

Supporting information

Marine Brominated Tyrosine Alkaloids as Promising Inhibitors of SARS-CoV-2

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Table of Contents

Table S1: Final docking validation	3
Three Dimensional Structures.....	5
Figure S1: 3D interactions between compounds 1-14 and the native ligand with M ^{Pro} (PDB ID: 6lu7).	5
Figure S2. 3D interactions of the 14 library compounds in addition to the native ligand with spike glycoprotein (PDB ID: 6VYB). ..	8
Figure S3. 3D interactions of the 14 library compounds plus the native ligand with nucleocapsid phosphoprotein (PDB ID: 6VYO).	11
Figure S4. 3D interactions between the 14 library compounds with membrane glycoprotein (PDB ID: 6M17).	14
Figure S5. 3D interactions of the 14 test compounds and the native ligand with the non-structural protein, nsp10 (PDB ID: 6W4H).	17

Table S1: Final docking validation

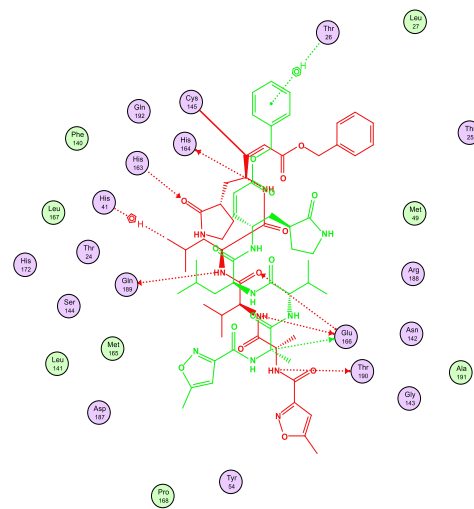
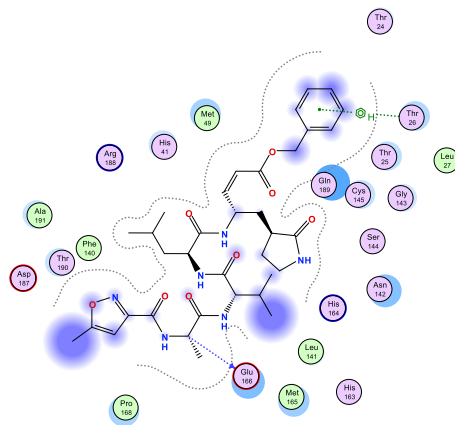
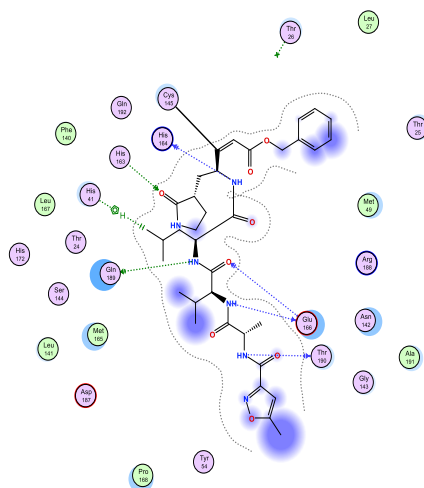
PDB
ID

Co-crystallized pose

Re-docked pose

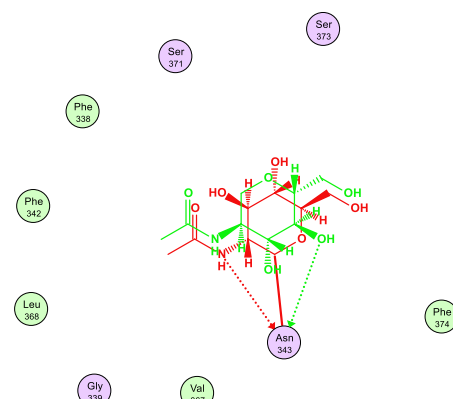
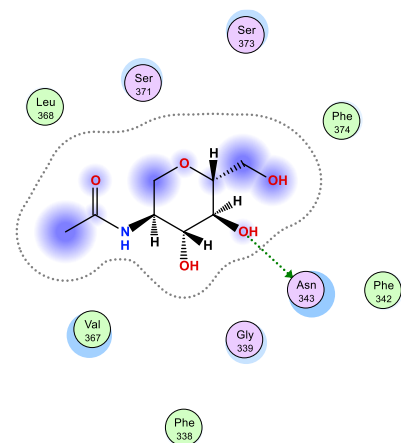
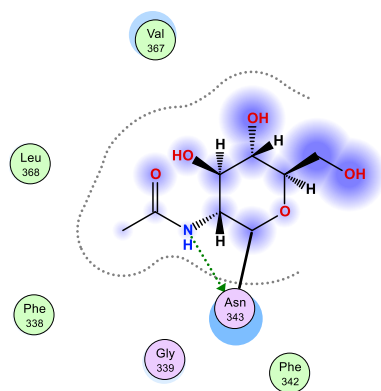
Overlay Complex/RMSD (kcal/mol)

