

Table S1. Structures (in smiles format), formulas, FlexX, Vina, HYDE, and ChemPLP docking scores

number	Canonical SMILES	Formula	Vina	Gold	FlexX	Hyde
1	<chem>S=C(Nc1ccccc1)NNC(=O)c1ccoc1C</chem>	C13H13N3O2S	-7.2	55.94	-24.516	-18.7
2	<chem>S=C(Nc1ccccc1)NNC(=O)c1[nH]cnc1C</chem>	C12H13N5OS	-7.1	56.29	-28.703	13.8
3	<chem>S=C(Nc1ccccc1)NNC(=O)c1ccc[nH]1</chem>	C12H12N4OS	-6.3	52.89	-27.769	4.9
4	<chem>S=C(Nc1ccccc1)NNC(=O)C1CCCC1</chem>	C13H17N3OS	-6.8	55.44	-23.732	-8.6
5	<chem>S=C(Nc1ccccc1)NNC(=O)C1=NC(=S)N=N1</chem>	C10H8N6OS2	-7.3	57.20	-28.149	24.0
6	<chem>S=C(Nc1ccccc1C)NNC(=O)c1ccoc1C</chem>	C14H15N3O2S	-7.6	61.90	-23.387	26.4
7	<chem>S=C(Nc1cccc(c1)C)NNC(=O)c1ccoc1C</chem>	C14H15N3O2S	-7.3	57.92	-24.901	-5.4
8	<chem>S=C(Nc1ccc(cc1)C)NNC(=O)c1ccoc1C</chem>	C14H15N3O2S	-6.9	58.27	-23.211	6.4
9	<chem>S=C(Nc1ccccc1C)NNC(=O)c1[nH]cnc1C</chem>	C13H15N5OS	-7.2	58.22	-28.015	-9.2
10	<chem>S=C(Nc1cccc(c1)C)NNC(=O)c1[nH]cnc1C</chem>	C13H15N5OS	-7.0	56.38	-31.507	12.1
11	<chem>S=C(Nc1ccc(cc1)C)NNC(=O)c1[nH]cnc1C</chem>	C13H15N5OS	-7.3	50.03	-27.066	-2.9
12	<chem>S=C(Nc1ccccc1C)NNC(=O)c1[nH]ccc1</chem>	C13H14N4OS	-6.7	52.58	-30.274	-2.7
13	<chem>S=C(Nc1cccc(c1)C)NNC(=O)c1ccc[nH]1</chem>	C13H14N4OS	-6.6	55.02	-32.008	27.2
14	<chem>S=C(Nc1ccc(cc1)C)NNC(=O)c1ccc[nH]1</chem>	C13H14N4OS	-6.5	54.86	-29.539	1.6
15	<chem>S=C(Nc1ccccc1C)NNC(=O)C1CCCC1</chem>	C14H19N3OS	-6.5	56.58	-25.723	-8.0
16	<chem>S=C(Nc1cccc(c1)C)NNC(=O)C1CCCC1</chem>	C14H19N3OS	-6.8	57.05	-24.785	-29.2
17	<chem>S=C(Nc1ccc(cc1)C)NNC(=O)C1CCCC1</chem>	C14H19N3OS	-6.7	54.27	-24.565	-9.8
18	<chem>S=C(Nc1ccccc1C)NNC(=O)C1=NC(=S)N=N1</chem>	C11H10N6OS2	-7.1	54.17	-30.008	-17.1
19	<chem>S=C(Nc1cccc(c1)C)NNC(=O)C1=NC(=S)N=N1</chem>	C11H10N6OS2	-7.2	52.47	-31.81	-10.4
20	<chem>S=C(Nc1ccc(cc1)C)NNC(=O)C1=NC(=S)N=N1</chem>	C11H10N6OS2	-7.4	44.27	-29.458	7.9
21	<chem>S=C(Nc1ccccc1N(=O)=O)NNC(=O)c1ccoc1C</chem>	C13H12N4O4S	-8.0	64.91	-35.976	8.4
22	<chem>S=C(Nc1cccc(c1)N(=O)=O)NNC(=O)c1ccoc1C</chem>	C13H12N4O4S	-7.4	61.32	-34.789	16.2
23	<chem>S=C(Nc1ccc(cc1)N(=O)=O)NNC(=O)c1ccoc1C</chem>	C13H12N4O4S	-7.4	55.62	-40.034	1.3
24	<chem>S=C(Nc1ccccc1N(=O)=O)NNC(=O)c1[nH]cnc1C</chem>	C12H12N6O3S	-7.6	66.15	-41.06	8.2
25	<chem>S=C(Nc1cccc(c1)N(=O)=O)NNC(=O)c1[nH]cnc1C</chem>	C12H12N6O3S	-7.3	58.24	-37.569	-12.6
26	<chem>S=C(Nc1ccc(cc1)N(=O)=O)NNC(=O)c1[nH]cnc1C</chem>	C12H12N6O3S	-7.3	54.40	-39.588	25.5
27	<chem>S=C(Nc1ccccc1N(=O)=O)NNC(=O)c1[nH]ccc1</chem>	C12H11N5O3S	-7.4	64.34	-40.891	15.4
28	<chem>S=C(Nc1cccc(c1)N(=O)=O)NNC(=O)c1ccc[nH]1</chem>	C12H11N5O3S	-6.8	55.82	-39.759	20.8

29	<chem>S=C(Nc1ccc(cc1)N(=O)=O)NNC(=O)c1ccc[nH]1</chem>	C12H11N5O3S	-7.2	47.56	-38.596	5.8
30	<chem>S=C(Nc1ccccc1N(=O)=O)NNC(=O)C1CCCC1</chem>	C13H16N4O3S	-7.3	60.99	-34.513	3.4
31	<chem>S=C(Nc1cccc(c1)N(=O)=O)NNC(=O)C1CCCC1</chem>	C13H16N4O3S	-7.4	56.67	-35.42	2.2
32	<chem>S=C(Nc1ccc(cc1)N(=O)=O)NNC(=O)C1CCCC1</chem>	C13H16N4O3S	-6.9	54.30	-37.114	5.6
33	<chem>S=C(Nc1ccccc1N(=O)=O)NNC(=O)C1=NC(=S)N=N1</chem>	C10H7N7O3S2	-6.8	57.75	-35.879	3.2
34	<chem>S=C(Nc1ccc(c1)N(=O)=O)NNC(=O)C1=NC(=S)N=N1</chem>	C10H7N7O3S2	-7.2	58.68	-37.396	19.2
35	<chem>S=C(Nc1ccc(cc1)N(=O)=O)NNC(=O)C1=NC(=S)N=N1</chem>	C10H7N7O3S2	-7.3	59.49	-44.163	19.2
