SABIO-RK

Heidelberger Institut für Theoretische Studien

HITS

Access to Biochemical Reaction Kinetics Data

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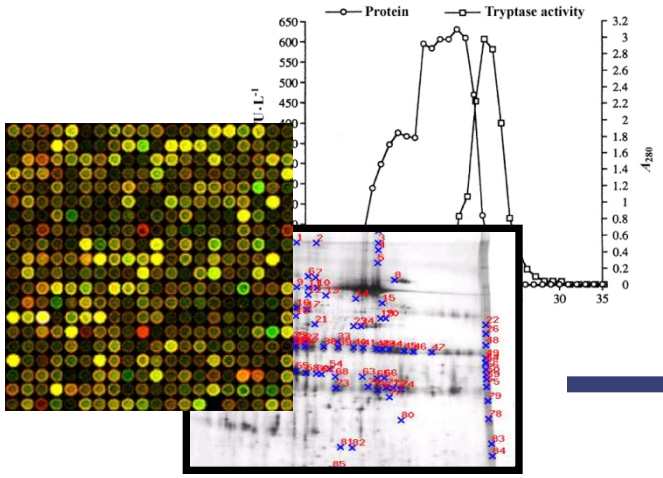
Heidelberg Institute for Theoretical Studies
HITS gGmbH, Germany

combine

COMBINE 2011, Heidelberg, Sept 3-7, 2011

Systems Biology



Experimental Data

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

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

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

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

Calculations

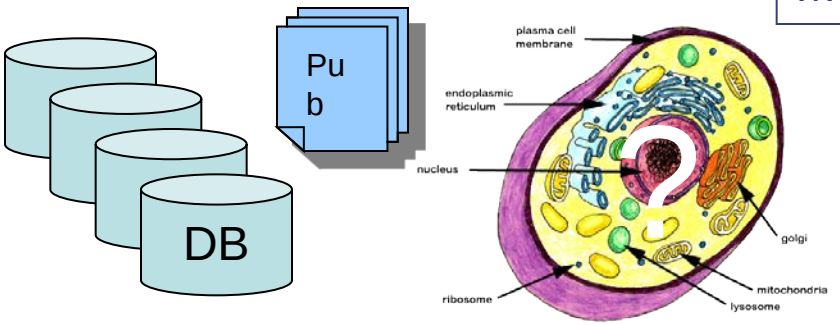
$$+ (Ca_{mit} - Ca_{cyt}) * k_{20}\frac{[Ca_{cyt}]}{([Ca_{cyt}]+K_{21})}$$

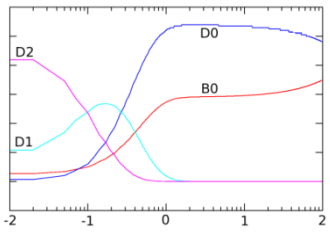
$$[Ca_{ER}]' = -(Ca_{ER} - Ca_{cyt}) * \frac{k_{10} * Ca_{cyt} * PLC^4}{PLC^4 + K_{11}^4} + k_{16}\frac{[Ca_{cyt}]}{([Ca_{cyt}]+K_{17})}$$

