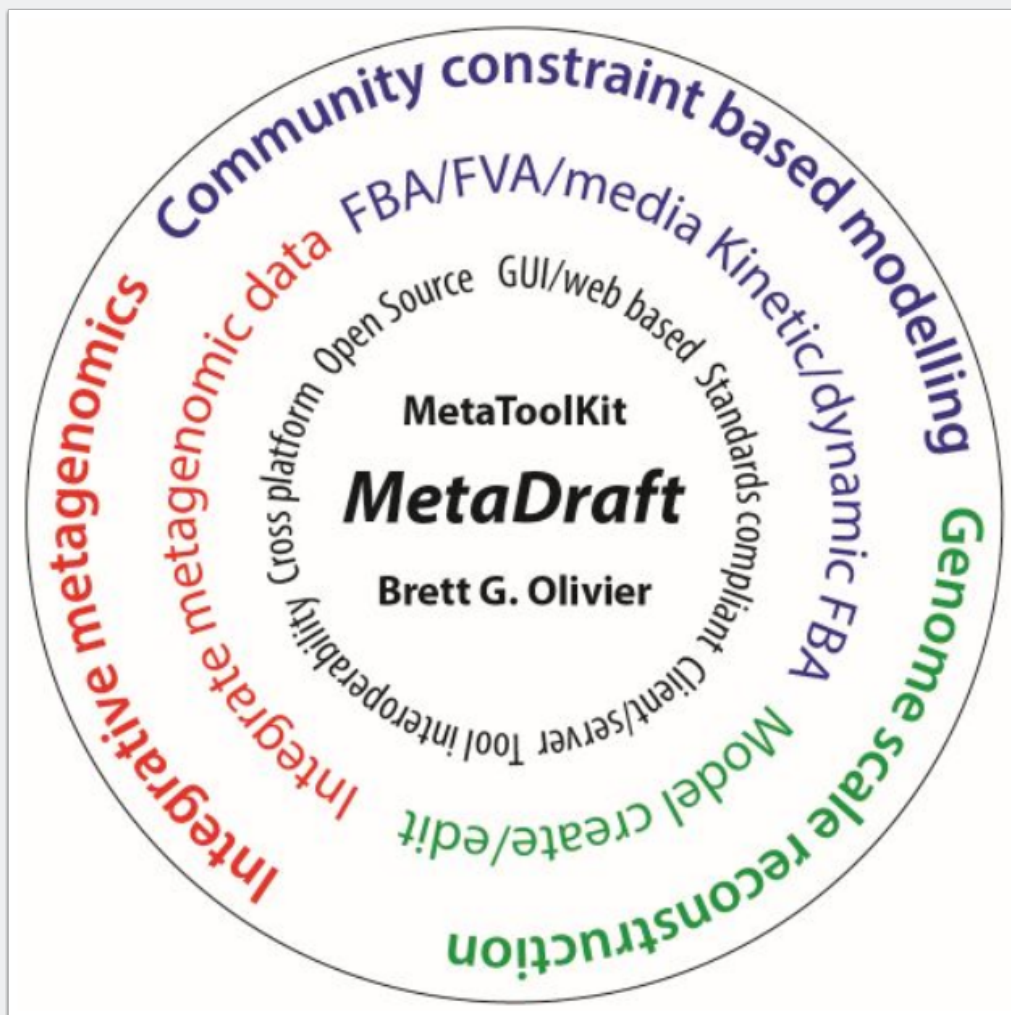


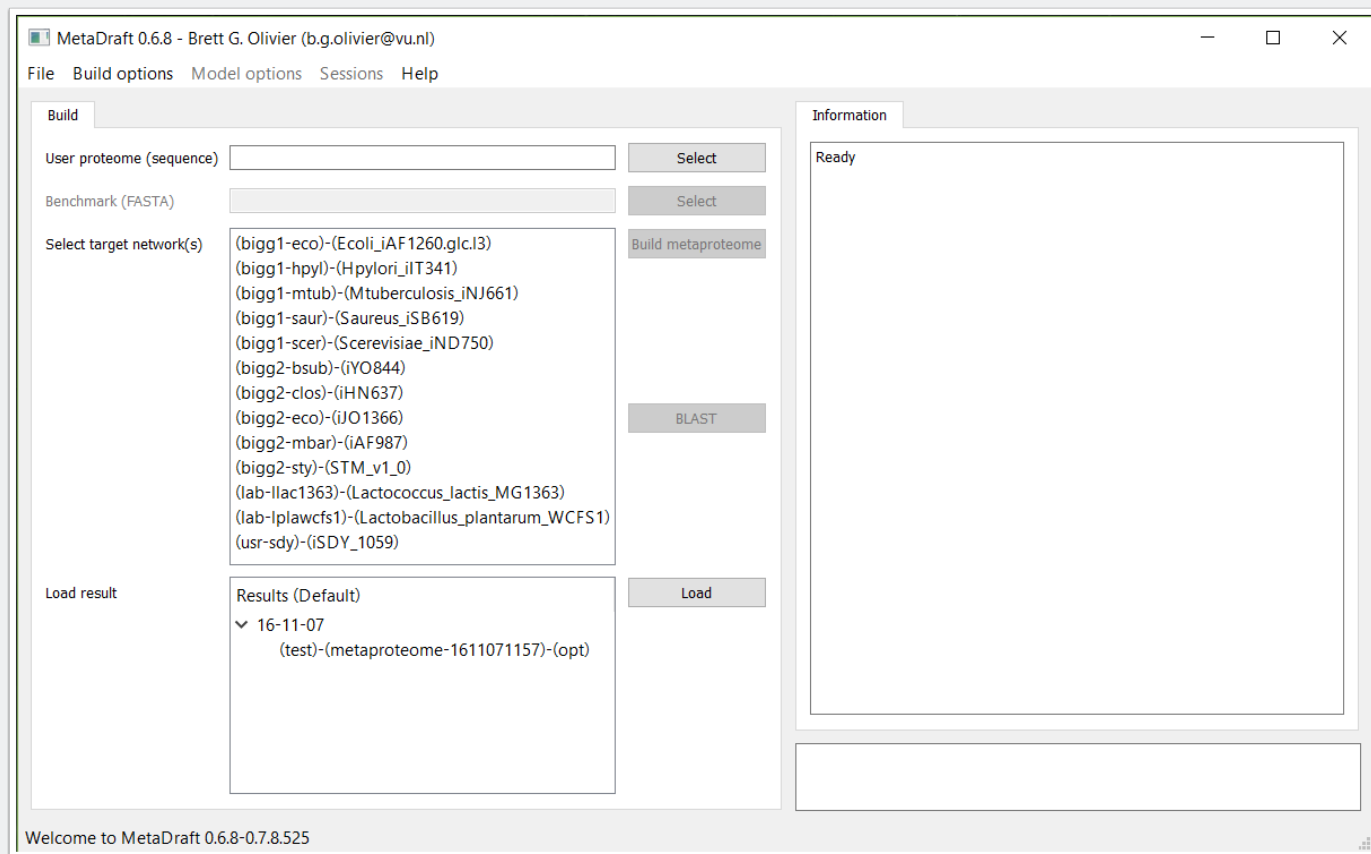
Welcome

Welcome to MetaDraft part of the MetaToolKit CBMPy software family
(<http://cbmpy.sourceforge.net>). MetaDraft has been designed and coded by Brett G. Olivier PhD (b.g.olivier@vu.nl)



