

Python Prescription

Virtual Screening Tool

sourceforge

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PyRx Binary Distribution



PyRx is open source software for Computer-Aided Drug Design distributed under Simplified BSD License.

System Requirements for PyRx are similar to Second Life.

Windows **Linux** **Mac OS X** **Source**

Instructions for Installing PyRx from Source

PyRx depends on many packages that might not be easy to install.

Please try binary installer corresponding to your OS first (see above).

If that fails, you'll need to install the following list of packages that PyRx depends on.

Please note that installing PyRx from source is challenging and requires expert Python programming experience.

- Python - a programming/scripting language - python.org.
- AutoDockTools, used to generate input files - mgltools.scripps.edu.
- wxPython for cross-platform GUI - wxpython.org.
- The Visualization ToolKit (VTK) for 3D computer graphics - vtk.org by Kitware, Inc.
- Enthought Tool Suite, including Traits, for application building blocks - code.enthought.com.
- Opal Toolkit for running AutoDock remotely using Web services - opal.nbcr.net.
You'll need to install [Python Opal Web Service Client](#). PyRx is set to use ws.nbcr.net servicer by default.
If you are planning to create your own grid/cloud, you'll need to install Opal Server as well.
- Open Babel for importing SDF files, removing salts and energy minimization - openbabel.org.
- AutoDock, used as a docking software - <http://autodock.scripps.edu> (optional).
Only remote execution mode is enabled if PyRx can't find autodock binaries.
- ePMV, embedded Python Molecular Viewer - epmv.scripps.edu.

Congratulations if you managed to install all the dependencies and read this far.

You are now only a few clicks away from using PyRx. Download and unpack [PyRx-0.9-Source.zip](#) (760 KB). The latest version of PyRx source code is also available at <https://sourceforge.net/projects/pyrx/develop> Now, do standard python install:

```
python setup.py install
```

Starting PyRx on Different Platforms

Windows Users - double click on runPyRx.py or run python runPyRx.py from command line.

Linux Users - add MGLTools to your PYTHONPATH:

```
csh - setenv PYTHONPATH/usr/local/MGLTools-$Version/MGLToolsPckgs:/usr/local/MGLTools
bash - PYTHONPATH="/usr/local/MGLTools-$Version/MGLToolsPckgs:/usr/local/MGLTools"
```

Run "python runPyRx.py" from command line.

Mac OS X Users - add MGLTools to your PYTHONPATH:

```
export PYTHONPATH="/Library/MGLTools/$Version/MGLToolsPckgs:/Library/MGLTools/$Version"
```

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Run pythonw runPyRx.py from command line.

Please see [PyRx 0.9.4 Release Announcement](http://sourceforge.net/projects/pyrx/files) for the list of new features and bug fixes. Older versions of PyRx are available for free from <http://sourceforge.net/projects/pyrx/files>.

[8 Comments](#)

Last Updated on Saturday, 15 October 2016 12:56

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Written by Sarkis Dallakian

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Last Updated on Monday, 13 February 2012 14:32

Known Issues and Feature Requests

Written by Sarkis Dallakian

- An incomplete download is the most common reason for non working installers. Make sure your download is complete before running installers.
- "Customize Filter" widget for table editor causes crash on Windows and Mac.
- PyRx crashes on Linux when there are no hardware 3D accelerated (OpenGL) drivers available. See [Using hardware accelerated 3D renderer on Linux](#) and [Installing Nvidia Driver on CentOS 6](#) for instructions on how to install OpenGL drivers.
- ~~On Mac OS X, 3D Scene tab needs to be resized when switching between different tabs, otherwise it doesn't redraw properly.~~

Please visit [FAQ](#) page for information on how to submit a bug or request a new feature.

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6 likes

