

Heidelberger Institut für Theoretische Studien



Upload of Kinetic Data into SABIO-RK via SBML

Martin Golebiewski Heidelberg Institute for Theoretical Studies HITS gGmbH, Germany

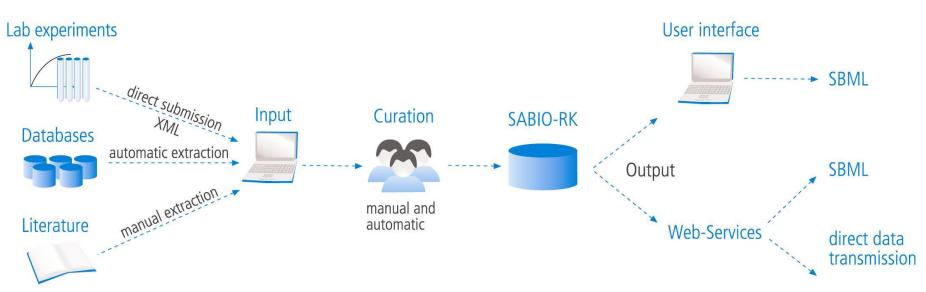
COMBINE 2014, Los Angeles, August 18-22



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- 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 <u>reaction mechanisms</u>
- > 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 spreadsheet and standard formats (SBML & BIOPAX)





SABIO-RK

http://sabiork.h-its.org

Unified

Structured

Normalized

Interrelated

Annotated

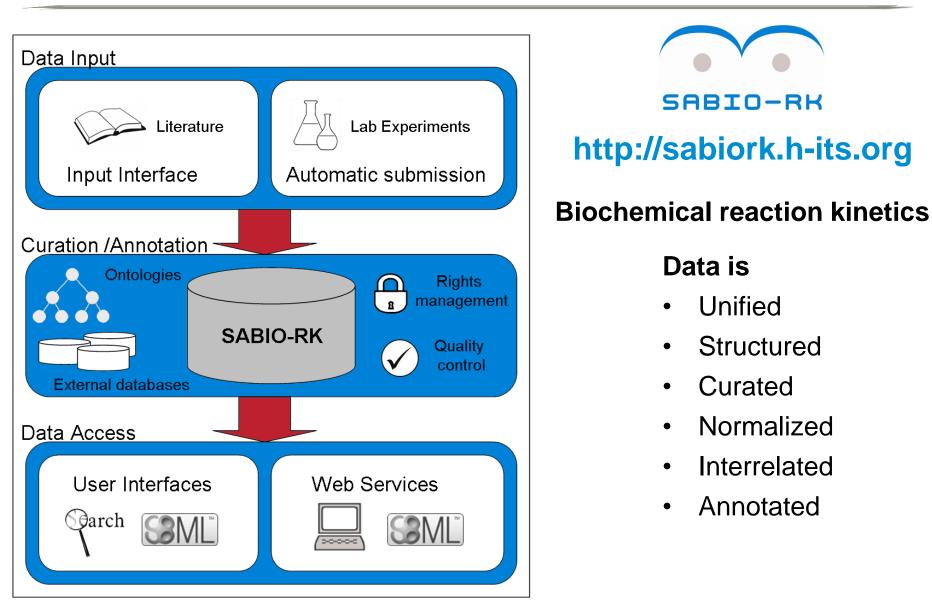
Curated

Data is

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В	D-Fractose 1,6-bisphosphate <- Exception of the second s	re- dialyze: [ALD1]*47	phate SRBIO-RH ielect	 Protein Reaktion kinetiso 	Standardized Coherent



Welcome!

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



News

COMBINE & ERASysAPP Tutorial

18-06-2014 SABIO-RK at the tutorial "Modelling and Simulation of Biological Models" on Sunday, September 14th, 2014 at the ICSB in Melbourne more≫

STRENDA Special Issue 16-06-2014

Special Issue: Reporting Enzymology Data – STRENDA Recommendations and Beyond – a highly educational, open access collection of 14 articles more»

http://sabiork.h-its.org

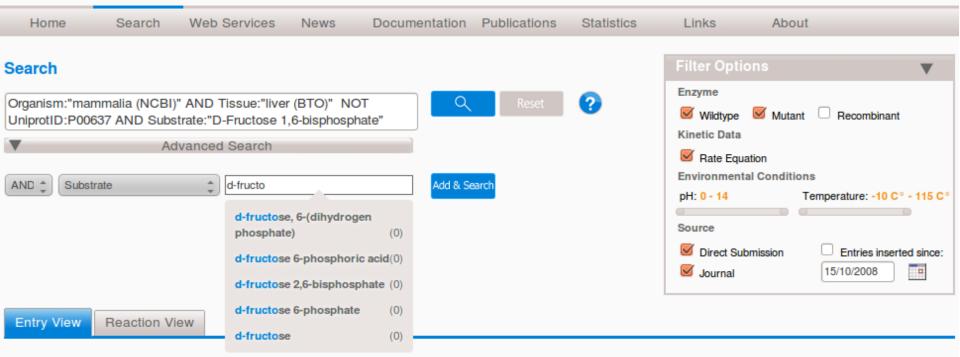
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SABIO-RK Biochemical Reaction Kinetics Database



Total number of kinetic law entries found: 40

1 2 3 Next

display 15 - entries per page

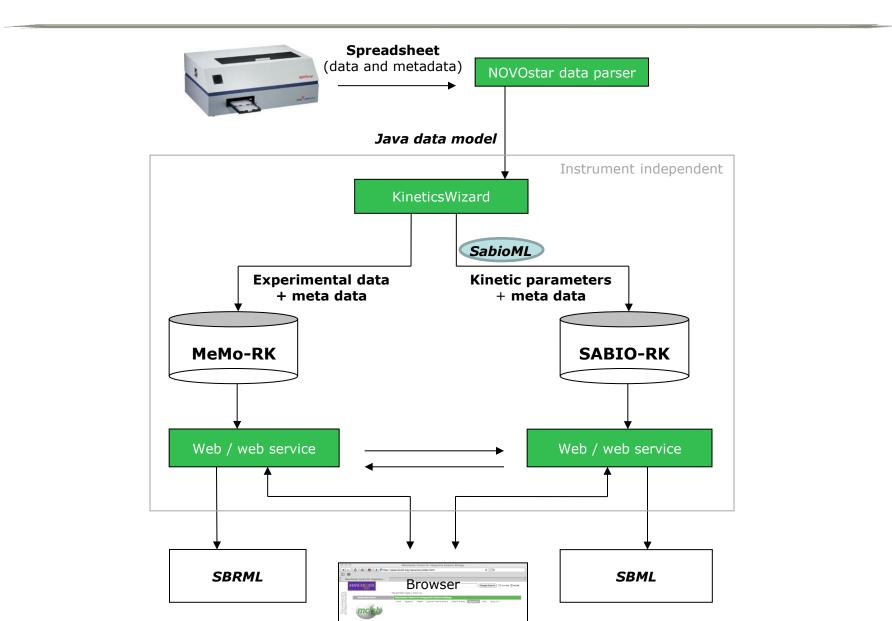
Login | Contact

Kinetic	Reaction		Enzyme		Tissue	Organism	Parameter (besides	Environment		Add to export
data D	neaction	ECNumber	Protein	Variant	1133 46	organishi	concentration)	°C	рН	cart?
	D-Fructose 1,6-bisphosphate + H2O = D-Fructose 6-phosphate + Orthophosphate	3.1.3.11	ר <u>ג Q9N0J6</u>	wildtype	liver '	Oryctolagus cuniculus	Kd Km Vmax	25.0	9.5	
	H2O + D-Fructose 1,6-bisphosphate =	3.1.3.11	ק ע3SZB7 ק	wildtype	liver ר	Bos taurus	Km Vmax	28.0	6.5	

