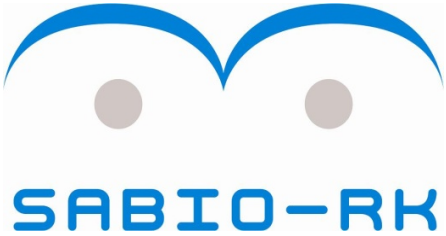

Heidelberger Institut für
Theoretische Studien

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

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Heidelberg Institute for Theoretical Studies
HITS gGmbH, Germany

COMBINE Tutorial 2017, August 6th, Blacksburg, Virginia

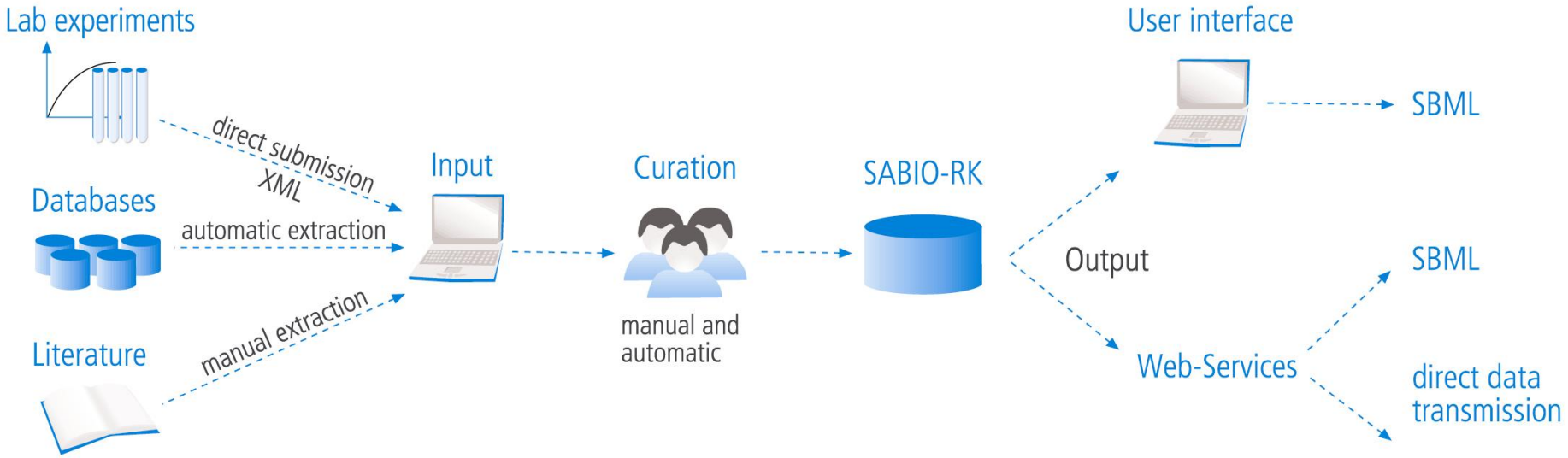
Data sources for modelling

Data sources for quantitative kinetics data including parameters, equations, …

can be obtained from:

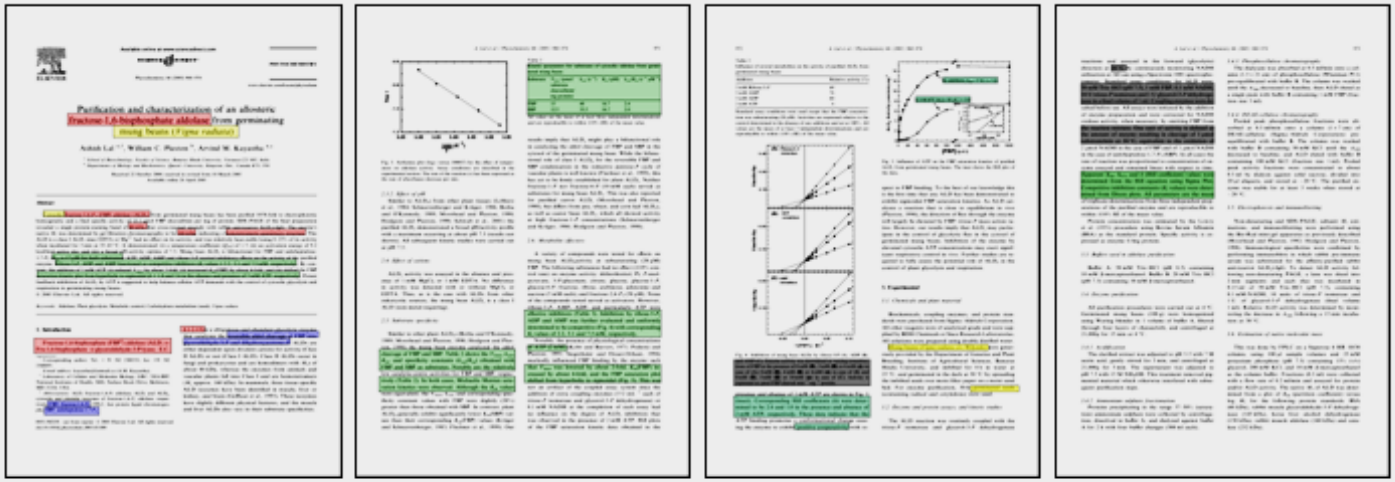
- experimenters
- literature
- kinetics databases

