Paxtools, a Java API for BioPAX

Paxtools: Basics

- A complete and consistent implementation of BioPAX specification:
 - POJO Beans
 - Getters/Setters

- Handles non-OO OWL constructs
 - Subproperties, reverse properties, anonymous classes

When to use Paxtools

- Develop BioPAX using software tools
- Extract simplified information
- Write Pathway specific algorithms
- Run complex searches:
 - Path, Pattern and Graph queries.
- Convert
 - BioPAX → SBGN
 - PSI-MI → BioPAX
 - BioPAX L1,L2 → L3
- Access PC2 web service















Pathway and interaction data (BioPAX/PSI-MI) from different data sources

Files



Web Service

Paxtools



Graph Queries



Algorithms



Export



Database Storage

Embed

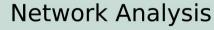
Use

Develop Software



ChiBE







Gene Set Enrichment Analysis



Validation Reports



Visualization

Getting started

- Hosted within SourceForge BioPAX project
 - "Fat" jars
 - Maven
 - Sources
- Documentation
 - Project documentation
 - API docs
 - Getting Started guide

Developing Paxtools

- If you get stuck or have questions, look for support in the Paxtools support mailing list: https://lists.sourceforge.net/lists/listinfo/biopax-paxtools.
- For general questions related to BioPAX, use BioPAX discuss mailing list: http://groups.google.com/group/biopax-discuss.

Module Structure

- Core
- Jena IO
- Query
- PathwayCommons client
- PSI-MI converter
- Sif, GSEA, SBGN converter
- BioPAX converter

My first model

```
BioPAXFactory factory =
BioPAXLevel.L3.getDefaultFactory();
Model model = factory.createModel();
Protein protein1 =
model.addNew(Protein.class,
"http://biopax.org/tutorial/protein1");
```

Adding fields

```
protein1.setStandardName("standard test");
protein1.setDisplayName("test");
BiochemicalReaction rxn1 =
model.addNew(BiochemicalReaction.class,
"http://biopax.org/tutorial/rxn1");
rxn1.addLeft(protein1);
```

Core Tools

- Editors
 - Flexible, reflection based property editors
- Accessors
 - Xpath like access/search
- Algorithms
 - Traverse, Normalize, Compare, Merge, Extract, Clone
- Persistence
 - Hibernate and Hibernate Search mappings

SIF and other reductions

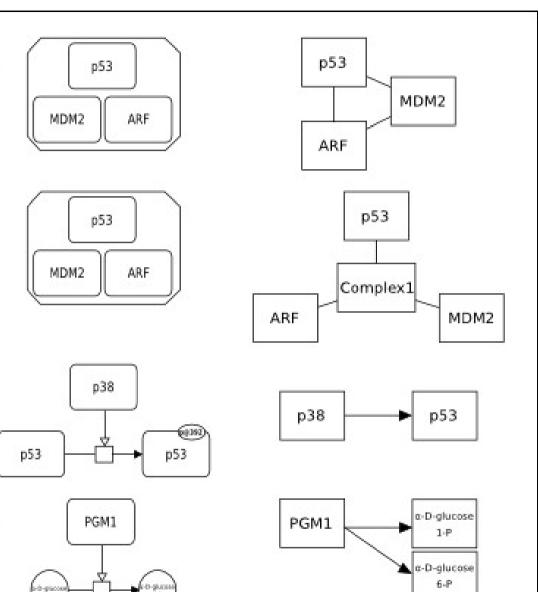
- Converts BioPAX to simpler formats
 - SIF to convert processes to binary relationships based on templates
 - SIFNX customizable SIF exporter
 - GSEA to get gene sets
 - Activity Network Format : PD → AF conversion for BioPAX (Work in Progress)