▼	1,6- Glyo D-G	cerone	osphate = e phosphat ildehyde	te +	4.1.2.1	13 <u>F</u>	<u>05062</u> -	aldo	lase B		<u>ver</u> יד	Homo sapiens	Vmax Km	22.0	7.6	8
	Entry ID: 2175															
Gener	General information															
Organi	sm		Homo	<u>sapiens</u>												
Tissue			liver T	1												
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SABIO	reactio	on id	1338													
Varian	t			e aldolase												
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s (D-Fructose								-	-						
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Glyce	rone p	hosphat	e						-			-				
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Expression, purification, and characterization of natural mutants of human aldolase B. Role of quaternary structure in catalysis.					Rellos I Sygusc Cox TN	hJ,	200	00	J Biol Chem		27	5114	45-51	<u>106</u>	62565	ד 2







Direct Data Submission





Enzyme kinetics informatics: from instrument to browser

Neil Swainston^{1,†}, Martin Golebiewski^{2,†}, Hanan L. Messiha¹, Naglis Malys¹, Renate Kania², Sylvestre Kengne², Olga Krebs², Saqib Mir², Heidrun Sauer-Danzwith², Kieran Smallbone¹, Andreas Weidemann², Ulrike Wittig², Douglas B. Kell¹, Pedro Mendes^{1,3}, Wolfgang Müller², Norman W. Paton¹, Isabel Rojas²

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Additional Information (Show All)