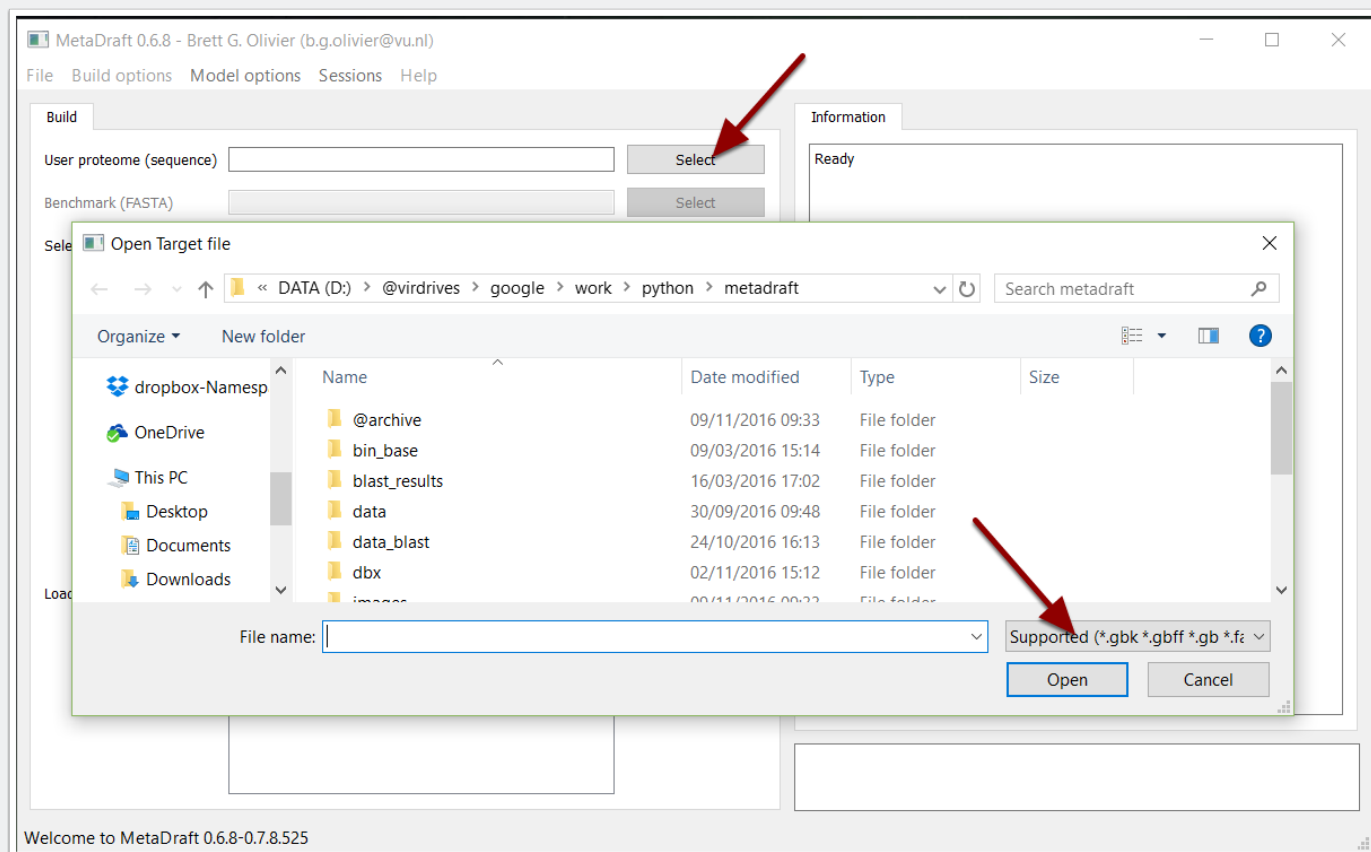
Main screen

This is the main program screen where you can create new draft reconstruction or load previously analysed results.



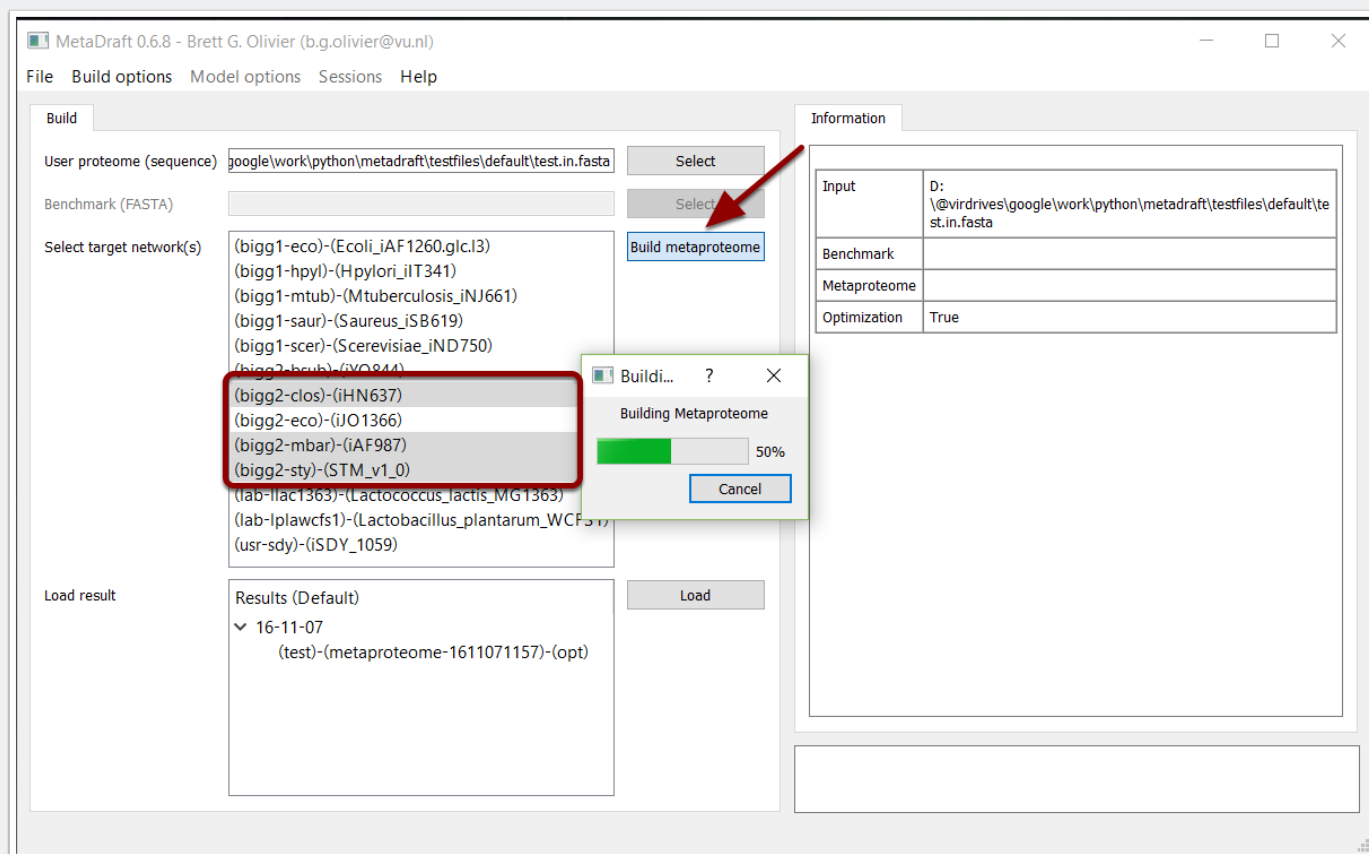
Sequence loading

To load your FASTA or GenBank sequence push "select".



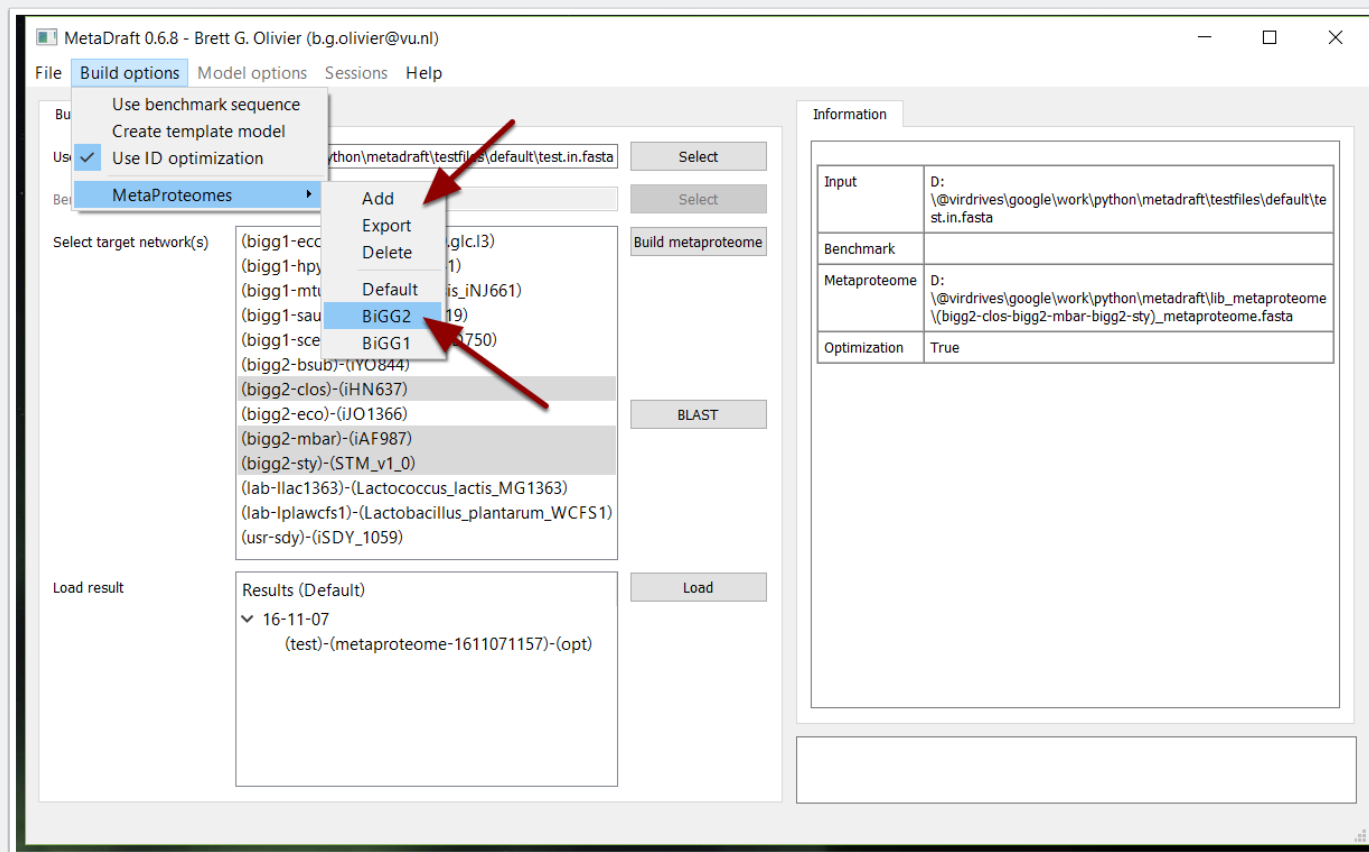
Build a metaproteome

Multiple organisms can be added to your metaproteome database, this list can be reordered to set its priority (higher is better).



