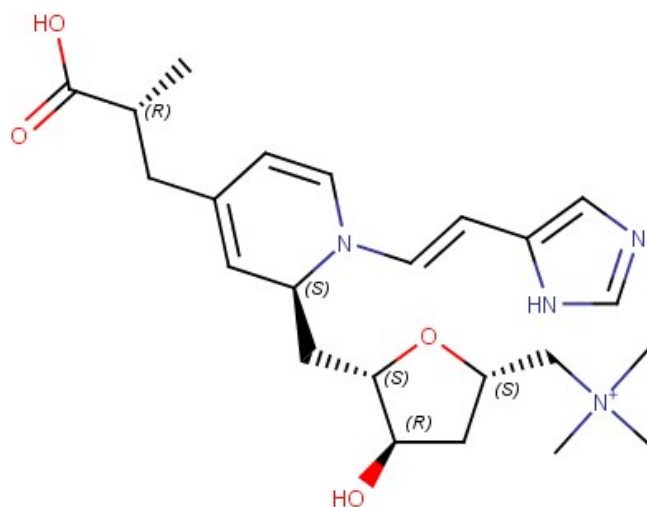


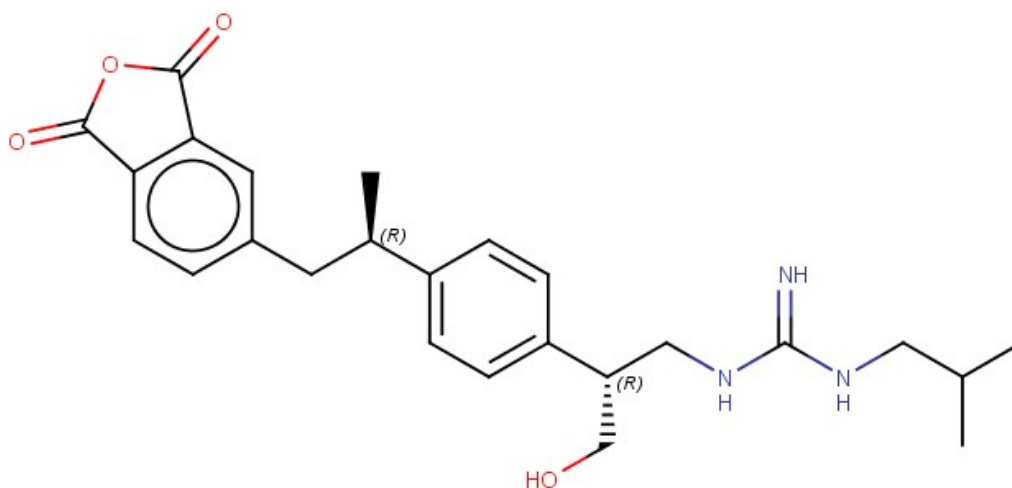
## Supporting Information

### *In silico* Identification of Potential SARS COV-2 2'-O-methyltransferase Inhibitor: Fragment-Based Screening Approach and MM-PBSA Calculations

A.



B.