Sabio-RK
Database Population and Access

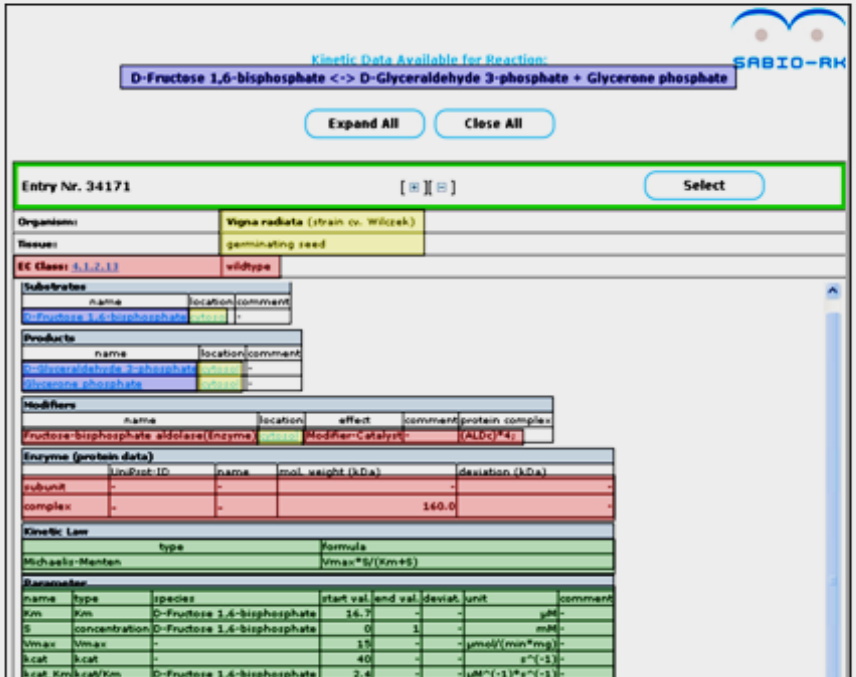


Biocuration: Adding Value to Data

A



B



Added Value:

- Clean
- Standardized
- Annotated
- Interlinked

→ **High quality data**

Protein- bzw. Enzymdaten
Reaktionen und chemische Verbindungen
kinetische Daten
experimentelle Bedingungen
biologische Quelle (Organismus, Gewebe, Zelltyp)

SABIO-RK
Biochemical Reaction Kinetics Database

Welcome!

http://sabiork.h-its.org

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

News

SABIO-RK at ICSB2017
05-29-2017
Tutorial at ICSB2017 in Blacksburg, Virginia
Modelling and Simulation Tools in Systems Biology

more>>

SABIO-RK Training Event
04-06-2017
Introduction and Hands-on Training on May 31st, 2017 in Heidelberg