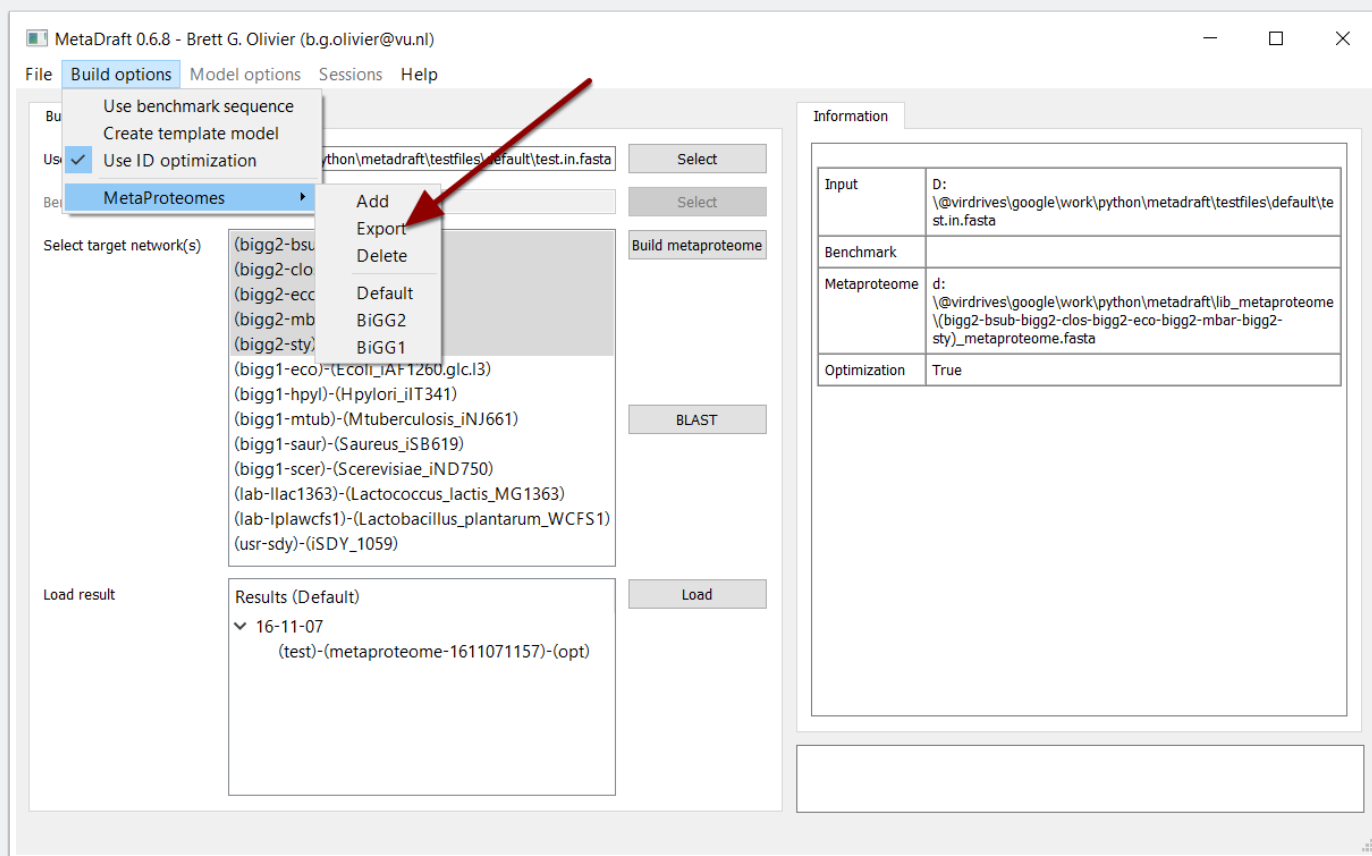
Predefined sets

Using the "Build options" menu it is possible to select predefined MetaProteomes. It is possible to "Add" or "Delete" predefined metaproteomes.



Metaproteome export

Export selected metaproteome in FASTA format.



Run sequence search

Pressing "BLAST" will use an inParanoid orthology search running multiple bi-directional BLAST's. This can take a while (minutes to hours).

MetaDraft 0.6.8 - Brett G. Olivier (b.g.olivier@vu.nl) (Not Responding)

File Build options Model options Sessions Help

Build

User proteome (sequence)

Benchmark (FASTA)

Select target network(s)

- (bigg2-eco)-(iJO1366)
- (bigg2-bsub)-(iYO844)
- (bigg2-clos)-(iHN637)
- (bigg2-mbar)-(iAF987)
- (bigg2-sty)-(STM_v1_0)
- (lab-llac1363)-(Lactococcus_lactis_MG1363)
- (lab-lplawcfs1)-(Lactobacillus_plantarum_WCFS1)
- (bigg1-eco)-(Ecoli_iAF1260.glc.l3)
- (bigg1-hpyl)-(Hpylori_iIT341)
- (bigg1-mtub)-(Mtuberculosis_iNJ661)
- (bigg1-saur)-(Saureus_iSB619)
- (bigg1-scer)-(Scerevisiae_iND750)
- (usr-sdy)-(iSDY_1059)

Load result

Results (Default)

- 16-11-07
 - (test)-(metaproteome-1611071157)-(opt)

Information

Input	D:\@virtdrives\google\work\python\metadraft\testfiles\default\test.in.fasta
Benchmark	
Metaproteome	d:\@virtdrives\google\work\python\metadraft\lib_metaproteome\bigg2-eco_metaproteome.fasta

Running sequence search

50%

Metaproteome: "d:\@virtdrives\google\work\python\metadraft\lib_metaproteome\bigg2-eco_metaproteome.fasta" created.

Search results

When the BLAST search completes the results are shown in the results panel.

MetaDraft 0.6.8 - Brett G. Olivier (b.g.olivier@vu.nl)

FileBuild optionsModel optionsSessionsHelp

Build

User proteome (sequence)

Select

Benchmark (FASTA)

Select

Select target network(s)

(bigg2-eco)-(iJO1366)
(bigg2-bsub)-(iYO844)
(bigg2-clos)-(iHN637)
(bigg2-mbar)-(iAF987)
(bigg2-sty)-(STM_v1_0)
(lab-llac1363)-(Lactococcus_lactis_MG1363)
(lab-lplawcfs1)-(Lactobacillus_plantarum_WCFS1)
(bigg1-eco)-(Ecoli_iAF1260.glcI3)
(bigg1-hpyl)-(Hpylori_iIT341)
(bigg1-mtub)-(Mtuberculosis_iNJ661)
(bigg1-saur)-(Saureus_iSB619)
(bigg1-scer)-(Scerevisiae_iND750)
(usr-sdy)-(iSDY_1059)

Build metaproteome

Load result

Results (Default)
11-09
(test)-(bigg2-eco)-(opt)
16-11-07
(test)-(metaproteome-1611071157)-(opt)

Load

BLAST

Information

Input	D:\@virddrives\google\work\python\metadraft\testfiles\default\test.in.fasta
Benchmark	
Metaproteome	d:\@virddrives\google\work\python\metadraft\lib_metaproteome\bigg2-eco_metaproteome.fasta
Optimization	True

BLAST run successful

METADRAFT

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Delete/rename results

Right-clicking on the result (and network) windows allows one to delete or rename files.

MetaDraft 0.6.8 - Brett G. Olivier (b.g.olivier@vu.nl)

File Build options Model options Sessions Help

Build

User proteome (sequence)

Benchmark (FASTA)

Select target network(s)

- (bigg2-eco)-(iJO1366)
- (bigg2-bsub)-(iYO844)
- (bigg2-clos)-(iHN637)
- (bigg2-mbar)-(iAF987)
- (bigg2-sty)-(STM_v1_0)
- (lab-llac1363)-(Lactococcus_lactis_MG1363)
- (lab-lplawcfs1)-(Lactobacillus_plantarum_WCFS1)
- (bigg1-eco)-(Ecoli_iAF1260.glc.l3)
- (bigg1-hpyl)-(Hpylori_iIT341)
- (bigg1-mtub)-(Mtuberculosis_iNJ661)
- (bigg1-saur)-(Saureus_iSB619)
- (bigg1-scer)-(Scerevisiae_iND750)
- (usr-sdy)-(iSDY_1059)

Load result

Results (Default)

- 16-11-09 (test)-(bigg2-eco)-(opt)
- 16-11-07 (test)-(bigg2-eco)-(opt) ⌵
 - 1611071157-(opt) ⌵
 - Rename
 - Delete

