



# Documentation

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## Introduction

The SABIO-Reaction Kinetics database (SABIO-RK) has as objective to provide data about the kinetics of biochemical reactions in different organisms, tissues and determined for or under diverse experimental conditions [1,2]. The database contains information about biochemical reactions, their compounds, their kinetics, and the pathways in which they participate. All this is related to information on enzymes, and organisms. The database allows the storage of multiple kinetic descriptions for the same reaction, according to factors such as the environmental conditions under which the experiments were done.

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## Reaction Search

In order to find kinetic data for biochemical reactions, characteristics of the reaction(s) can be specified. The user can combine different search criteria in one query. In doing so, at least one of the characteristics highlighted in blue must be included (Fig. 1).

Search

Return only reactions having kinetic data matching all criteria (blue and grey)

Search criteria in blue are used to define the search conditions for reactions, independently if there is or not kinetic data for these reactions.

Specify Search Criteria:

- Search criteria:  
No criteria selected

with **Reactant(s)** [ + ] [ - ]

in **Pathway(s)** [ + ] [ - ]

having **Enzyme(s)** [ + ] [ - ]

in **Publication** [ + ] [ - ]

related to **Protein** (UniProtID) [ + ] [ - ]

for **Signalling** [ + ] [ - ]

in **Organism(s)** [ + ] [ - ]

in **Tissue(s)/Cell Type(s)** [ + ] [ - ]

in **(Intra/Extra)Cellular Location(s)** [ + ] [ - ]

having **Kinetic Data** Determined for Specific Experimental Conditions [ + ] [ - ]

having **Kinetic data** [ + ] [ - ]

Fig. 1 Query page of SABIO-RK.

Details concerning the different characteristics:

- **Reactant(s)** (= chemical compounds) of the reactions and their functions (substrates, products, inhibitors, activators, cofactors)
- **Pathway(s)** in which the reaction participates, mainly based on KEGG definition
- **Enzyme(s)** catalysing the reaction by name or EC number, names are mainly due to IUBMB Nomenclature Committee Recommendations
- **Publication** in which kinetic data for the reaction were reported (Pubmed ID, author or title)
- **Protein** by defining UniProtID
  - wildtype or mutant
  - recombinant

- **Signalling** include signalling events and protein modification types
- **Organism(s)** in which the reaction takes place, due to NCBI taxonomy
- **Tissue(s)/Cell Type(s)** in which the reaction can take place
- having **Kinetic Data** (Fig. 2)
  - for defined experimental conditions (pH and temperature)
  - for defined parameter types (Km, Vmax etc.)
  - containing any rate law definition
  - containing a defined rate law
  - containing detailed mechanism steps

having **Kinetic Data** Determined for Specific Experimental Conditions [ + ] [ - ]

pH [ = ] [ > ] [ < ] [ 6 ] [ 7 ] [ 8 ] [ 9 ] [ 10 ]

Temperature [ = ] [ > ] [ < ] [ 37 ] °C

---

having **Kinetic data** [ + ] [ - ]

<input checked="" type="checkbox"/> Vmax	<input checked="" type="checkbox"/> Km	<input type="checkbox"/> Vmax/Km	<input type="checkbox"/> kcat
<input type="checkbox"/> kcat/Km	<input type="checkbox"/> Kd	<input type="checkbox"/> rate const.	<input type="checkbox"/> enz. activity
<input type="checkbox"/> EC50	<input type="checkbox"/> Hill coefficient	<input type="checkbox"/> Hill constant	<input type="checkbox"/> S_half
<input type="checkbox"/> Ki	<input type="checkbox"/> IC50	<input type="checkbox"/> Keq	

---

Rate law

---

Kinetic mechanism type

Michaelis-Menten ▼

---

Detailed mechanism data (single steps)

Fig. 2 Example for specifying kinetic details.

To submit a query, the following steps can be done (Fig. 3):

- 1 “Return only reactions having kinetic data matching all criteria (blue and grey) ”  
 clicked on views only those results for which there is kinetic data associated  
 exactly satisfying the search criteria. By deselecting the checkbox search results  
 will be displayed also for other search criteria like for example other organisms or  
 tissues.
- 2 Open search field using [ + ].

- 3 While typing in the search field, a selection list appears.
- 4 Select one or more items from the selection list. Selected items appear below the search field.
- 5 Use wildcard "%" to display e.g. all kinases in the selection list (type "%kinase" in the search field). Then again select one or more items from the list.
- 6 And/Or definition within one single search criterion.
- 7 "Submit search" button → [Search Results Overview](#)

The screenshot shows the SABIO-RK search interface. At the top, there is a login section with fields for Username and Password, and a 'remember me' checkbox. Below this is a navigation bar with links for HOME, CONTACT, HELP, and IMPRINT, and a 'Reaction Search' button (annotated with a red '1').

The main search area includes a search criteria section with a 'Specify Search Criteria:' label (annotated with a red '7'). Below this is a dropdown menu for search criteria, currently set to 'with Reactant(s)' (annotated with a red '2'). A search input field contains 'glucos', and a dropdown list of suggestions is visible, with 'Glucose' highlighted (annotated with a red '3').

Below the search criteria section, there is a 'Submit Search' button and a 'Reset Form' button. A search criteria list is shown on the left, including 'Reactant:', 'Pathway:', 'Enzyme:', 'Publication:', 'Protein:', 'Sign. modific.:', 'Sign. event:', 'Organism:', 'Tissue:', 'Cell. loc.:', 'Exp. cond.:', and 'Kin. data:'. The 'Protein:' criterion is set to 'P52792' (annotated with a red '4').

