Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Data

Computational Estimation of Potential Inhibitors from the Known Drugs against the Main Protease of SARS-CoV-2

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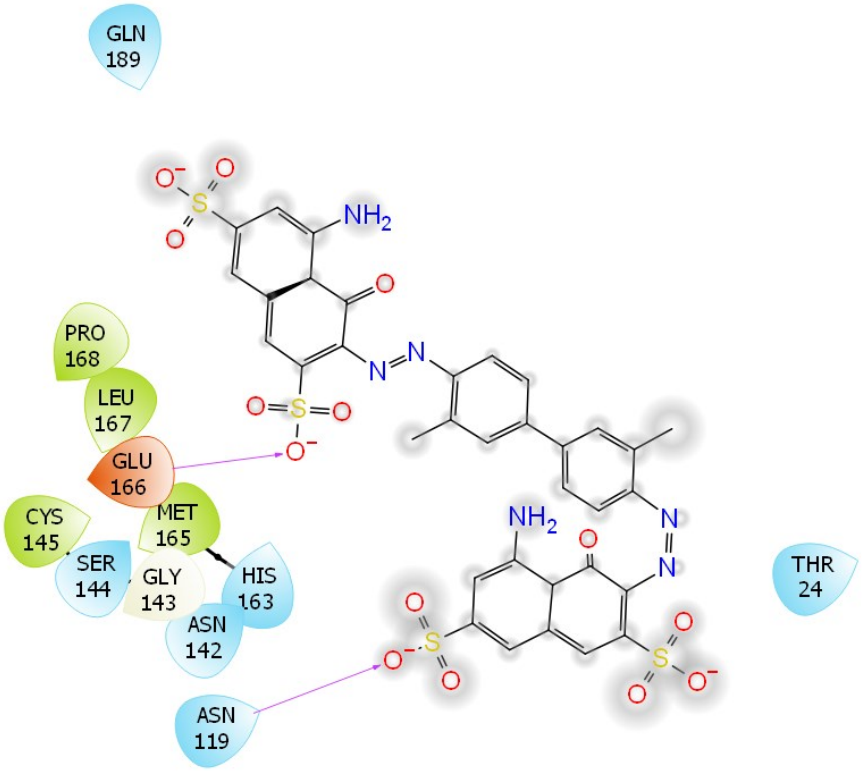

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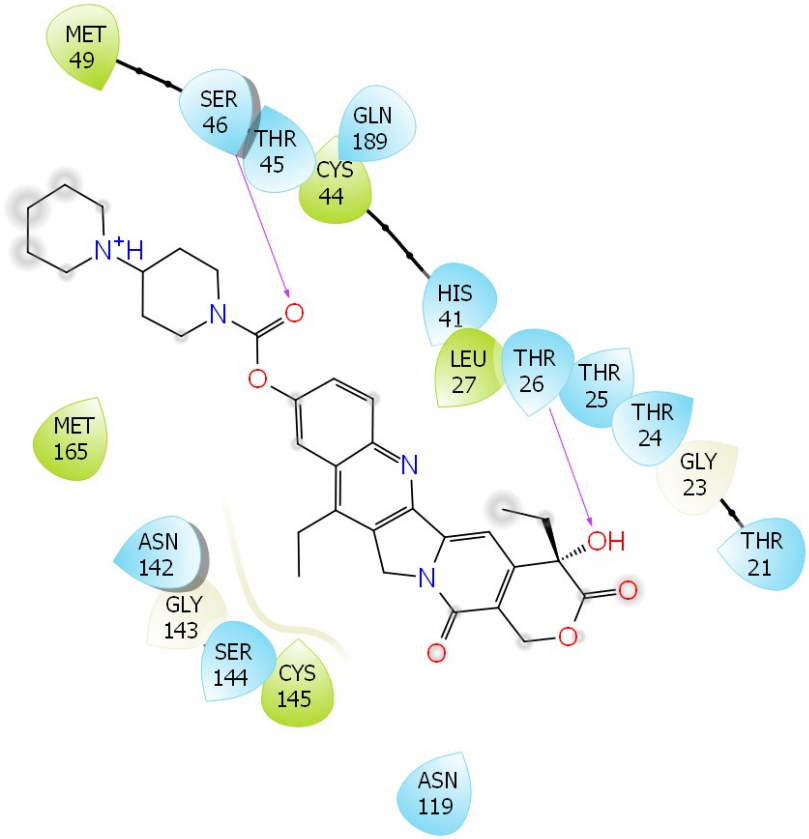

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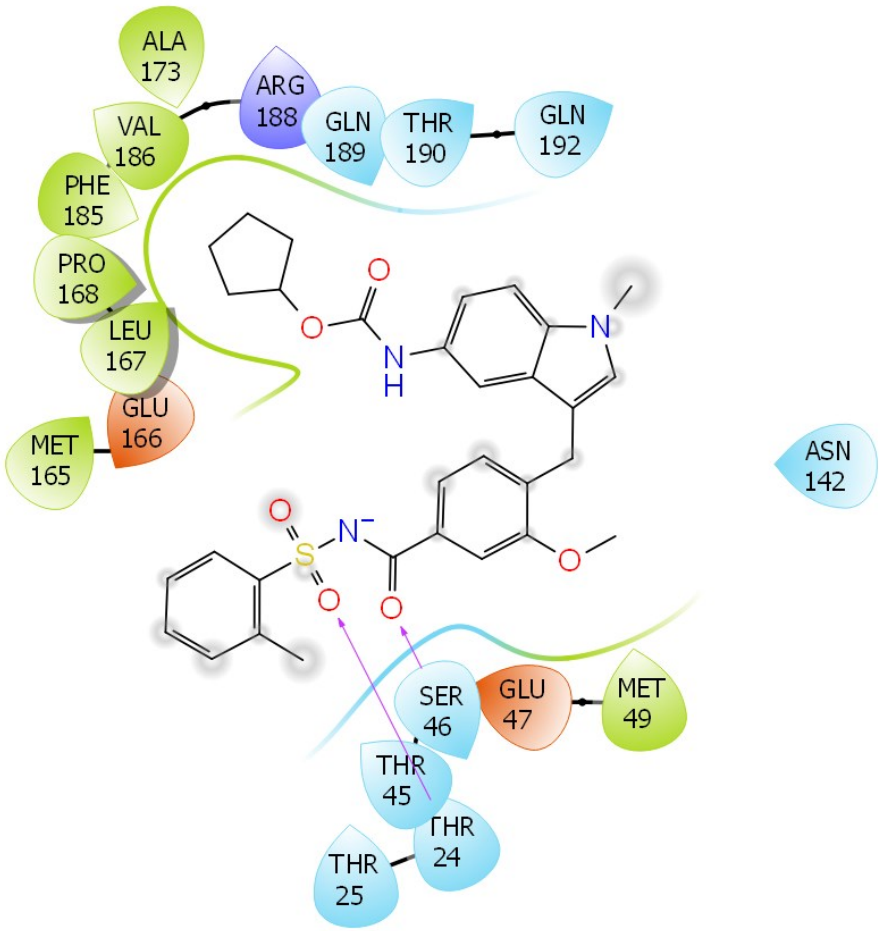

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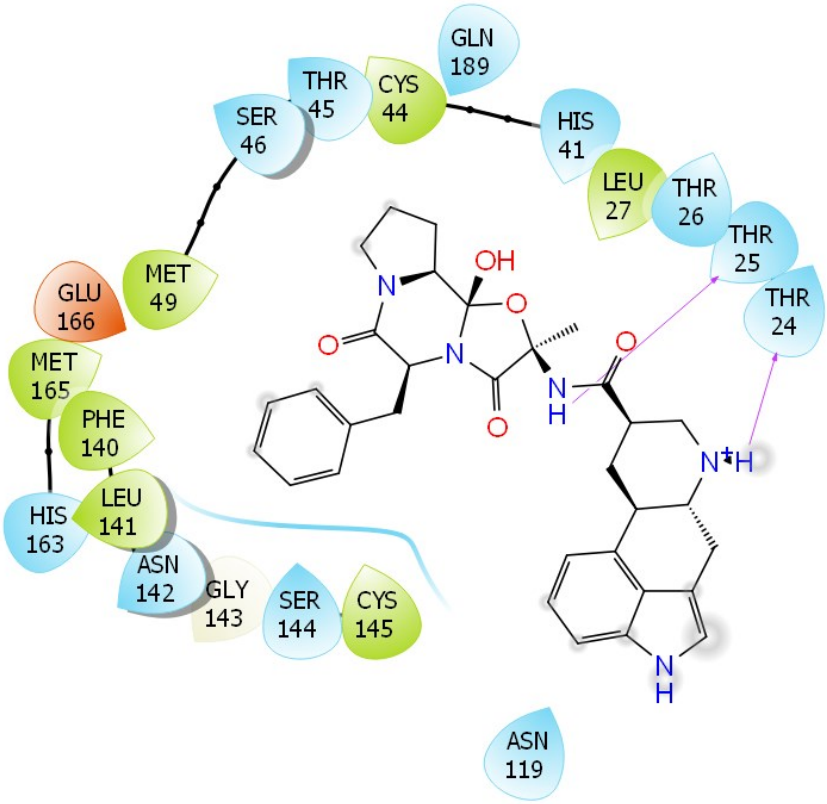

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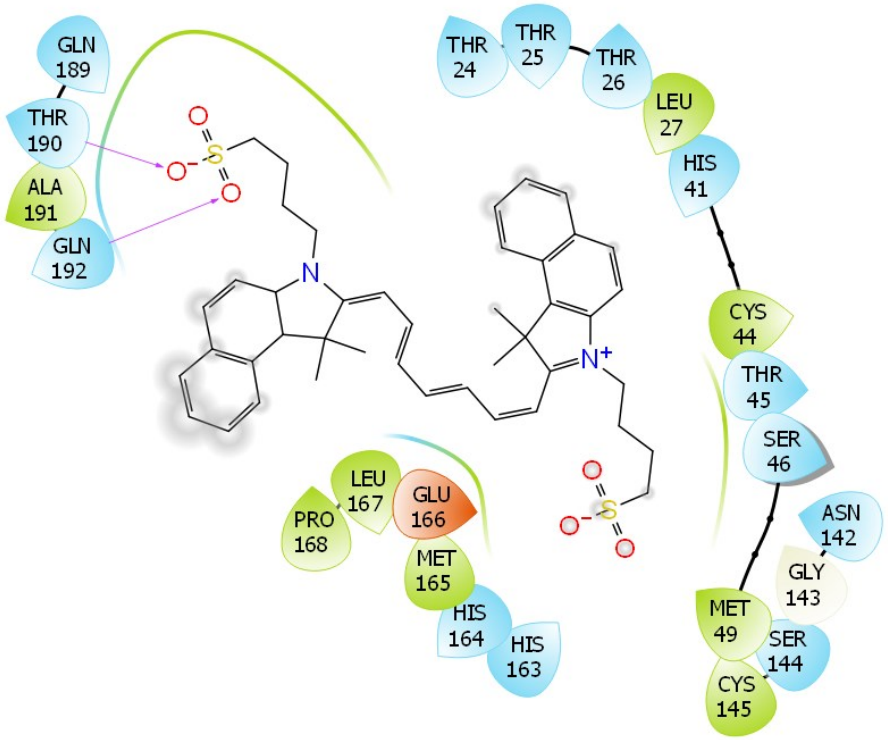

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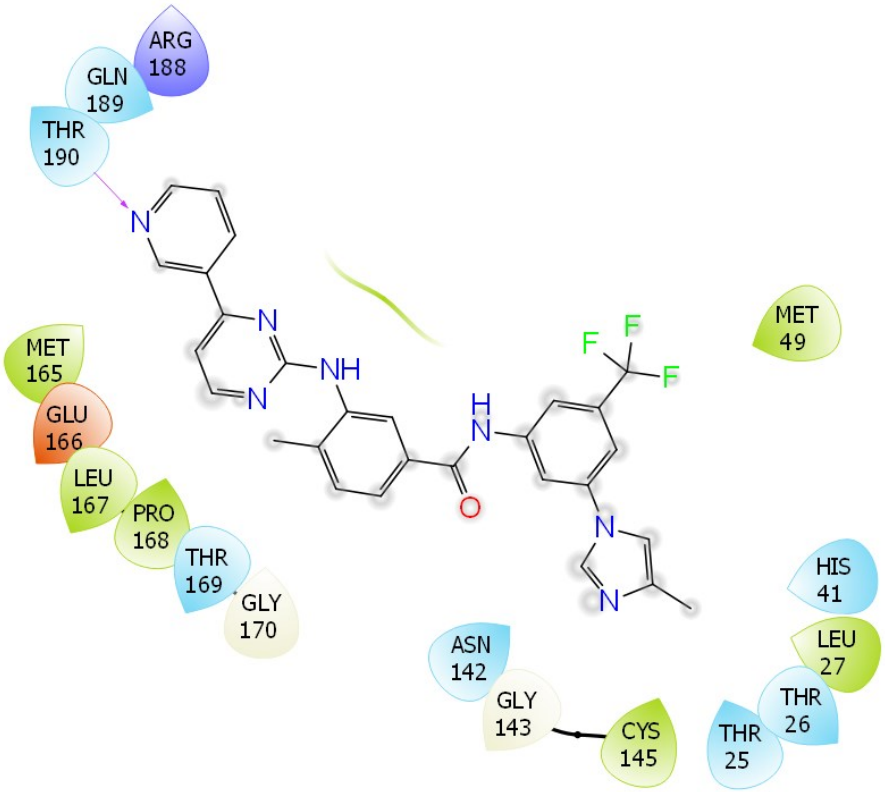

