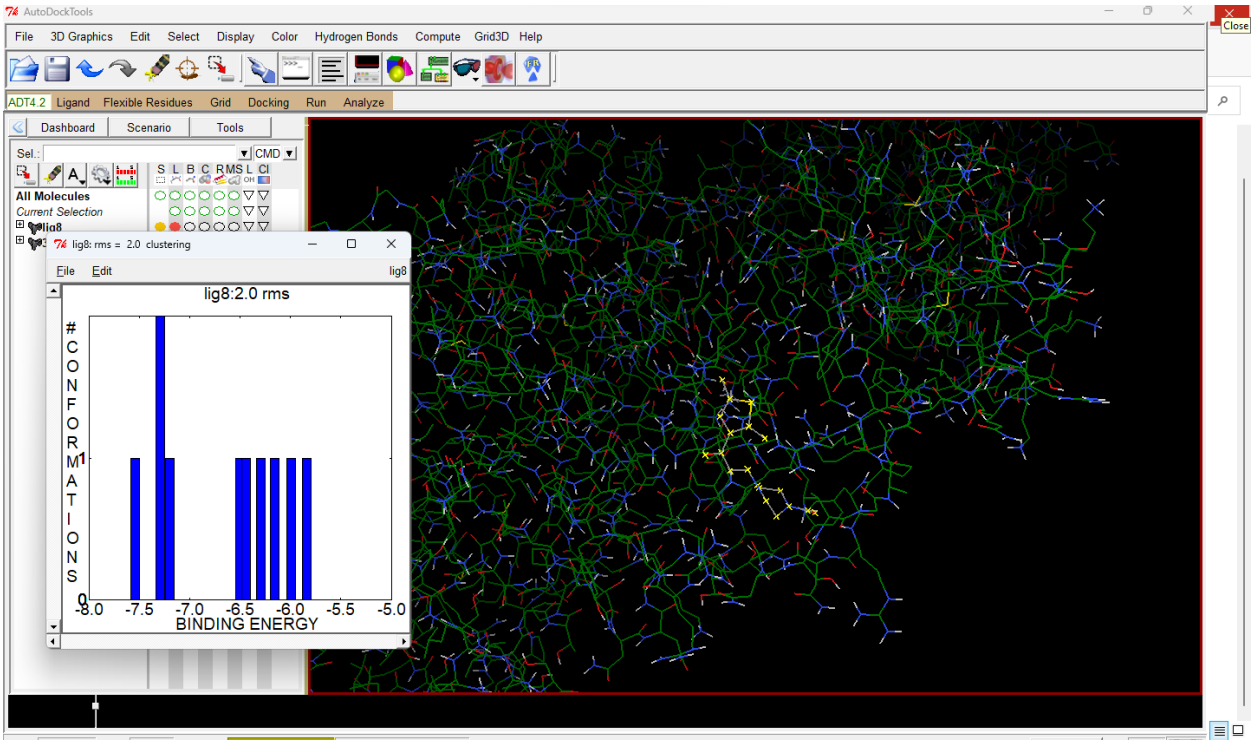
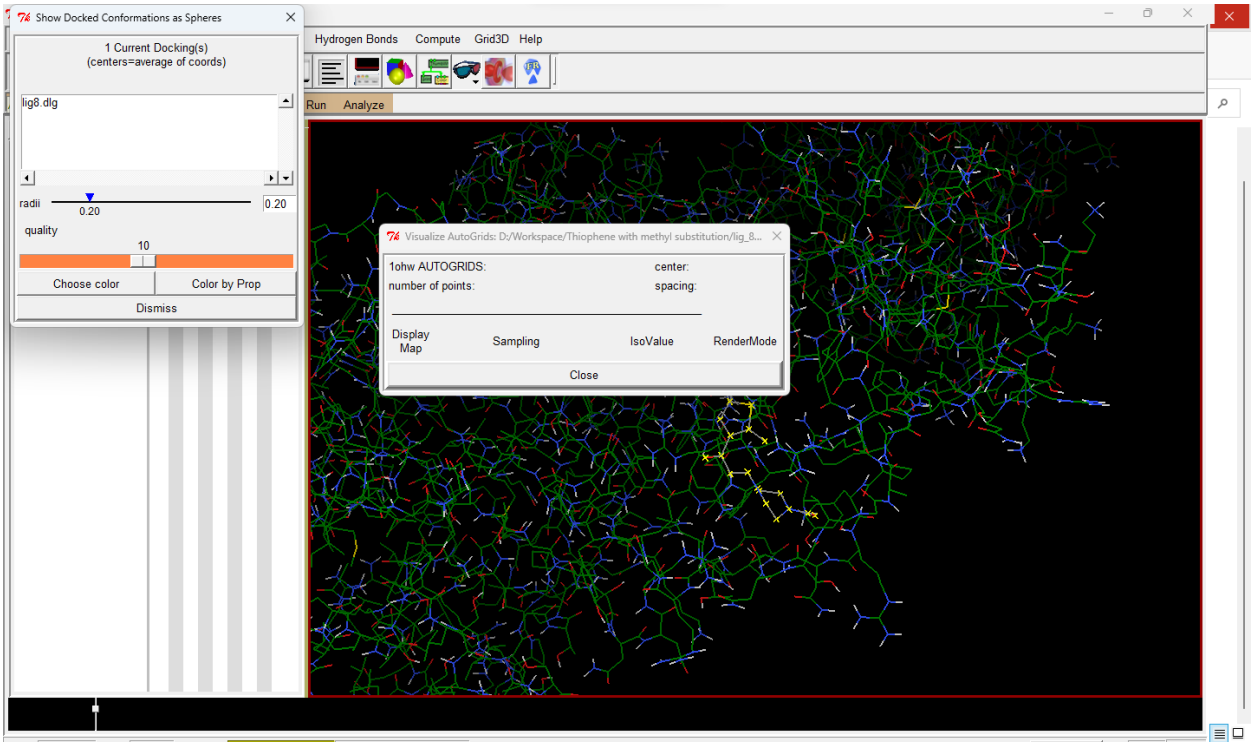
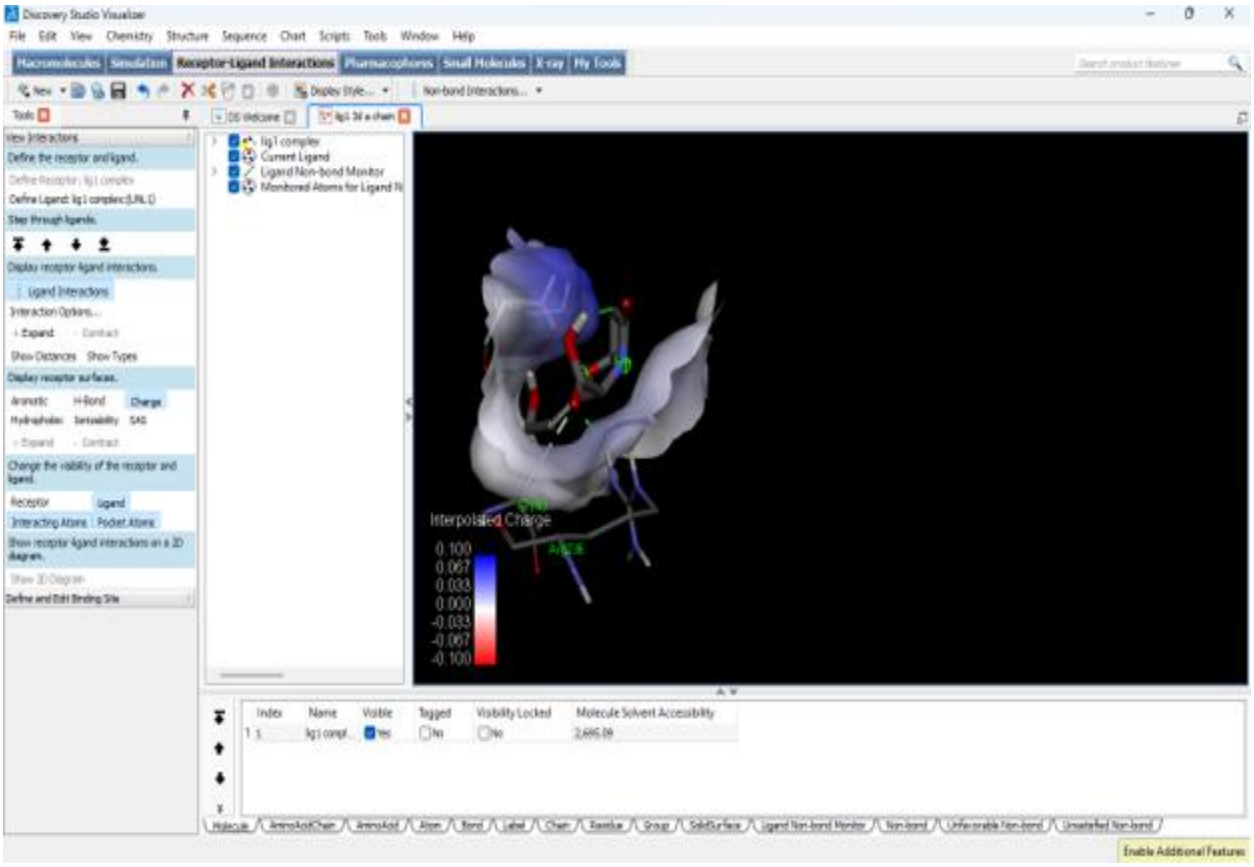
AD4


