cy3sbml: A Cytoscape App for SBML

Matthias König*, Nicolas Rodriguez & Andreas Dräger

*LiSyM Systems Medicine of the Liver
Humboldt University Berlin, Institute for Theoretical Biology
livermetabolism.com

DOI 10.5281/zenodo.59921 | build passing | codecov 36% | version 0.2.2 | license LGPLv3.0 | dependencies up to date

App store (v0.2.2 for Cy3.4)
http://apps.cytoscape.org/apps/cy3sbml

Source Code (v0.3.0-SNAPSHOT for Cy3.5-SNAPSHOT)
https://github.com/matthiaskoenig/cy3sbml

Bundesministerium
für Bildung
und Forschung

Cytoscape

- Open source software platform for visualizing complex networks

- Integrating networks with any type of attribute data.

- apps for implementation of additional features

- Large functionality out of the box
  - Visual Mappings
  - SubNetworks
  - Groups
  - Hierarchical Networks
  - NetworkAnalyzer

- Large community
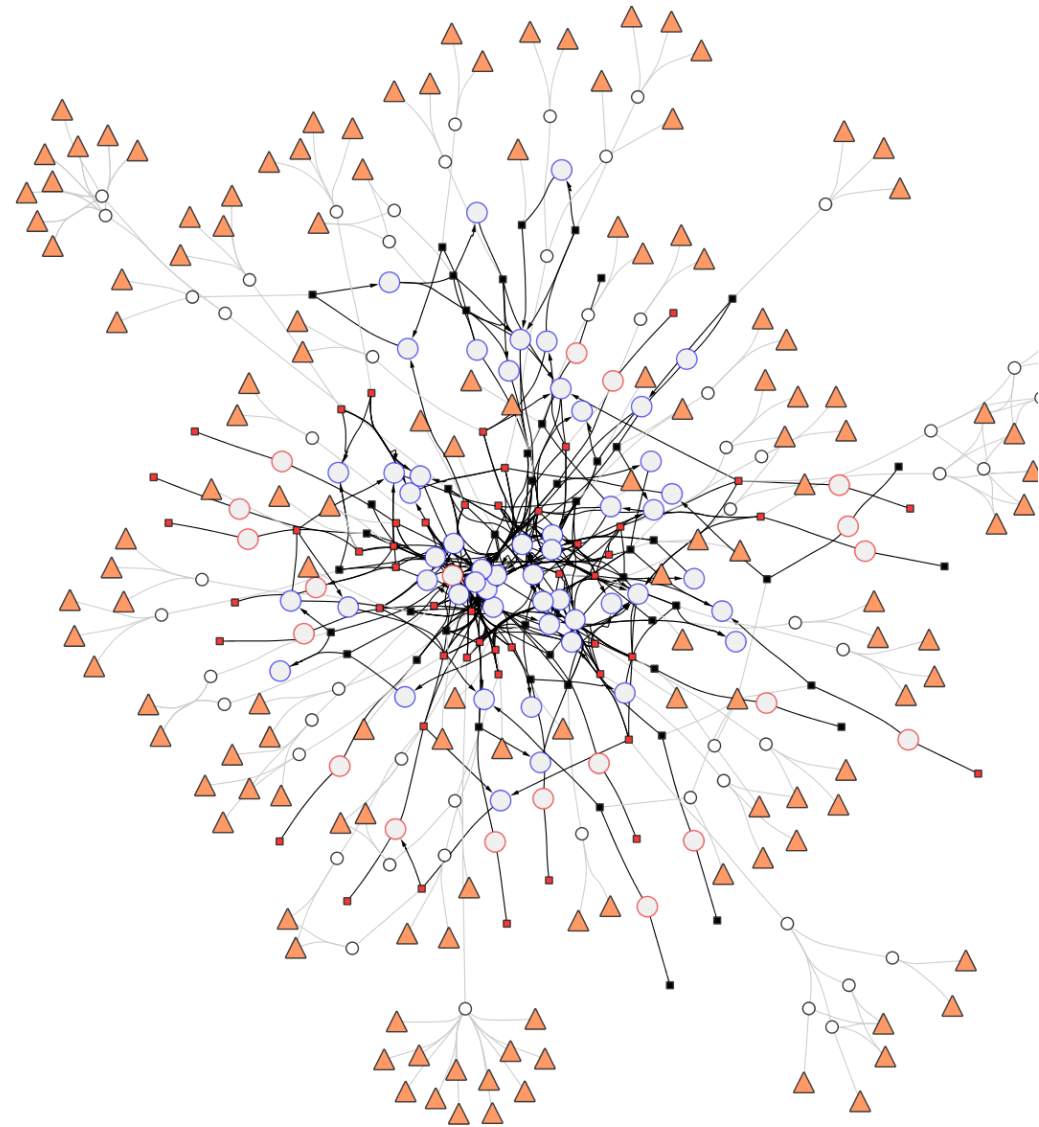
Cytoscape 3.4
http://www.cytoscape.org
Cytoscape 3.5-SNAPSHOT
http://code.cytoscape.org/