36	<chem>S=C(Nc1ccccc1O)NNC(=O)c1ccoc1C</chem>	C13H13N3O3S	-7.7	60.66	-31.865	-15.0
37	<chem>S=C(Nc1cccc(c1)O)NNC(=O)c1ccoc1C</chem>	C13H13N3O3S	-7.7	58.30	-30.912	1.5
38	<chem>S=C(Nc1ccc(cc1)O)NNC(=O)c1ccoc1C</chem>	C13H13N3O3S	-7.3	54.35	-28.263	20.9
39	<chem>S=C(Nc1ccccc1O)NNC(=O)c1[nH]cnc1C</chem>	C12H13N5O2S	-7.4	61.00	-32.248	5.6
40	<chem>S=C(Nc1ccc(c1)O)NNC(=O)c1[nH]cnc1C</chem>	C12H13N5O2S	-7.4	56.36	-35.526	-6.9
41	<chem>S=C(Nc1ccc(cc1)O)NNC(=O)c1[nH]cnc1C</chem>	C12H13N5O2S	-7.3	52.37	-29.489	-8.7
42	<chem>S=C(Nc1ccccc1O)NNC(=O)c1[nH]ccc1</chem>	C12H12N4O2S	-6.9	57.89	-32.183	2.6
43	<chem>S=C(Nc1ccc(c1)O)NNC(=O)c1ccc[nH]1</chem>	C12H12N4O2S	-6.8	53.72	-35.399	-1.8
44	<chem>S=C(Nc1ccc(cc1)O)NNC(=O)c1ccc[nH]1</chem>	C12H12N4O2S	-6.6	53.71	-30.773	21.8
45	<chem>S=C(Nc1ccccc1O)NNC(=O)C1CCCC1</chem>	C13H17N3O2S	-6.8	59.42	-29.221	10.6
46	<chem>S=C(Nc1ccc(c1)O)NNC(=O)C1CCCC1</chem>	C13H17N3O2S	-6.8	61.01	-29.641	15.0
47	<chem>S=C(Nc1ccc(cc1)O)NNC(=O)C1CCCC1</chem>	C13H17N3O2S	-6.4	53.34	-26.549	-20.3
48	<chem>S=C(Nc1ccccc1O)NNC(=O)C1=NC(=S)N=N1</chem>	C10H8N6O2S2	-7.3	59.23	-35.013	12.8
49	<chem>S=C(Nc1ccc(c1)O)NNC(=O)C1=NC(=S)N=N1</chem>	C10H8N6O2S2	-7.2	56.47	-30.621	-4.3
50	<chem>S=C(Nc1ccc(cc1)O)NNC(=O)C1=NC(=S)N=N1</chem>	C10H8N6O2S2	-7.0	47.46	-32.289	-0.6
51	<chem>COc1ccccc1NC(=S)NNC(=O)c1ccoc1C</chem>	C14H15N3O3S	-7.9	61.41	-28.368	13.7
52	<chem>COc1cccc(c1)NC(=S)NNC(=O)c1ccoc1C</chem>	C14H15N3O3S	-7.2	59.32	-32.886	-4.5
53	<chem>COc1ccc(cc1)NC(=S)NNC(=O)c1ccoc1C</chem>	C14H15N3O3S	-7.4	57.32	-30.367	3.3
54	<chem>COc1ccccc1NC(=S)NNC(=O)c1[nH]cnc1C</chem>	C13H15N5O2S	-7.8	57.49	-35.197	3.0
55	<chem>COc1cccc(c1)NC(=S)NNC(=O)c1[nH]cnc1C</chem>	C13H15N5O2S	-7.1	57.96	-36.426	1.6
56	<chem>COc1ccc(cc1)NC(=S)NNC(=O)c1[nH]cnc1C</chem>	C13H15N5O2S	-7.0	58.78	-32.143	-6.7
57	<chem>COc1ccccc1NC(=S)NNC(=O)c1[nH]ccc1</chem>	C13H14N4O2S	-6.7	52.33	-35.527	12.8
58	<chem>COc1cccc(c1)NC(=S)NNC(=O)c1ccc[nH]1</chem>	C13H14N4O2S	-6.5	52.35	-35.665	-12.7
59	<chem>COc1ccc(cc1)NC(=S)NNC(=O)c1ccc[nH]1</chem>	C13H14N4O2S	-6.4	54.48	-28.962	41.5

60	<chem>COc1cccc1NC(=S)NNC(=O)C1CCCC1</chem>	C14H19N3O2S	-6.7	55.84	-26.977	7.5
61	<chem>COc1cccc(c1)NC(=S)NNC(=O)C1CCCC1</chem>	C14H19N3O2S	-6.7	56.96	-28.675	-8.1
62	<chem>COc1ccc(cc1)NC(=S)NNC(=O)C1CCCC1</chem>	C14H19N3O2S	-7.3	52.76	-28.298	-8.3
63	<chem>COc1cccc1NC(=S)NNC(=O)C1=NC(=S)N=N1</chem>	C11H10N6O2S2	-7.3	59.32	-31.807	-9.8
64	<chem>COc1cccc(c1)NC(=S)NNC(=O)C1=NC(=S)N=N1</chem>	C11H10N6O2S2	-7.1	55.76	-33.763	4.8
65	<chem>COc1ccc(cc1)NC(=S)NNC(=O)C1=NC(=S)N=N1</chem>	C11H10N6O2S2	-7.2	53.29	-33.296	-10.1
66	<chem>S=C(Nc1cccc1F)NNC(=O)c1ccoc1C</chem>	C13H12FN3O2S	-7.7	56.33	-26.193	-0.6
67	<chem>S=C(Nc1cccc(c1)F)NNC(=O)c1ccoc1C</chem>	C13H12FN3O2S	-7.3	57.14	-25.226	1.1
68	<chem>S=C(Nc1ccc(cc1)F)NNC(=O)c1ccoc1C</chem>	C13H12FN3O2S	-7.6	57.83	-24.427	-5.3
69	<chem>S=C(Nc1cccc1F)NNC(=O)c1[nH]cnc1C</chem>	C12H12FN5OS	-7.4	56.90	-31.385	-5.8
70	<chem>S=C(Nc1cccc(c1)F)NNC(=O)c1[nH]cnc1C</chem>	C12H12FN5OS	-7.2	57.03	-29.171	4.6
71	<chem>S=C(Nc1ccc(cc1)F)NNC(=O)c1[nH]cnc1C</chem>	C12H12FN5OS	-7.1	56.15	-28.819	0.1
72	<chem>S=C(Nc1cccc1F)NNC(=O)c1[nH]ccc1</chem>	C12H11FN4OS	-7.0	56.81	-30.901	11.2