How to Cite Author Information Publication History

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Issue



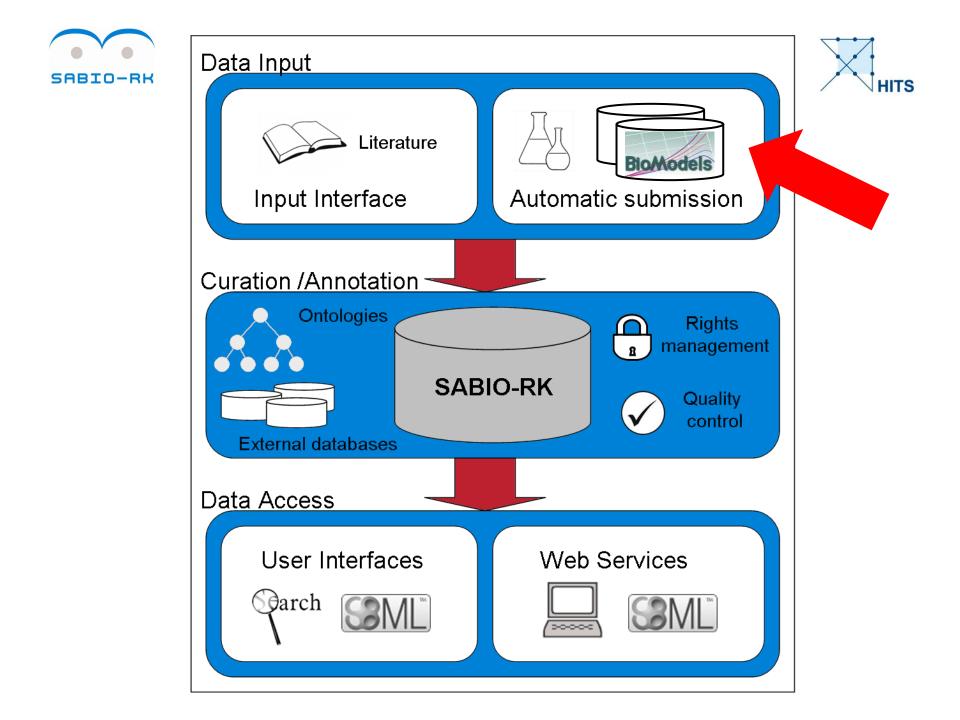
FEBS Journal

Volume 277, Issue 18, pages 3769–3779, September 2010



These authors contributed equally to this work

+*

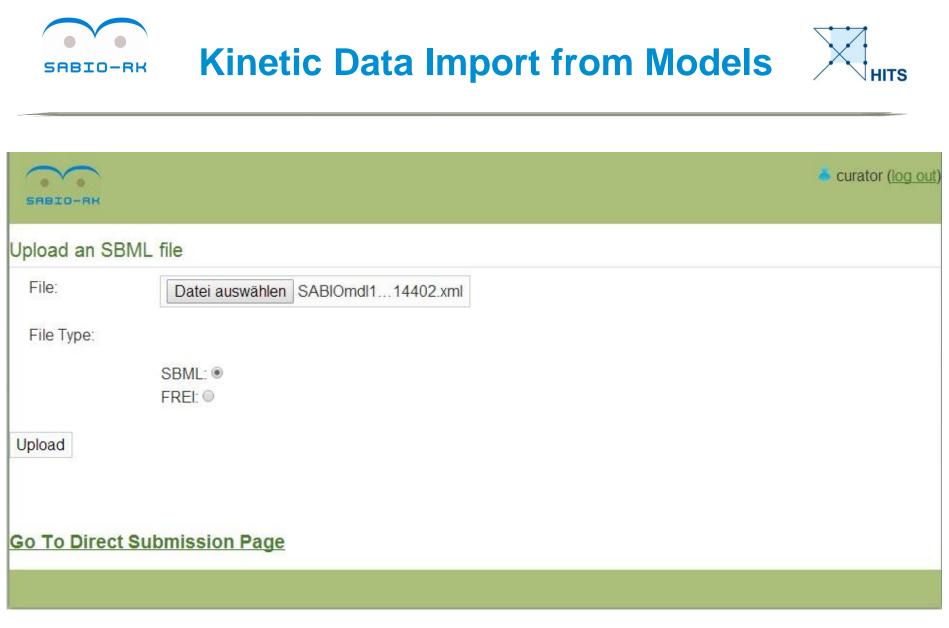


Kinetic Data Import from Models

SABIO-RK



MBL-EBI	Services Research Training About us
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BIOMD00000023 - Rohwer2001_Sucrose	
Download SBML I Other formats (auto- generated) I Actions I Send feedback	
Model Overview Math Physical entities Parameters Curation	
Reference Publication	
Publication ID: 11513743 Rohwer JM, Botha FC. Publication ID: 11513743 Analysis of sucrose accumulation in the sugar cane culm on the basis of in vitro kinetic data. Biochem. J. 2001 Sep; 358(Pt 2): 437-445 Department of Biochemistry, University of Stellenbosch, Private Bag X1, 7602 Matieland, South Africa. jr@maties.sun.ac.za [more]	
Model	
Original Model: <u>BIOMD000000023 xml.origin</u> set #1 bqbiol:is <u>KEGG Pathway map00500</u>	
Submitter: Nicolas Le Novère bqbiol:isVersionOf Gene Ontology sucrose biosynthetic process	
Submission ID: MODEL6618063111 bqbiol:occursIn Taxonomy Saccharum officinarum	
Submission Date: 13 Sep 2005 13:28:04 UTC	
Last Modification Date: 20 May 2012 12:43:33 UTC	
Creation Date: 03 May 2005 13:08:30 UTC	
Encoders: Jacky L Snoep	
Notes	
<u>SBML</u> Level 2 code generated for the JWS Online project by Jacky Snoep using <u>PySCeS</u> .	
Run this model online at http://iji.biochem.sun.acza.	
To cite JWS Online please refer to: Olivier, B.G. and Snoep, J.L. (2004) Web-based modelling using JWS Online, Bioinformatics, 20:2143-2144.	
This model originates from BioModels Database: A Database of Annotated Published Models. It is copyright (c) 2005-2010 The BioModels Team. For more information see the <u>terms of use</u> .	
To cite BioModels Database, please use Le Novère N. Bornstein B., Broicher A., Courtot M., Donizelli M., Dharuri H., Li L., Sauro H., Schilstra M., Shapiro B., Snoep J.L., Hucka M. (2006) BioModels Database: A Free, Centralized of Biochemical and Cellular Systems Nucleic Acids Res., 34: D689-D691.	d Database of Curated, Published, Quantitative Kinetic Models
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SABIO-RK SBML upload interface



Kinetic Data Import from Models



Publication entries

Publication ID 4864 (11 entries)

Reference

ID) Title	Authors	Journal	Volume	Pages	Year F	PubMed	Туре	Identifier	Organization	Responsible Person	Contact Email	Contact Phone	Base Url
486	Analysis of sucrose accumulation in the sugar cane culm on the basis of in vitro kinetic data.	Rohwer JM, Botha FC.	Biochem J	358(Pt 2)	437-45.	2001 1	1513743	BioModel	MODEL6618063111	Stellenbosh University;	Snoep,Jacky L;	jls@sun.ac.za;	null	http://www.ebi.ac.uk/biomodels- main/

					General							
ID	Organism	Org ID	Strain	Experiment Type	Pathway	Path ID	Mechanism	Tissue	Tiss ID	Comment	Select	Edit
63457	Saccharum officinarum	1541	strain	in silico	Starch and Sucrose metabolism	26	unknown	culm	1476	Bio Model Import		edit
63458	Saccharum officinarum	1541	strain	in silico	Starch and Sucrose metabolism	26	unknown	culm	1476	Bio Model Import		edit
63459	Saccharum officinarum	1541	strain	in silico	Starch and Sucrose metabolism	26	unknown	culm	1476	Bio Model Import		edit
63460	Saccharum officinarum	1541	strain	in silico	Starch and Sucrose metabolism	26	unknown	culm	1476	Bio Model Import		edit
63461	Saccharum officinarum	1541	strain	in silico	Starch and Sucrose metabolism 26 unknown cu		culm	1476	Bio Model Import		edit	
63462	Saccharum officinarum	<mark>1</mark> 541	strain	in silico	Starch and Sucrose metabolism	26	unknown	culm	1476	Bio Model Import		edit
63463	Saccharum officinarum	1541	strain	in silico	Starch and Sucrose metabolism	26	unknown	culm	1476	Bio Model Import		edit
63464	Saccharum officinarum	<mark>1</mark> 541	strain	in silico	Starch and Sucrose metabolism	26	unknown	culm	1476	Bio Model Import		edit
63465	Saccharum officinarum	<mark>1</mark> 541	strain	in silico	Starch and Sucrose metabolism	26	unknown	culm	1476	Bio Model Import		edit
63466	Saccharum officinarum	1541	strain	in silico	Starch and Sucrose metabolism	26	unknown	culm	1476	Bio Model Import		edit
63467	Saccharum officinarum	1541	strain	in silico	Starch and Sucrose metabolism	26	unknown	culm	1476	Bio Model Import		edit

ID	Reaction	Reaction ID	Transport	Select	Edit
63457	D-Fructose=D-Fructose	13415	true		edit
63458	D-Glucose=D-Glucose	7002	true		<u>edit</u>
63459	ATP + D-Glucose = D-Glucose 6-phosphate + ADP	793	1		edit
63460	D-Fructose + ATP = D-Fructose 6-phosphate + ADP	1116			<u>edit</u>
63461	D-Fructose + ATP = D-Fructose 6-phosphate + ADP	1116			edit
63462	D-Fructose 6-phosphate + UDP-D-glucose = UDP + Sucrose 6-phosphate	8678			<u>edit</u>
63463	Sucrose 6-phosphate + H2O = Sucrose + Phosphate	1150			edit
63464	UDP-D-glucose + D-Fructose = Sucrose + UDP	8404			<u>edit</u>
63465	Sucrose + H2O = D-Fructose + D-Glucose	1146			<u>edit</u>
63466	D-Fructose 6-phosphate + ATP = D-Fructose 1,6-bisphosphate + ADP	1113			edit
63467	Sucrose=Sucrose	13123	true		edit

SABIO-RK curation interface: Data source overview



Kinetic Data Import from Models



Kinetic law

ID	Туре	Type ID	Kinetic law	Reversible	Selec	t Edit
63457	Michaelis-Menten with product inhibition	0	vol*Vmax1*Fruex/(Km1Fruex*(1+Fru/Ki1Fru)+Fruex)	reversible		<u>edit</u>
	Michaelis-Menten with product inhibition	0	vol*Vmax2*Gicex/(Km2Gicex*(1+Gic/Ki2Gic)+Gicex)	reversible		<u>edit</u>
63459	irreversible random Bi	0	vol*Vmax3*Gic/Km3Gic*ATP/Km3ATP/((1+ATP/Km3ATP)*(1+Gic/Km3Gic+Fru/Km4Fru+0.113*HexP/Ki3G6P+0.0575*HexP/Ki4F6P))	reversible		edit
63460	irreversible random Bi	0	vol*Vmax4*Fru/Km4Fru*ATP/Km4ATP/((1+ATP/Km4ATP)*(1+Gic/Km3Gic+Fru/Km4Fru+0.113*HexP/Ki3G6P+0.0575*HexP/Ki4F6P))	reversible		edit
63461	irreversible random Bi	0	vol*Vmax5/(1+Fru/Ki5Fru)*Fru/Km5Fru*ATP/Km5ATP/(1+Fru/Km5Fru+ATP/Km5ATP+Fru*ATP/(Km5Fru*Km5ATP)+ADP/Ki5ADP)	reversible		edit
63462	reversible ordered Bi	0	vol*Vmax6f*(0.0575*HexP*0.8231*HexP-Suc6P*UDP/Keq6)/(0.0575*HexP*0.8231*HexP*(1+Suc6P/Ki6Suc6P)+Km6F6P*(1+phos/Ki6Pi)*(0.8231*HexP+Ki6UDPGic)+Km6UDPGic*0.0575*HexP+Vmax6f/(Vmax6r*Keq6)* (Km6UDP*Suc6P*(1+0.8231*HexP/Ki6UDPGic)+UDP*(Km6Suc6P*(1+Km6UDPGic*0.0575*HexP/(Ki6UDPGic*1+phos/Ki6Pi)))+Suc6P*(1+0.0575*HexP/Ki6UDPGic*0.0575*HexP+Vmax6f/(Vmax6r*Keq6)*	reversible		<u>edit</u>
63463	Michaelis-Menten	23	vol*Vmax7*Suc6P/(Km7Suc6P+Suc6P)	reversible		edit
63464	reversible ordered Bi		vol*(-Vmax8f)*(Suc*UDP-Fru*0.8231*HexP/Keq8)/(Suc*UDP*(1+Fru/Ki8Fru)+Km8Suc*(UDP+Ki8UDP)+Km8UDP*Suc+Vmax8f/(Vmax8r*Keq8)*(Km8UDPGic*Fru*(1+UDP/Ki8UDP)+0.8231*HexP*(Km8Fru* (1+Km8UDP*Suc/(Ki8UDP*Km8Suc))+Fru*(1+Suc/Ki8Suc))))	reversible		<u>edit</u>
	Michaelis-Menten with product inhibition	0	vol*Vmax9/(1+Glc/Ki9Glc)*Suc/(Km9Suc*(1+Fru/Ki9Fru)+Suc)	reversible		<u>edit</u>
63466	Michaelis-Menten	23	vol*Vmax10*0.0575*HexP/(Km10F6P+0.0575*HexP)	reversible		edit
63467	Michaelis-Menten	23	vol*Vmax11*Suc/(Km11Suc+Suc)	reversible		edit

