH AND NADP IS COUPLED TO RESPIRATION AND ATP HYDROLYSIS AND FUNCTIONS AS A PROTON PUMP ACROSS THE MEMBRANE**	**NADPH + NAD+ = NADP+ + NADH**	**Product:** **PROBABLE NAD(P) TRANSHYDROGENASE (SUBUNIT BETA) PNTB [INTEGRAL MEMBRANE PROTEIN] (PYRIDINE NUCLEOTIDE TRANSHYDROGENASE SUBUNIT BETA) (NICOTINAMIDE NUCLEOTIDE TRANSHYDROGENASE SUBUNIT BETA)** **KEGG GENES** mtu:Rv0157
Rv1389	**Guanylate kinase**	**gmk ,** KGUA_MYCTU, MT1434 , MTCY21B4.06	UniProtKB:P0A5I4	**ESSENTIAL FOR RECYCLING GMP AND INDIRECTLY, CGMP**	**ATP + GMP = ADP + GDP**	**Product:** **PROBABLE GUANYLATE KINASE GMK** **KEGG GENES** mtu:Rv1389

Gene	*Full Name*	*Synonyms*	*Database*	Function	Catalytic Activity	Pathway & Miscellaneous
Rv1862		**adhA**		**CATALYZES THE REVERSIBLE OXIDATION OF ETHANOL TO ACETALDEHYDE WITH THE CONCOMITANT REDUCTION OF NAD**		**Product:** **PROBABLE ALCOHOL DEHYDROGENASE ADHA** **KEGG GENES** mtu:Rv1862
Rv1530		**adh**		**CATALYZES THE REVERSIBLE OXIDATION OF ETHANOL TO ACETALDEHYDE WITH THE CONCOMITANT REDUCTION OF NAD**		**Product:** **PROBABLE ALCOHOL DEHYDROGENASE ADH** **KEGG GENES** mtu:Rv1530
Rv0162c		**adhE1**		**DEHYDROGENESES A ALCOHOL (OXIDO-REDUCTION)**	**AN ALCOHOL + NAD+ = AN ALDEHYDE OR KETONE + NADH**	**Product:** **PROBABLE ZINC-TYPE ALCOHOL DEHYDROGENASE (E SUBUNIT) ADHE** **KEGG GENES** mtu:Rv0162c
Rv0761c	**Alcohol dehydrogenase B**	**ADHB_MYCTU,** adhB, MTCY369.06c, Rv0761c, MT0786	UniProtKB:P71818	**DEHYDROGENESES A ALCOHOL (OXIDO-REDUCTION)**	**AN ALCOHOL + NAD+ = AN ALDEHYDE OR KETONE + NADH**	**Product:** **PROBABLE ZINC-TYPE ALCOHOL DEHYDROGENASE (E SUBUNIT) ADHE** **KEGG GENES** mtu:Rv0761c
Rv2445c	**Nucleoside diphosphate kinase**	**MT2521,** MTCY428.01, MTV008.01c ndk , ndkA , NDK_MYCTU	UniProtKB:P84284	**MAJOR ROLE IN THE SYNTHESIS OF NUCLEOSIDE TRIPHOSPHATES OTHER THAN ATP**	**ATP + NUCLEOSIDE DIPHOSPHATE = ADP + NUCLEOSIDE TRIPHOSPHATE**	**Product:** **PROBABLE NUCLEOSIDE DIPHOSPHATE KINASE NDKA (NDK) (NDP KINASE) (NUCLEOSIDE-2-P KINASE)** **KEGG GENES** mtu:Rv2445c
Rv2476c	**PROBABLE NAD-DEPENDENT GLUTAMATE DEHYDROGENASE GDH (NAD-GDH) (NAD-**	**O53203_MYCTU,** gdh	UniProtKB:O53203	**CATABOLIC GLUTDH INVOLVED IN THE UTILIZATION OF GLUTAMATE AND OTHER AMINO ACIDS OF THE GLUTAMATE FAMILY.**	**L-GLUTAMATE + H(2)O + NAD(+) = 2-OXOGLUTARATE + NH(3) + NADH**	**Product:** **PROBABLE NAD-DEPENDENT GLUTAMATE DEHYDROGENASE GDH (NAD-GDH) (NAD-DEPENDENT GLUTAMIC DEHYDROGENASE)**

Gene	*Full Name*	*Synonyms*	*Database*	Function	Catalytic Activity	Pathway & Miscellaneous
	DEPENDENT GLUTAMIC DEHYDROGENASE)			**GENERATES 2-OXOGLUTARATE FROM L-GLUTAMATE**		**KEGG GENES** mtu:Rv2476c
Rv2982c	**Glycerol-3-phosphate dehydrogenase [NAD(P)+]**	**gpdA2 ,** GPDA_MYCTU , gpsA , MT3060 , MTCY349.05	UniProtKB:P95113	**INVOLVED IN DE NOVO PHOSPHOLIPID BIOSYNTHESIS; GLYCEROL-3 PHOSPHATE FORMATION**	**SN-GLYCEROL 3-PHOSPHATE + NAD(P)(+) = GLYCERONE PHOSPHATE + NAD(P)H**	**ProductPROBABLE GLYCEROL-3-PHOSPHATE DEHYDROGENASE [NAD(P)+] GPDA2 (NAD(P)H- DEPENDENT GLYCEROL-3-PHOSPHATE DEHYDROGENASE)** **KEGG GENES** mtu:Rv2982c
Rv0564		**gpdA1, gpsA, glyC**		**NVOLVED IN DE NOVO PHOSPHOLIPID BIOSYNTHESIS; GLYCEROL-3 PHOSPHATE FORMATION**	**SN-GLYCEROL 3-PHOSPHATE + NAD(P)+ = GLYCERONE PHOSPHATE + NAD(P)H**	**Product: PROBABLE GLYCEROL-3-PHOSPHATE DEHYDROGENASE [NAD(P)+] GPDA1 (NAD(P)H-DEPENDENT GLYCEROL-3-PHOSPHATE DEHYDROGENASE) (NAD(P)H-DEPENDENT DIHYDROXYACETONE-PHOSPHATE REDUCTASE)** **KEGG GENES** mtu:Rv0564c
Rv3045	**NADP-dependent alcohol dehydrogenase C**	**adh,** adhC, ADHC_MYCTU, MT3130, MTV012.60	UniProtKB:P0A4X0	**GENERATES ALDEHYDE OR KETONE FROM ALCOHOL**	**ALCOHOL + NADP(+) = ALDEHYDE OR KETONE + NADPH**	**Product: PROBABLE NADP-DEPENDENT ALCOHOL DEHYDROGENASE ADHC** **KEGG GENES** mtu:Rv3045
Rv3436c	**Glucosamine--fructose-6-phosphate aminotransferase [isomerizing]**	**glmS,** GLMS_MYCTU, MT3542, MTCY77.08c	UniProtKB:P0A588	**CATALYZES THE FIRST STEP IN HEXOSAMINE METABOLISM, CONVERTING FRUCTOSE-6P INTO GLUCOSAMINE-6P USING GLUTAMINE AS A NITROGEN SOURCE**	**L-GLUTAMINE + D-FRUCTOSE 6-PHOSPHATE = L-GLUTAMATE + D-GLUCOSAMINE 6-PHOSPHATE**	**Product:PROBABLE GLUCOSAMINE--FRUCTOSE-6-PHOSPHATE AMINOTRANSFERASE [ISOMERIZING] GLMS (HEXOSEPHOSPHATE AMINOTRANSFERASE) (D-FRUCTOSE-6-PHOSPHATE AMIDOTRANSFERASE) (GFAT) (L-GLUTAMINE-D-FRUCTOSE-6-PHOSPHATE AMIDOTRANSFERASE) (GLUCOSAMINE-6-**

