



Heidelberger Institut für  
Theoretische Studien



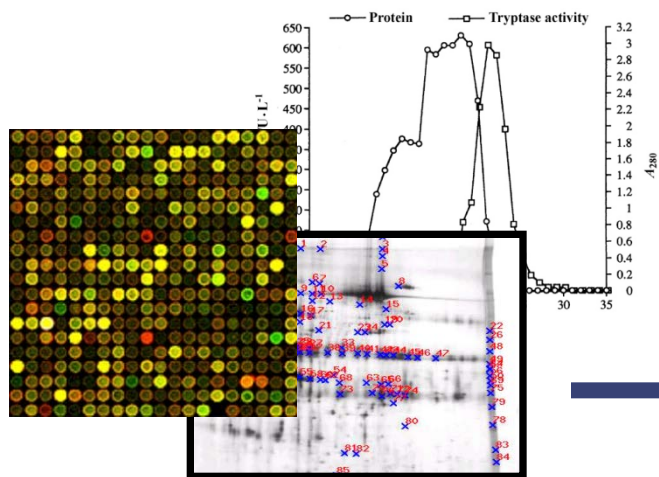
# Access to Biochemical Reaction Kinetics Data

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**Scientific Databases and Visualization Group  
Heidelberg Institute for Theoretical Studies  
HITS gGmbH, Germany**



COMBINE 2011, Heidelberg, Sept 3-7, 2011



Experimental Data

Calculations

$$[G\alpha]' = k_1 + (k_2[G\alpha]) - k_3 \frac{[G\alpha][PLC]}{([G\alpha] + K_4)} - k_5 \frac{[G\alpha][Ca_{cyt}]}{([G\alpha] + K_6)}$$

$$[PLC]' = k_7[G\alpha] - k_8 \frac{[PLC]}{([PLC] + K_9)}$$

$$[Ca_{cyt}]' = (Ca_{ER} - Ca_{cyt}) * \frac{k_{10} * Ca_{cyt} * PLC^4}{PLC^4 + K_{11}^4} + k_{12} * PLC + k_{13} * [G\alpha]$$

$$- k_{14} \frac{[Ca_{cyt}]}{([Ca_{cyt}] + K_{15})} - k_{16} \frac{[Ca_{cyt}]}{([Ca_{cyt}] + K_{17})} - k_{18} \frac{[Ca_{cyt}]^n}{([Ca_{cyt}]^n + K_{19}^n)}$$

$$+ (Ca_{mit} - Ca_{cyt}) * k_{20} \frac{[Ca_{cyt}]}{([Ca_{cyt}] + K_{21})}$$

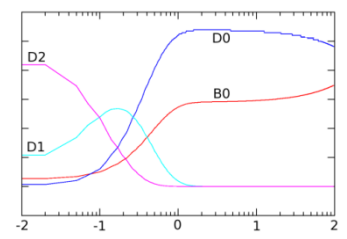
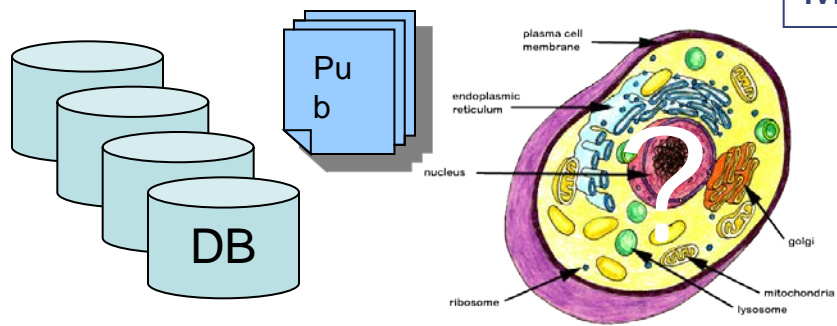
$$[Ca_{ER}]' = -(Ca_{ER} - Ca_{cyt}) * \frac{k_{10} * Ca_{cyt} * PLC^4}{PLC^4 + K_{11}^4} + k_{16} \frac{[Ca_{cyt}]}{([Ca_{cyt}] + K_{17})}$$

$$[Ca_{Mito}]' = k_{18} \frac{[Ca_{cyt}]^n}{([Ca_{cyt}]^n + K_{19}^n)} - (Ca_{mit} - Ca_{cyt}) * k_{20} \frac{[Ca_{cyt}]}{([Ca_{cyt}] + K_{21})}$$

