Docking Tutorial Documentation

Release 1.0

Noel O'Boyle

Nov 03, 2017

Contents

Contents:

CHAPTER 1

Overview of the AutoDock world

AutoDock is a docking program - Open Source, freely available

AutoGrid is part of AutoDock - Creates the grids for use in docking

Vina is another docking program - Faster (and claims to be more accurate) than AutoDock

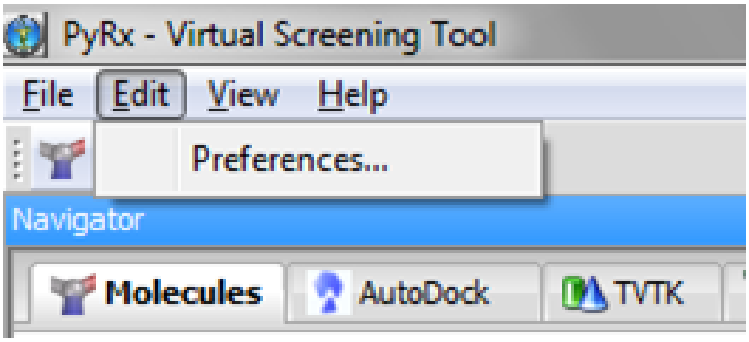
ADT (AutoDockTools) is a GUI for setting up and analysing AutoDock dockings - Been around a while - a bit clunky - quite powerful though

PyRx is a GUI for setting up and analysing AutoDock and Vina dockings - Relatively new - easy to use - works well - doesn't have all the features of ADT - If you are interested in new features, ask for them on the forum

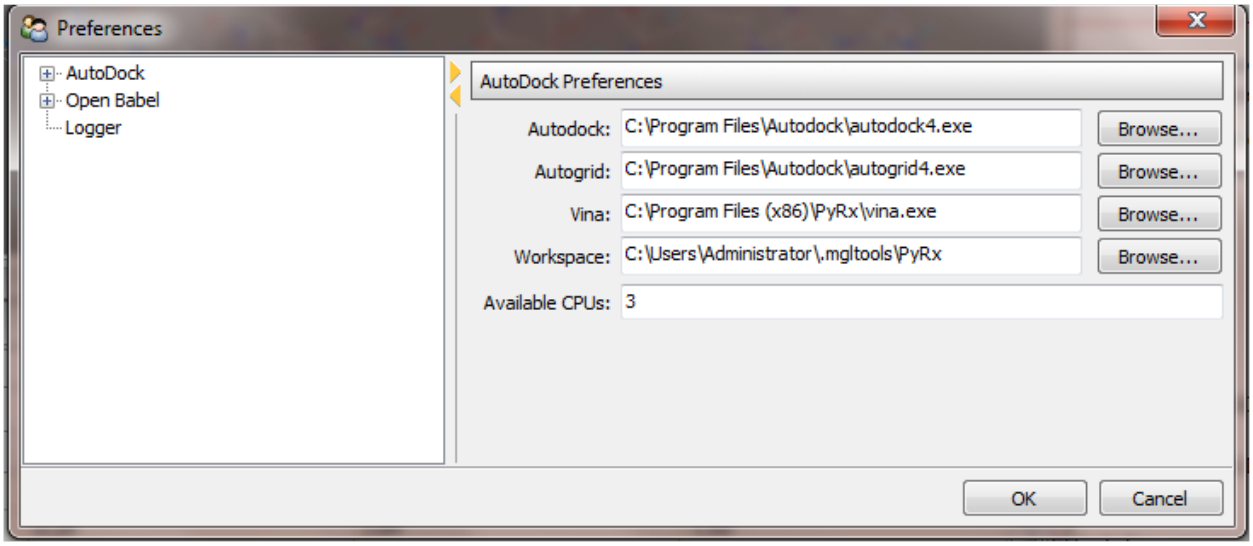
CHAPTER 2

Configure PyRx to find AutoDock

- Start PyRx
- Go to Edit/Preferences



- Set the preferences as follows:


Preferences
AutoDock
Open Babel
Logger
AutoDock Preferences
Autodock:
C:\Program Files\Autodock\autodock4.exe
Browse...
Autogrid:
C:\Program Files\Autodock\autogrid4.exe
Browse...
Vina:
C:\Program Files (x86)\PyRx\vina.exe
Browse...
Workspace:
C:\Users\Administrator\.mgltools\PyRx
Browse...
Available CPUs:
3
OK
Cancel

CHAPTER 3

Tutorial - Docking a HIV Protease Inhibitor

Indinavir is a HIV Protease Inhibitor. Going to dock against...a HIV Protease (iPDB code of 1hsg).

Follow the PyRx tutorial to run a docking experiment, and carry out a virtual screen. The notes below give extra information (or corrections) on each step of the tutorial.

Note: Part 1 of the tutorial using **AutoDock**, but Part 2 uses **Vina**. Make sure you are using the correct wizard in each case.

3.1 Part 1 Exercise 1

- **In the very first step, when you click *Next*, you need to wait about 2 minutes for the file to download**
  - Change address to http://pyrx.sf.net/sample.tar.gz
  - (If that doesn't work, choose local file and use sample.tar.gz)
- **"Click on the arrow next to hsg1" should be...** "Click on the plus sign next to hsg1"
- **Note that using the Molecules tab you can...**
  - Display/hide a molecule
  - Display/hide a particular chain
  - Label a particular protein residue
- Can zoom with mouse wheel (after clicking on the 3D view)
- Full screen very useful (Esc to exit)
- **Right click on a map (e.g. hsg1.A.map), and choose Display (MayaVi)**
  - In the MayaVi Panel, right click on Surface, and choose Hide/Show
  - Right click on it again, and choose Add Module, Isosurface

  - Once you are finishing, right click on IsoSurface, and choose Delete

3.2 Part 1 Exercise 2

- **Choose "Local (requires local AutoDock binaries)" at the bottom of the screen**
  - (We have installed both Autodock and Vina locally)

3.3 Part 1 Exercise 3

- **You will know when they are selected because it will list them at the bottom of the screen**
  - (as in the screenshot in the tutorial)

3.4 Part 1 Exercise 4

- Play around with the bounding box, then click Reset
- **The Grids already exist, but let's run AutoGrid anyway**
  - Instead of clicking Forward, click Run AutoGrid
  - It takes around 30s

3.5 Part 1 Exercise 5

- **Run AutoDock**
  - Takes about 5 minutes
- **FYI:**
  - dlg = docking log file
  - On Windows 7, all log files, etc. are placed in C:/Users/myname/.mgltools/PyRx

3.6 Part 1 Exercise 6

- **Click on Binding Energy to sort the ligands**
  - The one with the most negative binding energy is the strongest binder
- You can right click on a row, and choose Creating Clustering Histogram

3.7 Part 2 Exercise 1

- **Instead of opening "Desktop/PyRx2010/3D.sdf"** Use 3D.sdf from here (download and save it on your Desktop).
- **After you choose "Convert All to AutoDock Ligand"**

  - Right-click in the Ligands folder, and choose Refresh
  - The list of ligands should appear

3.8 Part 2 Exercise 2

- **When selecting the Molecules, instead of selecting them all, select only 5 or so.**
  - Each docking takes about a minute on these machines
- (You can ignore the text about computer clusters for this tutorial)

3.9 Part 2 Exercise 3

- ...we are not going to cover this now