Variables

ID	Name	Term	Not replaced	Comment	Edit

					Parame						
ID	Name	Role	Туре	Compound	Start	End	Deviation	Unit	Comment	Select	Edit
63457	vol	Constant	volume		1			I			edit
63457	Vmax1	Constant	Vmax		0.286			mM/min			edit
63457	Fruex	Variable	concentration	D-Fructose	5.0			mM			edit
63457	Km1Fruex	Constant	Km	D-Fructose	0.2			mM			edit
63457	Fru	Variable	concentration	D-Fructose	1.0			mM			edit
63457	Ki1Fru	Constant	Km	D-Fructose	1.0			mM	competitive		edit
63458	vol	Constant	volume		1			1			edit
63458	Vmax2	Constant	Vmax		0.286	•		mM/min			edit
63458	Glcex	Variable	concentration	D-Glucose	5.0	•		mM			edit
63458	Km2Glcex	Constant	Km	D-Glucose	0.2			mM			edit
63458	Glc	Variable	concentration	D-Glucose	1.0			mM		8	edit
63458	Ki2Glc	Constant	Km	D-Glucose	1.0			mM	competitive		edit
63459	vol	Constant	volume		1			1			edit
63459	Vmax3	Constant	Vmax		0.197			mM/min			edit
63459	Glc	Variable	concentration	D-Glucose	1.0			mM			edit
63459	Km3Glc	Constant	Km	D-Glucose	0.07			mM			edit
63459	ATP	Variable	concentration	ATP	1.0			mM			edit

Parameter



Edit entry

Publication ID: 4864 Entry ID: 63463

Pathwa	Ŋ	Starch and Sucrose meta	bolism	26								
Reaction	n	Sucrose 6-phosphate + H	20 = Sucrose + Phosphate	1150 Trans	port: 🔲 Reve	rse reaction						
Compou	nds											
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Stoech.	Name	Name	Role	Cell. location		Protein Identifier	Protein Name	Comment	Comp. ID			
1	Enzyme		Modifier-Catalyst 🔻	cytoplasm	54				0			
1	Sucrose 6-phosphate		Substrate •	cytoplasm	54				1373			
1	Sucrose		Product •	cytoplasm	54				1294			
1	Phosphate		Product •	cytoplasm	54				36			
1	H2O		Substrate	cytoplasm	54				40			
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		Choo	se location: Please Select	v		search locations						
		Choo	se pathway: Please Select		¥							
	ing avoid (manifest langed)		c	ear reaction fields								

Signalling event (reaction_b	ased)	
Event Description:		
Event type(s)		
Event type ID	Event type description	Event type annotation (GO)

SABIO-RK curation interface: Data entry editing



Kinetic Data Import from Models



Kinetic lav	v												
Туре		Michaelis-Menten							23				
Formula		vol*Vmax7*Suc6P/(Km7Suc6P+Suc6F	⊃)						reversible 🔻				
Variables													
Name	Term			Do not replace variable in formula	1			C	Comment				
								E					
Parameter					2		4						
Name	Role	Туре		Species	Value start	Value end	Deviation	U	Jnit	Unit ID	Unit def.	Comment	
vol	Constant V	volume 🔻		¥	1				I	64	-		
Vmax7	Constant V	Vmax •]	•	0.5				mM/min	11	- •	8	
Suc6P	Variable 🔻	concentration •]	Sucrose 6-phosphate 🔻	1.0				mM	29			
Km7Suc6P	Constant 🔻	Km 🔻]	Sucrose 6-phosphate 🔻	0.1				mM	29	. •		
	unknown 🔻	area bimolecular rate constant concentration						1		null	- •		
		EC50 enz. activity forward bimolecular rate constant forward rate constant forward unimolecular rate constant half-life Hill coefficient Hill coefficient Hill coefficient Kcat kcat/Km kcat/Km kcat/Km Kd	oose ki	netic law type: Please Select	add parameter rov	d variable row add 10 param kinetic law fields	eter rows			T			
Enzyme d		Keq Ki			T.								
Complex in	formation (UniProtID(s kinact Km			Q4FCW1								
Complex in	formation (names)		-		(enter com	plex information s	eparated <mark>b</mark> y semi	colon)	E				
EC number					3.1.3.24								
Protein	Protein						Rec	ombir	nant C Express	ed in			
Stoech.	Name				UniProt ID					Mo	I. weight (kDa)	Deviation (kDa)	
	native complex				Q4FCW1								
1													

add row add 5 rows

clear enzyme description fields

Experimental con	ditions			
pH		Temperature (°C)		Buffer
Start	End	Start	End	Composition



1000000015	Search Web Services News	Documentation	Publications Statistics	Links Ab	out
Search				Filter Options	
Rohwer		Q	Reset ?	Enzyme Ø Wildtype Ø Mut	ant Recombinant
V	Advanced Search			Kinetic Data	
OR • PubMe	edID 🔹	Add & Se	arch	Rate Equation	
				Transport Reaction	
				Environmental Cond	itions
				oH: 0 - 14	Temperature: -10 CP - 115
	SARIO-PK	nublic usor	interface	pH: 0 - 14	Temperature: -10 C° - 115
	SABIO-RK	public user	interface	pH: 0 - 14 Source	Temperature: -10 C° - 115

Total number of kinetic law entries found: 11

display 15 • entries per page

Kinetic	Reaction	Enzyme			Tissue	Organicm	Parameter (besides	Environment		LO
data	Reaction	ECNumber	Protein	Variant	TISSUE	Organism	concentration)	°C	pH	cart?
	D-Fructose = D-Fructose			wildtype	stem ר	Saccharum officinarum	Km Vmax Volume			
	D-Glucose = D-Glucose		2	wildtype	<u>stem</u> ्न	Saccharum officinarum	Km Vmax Volume			