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

Model

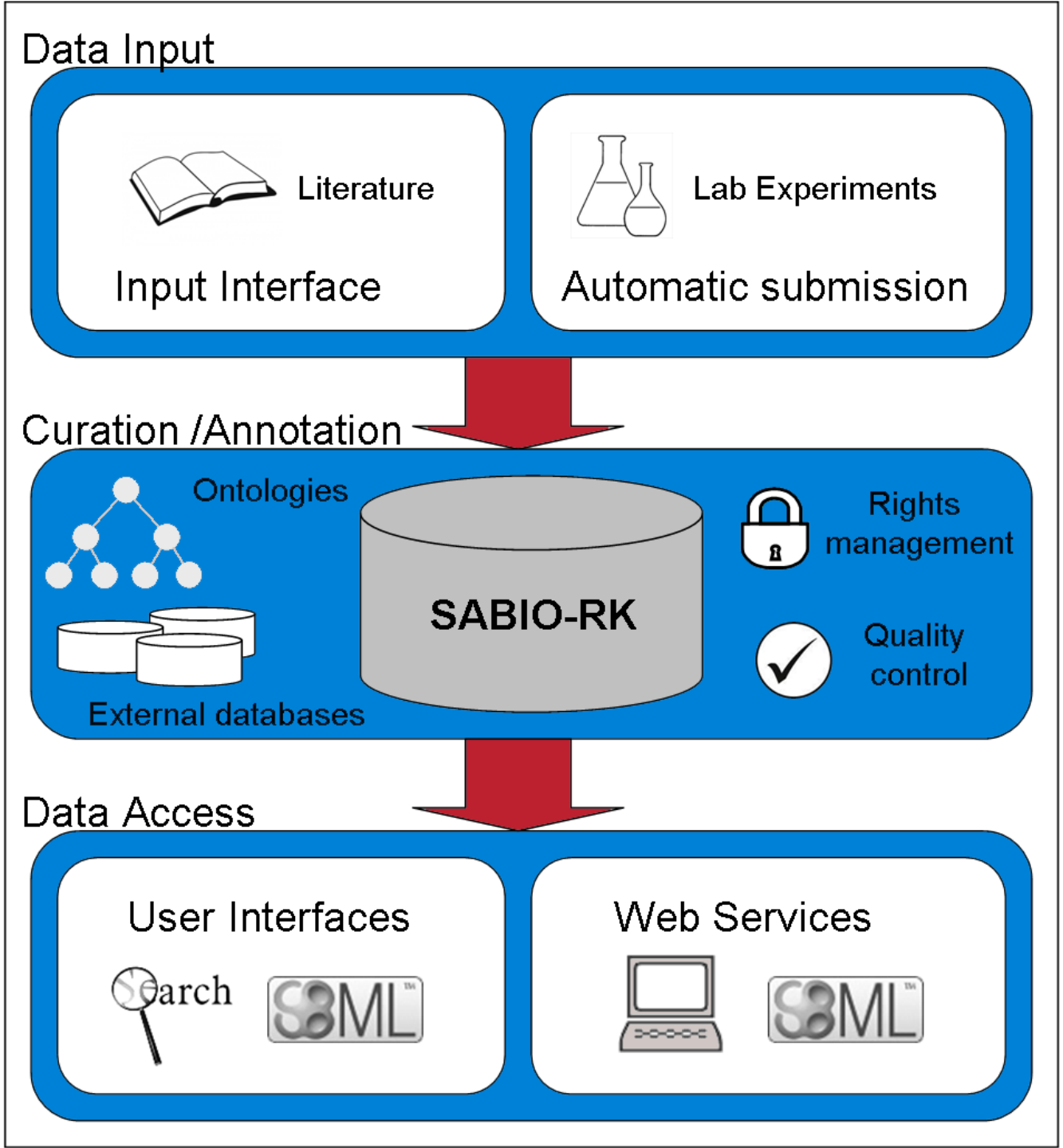
Simulation





Prediction

SABIO-RK



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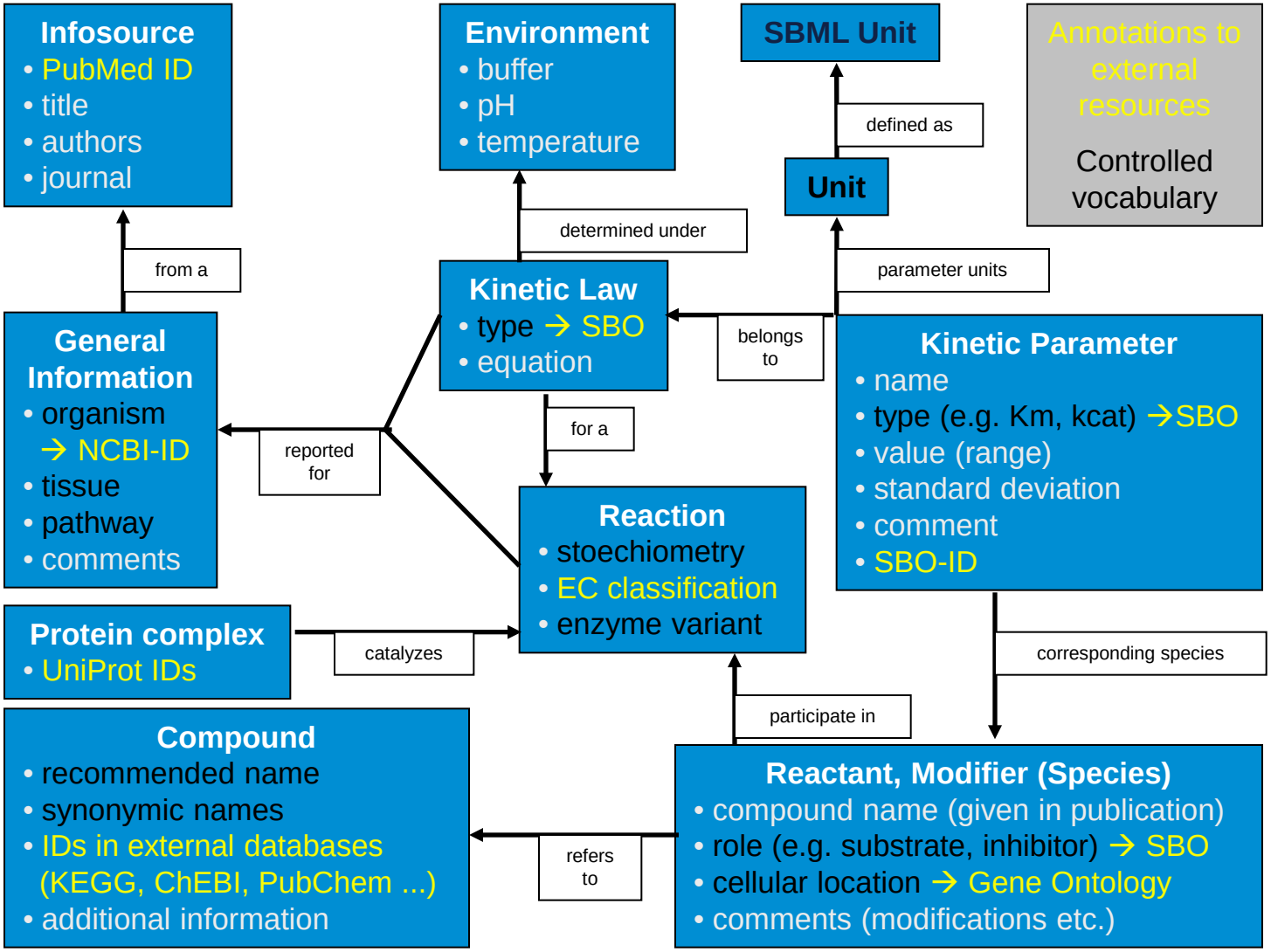
SABIO-RK Data Content



