

# sybilSBML – Quick Start

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January 16, 2013

## 1 Introduction

The package *sybilSBML* is an addition to *sybil* providing support for metabolic networks written in SBML (Systems Biology Markup Language), in particular those developed by Bernhard Ø. Palsson's lab<sup>1</sup> and those from the BiGG database<sup>2</sup> [Schellenberger et al., 2010].

The package *sybilSBML* requires one additional package *rsbml* available from Bioconductor<sup>3</sup>, which is itself powered by LibSBML [Bornstein et al., 2008] available from the SBML homepage<sup>4</sup> and pkg-config<sup>5</sup>.

## 2 Installation

The following sections describe the installation process of *sybilSBML* on various platforms.

### 2.1 Linux and Mac OS X

The package *sybilSBML* depends on a separate installation of *rsbml* and therefor of an installation of LibSBML and pkg-config (which should be available in a Linux distribution).

If pkg-config is installed in a non-standard directory, set the two environment variables PKG\_CONFIG\_PATH and PKG\_CONFIG to appropriate values. If LibSBML is installed in a non-standard directory, set the environment variables LIBSBML3\_CFLAGS and LIBSBML3\_LIBS, for example, if LibSBML is installed in your home directory:

```
$ export LIBSBML3_CFLAGS="-I$HOME/include"
```

```
$ export LIBSBML3_LIBS="-L$HOME/lib -lxml2 -lz -lm -lbz2 -lsbml -lstdc++"
```

For the installation of *rsbml*, start R and run

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<sup>1</sup><http://gcrg.ucsd.edu/>

<sup>2</sup><http://bigg.ucsd.edu/>

<sup>3</sup><http://www.bioconductor.org/>

<sup>4</sup><http://www.sbml.org/>

<sup>5</sup><http://pkg-config.freedesktop.org/wiki/>

```
> source("http://bioconductor.org/biocLite.R")
> biocLite("rsbml")
```

Now install the source code package from a Terminal command line

```
$ R CMD INSTALL sybilSBML_X.X.X.tar.gz
```

## 2.2 Windows

There is a precompiled binary version of *rsbml* available, no additional software is required. Start R and run

```
> source("http://bioconductor.org/biocLite.R")
> biocLite("rsbml")
```

Now install the Windows binary package *sybilSBML\_X.X.X.zip*.

## 3 Usage

The package *sybilSBML* provides the command `readSBMLmod()` which reads SBML formatted files and returns instances of class `modelorg`.

```
> library(sybil)
> library(sybilSBML)
> model <- readSBMLmod("<model>.xml")
```

## 4 Input files

The function `readSBMLmod()` reads metabolic network models written in SBML format (Systems Biology Markup Language). Among the models available in this de-facto standard format are in particular those developed by Bernhard Ø. Palsson's lab.

The metabolite id's are written in the format `M_<metabolite abbreviation>_<compartment abbreviation>`. The compartment abbreviation is a one letter abbreviation, e.g. `c` for cytosol. All metabolites outside the system boundary belong to compartment `b`. Those metabolites are transported into or outside the system. As long as they are mentioned, the network is closed. The function `readSBMLmod()` will remove them in order to produce an open network.

## References

- S. A. Becker et al. Quantitative prediction of cellular metabolism with constraint-based models: the COBRA Toolbox. *Nat Protoc*, 2(3):727–738, 2007. doi: 10.1038/nprot.2007.99.
- B. J. Bornstein et al. LibSBML: an API library for SBML. *Bioinformatics*, 24(6):880–881, Mar 2008. doi: 10.1093/bioinformatics/btn051.

- J. Schellenberger, J. O. Park, T. M. Conrad, and B. Ø. Palsson. BiGG: a biochemical genetic and genomic knowledgebase of large scale metabolic reconstructions. *BMC Bioinformatics*, 11:213, 2010. doi: 10.1186/1471-2105-11-213.
- J. Schellenberger, R. Que, R. M. T. Fleming, I. Thiele, J. D. Orth, A. M. Feist, D. C. Zielinski, A. Bordbar, N. E. Lewis, S. Rahmanian, J. Kang, D. R. Hyduke, and B. Ø. Palsson. Quantitative prediction of cellular metabolism with constraint-based models: the COBRA Toolbox v2.0. *Nat Protoc*, 6(9):1290–1307, 2011. doi: 10.1038/nprot.2011.308.