At the bottom, there is a section for 'Join entries with' options, with 'AND or OR' selected (annotated with a red '6'). Below this are radio buttons for 'wildtype', 'mutant', 'both', 'non-recomb.', 'recombinant', and 'both'.

Fig.3 Search for reactions by specifying their characteristics. The red numbers are explained in the text above.

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# Search Results Overview

In the search results overview (Fig. 4) the total number of reactions found for specified search criteria, which are shown on the left hand side control panel, is given together with a table containing:

The reaction equations satisfying the search criteria (a) together with the information whether (c) and how many (d) entries containing kinetic data are available. For each reaction all possible enzymes reported to catalyse this reaction is also be given (e) with information whether or not there is kinetic data available for the enzyme including other reactions (f) and how many entries are available (g). Green view buttons indicate that there is kinetic data available for all the criteria defined, yellow view buttons are given in the case of having kinetic information but not matching all the criteria, and red indicates that there is no kinetic data available.

**SABIO-RK**

You are logged in as anonymousUser

Username:  Password:   remember me

HOME | CONTACT | HELP | IMPRINT | Search Results

**Total number of reactions found for specified search criteria: 6**

Click here to view your search criteria

**Kinetic Data Availability:**

- Kinetic data available matching the search criteria
- Kinetic data available, but not matching all search criteria
- No kinetic data available

Number of results per page:

Show only reactions having kinetic data matching the search criteria

Reactions	Select only Reaction(s) (without kinetic data)	Kinetic Data for this reaction (Click to View)	#	Enzyme EC#	Kinetic data for enzymes (Click to View)	#
D-Glucose + ATP <-> D-Glucose 6-phosphate + ADP	<input type="checkbox"/>	<input type="button" value="view"/>	8	<a href="#">2.7.1.2</a>	<input type="button" value="view"/>	12
				<a href="#">2.7.1.1</a>	<input type="button" value="view"/>	616
				<a href="#">2.7.1.59</a>	<input type="button" value="view"/>	8
				<a href="#">2.7.1.4</a>	<input type="button" value="view"/>	26
				<a href="#">2.7.1.60</a>	<input type="button" value="view"/>	13
H2O + 3-beta-D-Glucosido lithocholic acid <-> beta-D-Glucose + 3alpha-Hydroxy-5beta-cholanate	<input type="checkbox"/>	<input type="button" value="view"/>	7	<a href="#">3.2.1.45</a>	<input type="button" value="view"/>	10
H2O + 4-Methylumbelliferyl-beta-D-glucoside <-> beta-D-Glucose + 4-Methylumbelliferol	<input type="checkbox"/>	<input type="button" value="view"/>	1	<a href="#">3.2.1.45</a>	<input type="button" value="view"/>	10
D-Glucose 6-phosphate + H2O <-> D-Glucose + Phosphate	<input type="checkbox"/>	<input type="button" value="view"/>	1	<a href="#">3.1.3.9</a>	<input type="button" value="view"/>	1
				<a href="#">3.1.3.2</a>	<input type="button" value="view"/>	143
				<a href="#">3.1.3.1</a>	<input type="button" value="view"/>	113
				<a href="#">3.1.3.25</a>	<input type="button" value="view"/>	30
H2O + 3-beta-D-Glucosido chenodeoxycholic acid <-> beta-D-Glucose + Chenodeoxycholate	<input type="checkbox"/>	<input type="button" value="view"/>	1	<a href="#">3.1.3.58</a>	<input type="button" value="view"/>	0
				<a href="#">3.2.1.45</a>	<input type="button" value="view"/>	10
beta-D-Glucose + NAD+ <-> NADH + D-Glucono-1,5-lactone + H+	<input type="checkbox"/>	<input type="button" value="view"/>	2	<a href="#">1.1.1.47</a>	<input type="button" value="view"/>	2

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Fig. 4 Search Results Overview including number of results (circled), list of search criteria (boxed), and a table containing reactions and more information (a-g).

→ “Show only reactions having kinetic data matching the search criteria” clicked on views only those results for which there is kinetic data associated exactly satisfying the search criteria (green view buttons). By deselecting the checkbox search results will be displayed also for other search criteria like for example other organisms or tissues (yellow view buttons). Also reactions without kinetic data (red cross) will be shown (Fig. 5). This checkbox has identical function with the checkbox in the → [Reaction Search](#) Page.

**SABIO-RK**

You are logged in as anonymousUser

Username:  Password:   remember me

HOME | CONTACT | HELP | IMPRINT | Search Results

**Total number of reactions found for specified search criteria: 195**

Click here to view your search criteria

**Kinetic Data Availability:**

- Kinetic data available matching the search criteria
- Kinetic data available, but not matching all search criteria
- No kinetic data available

Number of results per page:

Show only reactions having kinetic data matching the search criteria

Reactions	Select only Reaction(s) (without kinetic data)	Kinetic Data for this reaction (Click to View)	#	Enzyme EC#	Kinetic data for enzymes (Click to View)	#
<a href="#">beta-D-Glucose + NAD+ &lt;-&gt; NADH + D-Glucono-1,5-lactone + H+</a>	<input type="checkbox"/>		2	<a href="#">1.1.1.47</a>		2
<a href="#">ITP + D-Glucose &lt;-&gt; IDP + Glucose 6-phosphate</a>	<input type="checkbox"/>		1	<a href="#">2.7.1.1</a>		616
<a href="#">D-Glucose + dTTP &lt;-&gt; D-Glucose 6-phosphate + TDP</a>	<input type="checkbox"/>		1	<a href="#">2.7.1.1</a>		616
<a href="#">D-Glucose + Protein N(pi)-phospho-L-histidine &lt;-&gt; alpha-D-Glucose 6-phosphate + Protein histidine</a>	<input type="checkbox"/>		8	<a href="#">2.7.1.69</a>		52
<a href="#">H2O + Phenyl alpha-D-glucoside &lt;-&gt; alpha-D-Glucose + Phenol</a>	<input type="checkbox"/>		1	<a href="#">3.2.1.20</a>		146