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

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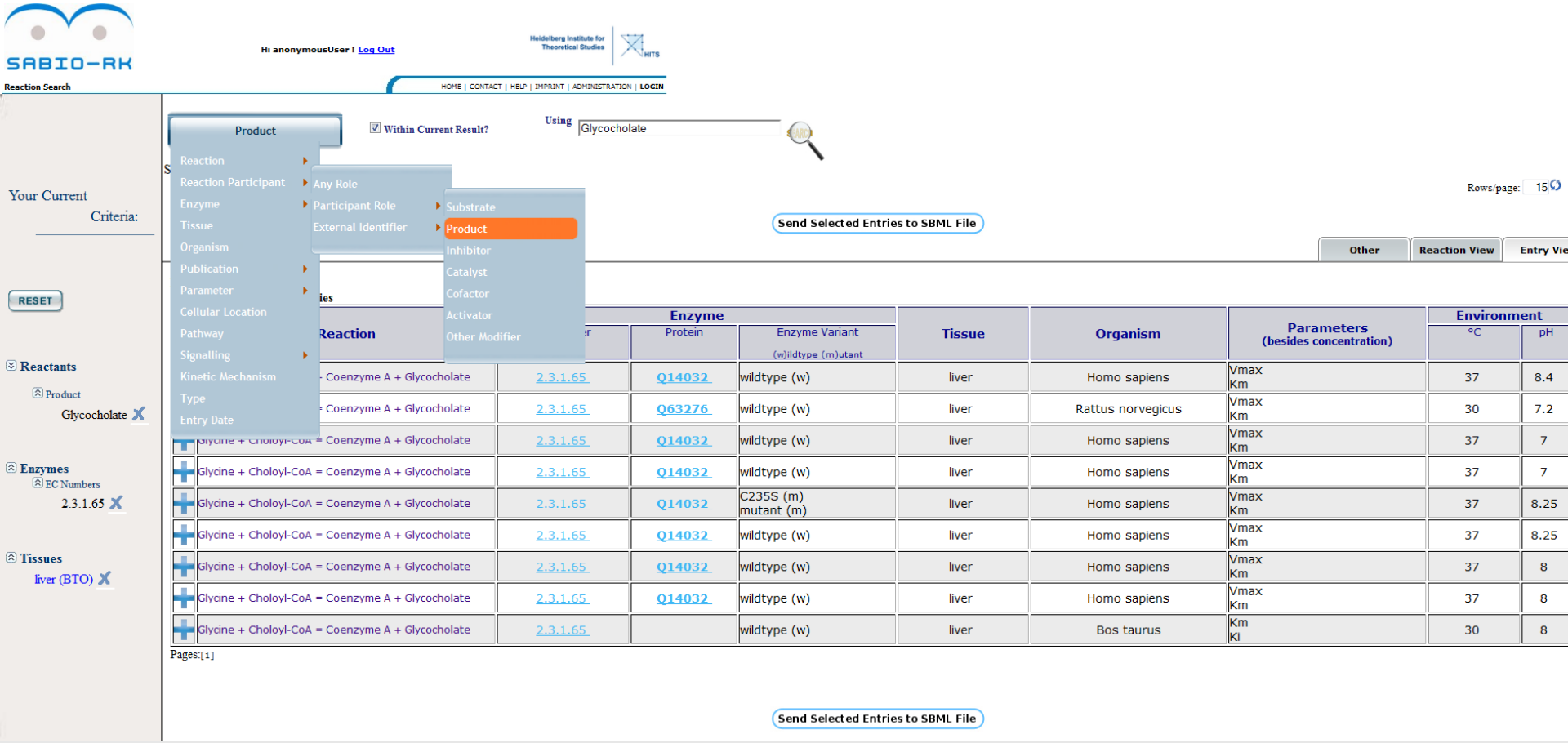
New user interface



HITS KTS DFG SysMO Systems Biology of Microorganisms virtual liver network

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Send Selected Entries to SBML File

Your Current Criteria:

RESET

Reactants
Product
Glycocholate

Enzymes
EC Numbers
2.3.1.65

Tissues
liver (BTO)

Pages:[1]

There are 9 Kinetic Law Entries

	Reaction	Enzyme			Tissue	Organism
		ECNumber	Protein	Enzyme Variant (w)ildtype (m)utant		
−	Glycine + Choloyl-CoA = Coenzyme A + Glycocholate	2.3.1.65	Q14032	wildtype (w)	liver	Homo sapiens

Entry ID: 37536

General information	
Organism	Homo sapiens
Tissue	liver
EC Class	2.3.1.65
SABIO reaction id	3479
Variant	wildtype

Substrates

name	location	comment
Glycine	cytosol	-
Choloyl-CoA	cytosol	-

Products

name	location	comment
Coenzyme A	cytosol	-
Glycocholate	cytosol	-

Modifiers

name	location	effect	comment	protein complex
Glycine N-choloyltransferase(Enzyme)	cytosol	Modifier-Catalyst	-	Q14032;

Enzyme (protein data)

	UniProt-ID	name	mol. weight (kDa)	deviation (kDa)
subunit	Q14032	-	-	-
complex	-	-	50.0	2.0

Kinetic Law

type	formula
Michaelis-Menten	Vmax*A/(Km+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	saturating
Vmax	Vmax	-	0.77	-	-	µmol/(min*mg)	purified enzyme
Km	Km	Glycine	5.8	-	-	mM	-

Experimental conditions

	start value	end value	unit
pH	8.4	-	-
temperature	37.0	-	°C
buffer	100 mM Potassium phosphate		

General comment

+	Glycine + Choloyl-CoA = Coenzyme A + Glycocholate	2.3.1.65	Q63276	wildtype (w)	liver	Rattus norvegicu
+	Glycine + Choloyl-CoA = Coenzyme A + Glycocholate	2.3.1.65	Q14032	wildtype (w)	liver	Homo sapiens

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Please Select Attribute

Within Current Result?

