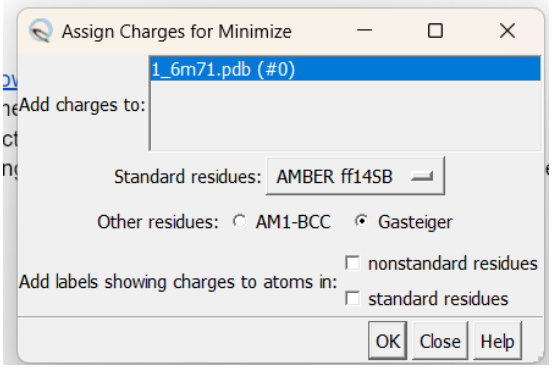
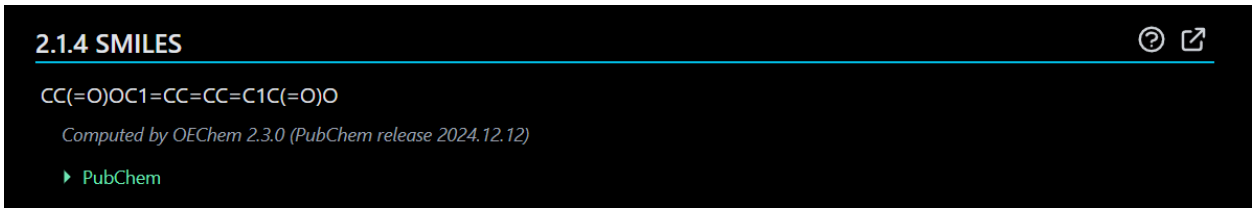
Steps:

1. PDB ID of rdrp receptor: 6M71: download in .pdb format
2. Open UCFS Chimera, open the 6M71 pdb file.
3. Go to tools > structure editing > minimize structure:
   Note: In proceeding (click ok), keep all settings by default aside from other residues: set it to “Gasteiger”.

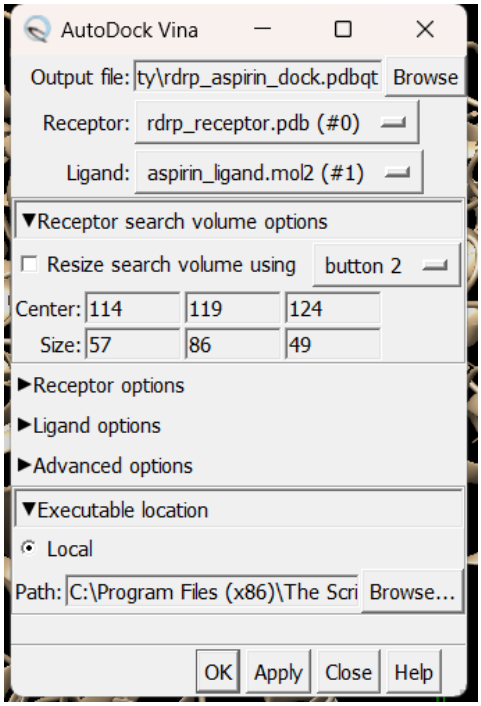


4. Go to files > save as pdb the minimized structure of the receptor.
5. Go to pubchem > search for aspirin (ligand) > go to “SMILES” > copy the structure

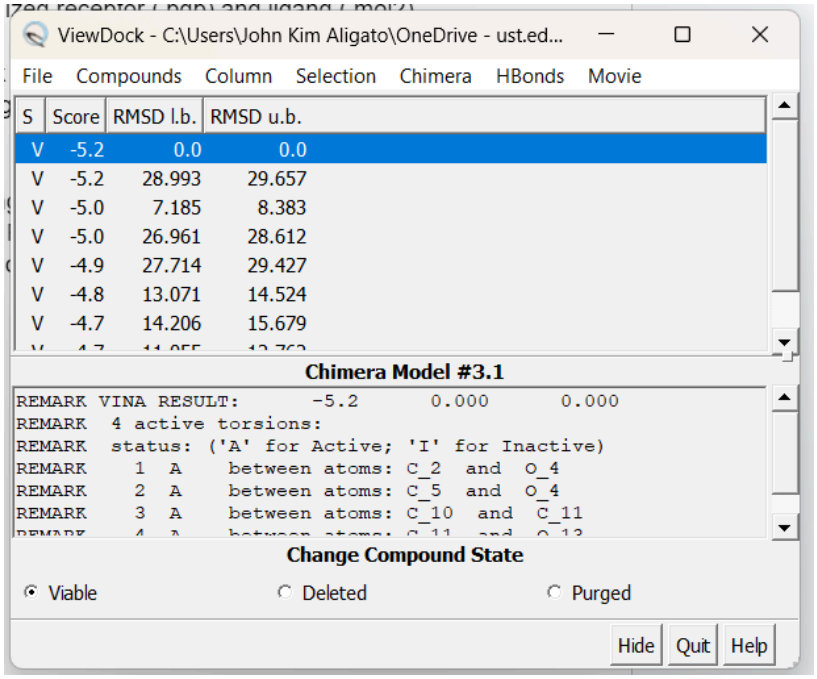


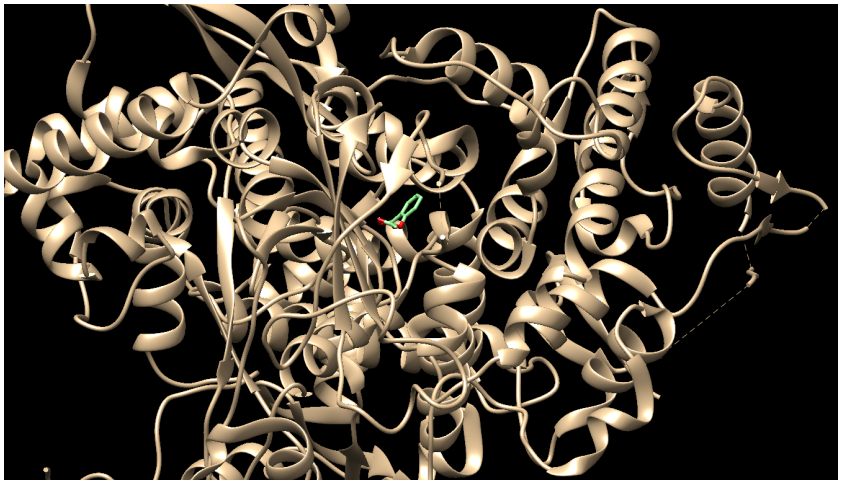
6. Open Avogadro > go to “Build” > insert > SMILES > Extension > Optimize geometry
7. Save the ligand file as sybyl mol2 (.mol2 format)
8. Go back to UCFS Chimera > open the minimized receptor (.pdb) and ligand (.mol2) simultaneously
9. Go to tools > surface binding/analysis > dock prep
   Note: In proceeding (click ok), keep all settings by default aside from other residues: set it to “Gasteiger”.
10. Save the file as .mol2 after dock prep
11. Go to tools > surface/binding analysis > autodock vina > set the following parameters **below** > executable location (set as local) > browse the path (C:\Program Files (x86)\The Scripps Research Institute\Vina\vina.exe > for the output file: click browse to set your location and save it as .pdbqt

Parameters:



12. View the results panel:





- The ligand has been bound to the receptor successfully -

13. Open BIOVIA > open the .pdbqt files
- Troubleshooting Phase (Version 2019 and version 2025 have different expected result) -