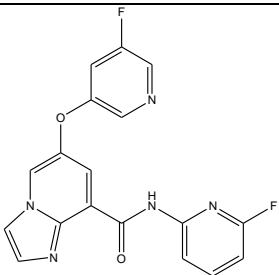
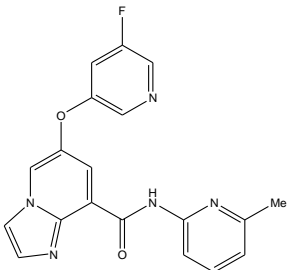
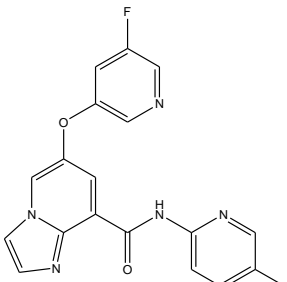
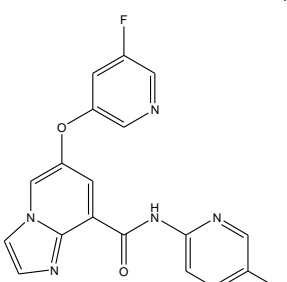
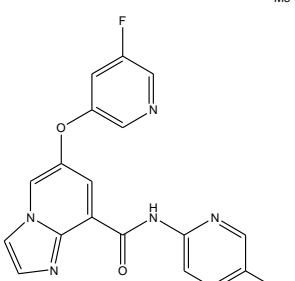
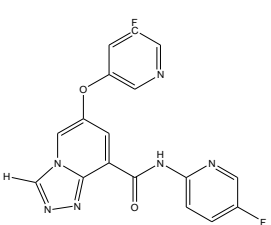
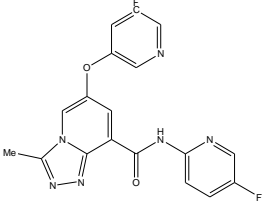
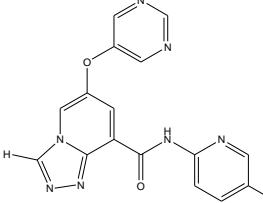
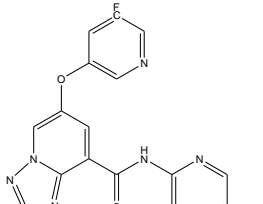
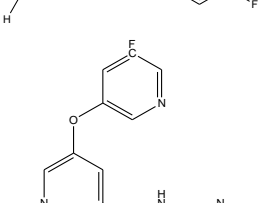
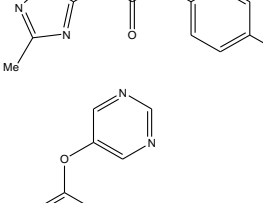
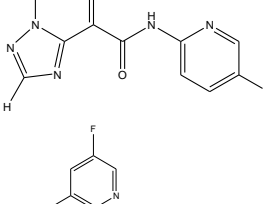
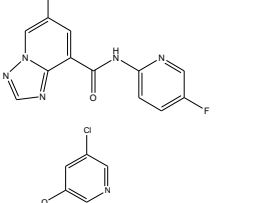
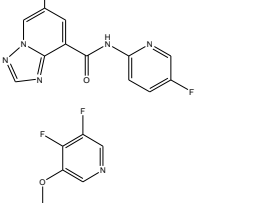
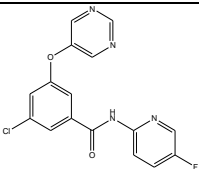
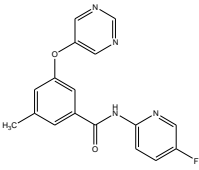
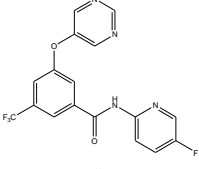
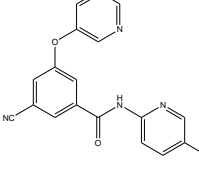
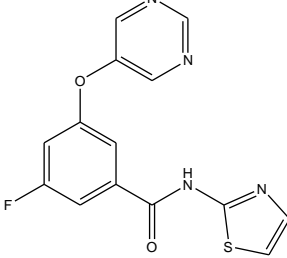
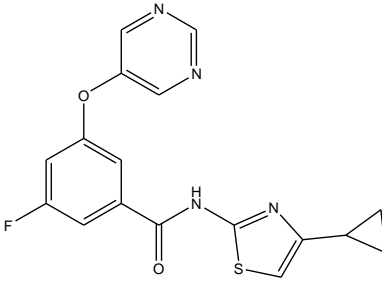
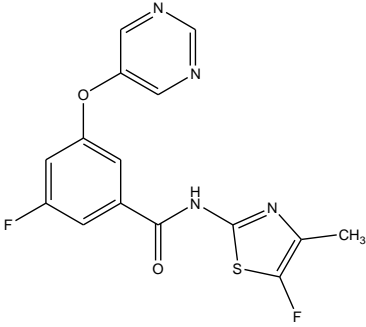


