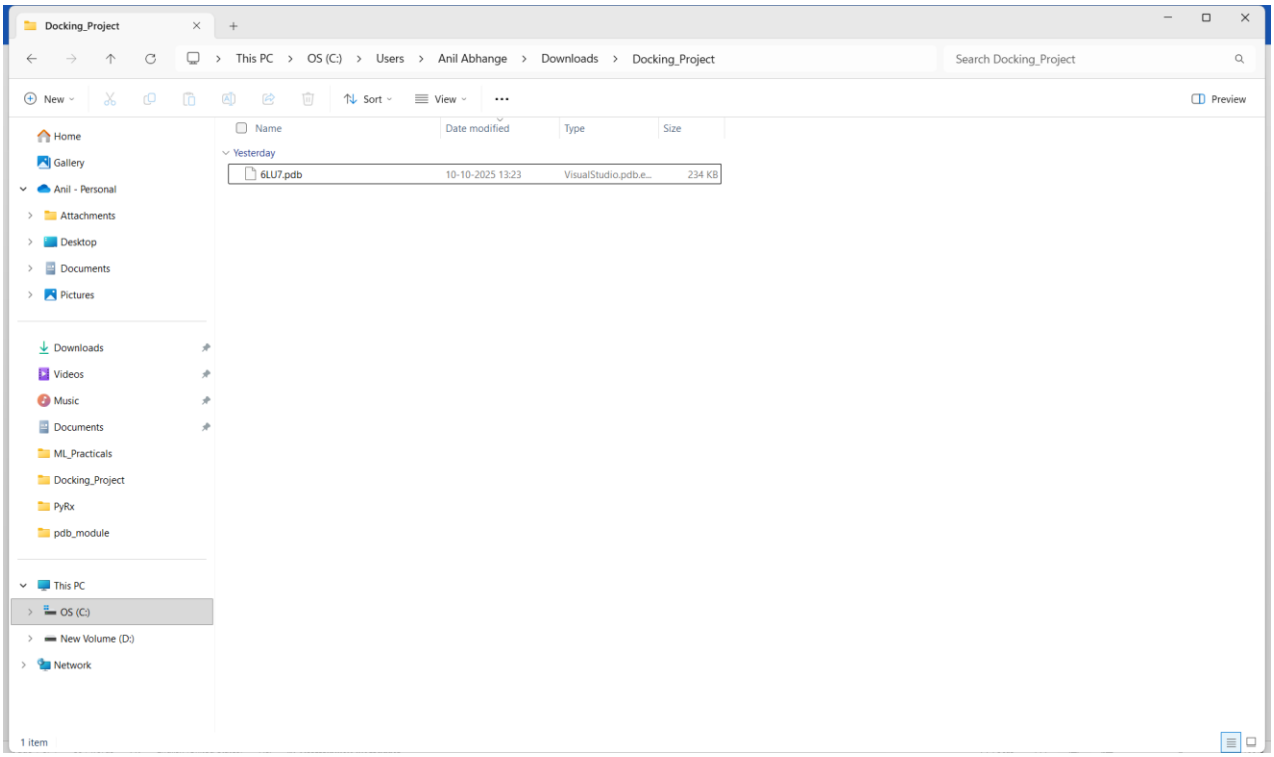
MOLECULAR DOCKING REPORT

Protein Target: 6LU7 (COVID-19 Main Protease)

