

Reaction kinetics database SABIO-RK

Andreas Weidemann
HITS Heidelberg, Germany
SDBV group

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SDBV group @ HITS

Data management for scientists in life sciences

Current major projects:

- SABIO-RK: reaction kinetics database
- SEEK: for sharing heterogeneous scientific research datasets, including models, data sheets, images...
- OperationExplorer: visualization of health data from German hospitals; in collaboration with investigative journalists
- Standards: NormSys (Martin)
- ...



Motivation for a reaction kinetics database

- quantitative data on reaction kinetics are required e.g. for modellers
- problem: hard to find in literature

=> 2005 / 2006 start of collecting reaction kinetics data, storage in a public accessible database

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

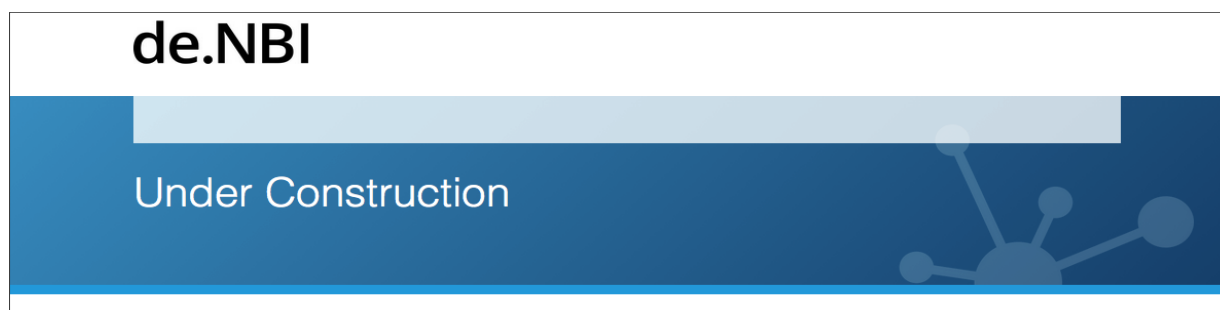
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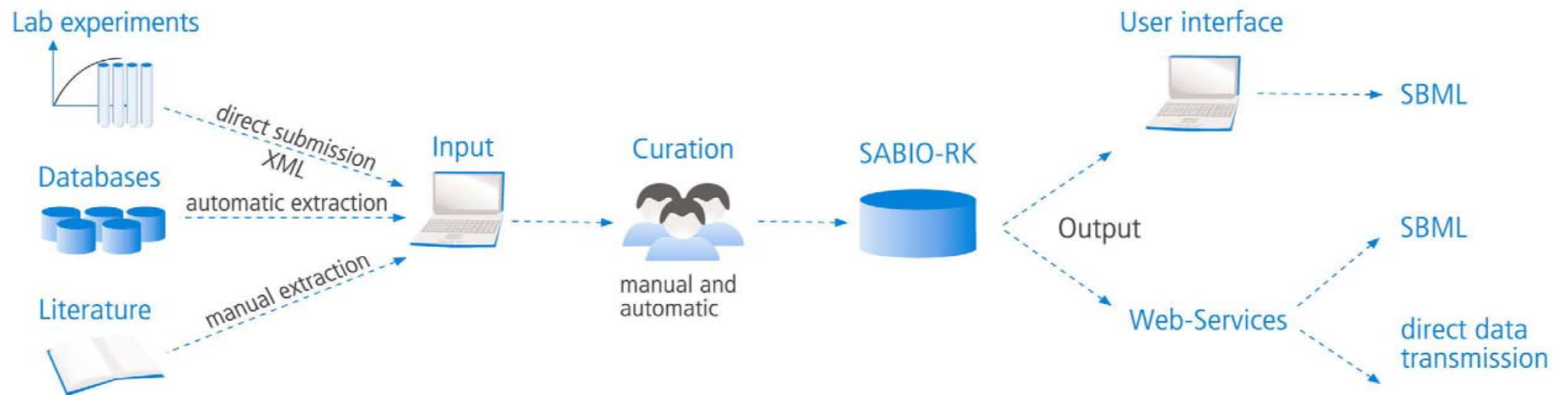
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<http://sabiork.h-its.org/>

- SABIO-RK is now part of 'The German Network for Bioinformatics Infrastructure' (de.NBI) which is still in consolidation phase:



SABIO-RK: data workflow



Data extraction from literature

- kinetics data from literature are manually entered via a web form => standardization
- the data are manually annotated, e.g. EC number and UniProtKB ID are added
- further automatic annotations performed: KEGG, PubChem,...
- in agreement with @ Pedro: many data are found in figures / figure legends and tables => not searchable in PubMed abstracts

Stored data I


| General information | | | | |
|---------------------------------------|---|--------------------|-------------------|-----------------|
| Organism | Homo sapiens | | | |
| Tissue | erythrocyte ↗ | | | |
| EC Class | 2.7.1.1 | | | |
| SABIO reaction id | 793 | | | |
| Variant | wildtype | | | |
| Experiment Type | in vitro | | | |
| Pathways | Glycolysis classical Glycolysis/Gluconeogenesis Starch and Sucrose metabolism | | | |
| Event Description | - | | | |
| Substrates | | | | |
| name | location | comment | | |
| ATP | - | - | | |
| D-Glucose | - | - | | |
| Products | | | | |
| name | location | comment | | |
| ADP | - | - | | |
| D-Glucose 6-phosphate | - | - | | |
| Modifiers | | | | |
| name | location | effect | comment | protein complex |
| N-Acetylglucosamine | - | Modifier-Inhibitor | - | - |
| hexokinase(Enzyme) | - | Modifier-Catalyst | - | HXX; |
| Enzyme (protein data) | | | | |
| | UniProtKB_AC | name | mol. weight (kDa) | deviation (kDa) |
| subunit | - | - | - | - |
| complex | - | - | 132.0 | 8.0 |

Stored data II

| Kinetic Law | | | | | | | |
|--|---|---------------------|-------------------------------|----------|---------|--------------------------|----------------|
| type | | formula | annotation | | | | |
| Competitive inhibition | | - | SBO:0000260 ↗ | | | | |
| Parameter | | | | | | | |
| name | type | species | start val. | end val. | deviat. | unit | comment |
| A | concentration ↗ | ATP | 5.0 | - | - | mM | - |
| Ki | Ki ↗ | N-Acetylglucosamine | 0.3 | 0.5 | - | mM | versus Glucose |
| Km2 | Km ↗ | D-Glucose | 0.048 | 0.08 | - | mM | - |
| Km1 | Km ↗ | ATP | 0.57 | 1.0 | - | mM | MgATP |
| Experimental conditions | | | | | | | |
| | start value | | end value | | | unit | |
| temperature | 37.0 | | | | | - | °C |
| pH | 7.25 | | | | | - | - |
| buffer | 0.033 M Tris/HCl, 10 mM MgCl2, 0.33 mM NADP+, 0.15 I.U. Glucose-6-phosphate dehydrogenase, 0.15 I.U. 6-Phosphogluconate dehydrogenase | | | | | | |
| comment | - | | | | | | |
| Reference | | | | | | | |
| title | author | year | journal | volume | pages | PubMed | |
| Purification and some properties of human erythrocyte hexokinase | Rijksen G, Staal GE | 1976 | Biochim Biophys Acta | 445 | 330-41 | 953036 ↗ | |

