SABIO-RK

Heidelberger Institut für Theoretische Studien

HITS

Bridging Experiments and Modelling: SABIO-RK - Reaction Kinetics Database

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HITS gGmbH, Germany

COMBINE 2012, Toronto, August 16

virtual liver network

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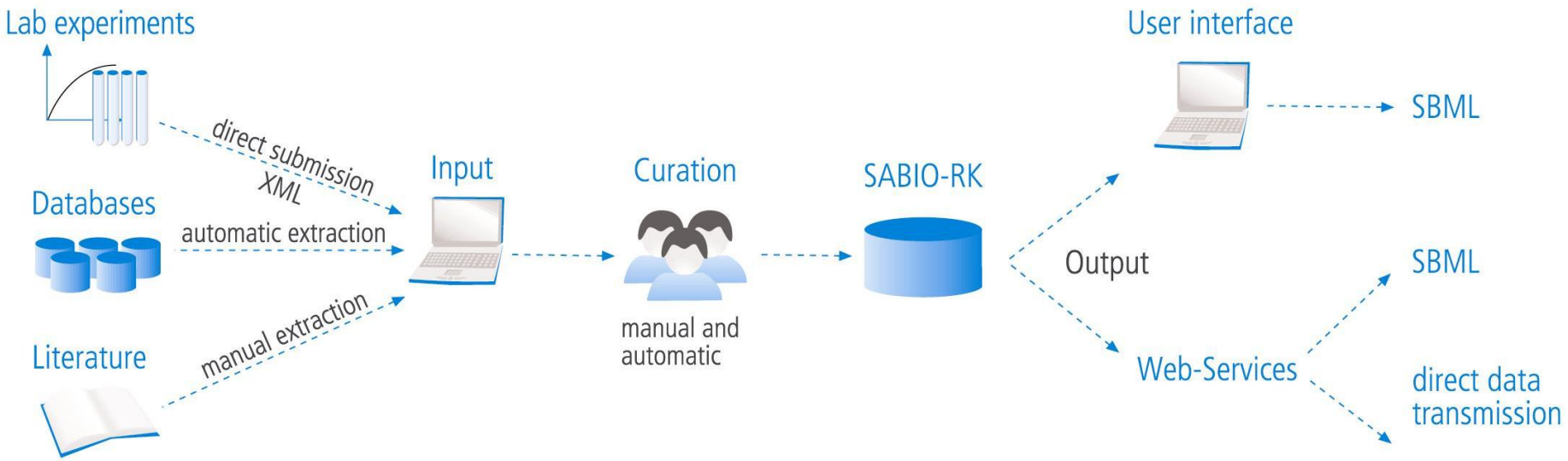
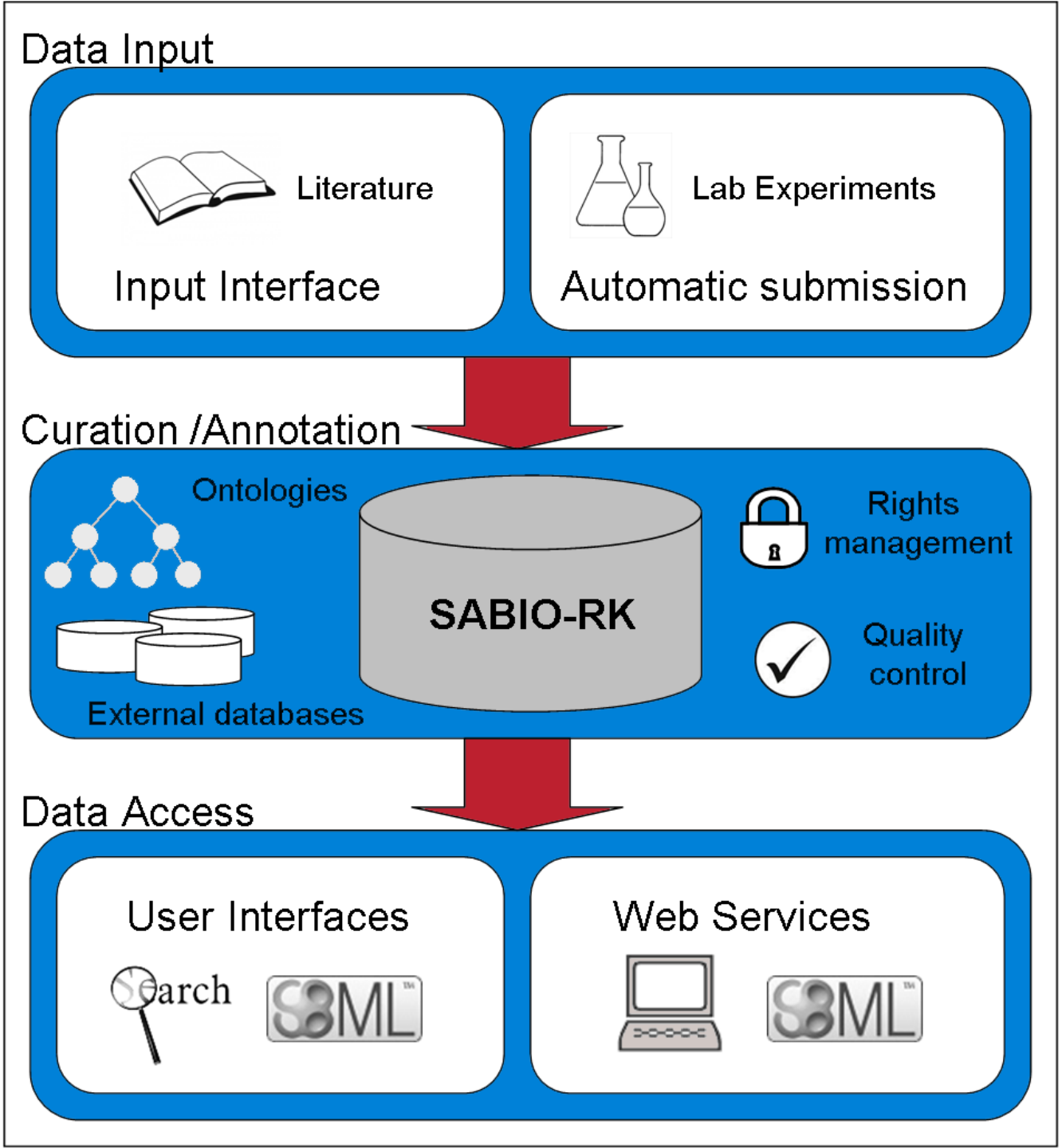
Federal Ministry of Education and Research

SABIO-RK
Database Population and Access



- Kinetic data from literature and directly from experiments merged with data describing biochemical reactions and pathways from other resources
- Data about metabolic and signalling reactions, as well as reaction mechanisms
- Data is unified, structured, normalized, interrelated and annotated
- Access through a web-based user interface and through web-services (API)
- Proprietary levels can be defined to restrict access to sensitive data
- Data export possible in standard formats (e.g. SBML and BIOPAX)

SABIO-RK



HITS

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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SABIO-RK
Biochemical Reaction Kinetics Database

Welcome!

