Curation & Analysis functions

Functions supported by PSAMM that are used for model curation and analysis. These function can be used to correct common errors and ensure that metabolic reconstructions are accurate representations of the metabolism of an organism, as well as perform various simulations of growth with metabolic models.

Choose model file (YAML format model)

Browse...	No file selected

Select functions you want to apply on your model

masscheck	▼

Search for reactions and compounds in the model(only used for 'search')

- ● reaction
- ○ compound

Enter reaction or compound ID (only used for 'search' function)

data

INFO: Consistent compounds: 72/72

compound_id	assigned_mass	compound_name
s7p_c	7.75	Sedoheptulose-7-phosphate
glc_D_e	7.50	D-Glucose
fru_e	7.50	D-Fructose
6pgc_c	7.00	6-Phospho-D-gluconate
g6p_c	6.50	D-Glucose-6-phosphate
f6p_c	6.50	D-Fructose-6-phosphate
6pgl_c	5.75	6-phospho-D-glucono-1-5-lactone
fdp_c	5.50	D-Fructose-1-6-bisphosphate
xu5p_D_c	5.25	D-Xylulose-5-phosphate
ru5p_D_c	5.25	D-Ribulose-5-phosphate
r5p_c	5.25	alpha-D-Ribose-5-phosphate
icit_c	4.50	Isocitrate
cit_c	4.50	Citrate
e4p_c	4.00	D-Erythrose-4-phosphate
mal_L_e	3.75	L-Malate
mal_L_c	3.75	L-Malate
3pg_c	3.25	3-Phospho-D-glycerate
2pg_c	3.25	D-Glycerate-2-phosphate
13dpg_c	3.25	3-Phospho-D-glyceroyl-phosphate
oaa_c	3.00	Oxaloacetate

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chargecheck ▼

Search for reactions and compounds in the model(only used for 'search')

🔘 reaction
⚪ compound

Enter reaction or compound ID (only used for 'search' function)

data

INFO: Model: Ecoli_core_model

INFO: Unbalanced reactions: 0/75

INFO: Unchecked reactions due to missing charge: 75/75

INFO: Reactions excluded from check: 0/75

Curation & Analysis functions

Functions supported by PSAMM that are used for model curation and analysis. These function can be used to correct common errors and ensure that metabolic reconstructions are accurate representations of the metabolism of an organism, as well as perform various simulations of growth with metabolic models.

Choose model file (YAML format model)

Browse...	No file selected

Select functions you want to apply on your model

formulacheck	▼

Search for reactions and compounds in the model(only used for 'search')

- ⦿ reaction
- ○ compound

Enter reaction or compound ID (only used for 'search' function)

data

INFO: Unbalanced reactions: 1/75

INFO: Unchecked reactions due to missing formula: 0/75

reaction_id	formula_left	formula_right
Biomass_Ecoli_core_w_GAM	C1088.0232H1471.1810N446.7617O1236.7018P240.5298S3.7478	C1045.4677H1395.2089N441.3

la: 0/75

	formula_right	number_of_atoms(left<right)	number_of_atoms(left>right)
471.1810N446.7617O1236.7018P240.5298S3.7478	C1045.4677H1395.2089N441.3089O1189.0281P236.8511S3.7478	NA	C42.5555H75.9721N5.4528O47.6737P3.6787

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Choose model file (YAML format model)

Browse...	No file selected

Select functions you want to apply on your model

fba	▼

Search for reactions and compounds in the model(only used for 'search')

● reaction
○ compound

Enter reaction or compound ID (only used for 'search' function)

data

INFO: Objective flux: 0.873921506968

INFO: Reactions at zero flux: 47/95

reaction_id	reaction_flux	equation	gene_associations
ACONTa	6.01	Citrate[c] <=> cis-Aconitate[c] + H2O[c]	(b0118 or b1276)
ACONTb	6.01	cis-Aconitate[c] + H2O[c] <=> Isocitrate[c]	(b0118 or b1276)
AKGDH	5.06	2-Oxoglutarate[c] + Coenzyme-A[c] + Nicotinamide-adenine-dinucleotide[c] => CO2[c] + Nicotinamide-adenine-dinucleotide-reduced[c] + Succinyl-CoA[c]	(b0116 and b0726 and b0727)
ATPM	8.39	ATP[c] + H2O[c] => ADP[c] + H[c] + Phosphate[c]	
ATPS4r	45.51	ADP[c] + (4) H[e] + Phosphate[c] <=> ATP[c] + H2O[c] + (3) H[c]	(((b3736 and b3737 and b3738) and (b3731 and b3732 and b3733 and b3734 and b3735)) or ((b3736 and b3737 and b3738) and (b3731 and b3732 and b3733 and b3734 and b3735) and b3739))
Biomass_Ecoli_core_w_GAM	0.87	(1.496) 3-Phospho-D-glycerate[c] + (3.7478) Acetyl-CoA[c] + (59.81) ATP[c] + (0.361) D-Erythrose-4-phosphate[c] + (0.0709) D-Fructose-6-phosphate[c] + (0.129) Glyceraldehyde-3-phosphate[c] + (0.205) D-Glucose-6-phosphate[c] + (0.2557) L-Glutamine[c] + (4.9414) L-Glutamate[c] + (59.81) H2O[c] +	

