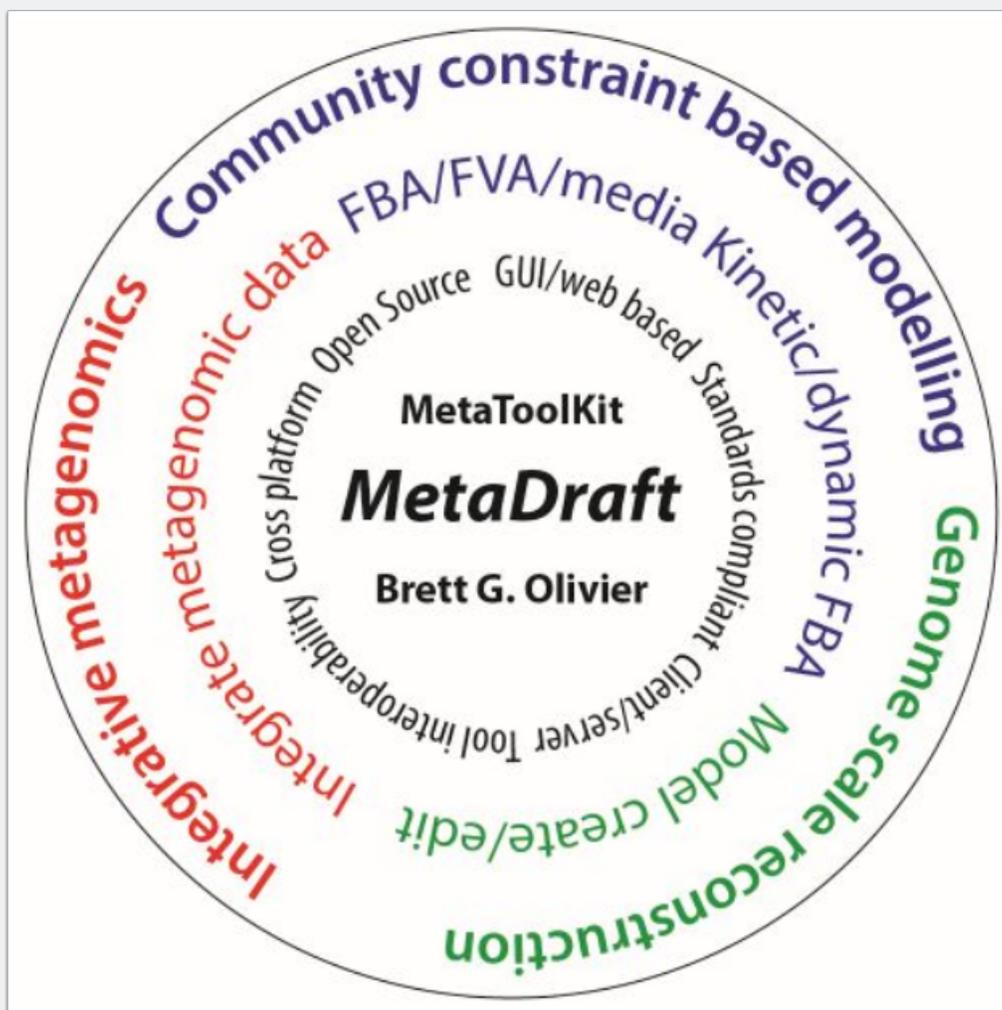


# MetaDraft

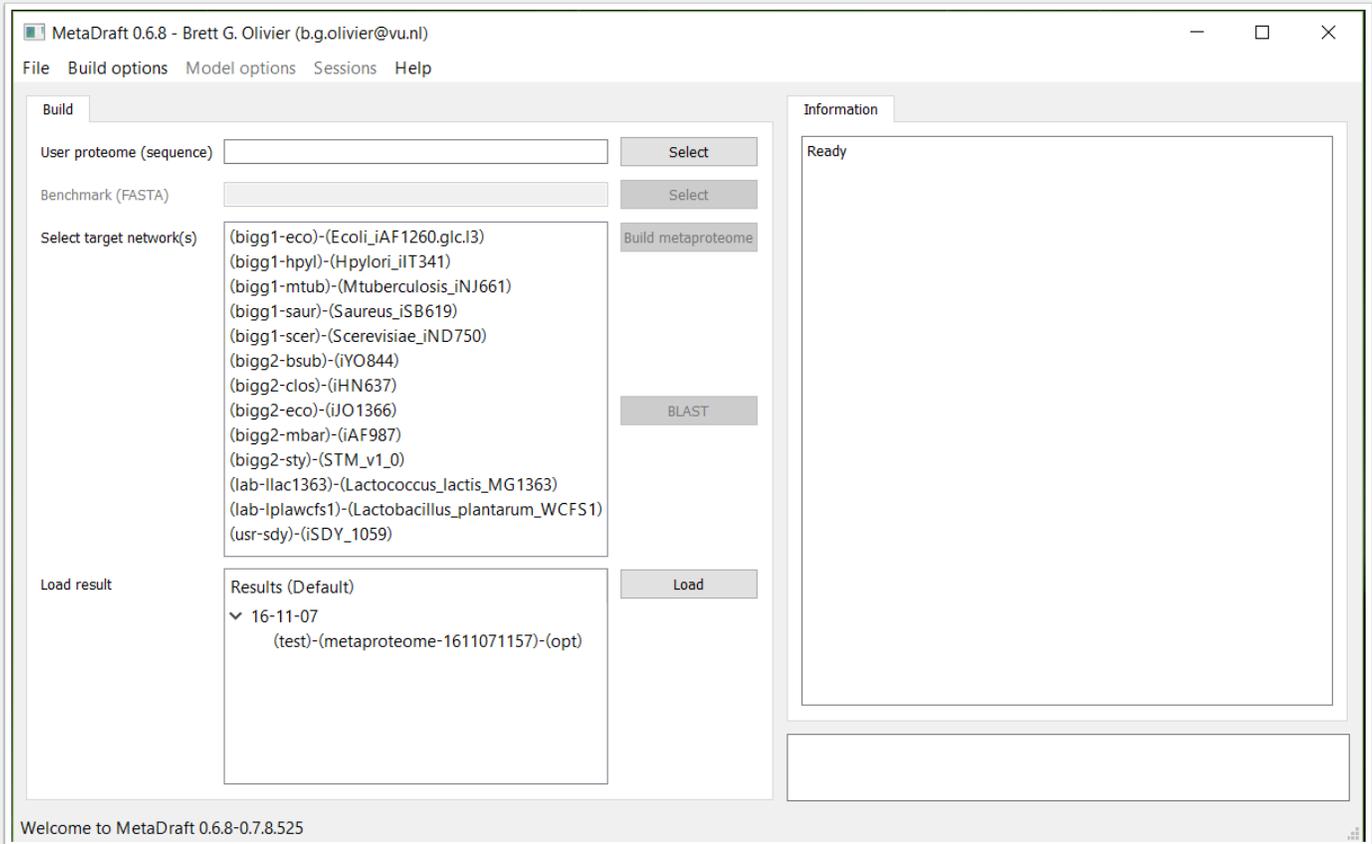
## Welcome

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)