6LU7



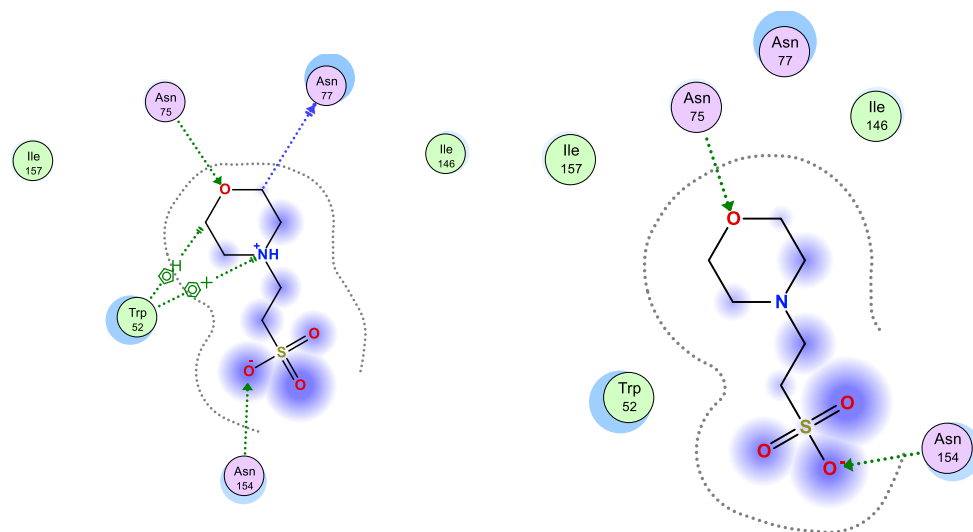
2.009

6VYB



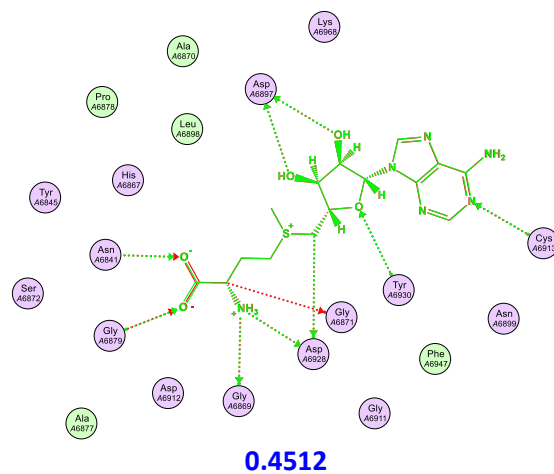
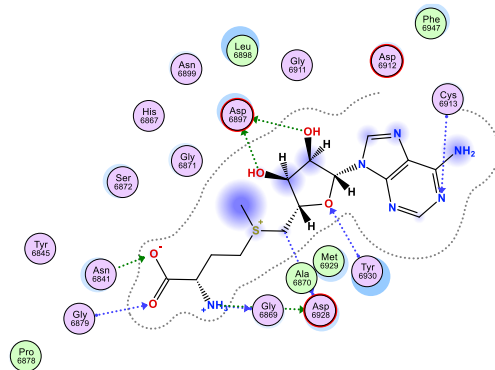
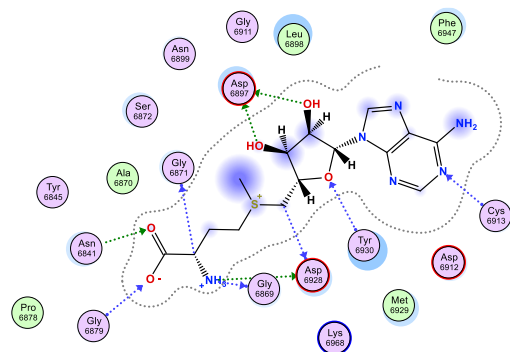
0.8360

6VYO



0.856

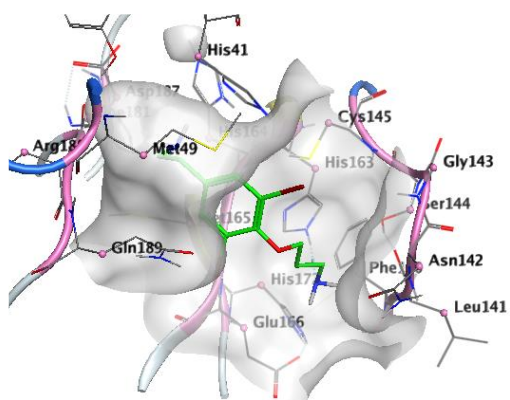
6W4
H



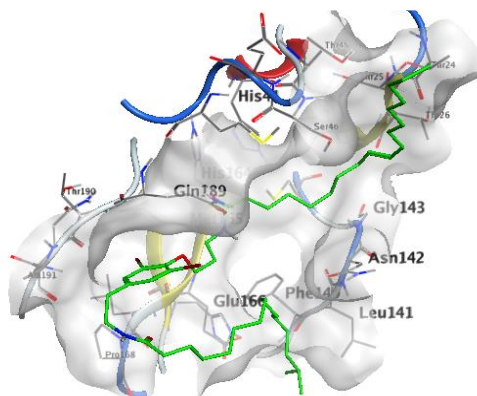
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Three Dimensional Structures

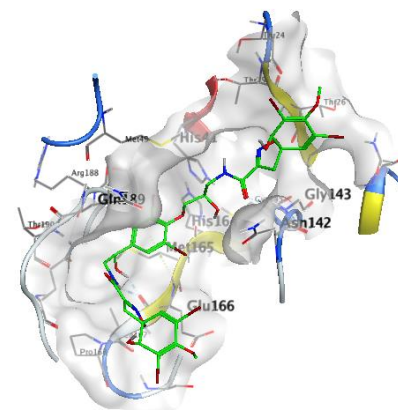
Figure S1: 3D interactions between compounds 1-14 and the native ligand with M^{Pro} (PDB ID: 6lu7).



