



# Tutorial For SabioRk New Interface

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## Kinetic Law Entries and Related Reactions Search

- **Single Query**

➤ **Step 1:** Select criteria attribute in the drop down menu (Fig.1)

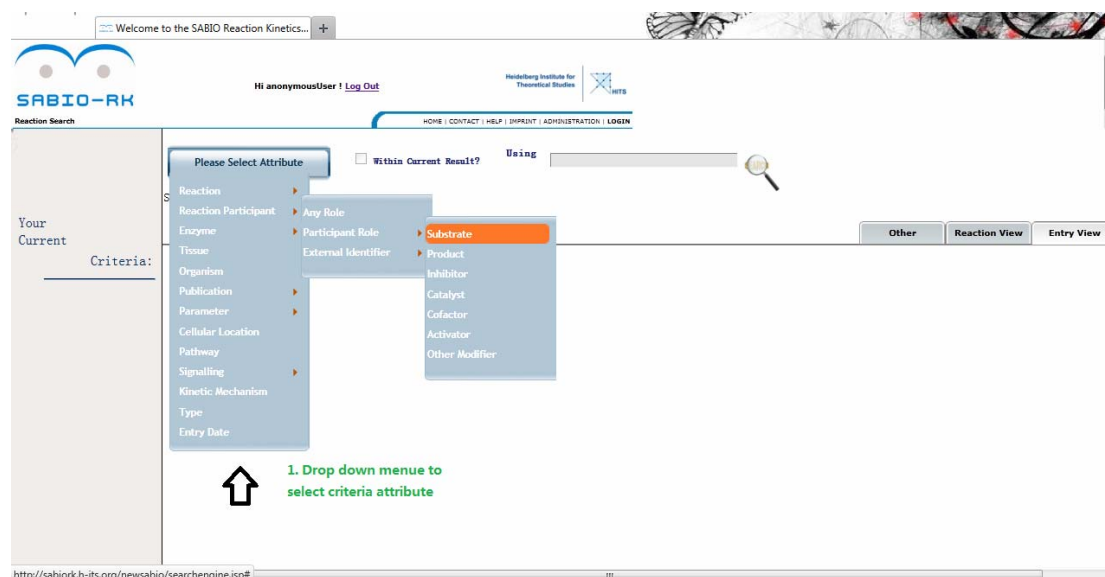


Fig. 1.

New features in this step:

(1) Simplify the interface, make the query area and later result area at the same page, which avoids users lose their searching context.

## ➤ Step 2: Autocomplete

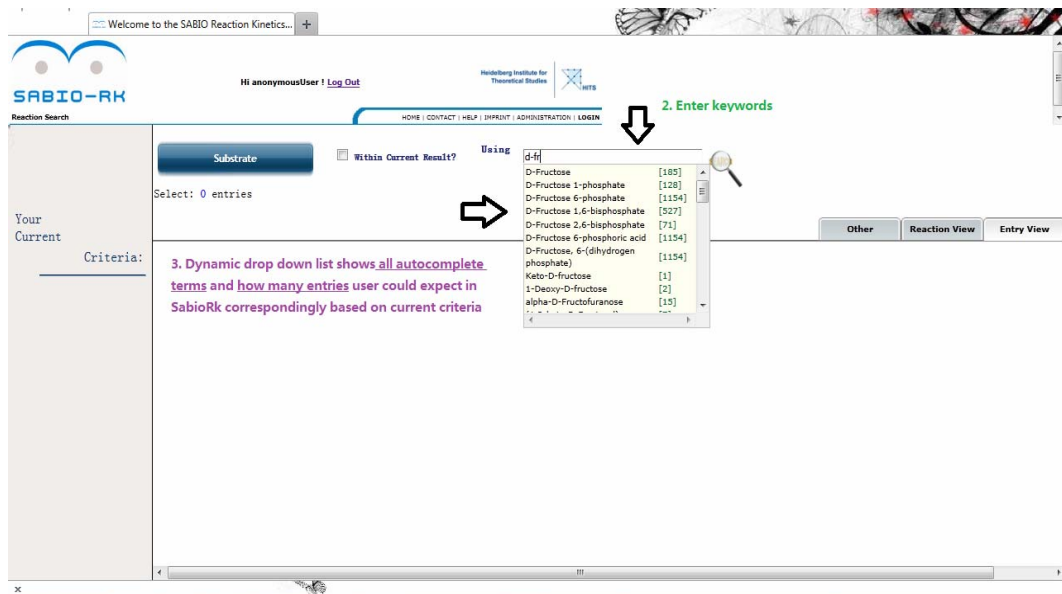


Fig.2.

