Model SEED Tutorial Part 3: Exploring, Comparing and Analyzing Metabolic Models in Model SEED

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Presented by: Christopher Henry

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Fellowship for Interpretation of Genomes







Exploring, Comparing and Analyzing Metabolic Models in Model SEED

- •Selecting a model
- •Comparing models
- •Viewing model data on maps and tables
- •Exploring the model predictions
- •Running flux balance analysis

Selecting a Model Using the Filter Select

	The Mo Welcome to the Model SEEI For more information about	del SE - a resource for the ger The SEED please visit <u>th</u>	ED Mod neration, optim <u>eSEED.org.</u>	el SEED version 1.0 ization, curation) I, and analysis of	genome-scale met	abolic models.			
»SEED Resources	»Account management							login		
Important Server 1.) We recommend Model SEED Tuto	Messages: using the Firefox browser to rials (Click here to view	o view this website.								
		,								
Selected models ar	nd run FBA Model construct	ion User models Mode	l statistics/Sele	ect Flux Balance	Results About	Model SEED				
You have arrived the SEED framework specific model for or you can brows in the tables belo type here to see a (Example search: 1) Map Reactions Co	You have arrived at the Biochemistry and Model database of the SEED framework for genome annotation. You can select a specific model for viewing using the model select box (below), or you can browse all the database compounds and reactions in the tables below. type here to see available models (Example search: 'bacillus', 'coli', 'Seed85962.1') The primary method for select Model filter select found on the home page.									
Man Coloct							dick to show	i/bide		
Name		Re	actions	Compound	ds E	C Numbers		71100		
Glycolysis / Glucor	neogenesis	47		31	4	-2				
Citrate cycle (TCA	cycle)	28		20	2	2				
Pentose phospha	te pathway	39		32	3	9				
Inositol metabolis	m	9		10	9					
Pentose and gluc	uronate interconversions	62		53	5	i6				
Fructose and man	inose metabolism	67		48	E	6				
		displaying	1 - 6 of 247			<u>next»</u>	<u>last»</u>			

Selecting a Model Using the Filter Select

Selected models and run FBA	Model construction	User models	Model statistics/Select	Flux Balance Results	About Model SEED	
You have arrived at the Bioch genome annotation. You can (below), or you can browse a	nemistry and Model of select a specific model all the database com	database of the del for viewing pounds and re	e SEED framework for using the model select actions in the tables bel	box ow.		
bac Acinetobacter baumannii ATCC Acinetobacter sp. ADP1 (Opt6 Acinetobacter sp. ADP1 (Seed Acinetobacter sp. ADP1 (iAbay	2 <u>17978 (Seed400667.</u> 2977.3) 62977.3) ylyiv4)	4)		Select Model		
Agrobacterium tumefaciens str Ma Anaeromyxobacter dehalogena	. C58 (Seed176299.3) ans 2CP-C (Seed29039) (7.13)				
Bacillus anthracis str. Ames Ar Bacillus anthracis str. Ames (S Bacillus subtilis subsp. subtilis	eed198094.1) str. 168 (Opt224308.	1)				
Bacillus subtilis subsp. subtilis Bacillus subtilis subsp. subtilis Bacillus subtilis subsp. subtilis	str. 168 (Seed224308 str. 168 (iAG612) str. 168 (iBsu1103)	.1)		Compounds	EC Numb	ers
Bacillus subtilis subsp. subtilis	str. 168 (iYO844)		4	31	42	
Citrate cycle (TCA cycle)	60293403.37		28	20	22	

• Models can be selected by typing the model ID (iJR904), genome ID (83333.1), or organism name (coli)