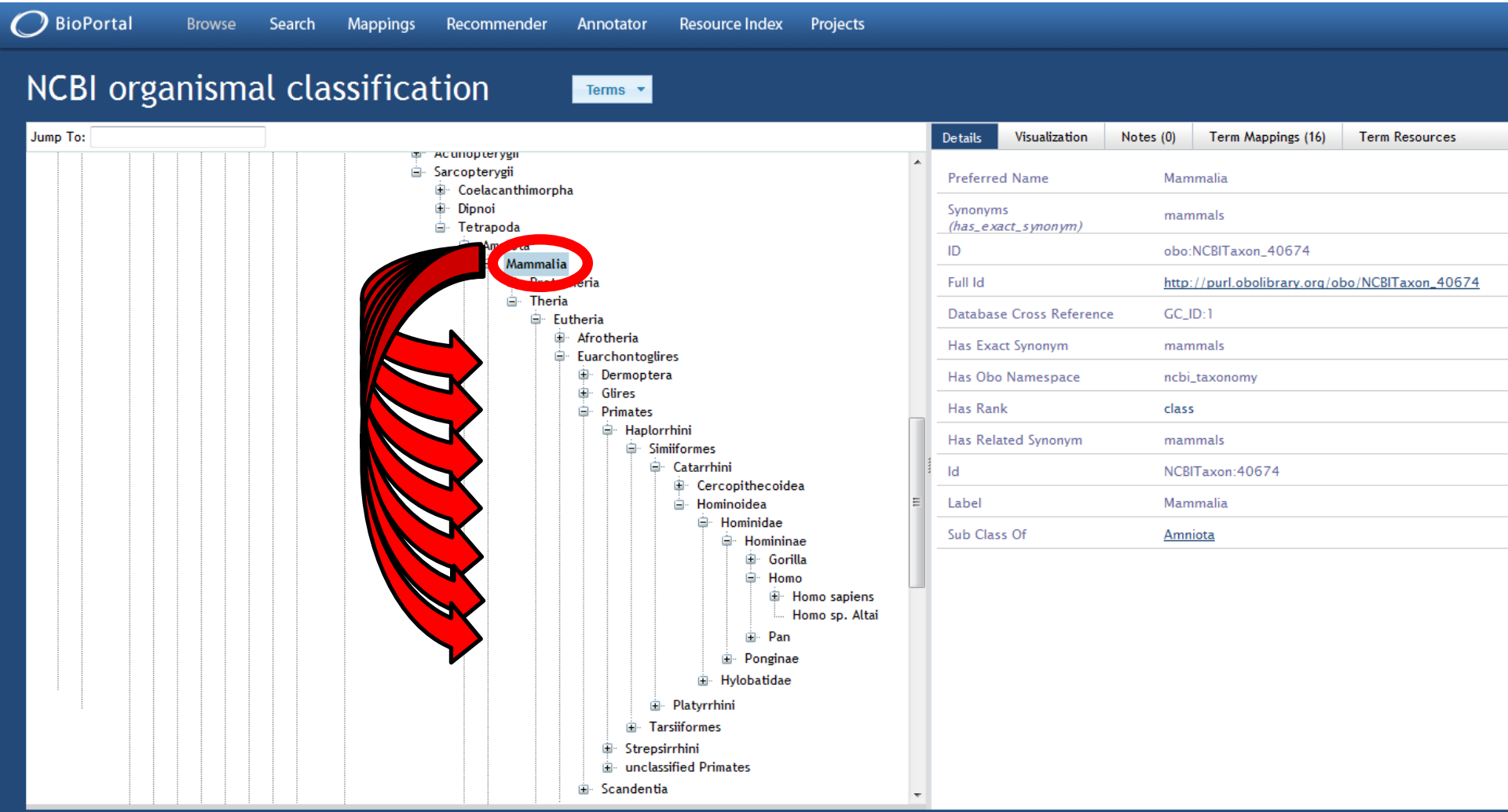
SABIO-RK is a curated database that contains information about biochemical reactions, their kinetic rate equations with parameters and experimental conditions.

News

SABIO-RK tutorial at ICSB2012
31-07-2012
SABIO-RK will be presented at the International Conference on Systems Biology (ICSB) on August 19, 2012, 9:00 am - 2:30 pm as part of the tutorial Modelling and Simulation of Quantitative Biological Models more≫

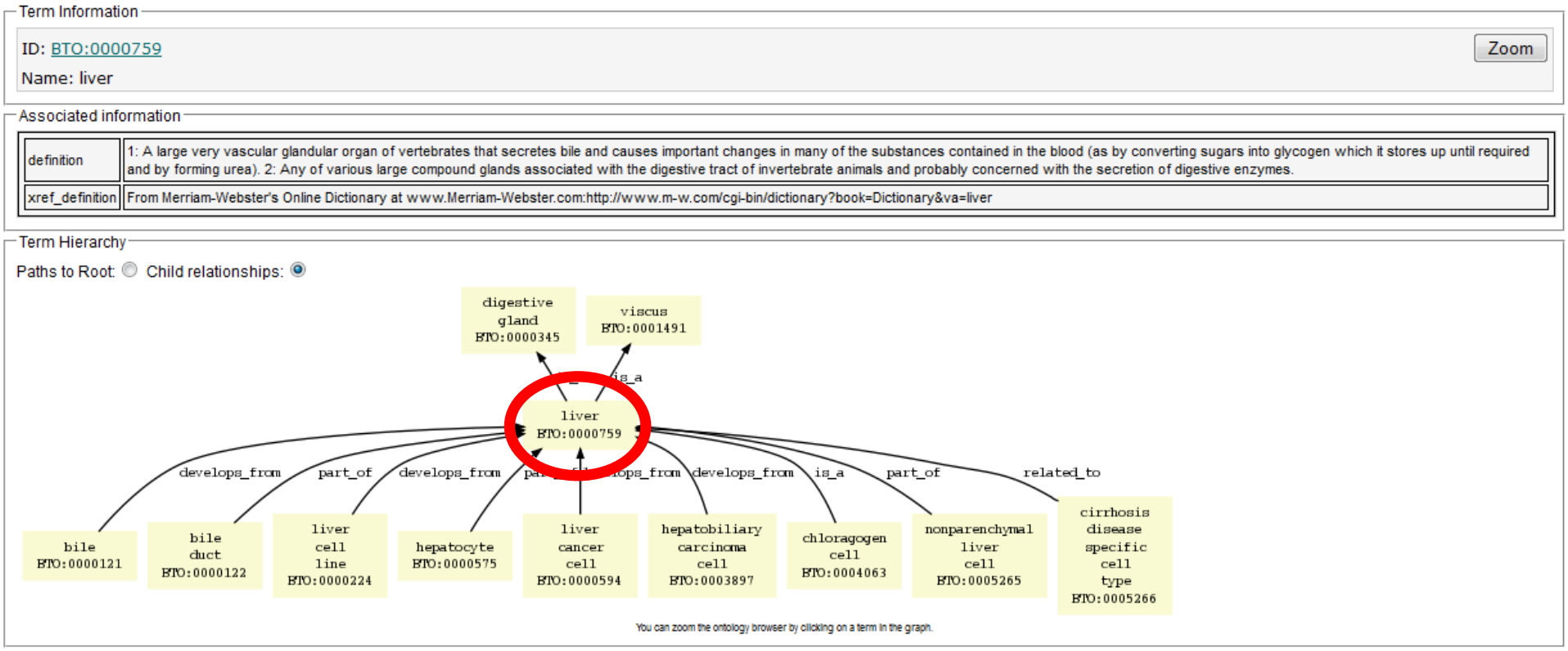
Web Services - User Survey
04-07-2012
To improve the SABIO-RK web services we prepared a short user survey which we would like to ask all web service users to fill in.
Click to start the survey! more≫

Organism Taxonomy Search



Tissue Ontology Search

SABIO-RK can be queried for all data referring to a tissue and all ontological childs



Source: http://www.ebi.ac.uk/ontology-lookup/browse.do?ontName=BTO&termId=BTO:0000759&termName=liver

Based on the BRENDA Tissue Ontology (BTO):
Nucleic Acids Research (2011) 39 (suppl 1): D507-D513

Search

Organism:"mammalia (NCBI)" AND Tissue:"liver (BTO)" NOT UniprotID:P00637 AND Substrate:"D-Fructose 1,6-bisphosphate"