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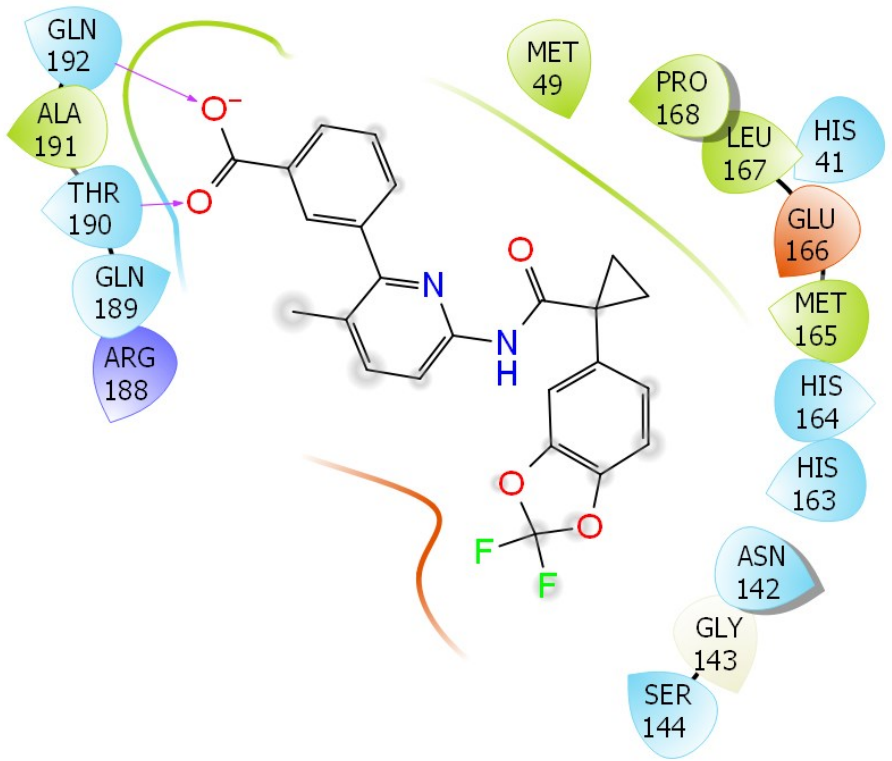

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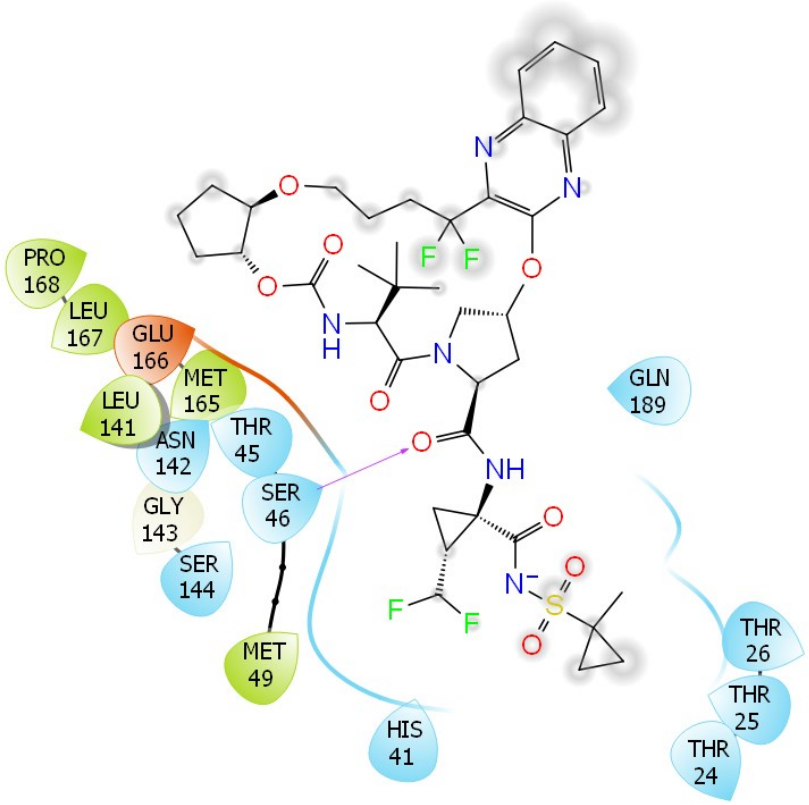

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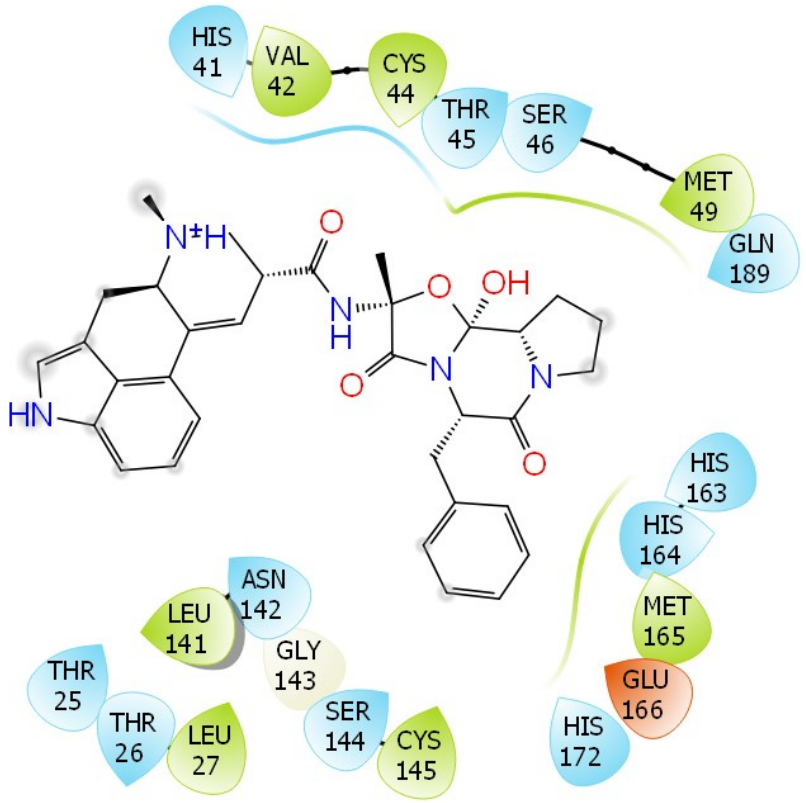

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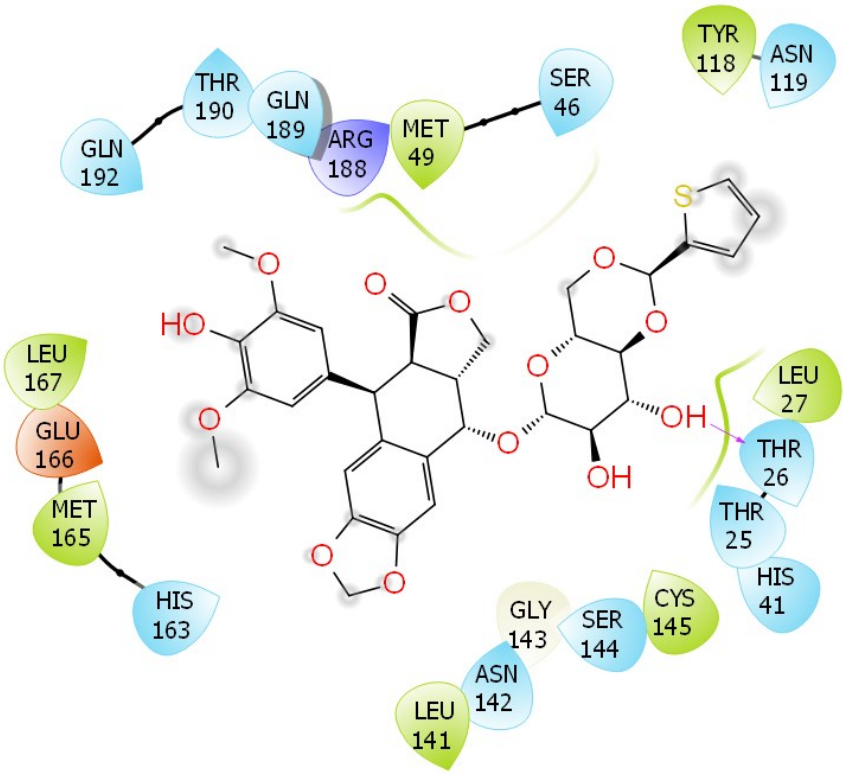

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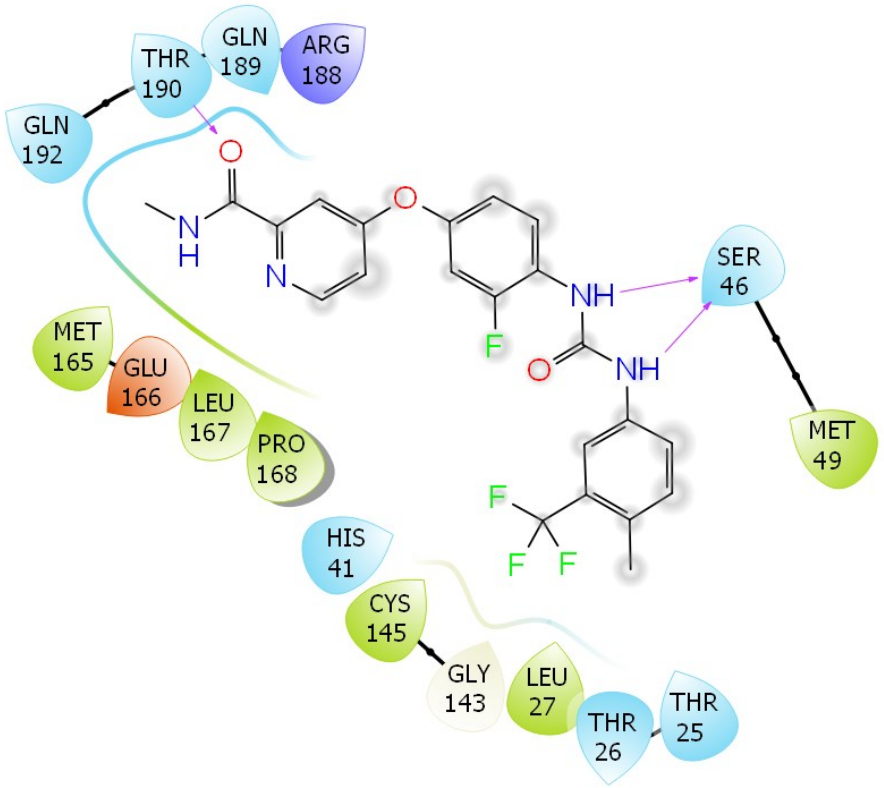

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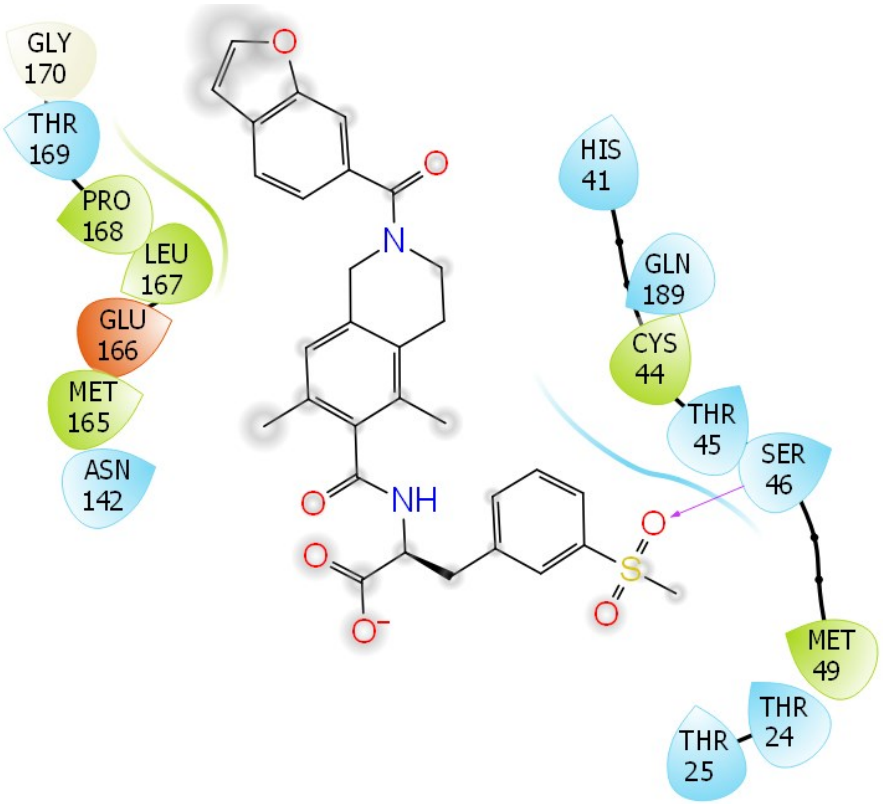

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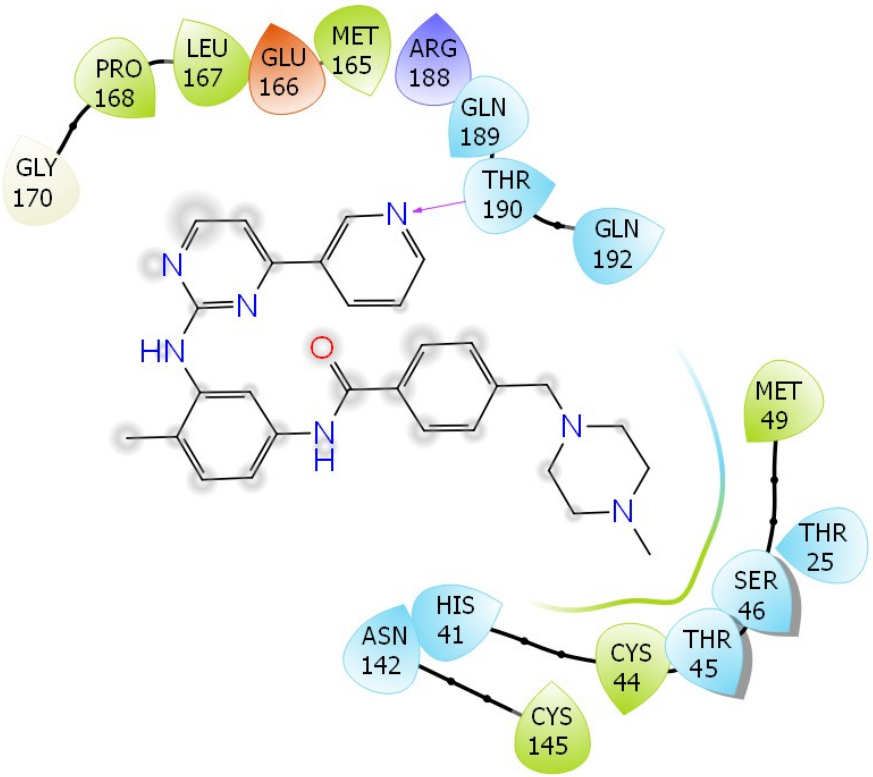