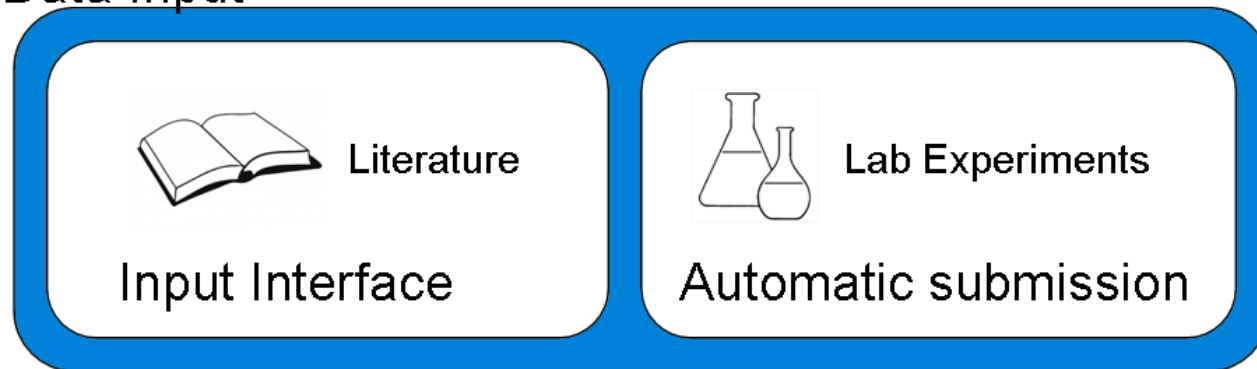
Model

Simulation

Prediction



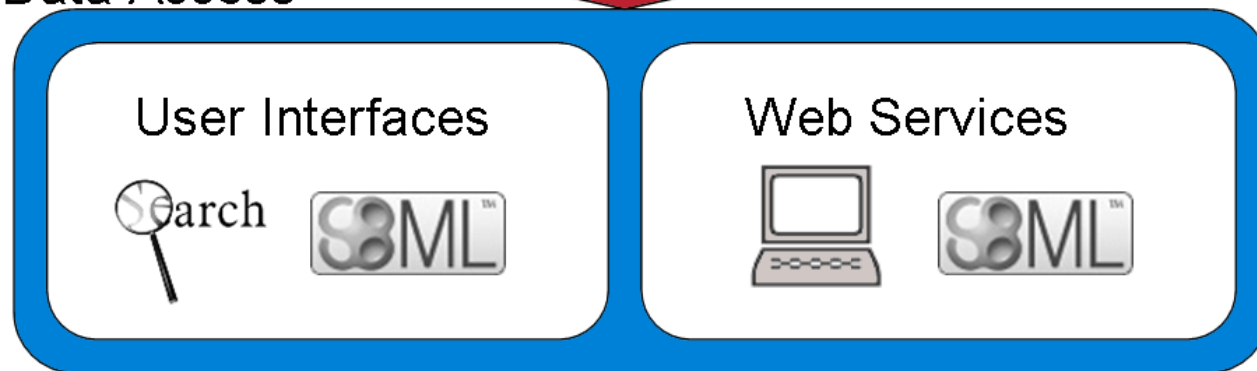
## Data Input

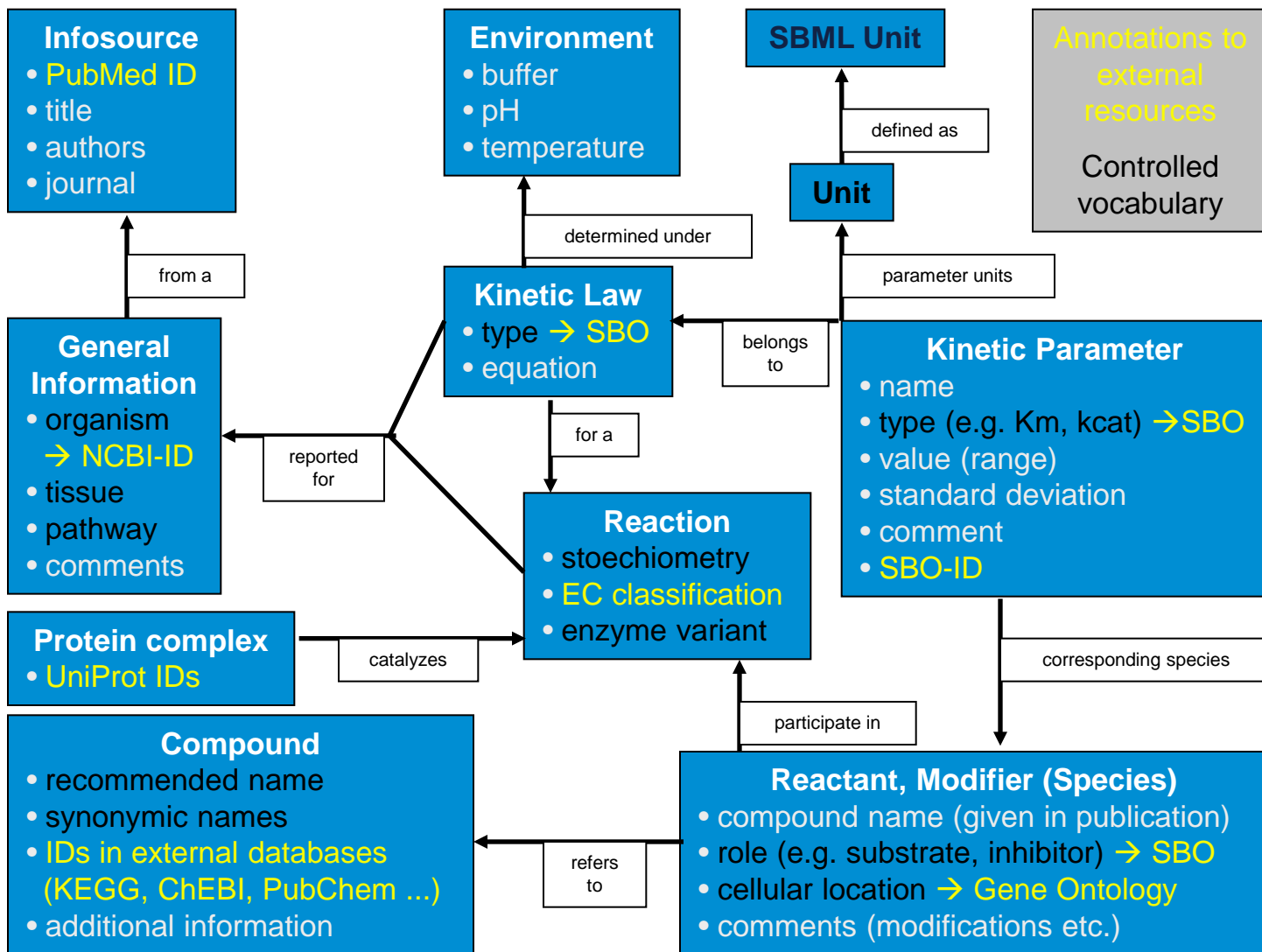


## Curation / Annotation



## Data Access






# SABIO-RK News


- **SABIO-RK: New user interface**, including new search features (e.g. Inhibitors/activators/cofactors as ligands)
- **Ontology/Taxonomy based search**, e.g. for organism (NCBI taxonomy) or tissue (Brenda tissue ontology)
- **New (RESTful) Web Services** for programmatic access to SABIO-RK (currently implemented by platforms like JWS online or Virtual Cell)
- **Access restriction** for sensitive data
- **Extended information** in exported SBML

# New user interface

Hi anonymousUser! [Log Out](#)

Heidelberg Institute for Theoretical Studies 

HOME | CONTACT | HELP | IMPRINT | ADMINISTRATION | LOGIN

Using  

Within Current Result?

[Send Selected Entries to SBML File](#)

Rows/page: 15

Criteria:

- Reaction
- Reaction Participant
  - Any Role
  - Participant Role
    - Substrate
    - Product
    - Inhibitor
    - Catalyst
    - Cofactor
    - Activator
    - Other Modifier
- Tissue
- Organism
- Publication
- Parameter
- Cellular Location
- Pathway
- Signalling
- Kinetic Mechanism
- Type
- Entry Date

Reaction	Enzyme		Tissue	Organism	Parameters (besides concentration)	Environment	
	Protein	Enzyme Variant (w)ldtype (m)mutant				°C	pH
Glycine + Cholesteryl-CoA = Coenzyme A + Glycocholate	<a href="#">2.3.1.65</a>	<a href="#">Q14032</a>	liver	Homo sapiens	Vmax Km	37	8.4
Glycine + Cholesteryl-CoA = Coenzyme A + Glycocholate	<a href="#">2.3.1.65</a>	<a href="#">Q63276</a>	liver	Rattus norvegicus	Vmax Km	30	7.2
Glycine + Cholesteryl-CoA = Coenzyme A + Glycocholate	<a href="#">2.3.1.65</a>	<a href="#">Q14032</a>	liver	Homo sapiens	Vmax Km	37	7
Glycine + Cholesteryl-CoA = Coenzyme A + Glycocholate	<a href="#">2.3.1.65</a>	<a href="#">Q14032</a>	liver	Homo sapiens	Vmax Km	37	8.25
Glycine + Cholesteryl-CoA = Coenzyme A + Glycocholate	<a href="#">2.3.1.65</a>	<a href="#">Q14032</a>	liver	Homo sapiens	Vmax Km	37	8.25
Glycine + Cholesteryl-CoA = Coenzyme A + Glycocholate	<a href="#">2.3.1.65</a>	<a href="#">Q14032</a>	liver	Homo sapiens	Vmax Km	37	8
Glycine + Cholesteryl-CoA = Coenzyme A + Glycocholate	<a href="#">2.3.1.65</a>	<a href="#">Q14032</a>	liver	Homo sapiens	Vmax Km	37	8
Glycine + Cholesteryl-CoA = Coenzyme A + Glycocholate	<a href="#">2.3.1.65</a>		liver	Bos taurus	Km KI	30	8