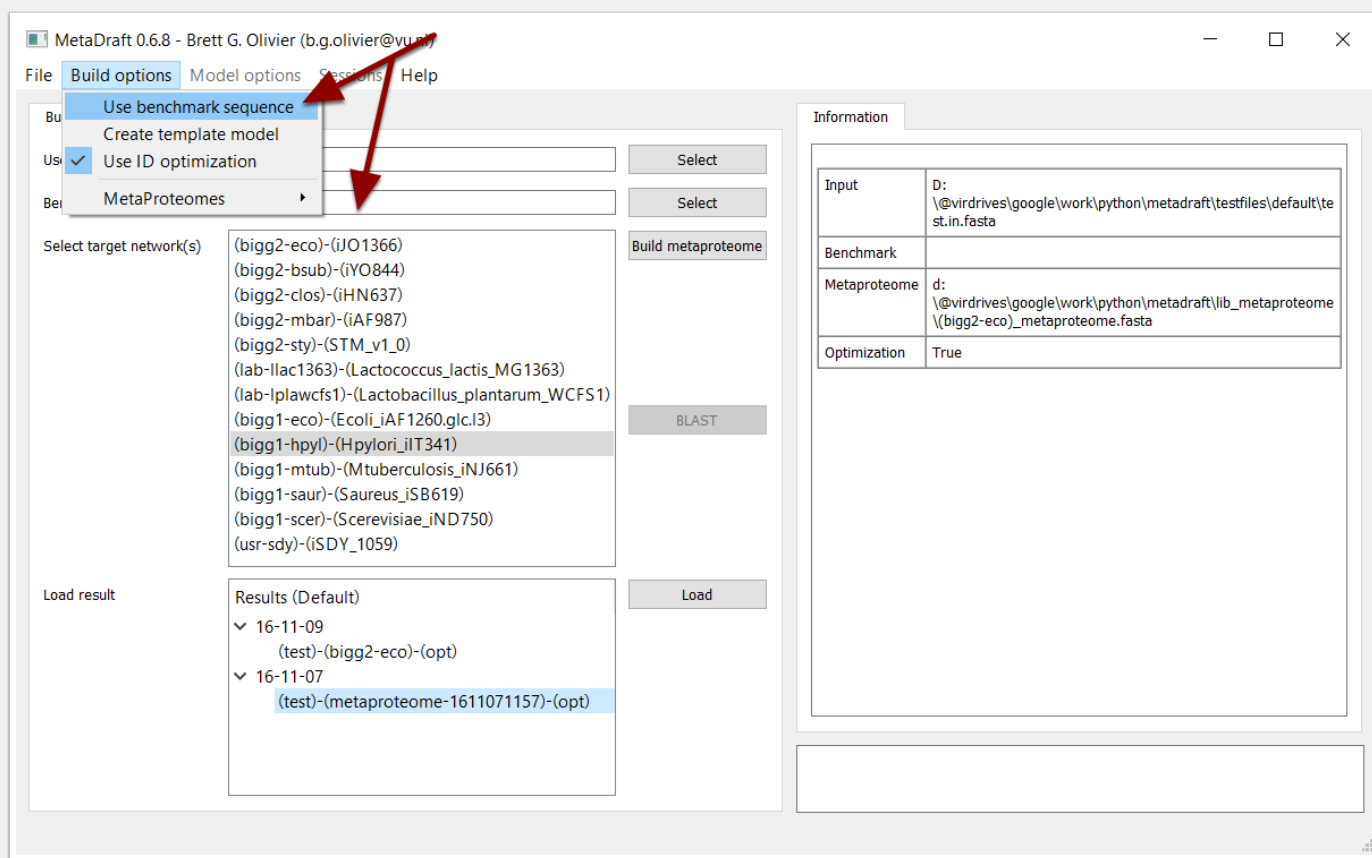
Information

Input	D:\@virtdrives\google\work\python\metadraft\testfiles\default\test.in.fasta
Benchmark	
Metaproteome	d:\@virtdrives\google\work\python\metadraft\lib_metaproteome\bigg2-eco_metaproteome.fasta
Optimization	True

BLAST run successful

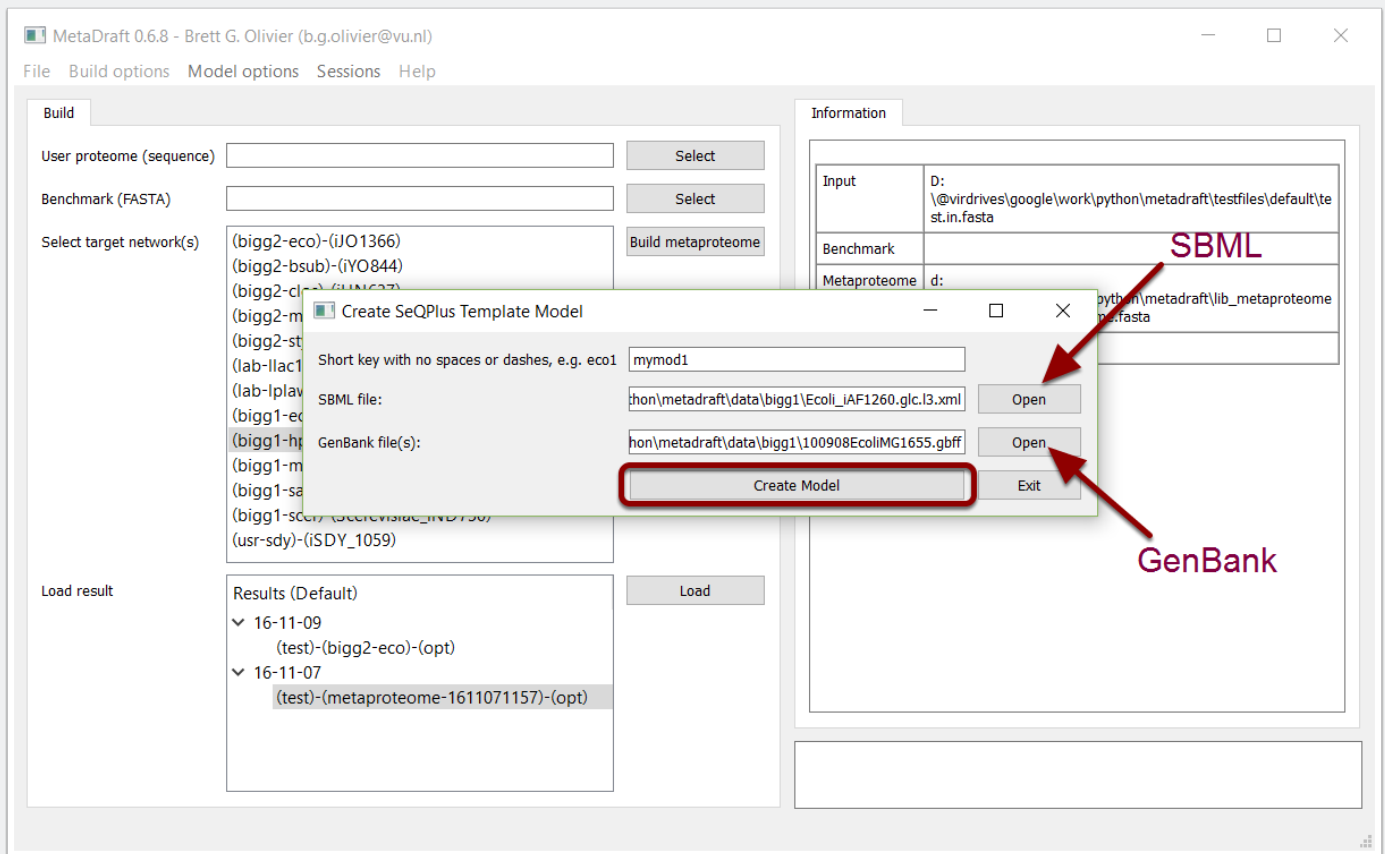
Optional: benchmark

Using the benchmark functionality you can include a sequence file that will be used as a benchmark for your sequence search. Only sequences with higher orthology than the benchmark will be included.



Option: create new template model

The creation of a new SeQPlus template model involves the merging of an SBML model which includes gene-protein-reaction associations and whose id's can be mapped to an associated GenBank file. A unique short alpha-numeric key is required.



Option: create new template model 2

Custom defined models are labelled as "usr-xxx" models

MetaDraft 0.6.8 - Brett G. Olivier (b.g.olivier@vu.nl)

File Build options Model options Sessions Help

Build

User proteome (sequence)

Benchmark (FASTA)

Select target network(s)

- (bigg1-hpyl)-(Hpylori_iIT341)
- (bigg1-mtub)-(Mtberculosis_iNJ661)
- (bigg1-saur)-(Saureus_iS8619)
- (bigg1-scer)-(Scerevisiae_iND750)
- (bigg2-bsub)-(iYO844)
- (bigg2-clos)-(iHN637)
- (bigg2-eco)-(iJO1366)
- (bigg2-mbar)-(iAF987)
- (bigg2-sty)-(STM_v1_0)
- (lab-llac1363)-(Lactococcus_lactis_MG1363)
- (lab-lplawcfs1)-(Lactobacillus_plantarum_WCFS)
- (usr-mymod1)-(Ecoli_iAF1260.glc.l3)**
- (usr-sdy)-(iSDY_1059)

Load result

Results (Default)

- 16-11-09
 - (test)-(bigg2-eco)-(opt)
- 16-11-07
 - (test)-(metaproteome-1611071157)-(opt)