Reset

Advanced Search

AND | Substrate | d-fructo | Add & Search

- d-fructose, 6-(dihydrogen phosphate) (0)
- d-fructose 6-phosphoric acid (0)
- d-fructose 2,6-bisphosphate (0)
- d-fructose 6-phosphate (0)
- d-fructose (0)

Filter Options

Enzyme
Wildtype Mutant Recombinant

Kinetic Data
Rate Equation

Environmental Conditions
pH: 0 - 14
Temperature: -10 C° - 115 C°

Source
Direct Submission
Journal
Entries inserted since: 15/10/2008

Entry View | Reaction View

Total number of kinetic law entries found: 40

1 2 3 Next

display 15 entries per page

Kinetic data	Reaction	Enzyme			Tissue	Organism	Parameter (besides concentration)	Environment		Add to export cart?
		ECNumber	Protein	Variant				°C	pH	
▶	D-Fructose 1,6-bisphosphate + H2O = D-Fructose 6-phosphate + Orthophosphate	3.1.3.11	Q9N0J6	wildtype	liver	Oryctolagus cuniculus	Kd Km Vmax	25.0	9.5	☐
▶	H2O + D-Fructose 1,6-bisphosphate =	3.1.3.11	Q3SZB7	wildtype	liver	Bos taurus	Km Vmax	28.0	6.5	☐

▼	D-Fructose 1,6-bisphosphate = Glycerone phosphate + D-Glyceraldehyde 3-phosphate	4.1.2.13	P05062	wildtype aldolase B	liver	Homo sapiens	Vmax Km	22.0	7.6	☑

Entry ID: 2175

General information	
Organism	Homo sapiens
Tissue	liver
EC Class	4.1.2.13
SABIO reaction id	1338
Variant	wildtype aldolase B
Recombinant	expressed in Escherichia coli BL21(DE3)

Substrates

name	location	comment
D-Fructose 1,6-bisphosphate	-	-

Products

name	location	comment
Glycerone phosphate	-	-
D-Glyceraldehyde 3-phosphate	-	-

Modifiers

name	location	effect	comment	protein complex
fructose-bisphosphate aldolase(Enzyme)	-	Modifier-Catalyst	-	(P05062)*4;

Enzyme (protein data)

	UniProt-ID	name	mol. weight (kDa)	deviation (kDa)
subunit	P05062	-	-	-
complex	-	-	-	-

Kinetic Law

type	formula
Michaelis-Menten	Vmax*S/(Km+S)

Parameter

name	type	species	start val.	end val.	deviat.	unit	comment
S	concentration	D-Fructose 1,6-bisphosphate	-	-	-	-	-
Km	Km	D-Fructose 1,6-bisphosphate	4.0	-	0.6	µM	-

Substrates		
name	**location**	**comment**
D-Fructose 1,6-bisphosphate	-	-

Products		
name	**location**	**comment**
Glycerone phosphate	-	-
D-Glyceraldehyde 3-phosphate	-	-

Modifiers				
name	**location**	**effect**	**comment**	**protein complex**
fructose-bisphosphate aldolase(Enzyme)	-	Modifier-Catalyst	-	(P05062)*4;

Enzyme (protein data)				
	UniProt-ID	**name**	**mol. weight (kDa)**	**deviation (kDa)**
subunit	P05062	-	-	-
complex	-	-	-	-

Kinetic Law	
type	**formula**
Michaelis-Menten	Vmax*S/(Km+S)

Parameter							
name	**type**	**species**	**start val.**	**end val.**	**deviat.**	**unit**	**comment**
S	concentration	D-Fructose 1,6-bisphosphate	-	-	-	-	-
Km	Km	D-Fructose 1,6-bisphosphate	4.0	-	0.6	µM	-
Vmax	Vmax	-	4.787	-	-	µmol/(min*mg)	-

Experimental conditions			
	start value	end value	unit
temperature	22.0	-	°C
pH	7.6	-	-
buffer	50 mM Tris-acetate, 0.15 mM NADH, 10 mM EDTA, 100 mg/ml bovine serum albumin, 2 mg/ml alpha-glycerophosphate dehydrogenase/triose phosphate isomerase		
comment	-		

Reference						
title	**author**	**year**	**journal**	**volume**	**pages**	**PubMed**
Expression, purification, and characterization of natural mutants of human aldolase B. Role of quaternary structure in catalysis.	Rellos P, Sygusch J, Cox TM.	2000	J Biol Chem	275	1145-51	10625657

Data Export

SABIO-RK

Biochemical Reaction Kinetics Database

Login | Contact

Entries to Export: 1

Home | Search | Web Services | News | Documentation | Publications | Statistics | Links | About

Save Model

Enter name of model: SABIOmdl16Aug20126(SBML level 3, version 1

- SBML level 3, version 1
- SBML level 2, version 4
- SBML level 2, version 3
- SBML level 2, version 2

Export parameters normalized to SI base units

Save Model on Disk as SBML

Save Model on Disk as PDF

Bioinformatics. 2009 June 1; 25(11): 1455–1456. PMCID: PMC2682517
Published online 2009 March 23. doi: 10.1093/bioinformatics/btp170.

SBML2LaTeX: Conversion of SBML files into human-readable reports

Andreas Dräger,[1*] Hannes Planatscher,[1] Dieudonné Motsou Wouamba,[1] Adrian Schröder,[1] Michael Hucka,[2] Lukas Endler,[3] Martin Golebiewski,[4] Wolfgang Müller,[4] and Andreas Zell[1]

Data Export in SBML

- Currently up to **SBML Level 3 Version 1**
- **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
- Export with **experimental conditions** (SABIO-RK specific namespace)
- Optional **normalization of kinetic parameters** to SI base units
- Export also as human readable PDF (only SBML level 2) → **SBML2LaTeX**

Data Export in SBML

```
<?xml version='1.0' encoding='UTF-8' standalone='no'?>
<sbml xmlns="http://www.sbml.org/sbml/level3/version1/core" level="3" version="1">
  <model name="SABIOmdl16Aug2012604">
<notes><body xmlns="http://www.w3.org/1999/xhtml">
<p>
This model has been created with the help of the SABIO-RK Database
(http://sabio.h-its.org/)
 (c) 2005-2012 HITS gGmbH http://www.h-its.org

</p><br/>
To cite SABIO-RK Database, please use
"http://www.ncbi.nlm.nih.gov/pubmed/22102587"
<br/>
SABIO-RK - database for biochemical reaction kinetics. Wittig U, Kania R, Golebiewski M, Rey M, Shi L, Jong L, Algaa E, Weidemann A, Sauer-Danzwith H, Mir S, Krebs O,
Bittkowski M, Wetsch E, Rojas I, Mueller W. Nucleic Acids Res. 2012;40(Database issue)790-6
</body></notes>
      <listOfFunctionDefinitions>
      <functionDefinition id="KL_2175" sboTerm="SBO:0000028">
        <math xmlns="http://www.w3.org/1998/Math/MathML">
          <lambda>
            <bvar>
              <ci> Km </ci>
            </bvar>
            <bvar>
              <ci> S </ci>
            </bvar>
            <bvar>
              <ci> Vmax </ci>
            </bvar>
            <apply>
              <divide/>
              <apply>
                <times/>
                <ci> Vmax </ci>
                <ci> S </ci>
              </apply>
              <apply>
                <plus/>
                <ci> Km </ci>
                <ci> S </ci>
              </apply>
            </apply>
          </lambda>
        </math>
      </functionDefinition>
    </listOfFunctionDefinitions>
    <listOfUnitDefinitions>
      <unitDefinition id="M" name="M">
        <listOfUnits>
```