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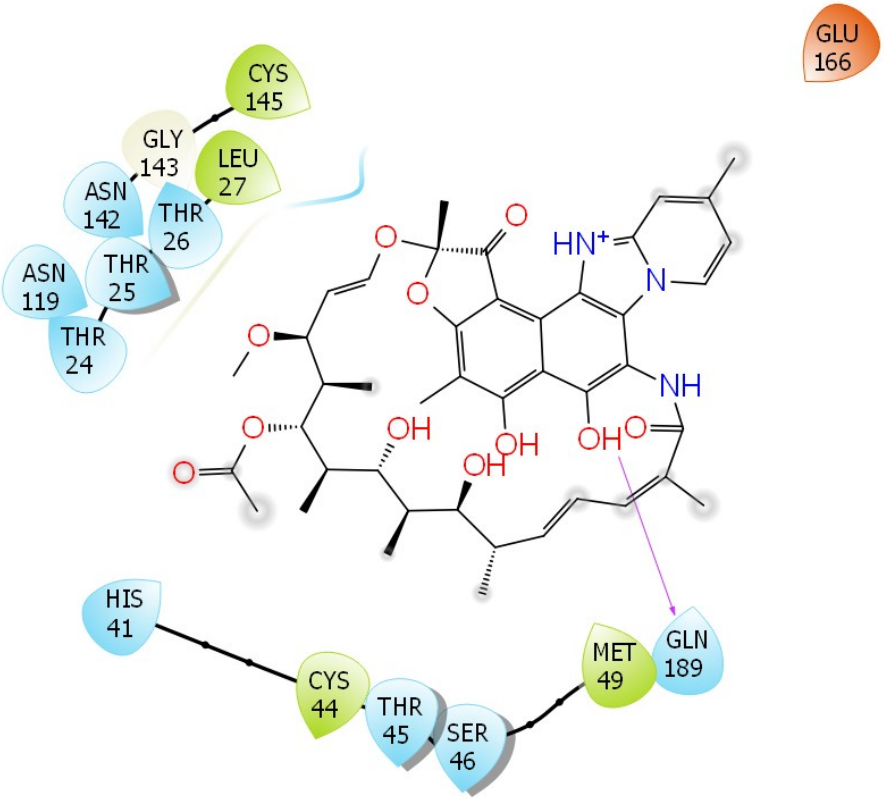

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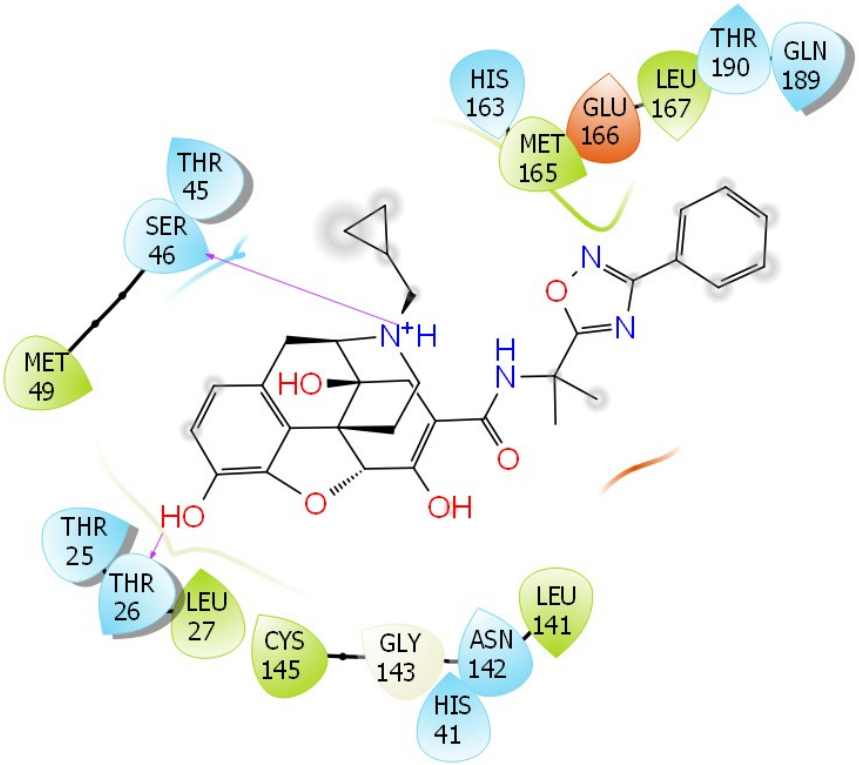

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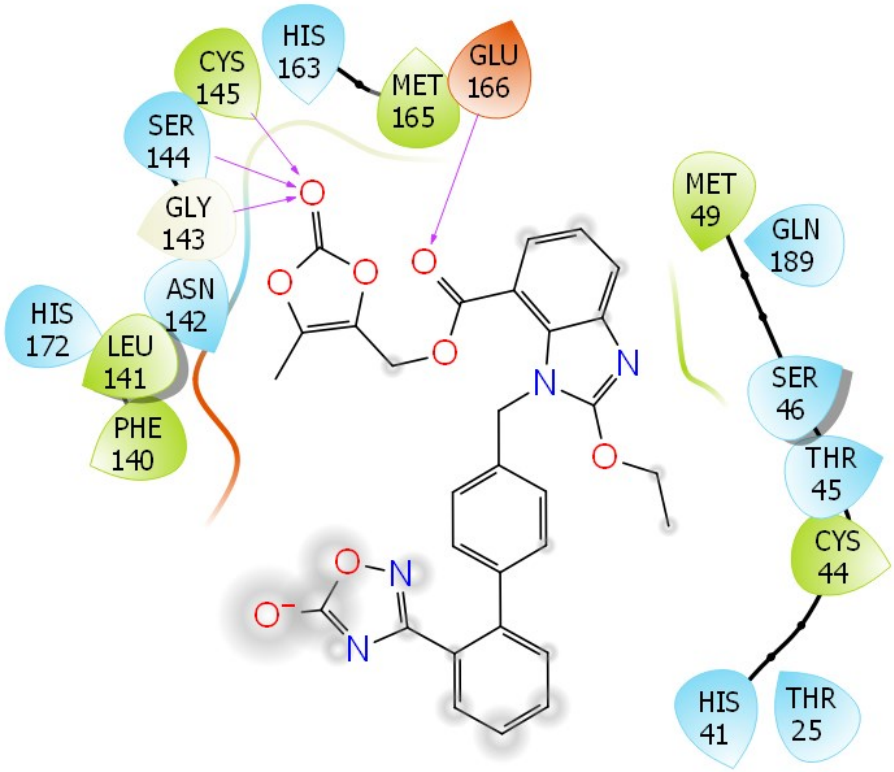

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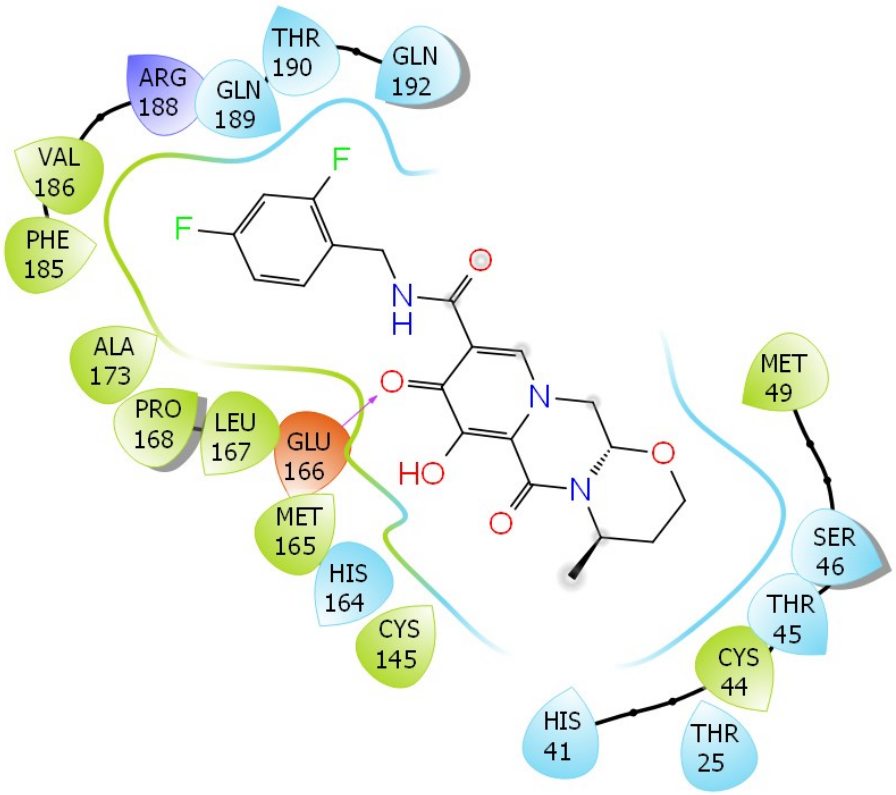

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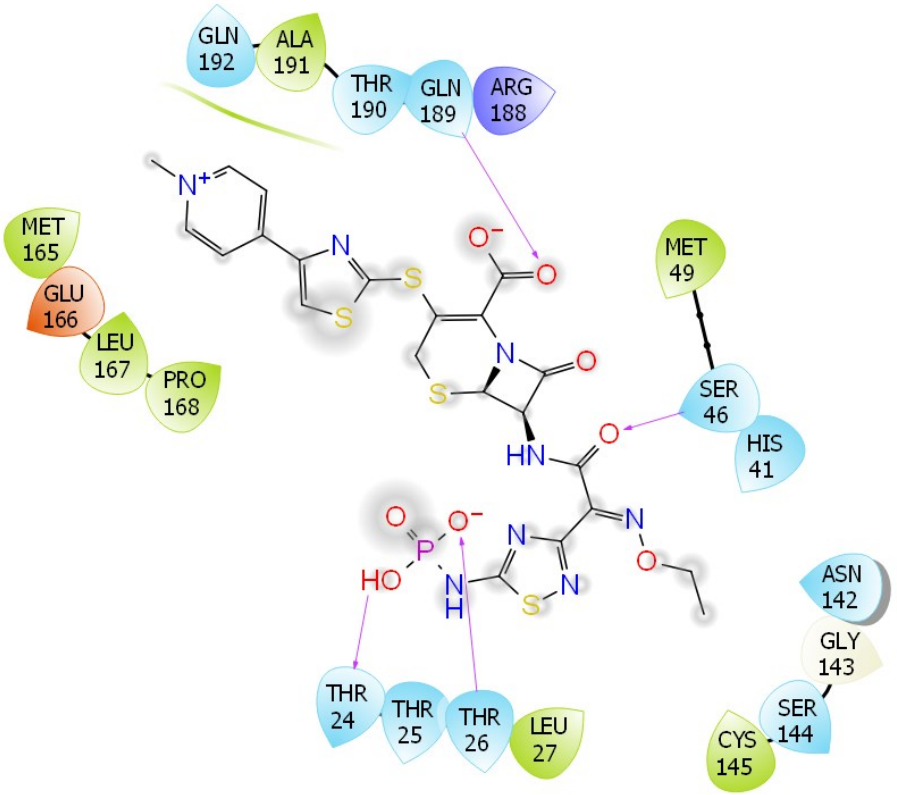

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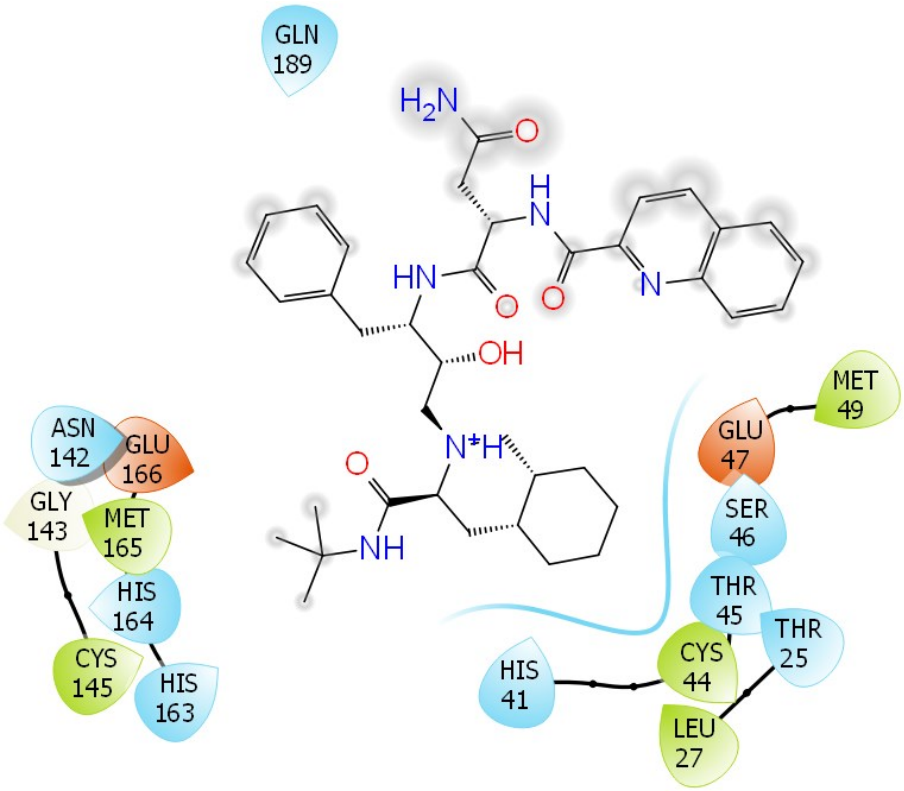