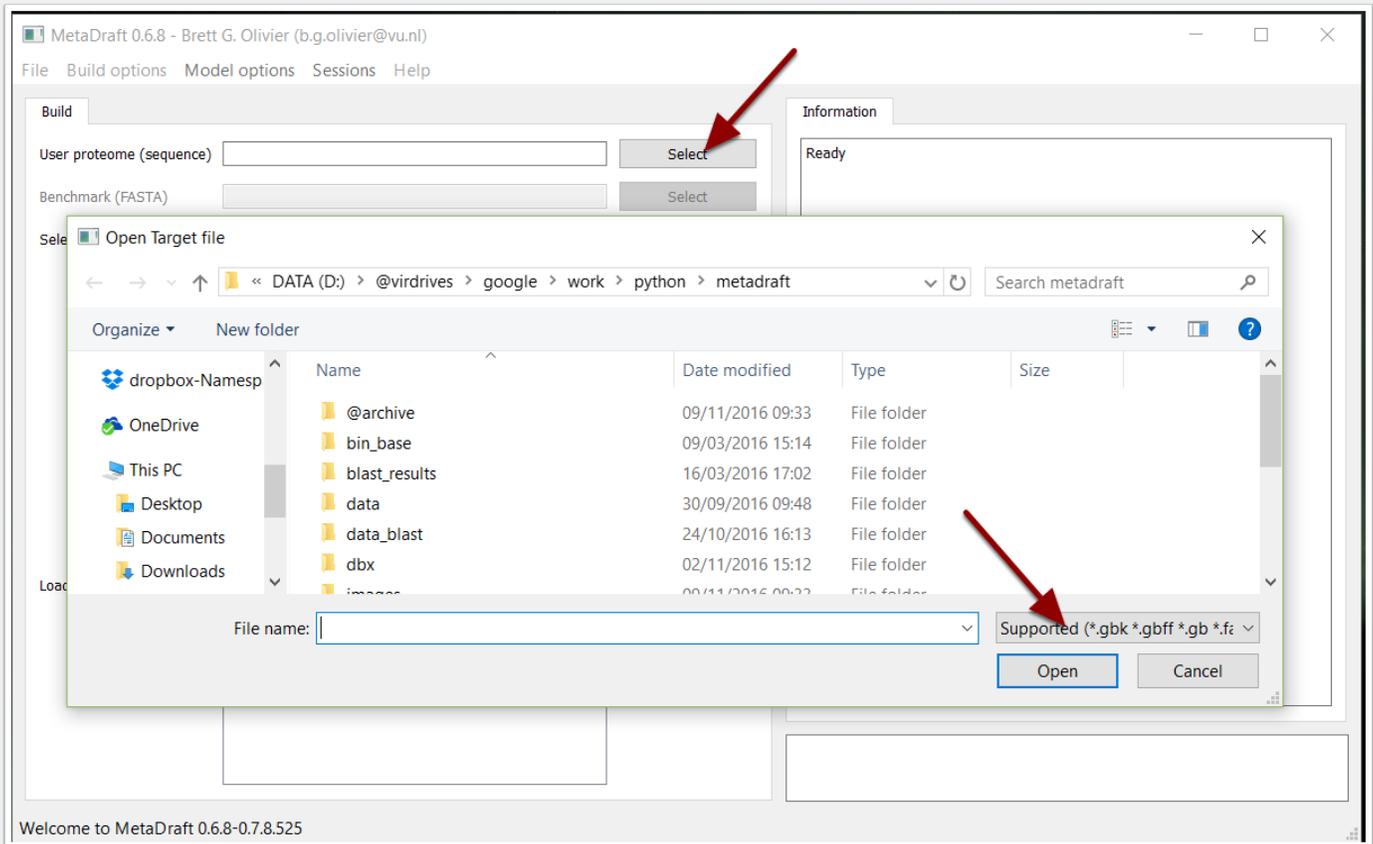
## Main screen

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).

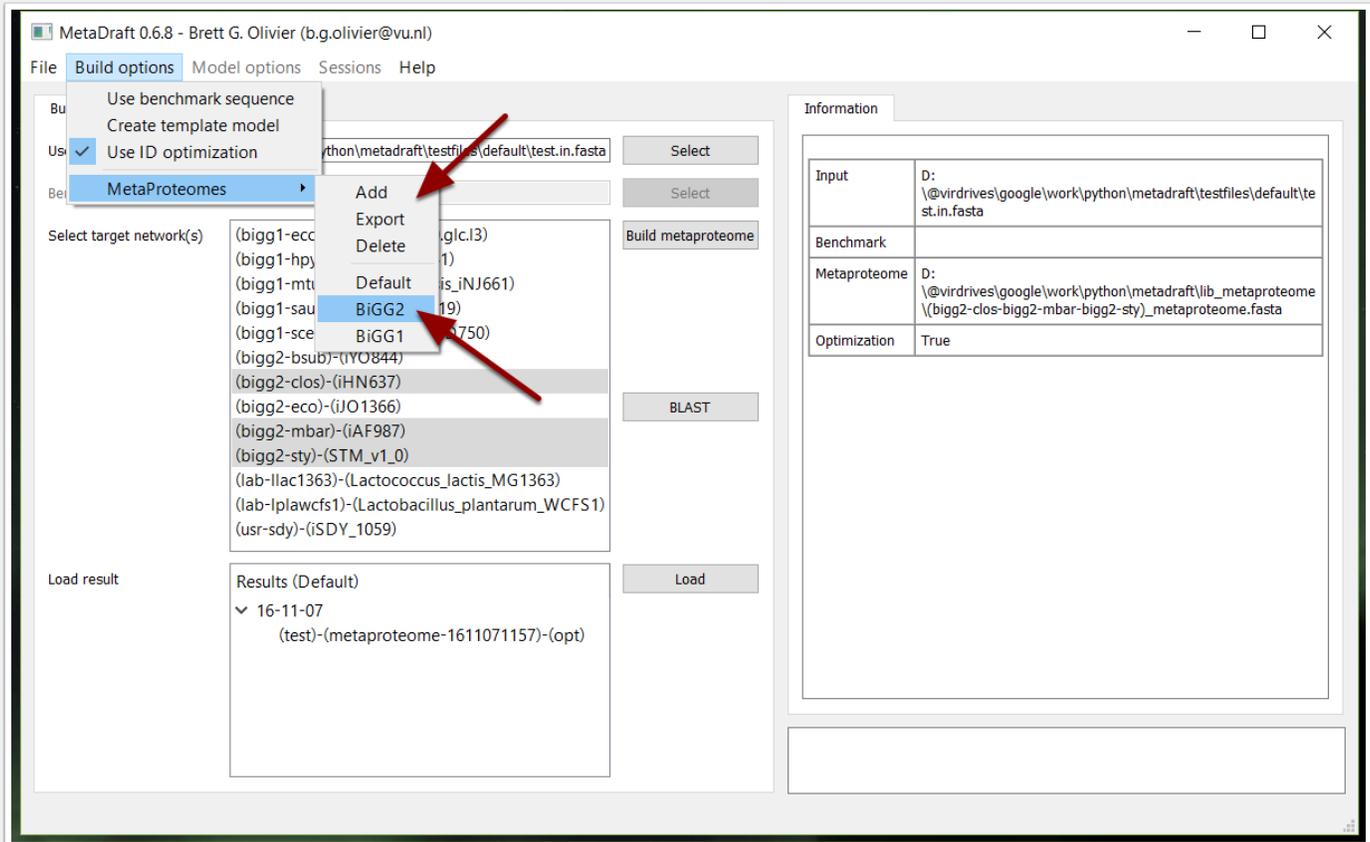
The screenshot shows the MetaDraft 0.6.8 interface. The 'Build' tab is active, displaying the 'Build metaproteome' workflow. The 'User proteome (sequence)' field contains the path `google\work\python\metadraft\testfiles\default\test.in.fasta`. The 'Benchmark (FASTA)' field is empty. The 'Select target network(s)' list includes several organisms, with `(bigg2-clos)-(iHN637)` highlighted in a red box. A red arrow points to the 'Build metaproteome' button. A 'Building Metaproteome' dialog box is open, showing a progress bar at 50% and a 'Cancel' button. The 'Information' tab on the right shows the input file path and optimization settings.