Kinetic Data Import from Models



						-			Keq	
	UDP-D-glucos phosphate = 1 phosphate			.4.1.14		wildtype	<u>stem</u> ר	Saccharum officinarum	Ki Km Vmax Volume	
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- L			6803		Entry	ID: 4936	4			
Genera	al information									
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Tissue		stem T								
EC Clas	ss	3.1.3.24								
SABIO (reaction id	1150								
Variant		wildtype								
	nent Type	in silico								
Pathwa		Starch and Sucr	rose metaboli	sm						
Event D	Description	-								
Substr	rates									
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Sucrose	<u>e 6-phosphate</u>		cytopla	asm 7	-	ŝ				
Produc	cts	100								
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Phosph	ate	cytoplasm	<u>ר</u>		-					
Modifi	ers									
name			location	effect	comm	nent protein comple	ex			
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SABIO-RK public user interface



Modifier	'S												
name				location	eff	ect	c	omme	nt protei	n ex			
	ohosphate ase(Enzyme)			<u>cytoplasm</u>		difier- alyst	-	ž.	<u>Q4FCW</u>	<u>ור 1;</u>			
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Parame	ter												
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6													
	UDP-D-gluco + Sucrose	se +	D-Fructos	e = UDP	2.4.1	.13	<u>Q9LK</u>	ר <u>R0</u>	wildtype	stem יר	Saccharum officinarum	Keq Ki Km Vmax Volume	

SABIO-RK public user interface



Data Export: Spreadsheets









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

SABIO-RK public user interface





Data Export: Spreadsheets



Back to Results

Save Excelsheet

Select Colums to Export

	Add all	5 items selected	Remove all	
(egg)(caccontb		EntryID		Export xls
KineticMechanism	+ 3	-		Export tou
Other Modifier	+	Reaction		Export tsv
Pathway	+	Organism	-	Reset
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Substrate	+ +			

Export Distinct Rows Only

SABIO-RK public user interface

Preview of the first 5 entries

		Sabio	Excel Export Prev	iew		
A	В	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
1049363	UDP-D-glucose	Saccharum offic	vol*Vmax6f*(0.0	Km	D-Fructose 6-p	6.0E-4



Data Export: Spreadsheets



A	В	С	D	E	F	G	Н	1	J	K
1 EntryID	Reaction	Organism	Rate Equation	parameter.ty	parameter.associated Speci	parameter.star	parameter.end	f parameter.st	a parameter.unit	Publication
2 49363	UDP-D-glucose + D-Fructose 6-phosphate = UDP + Sucrose 6-phosphate	Saccharum officinarum	vol*Vmax6f*(0.0575*HexP*0.8231*HexP-	SuKm	Sucrose 6-phosphate	1.0E-4		-	M	Rohwer JM, B
3 49363	UDP-D-glucose + D-Fructose 6-phosphate = UDP + Sucrose 6-phosphate	Saccharum officinarum	vol*Vmax6f*(0.0575*HexP*0.8231*HexP-	Suvolume		1.0		-	1	Rohwer JM, B
4 49363	UDP-D-glucose + D-Fructose 6-phosphate = UDP + Sucrose 6-phosphate	Saccharum officinarum	vol*Vmax6f*(0.0575*HexP*0.8231*HexP-	SuKm	D-Fructose 6-phosphate	6.0E-4		2	M	Rohwer JM, B
5 49363	UDP-D-glucose + D-Fructose 6-phosphate = UDP + Sucrose 6-phosphate	Saccharum officinarum	vol*Vmax6f*(0.0575*HexP*0.8231*HexP-	SuKeq		10.0		3	-	Rohwer JM, B
6 49363	UDP-D-glucose + D-Fructose 6-phosphate = UDP + Sucrose 6-phosphate	Saccharum officinarum	vol*Vmax6f*(0.0575*HexP*0.8231*HexP-	Su Vmax		3.33333333E-6			M*s^(-1)	Rohwer JM, B
7 49363	UDP-D-glucose + D-Fructose 6-phosphate = UDP + Sucrose 6-phosphate	Saccharum officinarum	vol*Vmax6f*(0.0575*HexP*0.8231*HexP-	Su Ki	Phosphate	0.003		-	M	Rohwer JM, B
8 49363	UDP-D-glucose + D-Fructose 6-phosphate = UDP + Sucrose 6-phosphate	Saccharum officinarum	vol*Vmax6f*(0.0575*HexP*0.8231*HexP-	SuKm	UDP	3.0E-4		-	M	Rohwer JM, B
9 49363	UDP-D-glucose + D-Fructose 6-phosphate = UDP + Sucrose 6-phosphate	Saccharum officinarum	vol*Vmax6f*(0.0575*HexP*0.8231*HexP-	SuKm	UDP-D-glucose	0.0018			M	Rohwer JM, B
10 49363	UDP-D-glucose + D-Fructose 6-phosphate = UDP + Sucrose 6-phosphate	Saccharum officinarum	vol*Vmax6f*(0.0575*HexP*0.8231*HexP-	Su concentration	Phosphate	0.0051		÷	M	Rohwer JM, B
11 49363	UDP-D-glucose + D-Fructose 6-phosphate = UDP + Sucrose 6-phosphate	Saccharum officinarum	vol*Vmax6f*(0.0575*HexP*0.8231*HexP-	SuVmax		6.31666667E-6			M*s^(-1)	Rohwer JM, B
12 49363	UDP-D-glucose + D-Fructose 6-phosphate = UDP + Sucrose 6-phosphate	Saccharum officinarum	vol*Vmax6f*(0.0575*HexP*0.8231*HexP-	Su Ki	D-Fructose 6-phosphate	4.0E-4		22 	M	Rohwer JM, B
13 49363	UDP-D-glucose + D-Fructose 6-phosphate = UDP + Sucrose 6-phosphate	Saccharum officinarum	vol*Vmax6f*(0.0575*HexP*0.8231*HexP-	Su concentration	UDP	2.0E-4		<u>_</u>	M	Rohwer JM, B
14 49363	UDP-D-glucose + D-Fructose 6-phosphate = UDP + Sucrose 6-phosphate	Saccharum officinarum	vol*Vmax6f*(0.0575*HexP*0.8231*HexP-	Su concentration	Sucrose 6-phosphate	0.001			M	Rohwer JM, B
15 49363	UDP-D-glucose + D-Fructose 6-phosphate = UDP + Sucrose 6-phosphate	Saccharum officinarum	vol*Vmax6f*(0.0575*HexP*0.8231*HexP-	Su Ki	UDP-D-glucose	0.0014			M	Rohwer JM, B
16 49363	UDP-D-glucose + D-Fructose 6-phosphate = UDP + Sucrose 6-phosphate	Saccharum officinarum	vol*Vmax6f*(0.0575*HexP*0.8231*HexP-	SuKi	Sucrose 6-phosphate	7.0E-5		-	M	Rohwer JM, B
17 49363	UDP-D-glucose + D-Fructose 6-phosphate = UDP + Sucrose 6-phosphate	Saccharum officinarum	vol*Vmax6f*(0.0575*HexP*0.8231*HexP-	Su concentration	D-Fructose 6-phosphate	0.001		-	M	Rohwer JM, B
18 49364	H2O + Sucrose 6-phosphate = Sucrose + Phosphate	Saccharum officinarum	vol*Vmax7*Suc6P/(Km7Suc6P+Suc6P)	volume		1.0		-	1	Rohwer JM, B
19 49364	H2O + Sucrose 6-phosphate = Sucrose + Phosphate	Saccharum officinarum	vol*Vmax7*Suc6P/(Km7Suc6P+Suc6P)	Vmax		8.33333333E-6		-	M*s^(-1)	Rohwer JM, B
20 49364	H2O + Sucrose 6-phosphate = Sucrose + Phosphate	Saccharum officinarum	vol*Vmax7*Suc6P/(Km7Suc6P+Suc6P)	concentration	Sucrose 6-phosphate	0.001		2	M	Rohwer JM, B
21 49364	H2O + Sucrose 6-phosphate = Sucrose + Phosphate	Saccharum officinarum	vol*Vmax7*Suc6P/(Km7Suc6P+Suc6P)	Km	Sucrose 6-phosphate	1.0E-4		2	M	Rohwer JM, B
22 3460	D-Glucose 1-phosphate = alpha-D-Glucose 6-phosphate	Rattus norvegicus	V*S/(Km+S)	concentration	D-Glucose 1-phosphate					Kashiwaya Y,
23 3460	D-Glucose 1-phosphate = alpha-D-Glucose 6-phosphate	Rattus norvegicus	V*S/(Km+S)	Km	D-Glucose 1-phosphate	4.5E-5		-	M	Kashiwaya Y,
24 3460	D-Glucose 1-phosphate = alpha-D-Glucose 6-phosphate	Rattus norvegicus	V*S/(Km+S)	Vmax		0.00193333333		2.76667E-4	M*s^(-1)	Kashiwaya Y,
25 12527	H2O + Sucrose 6-phosphate = beta-D-Fructose + alpha-D-Glucose 6-phosphate	Lactococcus lactis subsp. lactis	Vmax*S/(Km+S)	Km	Sucrose 6-phosphate	1.0E-4	1.1E-4		M	Thompson J, C
26 12527	H2O + Sucrose 6-phosphate = beta-D-Fructose + alpha-D-Glucose 6-phosphate	Lactococcus lactis subsp. lactis	Vmax*S/(Km+S)	Vmax		1.55E-4	1.71666667E-4		mol*s^(-1)*g^(-1)	Thompson J, (
27 12527	H2O + Sucrose 6-phosphate = beta-D-Fructose + alpha-D-Glucose 6-phosphate	Lactococcus lactis subsp. lactis	Vmax*S/(Km+S)	concentration	Sucrose 6-phosphate	0.0	0.002	-	M	Thompson J, 0
28 18577	alpha-D-Glucose 1-phosphate = alpha-D-Glucose 6-phosphate	Lactococcus lactis subsp. cremoris	Vmax*S/(Km+S)	concentration	Enzyme	0.0067		2	mg/ml	Neves AR, Po
29 18577	alpha-D-Glucose 1-phosphate = alpha-D-Glucose 6-phosphate	Lactococcus lactis subsp. cremoris	Vmax*S/(Km+S)	Vmax		0.0010883551		3.00006E-5	katal*g^(-1)	Neves AR, Po
30 18577	alpha-D-Glucose 1-phosphate = alpha-D-Glucose 6-phosphate	Lactococcus lactis subsp. cremoris	Vmax*S/(Km+S)	Km	alpha-D-Glucose 1-phosphate	7.14E-5		2.8E-6	M	Neves AR, Po
31 18577	alpha-D-Glucose 1-phosphate = alpha-D-Glucose 6-phosphate	Lactococcus lactis subsp. cremoris	Vmax*S/(Km+S)	concentration	Mg2+	0.005		-	M	Neves AR, Po
32 18577	alpha-D-Glucose 1-phosphate = alpha-D-Glucose 6-phosphate	Lactococcus lactis subsp. cremoris	Vmax*S/(Km+S)	concentration	alpha-D-Glucose 1-phosphate	0.0075		-	M	Neves AR, Po
33		1			10 D					
24										

