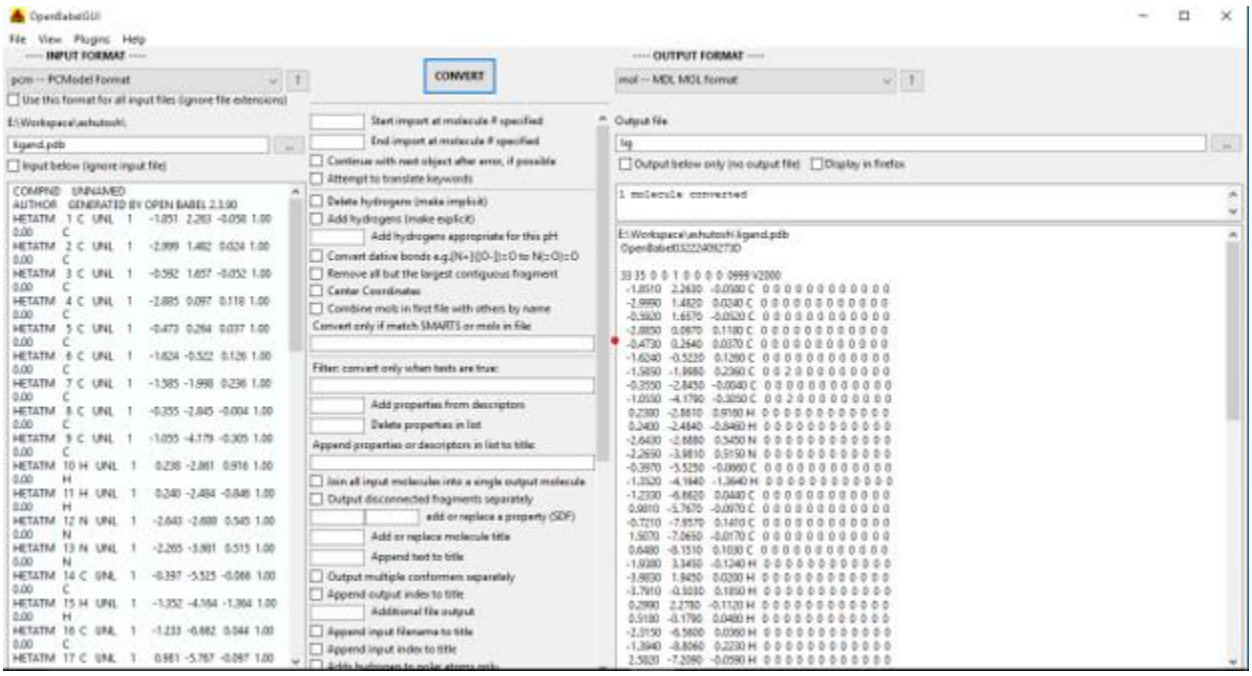
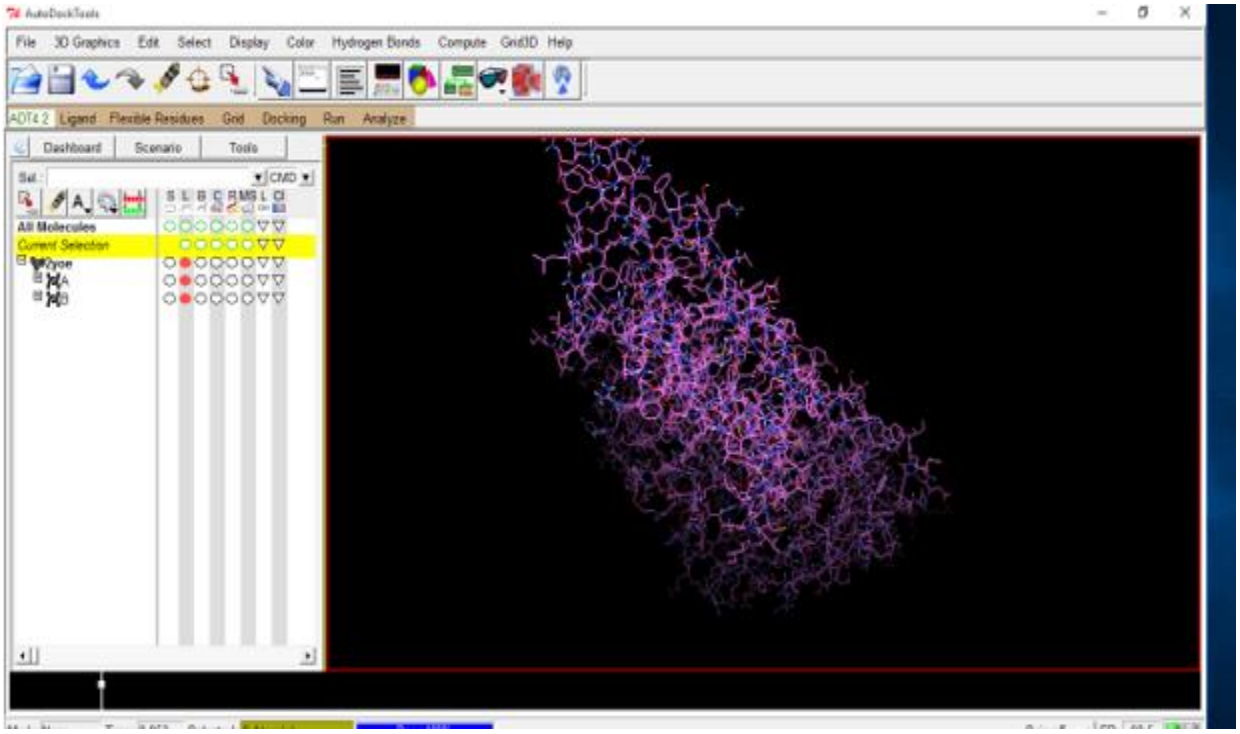
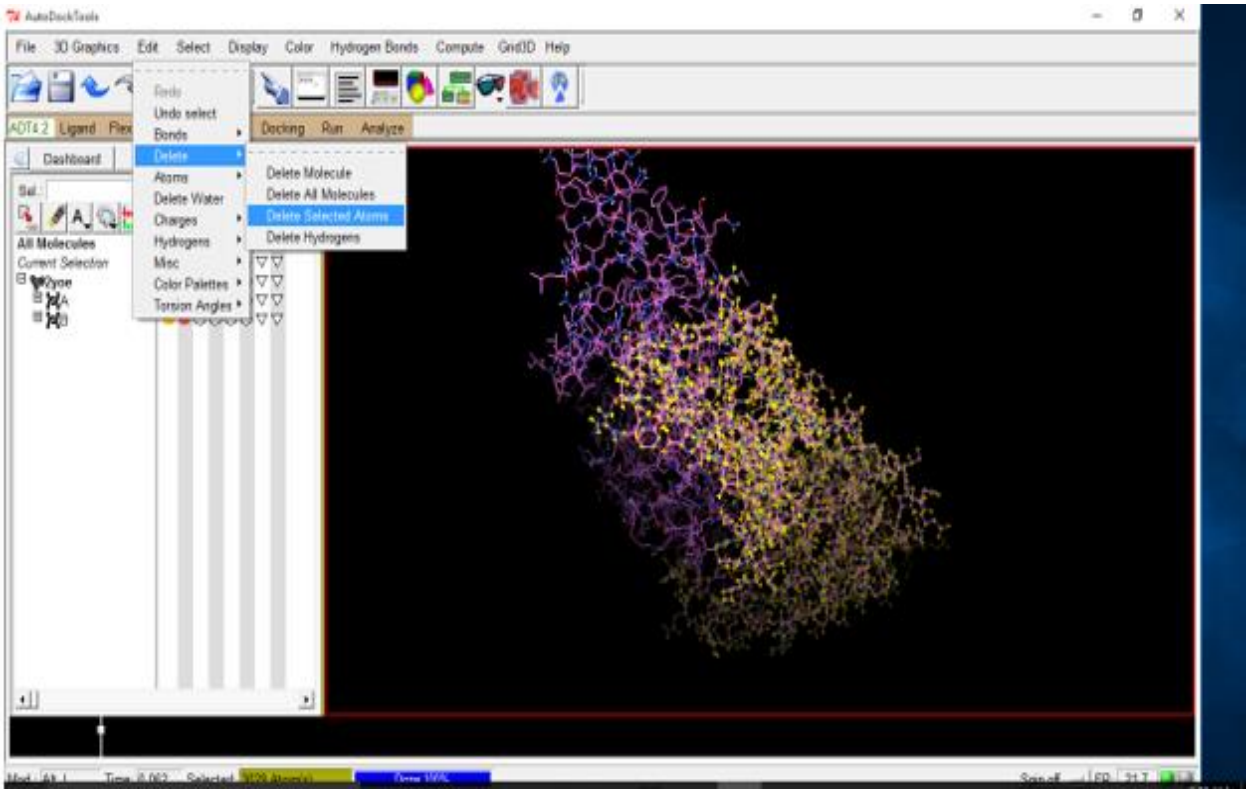
AD2