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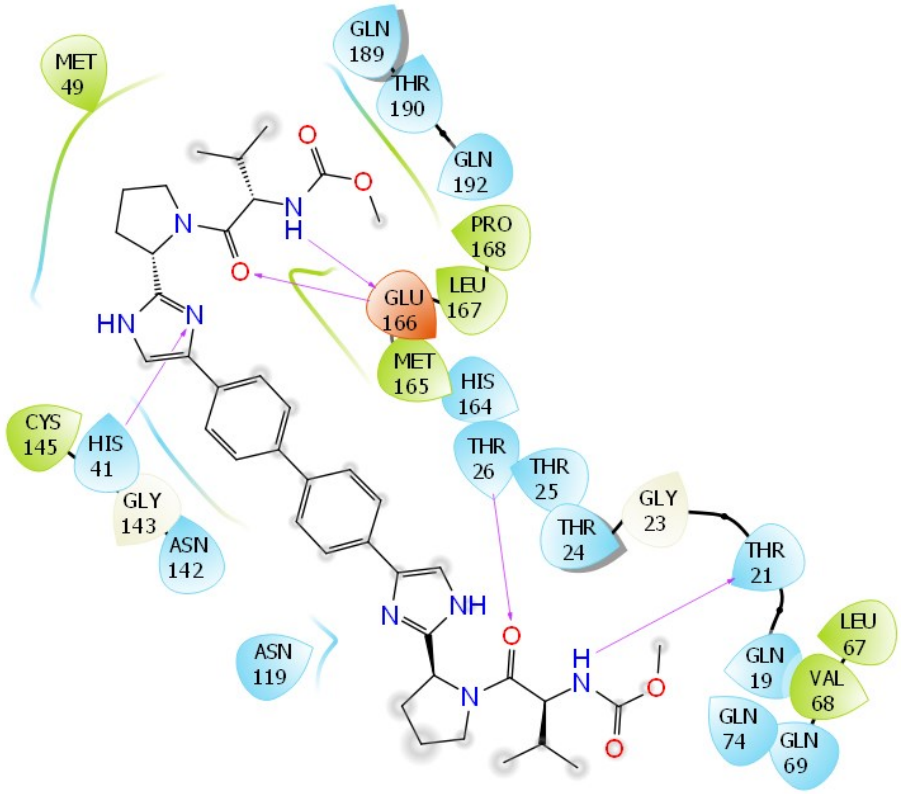

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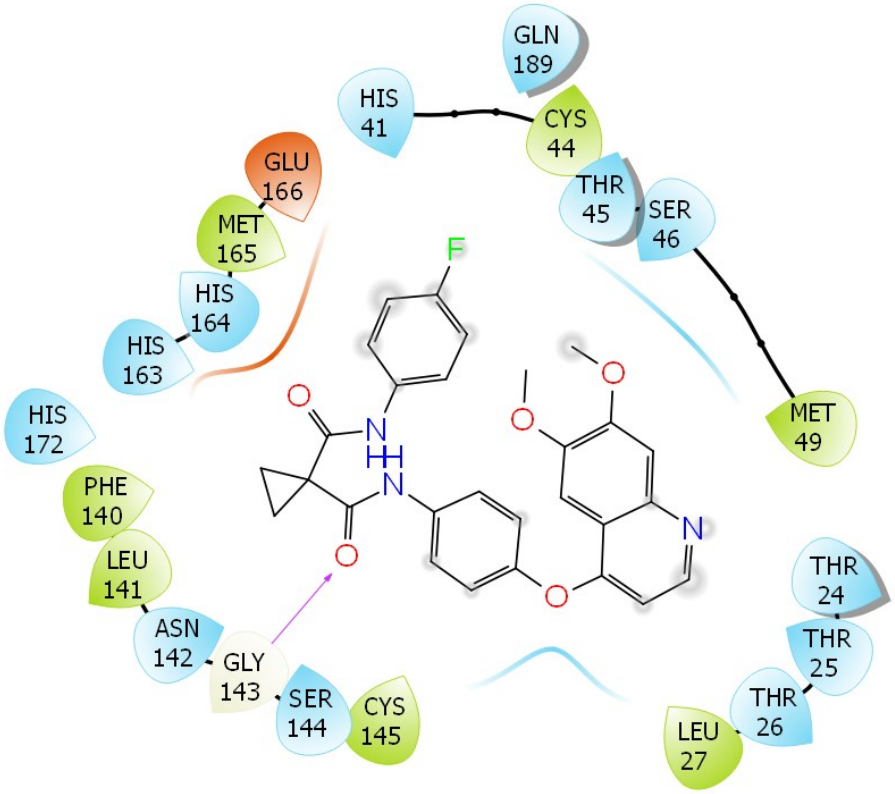

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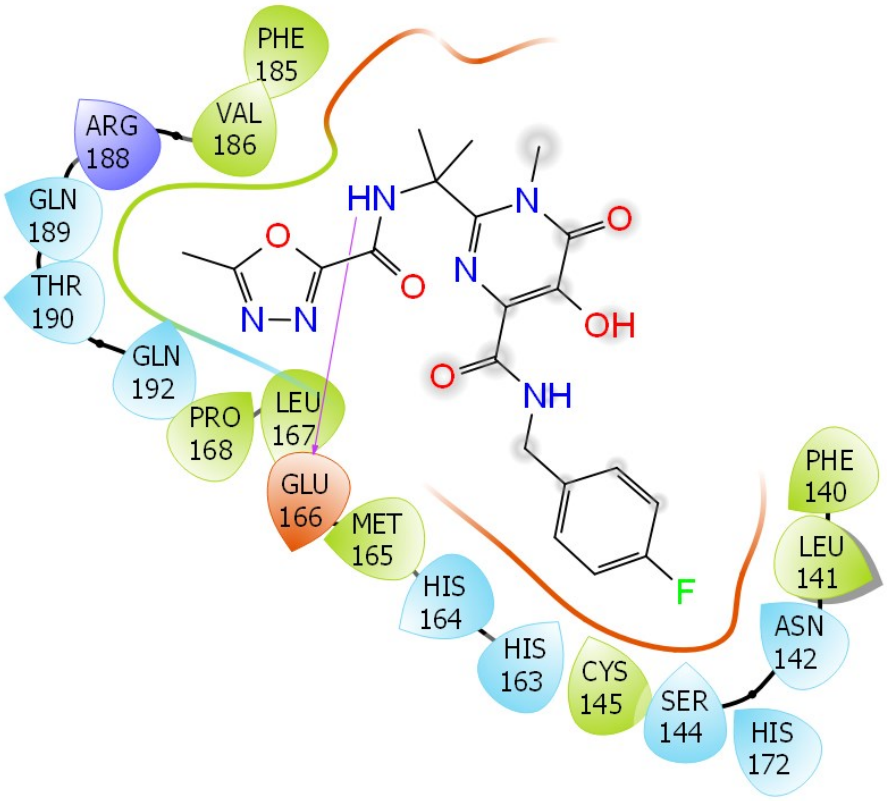

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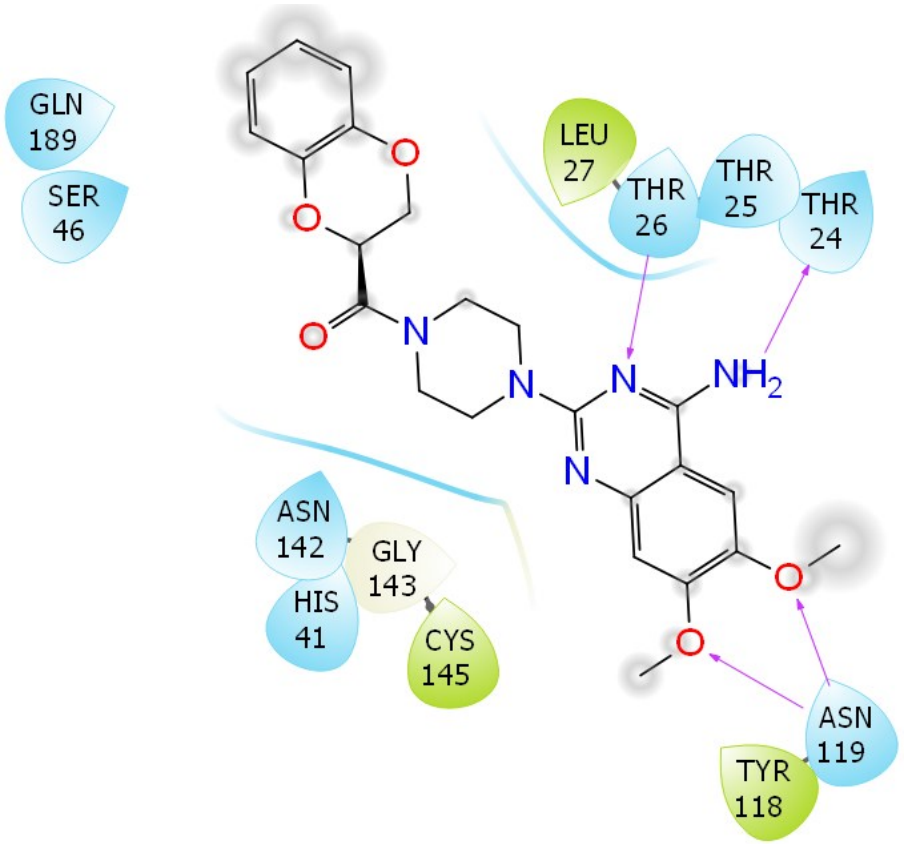

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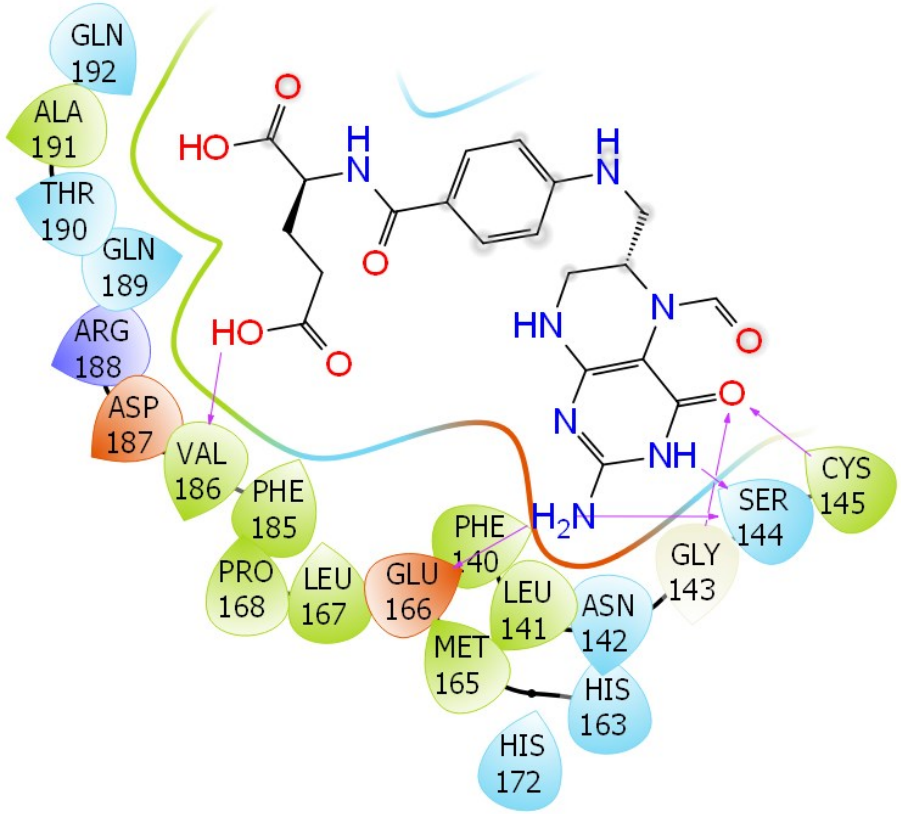

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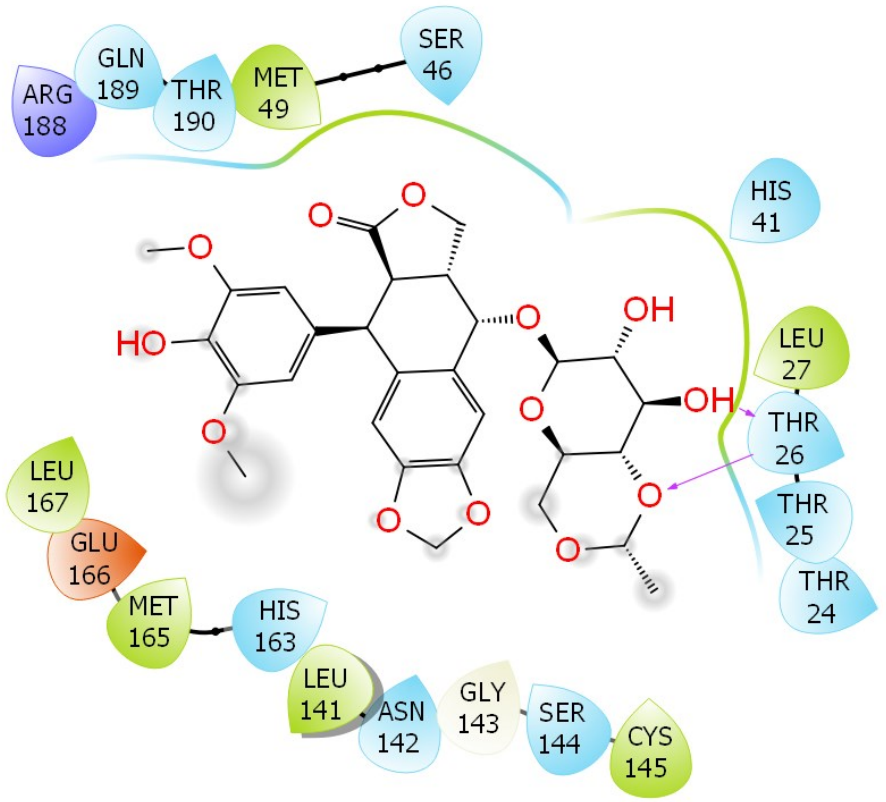

