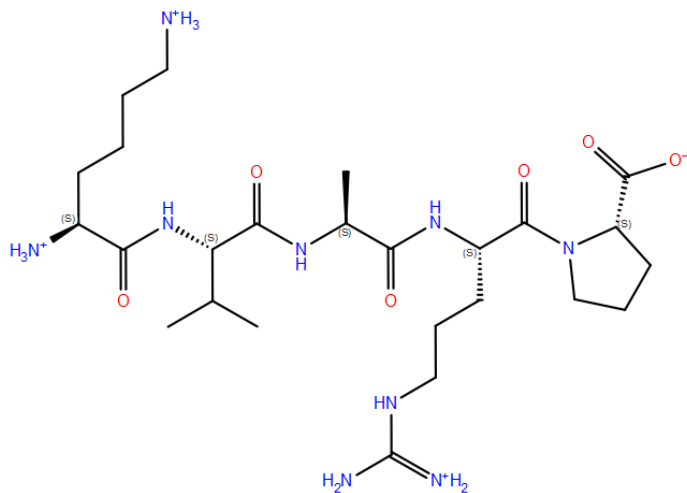


Supplement S1, binding energies

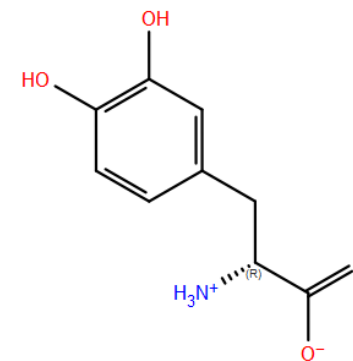
Binding score

| | | (kcal/mol) | |
|----------|------------|---------------|--------------|
| 2Y9X | | Docking score | MMGBSA score |
| Control | KVARP | -6.66 | -18.40 |
| Ligand01 | KGYSSYICDK | -8.64 | -19.35 |
| Ligand02 | L-TYROSINE | -9.01 | -14.60 |
| Ligand03 | L-DOPA | -8.39 | -15.08 |

