Frequently Asked Questions

10 Comments

Is there a user's manual for PyRx?

PyRx is designed to be intuitive to learn, with no manual required. Watching PyRx screencasts is the best way to get started. Please see the following documents for additional notes on how to use PyRx:

- http://www.slideshare.net/JohnCahill4/a-beginners-manual-for-pyrx
- https://faculty.missouri.edu/~gatesk/Docking_Assignment.pdf
- http://wiki.hpcvl.org/index.php/FAQ:PyRx
- http://pyrx.sourceforge.net/SI/2010/PyRx2010_rvsnALP_7122010.pdf

How to report a bug?

Please visit http://sourceforge.net/p/pyrx/tickets, click on Log In (if you have SourceForge account) or Join (if you don't have SourceForge account) and Create Ticket. Please provides steps required to reproduce the bug and attach all the input files needed. Also, take a screen capture and attach it as well; sometimes it's simpler to show someone what's on your screen than it is to explain it.

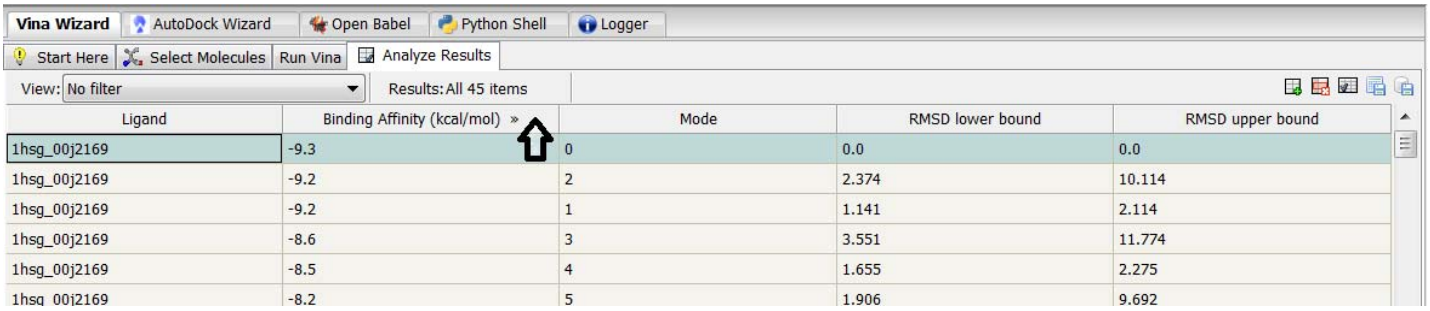
Bug Bounty: We offer $20 or more refunds for all original bug reports that are not listed under Known Issues. The exact amount depends on the severity of the bug and the percentage of impacted users.

- Bug reports that are too vague or unclear are not eligible for a bug bounty.
- Bug reports that include clearly written explanations and working code are more likely to get a bug bounty.

How to sort the table in Analyze Results tab?

The user can sort the items in the table based on the values in a column by clicking the header of that column as shown in the image below. Source: TableEditor#managing-items

- On the first click, the items are sorted in ascending order. The characters **>>** appear in the column header to indicate that the table is sorted ascending on this column's values.
- On the second click, the items are sorted descending order. The characters **<<** appear in the column header to indicate that the table is sorted descending on this column's values.
- On the third click, the items are restored to their original order, and the column header is undecorated.



How to reset perspective and restore the default PyRx arrangement?

Use *View -> Reset Perspective* menu. This is handy in case PyRx crashes and you want to restore the default view.

How to clean your PyRx workspace?

PyRx uses .PyRx_workspace in your home folder as the default workspace. You can rename/delete that folder and restart PyRx to have a new and clean workspace. See also: How can I get rid of old ligands?

Docking instance has no attribute 'ligMol'.

This error message shows up when there are no docked conformation in the docking log file. To troubleshoot this problem please open your dlg file and read it carefully to see why there were no docked conformation recorded there.

Too many torsions.

AutoDock sets the maximum number of torsions a ligand can have. When a ligand has more than this maximum number of torsions, you'll get "FATAL ERROR: PDBQT ERROR: too many torsions, maximum number of torsions is 32" error message. To run AutoDock with ligands that have too many torsions, limit the number of active torsions when making pdbqt files using Edit -> Preferences ->

AutoDock -> Ligand Preparation -> Number of torsion: option. Set this to, say, 32 and remake ligand pdbqt file(s). See this forum post for more info.

How to run PyRx on a cluster?

PyRx enables *Cluster* execution mode when, in addition to AutoDock binaries, you also have *qsub* (PBS or SGE) in your path. Please install PyRx on the head node and make sure that AutoDock binaries are available from all the nodes. PyRx creates individual job files for each protein-ligand docking and submit all the jobs to your cluster.

Location of PyRx source code in the binary distribution.