Step 1: Protein Download

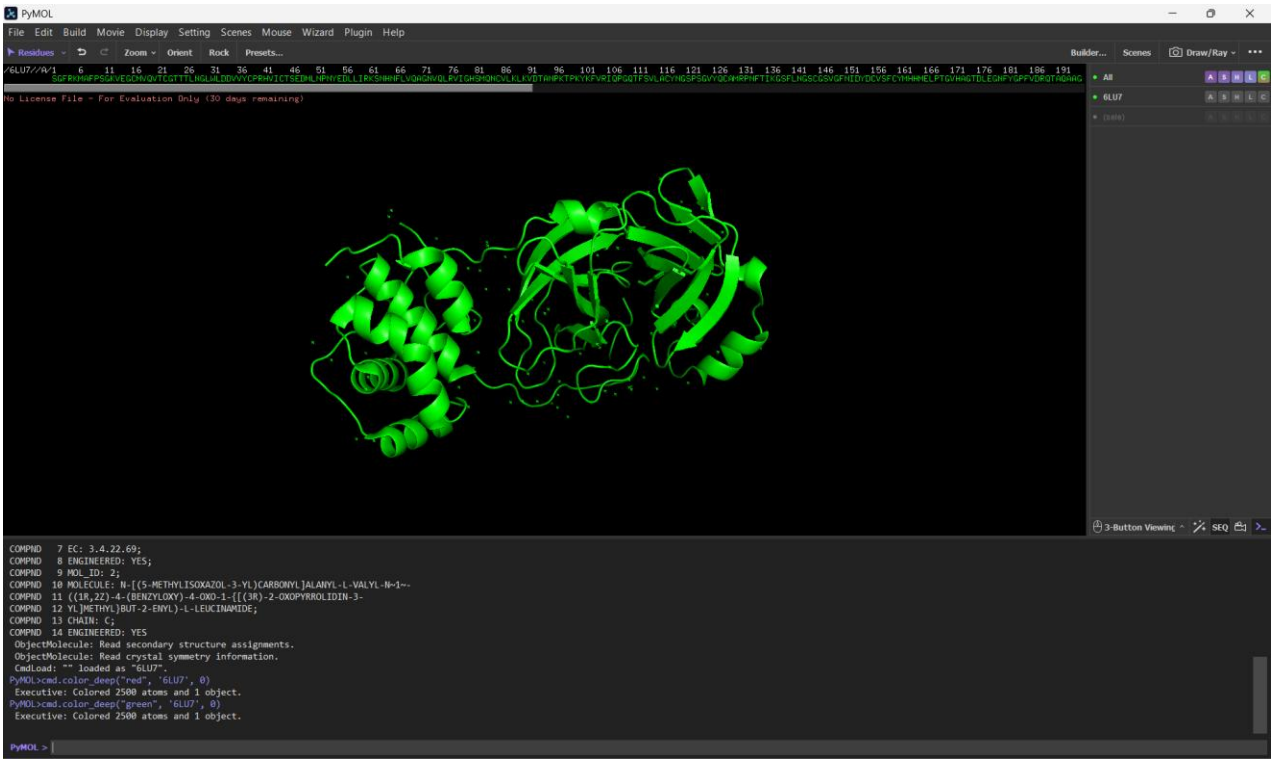
Downloaded 6LU7 from RCSB Protein Data Bank in PDB format.



