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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.



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.

Congradulations 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 uppack PyRx-0.9-Source.zip (760 KB). The latest version of PyRx source code is also available at

 $https://sourceforge.net/projects/pyrx/develop\ \textbf{Now},\ \textbf{do}\ standard\ python\ install:$

python setup.py install

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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/MGLT 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/MGLToolsPckgs/:/Library/MGLTools/\$Version/MGLToolsPckgs/:/Library/MGLTools/\$Version/MGLToolsPckgs/:/Library/MGLTools/\$Version/MGLToolsPckgs/:/Library/MGLTools/\$Version/MGLToolsPckgs/:/Library/MGLTools/\$Version/MGLToolsPckgs/:/Library/MGLTools/\$Version/MGLToolsPckgs/:/Library/MGLTools/\$Version/MGLToolsPckgs/:/Library/MGLTools/\$Version/MGLToolsPckgs/:/Library/MGLTools/\$Version/MGLToolsPckgs/:/Library/MGLTools/\$Version/MGLTools/\$Version/MGLToolsPckgs/:/Library/MGLTools/\$Version/MGLTools/\$Version/MGLToolsPckgs/:/Library/MGLTools/\$Version/MGLTools/\$Vers

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Run pythonw runPyRx.py from command line.

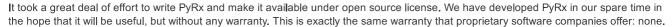
Please see PyRx 0.9.4 Release Announcement for the list of new features and bug fixes. Older versions of PyRx are available for free from http://sourceforge.net/projects/pyrx/files.

8 Comments

Last Updated on Saturday, 15 October 2016 12:56

Simplified BSD License

Written by Sarkis Dallakian



Please watch Which Open Source License is Best? to learn more about open source licenses. Here is the Simplified BSD License for PyRx which is short and permissive free software licence.

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3 Comments

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 avialable. See Using hardware accelerated 3D renderer on Linux and Installing Nvidia Driver on CentOS 6 for instuctions 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.

0 Comments

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