

## Supporting Information

### Indole-based compounds as potential drug candidates for SARS-CoV-2

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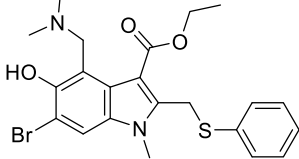
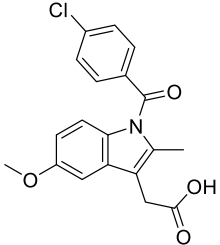
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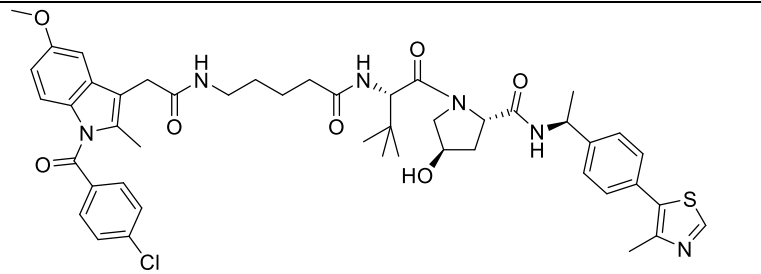
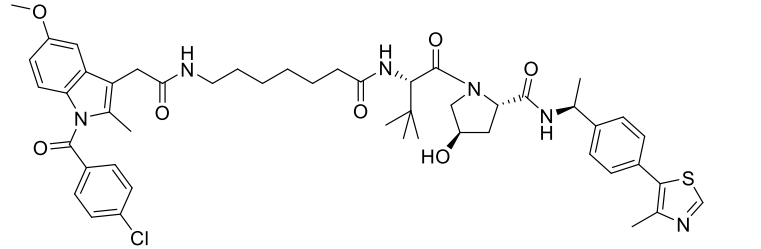
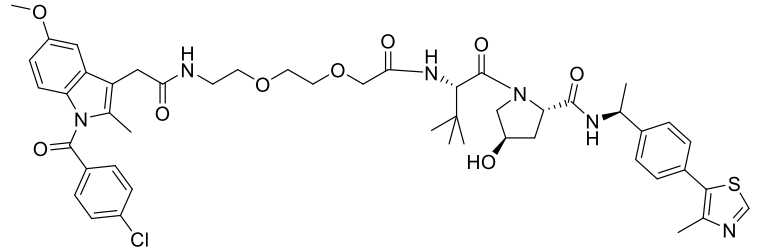
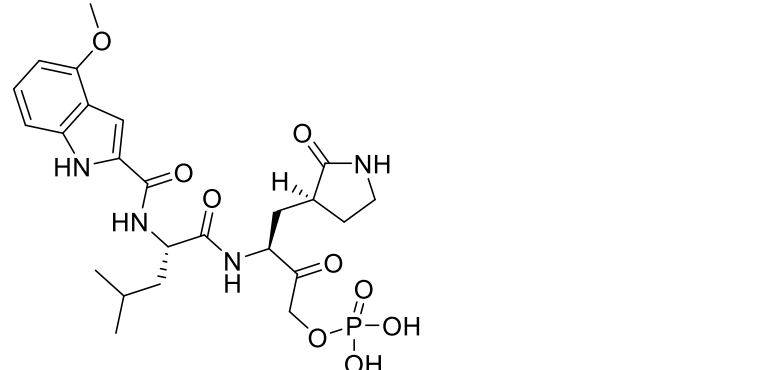
<sup>b</sup> *Department of Chemistry and Biochemistry, Augusta University, Augusta, GA 30912, USA*

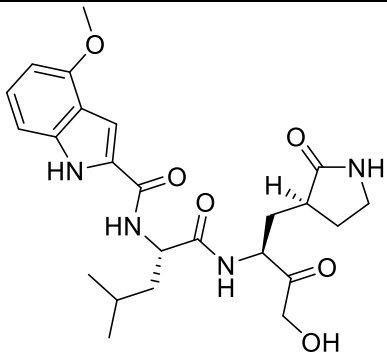
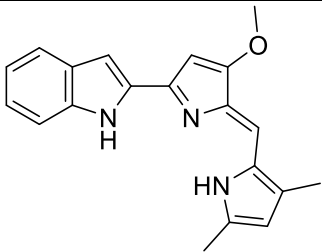
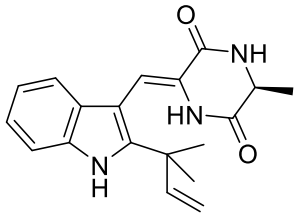
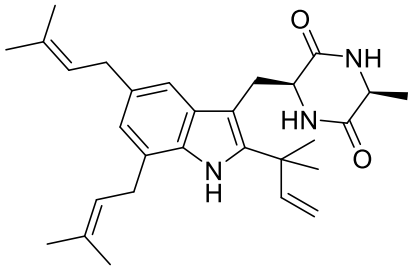
<sup>c</sup> *School of Chemistry, Cardiff University, Main Building, Park Place, Cardiff, CF10 3AT, UK*