Using

Select: 1 entries

Rows/page: 15

2

Send Selected Entries to SBML File

Other | Reaction View | Entry View

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	
+	Glycine + Choloyl-CoA = Coenzyme A + Glycocholate	2.3.1.65	Q14032	wildtype (w)	liver	Homo sapiens	Vmax Km	37	8.4	
+	Glycine + Choloyl-CoA = Coenzyme A + Glycocholate	2.3.1.65	Q14032	wildtype (w)	liver	Homo sapiens	Vmax Km	37	7	
+	Glycine + Choloyl-CoA = Coenzyme A + Glycocholate	2.3.1.65	Q14032	wildtype (w)	liver	Homo sapiens	Vmax Km	37	7	
+	Glycine + Choloyl-CoA = Coenzyme A + Glycocholate	2.3.1.65	Q14032	C235S (m) mutant (m)	liver	Homo sapiens	Vmax Km	37	8.25	
+	Glycine + Choloyl-CoA = Coenzyme A + Glycocholate	2.3.1.65	Q14032	wildtype (w)	liver	Homo sapiens	Vmax Km	37	8.25	
+	Glycine + Choloyl-CoA = Coenzyme A + Glycocholate	2.3.1.65	Q14032	wildtype (w)	liver	Homo sapiens	Vmax Km	37	8	
−	Glycine + Choloyl-CoA = Coenzyme A + Glycocholate	2.3.1.65	Q14032	wildtype (w)	liver	Homo sapiens	Vmax Km	37	8	☑

1

SABIO-RK SBML Export

Entry ID: 20147

Substrates

name	location	comment
Glycine	cytosol	-
Choloyl-CoA	cytosol	-

Products

name	location	comment
Coenzyme A	cytosol	-
Glycocholate	cytosol	-

Modifiers

name	location	effect	comment	protein complex
Glycine N-choloyltransferase(Enzyme)	cytosol	Modifier-Catalyst	-	Q14032;

Enzyme (protein data)

	UniProt-ID	name	mol. weight (kDa)	deviation (kDa)
subunit	Q14032	-	-	-
complex	-	-	50.0	-

Kinetic Law

type	formula
Michaelis-Menten	Vmax*B/(Km+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	-	µM	-
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	10884298

Pages:[1]

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SABIO-RK

2 Send Selected Entries to SBML File

You are logged in as anonymousUser

Username: Password: remember me

Daten absenden Zurücksetzen

HOME | CONTACT | HELP | IMPRINT | View Kinetic Data

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: My first model SBML level 2, version 4

Export parameters normalized to SI base units

Save Model on Disk as SBML

Back to Results

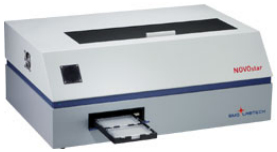
Sample File

SABIO-RK SBML Export

SBML Export

- 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**

Direct Data Submission



Spreadsheet
(data and metadata)

NOVOstar data parser

Java data model

Instrument independent

KineticsWizard

SabioML

Experimental data + meta data

Kinetic parameters + meta data

MeMo-RK

SABIO-RK

Web / web service

Web / web service

SBRML

SBML

Direct Data Submission

the FEBS Journal

Enzyme kinetics informatics: from instrument to browser

Neil Swainston[1,†], Martin Golebiewski[2,†], Hanan L. Messiha[1], Naglis Malys[1], Renate Kania[2], Sylvestre Kengne[2], Olga Krebs[2], Saqib Mir[2], Heidrun Sauer-Danzwith[2], Kieran Smallbone[1], Andreas Weidemann[2], Ulrike Wittig[2], Douglas B. Kell[1], Pedro Mendes[1,3], Wolfgang Müller[2], Norman W. Paton[1], Isabel Rojas[2]