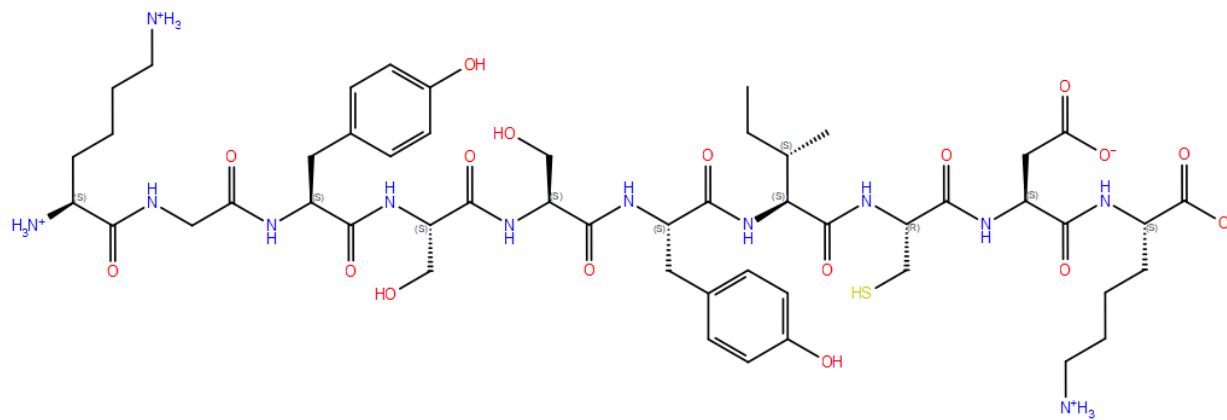
Ligand 2D



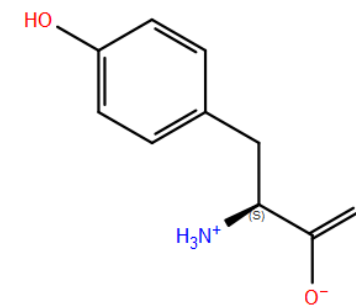
Control: KVARP



Ligand02: L-Tyrosine

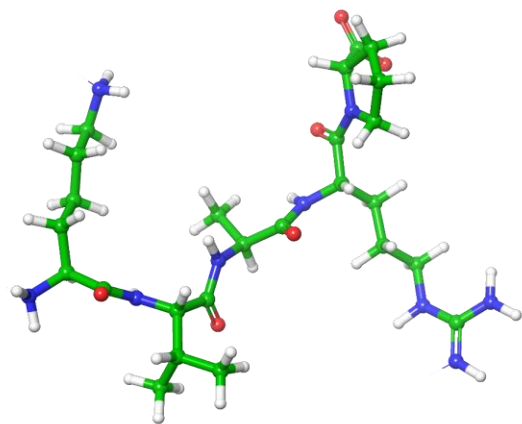


Ligand01: KGYSSYICDK

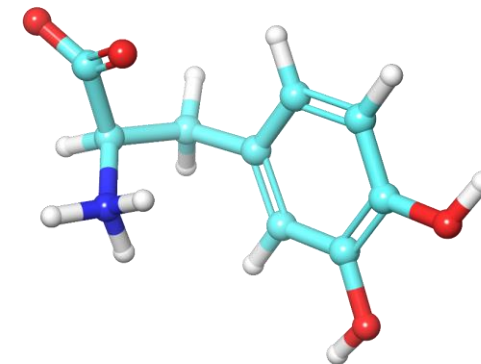


Ligand03: L-DOPA

