



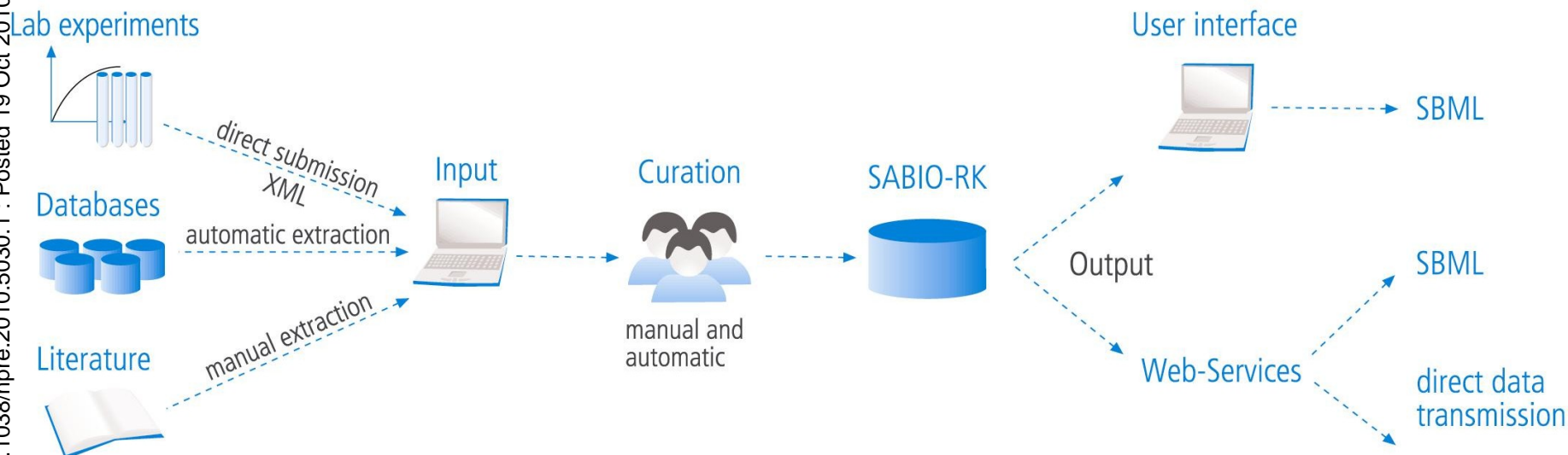
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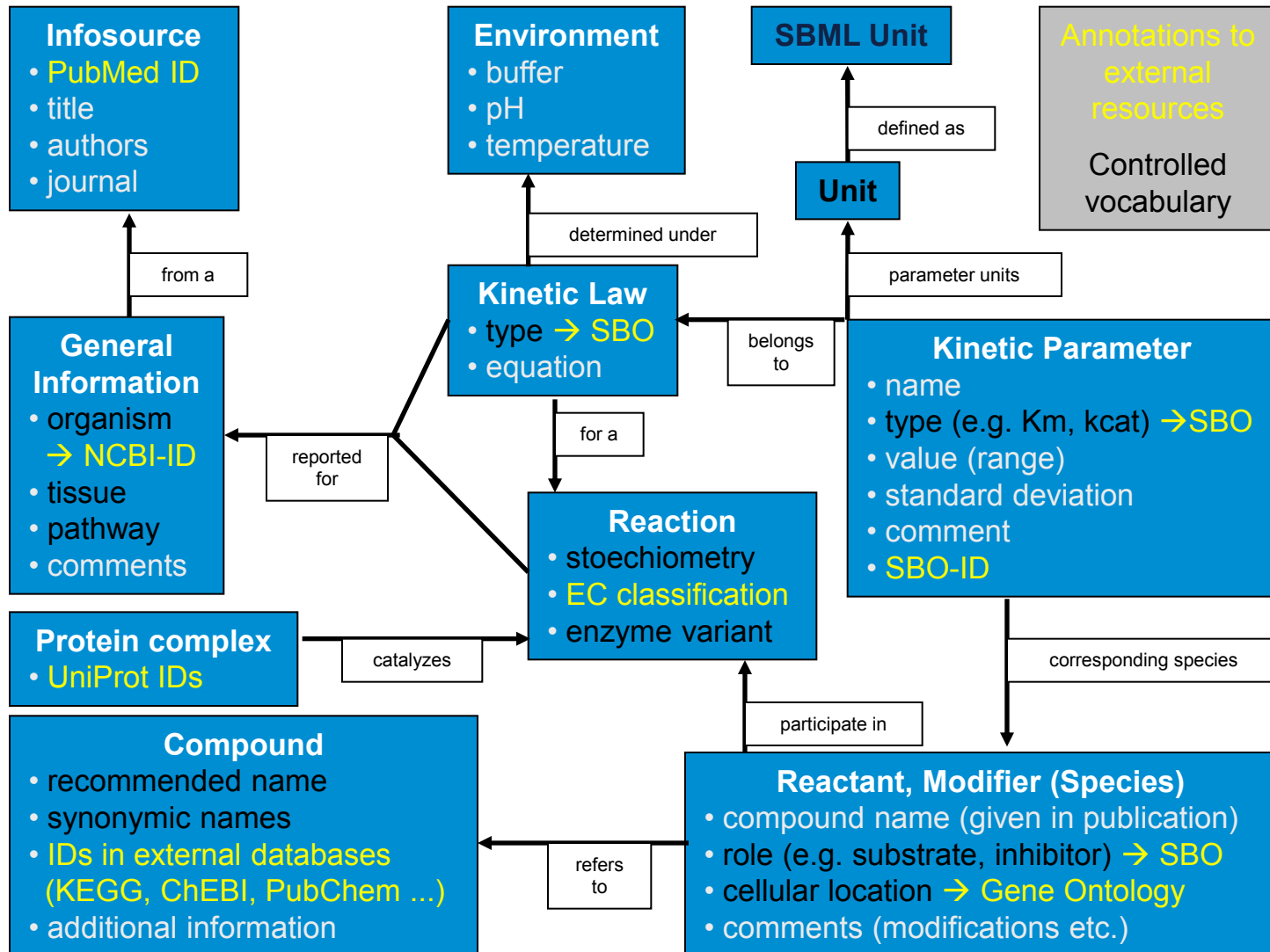
Exchanging Experimental Kinetic Data via SabioML

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HITS gGmbH, Germany

COMBINE Meeting 2010, October 6-9, Edinburgh (UK)

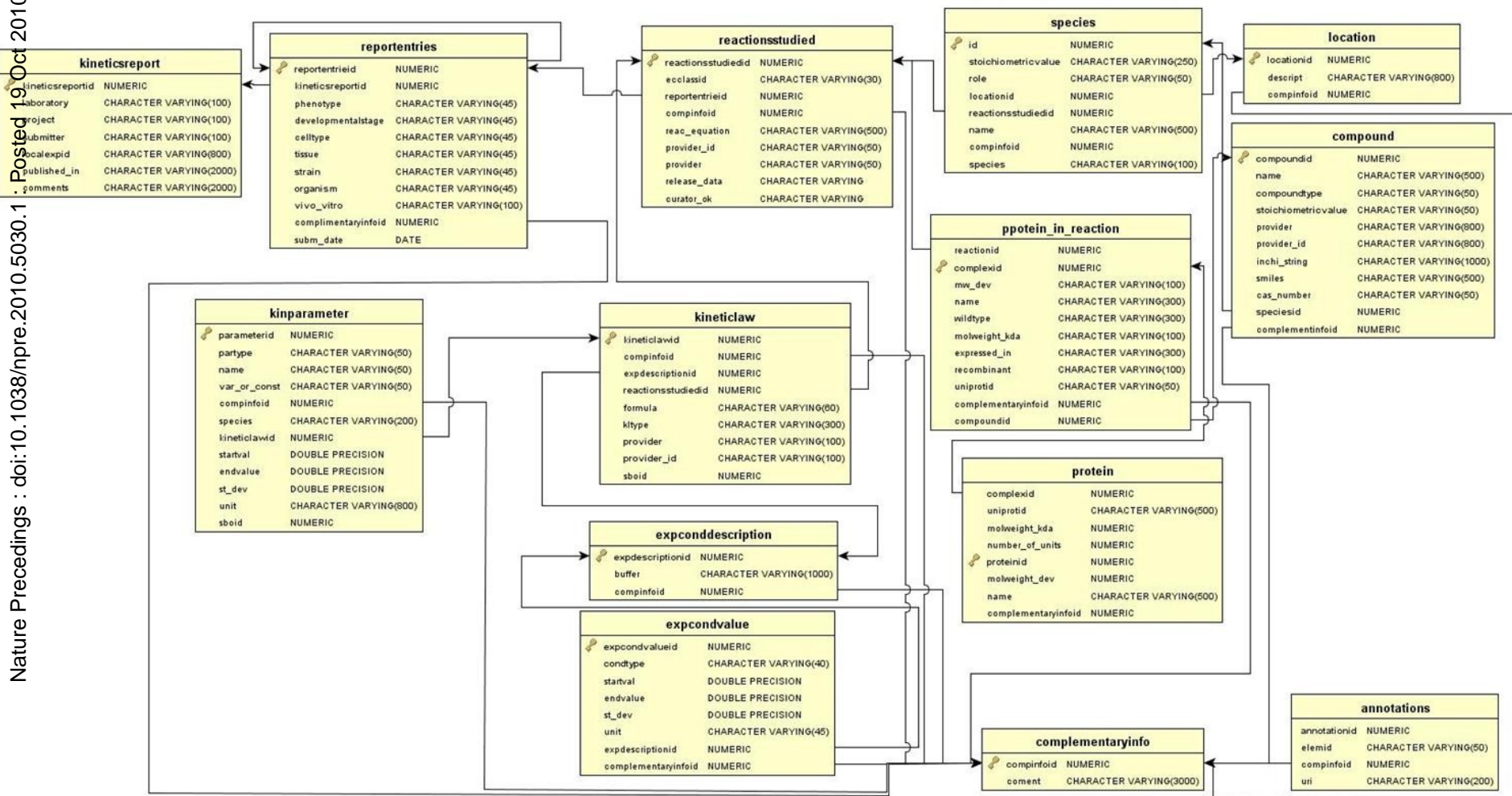


- Kinetic data from **literature** and directly from **experiments** merged with data describing biochemical reactions and pathways from **other resources**
- Data about **metabolic** and **signalling** reactions, as well as reaction mechanisms
- Data is unified, structured, normalized, interrelated 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 Systems Biology Markup Language (**SBML**)



Extensible Markup Language (XML) based exchange file format

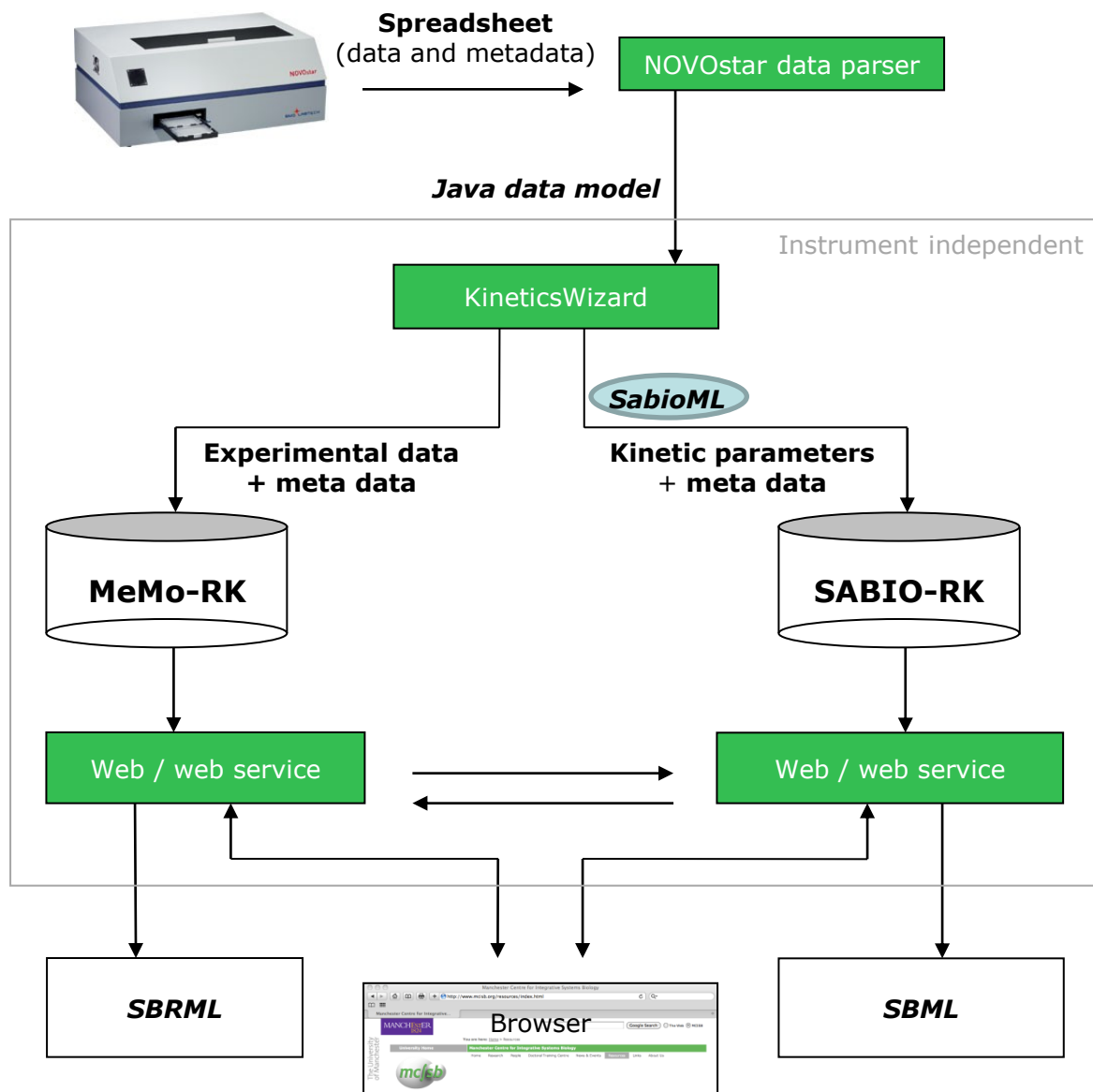
- Developed for data import into the SABIO-RK database
- Data schema mapped to the SABIO-RK database model
→ Data can be directly integrated into SABIO-RK
- Uses Controlled vocabulary (Constraints)
- Supports standardized annotations for many data types
→ Compliant with the MIRIAM standard (Minimal Information Required In the Annotation of Models)
- Data model flexible and conferrable for exchanging experimental kinetic data between databases and tools



```

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  5,7H2,1-3H3,(H4-,15,16,17,20,21,22,23,24)/p+1/fC14H23N4O8P2S/h20-21,23H,15H2/q+1">
