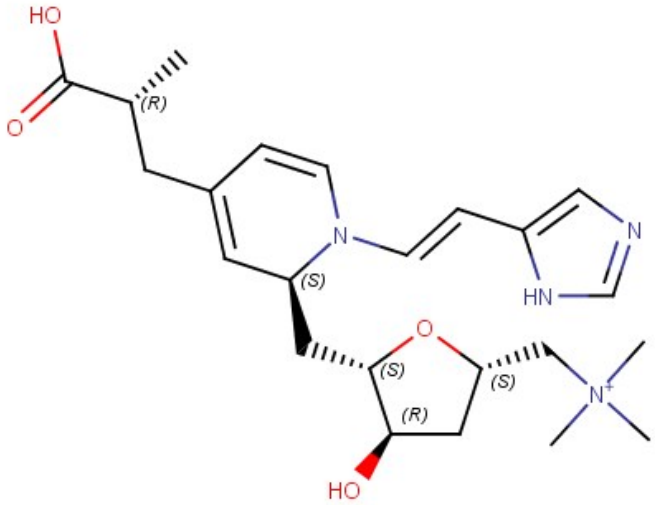
Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

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

A.



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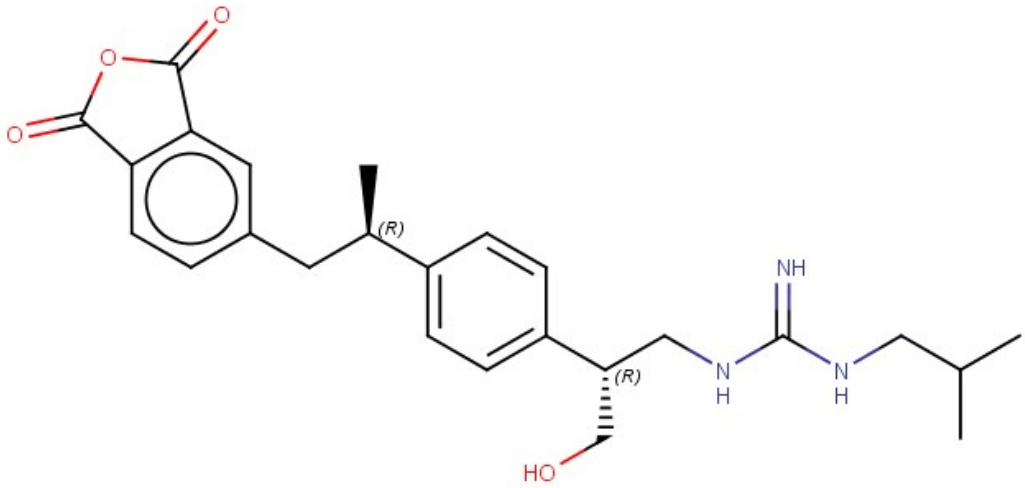

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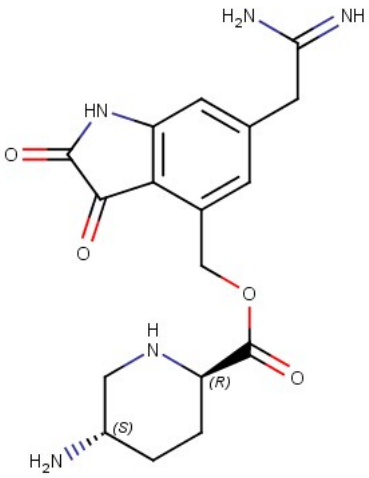

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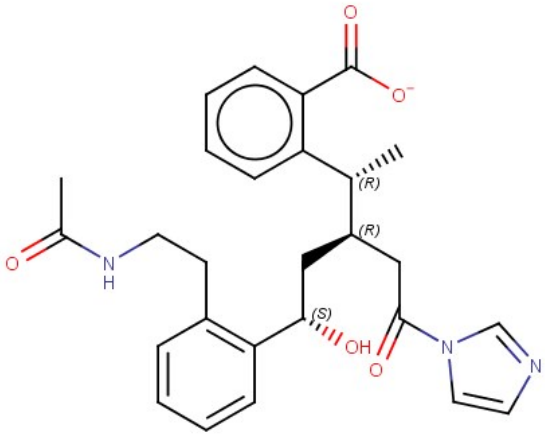