AutoDockTools
File 3D Graphics Edit Select Display Color Hydrogen Bonds Compute Grid3D Help
ADT4.2 Ligand Flexible Residues Grid Docking Run Analyze
Dashboard Scenario Tools
All Molecules
Current Selection
lig8: rms = 2.0 clustering
File Edit lig8
lig8:2.0 rms
CONFORMATIONS
BINDING ENERGY
-8.0 -7.5 -7.0 -6.5 -6.0 -5.5 -5.0


Show Docked Conformations as Spheres
1 Current Docking(s)
(centers=average of coords)
lig8.dlg
radii
0.20
quality
10
Choose color
Color by Prop
Dismiss
Hydrogen Bonds Compute Grid3D Help
Run Analyze
Visualize AutoGrids: D:/Workspace/Thiophene with methyl substitution/lig_8...
1ohw AUTOGRIDS:
number of points:
center:
spacing:
Display Map
Sampling
IsoValue
RenderMode
Close


Discovery Studio Visualizer
File Edit View Chemistry Structure Sequence Chart Scripts Tools Window Help
Macromolecules Simulation Receptor-Ligand Interactions Pharmacophores Small Molecules X-ray My Tools
lig1 complex
Current Ligand
Ligand Non-bond Monitor
Monitored Atoms for Ligand N
Interpolated Charge
0.100
0.067
0.033
0.000
-0.033
-0.067
-0.100
Index Name Visible Tagged Visibility Locked Molecule Solvent Accessibility
Enable Additional Features