(Only the reaction data will be included into the SBML file but no kinetics data; click on green or yellow images 'view' to select kinetics data)

Page: [1](#) [2](#) [3](#) [4](#) [5](#) [6](#) [7](#) [8](#) [9](#) [10](#) [11](#) [12](#) [13](#) [14](#) [15](#) [16](#) [17](#) [18](#) [19](#) [20](#) [21](#) [22](#) [23](#) [24](#) [25](#) [26](#) [27](#) [28](#) [29](#) [30](#) [31](#) [32](#) [33](#) [34](#) [35](#) [36](#) [37](#) [38](#) [39](#)

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Fig. 5 Results of the same query as in Fig. 4 after deselecting the checkbox.

From the list of reactions, the details of the reaction can be viewed in a separate window by clicking on its respective stoichiometric equation → [Reaction Details](#) (Fig. 6).

Reactions	Select only Reaction(s) (without kinetic data)	Kinetic Data for this reaction (Click to View)	#	Enzyme EC#	Kinetic data for enzymes (Click to View)	#
<a href="#">D-Glucose + ATP &lt;-&gt; D-Glucose 6-phosphate + ADP</a>	<input type="checkbox"/>	<input type="button" value="view"/>	8	<a href="#">2.7.1.2</a>	<input type="button" value="view"/>	12
				<a href="#">2.7.1.1</a>	<input type="button" value="view"/>	616
				<a href="#">2.7.1.59</a>	<input type="button" value="view"/>	8
				<a href="#">2.7.1.4</a>	<input type="button" value="view"/>	26
				<a href="#">2.7.1.60</a>	<input type="button" value="view"/>	13

Fig. 6 By clicking on a single reaction the Reaction Details window will open.

From the list of enzymes, general information about an enzyme can be viewed in a separate window by clicking on the EC number → [Enzyme Details](#) (Fig. 7).

Reactions	Select only Reaction(s) (without kinetic data)	Kinetic Data for this reaction (Click to View)	#	Enzyme EC#	Kinetic data for enzymes (Click to View)	#
<a href="#">D-Glucose + ATP &lt;-&gt; D-Glucose 6-phosphate + ADP</a>	<input type="checkbox"/>	<input type="button" value="view"/>	8	<a href="#">2.7.1.2</a>	<input type="button" value="view"/>	12
				<a href="#">2.7.1.1</a>	<input type="button" value="view"/>	616
				<a href="#">2.7.1.59</a>	<input type="button" value="view"/>	8
				<a href="#">2.7.1.4</a>	<input type="button" value="view"/>	26
				<a href="#">2.7.1.60</a>	<input type="button" value="view"/>	13

Fig. 7 By clicking on a single EC-number the Enzyme Details window will open.

To export reactions without kinetic data into an SBML file, click the checkbox “Select only Reaction(s) (without kinetic data)” (Fig. 8). For details about exporting data to SBML file go to → [Data Export](#).

Reactions	Select only Reaction(s) (without kinetic data)	Kinetic Data for this reaction (Click to View)	#	Enzyme EC#	Kinetic data for enzymes (Click to View)	#
<a href="#">D-Glucose + ATP &lt;-&gt; D-Glucose 6-phosphate + ADP</a>	<input checked="" type="checkbox"/>	<input type="button" value="view"/>	8	<a href="#">2.7.1.2</a>	<input type="button" value="view"/>	12
				<a href="#">2.7.1.1</a>	<input type="button" value="view"/>	616
				<a href="#">2.7.1.59</a>	<input type="button" value="view"/>	8
				<a href="#">2.7.1.4</a>	<input type="button" value="view"/>	26
				<a href="#">2.7.1.60</a>	<input type="button" value="view"/>	13

Fig. 8 By clicking on the checkbox reactions without kinetic data will be exported into an SBML file.

To view the kinetic data associated with a reaction or with its related enzyme(s) click on the respective “view” button (Fig. 9). The → [View Kinetic Data](#) Page will pop up in a new window.







Reactions	Select only Reaction(s) (without kinetic data)	Kinetic Data for this reaction (Click to View)	#	Enzyme EC#	Kinetic data for enzymes (Click to View)	#
<a href="#">D-Glucose + ATP &lt;-&gt; D-Glucose 6-phosphate + ADP</a>	<input type="checkbox"/>		8	<a href="#">2.7.1.2</a>		12
				<a href="#">2.7.1.1</a>		616
				<a href="#">2.7.1.59</a>		8
				<a href="#">2.7.1.4</a>		26
				<a href="#">2.7.1.60</a>		13

Fig. 9 By clicking on one of the view buttons the View Kinetic Data window will open.