Pages: [1]

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Nature Precedings : doi:10.1038/npre.2011.16506.1 Posted 7 October 2011

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Pages:[1]

 There are **9 Kinetic Law Entries**

	Reaction	Enzyme			Tissue	Organism
		ECNumber	Protein	Enzyme Variant (w)ildtype (m)utant		
<input checked="" type="checkbox"/>	Glycine + Choloyl-CoA = Coenzyme A + Glycocholate	<a href="#">2.3.1.65</a>	<a href="#">Q14032</a>	wildtype (w)	liver	Homo sapiens

Entry ID: 37536

General information	
Organism	<a href="#">Homo sapiens</a>
Tissue	liver
EC Class	<a href="#">2.3.1.65</a>
SABIO reaction id	3479
Variant	wildtype

Substrates		
name	location	comment
<a href="#">Glycine</a>	<a href="#">cytosol</a>	-
<a href="#">Choloyl-CoA</a>	<a href="#">cytosol</a>	-

Products		
name	location	comment
<a href="#">Coenzyme A</a>	<a href="#">cytosol</a>	-
<a href="#">Glycocholate</a>	<a href="#">cytosol</a>	-

Modifiers				
name	location	effect	comment	protein complex
Glycine N-choloyltransferase(Enzyme)	<a href="#">cytosol</a>	Modifier-Catalyst	-	<a href="#">Q14032</a> ;

Enzyme (protein data)				
	UniProt-ID	name	mol. weight (kDa)	deviation (kDa)
subunit	<a href="#">Q14032</a>	-	-	-
complex	-	-	50.0	2.0

Kinetic Law	
type	formula
Michaelis-Menten	$V_{max} \cdot A / (K_m + A)$

Parameter							
name	type	species	start val.	end val.	deviat.	unit	comment
A	concentration	Glycine	0.25	10.0	-	mM	-
B	concentration	Choloyl-CoA	1.15	-	-	mM	saturation
Vmax	Vmax	-	0.77	-	-	$\mu\text{mol}/(\text{min} \cdot \text{mg})$	purified enzyme
Km	Km	Glycine	5.8	-	-	mM	-

Experimental conditions			
	start value	end value	unit
pH	8.4	-	-
temperature	37.0	-	$^{\circ}\text{C}$
buffer	100 mM Potassium phosphate		

General comment

<input checked="" type="checkbox"/>	Glycine + Choloyl-CoA = Coenzyme A + Glycocholate	<a href="#">2.3.1.65</a>	<a href="#">Q63276</a>	wildtype (w)	liver	Rattus norvegicus
<input checked="" type="checkbox"/>	Glycine + Choloyl-CoA = Coenzyme A + Glycocholate	<a href="#">2.3.1.65</a>	<a href="#">Q14032</a>	wildtype (w)	liver	Homo sapiens

 Your Current Criteria:  
 Reactants  
 Product  
 Glycocholate X  
 Enzymes  
 EC Numbers  
 2.3.1.65 X  
 Issues  
 liver (BTO) X  
 Nature Precedings: doi:10.1038/npre.2011.6506.1 : Posted 7 Oct 2011

RESET



Please Select Attribute

Within Current Result?

Using



Rows/page:

2

[Send Selected Entries to SBML File](#)

Other

Reaction View

Entry View

doi:10.1038/npre.2011.6506.1 : Posted 7 Oct 2011

Select 1 entries

Pages:[1]

There are 7 Kinetic Law Entries

	Reaction	Enzyme			Tissue	Organism	Parameters (besides concentration)	Environment		
		ECNumber	Protein	Enzyme Variant (w)ildtype (m)utant				°C	pH	
<input type="checkbox"/>	Glycine + Choloyl-CoA = Coenzyme A + Glycocholate	<a href="#">2.3.1.65</a>	<a href="#">Q14032</a>	wildtype (w)	liver	Homo sapiens	Vmax Km	37	8.4	<input type="checkbox"/>
<input type="checkbox"/>	Glycine + Choloyl-CoA = Coenzyme A + Glycocholate	<a href="#">2.3.1.65</a>	<a href="#">Q14032</a>	wildtype (w)	liver	Homo sapiens	Vmax Km	37	7	<input type="checkbox"/>
<input type="checkbox"/>	Glycine + Choloyl-CoA = Coenzyme A + Glycocholate	<a href="#">2.3.1.65</a>	<a href="#">Q14032</a>	wildtype (w)	liver	Homo sapiens	Vmax Km	37	7	<input type="checkbox"/>
<input type="checkbox"/>	Glycine + Choloyl-CoA = Coenzyme A + Glycocholate	<a href="#">2.3.1.65</a>	<a href="#">Q14032</a>	C235S (m) mutant (m)	liver	Homo sapiens	Vmax Km	37	8.25	<input type="checkbox"/>
<input type="checkbox"/>	Glycine + Choloyl-CoA = Coenzyme A + Glycocholate	<a href="#">2.3.1.65</a>	<a href="#">Q14032</a>	wildtype (w)	liver	Homo sapiens	Vmax Km	37	8.25	<input type="checkbox"/>
<input type="checkbox"/>	Glycine + Choloyl-CoA = Coenzyme A + Glycocholate	<a href="#">2.3.1.65</a>	<a href="#">Q14032</a>	wildtype (w)	liver	Homo sapiens	Vmax Km	37	8	<input type="checkbox"/>
<input checked="" type="checkbox"/>	Glycine + Choloyl-CoA = Coenzyme A + Glycocholate	<a href="#">2.3.1.65</a>	<a href="#">Q14032</a>	wildtype (w)	liver	Homo sapiens	Vmax Km	37	8	<input checked="" type="checkbox"/>