Data annotation

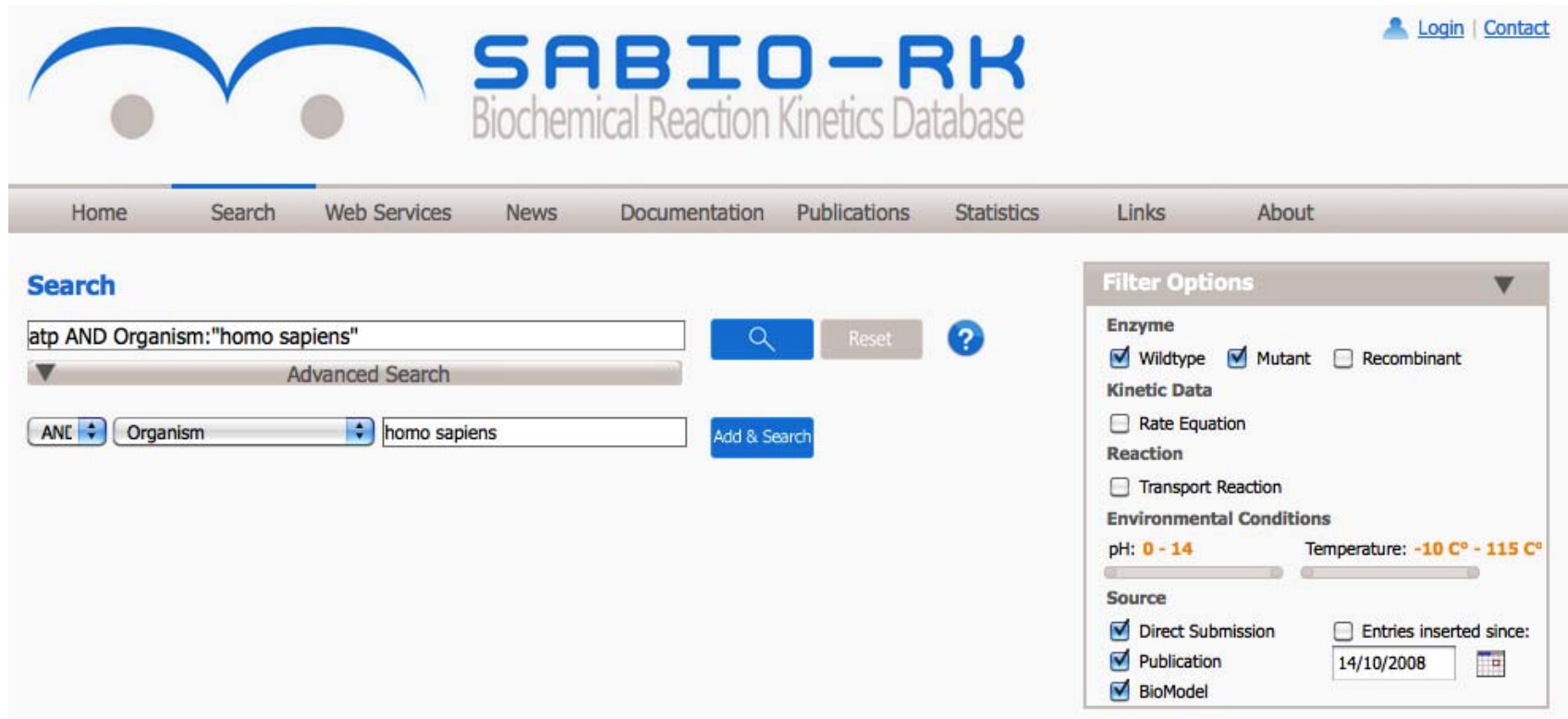
example 'ATP' as compound



| Compound Details | | List of Reactions |
|-------------------|--|-------------------|
| Common Name | ATP | |
| Synonyms | Adenosine 5'-triphosphate Adenosine triphosphate | |
| SABIO-Compound-ID | 34 | |
| InChI | InChI=1/C10H16N5O13P3 /c11-8-5-9(13-2-12-8)15(3-14-5)10-7(17)6(16)4(26-10)1-25-30(21,22)28-31(23,24)27-29(18, /h2-4,6-7,10,16-17H,1H2,(H,21,22)(H,23,24)(H2,11,12,13)(H2,18,19,20)/t4-,6-,7-,10-/m1/s1 | |
| SMILES | Nc3ncnc1c3(ncn1C2OC(COP(O)(=O)OP(O)(=O)OP(O)(O)=O)C(O)C2(O)) | |
| External Links | | |
| KEGG-ID | C00002 ↗ | |
| PUBCHEM-ID | 3304 ↗ | |
| ChEBI-ID | 15422 ↗ 30616 ↗ | |

Public search interface

provides many options for detailed search



The image shows the public search interface of the SABIO-RK Biochemical Reaction Kinetics Database. The header features the SABIO-RK logo and navigation links for Login and Contact. A horizontal menu bar contains links to Home, Search, Web Services, News, Documentation, Publications, Statistics, Links, and About. The main search area includes a text input field with the query "atp AND Organism: 'homo sapiens'", a search button, a Reset button, and a help icon. Below this is an "Advanced Search" section with a dropdown menu and a text input field containing "homo sapiens". To the right, a "Filter Options" panel allows users to refine their search by Enzyme (Wildtype, Mutant, Recombinant), Kinetic Data (Rate Equation), Reaction (Transport Reaction), Environmental Conditions (pH: 0 - 14, Temperature: -10 C° - 115 C°), and Source (Direct Submission, Publication, BioModel). The Source section also includes a date selector for "Entries inserted since: 14/10/2008".

