SABIO-RK User Interface



The **Search** field offers free text search. The complete word (no fragments) inserted in this field will be searched in the entire database's content, including comments.

The auto completion function makes suggestions and indicates how many results (entries) are in the database for the distinct search terms. Queries can be modified by using the following syntax in the **Search** field:

Search	Result							
rattus liver	entries containing both terms rattus and liver							
rattus AND liver								
(rattus OR liver)	entries containing either the term rattus or liver							
(rattus OR human) AND liver	entries containing the term liver and either rattus or human							
"homo sapiens"	entries containing both terms homo and sapiens in the exact order							
ratt* *kinase	wildcard search for more than one character entries containing terms starting with <i>ratt</i> (e.g. Rattus norvegicus) or ending with <i>kinase</i> (e.g. Hexokinase)							
"mammalia (NCBI)" NOT "homo sapiens" "liver (BTO)"	entries for all organisms of class <i>mammalia</i> (based on NCBI taxonomy) but not for <i>homo sapiens</i> entries for tissue <i>liver</i> including all tissue sub-parts and cell lines (based on BRENDA Tissue Ontology)							
Substrate:ATP	entries with reactions containing substrate <i>ATP</i> similar queries for specific attributes can be defined by using all other database attributes (see Advanced Search)							
Substrate:ATP AND Substrate:Pyruvate Substrate:(ATP AND Pyruvate)	entries with reactions containing both ATP and Pyruvate as substrates							
Year:[1990 TO 2012]	entries with publication years between 1990 and 2012							

More specific queries can additionally be defined by the Advanced Search.

Но	me Search	Services Web Service	s News	Documentation	Publications	Statistics Lin	nks About
	51					Filter Options	Ŧ
7	Advan	ced Search		Q Reset	0	Enzyme Wildtype Mu Kinetic Data Rate Equation Reaction	tant 🗌 Recombinant
ND ~	ECNumber	2.7.1.		Add & Search		Transport Reaction	
	SabioReactionID Signalling Modification Signalling Event Compound AnyRole Substrate Product Inhibitor Catalyst	2.7.1.1 2.7.1.3 2.7.1.4 2.7.1.8 2.7.1.5	(726) (42) (36) (3) (3)			Environmental Cond pH: 0-14 Source Direct Submission Publication BioModel	Itions Temperature: -10 C* - 118 C* Entries inserted since: 14/10/2008
Entry	Colactor Activator OtherModifier SabioCompoundID InChI Enzyme	sual Search (beta)					

To restrict search terms to specific attributes also the **Advanced Search** can be used. First an attribute from the list has to be selected. Then while typing terms a selection list with suggestions will appear containing the number of database entries related to them. Select a term from the list and click the **Add & Search** button to start the search. Wildcard search is not possible for the advanced search, the exact search term is needed.

Searches with different terms for the same attribute is possible using the OR boolean operator. For the specific attributes *Tissue* and *Organism* an ontology-based search can be defined by selecting terms with additional information (*BTO*) or (*NCBI*). By selecting BTO terms the search will include all subclasses of this term based on the BRENDA Tissue Ontology (http://bioportal.bioontology.org/ontologies/1005). By selecting NCBI terms the search will include all subclasses of this term based on the NCBI Organism Taxonomy (http://www.ncbi.nlm.nih.gov/taxonomy).

Time periods of publications in attribute Year can be defined:

>1990 <1990	entries with publication years from 1990 until today
	entries with publication years up to 1990

Queries can be specified additionally by setting different filters using the **Filter Options** box.



There are filters for the enzyme/protein. By default all entries containing Wildtype or Mutant proteins are displayed. By disabling one of these criteria only wildtype or only mutant data will be displayed. Selecting Recombinant will restrict the search output to entries resulting from experiments conducted with recombinant proteins.

Selecting the Rate Equation filter will display only data entries with a kinetic rate equation. Accordingly, selecting the Transport Reaction filter will restrict the search result to transport reactions.

Environmental conditions (pH value, Temperature) can be specified by moving the slider buttons to select a range.

Additionally the source of the data (Direct Submission, Publication, or BioModel (Model upload via SBML)) and the time of data insertion can be used to restrict the search.