Gene	*Full Name*	*Synonyms*	*Database*	Function	Catalytic Activity	Pathway & Miscellaneous
						PHOSPHATE SYNTHASE) **KEGG GENES** mtu:Rv3436c
Rv3565		**aspB**		**THOUGHT TO BE INVOLVED IN GLUTAMATE BIOSYNTHESIS**	**L-ASPARTATE + 2-OXOGLUTARATE = OXALOACETATE + L-GLUTAMATE**	**Product: POSSIBLE ASPARTATE AMINOTRANSFERASE ASPB (TRANSAMINASE A) (ASPAT) (GLUTAMIC--OXALOACETIC TRANSAMINASE) (GLUTAMIC--ASPARTIC TRANSAMINASE)** **KEGG GENES** mtu:Rv3565
Rv0337c	**Probable aspartate aminotransferase**	**AAT_MYCTU,** aspC , MT0351, MTCY279.04c	UniProtKB:P63498	**GENERATES OXALOACETATE AND L-GLUTAMATE FROM L-ASPARTATE AND 2-OXOGLUTARATE**	**L-ASPARTATE + 2-OXOGLUTARATE = OXALOACETATE + L-GLUTAMATE**	**Product: PROBABLE ASPARTATE AMINOTRANSFERASE ASPC (TRANSAMINASE A) (ASPAT)** **KEGG GENES** mtu:Rv0337c
Rv3859c	**PROBABLE FERREDOXIN-DEPENDENT GLUTAMATE SYNTHASE [NADPH] (LARGE SUBUNIT) GLTB (L-GLUTAMATE SYNTHASE) (L-GLUTAMATE SYNTHETASE) (NADH-GLUTAMATE SYNTHASE) (GLUTAMATE SYNTHASE (NADH))(NADPH-GOGAT)**	**GltB,** P96218_MYCTU	UniProtKB:P96218	**PROBABLY INVOLVED IN GLUTAMATE BIOSYNTHESIS**	**2 L-GLUTAMATE + NADP(+) = L-GLUTAMINE + 2-OXOGLUTARATE + NADPH**	**Product: PROBABLE FERREDOXIN-DEPENDENT GLUTAMATE SYNTHASE [NADPH] (LARGE SUBUNIT) GLTB (L-GLUTAMATE SYNTHASE) (L-GLUTAMATE SYNTHETASE) (NADH-GLUTAMATE SYNTHASE) (GLUTAMATE SYNTHASE (NADH))(NADPH-GOGAT)** **KEGG GENES** mtu:Rv3859c
Rv3858	**Glutamate synthase,**	**gltD ,** MT3973,	UniProtKB:P96219	**PROBABLY INVOLVED IN**	**2 L-GLUTAMATE +**	**Product: PROBABLE NADH-**

Gene	*Full Name*	*Synonyms*	*Database*	Function	Catalytic Activity	Pathway & Miscellaneous
c	**small subunit**	P96219_MYCTU		**GLUTAMATE BIOSYNTHESIS**	**NAD(+) = L-GLUTAMINE + 2-OXOGLUTARATE + NADH**	**DEPENDENT GLUTAMATE SYNTHASE (SMALL SUBUNIT) GLTD (L-GLUTAMATE SYNTHASE) (L-GLUTAMATE SYNTHETASE) (NADH-GLUTAMATE SYNTHASE) (GLUTAMATE SYNTHASE (NADH)) (GLTS BETA CHAIN) (NADPH-GOGAT)** **KEGG GENES** mtu:Rv3858c
Rv1449c	**Transketolase**	**MT1496 ,** MTCY493.05 , Rv1449c , tkt , TKT_MYCTU	UniProtKB:O06811	**THIS ENZYME, TOGETHER WITH TRANSALDOLASE, PROVIDES A LINK BETWEEN THE GLYCOLYTIC AND PENTOSE-PHOSPHATE PATHWAYS. IT CATALYZES THE REVERSIBLE TRANSFER OF A TWO-CARBON KETOL UNIT FROM XYLULOSE 5-PHOSPHATE TO AN ALDOSE RECEPTOR**	**SEDOHEPTULOSE 7-PHOSPHATE + D-GLYCERALDEHYDE 3-PHOSPHATE = D-RIBOSE 5-PHOSPHATE + D-XYLULOSE 5-PHOSPHATE**	**Product: PROBABLE TRANSKETOLASE TKT (TK)** **KEGG GENES** mtu:Rv1449c

Table-6: Results of Double knockout of non-essential genes and it's correlated genes

Gene	*Correlated genes (With biomass zero)*	
Rv0211	Rv1389	**0.0**
	Rv2445c	**0.0**
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**

Rv0244c	Rv1389	**0.0**
	Rv2445c	**0.0**
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**

Rv0363c	Rv1389	**0.0**

Gene	*Correlated genes (With biomass zero)*	
	Rv2445c	**0.0**
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**

Rv0467	Rv1389	**0.0**
	Rv2445c	**0.0**
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**

Rv0619	Rv1389	**0.0**
	Rv2445c	**0.0**
	Rv1449c	**0.0**

Rv0951	Rv1389	**0.0**
	Rv2445c	**0.0**
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**
Rv1553	Rv1389	**0.0**
	Rv2445c	**0.0**
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**

Rv1736c	Rv1389	**0.0**

Gene	*Correlated genes (With biomass zero)*	
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**

Rv1811	Rv1389	**0.0**
	Rv2445c	**0.0**
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**

Rv1854c	Rv1389	**0.0**
	Rv2445c	**0.0**
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**

Rv2029c	Rv1389	**0.0**
	Rv2445c	**0.0**
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**

Rv2380c	Rv1389	**0.0**
	Rv2445c	**0.0**
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**

Rv2381c	Rv1389	**0.0**

Gene	*Correlated genes (With biomass zero)*	
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**

Rv2383c	Rv1389	**0.0**
	Rv2445c	**0.0**
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**

Rv2385	Rv1389	**0.0**
	Rv2445c	**0.0**
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**

Rv2503c	Rv1389	**0.0**
	Rv2445c	**0.0**
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**

Rv2713	Rv1389	**0.0**
	Rv2445c	**0.0**
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**

Rv2764c	Rv1389	**0.0**

Gene	*Correlated genes (With biomass zero)*	
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**

Rv2930	Rv1389	**0.0**
	Rv2445c	**0.0**
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**

Rv3206c	Rv1389	**0.0**
	Rv2445c	**0.0**
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**

Rv3774	Rv1389	**0.0**
	Rv2445c	**0.0**
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**

Correlated genes and their corresponding reactions:

Genes	*Reactions*
Rv1079	R181, R240, R253, R254, R255, R256, R258
Rv2713 OR Rv3303c	R379
Rv3309c	R311, R312
Rv0155 AND Rv0157 AND Rv0156	R376

Genes	*Reactions*
Rv0162c	R3, R73
Rv0946c	R37, R39, R40
Rv1389	R327, R328, R357
Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c	R73
Rv2445c	R294, R299, R305, R306, R329, R354, R358, R361
Rv2476c	R198
Rv2982c OR Rv0564 OR Rv3045	R2
Rv3045	R74
Rv3436c	R712
Rv3565 OR Rv0337c	R190, R195, R225, R284, R286
Rv3859c AND Rv3858c	R197
Rv1449c	R93, R94, R95, R96

Table-7: Pathway information of Correlated genes:

Data surce: KEGG database (http://www.genome.jp/kegg/) & TB database (http://www.tbdb.org/)

Gene	***Pathways***
Rv1079	1. Cysteine and methionine metabolism Mtu00270 2. Selenocompound metabolism mtu00450 3. Sulfur metabolism mtu00920 4. Metabolic pathways mtu01100 *5.* Biosynthesis of secondary metabolites mtu01110

