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)
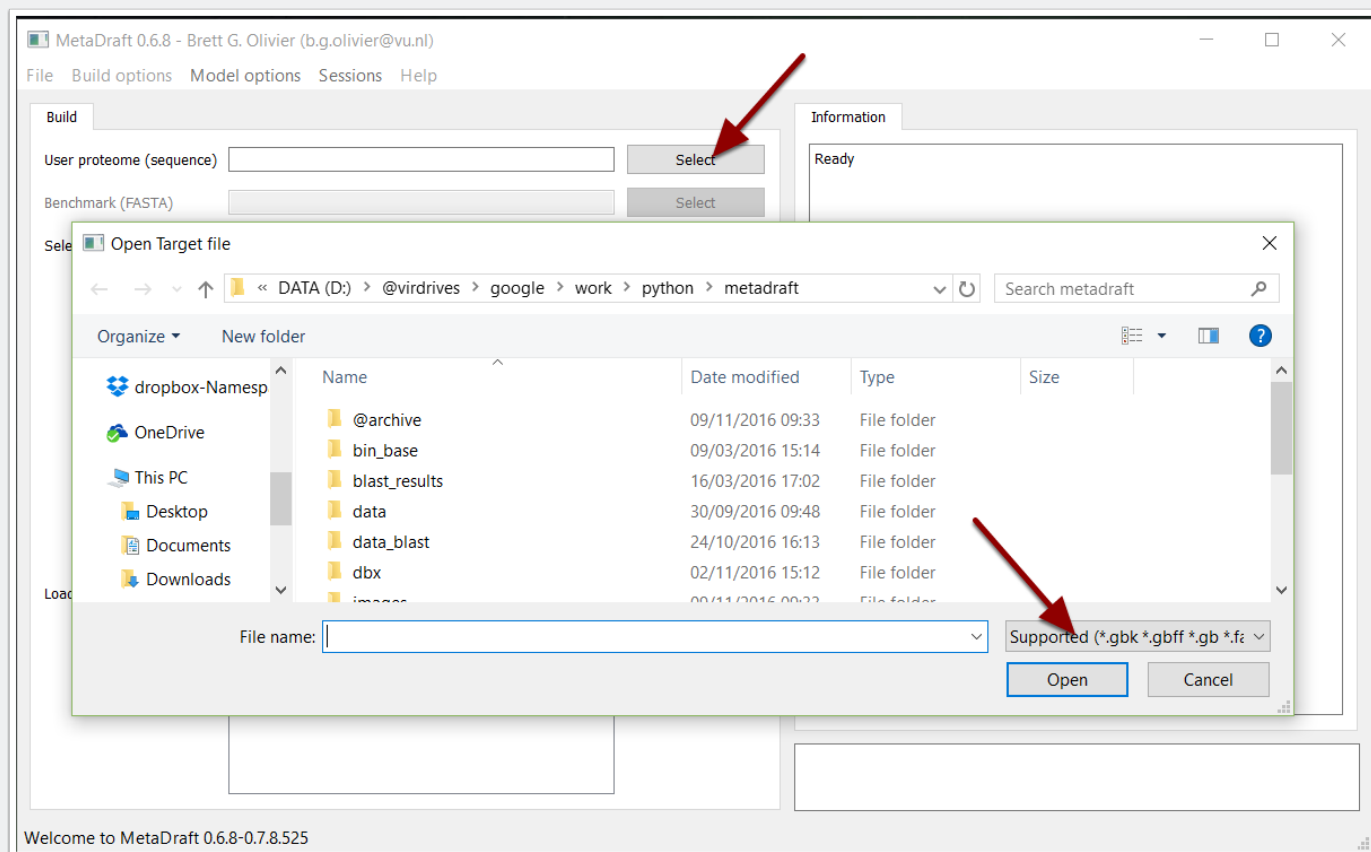
MetaDraft
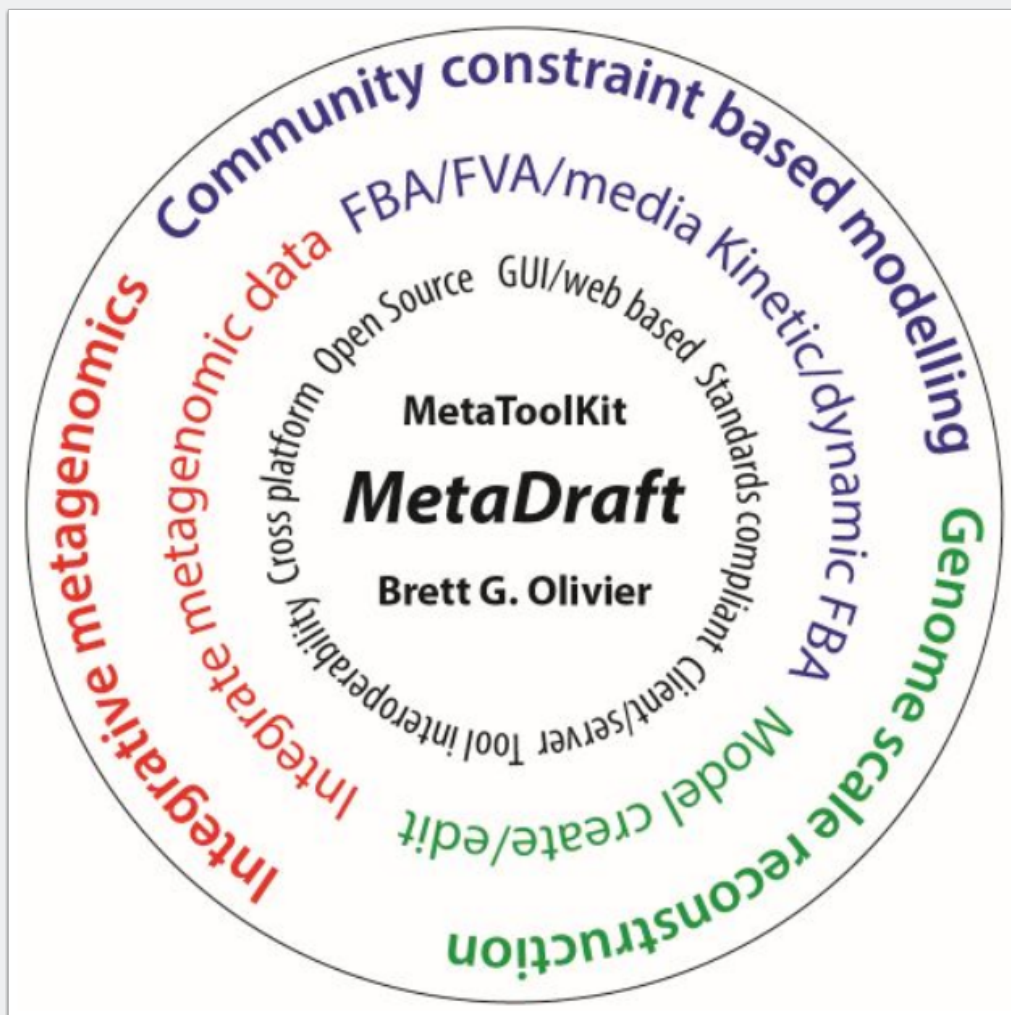
Main screen