SABIO-RK
Biochemical Reaction Kinetics Database

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Search

atp AND Organism: "homo sapiens"

Advanced Search

ANC Organism homo sapiens Add & Search

Filter Options

Enzyme

☒ Wildtype ☒ Mutant ☐ Recombinant

Kinetic Data

☐ Rate Equation

Reaction

☐ Transport Reaction

Environmental Conditions

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

Source

☒ Direct Submission ☐ Entries inserted since: 14/10/2008

☒ Publication

☒ BioModel

Search results

search for 'ATP' and 'homo sapiens'

Total number of kinetic law entries found: **1627**

1 2 3 4 5 6 7 8 9 10 .. 109 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-Glucose + ATP = ADP + D-Glucose 6-phosphate | 2.7.1.1 | | wildtype | erythrocyte ↗ | Homo sapiens | Ki Km | 37.0 | 7.25 | <input type="checkbox"/> |

Entry ID: 10716

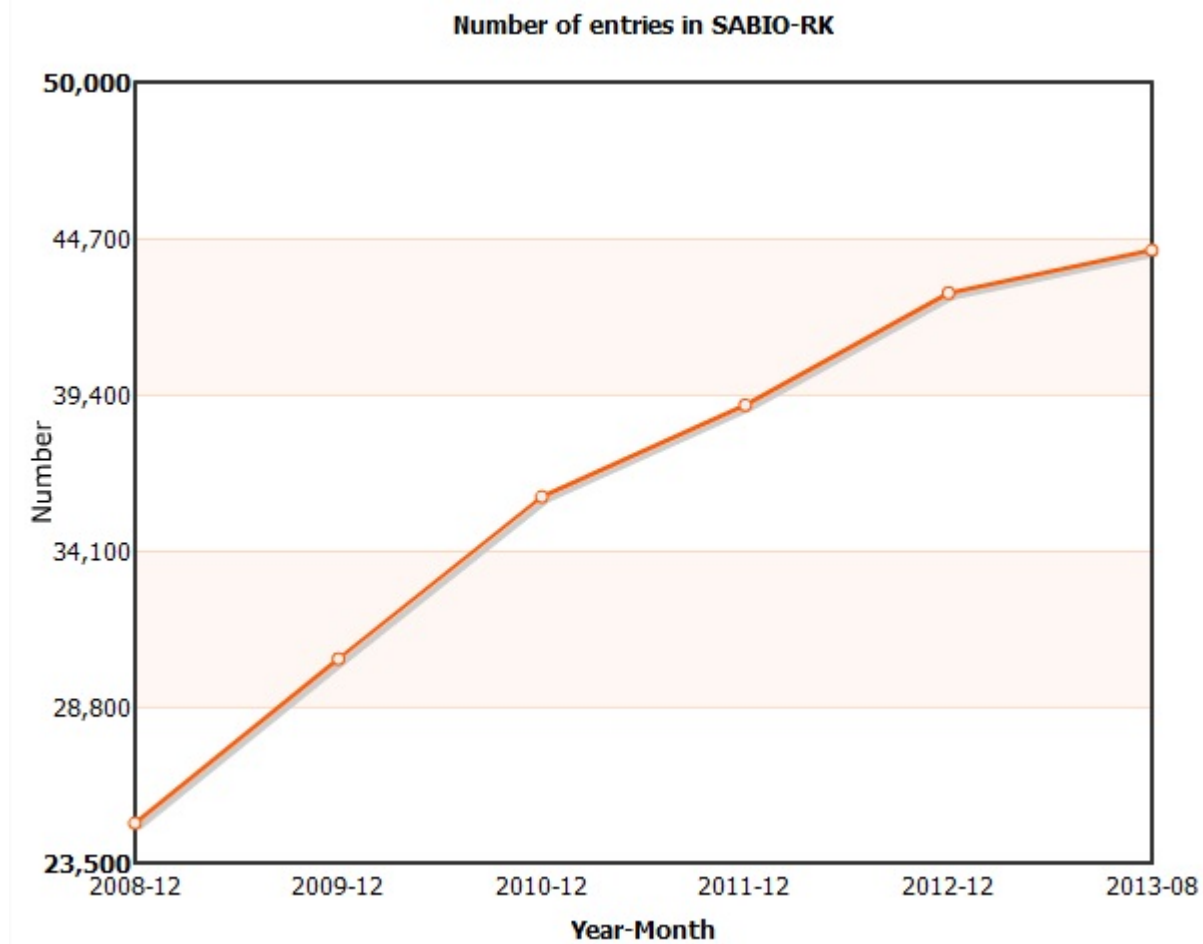
General information

| | |
|-------------------|---|
| Organism | Homo sapiens |
| Tissue | erythrocyte ↗ |
| EC Class | 2.7.1.1 |
| SABIO reaction id | 793 |
| Variant | wildtype |
| Experiment Type | in vitro |
| Pathways | Glycolysis classical Glycolysis/Gluconeogenesis Starch and Sucrose metabolism |
| Event Description | - |