• Once your model is selected, click "Select Model" to load your model data

Selecting a Model using the Model Select Table

	The Mo Welcome to the Model SEED For more information about	del S - a resource for the The SEED please vis	EED Model 8 9 generation, optimiza 9 it <u>theSEED.org.</u>	EED version 1.0 ition, curation, and ana	Ilysis of genome-scale	e metabolic mode	ls.
»SEED Resources	»Account management						login
Important Server	Messages:						
1.) We recommend	using the Firefox browser to	view this website.	You can load	a data table	containing a	ull availabl	Р
Model SEED Tuto	orials (Click here to view)			icking on this	toh in the h		
	· · · ·		models by cl	icking on this	tab in the n	omepage.	
Selected models ar	nd run FBA Model constructi	on User models M	lodel statistics/Select	Flux Balance Results	About Model SEED		
tou nave arrived the SEED framework specific model for or you can brows in the tables belo type here to see a (Example search:	at the Biochemistry and Moc ork for genome annotation." viewing using the model sel e all the database compoun- iw. available models 'bacillus', 'coli', 'Seed85962.1'	lei database of You can select a ect box (below), ds and reactions)	Sel	ect Model			
Map Reactions Co	ompounds Biomass Compo	nents Media formu	lations				
Map Select						click to :	show/hide
Name			Reactions	Compounds	EC Numbers		
Glycolysis / Glucor	neogenesis		47	31	42		
Citrate cycle (TCA	<u>, cycle)</u>		28	20	22		
Pentose phospha	<u>te pathway</u>		39	32	39		
Inositol metabolis	<u>sm</u>		9	10	9		
Pentose and gluci	uronate interconversions		62	53	56		
Fructose and man	inose metabolism		6/	48	66		
		displa	aying 1 - 6 of 247		1	<u>next» last»</u>	

Selecting a Model using the Model Select Table

Selected models and r		ion User mo		statistics/Selec		e Results Abo		Versi	on num	ibers: c	omple	ete
(export table)					displaying 1	- 20 of 199		anno befor	tation I e dot. I	reconst New ga	ructio p-fillir	n 1 <u>g after</u> .
Name	Organism	Genome ID	Class	Genes	Reactions	Gapfilling Reactions	Compounds	Source	Download links	Upload	Version	.ast Ipdate
<u>Seed99287.1</u>	Salmonella typhimurium LT2	99287.1	Gram negative	Based	on sub	system	1132 15	SEED	<u>SBML format</u> <u>Model SEED</u> format LP format	No curation permissions	V18.19	;/26/2009
Seed93062.4	Staphylococcus aureus subsp. aureus COL	93062.4	Gram positive	789/2622	Genes	s in mo	⁹⁸⁶ del / an	notate	SBML format Motiel SEED Consgene LP format	No curation	V16.16	5/26/2009
<u>Seed93061.3</u>	Staphylococcus aureus subsp. aureus NCTC 8325	93061.3	Gram positive	792/2893	1127	36	984	SEED	SBML format Model SEED format LP format	No curation permissions	V15.15	5/26/2009
<u>Seed85963.1</u>	Helicobacter pylori J99	85963.1	Gram negative	427/1517	735	57	732	SEED	SBML format Model SEED format LP format	No curation permissions	V13.11	5/26/2009
<u>Seed85962.1</u>	Helicobacter pylori 26695	85962.1	Gram negative	435/1620	775	80	754	SEED	SBML format Model SEED format LP format	No curation permissions	V17.15	5/26/2009
<u>Seed83333.1</u>	Escherichia coli K12	83333.1	Gram negative	1140/4310	1479	11	1120	SEED	SBML format Model SEED format LP format	No curation permissions	V20.21	5/26/2009
<u>Seed83332.1</u>	Mycobacterium tuberculosis H37Rv	83332.1	Gram positive	749/3931	1034	59	942	SEED	SBML format Model SEED format LP format	No curation permissions	V22.21	6/14/2010
Seed76869.3	Pseudomonas putida GB-1	76869.3	Gram negative	1148/5413	1320	26	1123	SEED	SBML format Model SEED format LP format	No curation permissions	V11.11	4/27/2010
<u>Seed76114.4</u>	Azoarcus sp. EbN1	76114.4	Gram negative	804/4607	1014	36	958	SEED	SBML format Model SEED format LP format	No curation permissions	V13.11	5/26/2009