more>>

SABIO-RK
Biochemical Reaction Kinetics Database

Login | Contact

Entries to Export: 1

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

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

SABIO-RK user interface: detailed search options

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)	-

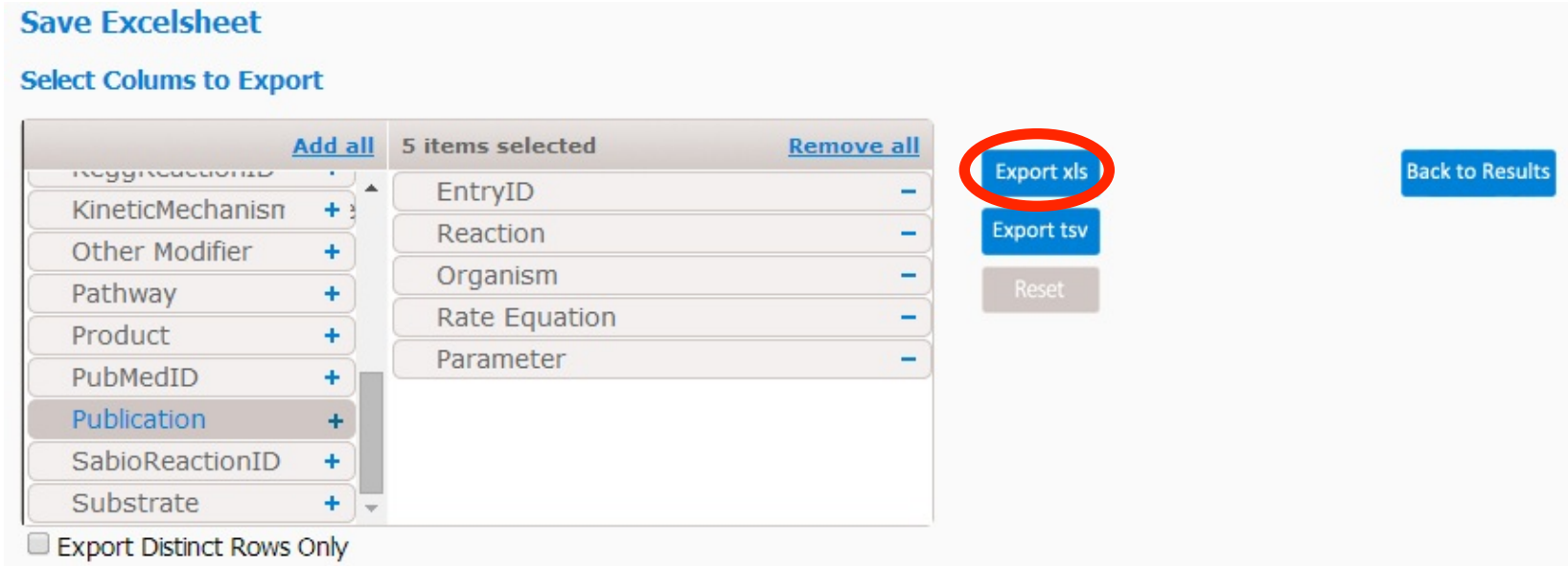
Experimental conditions			
	start value	end value	unit
temperature	22.0	-	°C
pH	7.6	-	-
buffer	50 mM Tris-acetate, 0.15 mM NADH, 10 mM EDTA, 100 mg/ml bovine serum albumin, 2 mg/ml alpha-glycerophosphate dehydrogenase/triose phosphate isomerase		
comment	-		

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: Spreadsheets

SABIO-RK public user interface

Data Export: Spreadsheets



SABIO-RK public user interface

Preview of the first 5 entries

Sabio Excel Export Preview

	A	B	C	D	E	F	G
1	EntryID	Reaction	Organism	Rate Equation	parameter.type	parameter.asso…	parameter.sta
2	49363	UDP-D-glucose …	Saccharum offic…	vol*Vmax6f*(0.0…	Km	Sucrose 6-phos…	1.0E-4
3	49363	UDP-D-glucose …	Saccharum offic…	vol*Vmax6f*(0.0…	concentration	D-Fructose 6-p…	0.001
4	49363	UDP-D-glucose …	Saccharum offic…	vol*Vmax6f*(0.0…	Keq		10.0
5	49363	UDP-D-glucose …	Saccharum offic…	vol*Vmax6f*(0.0…	Ki	Sucrose 6-phos…	7.0E-5
6	49363	UDP-D-glucose …	Saccharum offic…	vol*Vmax6f*(0.0…	Km	UDP	3.0E-4
7	49363	UDP-D-glucose …	Saccharum offic…	vol*Vmax6f*(0.0…	Km	UDP-D-glucose	0.0018
8	49363	UDP-D-glucose …	Saccharum offic…	vol*Vmax6f*(0.0…	concentration	UDP	2.0E-4
9	49363	UDP-D-glucose …	Saccharum offic…	vol*Vmax6f*(0.0…	Ki	Phosphate	0.003
10	49363	UDP-D-glucose …	Saccharum offic…	vol*Vmax6f*(0.0…	Km	D-Fructose 6-p…	6.0E-4