Table S1. The information of all 106 molecules.

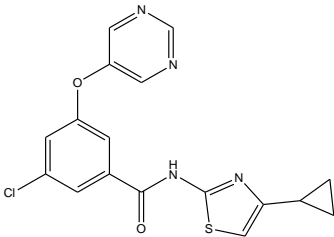
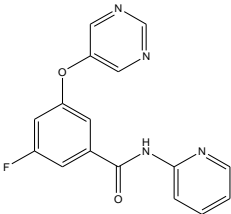
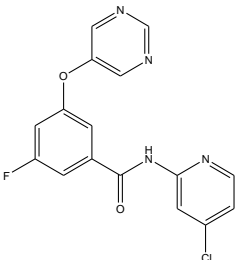
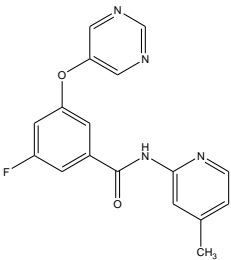
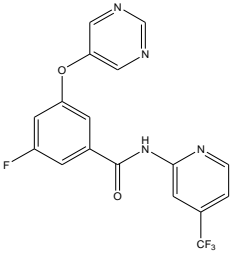
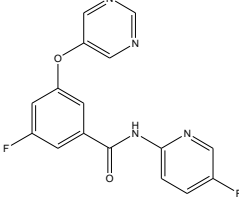
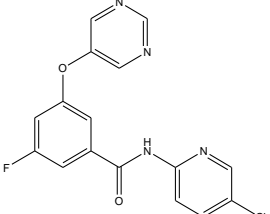
No.	Structure	mGlu5 pIC <sub>50</sub> ( $\pm$ SEM) %	Glu Max ( $\pm$ SEM) %
1		7.42 $\pm$ 0.02	1.5 $\pm$ 0.2
2		7.18 $\pm$ 0.01	1.5 $\pm$ 0.2
3		7.69 $\pm$ 0.15	1.6 $\pm$ 0.1
4		7.13 $\pm$ 0.10	1.4 $\pm$ 0.2
5		7.26 $\pm$ 0.08	1.6 $\pm$ 0.2
6		7.57 $\pm$ 0.11	2.3 $\pm$ 0.1

7		$6.43 \pm 0.01$	$2.7 \pm 0.9$
8		$6.49 \pm 0.15$	$1.6 \pm 0.2$
9		$7.69 \pm 0.05$	$1.5 \pm 0.2$
10		$5.85 \pm 0.33$	$3.3 \pm 1.6$
11		$7.13 \pm 0.05$	$1.5 \pm 0.2$
12		$7.69 \pm 0.05$	$1.5 \pm 0.2$
13		$7.05 \pm 0.18$	$1.1 \pm 0.2$
14		$7.39 \pm 0.02$	$2.0 \pm 0.1$