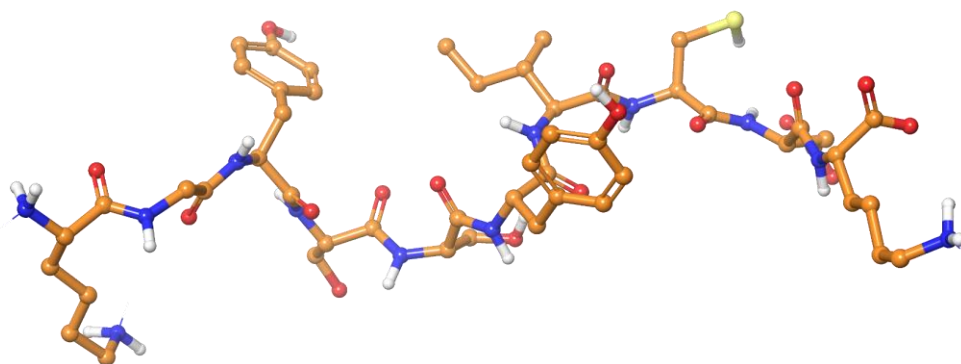
Ligand 3D



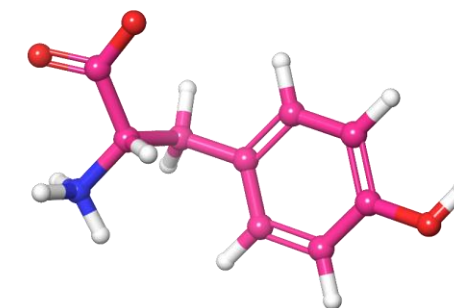
Control: KVARP



Ligand02: L-Tyrosine

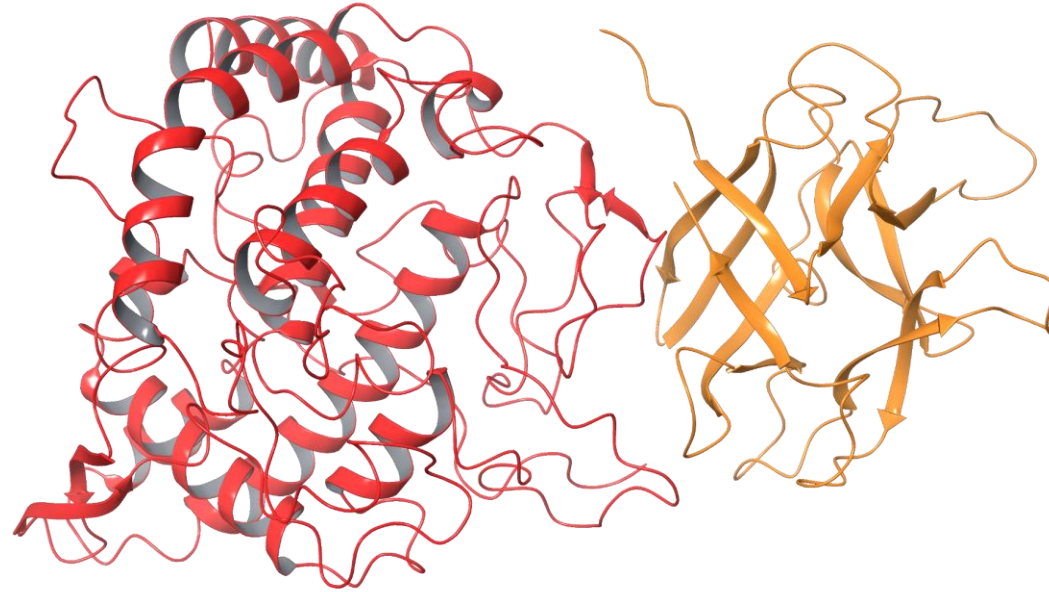


Ligand01: KGYSSYICDK



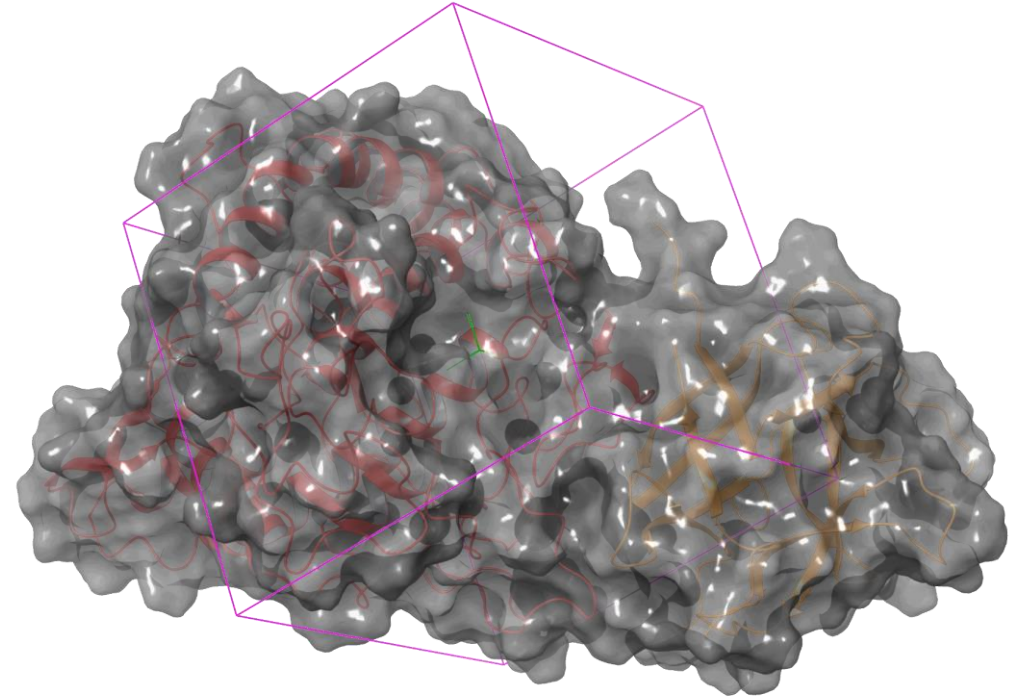
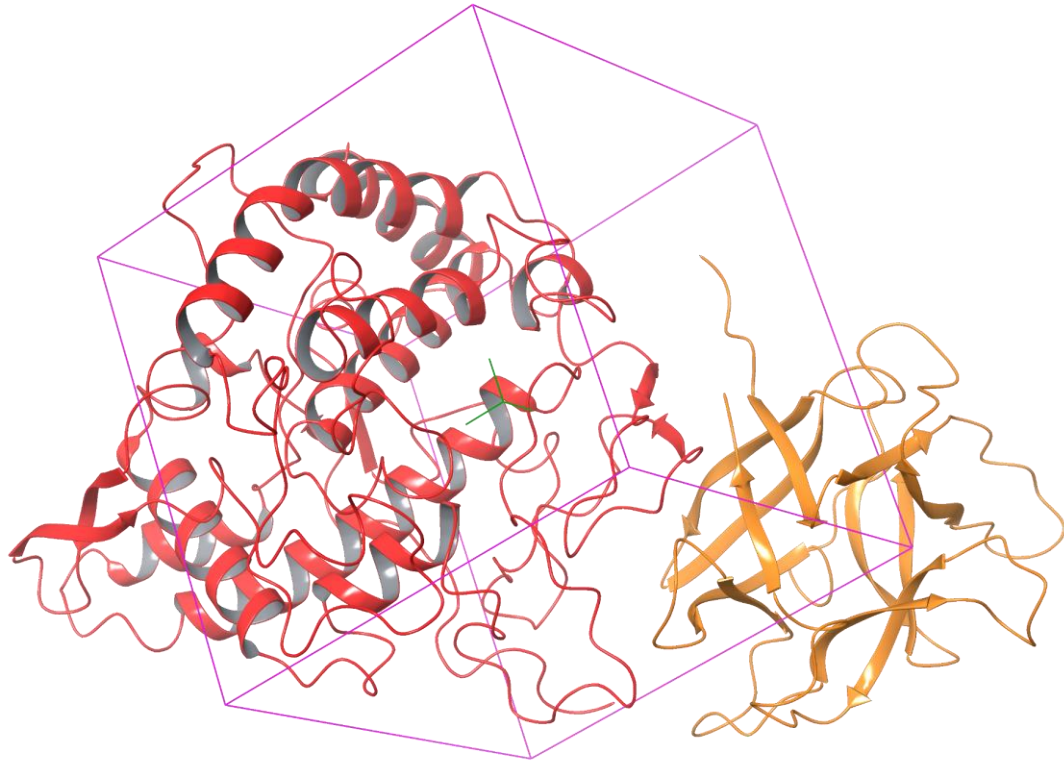
Ligand03: L-DOPA

