SABIO-RK Documentation

(December 2022)

Search

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:
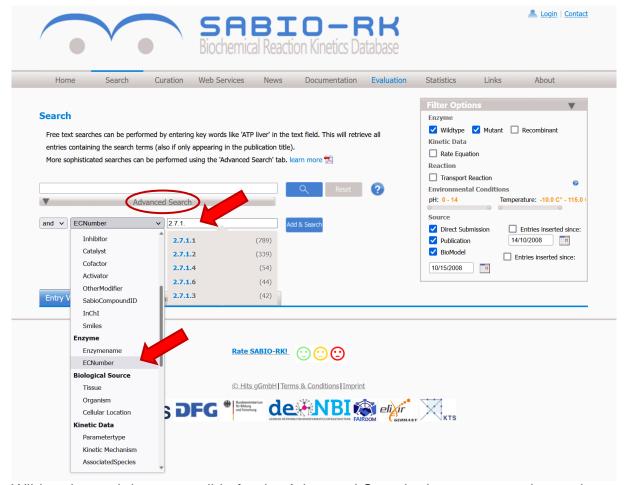
Search	Result
rattus liver rattus AND liver	entries containing both terms *rattus* and *liver*

Search	Result
(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 *ratt* (e.g. Rattus norvegicus) or ending with *kinase* (e.g. Hexokinase)
"mammalia (NCBI)" NOT "homo sapiens" "liver (BTO)"	entries for all organisms of class *mammalia* (based on NCBI taxonomy) but not for *homo sapiens* entries for tissue *liver* including all tissue sub-parts and cell lines (based on BRENDA Tissue Ontology)
Substrate:ATP	entries with reactions containing substrate *ATP* 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
ECNumber:1.* ECNumber: 1.3.1.?	All entries containing EC numbers starting with 1. wildcard search for exactly one character Entries containig EC numbers 1.3.1.1 to 1.3.1.9
Year:[2000 TO 2021]	entries with publication years between *1990* and *2012* (see also **Advanced Search**)

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

Advanced Search

To restrict search terms to specific attributes also the **Advanced Search** can be used. First an attribute from the list must 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 (https://bioportal.bioontology.org/ontologies/BTO) By selecting NCBI terms the search will include all subclasses of this term based on the NCBI Organism Taxonomy (https://www.ncbi.nlm.nih.gov/taxonomy).

Time periods of publications in attribute *Year* can be defined:

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

Filter Options

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

There are filters for the **Enzyme** (i.e. 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 recombinantly expressed 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. Filtering by temperature and pH values will exclude all entries from search without definition of those values (value = null).

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.

Search Result

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.

| Entry View | Reaction View | Bar Chart Search | Visual Search |

Total number of kinetic law entries found: **5415**   ☐ expand all displayed entries

Previous 1 .. 12 13 14 15 16 **17** 18 19 20 21 .. 361 Next   display 15 ⌄ entries per page

Kinetic data	Reaction	Enzyme			Tissue	Organism	Parameter (besides concentration)	Cond.		Add to export cart? ☐
		ECNumber	Protein	Variant				°C	pH	
▶	ATP + D-Fructose 6-phosphate = ADP + D-Fructose 1,6-bisphosphate	2.7.1.11	Q4E657	wildtype	epimastigote ⬑	Trypanosoma cruzi	Km Vmax	23.0	7.5	☐
▶	2-Phospho-D-glycerate = H2O + Phosphoenolpyruvate	4.2.1.11	P00924 P00925	wildtype	-	Saccharomyces cerevisiae	Ki	25.0	7.5	☐
▶	2-Phospho-D-glycerate = H2O + Phosphoenolpyruvate	4.2.1.11	P00925 P00924	wildtype	-	Saccharomyces cerevisiae	Ki	25.0	7.5	☐
▶	2-Phospho-D-glycerate = H2O + Phosphoenolpyruvate	4.2.1.11	P00924 P00925	wildtype	-	Saccharomyces cerevisiae	Ki	25.0	7.5	☐
▶	ATP + Pyruvate = ADP + Phosphoenolpyruvate	2.7.1.40	P11974	wildtype	muscle ⬑	Oryctolagus cuniculus	Km Vmax Vmax/Km	25.0	7.4	☐
▶	ATP + Pyruvate = ADP + Phosphoenolpyruvate	2.7.1.40	P11974	wildtype	muscle ⬑	Oryctolagus cuniculus	Km Vmax Vmax/Km	25.0	7.4	☐
▶	ATP + Pyruvate = ADP + Phosphoenolpyruvate	2.7.1.40	P11974	wildtype	muscle ⬑	Oryctolagus cuniculus	Ki	25.0	7.4	☐

Detailed information about kinetic data of a specific biochemical reaction determined in one experiment 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".