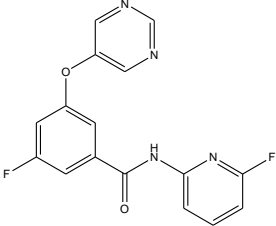
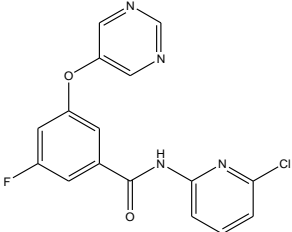
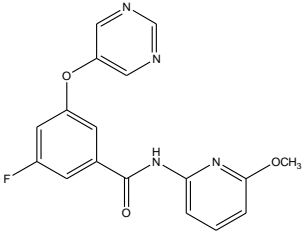
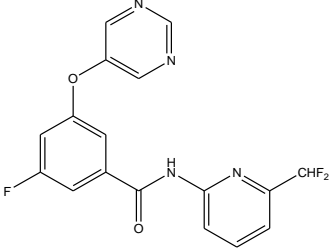
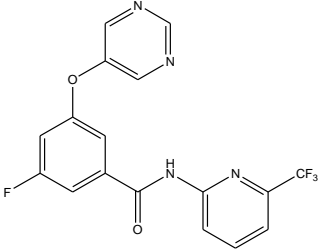
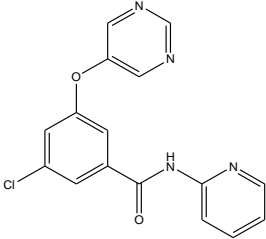
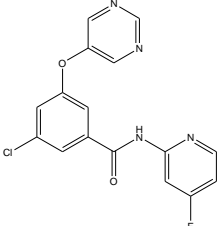
15		$7.25 \pm 0.08$	$1.6 \pm 0.3$
16		$6.93 \pm 0.07$	$2.2 \pm 0.6$
17		$7.36 \pm 0.14$	$2.3 \pm 0.4$
18		$6.89 \pm 0.02$	$1.7 \pm 0.2$
19		$6.69 \pm 0.25$	$1.7 \pm 0.3$
20		$7.62 \pm 0.03$	$1.2 \pm 0.1$
21		$7.94 \pm 0.19$	$1.4 \pm 0.2$
22		$6.55 \pm 0.10$	$1.7 \pm 0.2$
23		$6.52 \pm 0.07$	$1.3 \pm 0.3$

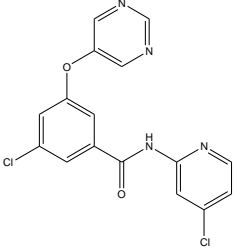
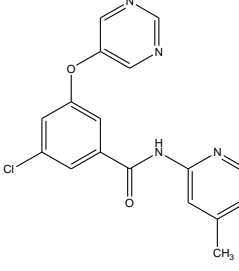
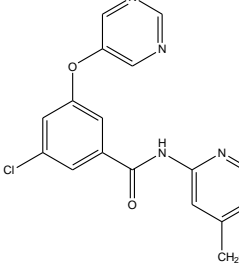
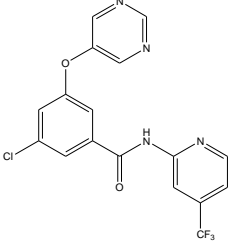
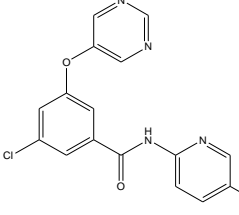
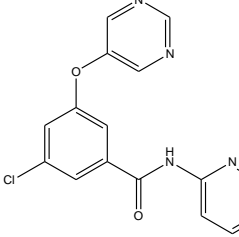
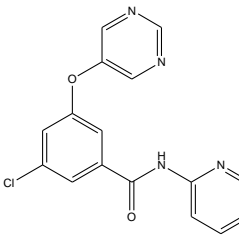
24		$7.49 \pm 0.02$	$1.2 \pm 0.2$
25		$7.72 \pm 0.06$	$0.8 \pm 0.2$
26		$5.26 \pm 0.01$	$3.2 \pm 0.3$
27		$6.50 \pm 0.08$	$1.1 \pm 0.4$
28		$5.75 \pm 0.25$	$3.2 \pm 1.2$
29		$6.62 \pm 0.08$	$1.7 \pm 0.3$
30		$7.27 \pm 0.03$	$1.5 \pm 0.1$

31		$6.66 \pm 0.03$	$1.6 \pm 0.4$
32		$5.66 \pm 0.06$	$1.7 \pm 0.4$
33		$5.49 \pm 0.05$	$1.5 \pm 0.5$
34		$7.09 \pm 0.19$	$1.7 \pm 0.2$
35		$7.44 \pm 0.09$	$1.4 \pm 0.2$
36		$7.01 \pm 0.08$	$1.3 \pm 0.2$
37		$6.51 \pm 0.07$	$1.2 \pm 0.2$