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Issue

FEBS Journal

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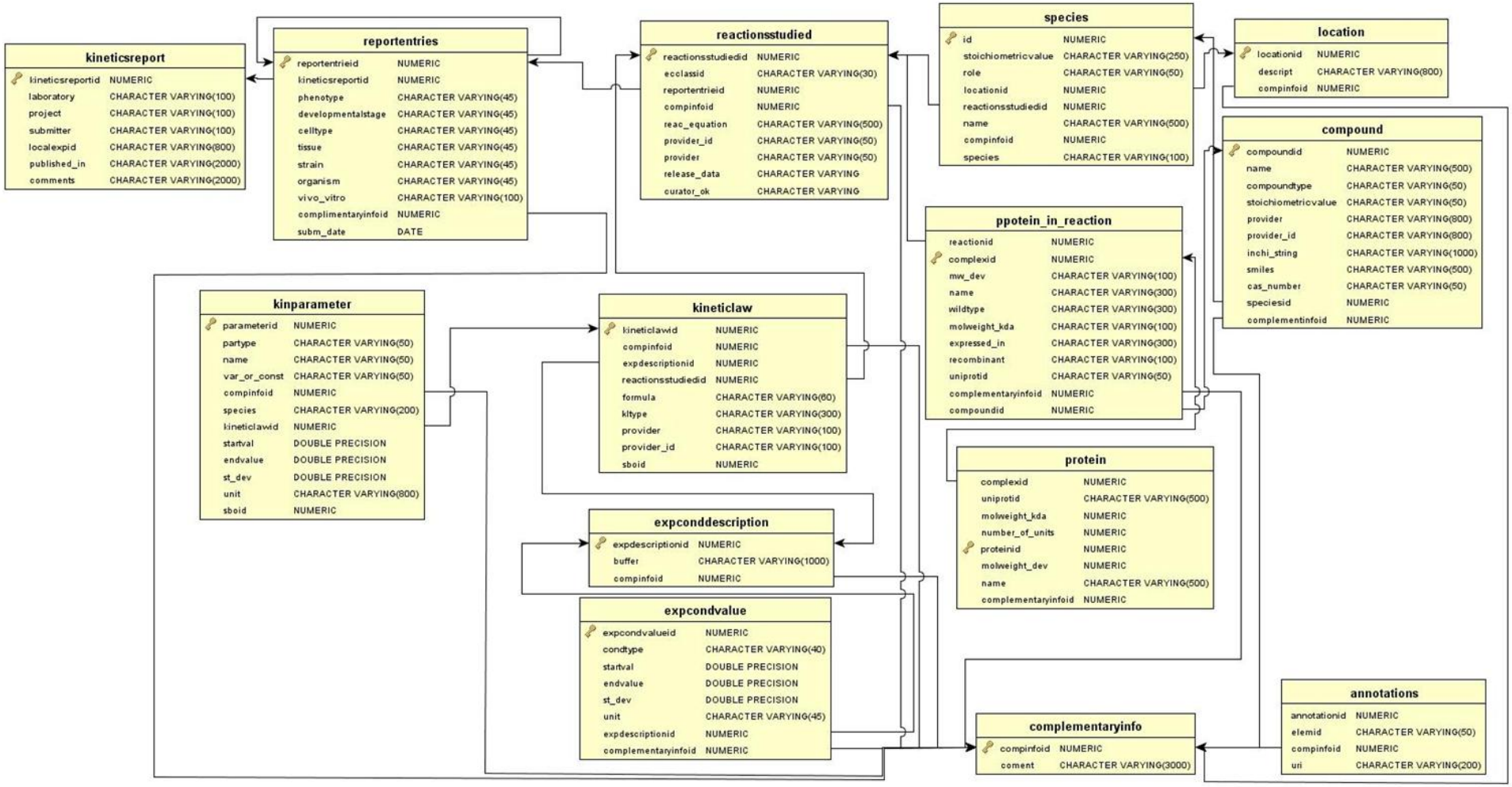
†* These authors contributed equally to this work