cy3sbml

- Small Tool Manifesto
  - Every single tool should do the smallest possible task really well

- cy3sbml is
  - **Mission**: visualization of SBML information within the network context
  - **Vision**: visualization tool for computational models and simulations which seamlessly integrates with computational modeling workflows and frameworks

- cy3sbml is NOT
  - NO model builder
  - NO simulator
  - NO analysis tool

cy3sbml A Cytoscape App for SBML

The main functions of cy3sbml are accessible from the Cytoscape menu bar above.

	Hide|show panel	Changes the visibility of the cy3sbml panel.
	Import SBML	Load SBML files via the File Import Dialogue. To import multiple files select multiple files.
	Validate SBML	Validate SBML files against the SBML specification. Select the network to validate and click the validation icon.
	SBML Examples	Load and explore the SBML examples.
	BioModel Import	Load SBML files from BioModels.
	Help	Display this help information.
	Cofactor nodes	Manage cofactor nodes in the network.
	Save layout	Save network layout information.
	Load layout	Load network layout information.

Support

	Forum	https://groups.google.com/forum/#!forum/cysbml-cyfluxviz
	Bug Tracker	https://github.com/matthiaskoenig/cy3sbml/issues
	Source code	https://github.com/matthiaskoenig/cy3sbml
	Email	konigmatt@googlemail.com

Small Tool Manifesto
https://github.com/pjotrp/bioinformatics

Model import

- Formats
  - SBML (all Levels & Versions)
  - Bundles
    - COMBINE Archive (OMEX)
    - ResearchObject bundle
    - Adobe Universal Container Format (UCF)
    - ePub OCF
    - Open Document package (ODF)
    - ZIP
  - Cytoscape Session Files
- Import via File or URL
- Batch support
- Dedicated Web services
 - BioModels Database

JWS online
http://jjj.biochem.sun.ac.za/rest/models/achcar1/sbml/?download=1
BiGG
http://bigg.ucsd.edu/static/models/iAB_RBC_283.xml
SEEK & Fairdom
https://fairdomhub.org/models/226/download?version=1

Networks

- **Nodes** correspond to SBases & **Edges** to links between them

- Supports
  - **core, fbc, groups, layout, comp***

- Small to genome-scale models

- Multiple views
  - full networks (all SBML)
  - kinetic networks (kinetic parts)
  - base networks (species, reactions, gene associations)