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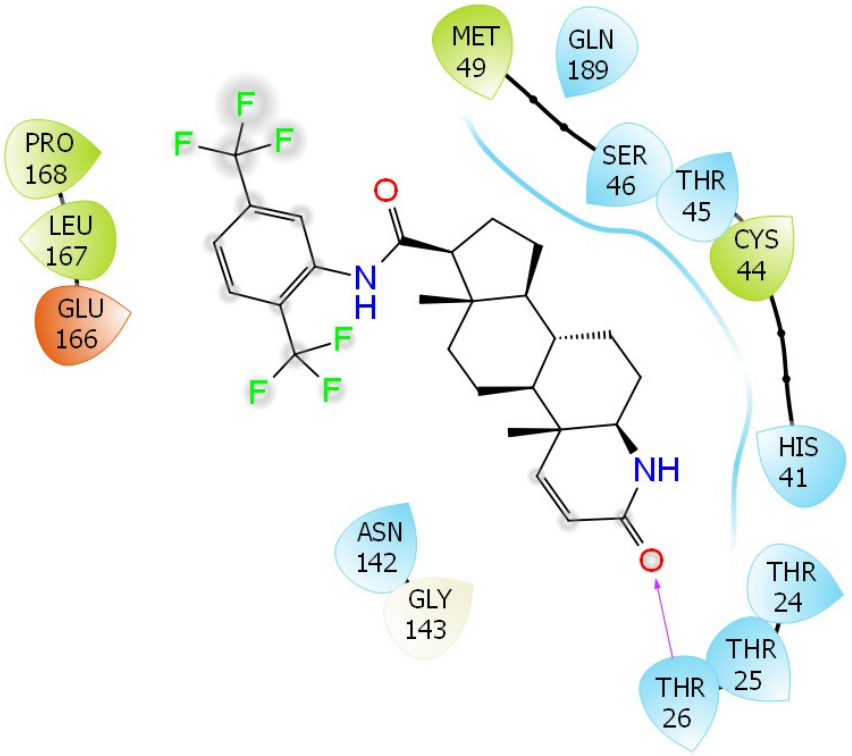

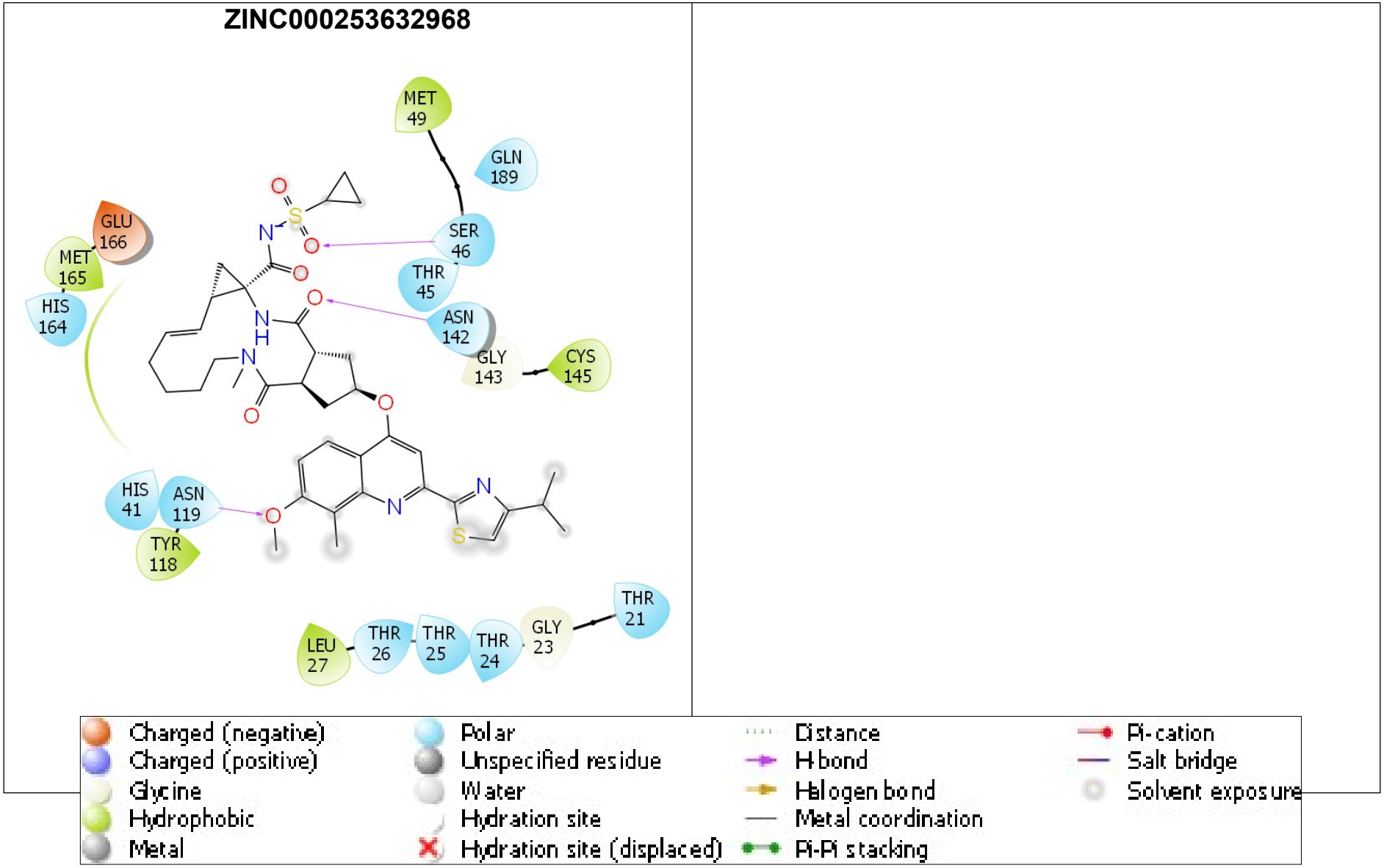

Figure S1. The detailed interaction of SARS-CoV-2 Mpro and the full top-lead compounds

The results are illustrated by the molecular modeling software Maestro, Schrödinger. Hydrogen bonds formed by residues of SARS-CoV-2 Mpro and ligands are indicated by purple arrows. Atoms of carbon, oxygen, nitrogen, and sulfur are presented in black, red, blue, and yellow, respectively.

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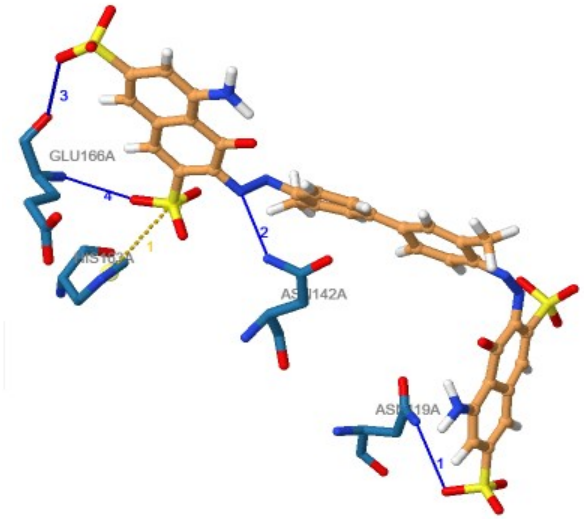

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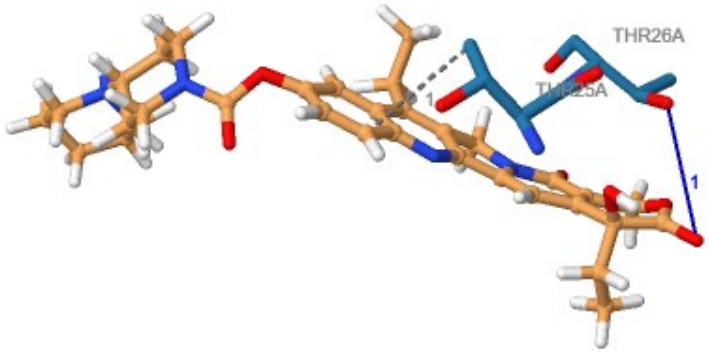

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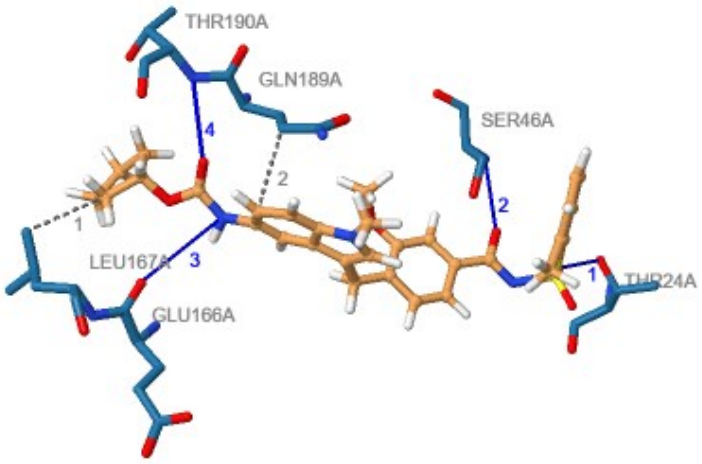

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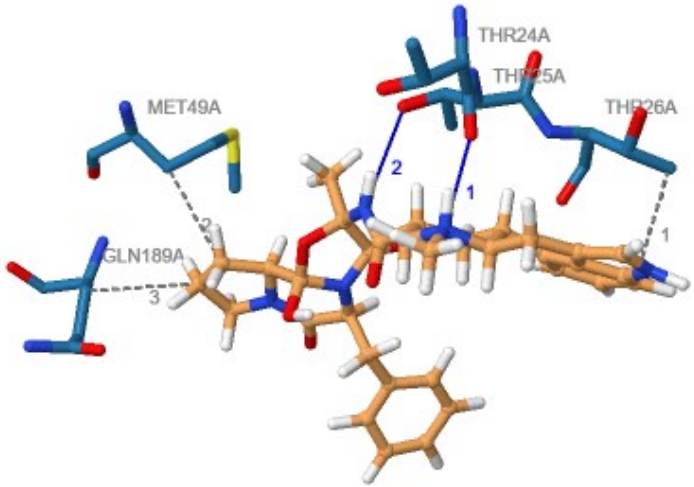

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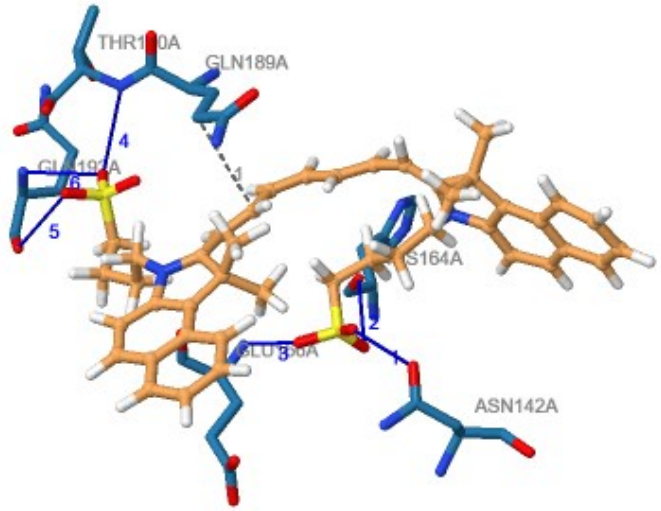

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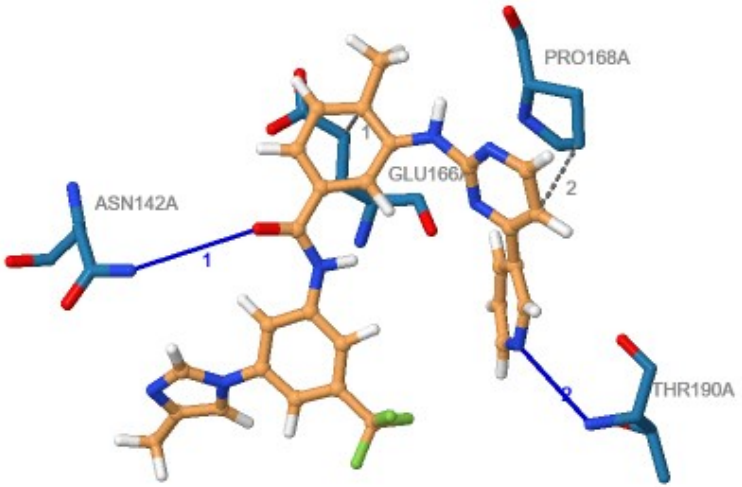

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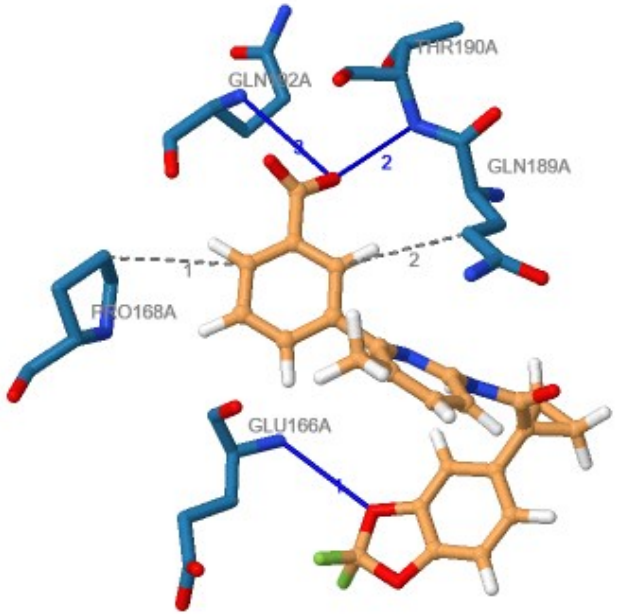

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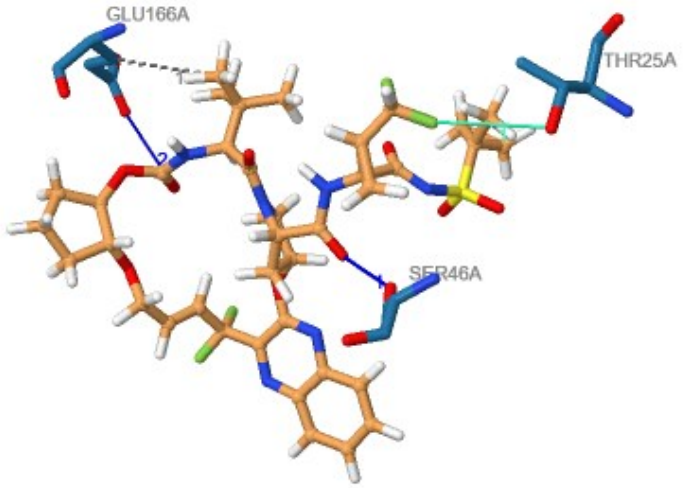