Entry View

The search result is represented by default in the **Entry View**, which is a table containing overview information of the database entries sorted by Sabio EntryID. The content of the table columns can be re-sorted by clicking on the column headers.

The number of entries per page can be varied.

Kinetic	Paastian		Enzyme		Tircuo	Oreanism	Parameter	Envir	onment	add to
data	Reaction	ECNumber	Protein	Variant	Tissue	organism	concentration)	۰c	рН	cart?
	NAD+ + D-Glyceraldehyde 3-phosphate + Phosphate = NADH + H+ + 3-Phospho- D-glyceroyi phosphate	1.2.1.12	<u>P04406</u>	? wildtype	lung P	Homo sapiens	Hill coefficient S_half			
	NAD+ + D-Glyceraldehyde 3-phosphate + Phosphate = NADH + H+ + 3-Phospho- D-glyceroyl phosphate	1.2.1.12	<u>P04406</u>	🤊 wildtype	lung. 🕫	Homo saplens	Hill coefficient S_half			
	D-Glyceraldehyde 3-phosphate + Phosphate + NAD+ = H+ + NADH + Glycerate 1,3-bisphosphate	1.2.1.12	<u>P04406</u>	? wildtype	erythrocyte. 7	Homo sapiens	Kd Km Vmax	23.0	8.6	
	ATP + 3-Phospho-D-glycerate = ADP + 3-Phospho- D-glyceroyl phosphate	2.7.2.3	P00558	7 mutant	muscle 🤿	Homo sapiens	Km Vmax	30.0	7.6	
	ATP + 3-Phospho-D-glycerate = ADP + 3-Phospho- D-glyceroyl phosphate	2.7.2.3	<u>P00558</u>	7 mutant	muscle 🤊	Homo sapiens	Km Vmax	30.0	7.6	
	ATP + 3-Phospho-D-glycerate = ADP + 3-Phospho- D-glyceroyl phosphate	2.7.2.3	P00558	🕈 wildtype	muscle *P	Homo sapiens	Km Vmax	30.0	7.6	
	ATP + 3-Phospho-D-glycerate = ADP + 3-Phospho- D-glyceroyi phosphate	2.7.2.3	P00558	7 wildtype	muscle ⁴¹	Homo sapiens	Km Vmax	30.0	7.6	
	ATP + D-Fructose 6-phosphate = ADP + D-Fructose 1,6-bisphosphate	2.7.1.11	P47857 P12382	n wildtype	liver 🕫	Mus musculus	IC50 Vmax	30.0	7.45	

Detailed information is given in the single database entries which can be displayed by clicking on the blue triangle to open an entry. Alternatively all entries can be opened at once by selecting "expand all displayed entries".

Entry View	Read	tion View	Visual Search	(beta)												
				-												
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data			Reaction								TISSUE	Organism	(Desides			cart?
						E	CNumber	Prot	tein	Variant			concentration)	°C	pH	
	NAD+ +	D-Glycerald	labuda 3-nh	osobate -	+ Ebornhati								Hill coefficient			
		No. of Street	and a D al			1	.2.1.12	P044	406. 7	wildtype	lung 🖓	Homo sapiens	C helf			
_	RADH +	n+ + 3-PR	vabuo-n-ĝi	ceroyi pri	ospnate								5_nair			
									Entry	ID: 2700	•					
Genera	l infor	nation														
Organis	m		Homo say	iens								-				
Tissue			ung 🗇									1				
EC Class	5		1.2.1.12													
SABIO r	eaction	id i	7844													
Variant		-	wildtype									-				
Experim	ient Typ	e	n vitro									-				
Pathway			Carbon fix Glucolusis	ation in	photosyn	thetic	organis	ms								
r a china a			Glycolysis.	Glucone	ogenesis											
Event D	escripti	on										1				
Substra	ates											1				
name							locat	tion		comme	int	-				
D-Glyce	raldehy	de 3-phosp	hate							-						
Phospha	ate									-						
NAD+										-						
Produc	ts															
name							loc	ation		comm	ent					
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<u>H+</u>										-		_				
3-Phosp	ho-D-gl	yceroyi ph	osphate				-									
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(phosph	orvlatir	-3-phospha (Enzyme)	ite denyar :)	ogenase	· .		Catalyst	.	-	(60	<u>4406</u> ¬ ?)*4;					
		also debel	/			_		· ·				-				
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Kinetic	type		formula						200	otation		-				
Hill Coo	perativi	ty	(Vmax*	5^n)/(S	half^n+S	^n)			SBO	:0000192	-P	-				
Barama	ter								-			1				
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s	conce	ntration 1	NAD+			-						-				
n	Hill co	efficient '	NAD+		1.	5		-				-				
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Vmax	Vmax	-9	-			-		-				1				
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buffer		50 mM Trie	thanolam	ine, 5 m	M EDTA,	0 mM	MgCI2					1				
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Genera	l comm	ent										-				
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title	nce				author		earlion	rnal v	alum		PubMed	-				
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human	diploid a	and SV40-t	ransforme	d	Jr, Smith	EC	Res	ľ	-	1410.2	1260723	1				
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SABIO-RK offers details about the Reaction, Organism, Enzyme, Pathway and Compound of an entry which are shown in additional pop-up windows after clicking on the appropriate term.