Kinetic Rate Equations

Data Export in SBML

```
    </listOfFunctionDefinitions>
    <listOfUnitDefinitions>
      <unitDefinition id="M" name="M">
        <listOfUnits>
          <unit scale="0" exponent="-1" multiplier="1" kind="litre"/>
          <unit scale="0" exponent="1" multiplier="1" kind="mole"/>
        </listOfUnits>
      </unitDefinition>
      <unitDefinition id="molswedgeonegwedgeone" name="mol*s^(-1)*g^(-1)">
        <listOfUnits>
          <unit scale="0" exponent="1" multiplier="1" kind="mole"/>
          <unit scale="0" exponent="-1" multiplier="1" kind="second"/>
          <unit scale="0" exponent="-1" multiplier="1" kind="gram"/>
        </listOfUnits>
      </unitDefinition>
    </listOfUnitDefinitions>
    <listOfCompartments>
      <compartment id="compart_Cell" constant="true" name="Cell"/>
    </listOfCompartments>
    <listOfSpecies>
      <species id="SPC_1465_Cell" initialConcentration="1" constant="false" hasOnlySubstanceUnits="false" name="D-Fructose 1,6-bisphosphate"
metaid="META_SPC_1465_Cell" boundaryCondition="false" compartment="compart_Cell">
        <annotation>
          <rdf:RDF xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#" xmlns:bqbiol="http://biomodels.net/biology-qualifiers/"
xmlns:bqmodel="http://biomodels.net/model-qualifiers/">
            <rdf:Description rdf:about="#META_SPC_1465_Cell">
              <bqbiol:is>
                <rdf:Bag>
                  <rdf:li rdf:resource="urn:miriam:obo.chebi:16905"/>
                  <rdf:li rdf:resource="urn:miriam:obo.chebi:37736"/>
                  <rdf:li rdf:resource="urn:miriam:kegg.compound:C00354"/>
                </rdf:Bag>
              </bqbiol:is>
            </rdf:Description>
          </rdf:RDF>
        </annotation>
</species>
      <species id="SPC_27_Cell" initialConcentration="1" constant="false" hasOnlySubstanceUnits="false" name="D-Glyceraldehyde 3-phosphate"
metaid="META_SPC_27_Cell" boundaryCondition="false" compartment="compart_Cell">
        <annotation>
          <rdf:RDF xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#" xmlns:bqbiol="http://biomodels.net/biology-qualifiers/"
```

Parameter Units

Reactants
(+ Annotations)

Data Export in SBML

```
      <species id="ENZ_140280_Cell" initialConcentration="1" constant="false" hasOnlySubstanceUnits="false" name="fructose-bisphosphate
aldolase(Enzyme) wildtype aldolase B" metaid="META_ENZ_140280_Cell" boundaryCondition="false" compartment="compart_Cell">
        <annotation bqbiol="http://biomodels.net/biology-qualifiers/" rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#/">
<sbrk:sabiork xmlns:sbrk="http://sabiork.h-its.org">
<sbrk:modifierType>Modifier-Catalyst</sbrk:modifierType>
</sbrk:sabiork>                  <rdf:RDF xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#" xmlns:bqbiol="http://biomodels.net/biology-
qualifiers/" xmlns:bqmodel="http://biomodels.net/model-qualifiers/">
            <rdf:Description rdf:about="#META_ENZ_140280_Cell">
              <bqbiol:is>
                <rdf:Bag>
                  <rdf:li rdf:resource="urn:miriam:uniprot:P05062"/>
                </rdf:Bag>
              </bqbiol:is>
            </rdf:Description>
          </rdf:RDF>
        </annotation>
</species>
    </listOfSpecies>
    <listOfReactions>
      <reaction id="REAC_0" metaid="META_REAC_0" reversible="true" fast="false">
        <annotation>
          <rdf:RDF xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#" xmlns:bqbiol="http://biomodels.net/biology-qualifiers/"
xmlns:bqmodel="http://biomodels.net/model-qualifiers/">
            <rdf:Description rdf:about="#META_REAC_0">
              <bqbiol:isVersionOf>
                <rdf:Bag>
                  <rdf:li rdf:resource="urn:miriam:ec-code:4.1.2.13"/>
                </rdf:Bag>
              </bqbiol:isVersionOf>
              <bqbiol:is>
                <rdf:Bag>
                  <rdf:li rdf:resource="urn:miriam:kegg.reaction:R01068"/>
                </rdf:Bag>
              </bqbiol:is>
              <bqbiol:occursIn>
                <rdf:Bag>
                  <rdf:li rdf:resource="urn:miriam:taxonomy:9606"/>
                </rdf:Bag>
              </bqbiol:occursIn>
              <bqbiol:is>
                <rdf:Bag>
                  <rdf:li rdf:resource="urn:miriam:sabiork.reaction:1338"/>
                </rdf:Bag>
```

Catalyzing Enzymes
(+ Annotations)

Reactions
(+ Annotations)

SABIO-RK
Annotations

Data Export in SBML

```
        <speciesReference constant="true" species="SPC_28_Cell" sboTerm="SBO:0000011" stoichiometry="1"/>
      </listOfProducts>
      <listOfModifiers>
        <modifierSpeciesReference species="ENZ_140280_Cell" sboTerm="SBO:0000460"/>
      </listOfModifiers>
      <kineticLaw metaid="META_KL_2175" sboTerm="SBO:0000028">
        <annotation sbrk="http://sabiork.h-its.org" bqbiol="http://biomodels.net/biology-qualifiers/" rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#/">
<sbrk:sabiork xmlns:sbrk="http://sabiork.h-its.org">
<sbrk:kineticLawID>2175</sbrk:kineticLawID>
<sbrk:experimentalConditions>
<sbrk:temperature>
<sbrk:startValueTemperature>22.0</sbrk:startValueTemperature>
<sbrk:temperatureUnit>°C</sbrk:temperatureUnit>
</sbrk:temperature>
<sbrk:pH>
<sbrk:startValuepH>7.6</sbrk:startValuepH>
</sbrk:pH>
<sbrk:buffer> 50 mM Tris-acetate, 0.15 mM NADH, 10 mM EDTA, 100 mg/ml bovine serum albumin, 2 mg/ml alpha-glycerophosphate dehydrogenase/triose phosphate isomerase
</sbrk:buffer>
</sbrk:experimentalConditions>
</sbrk:sabiork>                    <rdf:RDF xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#" xmlns:bqbiol="http://biomodels.net/biology-qualifiers/"
xmlns:bqmodel="http://biomodels.net/model-qualifiers/">
            <rdf:Description rdf:about="#META_KL_2175">
              <bqbiol:isDescribedBy>
                <rdf:Bag>
                  <rdf:li rdf:resource="urn:miriam:pubmed:10625657"/>
                </rdf:Bag>
              </bqbiol:isDescribedBy>
              <bqbiol:isDescribedBy>
                <rdf:Bag>
                  <rdf:li rdf:resource="urn:miriam:sabiork.kineticrecord:2175"/>
                </rdf:Bag>
              </bqbiol:isDescribedBy>
            </rdf:Description>
          </rdf:RDF>
        </annotation>
        <math xmlns="http://www.w3.org/1998/Math/MathML">
          <apply>
            <ci> KL_2175 </ci>
            <ci> Km_SPC_1465_Cell </ci>
            <ci> SPC_1465_Cell </ci>
            <ci> Vmax </ci>
          </apply>
        </math>
              <listOfLocalParameters>
          <localParameter id="Km_SPC_1465_Cell" name="Km_DFructose 16bisphosphate" value="4E-6" sboTerm="SBO:0000027" units="M"/>
          <localParameter id="Vmax" name="Vmax" value="7.97833E-5" sboTerm="SBO:0000186" units="molswedgeonegwedgeone"/>
        </listOfLocalParameters>
      </kineticLaw>
```

