

A web server to draft

Metabolic network reconstructions for Bacteria

Mr Bac



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HOW-TO

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Step 1. Select query and reference species

Select query species **Select reference species** Scroll bar for other species

*Select a query and a reference species: [Example]

Query Species:

- Salmonella enterica subsp. enterica serovar Heidelberg str. SL476
- Salmonella enterica subsp. enterica serovar Newport str. SL254
- Salmonella enterica subsp. enterica serovar Paratyphi A str. AKU_12601
- Salmonella enterica subsp. enterica serovar Paratyphi A str. ATCC 9150
- Salmonella enterica subsp. enterica serovar Paratyphi B str. SPB7
- Salmonella enterica subsp. enterica serovar Paratyphi C strain RKS4594
- Salmonella enterica subsp. enterica serovar Schwarzengrund str. CVM19633
- Salmonella enterica subsp. enterica serovar Typhi str. CT18
- Salmonella enterica subsp. enterica serovar Typhi str. Ty2
- Salmonella enterica subsp. enterica serovar Typhimurium str. LT2

Reference Species:

- Escherichia coli IAI39
- Escherichia coli O127:H6 str. E2348/69
- Escherichia coli O157:H7 EDL933
- Escherichia coli O157:H7 str. EC4115
- Escherichia coli O157:H7 str. Sakai
- Escherichia coli S88
- Escherichia coli SE11
- Escherichia coli SMS-3-5
- Escherichia coli str. K-12 substr. DH10B
- Escherichia coli str. K-12 substr. MG1655

*Choose Blast Settings: [Default / Select All]
E value: 1e-5 & Percent Identity: 50.0 %

Choose the blast columns to be shown: ?

Ref Query PercIden MLen mismatches gap openings q.start q.end r.start r.end EVAl BitScore

* indicates required input.

Submit Click to send Type in desired Blast parameters Click for column description Select columns to show

Step 2. One to one blastp best hits

Click to update the changes

Further change of parameters & the columns to show

Reciprocal Blast: Salmonella enterica subsp. enterica serovar Typhimurium str. LT2 vs Escherichia coli str. K-12 substr. MG1655

Setting Blast Filtering: [Default / Select All] Show columns: ? Ref Query PercIden MLen mismatches

E value: 1e-5 & Percent Identity: 50.0 % gap openings q.start q.end r.start r.end EVAl BitScore

Show filtered results **Proceed to annotation settings...** **Submit using current settings**

Save as .xls file **Enable Sorting** (*Memory and CPU consuming)

Click to enable browser sorting

Download result

Results of Reciprocal Blast

Query	Ref	PercIden	Eval	PercIden2	Eval2
STM0002	b0002	94.51	0.0	94.51	0.0
STM0003	b0003	93.51	2e-165	93.51	6e-154
STM0004	b0004	93.46	0.0	93.46	0.0
STM0005	b0006	86.38	6e-132	86.38	6e-132
STM0006	b0007	76.26	0.0	76.26	0.0
STM0007	b0008	94.64	0.0	94.64	0.0
STM0008	b0009	91.67	7e-101	91.67	6e-101
STM0009	b0010	90.43	1e-87	90.43	3e-95
STM0010	b0011	87.34	9e-96	87.34	4e-101
STM0011	b0012	81.24	1e-62	81.24	1e-62

2a. Sort Enabled

Total number of 1 to 1 protein matches to the reference genome: 3289 (out of 4525)
 Total number of 1 to 1 protein matches to the reference genome that pass through the filter: 3059

[Save as .xls file](#)

Sort Enabled.