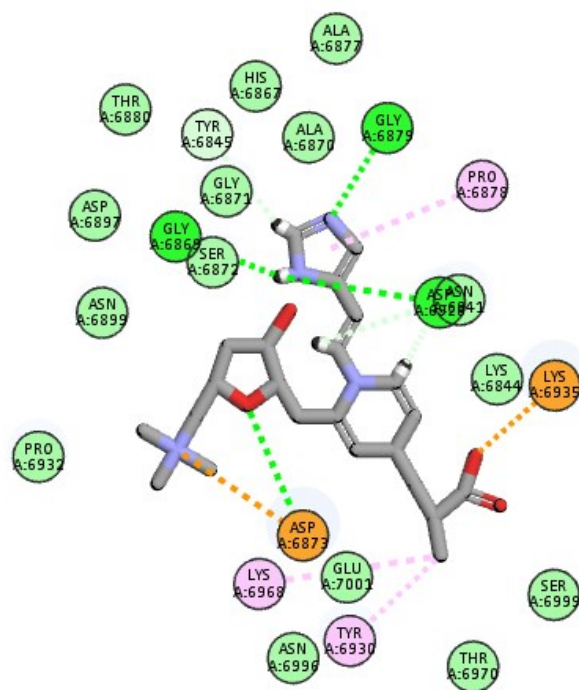


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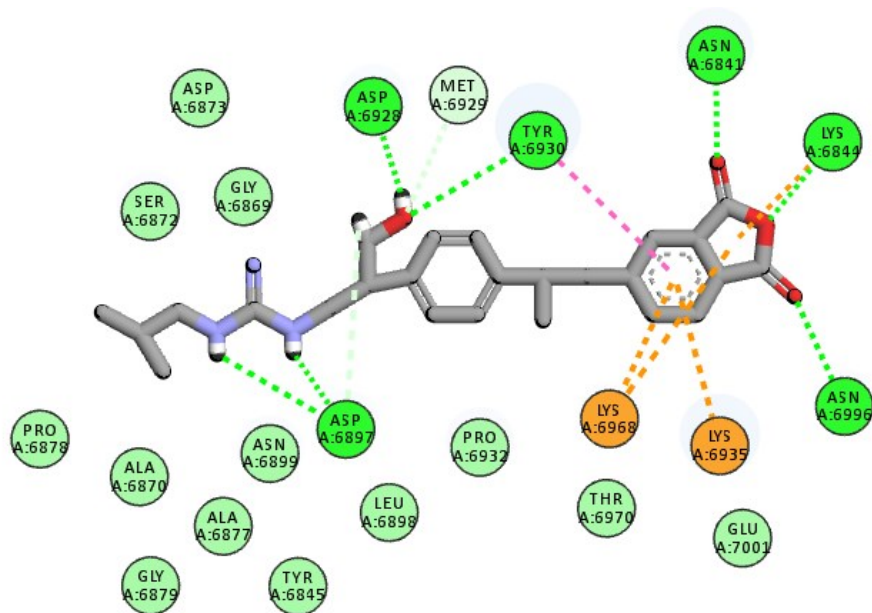
The chemical structure shows the active site of the enzyme. A benzyl derivative is bound to the active site, forming a covalent intermediate. The structure includes a benzyl group, a hydroxyl group, and a pyrazole ring. The stereochemistry is indicated with (R) and (S) labels.

2

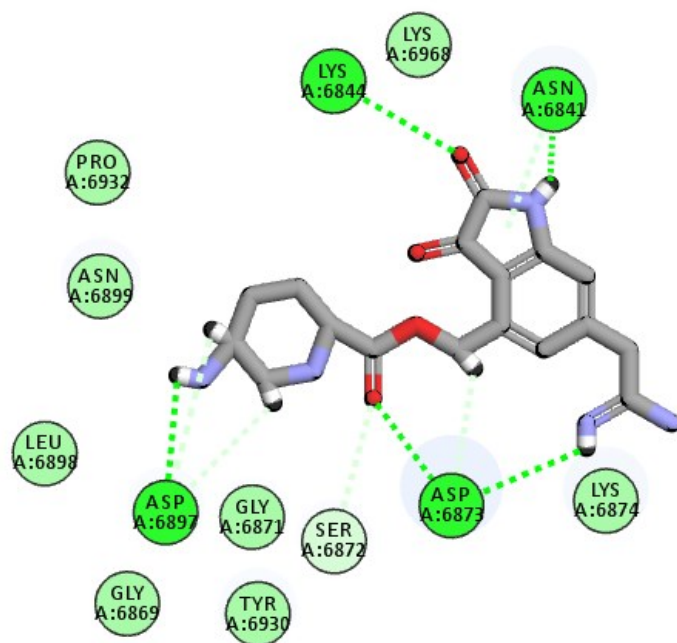
A.