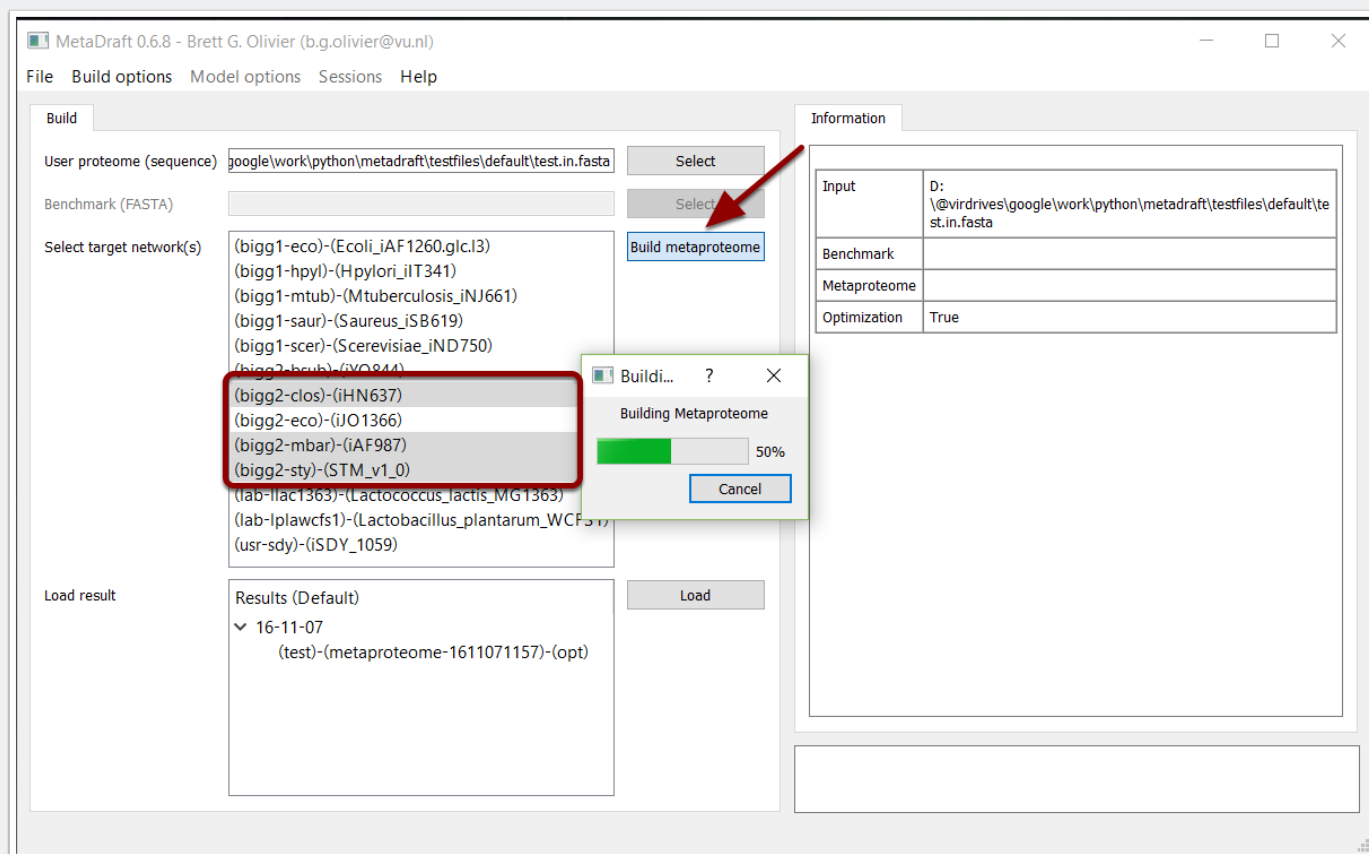This is the main program screen where you can create new draft reconstruction or load previously analysed results.