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## Reaction Details

The “Reaction Details” page contains several details of the selected reaction (Fig. 10). It shows the stoichiometric equation (1), the reactants (substrates and products) of the reaction (2) linked to → [Compound Details](#) and the pathway to which the reaction is associated (7) with a link to → [Pathway Details](#). EC Numbers of enzymes that are known from literature to catalyse the reaction are given (3) and linked to → [Enzyme Details](#). The organism (4) and the PubMed ID (6) associated with this information together with a link to the PubMed database are shown. A link to the UniProt database (5) is also provided by using the enzyme classification number and the organism name.

http://sabiork.h-its.org/reactdetails.jsp?reactid=1689

**Reaction Details**

Stoichiometric Equation **1** [beta-D-Glucose + NAD+ <-> NADH + D-Glucono-1,5-lactone + H+](#)

Substrates **2** [beta-D-Glucose](#)  
[NAD+](#)

Products [NADH](#)  
[D-Glucono-1,5-lactone](#)  
[H+](#)

EC Number	in Organism	UniProt Link	PubMedID
<a href="#">1.1.1.47</a>	Anas platyrhynchos	<a href="#">UniProt</a>	<a href="#">14342292</a>
<a href="#">1.1.1.47</a>	Bacillus subtilis	<a href="#">UniProt</a>	<a href="#">21162</a>
<a href="#">1.1.1.47</a>	Bos taurus	<a href="#">UniProt</a>	<a href="#">14342292</a>
<a href="#">1.1.1.47</a>	Bos taurus	<a href="#">UniProt</a>	<a href="#">6048806</a>
<a href="#">1.1.1.47</a>	Bos taurus	<a href="#">UniProt</a>	<a href="#">7092232</a>
<a href="#">1.1.1.47</a>	Cavia porcellus	<a href="#">UniProt</a>	<a href="#">14342292</a>
<a href="#">1.1.1.47</a>	Columba sp.	<a href="#">UniProt</a>	<a href="#">14342292</a>
<a href="#">1.1.1.47</a>	Gallus gallus	<a href="#">UniProt</a>	<a href="#">14342292</a>
<a href="#">1.1.1.47</a>	Homo sapiens <b>4</b>	<a href="#">UniProt</a> <b>5</b>	<a href="#">14342292</a> <b>6</b>
<a href="#">1.1.1.47</a>	Lagothrix lagothricha	<a href="#">UniProt</a>	<a href="#">14342292</a>
<a href="#">1.1.1.47</a>	Mus musculus	<a href="#">UniProt</a>	<a href="#">14342292</a>
<a href="#">1.1.1.47</a>	Paralabrax clathratus	<a href="#">UniProt</a>	<a href="#">14342292</a>
<a href="#">1.1.1.47</a>	Pituophis catenifer	<a href="#">UniProt</a>	<a href="#">14342292</a>
<a href="#">1.1.1.47</a>	Rattus sp.	<a href="#">UniProt</a>	<a href="#">14342292</a>
<a href="#">1.1.1.47</a>	Scomber scombus	<a href="#">UniProt</a>	<a href="#">14342292</a>
<a href="#">1.1.1.47</a>	Sulfolobus solfataricus	<a href="#">UniProt</a>	<a href="#">3827812</a>
<a href="#">1.1.1.47</a>	Sus scrofa	<a href="#">UniProt</a>	<a href="#">14342292</a>
<a href="#">1.1.1.47</a>	Sus scrofa	<a href="#">UniProt</a>	<a href="#">3350116</a>
<a href="#">1.1.1.47</a>	Sus scrofa	<a href="#">UniProt</a>	<a href="#">4392298</a>
<a href="#">1.1.1.47</a>	Sus scrofa	<a href="#">UniProt</a>	<a href="#">6641908</a>

Enzymes known to catalyse this reaction (curated information) **3**

Pathways **7** [Entner-Doudoroff-Pathway](#)  
[Pentose phosphate cycle](#)  
[non-phosphorylative Entner-Doudoroff-Pathway](#)

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Fig. 10 The Reaction Details page. The red numbers are explained in the text above.


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## Compound Details

The “Compound Details” page can be reached via the “Reaction Details” or the “Kinetic Data for this Reaction” page by clicking on a specific substrate, product, inhibitor, activator, or cofactor. It contains general information about a chemical compound (Fig. 11). It shows the names of the compound (1) and the SABIO-RK compound ID (2). Apart from that links to the external databases CAS (3), KEGG (4), PUBCHEM (5), ChEBI (6), and HepatoSys-Network (7) are given.

To view all reactions put in the database containing the compound of interest click on the “List of Reaction” button which is a direct link to → [Reaction Details](#).

Compound Details



[Back](#)      [List of Reactions](#)

<b>Common Name</b>	<b>1</b>	NAD+
<b>Synonyms</b>		NAD
		Nicotinamide adenine dinucleotide (oxidized)
		Diphosphopyridine nucleotide
		DPN
		Nadide
<b>SABIO-Compound-ID</b>	<b>2</b>	Nicotinamide adenine dinucleotide
<b>External Links</b>		37
<b>CAS-ID</b>	<b>3</b>	<a href="#">53-84-9</a>
<b>KEGG-ID</b>	<b>4</b>	<a href="#">C00003</a>
		<a href="#">C00004</a>
<b>PUBCHEM-ID</b>	<b>5</b>	<a href="#">3305</a>
<b>ChEBI-ID</b>	<b>6</b>	<a href="#">13389</a>
		<a href="#">44215</a>
		<a href="#">15846</a>
<b>HepatoSys-ID</b>	<b>7</b>	<a href="#">C00003</a> (Only accessible for HepatoSys project members)
		<a href="#">C00004</a> (Only accessible for HepatoSys project members)

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Fig. 11 The Compound Details page. The red numbers are explained in the text.