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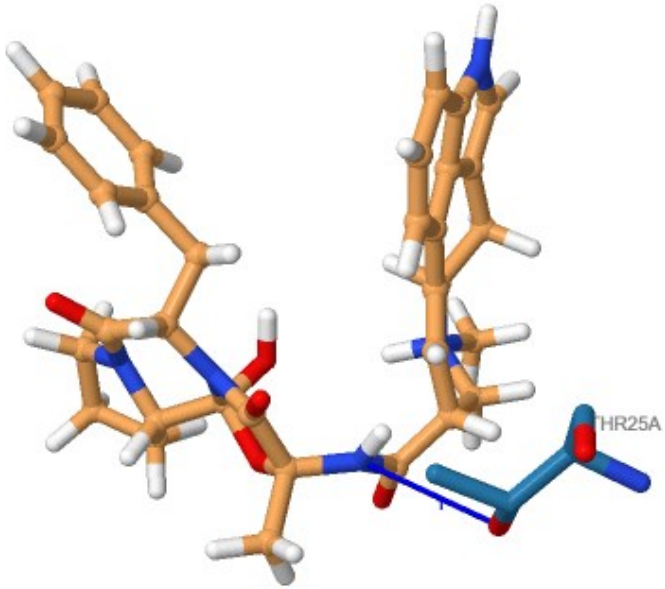

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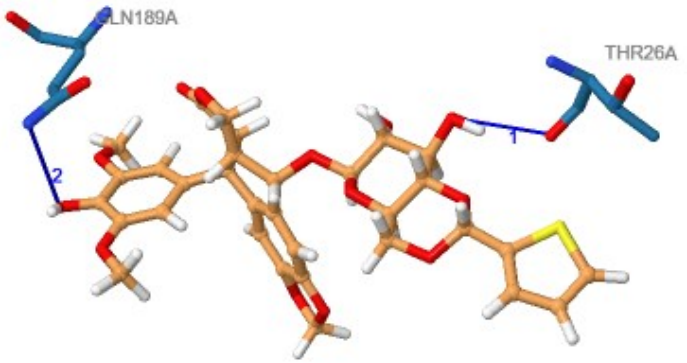

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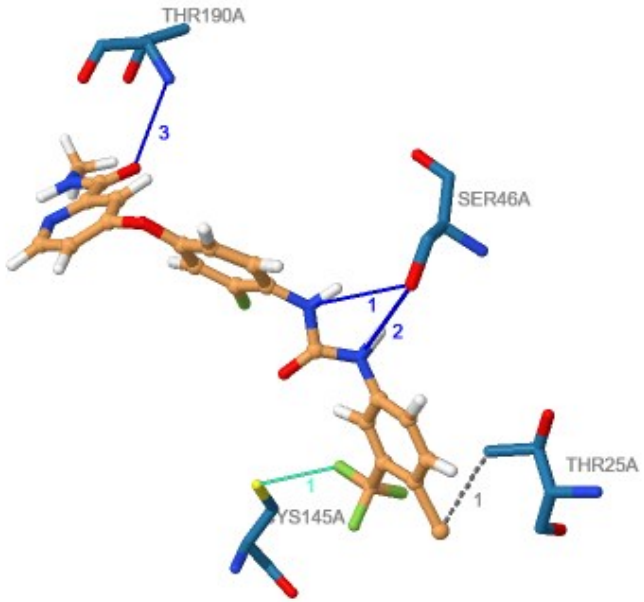

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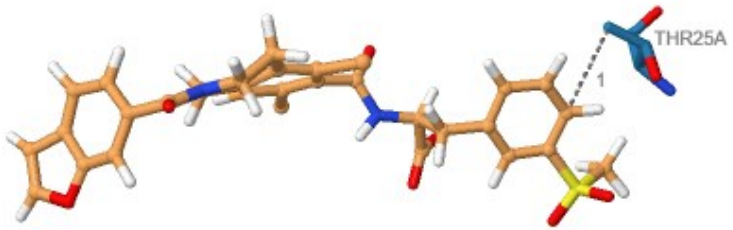

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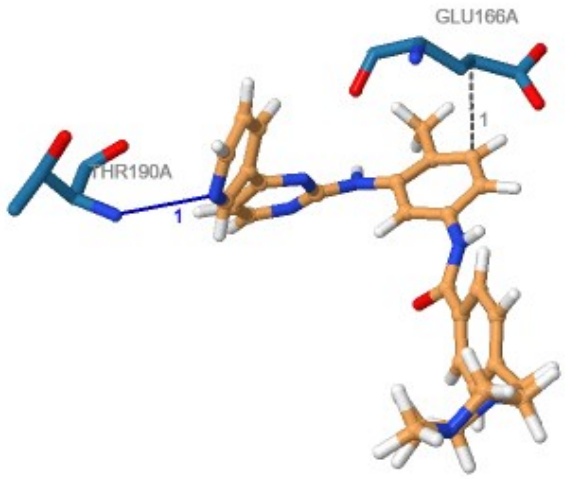

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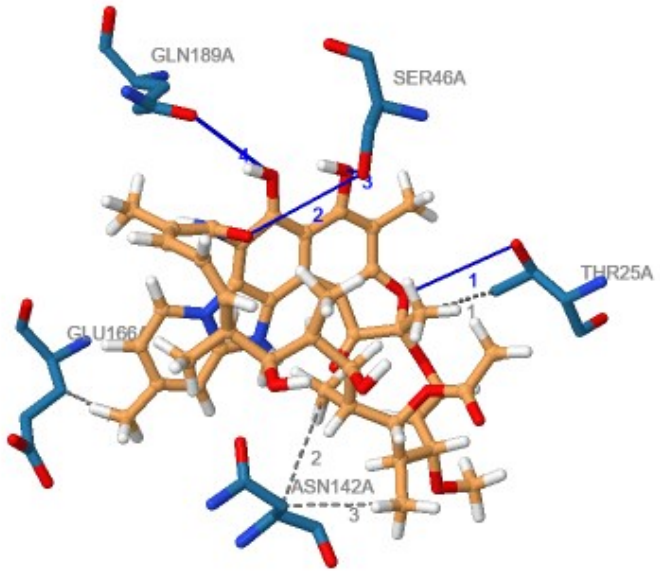

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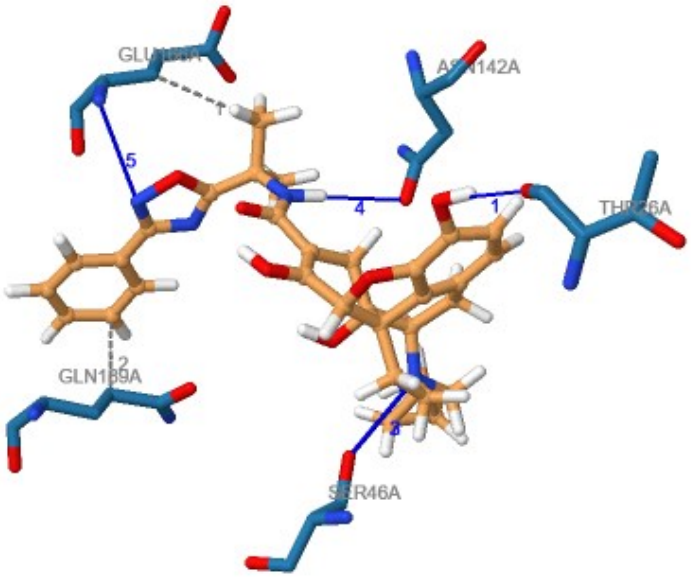

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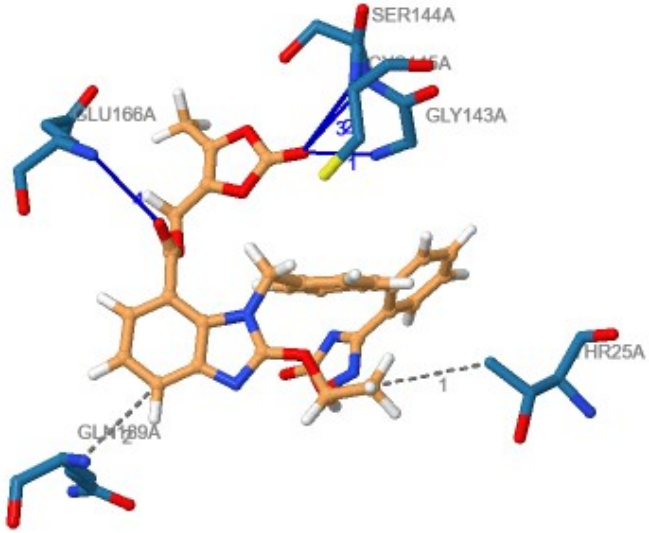

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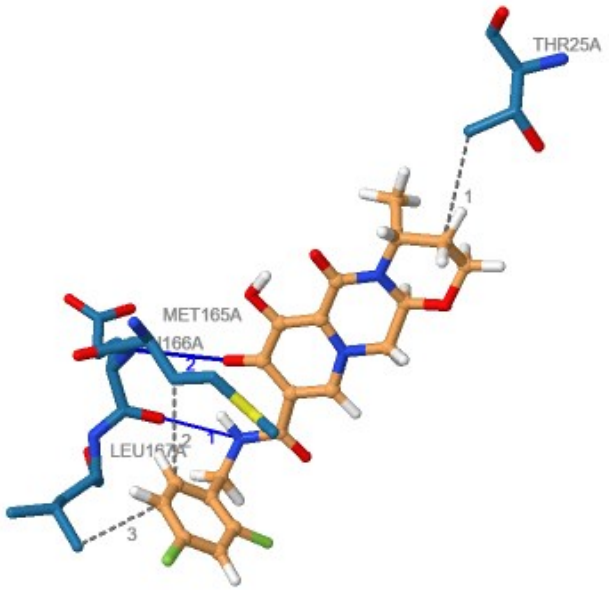

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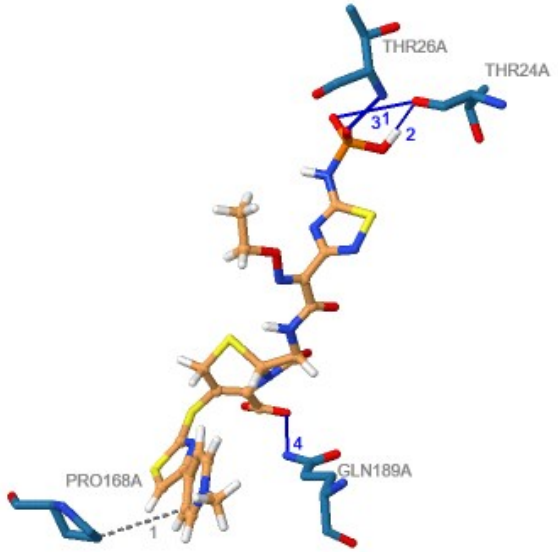

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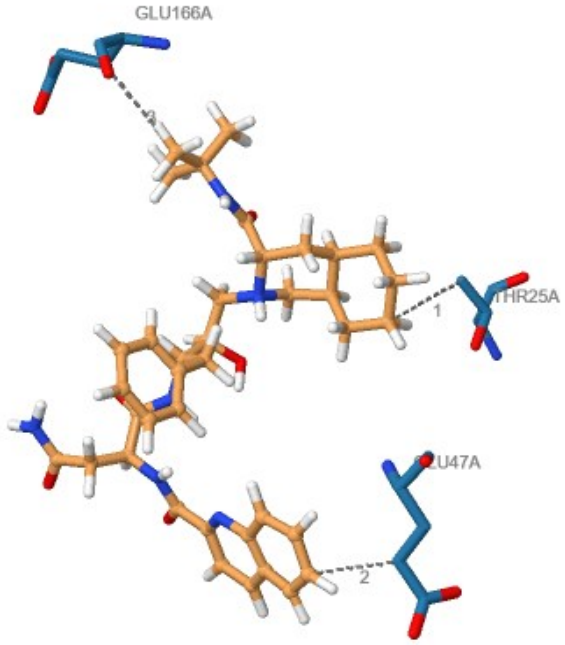

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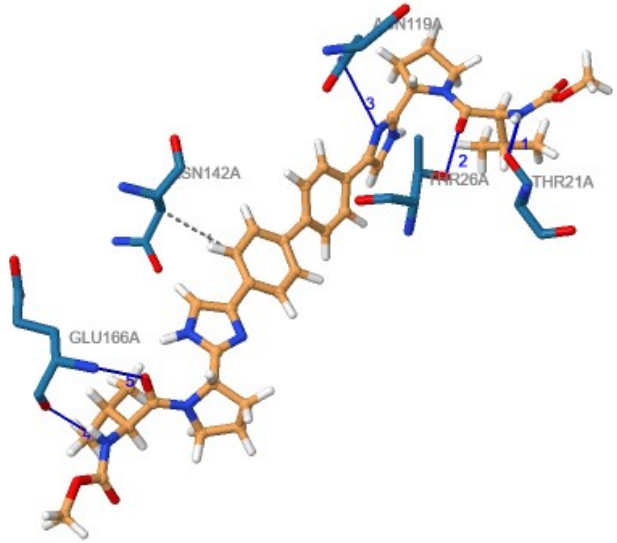