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```





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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Issue



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These authors contributed equally to this work



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Reaction Search

Search

- Search criteria:

Reactant:

Pathway:

- Enzyme:

[2.1.1.45:Thymidylate synthase](#)

Publication:

Protein:

Sign. modific.:

Sign. event:

Organism:

Tissue:

Cell. loc.:

Exp. cond.:

Kin. data:

with **Reactant(s)**

[+] [-]

in **Pathway(s)**

[+] [-]

having **Enzyme(s)**

[+] [-]

Use wildcard "%" to display e.g. all kinases in the selection list (type "%kinase%").

Join entries with

AND or OR

2.1.1.45:Thymidylate synthase

in **Publication**

[+] [-]

related to **Protein** (UniProtID)

[+] [-]

for **Signalling**

[+] [-]

in **Organism(s)**

[+] [-]

in **Tissue(s)/Cell Type(s)**

[+] [-]

in **(Intra/Extra)Cellular Location(s)**

[+] [-]



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Search Results

Search

- Search criteria:

Reactant:

Pathway:

- Enzyme:

[2.1.1.45:Thymidylate synthase](#)

Publication:

Protein:

Sign. modific.:

Sign. event:

Organism:

Tissue:

Cell. loc.:

Exp. cond.:

Kin. data:

Total number of reactions found for specified search criteria: 3

