AUTODOCK PROTOCOL

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Preface

Molecular Docking is a crucial process for most of the synthetic biology projects. Many iGEM Teams use molecular docking to screen molecules that exhibit the desired properties. One of the most prominent Molecular Docking software is Autodock. However, first time users may feel a bit lost while using the software. This short guide is a handy resource aimed at helping iGEM teams to perform molecule docking through Autodock.

Greetings,

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Autodock Protocols

Preliminary Preparation

A. Open Autodock Tools.
B. Go to File----Preferences----Set. Set the Startup Directory to the working directory. Click SET and MAKE DEFAULT.

Preparation of Macromolecule

1. Go to File---Read Molecule and select the macromolecule of interest.
2. Go to Edit---Delete Water.
3. Go to Edit---Hydrogens—Add.
4. Go to Edit---Hydrogens---Merge non-polar.
5. Go to Edit—Charges---Add Kollman Charges.
6. Go to Edit---Atoms---Assign AD4 type.
7. Go to Grid---Macromolecule---Choose and select the macromolecule.
8. Save the molecule in PDBQT format if asked.
9. Now the macromolecule is ready. The next step is to set up the ligand.

Preparation of Ligand:

1. Go to Ligand---Input---Open. The ligand should be selected from the working directory.
2. Select the ligand from the Dashboard and repeat step 4,5 and 6.
3. Go to Edit---Charges---Compute Gasteiger.
4. Go to Edit---Atoms---Assign AD4 type.
5. Go to Ligand---Torsion Tree---Detect Root.
6. Go to Ligand---Output----Save as PDBQT and save the ligand in PDBQT format.
7. Now the ligand is ready for docking.

Docking and Autogrid process:

1. Now go to Grid---Set Map Types---Choose Ligand and select the ligand from the list.
2. Now go to Grid---Grid Box and Set the grid box appropriately. After setting the grid box, go to File---Close Saving Current in the same dialog box.
3. Go to Grid---Output---Save GPF and save as name.gpf

4. Now the molecules are ready for Autogrid.
5. Go to Run---Autogrid and in the Program Pathname- set the Autogrid path from browse. Do the same for Parameter Filename to name.gpf. Log Filename should be automatically set if everything is fine. Click Launch. After the Autogrid gets completed, the terminal in the background will say if any errors are there.
6. Now go to Docking---Macromolecule---Set Rigid Filename and set the macromolecule.pdbqt
7. Go to Docking---Ligand---Choose and select the ligand from the dialog box and click ok again if you require random initial parameters.
8. Now select Docking---Search Parameters---Genetic Algorithm and set the required parameters and click Accept.
9. Lastly, select Docking---Output----Lamarckian GA (4.2) and save as dock.dpf.
10. Now the molecules are ready for docking.
11. Go to Run---Autodock and in the Program Pathname- set the Autodock path from browse. Do the same for Parameter Filename to dock.dpf. Log Filename should be automatically set if everything is fine. Click Launch. After the Autodock gets completed, the terminal in the background will say if any errors are there.
12. Now the docking is completed. To analyze the results, go to Analyze---Docking---Open and select the dock.dlg.
13. Select the macromolecule from Analyze---Macromolecule---Choose.
14. Now go to Analyze---Conformations---Play ranked by energy and analyze the confirmations as required.