Downloaded protein file in folder

Step 2: Protein Preparation

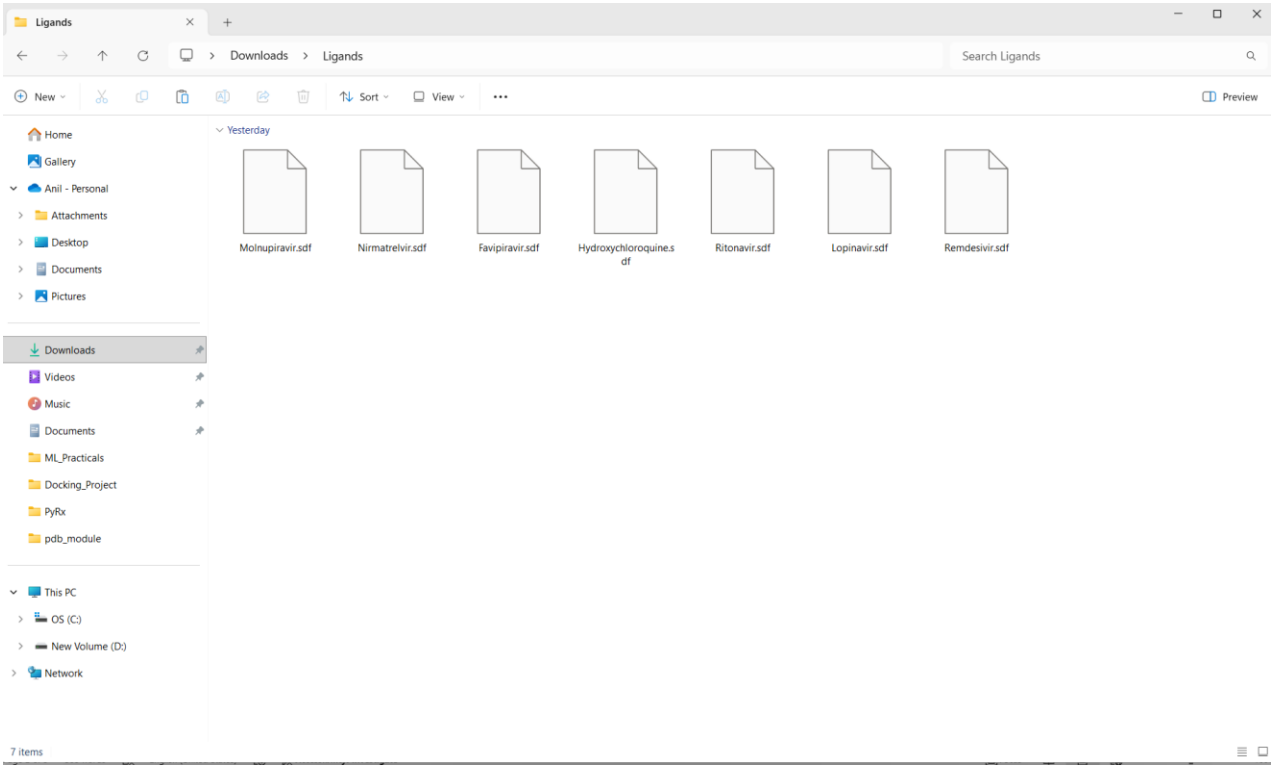
Cleaned protein using PyMOL - removed water, heteroatoms, extra chains.



PyMOL showing cleaned protein

Step 3: Ligand Download

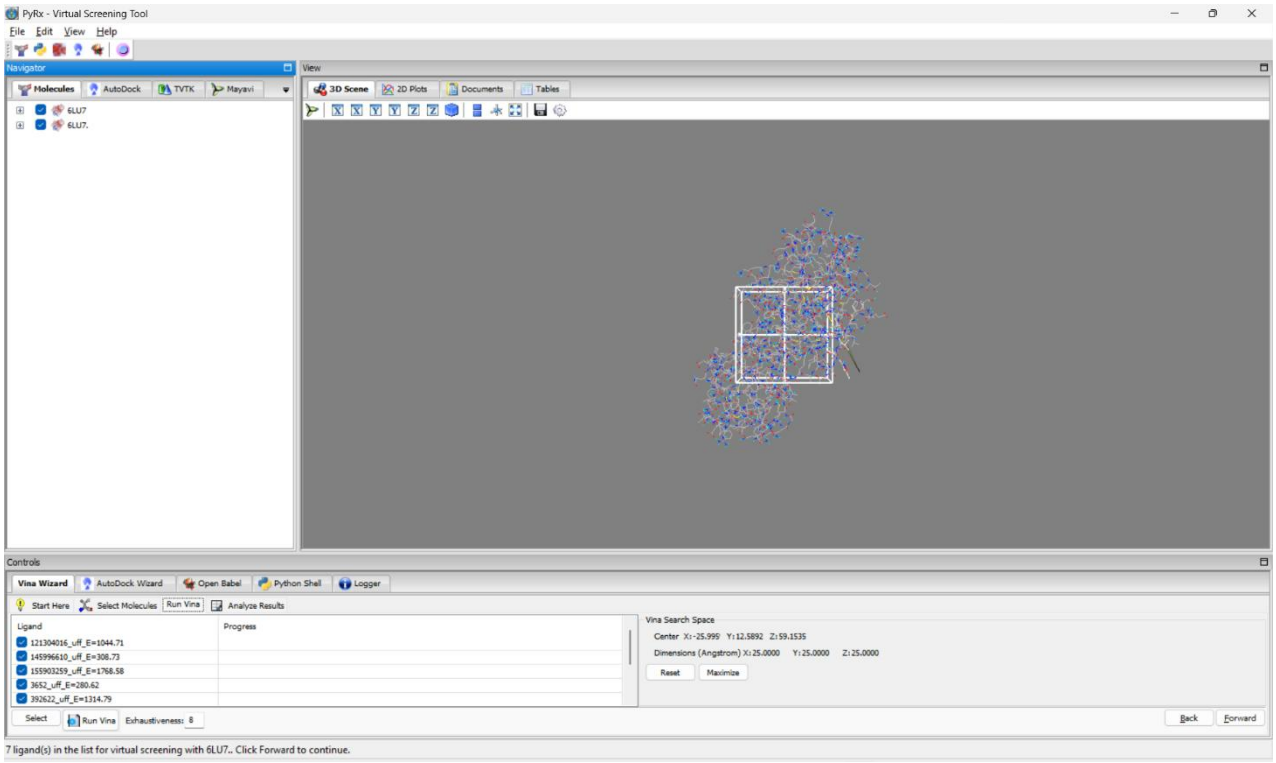
Downloaded 7 ligands from PubChem in SDF format.