Experimental Conditions (SABIO-RK namespace)

Data Sources: Primary source and SABIO-RK entry ID

Kinetic Parameters (+ SBO Annotations)

Data Export in BioPAX

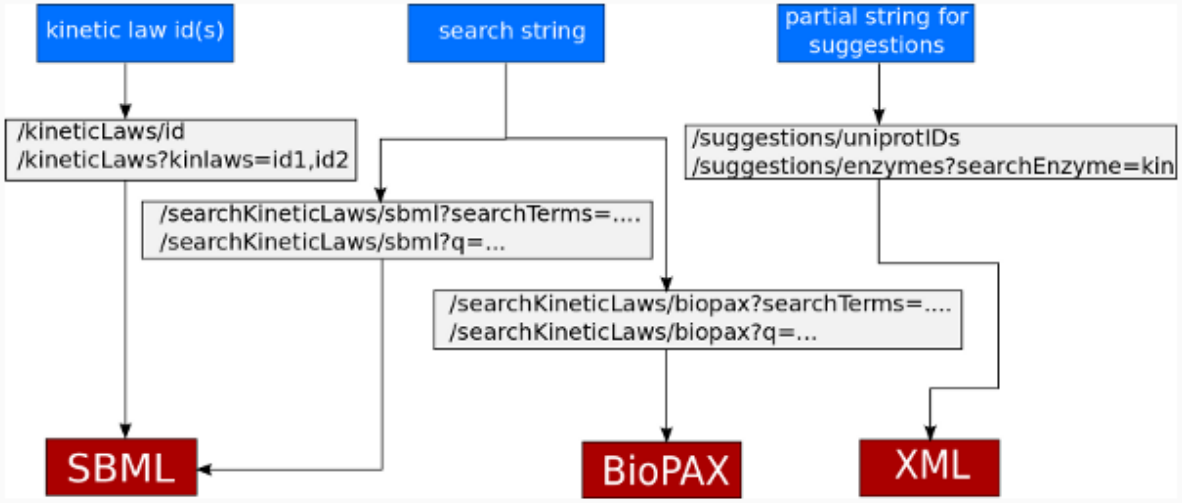
- **Reaction Kinetics Warehouse:**
  Reactions, kinetic equations and parameters (with corresponding units) from different database entries can be exported in one BioPAX file
- Data is annotated according to **MIRIAM**
- **SBPAX3** (Systems Biology Pathway Exchange) is used to represent the reaction kinetics data and experimental conditions (http://www.sbpax.org)
- Parameter units are described via the **UOME** (Units of Measurement Expressions) extension to BioPax (http://www.sbpax.org/uome/)
- BioPAX export is available in both web search interface and web services (http://sabio.h-its.org/sabioRestWebServices/searchKineticLaws/biopax endpoint)

Data Export in BioPAX

```
<?xml version="1.0" encoding="UTF-8"?>
<rdf:RDF
        xmlns:rdfs="http://www.w3.org/2000/01/rdf-schema#"
        xmlns:bp3="http://www.biopax.org/release/biopax-level3.owl#"
        xmlns:sbx3="http://vcell.org/sbpax3#"
        xmlns:xsd="http://www.w3.org/2001/XMLSchema#"
        xmlns:uome-core="http://www.sbpax.org/uome/core.owl#"
        xmlns:owl="http://www.w3.org/2002/07/owl#"
        xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
        xmlns:sabio="http://sabio.h-its.org/biopax#"
        xmlns:uome-list="http://www.sbpax.org/uome/list.owl#">
<owl:Ontology rdf:about="http://sabio.h-its.org/biopax">
        <owl:imports rdf:resource="http://vcell.org/sbpax3"/>
        <owl:imports rdf:resource="http://www.biopax.org/release/biopax-level3.owl"/>
        <owl:imports rdf:resource="http://www.sbpax.org/uome/core.owl"/>
        <owl:imports rdf:resource="http://www.sbpax.org/uome/list.owl"/>
</owl:Ontology>
<bp3:UnificationXref rdf:about="http://sabio.h-its.org/biopax#Brenda_Tissue_Ontology:BTO:0000424">
        <bp3:db rdf:datatype="http://www.w3.org/2001/XMLSchema#string">Brenda Tissue Ontology</bp3:db>
        <bp3:id rdf:datatype="http://www.w3.org/2001/XMLSchema#string">BTO:0000424</bp3:id>
</bp3:UnificationXref>
<bp3:SmallMolecule rdf:about="http://sabio.h-its.org/biopax#SmallMolecule_Glucose">
        <bp3:name rdf:datatype="http://www.w3.org/2001/XMLSchema#string">D-Glucose</bp3:name>
</bp3:SmallMolecule>
<sbx3:SBMeasurable rdf:about="http://sabio.h-its.org/biopax#temperature714">
        <sbx3:SBVocabulary rdf:resource="http://sabio.h-its.org/biopax#SBO:0000147"/>
        <sbx3:hasNumber rdf:datatype="http://www.w3.org/2001/XMLSchema#double">37.0</sbx3:hasNumber>
        <sbx3:hasUnit rdf:resource="http://www.sbpax.org/uome/list.owl#DegreeCelsius"/>
        <sbx3:sbTerm rdf:resource="http://sabio.h-its.org/biopax#SBO:0000147"/>
</sbx3:SBMeasurable>
<bp3:TissueVocabulary rdf:about="http://sabio.h-its.org/biopax#tissue_erythrocyte">
        <bp3:term rdf:datatype="http://www.w3.org/2001/XMLSchema#string">erythrocyte</bp3:term>
        <bp3:xref rdf:resource="http://sabio.h-its.org/biopax#Brenda_Tissue_Ontology:BTO:0000424"/>
</bp3:TissueVocabulary>
<uome-core:UnitOfMeasurement rdf:nodeID="node16t8bg47mx420">
        <uome-core:unitSymbol rdf:datatype="http://www.w3.org/2001/XMLSchema#string">M</uome-core:unitSymbol>
</uome-core:UnitOfMeasurement>
</rdf:RDF>
```

RESTful Web Services Introduction

RESTful Web Services are implemented offering data access via HTTP requests following a Representational State Transfer (REST) approach. Data can be accessed using simple http GET requests to either retrieve a complete SBML model, or a BioPAX/SBPAX3 representation of the requested entries, or pieces of information in a tailored format (in plain text or XML). Entries can be requested directly by using the database entry ID or can be searched for using the same format query built in user interface advanced search.



RESTFUL

- Introduction
- Manual - including request examples
- Search Keyword Vocabulary

SOAP

- Manual
- Sample Client Code
- WSDL

SABIO-RK RESTful Web Services Manual

API methods

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Error codes and their meaning

HTTP Response Code	Description
200	OK. The request to the web service completed successfully.
400	Bad request. The parameters passed to the API endpoint were invalid.
404	Not found. The resource corresponding to the supplied parameters does not exist.
500	Service unavailable. An internal problem prevented us from fulfilling your request.

SABIO REST api methods

Methods returning models of entries

Description: Get a single kinetic law entry by SABIO entry ID

RESTful Web Services

SABIO REST api methods

Methods returning models of entries

Description: Get a single kinetic law entry by SABIO entry ID

Input: N.A.