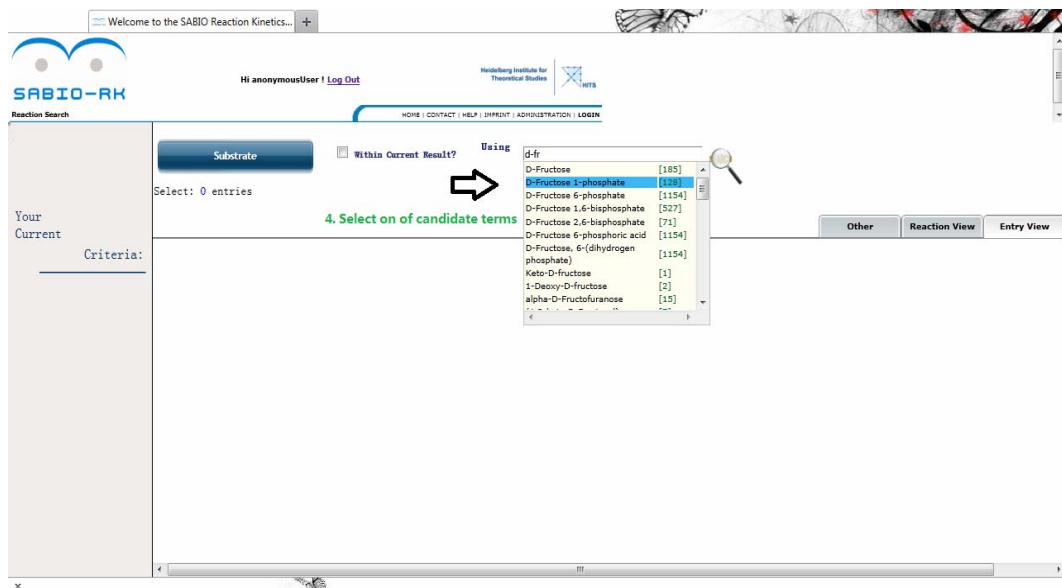


Fig.3.

### New features in this step:

(1) Providing dynamic overview of matching entry numbers to avoid „zero-hit“ and saving users query time. (Fig.4)

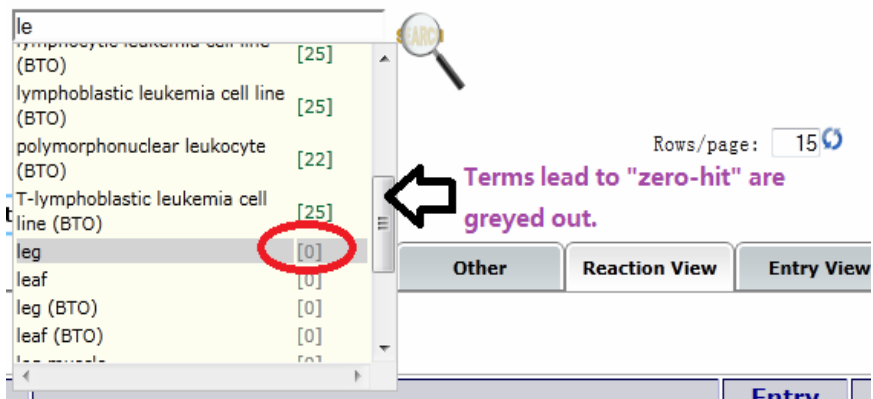


Fig.4.