38		$6.68 \pm 0.04$	$1.2 \pm 0.4$
39		$7.02 \pm 0.09$	$1.4 \pm 0.2$
40		$7.38 \pm 0.03$	$1.5 \pm 0.1$
41		$6.67 \pm 0.01$	$1.4 \pm 0.2$
42		$5.98 \pm 0.06$	$1.5 \pm 0.3$
43		$6.52 \pm 0.07$	$1.3 \pm 0.3$
44		$5.97 \pm 0.14$	$2.0 \pm 0.4$

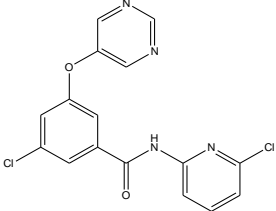
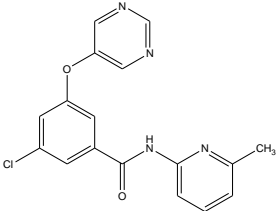
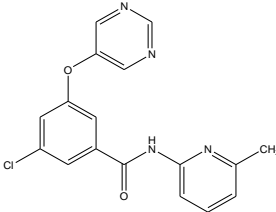
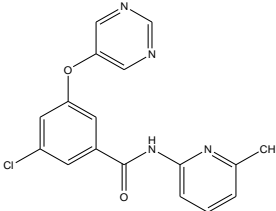
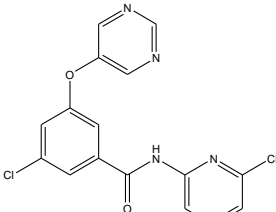
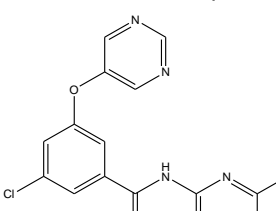
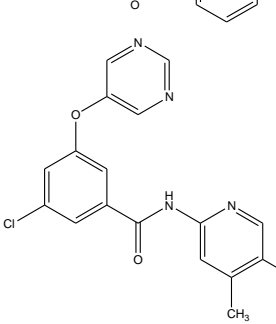
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45		$6.59 \pm 0.13$	$1.6 \pm 0.2$
46		$7.35 \pm 0.09$	$1.5 \pm 0.5$
47		$6.18 \pm 0.11$	$1.6 \pm 0.3$
48		$6.83 \pm 0.08$	$1.2 \pm 0.4$
49		$5.64 \pm 0.13$	$3.7 \pm 1.3$
50		$7.77 \pm 0.03$	$1.2 \pm 0.4$
51		$6.47 \pm 0.08$	$1.4 \pm 0.2$

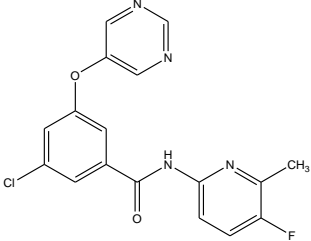
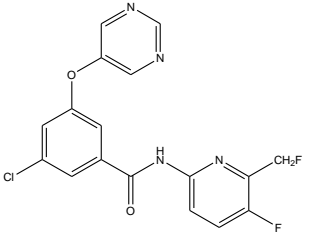
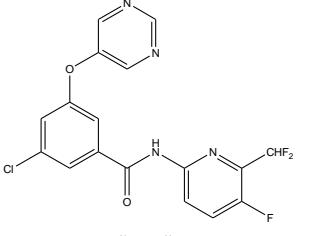
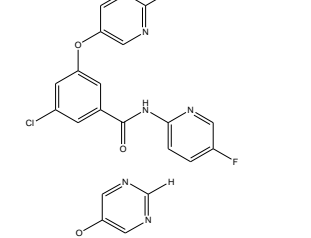
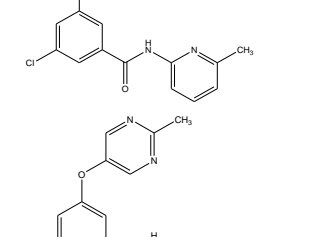
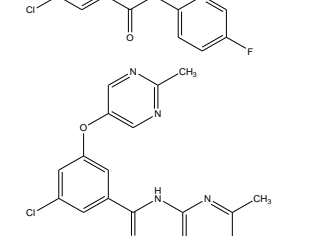
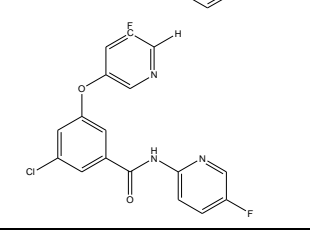