Total number of kinetic law entries found: **5415**   ☐ expand all displayed entries

Previous 1 .. 12 13 14 15 16 **17** 18 19 20 21 .. 361 Next   display [15 ∨] entries per page

Kinetic data	Reaction	Enzyme			Tissue	Organism	Parameter (besides concentration)	Cond.		Add to export cart? ☐
		ECNumber	Protein	Variant				°C	pH	
▼	ATP + D-Fructose 6-phosphate = ADP + D-Fructose 1,6-bisphosphate	2.7.1.11	Q4E657	wildtype	epimastigote ⌐	Trypanosoma cruzi	Km Vmax	23.0	7.5	☐

Entry ID: 12542

General information

Organism	Trypanosoma cruzi
Tissue	epimastigote ⌐
EC Class	2.7.1.11
SABIO reaction id	1113
Variant	wildtype
Experiment Type	in vitro
Pathways	Carbon metabolism Glycolysis classical Glycolysis/Gluconeogenesis Metabolic pathways Methane metabolism Microbial metabolism in diverse environments Starch and Sucrose metabolism

Substrates

name	location	comment
D-Fructose 6-phosphate	-	-
ATP	-	-

Products

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

Modifiers

name	location	effect	comment	protein complex
Mn2+	-	Modifier-Activator	-	-
6-phosphofructokinase(Enzyme)	-	Modifier-Catalyst	-	Q4E657;

Enzyme (protein data)

	UniProtKB_AC	name	mol. weight (kDa)	deviation (kDa)
subunit	Q4E657	-	-	-
complex	-	-	-	-

Kinetic Law

type	formula	annotation
Sequential Bi Bi	Vmax*A*B/(KmA*KmB+KmB*A+KmA*B+A*B)	SBO:0000151 ⌐

Other definitions

variable	variable formula

Parameter

name	type	species	start val.	end val.	deviat.	unit	comment
M	concentration ⌐	Mn2+	3.0	-	-	mM	saturated
A	concentration ⌐	ATP	0.0	500.0	-	µM	-
B	concentration ⌐	D-Fructose 6-phosphate	0.0	10.0	-	mM	-
KmB	Km ⌐	D-Fructose 6-phosphate	1.1	-	0.1	mM	-
KmA	Km ⌐	ATP	22.0	-	3	µM	equals Kia
Vmax	Vmax ⌐	-	7.9	-	0.5	µmol/(min*mg)	-

Experimental conditions

	start value	end value	unit
pH	7.5	-	-
temperature	23.0	-	°C
buffer	50 mM HEPES, 90 mM KCl, 5 mM mercaptoethanol, 0.2 mM NADH, 50 U/ml aldolase, 50 U/ml triosephosphate isomerase, 50 U/ml glycerol-3-phosphate dehydrogenase		
comment	-		

Reference

title	author	year	journal	volume	pages	PubMed
Involvement of a divalent cation in the binding of fructose 6-phosphate to Trypanosoma cruzi phosphofructokinase: kinetic and magnetic resonance studies	Urbina JA, Ysern X, Mildvan AS	1990	Arch Biochem Biophys	278	187-94	2138869 ⌐

report wrong or missing data

Furthermore SABIO-RK offers details about the Reaction, Organism, Enzyme, Protein, Pathway and Compound of an entry which are shown in additional pop-up windows after clicking on the appropiate 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, Stoichiometric Equation, Substrates, Products, Enzymes known to catalyse this reaction, Pathways and links to external databases.
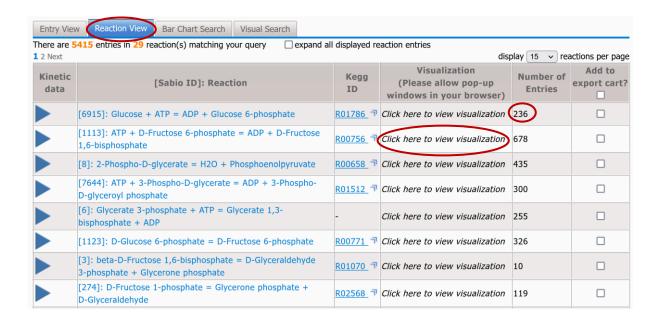
Reaction Details pop-up window with links to other data resources.

