



cy3sbml: A Cytoscape App for SBML

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Slides & Tutorial http://bit.ly/COMBINE2016_cy3sbml

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App store (v0.2.2 for Cy3.4)

<http://apps.cytoscape.org/apps/cy3sbml>

Source Code (v0.3.0-SNAPSHOT for Cy3.5-SNAPSHOT)

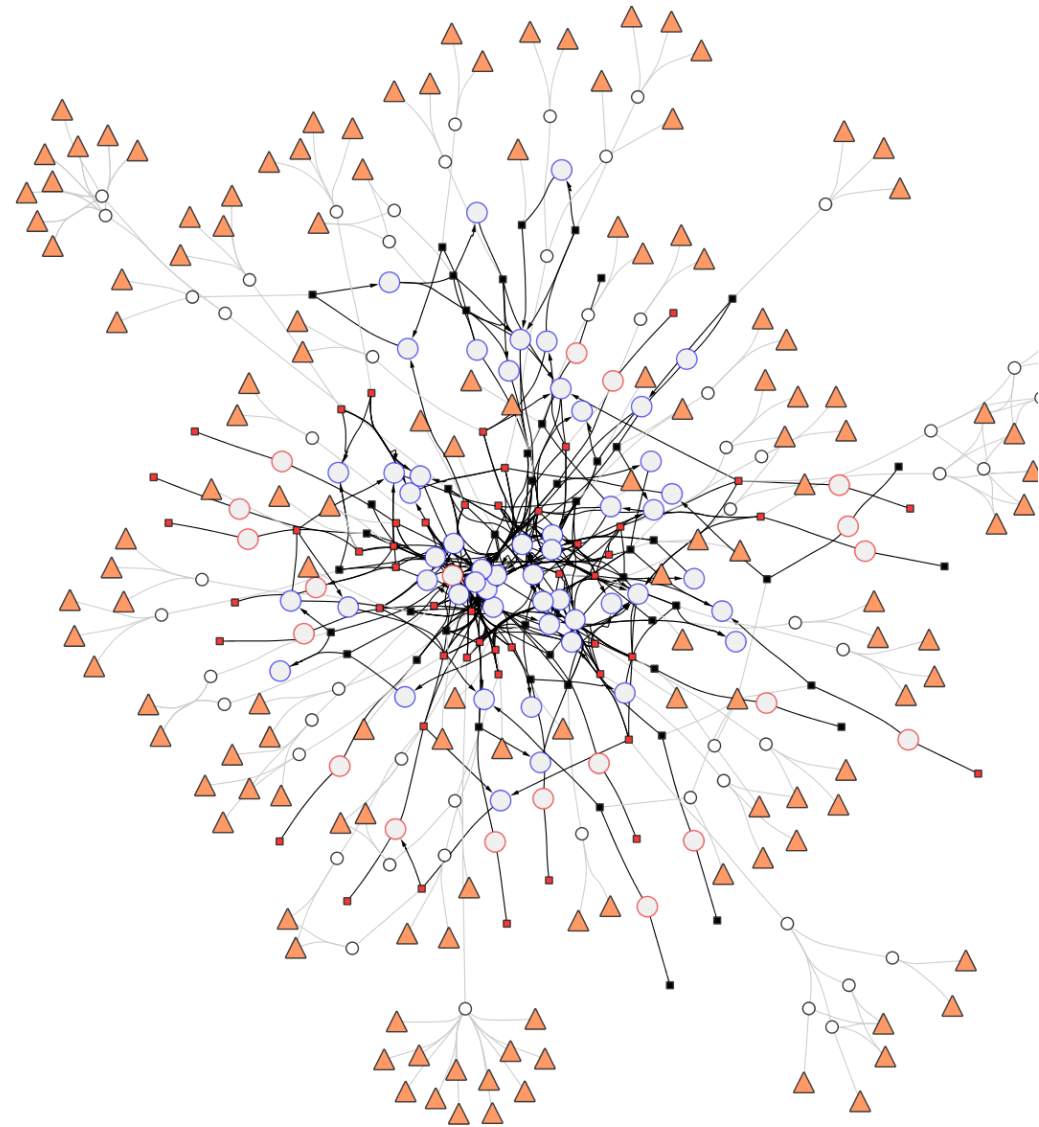
<https://github.com/matthiaskoenig/cy3sbml>