Please Keep Silence
Shot on OnePlus
By Dee


OpenBabelGUI
File View Plugins Help
INPUT FORMAT
OUTPUT FORMAT
CONVERT
pcm -- PCModel Format
mol -- MDL MOL format
Use this format for all input files (ignore file extensions)
E:\Workspace\ashutosh\
ligand.pdb
Input below (ignore input file)
Output file
lig
Output below only (no output file)
Display in firefox
1 molecule converted
Start import at molecule # specified
End import at molecule # specified
Continue with next object after error, if possible
Attempt to translate keywords
Delete hydrogens (make implicit)
Add hydrogens (make explicit)
Add hydrogens appropriate for this pH
Convert dative bonds e.g.[N+][O-]]=O to N(=O)=O
Remove all but the largest contiguous fragment
Center Coordinates
Combine mols in first file with others by name
Convert only if match SMARTS or mols in file
Filter: convert only when tests are true:
Add properties from descriptors
Delete properties in list
Append properties or descriptors in list to title:
Join all input molecules into a single output molecule
Output disconnected fragments separately
add or replace a property (SDF)
Add or replace molecule title
Append text to title
Output multiple conformers separately
Append output index to title
Additional file output
Append input filename to title
Append input index to title
E:\Workspace\ashutosh\ligand.pdb
OpenBabel03222409273D


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
2yce
A
B


AutoDockTools
File 3D Graphics Edit Select Display Color Hydrogen Bonds Compute Grid3D Help
Undo select
Bonds
Delete
Atoms
Delete Water
Charges
Hydrogens
Misc
Color Palettes
Torsion Angles
Delete Molecule
Delete All Molecules
Delete Selected Atoms
Delete Hydrogens
Docking Run Analyze
Dashboard
All Molecules
Current Selection
2yce
A
B