[Click here to view your search criteria](#)

Modify Search

Kinetic Data Availability:

view Kinetic data available matching the search criteria

view Kinetic data available, but not matching all search criteria

No kinetic data available

Number of results per page:

Display

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)	#
5,10-Methylenetetrahydrofolate + dUMP <-> dTMP + Dihydrofolate	<input type="checkbox"/>	<input checked="" type="radio"/> view	25	2.1.1.45	<input checked="" type="radio"/> view	31
2-Mercaptoethanol + E-5-(2-Bromovinyl)-2'-deoxyuridine monophosphate <-> 1-(3-Hydroxy-4-hydroxymethyl-cyclopentyl)-5-[1,4]oxathian-2-yl-1H-pyrimidine-2,4-dione	<input type="checkbox"/>	<input checked="" type="radio"/> view	3	2.1.1.45	<input checked="" type="radio"/> view	31
1,4-Dithiothreitol + 5-Bromo-dUMP <-> Oxidized dithiothreitol + Hydrobromic acid + dUMP	<input type="checkbox"/>	<input checked="" type="radio"/> view	3	2.1.1.45	<input checked="" type="radio"/> view	31

Kinetic Data Available for Reaction:

D-Glucose 6-phosphate <-> D-Fructose 6-phosphate

Show only kinetic data matching the search criteria



Expand All

Close All

Entry Nr. 29390

[+][−]

Select

Organism:	Saccharomyces cerevisiae (strain BY4700 transformed in Y258)
Tissue:	-
EC Class: 5.3.1.9	wildtype Glucose-6-phosphate isomerase
Recombinant	expressed in Saccharomyces cerevisiae

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