MetaDraft
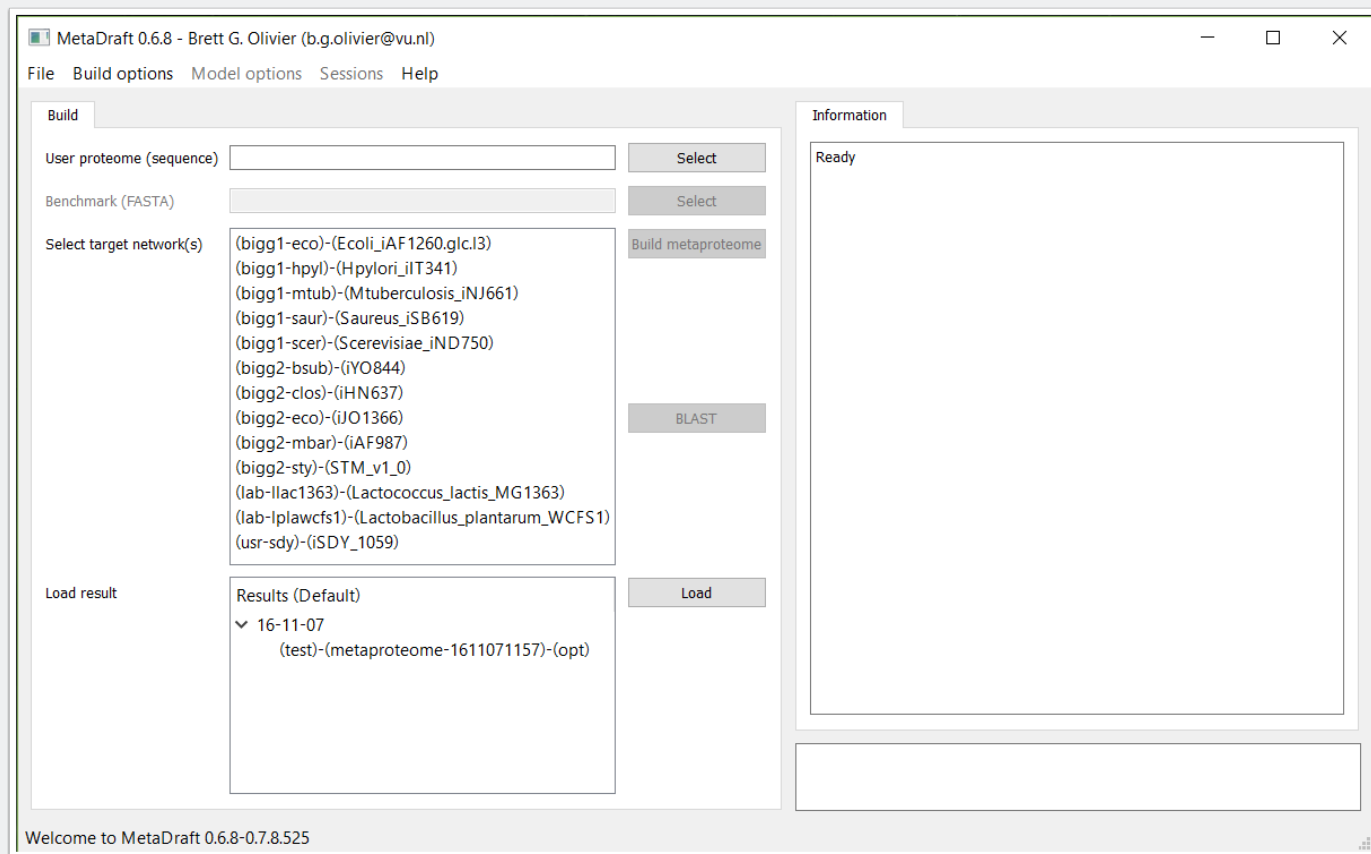
Sequence loading

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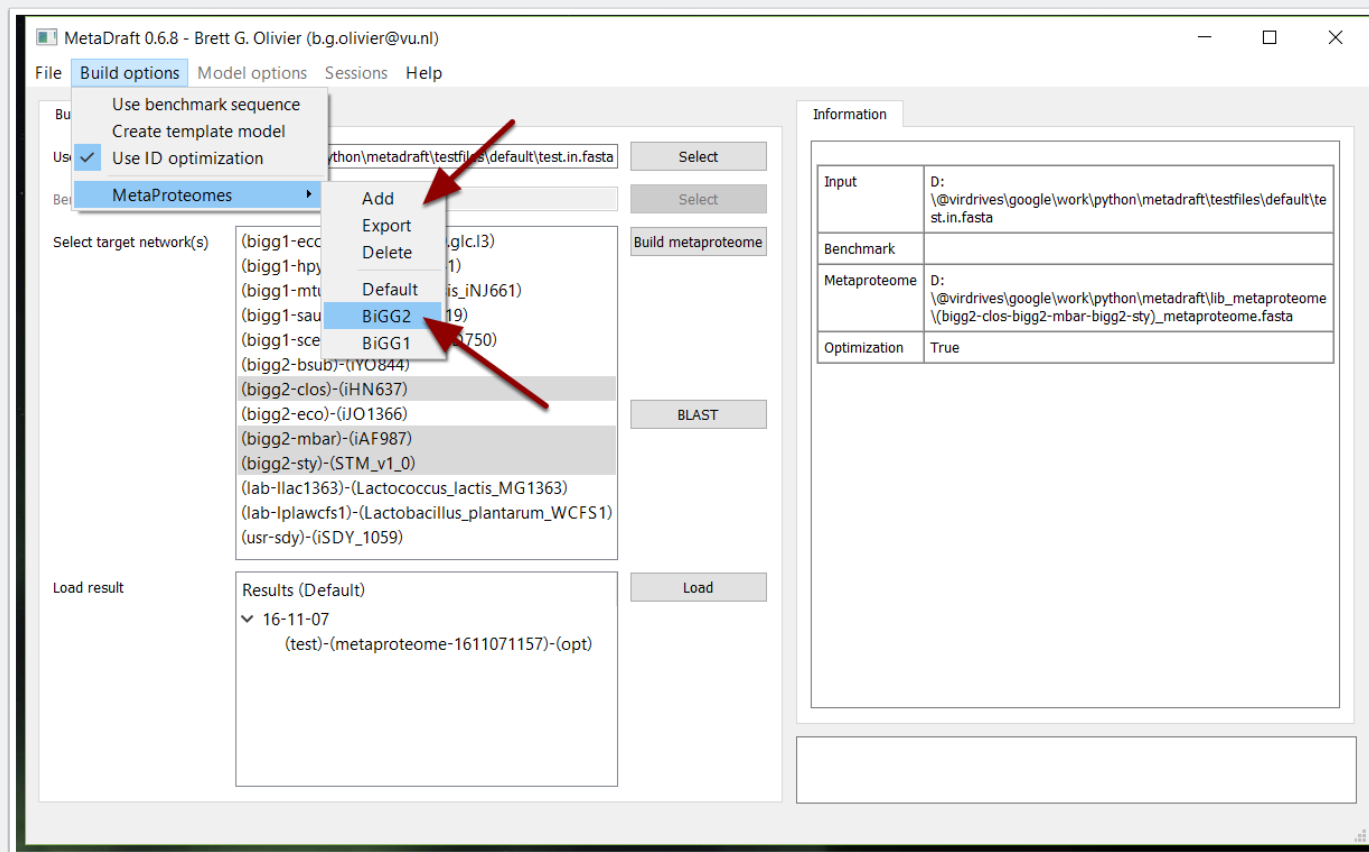