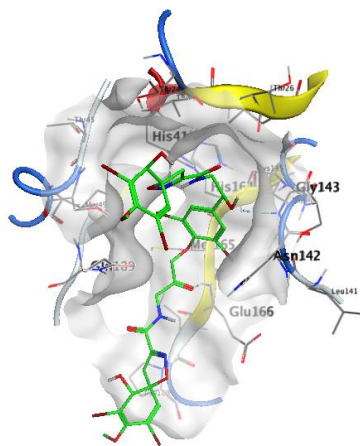
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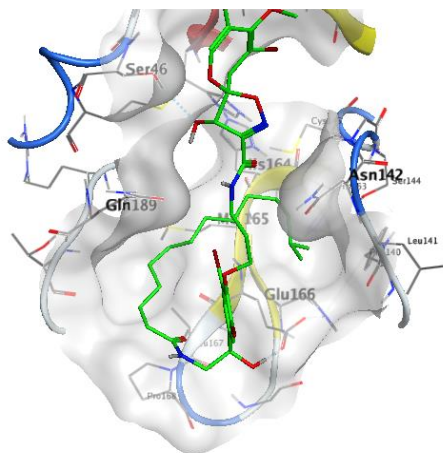
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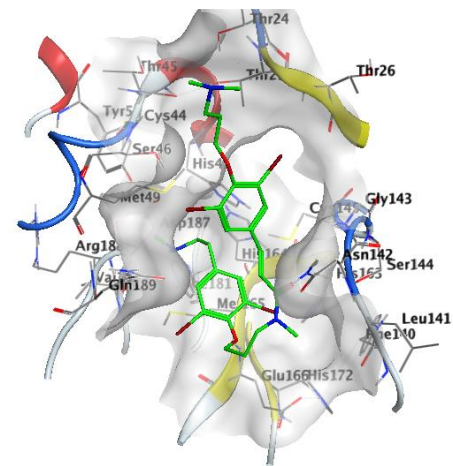
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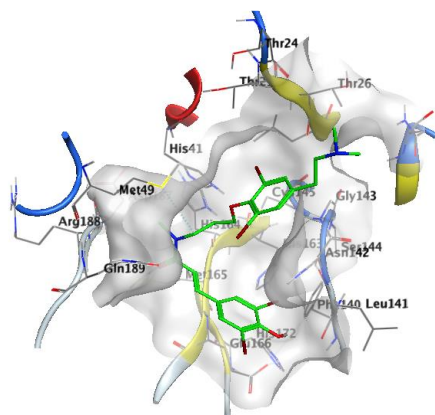
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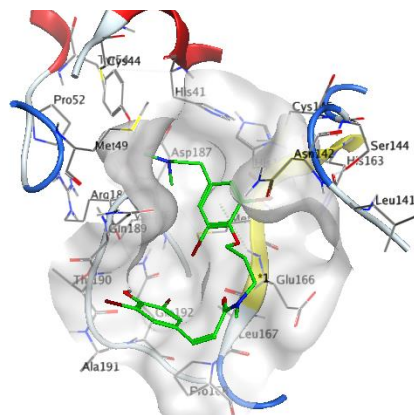
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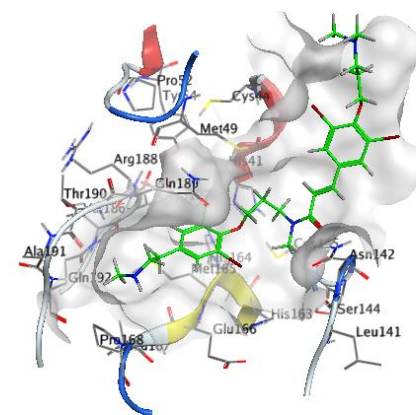
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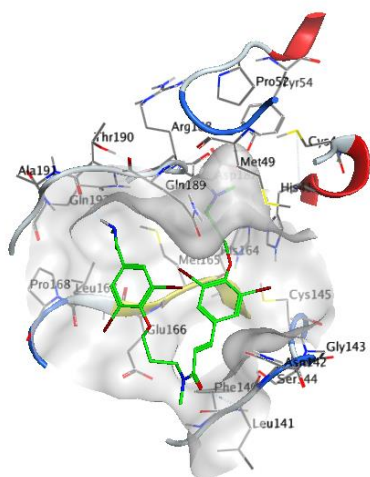
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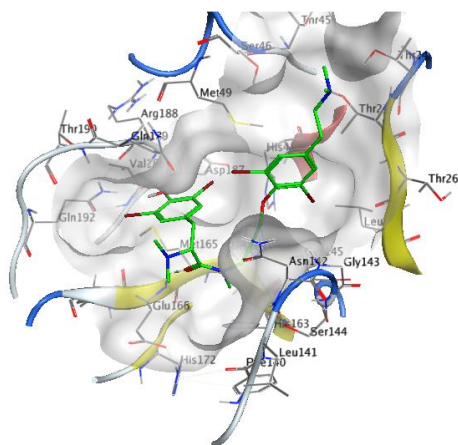
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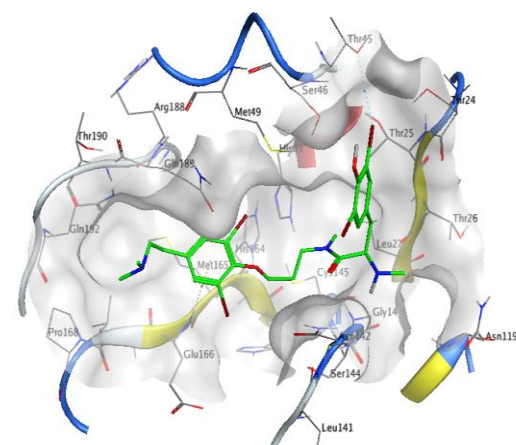
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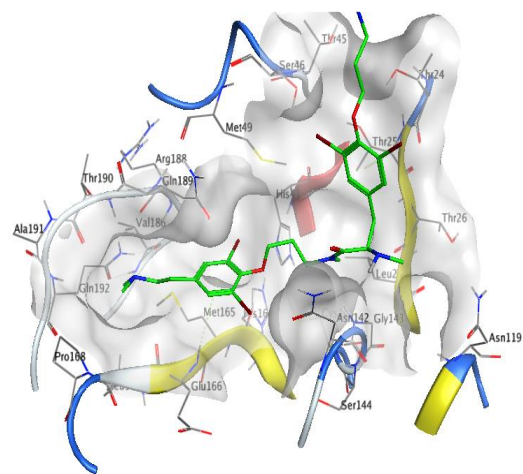
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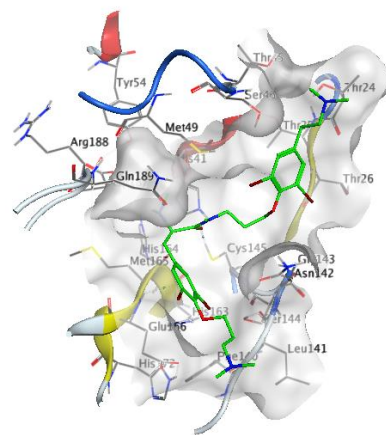