Input	D:\@virdrives\google\work\python\metadraft\testfiles\default\test.in.fasta
Benchmark	
Metaproteome	
Optimization	True

Building Metaproteome  
50%  
Cancel

## 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.

The screenshot shows the MetaDraft 0.6.8 application window. The 'Build options' menu is open, and the 'MetaProteomes' sub-menu is visible. A red arrow points to the 'Export' option. The main interface displays a list of target networks and a 'Load result' section.

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

File Build options Model options Sessions Help

- Use benchmark sequence
- Create template model
- Use ID optimization
- MetaProteomes**
  - Add
  - Export**
  - Delete
  - Default
  - BiGG2
  - BiGG1

Select target network(s)

- (bigg2-bsu)
- (bigg2-clo)
- (bigg2-eco)
- (bigg2-mb)
- (bigg2-sty)
- (bigg1-eco)-(Ecoli\_AF1260.glc.l3)
- (bigg1-hpyl)-(Hpylori\_iIT341)
- (bigg1-mtub)-(Mtberculosis\_iNJ661)
- (bigg1-saur)-(Saureus\_iSB619)
- (bigg1-scer)-(Scerevisiae\_iND750)
- (lab-llac1363)-(Lactococcus\_lactis\_MG1363)
- (lab-lplawcfs1)-(Lactobacillus\_plantarum\_WCFS1)
- (usr-sdy)-(iSDY\_1059)

Build metaproteome

BLAST

Load result

Results (Default)

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

Load

Information

Input	D:\@virdrives\google\work\python\metadraft\testfiles\default\test.in.fasta
Benchmark	
Metaproteome	d:\@virdrives\google\work\python\metadraft\lib_metaproteome\bigg2-bsu-big2-clo-big2-eco-big2-mbar-big2-sty_metaproteome.fasta
Optimization	True

## 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).

The screenshot displays the MetaDraft 0.6.8 application window. The 'Build' tab is active, showing a list of target networks. The network '(bigg2-eco)-(iJO1366)' is selected, and a red arrow points from it to the 'BLAST' button. The 'Information' tab on the right shows the input and benchmark paths. A 'Running sequence search' dialog box is overlaid on top, indicating that the search is in progress at 50% completion.

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)-(Mtberculosis\_iNJ661)
- (bigg1-saur)-(Saureus\_jSB619)
- (bigg1-scer)-(Scerevisiae\_iND750)
- (usr-sdy)-(iSDY\_1059)

Load result

Results (Default)

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

Information

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

Running sequence search

50%

Metaproteome: "d:\@virdrives\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.

The screenshot shows the MetaDraft 0.6.8 interface. The 'Build' tab is active, displaying a list of target networks under 'Select target network(s)'. A red arrow points to the selected result '(test)-(metaproteome-1611071157)-(opt)' in the 'Load result' section. The 'Information' tab is also visible, showing details about the input, benchmark, metaproteome, and optimization.

**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.I3)
- (bigg1-hpyl)-(Hpylori\_iIT341)
- (bigg1-mtub)-(Mtuberculosis\_iNJ661)
- (bigg1-saur)-(Saureus\_jSB619)
- (bigg1-scer)-(Scerevisiae\_iND750)
- (usr-sdy)-(iISDY\_1059)

Load result

Results (Default)

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

**Information**

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

BLAST run successful

## Delete/rename results

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

The screenshot shows the MetaDraft 0.6.8 interface. The 'Build' panel on the left contains fields for 'User proteome (sequence)', 'Benchmark (FASTA)', and a list of 'Select target network(s)'. A 'Load result' section shows a tree view of results. A red arrow points to a right-click context menu over the entry '(test)-(bigg1-1611071157)-(opt)'. The context menu has 'Rename' and 'Delete' options. The 'Information' panel on the right shows a table with the following data:

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

At the bottom left, a status bar indicates 'BLAST run successful'.