Products		
name	location	comment
D-Glucose 6-phosphate	-	-

Modifiers					
name	location	effect	comment	protein complex	
Glucose-6-phosphate isomerase(Enzyme)	-	Modifier-Catalyst	-	(P12709)*2;	

Kinetic Law	
type	formula
Michaelis-Menten	$k_{cat} * E_t * S / (K_s + S)$

Parameter

D-Glucose 6-phosphate	-	-
---------------------------------------	---	---

Modifiers				
name	location	effect	comment	protein complex
Glucose-6-phosphate isomerase(Enzyme)	-	Modifier-Catalyst	-	(P12709)*2;

Kinetic Law	
type	formula
Michaelis-Menten	$k_{cat} * E_t * S / (K_s + S)$

Parameter							
name	type	species	start val.	end val.	deviat.	unit	comment
kcat	kcat	-	247.2	-	5.1	s ⁽⁻¹⁾	-
Ks	Km	D-Fructose 6-phosphate	0.307	-	0.021	mM	-
S	concentration	D-Fructose 6-phosphate	-	2.0	-	mM	-
Et	concentration	Enzyme	6.67E-7	-	-	mM	-

Experimental conditions			
	start value	end value	unit
pH	6.5	-	-
temperature	30.0	-	°C
buffer	0.0mM Glucose-6-phosphate 1-dehydrogenase, 100.0mM 2-(N-morpholino)ethanesulfonic acid, 5.0mM magnesium dichloride, 100.0mM potassium chloride, 0.4mM NADP		

Reference				
SABIORK id	title	author	year	direct submission link
2459	Glycolysis	Hanan Messiha and Naglis Malys, Manchester Centre for Integrative Systems Biology (MCISB), UK	2009	http://maureen.mib.manchester.ac.uk:8080/mcisb-web/index.jsp?application=MeMo-RK&directory=Home&experimentId=_14795743_9a81_45eb_ab79_d779a61fa41b