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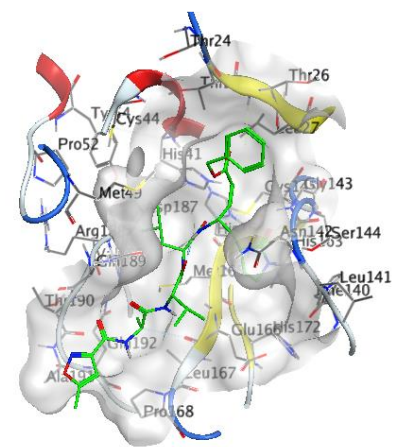
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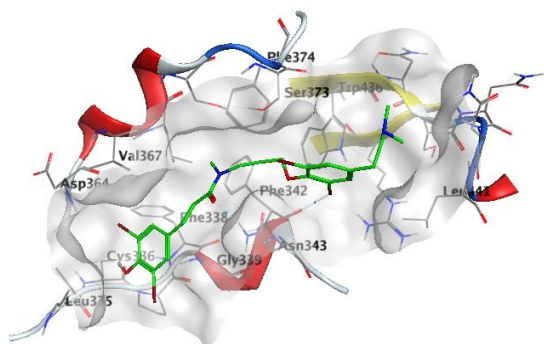
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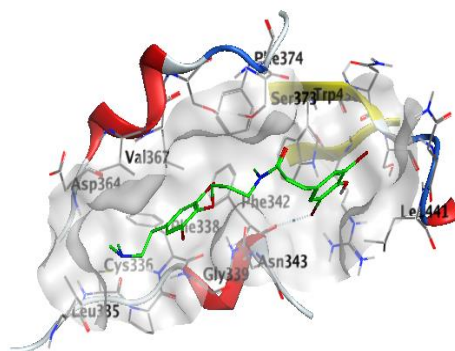
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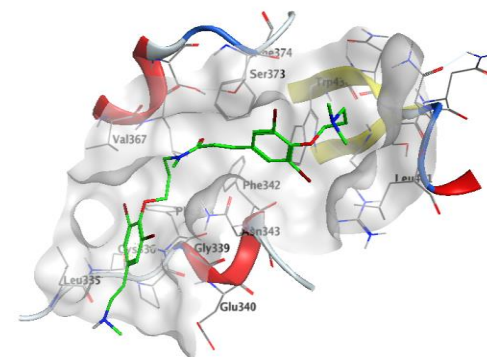
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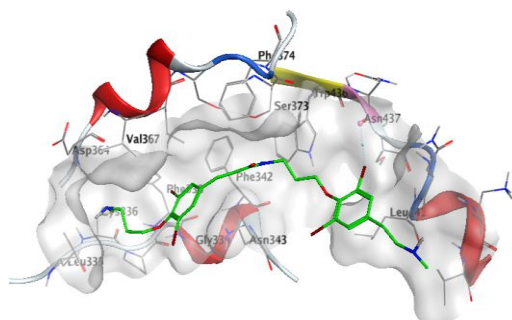
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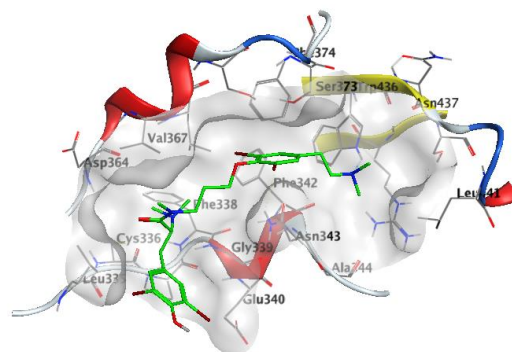
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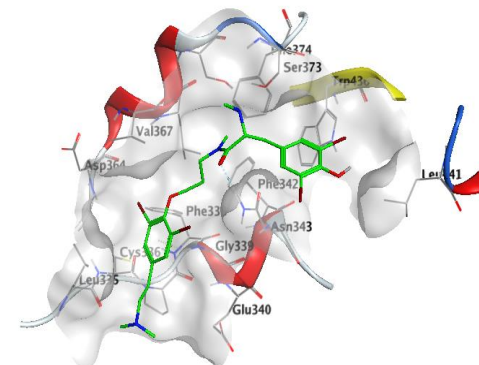
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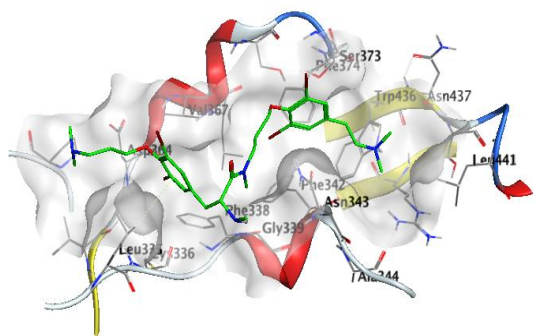
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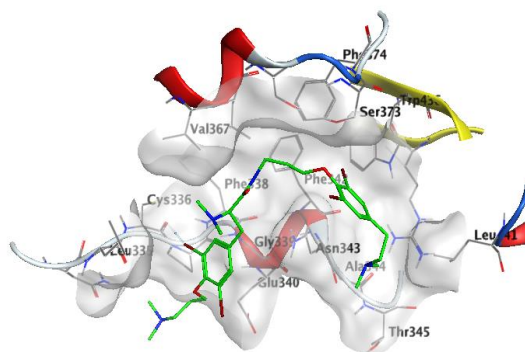
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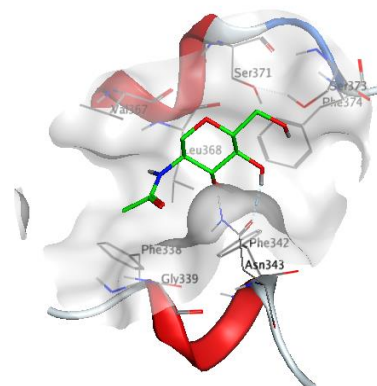
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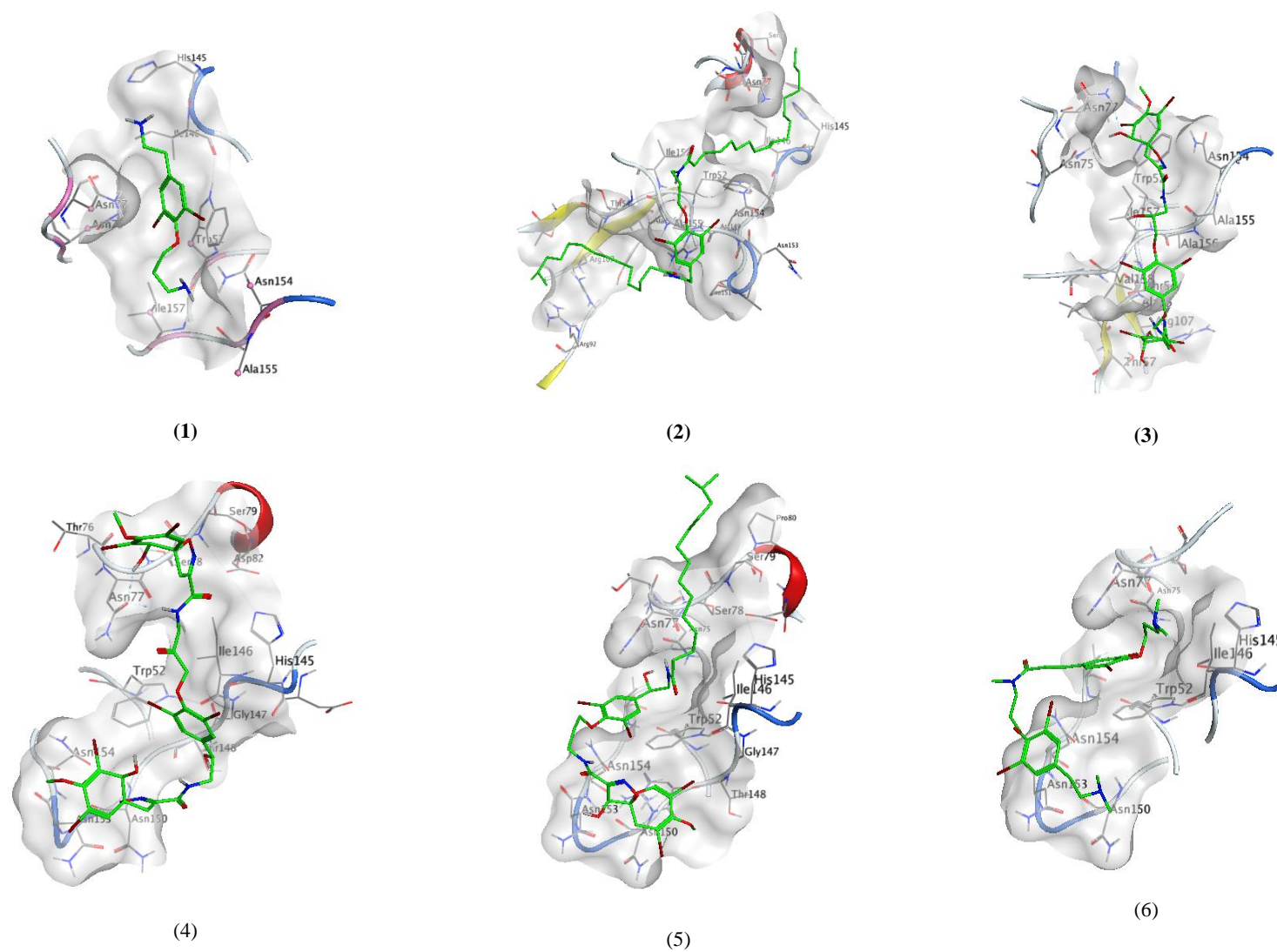