52		$6.77 \pm 0.02$	$1.2 \pm 0.2$
53		$6.85 \pm 0.05$	$1.7 \pm 0.2$
54		$5.35 \pm 0.02$	$2.0 \pm 0.7$
55		$5.36 \pm 0.12$	$2.0 \pm 0.0$
56		$7.49 \pm 0.02$	$1.2 \pm 0.2$
57		$6.99 \pm 0.11$	$1.3 \pm 0.4$
58		8.00d	0.8d

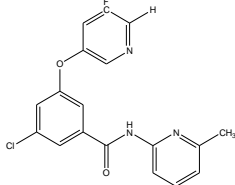
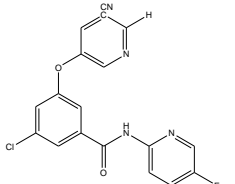
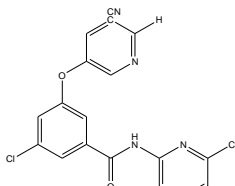
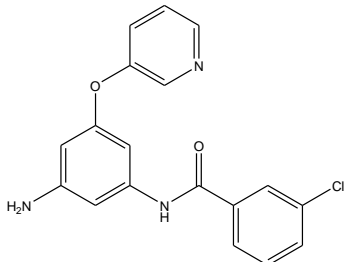
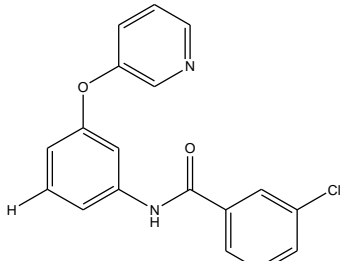
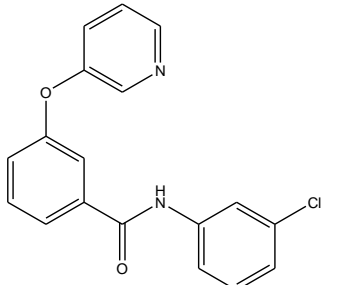
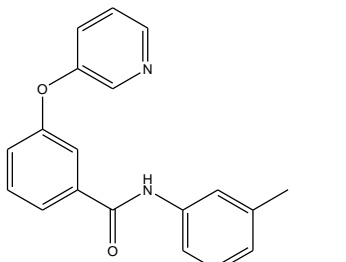


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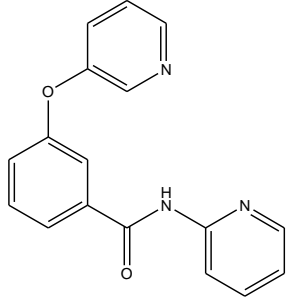
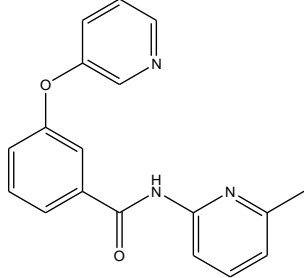
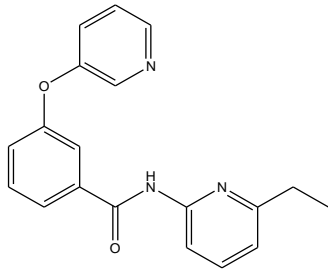
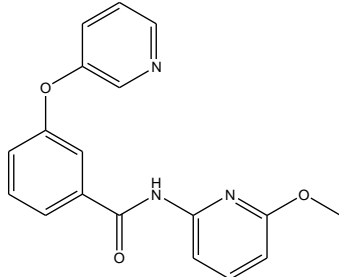
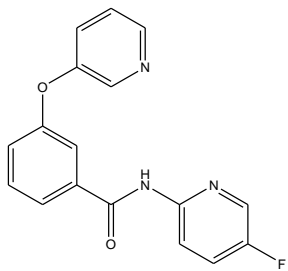
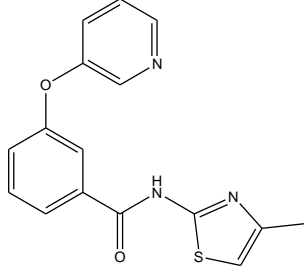
59		$7.86 \pm 0.06$	$1.2 \pm 0.3$
60		$7.75 \pm 0.13$	$1.1 \pm 0.3$
61		$7.74 \pm 0.04$	$1.4 \pm 0.4$
62		$7.44 \pm 0.15$	$1.1 \pm 0.4$
63		$6.51 \pm 0.14$	$1.5 \pm 0.2$
64		$7.27 \pm 0.04$	$1.3 \pm 0.2$
65		$5.49 \pm 0.04$	$10.2 \pm 7.7$