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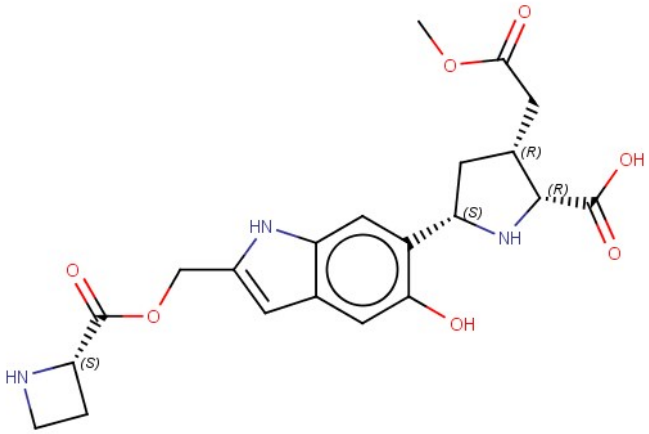
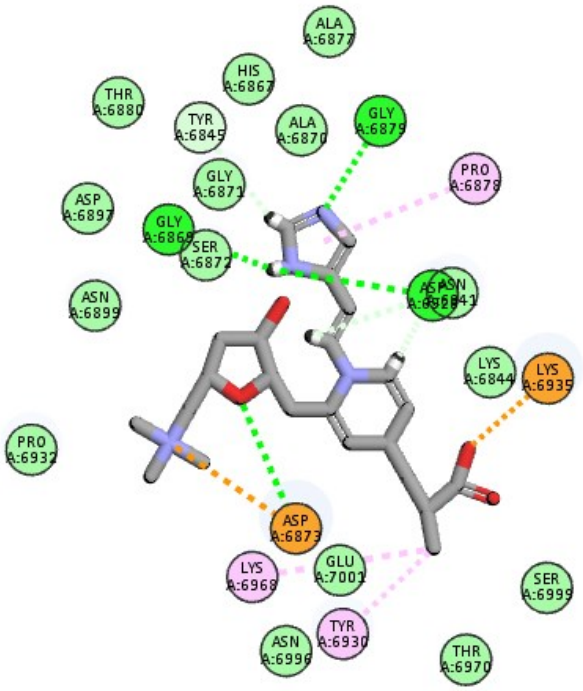


Figure S1. The 2D structures of the other five designed compounds (**A**) **W-1** (**B**) **W-2** (**C**) **W-3** (**D**) **W-4** and (**E**) **W-5**.

A.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THR A:6880
TYR A:6845
ALA A:6870
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ASP A:6897
GLY A:6868
SER A:6872
ASN A:6899
LYS A:6844
LYS A:6935
PRO A:6932
ASP A:6873
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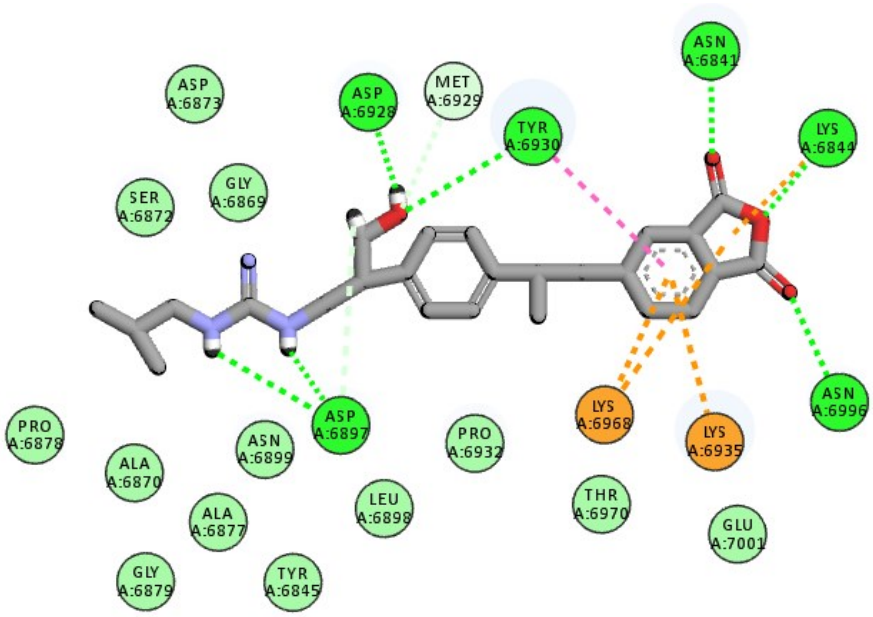
SER A:6999
TYR A:6930
ASN A:6996
THR A:6970