SABIO-RK

Reaction Details

Reaction ID	7
Stochiometric Equation	2-Phosphoglycerate <-> Glycerate 3-phosphate
Substrates	2-Phosphoglycerate
Products	Glycerate 3-phosphate

	EC Number	in Organism	UniProtKB Link	PubMedID
	5.4.2.11	Amycolatopsis methanolica	UniProtKB	7961441
	5.4.2.11	Equus caballus	UniProtKB	8447
	5.4.2.11	Gallus gallus	UniProtKB	213437
	5.4.2.11	Gallus gallus	UniProtKB	8447
Enzymes known to catalyse this reaction (curated information)	5.4.2.11	Homo sapiens	UniProtKB	15949708
	5.4.2.11	Rattus norvegicus	UniProtKB	6450416
	5.4.2.11	Rattus norvegicus	UniProtKB	7929251
	5.4.2.11	Saccharomyces cerevisiae	UniProtKB	1386023
	5.4.2.11	Saccharomyces cerevisiae	UniProtKB	23856461
	5.4.2.11	Sus scrofa	UniProtKB	6293580
	5.4.2.12	Entamoeba histolytica	UniProtKB	15794763

Pathways	Biosynthesis of amino acids Biosynthesis of secondary metabolites Carbon metabolism Glycine, Serine and Threonine metabolism Glycolysis classical Glycolysis/Gluconeogenesis Metabolic pathways Methane metabolism Microbial metabolism in diverse environments

External Links

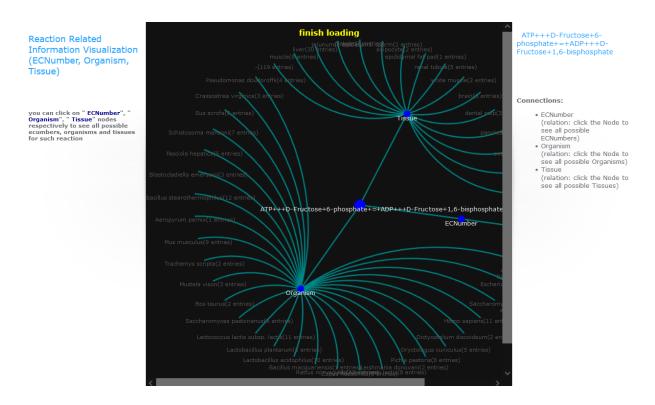| KEGG-Pathway-ID	map01230 map01110 map01200 map00260 map00010 map01100 map00680 map01120
KEGG-Reaction-ID	R01518
MetaNetX-Reaction-ID	MNXR102547
Rhea-Reaction-ID	15903 15904 15901 15902
Reactome-Reaction-ID	R-DRE-71654 R-SSC-71445 R-SPO-71654 R-DME-71445 R-DRE-71445 R-ATH-71445 R-PFA-71654 R-DDI-71654 R-CFA-71445 R-MMU-71654 R-SCE-71654 R-BTA-71445 R-DME-71654 R-HSA-71445 R-SCE-71445 R-XTR-71445 R-RNO-71445 R-BTA-71654 R-TGU-71445 R-CFA-71654 R-MMU-71445 R-HSA-71654 R-OSA-71654 R-GGA-71445 R-TGU-71654 R-DDI-71445 R-ATH-71654 R-PFA-71445 R-XTR-71654 R-SSC-71654 R-SPO-71445 R-RNO-71654 R-OSA-71445 R-GGA-353014 R-GGA-71654 R-GGA-352994
MetaCyc-Reaction-ID	3PGAREARR-RXN

Reaction View

In addition to the Entry View table there is the Reaction View table which groups the entries based on the biochemical reaction and shows the number of entries per 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**	Bar Chart Search	Visual Search

There are **5415** entries in **29** reaction(s) matching your query ☐ expand all displayed reaction entries