73	<chem>S=C(Nc1cccc(c1)F)NNC(=O)c1ccc[nH]1</chem>	C12H11FN4OS	-7.0	55.38	-29.003	31.0
74	<chem>S=C(Nc1ccc(cc1)F)NNC(=O)c1ccc[nH]1</chem>	C12H11FN4OS	-6.5	54.26	-28.732	-2.8
75	<chem>S=C(Nc1cccc1F)NNC(=O)C1CCCC1</chem>	C13H16FN3OS	-6.9	53.72	-27.717	-6.7
76	<chem>S=C(Nc1cccc(c1)F)NNC(=O)C1CCCC1</chem>	C13H16FN3OS	-7.1	58.33	-23.863	-25.2
77	<chem>S=C(Nc1ccc(cc1)F)NNC(=O)C1CCCC1</chem>	C13H16FN3OS	-6.7	53.73	-22.957	-4.6
78	<chem>S=C(Nc1cccc1F)NNC(=O)C1=NC(=S)N=N1</chem>	C10H7FN6OS2	-7.0	58.16	-29.738	47.4
79	<chem>S=C(Nc1cccc(c1)F)NNC(=O)C1=NC(=S)N=N1</chem>	C10H7FN6OS2	-7.2	55.25	-31.654	2.4
80	<chem>S=C(Nc1ccc(cc1)F)NNC(=O)C1=NC(=S)N=N1</chem>	C10H7FN6OS2	-6.6	58.51	-31.311	-9.6
81	<chem>S=C(Nc1cccc1Cl)NNC(=O)c1ccoc1C</chem>	C13H12ClN3O2S	-7.7	62.43	-23.243	17.7
82	<chem>S=C(Nc1cccc(c1)Cl)NNC(=O)c1ccoc1C</chem>	C13H12ClN3O2S	-7.5	57.87	-25.586	-3.4
83	<chem>S=C(Nc1ccc(cc1)Cl)NNC(=O)c1ccoc1C</chem>	C13H12ClN3O2S	-7.5	57.74	-23.984	-11.1
84	<chem>S=C(Nc1cccc1Cl)NNC(=O)c1[nH]cnc1C</chem>	C12H12ClN5OS	-7.3	55.84	-29.518	0.5
85	<chem>S=C(Nc1cccc(c1)Cl)NNC(=O)c1[nH]cnc1C</chem>	C12H12ClN5OS	-7.3	57.09	-30.297	5.2
86	<chem>S=C(Nc1ccc(cc1)Cl)NNC(=O)c1[nH]cnc1C</chem>	C12H12ClN5OS	-7.3	55.95	-27.135	-23.9
87	<chem>S=C(Nc1cccc1Cl)NNC(=O)c1[nH]ccc1</chem>	C12H11ClN4OS	-7.0	54.85	-28.537	23.9
88	<chem>S=C(Nc1cccc(c1)Cl)NNC(=O)c1ccc[nH]1</chem>	C12H11ClN4OS	-6.5	53.27	-29.095	26.8
89	<chem>S=C(Nc1ccc(cc1)Cl)NNC(=O)c1ccc[nH]1</chem>	C12H11ClN4OS	-6.6	55.39	-29.211	-6.4
90	<chem>S=C(Nc1cccc1Cl)NNC(=O)C1CCCC1</chem>	C13H16ClN3OS	-7.1	56.72	-27.436	-7.8

91	<chem>S=C(Nc1cccc(c1)Cl)NNC(=O)C1CCCC1</chem>	C13H16ClN3OS	-6.5	55.79	-23.133	-21.4
92	<chem>S=C(Nc1ccc(cc1)Cl)NNC(=O)C1CCCC1</chem>	C13H16ClN3OS	-6.7	54.26	-22.752	-11.8
93	<chem>S=C(Nc1cccc1Cl)NNC(=O)C1=NC(=S)N=N1</chem>	C10H7ClN6OS2	-7.5	60.09	-29.435	2.6
94	<chem>S=C(Nc1cccc(c1)Cl)NNC(=O)C1=NC(=S)N=N1</chem>	C10H7ClN6OS2	-6.8	56.57	-28.794	10.6
95	<chem>S=C(Nc1ccc(cc1)Cl)NNC(=O)C1=NC(=S)N=N1</chem>	C10H7ClN6OS2	-6.4	49.66	-28.636	2.7
96	<chem>S=C(Nc1cccc1Br)NNC(=O)c1ccoc1C</chem>	C13H12BrN3O2S	-7.7	61.97	-24.05	24.9
97	<chem>S=C(Nc1cccc(c1)Br)NNC(=O)c1ccoc1C</chem>	C13H12BrN3O2S	-7.5	58.81	-25.474	-9.4
98	<chem>S=C(Nc1ccc(cc1)Br)NNC(=O)c1ccoc1C</chem>	C13H12BrN3O2S	-7.4	58.21	-23.717	-12.2
99	<chem>S=C(Nc1cccc1Br)NNC(=O)c1[nH]cnc1C</chem>	C12H12BrN5OS	-7.3	55.97	-28.915	-2.4
100	<chem>S=C(Nc1cccc(c1)Br)NNC(=O)c1[nH]cnc1C</chem>	C12H12BrN5OS	-7.1	57.69	-29.793	-1.2
101	<chem>S=C(Nc1ccc(cc1)Br)NNC(=O)c1[nH]cnc1C</chem>	C12H12BrN5OS	-7.0	57.11	-27.372	2.7
102	<chem>S=C(Nc1cccc1Br)NNC(=O)c1[nH]ccc1</chem>	C12H11BrN4OS	-6.7	51.44	-27.267	-3.5
103	<chem>S=C(Nc1cccc(c1)Br)NNC(=O)c1ccc[nH]1</chem>	C12H11BrN4OS	-6.4	57.65	-29.681	-2.2
104	<chem>S=C(Nc1ccc(cc1)Br)NNC(=O)c1ccc[nH]1</chem>	C12H11BrN4OS	-6.6	52.58	-29.144	5.9
105	<chem>S=C(Nc1cccc1Br)NNC(=O)C1CCCC1</chem>	C13H16BrN3OS	-6.6	54.70	-26.064	-7.4
106	<chem>S=C(Nc1cccc(c1)Br)NNC(=O)C1CCCC1</chem>	C13H16BrN3OS	-6.6	55.52	-22.93	-23.2
107	<chem>S=C(Nc1ccc(cc1)Br)NNC(=O)C1CCCC1</chem>	C13H16BrN3OS	-6.9	55.30	-25.342	-7.7
108	<chem>S=C(Nc1cccc1Br)NNC(=O)C1=NC(=S)N=N1</chem>	C10H7BrN6OS2	-6.8	51.95	-32.5	-7.8
