# Model SEED Tutorial Part 2: Model SEED Biochemistry Database

Christopher Henry, Scott Devoid, Matt DeJongh, Aaron Best, Ross Overbeek, and Rick Stevens

Presented by: Christopher Henry

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### Model SEED Biochemistry Database

- Model SEED Homepage
- Viewing reactions/compound on KEGG maps
- Reactions and Compound pages
- Reaction data table
- Compound data table
- Media data table

#### http://www.theseed.org/models/



### The Model SEED

Model SEED version 1.0

You should log in here using your RAST account

Welcome to the Model SEED - a resource for the generation, optimization, curation, and analysis of genome-scale metabolic models.

For more information about The SEED please visit the SEED.org.

»SEED Resources

»Account management

Use this menu to create an account

login

#### Important Server Messages:

1.) We recommend using the Firefox browser to view this website.

Important server messages show up here

Model SEED Tutorials (Click here to view)

Click here for links to site tutorials

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

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')

Select Model

With no models selected, the site shows all reactions and compounds found in the Model SEED biochemistry database

Map | Reactions | Compounds | Biomass Components | Media formulations

Map Select

click to show/hide

Name	Reactions	Compounds	EC Numbers
Glycolysis / Gluconeogenesis	47	31	42
Citrate cycle (TCA cycle)	28	20	22
Pentose phosphate pathway	39	32	39
Inositol metabolism	9	10	9
Pentose and glucuronate interconversions	62	53	56
Fructose and mannose metabolism	67	48	66

displaying 1 - 6 of 247

next» last»

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Select Model

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Map Reactions | Compounds | Biomass Components | Media formulations

Click on this tab to view reaction and compound data overlaid on KEGG maps

Map Select

click to show/hide

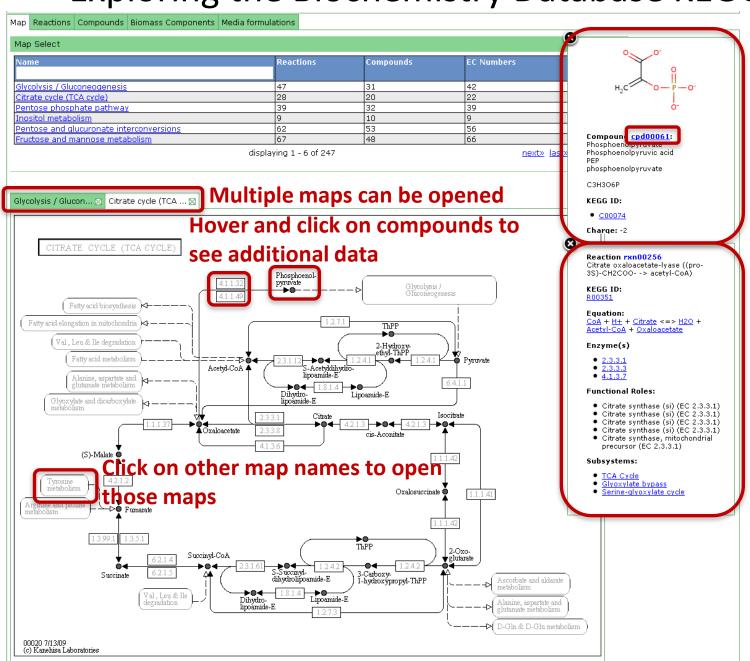
Search maps by name here	Reactions	Compounds	EC Numbers
<u> Alycolysis / Gluconeogenesis</u>	47	31	42
Citrate cycle (TCA cycle)	28	20	22
Pentose phosphate pathway	39	32	39
Inositol metabolism	9	10	9
Pentose and glucuronate interconversions	62	53	56
ructose and mannose metabolism	67	48	66

displaying 1 - 6 of 247

Click on link to select a single map

next» last»