- Currently up to **SBML Level 2 Version 4**
- **Reaction Kinetics Warehouse:**
Reactions, kinetic equations and parameters (with corresponding units) from different database entries can be exported in one SBML file
- Data is annotated (RDF and SBOterms) according to **MIRIAM**
- Annotations include **SABIO-RK Ids** (reaction and kineticlaw) for tracking
- Optional **normalization of kinetic parameters** to SI base units
- Model can also be exported as human readable PDF → **SBML2LaTeX**

<http://www.ra.cs.uni-tuebingen.de/software/SBML2LaTeX/>



Conversion of SBML files into human-readable reports

Andreas Dräger¹, Hannes Planatscher¹, Dieudonné Moutsou Wouamba¹, Adrian Schröder¹, Michael Hucka², Lukas Endler³, Martin Golebiewski⁴,
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Short description: SBML2LaTeX is a tool to convert files in the System Biology Markup Language (SBML) format into LaTeX files. A convenient [web service](#) is available, which allows the user to directly generate various file types from SBML including PDF, TeX, DVI, PS, EPS, GIF, JPG or PNG. SBML2LaTeX can also be downloaded and used locally in batch mode or interactively with its Graphical User Interface or several command line options. The purpose of SBML2LaTeX is to provide a way to read the contents of XML-based SBML files. This is helpful and important for, e.g., error detection, proofreading and model communication.