- Creation of subnetworks
  - Filter based on SBML & graph attributes
  - Filter based on neighbors
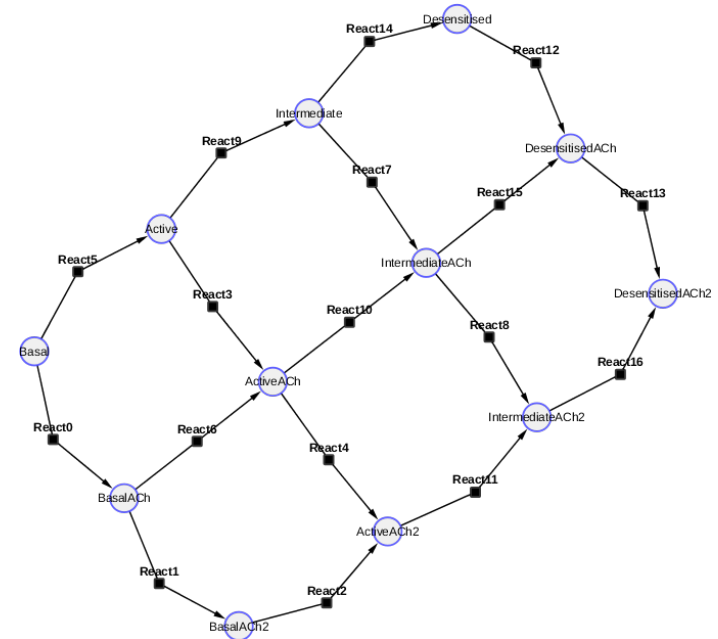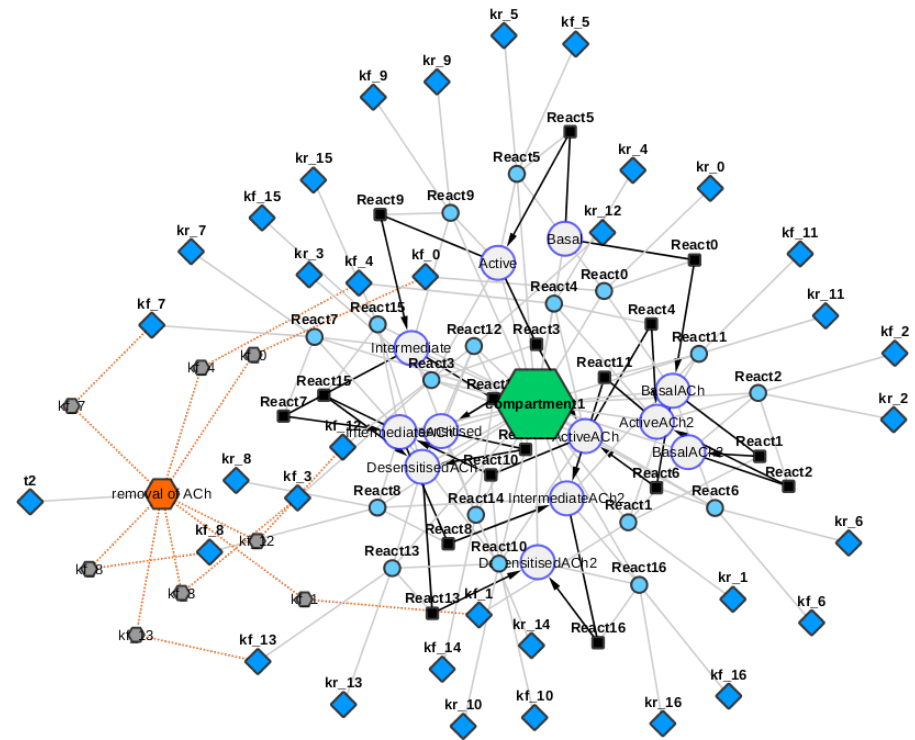
Annotations

- Information about respective SBMLObject

  - History

  - Attributes

  - Node table with attributes (for mapping)

- Annotations (RDF)

  - Resolution via Ontology Lookup Service (OLS)

  - Secondary information for subset of databases

    - UniProt, ChEBI

  - Export of HTML information

Validation

- Validation report
- Table with filtering & sorting
- Network selections from validation results

Data mapping

- Data mapped to network via node & edge attributes

  - sid, metaId

  - Usage of attributes in Visual Mappings

- Data import via CSV

	Fill Color	
Column	sbml type ext	
Mapping Type	Discrete Mapping	
algebraicRule		R:0 G:153 B:51 - #009933
assignmentRule		R:0 G:153 B:51 - #009933
compartment		R:0 G:204 B:102 - #00CC66
event		R:255 G:102 B:0 - #FF6600
eventAssignment		R:153 G:153 B:153 - #999999
fbc_and		
fbc_geneProduct		R:255 G:153 B:102 - #FF9966
fbc_or		
initialAssignment		R:255 G:102 B:102 - #FF6666
kineticLaw		R:102 G:204 B:255 - #66CCFF
localParameter		R:0 G:153 B:255 - #0099FF
parameter		R:0 G:153 B:255 - #0099FF
qual_species		R:240 G:240 B:240 - #F0F0F0
qual_transition		R:153 G:153 B:153 - #999999
rateRule		R:0 G:153 B:51 - #009933
reaction irreversible		R:255 G:51 B:51 - #FF3333
reaction reversible		R:0 G:0 B:0 - #000000
species		R:240 G:240 B:240 - #F0F0F0
unit		R:255 G:255 B:255 - #FFFFFF
unitDefinition		R:204 G:204 B:204 - #CCCCCC