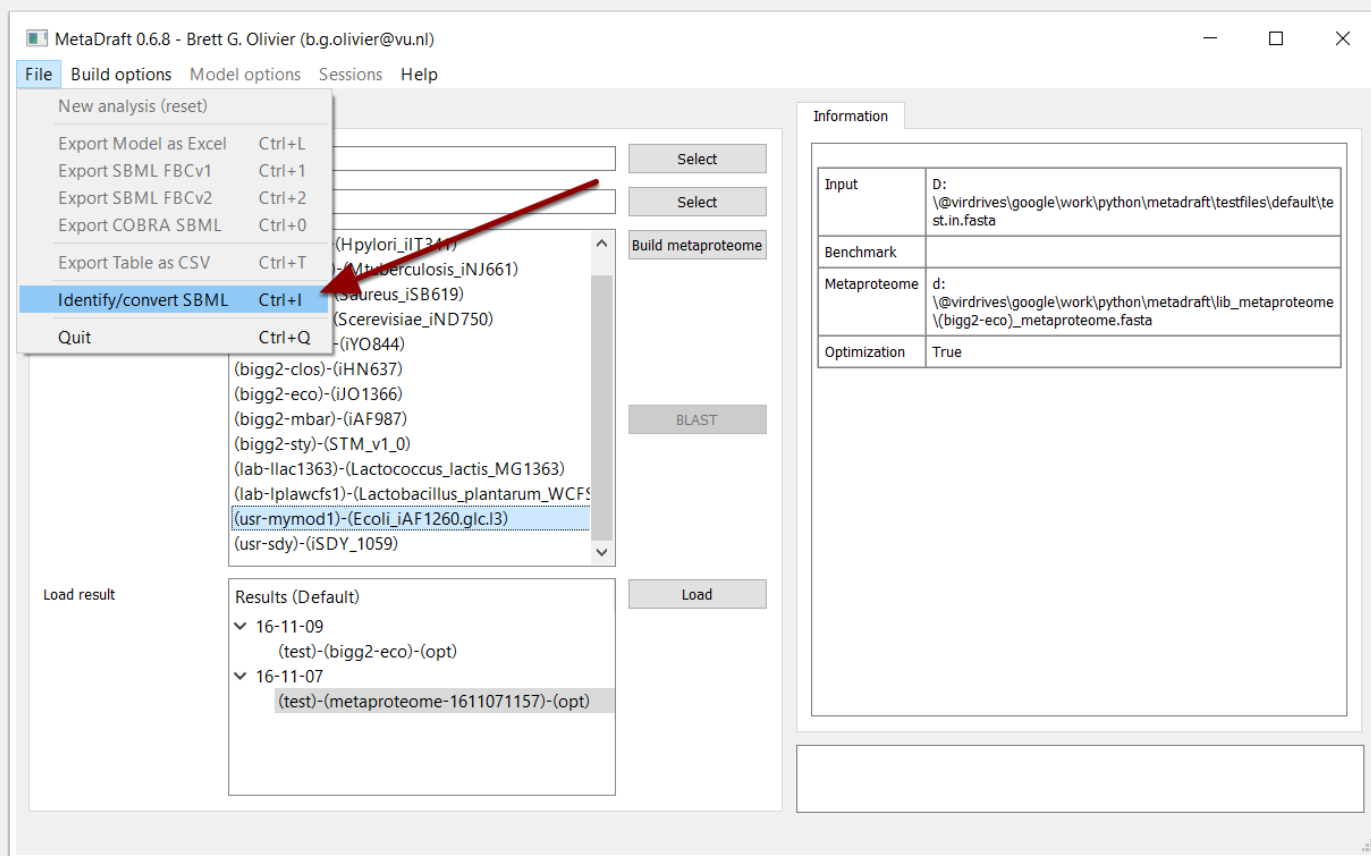
Information

Input	D: \\@virtdrives\google\work\python\metadraft\testfiles\default\test.in.fasta
Benchmark	
Metaproteome	d: \\@virtdrives\google\work\python\metadraft\lib_metaproteome \\(bigg2-eco)_metaproteome.fasta
Optimization	True

Created new SeqPlus template model: (usr-mymod1)-(Ecoli_iAF1260.glc.l3.xml)

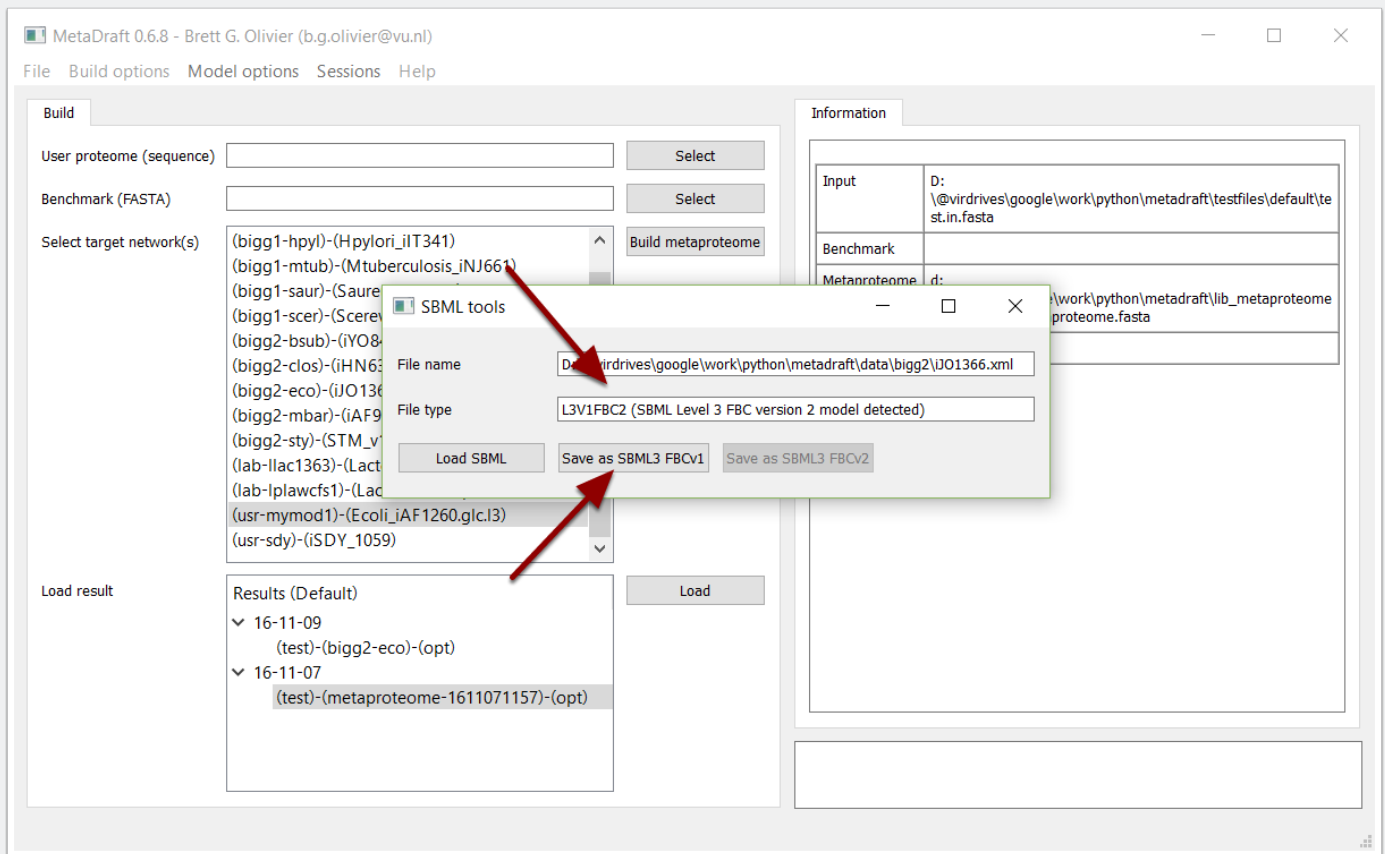
Option: analyse SBML model

To analyse, identify and optionally convert an SBML the model, use the File menu.



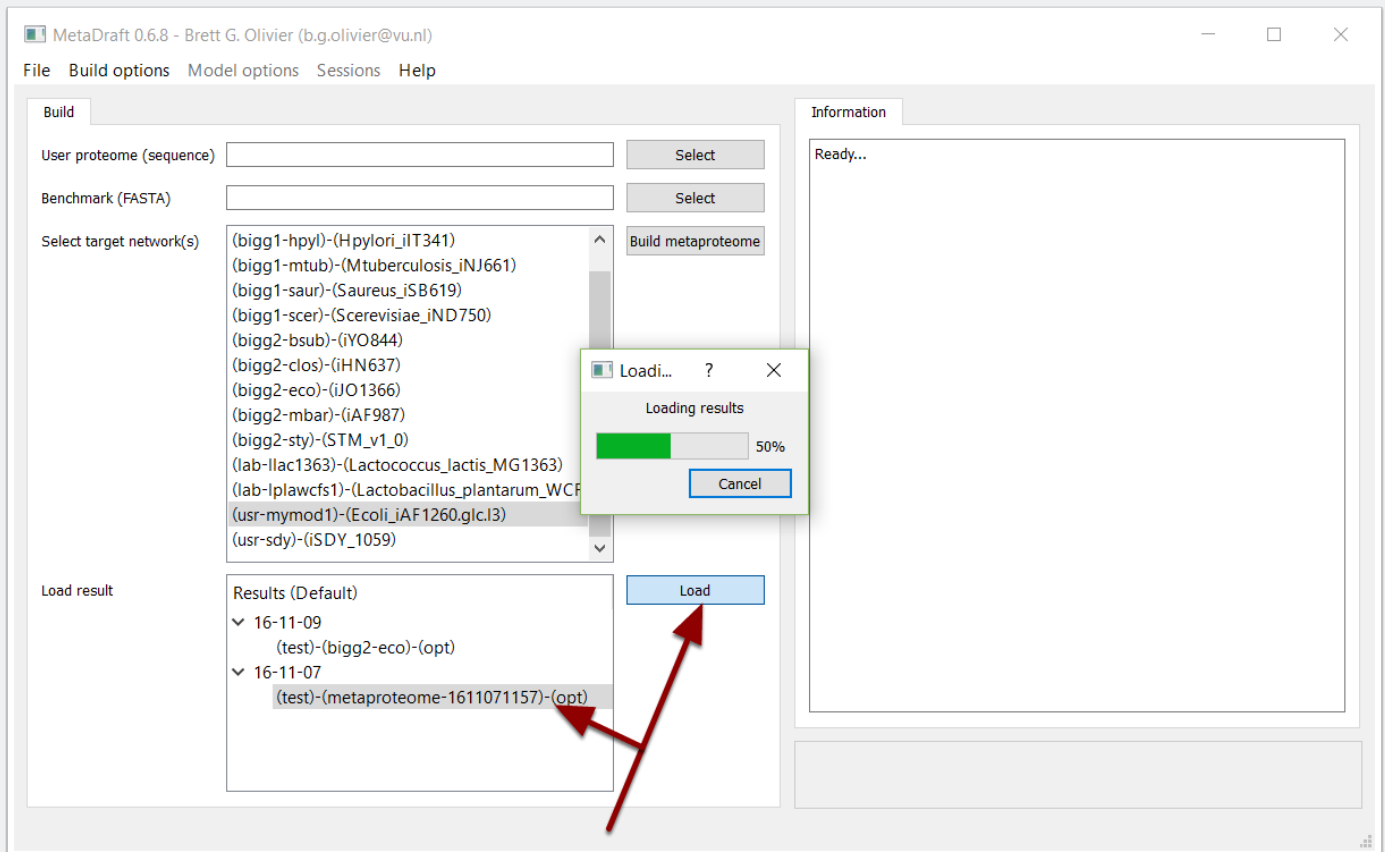
Option: analyse SBML model 2

Load an SBML file and MetaToolKit will try and identify it's encoding. Once the type of model encoding is identified the model can be converted to either of the new standard model encoding formats SBML3 FBC version 1 or 2.