Number of gap-filled reactions

Genome Annotation: the Subsystems Approach



www.theseed.org/models/

Selecting a Model using the Model Select Table

Selected models an	d run FBA Model construct	ion User m	odels Model	statistics/Sele	ect Flux Balan	ce Results Ab	out Model SEED					
export table					displaying 1	L - 20 of 199						<u>next»</u> last»
Name	Organism	Genome ID	Class	Genes	Reactions	Gapfilling Reactions	Compounds	Source	Download links	Upload	Version	Last update
<u>Seed99287.1</u>	Salmonella typhimurium LT2	99287.1	Gram negative	1141/4534	1462	14	1132	SEED	SBML format Model SEED format LP format	No curation permissions	V18.19	5/26/2009
Seed93062.4	Staphylococcus aureus subsp. aureus COL	93062.4	Gram positive	789/2622	1143	49	986	SEED	SBML format Model SEED format LP format	No curation permissions	V16.16	5/26/2009
Seed93061.3	Staphylococcus aureus subsp. aureus NCTC 8325	93061.3	Gram positive	792/2893	1127	36	984	SEED	SBML format Model SEED format LP format	No curation permissions	V15.15	5/26/2009
<u>Seed85963.1</u>	Helicobacter pylori J99	85963.1	Gram negative	427/1517	735	57	732	SEED	SBML format Model SEED format LP format	No curation permissions	V13.11	5/26/2009
Seed85962.1	Helicobacter pylori 26695	85962.1	Gram negative	435/1620	775	80	754	SEED	SBML format Model SEED format LP format	No curation permissions	V17.15	5/26/2009
<u>Seed83333.1</u>	Escherichia coli K12	83333.1	Gram negative	1140/4310	1479	11	1120	SEED	SBML format Model SEED format LP format	No curation permissions	V20.21	5/26/2009
<u>Seed83332.1</u>	Mycobacterium tuberculosis H37Rv	83332.1	Gram positive	749/3931	1034	59	942	SEED	SBML format Model SEED format LP format	No curation permissions	V22.21	6/14/2010
<u>Seed76869.3</u>	Pseudomonas putida GB-1	76869.3	Gram negative	1148/5413	1320	26	1123	SEED	SBML format Model SEED format	No curation permissions	V11.11	4/27/2010
Seed76114.4	Azoarcus sp. EbN1	76114.4	Gram negative	804/4607	1014	36	958	SEED	SBML format Model SEED format LP format	No curation permissions	V13.11	5/26/2009

Click on link to select model

Three model files available for download...

Downloading Model Data

Source	Download links	Upload
SEED	SBML format Model SEED format LP format	No curation permissions

Three download formats:

- SBML format
- Model SEED format
- LP Format



```
<?xml version="1.0" encoding="UTF-8"?>
<sbml xmlns="http://www.sbml.org/sbml/level2" level="2" version="1" xmlns:html="http://www.w3.org/1999/xhtml">
<model id="Seed99287_1" name="Salmonella typhimurium LT2 SEED model">
<listOfUnitDefinitions>
<unitDefinition id="mmol_per_gDW_per_hr">
<listOfUnitS>
<unit kind="mole" scale="-3"/>
<unit kind="gram" exponent="-1"/>
<unit kind="gram" exponent="-1"/>
</listOfUnits>
</unitDefinition>
</continued ... />
```

Downloading Model Data

Model SEED Format: Tab delimited file linking reaction IDs to gene IDs

DATABASE	DIRE	CTIONA	ALITY COMPARTMENT ASSOCIATED PEG NOTES	
rxn12008	<=	с	peg. 3191 NONE Genes are gene-sets: e.g.	
rxn10155	<=>	с	peg.4139+peg.4162 NONE peg 4139 AND peg 4162	
rxn00225	<=>	с	peg.2260 peg.3132 NONE PCG.4105 AND PCG.4102,	
rxn00541	<=>	с	Peg.901 NONE Peg.2260 OR peg.3132	
rxn08954	<=>	С	peg.3591 NONE	
rxn01674	<=>	С	peg.2047 NONE	
rxn00966	<=	С	peg.4071 NONE	
rxn05572	<=>	С	peg.2859 NONE	
rxn01199	<=>	С	peg.3536 NONE	
rxn10215	=>	С	peg.3064 NONE	
rxn01451	<=>	с	peg.2311 peg.3842 NONE	
rxn00785	<=>	с	peg.2263+peg.2264 peg.2390 peg.2969 NONE	
rxn00802	<=>	с	peg.3976 NONE	
rxn03638	=>	с	peg. 3735 NONE Reactions have directionality and cor	npartment:
rxn08851	<->	C	peg. 3820 NONE	
rxn08842	<=>	С	peg. 3820 NONE -> C IS IOF Ward and Cytopiasm	
rxn05323	<=	С	peg.1646 NONE	
rxn03084	=>	С	peg.2479 NONE	
rxn03887	=>	с	peg.3139 NONE	
rxn00868	<=	С	peg.299 NONE	
rxn00011	<=	С	peg.114+peg.115 peg.150 peg.2327 peg.3669+peg.3670 peg.3766	5+peg.3767 NONE
rxn00292	<=>	с	peg.3784 NONE	
nvn03051	<->	C	peg.4312 NONE	
1 ×1105954	<->	C	P-8	
rxn10378	<=>	c	peg.3816 NONE	
rxn10378 rxn01675	<=> <=>	c c	peg.3816 NONE peg.2020 NONE	