109	<chem>S=C(Nc1cccc(c1)Br)NNC(=O)C1=NC(=S)N=N1</chem>	C10H7BrN6OS2	-7.3	58.68	-29.316	8.6
110	<chem>S=C(Nc1ccc(cc1)Br)NNC(=O)C1=NC(=S)N=N1</chem>	C10H7BrN6OS2	-7.4	49.83	-31.908	-3.9
111	<chem>S=C(Nc1cccc1I)NNC(=O)c1ccoc1C</chem>	C13H12IN3O2S	-7.2	57.90	-24.512	20.7
112	<chem>S=C(Nc1cccc(c1)I)NNC(=O)c1ccoc1C</chem>	C13H12IN3O2S	-7.3	58.24	-26.781	-0.5
113	<chem>S=C(Nc1ccc(cc1)I)NNC(=O)c1ccoc1C</chem>	C13H12IN3O2S	-7.3	57.93	-23.646	-0.3
114	<chem>S=C(Nc1cccc1I)NNC(=O)c1[nH]cnc1C</chem>	C12H12IN5OS	-7.3	55.99	-27.932	1.5
115	<chem>S=C(Nc1cccc(c1)I)NNC(=O)c1[nH]cnc1C</chem>	C12H12IN5OS	-7.3	56.77	-30.284	-0.3
116	<chem>S=C(Nc1ccc(cc1)I)NNC(=O)c1[nH]cnc1C</chem>	C12H12IN5OS	-7.2	54.78	-26.61	-26.1
117	<chem>S=C(Nc1cccc1I)NNC(=O)c1[nH]ccc1</chem>	C12H11IN4OS	-6.4	49.04	-28.393	-10.1
118	<chem>S=C(Nc1cccc(c1)I)NNC(=O)c1ccc[nH]1</chem>	C12H11IN4OS	-6.6	55.97	-30.666	26.6
119	<chem>S=C(Nc1ccc(cc1)I)NNC(=O)c1ccc[nH]1</chem>	C12H11IN4OS	-6.4	52.35	-29.053	-10.2
120	<chem>S=C(Nc1cccc1I)NNC(=O)C1CCCC1</chem>	C13H16IN3OS	-6.3	56.80	-26.08	-6.8
121	<chem>S=C(Nc1cccc(c1)I)NNC(=O)C1CCCC1</chem>	C13H16IN3OS	-6.6	55.73	-22.01	9.4

122	<chem>S=C(Nc1ccc(cc1)I)NNC(=O)C1CCCC1</chem>	C13H16IN3OS	-6.8	54.94	-25.503	-7.0
123	<chem>S=C(Nc1ccccc1I)NNC(=O)C1=NC(=S)N=N1</chem>	C10H7IN6OS2	-6.6	48.10	-28.303	-9.0
124	<chem>S=C(Nc1ccc(cc1)I)NNC(=O)C1=NC(=S)N=N1</chem>	C10H7IN6OS2	-7.2	52.26	-29.191	2.7
125	<chem>S=C(Nc1ccc(cc1)I)NNC(=O)C1=NC(=S)N=N1</chem>	C10H7IN6OS2	-7.2	51.41	-29.223	7.9
126	<chem>S=C(Nc1ccc(cc1F)F)NNC(=O)c1ccoc1C</chem>	C13H11F2N3O2S	-7.9	58.58	-25.86	-6.1
127	<chem>S=C(Nc1ccc(cc1F)F)NNC(=O)c1[nH]cnc1C</chem>	C12H11F2N5OS	-7.7	60.95	-30.751	-5.5
128	<chem>S=C(Nc1ccc(cc1F)F)NNC(=O)c1ccc[nH]1</chem>	C12H10F2N4OS	-6.8	47.83	-30.515	-1.1
129	<chem>S=C(Nc1ccc(cc1F)F)NNC(=O)C1CCCC1</chem>	C13H15F2N3OS	-6.8	55.26	-26.775	-27.7
130	<chem>S=C(Nc1ccc(cc1F)F)NNC(=O)C1=NC(=S)N=N1</chem>	C10H6F2N6OS2	-7.6	34.22	-31.805	-2.8
131	<chem>S=C(Nc1ccc(cc1F)Cl)NNC(=O)c1ccoc1C</chem>	C13H11ClFN3O2S	-7.9	57.07	-24.044	5.4
132	<chem>S=C(Nc1ccc(cc1F)Cl)NNC(=O)c1[nH]cnc1C</chem>	C12H11ClFN5OS	-7.5	58.99	-29.892	-1.9
133	<chem>S=C(Nc1ccc(cc1F)Cl)NNC(=O)c1ccc[nH]1</chem>	C12H10ClFN4OS	-6.8	54.63	-29.932	14.7
134	<chem>S=C(Nc1ccc(cc1F)Cl)NNC(=O)C1CCCC1</chem>	C13H15ClFN3OS	-7.1	56.23	-25.693	-6.2
135	<chem>S=C(Nc1ccc(cc1F)Cl)NNC(=O)C1=NC(=S)N=N1</chem>	C10H6ClFN6OS2	-7.6	55.84	-30.918	-2.3
136	<chem>S=C(Nc1ccc(cc1F)Br)NNC(=O)c1ccoc1C</chem>	C13H11BrFN3O2S	-7.8	63.62	-25.852	-28.3
137	<chem>S=C(Nc1ccc(cc1F)Br)NNC(=O)c1[nH]cnc1C</chem>	C12H11BrFN5OS	-7.1	60.19	-29.483	-4.1
138	<chem>S=C(Nc1ccc(cc1F)Br)NNC(=O)c1ccc[nH]1</chem>	C12H10BrFN4OS	-6.8	56.83	-29.827	15.5
139	<chem>S=C(Nc1ccc(cc1F)Br)NNC(=O)C1CCCC1</chem>	C13H15BrFN3OS	-7.0	58.97	-27.667	-4.6
140	<chem>S=C(Nc1ccc(cc1F)Br)NNC(=O)C1=NC(=S)N=N1</chem>	C10H6BrFN6OS2	-7.6	50.14	-32.178	0.8
141	<chem>S=C(Nc1ccc(cc1F)I)NNC(=O)c1ccoc1C</chem>	C13H11FIN3O2S	-7.7	62.52	-23.183	1.0
142	<chem>S=C(Nc1ccc(cc1F)I)NNC(=O)c1[nH]cnc1C</chem>	C12H11FIN5OS	-7.4	54.48	-29.989	-4.5
143	<chem>S=C(Nc1ccc(cc1F)I)NNC(=O)c1ccc[nH]1</chem>	C12H10FIN4OS	-7.0	53.33	-29.704	16.2
144	<chem>S=C(Nc1ccc(cc1F)I)NNC(=O)C1CCCC1</chem>	C13H15FIN3OS	-7.0	57.73	-25.741	-6.6