Tyrosinase PDB

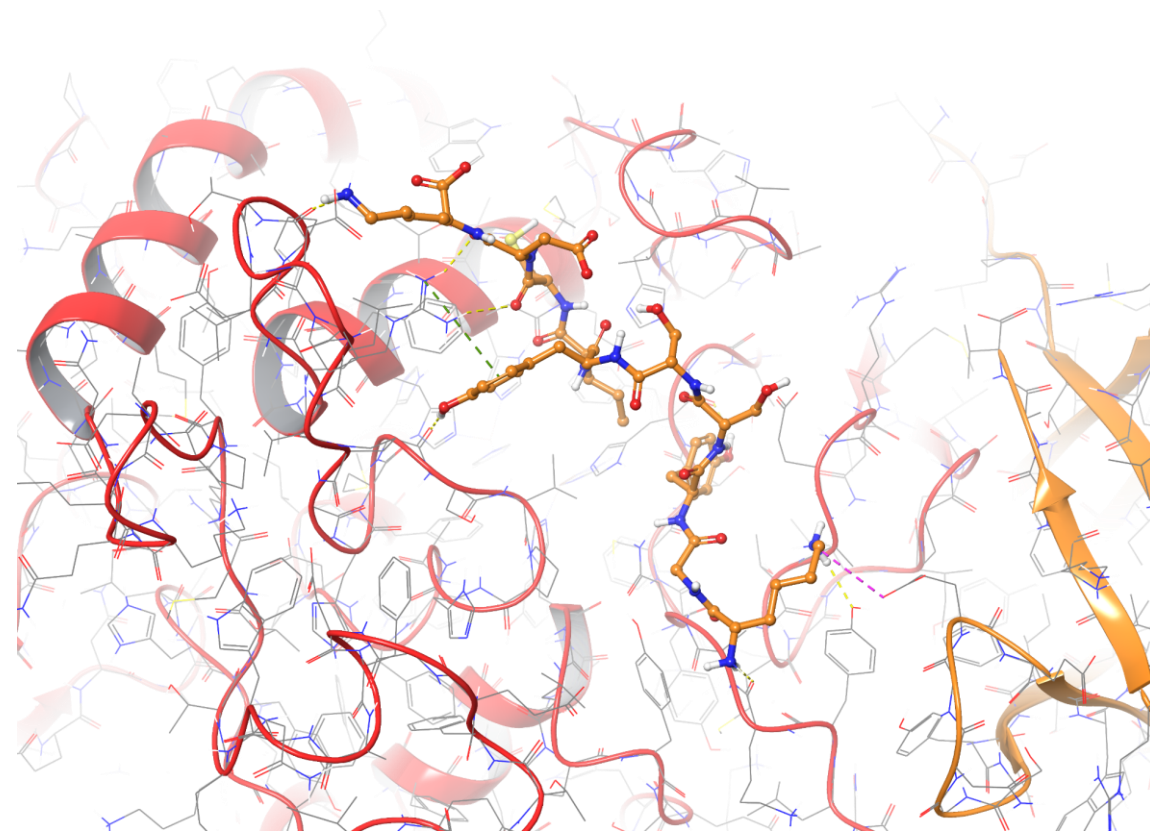
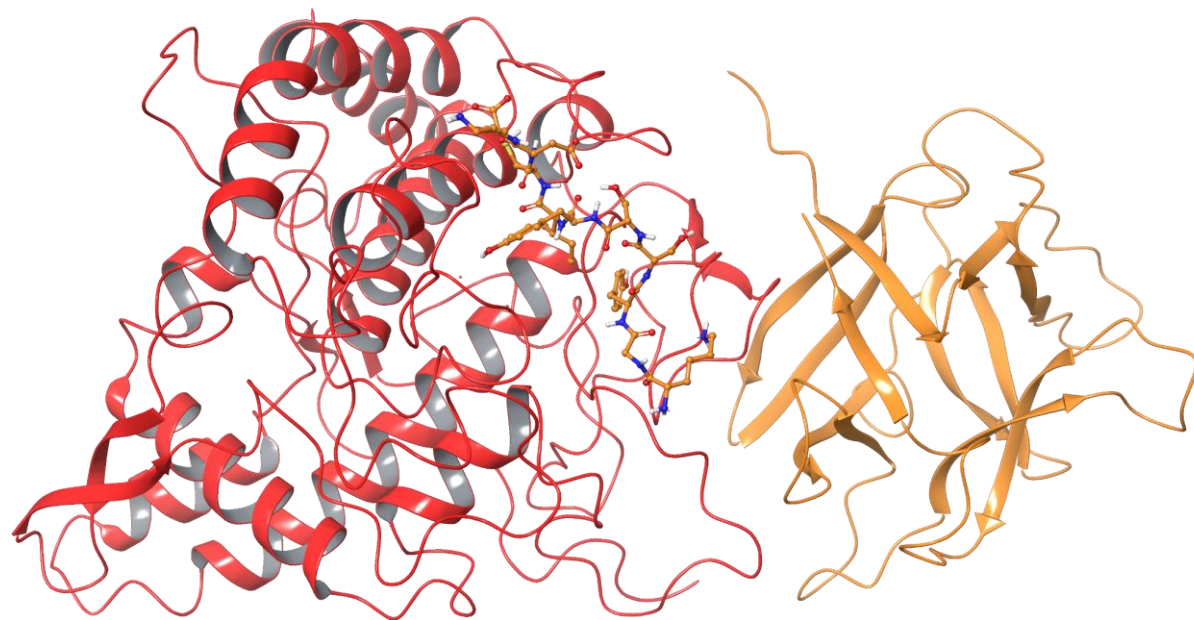