Output: SBML model

Example URL: http://sabiork.h-its.org/sabioRestWebServices/kineticLaws/123

Optional Parameters:

level - SBML level, default value:3
version - SBML version, default value:1
normalized - Export parameters with normalized units, default:true

Description: Get kinetic law entries by SABIO entry IDs

Input: list of SABIO entry IDs

Output: SBML model

Example URL: http://sabiork.h-its.org/sabioRestWebServices/kineticLaws?kinlawids=123,234

Optional Parameters:

level - SBML level, default value:3
version - SBML version, default value:1
normalized - Export parameters with normalized units, default:true

RESTful Web Services

Description: Search for kinetic law entries by SABIO entry by a query string
Input: query string, see Search Keyword Vocabulary for how to form a query
Output: SBML model
Example URL: http://sabiork.h-its.org/sabioRestWebServices/searchKineticLaws/sbml?q=Tissue:liver AND Organism:Homo sapiens
Optional Parameters:

level - SBML level, default:3
version - SBML version, default:1
normalized - Export parameters with normalized units, default:true

Description: Search for kinetic law entries by SABIO entry by a query string
Input: query string, see Search Keyword Vocabulary for how to form a query
Output: BioPAX model
Example URL: http://sabiork.h-its.org/sabioRestWebServices/biopax?q=Tissue:liver AND Organism:Homo sapiens

Description: Search for kinetic law entries by SABIO entry by a query string, return only the number of the matching entries
Input: query string, see Search Keyword Vocabulary for how to form a query
Output: XML or plain text
Example URL: http://sabiork.h-its.org/sabioRestWebServices/count?q=Tissue:liver AND Organism:Homo sapiens
Optional Parameters:

format - format for export "xml" or "txt", default:xml

RESTful Web Services Search Keyword Vocabulary

The following vocabulary may be used to form queries to search for entries. These terms are identical to those used in the web interface for forming queries. An xml document containing all possible search fields is also accessible at http://sabiork.h-its.org/sabioRestWebServices/searchKineticLaws . Queries are formed using one or more of the fields below and should be passed as a request parameter named "q". Fields may be combined using the boolean AND operator to form complex queries.

Entry

EntryID - SABIO-RK entry ID (eg EntryID:123)

Reaction/Pathway

Pathway - The name of the reaction pathway (eg, Pathway:urea Cycle)

KeggReactionID - KEGG ID for the reaction (eg KeggReactionID:R00782)

SabioReactionID- SABIO-RK ID for the reaction (eg SabioReactionID:14

Compound

AnyRole - Compound found in any role in a reaction eg (AnyRole:oxygen)

Substrate - Compound acting as a substrate in a reaction eg (Substrate:ATP)

Product - Compound acting as a product in a reaction

Inhibitor - Compound acting as an inhibitor modifier in a reaction

Catalyst - Compound acting as a catalyst modifier in a reaction

Cofactor - Compound acting as a cofactor in a reaction

Activator - Compound acting as an activator in a reaction

OtherModifier - Compound acting as a modifier not specified above, in a reaction

PubChemID - PubChem ID number of a compound

KeggID - KEGG ID number of a compound

ChebiID - Chebi ID number of a compound

SabioCompoundID

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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

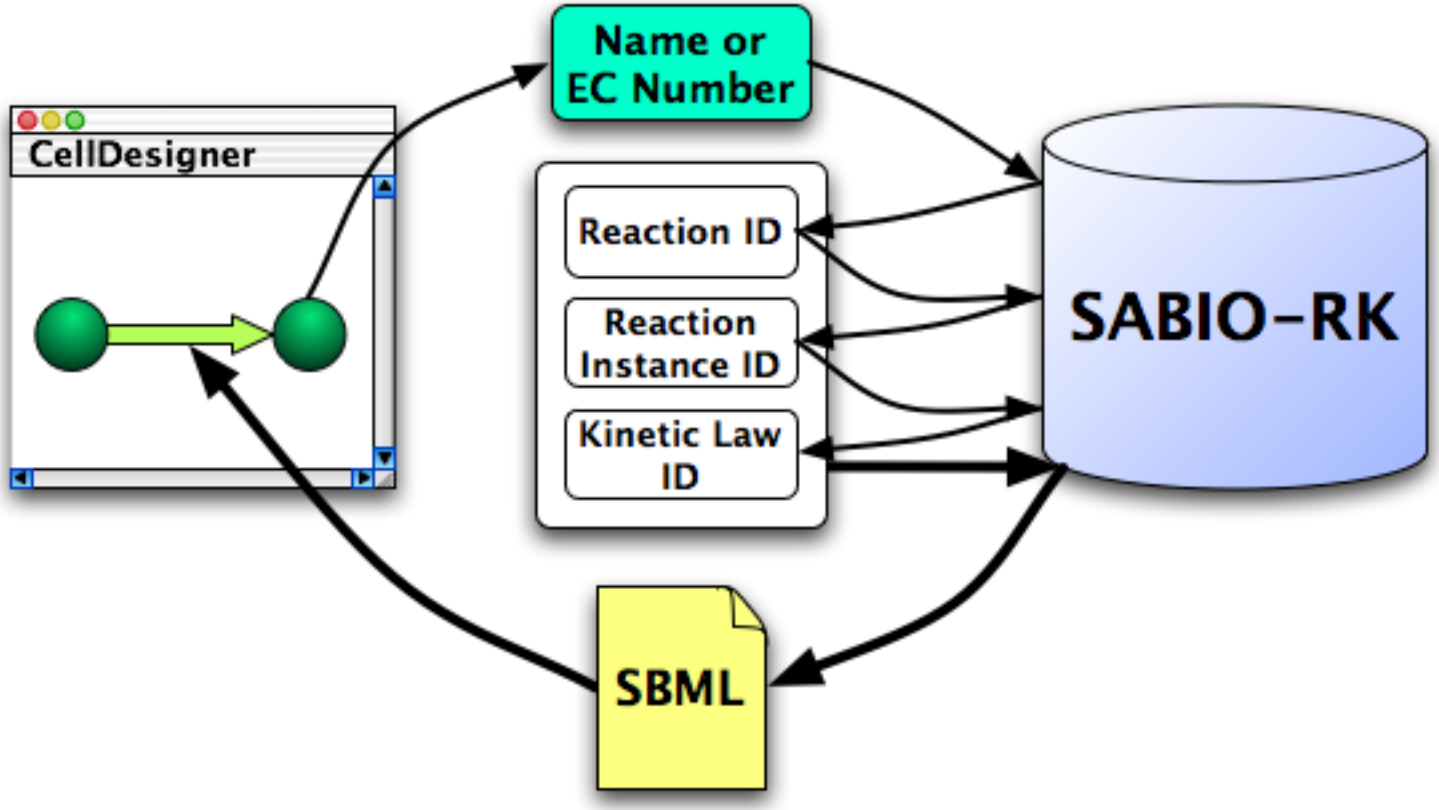
Entries may be searched for using the same search options available in the browser search interface