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## Enzyme Details

The “Enzyme Details” page can be reached via the “Reaction Details” or the “Kinetic Data for this Reaction” page.

It contains general information about an enzyme (Fig. 12). It shows the recommended (1) and alternative names (2) of the enzyme, the EC number (3) and the definition of the enzyme classification based on the IUBMB recommendations (4). A list of stoichiometric equations contains the reactions, which are known to be catalysed by this enzyme (5). To view the → [Reaction Details](#) of a single reaction, click on it. Apart from that links to the external databases EXPASY, KEGG, IntEnz, IUBMB, Reactome, and HepatoSys-Network are given (6).



Enzyme Details	
<b>Enzyme (recommended) name</b>	<b>1</b> Glucose 1-dehydrogenase
<b>Alternative names</b>	<b>2</b> beta-D-glucose:NAD(P) 1-oxidoreductase D-glucose dehydrogenase (NAD(P)) Hexose phosphate dehydrogenase
<b>EC Classification</b>	<b>3</b> 1.1.1.47
<b>Classification</b>	<b>4</b> Oxidoreductases Acting on the CH-OH group of donors With NAD(+) or NADP(+) as acceptor
<b>Catalyses reactions</b>	<b>5</b> <a href="#">Glucose 6-phosphate + NADP+ &lt;-&gt; 6-Phospho-D-glucono-1,5-lactone + H+ + NADPH</a> <a href="#">D-Galactose 6-phosphate + NADP+ &lt;-&gt; H+ + 6-Phospho-D-galactono-1,5-lactone + NADPH</a> <a href="#">Glucose 6-phosphate + NAD+ &lt;-&gt; 6-Phospho-D-glucono-1,5-lactone + NADH + H+</a> <a href="#">NAD+ + 6-Deoxy-D-glucose &lt;-&gt; NADH + H+ + 6-Deoxy-D-glucono-1,5-lactone</a> <a href="#">2-Deoxy-D-glucose 6-phosphate + NADP+ &lt;-&gt; H+ + 2-Deoxy-6-phospho-D-glucono-1,5-lactone + NADPH</a> <a href="#">D-Glucose + NAD+ &lt;-&gt; NADH + D-Glucono-1,5-lactone + H+</a> <a href="#">D-Galactose + NADP+ &lt;-&gt; NADPH + D-Galactono-1,5-lactone + H+</a> <a href="#">D-Xylose + NAD+ &lt;-&gt; NADH + D-Xylonolactone + H+</a> <a href="#">D-Xylose + NADP+ &lt;-&gt; H+ + NADPH + D-Xylonolactone</a> <a href="#">beta-D-Glucose + NAD+ &lt;-&gt; NADH + D-Glucono-1,5-lactone + H+</a> <a href="#">beta-D-Glucose + NADP+ &lt;-&gt; NADPH + D-Glucono-1,5-lactone + H+</a> <a href="#">D-Galactose + NAD+ &lt;-&gt; NADH + H+ + D-Galactonate</a> <a href="#">D-Galactose + NADP+ &lt;-&gt; H+ + NADPH + D-Galactonate</a> <a href="#">D-Glucose + NAD+ &lt;-&gt; NADH + H+ + D-Gluconate</a> <a href="#">D-Glucose + NADP+ &lt;-&gt; H+ + NADPH + D-Gluconate</a> <a href="#">D-Glucose + NADP+ &lt;-&gt; D-Glucono-1,5-lactone + H+ + NADPH</a> <a href="#">D-Galactose + NAD+ &lt;-&gt; NADH + D-Galactono-1,5-lactone + H+</a> <a href="#">D-Glucose 6-phosphate + NADP+ &lt;-&gt; 6-Phospho-D-glucono-1,5-lactone + H+ + NADPH</a> <a href="#">NAD+ + 2-Deoxy-D-glucose &lt;-&gt; H+ + NADH + 2-deoxy-D-Glucono-1,5-lactone</a>
<b>External links</b>	<b>6</b> <a href="#">Expasy</a> <a href="#">KEGG</a> <a href="#">IntEnz (EBI)</a> <a href="#">IUBMB</a> <a href="#">Reactome</a> <a href="#">HepatoSys</a> (Only accessible for HepatoSys project members)

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Fig. 12 The Enzyme Details page. The red numbers are explained in the text above.

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## Pathway Details

The Pathway Details page gives the recommended (1) and alternative names (2) together with a list of all available reactions for the pathway in which the reaction of interest is involved (3).



Pathway Details

<b>Recommended name</b>	<b>1</b> non-phosphorylative Entner-Doudoroff-Pathway
<b>Alternative names</b>	<b>2</b> non-phosphorylative Entner-Doudoroff Pathway
<b>Reactions</b>	<b>3</b> <a href="#">CO2 + Acetyl-CoA + Reduced ferredoxin &lt;-&gt; Coenzyme A + Pyruvate + Oxidized ferredoxin</a> <a href="#">Pyruvate + ATP &lt;-&gt; Phosphoenolpyruvate + ADP</a> <a href="#">ATP + D-Glycerate &lt;-&gt; ADP + 3-Phospho-D-glycerate</a> <a href="#">alpha-D-Glucose &lt;-&gt; beta-D-Glucose</a> <a href="#">beta-D-Glucose + NADP+ &lt;-&gt; NADPH + D-Glucono-1,5-lactone + H+</a> <a href="#">H2O + D-Glucono-1,5-lactone &lt;-&gt; D-Gluconate</a> <a href="#">2-Phospho-D-glycerate &lt;-&gt; Phosphoenolpyruvate + H2O</a> <a href="#">D-Galactonate &lt;-&gt; H2O + 2-Dehydro-3-deoxy-D-galactonate</a> <a href="#">2-Dehydro-3-deoxy-D-gluconate &lt;-&gt; Glyceraldehyde + Pyruvate</a> <a href="#">D-Glyceraldehyde + H2O + NAD+ &lt;-&gt; NADH + H+ + D-Glycerate</a> <a href="#">D-Gluconate &lt;-&gt; H2O + 2-Dehydro-3-deoxy-D-gluconate</a> <a href="#">beta-D-Glucose + NAD+ &lt;-&gt; NADH + D-Glucono-1,5-lactone + H+</a>
<b>Classification</b>	