PDB 2Y9X

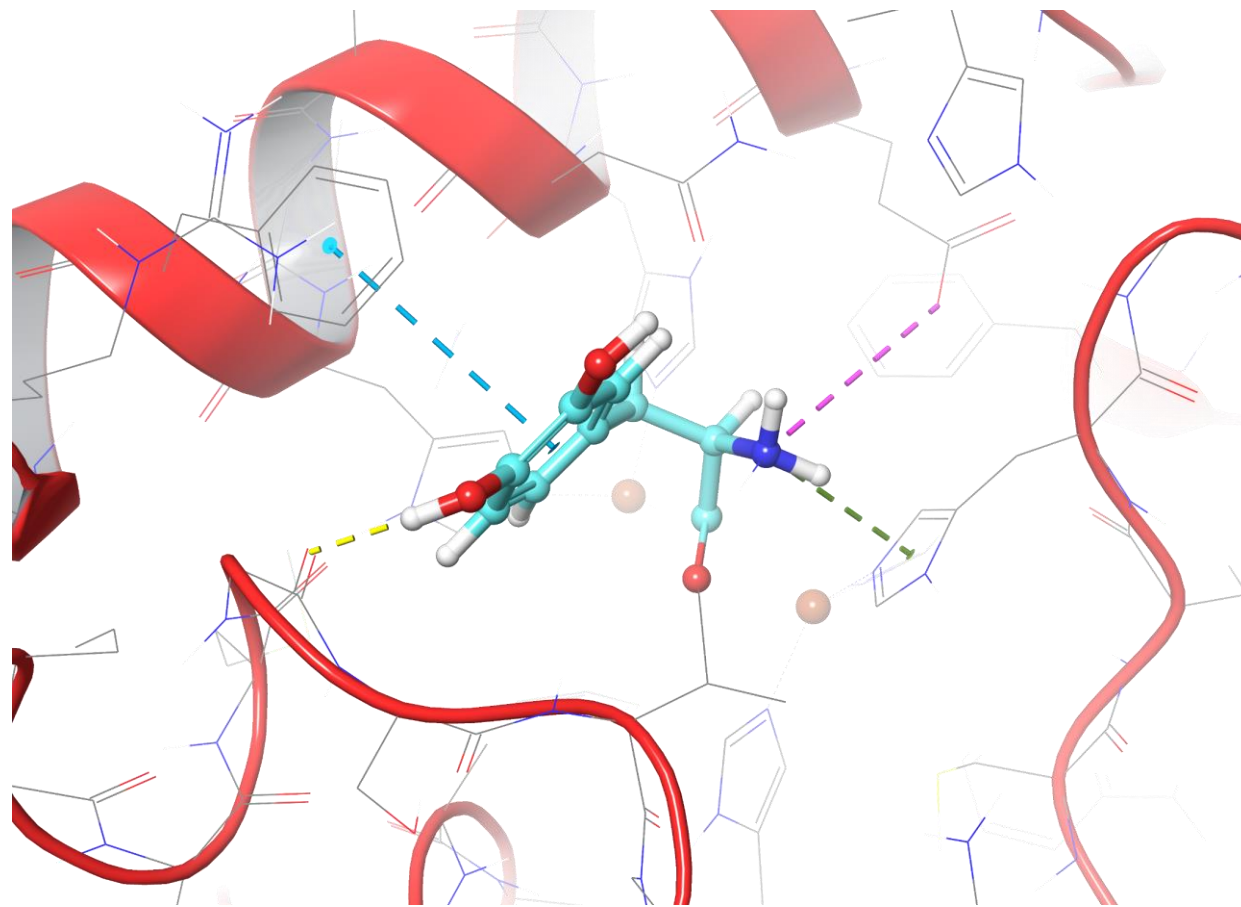
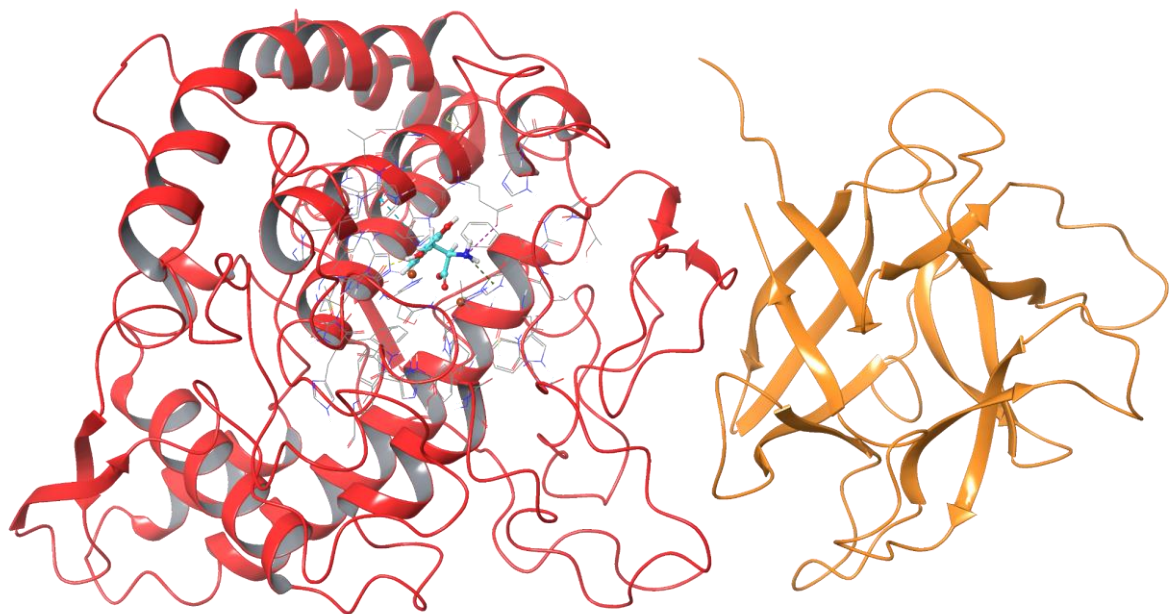
Grid box in this experiment



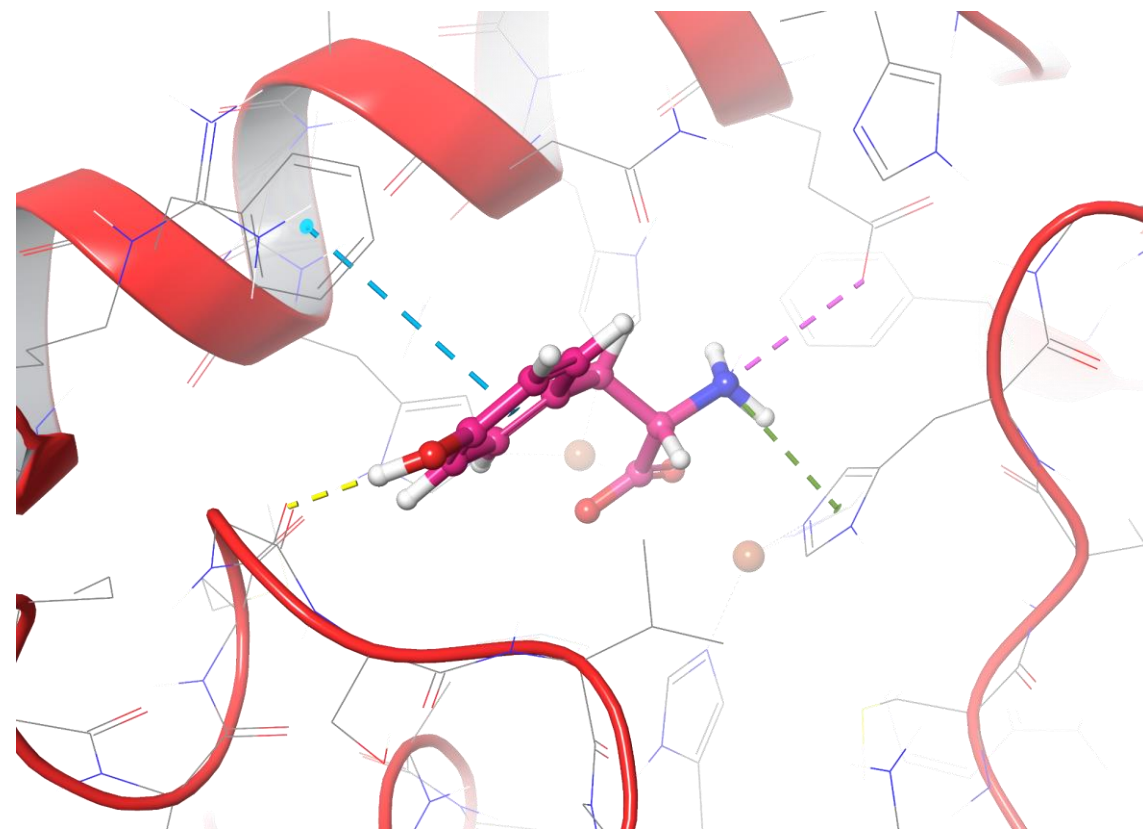
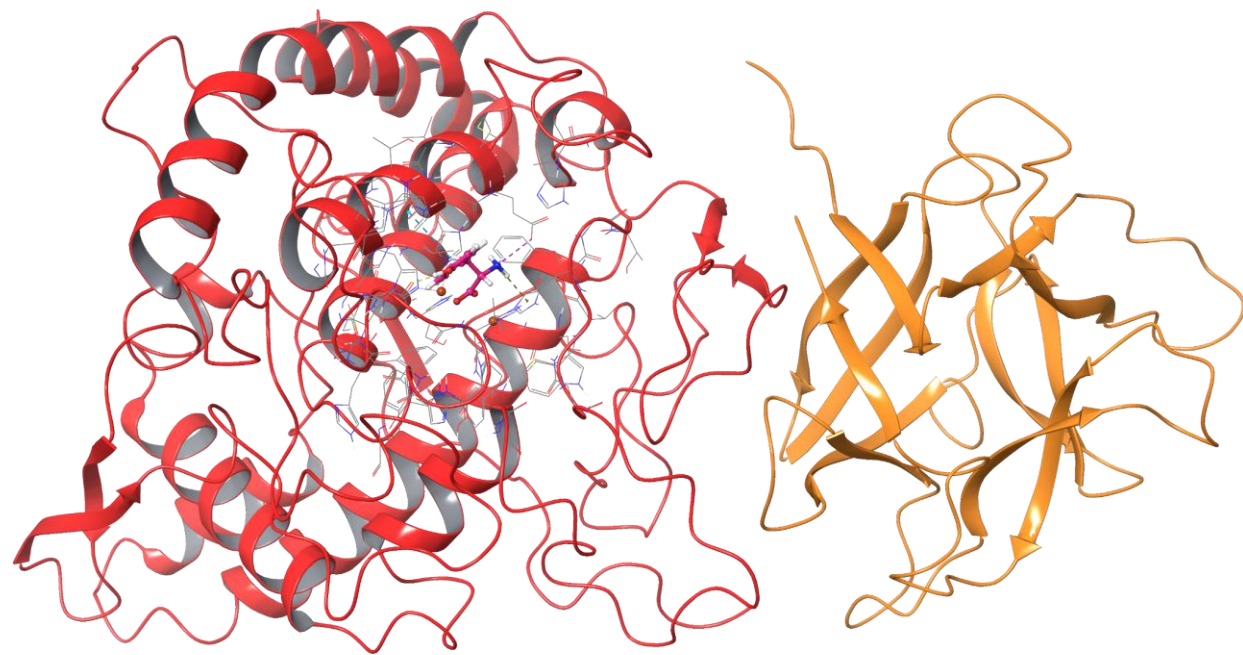
Docking result – Ligand01