## Optional: benchmark

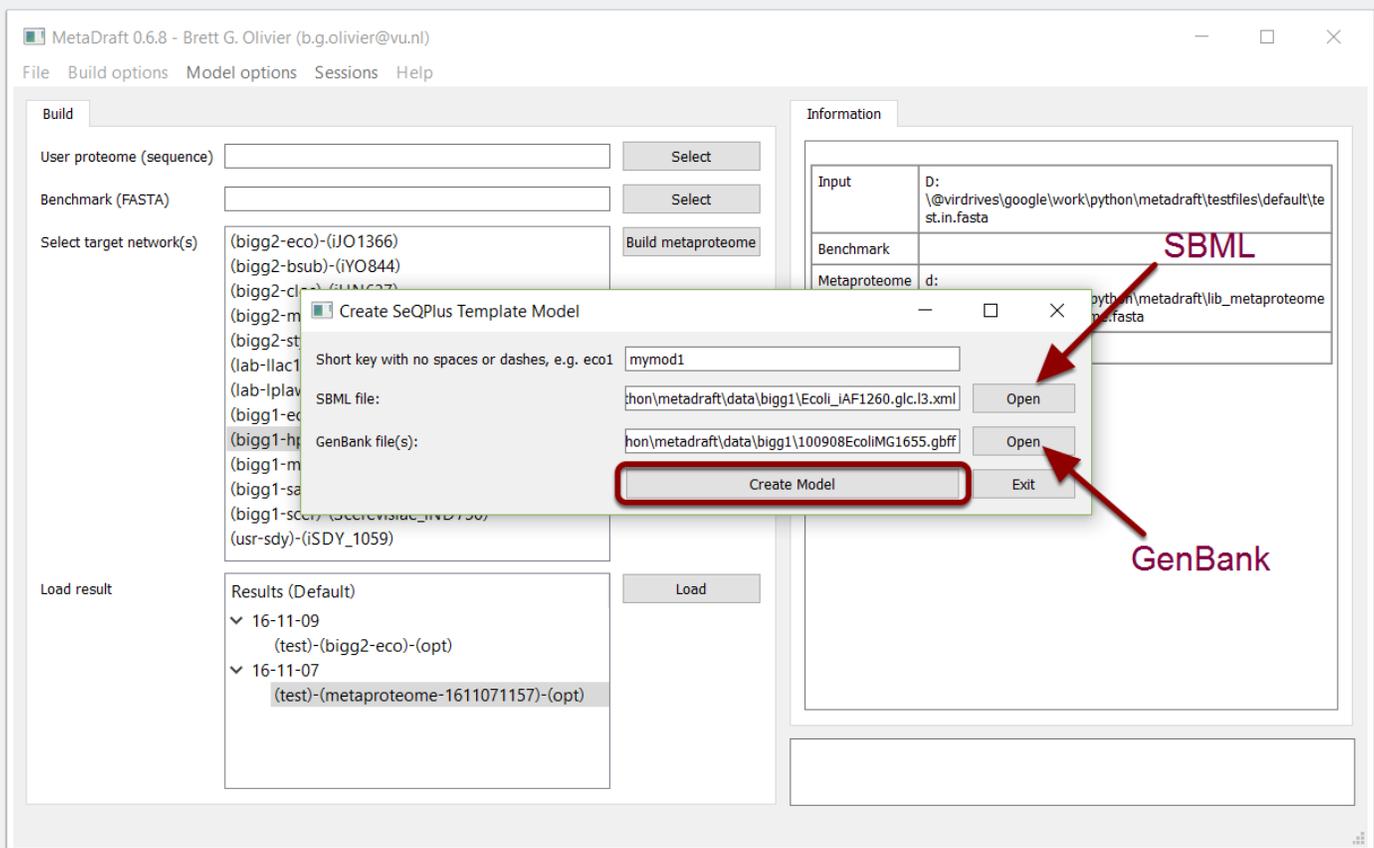
Using the benchmark functionality you can include a sequence file that will be used as a benchmark for your sequence search. Only sequences with higher orthology than the benchmark will be included.

The screenshot shows the MetaDraft 0.6.8 application window. The 'Build options' menu is open, with 'Use benchmark sequence' highlighted. The main workspace contains a list of target networks and a 'Load result' section. The 'Information' panel on the right displays the following data:

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

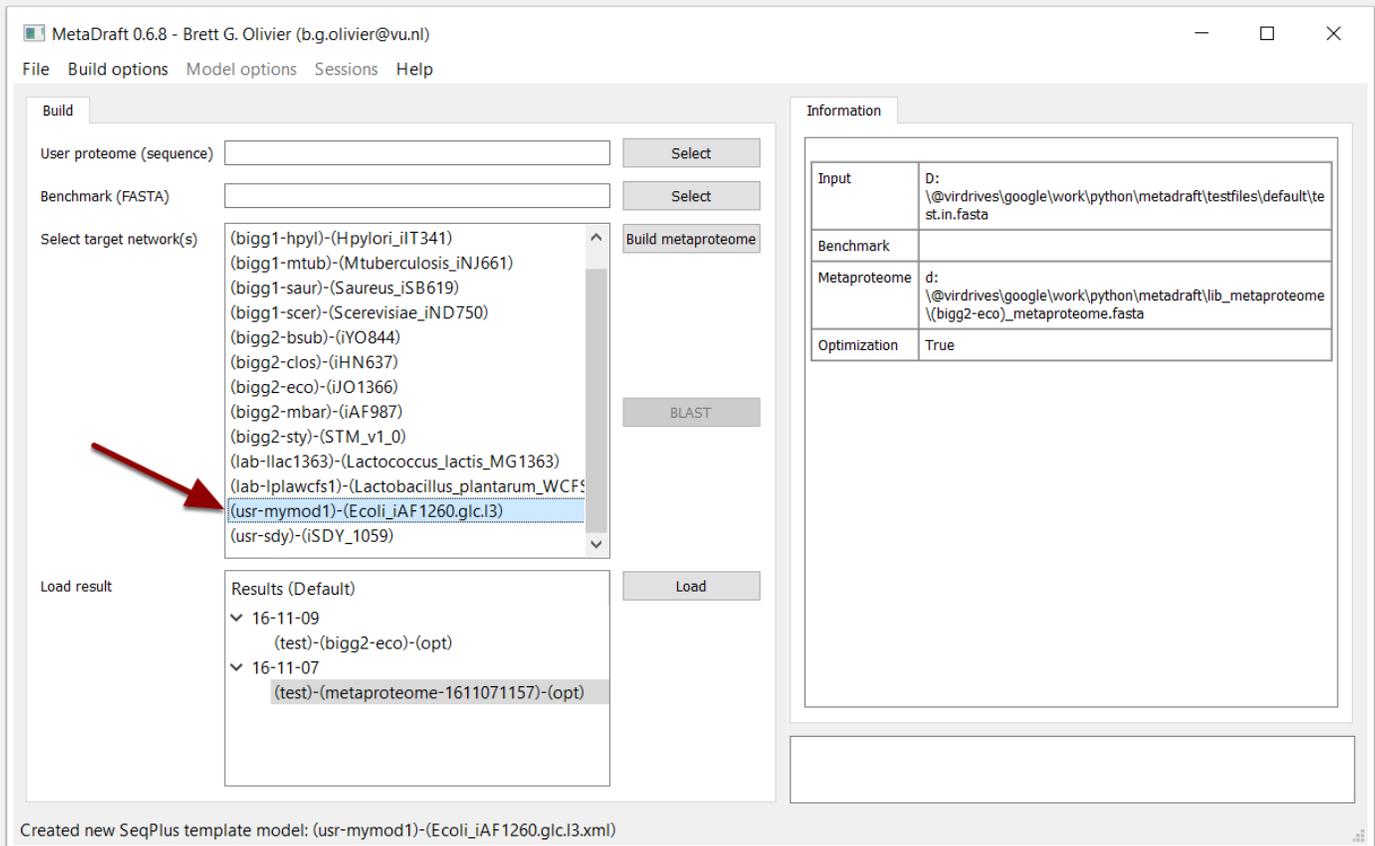
## Option: create new template model

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\_iSB619)
- (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\_WCF5)
- (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)