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

Suggestions for search terms can be done

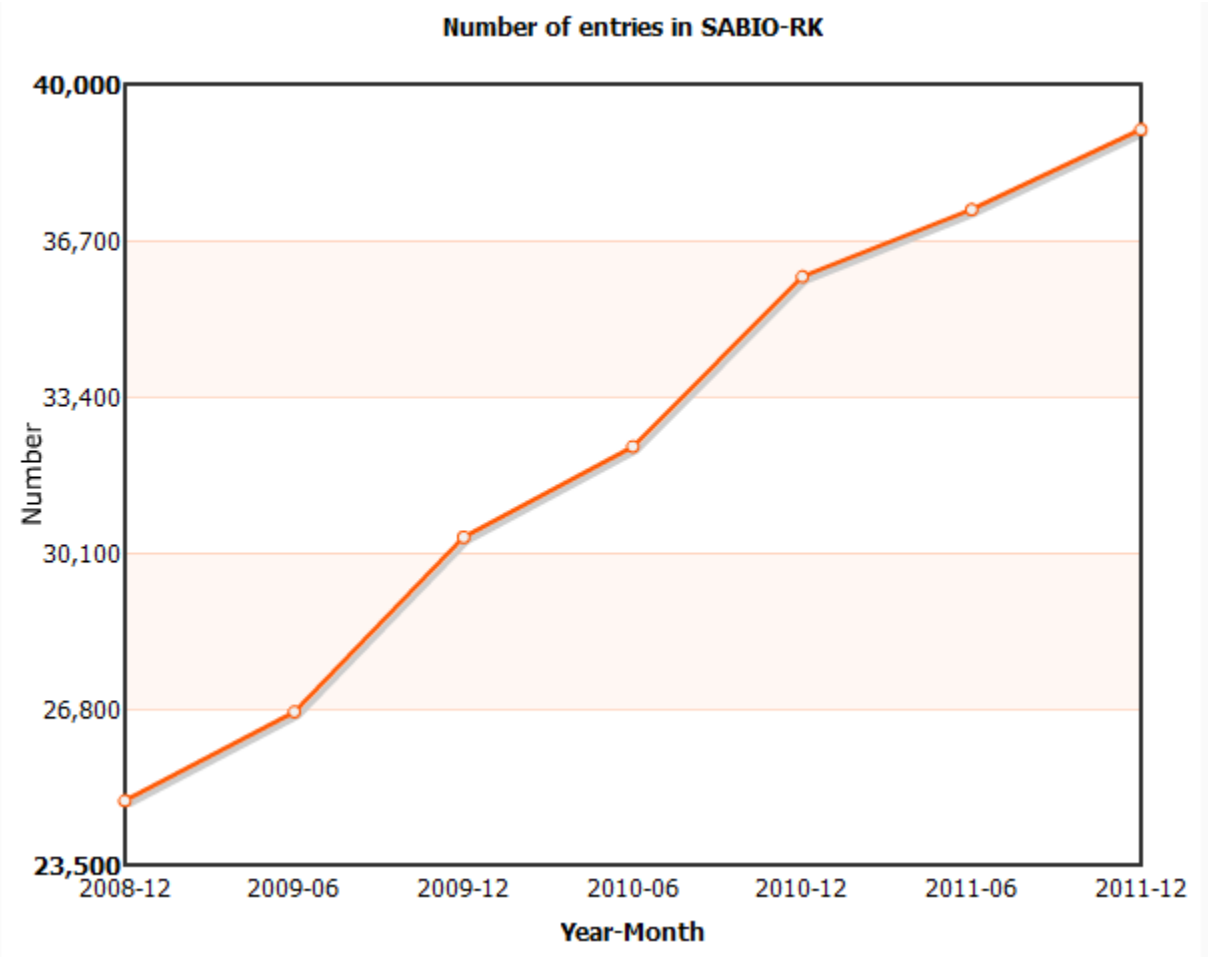
http://sabio.h-its.org/sabioRestWebServices/suggestions/compounds?searchCompounds=glycoch

SABIO-RK API Access
Integration into Modeling Tools



http://www.celldesigner.org

SABIO-RK Content



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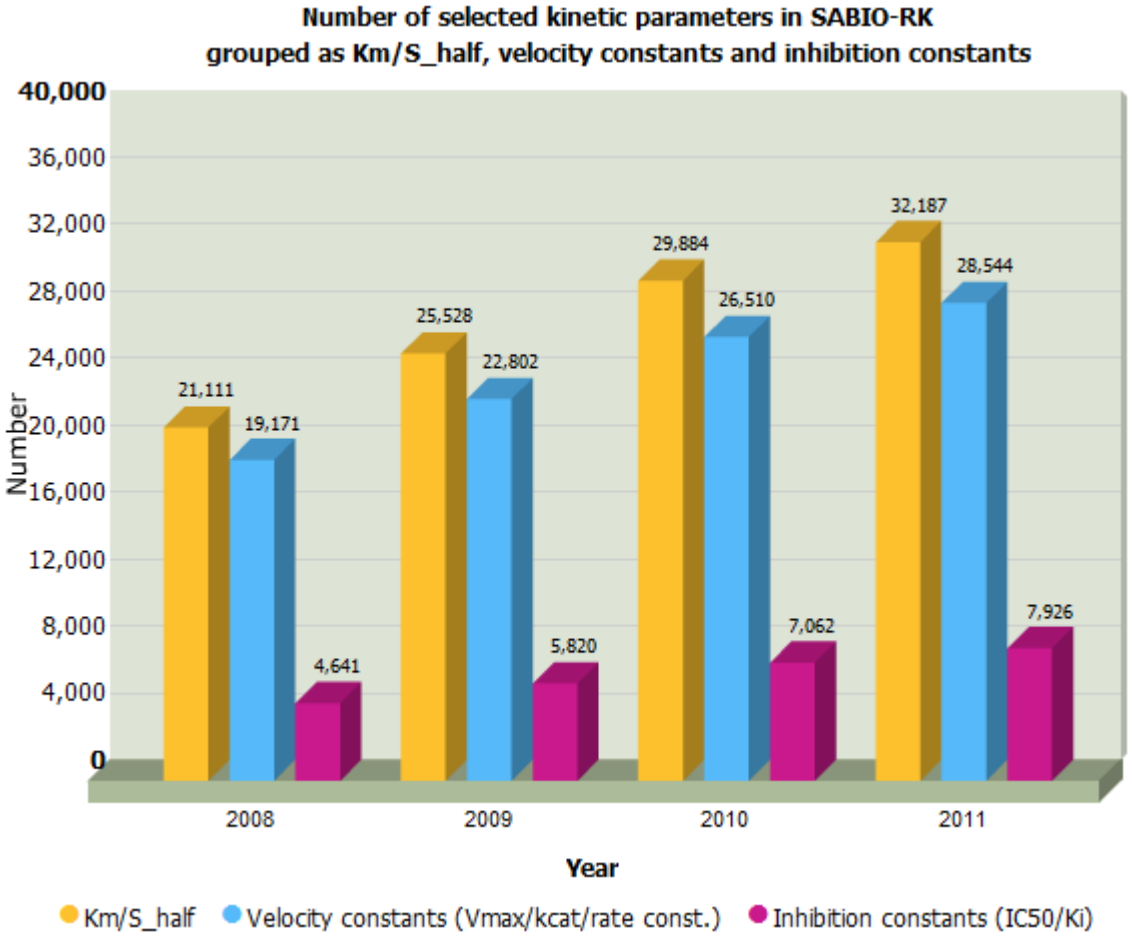
SABIO-RK Content



