sybilSBML – Quick Start

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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[1] and those from the BiGG database[2][Schellenberger et al., 2010].

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

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 instalation 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

[1] `http://gcrg.ucsd.edu/`
[2] `http://bigg.ucsd.edu/`
[3] `http://www.bioconductor.org/`
[4] `http://www.sbml.org/`
[5] `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 formated 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

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