All ligand files in folder

Step 4: Load Protein in PyRx

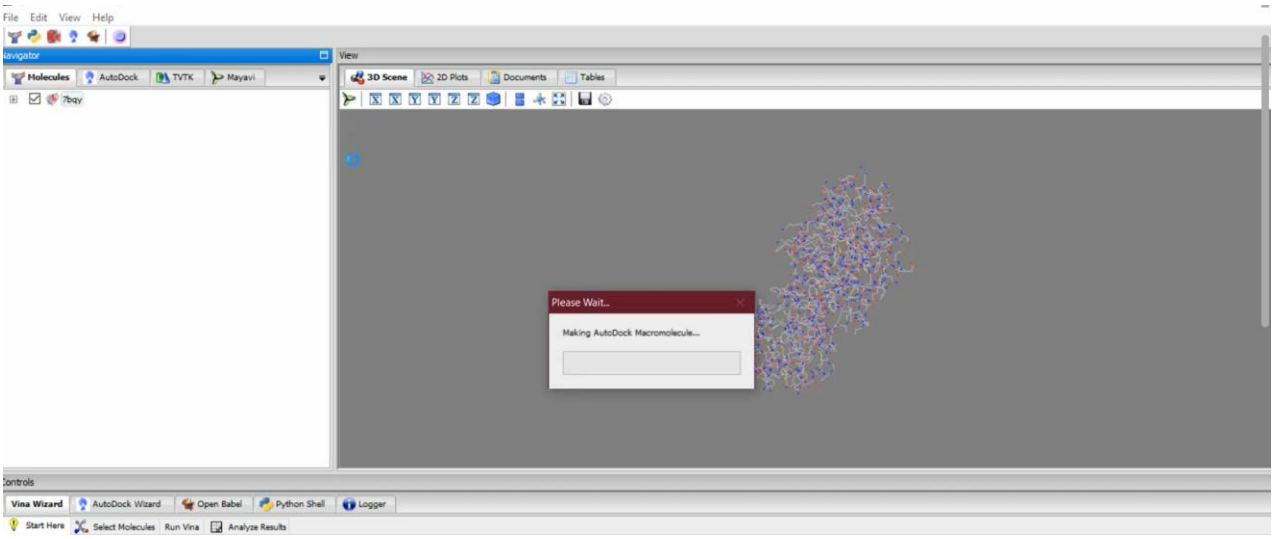
Opened PyRx and loaded cleaned protein file.