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Choose model file (YAML format model)

Browse...	No file selected

Select functions you want to apply on your model

fva	▼

Search for reactions and compounds in the model(only used for 'search')

● reaction
○ compound

Enter reaction or compound ID (only used for 'search' function)

[   ]

data

INFO: Using Biomass_Ecoli_core_w_GAM as objective

INFO: Setting objective threshold to 100.0% of 0.873921506968 = 0.873921506968

reaction_id	lowest_reaction_flux	highest_reaction_flux	equation
G6PDH2r	4.96	4.96	D-Glucose-6-phosphate[c] + Nicotinamide-adenine-dinucleotide-phosphate[c] <=> 6-phospho-D-glucono-1-5-lactone[c] + H[c] + Nicotinamide-adenine-dinucleotide-phosphate-reduced[c]
AKGDH	5.06	5.06	2-Oxoglutarate[c] + Coenzyme-A[c] + Nicotinamide-adenine-dinucleotide[c] => CO2[c] + Nicotinamide-adenine-dinucleotide-reduced[c] + Succinyl-CoA[c]
GLNS	0.22	0.22	ATP[c] + L-Glutamate[c] + Ammonium[c] => ADP[c] + L-Glutamine[c] + H[c] + Phosphate[c]
ADK1	0.00	0.00	AMP[c] + ATP[c] <=> (2) ADP[c]
PYRt2r	0.00	0.00	H[e] + Pyruvate[e] <=> H[c] + Pyruvate[c]
EX_co2_e	22.81	22.81	CO2[e] <=>
ATPM	8.39	8.39	ATP[c] + H2O[c] => ADP[c] + H[c] + Phosphate[c]
SUCCt2_2	0.00	0.00	(2) H[e] + Succinate[e] => (2) H[c] + Succinate[c]
PIt2r	3.21	3.21	H[e] + Phosphate[e] <=> H[c] + Phosphate[c]
EX_lac_D_e	0.00	0.00	D-Lactate[e] <=>
GAPD	16.02	16.02	Glyceraldehyde-3-phosphate[c] + Nicotinamide-adenine-dinucleotide[c] + Phosphate[c] <=> 3-Phospho-D-glyceroyl-phosphate[c] + H[c] + Nicotinamide-adenine-dinucleotide-reduced[c]
ACALDt	0.00	0.00	Acetaldehyde[e] <=> Acetaldehyde[c]

Result:

id: PGI

equation: g6p_c[c] <=> f6p_c[c]

equation (compound names): D-Glucose-6-phosphate[c] <=> D-Fructose-6-phosphate[c]

genes: b4025

name: glucose-6-phosphate isomerase

subsystem: Glycolysis/Gluconeogenesis

Defined in ./E_coli_yaml/reactions.yaml

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Choose model file (YAML format model)

Browse...	No file selected

Select functions you want to apply on your model

search ▼

Search for reactions and compounds in the model(only used for 'search')

● reaction
○ compound

Enter reaction or compound ID (only used for 'search' function)

PGI

Curation & Analysis functions

Functions supported by PSAMM that are used for model curation and analysis. These function can be used to correct common errors and ensure that metabolic reconstructions are accurate representations of the metabolism of an organism, as well as perform various simulations of growth with metabolic models.

Choose model file (YAML format model)

Browse...	No file selected

Select functions you want to apply on your model

search	▼

Search for reactions and compounds in the model(only used for 'search')

○ reaction

● compound

Enter reaction or compound ID (only used for 'search' function)

g6p_c

Result:

id: g6p_c

formula: C6H11O9P

name: D-Glucose-6-phosphate

Defined in ./E_coli_yaml/compounds.yaml