➤ **Step 3: Search and get the result**

5. Press "search" button

8. Get Entry / Reaction Numbers

6. Get result table (either in Entry/ Reaction view)

7. Get overview of users' current criteria

Reaction	ECNumber	Enzyme		Tissue	Organism	Parameters (besides concentration)	Environment	
		Protein	Enzyme Variant (wildtype (w), mutant (m))				°C	pH
D-Fructose 1-phosphate = D-Glyceraldehyde + Glycerone phosphate	4.1.2.13	Q8J308	class IA (w) wildtype (w)		Thermococcus kodakaraensis	Km	70	6.5
D-Fructose 1-phosphate = D-Glyceraldehyde + Glycerone phosphate	4.1.2.13	P05062	wildtype (w)		Homo sapiens	kcat Km	10	7.4
D-Fructose 1-phosphate = D-Glyceraldehyde + Glycerone phosphate	4.1.2.13	P05062	mutant (m) AP (m)		Homo sapiens	kcat Km	10	7.4
D-Fructose 1-phosphate = D-Glyceraldehyde + Glycerone phosphate	4.1.2.13	P05062	mutant (m) AP (m)		Homo sapiens	kcat Km	30	7.4
D-Fructose 1-phosphate = D-Glyceraldehyde + Glycerone phosphate	4.1.2.13	P05062	wildtype (w)		Homo sapiens	kcat Km	30	7.4

Fig.5.

Welcome to the SABIO Reaction Kinetics... +

HI anonymousUser | Log Out

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Reaction Search

Substrate: D-Fructose 1-phosphate

Within Current Result?

Using: D-Fructose 1-phosphate

Select: 0 entries

Send Selected Entries to SBML File

Other Reaction View **Entry View**

10. Users can customize how many records per page

Rows/page: 15

11. User can expand to see entry/reaction details

9. Users can change different result view

There are 128 Kinetic Law Entries

Reaction	Enzyme			Tissue	Organism	Parameters (besides concentration)	Environment	
	ECNumber	Protein	Enzyme Variant (wildtype (w)/mutant (m))				°C	pH
D-Fructose 1-phosphate = D-Glyceraldehyde + Glycerone phosphate	4.1.2.13	Q8J308	class IA (w) wildtype (w)		Thermococcus kodakaraensis	Km	70	6.5
D-Fructose 1-phosphate = D-Glyceraldehyde + Glycerone phosphate	4.1.2.13	P05062	wildtype (w)		Homo sapiens	kcat Km	10	7.4
D-Fructose 1-phosphate = D-Glyceraldehyde + Glycerone phosphate	4.1.2.13	P05062	mutant (m) AP (m)		Homo sapiens	kcat Km	10	7.4
D-Fructose 1-phosphate = D-Glyceraldehyde + Glycerone phosphate	4.1.2.13	P05062	mutant (m) AP (m)		Homo sapiens	kcat Km	30	7.4
D-Fructose 1-phosphate = D-Glyceraldehyde + Glycerone phosphate	4.1.2.13	P05062	wildtype (w)		Homo sapiens	kcat Km	30	7.4

Fig.6.

Welcome to the SABIO Reaction Kinetics... +

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Reaction Search

Send Selected Entries to SBML File

Other Reaction View **Entry View**

Pages: 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10

There are 128 Kinetic Law Entries

Reaction	Enzyme			Tissue	Organism	Parameters (besides concentration)	Environment	
	ECNumber	Protein	Enzyme Variant (wildtype (w)/mutant (m))				°C	pH
D-Fructose 1-phosphate = D-Glyceraldehyde + Glycerone phosphate	4.1.2.13	Q8J308	class IA (w) wildtype (w)		Thermococcus kodakaraensis	Km	70	6.5

Entry ID: 39699

General information

Organism	Thermococcus kodakaraensis
Strain	KOD1
Tissue	-
EC Class	4.1.2.13
SABIO reaction id	274
Variant	wildtype class IA
Recombinant	expressed in Escherichia coli BL21-CodonPlus (DE3)-RIL

Substrates

name	location	comment
D-Fructose 1-phosphate	-	-

Products

name	location	comment
D-Glyceraldehyde	-	-
Glycerone phosphate	-	-

Modifiers

name	location	effect	comment	protein complex
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Expanded entry detail

Fig.7.

New features in this step:

(1) Users can customize different result views according to their needs. (Fig.6, Fig.8)

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Heidelberg Institute for Theoretical Studies

Reaction Search

Substrate:  Within Current Result? Using: D-Fructose 1-phosphate

Select: 0 entries

Rows/page: 15

Send Selected Entries to SBML File

Other **Reaction View** Entry View

Pages: [1]

There are 2 Reactions

[Sabio ID]: Reaction	Kegg ID	Visualization	Entry Numbers
[7171]: ATP + D-Fructose 1-phosphate = D-Fructose 1,6-bisphosphate + ADP		Double Click to Get the View	13
[274]: D-Fructose 1-phosphate = D-Glyceraldehyde + Glycerone phosphate	R02568	Double Click to Get the View	115

Pages: [1]

↑ Changed result view (Reaction View)

Send Selected Entries to SBML File

↑ 12. User can double click to visualize the reaction overview

http://sabiorkh-its.org/newsabio/searchengine.jsp#second

Fig.8.