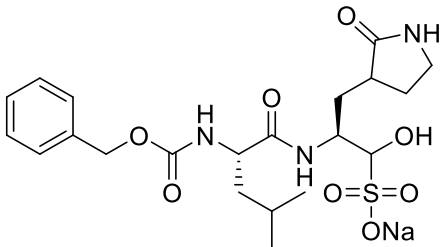
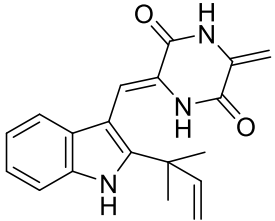
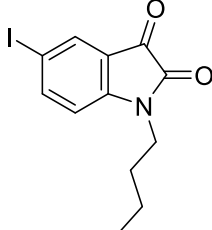
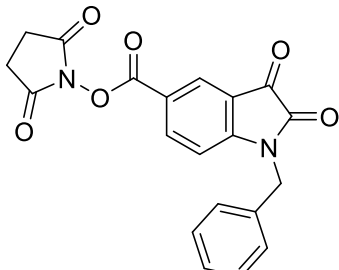
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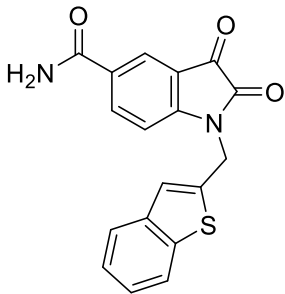
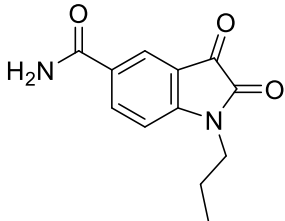
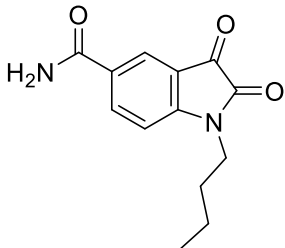
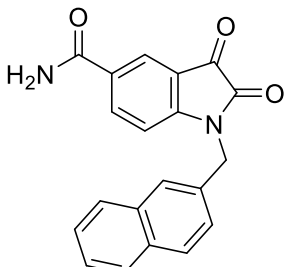
Table S1: List of potential Indole-based compounds and their activities (IC<sub>50</sub>/EC<sub>50</sub>) against SARS-CoV-2

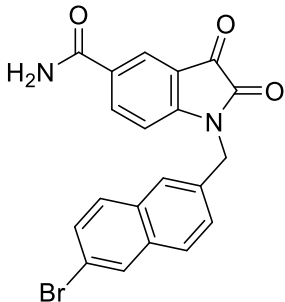
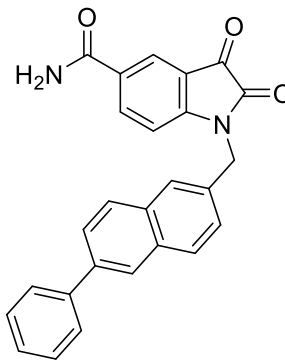
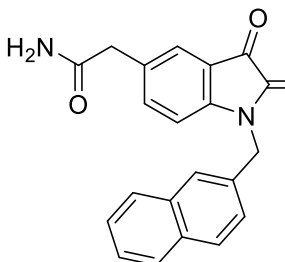
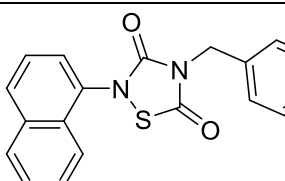
S.No.	Compound Name	Compound Structure	IC <sub>50</sub> /EC <sub>50</sub>	Virus/Enzyme
1	Arbidol		IC <sub>50</sub> = 4.11 μM	SARS-CoV-2
2	Indomethacin		EC <sub>50</sub> = 94.9 μM	SARS-CoV 2/NL/2020

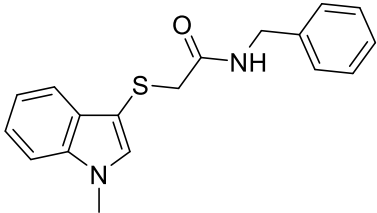
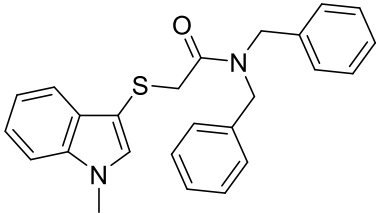
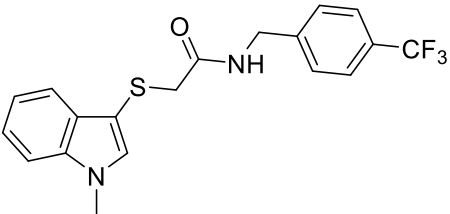
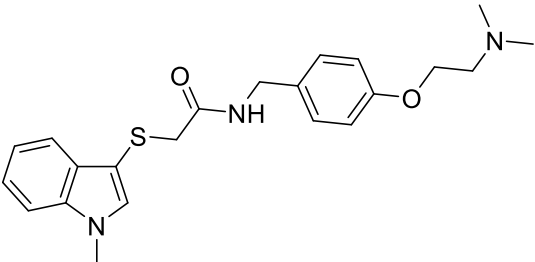
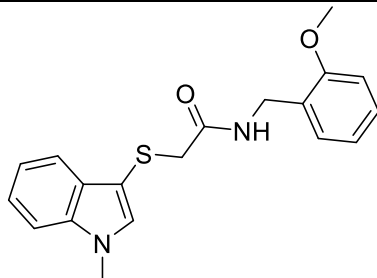
3	<b>B1</b>		EC <sub>50</sub> = >50 μM EC <sub>50</sub> = >50 μM	SARS-CoV 2/NL/2020 SARS-CoV-2/Padova/2021
4	<b>B2</b>		EC <sub>50</sub> = 18.1 μM EC <sub>50</sub> = 25.4 μM	SARS-CoV 2/NL/2020 SARS-CoV-2/Padova/2021
5	<b>B3</b>		EC <sub>50</sub> = >50 μM EC <sub>50</sub> = >50 μM	SARS-CoV 2/NL/2020 SARS-CoV-2/Padova/2021
6	<b>Lufotrelvir (PF-07304814)</b>		IC <sub>50</sub> = 0.692 μM	M <sup>pro</sup> SARSCoV-2