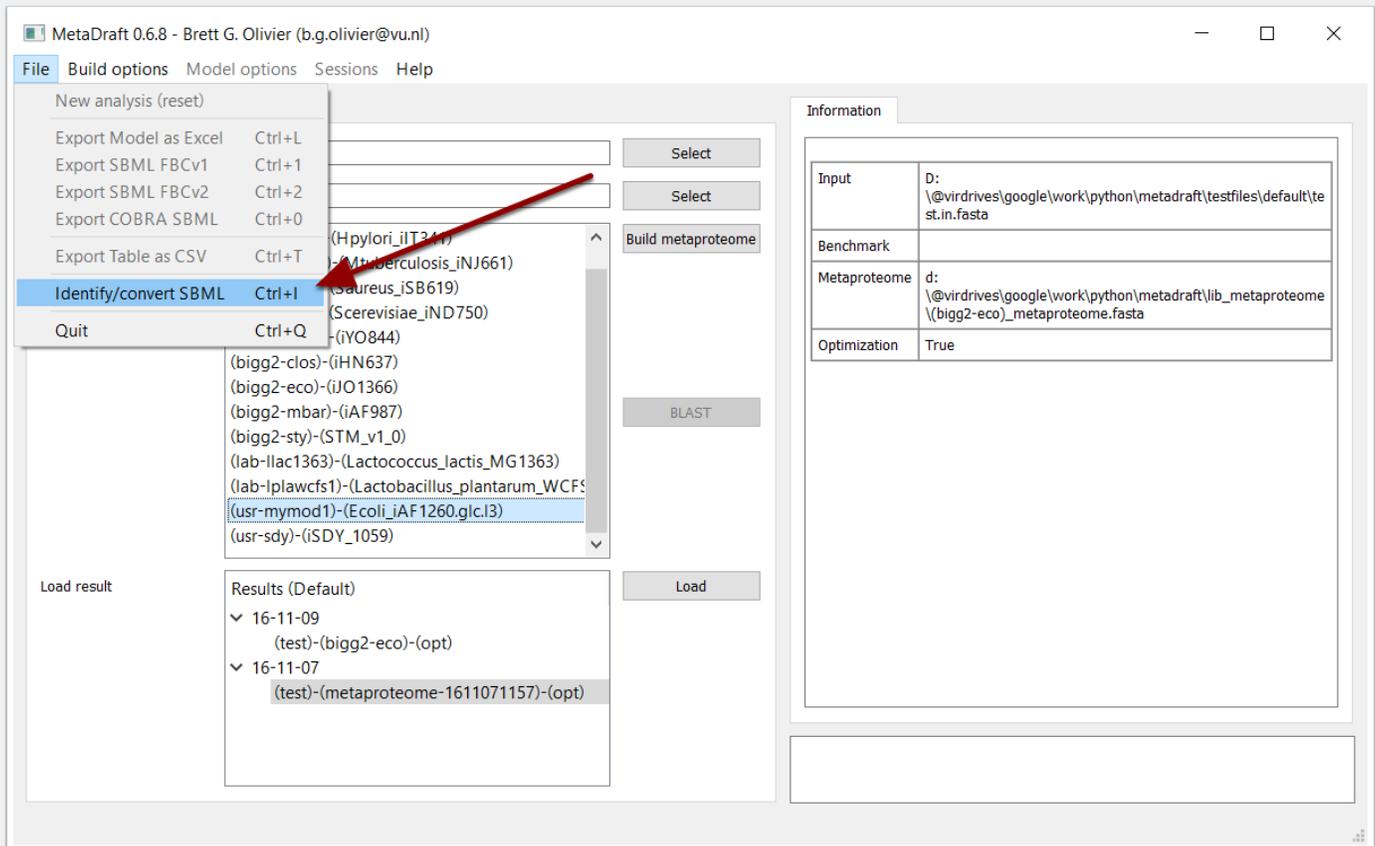
**Information**

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

Created new SeqPlus template model: (usr-mymod1)-(Ecoli\_iAF1260.glc.l3.xml)