1



# SABIO-RK SBML Export

Nature Precedings : doi:10.1038/npre.2011.6506.1 : Posted 7 Oct 2011

Substrates							
name	location	comment					
<a href="#">Glycine</a>	<a href="#">cytosol</a>	-					
<a href="#">Choloyl-CoA</a>	<a href="#">cytosol</a>	-					
Products							
name	location	comment					
<a href="#">Coenzyme A</a>	<a href="#">cytosol</a>	-					
<a href="#">Glycocholate</a>	<a href="#">cytosol</a>	-					
Modifiers							
name	location	effect	comment	protein complex			
Glycine N-choloyltransferase(Enzyme)	<a href="#">cytosol</a>	Modifier-Catalyst	-	<a href="#">Q14032</a> ;			
Enzyme (protein data)							
	UniProt-ID	name	mol. weight (kDa)		deviation (kDa)		
subunit	Q14032	-			-		
complex	-	-			50.0		
Kinetic Law							
type				formula			
Michaelis-Menten				$V_{max} * B / (K_m + B)$			
Parameter							
name	type	species	start val.	end val.	deviat.	unit	comment
B	concentration	Glycine	0.0	20.0	-	mM	-
Km	Km	Glycine	0.02	-	-	M	-
A	concentration	Choloyl-CoA	200.0	300.0	-	$\mu$ M	-
Vmax	Vmax	-	15.3	-	-	nmol/(min*mg)	cytosolic protein
E	concentration	Enzyme	0.2	-	-	mg/ml	-
Experimental conditions							
	start value	end value	unit				
temperature		37.0	- °C				
pH		8.0	-				
buffer	50 mM potassium phosphate						
comment	-						
Reference							
title	author	year	journal	volume	pages	PubMed	
Subcellular organization of bile acid amidation in human liver: a key issue in regulating the biosynthesis of bile salts	Solaas K, Ulvestad A, Soreide O, Kase BF	2000	J Lipid Res	41	1154-62	<a href="#">10884298</a>	

Pages:[1]



2

Send Selected Entries to SBML File

Nature Precedings : doi:10.1038/npre.2011.6506.1.1 Posted 7 Oct 2011

Search

3

Search criteria:

Reactant:

Pathway:

[Glycolysis classical](#)

Enzyme:

Publication:

Protein:

Sign. modific.:

Sign. event:

Organism:

[Homo sapiens](#)

Tissue:

[liver](#)

Cell. loc.:

Exp. cond.:

Kin. data:

[Save Model](#)

Enter name of model:

▾

Export parameters normalized to SI base units

[Save Model on Disk as SBML](#)

[Back to Results](#)



[Sample File](#)

# SABIO-RK SBML Export

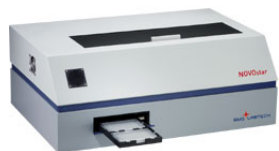
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      <body xmlns="http://www.w3.org/1999/xhtml">
        <p>
          This model has been created with the help of the SABIO-RK Database
          (http://sabiork.h-its.org/)
          (c) 2005-2010 HITS gGmbH http://www.h-its.org
        </p><br/>
        To cite SABIO-RK Database, please use
        "http://www.ncbi.nlm.nih.gov/pubmed/17822389"
        <br/>
        Wittig U., Golebiewski M., Kania R., Krebs O., Mir S., Weidemann A., Anstein S., Sar...
        Lecture Notes in Computer Science, 4075: 94-103.
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    </notes>
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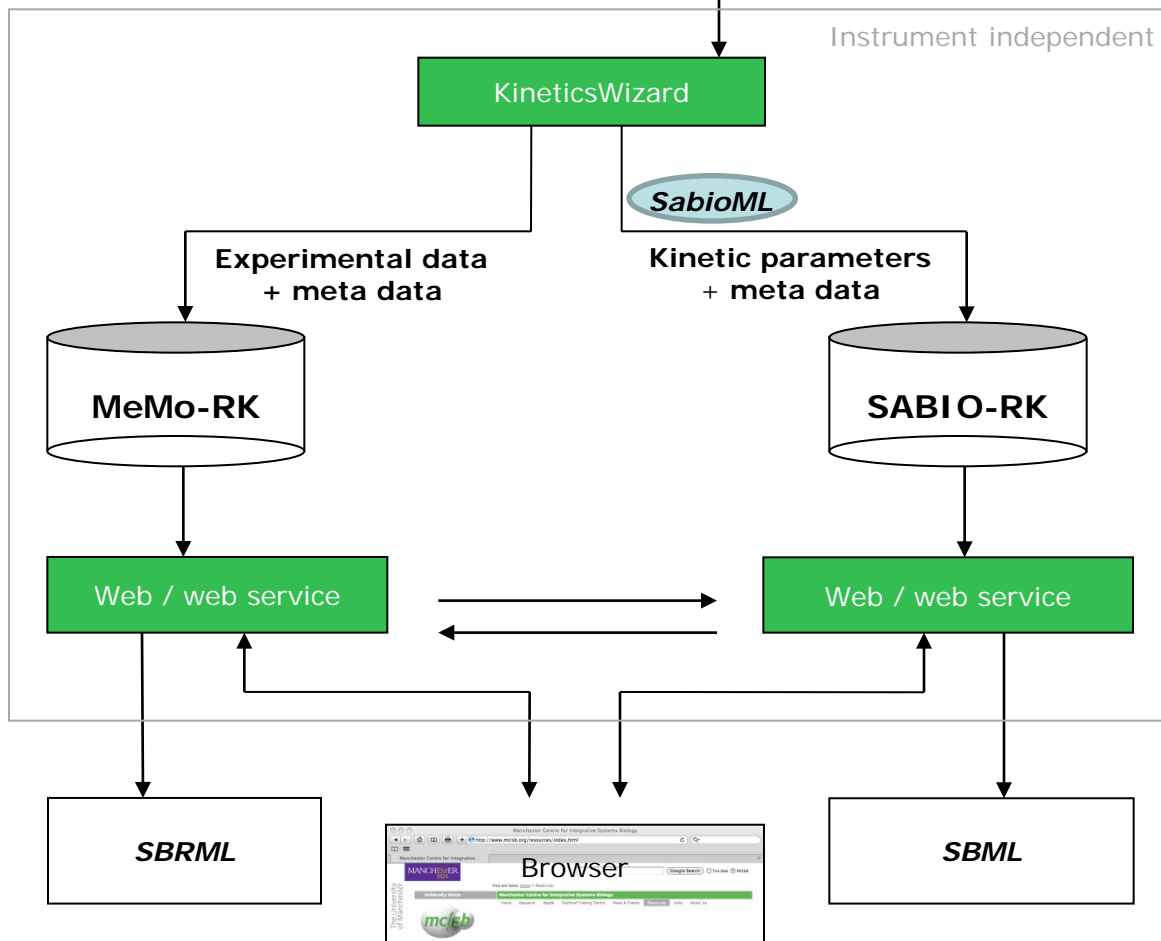
- Currently up to **SBML Level 2 Version 4**
- **Reaction Kinetics Warehouse:**  
Reactions, kinetic equations and parameters (with corresponding units) from different database entries can be exported in one SBML file
- Data is annotated (RDF and SBOterms) according to **MIRIAM**
- Annotations include **SABIO-RK Ids** (reaction and kineticlaw) for tracking
- Optional **normalization of kinetic parameters** to SI base units
- Model can also be exported as human readable PDF → **SBML2LaTeX**