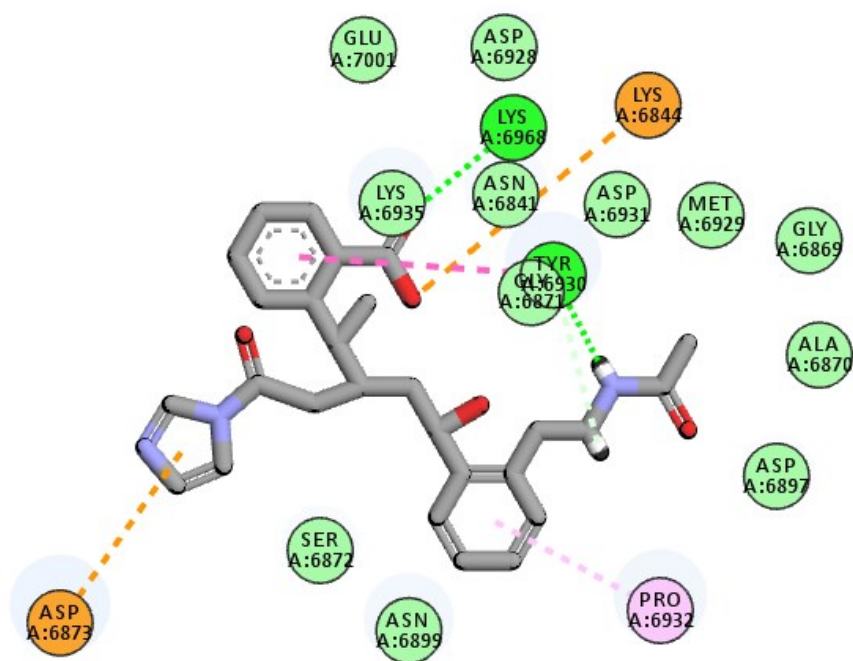
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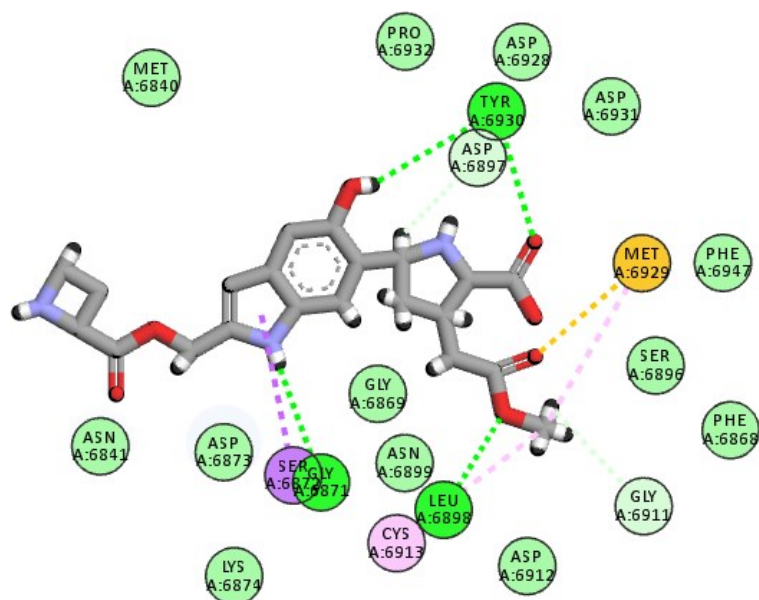
C.



D.



E.



**Figure S2.** 2D interactions diagram for compounds (A) W-1 (B) W-2 (C) W-3 (D) W-4 and (E) W-5.

**The protocol used for conducting the docking study:**

receptor = 6wkq.pdbqt

ligand = AP-20.pdbqt

out= AP-20 out.pdbqt

center\_x= 83

center\_y= 13

center\_z= -0.5

size\_x= 22

size\_y= 22

size\_z= 22

exhaustiveness= 64

**Table S1. Physico-chemical properties and medicinal chemistry friendliness of AP-20**

<b>GIA</b>	Low
<b>BBB</b>	No
<b>P-gP substrate</b>	Yes
<b>CYP1A2 inhibitor</b>	No
<b>CYP2C19 inhibitor</b>	No
<b>CYP2C9 inhibitor</b>	No
<b>CYP2D6 inhibitor</b>	No
<b>CYP3A4 inhibitor</b>	No
<b>PAINS Alerts</b>	0
<b>Egan violations</b>	1
<b>Lipinski Violations</b>	3