Downloading Model Data

LP Format: Mixed linear optimization file format. Like SBML, useful for some applications. Used for running gap-filling and flux balance analysis.

* Problem: Unknown *\
Maximize
obj: - D cpd11416 c

Subject To

r_1: - F_rxn00533 - F_rxn10447 + F_rxn10821 - F_rxn05029 - F_rxn03536 - F_rxn00379 - F_rxn00340 -40.0531394085024 F_bio00236 - F_rxn05195 - F_rxn10571 - F_rxn00062 - F_rxn00851 - F_rxn05540 + F_rxn01987 -F_rxn01517 - F_rxn01210 - F_rxn08295 - F_rxn00114 - F_rxn00237 - F_rxn05146 - F_rxn00392 - F_rxn03108 -F_rxn05538 - F_rxn05528 - F_rxn03075 - 24 F_rxn10323 - F_rxn05183 - F_rxn02175 - F_rxn05545 - F_rxn10254 -F_rxn08300 - F_rxn05515 - F_rxn01603 - F_rxn05163 - F_rxn01100 - F_rxn01917 - F_rxn03147 - F_rxn09450 -F_rxn00247 - F_rxn00077 - F_rxn05159 - F_rxn01353 - F_rxn05177 - F_rxn06672

Select User / Private models

Selected models and run FBA Model construction User models Model statistics/Select Flux Balance Results About Model SEED

Complete and incomplete models currently owned by user:

export table

Name	Organism	Genome ID	Status	Download links	Upload	Version	Last update
Seed224308.50.26152	Bacillus subtilis subsp. subtilis str. 168	224308.50	Auto completion successfully finished	SBML format Model SEED format LP format	Upload curated model file	V1.1	8/19/2010
Seed511145.18.26152	Escherichia coli str. K-12 substr. MG1655	511145.18	Auto completion successfully finished	SBML format Model SEED format LP format	Upload curated model file	V1.1	8/19/2010
Seed1148.37.26152	Synechocystis sp. PCC 6803	1148.37	Auto completion successfully finished	SBML format Model SEED forma LP format	<u>Upload curated</u> model file	1.1	8/19/2010

displaying 1 - 3 of 3

select model for viewing

link to genome page

model curation tools available, we'll cover later

Selecting multiple models for comparison

Selected models an	d run FBA	Model construction	User models	Model statist	ics/Select	Flux Balance Result	About Mo	del SEED		
type here to see a	vailable mod	els			S	elect Model				
(Example search:	'bacillus',	'coli', 'Seed85962.1',)							
Model ID	Organis	m Ve	ersion S	ource	Class	Genome size	Model genes	Reactions with genes	Gapfilling Reactions	Gapfil Media
iJR904	Escherich (<u>83333.1</u>	ia toli K12 V1)	.1 <u>PN</u>	MID12952533	Gram negative	4,639 KB	892 4,310	854 /921	68/921	Carbon D-Gluce
Seed83333.1	Escherich (<u>83333.1</u>	ia xoli K12 V2)	0.21 SE	EED	Gram negative	4,639 KB	,140 4,310	1,454 /1,482	11/1,482	Carbon- D-Gluce
Click here to	run FBA o	n selected mode	ls							