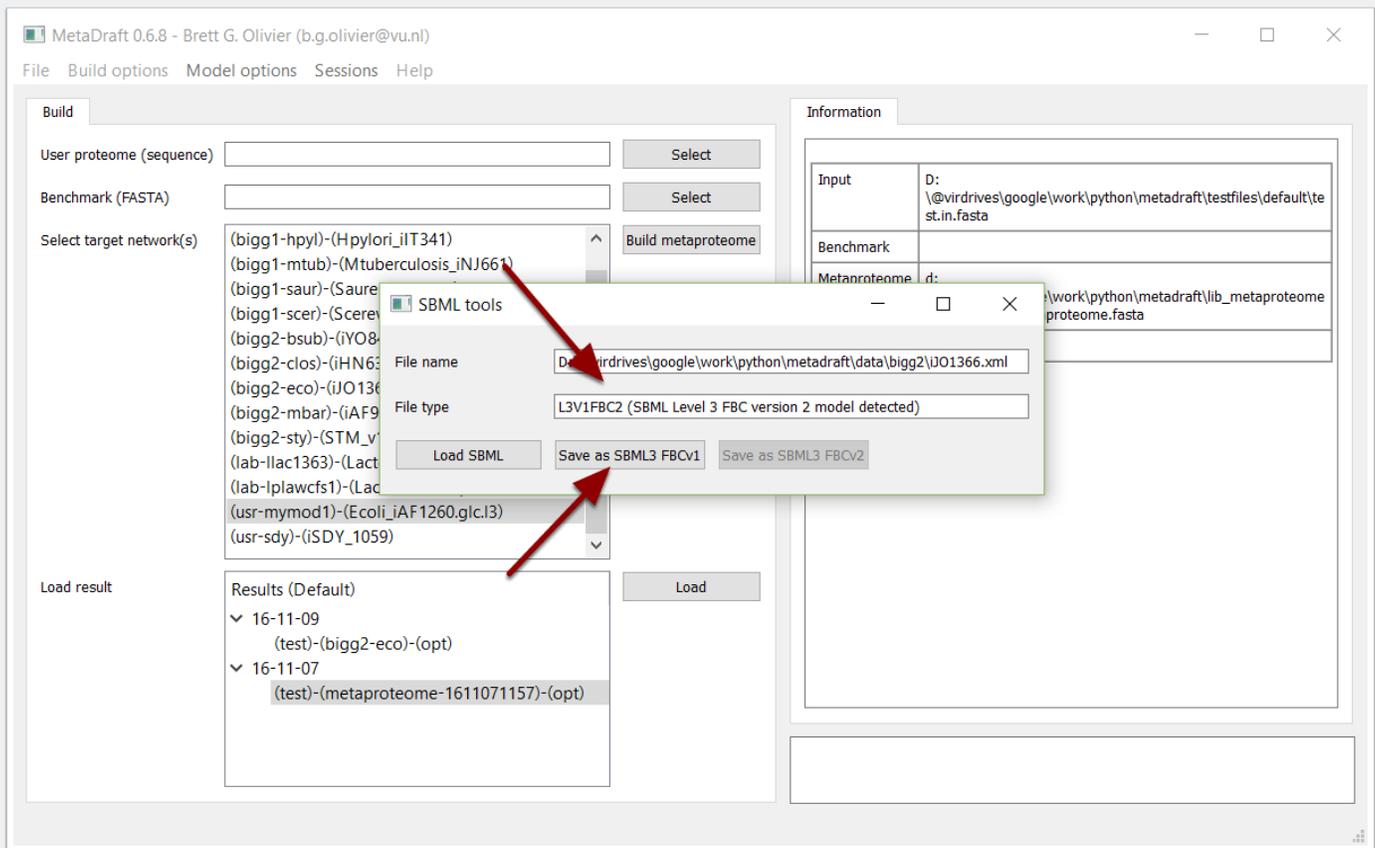
## Option: analyse SBML model

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



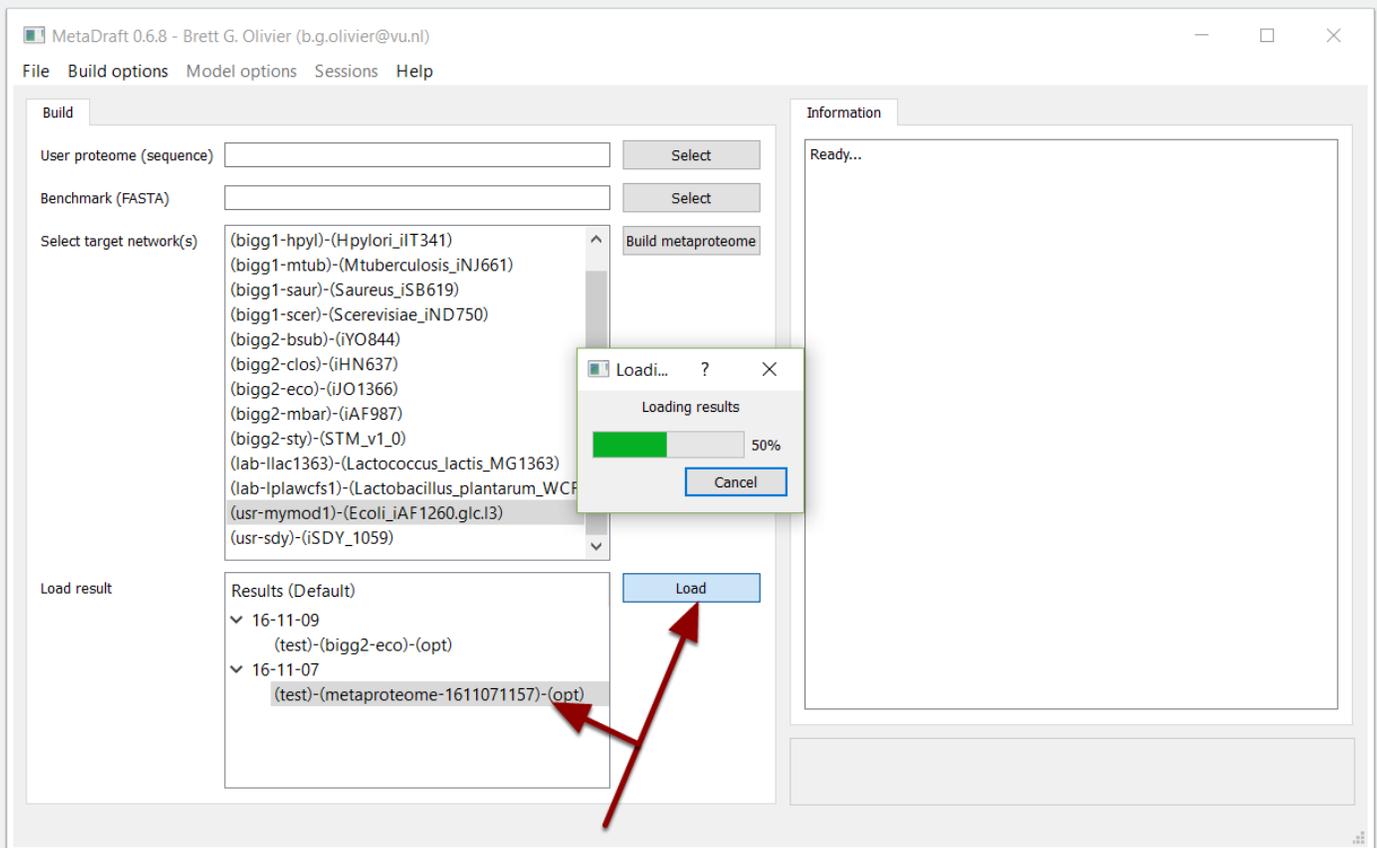
## Option: analyse SBML model 2

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

# MetaDraft

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	1.0	<input checked="" type="checkbox"/>	bigg2-bsub
9	in_stu0590	BSU38550	1.0	<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	<a href="http://GeneID:504547912">GI:504547912</a>
Associated reaction(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 <b>LLMG_RS06045</b> )	
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 <b>LLMG_RS06045</b> )	

Loaded results: "d:\@virdrives\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.

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

File Build options Model options Sessions Help

	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	0.219	<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	BSU02390	1.0	<input checked="" type="checkbox"/>	bigg1-eco
9	in_stu0590	YHR208W	0.463	<input type="checkbox"/>	bigg1-eco
10	in_stu0590	BSU38550	0.463	<input type="checkbox"/>	bigg1-eco
11	in_stu0596			<input type="checkbox"/>	bigg1-eco
12	in_stu0603			<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

Filter selected genes

Minimum score: 0.8 Maximum score: 1.0

Apply

Information

GeneMatch: in\_stu0590 --> BSU02390

Matching Gene Information	
function	16.2: Construct biomass (Anabolism) 16.11: Scavenge (Catabolism)
EC_number	<a href="#">2.6.1.42</a>
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	<a href="#">GI:2632525</a> EnsemblGenomes-Gn:BSU02390 EnsemblGenomes-Tr:CAB12033 GOA:O31461 InterPro:IPR001544 InterPro:IPR005786 InterPro:IPR018300 SubtilList: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.