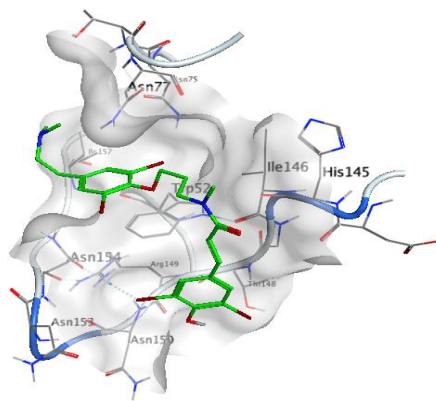
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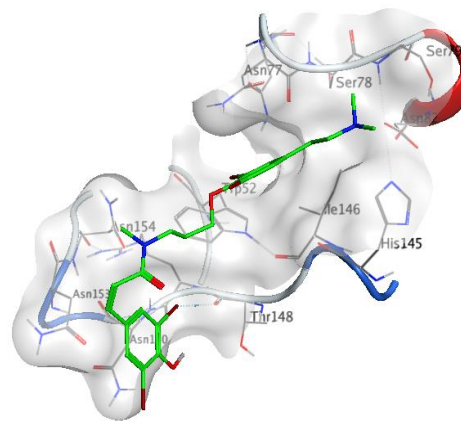
(Native)