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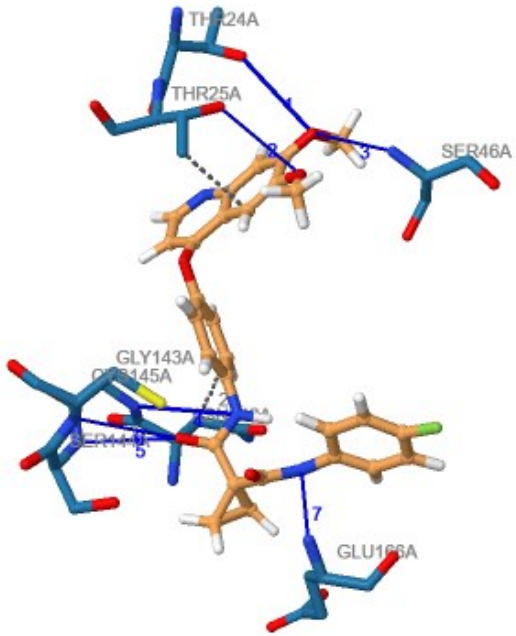	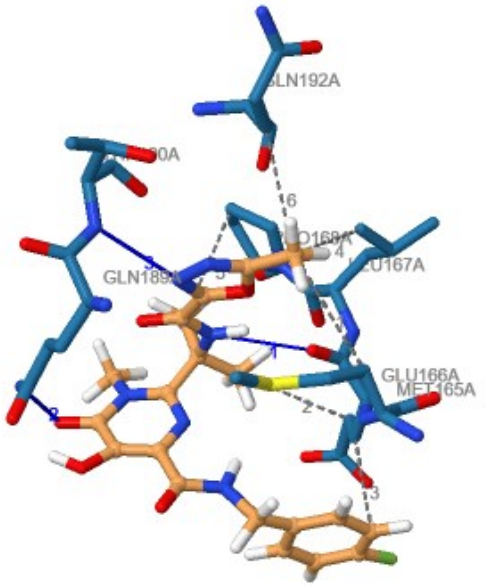
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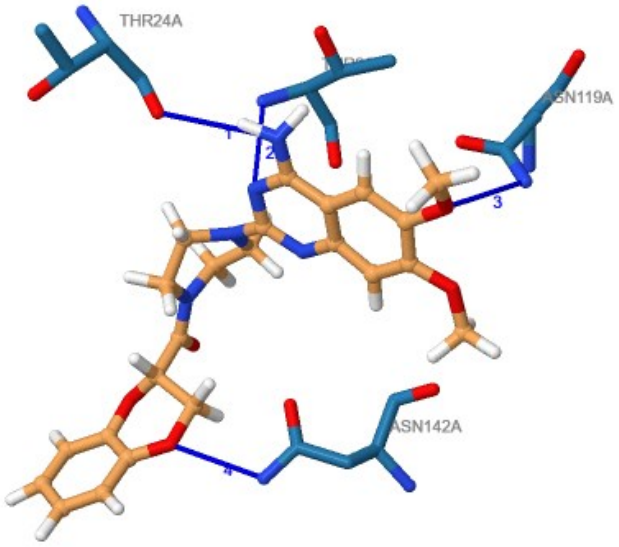	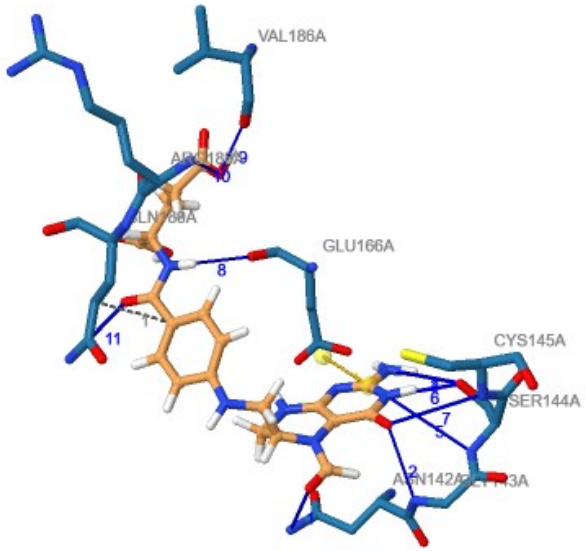

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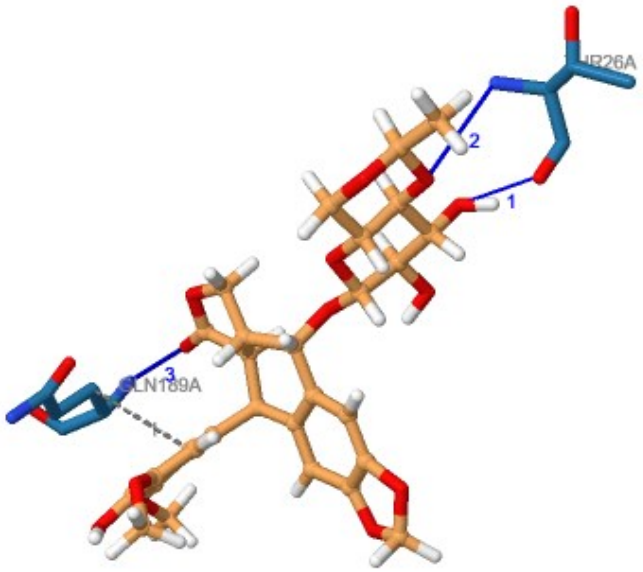

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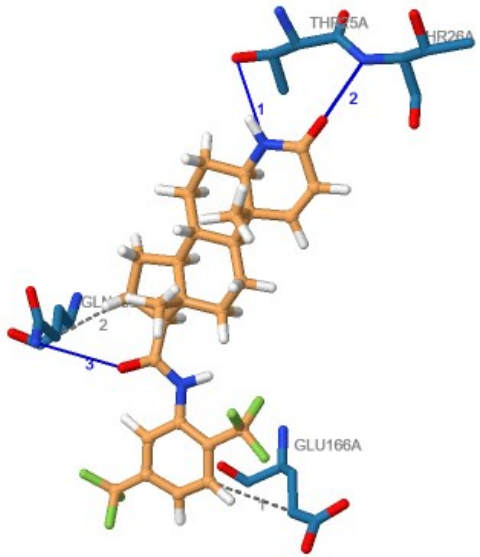

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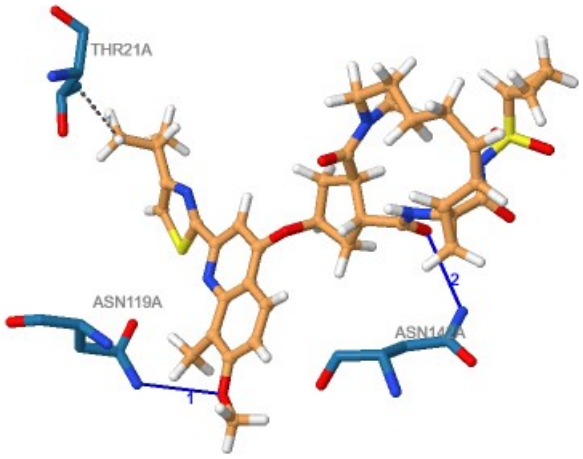
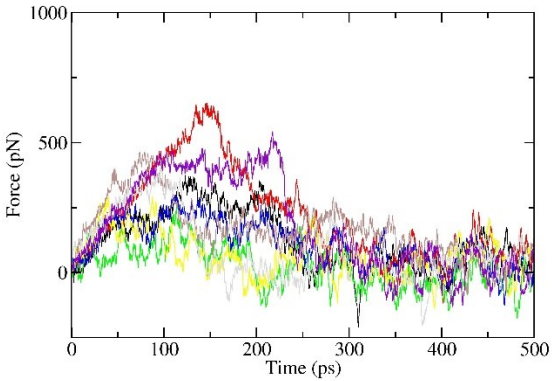


Figure S2. The dominant conformation of the top-lead compounds in the complex with SARS-CoV-2 Mpro

The result was obtained by all-atom clustering with a cut-off of 0.3 nm over the last NPT. Blue and green lines indicate hydrogen and halogen bonds between the ligand and the residues of SARS-CoV-2 Mpro, respectively. Grey and yellow dots indicate hydrophobic interactions and salt bridges between the ligand and the residues of SARS-CoV-2 Mpro, respectively. The figure was generated using a PLIP web service.[1]



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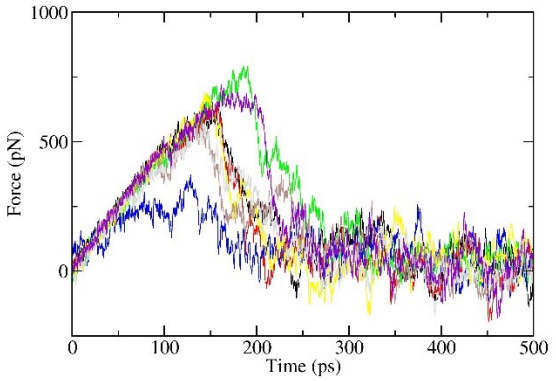

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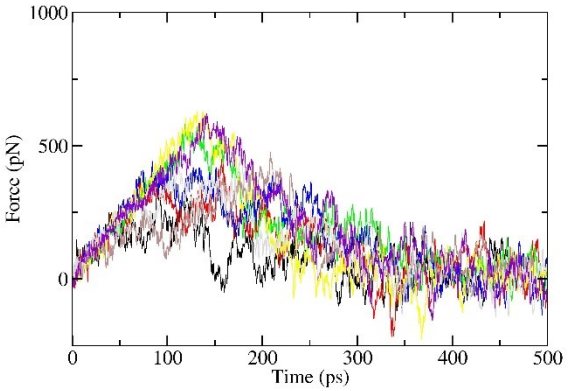

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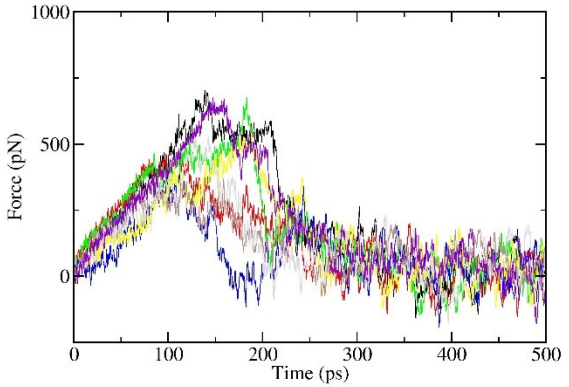

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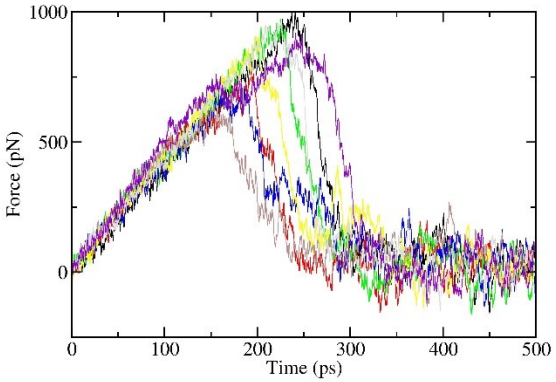

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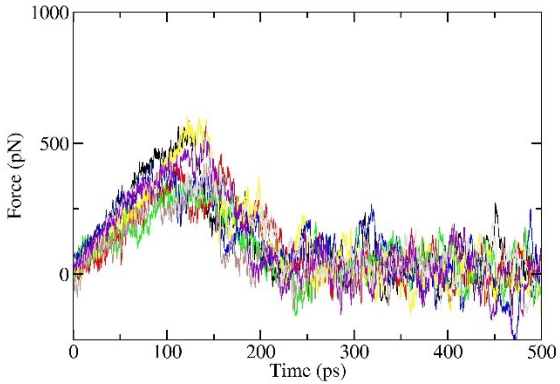

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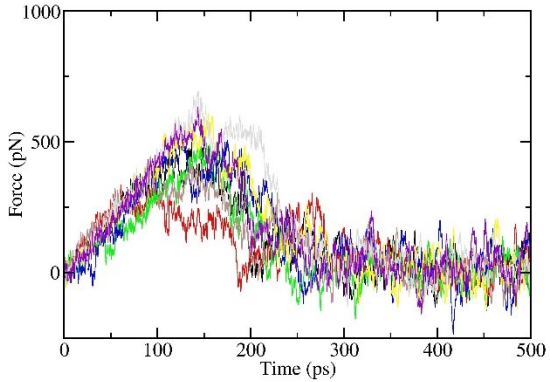

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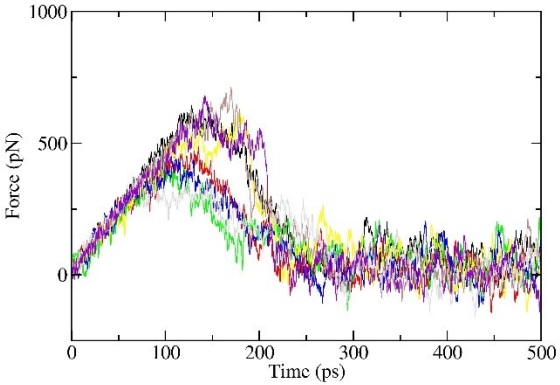

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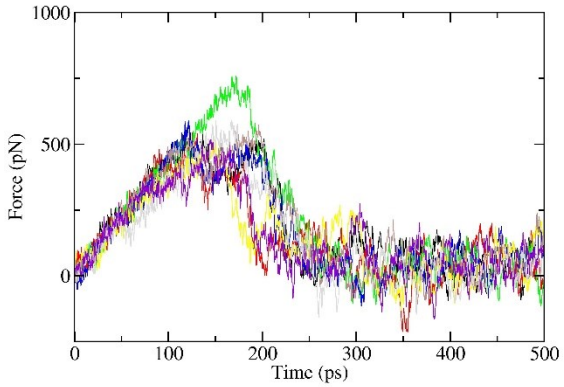

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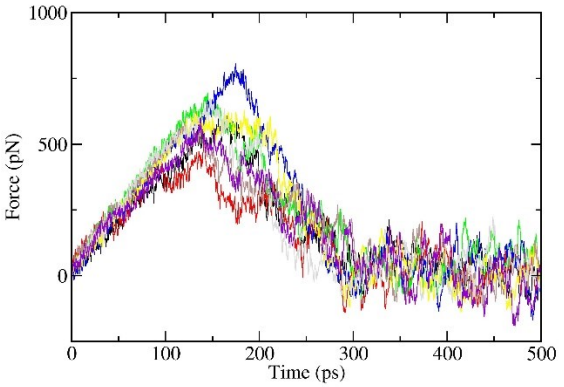