link to SEED genome annotation page

About Model SEED

lodel enes	Reactions with genes	Gapfilling Reactions	Gapfilling Media	Compounds	Download	(<u>clear all</u>)	
92 ,310	854 /921	68/921	Carbon- D-Glucose	627	SBML format Model SEED forma LP format	(<u>remove</u>)	remove from page
140 ,310	1,454 /1,482	11/1,482	Carbon- D-Glucose	1,120	<u>SBML format</u> <u>Model SEED forma</u> <u>LP format</u>	(<u>remove</u>)	

download model

KEGG Map details on multiple models



KEGG Map details on multiple models

Citrate cycle (TCA ... 🖂



KEGG Map details on multiple models



Compare model reactions

Map Reactio	ns Compounds Biomass Compo	nents Genes Media formulations					
			display 50 ite	ms per page			
			displaying 1	0 07 107 1			
P⊿action	Name	Equation	Roles	Subsystems	KEGG MAP	UR904	Seed83333.1
rxn00191	L-Alanine: 2-oxoglutarate aminotransferase, L-alanine transaminase, L-alanine transaminase, mitochondrial, Alanine transaminase, alanine aminotransferase	2-Oxoglutarate + L-Alanine <=> Pyruvate + L-Glutamate	Glutamate-pyruvate aminotransferase (EC 2.6.1.2)	Alanine biosynthesis	Glutamate meta polism Alanine and asp rtate metabolism Carbon fixation n photosynthetic organisms	Complete:Active <=> [Flu.: -100 to 100] Cart on- D-G ucose:Essential <= [Flu: -0.0269573 to -100] Cart on- Glyc ne:Essential <= [Flu: -0.0036747 to -100] Gap filling:UNKNOWN	Not in model
rxn00283	L-Alanine racemase, alanine racemase, alanine racemase (irreversible), L-Alanine racemase, ALAR, alanineracemase, alanine racemase	L-Alanine <=> D-Alanine	Alanine racemase, biosynthetic (EC 5.1.1.1) Alanine racemase, catabolic (EC 5.1.1.1) Alanine racemase (EC 5.1.1.1)	Pyruvate Alanine Serine Interconversions Alanine biosynthesis	Alanine and asp irtate metabolism D-Alanine meta olism	Complete:Active <=> [Flu: -99.9446 to 100] Carton- D-Gucose:Essential => [Flu: 0.00260695 to 56.557] Carton- Glyc ne:Essential => [Flu: 0.000355367 to 9.3/119] prg.1176, peg.3963	Complete:Active <=> [Flux: -100 to 100] Carbon-D-Glucose:Active <=> [Flux: -99.9972 to 99.9554] ArgonneLBMedia:Active <=> [Flux: -99.9998 to 100] Carbon-Glycine:Active <=> [Flux: -100 to 99.9747] peg.1176, peg.3963

- •View reaction details; search and sort by reaction details.
- •Compare reaction predictions for two models
- •Additional columns available under dropdown menu.

Compare model reactions: looking at predictions

		110700	<u></u>
	iJR904	Seed83333.1	-
			Predictio
			various
(Complete:Active <=> [Flux: -100 to 100]	Not in model	Active, E Reaction
	ArgonneLBMedia:Active <=> [Flux: -100 to 99.4511]		"<=" bac
	Carbon-D-Glucose:Essential <= [Flux: -0.0269573 to -100]		
	Carbon-Glycine:Essential <= [Flux: -0.0036747 to -100]		
ſ	Gap filling:UNKNOWN		
	Complete:Active <=> [Flux: -99.9446 to 100]	Complete:Active <=> [Flux: -100 to 100]	
	ArgonneLBMedia:Essential => [Flux: 0.0530814 to 100]	Carbon-D-Glucose:Active <=> [Flux: -99.9972 to 99.9554]	Reaction
	Carbon-D-Glucose:Essential => [Flux: 0.00260695 to 56.557]	ArgonneLBMedia:Active <=> [Flux: -99.9998 to 100]	reaction
	Carbon-Glycine:Essential =>	Carbon-Glycine:Active <=> [Flux: -100 to 99.9747]	
	9.34119]	<u>peg.1176,</u> <u>peg.3963</u>	
	peg.1176, peg.3963		

Predictions for reaction activity under various media conditions. Can be: Active, Essential or Inactive. Reaction directionality "=>" forward, "<=" backward and "<=>" reversible

Reaction added to model via gapfilling or based on a set of genes that enable the reaction.