Data Export: SBML

Login | Contact

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: ☐)
49364	H2O + Sucrose 6-phosphate <-> Phosphate + Sucrose	Saccharum officinarum	stem	Michaelis-Menten	view	☐
49363	UDP-D-glucose + D-Fructose 6-phosphate <-> UDP + Sucrose 6-phosphate	Saccharum officinarum	stem	reversible ordered Bi	view	☐
12527	H2O + Sucrose 6-phosphate <-> alpha-D-Glucose 6-phosphate + beta-D-Fructose	Lactococcus lactis subsp. lactis	-	Michaelis-Menten	view	☐
18577	alpha-D-Glucose 1-phosphate <-> alpha-D-Glucose 6-phosphate	Lactococcus lactis subsp. cremoris	-	Michaelis-Menten	view	☐
3460	D-Glucose 1-phosphate <-> alpha-D-Glucose 6-phosphate	Rattus norvegicus	heart	Michaelis-Menten	view	☐

remove selected Reactions

Back to Results | Write spreadsheet | Write SBML | Write BioPAX (beta)

Data Export: SBML
(Systems Biology Markup Language)

Login | Contact

Entries to Export: 5

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

Save Model

Enter name of model: SABIOmdl15Aug20143 | SBML level 3, version 1

Export parameters normalized to SI base units

Choose the annotation schema *: identifier.org
- identifier.org
- Miriam URI

Save Model on Disk as SBML

Save Model on Disk as PDF

Back to Results

SBML

SBML LATEX

* For details please refer to http://identifiers.org/ or http://co.mbine.org/standards/miriam_uris .