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>

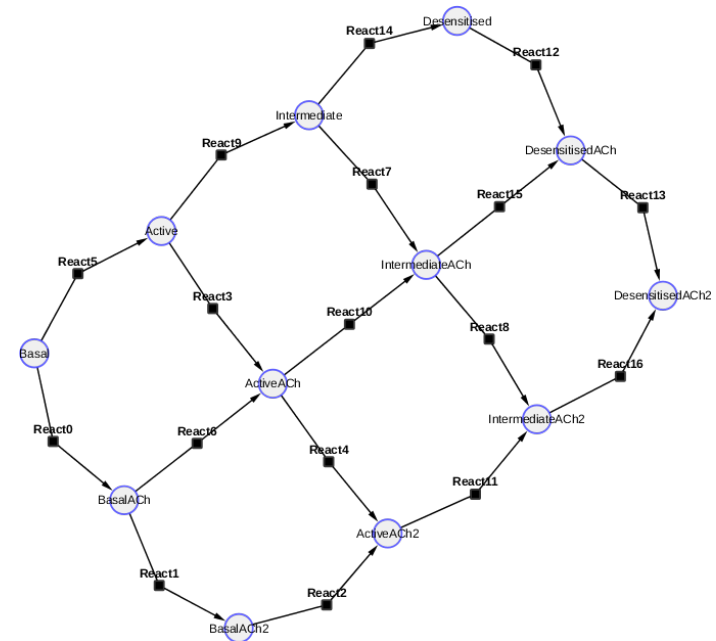
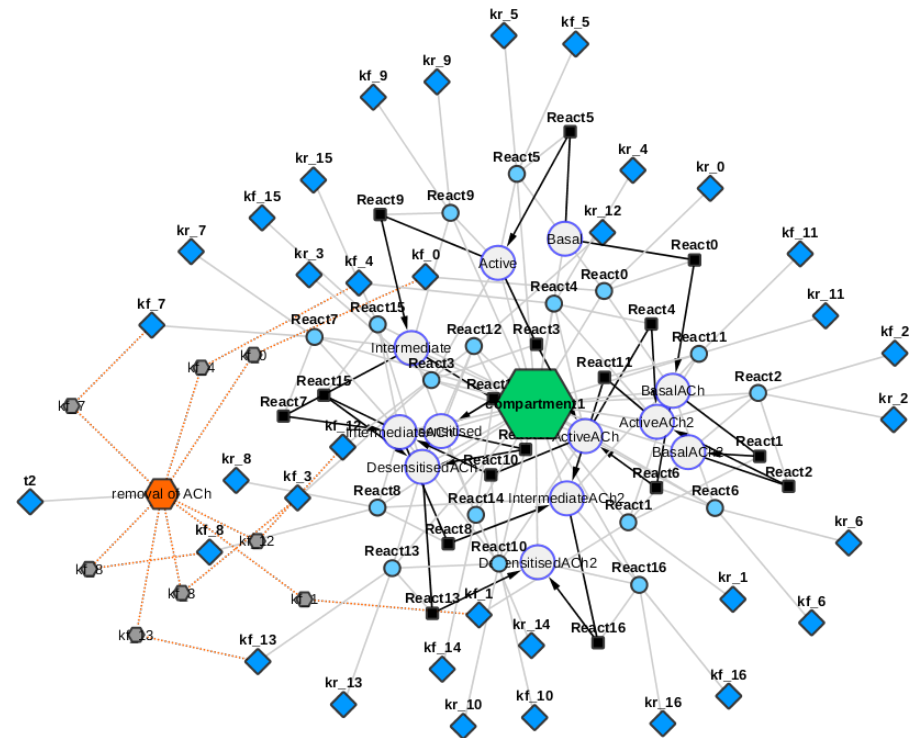
BiGG

http://bigg.ucsd.edu/static/models/iAB_RBC_283.xml

SEEK & Fairdom

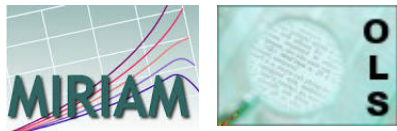
<https://fairdomhub.org/models/226/download?version=1>

- **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



Model BIOMD0000000001

L2V4



id	BIOMD0000000001
name	Edelstein1996 - EPSP ACh event
metaId	_000001

Nicolas Le Novère (lenov@ebi.ac.uk), EMBL-EBI
created: Wed Feb 02 15:56:11 CET 2005
modified: Fri Oct 31 18:17:46 CET 2014

BQM_IS BioModels Database MODEL6613849442

✓ BioModels Database
Caltech mirror
Bio2RDF

BQM_IS BioModels Database BIOMD0000000001

✓ BioModels Database
Caltech mirror
Bio2RDF

BQM_IS DESCRIBED_BY PubMed 8983160

✓ NCBI PubMed
HubMed
Europe PMC
Bio2RDF
PubMed through Linkedlife data

BQB_IS_VERSION_OF Gene Ontology GO:0007274

GO neuromuscular synaptic transmission

http://purl.obolibrary.org/obo/GO_0007274

The process of communication from a neuron to a muscle, across a synapse.
QuickGO (Gene Ontology browser)