The screenshot displays the MetaDraft 0.6.8 interface. The main window shows a table of reactions with columns for reaction ID, name, status, organism, genes, and source. Reaction R\_VALTA (Valine transaminase) is highlighted in blue. The right-hand panel shows detailed information for this reaction, including its organism (bigg2-bsub), enzyme name (Valine transaminase), and associated genes (M\_alk\_c, M\_val\_c, M\_val\_L\_c, M\_glu\_L\_c, M\_3mob\_c). A tooltip for the gene M\_val\_L\_c (Valine) is visible, showing its function (Construct biomass) and other details.

reaction	name	org	genes	src
44	R_PRPPS	phosphoribos...	bigg1-eco	b1207 stu1460
45	R_PSUDS	R_pseudouridy...	lab-llac1363	LLMG_RS0... stu0262
46	R_PTPAT	R_pantetheine...	lab-llac1363	LLMG_RS1... stu1648
47	R_SBTpts	R_D_sorbitol_tr...	lab-llac1363	LLMG_RS0... stu1264,stu1...
48	R_SERAT	serine O-acetyl...	bigg1-eco	b3607 stu0848
49	R_SHSL1r	O-succinylhom...	bigg1-hpyl	HP0106 stu0847
50	R_SHSL2r	O-succinylhom...	bigg1-hpyl	HP0106 stu0847
51	R_SHSL2r	SHSL2r	bigg2-clos	CLUJ_RS03... stu0987
52	R_SHSL4r	O-succinylhom...	bigg1-hpyl	HP0106 stu0847
53	R_SODr	Superoxide dis...	bigg2-bsub	BSU25020 stu0720
54	R_SUCpts	R_sucrose_tran...	lab-llac1363	LLMG_RS0... stu1264,stu1...
55	R_TECA1S45	Glycerol teicho...	bigg2-bsub	BSU35530 stu0163
56	R_TECA2S45	Glycerol teicho...	bigg2-bsub	BSU35530 stu0163
57	R_TECA3S45	Glycerol teicho...	bigg2-bsub	BSU35530 stu0163
58	R_TREpts	R_trehalose_tra...	lab-llac1363	LLMG_RS0... stu1264,stu1...
59	R_UDC...	R_undecapren...	lab-llac1363	LLMG_RS1... stu0160
60	R_VALTA	Valine transami...	bigg2-bsub	BSU02390 stu0590
61	R_YUMPS	R_yUMP_synth...	lab-llac1363	LLMG_RS0... stu0262

Information panel for R\_VALTA:

- Organism: bigg2-bsub
- R\_VALTA: Valine transaminase (reversible)
- Association: (BSU38550 or BSU02390)
- Association: (stu0590)
- Equation ID: M\_alk\_c + M\_val\_c
- Equation Name: 2-Oxoglutarate + oxobutanoate
- M\_alk\_c: 2-Oxoglutarate (charge: -2, C5H4O5)
- M\_val\_L\_c: Valine (charge: 0, C5H11NO2)
- M\_glu\_L\_c: 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

Genes: 38 Reactions: 61 Metabolites: 137

## 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 shows the MetaDraft 0.6.8 interface. The left panel displays a table of metabolites, and the right panel shows the information for the selected metabolite, M\_ac\_c.

metabolite	name	org	fix
1 M_23dhb_c	2,3-Dihydroxybenzoate	bigg2-eco	<input type="checkbox"/>
2 M_23dhba_c	(2,3-Dihydroxybenzoyl)adenylate	bigg2-eco	<input type="checkbox"/>
3 M_2fe1s_c	[2Fe-1S] desulfurated iron-sulfur cl...	bigg2-eco	<input type="checkbox"/>
4 M_2mci_c	2-Methylcitrate	bigg2-eco	<input type="checkbox"/>
5 M_2obut_c	2-Oxobutanoate	bigg2-eco	<input type="checkbox"/>
6 M_2pg_c	D-Glycerate 2-phosphate	bigg2-eco	<input type="checkbox"/>
7 M_3mob_c	3-Methyl-2-oxobutanoate	bigg2-eco	<input type="checkbox"/>
8 M_3mop_c	(S)-3-Methyl-2-oxopentanoate	bigg2-eco	<input type="checkbox"/>
9 M_3pg_c	3-Phospho-D-glycerate	bigg2-eco	<input type="checkbox"/>
10 M_4mop_c	4-Methyl-2-oxopentanoate	bigg2-eco	<input type="checkbox"/>
11 M_4mpetz_c	4-Methyl-5-(2-phosphoethyl)-thia...	bigg2-eco	<input type="checkbox"/>
12 M_5mthf_c	5-Methyltetrahydrofolate	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-glucosamine	bigg2-eco	<input type="checkbox"/>
17 M_acgam6p_c	N-Acetyl-D-glucosamine 6-phosp...	bigg2-eco	<input type="checkbox"/>

The right panel shows the information for the selected metabolite, M\_ac\_c:

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

## 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 displays the MetaDraft 0.6.8 application window. The 'Sessions' menu is open, showing options: 'Save current session', 'Saved sessions' (with a sub-menu containing '2016-11-11-15-12-03'), and 'Clear all sessions'. The main window is divided into several panels:

- Build**: A table listing metabolites and their associated genes and reactions.
- Information**: A detailed view of the selected metabolite, M\_23dhb\_c.

metabolite	name	bigg2-eco	
1 M_23dhb_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_2mci_c	2-Methylcitr...	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_23dhb_c
Name	2,3-Dihydroxybenzoate
Charge	-1
Formula	C7H5O4
ReagentOf	R_DHBS
RDF references (opens in browser)	
is	<a href="http://identifiers.org/bigg.metabolite/23dhb">http://identifiers.org/bigg.metabolite/23dhb</a>
is	<a href="http://identifiers.org/chebi/11427">http://identifiers.org/chebi/11427</a>
is	<a href="http://identifiers.org/chebi/18026">http://identifiers.org/chebi/18026</a>
is	<a href="http://identifiers.org/chebi/19319">http://identifiers.org/chebi/19319</a>
is	<a href="http://identifiers.org/chebi/19320">http://identifiers.org/chebi/19320</a>
is	<a href="http://identifiers.org/biocyc/2-3-DIHYDROXYBENZOATE">http://identifiers.org/biocyc/2-3-DIHYDROXYBENZOATE</a>
is	<a href="http://identifiers.org/chebi/36654">http://identifiers.org/chebi/36654</a>
is	<a href="http://identifiers.org/chebi/41901">http://identifiers.org/chebi/41901</a>
is	<a href="http://identifiers.org/chebi/885">http://identifiers.org/chebi/885</a>
is	<a href="http://identifiers.org/brenda/BG24972">http://identifiers.org/brenda/BG24972</a>
is	<a href="http://identifiers.org/kegg.compound/C00196">http://identifiers.org/kegg.compound/C00196</a>

## Model options: reports

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

The screenshot shows the MetaDraft 0.6.8 interface. The 'Model options' menu is open, highlighting 'Gene report', 'Reaction report', and 'Metabolite report'. The main window displays a table of metabolites and an 'Information' panel for the selected metabolite M\_23dhb\_c.

