

## 1. Starting SyBiL

- a) Connect to the internet.
- b) Go to <http://vcell.org/sybil>
- c) Click on Run SyBiL on the right

## 2. Get sample files

- a) Go to <http://vcell.org/sybil/samples.html>. The "BioPAX" links lead to sample files, the "Reactome" links to their origin on Reactome.
- b) Download sample files to your computer.
- c) Go to Reactome and download any .owl file

## 3. Visualize BioPAX files

- a) Switch to Data tab in the second raw menu bar.
- b) If you opened a file previously, first do Menu > File > New to clear, otherwise new data will be added to the existing
- c) Menu > File > Open and open .owl file from your computer
- d) BioPAX source code is in tab Data > BioPAX Source
- e) Graph representation is in tab Data > Graph
- f) Click on buttons on the left toolbar to show (from top to bottom; leave mouse over a button for 5 seconds to see tips):
  - i) zoom in and out,
  - ii) view various layouts,
  - iii) view various levels of detail : 1 dot - see reactions only; 2 dots - reaction network; 3 dots – view components of reaction participants.
- g) Click on buttons on the toolbar above graph to select nodes by type. New selections are added to the old. Deselect by clicking on empty space n a graph.

## 4. Study the content of BioPAX data.

- a) Select nodes by mouse, individually or drag or shift/control.
- b) Edges can be selected, too
- c) Resources associated with selected graph elements are listed right to graph. One resource is selected and certain properties show in the table below.

## 5. Export to SBML.

- a) Tab "BioPAX to SBML Conversion" > Conversion Criteria
- b) Conversion criteria: whether substances have modifications (e.g. phosphorylations).
  - i) Choosing "none" means all substances are mapped to species types.
  - ii) Choosing "Some" converts only selected substances to Species Types. For others, user will assign

species types manually later on.

iii) Choosing “All” means no substances are assigned to species types automatically.

- c) Button “Process and Proceed”, leads to Tab “Reactions and Participants”.
- d) SBML terms are red, BioPAX terms are blue
- e) If you selected in the previous panel “All” or “Some”, some cells in the species type column will be empty (“[none]”) and should be filled.
- f) Check all columns for “none”. Select the proper name from drop-down menu.
- g) Check right column (locations) for empty cells (“[none]”) and select a location. For files from Reactome (as are all our sample files), the participant name often contains the location. Leaving a location empty will lead to an error if you proceed.
- h) Button “Process and proceed” leads to tab “Compartments”.
- i) Set dimensions and surrounding compartment. Default is “2” if the location contains the string “membrane” and “3” otherwise.
- j) Button “Process for SBML”.
- k) Button “Browser” displays SBML file in your default browser. To save, specify name and click “Save”.

## 6. Advanced features. Data and SPARQL queries

- a) Tab Advanced > Query > Query for SPARQL queries. SPARQL is an SQL-style standard query format for OWL.
- b) There are editable sample queries. Recommended are B, D, E and G.

## 7. Miscellaneous

Tab Advanced > Schemas has a few sample ontologies in N3 format such as BioPAX (pathways), SBPAX (bridging pathways and models), Dublin Core (general purpose annotations) and Basic Formal Ontology (high level ontology)

## 8. Import EGFR Pathway (not finished)

- a) If you previously opened or imported another file, do Menu > File > New first to clear, since import is accumulative.)
- b) Type some search string in the “search keyword” field, such as “egfr”, click search
- c) The results are hits by Pathway Commons representing records. Each comes with a number of related substance and pathway entries, whose number is on the tab. For example tab “Hit 2 (20S, 16P)” means hit 2 has 20 related substances and 16 pathways.
- d) Select hit 2 and select the pathways. Each pathway can be obtained unaltered (“raw”) or processed to optimize the data (“smelted”) - removed duplicated entities. Choose the second from the top “Grb2 events in EGFR signaling” from Reactome, smelted.
- e) Choose some entities, preferably reactions and their participants. If you choose reactions, participants will be included, but not their properties, unless you select those participants, too.