SABIO-RK Biochemical Reaction Kinetics Database



Entries to Export:

	Home	Search	Web Services	News	Documentation	Publications	Statistics	Links	About
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Selected kinetics data

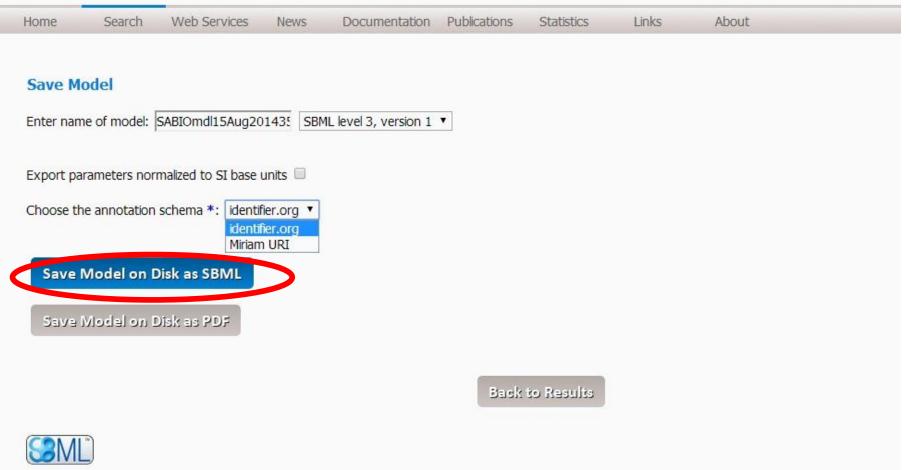
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<mark>4</mark> 9363	UDP-D-glucose + D-Fructose 6-phosphate <-> UDP + Sucrose 6-phosphate	Saccharum officinarum	stem	reversible ordered Bi	(view)	
12527	H2O + Sucrose 6-phosphate <-> alpha-D-Glucose 6-phosphate + beta-D-Fructose	Lactococcus lactis subsp. 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