(2) Users could visualize the general information about certain reaction to get the quick impression. (Fig. 9, Fig.10)

Reaction Related Information Visualization (ECNumber, Organism, Tissue)

you can click on "ECNumber", "Organism", "Tissue" nodes respectively to see all possible ecumbers, organisms and tissues for such reaction

finish loading

Organism + D-Fructose 1-phosphate = D-Fructose 1,6-bisphosphate + ADP

ECNumber

Tissue

Connections:

- ECNumber (relation: click the Node to see all possible ECNumbers)
- Organism (relation: click the Node to see all possible Organisms)
- Tissue (relation: click the Node to see all possible Tissues)

13. User could click on either "Organism", or "Tissue" or "ECNumber"

Fig.9.

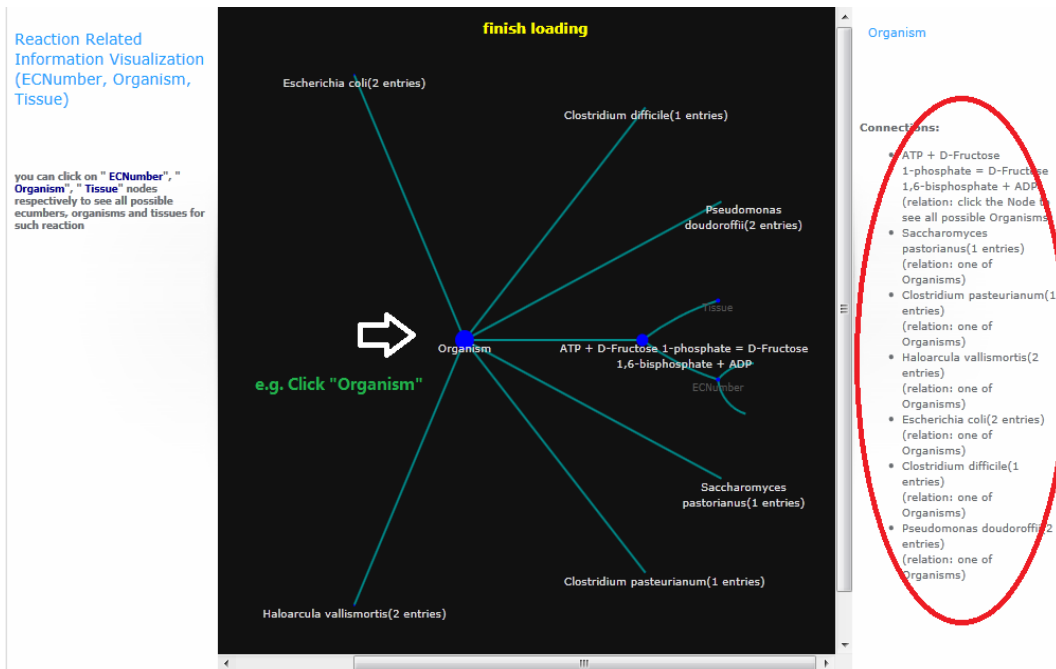


Fig.10.