Gene	*Pathways*
Rv2713	1. Nicotinate and nicotinamide metabolism Mtu00760 *2.* Metabolic pathways mtu01100
Rv3303c	1. Glycolysis / Gluconeogenesis Mtu00010 2. Citrate cycle (TCA cycle) mtu00020 3. Glycine, serine and threonine metabolism mtu00260 4. Valine, leucine and isoleucine degradation mtu00280 5. Pyruvate metabolism mtu00620 6. Metabolic pathways mtu01100 7. Biosynthesis of secondary metabolites mtu01110 *8.* Microbial metabolism in diverse environments mtu01120
Rv0155, Rv0156, Rv0157	1. Nicotinate and nicotinamide metabolism Mtu00760 *2.* Metabolic pathways mtu01100
Rv1389	1. Purine metabolism Mtu00230 *2.* Metabolic pathways mtu01100
Rv1862, Rv1530, Rv0162c, Rv0761c	1. Glycolysis / Gluconeogenesis Mtu00010 2. Fatty acid metabolism mtu00071 3. Tyrosine metabolism mtu00350 4. Chloroalkane and chloroalkene degradation mtu00625 5. Naphthalene degradation mtu00626 6. Metabolic pathways mtu01100 7. Biosynthesis of secondary metabolites mtu01110 *8.* Microbial metabolism in diverse environments mtu01120
Rv2445c	1. Purine metabolism Mtu00230 2. Pyrimidine metabolism mtu00240 3. Metabolic pathways mtu01100 *4.* Biosynthesis of secondary metabolites mtu01110
Rv2476c	1. Alanine, aspartate and glutamate metabolism Mtu00250 2. Arginine and proline metabolism mtu00330 3. Taurine and hypotaurine metabolism mtu00430 4. Nitrogen metabolism mtu00910 *5.* Metabolic pathways mtu01100
Rv2982c	*1.* Glycerophospholipid metabolism Mtu00564
Rv0564	1. phospholipid biosynthesis I 2. CDP-diacylglycerol biosynthesis I 3. CDP-diacylglycerol biosynthesis II 4. phosphatidylglycerol biosynthesis I (plastidic) 5. phosphatidylglycerol biosynthesis II (non-plastidic)
Rv3436c, Rv0337c	1. Alanine, aspartate and glutamate metabolism Mtu00250 2. Amino sugar and nucleotide sugar metabolism mtu00520 3. Metabolic pathways mtu01100 *4.* Biosynthesis of secondary metabolites mtu01110
Rv3565	1. alanine degradation III

Gene	*Pathways*
	2. alanine biosynthesis II 3. superpathway of alanine biosynthesis
Rv3858c, Rv3859c	1. Alanine, aspartate and glutamate metabolism Mtu00250 2. Nitrogen metabolism mtu00910 3. Metabolic pathways mtu01100 4. Biosynthesis of secondary metabolites mtu01110 5. Microbial metabolism in diverse environments mtu01120
Rv1449c	1. Pentose phosphate pathway Mtu00030 2. Metabolic pathways mtu01100 3. Biosynthesis of secondary metabolites mtu01110 4. Microbial metabolism in diverse environments mtu01120

Results:

Result generated after knockout studies of all 100 genes, in four models is as follows:

Genes	*Model(1)*	*Model(2)*	*Model(3)*	*Model(4)*
Rv0046c	Essential	Essential	Essential	Essential
Rv0070c	Non-essential	Non-essential	Non-essential	Non-essential
Rv0112	Non-essential	Non-essential	Non-essential	Non-essential
Rv0183	Non-essential	Non-essential	Non-essential	Non-essential
Rv0186	Non-essential	Non-essential	Non-essential	Non-essential
Rv0211	Non-essential	Non-essential	Non-essential	Non-essential
Rv0244c	Non-essential	Non-essential	Non-essential	Non-essential
Rv0363c	Non-essential	Non-essential	Non-essential	Non-essential
Rv0404	Non-essential	Non-essential	Non-essential	Non-essential
Rv0467	Non-essential	Non-essential	Non-essential	Non-essential
Rv0503c	Essential	Essential	Essential	Essential
Rv0619	Non-essential	Non-essential	Non-essential	Non-essential
Rv0753c	Non-essential	Non-essential	Non-essential	Non-essential
Rv0780	Non-essential	Non-essential	Non-essential	Non-essential
Rv0809	Essential	Essential	Essential	Essential

Genes	*Model(1)*	*Model(2)*	*Model(3)*	*Model(4)*
Rv0886	Non-essential	Non-essential	Non-essential	Non-essential
Rv0951	Non-essential	Non-essential	Non-essential	Non-essential
Rv0973c	Essential	Essential	Essential	Essential
Rv0974c	Essential	Essential	Essential	Essential
Rv1144	Non-essential	Non-essential	Non-essential	Non-essential
Rv1285	Non-essential	Non-essential	Non-essential	Non-essential
Rv1348	Essential	Essential	Essential	Essential
Rv1464	Essential	Essential	Essential	Essential
Rv1475c	Non-essential	Non-essential	Non-essential	Non-essential
Rv1500	Essential	Essential	Essential	Essential
Rv1525	Essential	Essential	Essential	Essential
Rv1553	Non-essential	Non-essential	Non-essential	Non-essential
Rv1623c	Essential	Essential	Essential	Essential
Rv1736c	Non-essential	Essential	Essential(non-feasible)	Essential(non-feasible)
Rv1811	Non-essential	Non-essential	Non-essential	Non-essential
Rv1832	Non-essential	Non-essential	Non-essential	Non-essential
Rv1854c	Non-essential	Non-essential	Non-essential	Non-essential
Rv2006	Essential	Essential	Essential	Essential
Rv2029c	Non-essential	Non-essential	Non-essential	Non-essential
Rv2121c	Non-essential	Non-essential	Non-essential	Non-essential
Rv2225	Essential	Essential	Essential	Essential
Rv2246	Essential	Essential	Essential	Essential
Rv2380c	Non-essential	Non-essential	Non-essential	Non-essential
Rv2381c	Non-essential	Non-essential	Non-essential	Non-essential

Genes	*Model(1)*	*Model(2)*	*Model(3)*	*Model(4)*
Rv2383c	Non-essential	Non-essential	Non-essential	Non-essential
Rv2385	Non-essential	Non-essential	Non-essential	Non-essential
Rv2386c	Essential	Essential	Essential	Essential
Rv2482c	Essential	Essential	Essential	Essential
Rv2503c	Non-essential	Non-essential	Non-essential	Non-essential
Rv2713	Non-essential	Non-essential	Non-essential	Non-essential
Rv2764c	Non-essential	Non-essential	Non-essential	Non-essential
Rv2780	Non-essential	Non-essential	Non-essential	Non-essential
Rv2930	Non-essential	Non-essential	Non-essential	Non-essential
Rv2931	Non-essential	Non-essential	Non-essential	Non-essential
Rv2940c	Essential	Essential	Essential	Essential
Rv2959c	Non-essential	Non-essential	Non-essential	Non-essential
Rv3001c	Non-essential	Non-essential	Non-essential	Non-essential
Rv3002c	Non-essential	Non-essential	Non-essential	Non-essential
Rv3048c	Essential	Essential	Essential	Essential
Rv3206c	Non-essential	Essential	Essential(non-feasible)	Essential(non-feasible)
Rv3601c	Essential	Essential	Essential	Essential
Rv3774	Non-essential	Non-essential	Non-essential	Non-essential
Rv3913	Essential	Essential	Essential	Essential
Rv0752c	Non-essential	Non-essential	Non-essential	Non-essential
Rv0859	Non-essential	Non-essential	Non-essential	Non-essential
Rv1467c	Non-essential	Non-essential	Non-essential	Non-essential
Rv1737c	Non-essential	Essential	Essential	Essential
Rv2497c	Non-essential	Non-essential	Non-essential	Non-essential