Figure S3. 3D interactions of the 14 library compounds plus the native ligand with nucleocapsid phosphoprotein (PDB ID: 6VYO).

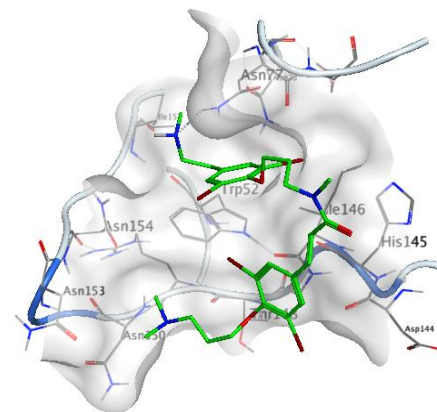




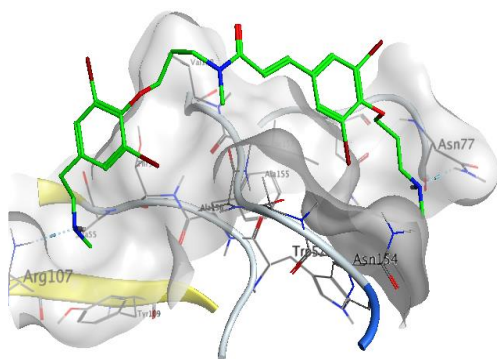
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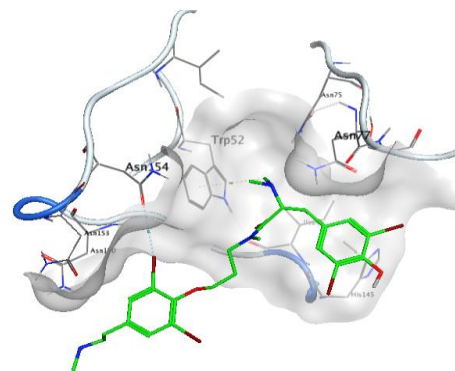
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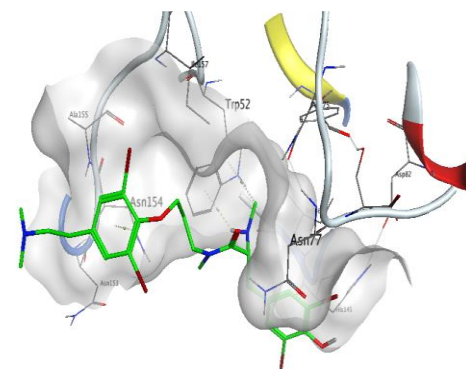
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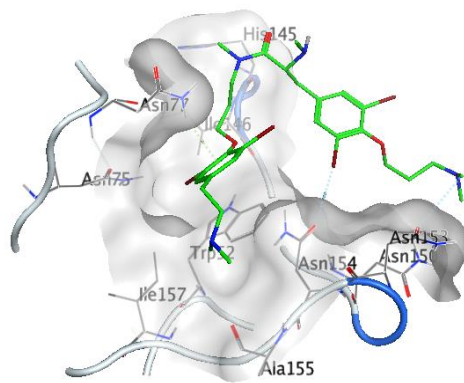
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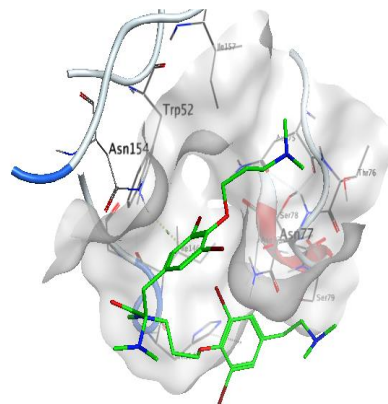
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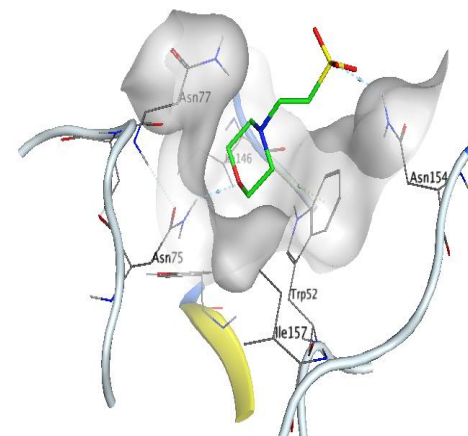
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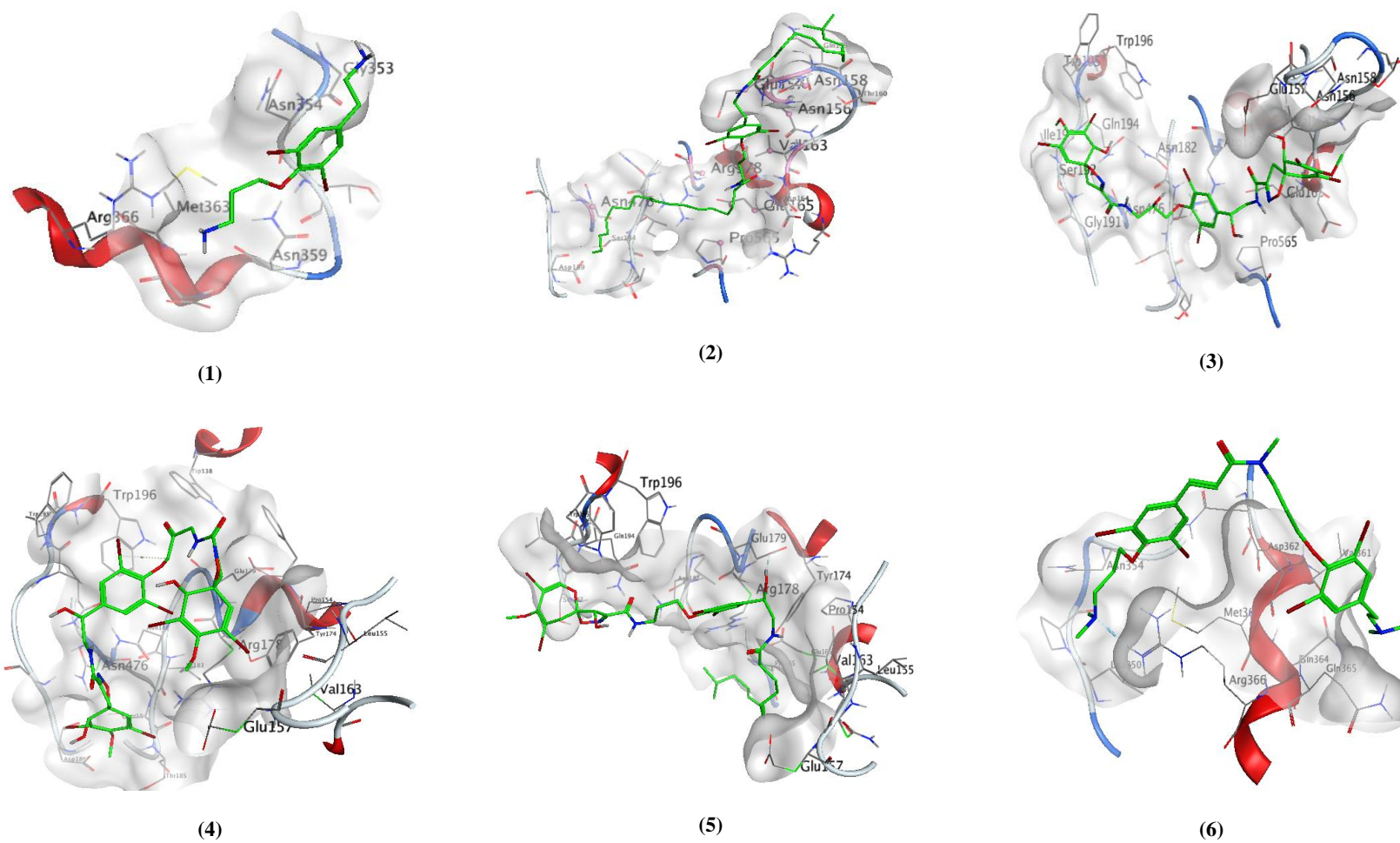


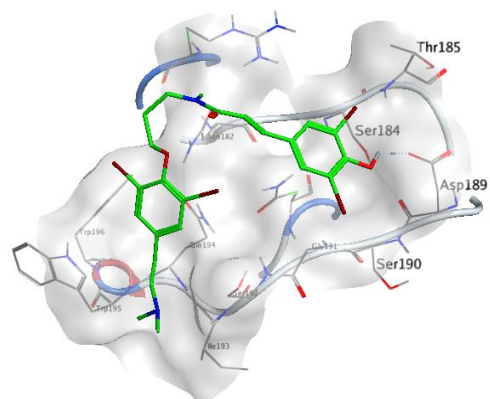
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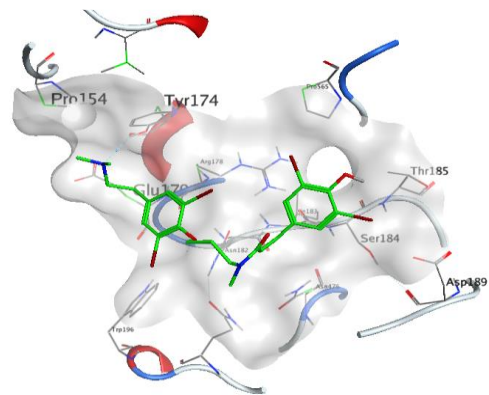
(Native)

Figure S4. 3D interactions between the 14 library compounds with membrane glycoprotein (PDB ID: 6M17).