Data Export: SBML

```
This model has been created with the help of the SABIO-RK Database
(http://sabio.h-its.org/)
 (c) 2005-2014 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
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              </apply>
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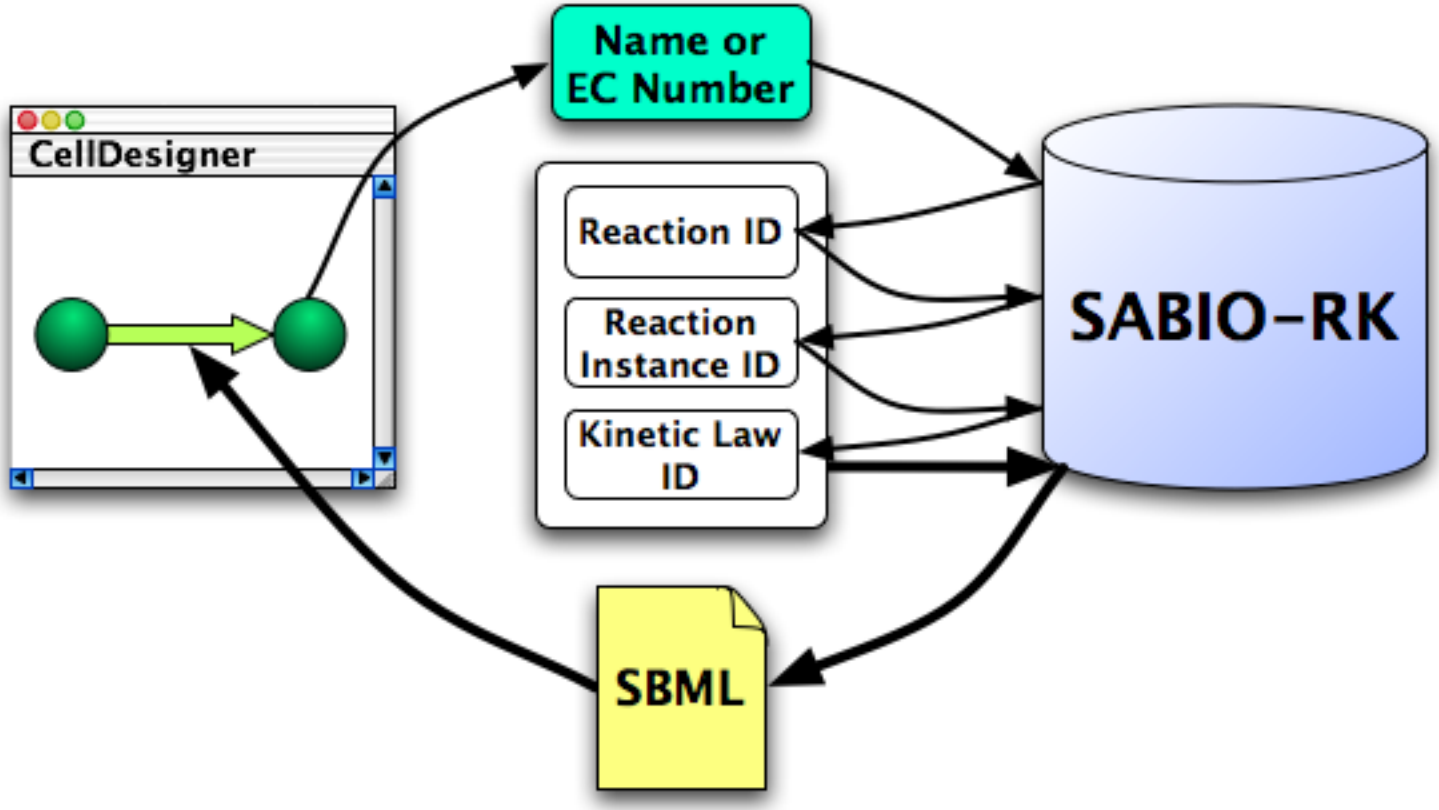
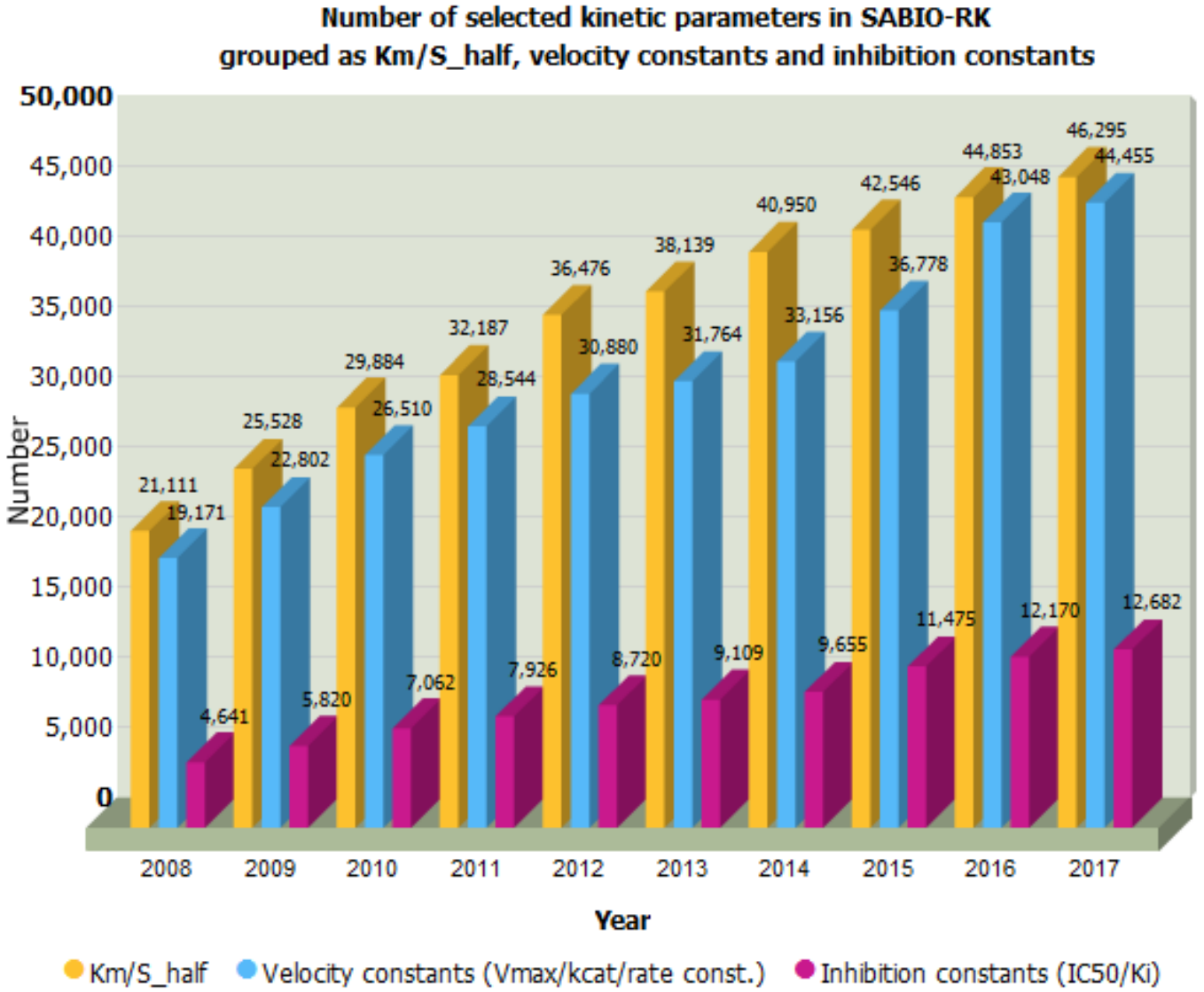
Kinetic Rate Equations
(… and all other relevant data)

SABIO-RK API Access
Integration into Modeling Tools