### **Exploring the Biochemistry Database KEGG Maps**

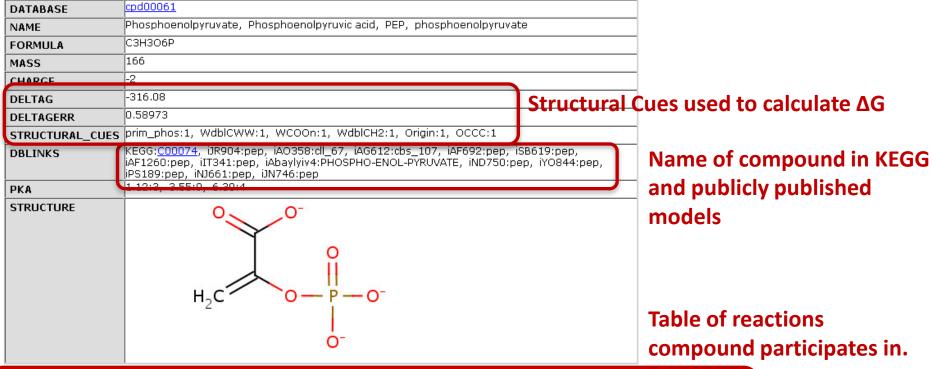


Click on compound link to visit compound page

Hover and click on reactions to see additional reaction data

### Compound Page of Model SEED Database

#### Viewing data for compound cpd00061



Reaction:	s involving compound cpd00061							
		display 50	items per page					
		displayi	ing 1 - 50 of 69			<u>n</u>	iext» <u>las</u>	st»
Reaction	Name	Equation	Roles	Subsystems	KEGG Map	Enzyme	KEGG RID	
	phosphotransferase, phosphoenolpyruvate synthase,	H2O + ATP + Pyruvate => Orthophosphate + AMP + Phosphoenolpyruvate + H+	Phosphoenolpyruvate synthase (EC 2.7.9.2)	Pyruvate metabolism I: anaplerotic reactions, PEP Glycolysis and Gluconeogenesis, including Archaeal enzymes	00620 00720	2.7.9.2	R00199	

### Group contribution method for estimating $\Delta_f G^{'\hat{i}}$

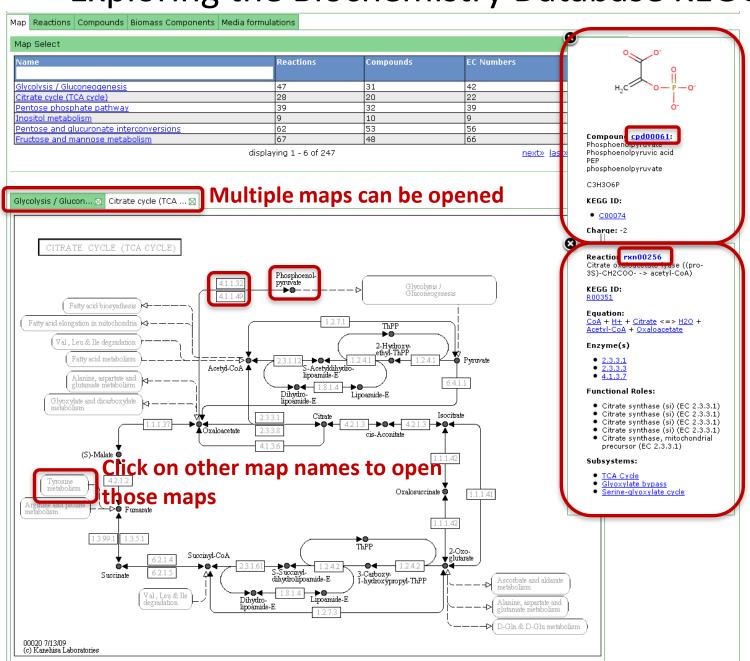
•In the group contribution method, the estimated  $\Delta_f G^{'^\circ}$  of a molecular is equal to the sum of the estimated energies for the molecular substructures that make up the molecule

	otiiii atea e		Group	$\Delta_{ m f} G_{ m group}^{'\circ}$	Count		
		O	[-COO <sup>-</sup> ]	-82.2	2	0.3	
			[-OH] <sub>sec</sub>	-42.2	1	0.4	
	XX	<b>1</b> 0	[-CH=] <sub>ring</sub>	4.6	3	0.5	
			[-O-]	-24.9	1	0.9	
			[>C=]	14.5	1	0.7	
HU	W.		[>CH-] <sub>ring</sub>	5.5	2	0.6	
	Ó		[-CH <sub>2</sub> -]	0.9	1	0.1	
			[>C=] <sub>ring</sub>	9.7	1	1.0	
			[=CH <sub>2</sub> ]	4.8	1	1.1	
		<u>``</u> O	Chorismate:	-176.8 ±	2.3 kcal,	/mol	

Uncertainty 
$$\sum_{\Delta_r G^{\circ}}^{\text{Number of groups}} \left( n_i \mathcal{E}_{\Delta_g G_i^{\circ}} \right)^2$$