MetaDraft

Build a metaproteome

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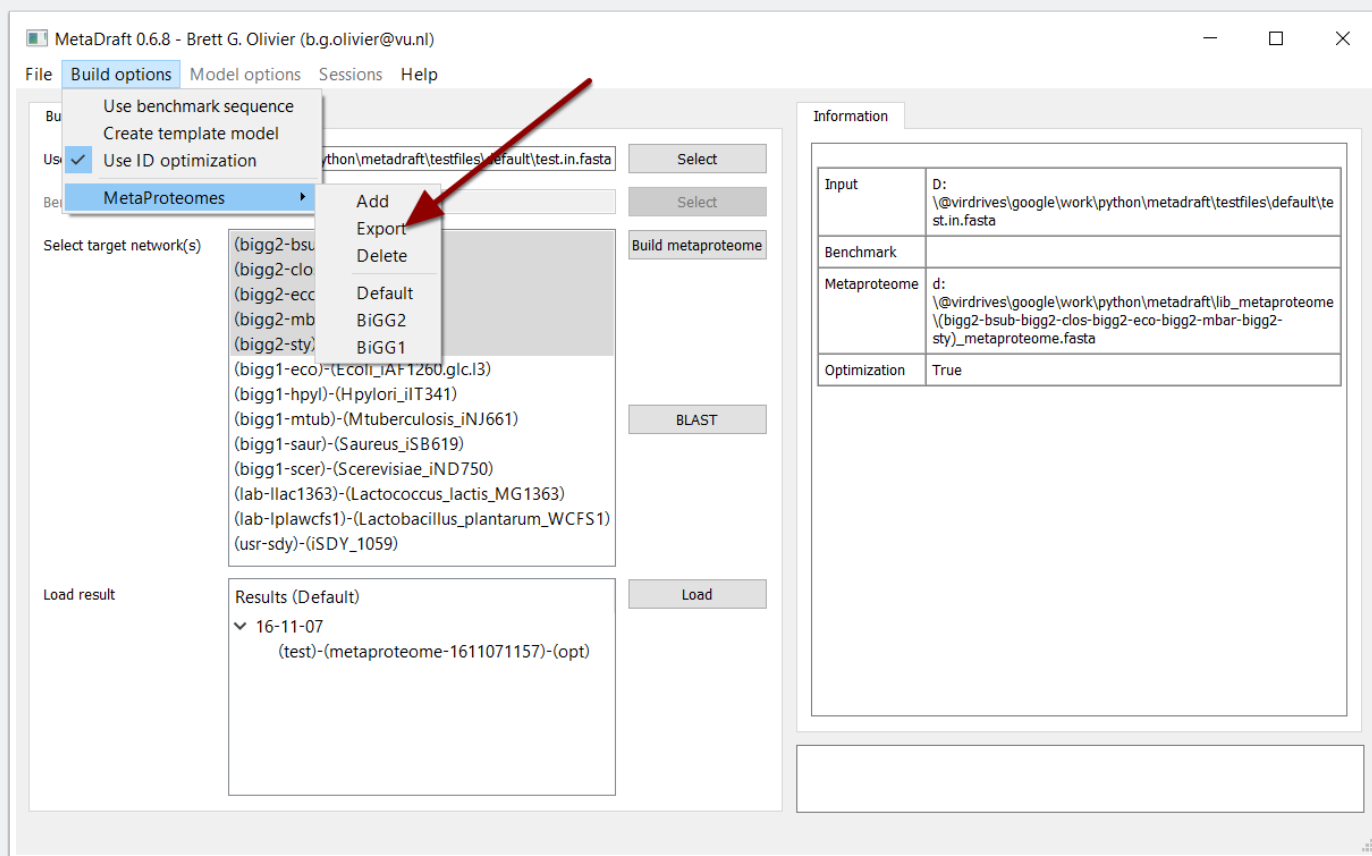
Predefined sets