145	<chem>S=C(Nc1ccc(cc1F)I)NNC(=O)C1=NC(=S)N=N1</chem>	C10H6FIN6OS2	-7.5	56.97	-31.235	-0.4
146	<chem>S=C(Nc1ccc(cc1Cl)F)NNC(=O)c1ccoc1C</chem>	C13H11ClFN3O2S	-8.1	61.30	-24.356	7.8
147	<chem>S=C(Nc1ccc(cc1Cl)F)NNC(=O)c1[nH]cnc1C</chem>	C12H11ClFN5OS	-7.2	62.24	-28.111	-3.5
148	<chem>S=C(Nc1ccc(cc1Cl)F)NNC(=O)c1ccc[nH]1</chem>	C12H10ClFN4OS	-7.0	58.25	-28.174	-6.3
149	<chem>S=C(Nc1ccc(cc1Cl)F)NNC(=O)C1CCCC1</chem>	C13H15ClFN3OS	-7.2	60.05	-27.457	-6.6
150	<chem>S=C(Nc1ccc(cc1Cl)F)NNC(=O)C1=NC(=S)N=N1</chem>	C10H6ClFN6OS2	-7.8	61.46	-28.252	13.7
151	<chem>S=C(Nc1ccc(cc1Cl)Cl)NNC(=O)c1ccoc1C</chem>	C13H11Cl2N3O2S	-7.9	63.51	-24.56	-2.1
152	<chem>S=C(Nc1ccc(cc1Cl)Cl)NNC(=O)c1[nH]cnc1C</chem>	C12H11Cl2N5OS	-7.7	53.42	-28.103	-1.8

153	<chem>S=C(Nc1ccc(cc1Cl)Cl)NNC(=O)c1ccc[nH]1</chem>	C12H10Cl2N4OS	-6.8	58.01	-29.231	19.0
154	<chem>S=C(Nc1ccc(cc1Cl)Cl)NNC(=O)C1CCCC1</chem>	C13H15Cl2N3OS	-6.9	58.79	-24.989	-28.7
155	<chem>S=C(Nc1ccc(cc1Cl)Cl)NNC(=O)C1=NC(=S)N=N1</chem>	C10H6Cl2N6OS2	-6.8	64.15	-29.379	-7.1
156	<chem>S=C(Nc1ccc(cc1Cl)Br)NNC(=O)c1ccoc1C</chem>	C13H11BrClN3O2S	-8.0	56.83	-25.755	-1.5
157	<chem>S=C(Nc1ccc(cc1Cl)Br)NNC(=O)c1[nH]cnc1C</chem>	C12H11BrClN5OS	-7.2	59.13	-29.369	-6.6
158	<chem>S=C(Nc1ccc(cc1Cl)Br)NNC(=O)c1ccc[nH]1</chem>	C12H10BrClN4OS	-6.9	55.22	-27.6487	-14.0
159	<chem>S=C(Nc1ccc(cc1Cl)Br)NNC(=O)C1CCCC1</chem>	C13H15BrClN3OS	-6.9	56.33	-28.269	-7.2
160	<chem>S=C(Nc1ccc(cc1Cl)Br)NNC(=O)C1=NC(=S)N=N1</chem>	C10H6BrClN6OS2	-7.7	47.01	-30.052	1.0
161	<chem>S=C(Nc1ccc(cc1Cl)I)NNC(=O)c1ccoc1C</chem>	C13H11ClIN3O2S	-7.3	60.19	-26.572	-11.2
162	<chem>S=C(Nc1ccc(cc1Cl)I)NNC(=O)c1[nH]cnc1C</chem>	C12H11ClIN5OS	-7.3	62.37	-28.548	-4.0
163	<chem>S=C(Nc1ccc(cc1Cl)I)NNC(=O)c1ccc[nH]1</chem>	C12H10ClIN4OS	-6.8	59.98	-29.146	-0.1
164	<chem>S=C(Nc1ccc(cc1Cl)I)NNC(=O)C1CCCC1</chem>	C13H15ClIN3OS	-6.9	56.38	-25.065	-26.9
165	<chem>S=C(Nc1ccc(cc1Cl)I)NNC(=O)C1=NC(=S)N=N1</chem>	C10H6ClIN6OS2	-7.7	45.95	-32.315	3.2
166	<chem>S=C(Nc1ccc(cc1Br)F)NNC(=O)c1ccoc1C</chem>	C13H11BrFN3O2S	-8.0	63.77	-24.167	23.4
167	<chem>S=C(Nc1ccc(cc1Br)F)NNC(=O)c1[nH]cnc1C</chem>	C12H11BrFN5OS	-7.3	60.85	-27.476	0.6
168	<chem>S=C(Nc1ccc(cc1Br)F)NNC(=O)c1ccc[nH]1</chem>	C12H10BrFN4OS	-6.8	51.19	-27.987	3.7
169	<chem>S=C(Nc1ccc(cc1Br)F)NNC(=O)C1CCCC1</chem>	C13H15BrFN3OS	-6.8	52.27	-28.6	-6.0
170	<chem>S=C(Nc1ccc(cc1Br)F)NNC(=O)C1=NC(=S)N=N1</chem>	C10H6BrFN6OS2	-6.6	55.79	-28.444	22.5
171	<chem>S=C(Nc1ccc(cc1Br)Cl)NNC(=O)c1ccoc1C</chem>	C13H11BrClN3O2S	-7.9	58.31	-23.062	-20.4
172	<chem>S=C(Nc1ccc(cc1Br)Cl)NNC(=O)c1[nH]cnc1C</chem>	C12H11BrClN5OS	-7.2	60.96	-28.029	-7.6
173	<chem>S=C(Nc1ccc(cc1Br)Cl)NNC(=O)c1ccc[nH]1</chem>	C12H10BrClN4OS	-6.7	58.31	-29.85	-6.6
174	<chem>S=C(Nc1ccc(cc1Br)Cl)NNC(=O)C1CCCC1</chem>	C13H15BrClN3OS	-6.9	52.62	-28.656	-8.8
175	<chem>S=C(Nc1ccc(cc1Br)Cl)NNC(=O)C1=NC(=S)N=N1</chem>	C10H6BrClN6OS2	-6.2	45.36	-28.846	-13.2
176	<chem>S=C(Nc1ccc(cc1Br)Br)NNC(=O)c1ccoc1C</chem>	C13H11Br2N3O2S	-7.8	60.01	-26.038	-2.2
177	<chem>S=C(Nc1ccc(cc1Br)Br)NNC(=O)c1[nH]cnc1C</chem>	C12H11Br2N5OS	-7.3	60.47	-27.432	-28.3
178	<chem>S=C(Nc1ccc(cc1Br)Br)NNC(=O)c1ccc[nH]1</chem>	C12H10Br2N4OS	-6.6	60.34	-29.288	27.8
179	<chem>S=C(Nc1ccc(cc1Br)Br)NNC(=O)C1CCCC1</chem>	C13H15Br2N3OS	-7.0	55.70	-28.753	-9.6