Compare compounds present in model

Map Reactions	Compounds Biomass Components Genes Media fo	rmulations						
export table			c	display 50 items per page	leade	r to sort table	by c	olumn.
				displaying 1 - 50 of 1163				<u>next»</u> <u>last»</u>
Compound	Name	Formula Ma	ass	KEGG MAP	KEGG CID	Model ID	iJR904	eed83333.1
cpd00001	H2O, Water, HO-, OH-, h2o	H2O 18	3	Oxidative phosphorylation Photosynthesis Carbon fixation in photosynthetic organisms Riboflavin metabolism Amyotrophic lateral sclerosis (ALS)	C01328 C00001	C01328 C00001 cpd00969 WATER h2o cbs_1 cbs_152 cll_9	yes	yes
cpd00002	ATP, Adenosine 5'-triphosphate, atp	C10H13N5O13P3 504)4	Oxidative phosphorylation Photosynthesis Purine metabolism Puromycin biosynthesis Zeatin biosynthesis Calcium signaling pathway Neuroactive ligand-receptor interaction Type II diabetes mellitus Parkinson's disease	C00002	C00002 ATP atp cbs_274 cbs_42 cll_0	yes	yes
cpd00003	NAD+, NAD, Nicotinamide adenine dinucleotide, DPN, Diphosphopyridine nucleotide, Nadide	C21H26N7O14P2 662	52	<u>Oxidative phosphorylation</u> <u>Glutamate metabolism</u> <u>Nicotinate and nicotinamide metabolism</u>	C00003	C00003 NAD nad cbs_61 cbs_35 cbs_150	yes	yes

Compound table shows whether compound is included in model

Compare biomass objective functions of each model

Map Reactions	Compounds Biomass Components Genes Medi	a formulations		Select addition	nal biom	ass
Biomass Sele	ect (Click this title bar to select biomass reaction	ns for comparison)		reactions		
		85				
Compound	Name	Formula	Mass	Kegg Map	Kegg ID	Seed83333.1: (bio00179)
cpd00001	OH- HO- Water H2O	H2O	18	<u>00190</u>	<u>C01328</u> <u>C00001</u>	34.796
cpd00002	Adenosine 5'-triphosphate ATP	C10H13N5O13P3	504	00190	<u>C00002</u>	40.17
cpd00003	Nicotinamideadeninedinucleotide Nadide Diphosphopyridine nucleotide DPN Nicotinamide adenine dinucleotide NAD NAD+	C21H26N7O14P2	662	This is m gram bio	coooos mol cons mass pro	^{3.409e-3} umed per duced
cpd00006	Nicotinamideadeninedinucleotidephosphate Nicotinamide adenine dinucleotide phosphate - Triphosphopyridine nucleotide TPN beta-Nicotinamide adenine dinucleotide phosphate Nicotinamide adenine dinucleotide phosphate NADP NADP+	C21H26N7O17P3	741	<u>00195</u>	<u>C00006</u>	3.409e-3