Build	Genes	metabolite	fixed
1	M_23dhb_c	2,3-Dihydro...	bigg2-eco <input type="checkbox"/>
2	M_23dhaba_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-Methylcitr...	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_23dhb_c
Name	2,3-Dihydroxybenzoate
Charge	-1
Formula	C7H5O4
ReagentOf	R_DHBS
RDF references (opens in browser)	
is	<a href="http://identifiers.org/bigg.metabolite/23dhb">http://identifiers.org/bigg.metabolite/23dhb</a>
is	<a href="http://identifiers.org/chebi/11427">http://identifiers.org/chebi/11427</a>
is	<a href="http://identifiers.org/chebi/18026">http://identifiers.org/chebi/18026</a>
is	<a href="http://identifiers.org/chebi/19319">http://identifiers.org/chebi/19319</a>
is	<a href="http://identifiers.org/chebi/19320">http://identifiers.org/chebi/19320</a>
is	<a href="http://identifiers.org/biocyc/2-3-DIHYDROXYBENZOATE">http://identifiers.org/biocyc/2-3-DIHYDROXYBENZOATE</a>
is	<a href="http://identifiers.org/chebi/36654">http://identifiers.org/chebi/36654</a>
is	<a href="http://identifiers.org/chebi/41901">http://identifiers.org/chebi/41901</a>
is	<a href="http://identifiers.org/chebi/885">http://identifiers.org/chebi/885</a>
is	<a href="http://identifiers.org/brenda/BG24972">http://identifiers.org/brenda/BG24972</a>
is	<a href="http://identifiers.org/kegg.compound/C00196">http://identifiers.org/kegg.compound/C00196</a>

## 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

# MetaDraft

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

The screenshot displays the MetaDraft 0.6.8 interface. The main window shows a list of reactions under the 'Reactions' tab. A 'MetaDraft Report' window is open, displaying the following information:

### 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
<a href="#">stu0160</a>	b3057	1.0	bigg2-eco
<a href="#">stu0163</a>	b3784	1.0	bigg2-eco
<a href="#">stu0246</a>	b0968	1.0	bigg2-eco
<a href="#">stu0264</a>	b3849	1.0	bigg2-eco
<a href="#">stu0265</a>	b3290	1.0	bigg2-eco
<a href="#">stu0505</a>	b3560	1.0	bigg2-eco
<a href="#">stu0590</a>	b3770	1.0	bigg2-eco

Buttons: View in browser, Export (HTML)

The background window shows a list of reactions with columns for 'reaction', 'name', and a checkbox. The 'Information' tab is active, showing details for a reaction involving 'glucosamine:undecaprenylphosphate N-acetyltransferase'.

## 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 interface. The main window shows a table of reactions with columns for reaction ID, name, and a checkbox. A 'MetaDraft Report' window is open, showing detailed information for a gene match.

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-acetylm... <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	
<b>function</b>	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)
<b>gene</b>	rfe
<b>GO_function</b>	<a href="#">GO:0042280</a> - cell surface antigen activity, host-interacting
<b>gene_synonym</b>	ECK3776; JW3758; wecA
<b>EC_number</b>	<a href="#">2.4.1.-</a>
<b>product</b>	UDP-GlcNAc:undecaprenylphosphate GlcNAc-1-phosphate transferase
<b>GO_process</b>	<a href="#">GO:0009246</a> - 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.

The screenshot displays the MetaDraft 0.6.8 interface. A 'MetaDraft Report' window is open, showing details for reaction R\_ACGAMT. The main window has tabs for 'Build', 'Genes', 'Reactions', and 'Metabolites'. The 'Reactions' tab is active, showing a list of reactions. The report window provides the following information:

- Reaction ID:** R\_ACGAMT
- Name:** UDP-N-acetylglucosamine:undecaprenylphosphate N-acetylglucosamine -1-phosphate transferase
- Organism:** bigg2-eco
- Reaction Name:** N-Acetyl-D-glucosamine transport via PEP:Pyruvate PTS (periplasm) (irreversible)
- Association:** ((b2415 and b2417 and b1101 and b2416) or (b2415 and b0679 and b2416))
- 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:** <http://identifiers.org/bigg.reaction/ACGAptspp>

Buttons for 'View in browser' and 'Export (HTML)' are visible at the bottom of the report window.

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The screenshot displays the MetaDraft 0.6.8 interface. The main window has a menu bar (File, Build options, Model options, Sessions, Help) and a tabbed interface with 'Build', 'Genes', 'Reactions', and 'Metabolites' tabs. The 'Reactions' tab is active, showing a table of reactions with columns for reaction ID, name, a checkbox, organism, genes, and source. An 'About MetaDraft' dialog box is open, providing version information and contact details. The 'Information' panel on the right shows details for reaction R\_APH120, including its organism (bigg2-eco), name (Acylphosphatase (C12:0)), and association (b0968, stu0246). Below this, a chemical reaction is partially visible, showing substrates and products.

reaction	name		org	genes	src	
1	R_ACGAMT	UDP-N-ace...	<input type="checkbox"/>	bigg2-eco	b3784	stu0163
2	R_ACGApts...	N-Acetyl-D...	<input checked="" type="checkbox"/>	bigg2-eco	b2416,b2415	stu1264,stu1.
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"/>	bigg2-eco	b0968	stu0246
15	R_APH140	Acylphosph...	<input checked="" type="checkbox"/>	bigg2-eco	b0968	stu0246
16	R_APH141	Acylphosph...	<input checked="" type="checkbox"/>	bigg2-eco	b0968	stu0246
17	R_APH160	Acylphosph...	<input checked="" type="checkbox"/>	bigg2-eco	b0968	stu0246

**About MetaDraft**

This is the MetaDraft component of MetaToolkit version 0.6.8-(0.7.8.525) (rc1). MetaDraft uses PySCeS-CBMPy (<http://cbmpy.sourceforge.net>) technology.

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For help and support please contact Brett Olivier:  
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OK

**Information**

Organism **bigg2-eco**  
**R\_APH120** Acylphosphatase (C12:0)  
(irreversible)  
Association **b0968**  
Association (stu0246)

ddcap\_c > M\_pl\_c + (2.0) M\_h\_c + M\_ddca\_c  
anolyl-phosphate (n-C12:0) > Phosphate + (2.0) H+ +  
(n-C12:0)

**Substrates**

phosphate (n-C12:0)

**Products**

e (n-C12:0)