Genes	*Model(1)*	*Model(2)*	*Model(3)*	*Model(4)*
Rv2933	Non-essential	Non-essential	Non-essential	Non-essential
Rv2950c	Non-essential	Non-essential	Non-essential	Non-essential
Rv2332	Non-essential	Non-essential	Non-essential	Non-essential
Rv3515c	Non-essential	Non-essential	Non-essential	Non-essential
Rv0468	Non-essential	Non-essential	Non-essential	Non-essential
Rv0551c	Non-essential	Non-essential	Non-essential	Non-essential
Rv0952	Non-essential	Non-essential	Non-essential	Non-essential
Rv1345	Non-essential	Non-essential	Non-essential	Non-essential
Rv2724c	Non-essential	Non-essential	Non-essential	Non-essential
Rv2932	Non-essential	Non-essential	Non-essential	Non-essential
Rv2935	Non-essential	Non-essential	Non-essential	Non-essential
Rv3003c	Non-essential	Non-essential	Non-essential	Non-essential
Rv3061c	Non-essential	Non-essential	Non-essential	Non-essential
Rv3516	Non-essential	Non-essential	Non-essential	Non-essential
Rv3546	Non-essential	Non-essential	Non-essential	Non-essential
Rv3804c	Essential	Essential	Essential	Essential
Rv0166	Non-essential	Non-essential	Non-essential	Non-essential
Rv0408	Non-essential	Non-essential	Non-essential	Non-essential
Rv0694	Non-essential	Non-essential	Non-essential	Non-essential
Rv1497	Non-essential	Non-essential	Non-essential	Non-essential
Rv1613	Non-essential	Non-essential	Non-essential	Non-essential
Rv3084	Non-essential	Non-essential	Non-essential	Non-essential
Rv3145	Non-essential	Non-essential	Non-essential	Non-essential
Rv3146	Non-essential	Non-essential	Non-essential	Non-essential

Genes	*Model(1)*	*Model(2)*	*Model(3)*	*Model(4)*
Rv3147	Non-essential	Non-essential	Non-essential	Non-essential
Rv3148	Non-essential	Non-essential	Non-essential	Non-essential
Rv3149	Non-essential	Non-essential	Non-essential	Non-essential
Rv3150	Non-essential	Non-essential	Non-essential	Non-essential
Rv3152	Non-essential	Non-essential	Non-essential	Non-essential
Rv3153	Non-essential	Non-essential	Non-essential	Non-essential
Rv3154	Non-essential	Non-essential	Non-essential	Non-essential
Rv3155	Non-essential	Non-essential	Non-essential	Non-essential
Rv3156	Non-essential	Non-essential	Non-essential	Non-essential
Rv3157	Non-essential	Non-essential	Non-essential	Non-essential
Rv3158	Non-essential	Non-essential	Non-essential	Non-essential
Rv3322c	Non-essential	Essential	Essential	Essential
Rv1349	Essential	Essential	Essential	Essential

Growth rate (Biomass production) after gene knock outs:

Genes	***Model-1***	***Model-2***	***Model-3***	***Model-4***
Rv0046c	0.000000	0.000000	0.000000	0.000000
Rv0070c	0.000711	0.000711	0.000711	0.000711
Rv0112	0.054775	0.013069	0.013069	0.013069
Rv0183	0.054419	0.013069	0.013069	0.013069
Rv0186	0.054676	0.013069	0.013069	0.013069
Rv0211	0.054775	0.013069	0.013069	0.013069
Rv0244c	0.05319	0.013069	0.013069	0.013069
Rv0363c	0.052487	0.002163	0.002163	0.002163

Genes	*Model-1*	*Model-2*	*Model-3*	*Model-4*
Rv0404	0.052379	0.013069	0.013069	0.013069
Rv0467	0.052752	0.013069	0.013069	0.013069
Rv0503c	0.000000	0.000000	0.000000	0.000000
Rv0619	0.054725	0.013069	0.013069	0.013069
Rv0753c	0.054775	0.013069	0.013069	0.013069
Rv0780	0.000680	0.000680	0.000680	0.000680
Rv0809	0.000000	0.000000	0.000000	0.000000
Rv0886	0.025964	0.003161	0.003161	0.003161
Rv0951	0.054772	0.013069	0.013069	0.013069
Rv0973c	0.000000	0.000000	0.000000	0.000000
Rv0974c	0.000000	0.000000	0.000000	0.000000
Rv1144	0.050816	0.013069	0.013069	0.013069
Rv1285	0.025961	0.003161	0.003161	0.003161
Rv1348	0.000000	0.000000	0.000000	0.000000
Rv1464	0.000000	0.000000	0.000000	0.000000
Rv1475c	0.010905	0.004630	0.004630	0.004630
Rv1500	0.000000	0.000000	0.000000	0.000000
Rv1525	0.000000	0.000000	0.000000	0.000000
Rv1553	0.053562	0.013069	0.013069	0.013069
Rv1623c	0.000000	0.000000	0.000000	0.000000
Rv1736c	0.054775	0.000000	0.000000	0.000000
Rv1811	0.055743	0.013069	0.013069	0.013069
Rv1832	0.000694	0.000694	0.000694	0.000694
Rv1854c	0.054775	0.013069	0.013069	0.013069
Rv2006	0.000000	0.000000	0.000000	0.000000

Genes	*Model-1*	*Model-2*	*Model-3*	*Model-4*
Rv2029c	0.052538	0.013069	0.013069	0.013069
Rv2121c	0.044932	0.013069	0.013069	0.013069
Rv2225	0.000000	0.000000	0.000000	0.000000
Rv2246	0.000000	0.000000	0.000000	0.000000
Rv2380c	0.054775	0.013069	0.013069	0.013069
Rv2381c	0.054775	0.013069	0.013069	0.013069
Rv2383c	0.054775	0.013069	0.013069	0.013069
Rv2385	0.054415	0.013069	0.013069	0.013069
Rv2386c	0.000000	0.000000	0.000000	0.000000
Rv2482c	0.000000	0.000000	0.000000	0.000000
Rv2503c	0.054775	0.013069	0.013069	0.013069
Rv2713	0.054775	0.013069	0.013069	0.013069
Rv2764c	0.054775	0.054775	0.013069	0.013069
Rv2780	0.004619	0.004619	0.004619	0.004619
Rv2930	0.052379	0.013069	0.013069	0.013069
Rv2931	0.025961	0.013069	0.013069	0.013069
Rv2940c	0.000000	0.000000	0.000000	0.000000
Rv2959c	0.054775	0.013069	0.013069	0.013069
Rv3001c	0.012718	0.012718	0.012718	0.012718
Rv3002c	0.012718	0.012718	0.012718	0.012718
Rv3048c	0.000000	0.000000	0.000000	0.000000
Rv3206c	0.054775	0.000000	0.000000	0.000000
Rv3601c	0.000000	0.000000	0.000000	0.000000
Rv3774	0.048973	0.013069	0.013069	0.013069
Rv3913	0.000000	0.000000	0.000000	0.000000

Genes	*Model-1*	*Model-2*	*Model-3*	*Model-4*
Rv0752c	0.05319	0.013069	0.013069	0.013069
Rv0859	0.05319	0.013069	0.013069	0.013069
Rv1467c	0.05319	0.013069	0.013069	0.013069
Rv1737c	0.054775	0.000000	0	0
Rv2497c	0.050816	0.013069	0.013069	0.013069
Rv2933	0.054775	0.013069	0.013069	0.013069
Rv2950c	0.052379	0.013069	0.013069	0.013069
Rv2332	0.054775	0.013069	0.013069	0.013069
Rv3515c	0.052379	0.013069	0.013069	0.013069
Rv0468	0.05319	0.013069	0.013069	0.013069
Rv0551c	0.052379	0.013069	0.013069	0.013069
Rv0952	0.054772	0.013069	0.013069	0.013069
Rv1345	0.052379	0.013069	0.013069	0.013069
Rv2724c	0.05319	0.013069	0.013069	0.013069
Rv2932	0.054775	0.013069	0.013069	0.013069
Rv2935	0.054775	0.013069	0.013069	0.013069
Rv3003c	0.012718	0.012718	0.012718	0.012718
Rv3061c	0.05319	0.013069	0.013069	0.013069
Rv3516	0.05319	0.013069	0.013069	0.013069
Rv3546	0.05319	0.013069	0.013069	0.013069
Rv3804c	0	0.000000	0	0
Rv0166	0.052379	0.013069	0.013069	0.013069
Rv0408	0.05477	0.013069	0.013069	0.013069
Rv0694	0.054751	0.013069	0.013069	0.013069
Rv1497	0.054415	0.013069	0.013069	0.013069