5





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

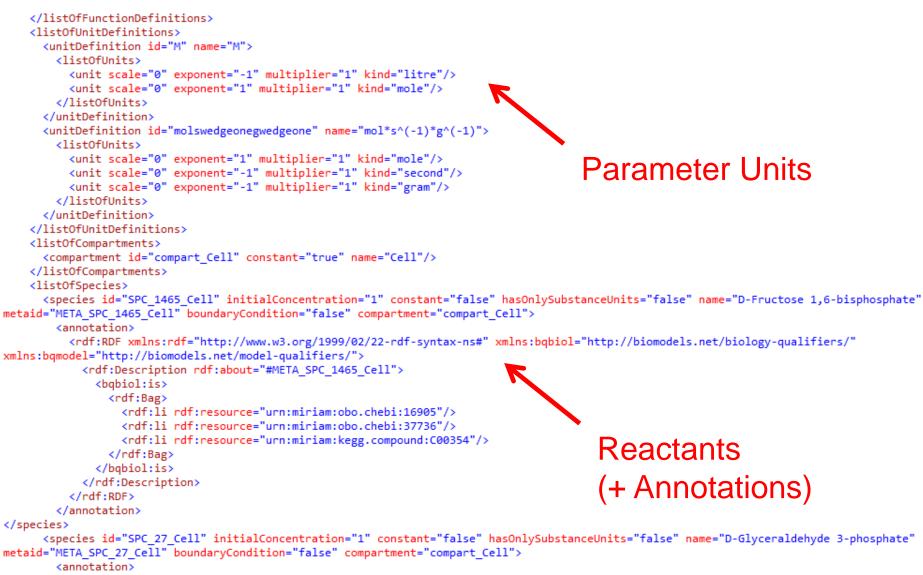




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This model has been created with the help of the SABIO-RK Database
(http://sabio.h-its.org/)
(c) 2005-2014 HITS gGmbH http://www.h-its.org
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To cite SABIO-RK Database, please use
"http://www.ncbi.nlm.nih.gov/pubmed/22102587"
<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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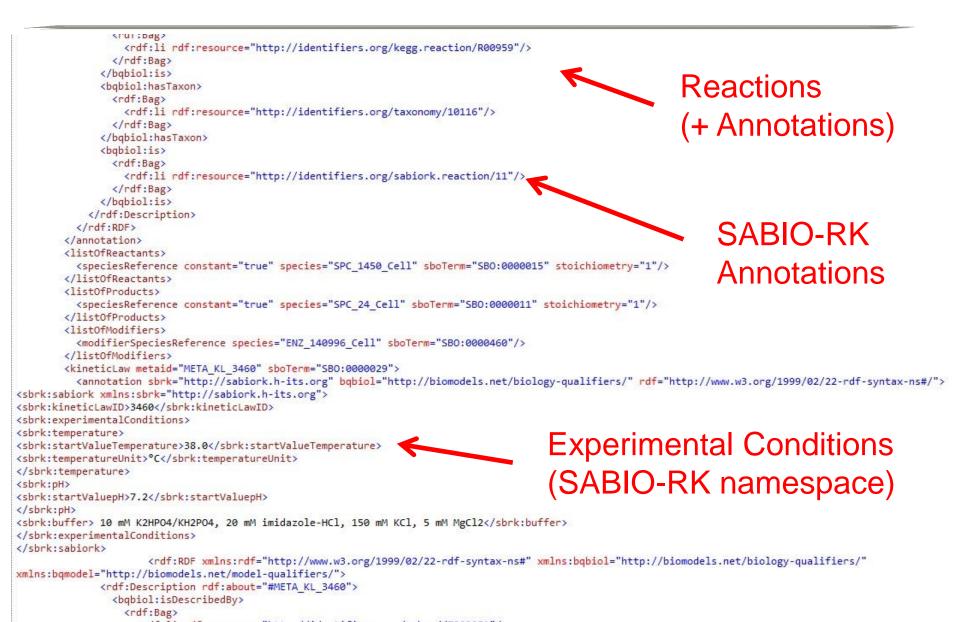




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SABIO-RK









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- 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 annotated (RDF) with **identifiers.org** or **MIRIAM** URIs:
 - Annotations to reaction, protein and chemical compound databases
 - Annotations of reactions to organism and tissue databases
 - Annotations to <u>SABIO-RK Ids</u> (reaction and kinetic data entry) for tracking
 - Annotations to primary data source: Publications (PubMed Ids)
 - Content fully annotated to Systems Biology Ontology (SBO)
- 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







Home	Search	Web Services	News	Documentation	Publications	Statistics	Links	About	
Save Mod	lel								
Enter name	of model:	SABIOmdl15Aug20	SBM	IL level 2, version 4 IL level 3, version 1 IL level 2, version 4	•				
Export parar	meters nor	malized to SI base	units SBM	IL level 2, version 3 IL level 2, version 2					
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		Copyright © 2009	The Author(s	3)					
SML)				ersion of SBN	AL files into	human-			
		readable re	pons						

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



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 (<u>http://www.sbpax.org</u>)
- Parameter units are described via the UOME (Units of Measurement Expressions) extension to BioPax (<u>http://www.sbpax.org/uome/</u>)
- 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

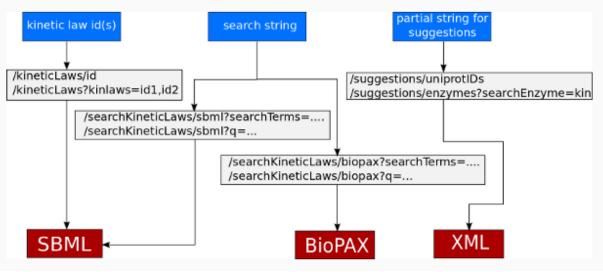


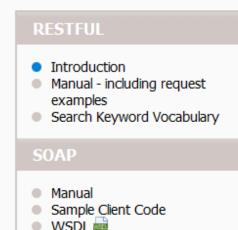
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	3: Sha (tho tecute>
<sdx< td=""><td>3:SBMeasurable rdf:about="http://sabio.h-its.org/biopax#temperature714"></td></sdx<>	3:SBMeasurable rdf:about="http://sabio.h-its.org/biopax#temperature714">
	<sbx3:sbvocabulary rdf:resource="http://sabio.h-its.org/biopax#SBO:0000147"></sbx3:sbvocabulary>
	<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:sbterm>
	x3:SBMeasurable>
	x3:SBMeasurable> :TissueVocabulary rdf:about="http://sabio.h-its.org/biopax#tissue_erythrocyte">
	<pre>x3:SBMeasurable> :TissueVocabulary rdf:about="http://sabio.h-its.org/biopax#tissue_erythrocyte"></pre>
 bp3	<pre>x3:SBMeasurable> :TissueVocabulary rdf:about="http://sabio.h-its.org/biopax#tissue_erythrocyte"></pre>
<bp3< td=""><td><pre>x3:SBMeasurable> :TissueVocabulary rdf:about="http://sabio.h-its.org/biopax#tissue_erythrocyte"></pre></td></bp3<>	<pre>x3:SBMeasurable> :TissueVocabulary rdf:about="http://sabio.h-its.org/biopax#tissue_erythrocyte"></pre>
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<bp3 <uom< td=""><td><pre>x3:SBMeasurable> :TissueVocabulary rdf:about="http://sabio.h-its.org/biopax#tissue_erythrocyte"></pre></td></uom<></bp3 	<pre>x3:SBMeasurable> :TissueVocabulary rdf:about="http://sabio.h-its.org/biopax#tissue_erythrocyte"></pre>
<bp3 <uom< td=""><td><pre>x3:SBMeasurable> :TissueVocabulary rdf:about="http://sabio.h-its.org/biopax#tissue_erythrocyte"></pre></td></uom<></bp3 	<pre>x3:SBMeasurable> :TissueVocabulary rdf:about="http://sabio.h-its.org/biopax#tissue_erythrocyte"></pre>





Home Search Web Services News Documentation Publications Statistics Links About **RESTful Web Services Introduction** RESTFUL RESTful Web Services are implemented offering data access via HTTP requests following a Introduction Representational State Transfer (REST) approach. Data can be accessed using simple http GET Manual - including request requests to either retrieve a complete SBML model, or a BioPAX/SBPAX3 representation of the examples 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 SOAP query built in user interface advanced search.