SabioML: Exchange Format for Experimental Kinetic Data



SabioML: Exchange Format for Experimental Kinetic Data

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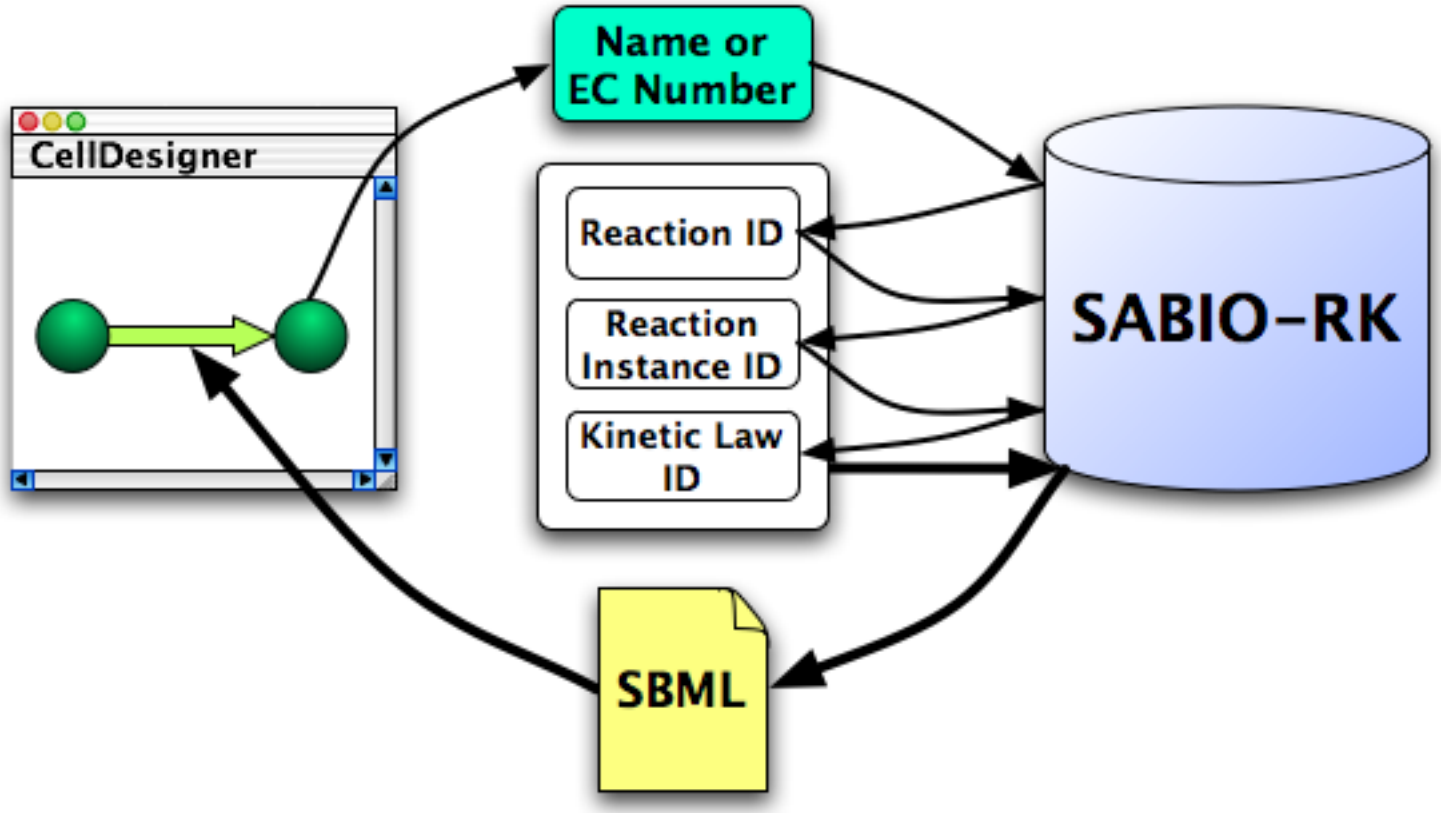
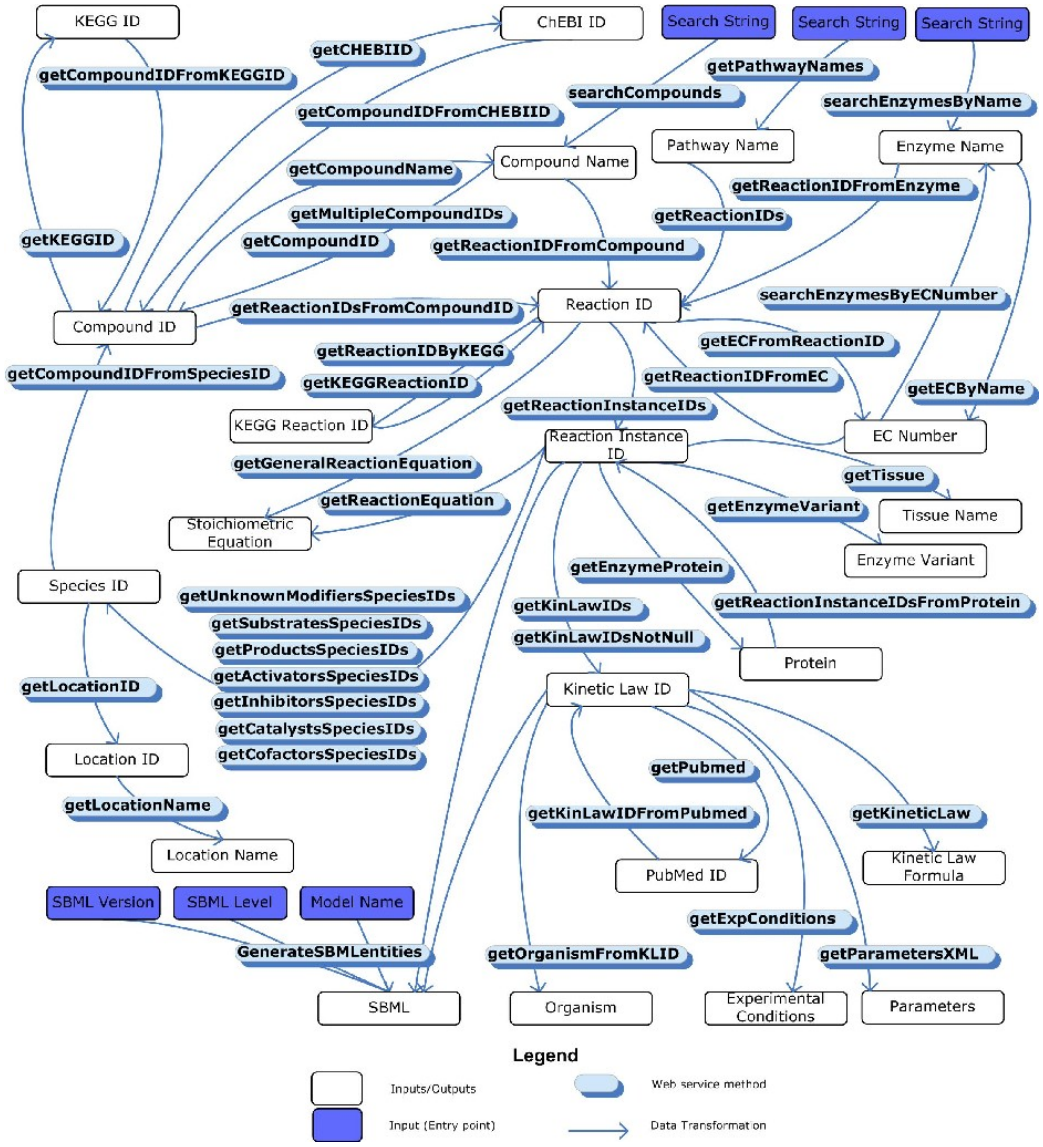
SABIO-RK API Access
Integration into Modeling Platforms