1 2 Next

display 15 ∨ reactions per page

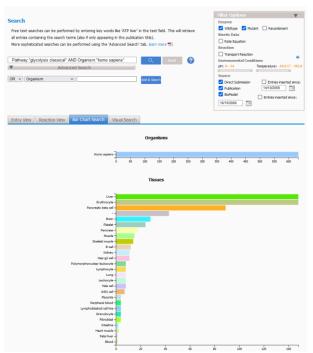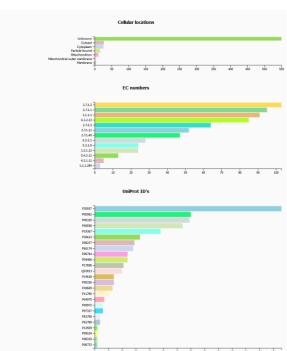| Kinetic data	[Sabio ID]: Reaction	Kegg ID	Visualization (Please allow pop-up windows in your browser)	Number of Entries	Add to export cart? ☐
▶	[6915]: Glucose + ATP = ADP + Glucose 6-phosphate	R01786 ⬏	Click here to view visualization	236	☐
▶	[1113]: ATP + D-Fructose 6-phosphate = ADP + D-Fructose 1,6-bisphosphate	R00756 ⬏	Click here to view visualization	678	☐
▶	[8]: 2-Phospho-D-glycerate = H2O + Phosphoenolpyruvate	R00658 ⬏	Click here to view visualization	435	☐
▶	[7644]: ATP + 3-Phospho-D-glycerate = ADP + 3-Phospho-D-glyceroyl phosphate	R01512 ⬏	Click here to view visualization	300	☐
▶	[6]: Glycerate 3-phosphate + ATP = Glycerate 1,3-bisphosphate + ADP	-	Click here to view visualization	255	☐
▶	[1123]: D-Glucose 6-phosphate = D-Fructose 6-phosphate	R00771 ⬏	Click here to view visualization	326	☐
▶	[3]: beta-D-Fructose 1,6-bisphosphate = D-Glyceraldehyde 3-phosphate + Glycerone phosphate	R01070 ⬏	Click here to view visualization	10	☐
▶	[274]: D-Fructose 1-phosphate = Glycerone phosphate + D-Glyceraldehyde	R02568 ⬏	Click here to view visualization	119	☐

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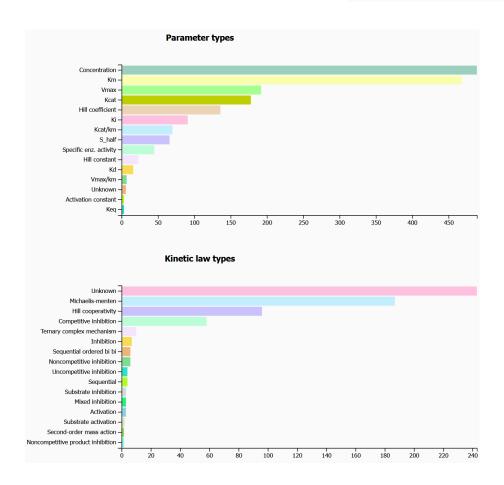
Bar Chart Search

A visual overview of the frequency distribution of single attributes within a search result is given in the Bar Chart Search. Here the user can confine the search to one specific Organism, Tissue, Cellular location, EC number, Uniprot ID, Parameter type or Kinetic law type by clicking on the corresponding bar.
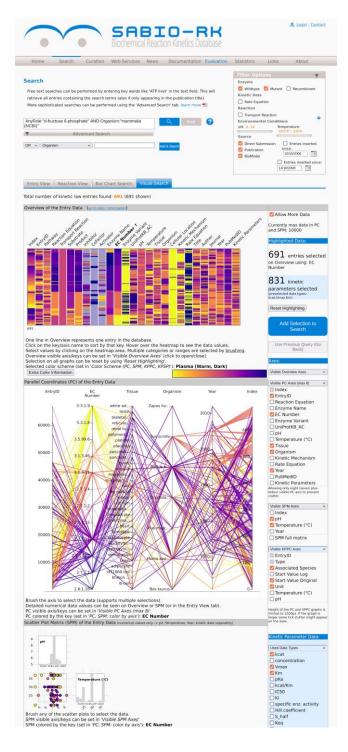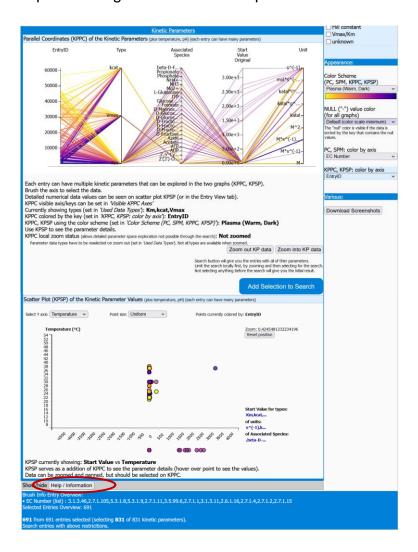
Visual Search

Visual search is a graphical interface that is customizable and allows interactive navigation of search results.