PyRx with protein loaded in Navigator panel

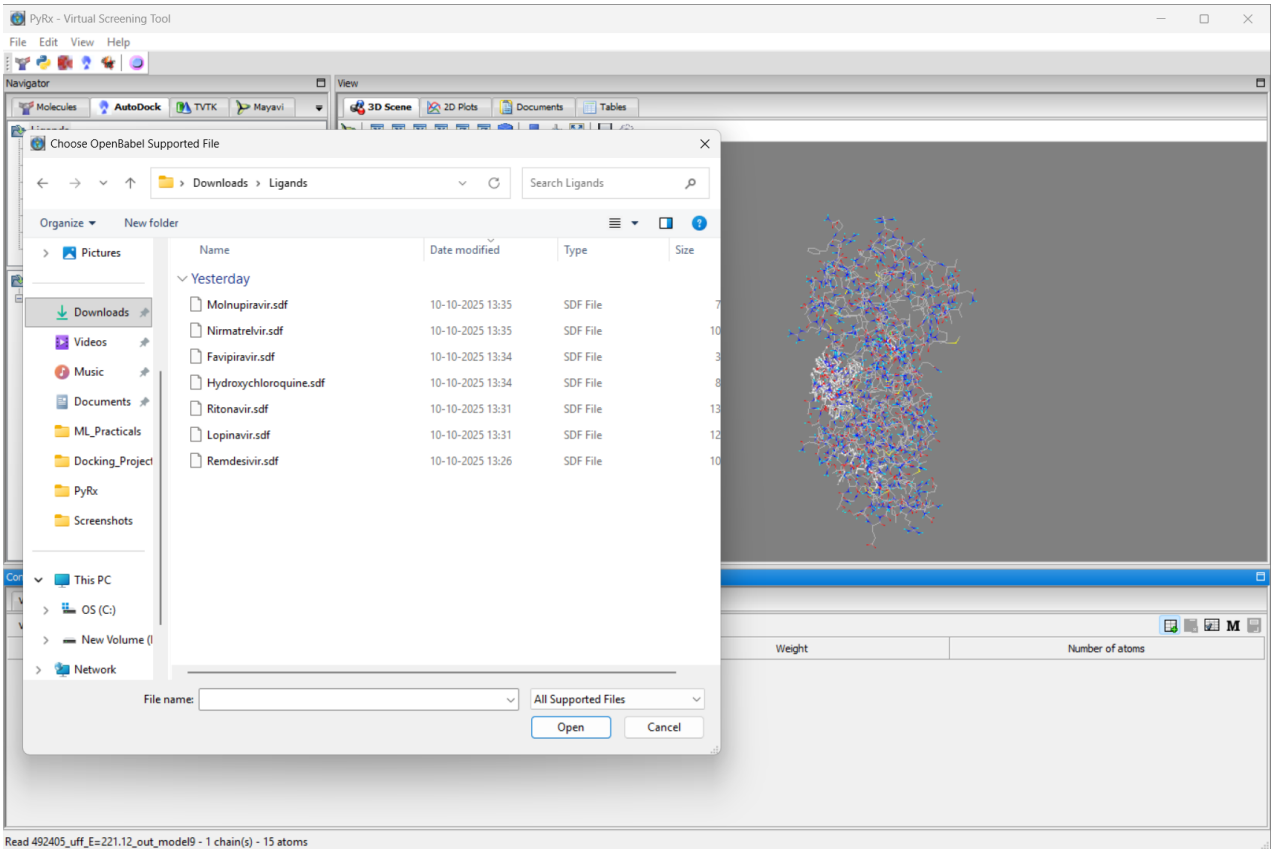
Step 5: Convert Protein to Macromolecule

Right-click protein → AutoDock → Make Macromolecule.



Step 6: Load Ligands in PyRx

Clicked Open Babel tab, added all ligand files.