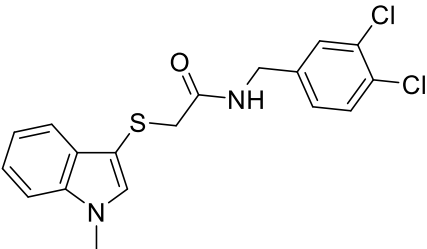
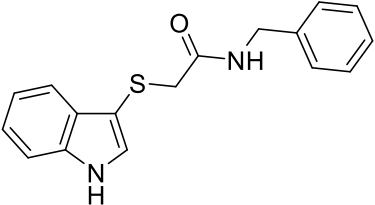
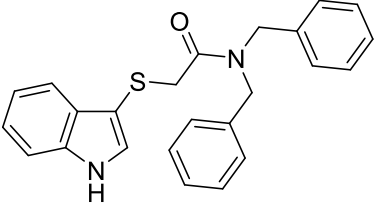
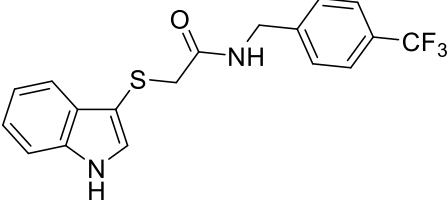
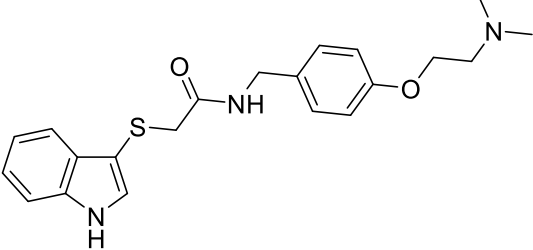
7	<b>PF-00835231</b>		$IC_{50} = 0.009 \mu M$	M <sup>pro</sup> SARSCoV-2
8	<b>Obatoclax (GX15-070)</b>		$EC_{50}: 23.2 \mu M$	Nijmegen1
9	<b>Neoechinulin A</b>		$IC_{50} = 0.47 \mu M$	M <sup>pro</sup> -SARS-CoV-2
10	<b>Echinulin</b>		$IC_{50} = 3.90 \mu M$	M <sup>pro</sup> -SARS-CoV-2

11	<b>GC376</b>		$IC_{50} = 0.36 \mu M$	M <sup>pro</sup> -SARS-CoV-2
12	<b>Neoechinulin B</b>		$IC_{50} = 32.9 \mu M$	Vero E6
13	<b>C9</b>		$IC_{50} = 41.8 \pm 8.0 \mu M$	M <sup>pro</sup> -SARS-CoV-2
14	<b>C17</b>		$IC_{50} = 15.5 \pm 1.2 \mu M$	M <sup>pro</sup> -SARS-CoV-2

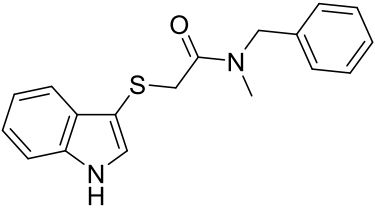
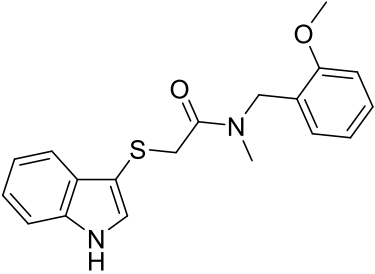
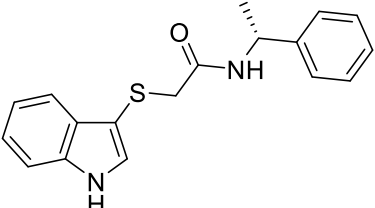
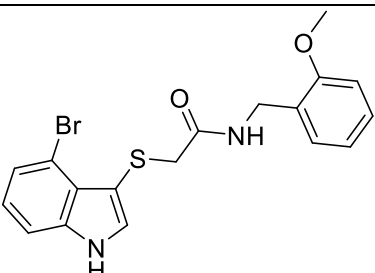
15	<b>C23</b>		$IC_{50} = 0.053 \pm 0.01 \mu M$	M <sup>pro</sup> -SARS-CoV-2
16	<b>C24</b>		$IC_{50} = 10.2 \pm 1.0 \mu M$	M <sup>pro</sup> -SARS-CoV-2
17	<b>C25</b>		$IC_{50} = 17.8 \pm 0.7 \mu M$	M <sup>pro</sup> -SARS-CoV-2
18	<b>C26</b>		$IC_{50} = 0.045 \pm 0.007 \mu M$	M <sup>pro</sup> -SARS-CoV-2

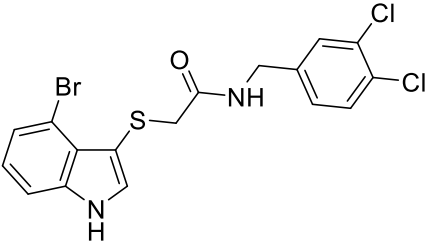
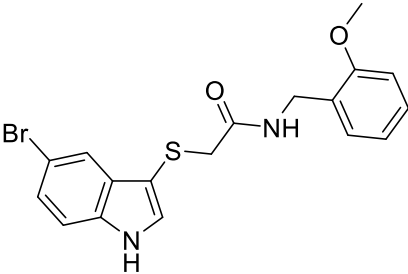
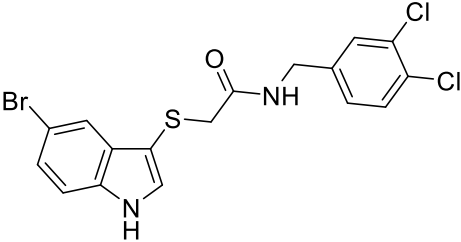
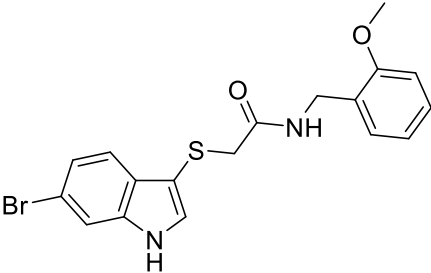
19	<b>C27</b>		$IC_{50} = 0.047 \pm 0.007 \mu M$	SARS-CoV-2 RdRp
20	<b>C28</b>		$IC_{50} = 24.9 \pm 4.6 \mu M$	SARS-CoV-2 RdRp
21	<b>C29</b>		$IC_{50} = 39.2 \pm 10.5 \mu M$	SARS-CoV-2 RdRp
22	<b>Tideglusib</b>		$IC_{50} = 1.91 \pm 0.16 \mu M$	SARS-CoV-2 RdRp