180	<chem>S=C(Nc1ccc(cc1Br)Br)NNC(=O)C1=NC(=S)N=N1</chem>	C10H6Br2N6OS2	-6.7	47.92	-32.423	-17.5
181	<chem>S=C(Nc1ccc(cc1Br)I)NNC(=O)c1ccoc1C</chem>	C13H11BrIN3O2S	-7.8	62.98	-26.331	0.9
182	<chem>S=C(Nc1ccc(cc1Br)I)NNC(=O)c1[nH]cnc1C</chem>	C12H11BrIN5OS	-7.5	61.38	-28.828	-2.3
183	<chem>S=C(Nc1ccc(cc1Br)I)NNC(=O)c1ccc[nH]1</chem>	C12H10BrIN4OS	-6.7	56.96	-27.837	-8.3

184	<chem>S=C(Nc1ccc(cc1Br)I)NNC(=O)C1CCCC1</chem>	C13H15BrIN3OS	-6.7	58.44	-25.268	-27.7
185	<chem>S=C(Nc1ccc(cc1Br)I)NNC(=O)C1=NC(=S)N=N1</chem>	C10H6BrIN6OS2	-7.6	52.04	-32.131	-15.9
186	<chem>S=C(Nc1ccc(cc1I)F)NNC(=O)c1ccoc1C</chem>	C13H11FIN3O2S	-7.2	64.02	-26.369	1.4
187	<chem>S=C(Nc1ccc(cc1I)F)NNC(=O)c1[nH]cnc1C</chem>	C12H11FIN5OS	-7.2	62.14	-27.552	17.8
188	<chem>S=C(Nc1ccc(cc1I)F)NNC(=O)c1ccc[nH]1</chem>	C12H10FIN4OS	-6.7	52.08	-27.508	4.3
189	<chem>S=C(Nc1ccc(cc1I)F)NNC(=O)C1CCCC1</chem>	C13H15FIN3OS	-6.8	55.50	-28.921	-9.8
190	<chem>S=C(Nc1ccc(cc1I)F)NNC(=O)C1=NC(=S)N=N1</chem>	C10H6FIN6OS2	-7.1	62.92	-31.032	-6.3
191	<chem>S=C(Nc1ccc(cc1I)Cl)NNC(=O)c1ccoc1C</chem>	C13H11ClIN3O2S	-7.1	62.18	-25.239	-3.1
192	<chem>S=C(Nc1ccc(cc1I)Cl)NNC(=O)c1[nH]cnc1C</chem>	C12H11ClIN5OS	-7.2	61.76	-26.066	3.7
193	<chem>S=C(Nc1ccc(cc1I)Cl)NNC(=O)c1ccc[nH]1</chem>	C12H10ClIN4OS	-6.6	58.73	-27.814	-22.2
194	<chem>S=C(Nc1ccc(cc1I)Cl)NNC(=O)C1CCCC1</chem>	C13H15ClIN3OS	-6.5	55.28	-24.117	-29.0
195	<chem>S=C(Nc1ccc(cc1I)Cl)NNC(=O)C1=NC(=S)N=N1</chem>	C10H6ClIN6OS2	-7.0	49.08	-28.832	-6.7
196	<chem>S=C(Nc1ccc(cc1I)Br)NNC(=O)c1ccoc1C</chem>	C13H11BrIN3O2S	-7.2	62.65	-25.124	-6.7
197	<chem>S=C(Nc1ccc(cc1I)Br)NNC(=O)c1[nH]cnc1C</chem>	C12H11BrIN5OS	-7.2	61.87	-25.764	12.1
198	<chem>S=C(Nc1ccc(cc1I)Br)NNC(=O)c1ccc[nH]1</chem>	C12H10BrIN4OS	-6.7	49.01	-28.111	-25.5
199	<chem>S=C(Nc1ccc(cc1I)Br)NNC(=O)C1CCCC1</chem>	C13H15BrIN3OS	-6.7	57.96	-24.031	-10.2
200	<chem>S=C(Nc1ccc(cc1I)Br)NNC(=O)C1=NC(=S)N=N1</chem>	C10H6BrIN6OS2	-7.1	61.25	-33.307	-5.2
201	<chem>S=C(Nc1ccc(cc1I)I)NNC(=O)c1ccoc1C</chem>	C13H11I2N3O2S	-7.2	62.93	-26.732	3.0
202	<chem>S=C(Nc1ccc(cc1I)I)NNC(=O)c1[nH]cnc1C</chem>	C12H11I2N5OS	-7.3	48.53	-27.784	-8.8
203	<chem>S=C(Nc1ccc(cc1I)I)NNC(=O)c1ccc[nH]1</chem>	C12H10I2N4OS	-6.7	55.29	-28.342	31.1
204	<chem>S=C(Nc1ccc(cc1I)I)NNC(=O)C1CCCC1</chem>	C13H15I2N3OS	-6.8	59.12	-25.491	-10.5
205	<chem>S=C(Nc1ccc(cc1I)I)NNC(=O)C1=NC(=S)N=N1</chem>	C10H6I2N6OS2	-7.2	64.34	-33.23	-3.1
206	<chem>S=C(Nc1cc(F)cc(c1)F)NNC(=O)c1ccoc1C</chem>	C13H11F2N3O2S	-7.6	58.32	-25.175	0.7
207	<chem>S=C(Nc1cc(F)cc(c1)F)NNC(=O)c1[nH]cnc1C</chem>	C12H11F2N5OS	-7.3	57.27	-27.889	-0.1
208	<chem>S=C(Nc1cc(F)cc(c1)F)NNC(=O)c1ccc[nH]1</chem>	C12H10F2N4OS	-7.0	57.33	-29.271	18.1
209	<chem>S=C(Nc1cc(F)cc(c1)F)NNC(=O)C1CCCC1</chem>	C13H15F2N3OS	-7.3	57.23	-24.323	-10.8
210	<chem>S=C(Nc1cc(F)cc(c1)F)NNC(=O)C1=NC(=S)N=N1</chem>	C10H6F2N6OS2	-7.2	56.92	-29.047	-3.3
211	<chem>S=C(Nc1cc(F)cc(c1)Cl)NNC(=O)c1ccoc1C</chem>	C13H11ClFN3O2S	-7.3	58.34	-25.72	-4.6
212	<chem>S=C(Nc1cc(F)cc(c1)Cl)NNC(=O)c1[nH]cnc1C</chem>	C12H11ClFN5OS	-7.3	57.15	-29.589	8.0
213	<chem>S=C(Nc1cc(F)cc(c1)Cl)NNC(=O)c1[nH]ccc1</chem>	C12H10ClFN4OS	-7.0	56.96	-29.264	2.7
214	<chem>S=C(Nc1cc(F)cc(c1)Cl)NNC(=O)C1CCCC1</chem>	C13H15ClFN3OS	-7.4	58.28	-24.536	-9.7