Demo

Programmatic access via REST API

- cyREST
  - language-agnostic, low-level RESTful API module for Cytoscape
  - driving Cytoscape and cy3sbml from R/python/Julia/Node.js/Matlab/...
  - access all Cytoscape data objects, including networks, tables, and Visual Styles
  - Automatic layouts, image generation, ...
  - Use Cytoscape from Jupyter Notebook or Rstudio
  - Connect your services to Cytoscape with programming language of your choice
- py2cytoscape & RCy3
- Examples
  - Integration of cy3sbml with simulators & analysis workflows
  - Coupling to roadrunner & tellurium for visualization of numerical results

Ono, Keiichiro, et al. "
CyREST: Turbocharging Cytoscape Access for External Tools via a RESTful API."
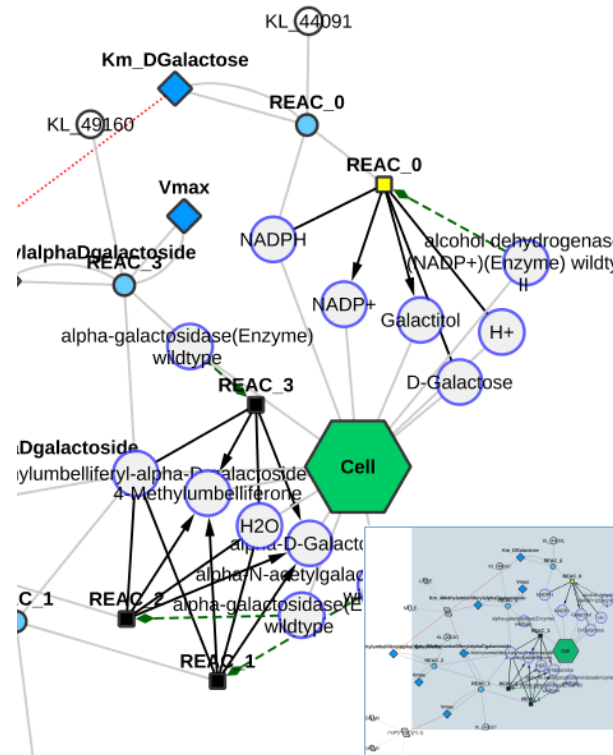F1000Research 4 (2015).

Demo

Integration with other apps

- cy3sabiork
  - Kinetic information from SABIO-RK

- cy3fluxviz
  - Visualization of FluxDistributions

cy3sabiork
https://github.com/matthiaskoenig/cy3sabiork
cy3fluxviz
https://github.com/matthiaskoenig/cy3fluxviz

Things to come

- comp*

  - Model flattening in JSBML #186

- groups browsing #171, #172

  - Groups subnetworks & navigation tree

- layout

  - Escher Layouts #42

  - Layout export #71

- offline modus #138

  - Cache webservice info locally

- Improved cofactor node, clone marker

- Finalize REST API #18

  - documentation, examples, finalization

- SEDML networks #193

- model databases via web services

  - JWS online #10

  - BiGG #104

- Your feature request? https://github.com/matthiaskoenig/cy3sbml/issues

Manuscript Draft
http://bit.ly/2cg7p8u

Acknowledgements

- JSBML
  - Nicolas Rodriguez
  - Andreas Dräger
- SBML
  - Frank Bergmann
  - Mike Hucka
  - Sarah Keating
- Biomodels & MIRIAM
  - Nicolas Le Novère
  - Nick Juty
- Cytoscape
  - Barry Demchak
  - Lopes
  - Scooter Morris
- Tellurium & Roadrunner
  - Kyle Medley
  - Kiri Choi
  - Herbert Sauro