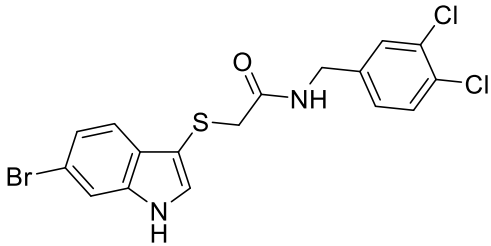
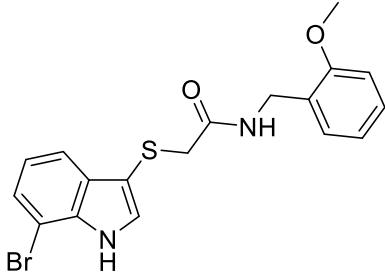
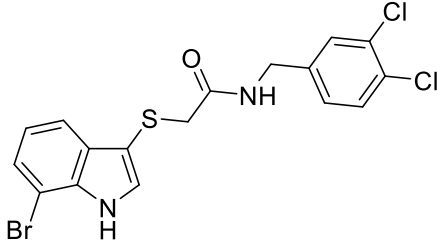
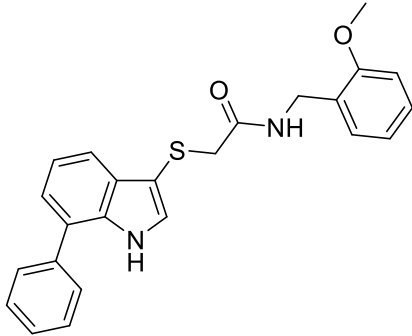
23	<b>D1</b>		$IC_{50} = 26.92 \pm 3.54 \mu M$	SARS-CoV-2 RdRp
24	<b>D2</b>		$IC_{50} = 12.3 \pm 1.40 \mu M$	SARS-CoV-2 RdRp
25	<b>D3</b>		Not active	SARS-CoV-2 RdRp
26	<b>D4</b>		$IC_{50} = 8.91 \pm 0.87 \mu M$	SARS-CoV-2 RdRp
27	<b>D5</b>		$IC_{50} = 9.82 \pm 0.96 \mu M$	SARS-CoV-2 RdRp

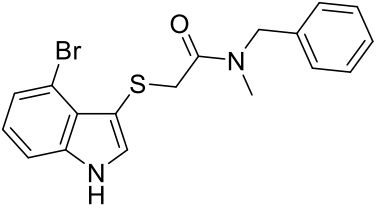
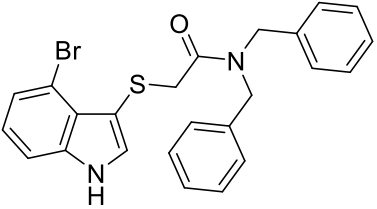
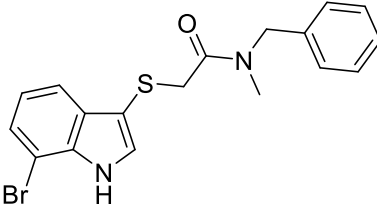
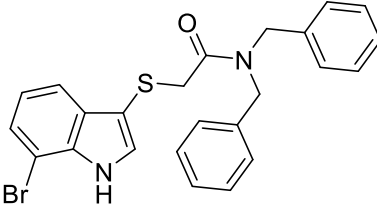
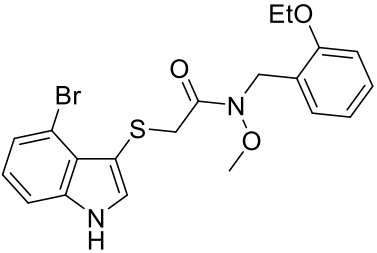
28	<b>D6</b>		$IC_{50} = 7.50 \pm 1.68 \mu M$	SARS-CoV-2 RdRp
29	<b>D7</b>		$IC_{50} = 6.81 \pm 1.03 \mu M$	SARS-CoV-2 RdRp
30	<b>D8</b>		$IC_{50} = 3.35 \pm 0.21 \mu M$	SARS-CoV-2 RdRp
31	<b>D9</b>		$IC_{50} = 7.94 \pm 1.02 \mu M$	SARS-CoV-2 RdRp
32	<b>D10</b>		$IC_{50} = 9.08 \pm 1.38 \mu M$	SARS-CoV-2 RdRp

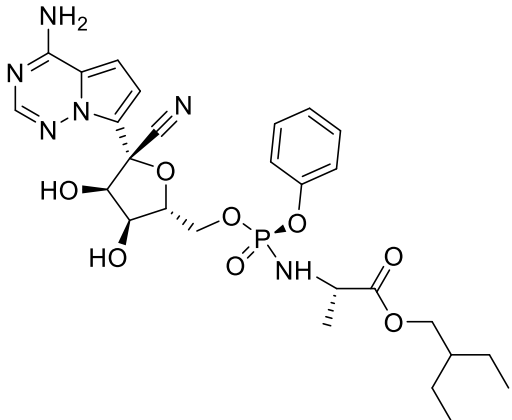
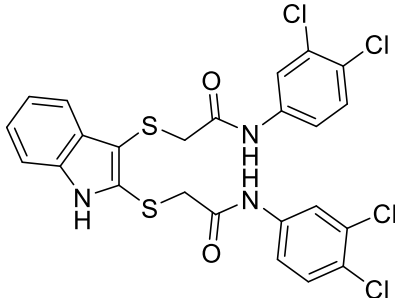
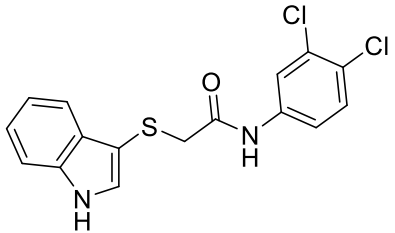
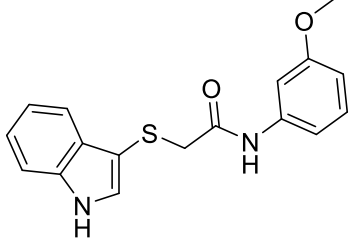