Load results

To continue the analysis select a results set and click "Load".



Results: genes

The results are displayed on three interlinked tabs on the left. In all cases select components annotation is displayed on the right panel. Source genes are those in your input file, while matches from the metaproteome are displayed next. next, the "score" column provides the orthology match score which ranges from 0 to 1. Finally, the

selection column allows genes to be (un)selected as required (100% match is automatically selected) and source genes with multiple matches are grouped by colour for easy identification. On the right hand side the "Information" panel displays all known annotation about the matching gene and the reactions associated with it while the GPR association is colour coded such that green is matched and selected, red is matched and not selected while black is not matched.

MetaDraft 0.6.8 - Brett G. Olivier (b.g.olivier@vu.nl)

File Build options Model options Sessions Help

Build Genes Reactions Metabolites

	source	match	score		org
1	in_stu0160	LLMG_RS1...	1.0	<input checked="" type="checkbox"/>	lab-llac1363
2	in_stu0163	BSU35530	1.0	<input checked="" type="checkbox"/>	bigg2-bsub
3	in_stu0246	lp_1554	1.0	<input checked="" type="checkbox"/>	lab-lplawcfs1
4	in_stu0262	LLMG_RS0...	1.0	<input checked="" type="checkbox"/>	lab-llac1363
5	in_stu0264	b1363	0.9	<input type="checkbox"/>	bigg1-eco
6	in_stu0264	b3849	1.0	<input checked="" type="checkbox"/>	bigg1-eco
7	in_stu0265	b3290	1.0	<input checked="" type="checkbox"/>	bigg1-eco
8	in_stu0590	BSU38550	0.463	<input type="checkbox"/>	bigg2-bsub
9	in_stu0590	BSU38550	0.463	<input type="checkbox"/>	bigg1-scer
10	in_stu0590	BSU38550	0.463	<input type="checkbox"/>	bigg2-bsub
11	in_stu0596			<input type="checkbox"/>	
12	in_stu0603	b4254	1.0	<input checked="" type="checkbox"/>	bigg1-eco
13	in_stu0603	b0273	0.801	<input type="checkbox"/>	bigg1-eco
14	in_stu0606	LLMG_RS0...	1.0	<input checked="" type="checkbox"/>	lab-llac1363
15	in_stu0692	b4129	0.82	<input type="checkbox"/>	bigg1-eco
16	in_stu0692	b2890	1.0	<input checked="" type="checkbox"/>	bigg1-eco
17	in_stu0697	b4395	1.0	<input checked="" type="checkbox"/>	bigg1-eco
18	in_stu0720	BSU25020	1.0	<input checked="" type="checkbox"/>	bigg2-bsub

gene homology model

Information

GeneMatch: in_stu0262 --> LLMG_RS06045

Matching Gene Information	
inference	EXISTENCE: similar to AA sequence:RefSeq:WP_014735014.1
product	ribosomal large subunit pseudouridine synthase B
note	Derived by automated computational analysis using gene prediction method: Protein Homology.
old_locus_tag	llmg_1194
protein_id	WP_014735014.1
db_xref	GI:504547912
Associated reactions(s)	
R_PSUDS (lab-llac1363)	R_pseudouridylate_synthase
(LLMG_RS02350 or LLMG_RS07220 or llmg_2518 or LLMG_RS01970 or LLMG_RS07670 or LLMG_RS12010 or LLMG_RS06045)	
R_YUMPS (lab-llac1363)	R_yump_synthetase
(LLMG_RS02350 or LLMG_RS07220 or llmg_2518 or LLMG_RS01970 or LLMG_RS07670 or LLMG_RS12010 or LLMG_RS06045)	

Loaded results: "d:\@viridives\google\work\python\metadraft\blast_results\default\16-11-07\test-(metaproteome-1611071157)-(opt)_metalink.resplu.json".

Results: genes score filter

Right clicking on the "gene" table allows the selection of the "Gene Filter" tool where a user defined range can be set (between 0 and 1) and applied to quickly select multiple genes matching the selection criteria.

The screenshot shows the MetaDraft 0.6.8 interface. The 'Genes' table is displayed with columns: source, match, score, and org. A 'Filter selected genes' dialog box is open, allowing users to set a minimum and maximum score. The 'score' column in the table is highlighted in green for scores above 0.8 and yellow for scores below 0.8. A red arrow points to the 'score' column header with the text 'Right Click'.

	source	match	score	org
1	in_stu0160	LLMG_RS1...	1.0	lab-llac1363
2	in_stu0163	BSU35530	1.0	bigg2-bsub
3	in_stu0246	lp_1554	1.0	lab-lplawcfs1
4	in_stu0262	LLMG_RS0...	1.0	lab-llac1363
5	in_stu0264	b1363	0.219	bigg1-eco
6	in_stu0264	b3849	1.0	bigg1-eco
7	in_stu0265	b3290	1.0	bigg1-eco
8	in_stu0590	BSU02390	1.0	bigg1-eco
9	in_stu0590	YHR208W	0.46	bigg1-eco
10	in_stu0590	BSU38550	0.463	bigg1-eco
11	in_stu0596			
12	in_stu0603			bigg1-eco
13	in_stu0603	b0273	0.801	bigg1-eco
14	in_stu0606	LLMG_RS0...	1.0	lab-llac1363
15	in_stu0692	b4129	0.82	bigg1-eco
16	in_stu0692	b2890	1.0	bigg1-eco
17	in_stu0697	b4395	1.0	bigg1-eco
18	in_stu0720	BSU25020	1.0	bigg2-bsub

Filter selected genes dialog box:

Minimum score: 0.8 Maximum score: 1.0

Apply

Information panel:

GeneMatch: in_stu0590 --> BSU02390

Matching Gene Information

function	16.2: Construct biomass (Anabolism) 16.11: Scavenge (Catabolism)
EC_number	2.6.1.42
note	Evidence 1a: Function experimentally demonstrated in the studied strain; PubMedId: 12670965, 15060025, 15102328; Product type e: enzyme
experiment	publication(s) with functional evidences, PMID:12670965, 15060025, 15102328
gene	ilvE
product	ketomethiobutyrate-branched-chain/aromatic amino acid aminotransferase
protein_id	CAB12033.1
db_xref	GI:2632525 EnsemblGenomes-Gn:BSU02390 EnsemblGenomes-Tr:CAB12033 GOA:O31461 InterPro:IPR001544 InterPro:IPR005786 InterPro:IPR018300 Subtilist:8G12749

Genes: 36 Reactions: 61 Metabolites: 137

Results: reactions

The reactions displayed in the "Reaction" table are dynamically generated based on the gene selections made in the "Gene" panel. Information displayed in the table include id,

name organism as well as associated source and match genes. Any annotation associated with the reaction is displayed on the right as well as the GPR association in terms of the source and match reactions (using the colour scheme discussed in the "Genes" table). Hovering over the gene displays the gene annotation as a tooltip. In addition to the gene selection you may now unselect specific reactions based on the annotation, GPR association resolution.

MetaDraft 0.6.8 - Brett G. Olivier (b.g.olivier@vu.nl)

File Build options Model options Sessions Help

Build Genes Reactions Metabolites

reaction	name		org	genes	src
44	R_PRPPS	phosphoribos...	<input checked="" type="checkbox"/>	bigg1-eco	b1207 stu1460
45	R_PSUDS	R_pseudouridy...	<input checked="" type="checkbox"/>	lab-Ilac1363	LLMG_RS0... stu0262
46	R_PTPAT	R_pantetheine...	<input checked="" type="checkbox"/>	lab-Ilac1363	LLMG_RS1... stu1648
47	R_SBTpts	R_D_sorbitol_tr...	<input checked="" type="checkbox"/>	lab-Ilac1363	LLMG_RS0... stu1264,stu1...
48	R_SERAT	serine O-acetyl...	<input checked="" type="checkbox"/>	bigg1-eco	b3607 stu0848
49	R_SHSL1r	O-succinylhom...	<input checked="" type="checkbox"/>	bigg1-hpyl	HP0106 stu0847
50	R_SHSL2r	O-succinylhom...	<input checked="" type="checkbox"/>	bigg1-hpyl	HP0106 stu0847
51	R_SHSL2r	SHSL2r	<input checked="" type="checkbox"/>	bigg2-clos	CLJU_RS03... stu0987
52	R_SHSL4r	O-succinylhom...	<input checked="" type="checkbox"/>	bigg1-hpyl	HP0106 stu0847
53	R_SODr	Superoxide dis...	<input checked="" type="checkbox"/>	bigg2-bsub	BSU25020 stu0720
54	R_SUCpts	R_sucrose_tran...	<input checked="" type="checkbox"/>	lab-Ilac1363	LLMG_RS0... stu1264,stu1...
55	R_TECA1S45	Glycerol teicho...	<input checked="" type="checkbox"/>	bigg2-bsub	BSU35530 stu0163
56	R_TECA2S45	Glycerol teicho...	<input checked="" type="checkbox"/>	bigg2-bsub	BSU35530 stu0163
57	R_TECA3S45	Glycerol teicho...	<input checked="" type="checkbox"/>	bigg2-bsub	BSU35530 stu0163
58	R_TREpts	R_trehalose_tra...	<input checked="" type="checkbox"/>	lab-Ilac1363	LLMG_RS0... stu1264,stu1...
59	R_UDC...	R_undecapren...	<input checked="" type="checkbox"/>	lab-Ilac1363	LLMG_RS1... stu0160
60	R_VALTA	Valine transami...	<input checked="" type="checkbox"/>	bigg2-bsub	BSU02390 stu0590
61	R_YUMPS	R_yUMP_synth...	<input checked="" type="checkbox"/>	lab-Ilac1363	LLMG_RS0... stu0262