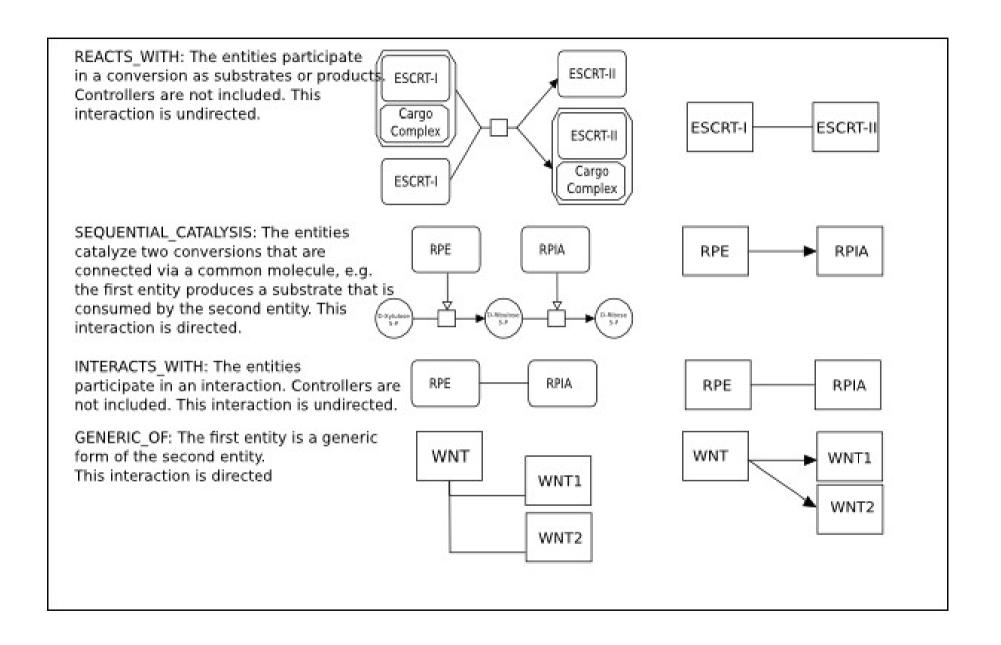
COMPONENT_OF: The first entity is a component of the second entity, which is a complex. This interaction is transient in the sense that A component_of B and B component_of C implies A component_of C. This interaction is directed.

IN_SAME_COMPONENT: Two entities belong to the same molecular complex. This does not necessarily mean they interact directly. In a complex with n molecules, this rule will create a clique composed of n(n-1)/2 interactions. This interaction is undirected.

STATE_CHANGE: The first entity controls a reaction that changes the state of the second entity, e.g. by phosphorylation or other posttranslational modification, or by a change in subcellular location. This interaction is directed.

METABOLIC_CATALYSIS: The first entity catalyzes a reaction that either consumes or produces the second entity. This interaction is directed.



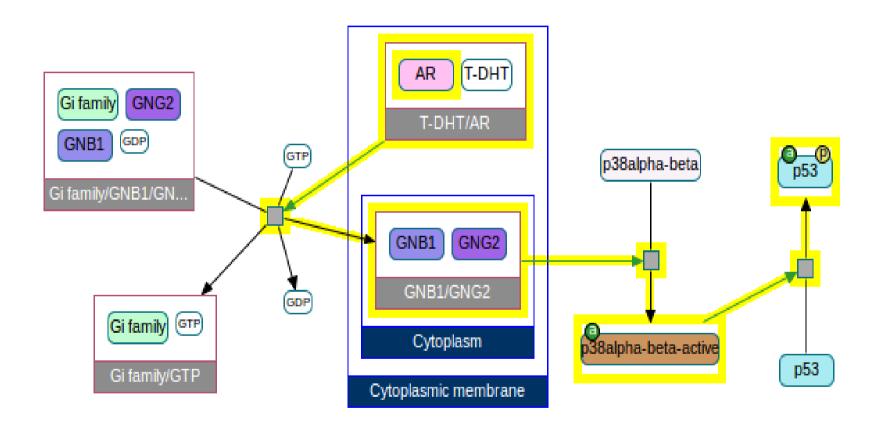


Graph Searches

- Neighborhood
- Graph-of-interest
- Common upstream/downstream
- Shortest Path
- New powerful Pattern search system
 - Regular expressions for pathways

Accessing Pathway Commons

- PC client distributed as a seperate Maven project.
- Seamless access to full PC2 web service
- Filters, simple and graph searches, Xpath like acessors.



Paxtools from the command line

- merge file1 file2 output
- toSif file1 output
- toSifnx file1 outEdges outNodes prop1,prop2,...
- validate path out [xml|html|biopax] [auto-fix] [normalize] [only-errors] [maxerrors=n]
- integrate file1 file2 output
- toLevel3 file1 output
- fromPsimi level file1 output
- toGSEA file1 output database crossSpeciesCheck
- fetch file1 id1,id2,.. output
- getNeighbors file1 id1,id2,.. output

Get Involved

- Use Paxtools and report issues and feature requests.
 See: http://biopax.sourceforge.net/paxtools/issuetracking.html
- Respond to questions by other users at biopaxpaxtools
- Try your hand at fixing bugs and implementing requests
- Improve this documentation.
- Spread the word. Let other people know about BioPAX and Paxtools.

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BioPAX Community

