

FAQ:PyRx

From HPCVL Support Wiki

This is a quick introduction to the usage of the screening software PyRx that is installed on the HPCVL clusters. It is meant as an initial pointer to more detailed information. It also explains a few specific details about local usage.

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What is PyRx ?

PyRx is a Virtual Screening software for Computational Drug Discovery that can be used to screen libraries of compounds against potential drug targets. It is a GUI that uses a large body of established open source software such as:

- AutoDock 4 and AutoDock Vina are used as a docking software.
- AutoDockTools, used to generate input files.
- Python as a programming/scripting language.
- wxPython for cross-platform GUI.
- The Visualization ToolKit (VTK) by Kitware, Inc.
- Enthought Tool Suite, including Traits, for application building blocks.
- Opal Toolkit for running AutoDock remotely using web services.
- Open Babel for importing SDF files, removing salts and energy minimization.
- matplotlib for 2D plotting.

Where is the program located ?

The binary executable is in /opt/PyRx on the SW (Linux) Cluster. The present version of the program is 0.9.2, and it is available on the Linux platform in its 64 bit version. Therefore, all the relevant executables are in /opt/PyRx/0.9.2. Documentation can be found at at the main PyRx site (<http://pyrx.sourceforge.net/>).

How do I set up my environment for PyRx ?

You can run PyRx only on the swlogin1 Linux login node (it won't run on Solaris). From there, the setup for PyRx is very simple. It is only necessary type :

```
source PyRx
```

This will enter the proper directory into your PATH and off you go.

How do I run PyRx interactively ?

Issuing the command

```
PyRx
```

will pop up the GUI. All operations are performed from within that interface. At a minimum, you will have to specify a macromolecule and at least one compound that you want to "dock". These molecules can be specified in several formats such as *pdb*, *pdbq*, *cif*, *mol2*. You can Import or Load molecules from the

```
File -> Load Molecule
```

or the

```
File -> Import ...
```

tab.

The actual Analysis is performed using various tabs on the GUI. As an example we outlined the steps using the "Vina Wizard" which runs a software called "Autodock Vina" for the Analysis:

```
Vina Wizard -> Start Here -> (select /opt/PyRx/0.9.2/bin/vina) -> Start  
(highlight Ligands and Macromolecule(s)) -> Forward  
(adjust values for Search Space) -> Forward  
(check results in bottom window)
```

There's of course a lot more to it. But the authors of the software claim that it is intuitive enough that you can figure anything out while doing it. Your mileage may vary.

How do I run PyRx on a cluster ?

If you are screening hundreds (or even thousands) of molecules using PyRx the time required may be too much for interactive usage. PyRx offers some basic interface with a scheduler, but the default settings are too non-specific to work with our systems.

For the Vina Wizard, we have provided a work-around that allows you to work through a large number of runs using the machines on the SW cluster in parallel. **Before you are trying to do this read through our Grid Engine FAQ to learn how jobs are submitted to our production clusters.**

The procedure for this starts off the same as for the interactive approach:

```
Vina Wizard -> Start Here -> (select Cluster(Portable Batch System)) -> Start  
(highlight Ligands and Macromolecule(s)) -> Forward  
(adjust values for Search Space) -> Forward
```

However, in this case the "Cluster" setting was selected and as a result, the program is not actually running any docking software, but rather generates a large number of scripts in a directory

```
~/PyRx_workspace/Macromolecules/MACRO
```

where "MACRO" stands for the name of the macromolecule you are using, and "~" is short for the name of your home directory. To run the actual analysis on our cluster, you now need to go into that directory and execute a "perl" script that we have provided for this purpose:

```
cd ~/.PyRx_workspace/Macromolecules/MACRO
PyRxVinaArray.pl
```

This will generate two new sub-directories "jobs" and "logs" and copy the scripts mentioned earlier, then produce a job for our scheduler "Grid Engine", and submit it. Using the qstat command, you should then be seeing something like:

```
$ qstat
job-ID prior name user state submit/start at queue slots ja-task-ID
-----
952371 0.50734 runVina.sh hpcXXXX r 11/17/2015 12:59:29 abaqus.q@sw0013.hpcvl.org 8 64
952371 0.50734 runVina.sh hpcXXXX r 11/17/2015 12:48:59 abaqus.q@sw0020.hpcvl.org 8 60
952371 0.50734 runVina.sh hpcXXXX r 11/17/2015 12:58:29 abaqus.q@sw0044.hpcvl.org 8 62
952371 0.50734 runVina.sh hpcXXXX r 11/17/2015 12:58:59 abaqus.q@sw0047.hpcvl.org 8 63
952371 0.50734 runVina.sh hpcXXXX r 11/17/2015 13:05:59 abaqus.q@sw0048.hpcvl.org 8 65
952371 0.50734 runVina.sh hpcXXXX r 11/17/2015 13:09:29 abaqus.q@sw0054.hpcvl.org 8 66
952371 0.50734 runVina.sh hpcXXXX qw 11/17/2015 09:30:03 8 67-511:1
```

As you can see, it's working on 6 "Vina" jobs simultaneously, with 8 processors each for a total of 48.

Once the "qstat" command does not show anything anymore, the analyses are finished, and you can go back to your PyRX GUI:

```
--> Forward
(check results in bottom window)
```

Note that this works only for the analysis with *Vina*. If you want to do something similar with a different analysis (for instance Autodock4), please get in touch with us. We can probably come up with a solution.

Are there licensing issues with PyRx ?

No. PyRx is distributed through SourceForge. We have paid for a license, but the number of Users is not limited by this.

Where can I get more detailed information ?

The obvious "goto" place is the PyRx Homepage (<http://pyrx.sourceforge.net>). They do not provide a manual for the software, but there is a FAQ file (<http://pyrx.sourceforge.net/faq>) that answers basic questions, a forum (<http://mgl.scripps.edu/forum/viewforum.php?f=25>) that may help you out, and even some videos (<http://pyrx.sourceforge.net/videos>) that demonstrate how the software is used. If you run into issues you can't resolve, please send email to help@hpcvl.org (<mailto:help@hpcvl.org>).

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