Genes	*Model-1*	*Model-2*	*Model-3*	*Model-4*
Rv1613	0.035401	0.013069	0.013069	0.013069
Rv3084	0.054415	0.013069	0.013069	0.013069
Rv3145	0.050417	0.013069	0.013069	0.013069
Rv3146	0.050417	0.013069	0.013069	0.013069
Rv3147	0.050417	0.013069	0.013069	0.013069
Rv3148	0.050417	0.013069	0.013069	0.013069
Rv3149	0.050417	0.013069	0.013069	0.013069
Rv3150	0.050417	0.013069	0.013069	0.013069
Rv3152	0.050417	0.013069	0.013069	0.013069
Rv3153	0.050417	0.013069	0.013069	0.013069
Rv3154	0.050417	0.013069	0.013069	0.013069
Rv3155	0.050417	0.013069	0.013069	0.013069
Rv3156	0.050417	0.013069	0.013069	0.013069
Rv3157	0.050417	0.013069	0.013069	0.013069
Rv3158	0.050417	0.013069	0.013069	0.013069
Rv3322c	0.054775	0.000000	0	0
Rv1349	0	0.000000	0	0

Here in this plot (Figure-7) Y-axes represents all the genes corresponding to all reactions, and the X-axes represents the values of maximum flux, this plot is FVA result of gene Rv0211, for which there are 16 correlated genes, which having highest maximum flux value (100000.0). this cluster of 16 genes, is selected as the set of correlated genes for the non-essential gene Rv0211. This process repeated similarity for all 23 genes.

Results:

Gene	*Correlated genes*
Rv0183	**Rv1079 ,Rv2713 OR Rv3303c, Rv3309c ,Rv0155 AND Rv0157 AND Rv0156, Rv0162c, Rv0946c, Rv1389, Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c, Rv2445c, Rv2476c, Rv2982c OR Rv0564 OR Rv3045, Rv1449c**

Gene	*Correlated genes*
	Rv3045, Rv3436c, Rv3565 OR Rv0337c, Rv3859c AND Rv3858c
Rv0186	**Rv3859c AND Rv3858c , Rv3565 OR Rv0337c, Rv3436c, Rv3309c , Rv3045, Rv2982c OR Rv0564 OR Rv3045, Rv2713 OR Rv3303c, Rv2476c, Rv2445c, Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c, Rv1389 , Rv1079, Rv0946c, Rv0162c , v0155 AND Rv0157 AND Rv0156,** **Rv1449c**
Rv0211	**Rv0155 AND Rv0157 AND Rv0156 , Rv0162c , R v0946c , Rv1079** **Rv1389 , Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c, Rv2445c , Rv2476c, Rv2713 OR Rv3303c , Rv2982c OR Rv0564 OR Rv3045,** **Rv3045 , Rv3309c , Rv3436c , Rv3565 OR Rv0337c ,** **Rv3859c AND Rv3858c, Rv1449c**
Rv0244c	**Rv3859c AND Rv3858c , Rv3565 OR Rv0337c, Rv3436c, Rv3309c, Rv3045, Rv2982c OR Rv0564 OR Rv3045, Rv2713 OR Rv3303c , Rv2476c, Rv2445c, Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c , Rv1389, Rv1079, Rv0946c, Rv0162c, Rv0155 AND Rv0157 AND Rv0156, Rv1449c**
Rv0363c	**Rv3859c AND Rv3858c, Rv3565 OR Rv0337c, Rv3436c, Rv3309c, Rv3045, Rv2982c OR Rv0564 OR Rv3045 , Rv2713 OR Rv3303c, Rv2476c, Rv2445c, Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c ,Rv1389, Rv1079, Rv0946c, Rv0162c , Rv0155 AND Rv0157 AND Rv0156 , Rv1449c**
Rv0467	**Rv0155 AND Rv0157 AND Rv0156 ,Rv0162c,Rv0946c,Rv1079,Rv1389,Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c ,Rv2445c,Rv2476c,Rv2713 OR Rv3303c,** **Rv2982c OR Rv0564 OR Rv3045 ,Rv3045,Rv3309c,Rv3436c, Rv3565 OR Rv0337c, Rv3859c AND Rv3858c, Rv1449c**
Rv0619	**Rv2982c OR Rv0564 OR Rv3045,Rv0162c, Rv0946c ,Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c ,Rv3045, Rv1079, Rv3565 OR Rv0337c ,Rv3859c AND Rv3858c ,Rv2476c, Rv1449c,Rv3436c,Rv3309c,Rv1389, Rv2445c, Rv1389, Rv0155 AND Rv0157 AND Rv0156, Rv2713 OR Rv3303c**
Rv0951	**Rv2982c OR Rv0564 OR Rv3045, Rv0162c, Rv0946c, Rv1862 OR Rv1530 OR Rv0162c OR**

Gene	*Correlated genes*
	Rv0761c , Rv3045, Rv1079, Rv3859c AND Rv3858c, Rv2476c, Rv3565 OR Rv0337c, Rv3309c, Rv1389, Rv2445c, Rv0155 AND Rv0157 AND Rv0156, Rv2713 OR Rv3303c, Rv3436c , Rv1449c
Rv1553	**Rv0155 AND Rv0157 AND Rv0156 , Rv0162c, Rv0946c, Rv1079, Rv1389, Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c , Rv2445c , Rv2476c , Rv2713 OR Rv3303c , Rv2982c OR Rv0564 OR Rv3045, Rv3045, Rv3309c, Rv3436c , Rv3565 OR Rv0337c, Rv3859c AND Rv3858c, Rv1449c**
Rv1736c	**Rv0155 AND Rv0157 AND Rv0156, Rv0162c, Rv0946c, Rv1079, Rv1389, Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c , Rv2445c, Rv2476c , Rv2713 OR Rv3303c , Rv2982c OR Rv0564 OR Rv3045, Rv3045, Rv3309c , Rv3436c, Rv3565 OR Rv0337c , Rv3859c AND Rv3858c, Rv1449c**
Rv1811	**Rv2982c OR Rv0564 OR Rv3045, Rv0162c, Rv0946c, Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c , Rv3045, Rv1079, Rv3565 OR Rv0337c,Rv3859c AND Rv3858c ,Rv2476c, Rv3309c, Rv2445c , Rv1389, Rv0155 AND Rv0157 AND Rv0156, Rv2713 OR Rv3303c, Rv3436c, Rv1449c**
Rv1854c	**Rv3859c AND Rv3858c, Rv3565 OR Rv0337c, Rv3436c, Rv3309c, Rv3045, Rv2982c OR Rv0564 OR Rv3045, Rv2713 OR Rv3303c, Rv2476c, Rv2445c, Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c, Rv1389, Rv1079, Rv0946c, Rv0162c, Rv0155 AND Rv0157 AND Rv0156, Rv1449c**
Rv2029c	**Rv3859c AND Rv3858c, Rv3565 OR Rv0337c, Rv3436c ,Rv3309c , Rv3045 ,Rv2982c OR Rv0564 OR Rv3045, Rv2713 OR Rv3303c, Rv2476c , Rv2445c , Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c, Rv1389 , Rv1079 , Rv0946c , Rv0162c , Rv0155 AND Rv0157 AND Rv0156, Rv1449c**
Rv2380c	**Rv0155 AND Rv0157 AND Rv0156 , Rv0162c , Rv0946c, Rv1079,Rv1389, Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c, Rv2445c, Rv2476c,Rv2713 OR Rv3303c, Rv2982c OR Rv0564 OR Rv3045, Rv3045, Rv3309c, Rv3436c, Rv3565 OR Rv0337c, Rv3859c AND Rv3858c, Rv1449c**
Rv2381c	**Rv0155 AND Rv0157 AND Rv0156,Rv0162c, Rv0946c, Rv1079, Rv1389,Rv1862 OR Rv1530**