Jankowski et al, Biophysical Journal, 2008

### **Exploring the Biochemistry Database KEGG Maps**



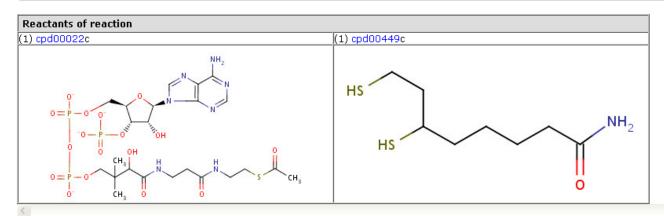
Click on compound link to visit compound page

Click on reaction link to visit reaction page

### Reaction Page of Model SEED Database

#### Viewing data for reaction rxn01871

DATABASE	<u>rxn01871</u>
NAME	acetyl-CoA:enzyme N6-(dihydrolipoyl)lysine S-acetyltransferase, pyruvate dehydrogenase (dihydrolipoamide) reversible, dihydrolipoamide acetyltransferase component of DDH compley, dihydrolipoamide acetyltransferase component of DDH compley, dihydrolipoamide acetyltransferase component of DDH compley, dihydrolipoamide acetyltransferase component of DDH compley.
EQUATION	Acetyl-CoA + Dihydrolipoamide <=> CoA + S-Acetyldihydrolipoamide
ENZYME	pages
PATHWAY	Glycolysis / Gluconeogenesis, Alanine and aspartate metabolism, Pyruvate metabolism, Glycolysis, Gluconeogenesis, rn00010,
DBLINKS	ARGONNE: <u>rxn01871:rxn06179</u> , KEGG: <u>R02569</u> , iAO358:rll_310, iNJ661:PDHbr, iJN746:PDHbr Name of reaction in
DELTAG	VECC and published
DELTAGERR	KEGG and published
THERMODYNAMIC REVERSIBILITY	models.
MAIN EQUATION	<u>cpd00022</u> + <u>cpd00449</u> <=> <u>cpd00836</u>