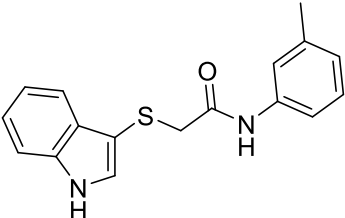
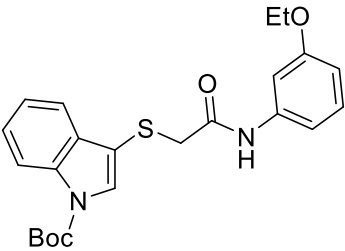
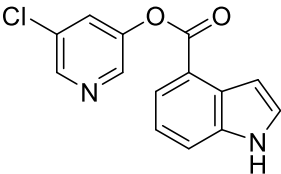
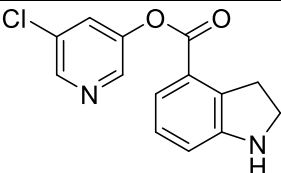
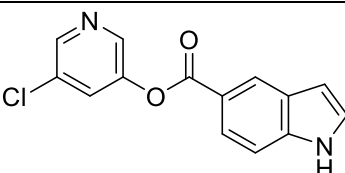
33	<b>D11</b>		$IC_{50} = 4.55 \pm 0.23 \mu M$	SARS-CoV-2 RdRp
34	<b>D12</b>		$IC_{50} = 7.64 \pm 0.54 \mu M$	SARS-CoV-2 RdRp
35	<b>D13</b>		$IC_{50} = 6.68 \pm 0.86 \mu M$	SARS-CoV-2 RdRp
36	<b>D14</b>		$IC_{50} = 8.71 \pm 0.33 \mu M$	SARS-CoV-2 RdRp

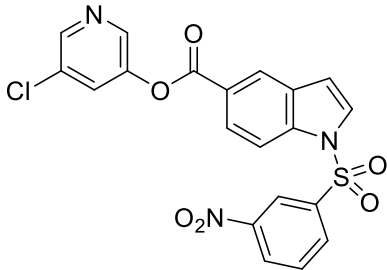
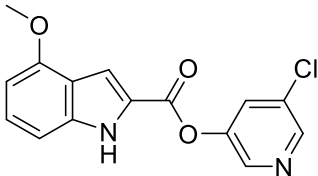
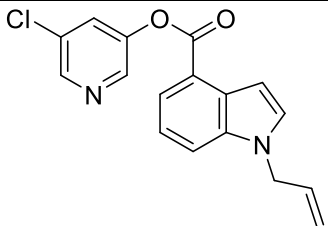
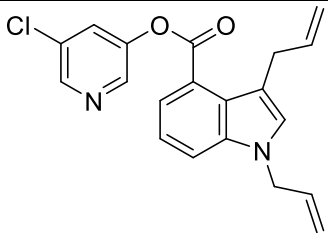
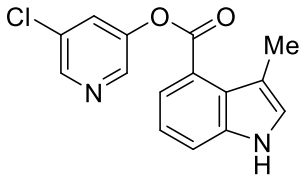
37	<b>D25</b>		$IC_{50} = 7.21 \pm 0.59 \mu M$	SARS-CoV-2 RdRp
38	<b>D16</b>		$IC_{50} = 10.72 \pm 1.11 \mu M$	SARS-CoV-2 RdRp
39	<b>D17</b>		$IC_{50} = 9.77 \pm 0.46 \mu M$	SARS-CoV-2 RdRp
40	<b>D18</b>		$IC_{50} = 10.01 \pm 0.95 \mu M$	SARS-CoV-2 RdRp

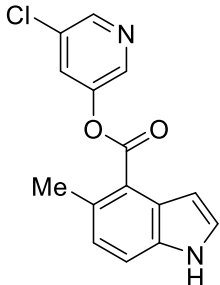
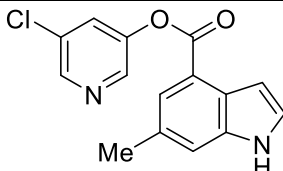
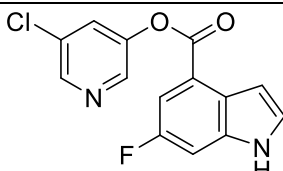
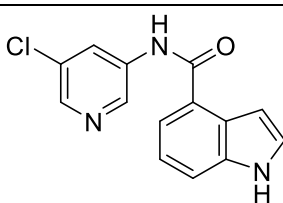
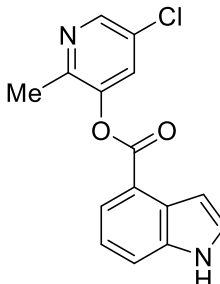
41	<b>D19</b>		$IC_{50} = 8.71 \pm 0.63 \mu M$	SARS-CoV-2 RdRp
42	<b>D20</b>		$IC_{50} = 7.08 \pm 0.65 \mu M$	SARS-CoV-2 RdRp
43	<b>D21</b>		$IC_{50} = 4.55 \pm 0.25 \mu M$	SARS-CoV-2 RdRp
44	<b>D22</b>		$IC_{50} = 1.65 \pm 0.05 \mu M$	SARS-CoV-2 RdRp

45	<b>D23</b>		$IC_{50} = 4.73 \pm 0.67 \mu M$	SARS-CoV-2 RdRp
46	<b>D24</b>		$IC_{50} = 3.76 \pm 0.79 \mu M$	SARS-CoV-2 RdRp
47	<b>D25</b>		$IC_{50} = 20.89 \pm 2.68 \mu M$	SARS-CoV-2 RdRp
48	<b>D26</b>		$IC_{50} = 7.08 \pm 0.32 \mu M$	SARS-CoV-2 RdRp
49	<b>D27</b>		$IC_{50} = 1.11 \pm 0.05 \mu M$	SARS-CoV-2 RdRp