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Fig. 13 The Pathway Details page. The red numbers are explained in the text above.


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## View Kinetic Data

By clicking on a “view” button on the search results overview page associated with a reaction (Fig. 4, c), first the system will present an overview of all the kinetic data available for the given reaction. The summary view (Fig. 14) shows general entry information including the entry ID (1), organism (2), tissue/cell type (3), EC number and protein information (wildtype, mutant etc.) (4). The summary view can be expanded completely (by clicking the “Expand All” button), showing all the details of all the entries, or partially (by clicking the “+” of each entry), only expanding selected entries.



**Kinetic Data Available for Reaction:**  
 beta-D-Glucose + NAD+ <-> NADH + D-Glucono-1,5-lactone + H+  
 Show only kinetic data matching the search criteria



<b>Entry Nr. 12019</b>	<b>1</b>	 <input type="checkbox"/> <input type="checkbox"/>	<input type="button" value="Select"/>
<b>Organism:</b>	<b>2</b>	Homo sapiens	
<b>Tissue:</b>	<b>3</b>	liver	
<b>EC Class:</b> <a href="#">1.1.1.47</a>	<b>4</b>	wildtype Newborn	
<b>Entry Nr. 12020</b>		<input type="checkbox"/> <input type="checkbox"/>	<input type="button" value="Select"/>
<b>Organism:</b>		Homo sapiens	
<b>Tissue:</b>		liver	
<b>EC Class:</b> <a href="#">1.1.1.47</a>		wildtype 4-year old	

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Fig. 14 Summary view of the View Kinetic Data window. The red numbers are explained in the text above.

The entry details (Fig. 15), additionally to the summary view information, presents substrates (5), products (6) and modifiers (inhibitors, activators, cofactors, catalysts) (7), their cellular locations and related comments. The enzyme information (8) include the definition of the protein complex, UniProtIDs and molecular weights of the subunits and the protein complex if available in the publication. The kinetic law (9) can be defined by the kinetic law type and the kinetic law formula. Parameters (10) are shown with their names, types, related compound-species, start and endvalues, deviations, unit descriptions and comments. The experimental conditions (11) contain pH value, temperature and the buffer description. The comment gives general information about the entry if available. At the end of the entry the publication details (12) (authors, title etc.) are given.

Kinetic Data Available for Reaction:  
 $\beta\text{-D-Glucose} + \text{NAD}^+ \leftrightarrow \text{NADH} + \text{D-Glucono-1,5-lactone} + \text{H}^+$   
 Show only kinetic data matching the search criteria

Expand All

Close All

Entry Nr. 12019		[ + ] [ - ]		Select			
Organism:	Homo sapiens						
Tissue:	liver						
EC Class: <a href="#">1.1.1.47</a>	wildtype Newborn						
<b>Substrates</b> 5							
name	location	comment					
<a href="#">beta-D-Glucose</a>	<a href="#">microsome</a>	-					
<a href="#">NAD+</a>	<a href="#">microsome</a>	-					
<b>Products</b> 6							
name	location	comment					
<a href="#">D-Glucono-1,5-lactone</a>	<a href="#">microsome</a>	-					
<a href="#">NADH</a>	<a href="#">microsome</a>	-					
<b>Modifiers</b> 7							
name	location	effect	comment	protein complex			
Glucose 1-dehydrogenase(Enzyme)	<a href="#">microsome</a>	Modifier-Catalyst	-	<a href="#">O95479</a> ;			
<b>Enzyme (protein data)</b> 8							
	UniProt-ID	name	mol. weight (kDa)	deviation (kDa)			
subunit	O95479	-	-	-			
complex	-	-	-	-			
<b>Kinetic Law</b> 9							
	type	formula					
-							
<b>Parameter</b> 10							
name	type	species	start val.	end val.	deviat.	unit	comment
Vmax	Vmax	-	0.28	-	-	$\mu\text{mol}/(\text{min} \cdot \text{mg})$	-
Km	Km	beta-D-Glucose	0.17	-	-	M	-
<b>Experimental conditions</b> 11							
	start value	end value		unit			
pH		7.8		-			
temperature		25.0		°C			
buffer	0.05 M phosphate						
comment	-						
<b>Reference</b> 12							
SABIO id	title	author	year	journal	volume	pages	PubMed
1073	SUBCELLULAR DISTRIBUTION AND PROPERTIES OF HEPATIC GLUCOSE DEHYDROGENASES OF SELECTED VERTEBRATES	METZGER RP, WILCOX SS, WICK AN	1965	J Biol Chem	240	2767-71	<a href="#">14342292</a>

Fig. 15 The Entry Details of the View Kinetic Data Window. The red numbers are explained in the text above.

By clicking on the “Select” button of single entries the entry information will be selected for export and added to the list for data export (for details go to [→ Data Export](#)).