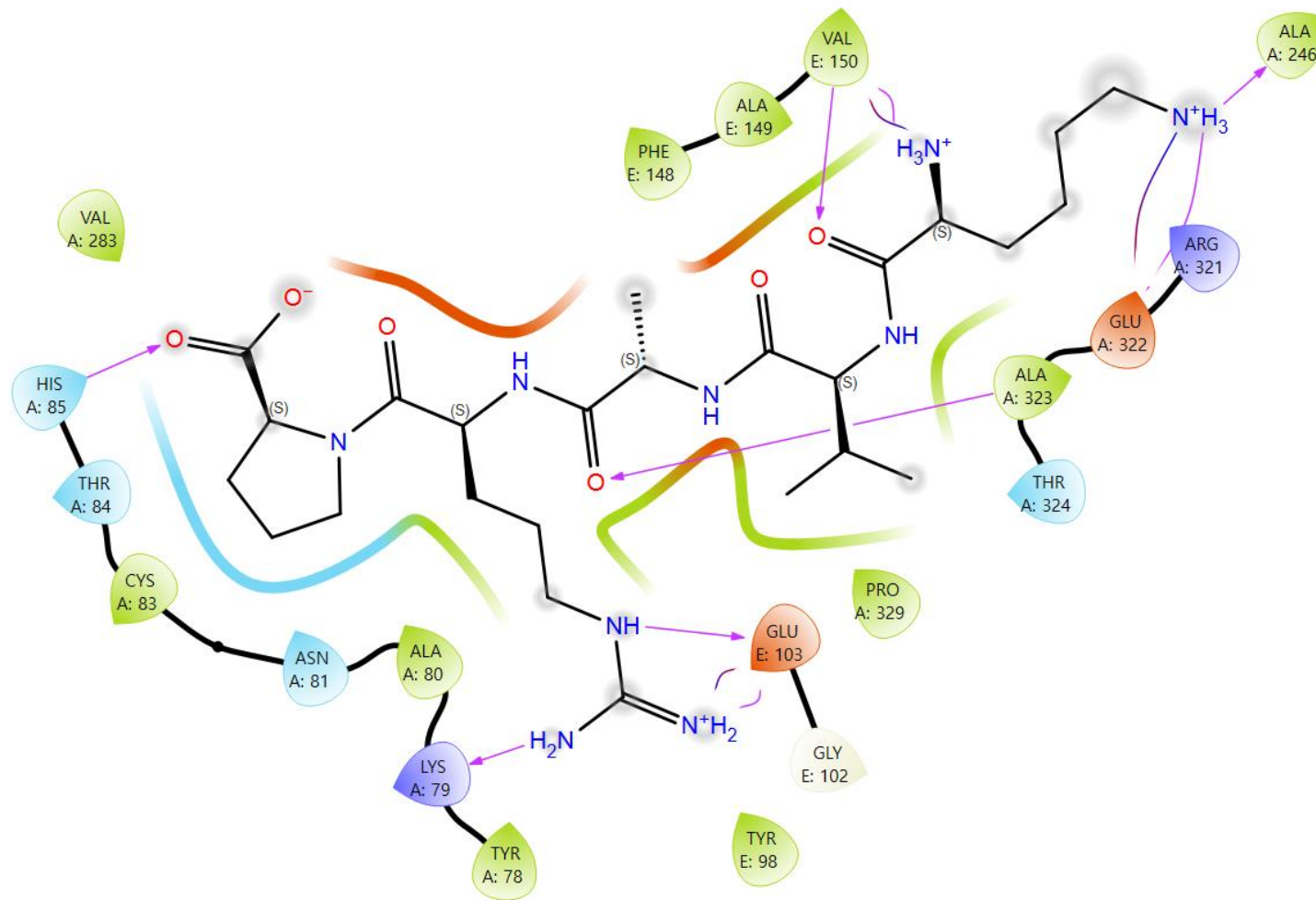
Docking result – Ligand02



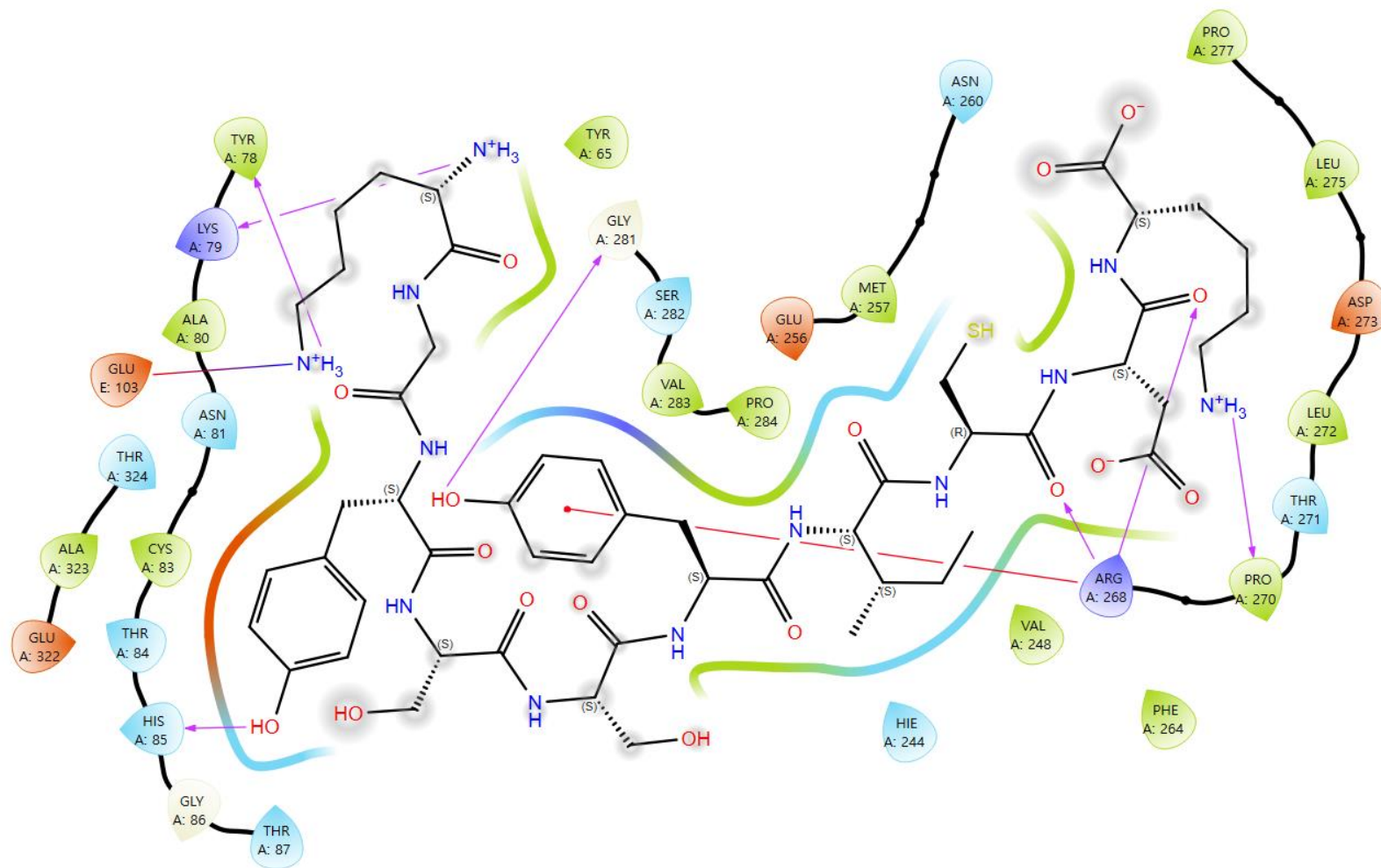
Docking result – Ligand03



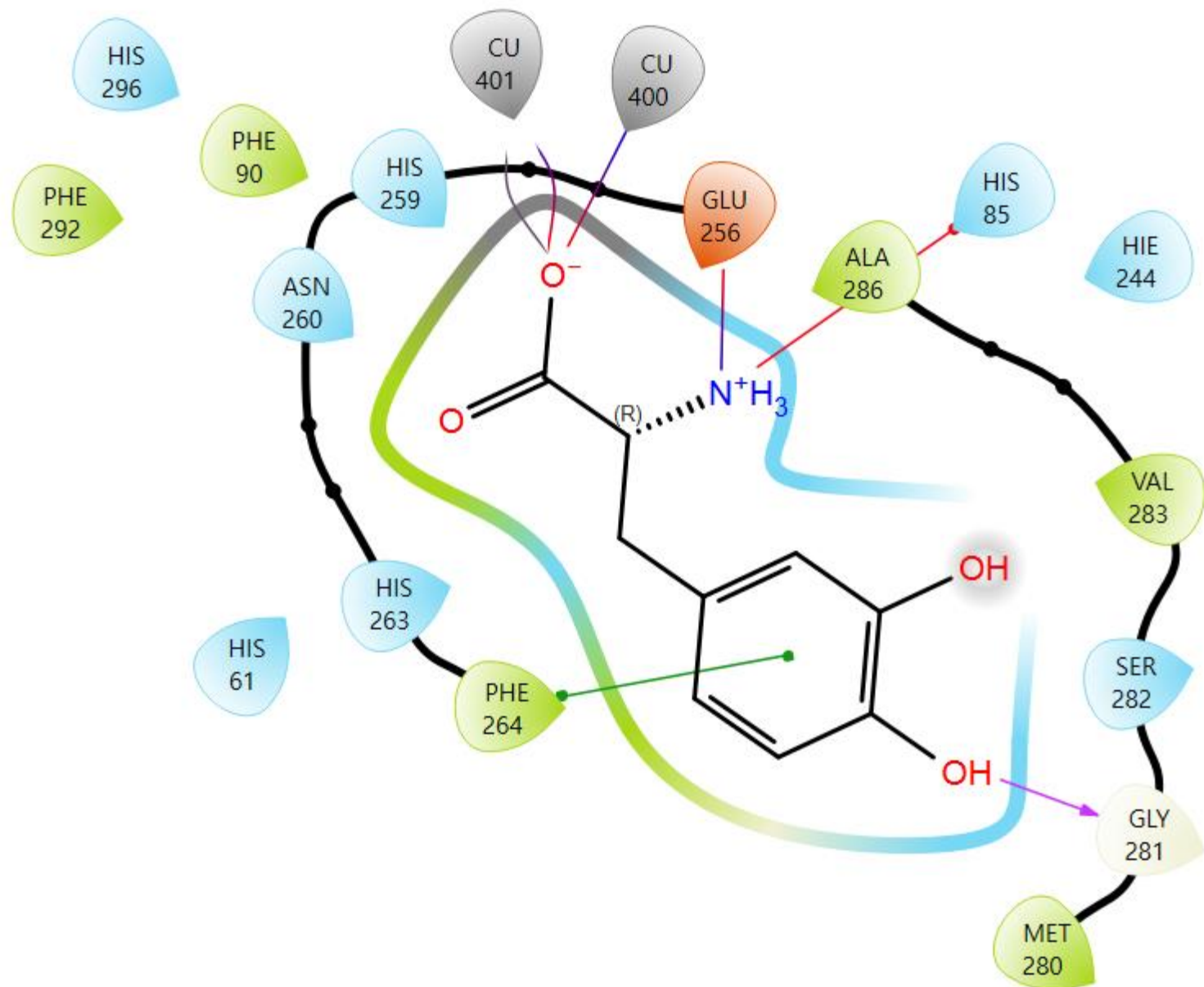
Docking result – Control (2D)