Gene	*Correlated genes*
	OR Rv0162c OR Rv0761c,Rv2445c, Rv2476c, Rv2713 OR Rv3303c, Rv2982c OR Rv0564 OR Rv3045, Rv3045, Rv3309c, Rv3436c, Rv3565 OR Rv0337c, Rv3859c AND Rv3858c, Rv1449c
Rv2383c	**Rv2982c OR Rv0564 OR Rv3045, Rv0162c, Rv0946c, Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c, Rv3045, Rv1079, Rv3565 OR Rv0337c, Rv3859c AND Rv3858c, Rv2476c, Rv1079, Rv3565 OR Rv0337c, Rv3309c, Rv2445c, Rv1389, Rv0155 AND Rv0157 AND Rv0156, Rv2713 OR Rv3303c, Rv3436c, Rv1449c**
Rv2385	**Rv2982c OR Rv0564 OR Rv3045, Rv0162c, Rv0946c, Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c, Rv3045, Rv1079, Rv3565 OR Rv0337c, Rv3859c AND Rv3858c, Rv2476c, Rv1079, Rv3565 OR Rv0337c , Rv3309c, Rv2445c, Rv1389, Rv0155 AND Rv0157 AND Rv0156 , Rv2713 OR Rv3303c, Rv3436c , Rv1449c**
Rv2503c	**Rv2982c OR Rv0564 OR Rv3045 , Rv0162c, Rv0946c, Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c , Rv3045, Rv1079, Rv3859c AND Rv3858c , Rv2476c, Rv1079 , Rv3565 OR Rv0337c, Rv3309c, Rv1389 , Rv2445c, Rv0155 AND Rv0157 AND Rv0156, Rv2713 OR Rv3303c, Rv3436c, Rv1449c**
Rv2713	**Rv2982c OR Rv0564 OR Rv3045, Rv0162c , Rv0946c , Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c , Rv3045, Rv1079, Rv3565 OR Rv0337c, Rv3859c AND Rv3858c, Rv2476c, Rv1079, Rv3309c, Rv1389, Rv2445c, Rv0155 AND Rv0157 AND Rv0156, Rv3436c, Rv1449c**
Rv2764c	**Rv2982c OR Rv0564 OR Rv3045 ,Rv0162c, Rv0946c, Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c , Rv3045, Rv1079, Rv3859c AND Rv3858c, Rv2476c, Rv1079 , Rv3565 OR Rv0337c, Rv3309c, Rv1389, Rv2445c , Rv1389, Rv0155 AND Rv0157 AND Rv0156 , Rv2713 OR Rv3303c, Rv3436c, Rv1449c**
Rv2930	**Rv2982c OR Rv0564 OR Rv3045, Rv0162c , Rv0946c , Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c , Rv3045 , Rv1079 ,Rv3859c AND Rv3858c, Rv2476c , Rv3565 OR Rv0337c , Rv3309c , Rv1389 ,Rv2445c ,Rv0155 AND Rv0157 AND Rv0156 ,Rv2713 OR Rv3303c, Rv3436c , Rv1449c**
Rv3206c	**Rv2982c OR Rv0564 OR Rv3045, Rv0162c, Rv0946c, Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c , Rv3045, Rv1079, Rv3859c AND Rv3858c, Rv2476c , Rv1079, Rv3565 OR Rv0337c,**

Gene	*Correlated genes*
	Rv3309c, Rv1389, Rv2445c ,Rv0155 AND Rv0157 AND Rv0156 , Rv2713 OR Rv3303c, Rv3436c, Rv1449c
Rv3774	**Rv2982c OR Rv0564 OR Rv3045 ,Rv0162c, Rv0946c, Rv1862 OR Rv1530 OR Rv0162c OR Rv0761c ,Rv3045, Rv1079, Rv3565 OR Rv0337c, Rv3859c AND Rv3858c , Rv2476c, Rv1079, Rv3309c, Rv1389 , Rv2445c, Rv0155 AND Rv0157 AND Rv0156 , Rv2713 OR Rv3303c , Rv3436c, Rv1449c**

Properties of correlated genes:

Gene	*Full Name*	*Synonyms*	*Database*	Function	Catalytic Activity	Pathway & Miscellaneous
Rv1079 Nonessential model1	**Cystathionine gamma-synthase**	**METB_MYCTU,** MTV017.32, metB, MT1110	UniProtKB:P66875	**INVOLVED IN METHIONINE BIOSYNTHESIS: CONVERTS O-SUCCINYL-L-HOMOSERINE TO CYSTATHIONINE**	**O-SUCCINYL-L-HOMOSERINE + L-CYSTEINE = CYSTATHIONINE + SUCCINATE (CAN ALSO USE HYDROGEN SULFIDE AND METHANETHIOL AS SUBSTRATES)**	**Product:** **PROBABLE CYSTATHIONINE GAMMA-SYNTHASE METB (CGS) (O-SUCCINYLHOMOSERINE [THIOL]-LYASE)** **KEGG GENES** mtu:Rv1079
Rv2713	**Probable soluble pyridine nucleotide transhydrogenase**	**SthA MT2786** MTCY05A6.34 STHA_MYCTU	UniProtKB:P66006	**CONVERSION OF NADPH, GENERATED BY PERIPHERAL CATABOLIC PATHWAYS, TO NADH, WHICH CAN ENTER THE RESPIRATORY CHAIN FOR ENERGY GENERATION**	**NADPH + NAD(+) = NADP(+) + NADH**	**Product:** **PROBABLE SOLUBLE PYRIDINE NUCLEOTIDE TRANSHYDROGENASE STHA (STH) (NAD(P)(+) TRANSHYDROGENASE [B-SPECIFIC]) (NICOTINAMIDE NUCLEOTIDE TRANSHYDROGENASE)** **KEGG GENES** mtu:Rv2713
Rv3303c	**NAD(P)H dehydrogenase (quinone)**	**lpdA ,** lpdA-2, LPDA_MYCTU , MT3402	UniProtKB:O53355	**INVOLVED IN ENERGY METABOLISM. CAN CATALYZE THE REDUCTION OF ELECTRON ACCEPTORS SUCH AS 2,6-DIMETHYL-1,4-BENZOQUINONE (DMBQ) AND 5-HYDROXY-1,4-NAPTHAQUINONE (5-HNQ)**	**CATALYTIC ACTIVITY: NAD(P)H + A QUINONE + H+ -> A QUINOL + NAD(P)+**	**Product:** **NAD(P)H QUINONE REDUCTASE LPDA** **KEGG GENES** mtu:Rv3303c