Please click the desired column name to sort

(*Memory and CPU consuming)

Query	Ref	PercIden	EVal	PercIden2	EVal2
STM0485	b0471	100.00	1e-38	100.00	9e-39
STM0953	b0884	100.00	5e-38	100.00	5e-38
STM1191	b1089	100.00	2e-28	100.00	2e-28
STM1196	b1094	100.00	3e-30	100.00	3e-30
STM1336	b1716	100.00	1e-52	100.00	1e-52
STM1335	b1717	100.00	5e-19	100.00	5e-19
STM1837	b1823	100.00	6e-35	100.00	5e-35
STM1966	b1930	100.00	4e-41	100.00	3e-41
STM2431	b2415	100.00	3e-44	100.00	2e-44
STM2561	b2553	100.00	4e-48	100.00	4e-48

Click on column name to sort the specific column

2b. Changed blastp settings

Reciprocal Blast: *Salmonella enterica subsp. enterica serovar Typhimurium str. LT2* vs *Escherichia coli str. K-12 substr. MG1655*

Setting Blast Filtering: [Default/Select All](#)

E value: 1e-5 & Percent Identity: 80.0 %

Show columns: Ref Query PercIden MLen mismatches
 gap openings q.start q.end r.start r.end EVal BitScore

Show filtered results

Proceed to annotation settings...

Total number of 1 to 1 protein matches to the reference genome: 3289 (out of 4525)
 Total number of 1 to 1 protein matches to the reference genome that pass through the filter: 2638

[Save as .xls file](#)

[Enable Sorting](#)

(*Memory and CPU consuming)

Query	Ref	PercIden	MLen	EVal	PercIden2	MLen2	EVal2
STM0002	b0002	94.51	820	0.0	94.51	820	0.0
STM0003	b0003	93.51	308	2e-165	93.51	308	6e-154
STM0004	b0004	93.46	428	0.0	93.46	428	0.0
STM0005	b0006	86.38	257	6e-132	86.38	257	6e-132
STM0007	b0008	94.64	317	0.0	94.64	317	0.0
STM0008	b0009	91.67	192	7e-101	91.67	192	6e-101
STM0009	b0010	90.43	188	1e-87	90.43	188	3e-95
STM0010	b0011	87.34	237	9e-96	87.34	237	4e-101
STM0011	b0013	81.34	134	1e-62	81.34	134	1e-62

Results of reciprocal Blast from the update

Step 3. Annotation Selection



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Salmonella enterica subsp. enterica serovar Typhimurium str. LT2 versus *Escherichia coli str. K-12 substr. MG1655*

Your current blast settings are

Evalue: 1e-5
 PercIden: 50.0

Show all Query Genes: Yes No

Click No to list only filtered genes
 Yes to list all Query genes in genome

Click for column description

*Choose the annotation columns to be shown for both query and reference: ?

- QueryID gene
- 5'Coordinate 3'Coordinate Product ProteinLength
- KO: KONum KODEFIN KOCLASS
- EC: ECNum ECNAME ECCLASS ECSYSNAME
- COG: FunID FUNCategory FUNDesc
- MT: TransporterType FamilyName Substrate
- ReferenceID gene
- KO: KONum KODEFIN KOCLASS
- EC: ECNum ECNAME ECCLASS ECSYSNAME
- COG: FunID FUNCategory FUNDesc
- MT: TransporterType FamilyName Substrate

Select desired annotations to view

[Back to blast filtering](#)

Proceed to annotation matching...

Submit to obtain annotations of both species

Step 4. Annotation retrieval

Salmonella enterica subsp. enterica serovar Typhimurium str. LT2 versus Escherichia coli str. K-12 substr. MG1655

Evalue: 1e-5 Percent Identity: 50.0

Download annotation Input for SBML Generator

Back to settings Save as .xls file Save Gene Pair File Metabolic Network Generator