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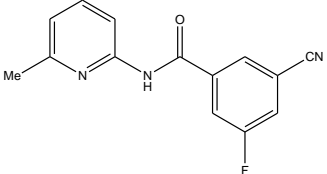
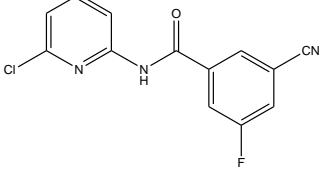
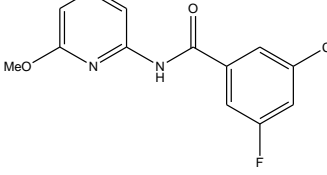
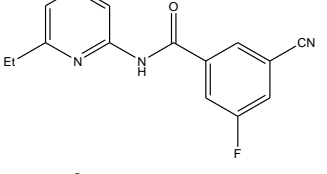
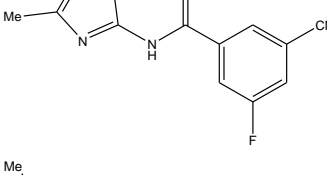
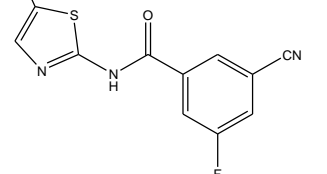
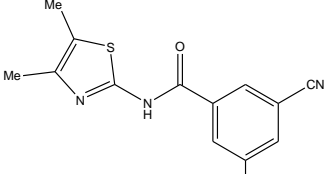
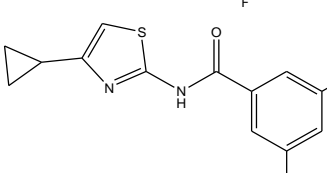
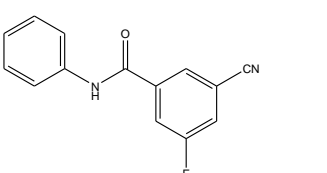
66		$7.30 \pm 0.08$	$1.1 \pm 0.3$
67		$6.84 \pm 0.10$	$1.2 \pm 0.3$
68		$6.30 \pm 0.11$	$1.6 \pm 0.3$
69		$7.49 \pm 0.02$	$1.2 \pm 0.2$
70		$7.75 \pm 0.13$	$1.1 \pm 0.3$
71		$5.35 \pm 0.04$	$2.6 \pm 0.1$
72		$7.02 \pm 0.06$	$1.6 \pm 0.2$
73		$7.61 \pm 0.04$	$1.1 \pm 0.1$