215	<chem>S=C1N=NC(=N1)C(=O)NNC(=S)Nc1cc(F)cc(c1)Cl</chem>	C10H6ClFN6OS2	-7.5	53.32	-31.051	-1.3
216	<chem>S=C(Nc1cc(F)cc(c1)Br)NNC(=O)c1ccoc1C</chem>	C13H11BrFN3O2S	-7.3	58.27	-26.607	12.4
217	<chem>S=C(Nc1cc(F)cc(c1)Br)NNC(=O)c1[nH]cnc1C</chem>	C12H11BrFN5OS	-7.3	56.97	-29.467	-2.6
218	<chem>S=C(Nc1cc(F)cc(c1)Br)NNC(=O)c1[nH]ccc1</chem>	C12H10BrFN4OS	-6.7	56.29	-29.081	-4.9
219	<chem>S=C(Nc1cc(F)cc(c1)Br)NNC(=O)C1CCCC1</chem>	C13H15BrFN3OS	-7.0	56.89	-24.693	-14.5
220	<chem>S=C1N=NC(=N1)C(=O)NNC(=S)Nc1cc(F)cc(c1)Br</chem>	C10H6BrFN6OS2	-7.1	50.39	-31.124	-0.8
221	<chem>S=C(Nc1cc(F)cc(c1)I)NNC(=O)c1ccoc1C</chem>	C13H11FIN3O2S	-7.3	57.78	-26.484	-9.2
222	<chem>S=C(Nc1cc(F)cc(c1)I)NNC(=O)c1[nH]cnc1C</chem>	C12H11FIN5OS	-7.2	56.99	-29.708	-1.6
223	<chem>S=C(Nc1cc(F)cc(c1)I)NNC(=O)c1[nH]ccc1</chem>	C12H10FIN4OS	-6.8	55.56	-28.828	-1.3
224	<chem>S=C(Nc1cc(F)cc(c1)I)NNC(=O)C1CCCC1</chem>	C13H15FIN3OS	-6.8	57.84	-24.853	-12.2
225	<chem>S=C1N=NC(=N1)C(=O)NNC(=S)Nc1cc(F)cc(c1)I</chem>	C10H6FIN6OS2	-7.1	51.24	-30.997	0.7
226	<chem>S=C(Nc1cc(Cl)cc(c1)Cl)NNC(=O)c1ccoc1C</chem>	C13H11Cl2N3O2S	-7.2	58.57	-25.224	21.3
227	<chem>S=C(Nc1cc(Cl)cc(c1)Cl)NNC(=O)c1[nH]cnc1C</chem>	C12H11Cl2N5OS	-7.2	56.25	-30.63	5.9
228	<chem>S=C(Nc1cc(Cl)cc(c1)Cl)NNC(=O)c1ccc[nH]1</chem>	C12H10Cl2N4OS	-6.8	55.16	-30.256	1.7
229	<chem>S=C(Nc1cc(Cl)cc(c1)Cl)NNC(=O)C1CCCC1</chem>	C13H15Cl2N3OS	-6.7	54.88	-24.535	-10.8
230	<chem>S=C(Nc1cc(Cl)cc(c1)Cl)NNC(=O)C1=NC(=S)N=N1</chem>	C10H6Cl2N6OS2	-7.1	53.89	-31.13	1.6
231	<chem>S=C(Nc1cc(Cl)cc(c1)Br)NNC(=O)c1ccoc1C</chem>	C13H11BrClN3O2S	-7.3	56.28	-25.309	21.2
232	<chem>S=C(Nc1cc(Cl)cc(c1)Br)NNC(=O)c1[nH]cnc1C</chem>	C12H11BrClN5OS	-7.3	59.29	-30.341	5.9
233	<chem>S=C(Nc1cc(Cl)cc(c1)Br)NNC(=O)c1[nH]ccc1</chem>	C12H10BrClN4OS	-6.7	57.42	-29.963	1.2
234	<chem>S=C(Nc1cc(Cl)cc(c1)Br)NNC(=O)C1CCCC1</chem>	C13H15BrClN3OS	-6.6	54.94	-24.69	-12.5
235	<chem>S=C1N=NC(=N1)C(=O)NNC(=S)Nc1cc(Cl)cc(c1)Br</chem>	C10H6BrClN6OS2	-7.1	53.10	-31.316	1.2
236	<chem>S=C(Nc1cc(Cl)cc(c1)I)NNC(=O)c1ccoc1C</chem>	C13H11ClIN3O2S	-7.4	57.57	-25.61	0.4
237	<chem>S=C(Nc1cc(Cl)cc(c1)I)NNC(=O)c1[nH]cnc1C</chem>	C12H11ClIN5OS	-7.3	56.48	-29.923	6.0
238	<chem>S=C(Nc1cc(Cl)cc(c1)I)NNC(=O)c1[nH]ccc1</chem>	C12H10ClIN4OS	-6.5	54.98	-29.634	1.1
239	<chem>S=C(Nc1cc(Cl)cc(c1)I)NNC(=O)C1CCCC1</chem>	C13H15ClIN3OS	-6.8	53.62	-24.852	-11.4
240	<chem>S=C1N=NC(=N1)C(=O)NNC(=S)Nc1cc(Cl)cc(c1)I</chem>	C10H6ClIN6OS2	-7.2	50.90	-31.093	-6.2
241	<chem>S=C(Nc1cc(Br)cc(c1)Br)NNC(=O)c1ccoc1C</chem>	C13H11Br2N3O2S	-7.2	58.91	-24.337	1.6
242	<chem>S=C(Nc1cc(Br)cc(c1)Br)NNC(=O)c1[nH]cnc1C</chem>	C12H11Br2N5OS	-7.3	59.53	-30.609	6.4
243	<chem>S=C(Nc1cc(Br)cc(c1)Br)NNC(=O)c1ccc[nH]1</chem>	C12H10Br2N4OS	-6.7	55.94	-30.094	1.0
244	<chem>S=C(Nc1cc(Br)cc(c1)Br)NNC(=O)C1CCCC1</chem>	C13H15Br2N3OS	-6.5	54.00	-24.738	-13.7
245	<chem>S=C(Nc1cc(Br)cc(c1)Br)NNC(=O)C1=NC(=S)N=N1</chem>	C10H6Br2N6OS2	-7.2	49.17	-31.219	0.1

246	<chem>S=C(Nc1cc(Br)cc(c1)I)NNC(=O)c1ccoc1C</chem>	C13H11BrIN3O2S	-7.3	56.04	-24.191	-0.1
247	<chem>S=C(Nc1cc(Br)cc(c1)I)NNC(=O)c1[nH]cnc1C</chem>	C12H11BrIN5OS	-7.3	53.10	-30.193	6.4
248	<chem>S=C(Nc1cc(Br)cc(c1)I)NNC(=O)c1[nH]ccc1</chem>	C12H10BrIN4OS	-6.4	50.47	-29.77	1.0
