AutoDock Tutorial

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AUTODOCK TUTORIAL

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- *At the start of this tutorial, all you need is a directory (e.g., "Docking") which consists of two files; protein.pdb and ligand.mol2.*
- 1. **Open** ADT tool of AutoDock.
- 2. **File -> Preferences -> Set**: change the startup directory.
- 3. **Ligand -> Input -> Open**: open your ligand mol2 file.
- 4. **Ligand -> Torsion Tree -> Choose Torsions**: decide on the rotatable bonds to be considered.
- 5. **Ligand -> Output -> Save as PDBQT**: save your ligand file with "pdbqt" extension (e.g. ligand.pdbqt). Type in the extension manually.

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- 6. **Grid -> Macromolecule -> Open**: Open your protein pdb file (e.g. protein.pdb), and ADT tool will prompt a new window to save your protein into pdbqt file.
- 7. **Grid -> Set Map Types -> Choose Ligand**: select the ligand molecule from the list shown.
- 8. **Grid -> Grid Box**: Select the number of grid points in x, y and z directions. Usually, the default 40 is taken. However, you can increase or decrease that number in any direction. From "**Center**" menu, select "**Center on ligand**". Leave other parameters on default.

(*Observe your grid box. Make sure that it covers the whole ligand as well as the binding site*).

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- **File -> Close saving current**: save your settings before closing. Otherwise, your settings will be lost if the program is closed.
- 10. **Grid -> Output -> Save GPF**: save your gpf file (e.g. docking.gpf). Type in the extension manually.
- 11. **Check out** the content of Grid Parameter File, docking.gpf (by Notepad).
- 12. **Docking -> Macromolecule -> Set Rigid Filename**: Select your macromolecule protein file (e.g. protein.pdbqt).
- 13. **Docking -> Ligand -> Choose**: select your ligand. Leave everything on default and select **Accept**.

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- 14. **Docking -> Search Parameters -> Genetic Algorithm**: set the number of GA Runs as 20.
- Also, set the maximum number of “evals” to *long = 25000000* depending on the number rotatable bonds. Leave other parameters on default and select **Accept**.
- 15. **Docking -> Docking Parameters**: Leave on default.
- 16. **Docking -> Output -> Lamarckian GA**: save your dpf file (e.g. docking.dpf). Type in the extension manually.
- 17. **Close** your ADT tool.

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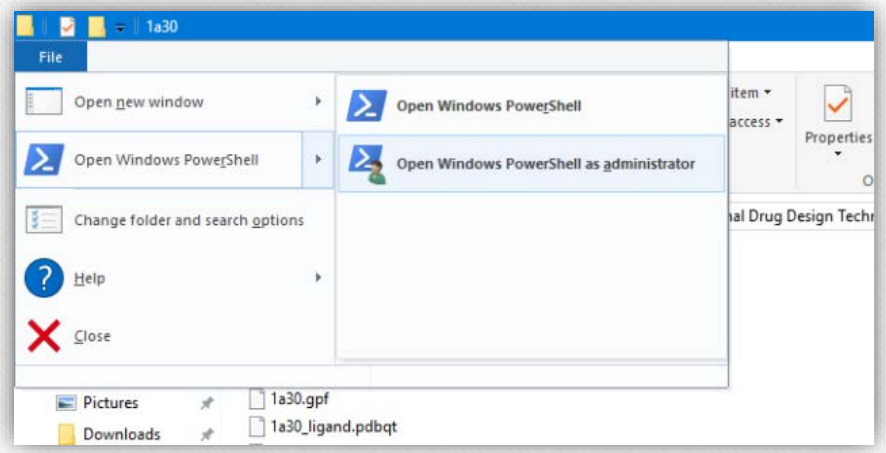
- In your working directory you should now have the following four files:
  - ligand.pdbqt • receptor.pdbqt • docking.gpf • docking.dpf
- 18. **Open** “Windows PowerShell”: **File -> Open Windows PowerShell -> Open Windows PowerShell as administrator**.



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- While you are inside your working directory, type the following Win/unix command:

Windows:

.\autogrid4.exe -p docking.gpf -l docking.glg

Unix:

autogrid4 -p docking.gpf -l docking.glg

- Once the program is completed, new files should appear in your working directory including the map files.

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- These grid map files are necessary for the docking run. Now you are ready to dock. Type the following:

Windows:

.\autodock4.exe -p docking.dpf -l docking.dlg

Unix:

autodock4 -p docking.dpf -l docking.dlg

HAPPY DOCKING