<< Back to blast filtering
< Back to column selection

Query	gene	ECNum	Ref	gene	ECNum
PSLT067	--	--	b0249	ykfF	--
STM0002	thrA	1.1.1.13;; 1.1.1.13;; 2.7.2.4	b0002	thrA	1.1.1.13;; 2.7.2.4
STM0003	thrB	2.7.1.39	b0003	thrB	2.7.1.39
STM0004	thrC	4.2.3.1	b0004	thrC	4.2.3.1
STM0005	yaaA	--	b0006	yaaA	--
STM0006	yaaJ	--	b0007	yaaJ	--
STM0007	talB	2.2.1.2	b0008	talB	2.2.1.2
STM0008	mogA	--	b0009	mog	--
STM0009	yaaH	--	b0010	yaaH	--
STM0010	htgA	--	b0011	yaaW	--
STM0011	yaaI	--	b0013	yaaI	--
STM0012	dnaK	--	b0014	dnaK	--

Link to the generator

Annotation list of query and reference species

Step 5. Network draft generation

Metabolic Network Draft Generation

Upload the reference reconstruction

Upload a reference SBML file (sample, iAF1260) ?
SBML File:

Upload the gene pair file

Upload a one to one gene pair file (sample, SLT2vsECO) ?
Gene Pair File:

Name the model

Type in a model name
New Model Name:

Submit Query

Submit to obtain the draft

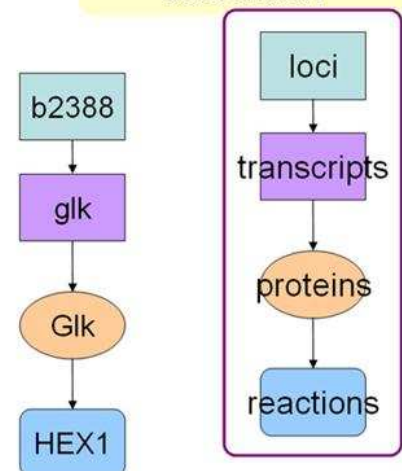
5a. sample reaction tag in SBML

```
<reaction id="R_HEX1" name="R_hexokinase_D_glucose&ATP_" reversible="false">
  <notes>
    <html:p>GENE_ASSOCIATION: b2388</html:p>
    <html:p>PROTEIN_ASSOCIATION: Glk</html:p>
    <html:p>SUBSYSTEM: S_GlycolysisGluconeogenesis</html:p>
    <html:p>PROTEIN_CLASS: 2.7.1.1</html:p>
  </notes>
  <listOfReactants>
    <speciesReference species="H_atp_c" stoichiometry="1.000000"/>
    <speciesReference species="H_glc_D_c" stoichiometry="1.000000"/>
  </listOfReactants>
  <listOfProducts>
    <speciesReference species="H_adp_c" stoichiometry="1.000000"/>
    <speciesReference species="H_g6p_c" stoichiometry="1.000000"/>
    <speciesReference species="H_h_c" stoichiometry="1.000000"/>
  </listOfProducts>
  <kineticLaw>
```

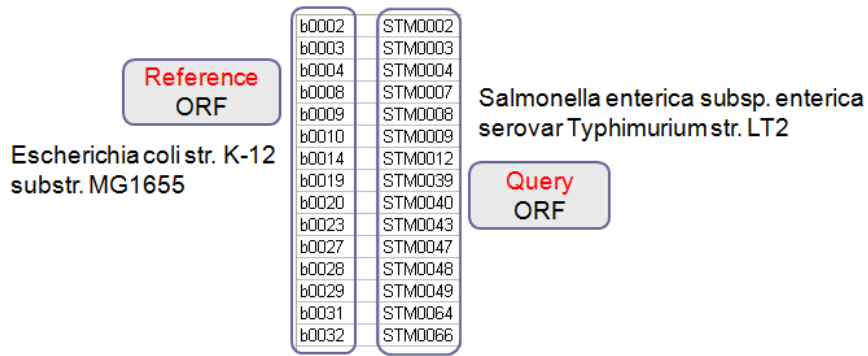
HEX1: [c] glc_D + atp → g6p + adp + h

i.e. D-Glucose + ATP → D-Glucose 6-phosphate + ADP + H

Gene-protein-reaction association



5b. One to one gene pair .txt file format: first column lists the reference gene id; second column lists the corresponding query id.



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