Spreadsheet  
(data and metadata)

NOVOstar data parser

Java data model





## Enzyme kinetics informatics: from instrument to browser

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Issue



FEBS Journal

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 3769–3779, September 2010

### SEARCH

In this issue

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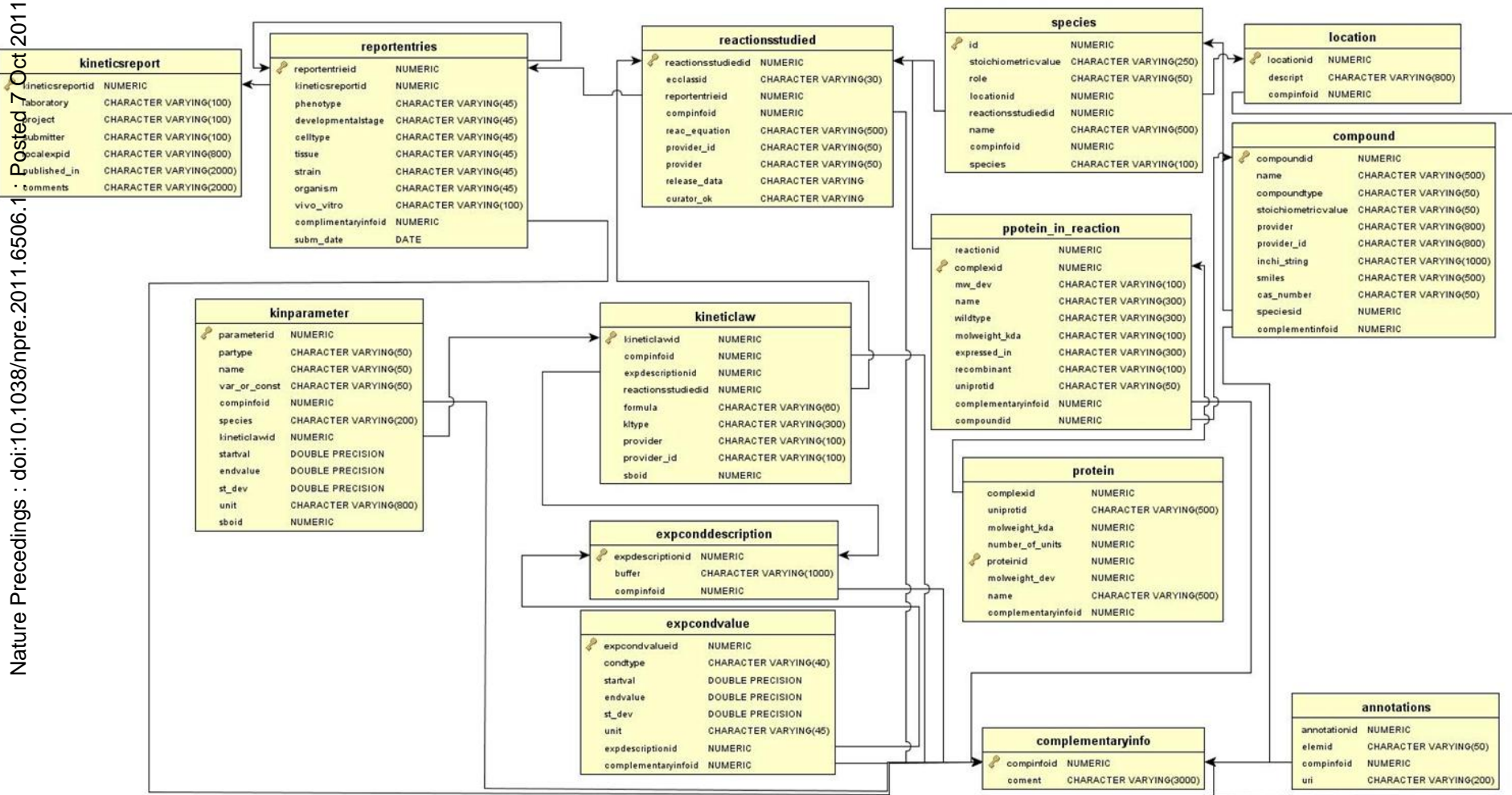
\*Correspondence: N. Swainston, Manchester Centre for Integrative Systems Biology, University of Manchester, Manchester M1 7DN, UK Fax: +44 161 306 8918 Tel:  +44 161 306 5146  E-mail: [neil.swainston@manchester.ac.uk](mailto:neil.swainston@manchester.ac.uk) Website: <http://www.mcisb.org>

