Methodology for Autodock 4 (Using Defaults)

When Functional Site of Receptor in Known

1. Start →All Programs→MGL Tools→Autodock1.5→Enter
   (It opens ADT window)
2. PMV Molecules→Right Click
   It opens Open Widget for Macromolecule
3. Select Macromolecule→Open

Preparing Macromolecule First

1. Edit→Hydrogen's→Add→Select radio button of All Hydrogen's→OK
2. File→Save→Write PDB→Select macromolecule→OK→Overwrite→Yes

Preparing Ligand Molecule Second

1. Ligand→ Input→Open→(Open Ligand Widget opens) →Change to All Files from PDBQT→ Select Ligand File to open→ Open →OK
2. Ligand→ Torsion Tree→Detect Root
3. Ligand→Torsion Tree→ Choose Torsion→Done
4. Ligand→ Torsion Tree →Set No of Torsions→set value→ Dismiss
5. Ligand→ Output → Save As PDBQT→ Provide file name with (dot)PDBQT extension
6. Ligand → Torsion Tree→ Show/Hide Root Markers

Preparing Flexible Residue File Third

1. Flexible Residues →Input → Choose Macromolecule → Select Macromolecule → OK
2. Select → Select From String → Selection Menu Opens → Clear Form → Type Residue Name in Residue Name Field; that has to be consider as flexible residue during docking calculation → Add → Dismiss
3. Flexible Residues → Choose Torsions in Currently Selected Residue/s → Close
4. Flexible Residues → Output → Save Flexible PDBQT → add (_flex.pdbqt) with saving file name → Save
5. Flexible Residues → Output → Save Rigid PDBQT → add (_rigid.pdbqt) with saving file name → Save
6. Edit →Delete → Delete Macromolecule → Select Macromolecule → Delete Molecule → Dismiss

Preparing Grid Maps Fourth

1. Grid → Macromolecule → Open → select macromolecule_rigid.pdbqt → Open → if warn click on Yes → OK
2. Grid → Set Map Types → Choose Ligand →select ligand molecule → Accept → OK
3. Grid → Grid Box → set grid center point → Close Saving Current
4. Grid → Output → Save GPF → save file with (dot)gpf → Save

Execution of Gridding for Grid Log Generation Fifth

1. (For Windows Operation)Start → All Programs → Cygwin → Cygwin Bash Shell →Cygwin Bash Shell Command Line Opens
2. Change to your current home directory on command line → (**ls**) check for the files you have prepared by using MGL Tools → Make sure you have PDBQT file of ligand, Rigid residue file and Flexible residue file of Macromolecule and Ligand(dot)gpf
3. Now execute the Grid by typing the following command in command line
   Autogrid4(space)-p(space)Ligand(dot)gpf(space)-l(space)Ligand(dot)glg

4. Now wait and Do Not Close the command line window untill the execution display the message of Successful Completion
5. Time taken for execution will depends on systems configuration and Macromolecule-Ligand complex complexity.
6. After completion Check for (dot)glg file in your current Home directory
7. (For Linux Operation) Use Linux Command Line Window instead Cygwin Bash Shell and the rest will remain same.

Preparing Docking Parameter File Sixth

1. Docking → Macromolecule → Set Rigid ResidueFile Name → select macromolecule_rigid.pdbqt → Open
2. Docking →Ligand →Choose → select ligand file→ Select Ligand→ Accept
3. Docking → Macromolecule → Set Flexible Residue File Name→ select macromolecule_flex.pdbqt → Open
4. Docking → Search Parameters → Genetic Algorithm → Accept
5. Docking → Docking Parameters → Accept
6. Docking → Output → Lamarckian GALS → save file with (dot)dpf → Save

Execution of Docking for Docking Log Generation Seventh

1. (For Windows Operation)Start → All Programs → Cygwin → Cygwin Bash Shell →Cygwin Bash Shell Command Line Opens
2. Change to your current home directory on command line → (ls) check for the files you have prepared by using MGL Tools → Make sure you have Ligand(dot)dpf
3. Now execute the Dock by typing the following command in command line
   Autodock4(space)-p(space)Ligand(dot)dpf(space)-l(space)Ligand(dot)dlg

4. Now wait and Do Not Close the command line window untill the execution display the message of Successful Completion
5. Time taken for execution will depends on systems configuration and Macromolecule-Ligand complex complexity.
6. After completion Check for (dot)dlg file in your current Home directory
7. (For Linux Operation) Use Linux Command Line Window instead Cygwin Bash Shell and the rest will remain same.