✓ AmiGO 2
GO Browser
GO through BioPortal
GO through PANTHER

Validation























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

Goldbeter1995

This document is valid SBML							
Show 10 entries		Search:					
metaid	severity	line	category	code	package	excerpt	message
_289389	Warning	286	Units consistency	99505	core	<kineticLaw metaid="_289389">	(LibSBML Check #99505) Missing unit declarations on parameters or literal numbers in expression
_289401	Warning	321	Modeling practice	80701	core	<parameter metaid="_289401" id="rM_Vs" value="0.76"/>	(Modeling Practice Guideline #80701) It's best to declare units for every parameter in a model
_289413	Warning	322	Modeling practice	80701	core	<parameter metaid="_289413" id="rM_KI" value="1"/>	(Modeling Practice Guideline #80701) It's best to declare units for every parameter in a model
_289425	Warning	323	Modeling practice	80701	core	<parameter metaid="_289425" id="rM_n" value="4"/>	(Modeling Practice Guideline #80701) It's best to declare units for every parameter in a model
_289473	Warning	348	Units consistency	99505	core	<kineticLaw metaid="_289473">	(LibSBML Check #99505) Missing unit declarations on parameters or literal numbers in expression
_289485	Warning	363	Modeling practice	80701	core	<parameter metaid="_289485" id="rTL_ks" value="0.38"/>	(Modeling Practice Guideline #80701) It's best to declare units for every parameter in a model
_289521	Warning	386	Units consistency	99505	core	<kineticLaw metaid="_289521">	(LibSBML Check #99505) Missing unit declarations on parameters or literal numbers in expression
_289533	Warning	409	Modeling practice	80701	core	<parameter metaid="_289533" id="rP01_V1" value="3.2"/>	(Modeling Practice Guideline #80701) It's best to declare units for every parameter in a model
_289545	Warning	410	Modeling practice	80701	core	<parameter metaid="_289545" id="rP01_K1" value="2"/>	(Modeling Practice Guideline #80701) It's best to declare units for every parameter in a model
_289581	Warning	433	Units consistency	99505	core	<kineticLaw metaid="_289581">	(LibSBML Check #99505) Missing unit declarations on parameters or literal numbers in expression

Data mapping

- Data mapped to network via node & edge attributes
 - sid, metald
 - 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).

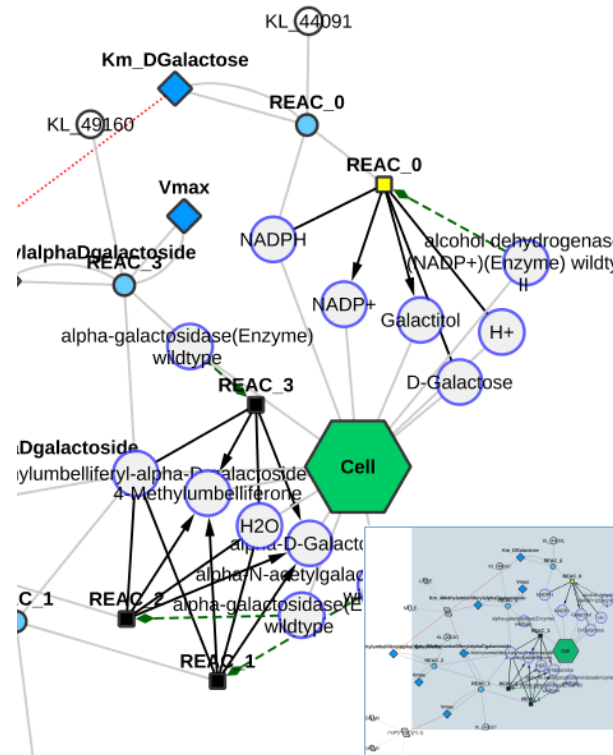


Demo

Integration with other apps



- cy3sabiork
 - Kinetic information from SABIO-RK
- cy3fluxviz
 - Visualization of FluxDistributions



Reaction REAC_0

id	REAC_0
name	
metald	META_REAC_0
compartment	
reversible	<input checked="" type="checkbox"/>
fast	<input checked="" type="checkbox"/>
kineticLaw	KL_44091(REAC_0_Km_SPC_1661_Cell, SPC_1262_Cell) %
units	invalid

BQB_IS_VERSION_OF Enzyme Nomenclature 1.1.1.2
 IntEnZ (Integrated relational Enzyme database)
 KEGG Ligand Database for Enzyme Nomenclature
 Enzyme nomenclature database, ExPASy (Expert Protein Analysis System)
 ExploreEnz at Trinity College

BQB_HAS_TAXON Taxonomy 9606
 NCBITAXON Homo sapiens http://purl.obolibrary.org/obo/NCBITaxon_9606
 Synonyms man; human;
 ✓ NCBI Taxonomy
 Taxonomy through UniProt PURL
 European Nucleotide Archive (ENA)
 BioPortal
 Bio2RDF

BQB_IS SABIO-RK Reaction 1357
 SABIO-RK reaction

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>

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 - Lopes
 - Scooter Morris
- Tellurium & Roadrunner
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 - Kiri Choi
 - Herbert Sauro



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