Gene	*Full Name*	*Synonyms*	*Database*	Function	Catalytic Activity	Pathway & Miscellaneous
Rv0155	**PROBABLE NAD(P) TRANSHYDROGENASE (SUBUNIT ALPHA) PNTAA [FIRST PART; CATALYTIC PART] (PYRIDINE NUCLEOTIDE TRANSHYDROGENASE SUBUNIT ALPHA) (NICOTINAMIDE NUCLEOTIDE TRANSHYDROGENASE SUBUNIT ALPHA)**	**P96832_MYCTU,** pntAa	UniProtKB:P96832	**THE TRANSHYDROGENATION BETWEEN NADH AND NADP IS COUPLED TO RESPIRATION AND ATP HYDROLYSIS AND FUNCTIONS AS A PROTON PUMP ACROSS THE MEMBRANE**	**NADPH + NAD+ = NADP+ + NADH**	**Product:** **PROBABLE NAD(P) TRANSHYDROGENASE (SUBUNIT ALPHA) PNTAA [FIRST PART; CATALYTIC PART] (PYRIDINE NUCLEOTIDE TRANSHYDROGENASE SUBUNIT ALPHA) (NICOTINAMIDE NUCLEOTIDE TRANSHYDROGENASE SUBUNIT ALPHA)** **KEGG GENES** mtu:Rv0155
Rv0156	**PROBABLE NAD(P) TRANSHYDROGENASE (SUBUNIT ALPHA) PNTAB [SECOND PART; INTEGRAL MEMBRANE PROTEIN] (PYRIDINE NUCLEOTIDE TRANSHYDROGENASE SUBUNIT ALPHA) (NICOTINAMIDE NUCLEOTIDE TRANSHYDROGENASE SUBUNIT ALPHA)**	**P96833_MYCTU,** pntAb	UniProtKB:P96833	**THE TRANSHYDROGENATION BETWEEN NADH AND NADP IS COUPLED TO RESPIRATION AND ATP HYDROLYSIS AND FUNCTIONS AS A PROTON PUMP ACROSS THE MEMBRANE**	**NADPH + NAD+ = NADP+ + NADH**	**Product:** **PROBABLE NAD(P) TRANSHYDROGENASE (SUBUNIT ALPHA) PNTAB [SECOND PART; INTEGRAL MEMBRANE PROTEIN] (PYRIDINE NUCLEOTIDE TRANSHYDROGENASE SUBUNIT ALPHA) (NICOTINAMIDE NUCLEOTIDE TRANSHYDROGENASE SUBUNIT ALPHA)** **KEGG GENES** mtu:Rv0156
Rv0157	**NAD(P) transhydrogenase subunit beta**	**MT0165 ,** P96834_MYCTU , pntB	UniProtKB:P96834	**THE TRANSHYDROGENATION BETWEEN NADH AND NADP IS COUPLED TO RESPIRATION AND ATP HYDROLYSIS**	**NADPH + NAD+ = NADP+ + NADH**	**Product:** **PROBABLE NAD(P) TRANSHYDROGENASE (SUBUNIT BETA) PNTB [INTEGRAL MEMBRANE PROTEIN] (PYRIDINE NUCLEOTIDE**

Gene	*Full Name*	*Synonyms*	*Database*	Function	Catalytic Activity	Pathway & Miscellaneous
				AND FUNCTIONS AS A PROTON PUMP ACROSS THE MEMBRANE		**TRANSHYDROGENASE SUBUNIT BETA) (NICOTINAMIDE NUCLEOTIDE TRANSHYDROGENASE SUBUNIT BETA)** **KEGG GENES** mtu:Rv0157
Rv1389	**Guanylate kinase**	**gmk ,** KGUA_MYCTU, MT1434 , MTCY21B4.06	UniProtKB:P0A5I4	**ESSENTIAL FOR RECYCLING GMP AND INDIRECTLY, CGMP**	**ATP + GMP = ADP + GDP**	**Product:** **PROBABLE GUANYLATE KINASE GMK** **KEGG GENES** mtu:Rv1389
Rv1862		**adhA**		**CATALYZES THE REVERSIBLE OXIDATION OF ETHANOL TO ACETALDEHYDE WITH THE CONCOMITANT REDUCTION OF NAD**		**Product:** **PROBABLE ALCOHOL DEHYDROGENASE ADHA** **KEGG GENES** mtu:Rv1862
Rv1530		**adh**		**CATALYZES THE REVERSIBLE OXIDATION OF ETHANOL TO ACETALDEHYDE WITH THE CONCOMITANT REDUCTION OF NAD**		**Product:** **PROBABLE ALCOHOL DEHYDROGENASE ADH** **KEGG GENES** mtu:Rv1530
Rv0162c		**adhE1**		**DEHYDROGENESES A ALCOHOL (OXIDO-REDUCTION)**	**AN ALCOHOL + NAD+ = AN ALDEHYDE OR KETONE + NADH**	**Product:** **PROBABLE ZINC-TYPE ALCOHOL DEHYDROGENASE (E SUBUNIT) ADHE** **KEGG GENES** mtu:Rv0162c
Rv0761c	**Alcohol dehydrogenase B**	**ADHB_MYCTU,** adhB, MTCY369.06c, Rv0761c, MT0786	UniProtKB:P71818	**DEHYDROGENESES A ALCOHOL (OXIDO-REDUCTION)**	**AN ALCOHOL + NAD+ = AN ALDEHYDE OR KETONE + NADH**	**Product:** **PROBABLE ZINC-TYPE ALCOHOL DEHYDROGENASE (E SUBUNIT) ADHE** **KEGG GENES** mtu:Rv0761c
Rv2445	**Nucleoside diphosphate**	**MT2521,** MTCY428	UniProtKB:P84284	**MAJOR ROLE IN THE SYNTHESIS**	**ATP + NUCLEOSIDE**	**Product:** **PROBABLE**

Gene	*Full Name*	*Synonyms*	*Database*	Function	Catalytic Activity	Pathway & Miscellaneous
c	**kinase**	.01, MTV008.01c ndk , ndkA , NDK_MYCTU		**OF NUCLEOSIDE TRIPHOSPHATES OTHER THAN ATP**	**DIPHOSPHATE = ADP + NUCLEOSIDE TRIPHOSPHATE**	**NUCLEOSIDE DIPHOSPHATE KINASE NDKA (NDK) (NDP KINASE) (NUCLEOSIDE-2-P KINASE)** **KEGG GENES** mtu:Rv2445c
Rv2476c	**PROBABLE NAD-DEPENDENT GLUTAMATE DEHYDROGENASE GDH (NAD-GDH) (NAD-DEPENDENT GLUTAMIC DEHYDROGENASE)**	**O53203_MYCTU,** gdh	UniProtKB:O53203	**CATABOLIC GLUTDH INVOLVED IN THE UTILIZATION OF GLUTAMATE AND OTHER AMINO ACIDS OF THE GLUTAMATE FAMILY. GENERATES 2-OXOGLUTARATE FROM L-GLUTAMATE**	**L-GLUTAMATE + H(2)O + NAD(+) = 2-OXOGLUTARATE + NH(3) + NADH**	**Product: PROBABLE NAD-DEPENDENT GLUTAMATE DEHYDROGENASE GDH (NAD-GDH) (NAD-DEPENDENT GLUTAMIC DEHYDROGENASE)** **KEGG GENES** mtu:Rv2476c
Rv2982c	**Glycerol-3-phosphate dehydrogenase [NAD(P)+]**	**gpdA2 ,** GPDA_MYCTU , gpsA , MT3060 , MTCY349.05	UniProtKB:P95113	**INVOLVED IN DE NOVO PHOSPHOLIPID BIOSYNTHESIS; GLYCEROL-3 PHOSPHATE FORMATION**	**SN-GLYCEROL 3-PHOSPHATE + NAD(P)(+) = GLYCERONE PHOSPHATE + NAD(P)H**	**ProductPROBABLE GLYCEROL-3-PHOSPHATE DEHYDROGENASE [NAD(P)+] GPDA2 (NAD(P)H- DEPENDENT GLYCEROL-3-PHOSPHATE DEHYDROGENASE)** **KEGG GENES** mtu:Rv2982c
Rv0564		**gpdA1, gpsA, glyC**		**NVOLVED IN DE NOVO PHOSPHOLIPID BIOSYNTHESIS; GLYCEROL-3 PHOSPHATE FORMATION**	**SN-GLYCEROL 3-PHOSPHATE + NAD(P)+ = GLYCERONE PHOSPHATE + NAD(P)H**	**Product: PROBABLE GLYCEROL-3-PHOSPHATE DEHYDROGENASE [NAD(P)+] GPDA1 (NAD(P)H-DEPENDENT GLYCEROL-3-PHOSPHATE DEHYDROGENASE) (NAD(P)H-DEPENDENT DIHYDROXYACETONE-PHOSPHATE REDUCTASE)** **KEGG GENES** mtu:Rv0564c
Rv3045	**NADP-dependent alcohol dehydrogenase C**	**adh,** adhC, ADHC_MYCTU, MT3130, MTV012.	UniProtKB:P0A4X0	**GENERATES ALDEHYDE OR KETONE FROM ALCOHOL**	**ALCOHOL + NADP(+) = ALDEHYDE OR KETONE + NADPH**	**Product: PROBABLE NADP-DEPENDENT ALCOHOL DEHYDROGENASE ADHC** **KEGG GENES**