http://www.celldesigner.org

SABIO-RK Content



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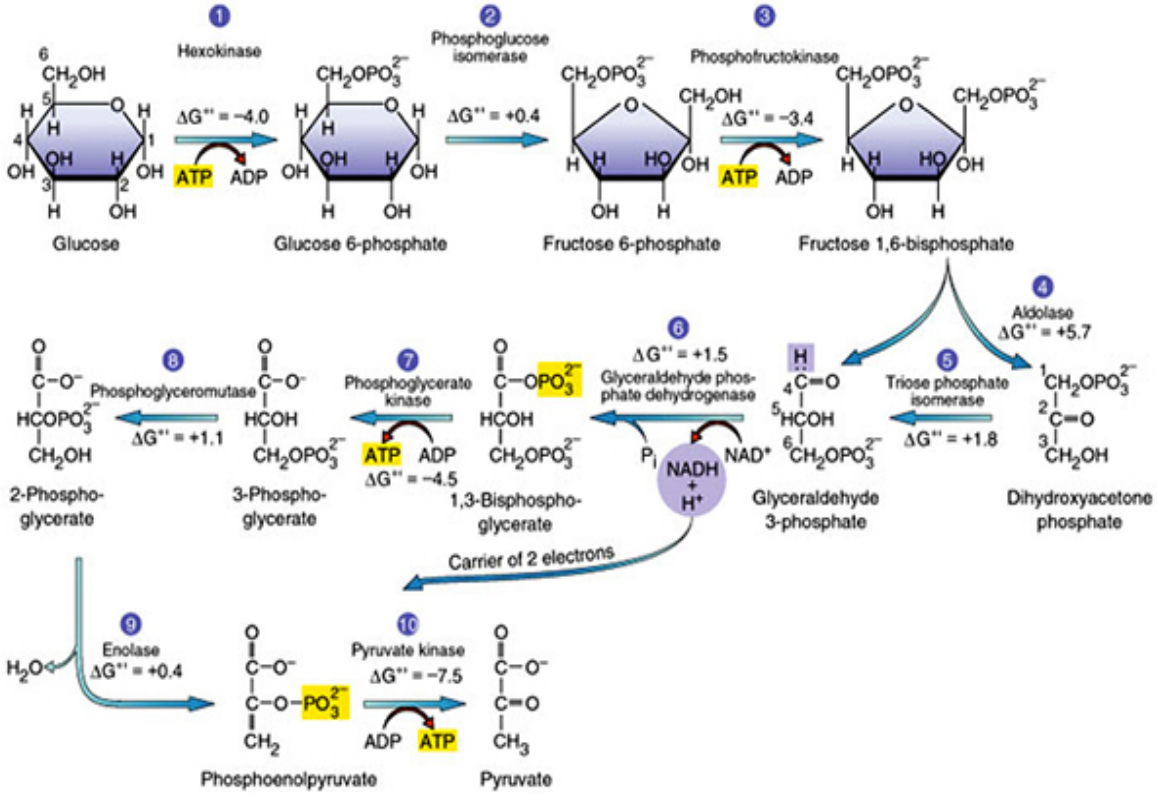
Hands-on



- perform distinct searches for first 3 steps in Glycolysis
'Hexokinase: Gluc + ATP → Gluc-6-P + ADP
'Phosphoglucose isomerase': Gluc-6-P → Fruc-6-P
'Phosphofructokinase': Fruc-6-P + ATP → Fruc-1,6-P + ADP
- collect entries in 'basket'
- export entries as SBML file (save on disk)

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