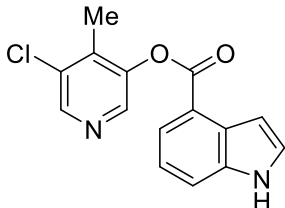
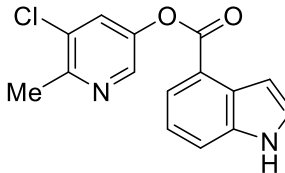
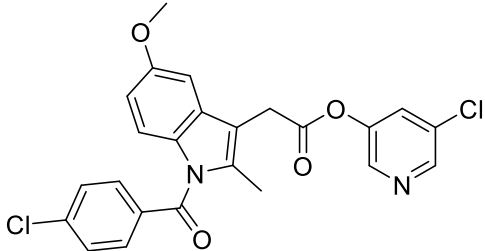
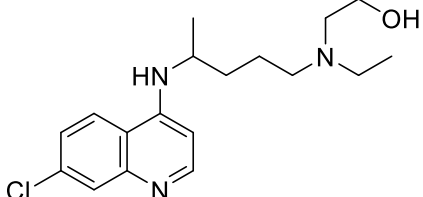
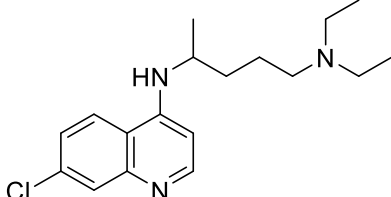
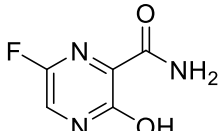
50	<b>Remdesivir</b>		$IC_{50} = 1.56 \pm 0.12 \mu M$ $EC_{50} = 1.05 \mu M$	SARS-CoV-2 RdRp
51	<b>E1</b>		$EC_{50} = 3.07 \mu M$	SARS-CoV-2 RdRp
52	<b>E2</b>		$EC_{50} = 2.75 \mu M$	SARS-CoV-2 RdRp
53	<b>E3</b>		$EC_{50} = 1.70 \mu M$	SARS-CoV-2 RdRp

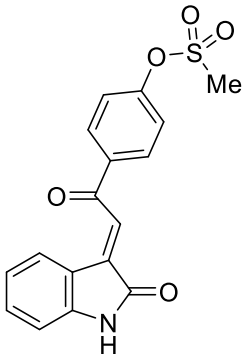
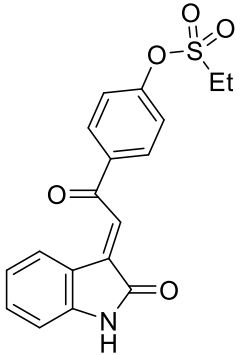
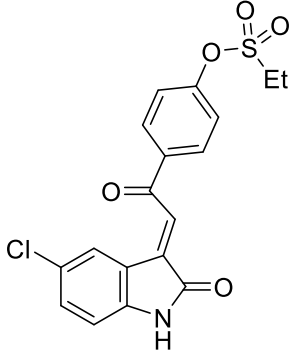
54	<b>E4</b>		$EC_{50} = 2.53 \mu\text{M}$	SARS-CoV-2 RdRp
55	<b>E5</b>		$EC_{50} = 1.41 \mu\text{M}$	SARS-CoV-2 RdRp
56	<b>F1</b>		$EC_{50} = 2.8 \mu\text{M}$ $IC_{50} = 0.25 \mu\text{M}$	SARS-CoV-2 M <sup>pro</sup> -SARS-CoV-2
57	<b>F2</b>		$EC_{50} = 15 \mu\text{M}$ $IC_{50} = 0.32 \mu\text{M}$	SARS-CoV-2 M <sup>pro</sup> -SARS-CoV-2
58	<b>F3</b>		$EC_{50} = 43.7 \mu\text{M}$ $IC_{50} = 0.31 \mu\text{M}$	SARS-CoV-2 M <sup>pro</sup> -SARS-CoV-2

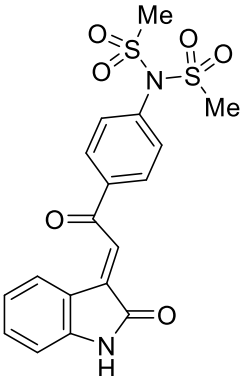
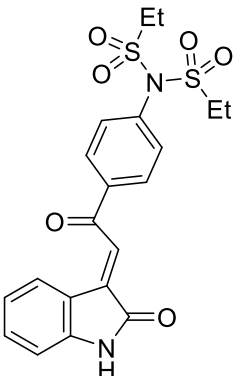
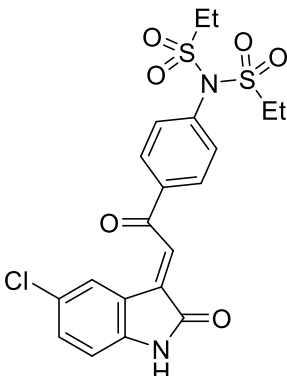
59	<b>F4</b>		$EC_{50} = 69.8 \mu\text{M}$ $IC_{50} = 0.12 \mu\text{M}$	SARS-CoV-2 M <sup>pro</sup> -SARS-CoV-2
60	<b>F5</b>		$EC_{50} = 8.1 \mu\text{M}$ $IC_{50} = 0.90 \mu\text{M}$	SARS-CoV-2 M <sup>pro</sup> -SARS-CoV-2
61	<b>F6</b>		$EC_{50} = 15 \mu\text{M}$ $IC_{50} = 0.073 \mu\text{M}$	SARS-CoV-2 M <sup>pro</sup> -SARS-CoV-2
62	<b>F7</b>		$EC_{50} = 11.5 \mu\text{M}$ $IC_{50} = 0.38 \mu\text{M}$	SARS-CoV-2 M <sup>pro</sup> -SARS-CoV-2
63	<b>F8</b>		$EC_{50} = 56 \mu\text{M}$ $IC_{50} = 0.47 \mu\text{M}$	SARS-CoV-2 M <sup>pro</sup> -SARS-CoV-2