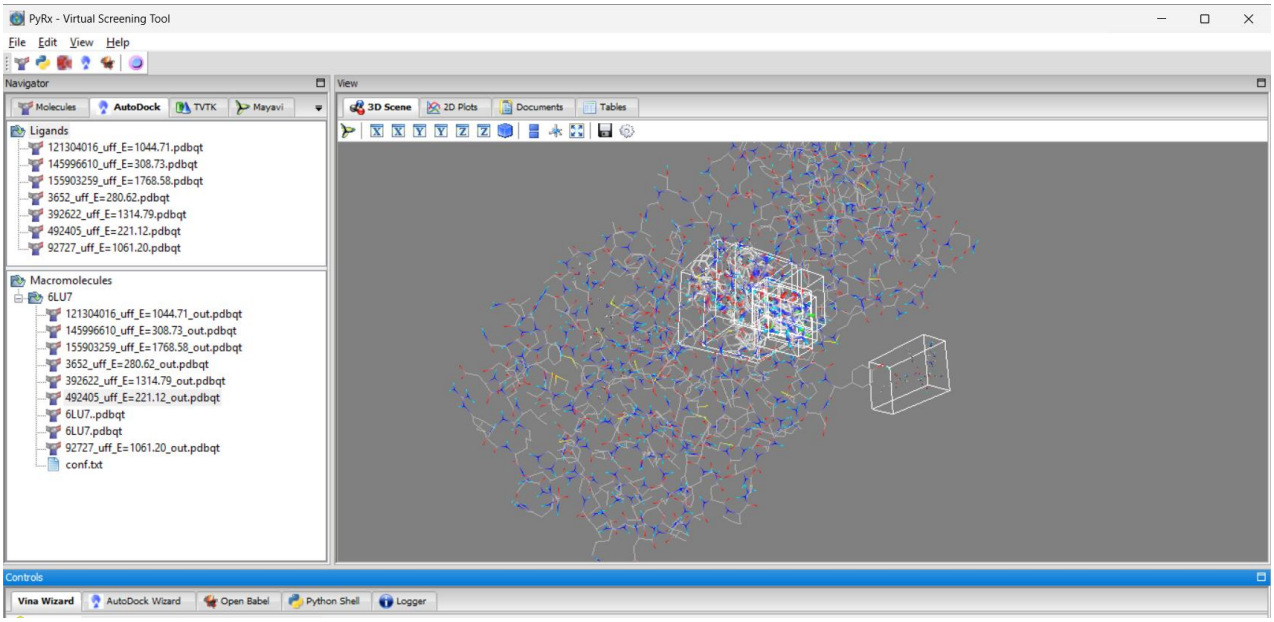
Ligands Uploading in Open Babel panel

Step 7: Energy Minimization

Selected all ligands → Right-click → Minimize All using UFF.

Step 8: Convert Ligands to PDBQT

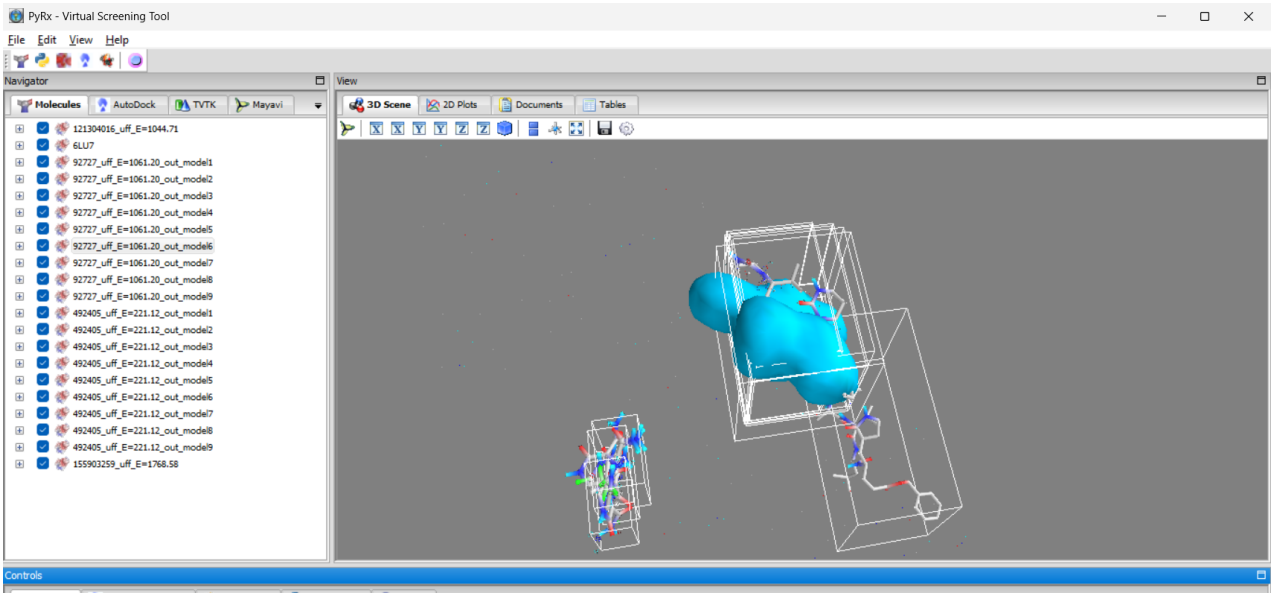
Right-click ligands → AutoDock → Make Ligand.