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

MetaDraft

Metaproteome export

Export selected metaproteome in FASTA format.

Run sequence search

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

MetaDraft

Search results

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

Delete/rename results

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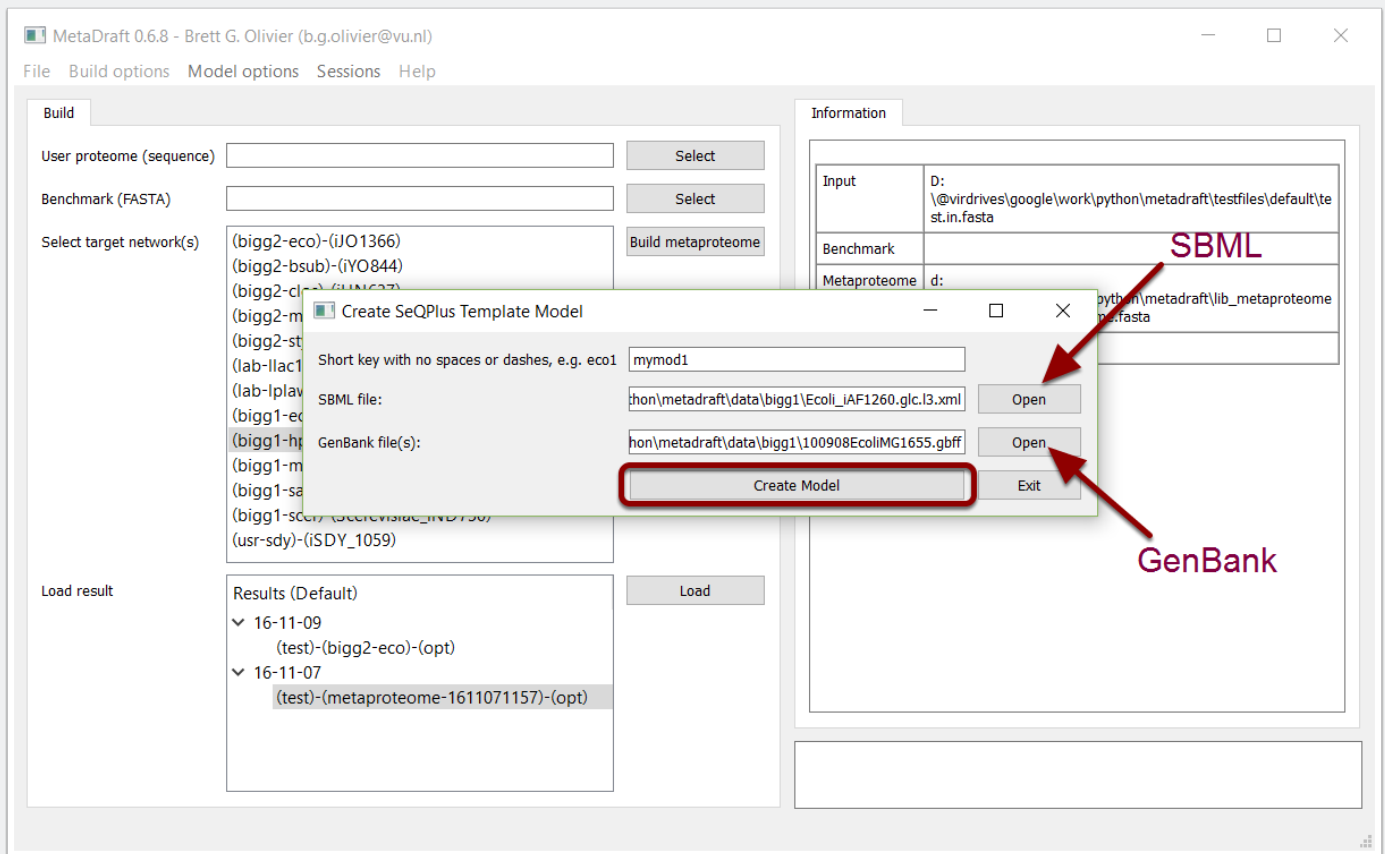
Optional: benchmark