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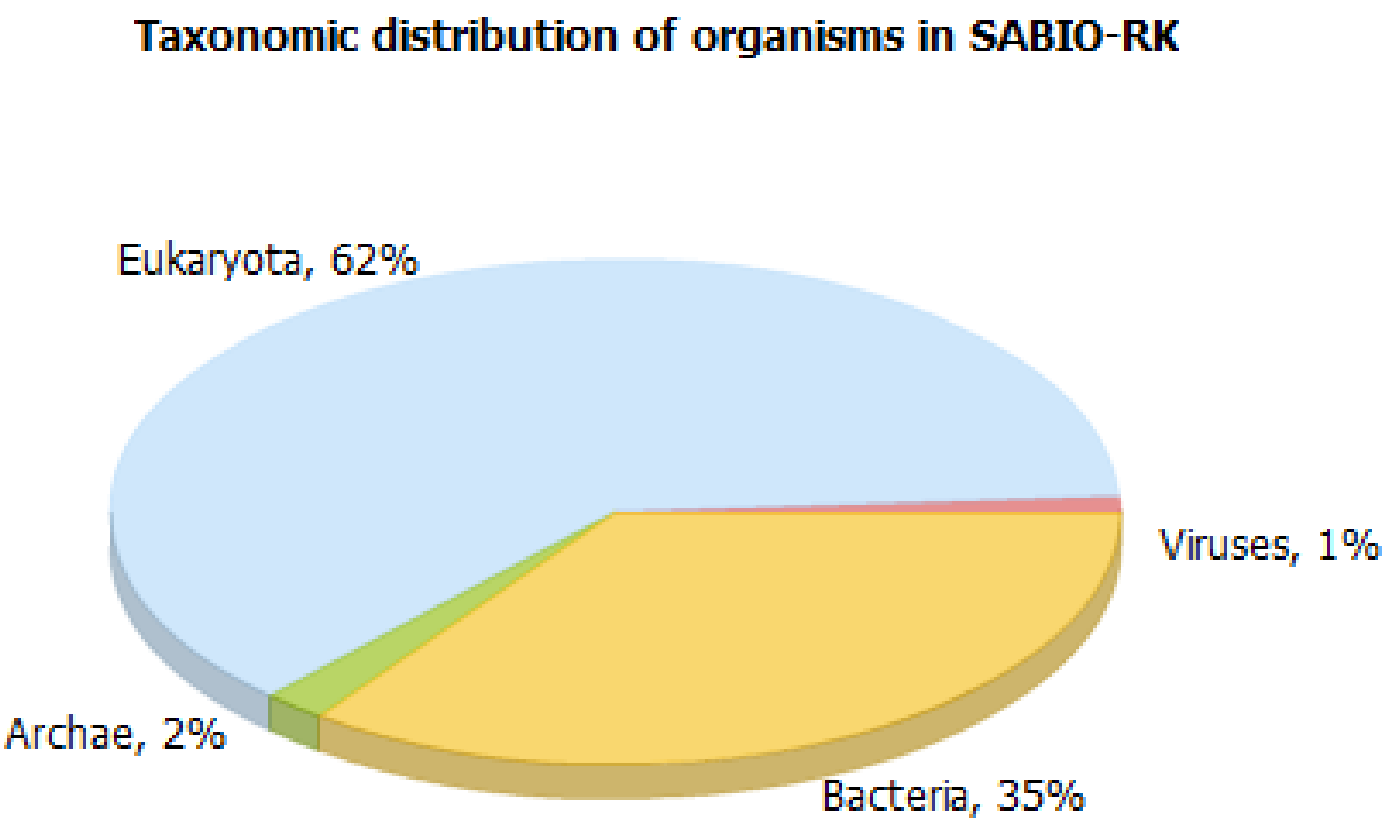
SABIO-RK Content



SABIO-RK Content

Organism Tissue	Publications (distinct)	Entries (total)	Reactions (distinct)	EC numbers (distinct)	Velocity constants (total)	Km/S-half (total)	Rate equations (total)
All organisms all tissues	3521	39025	5188	1135	28544	32187	20433
All organisms Liver (BTO)	753	7344	1463	377	4893	6019	3887
Rattus norvegicus Liver (BTO)	355	2869	685	246	1786	2227	1514
Homo sapiens Liver (BTO)	208	1973	523	138	1519	1648	1148

Additional 2400 data entries are already curated, but not yet released to the public

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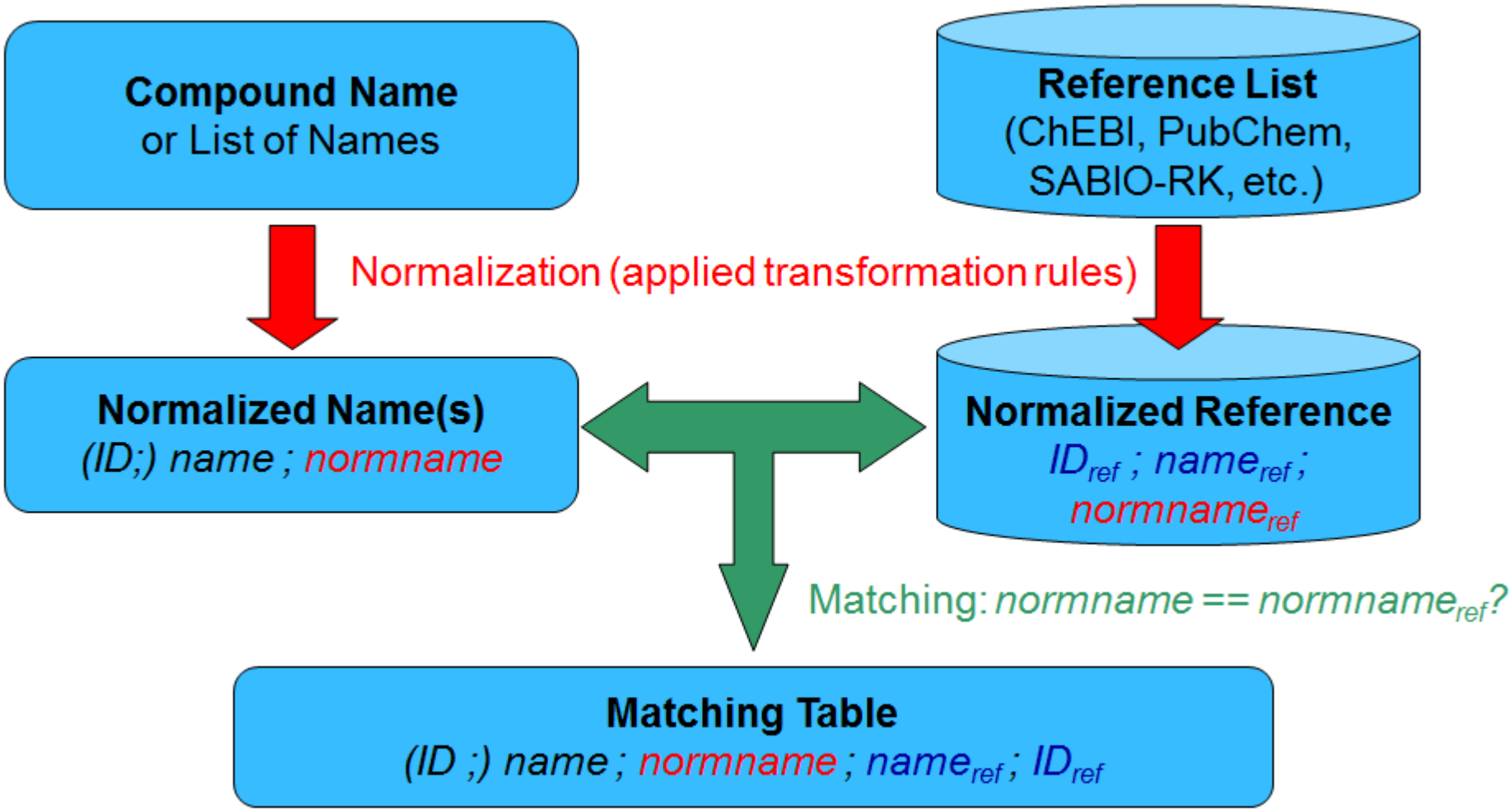
Chemical Name Matching



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HITS

ChemHits

http://sabio.h-its.org/chemHits/

chemical compound name normalization and matching

Short Documentation

Match

Results in chebi060312 for *2-aminoprop-2-enoic acid*

ID (chebi060312)	Name (chebi060312)
17123	2-aminoacrylic acid
58020	2-aminoacrylate

Back to ChemHits Search Save Results

Name of C

Select Da

Perform A

Search for

Match Name

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Wittig U, Kania R, Golebiewski M, Rey M, Shi L, Jong L, Algaa E, Weidemann A, Sauer-Danzwith H, Mir S, Krebs O, Bittkowski M, Wetsch E, Rojas I, Müller W

Nucleic Acids Research (2012) 40 (D1): D790-D796 *(doi: 10.1093/nar/gkr1046)*

Tutorial video: http://sabio.h-its.org/redesign/files/SABIORKtutorial.mp4

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