†\*

These authors contributed equally to this work

# SabioML: Exchange Format for Experimental Kinetic Data

Nature Precedings : doi:10.1038/npre.2011.6506.1 Posted 7 Oct 2011



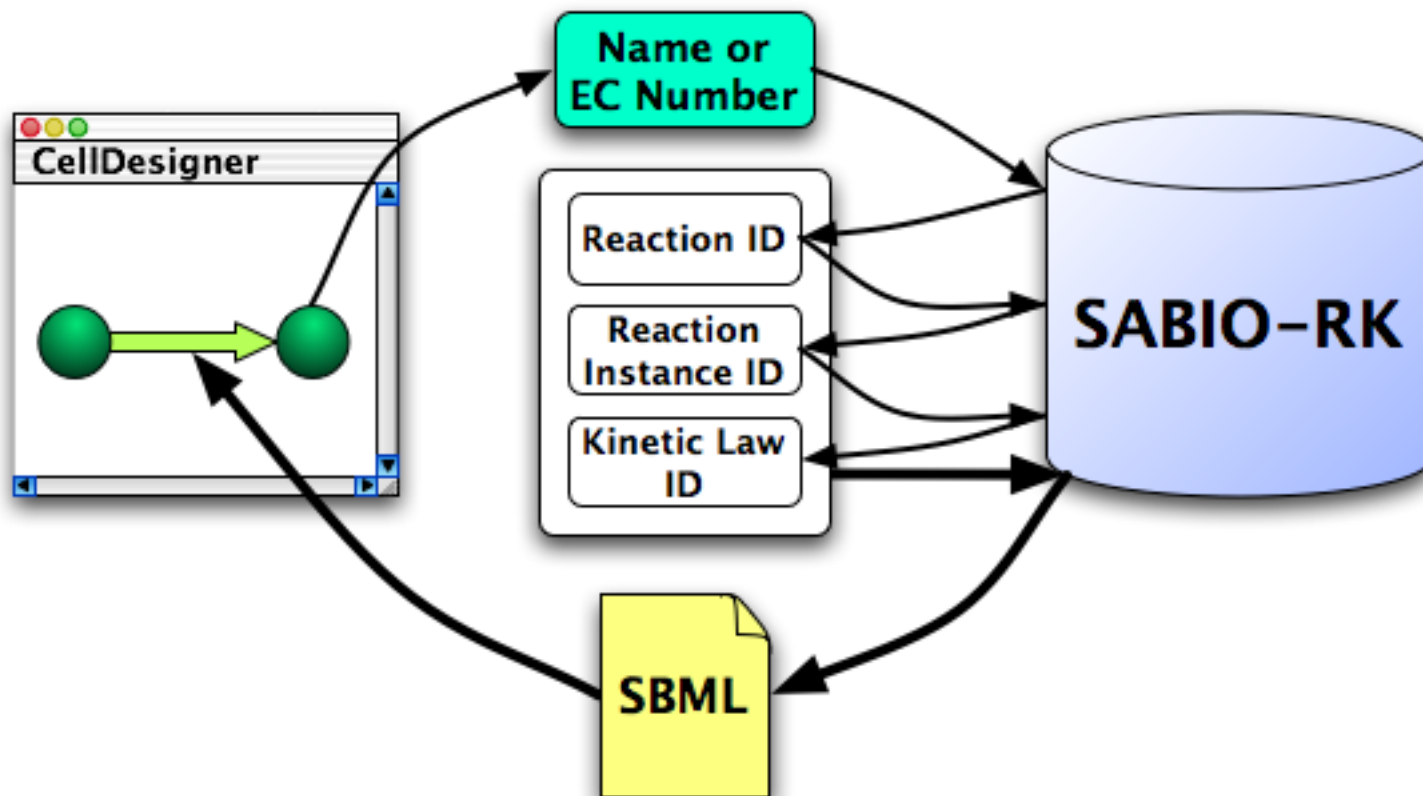
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  5,7H2,1-3H3,(H4-,15,16,17,20,21,22,23,24)/p+1/fC14H23N4O8P2S/h20-21,23H,15H2/q+1">
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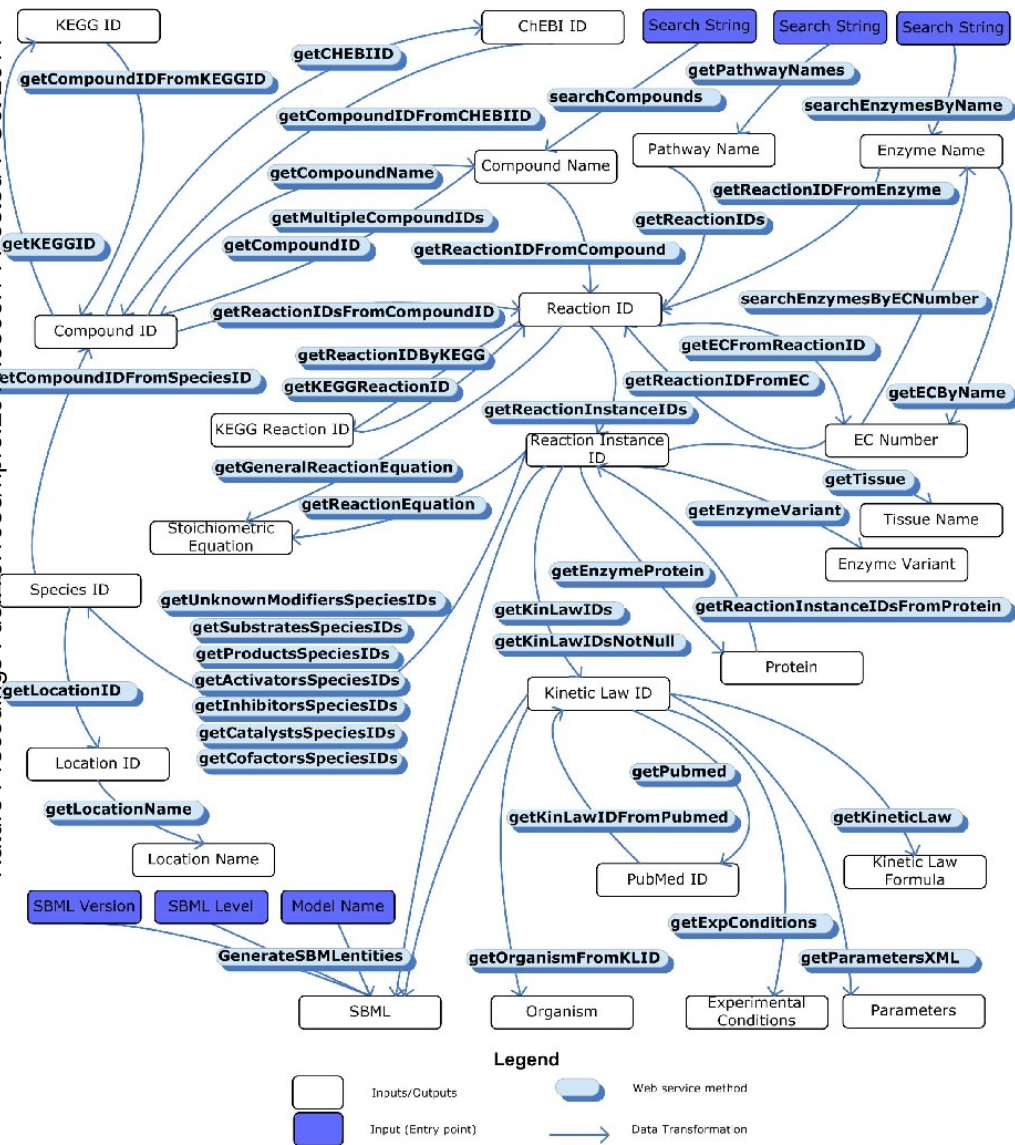