The offered graphs consist of a heat map representing an Overview of the Entry Data, Parallel Coordinates (PC) of the Entry Data and Scatter Plot Matrix of the Entry Data with histograms (SPM). These entry based graphs contain all entry information except the kinetic parameter values of the Search result.

Since each entry can contain several kinetic parameters, the kinetic parameters are represented separately in the KPPC (Parallel Coordinates of the Kinetic Parameters)
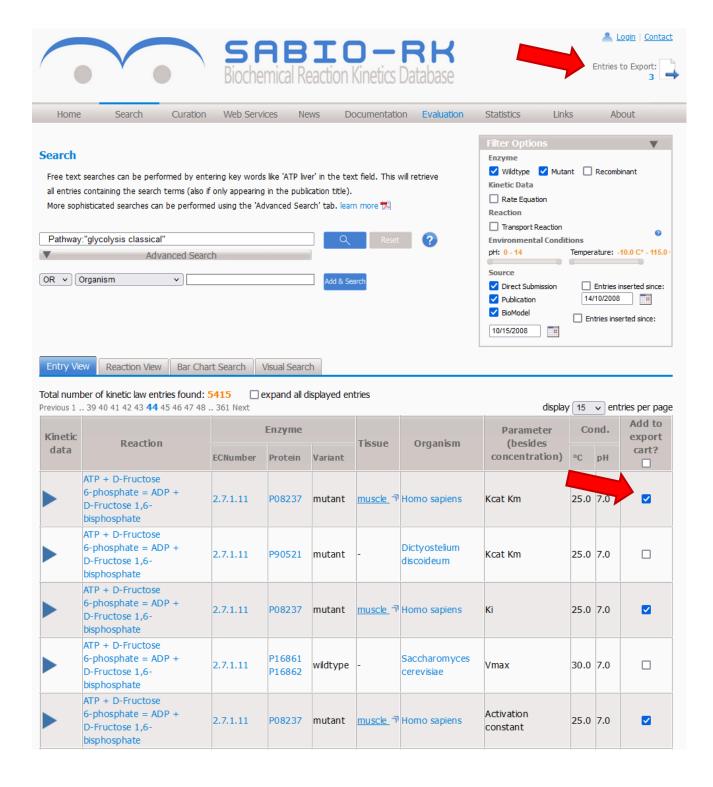
and the KPSP (Scatter Plot of the Kinetic Parameter Values) graphs, which allow to explore through the kinetic data space.
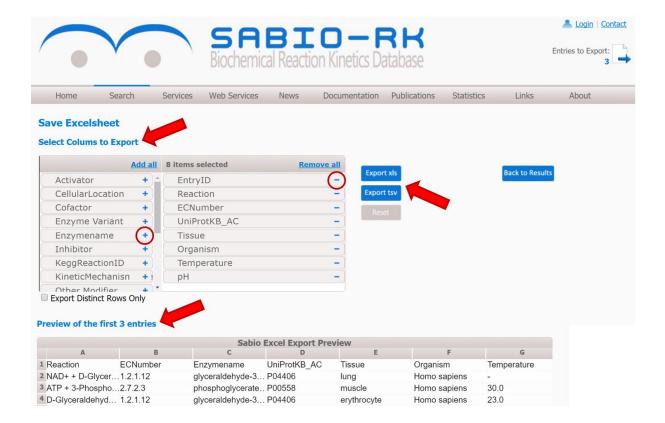

By pressing the Help/Information button detailed explanation of all the functionalities in the Visual Search is shown in detail.

Data Export

To export data in SBML, spreadsheet or other formats 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.

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.

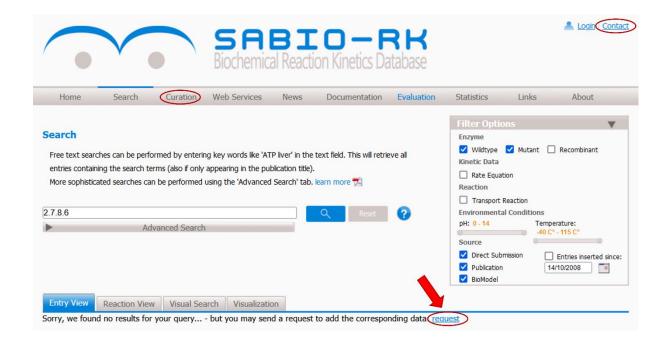The order of the columns can easily be changed by shifting them up and down.

After finishing the selection and the order of the favoured 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.

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