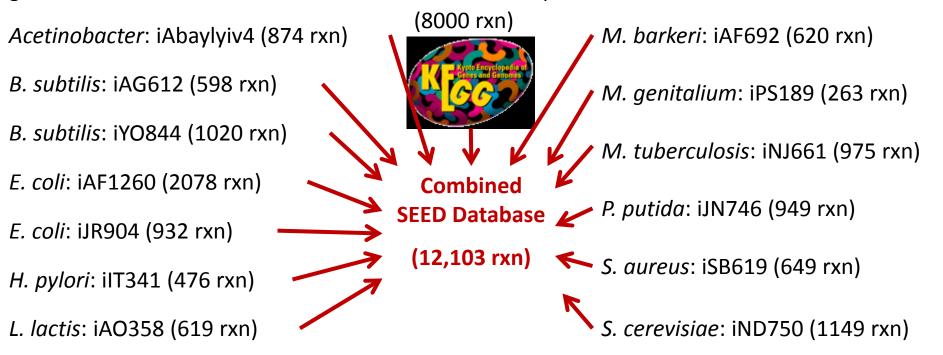


## Model SEED Reaction Table Click on this tab to view a table of all reactions in the Model SEED database

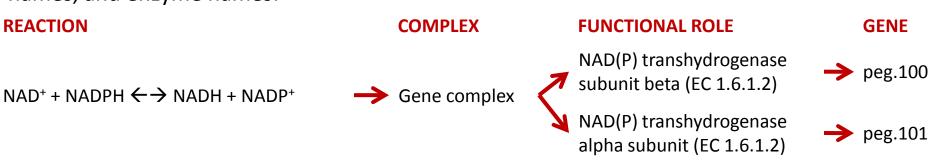
1a Reactions	compounds Biomass Components Media formulations				
		lay 50 items per page	'13,000 reaction	ns in da	atabase
Reaction	Equation	Roles	KEGG MAP	Enzyme	KEGG RID
rxn00001	H2O + Pyrophosphate => (2) Orthophosphate + (2) H+	Inorganic pyrophosphatase (EC 3.6.1.1)		3.6.1.1	R00004
		Manganese-dependent inorganic pyrophosphatase (EC 3.6.1.1)			
		Inorganic pyrophospatase PpaX			
xn00002	H2O + (3) H+ + Urea-1-carboxylate => (2) CO2 + (2) NH3	Allophanate hydrolase 2 subunit 1 (EC 3.5.1.54)	Urea cycle and metabolism of amino groups Atrazine degradation	3.5.1.54	R00005
		Allophanate hydrolase (EC 3.5.1.54)	Actazina degradadon		
		Allophanate hydrolase 2 subunit 2 (EC 3.5.1.54)			
xn00003	CO2 + 2-Acetolactate <= (2) Pyruvate + H+		C5-Branched dibasic acid metabolism Pantothenate and CoA biosynthesis	2.2.1.6 4.1.3.18	R00006 R00226
kn00004	4-Hydroxy-4-methyl-2-oxoglutarate <=> (2) Pyruvate		Benzoate degradation via hydroxylation C5-Branched dibasic acid metabolism	4.1.3.17	R00008
m00006	(2) H2O2 => (2) H2O + Oxygen	Catalase (EC 1.11.1.6)		1.11.1.6	R00009
:n00007	H2O + alpha,alpha-Trehalose <=> (2) D-Glucose	Trehalase (EC 3.2.1.28) Cytoplasmic trehalase (EC 3.2.1.28)	Starch and sucrose metabolism	3.2.1.28	R00010
n00008	(2) H2O <= H2O2 + (2) H+	012121207		1.11.1.13	R00011
m00009	(2) GTP <=> Pyrophosphate + P1,P4-Bis(5'-guanosyl) tetraphosphate			2.7.7.45	R00012
kn00010	(2) Glyoxylate + H+ => CO2 + 2-Hydroxy-3-oxopropanoate	Glyoxylate carboligase (EC 4.1.1.47)	Glyoxylate and dicarboxylate metabolism	4.1.1.47	R00013
kn00011	CO2 + 2-(alpha-Hydroxyethyl)thiamine diphosphate <= Pyruvate + Thiamin diphosphate + H+	Acetolactate synthase small subunit (EC 2.2.1.6), predicted, Archaeal type	Glycolysis / Gluconeogenesis Citrate cycle (TCA cycle) Valine, leucine and isoleucine biosynthesis	1.2.4.1 2.2.1.6 4.1.1.1	R00014
		Pyruvate dehydrogenase E1 component (EC 1.2.4.1)	Pyruvate metabolism Butanoate metabolism		
		Acetolactate synthase small subunit (EC 2.2.1.6), predicted, Archaeal type 2			
		Acetolactate synthase, catabolic (EC 2.2.1.6)			
		Pyruvate decarboxylase (EC 4.1.1.1)			

#### Biochemistry Database in the SEED

•A biochemistry database was constructed combining content from the **KEGG** and **13** published genome-scale models into a non-redundant set of compounds and reactions



•Reactions were then mapped to the functional roles in the SEED based on EC number, substrate names, and enzyme names:



www.theseed.org/models/

# Model SEED Reaction Table Click on this tab to view a table of all reactions in the Model SEED database

Reaction	ompounds Biomass Components Media formulations				
	di	splay 50 items per page	Table is pa	ginated	
		lisplaying 1 - 50 of 12980	lable is pa	gillateu	<u>next»</u> <u>la</u>
action	Equation	Roles	KEGG MAP	Enzyme	KEGG RID
00001	Search by compound name	Inorganic pyrophosphatase (EC 3.6.1.1)		3.6.1.1	R00004
	Scarcin by compound name	Manganese-dependent inorganic pyrophosphatase (EC 3.6.1.1)	Links to KEGG		
		Inorganic pyrophospatase PpaX	Map in Map ta		
00002	H2O + (3) H+ + Urea-1-carboxylate => (2) CO2 + (2) NH3	Allophanate hydrolase 2 subunit 1 (EC 3.5.1.54)	<u>Urea cycle and metabolism of</u> <u>amino groups</u> Atrazine degradation	3.5.1.54	R00005
		Allophanate hydrolase (EC 3.5.1.54)	Act desired desired desired	J	
		Allophanate hydrolase 2 subunit 2 (EC 3.5.1.54)			
00003	CO2 + 2-Acetolactate <= (2) Pyruvate + H+		C5-Branched dibasic acid metabolism Pantothenate and CoA biosynthesis	2.2.1.6 4.1.3.18	R00006 R00226
00004	4-Hydroxy-4-methyl-2-oxoglutarate <=> (2) Pyruvate		Benzoate degradation via hydroxylation C5-Branched dibasic acid metabolism	4.1.3.17	R00008
00006	(2) H2O2 => (2) H2O + Oxygen	Catalase (EC 1.11.1.6)		1.11.1.6	R00009
00007	H2O + alpha,alpha-Trehalose <=> (2) D-Glucose	Trehalase (EC 3.2.1.28)  Cytoplasmic trehalase (EC 3.2.1.28)	SEED Function	al roles	of react
00008	(2) H2O <= H2O2 + (2) H+			1.11.1.13	R00011
100009	(2) GTP <=> Pyrophosphate + P1,P4-Bis(5'-guanosyl) tetraphosphate			2.7.7.45	R00012
100010	(2) Glyoxylate + H+ => CO2 + 2-Hydroxy-3-oxopropanoate	Glyoxylate carboligase (EC 4.1.1.47)	Glyoxylate and dicarboxylate metabolism	4.1.1.47	R00013
100011	CO2 + 2-(alpha-Hydroxyethyl)thiamine diphosphate <= Pyruvate + Thiamin diphosphate + H+	Acetolactate synthase small subunit (EC 2.2.1.6), predicted, Archaeal type	Glycolysis / Gluconeogenesis Citrate cycle (TCA cycle) Valine, leucine and isoleucine biosynthesis	1.2.4.1 2.2.1.6 4.1.1.1	R00014
		Pyruvate dehydrogenase E1 component (EC 1.2.4.1)	Pyruvate metabolism Butanoate metabolism		
		Acetolactate synthase small subunit (EC 2.2.1.6), predicted, Archaeal type 2			
		Acetolactate synthase, catabolic (EC 2.2.1.6)			
		Pyruvate decarboxylase (EC 4.1.1.1)			