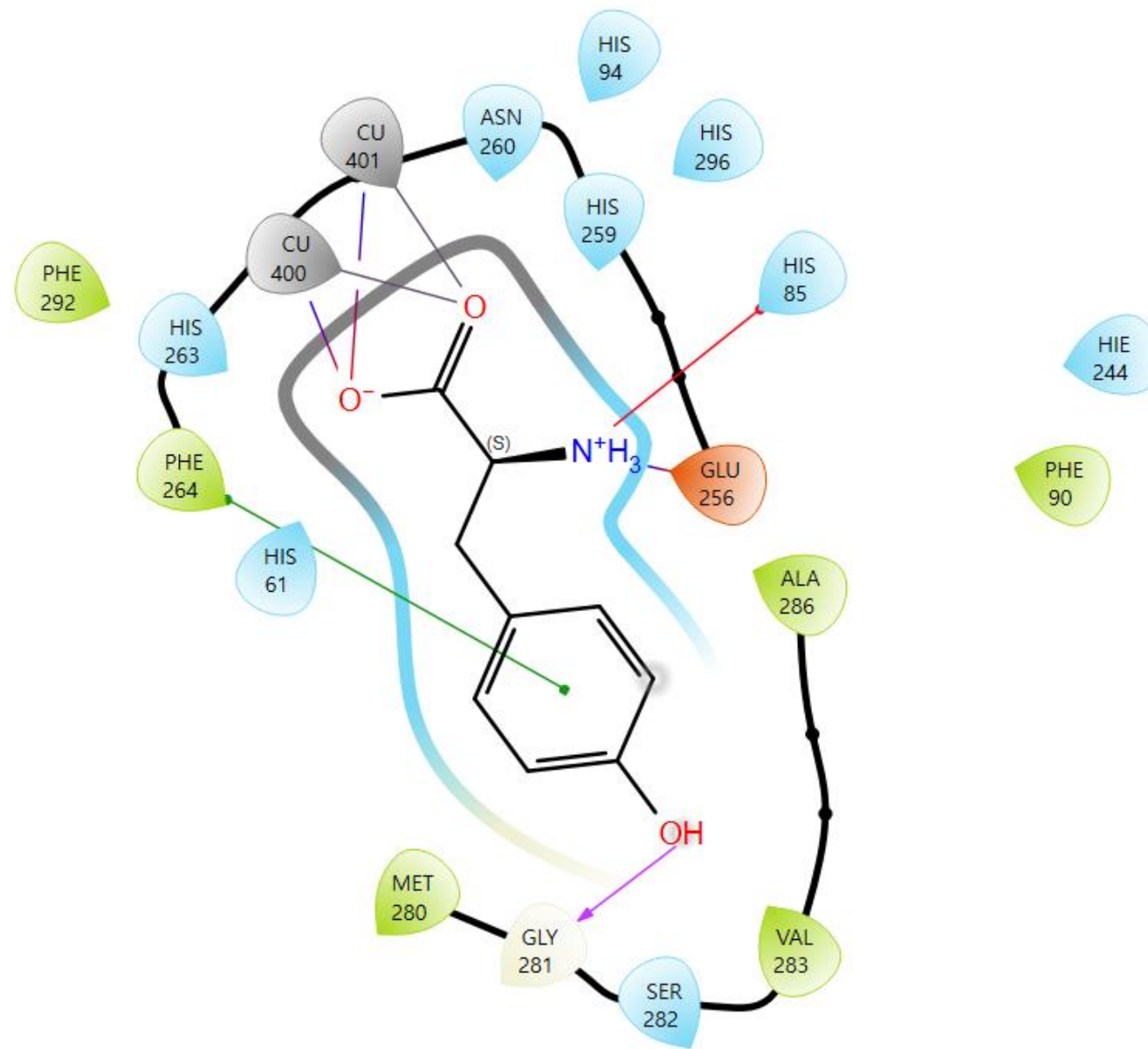
Docking result – Ligand01 (2D)



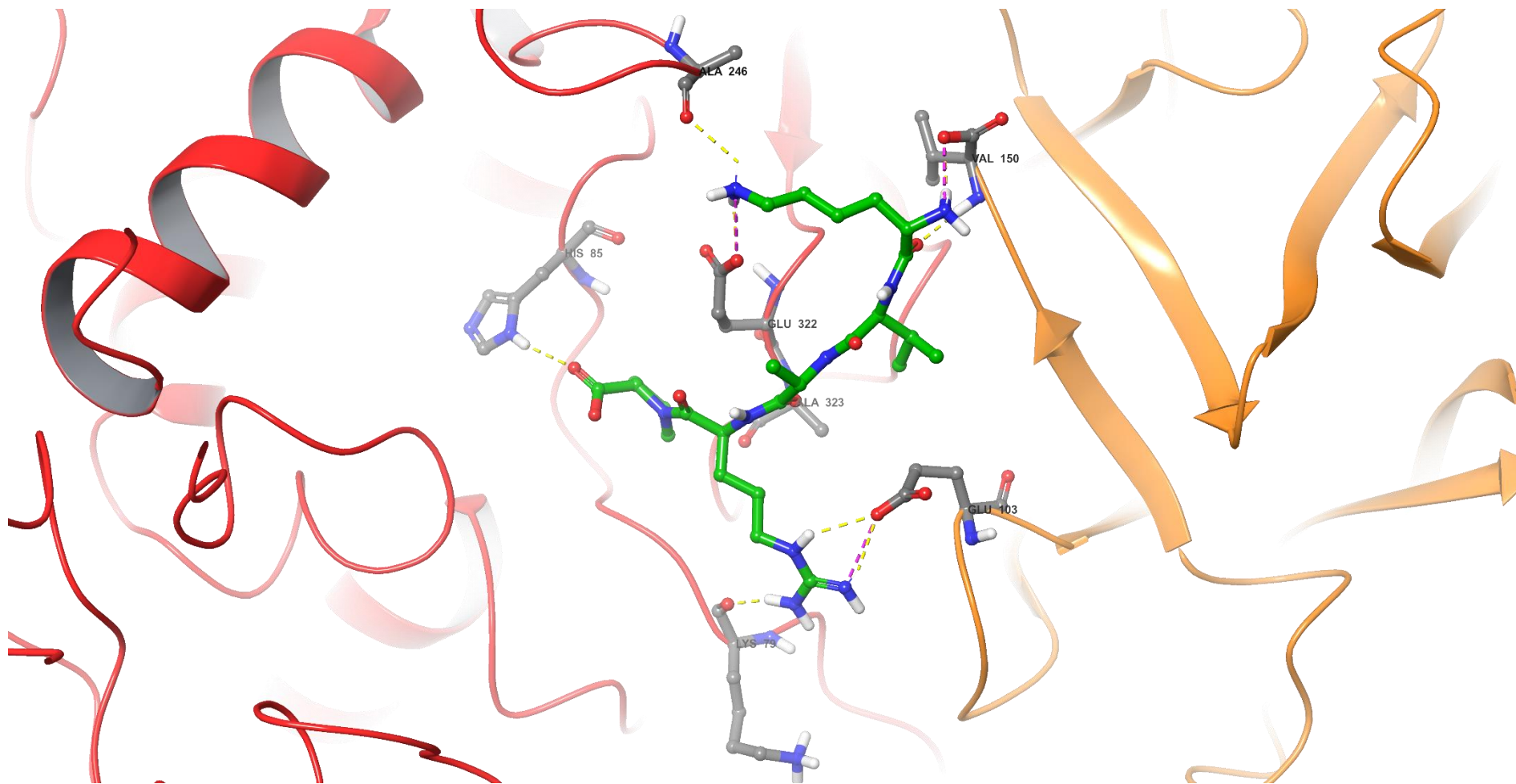
Docking result – Ligand02 (2D)