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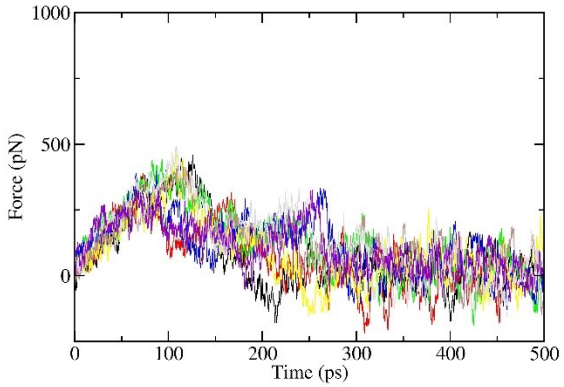

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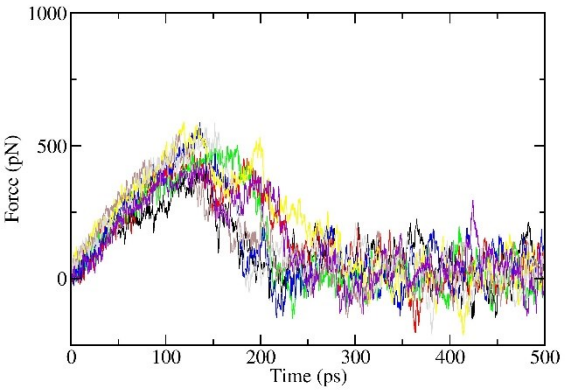

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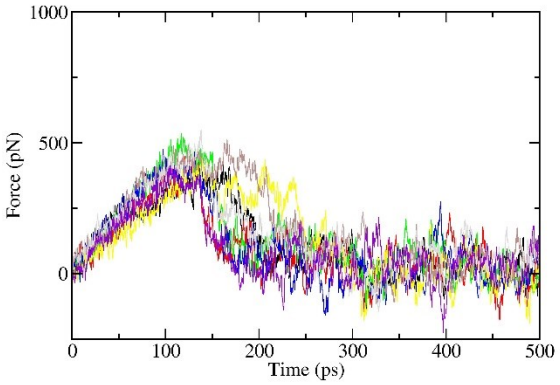

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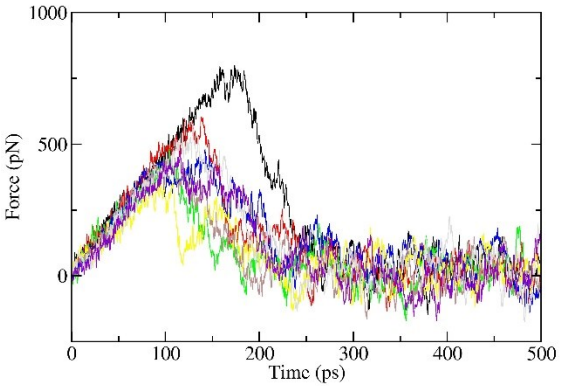

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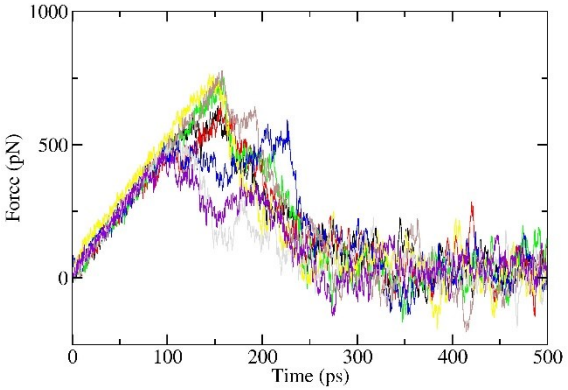

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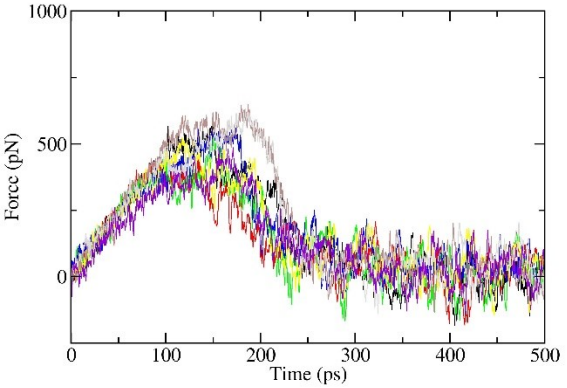

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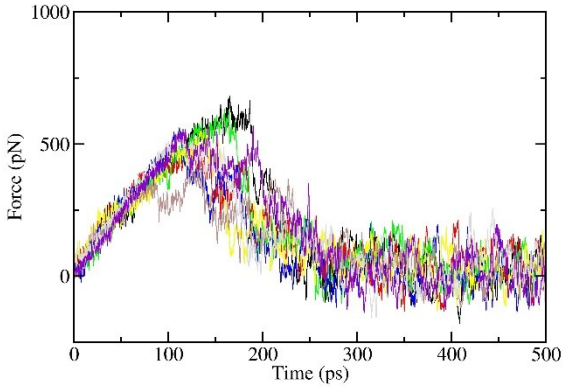

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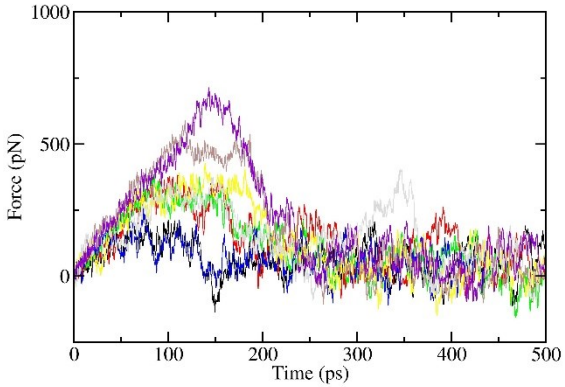

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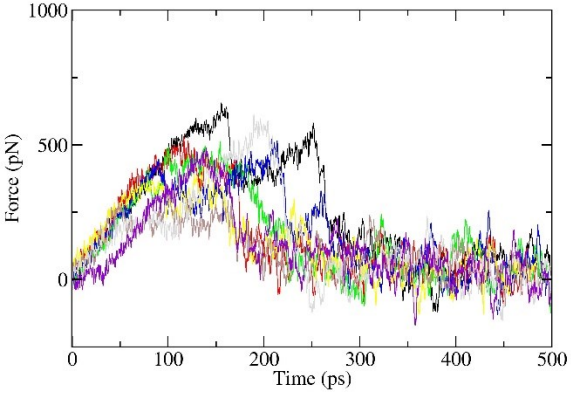

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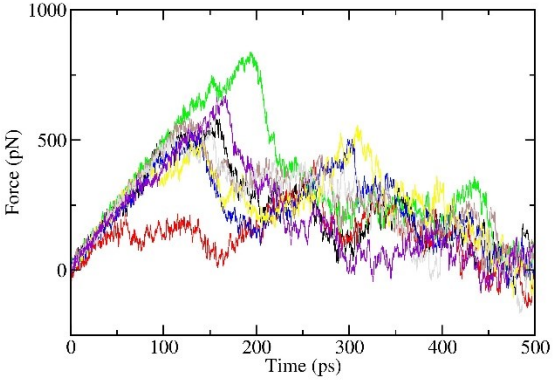

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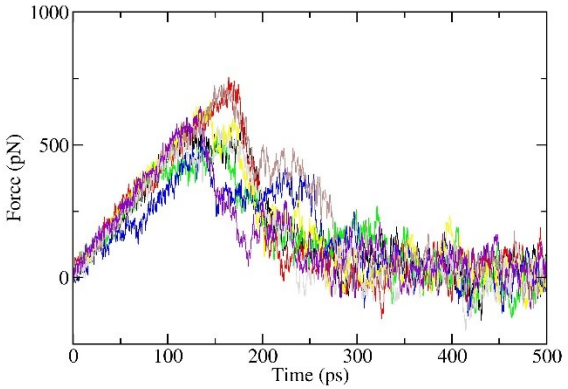

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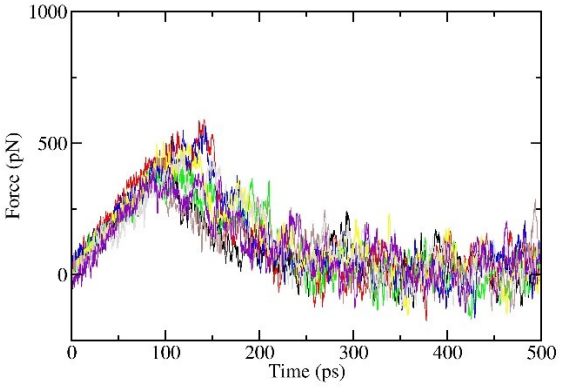

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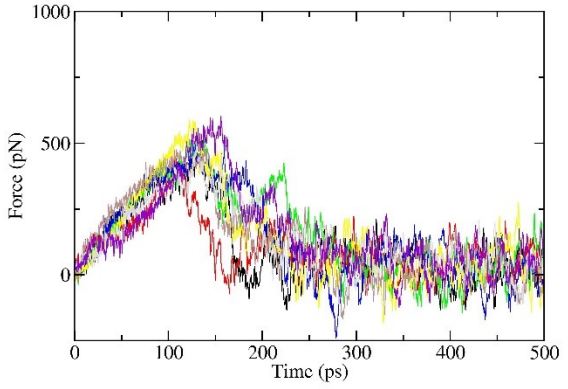

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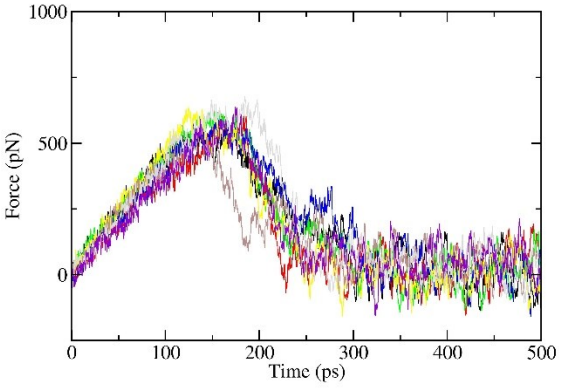

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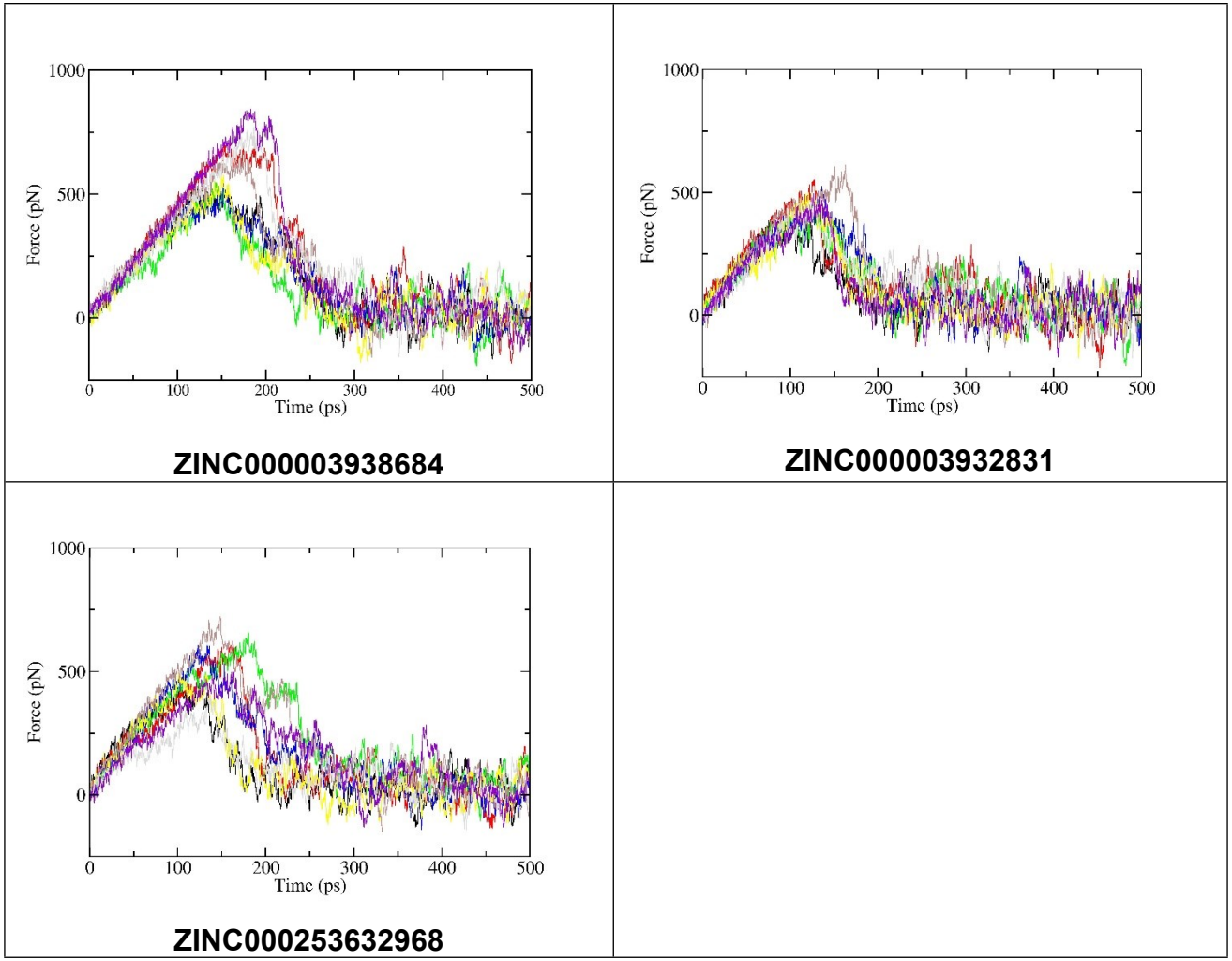

Figure S3. The pulling force in time-dependence over 8 independent SMD trajectories. Each interaction force is reported every 0.02 ps and is the 8 independent trajectories average value. Each interaction work is reported every 10 ps and is the 8 independent trajectories average value. The figure was prepared using PyMOL 1.3 open source.

References

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