SBML tools in Python

Here I compare the different python tools for SBML manipulation

Website for collected packages/software information: https://biosimulators.org

Online tool to validate SBML model: http://constraint.caltech.edu:8888/validator\_servlet/index.jsp

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| --- | --- | --- | --- | --- | --- | --- |
| Status | Name of Package | Advantages | Disadvantages | | Description | |
| X, 1 | [Tellurium](http://tellurium.analogmachine.org/) | Import successful, simulation up and running. | Crashes program when errors in matlab file. | Relies on Roadrunner | |
| X, 0 | [SimpleSBML](https://simplesbml.readthedocs.io/en/latest/) | Import successful. No simulation possible, use of tellurium in documentation. |  | | Intended Use with tellurium. | |
| X, 0 | [sbmlutils](https://github.com/matthiaskoenig/sbmlutils) | Manipulation tool, Intended use is creating and manipulating sbml files. Great error messages. | No direct support to extract species or reaction data | | Relies on <https://sbmlutils.readthedocs.io/en/latest/notebooks/sbml_interpolation.html> other packages for simulations | |
| o | [SBMLmod](https://bmcbioinformatics.biomedcentral.com/articles/10.1186/s12859-017-1722-9) | Manipulation tool | Only intended for GUI use, code in component Pascal | |  | |
| X, 1 | [SBMLtoODE](https://joss.theoj.org/papers/10.21105/joss.01643) | Manipulation tool, up and running, accessing species requires string of name of species. | Access to species ect. Requires exact names. Conversion from matlab export removes these name informations, thus making it very difficult to use. | | Prints second file with “python readable” model file | |
| X,0 | LibSBML | Manipulation tool, Import successful. Intended Use: Validation of Model. |  | |  | |
| o | pyVipr |  |  | | Widget for visualization in jupyter notebook | |
| X, 1 | [libRoadRunner](https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4607739/) | Simulation tool, import & simulation successful |  | | Very bad documentation | |
| o | [CompuCell3d](https://pythonscriptingmanual.readthedocs.io/en/latest/sbml_solver.html) | Simulation tool |  | | Intended Use as GUI | |
| o | [LibSBMLSim](https://fun.bio.keio.ac.jp/software/libsbmlsim/) | Simulation tool | Couldn’t find installer file Download libSBMLSim Installer for Windows (libsbmlsim-1.4.0-win{32,64}.exe) | | Depends on libsbml, C code | |
| o | [MASSpy](https://journals.plos.org/ploscompbiol/article?id=10.1371/journal.pcbi.1008208) | Simulation tool | Failed to install | | pip install masspy  pip install biosimulators-masspy  Intended use with Cobrapy, relies on libroadrunner | |
| o | [SBMLToolbox](http://model.caltech.edu/software/sbmltoolbox/) | Simulation tool |  | | For matlab, octave | |
|  | deSolve, ODE solver | Simulation tool |  | | Check which packages can spit out system of ODEs | |
| x | [biosimulators-libsbmlsim 0.0.3](https://pypi.org/project/biosimulators-libsbmlsim/) |  |  | | Depends on libsbmlsim, libsbml | |
| x | bioconductor |  | https://pythonhosted.org/rpy2-bioconductor-extensions/introduction.html#installing-bioconductor-packages | | Intended use with R | |
|  | [Bionetgen](https://pypi.org/project/biosimulators-bionetgen/) |  |  | |  | |

0 Github private repository

1. Plot same as Matlab
2. Difference between matlab results & python results would be great

Virtual-pip (alternative to conda?)