Gene	*Full Name*	*Synonyms*	*Database*	Function	Catalytic Activity	Pathway & Miscellaneous
		60				mtu:Rv3045
Rv3436c	**Glucosamine--fructose-6-phosphate aminotransferase [isomerizing]**	**glmS,** GLMS_MYCTU, MT3542, MTCY77.08c	UniProtKB:P0A588	**CATALYZES THE FIRST STEP IN HEXOSAMINE METABOLISM, CONVERTING FRUCTOSE-6P INTO GLUCOSAMINE-6P USING GLUTAMINE AS A NITROGEN SOURCE**	**L-GLUTAMINE + D-FRUCTOSE 6-PHOSPHATE = L-GLUTAMATE + D-GLUCOSAMINE 6-PHOSPHATE**	**Product:PROBABLE GLUCOSAMINE--FRUCTOSE-6-PHOSPHATE AMINOTRANSFERASE [ISOMERIZING] GLMS (HEXOSEPHOSPHATE AMINOTRANSFERASE) (D-FRUCTOSE-6-PHOSPHATE AMIDOTRANSFERASE) (GFAT) (L-GLUTAMINE-D-FRUCTOSE-6-PHOSPHATE AMIDOTRANSFERASE) (GLUCOSAMINE-6-PHOSPHATE SYNTHASE)** KEGG GENES mtu:Rv3436c
Rv3565		**aspB**		**THOUGHT TO BE INVOLVED IN GLUTAMATE BIOSYNTHESIS**	**L-ASPARTATE + 2-OXOGLUTARATE = OXALOACETATE + L-GLUTAMATE**	**Product: POSSIBLE ASPARTATE AMINOTRANSFERASE ASPB (TRANSAMINASE A) (ASPAT) (GLUTAMIC--OXALOACETIC TRANSAMINASE) (GLUTAMIC--ASPARTIC TRANSAMINASE)** KEGG GENES mtu:Rv3565
Rv0337c	**Probable aspartate aminotransferase**	**AAT_MYCTU,** aspC , MT0351, MTCY279.04c	UniProtKB:P63498	**GENERATES OXALOACETATE AND L-GLUTAMATE FROM L-ASPARTATE AND 2-OXOGLUTARATE**	**L-ASPARTATE + 2-OXOGLUTARATE = OXALOACETATE + L-GLUTAMATE**	**Product: PROBABLE ASPARTATE AMINOTRANSFERASE ASPC (TRANSAMINASE A) (ASPAT)** KEGG GENES mtu:Rv0337c
Rv3859c	**PROBABLE FERREDOXIN-DEPENDENT GLUTAMATE SYNTHASE [NADPH] (LARGE SUBUNIT) GLTB (L-GLUTAMAT**	**GltB,** P96218_MYCTU	UniProtKB:P96218	**PROBABLY INVOLVED IN GLUTAMATE BIOSYNTHESIS**	**2 L-GLUTAMATE + NADP(+) = L-GLUTAMINE + 2-OXOGLUTARATE + NADPH**	**Product: PROBABLE FERREDOXIN-DEPENDENT GLUTAMATE SYNTHASE [NADPH] (LARGE SUBUNIT) GLTB (L-GLUTAMATE SYNTHETASE) (NADH-GLUTAMATE**

Gene	*Full Name*	*Synonyms*	*Database*	Function	Catalytic Activity	Pathway & Miscellaneous
	E SYNTHASE) (L-GLUTAMATE SYNTHETASE) (NADH-GLUTAMATE SYNTHASE) (GLUTAMATE SYNTHASE (NADH))(NADPH-GOGAT)					**SYNTHASE) (GLUTAMATE SYNTHASE (NADH))(NADPH-GOGAT)** **KEGG GENES** mtu:Rv3859c
Rv3858c	**Glutamate synthase, small subunit**	**gltD ,** MT3973, P96219_MYCTU	UniProtKB:P96219	**PROBABLY INVOLVED IN GLUTAMATE BIOSYNTHESIS**	**2 L-GLUTAMATE + NAD(+) = L-GLUTAMINE + 2-OXOGLUTARATE + NADH**	**Product:** **PROBABLE NADH-DEPENDENT GLUTAMATE SYNTHASE (SMALL SUBUNIT) GLTD (L-GLUTAMATE SYNTHASE) (L-GLUTAMATE SYNTHETASE) (NADH-GLUTAMATE SYNTHASE) (GLUTAMATE SYNTHASE (NADH)) (GLTS BETA CHAIN) (NADPH-GOGAT)** **KEGG GENES** mtu:Rv3858c
Rv1449c	**Transketolase**	**MT1496 ,** MTCY493.05 , Rv1449c , tkt , TKT_MYCTU	UniProtKB:O06811	**THIS ENZYME, TOGETHER WITH TRANSALDOLASE, PROVIDES A LINK BETWEEN THE GLYCOLYTIC AND PENTOSE-PHOSPHATE PATHWAYS. IT CATALYZES THE REVERSIBLE TRANSFER OF A TWO-CARBON KETOL UNIT FROM XYLULOSE 5-PHOSPHATE TO AN ALDOSE RECEPTOR**	**SEDOHEPTULOSE 7-PHOSPHATE + D-GLYCERALDEHYDE 3-PHOSPHATE = D-RIBOSE 5-PHOSPHATE + D-XYLULOSE 5-PHOSPHATE**	**Product:** **PROBABLE TRANSKETOLASE TKT (TK)** **KEGG GENES** mtu:Rv1449c

Result:

Gene	*Correlated genes (With biomass zero)*	
Rv0211	Rv1389	**0.0**
	Rv2445c	**0.0**
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**

Rv0244c	Rv1389	**0.0**
	Rv2445c	**0.0**
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**

Rv0363c	Rv1389	**0.0**
	Rv2445c	**0.0**
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**

Rv0467	Rv1389	**0.0**
	Rv2445c	**0.0**
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**

Rv0619	Rv1389	**0.0**
	Rv2445c	**0.0**
	Rv1449c	**0.0**

	Rv1389	**0.0**

Gene	*Correlated genes (With biomass zero)*	
Rv0951	Rv2445c	**0.0**
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**
Rv1553	Rv1389	**0.0**
	Rv2445c	**0.0**
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**
Rv1736c	Rv1389	**0.0**
	Rv2445c	**0.0**
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**
Rv1811	Rv1389	**0.0**
	Rv2445c	**0.0**
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**
Rv1854c	Rv1389	**0.0**
	Rv2445c	**0.0**
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**
Rv2029c	Rv1389	**0.0**

Gene	*Correlated genes (With biomass zero)*	
	Rv2445c	**0.0**
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**

Rv2380c	Rv1389	**0.0**
	Rv2445c	**0.0**
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**

Rv2381c	Rv1389	**0.0**
	Rv2445c	**0.0**
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**

Rv2383c	Rv1389	**0.0**
	Rv2445c	**0.0**
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**

Rv2385	Rv1389	**0.0**
	Rv2445c	**0.0**
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**

Rv2503c	Rv1389	**0.0**

Gene	*Correlated genes (With biomass zero)*	
	Rv2445c	**0.0**
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**

Rv2713	Rv1389	**0.0**
	Rv2445c	**0.0**
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**

Rv2764c	Rv1389	**0.0**
	Rv2445c	**0.0**
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**

Rv2930	Rv1389	**0.0**
	Rv2445c	**0.0**
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**

Rv3206c	Rv1389	**0.0**
	Rv2445c	**0.0**
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**

Rv3774	Rv1389	**0.0**

Gene	*Correlated genes (With biomass zero)*	
	Rv2445c	**0.0**
	Rv3565 OR Rv0337c	**0.000785**
	Rv1449c	**0.0**