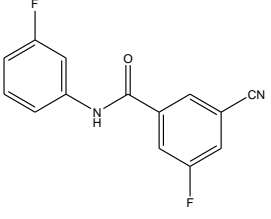
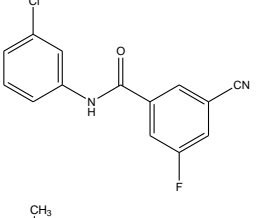
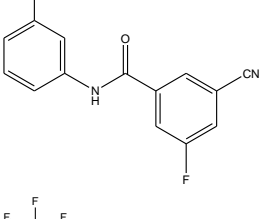
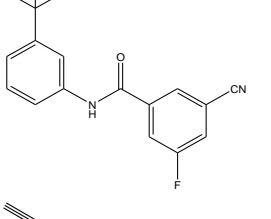
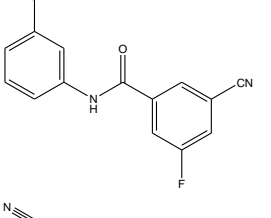
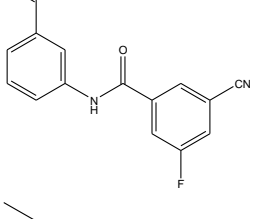
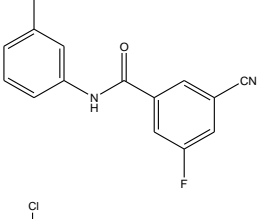
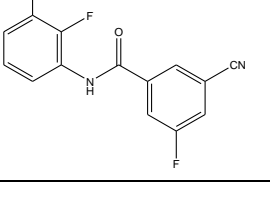
74		$8.13 \pm 0.08$	$1.8 \pm 0.4$
75		$7.57 \pm 0.08$	$1.7 \pm 0.2$
76		$7.99 \pm 0.15$	$1.6 \pm 0.1$
77		$6.55 \pm 0.19$	$1.3 \pm 0.2$
78		$7.09 \pm 0.07$	$1.0 \pm 0.2$
79		$5.71 \pm 0.14$	$1.6 \pm 0.4$
80		$5.66 \pm 0.11$	$1.4 \pm 0.1$

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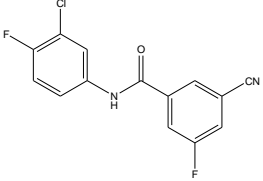
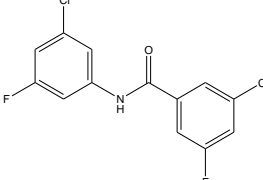
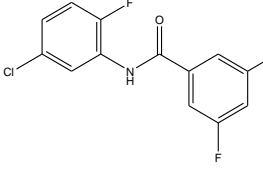
81		$6.07 \pm 0.13$	$1.6 \pm 0.6$
82		$6.45 \pm 0.16$	$1.3 \pm 0.4$
83		$5.73 \pm 0.13$	$1.9 \pm 0.2$
84		$5.44 \pm 0.11$	$3.2 \pm 0.9$
85		$5.17 \pm 0.05$	$6.8 \pm 0.9$
86		$6.11 \pm 0.12$	$1.7 \pm 0.2$

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87		$7.18 \pm 0.13$	$1.2 \pm 0.7$
88		$6.60 \pm 0.06$	$2.2 \pm 0.2$
89		$5.82 \pm 0.05$	$17.3 \pm 0.4$
90		$6.29 \pm 0.11$	$1.7 \pm 0.5$
91		$7.22 \pm 0.09$	$1.0 \pm 0.3$
92		$6.06 \pm 0.07$	$17.5 \pm 6.8$
93		$6.22 \pm 0.07$	$2.4 \pm 0.4$
94		$6.05 \pm 0.11$	$1.5 \pm 0.5$
95		$5.26 \pm 0.10$	$12.5 \pm 4.7$

96		$5.67 \pm 0.01$	$22.1 \pm 1.1$
97		$7.35 \pm 0.17$	$0.6 \pm 0.2$
98		$6.91 \pm 0.09$	$2.1 \pm 0.2$
99		$6.27 \pm 0.05$	$0.9 \pm 0.3$
100		$6.31 \pm 0.06$	$1.4 \pm 0.3$
101		$6.48 \pm 0.08$	$2.3 \pm 0.3$
102		$5.31 \pm 0.10$	$2.4 \pm 0.2$
103		$6.46 \pm 0.09$	$2.5 \pm 0.5$

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104		$6.42 \pm 0.05$	$43.0 \pm 8.0$
105		$5.74 \pm 0.10$	$38.5 \pm 5.2$
106		$5.42 \pm 0.05$	$29.8 \pm 6.6$

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