Genes: 38 Reactions: 61 Metabolites: 137

Information

Organism **bigg2-bsub**
R_VALTA Valine transaminase
 (reversible)
Association (BSU38550 or BSU02390)
Association (stu0590)
 new
Equation ID M_akg_c + M_val
Equation Name 2-Oxoglutarate + oxobutanoate
M_akg_c 2-Oxoglutarate
 charge: -2 C5H4O5
M_val_L_cL-Valine
 charge: 0 C5H11NO2
M_glu_L_cL-Glutamate
 charge: -1 C5H8NO4
M_3mob_c 3-Methyl-2-oxo
 charge: -1 C5H7O3

function: 16.2: Construct biomass (Anabolism)
locus_tag: BSU02390
raw_location: 259016..260086
codon_start: 1
EC_number: 2.6.1.42
transl_table: 11
note: Evidence 1a: Function experimentally de strain; PubMedId: 12670965, 15060025, 15102: experiment: publication(s) with functional evi 15060025, 15102328
gene: ilvE
product: ketomethiobutyrate-branched-chain, aminotransferase
protein_id: CAB12033.1

Results: metabolites

The metabolite panel is dynamically generated from the selected reactions on the "Reaction" panel. The lefthand panel contains metabolite id, name and source organism. On the right hand side metabolite properties and associated annotation (as defined in the model) is displayed, where possible URL's are made live and can be opened in a webbrowser.

The screenshot displays the MetaDraft 0.6.8 application window. The 'Metabolites' tab is selected in the top navigation bar. The left panel shows a list of metabolites with columns for 'metabolite', 'name', 'org', and 'fix'. The right panel, titled 'Information', shows detailed properties for the selected metabolite, M_ac_c (Acetate).

metabolite	name	org	fix
1	M_23dhb_c	2,3-Dihydroxybenzoate	bigg2-eco
2	M_23dha_c	(2,3-Dihydroxybenzoyl)adenylate	bigg2-eco
3	M_2fe1s_c	[2Fe-1S] desulfurated iron-sulfur cl...	bigg2-eco
4	M_2mcit_c	2-Methylcitrate	bigg2-eco
5	M_2obut_c	2-Oxobutanoate	bigg2-eco
6	M_2pg_c	D-Glycerate 2-phosphate	bigg2-eco
7	M_3mob_c	3-Methyl-2-oxobutanoate	bigg2-eco
8	M_3mop_c	(S)-3-Methyl-2-oxopentanoate	bigg2-eco
9	M_3pg_c	3-Phospho-D-glycerate	bigg2-eco
10	M_4mop_c	4-Methyl-2-oxopentanoate	bigg2-eco
11	M_4mpetz_c	4-Methyl-5-(2-phosphoethyl)-thia...	bigg2-eco
12	M_5mthf_c	5-Methyltetrahydrofolate	bigg2-eco
13	M_ac_c	Acetate	bigg2-eco
14	M_acald_c	Acetaldehyde	bigg2-eco
15	M_accoa_c	Acetyl-CoA	bigg2-eco
16	M_acgam_p	N-Acetyl-D-glucosamine	bigg2-eco
17	M_acgam6p_c	N-Acetyl-D-glucosamine 6-phosp...	bigg2-eco

Id	M_ac_c
Name	Acetate
Charge	-1
Formula	C2H3O2
ReagentOf	R_CYSS
RDF reference (opens in browser)	
is	http://identifiers.org/bigg.metabolite/ac
is	http://identifiers.org/reactome/113539
is	http://identifiers.org/chebi/13704
is	http://identifiers.org/reactome/1524044
is	http://identifiers.org/chebi/15366
is	http://identifiers.org/reactome/2022890
is	http://identifiers.org/chebi/22165
is	http://identifiers.org/chebi/22169
is	http://identifiers.org/chebi/2387
is	http://identifiers.org/reactome/29416
is	http://identifiers.org/chebi/30089

Sessions

MetaDraft has multi-session support, opening the "Sessions" menu allows you to save, load or clear the current selection state of both the "Gene" and "Reaction" panels.

The screenshot shows the MetaDraft 0.6.8 application window. The 'Sessions' menu is open, displaying options: 'Save current session', 'Saved sessions' (with a dropdown arrow), and 'Clear all sessions'. The 'Saved sessions' dropdown shows a single session named '2016-11-15-12-03'. The main panel displays a table of metabolites with columns for 'metabolite', 'name', and 'bigg2-eco'. The 'Information' panel on the right shows details for the selected metabolite 'M_23dhhb_c'.

metabolite	name	bigg2-eco
1 M_23dhhb_c	2,3-Dihydro...	bigg2-eco <input type="checkbox"/>
2 M_23dhba_c	(2,3-Dihydr...	bigg2-eco <input type="checkbox"/>
3 M_2fe1s_c	[2Fe-1S] de...	bigg2-eco <input type="checkbox"/>
4 M_2mcit_c	2-Methylcit...	bigg2-eco <input type="checkbox"/>
5 M_2obut_c	2-Oxobutan...	bigg2-eco <input type="checkbox"/>
6 M_2pg_c	D-Glycerate...	bigg2-eco <input type="checkbox"/>
7 M_3mob_c	3-Methyl-2-...	bigg2-eco <input type="checkbox"/>
8 M_3mop_c	(S)-3-Methy...	bigg2-eco <input type="checkbox"/>
9 M_3pg_c	3-Phospho-...	bigg2-eco <input type="checkbox"/>
10 M_4mop_c	4-Methyl-2-...	bigg2-eco <input type="checkbox"/>
11 M_4mpetz_c	4-Methyl-5-...	bigg2-eco <input type="checkbox"/>
12 M_5mthf_c	5-Methyltet...	bigg2-eco <input type="checkbox"/>
13 M_ac_c	Acetate	bigg2-eco <input type="checkbox"/>
14 M_acald_c	Acetaldehyde	bigg2-eco <input type="checkbox"/>
15 M_accoa_c	Acetyl-CoA	bigg2-eco <input type="checkbox"/>
16 M_acgam_p	N-Acetyl-D...	bigg2-eco <input type="checkbox"/>
17 M_acgam6...	N-Acetyl-D...	bigg2-eco <input type="checkbox"/>
18 M_acmana_p	N-Acetyl-D...	bigg2-eco <input type="checkbox"/>

Id	M_23dhhb_c
Name	2,3-Dihydroxybenzoate
Charge	-1
Formula	C7H5O4
ReagentOf	R_DHBS
RDF references (opens in browser)	
is	http://identifiers.org/bigg.metabolite/23dhhb
is	http://identifiers.org/chebi/11427
is	http://identifiers.org/chebi/18026
is	http://identifiers.org/chebi/19319
is	http://identifiers.org/chebi/19320
is	http://identifiers.org/biocyc/2-3-DIHYDROXYBENZOATE
is	http://identifiers.org/chebi/36654
is	http://identifiers.org/chebi/41901
is	http://identifiers.org/chebi/885
is	http://identifiers.org/brenda/BG24972
is	http://identifiers.org/kegg.compound/C00196

Model options: reports

The current model options include the generation of reports on the various model components used in the draft reconstruction.

MetaDraft 0.6.8 - Brett G. Olivier (b.g.olivier@vu.nl)

File Build options **Model options** Sessions Help

Build Genes

metabolite

	metabolite	bigg2-eco	fixed
1	M_23dhhb_c	2,3-Dihydroxybenzoate	<input type="checkbox"/>
2	M_23dhhba_c	(2,3-Dihydroxybenzoate)	<input type="checkbox"/>
3	M_2fe1s_c	[2Fe-1S] dehydrogenase	<input type="checkbox"/>
4	M_2mci_c	2-Methylcitrate	<input type="checkbox"/>
5	M_2obut_c	2-Oxobutanal	<input type="checkbox"/>
6	M_2pg_c	D-Glycerate	<input type="checkbox"/>
7	M_3mob_c	3-Methyl-2-oxobutanal	<input type="checkbox"/>
8	M_3mop_c	(S)-3-Methyl-2-oxobutanal	<input type="checkbox"/>
9	M_3pg_c	3-Phosphoglycerate	<input type="checkbox"/>
10	M_4mop_c	4-Methyl-2-oxobutanal	<input type="checkbox"/>
11	M_4mpetz_c	4-Methyl-5-oxopentanoate	<input type="checkbox"/>
12	M_5mthf_c	5-Methyltetrahydrofuran	<input type="checkbox"/>
13	M_ac_c	Acetate	<input type="checkbox"/>
14	M_acald_c	Acetaldehyde	<input type="checkbox"/>
15	M_accoa_c	Acetyl-CoA	<input type="checkbox"/>
16	M_acgam_p	N-Acetyl-D-glucosamine	<input type="checkbox"/>
17	M_acgam6_p	N-Acetyl-D-glucosamine	<input type="checkbox"/>
18	M_acmana_p	N-Acetyl-D-glucosamine	<input type="checkbox"/>

Information

Id	M_23dhhb_c
Name	2,3-Dihydroxybenzoate
Charge	-1
Formula	C7H5O4
ReagentOf	R_DHBS
RDF references (opens in browser)	
is	http://identifiers.org/bigg.metabolite/23dhhb
is	http://identifiers.org/chebi/11427
is	http://identifiers.org/chebi/18026
is	http://identifiers.org/chebi/19319
is	http://identifiers.org/chebi/19320
is	http://identifiers.org/biocyc/2-3-DIHYDROXYBENZOATE
is	http://identifiers.org/chebi/36654
is	http://identifiers.org/chebi/41901
is	http://identifiers.org/chebi/885
is	http://identifiers.org/brenda/BG24972
is	http://identifiers.org/kegg.compound/C00196

Report: genes

The "Gene Report" provides details of the input file, metaproteome composition. Source genes with no orthology to the metaproteome are provided together with a table of

genes includes in draft reconstruction and their score. In addition the report can be viewd directly in your browser as well as saved as an HTML file.