## Query Refinement

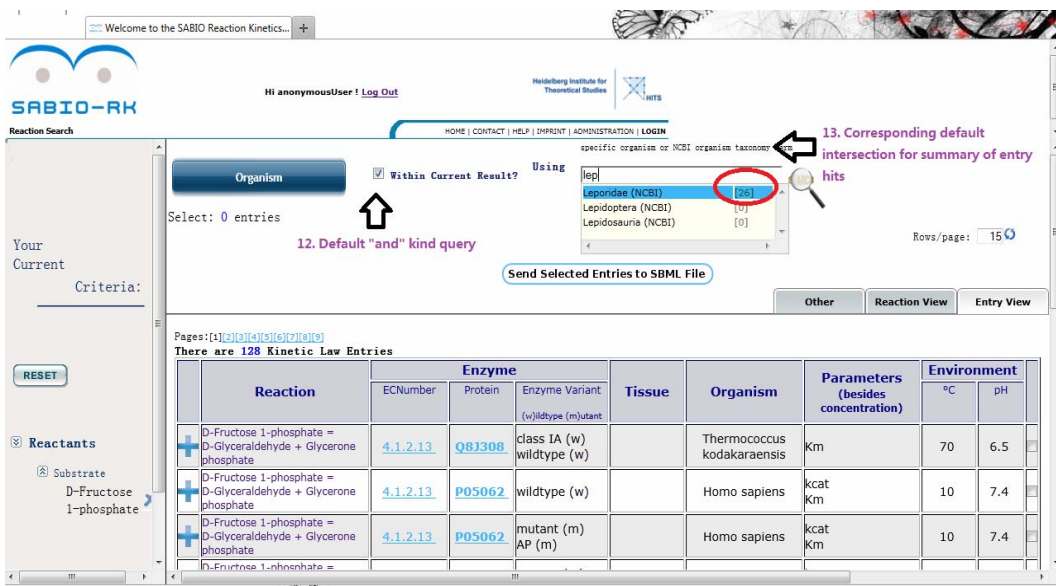


Fig.11.

Reaction Search

Organism  Within Current Results? Using Leporidae (NCBI)

Select: 0 entries

Rows/page: 15

Send Selected Entries to SBML File

Other Reaction View Entry View

Pages: [1/23]

There are 26 Kinetic Law Entries

Reaction	ECNumber	Enzyme		Tissue	Organism	Parameters (besides concentration)	Environment	
		Protein	Enzyme Variant (w/wildtype (w) / (m)mutant)				°C	pH
D-Fructose 1-phosphate = D-Glyceraldehyde + Glycerone phosphate	4.1.2.13	P00883	A (w) wildtype (w)	muscle	Oryctolagus cuniculus	Vmax Km	30	7.4
D-Fructose 1-phosphate = D-Glyceraldehyde + Glycerone phosphate	4.1.2.13	P00883	A (w) wildtype (w)	muscle	Oryctolagus cuniculus	Vmax Km	30	7.4
D-Fructose 1-phosphate = D-Glyceraldehyde + Glycerone phosphate	4.1.2.13	P00883	wildtype (w) aldolase A (w)	skeletal muscle	Oryctolagus cuniculus	kcat Km	20	8.5

Fig.12.

**New features in this part:**

(1) Automatic intersection to show the summary of entry hits will again save the time which users might spend on those „zero-hits“ queries during their query refinement. (Fig.11.)

(2) More informative result table will conduct users for their further query refinements.

(3). Supports for „Ontology“ terms also conduct users' choice of further query terms. Such support is valid for both Brenda tissue terms with (BTO) surffix and NCBI organism taxonomy terms with (NCBI) surffix. (Fig.13)

Reaction Search

Organism  Within Current Results? Using Lactobacillus (NCBI)

Select: 0 entries

Rows/page: 15

Other Reaction View Entry View

Pages: [1/1]

There are 326 Kinetic Law Entries

Reaction	ECNumber	Protein	Enzyme Variant (w/wildtype (w) / (m)mutant)	Tissue	Organism	Parameters (besides concentration)	Environment	
							°C	pH
H2O + Propyl-p-nitroaniline = 4-Nitroaniline + Proline	3.4.11.5	P41			Lactobacillus casei subsp. roussoi	Vmax Km	30	7
4-Hydroxyphenylpyruvate + H2O = 4-Hydroxyphenylacetate + Pyruvate	17.4.2	Q5			Lactobacillus casei subsp. roussoi	Km	37	7.5
Ethyl pentanoate + H2O = Ethanol + Pentanoate	3.1.1.1	Q8KT44	wildtype (w) isoenzyme ESTC (w)		Lactobacillus casei	Vmax Km Vmax/Km	25	5.5

Get the list of all counted specific terms

Click on "Ontology" Term

Lactobacillus (NCBI)

Within current criteria, following organisms have entries:

- Lactobacillus casei;
- Lactobacillus leichmannii;
- Lactobacillus fermentum;
- Lactobacillus delbrueckii subsp. bulgaricus;
- Lactobacillus reuteri;
- Lactobacillus acidophilus;
- Lactobacillus plantarum;

Fig.13.

## Kinetic Law Entries Selection and Export

- **Step 1:** Users could either select entry one by one from „Entry View“ (Fig.14.) or select entries based on reactions at once from „Reaction View“ (Fig.15).