### Model SEED Compound Table

#### Click on this tab to view a table of all compounds in the Model SEED database

Map Reaction	ns Compounds Biomass Components Media formulat	tions				
export table				Sort by Column hea	aders e	.g. largest
		display 5	0 iten			-0-10-000
		display	pg 1 - 50	and smallest mass		<u>next» last»</u>
Compound	Name	Formula	Mass	EGG MAP	KEGG CID	Model ID
cpd00001	H2O, Water, HO-, OH-, h2o	H2O	18	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
cpd00002	ATP, Adenosine 5'-triphosphate, atp	C10H13N5O13P3	504	Oxidative phosphorylation Photosynthesis Purine metabolism Puromycin biosynthesis Zeatin biosynthesis Calcium signaling pathway Neuroactive ligand-receptor interaction Type II diabetes mellitus Parkinson's disease	Maps	to KEGG
cpd00003	NAD+, NAD, Nicotinamide adenine dinucleotide, DPN, Diphosphopyridine nucleotide, Nadide, Nicotinamideadeninedinucleotide, nad	C21H26N7O14P2	662	Oxidadive priosprior viadori Glutamate metabolism Nicotinate and nicotinamide metabolism	C00003	C00003 NAD nad cbs_61 cbs_35 cbs_150 cll_22 nad+
cpd00004	NADH, DPNH, Nicotinamide adenine dinucleotide - reduced, Nicotinamideadeninedinucleotide-reduced, nadh	C21H27N7O14P2	663	Oxidative phosphorylation Calcium signaling pathway	C00004	C00004 cpd15266 NADH nadh cbs_37 cll_23 cll_19
cpd00005	NADPH, TPNH, Nicotinamide adenine dinucleotide phosphate - reduced, Nicotinamideadeninedinucleotidephosphate- reduced, nadph	C21H27N7O17P3	742	Photosynthesis Glutathione metabolism	C00005	cpd15267 C00005 NADPH nadph cbs_23 cbs_63 cll_61
cpd00006	NADP+, NADP, Nicotinamide adenine dinucleotide phosphate, beta-Nicotinamide adenine dinucleotide phosphate, TPN, Triphosphopyridine nucleotide, Nicotinamide adenine dinucleotide phosphate -, Nicotinamideadeninedinucleotidephosphate, nadp		741	Photosynthesis Glutathione metabolism Nicotinate and nicotinamide metabolism	C00006	C00006 NADP nadp cbs_26 cll_63 nadp+
cpd00007	Oxygen,	02	32	Oxidative phosphorylation	C00007	C00007

#### Model SEED Media Table

Click on this tab to view a table of all media formulations in the Model SEED database



Compound name and ID link to compound page

### Acknowledgements

#### ANL/U. Chicago Team

- Robert Olson
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- Daniela Bartels
- Tobias Paczian
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- Ross Overbeek
- Gordon Pusch
- Bruce Parello
- Veronika Vonstein
- Andrei Ostermann
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- Olga Zagnitzko
- Svetlana Gerdes

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- Matt DeJongh
- Nathan Tintle
- Hope college students