Compare gene essentiality in models

Model annotation of genes:								nes:				
Map Rea	ctions Compound	ds Bioma	ss Comp	onents Ge	enes Media formulations	"A" is active	e. "E" is esse	ntial and				
export ta	(isplay 50 items per page displaying 1 - 36 of 36 (items per page displaying 1 - 36 of 36) (items per page displaying 1 - 36 of 36) (items per page displaying 1 - 36 of 36)											
Gene ID	Alias	Start (BP)	Length (BP)	Directior	n Functional Assignment	Essentiality	iJR904	Seed83333.1				
peg.115	aceF, b0115, NP_414657.1, gi 16128108, GeneID:944794	125695	1892	for	Dihydrolipoamide acetyltransferase component of pyruvate dehydrogenase complex (EC 2.3.1.12)	Essential Nonessential	False positive Nonessential Correct positive rxn00154(A=>)	False positive Nonessential rxn01871(A)				
<u>peg.116</u>	lpdA, b0116, NP_414658.1, gi 16128109, GeneID:944854	127912	1424	for	Dihydrolipoamide dehydrogenase (EC 1.8.1.4) Dihydrolipoamide dehydrogenase of pyruvate dehydrogenase complex (EC 1.8.1.4)	Essential Nonessential	False positive Nonessential Correct positive rxn00908(E=>,A=>) rxn00154(A=>)	False positive Nonessential rxn06493(A=>) rxn01241(A)				
peg.1795	pabB, b1812, NP_416326.1, gi 16129766, GeneID:946337	1892829	1361	for	Para-aminobenzoate synthase, aminase component 2.6.1.85)	t (EC Essential Nonessential	False positive Nonessential Correct positive rxn01257(E=>) rxn00189(A=>)	False positive Nonessential rxn01257(E=>)				
<u>peg.2</u>	thrA, b0002, NP_414543.1, gi 16127996, GeneID:945803	337	2462	for N	Aspartokinase (EC 2.7.2.4) Homoserine dehydrogenase (EC 1.1.1.3) Aultiple annotations for diffe onditions: hover over "A=>"	Essential Nonessential rent media for media	False positive Nonessential Correct positive rxn01302(E<=,A<=) rxn00337(E=>,A=>)	False positive Nonessential rxn01302(A) rxn01301(A) rxn00337(E=>)				
peg.237	proB, b0242, NP_414777.1, gi 16128228, GeneID:946425	259612	1103	for C	Glutamate 5-kinase (EC 2.7.2.11) Ondition name.	Essential Nonessential	False positive Nonessential Correct positive rxn00179(A=>)	False positive Nonessential rxn00179(A=>)				
peg.238	proA, b0243, NP_414778.1, gi 16128229, GeneID:946680	260727	1253	for	Gamma-glutamyl phosphate reductase (EC 1.2.1.4	1) Essential Nonessential	False positive Nonessential Correct positive rxn02373(A<=)	False positive Nonessential rxn02373(A<=)				

Currently only works when compared models use the same genome.

Run flux balance analysis on models

Selected models and	d run FBA	Model construct	ion User mode	els Model statis	tics/Select	Flux Balance Results	About Mode	I SEED	
type here to see available models Select Model									
(Example search: 'bacillus', 'coli', 'Seed85962.1')									
Model ID	Organis	m	Version	Source	Class	Genome size	Model genes	Reactions with gene	
iJR904	Escherich (83333.1)	ia coli K12)	V1.1	PMID12952533	Gram negative	4,639 KB 8	92 4,310	854 /921	
Seed83333.1	Escherich (83333.1)	ia coli K12)	V20.21	SEED	Gram negative	4,639 KB 1 /	,140 4,310	1,454 /1,482	
Click here to run FBA on selected models									
Select media condition: Complete									

Click on green "blind" to open FBA panel.

Begin typing media name to select, then click "Run".

Select Flux Results

Select	ed n	nodels and run FBA	Model construction	User models	Model statistics/Select	Flux Balance Results	About Model SEED			
Select Time		Time	Model Method		Media	Growt	Growth			
		August 30, 2010	iJR904	SINGLEGR	OWTH Complete	Model g	rew with biomass flux of: 100			
		August 30, 2010	Seed83333.1	SINGLEGR	OWTH Complete	Model g	rew with biomass flux of: 100			
		August 23, 2010	Seed224308.1	SINGLEGR	OWTH Carbon-a-D	-Lactose No grov	vth predicted in input conditions.			
		August 23, 2010	Seed83333.1	SINGLEGR	OWTH Carbon-a-D	-Lactose Model g	rew with biomass flux of: 100			
		August 23, 2010	Seed269798.12	SINGLEGR	OWTH Carbon-a-D	-Lactose Model g	rew with biomass flux of: 56.6735			

Eventually we'll offer different Flux methods, e.g. gene and/or Reaction knockout.

Delete Selected Results

View Selected Results

Growth is a bit arbitrary, but peaks around 100g biomass.