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 th benchmark will be included.
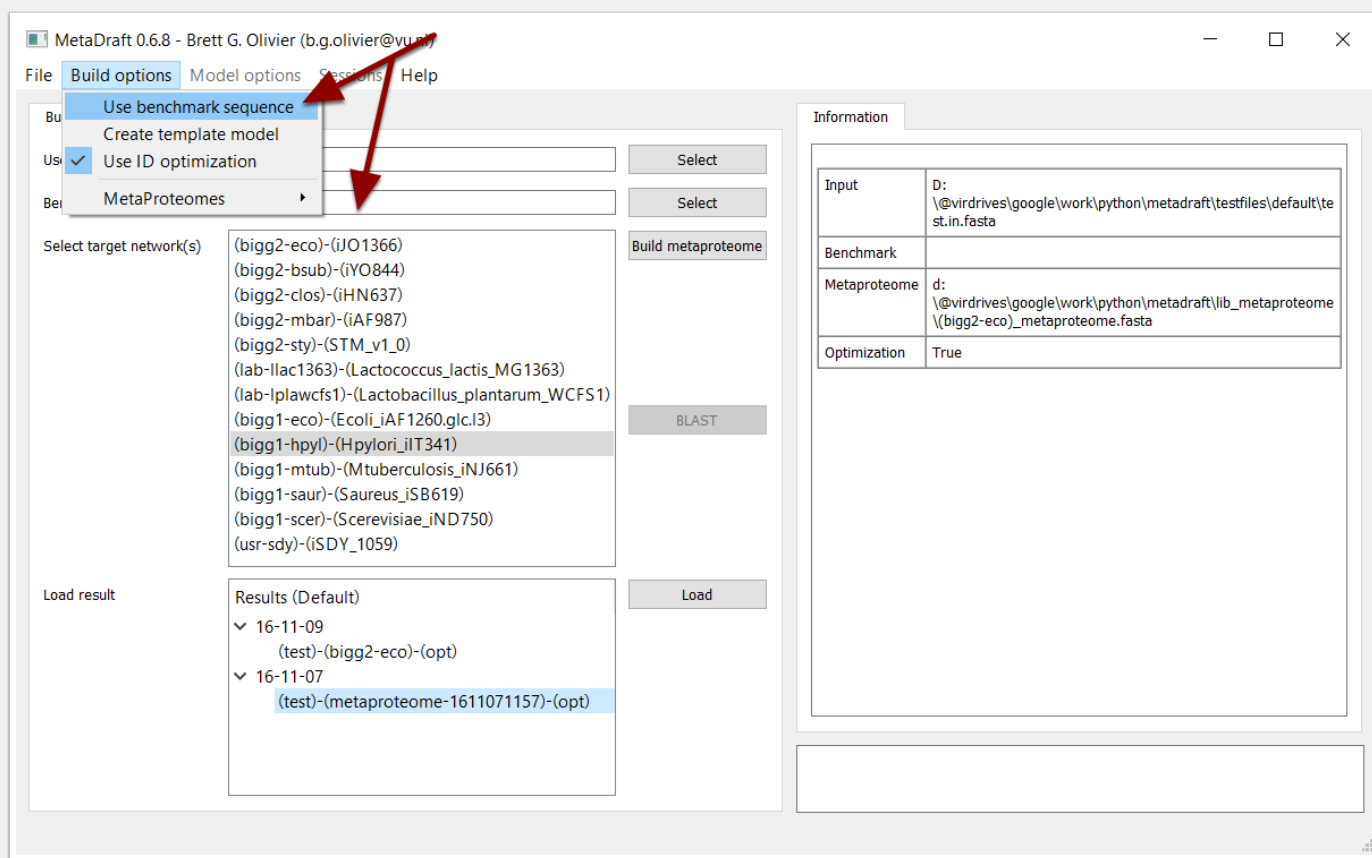
Option: create new template model