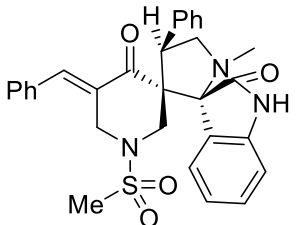
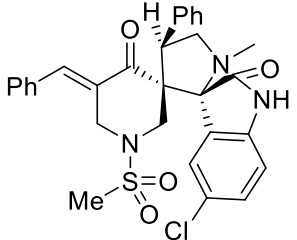
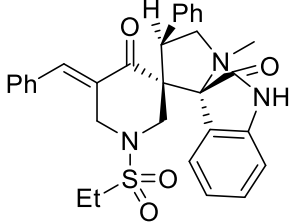
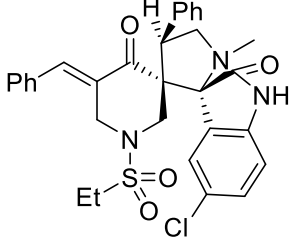
64	<b>F9</b>		EC <sub>50</sub> = >100 μM IC <sub>50</sub> = 10.3 μM	SARS-CoV-2 M <sup>pro</sup> -SARS-CoV-2
65	<b>F10</b>		EC <sub>50</sub> = 3.1 μM IC <sub>50</sub> = 0.59 μM	SARS-CoV-2 M <sup>pro</sup> -SARS-CoV-2
66	<b>F11</b>		EC <sub>50</sub> = 14 μM IC <sub>50</sub> = 0.87 μM	SARS-CoV-2 M <sup>pro</sup> -SARS-CoV-2
67	<b>F12</b>		EC <sub>50</sub> = >100 μM IC <sub>50</sub> = 100 μM	SARS-CoV-2 M <sup>pro</sup> -SARS-CoV-2
68	<b>F13</b>		EC <sub>50</sub> = >100 μM IC <sub>50</sub> = >100 μM	SARS-CoV-2 M <sup>pro</sup> -SARS-CoV-2

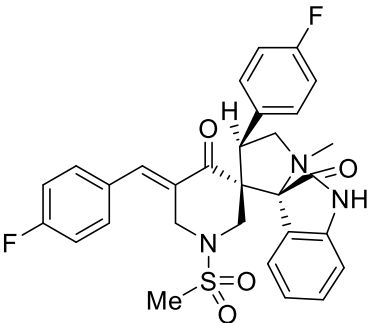
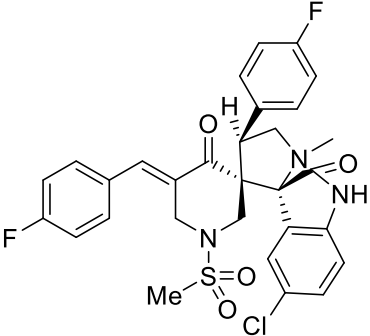
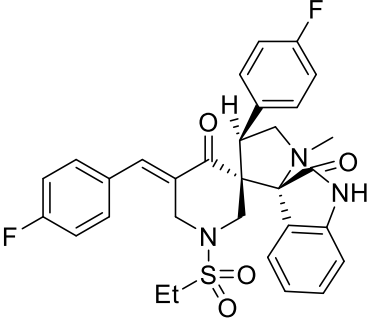


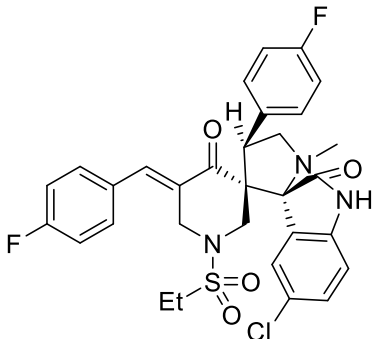
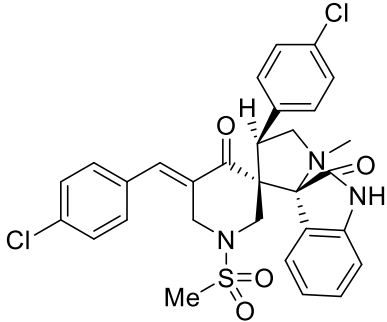
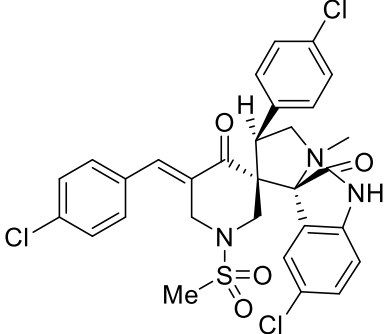
69	<b>F14</b>		EC <sub>50</sub> = 19.3 μM IC <sub>50</sub> = 2.2 μM	SARS-CoV-2 M <sup>pro</sup> -SARS-CoV-2
70	<b>F15</b>		EC <sub>50</sub> = 30 μM IC <sub>50</sub> = 15.3 μM	SARS-CoV-2 M <sup>pro</sup> -SARS-CoV-2
71	<b>16</b>		EC <sub>50</sub> = 30.2 μM IC <sub>50</sub> = 5.32 μM	SARS-CoV-2 M <sup>pro</sup> -SARS-CoV-2
72	<b>Hydroxychloroquine</b>		IC <sub>50</sub> = 29.25 μM	Vero E6
73	<b>Chloroquine</b>		IC <sub>50</sub> = 19.78 μM	Vero E6
74	<b>Favipiravir</b>		IC <sub>50</sub> = 1382 μM	Vero E6