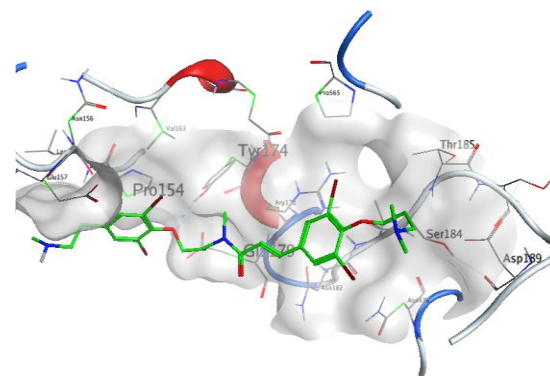




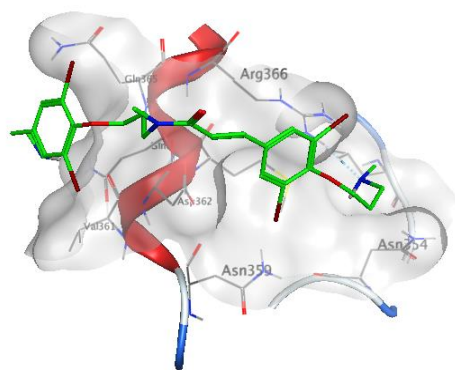
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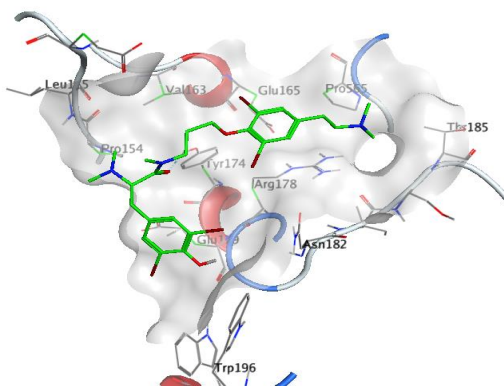
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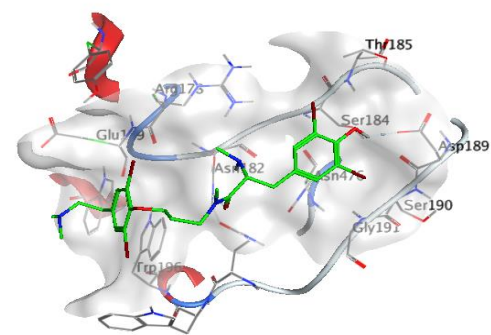
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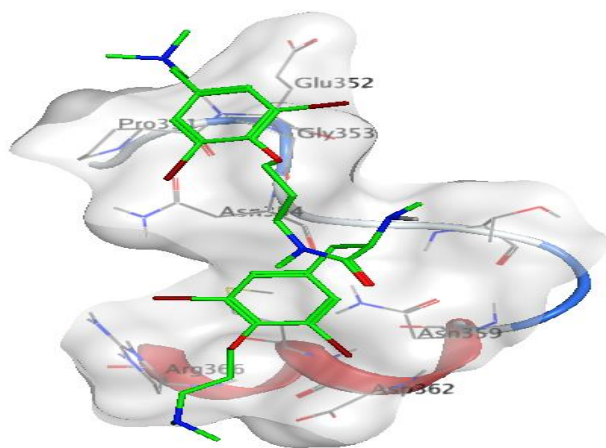
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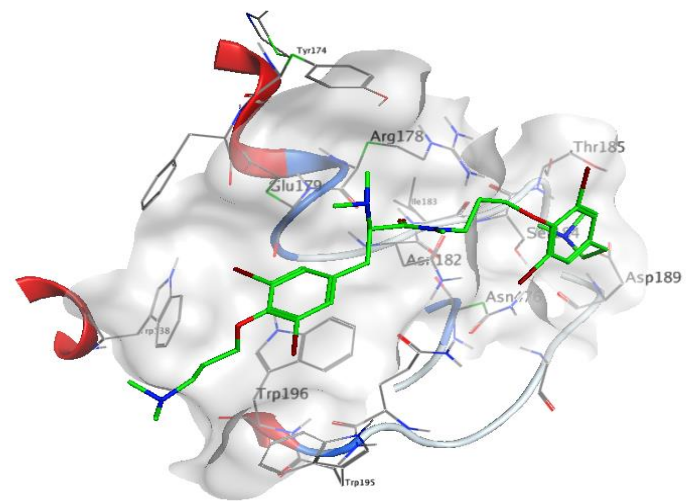
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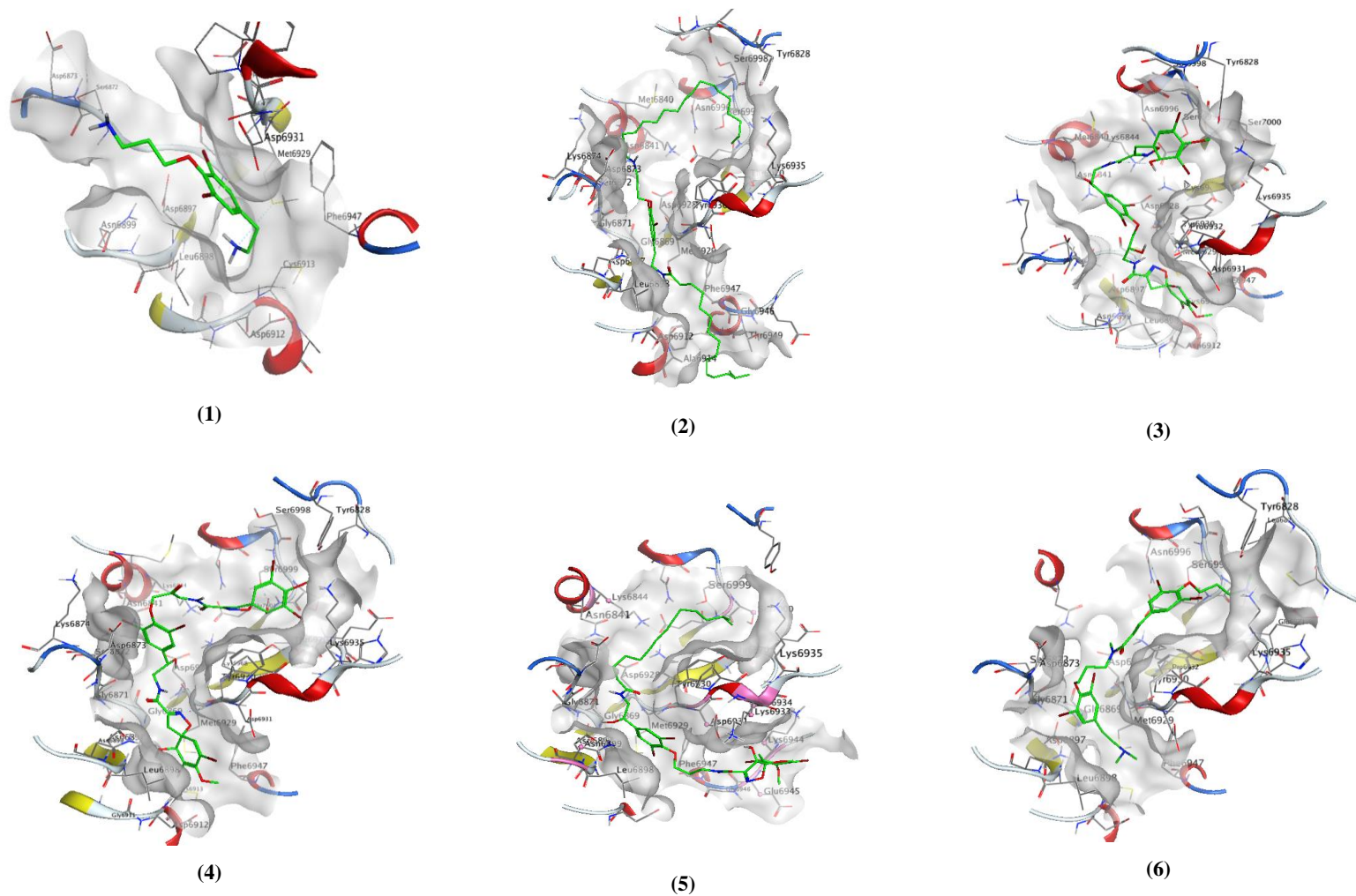


