

Oral presentation

## **SABIO-RK: a database for biochemical reactions and their kinetics**

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### **The system**

SABIO-RK is a web-accessible curated database offering information about biochemical reactions and their kinetic properties. It integrates information about reactions, such as reactants, effectors, and catalyzing enzymes, with information about organisms, tissues and cellular locations where the reactions take place, and with the kinetic properties of these reactions (type of the kinetic mechanism, modes of inhibition or activation and rate equations together with their parameters and measured values). As kinetic constants highly depend on environmental conditions used for their determination these are given together with the description of the kinetics. This also facilitates the comparison of data sets based on experiments assayed under similar experimental conditions.

### **User interface**

Users can access the SABIO-RK database by a web-based interface that allows the search for biochemical reactions and their kinetics by specifying characteristics of the reactions of interest (such as reactants, enzymes or pathways) as well as of the kinetic data searched (e.g. from a particular tissue, determined under certain experimental conditions or having certain parameter type). All reactions matching the search criteria are shown. Details about the reactions, catalyzing enzymes and the corresponding kinetic data can be displayed upon selection. Links to several external databases enable the user to gather further information about compounds, enzymes and reactions, and to refer to the original publications. These links

together with the use of synonymic notations for compounds and enzymes, as well as with the use of controlled vocabularies and ontologies, facilitate the comparison and integration of the data. Data about biochemical reactions and their kinetics (including parameters with their respective rate equations) can be exported in SBML (Systems Biology Mark-up Language) [1] format, allowing its import into simulation and modeling programs supporting SBML. Apart from the graphical interface we recently started offering web services to allow users' applications to directly query the database without having to go manually through the web-interface. These web services provide customizable points of entry for an automatic access to the SABIO-RK database in a language-independent fashion.

### **Database population**

The database is populated by merging data from several sources. The general information about the reactions is mainly obtained from external databases such as KEGG (Kyoto Encyclopedia of Genes and Genomes)[2]. In contrast, the kinetic data along with descriptions of the experimental conditions under which they were determined are primarily manually extracted from literature and curated by a team of scientists. This is supported by a tailored input interface that is now been adapted to allow external users to directly submit their information and results from their experiments to SABIO-RK, avoiding the possible loss of information during publication and information extraction. The interface employs controlled vocabularies

and ontologies to avoid the introduction of errors and duplications through misspelling or variants in spellings. Other problems faced in the population process are the identification and unambiguous description of compounds (identification of synonyms), enzymes and reactions, as well as missing specifications of experimental conditions or the multiplicity of parameter units

### Future work

Currently the system mainly contains information about metabolic reactions, thus one of our main extension plans is to incorporate more information for signalling and regulation reactions. This will require some changes in the database model and to the user interface to offer an appropriate storage and access to this information. We are also working on the extensions to system to provide data about the elementary reactions describing the mechanisms of reactions.

### Availability

SABIO-RK can be freely accessed for academic use at <http://sabio.villa-bosch.de/SABIORK/>.

### References

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2. Kanehisa M, Goto S: **KEGG: Kyoto Encyclopedia of Genes and Genomes.** *Nucleic Acids Res* 2000, **28**:27-30.

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