Reaction Search

Organism  Within Current Result? Using

Select: 2 entries

16. Export to SBML FILE

Send Selected Entries to SBML File

Rows/page: 15

Other Reaction View Entry View

Pages: [1] [2] [3] [4] [5] [6] [7] [8] [9] [10] [11] [12] [13] [14] [15] [16] [17] [18] [19] [20] [21] [22]

There are 325 Kinetic Law Entries

Reaction	Enzyme		Tissue	Organism	Parameters (besides concentration)	Environment	
	ECNumber	Protein				Enzyme Variant (wildtype (w) mutant)	°C
<input checked="" type="checkbox"/> H2O + Prolyl-p-nitroanilide = 4-Nitroaniline + Proline	3.4.11.5	P46544	wildtype (w)	Lactobacillus delbrueckii subsp. bulgaricus	Vmax Km	15. Entries selection	30 <input checked="" type="checkbox"/>
<input checked="" type="checkbox"/> ATP + 1,4-Dithiothreitol = H2O + dATP + Oxidized dithiothreitol	1.17.4.2	Q59490	wildtype (w)	Lactobacillus leichmannii	Km		37 7.5 <input checked="" type="checkbox"/>
<input checked="" type="checkbox"/> Ethyl pentanoate + H2O = Ethanol + Pentanoate	3.1.1.1	Q8KT44	wildtype (w) isoenzyme EstC (w)	Lactobacillus casei	Vmax Km Vmax/Km		25 5.5 <input type="checkbox"/>

Fig.14.

Reaction Search

Organism  Within Current Result? Using

Select: 6 entries

16. Export to SBML file

Send Selected Entries to SBML File

Rows/page: 15

Other Reaction View Entry View

Pages: [1] [2] [3] [4] [5] [6] [7]

There are 96 Reactions

[Sabio ID]: Reaction	Kegg ID	Visualization	Entry Numbers
<input checked="" type="checkbox"/> [7703]: H2O + Amylose = Amylose + Amylose		Double Click to Get the View	6 <input checked="" type="checkbox"/>
<input checked="" type="checkbox"/> [240]: H2O + Oxidized thioredoxin + dCDP = CDP + Reduced thioredoxin	R02024	Double Click to Get the View	2 <input type="checkbox"/>
<input checked="" type="checkbox"/> [1147]: H2O + Sucrose = alpha-D-Glucose + beta-D-Fructose	R00802	Double Click to Get the View	2 <input type="checkbox"/>
<input checked="" type="checkbox"/> [800]: D-Glucose = D-Fructose		Double Click to Get the View	13 <input type="checkbox"/>
<input checked="" type="checkbox"/> [2051]: H2O + dATP + Oxidized thioredoxin = ATP + Reduced thioredoxin	R02014	Double Click to Get the View	12 <input type="checkbox"/>

Fig.15.

## ➤ Step 2: Export selected entries in SBML

View Kinetic Data

Selected kinetics data

Entry ID	Selected Reaction	Organism	Tissue	Kinetic law type	View details	Remove entry
39485		Lactobacillus plantarum		Uncompetitive inhibition	<a href="#">View</a>	<input type="checkbox"/>
39488		Lactobacillus plantarum		Michaëlis-Menten	<a href="#">View</a>	<input type="checkbox"/>
39487		Lactobacillus fermentum		Mixed noncompetitive inhibition	<a href="#">View</a>	<input type="checkbox"/>
38875		Lactobacillus amylovorus		Michaëlis-Menten	<a href="#">View</a>	<input type="checkbox"/>
39490		Lactobacillus fermentum		Michaëlis-Menten	<a href="#">View</a>	<input type="checkbox"/>
38880		Lactobacillus plantarum		Michaëlis-Menten	<a href="#">View</a>	<input type="checkbox"/>

Remove selected entries

Back to Results Write SBML

17. Write into SBML model

Fig.16.

Save Model

Enter name of model: SABIOmdl30Aug2011: SBML level 2, version 4

Export parameters normalized to SI base units

Save Model on Disk as SBML

Save Model on Disk as PDF

Back to Results

18. Choose the model

19. Export it either in XML file or PDF file

SABIOmdl30Aug2011213.pdf  
237 kB — h-its.org

Fig.17.

(updated on Aug.30th.2011)