MetaDraft 0.6.8 - Brett G. Olivier (b.g.olivier@vu.nl)

FileBuild optionsModel optionsSessionsHelp

BuildGenesReactionsMetabolites

	reaction	name	
1	R_ACGAMT	UDP-N-ace...	<input checked="" type="checkbox"/>
2	R_ACGApts...	N-Acetyl-D...	<input checked="" type="checkbox"/>
3	R_ACMAN...	N-acetyl-D...	<input checked="" type="checkbox"/>
4	R_ACMUM...	N-acetylmu...	<input checked="" type="checkbox"/>
5	R_ACONTa	Aconitase (...)	<input checked="" type="checkbox"/>
6	R_ACONTb	Aconitase (...)	<input checked="" type="checkbox"/>
7	R_ALAALAr	D-alanine-...	<input checked="" type="checkbox"/>
8	R_ALCD19	Alcohol deh...	<input checked="" type="checkbox"/>
9	R_ALCD2x	Alcohol deh...	<input checked="" type="checkbox"/>
10	R_AMALT1	Amylomalt...	<input checked="" type="checkbox"/>
11	R_AMALT2	Amylomalt...	<input checked="" type="checkbox"/>
12	R_AMALT3	Amylomalt...	<input checked="" type="checkbox"/>
13	R_AMALT4	Amylomalt...	<input checked="" type="checkbox"/>
14	R_APH120	Acylphosph...	<input checked="" type="checkbox"/>
15	R_APH140	Acylphosph...	<input checked="" type="checkbox"/>
16	R_APH141	Acylphosph...	<input checked="" type="checkbox"/>
17	R_APH160	Acylphosph...	<input checked="" type="checkbox"/>
18	R_APH161	Acylphosph...	<input checked="" type="checkbox"/>

Information

MetaDraft Report

MetaDraft Gene Report

Analysis

Input fasta: test.fasta

Metaproteome used: bigg2-eco

Report date: 16-11-11

MetaDraft version: 0.6.8

Genes (35)

Input genes not matched

stu0987, stu0596, stu0763, stu0762, stu1886, stu0262, stu0117, stu15

Genes selected

Source	Target	Score	Model
stu0160	b3057	1.0	bigg2-eco
stu0163	b3784	1.0	bigg2-eco
stu0246	b0968	1.0	bigg2-eco
stu0264	b3849	1.0	bigg2-eco
stu0265	b3290	1.0	bigg2-eco
stu0505	b3560	1.0	bigg2-eco
stu0590	b3770	1.0	biaa2-eco

View in browser

Export (HTML)

glucosamine:undecaprenylphosphate N-acetylglucosamine-1-phosphate transferase

uacgam_c > M_ump_c + M_unaga_c

osphate + UDP-N-acetyl-D-glucosamine > UMP +

hospho N-acetyl-glucosamine

Substrates

osphate

glucosamine

Products

iphospho N-acetyl-glucosamine

Report: genes 2

Gene id's are hyperlinked to extended gene annotation which may provide links to additional annotation. Please note that hyperlinking is only active when viewed in a web-browser.

The screenshot displays the MetaDraft 0.6.8 web interface. The main window shows a table of genes with columns for reaction, name, and a checkbox. A 'MetaDraft Report' window is open, showing detailed information for gene [stu0163](#).

reaction	name	
1 R_ACGAMT	UDP-N-ace...	<input checked="" type="checkbox"/>
2 R_ACGApts...	N-Acetyl-D...	<input checked="" type="checkbox"/>
3 R_ACMAN...	N-acetyl-D...	<input checked="" type="checkbox"/>
4 R_ACMUM...	N-acetylmu...	<input checked="" type="checkbox"/>
5 R_ACONTa	Aconitase (...)	<input checked="" type="checkbox"/>
6 R_ACONtb	Aconitase (...)	<input checked="" type="checkbox"/>
7 R_ALAALAr	D-alanine...	<input checked="" type="checkbox"/>
8 R_ALCD19	Alcohol deh...	<input checked="" type="checkbox"/>
9 R_ALCD2x	Alcohol deh...	<input checked="" type="checkbox"/>
10 R_AMALT1	Amylomalt...	<input checked="" type="checkbox"/>
11 R_AMALT2	Amylomalt...	<input checked="" type="checkbox"/>
12 R_AMALT3	Amylomalt...	<input checked="" type="checkbox"/>
13 R_AMALT4	Amylomalt...	<input checked="" type="checkbox"/>
14 R_APH120	Acylphosph...	<input checked="" type="checkbox"/>
15 R_APH140	Acylphosph...	<input checked="" type="checkbox"/>
16 R_APH141	Acylphosph...	<input checked="" type="checkbox"/>
17 R_APH160	Acylphosph...	<input checked="" type="checkbox"/>

Matching Gene Information	
function	enzyme; Central intermediary metabolism: Sugar-nucleotide biosynthesis, conversions 1.6.4 metabolism; macromolecules (cellular constituent) biosynthesis; enterobacterial common antigen (surface glycolipid) 6.3 cell structure; surface antigens (ECA, O antigen of LPS)
gene	rfe
GO_function	GO:0042280 - cell surface antigen activity, host-interacting
gene_synonym	ECK3776; JW3758; wecA
EC_number	2.4.1.-
product	UDP-GlcNAc:undecaprenylphosphate GlcNAc-1-phosphate transferase
GO_process	GO:0009246 - enterobacterial common antigen biosynthetic process

Buttons: [View in browser](#) [Export \(HTML\)](#)

Report: reactions

The reaction report also contains details of the selected reactions and their annotation.

MetaDraft 0.6.8 - Brett G. Olivier (b.g.olivier@vu.nl)

FileBuild optionsModel optionsSe

BuildGenesReactionsMetabolites

	reaction	name	
1	R_ACGAMT	UDP-N-ace...	<input type="checkbox"/>
2	R_ACGApts...	N-Acetyl-D...	<input checked="" type="checkbox"/>
3	R_ACMAN...	N-acetyl-D...	<input checked="" type="checkbox"/>
4	R_ACMUM...	N-acetylmu...	<input checked="" type="checkbox"/>
5	R_ACONTa	Aconitase (...)	<input checked="" type="checkbox"/>
6	R_ACONtb	Aconitase (...)	<input checked="" type="checkbox"/>
7	R_ALAALAR	D-alanine-...	<input checked="" type="checkbox"/>
8	R_ALCD19	Alcohol deh...	<input checked="" type="checkbox"/>
9	R_ALCD2x	Alcohol deh...	<input checked="" type="checkbox"/>
10	R_AMALT1	Amylomalt...	<input checked="" type="checkbox"/>
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12	R_AMALT3	Amylomalt...	<input checked="" type="checkbox"/>
13	R_AMALT4	Amylomalt...	<input checked="" type="checkbox"/>
14	R_APH120	Acylphosph...	<input checked="" type="checkbox"/>
15	R_APH140	Acylphosph...	<input checked="" type="checkbox"/>
16	R_APH141	Acylphosph...	<input checked="" type="checkbox"/>
17	R_APH160	Acylphosph...	<input checked="" type="checkbox"/>

MetaDraft Report

R_ACGAMT

UDP-N-acetylglucosamine:undecaprenylphosphate N-acetylglucosamine -1-phosphate transferasebigg2-eco stu0163

Annotation

R_ACGAptspp

top

bigg2-eco

R_ACGAptspp

N-Acetyl-D-glucosamine transport via PEP:Pyr PTS (periplasm)

(irreversible)

Association

((b2415 and b2417 and b1101 and b2416) or (b2415 and b0679 and b2416))

Association new

Equation ID

M_pep_c + M_acgam_p > M_pyr_c + M_acgam6p_c

Equation Name

Phosphoenolpyruvate + N-Acetyl-D-glucosamine > Pyruvate + N-Acetyl-D-glucosamine 6-phosphate

Substrates

M_pep_c

Phosphoenolpyruvate

charge: -3

C3H2O6P

M_acgam_p

N-Acetyl-D-glucosamine

charge: 0

C8H15NO6

Products

M_pyr_c

Pyruvate

charge: -1

C3H3O3

M_acgam6p_c

N-Acetyl-D-glucosamine 6-phosphate

charge: -2

C8H14NO9P

RDF references (opens in browser)

is

<http://identifiers.org/bigg.reaction/ACGAptspp>

View in browser

Export (HTML)

transport via PTS

and b1819 and b2416)

L_pyr_c + M_acmanap_c

phosphoenolpyruvate >

samine 6-phosphate

6-phosphate

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