Substrates

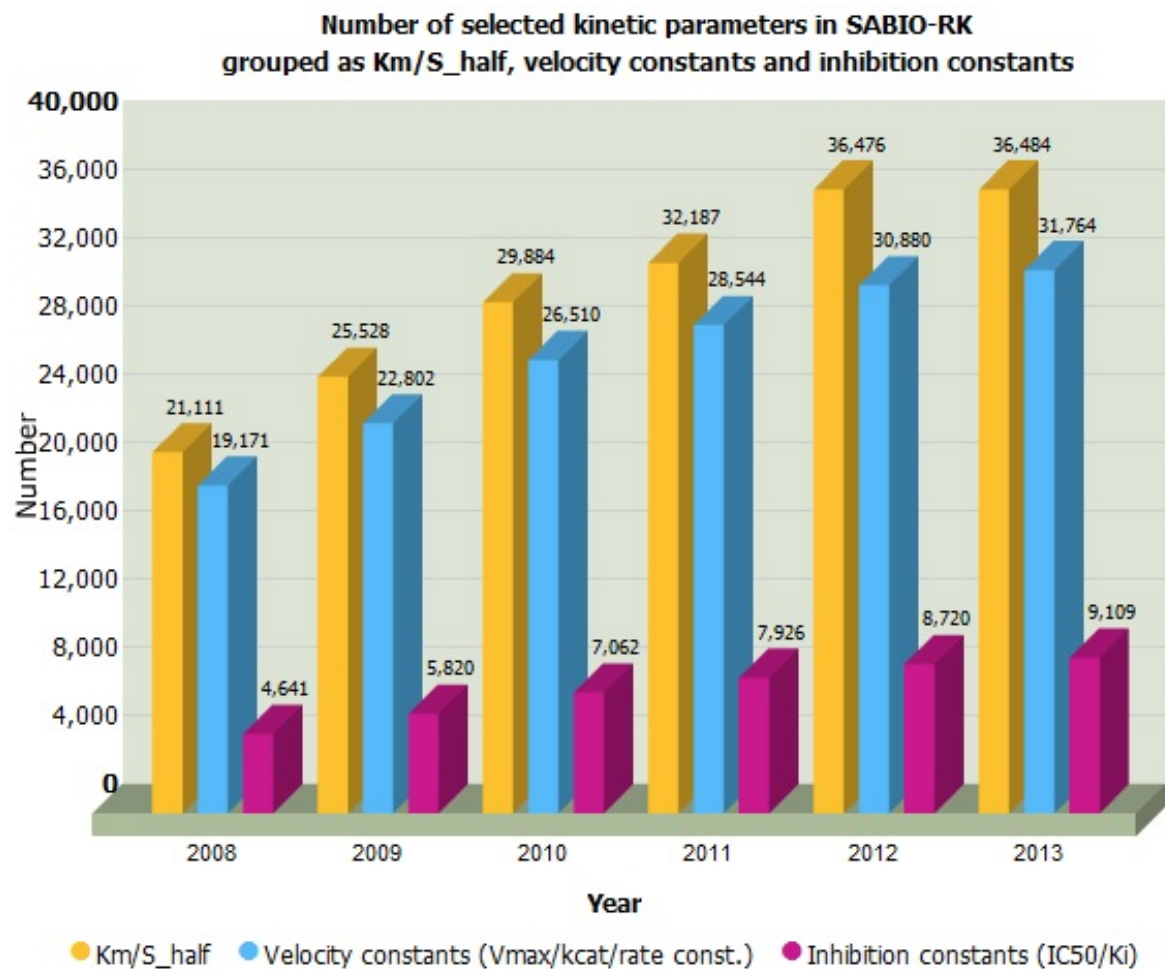
| name | location | comment |
|---------------------------|----------|---------|
| ATP | - | - |
| D-Glucose | - | - |

Statistics I



as of October 2015: 52.672 single entries

Statistics II



kinetic parameter as of October 2015: 116.287

Data upload and data import into SABIO-RK

- direct submission of experimental data
- kinetics data in SBML format:



Upload an SBML file

File: SABIOmdl1... 14402.xml

File Type:

SBML: ☒

FREI: ☐

upload of SBML file

↓
parsing & mapping of entities

↓
annotation

↓
storage in database



RESTfull webservices I

- allows programmatic access of data
- example: get the list of SABIO kinetic law entries:

[http://sabiork.hits.org/sabioRestWebServices/searchKineticLaws/entryIDs?q=Tissue:"spleen" AND Organism:"Homo sapiens"](http://sabiork.hits.org/sabioRestWebServices/searchKineticLaws/entryIDs?q=Tissue:)

- returns SBML document

RESTfull webservices II

application and tools using SABIO-RK webservices:

- CellDesigner
- JWS Online (Jacky Snoep)
- Virtual Cell (VCell, Ion Moraru)
- CySABIO-RK-Plugin for Cytoscape (Matthias König)
- BioUML (Mandrik, Kiselev,...)
- Path2Models
- Bio2RDF
- Virtual Liver Network (Matthias König)
- University of Manchester (integrated into Taverna workflows)
- Systems Biology Metabolic Modeling Assistant SBMM (Univ. Malaga)
- SBMLsqueezer (Andreas Dräger)
-

Data export

- spreadsheets (tables, PDF)
- BioPax (main entities, mapping coded by Oliver Ruebenacker)
- SBML:



The screenshot displays the SABIO-RK Biochemical Reaction Kinetics Database interface. At the top, there is a navigation bar with links for Home, Search, Web Services, News, Documentation, Publications, Statistics, Links, and About. The main content area shows a table of selected kinetics data with columns for Entry ID, Selected Reaction, Organism, Tissue, Kinetic law type, View details, and Remove entry (Select all: ☐). The table lists five entries, each with a reaction equation, organism, tissue, and kinetic law type. Below the table, there is a button labeled 'remove selected Reactions'. At the bottom, there are buttons for 'Back to Results', 'Write spreadsheet', 'Write SBML', and 'Write BioPAX', along with a 'beta' badge.

SABIO-RK
Biochemical Reaction Kinetics Database

Entries to Export: 5

Home Search Web Services News Documentation Publications Statistics Links About

Selected kinetics data

| Entry ID | Selected Reaction | Organism | Tissue | Kinetic law type | View details | Remove entry (Select all: <input type="checkbox"/>) |
|----------|--|------------------------------------|--------|-----------------------|----------------------|--|
| 49364 | H ₂ O + Sucrose 6-phosphate <-> Phosphate + Sucrose | Saccharum officinarum | stem | Michaelis-Menten | view | <input type="checkbox"/> |
| 49363 | UDP-D-glucose + D-Fructose 6-phosphate <-> UDP + Sucrose 6-phosphate | Saccharum officinarum | stem | reversible ordered Bi | view | <input type="checkbox"/> |
| 12527 | H ₂ O + Sucrose 6-phosphate <-> alpha-D-Glucose 6-phosphate + beta-D-Fructose | Lactococcus lactis subsp. lactis | - | Michaelis-Menten | view | <input type="checkbox"/> |
| 18577 | alpha-D-Glucose 1-phosphate <-> alpha-D-Glucose 6-phosphate | Lactococcus lactis subsp. cremoris | - | Michaelis-Menten | view | <input type="checkbox"/> |
| 3460 | D-Glucose 1-phosphate <-> alpha-D-Glucose 6-phosphate | Rattus norvegicus | heart | Michaelis-Menten | view | <input type="checkbox"/> |

[remove selected Reactions](#)

[Back to Results](#) [Write spreadsheet](#) [Write SBML](#) [Write BioPAX](#) [beta](#)



Data export in SBML format – problems

- issues encountered eg:
 - concentration ranges as boundary conditions
 - enzyme
 - compounds
 - experimental conditions (pH, temp., ...) only in SABIO_RK namespace exported
 - description of enzyme complexes

Data import from SBML files – challenges

- most of the information in SBML is optional (e.g. units, names)
- global and local attributes (e.g. global parameters for whole model and local parameters for single reactions)
- sometimes missing organism (e.g. „cellular organisms“ in 74 curated models in BioModels DB)
- frequently missing annotations to UniprotKB for enzymes/catalysts (only EC number)
- missing parameter definitions (Km, Vmax etc.)
- abbreviations for compound names (used only within the model – no standard controlled vocabulary)



Your data ...

if you are interested ...

- we could focus on your specific research topic and insert relevant publications
- please feel free to send us your data as SMBL
- talk to us about uploading and storage of your data in other formats



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