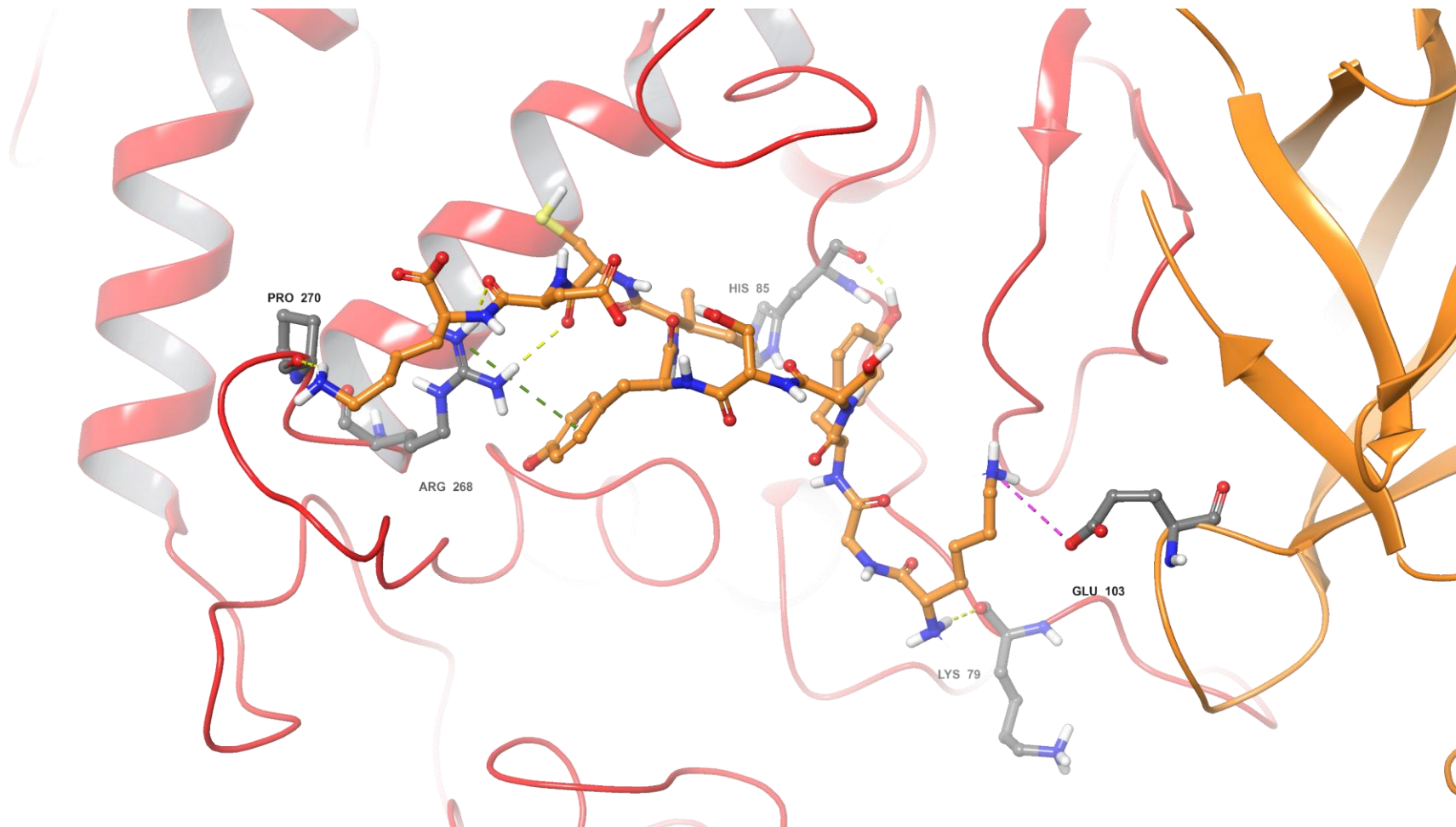
Docking result – Ligand03 (2D)



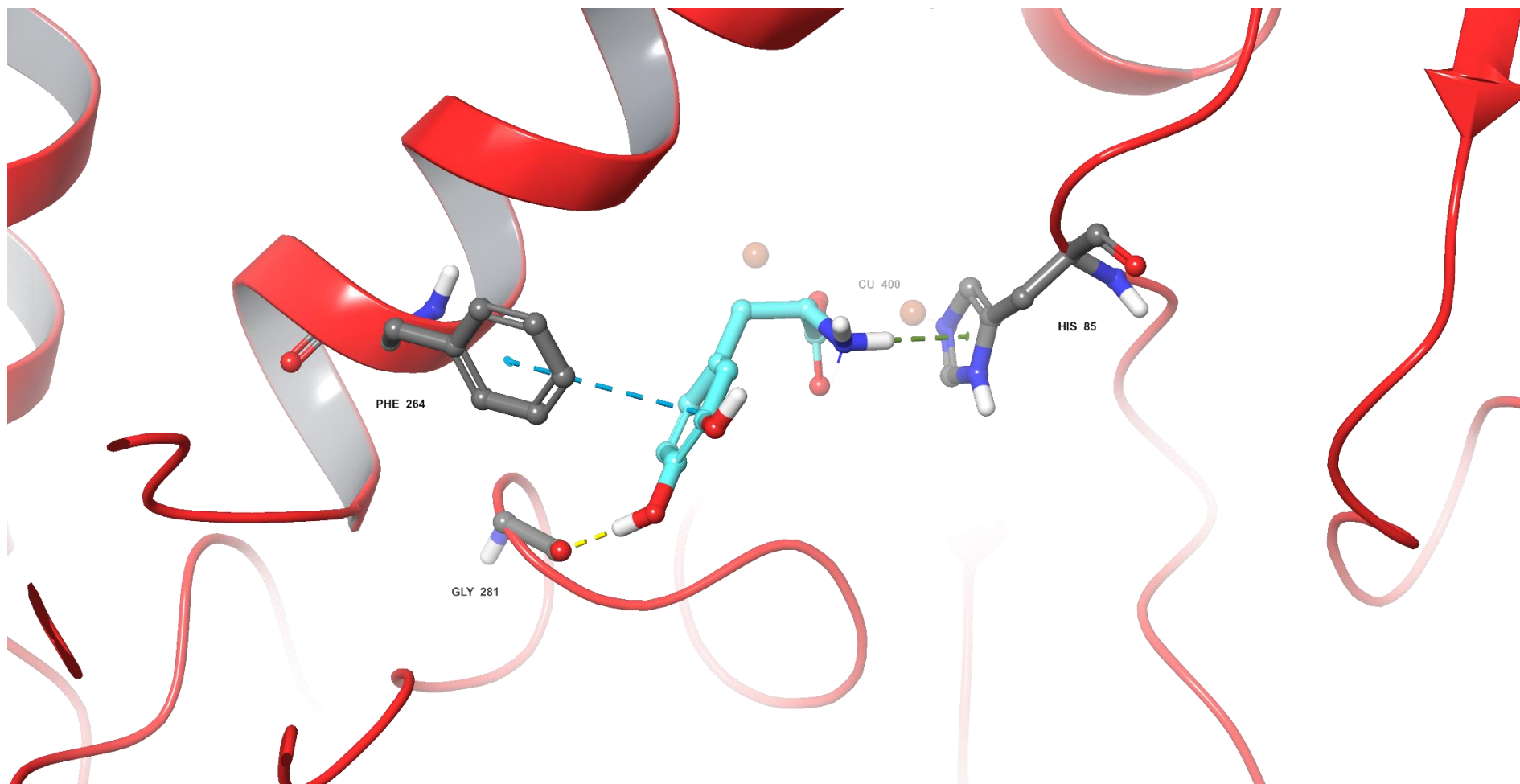
Docking result – Control (binding site)



Docking result – Ligand01 (binding site)



Docking result – Ligand02 (binding site)



Docking result – Ligand03 (binding site)