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

Option: analyse SBML model

To analyse, identify and optionally convert an SBML the model, use the File menu.
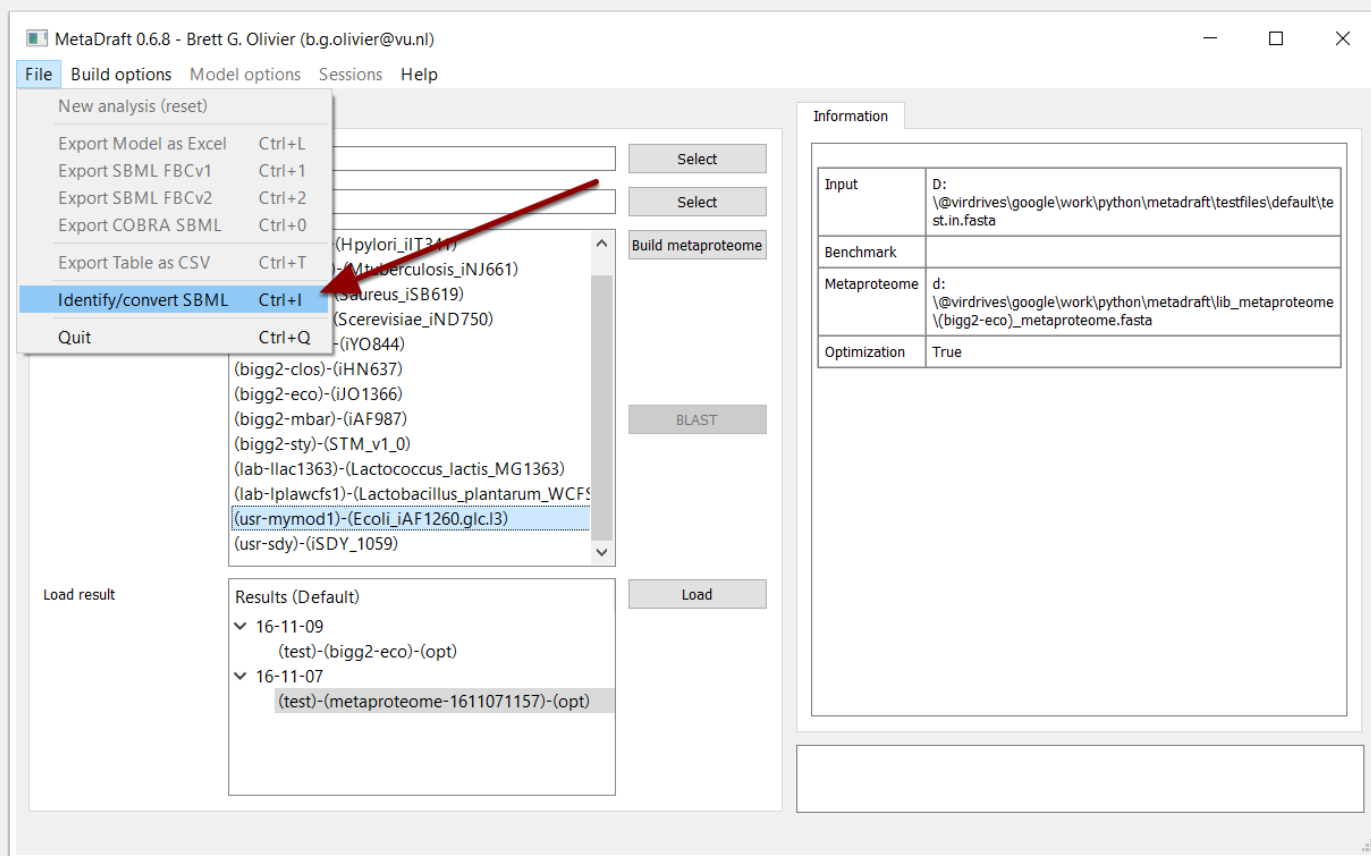
Option: analyse SBML model 2

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.
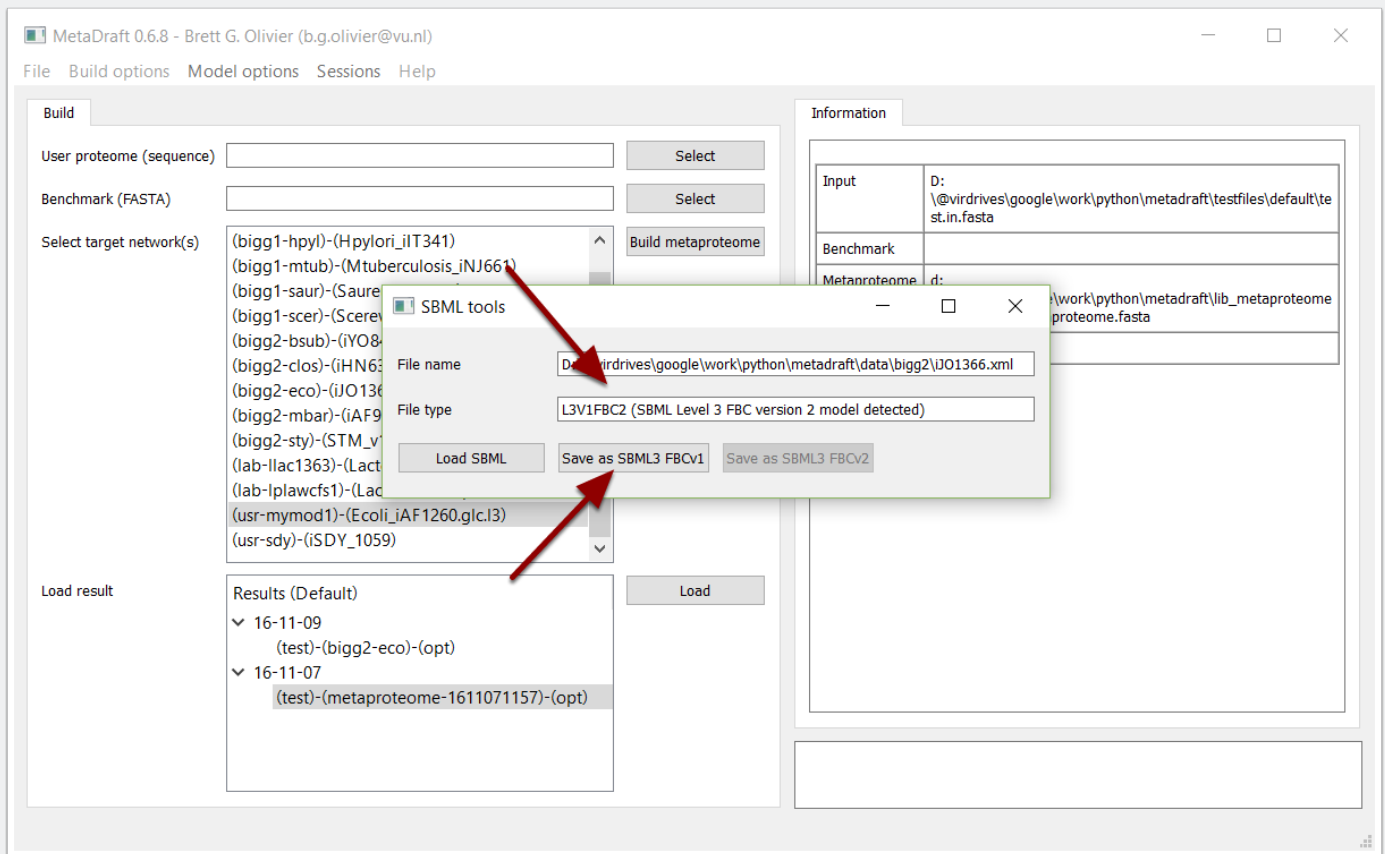
Load results