Check results and click "View Selected Results to load them into the Reaction table.

View Fluxes in Reaction Table

Map Reactions	Compounds Biomass Component	s Genes Media formulations				
		display 50	items per page			
		displayin	g 1 - 50 of 1673			next» last»
Reaction	Name	KEGG MAP	iJR904	Seed83333.1	Flux #1	Flux #2
rxn00191	L-Alanine:2-oxoglutarate aminotransferase,	Glutamate metabolism Alanine and aspartate	Complete:Active <=> [Flux: -100 to 100]	Not in model	-1000	Not in model
	L-alanine transaminase, L-alanine transaminase,	Carbon fixation in photosynthetic	ArgonneLBMedia:Active <=>	Fluxes are		
	mitochondrial, Alanine transaminase,	organisms	[Flux: -100 to 99.4511]	numbered base	ed on	
	alanine aminotransferase		Carbon-D-Glucose:Essential <=	their order in th		
			[Flux: -0.0209575 to -100]		C	
			Carbon-Glycine:Essential <= [Flux: -0.0036747 to -100]	results table.		
			Gap filling:UNKNOWN			
rxn00283	L-Alanine racemase, alanine racemase, alanine racemase, (irreversible)	Alanine and aspartate metabolism	Complete:Active <=> [Flux: -99.9446 to 100]	Complete:Active <=> [Flux: -100 to 100]	-994.48	5.81758
	L-Alanine racemase (in everyble), ALAR, alanineracemase		ArgonneLBMedia:Essential => [Flux: 0.0530814 to 100]	Carbon-D-Glucose:Active <=> [Flux: -99.9972 to 99.9554]		
	alanine racemase		Carbon-D-Glucose:Essential => [Flux: 0.00260695 to 56.557]	ArgonneLBMedia:Active <=> [Flux: -99.9998 to 100]		
			Carbon-Glycine:Essential => [Flux: 0.000355367 to 9.34119]	Carbon-Glycine:Active <=> [Flux: -100 to 99.9747]		
			peg.1176, peg.3963	peg.1176, peg.3963		

Negative numbers are reactions running in reverse. Still mmol/gram cell dry weight hour

View Fluxes in Reaction Table

Мар	Reactions	Compounds Biomass Component	s Genes Media formulations									
	display 50 items per page											
			displayin	ig 1 - 50 of 1673			next» last»	2				
Rea	ction	Name	KEGG MAP	iJR904	Seed83333.1	Flux #1	Flux #2					
rxn0	0191	L-Alanine:2-oxoglutarate aminotransferase,	Glutamate metabolism Alanine and aspartate	Complete:Active <=> [Flux: -100 to 100]	Not in model	-1000	Not in model					
	L-a L-a mit Ala ala	L-alanine transaminase, L-alanine transaminase, mitochondrial, Alanine transaminase, alanine aminotransferase	metabolism Carbon fixation in photosynthetic organisms	ArgonneLBMedia:Active <=>	Additional colu	mns						
				[Flux: -100 to 99.4511]	are available u	nder						
				Carbon-D-Glucose:Essential <= [Flux: -0.0269573 to -100]	the dropdown							
				Carbon-Glycine:Essential <= [Flux: -0.0036747 to -100]	menu.							
				Gap filling:UNKNOWN								
rxn0	0283	L-Alanine racemase, alanine racemase,	Alanine and aspartate metabolism	Complete:Active <=> [Flux: -99.9446 to 100]	Complete:Active <=> [Flux: -100 to 100]	-994.48	5.81758					
		L-Alanine racemase, ALAR, alanineracemase		ArgonneLBMedia:Essential => [Flux: 0.0530814 to 100]	Carbon-D-Glucose:Active <=> [Flux: -99.9972 to 99.9554]							
		alanine racemase		Carbon-D-Glucose:Essential => [Flux: 0.00260695 to 56.557]	ArgonneLBMedia:Active <=> [Flux: -99.9998 to 100]							
				Carbon-Glycine:Essential => [Flux: 0.000355367 to 9.34119]	Carbon-Glycine:Active <=> [Flux: -100 to 99.9747]							
				<u>peg.1176</u> , peg.3963	peg.1176, peg.3963							

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