Bioinformatics. 2009 June 1; 25(11): 1455–1456.

PMCID: PMC2682517

Published online 2009 March 23. doi: [10.1093/bioinformatics/btp170](https://doi.org/10.1093/bioinformatics/btp170).

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SBML2L^AT_EX: Conversion of SBML files into human-readable reports

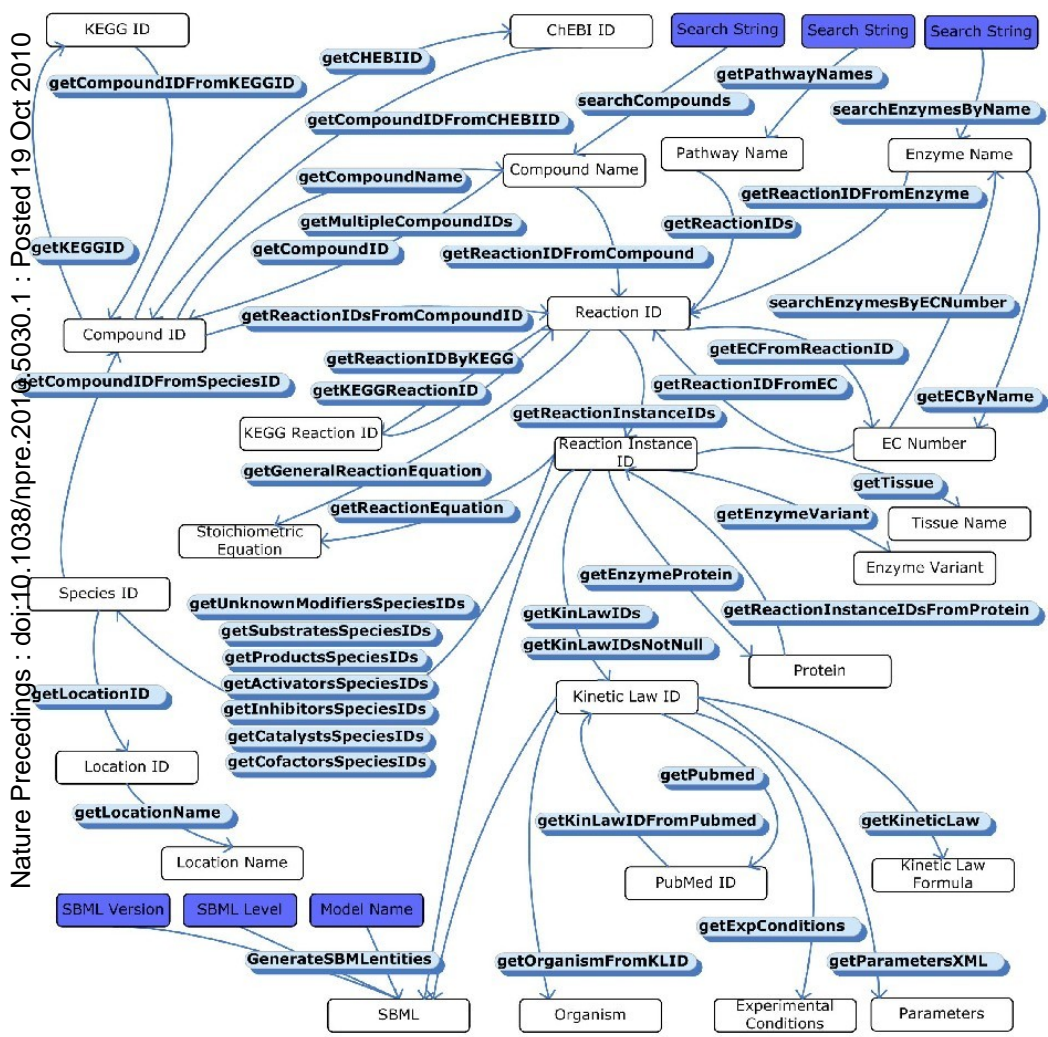
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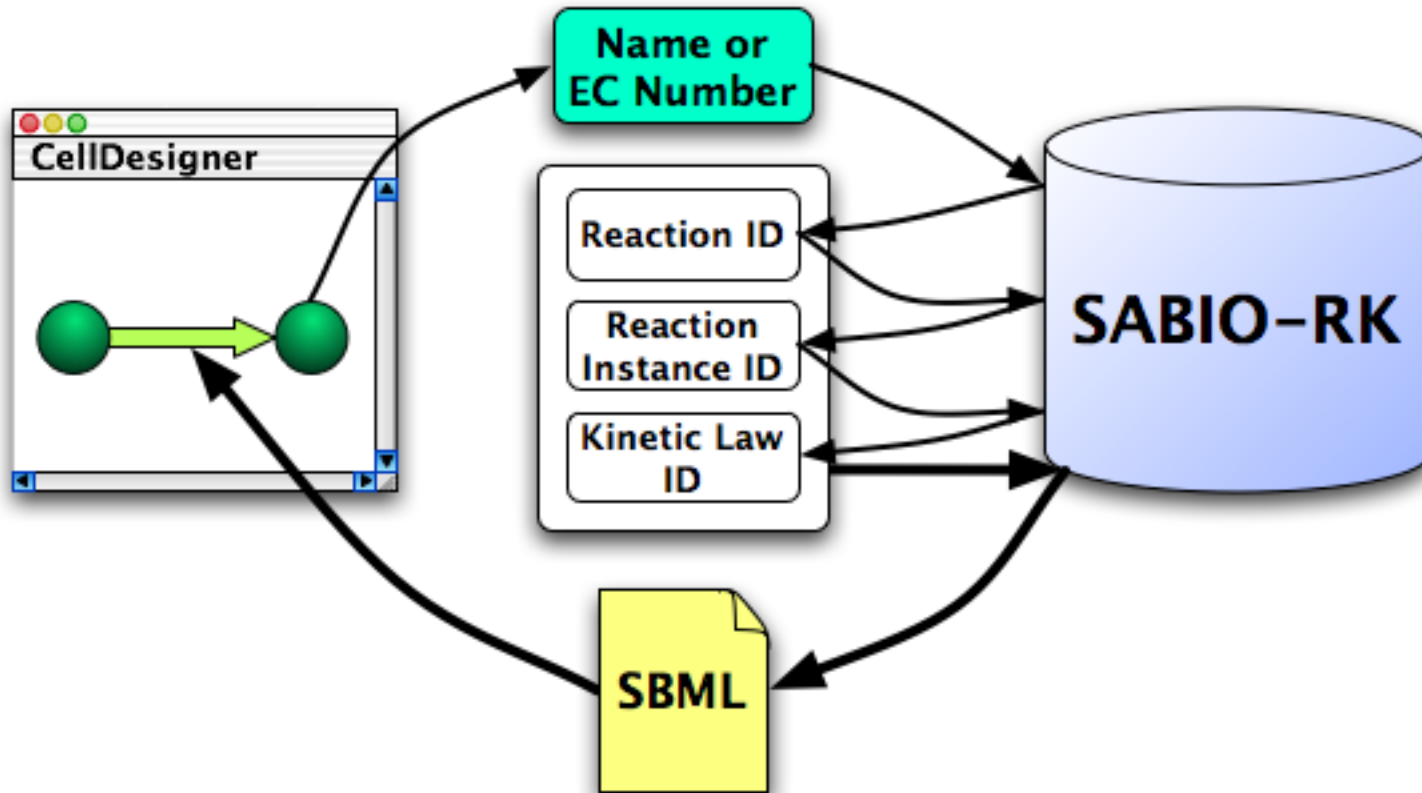
[SBML export of literature data](#)

[SBML export of direct submission data](#)

Nature Precedings : doi:10.1038/npre.2010.5030.1 : Posted 19 Oct 2010



- JAW-WS based
- Integration possible in modeling platforms or simulation tools (e.g. CellDesigner)
- Cross-linking with other databases (e.g. ChEBI)
- Data export in **SBML** supported



<http://www.celldesigner.org>

Heidelberg Institute for
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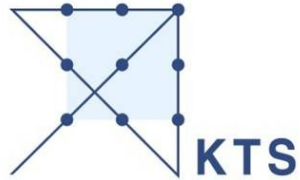
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<http://www.virtual-liver.de/>



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If you want to speed up SABIO-RK development

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**Two software developer positions available in the research group "Scientific
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To apply, please send CV by 31 October 2010



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