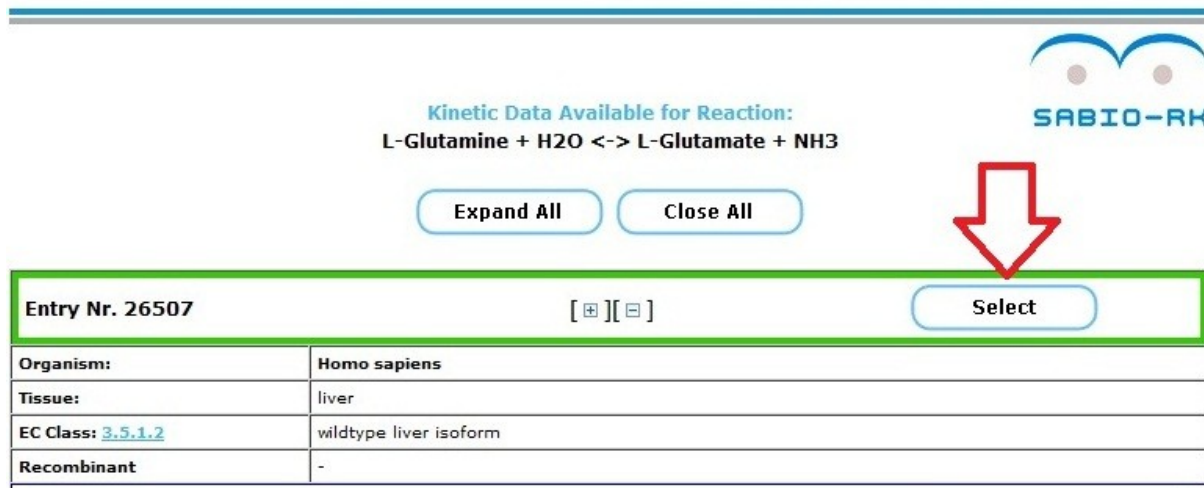
Apart from that there are given internal links to the EC Class → [Enzyme Details](#), compound → [Compound Details](#), and links to external databases UniProt (protein complex) and Pub Med.

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## Data Export

Reactions with selected kinetic data can be exported in SBML (Systems Biology Markup Language [3]) for exchange with other systems or programs, e.g. allowing its import into simulation and modelling programs supporting SBML like COPASI [4] or CellDesigner [5]. The data is described in SBML together with annotations of entities and expressions to other resources and biological ontologies. These annotations comply with the MIRIAM standard (Minimal Information Requested In the Annotation of biochemical Models [6]). For better tracking the exported SBML also contains SABIO-RK specific identifiers (e.g. for a reaction or a kinetic record) that are compliant with MIRIAM.

To export data from SABIO-RK, the data entries to be exported in one SBML file have to be selected. For selection of a dataset with kinetic data, the *SELECT* button in the header of the entry on the View Kinetic Data page should be used (Fig. 16).



Kinetic Data Available for Reaction:  
L-Glutamine + H2O <-> L-Glutamate + NH3

Expand All Close All

SELECT


Entry Nr. 26507	[+][−]	Select
Organism:	Homo sapiens	
Tissue:	liver	
EC Class: <a href="#">3.5.1.2</a>	wildtype liver isoform	
Recombinant	-	

Fig. 16 To export a dataset containing kinetic data press the select button.

To include reactions with **no** kinetic data a reaction can be chosen from the search results overview page and then by clicking the checkbox “Select only Reaction(s) (without kinetic data)” to send it to the list of reactions to be included in the SBML file (Fig. 17).

Search

Total number of reactions found for specified search criteria: **7**

Click here to view your search criteria 

Modify Search

Kinetic Data Availability:

-  Kinetic data available matching the search criteria
-  Kinetic data available, but not matching all search criteria
-  No kinetic data available

Number of results per page:

Display

- Search criteria:
- Reactant:
- Pathway: Glycolysis classical
- Enzyme:
- Publication:
- Protein:
- Sign. modific.:
- Sign. event:
- Organism: Homo sapiens
- Tissue: liver
- Cell. loc.:
- Exp. cond.:
- Kin. data:

Show only reactions having kinetic data matching the search criteria












Reactions	Select only Reaction(s) (without kinetic data)	Kinetic Data for this reaction (Click to View)	#	Enzyme EC#	Kinetic data for enzymes (Click to View)	#
D-Glucose + ATP <-> D-Glucose 6-phosphate + ADP	<input type="checkbox"/>		8	2.7.1.2		12
				2.7.1.1		616
				2.7.1.59		8
				2.7.1.4		26
				2.7.1.60		13
D-Glucose 6-phosphate <-> D-Fructose 6-phosphate	<input type="checkbox"/>		2	5.3.1.9		2
D-Glyceraldehyde 3-phosphate <-> Glycerone phosphate	<input type="checkbox"/>		2	5.3.1.1		2
D-Fructose 1,6-bisphosphate <-> D-Glyceraldehyde 3-phosphate + Glycerone phosphate	<input type="checkbox"/>		22	4.1.2.13		45
				4.3.1.17		16
				4.1.2.40		34

Fig. 17 To export reactions without kinetic data click on the marked checkbox.

All selected datasets are summarized in a list and shown in the export cart accessible from the left hand side control panel. The number of selected entries is shown (Fig. 18).