After installing PyRx using binary distribution you can find PyRx source code at:

- Windows - C:\Program Files (x86)\PyRx\$Version\Lib\site-packages\PyRx
- Linux - /usr/local/PyRx-$Version/lib/python2.6/site-packages/PyRx
- Mac - /Library/PyRx-$Version/Python.framework/Versions/2.6/lib/python2.6/site-packages/PyRx

where $Version is version number for PyRx binary distribution.

How to remove/uninstall update?

If you experience problems after updating PyRx using Help -> *Check for Updates...* menu, please remove the following folder to disable this update:

- Windows - C:\Users\$UserName\.PyRx_workspace\update (Windows Vista and higher)
- Linux - /home/$UserName/.PyRx_workspace/update
- Mac - /Users/$UserName/.PyRx_workspace/update

where $UserName is your user name.

How many jobs can I run at once?

This depends if you are using AutoDock 4 or Vina, and the execution mode you select for the corresponding wizards.

- If *Local* execution mode is selected when you start AutoDock Wizard, then PyRx would use the number of available CPUs to decide how many docking jobs to run at once. By default, this number is set to the number of CPU cores minus one (or one, if there is only one CPU core available). For instance, if you have a PC with 8 CPU cores, PyRx runs 7 docking jobs at once. This number can be changed using PyRx > Edit > Preferences... menu. For Vina jobs, PyRx submits one job at a time, since Vina can utilize all available CPUs.
- If you select *Remote* execution mode, PyRx submits all the jobs at once for both AutoDock 4 and Vina. However, there is a limit of 35 jobs per IP per hour for the default Web services PyRx is currently using (http://nbcr-222.ucsd.edu). If you exceed this limit, your remote jobs will error out until the next hour.
- On a Linux cluster, there is additional execution mode available called *Cluster*. If you select that, PyRx would submit all the jobs at once to your cluster.

How do I cite PyRx?

Please refer to the following publication if you'd like to cite PyRx in your article:

Small-Molecule Library Screening by Docking with PyRx. Dallakyan S, Olson AJ. *Methods Mol Biol.* 2015;1263:243-50. The full-text is available at https://www.researchgate.net/publication/273954875_Small-Molecule_Library_Screening_by_Docking_with_PyRx

how to fix this problem?
i can't docking more than 10 molecule with Autodock (LGA GA SA)
thanks for help

fakhmi

Reply • Share ›

Sarkis Dallakian Mod → nurul fakhmi • 5 months ago

Dear nurul,

Thank you for the screenshot. It seems that this problems is because there are too many atom types in your molecules. We have fixed this in the latest release of PyRx following - http://mgl.scripps.edu/forum/v...

Please update your version of PyRx using Help->Check for Updates... option. If the problem persist after updating PyRx, please create a new ticket following How to report a bug? - http://pyrx.sourceforge.net/fa.... You can upload your molecules as attachments for the tickets. That way, I'll be able to reproduce this on my end.

Thank you for using PyRx!

Reply • Share ›

Learner • a year ago

How to save complex pdf file after docking using autodock vina on Pyrx? Is there any way to know which is the complex file after sucessful docking?

Reply • Share ›

Sarkis Dallakian Mod → Learner • a year ago

I have implemented *save docked complex as pdb* (not pdf) for the upcoming 0.9.3 release:
https://sourceforge.net/p/pyrx...
I'm not sure I understand your second question. What do you mean?

Reply • Share ›

Deena Das1 • 5 years ago

sir,
whenever i am loading more than 50 compounds in sdf format using open barbel ,it is going wrong in between.The software proceeds till autogrid step but after clicking autodock the software does not perform docking and so i am not the binding energy.how do i tackle this problem? please give me a solution so that i can load more than 100 compounds at a single step using open barbel.

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Sarkis Dallakian Mod → Deena Das1 • 5 years ago

Thanks for the comment Deena. Please visit PyRx Forum and post any error messages you see there. You can also attach screenshots and the input sdf file, if needed. Please also mention OS and PyRx version you are using. Thank you.

Reply • Share ›

Rgopalas • 5 years ago

How do I use an old config file (that was generated in a previous run) for a new ligand to be docked?

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Sarkis Dallakian Mod ➚ Rgopalas • 5 years ago

Thanks for the question. I'll need some more information to make sure that I understand this question correctly. Do you want to use ligands generated in a previous run as a starting point for a new run? If so, you can copy/past ligands from config file or save them as pdb and then use them as a starting point for the next run.

^ | v • Reply • Share ›

Nedavaghefi • 5 years ago

how prepare flexible residues?

^ | v • Reply • Share ›

Sarkis Dallakian Mod ➚ Nedavaghefi • 5 years ago

Please see the following video http://www.youtube.com/embed/9...
It shows how to prepare flexible residues and other new features introduced in PyRx 0.5. See also: http://pyrx.scripps.edu/blog/6... and http://pyrx.scripps.edu/blog/9...

Thanks!

^ | v • Reply • Share ›

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