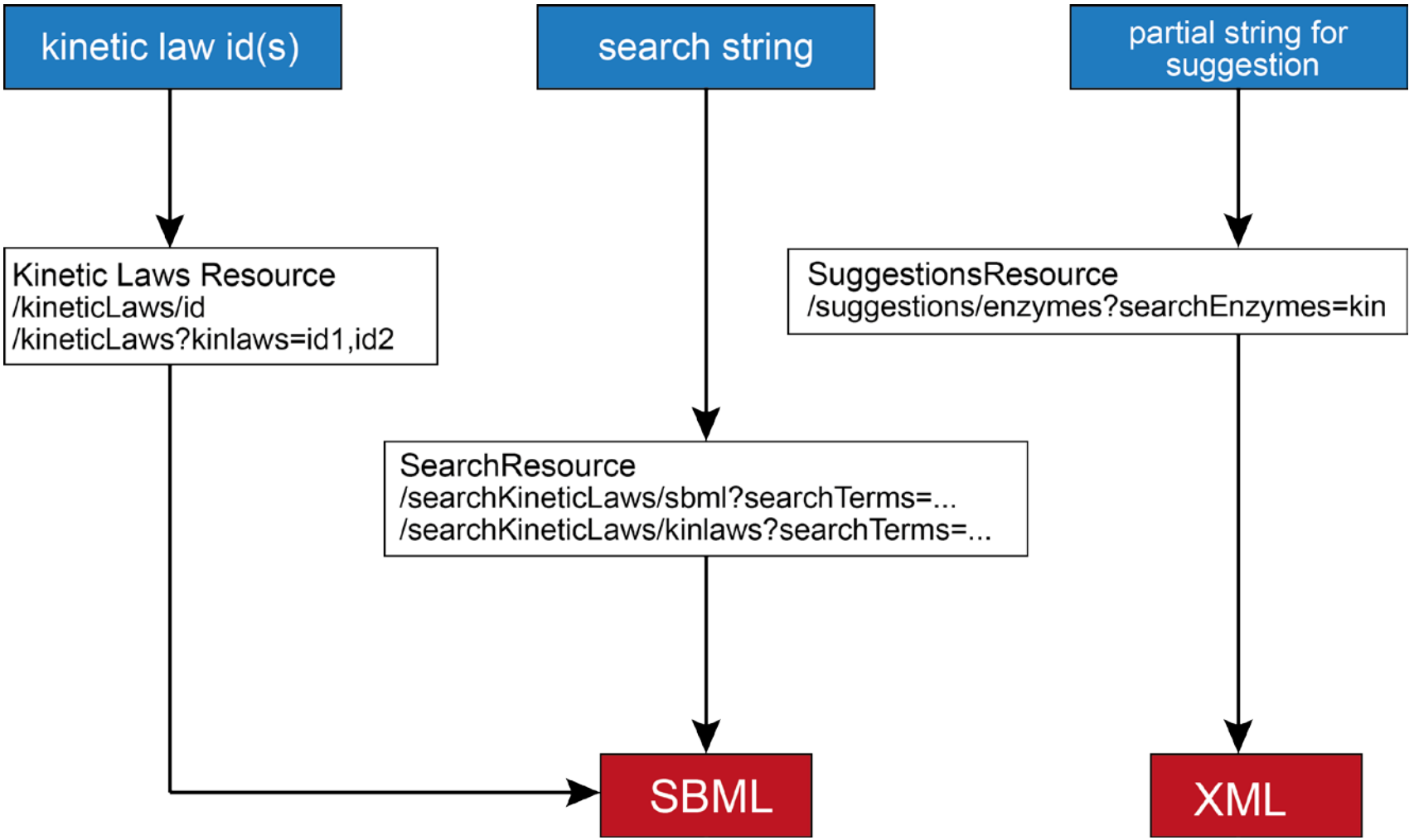
http://www.celldesigner.org

SABIO-RK API Access (Web Services)



- 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

New (RESTful) Web Services



New (RESTful) Web Services

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

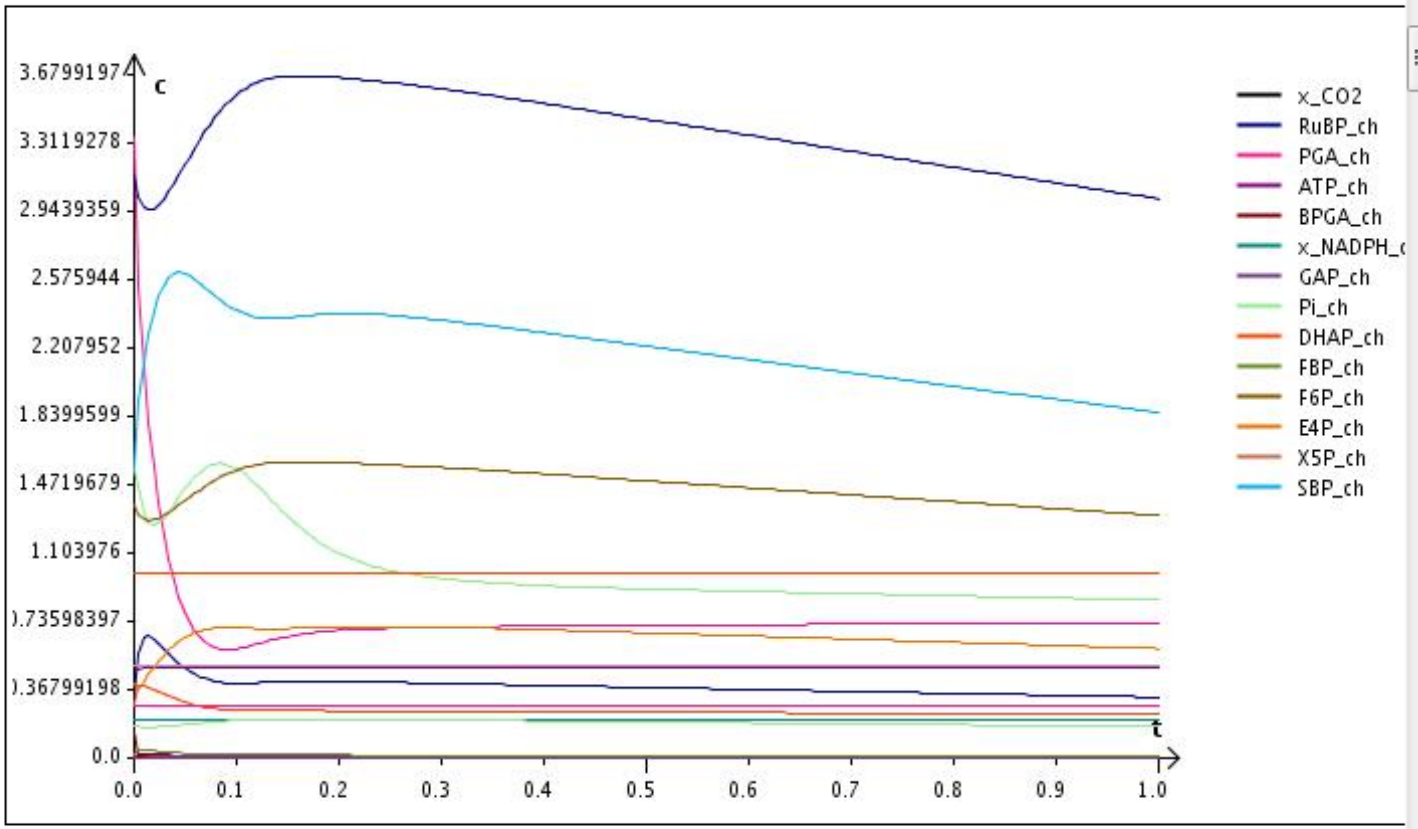
Seamless Data Transfer to SYCAMORE for Modelling