## Export cart



Search

- Search criteria:

Reactant:

- Pathway:

Glycolysis classical

Enzyme:

Publication:

Protein:

Sign. modific.:

Sign. event:

- Organism:

Homo sapiens

- Tissue:

liver

Cell. loc.:

Exp. cond.:

Kin. data:

### Selected kinetics data

Entry ID	Selected Reaction	Organism	Tissue	Kinetic law type	View details	Remove entry
26507	L-Glutamine + H <sub>2</sub> O <-> L-Glutamate + NH <sub>3</sub>	Homo sapiens	liver	Hill Cooperativity	<a href="#">view</a>	<input type="checkbox"/>
32924	L-Ornithine + 2-Oxoglutarate <-> L-Glutamate + L-Glutamate 5-semialdehyde	Homo sapiens	liver	-	<a href="#">view</a>	<input type="checkbox"/>

Remove selected entries

### Selected reactions (without kinetics data)

Reaction ID	Reaction equation	Remove reaction
793	D-Glucose + ATP <-> D-Glucose 6-phosphate + ADP	<input type="checkbox"/>

Remove selected reactions

Clear

Write SBML

Back to Results

Fig. 18 List of selected data to be exported in SBML.

Selected entries could also be removed from the selection list (→ Remove selected entries). A click on the button 'Write SBML' leads to the export page (Fig. 19).

On the export page you have different options:

- Enter a name for the exported SBML file.  
With this name the file will be saved on your hard disk.
- Select the SBML version for the export (currently only SBML level 2 versions 2, 3 and 4 are supported).  
We recommend using SBML level 2 version 4 to fully benefit from annotations for the data.
- To choose whether all parameter values should be normalized to SI base units before export.  
To make data from different sources, described in different units

comparable, it is important to transform them to the same scaling. We offer such a transformation to SI base units (e.g.  $\mu\text{M}$  and  $\text{mM}$  to  $\text{M}$ ).

- To actually proceed with the export by clicking on the button 'Save model on disk as SBML'.  
You will have the option to either save the file or open it.

You are logged in as anonymousUser

Username:  Password:   remember me

Daten absenden Zurücksetzen

HOME | CONTACT | HELP | IMPRINT | [View Kinetic Data](#)

Search [Save Model](#)

3

– Search criteria:

- Reactant:
- Pathway: [Glycolysis classical](#)
- Enzyme:
- Publication:
- Protein:
- Sign. modific.:
- Sign. event:
- Organism: [Homo sapiens](#)
- Tissue: [liver](#)
- Cell. loc.:
- Exp. cond.:
- Kin. data:

Enter name of model:

Export parameters normalized to SI base units

[Save Model on Disk as SBML](#)

[Back to Results](#)

Fig. 19 The export page of SABIO-RK.

The SBML export file includes:

- Header (with model name and reference to SABIO-RK)
- Mathematical functions (kinetic rate equations) → listOfFunctionDefinitions
- Parameter unit definition → listOfUnitDefinitions
- Cellular compartments where reactions take place → listOfCompartments
- Species: substrates, products and modifiers (e.g. enzymes, inhibitors, activators, cofactors) → listOfSpecies

- Reactions (with reactants and modifiers) → listOfReactions
- Kinetic record (kinetic rate equation and corresponding data) → kineticLaw
- Kinetic parameters → listOfParameters

### **Annotations included in SBML (if applicable):**

#### Reactions:

- SABIO-RK Reaction  
<http://sabio.h-its.org/>  
MIRIAM: <http://www.ebi.ac.uk/miriam/main/datatypes/MIR:00000038>
- KEGG Reaction  
<http://www.genome.jp/kegg/reaction/>  
MIRIAM: <http://www.ebi.ac.uk/miriam/main/datatypes/MIR:00000014>
- Enzyme Nomenclature  
<http://us.expasy.org/enzyme/>  
MIRIAM: <http://www.ebi.ac.uk/miriam/main/datatypes/MIR:00000004>

#### Chemical entities (Substrates, Products, Modifier, etc.):

- ChEBI (Chemical Entities of Biological Interest)  
<http://www.ebi.ac.uk/chebi/>  
MIRIAM: <http://www.ebi.ac.uk/miriam/main/datatypes/MIR:00000002>
- KEGG Compound  
<http://www.genome.jp/kegg/ligand.html>  
MIRIAM: <http://www.ebi.ac.uk/miriam/main/datatypes/MIR:00000013>

#### SABIO-RK Kinetic Record (kinetic rate equation and corresponding data):

- SABIO-RK Kinetic Record  
<http://sabio.h-its.org/>  
MIRIAM: <http://www.ebi.ac.uk/miriam/main/datatypes/MIR:00000086>
- PubMed (Publication describing the data source)  
<http://www.ncbi.nlm.nih.gov/PubMed/>  
MIRIAM: <http://www.ebi.ac.uk/miriam/main/datatypes/MIR:00000015>
- Systems Biology Ontology (SBO)  
<http://www.ebi.ac.uk/sbo/>  
MIRIAM: <http://www.ebi.ac.uk/miriam/main/datatypes/MIR:00000024>

#### Kinetic parameters, mathematical functions, species role:

- Systems Biology Ontology (SBO)  
<http://www.ebi.ac.uk/sbo/>  
MIRIAM: <http://www.ebi.ac.uk/miriam/main/datatypes/MIR:00000024>

The SBML file is generated using the libSBML library. Given the restrictions of the SBML format, the system includes the kinetic data into the SBML file by making

certain unilateral decision such as: if a parameter value is defined as a range, the system takes the middle value of this range as the parameter's value in SBML, given that the SBML file does not support the definition of ranges for parameter values.

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## References

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