These Details are partially interlinked, and contain additionally links to external databases, e.g., clicking on the Reaction (in the Entry View or in the Reaction View) opens the Reaction Details containing the SABIO ReactionID, Stochiometric Equation, Substrates, Products, Enzymes known to catalyze this reaction, Pathways and links to external databases.

				SABIO-R
eaction Details				
eacting 10	7644			
tochiometric Equation	D-Gyceraldehode 3-phose	hate + Phosphate + MAD+ <-> NADH + H+ + 3-Phospho-D-dur	ero/ shosshate	
	NAD+			
ubstrates	D-Gyomaldehede 3-photo	hato		
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roducts	He			
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	1,2,1,12	Geobacilius stearothermiphilus	Unifratsit 19	10799425 -9
	12.1.12	Homo sapiens	UnExcite 1	1295515 19
	1.2.1.12	Homo sapiona	Uniferences 19	4329735 19
	1.2.1.12	Jacoka priestalis	UniPostA P	8547342 -9
	12.1.32	Lactococcus lactis subsp. cremoria	UniProteit 19	11559999 4
	12.1.12	Lactococcus lactis subsp. cremoris	Unitration -P	2025452 -9
	1.2.1.12	Lactococcus lactis subsp. lectis.	Unifratility 19	10937934 19
	1.2.1.32	Lactococcus lactis subsp. lactis	UniProteit 19	11395443 **
	1.2.1.12	Lactococcus lactis subsp. lactis	UniProteit (P	9200977 9
	1.7.1.12	Mue musculue	UniPrototil 19	10339623 **
	1.2.1.12	Mus musculus	UniFrancis 19	14114000 19
	1.2.1.12	Mus musculus	UniPotes 1	18721135 1
aymes known to	1.2.1.12	Oncorhynchus mykiss	UniProtKB 19	4522902 10
wrated information)	1.2.1.12	Oryctologus cuniculus	Particos 7	4353270 19
	1.2.1.12	Plasmodium falciparum	Un Proteit - P	25693925 19
	12132	Rattus norvegicus	101/51055 ·P	20092392 9
	1.2.1.12	Saccharomyces cerevisiae	UniProteit 19	: *
	1.2.1.12	Saccharomyces cerevisiae	Unifrantia 19	1149170 9
	1.2.1.12	Saccharomyces cerevisiae	UniProteit 19	4353270 -9
	12.1.12	Spinacia oleracea	Unifritos 1	202224 -9
	1.2.1.32	Streptococcus mutans	MiniFrankik -W	32103 **
	12132	Streptomyces annae	United at the second se	8822490 -9
	1,2,1,32	Zymomonas mobilis	UniCratical -9	2025243 -9
	1.2.1.33	Spinacia oleracea	Uniformit - P	12793828 19
	1.2.1.33	Spinacia oleracea	UniFrat/3 -1	#554310 -9
	12159	Bacillus subtilis	University 4	10799421 19
	1.2.1.59	Hethandhemus fervidus	UniFranks /#	3569291 19
	12.159	Synechocystia sp.	Uniference 4	9726260 -9
Cways	Gassivali denisal Gasten fusion in shoten Gasten/Gastenenen	State organism		
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	and the second se			

Reaction View

In addition to the **Entry View** table there is the **Reaction View** table which groups the entries based on the biochemical reaction.