http://sycamore.eml.org/sycamore/submission.jsp

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



SABIO-RK Content

Organism	Entries (total)	Mutants	Reactions (distinct)	EC number (distinct)	Reaction rates	Km	Kinetic laws
Total 660	37343	10616	4951	1070	27305	29852	17673
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
Oryctolagus cuniculus	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
Enterococcus faecalis	538	42	155	51	320	157	478
Gallus gallus	487	167	78	35	405	521	217

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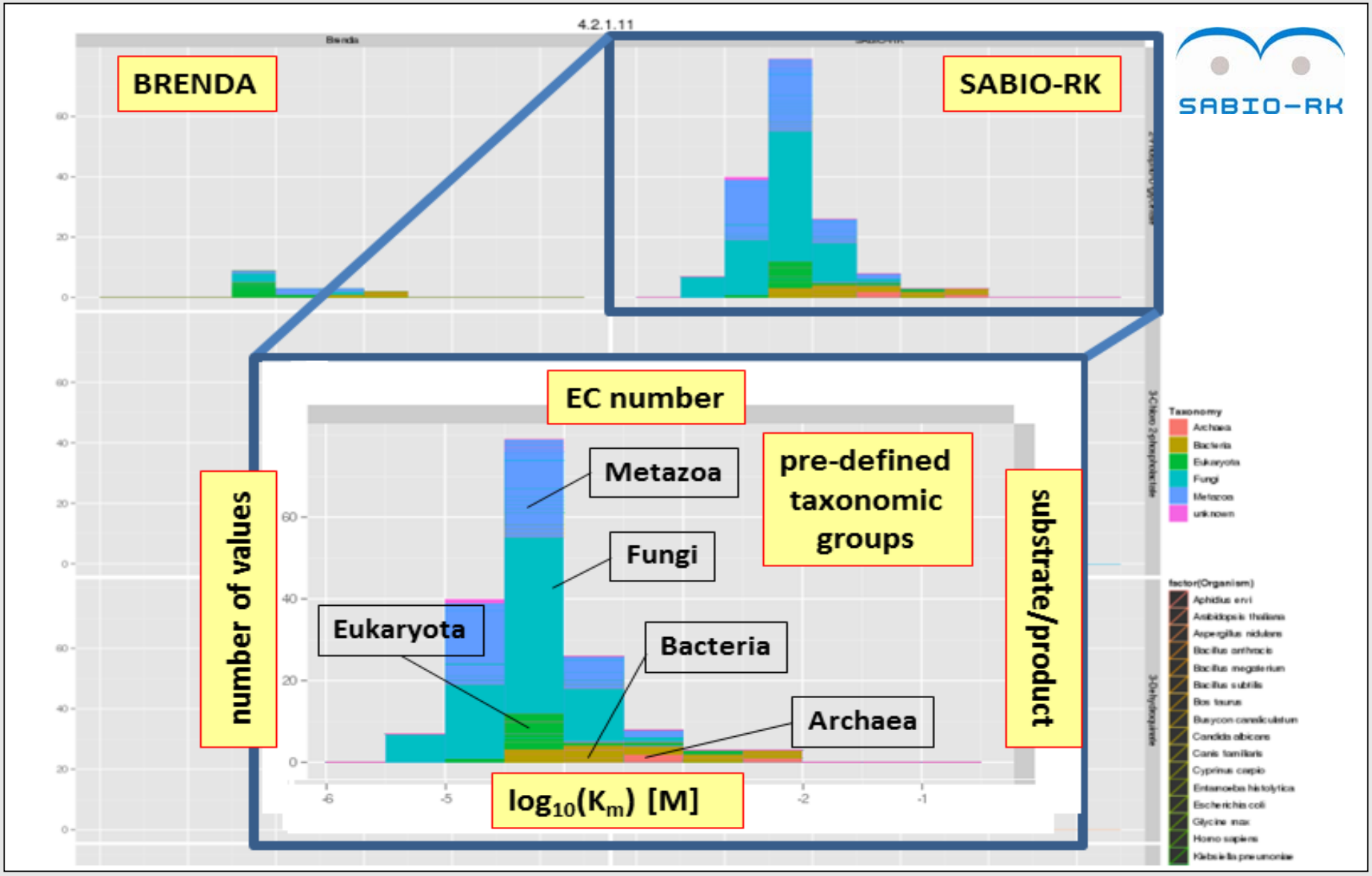

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