AUTODOCK PROTOCOL

. **INPUT FILES:**

MACROMOLECULE : hsg1.pdb (Protein)
SMALL MOLECULE : ind.pdb (Ligand)

BEFORE STARTING : SET STARTUP DIRECTORY

- File → Preferences → Set (Working Directory) → Set → Dismiss

V) PROTEIN PREPARATION:

- File → Read Molecule → Open (**hsg1.pdb**).
- Edit → Delete Water.
- Edit → Hydrogens→ Add → Default.
- Edit → Charges → (Click- Gasteiger charges.)

V) LIGAND PREPARATION:

- Ligand → Input → Open → (File Name: **ind.pdb**, File Type: pdb).
- Ligand → Torsion Tree → Detect Root
- Ligand → Torsion Tree → Choose Torsions
- Ligand → Torsion Tree → Set Number Of Torsions → Dismiss
- Ligand → Output → Save As **ind**.**pdbqt**

V) a) PREPARING THE AUTOGRID PARAMETER FILE (GPF):

- Grid → Macromolecule → Choose→ **hsg1**→Select Molecule Save (**hsg1.pdbqt**).
- Grid →Set Map Types →Choose Ligand→ **ind** →Select Ligand
- Grid → Grid Box → Center On Ligand
- File → Output Grid Dimensions File.
- File → Save As **grid.txt**.
- File → Close Saving Current.
- Grid → Output → Save GPF (Grid Parameter File) File Name: **hsg1.gpf**:
- File Type: GPF File→ Click Save.
- Grid → Edit GPF→ Read→ Ok.

b) LAUNCH AUTOGRID 4 (GLG)

- Run → Run autogrid4.
  - Program path name: **autogrid4.exe**
  - Parameter file name: **hsg1.gpf**
  - Log filename: **hsg1.glg**

- Launch (Autodock process manager will be opens till the job completes and the generated files can be verified from the start up directory)

· **IV) a) PREPARING THE AUTODOCK PARAMETER FILE (DPF):**

- Docking → Macromolecule → Set Rigid File Name… (**hsg1.pdbqt**) →click.
- Docking → Ligand→ Choose→ Select Ligand→ Accept
- Docking → Search Parameters→ Genetic Algorithm→ Accept
- Docking → Docking Parameter→ Accept.
- Docking → Output → Lamarckian GA→ **ind.dpf**→ Save
- Docking → Edit DPF→ Read → Ok.

b) LAUNCH AUTODOCK4 (DLG)

- Run → Run Autodock.
  - Program pathname : **autodock4.exe**
  - Parameter file name: **ind.dpf**
  - Log filename: **ind.dlg**
- Launch→ Click (we can get the result for conformations).

V) ANALYZING AND VISUALIZING AUTODOCK4 RESULTS:

- Analyze → Dockings → Open (**ind.dlg**).
- Analyze → Macromolecule → Choose (**hsg1**).
- Analyze → Clusterings → show → conformation graph opens.
- Click the histogram → play via conformation player window.
- Click Ampersand symbol [set play options] for docking information.

RESULTS FILES:

Ligand
ind.pdbqt
Macromolecule
hsg1.pdbqt
Autogrid
hsg1.gpf
hsg1.glg
hsg1.*.map
hsg1.maps.fld,
hsg1.maps.xyz
AutoDock
hsg1.dpf
ind.dlg