# SABIO-RK API Access Integration into Modeling Platforms

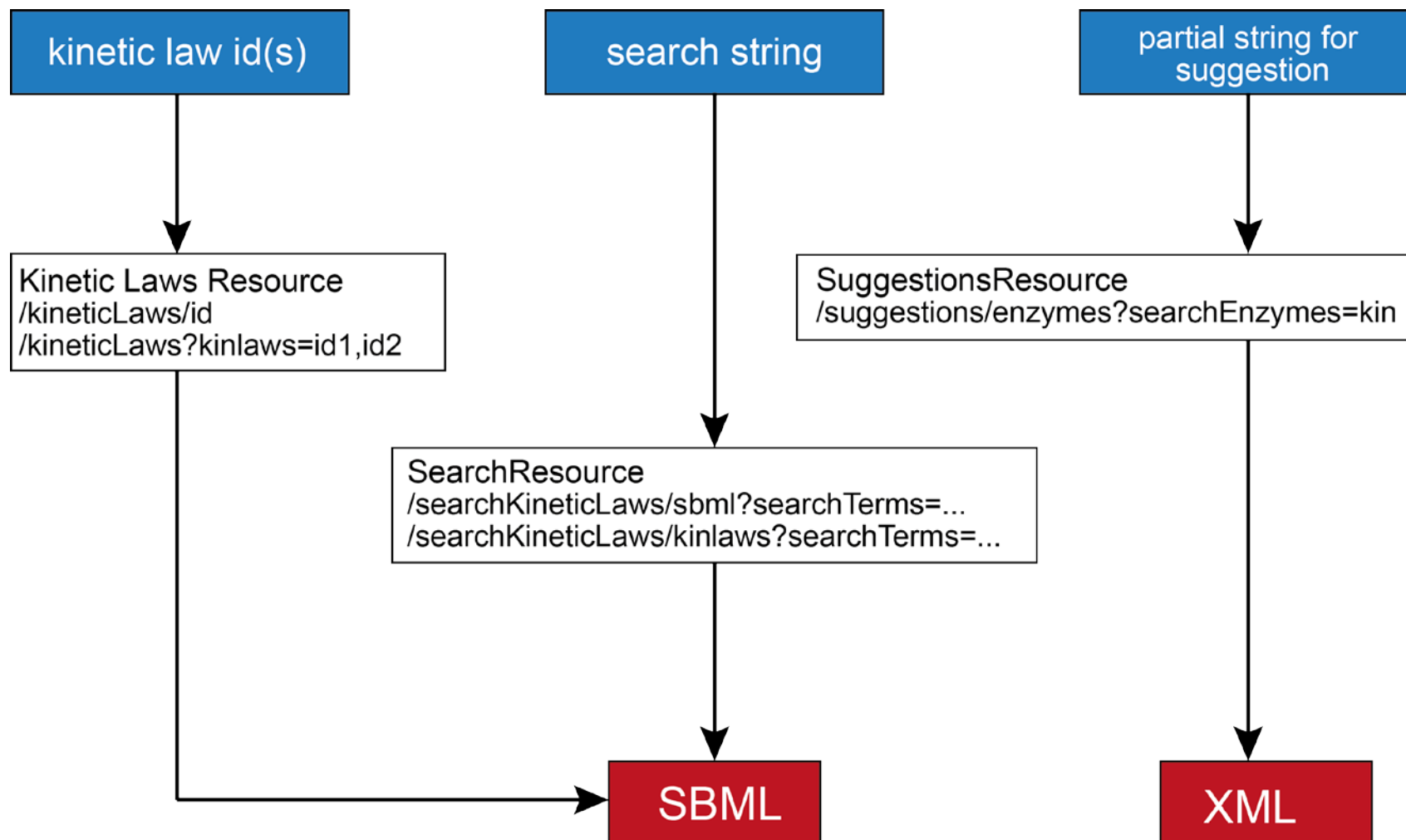


<http://www.celldesigner.org>

Nature Precedings : doi:10.1038/npre.2011.6506.1 : Posted 7 Oct 2011



- JAW-WS based
- Integration possible in modeling platforms or simulation tools (e.g. CellDesigner)
- Cross-linking with other databases (e.g. ChEBI)
- Data export in **SBML** supported



## Example requests:

Entries may be requested directly if the database entry ID is known

<http://sabio.h-its.org/sabioRestWebServices/kineticLaws/20147>

Entries may be searched for using the same search options available in the browser search interface

<http://sabio.h-its.org/sabioRestWebServices/searchKineticLaws/sbml?searchTerms=ORGANISM=Homo sapiens;TISSUE=liver>


Suggestions for search terms can be done

<http://sabio.h-its.org/sabioRestWebServices/suggestions/compounds?searchCompounds=glycoch>

Browser address bar: <http://sycamore.eml.org/sycamore/submission.jsp>

Navigation: Deaktivieren, Cookies, Keine CSS-Fehler, Formulare, Grafiken, Informationen, Verschiedenes, Hervorheben, Größer, Extras, Quelle

Page Title: SYCAMORE HITS gGmbH



**SYCAMORE**

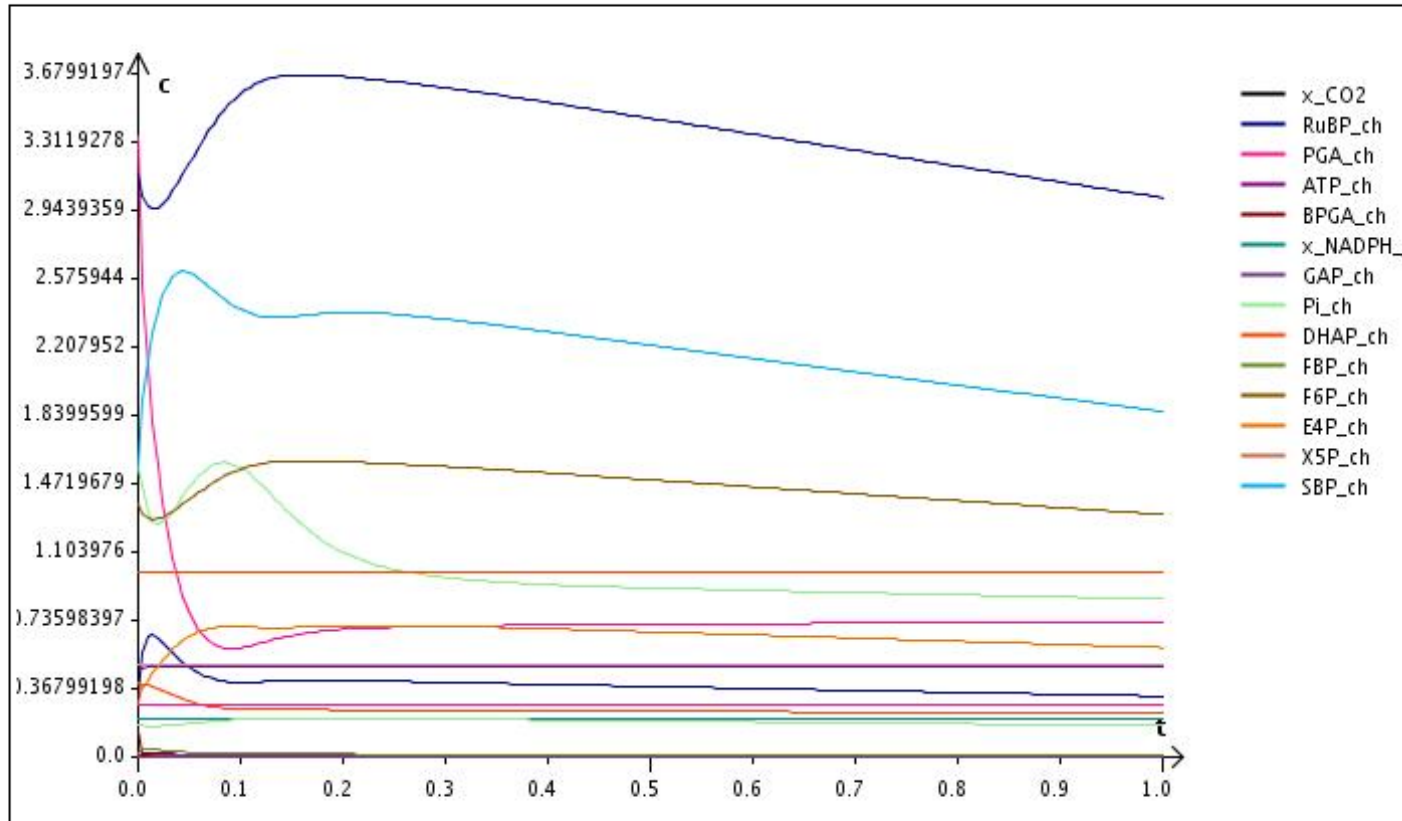
- SYCAMORE
- Home
- Startpage
- Registration
- Workflow
- User guide
- Use case