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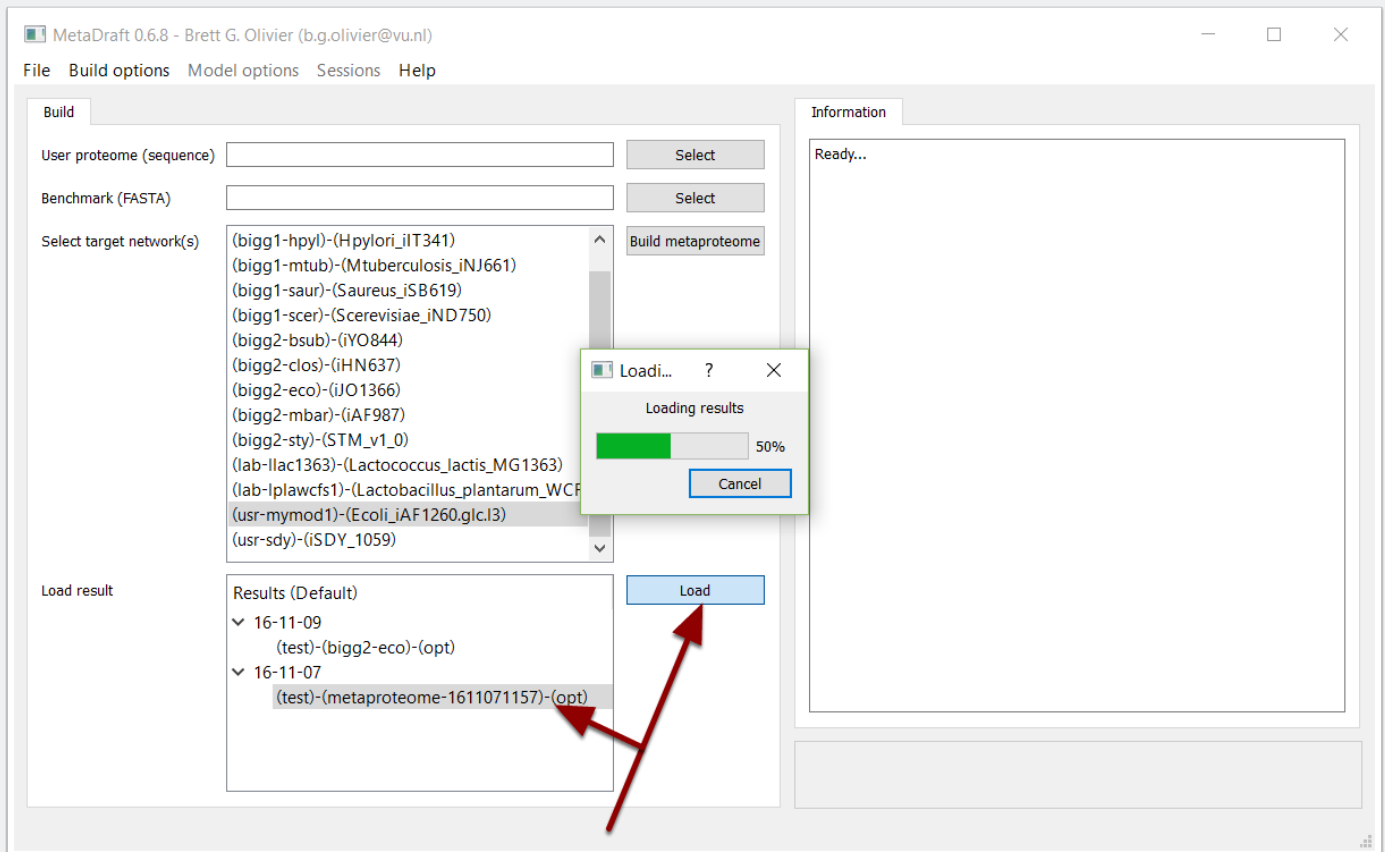
Results: genes

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 otrthology 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.

Results: genes score filter

Right clickingon 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.

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

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.

Sessions

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

MetaDraft

Model options: reports

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

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.

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 viewd in a web-browser.

MetaDraft

Report: reactions

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

Copyright

(C) Brett G. Olivier, Systems Bioinformatics, Vrije Universiteit Amsterdam, Amsterdam 2016.