

PANTHER software developments

Mapping BioPAX to SBGN
process description

Goals

- Save SBGN PD map to BioPAX
- Read BioPAX and generate SBGN PD

CellDesigner to BioPAX conversion

Generate OWL files from
CellDesigner files

CellDesigner to BioPAX converter

- Java application
- Uses the PAXTools library to output an OWL file.
- Currently it uses the CellDesigner code directly. In the future this will be converted to a plugin.

Information from CellDesigner that is captured in BioPAX

- Model Information
- Compartment Information
- Species Information
- Reactions Information

CellDesigner to BioPAX mapping (model and compartment information)

Model Information	Pathway Object
Compartment	Cellular Location Vocabulary object

CellDesigner to BioPAX mapping (Species)

Protein	Protein
RNA and AntiSenseRNA	RNA
Gene	DNA
Simple Molecule and Ion	Small molecule
Unknown, Degraded, Phenotype	Physical Entity

CellDesigner to BioPAX mapping (Species cont.,)

Heterodimer	Complex
Modification Features	Sequence Modification Vocabulary
Binding region	Binding Feature

CellDesigner to BioPAX mapping (Reaction)

State Transition, Truncation, Transcription and Translation	BiochemicalReaction or Degradation if all products are degraded
DimerFormation or Dissociation	ComplexAssembly
Transport	Transport With Biochemical Reaction

Once converted to OWL file, it can be viewed using Protege

The screenshot displays the Protege software interface, which is used for editing OWL (Web Ontology Language) files. The interface is divided into several panes:

- Class Browser:** Shows the class hierarchy for the project "Apoptosis_signaling_pathway". The hierarchy starts with "owl:Thing" and includes various biological classes such as "bp:Entity", "bp:Gene", "bp:Interaction", "bp:Control", "bp:Conversion", "bp:BiochemicalReaction", "bp:Complex", "bp:Dna", "bp:Protein", "bp:Rna", and "bp:SmallMolecule".
- Instance Browser:** Shows a list of instances for the class "bp:BiochemicalReaction". The instances are labeled with file paths, such as "/pathway_files/set6_output/r101", "/pathway_files/set6_output/r103", and "/pathway_files/set6_output/r104".
- Individual Editor:** Shows the details for the instance "file:/Users/muruganu/pathway_files/set6_output/r101". The editor is divided into several sections, each representing a property of the instance. The properties and their values are:
 - bp:conversionDirection:** Value: [empty]
 - bp:CNumber:** Value: [empty], Lang: [empty]
 - bp:kEQ:** Value: [empty]
 - bp:displayName:** Value: [empty], Lang: [empty]
 - bp:standardName:** Value: [empty], Lang: [empty]
 - bp:name:** Value: [empty], Lang: [empty]
 - bp:left:** Value: file:/Users/muruganu/pathway_files/set6_output/s
 - bp:spontaneous:** Value: undefined
 - bp:availability:** Value: [empty], Lang: [empty]
 - bp:dataSource:** Value: [empty], Lang: [empty]
 - bp:participant:** Value: file:/Users/muruganu/pathway_files/set6_output/s, file:/Users/muruganu/pathway_files/set6_output/s
 - bp:comment:** Value: REACTION_REVERSIBLE=false, Lang: [empty]
 - bp:deltaG:** Value: [empty], Lang: [empty]
 - bp:participantStoichiometry:** Value: file:/Users/muruganu/pathway_files/set6_output/s, file:/Users/muruganu/pathway_files/set6_output/s
 - bp:deltaH:** Value: [empty], Type: [empty]
 - bp:previdence:** Value: [empty], Lang: [empty]
 - bp:right:** Value: file:/Users/muruganu/pathway_files/set6_output/s

Issues to be addressed

- Logical Operators
- Activation status
- Some CellDesigner component types do not have a corresponding type in BioPAX

Future development

- Read BioPAX file and create SBGN PD diagrams
 - Through CellDesigner
 - Directly after libSBGN is available
 - Auto layout is the key