Load existing model

- Model from disk
- Model from projects
- Example models

Build new model

- SYCAMORE
  - New model
- SABIORK
  - Reaction Search



The graph displays the time course of various metabolites. RuBP\_ch (dark blue) shows the highest concentration, peaking around 3.68. x\_CO2 (black) remains near zero. Other metabolites like Pi\_ch (green) and FBP\_ch (olive) show intermediate concentrations that slightly decrease over time. The x-axis represents time (t) from 0.0 to 1.0, and the y-axis represents concentration (c).

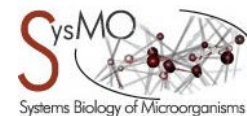
Vertical text on the left: Nature Precedings : doi:10.1038/npre.2011.6506.1 : Posted 7 Oct 2011

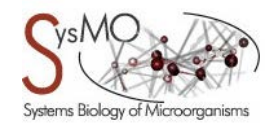
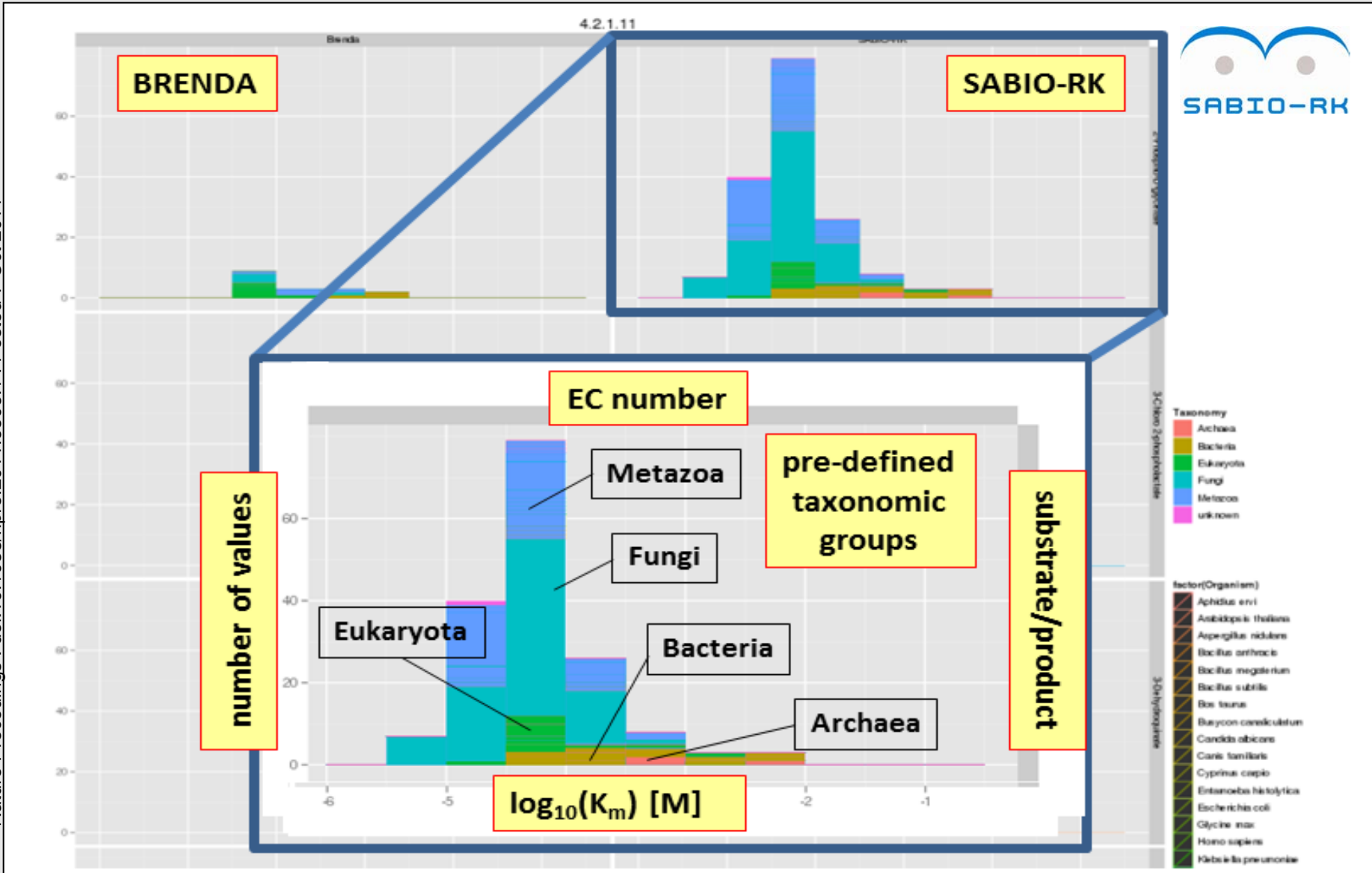


# SABIO-RK Content

Posted 7 Oct 2011  
doi:10.1098/rstb.2011.0150

<b>Organism</b>	<b>Entries (total)</b>	<b>Mutants</b>	<b>Reactions (distinct)</b>	<b>EC number (distinct)</b>	<b>Reaction rates</b>	<b>Km</b>	<b>Kinetic laws</b>
<b>Total 660</b>	<b>37343</b>	<b>10616</b>	<b>4951</b>	<b>1070</b>	<b>27305</b>	<b>29852</b>	<b>17673</b>
Homo sapiens	7028	2156	1233	348	5353	5757	3738
Rattus norvegicus	4286	759	821	285	2723	3188	2178
Escherichia coli	3828	1912	577	188	2976	3155	1988
Saccharomyces cerevisiae	1518	451	220	76	1044	1300	805
Bos taurus	982	59	276	86	579	722	471
Dryctolagus uniculus	849	125	180	50	450	626	322
Sus scrofa	842	295	158	68	669	434	750
Mus musculus	809	92	236	92	456	290	603
Streptococcus faecalis	538	42	155	51	320	157	478
Gallus gallus	487	167	78	35	405	521	217





Nature Precedings : doi:10.1038/npre.2011.6506.1 : Posted 7 Oct 2011







<http://sabio.h-its.org>