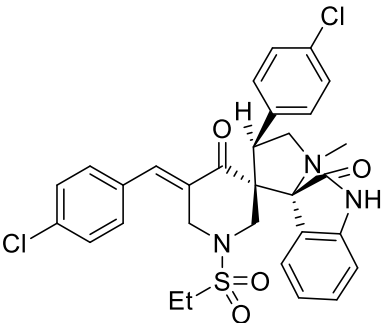
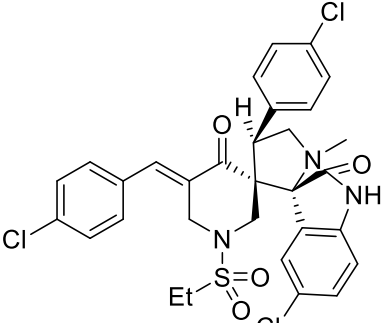
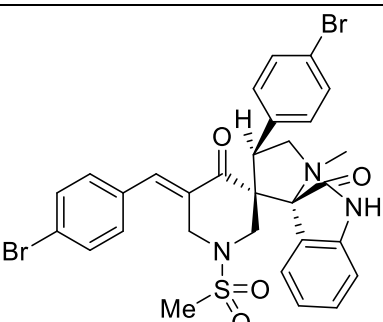
75	<b>G1</b>		$IC_{50} = 3.799 \mu M$	Vero E6
76	<b>G2</b>		$IC_{50} = 55.14 \mu M$	Vero E6
77	<b>G3</b>		$IC_{50} = 13.52 \mu M$	Vero E6

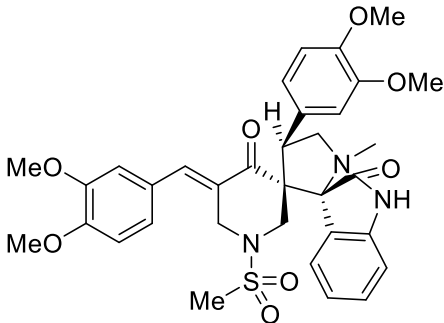
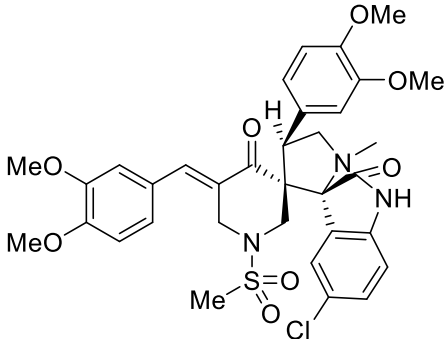
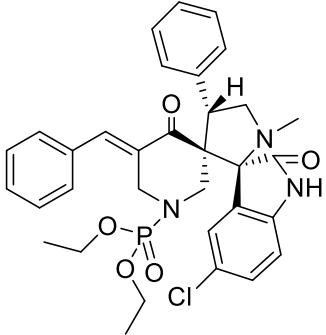
78	<b>H1</b>		$IC_{50} = 219 \mu M$	Vero E6
79	<b>H2</b>		$IC_{50} = 3.417 \mu M$	Vero E6
80	<b>H3</b>		$IC_{50} = 20.1 \mu M$	Vero E6

81	<b>I1</b>		$IC_{50} = 34.26 \mu M$	Vero E6
82	<b>I2</b>		$IC_{50} = 9.628 \mu M$	Vero E6
83	<b>I3</b>		$IC_{50} = 102.6 \mu M$	Vero E6
84	<b>I4</b>		$IC_{50} = 171.3 \mu M$	Vero E6

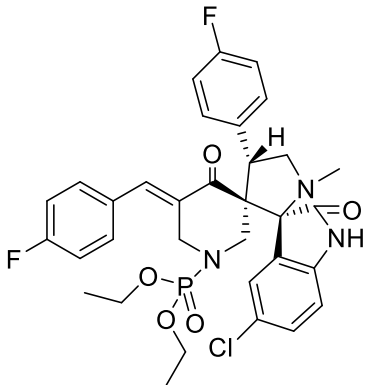
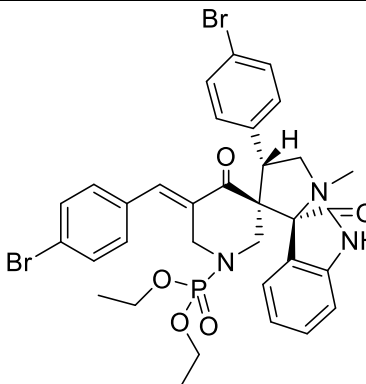
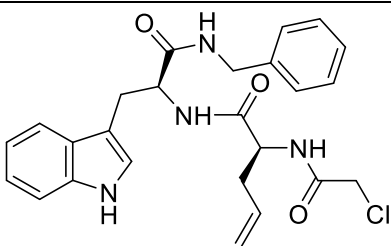
85	<b>I5</b>		$IC_{50} = 27.85 \mu M$	Vero E6
86	<b>I6</b>		$IC_{50} = 7.666 \mu M$	Vero E6
87	<b>I7</b>		$IC_{50} = 16.91 \mu M$	Vero E6

88	<b>I8</b>		$IC_{50} = 7.689 \mu M$	Vero E6
89	<b>I9</b>		$IC_{50} = 113.3 \mu M$	Vero E6
90	<b>I10</b>		$IC_{50} = 27.09 \mu M$	Vero E6

91	<b>I11</b>		$IC_{50} = 55.45 \mu M$	Vero E6
92	<b>I12</b>		$IC_{50} = 31.45 \mu M$	Vero E6
93	<b>I13</b>		$IC_{50} = 8.924 \mu M$	Vero E6

94	<b>I14</b>		$IC_{50} = 35.89 \mu M$	Vero E6
95	<b>I15</b>		$IC_{50} = 88.25 \mu M$	Vero E6
96	<b>J1</b>		$IC_{50} = 10.39 \mu M$ $IC_{50} = 9.605 \pm 0.66 \mu M$	SARS-CoV-2 M <sup>pro</sup> -SARS-CoV-2



97	<b>J2</b>		$IC_{50} = 13.53 \mu M$ $IC_{50} = 42.82 \pm 2.53 \mu M$	SARS-CoV-2 M <sup>pro</sup> -SARS-CoV-2
98	<b>J3</b>		$IC_{50} = 8.88 \mu M$ $IC_{50} = 15.59 \pm 1.02 \mu M$	SARS-CoV-2 M <sup>pro</sup> -SARS-CoV-2
99	<b>22</b>		$IC_{50} = 1.72 \pm 0.75 \mu M$ $IC_{50} = 0.67 \pm 0.59 \mu M$	M <sup>pro</sup> -SARS-CoV-2 PL <sup>pro</sup> -SARS-CoV-2