Ligands in AutoDock tab

Step 9: Grid Box Setup

Opened Vina Wizard, set grid box around protein.



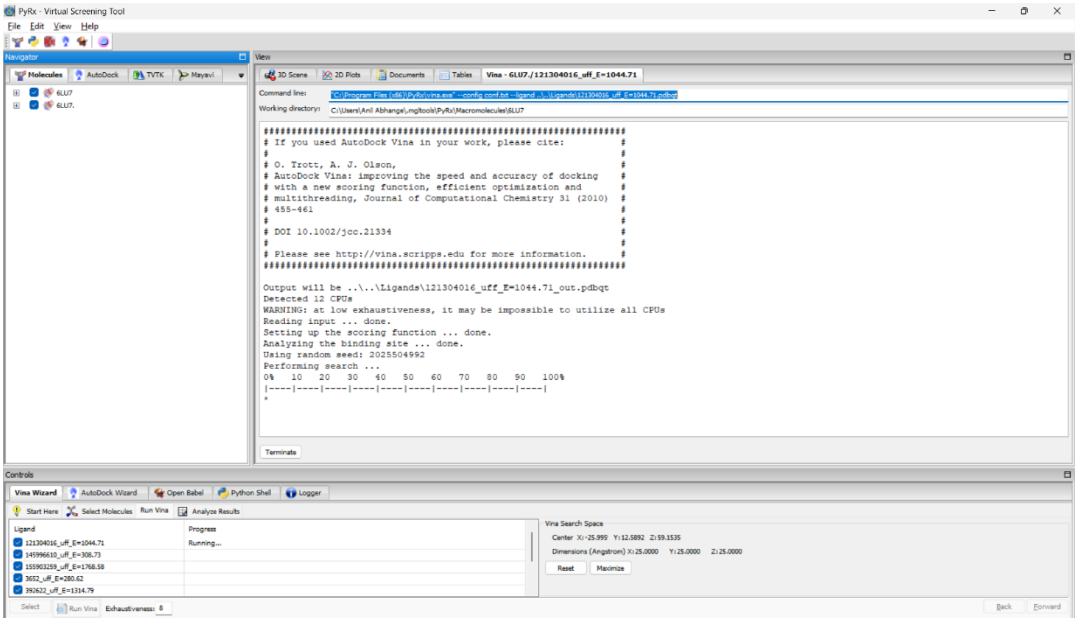
Grid box visualization in 3D viewer

Grid Parameters:

- Center: X = [value], Y = [value], Z = [value]
- Dimensions: 25 Å × 25 Å × 25 Å

Step 10: Run Docking

Selected macromolecule and all ligands, set exhaustiveness = 8, clicked Forward.



Step 11 : Interaction of ligand with Protein Molecule

RESULTS

Binding Affinity Table

Rank	Ligand ID (PubChem)	Binding Affinity (kcal/mol)
1	121304016	-1044.71
2	92727	-1061.20
3	155903259	-1768.58
4	392622	-1314.79
5	145996610	-308.73
6	3652	-280.62
7	492405	-221.12

PyRx results panel showing all binding scores

Top 3 Compounds

Compound 1: 121304016

Binding Affinity: -1044.71 kcal/mol

Compound 2: 92727

Binding Affinity: -1061.20 kcal/mol

Compound 3: 155903259

Binding Affinity: -1768.58 kcal/mol

These show promise as COVID-19 main protease inhibitors.