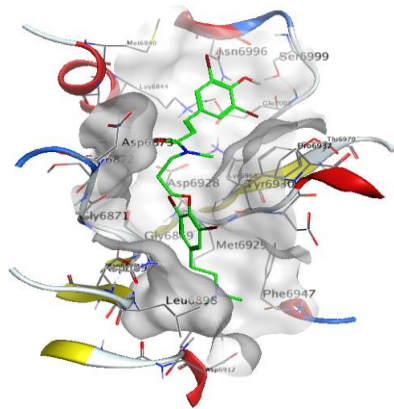
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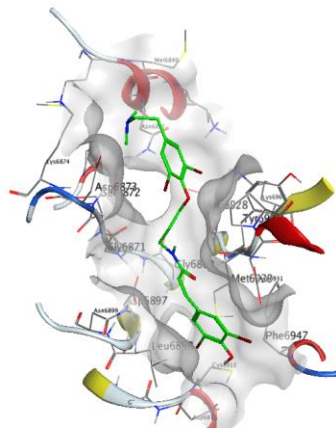
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Figure S5. 3D interactions of the 14 test compounds and the native ligand with the non-structural protein, nsp10 (PDB ID: 6W4H).

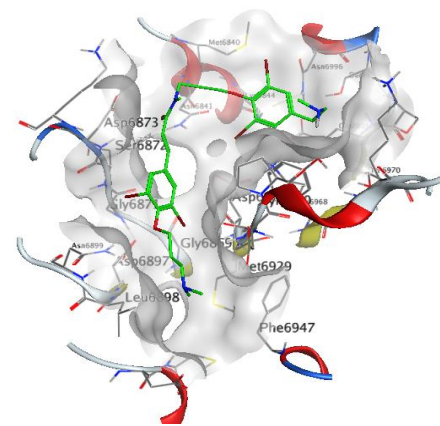




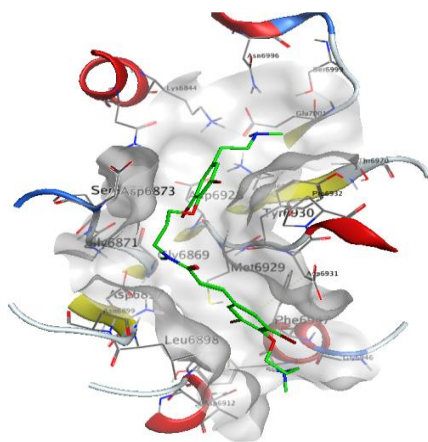
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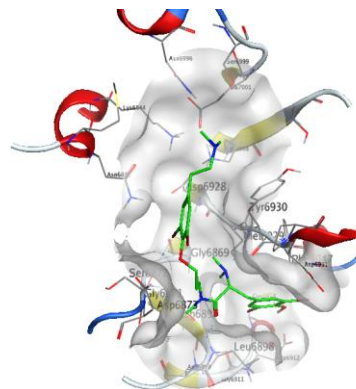
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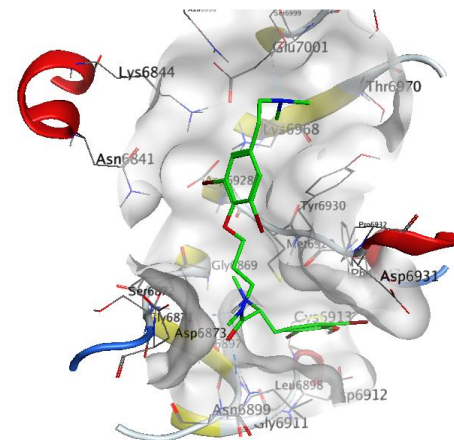
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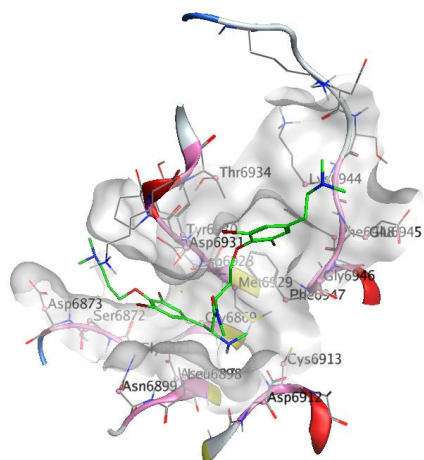
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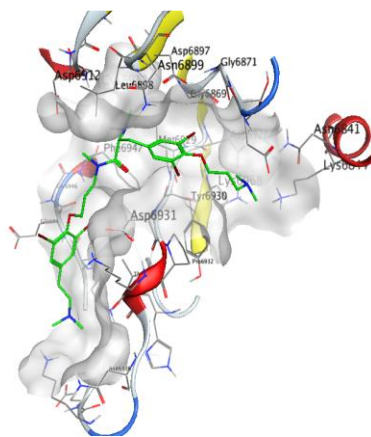
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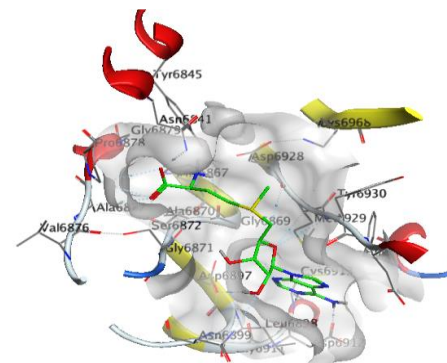
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(13)



(14)



(Native)