B.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ASP A:6873
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LYS A:6844
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LYS A:6968
LYS A:6935
PRO A:6878
ASP A:6897
ASN A:6899
PRO A:6932
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LEU A:6898
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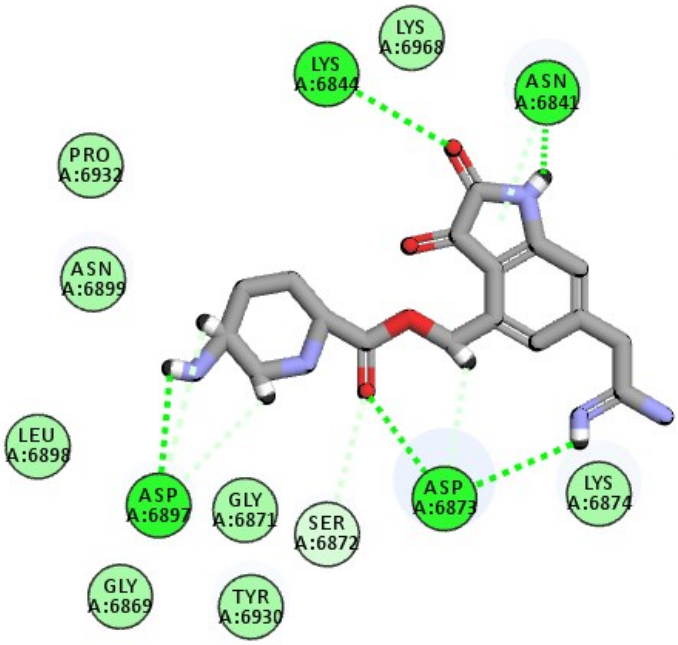
GLY A:6879
TYR A:6845

C.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LYS A:6844
ASN A:6841
PRO A:6932
ASN A:6899
LEU A:6898
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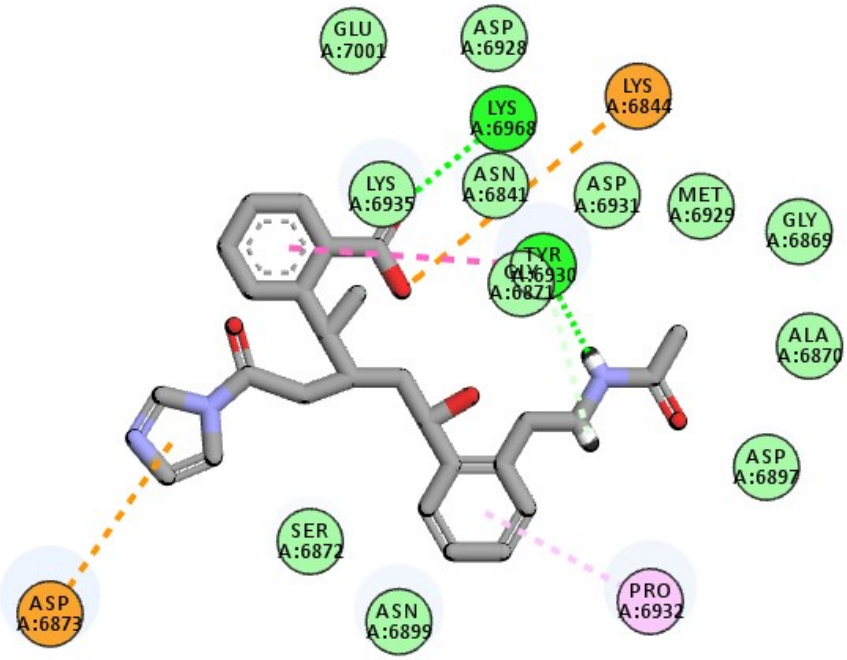
ASP A:6873
LYS A:6874
GLY A:6869
TYR A:6930

D.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ASP A:6928
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TYR A:6930
GLY A:6871
ALA A:6870
ASP A:6897
SER A:6872
PRO A:6932
ASP A:6873
ASN A:6899

E.

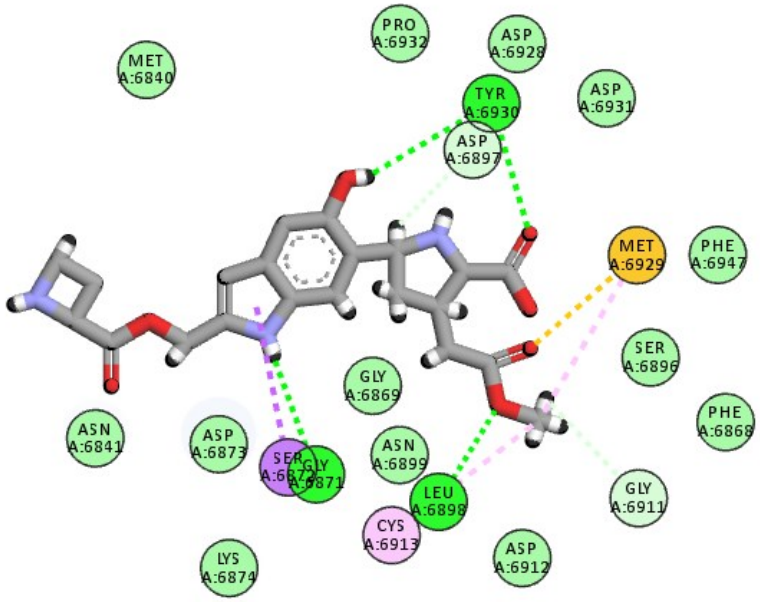

Figure S2. 2D interactions diagram for compounds (**A**) **W-1** (**B**) **W-2** (**C**) **W-3** (**D**) **W-4** and (**E**) **W-5**.

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

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