In the Entry and in the Reaction View data can be exported in spreadsheet, SBML or BioPAX format. Entries can be selected either by clicking the checkbox at the end of each entry row in the overview table or by clicking the checkbox in the last column header to select all displayed entries per page (see also **Data Export**).

Entry View	Reaction View Visual Search (beta)				
There are 1 1 2 Next	406 entries in 23 reaction(s) matching your query	ayed reaction	entries d	isplay 15 -	reactions per page
Kinetic data	[Sabio ID]: Reaction	Kegg ID	Visualization (Please allow pop-up windows in your browser)	Number of Entries	Add to export cart?
	(1): alpha-D-Glucose 6-phosphate = beta-D-Fructose 6-phosphate	R02740	Click here to view visualization	э	
	[10]: ATP + alpha-D-Glucose = ADP + alpha-D-Glucose 6-phosphate	R01786 7	Click here to view visualization	4	
	[1113]: ATP + D-Fructose 6-phosphate - ADP + D-Fructose 1,6-bisphosphate	R00756. 77	Click here to view visualization	225	
	[1123]: D-Glucose 6-phosphate = D-Fructose 6-phosphate	800771 7	Click here to view visualization	187	
	[1338]: D-Fructose 1,6-bisphosphate = D-Glyceroldehyde 3-phosphate + Glycerone phosphate	801068 7	Click here to view visualization	51	
	[22]: UTP + D-Fructose 6-phosphate = UDP + D-Fructose 1,6-bisphosphate	R00769 7	Click here to view visualization	24	
	[23]: CTP + D-Fructose 6-phosphate = CDP + D-Fructose 1,6-bisphosphate	R00767. 7	Click here to view visualization	24	
	[24]: ITP + D-Fructose 6-phosphate = IDP + D-Fructose 1,6-bisphosphate	R00270. 🐨	Click here to view visualization	22	
	[274]: D-Fructose 1-phosphate = Glycerone phosphate + D-Glyceraldehyde	H02568 - P	Click here to view visualization	22	

To get a quick impression about a certain reaction and to understand the connections between reaction, enzymes, organisms, and tissues a visualization is available.



Visual Search

Finally **Visual Search** gives an visual overview of the Search Result together with the opportunity to confine the search, e.g. to an organism, a tissue or a special kind of kinetic parameter or kinetic rate law.



Data Export

To export data in SBML, BioPAX, or spreadsheet format entries can be selected either in the **Entry View** or **Reaction View** by clicking the checkbox at the end of each entry row in the overview table or by clicking the checkbox in the last column header to select all displayed entries per page.

		S Bioche	R B emical R	E I C	D — F Kinetics Da	RH			Entries to f	n. Contac Export: 3 =
Home	e Search Services	Web Serv	rices N	levs D	ocumentation	Publications	Statistics Lini	la 📢	Abou	t.
Search							Filter Options			v
glycolyski Entry Vi Total nun	a dassical Advanced Scarr Reaction View Visual S aber of kinetic law entries found:	h earch (beta) 1496			Feat	0	Exzyme versyne here Equation Reaction Reaction Reaction Environmental Condit pt 3 - 16 Source Deet Sutmission Mathicale	ions Tempe	Recombinan rature: -10 0 Entries inse 16/2008	x P - est C ¹ read since:
Vinatic	- 9 10 11 12 13 14 15 15 17 18 . 0	o nex	Enzyme				Parameter	Environment		Add to
data	Reaction	ECNumber	Protein	Variant	Tissue	Organism	(besides concentration)	°C	pH	cart?
•	NAD+ + D-Glyceraldehyde 3-phosphate + Phosphate = NADH + H+ + 3-Phospho-D- glyceroyl phosphate	1.2.1.12	P04406	*wildtype	lung. *	Homo sapiens	Hill coefficient S_half			0
	NAD+ + D-Glyceraldehyde 3-phosphate + Phosphate = NADH + H+ + 3-Phospho-D- glyceroyl phosphate	1.2.1.12	P04406	P wildtype	lung '7	Homo sapiens	Hill coefficient S_helf			
	D-Glyceraldehyde 3-phosphate + Phosphate + NAD+ = H+ + NADH + Glycerate 1,3-bisphosphate	1.2.1.12	P04406	* wildtype	erythrocyte.	PHomo saplens	Kd Km Vmax	23.0	8.6	
	ATP + 3-Phospho-D-glycerate = ADP + 3-Phospho-D- glyceroyl phosphate	2.7.2.3	P00558	mutant	muscie, 7	Homo sapiens	Km Vmax	30.0	7.6	Ø