Example requests:

Entries may be requested directly if the database entry ID is known http://sabio.h-its.org/sabioRestWebServices/kineticLaws/20147

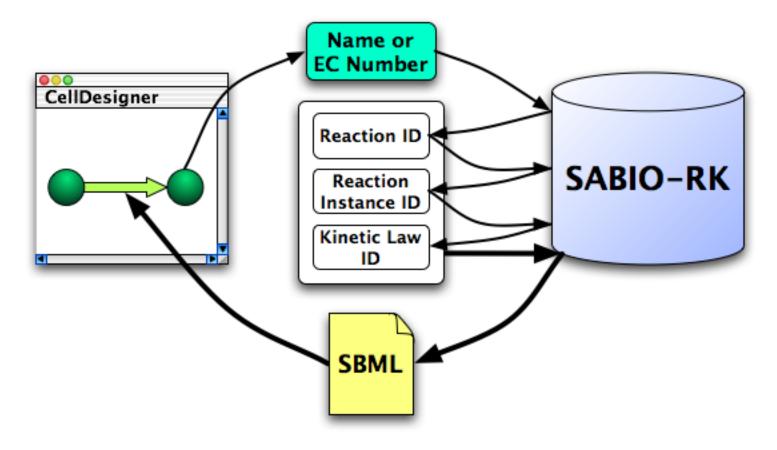
Entries may be searched for using the same search options available in the browser search interface

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?search Compounds=glycoch

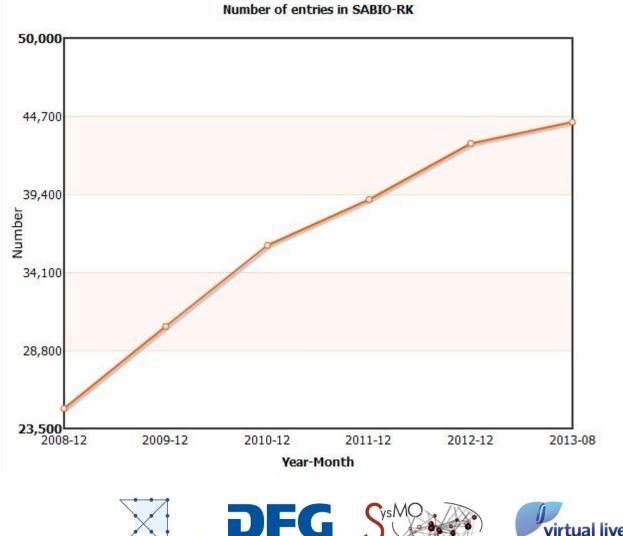




http://www.celldesigner.org







ктѕ



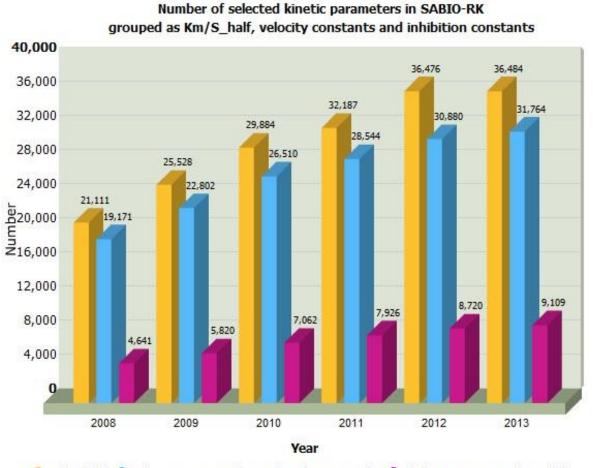


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Km/S_half 🔍 Velocity constants (Vmax/kcat/rate const.) 🔎 Inhibition constants (IC50/Ki)









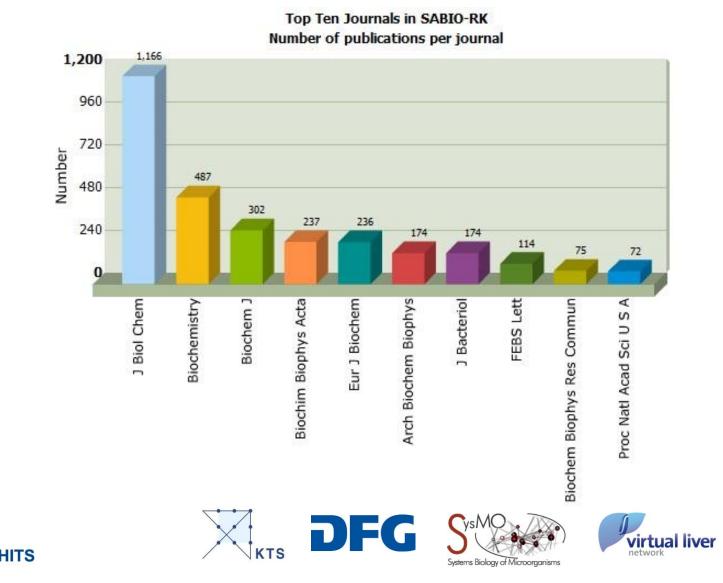
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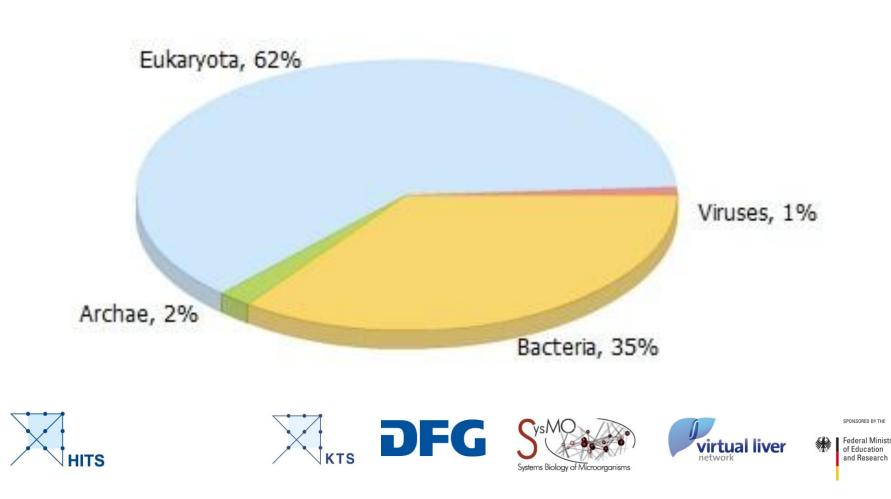
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Taxonomic distribution of organisms in SABIO-RK



Heidrun Sauer-Danzwith

Wolfgang Müller Martin Golebiewski Lenneke Jong

Lei Shi Enkhjargal Algaa

Ulrike Wittig

Renate

Kania

Andreas Maja Weidemann Rey

> Meik Bittkowski (no image)











Isabel

Rojas

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http://sabiork.h-its.org

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)



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