Selected entries are stored in the **Export Cart** ("Entries to Export") and the total number of selected entries is given. By clicking on "Entries to Export" a table gives an overview about selected entries for export in SBML, BioPAX or spreadsheet format. Single entries can be removed afterwards from the export table by checking them and clicking on the remove button.

Entry ID	metics data	s	elected Reactio	n		Organism	Tissue	Kinetic law type	View details	Remove entry (Select all:
27001 D-G	ilyceraldehyde spho-D-glycer	3-phosphate - ovl phosphate	+ Phosphate + NA	D+ <-> NA	DH + H+ + 3-	Homo sapiens	lung	Hill Cooperativity	-	
2723 D-G	ilyceraldehyde hosphate + N	3-phosphate - ADH + H+	Phosphate + NA	D+ <-> Ghy	vcerate 1,3-	Homo sapiens	erythrocyte	Michaelis- Menten		0
27402 ATP	+ 3-Phospho-	-D-glycerate <	-> ADP + 3-Phosp	ho-D-glyce	royl phosphate	Homo sapiens	muscle	Michaelis- Menten	-	.0
								remove sel	acted Re	actions

There are three different exports methods: Write spreadsheet, SBML, and BioPAX **Write spreadsheet** allows to export the data in a table format (xls or tsv).

•	•	Biochem	ical Reaction I	(inetics Dat	abase		Entries to Export:
Home Searc	n	services Web Services	News Do	cumentation I	Publications Statisti	cs Links	About
Save Excelsheet	M						
elect Colums to Expo	ort 🔨						
	Add all	8 items selected	Remove	all		PERMIT	1
Activator	+ -	EntryID	(-) Export x		Back to Result	
CellularLocation	+	Reaction		Export to			
Cofactor		ECNumber		-			
Enzyme Variant		UniProtKB_AC		-			
Enzymename	\bigcirc	Tissue		-			
Inhibitor	¥	Organism		-			
KeggReactionID	+	Temperature		-			
KineticMechanisn	+1	pH		-			
Other Morlifier Export Distinct Rows	Only						
review of the first 3 of	entries						
		Sabi	o Excel Export Pre	view			
A	8	c	D	E	F	G	
NAD+ + D-Glycer1.2	Number 2.1.12	Enzymename glyceraldehyde-3	UniProtKB_AC	lung	Organism Homo sapiens	Temperature	

The user can choose which entry information should be exported by selecting the columns to be exported.

As a default choice 8 items are selected (right column) which can easily be removed by clicking on the minus. To include additional columns in the export table the appropriate items on the left side should be included by clicking on the plus.

The order of the columns can easily be changed by shifting them up and down.

After finishing the selection and the order of the favored columns, which are previewed for the first 3 entries, the Export xls or Export tsv button should be pressed to execute the export.

Write SBML allows to export the selected entries as a model in the Systems Biology Markup Language (SBML)-format or as pdf. Different SBML versions and annotation schema could be selected and a user-defined name could be given to the SBML file.



No Search Result

If the **Search** did not give any results, a link to a pre-filled request form is given (see below).



User feedback can also be given via the contact button or within Services as Request for SABIO-RK curation service. Any feedback is highly appreciated.



The search term is already filled in, so that the user can request, e.g., for the addition of special publications, pathways or kinetic data for the search term.

This request is for free, will be edited by a SABIO curator and shown subsequently in the Public Curation List, if the user allowed it by choosing false in the Details Hidden section.