249	<chem>S=C(Nc1cc(Br)cc(c1)I)NNC(=O)C1CCCC1</chem>	C13H15BrIN3OS	-6.7	55.96	-24.909	-13.3
250	<chem>S=C1N=NC(=N1)C(=O)NNC(=S)Nc1cc(Br)cc(c1)I</chem>	C10H6BrIN6OS2	-7.2	52.10	-31.285	-0.4
251	<chem>S=C(Nc1cc(I)cc(c1)I)NNC(=O)c1ccoc1C</chem>	C13H11I2N3O2S	-7.4	54.31	-23.328	-5.7
252	<chem>S=C(Nc1cc(I)cc(c1)I)NNC(=O)c1[nH]cnc1C</chem>	C12H11I2N5OS	-7.4	59.07	-29.08	13.2
253	<chem>S=C(Nc1cc(I)cc(c1)I)NNC(=O)c1ccc[nH]1</chem>	C12H10I2N4OS	-6.6	54.33	-28.545	7.8
254	<chem>S=C(Nc1cc(I)cc(c1)I)NNC(=O)C1CCCC1</chem>	C13H15I2N3OS	-6.8	53.17	-24.885	-14.4
255	<chem>S=C(Nc1cc(I)cc(c1)I)NNC(=O)C1=NC(=S)N=N1</chem>	C10H6I2N6OS2	-7.2	49.82	-31.112	-0.8
256	<chem>S=C(Nc1c(F)cc(cc1F)F)NNC(=O)c1ccoc1C</chem>	C13H10F3N3O2S	-7.8	60.31	-25.335	-4.7
257	<chem>S=C(Nc1c(F)cc(cc1F)F)NNC(=O)c1[nH]cnc1C</chem>	C12H10F3N5OS	-7.4	55.64	-27.526	-7.1
258	<chem>S=C(Nc1c(F)cc(cc1F)F)NNC(=O)c1ccc[nH]1</chem>	C12H9F3N4OS	-6.9	49.29	-30.507	-6.9
259	<chem>S=C(Nc1c(F)cc(cc1F)F)NNC(=O)C1CCCC1</chem>	C13H14F3N3OS	-7.1	51.36	-25.647	-0.4
260	<chem>S=C(Nc1c(F)cc(cc1F)F)NNC(=O)C1=NC(=S)N=N1</chem>	C10H5F3N6OS2	-7.7	58.44	-31.505	-6.2
261	<chem>S=C(Nc1c(F)cc(cc1F)Cl)NNC(=O)c1ccoc1C</chem>	C13H10ClF2N3O2S	-7.7	58.15	-25.071	-6.8
262	<chem>S=C(Nc1c(F)cc(cc1F)Cl)NNC(=O)c1[nH]cnc1C</chem>	C12H10ClF2N5OS	-7.5	56.22	-27.405	11.5
263	<chem>S=C(Nc1c(F)cc(cc1F)Cl)NNC(=O)c1ccc[nH]1</chem>	C12H9ClF2N4OS	-6.7	52.65	-30.098	12.5
264	<chem>S=C(Nc1c(F)cc(cc1F)Cl)NNC(=O)C1CCCC1</chem>	C13H14ClF2N3OS	-7.0	55.43	-25.725	-15.7
265	<chem>S=C(Nc1c(F)cc(cc1F)Cl)NNC(=O)C1=NC(=S)N=N1</chem>	C10H5ClF2N6OS2	-7.1	31.56	-30.468	2.0
266	<chem>S=C(Nc1c(F)cc(cc1F)Br)NNC(=O)c1ccoc1C</chem>	C13H10BrF2N3O2S	-7.5	60.83	-25.155	-28.9
267	<chem>S=C(Nc1c(F)cc(cc1F)Br)NNC(=O)c1[nH]cnc1C</chem>	C12H10BrF2N5OS	-7.5	48.83	-29.098	-5.7
268	<chem>S=C(Nc1c(F)cc(cc1F)Br)NNC(=O)c1ccc[nH]1</chem>	C12H9BrF2N4OS	-6.9	50.24	-30.057	12.9
269	<chem>S=C(Nc1c(F)cc(cc1F)Br)NNC(=O)C1CCCC1</chem>	C13H14BrF2N3OS	-7.0	50.72	-25.792	-11.2
270	<chem>S=C(Nc1c(F)cc(cc1F)Br)NNC(=O)C1=NC(=S)N=N1</chem>	C10H5BrF2N6OS2	-7.5	51.86	-29.036	30.9
271	<chem>S=C(Nc1c(F)cc(cc1F)I)NNC(=O)c1ccoc1C</chem>	C13H10F2IN3O2S	-7.4	59.16	-25.341	-6.7
272	<chem>S=C(Nc1c(F)cc(cc1F)I)NNC(=O)c1[nH]cnc1C</chem>	C12H10F2IN5OS	-7.3	54.79	-27.249	-3.9
273	<chem>S=C(Nc1c(F)cc(cc1F)I)NNC(=O)c1ccc[nH]1</chem>	C12H9F2IN4OS	-6.9	51.28	-29.943	13.6
274	<chem>S=C(Nc1c(F)cc(cc1F)I)NNC(=O)C1CCCC1</chem>	C13H14F2IN3OS	-7.2	52.70	-25.729	-14.8
275	<chem>S=C(Nc1c(F)cc(cc1F)I)NNC(=O)C1=NC(=S)N=N1</chem>	C10H5F2IN6OS2	-6.9	37.04	-32.005	-7.5
276	<chem>S=C(Nc1c(F)cc(cc1Cl)F)NNC(=O)c1ccoc1C</chem>	C13H10ClF2N3O2S	-7.6	60.16	-25.399	0.2

277	<chem>S=C(Nc1c(F)cc(cc1Cl)F)NNC(=O)c1[nH]cnc1C</chem>	C12H10ClF2N5OS	-7.6	58.27	-27.181	6.3
278	<chem>S=C(Nc1c(F)cc(cc1Cl)F)NNC(=O)c1[nH]ccc1</chem>	C12H9ClF2N4OS	-7.1	51.41	-30.059	-8.0
279	<chem>S=C(Nc1c(F)cc(cc1Cl)F)NNC(=O)C1CCCC1</chem>	C13H14ClF2N3OS	-7.1	54.60	-25.966	-4.7
280	<chem>S=C1N=NC(=N1)C(=O)NNC(=S)Nc1c(F)cc(cc1Cl)F</chem>	C10H5ClF2N6OS2	-7.4	40.39	-32.304	-6.4
281	<chem>S=C(Nc1c(F)cc(cc1Cl)Cl)NNC(=O)c1ccoc1C</chem>	C13H10Cl2FN3O2S	-7.8	61.98	-26.047	-4.4
282	<chem>S=C(Nc1c(F)cc(cc1Cl)Cl)NNC(=O)c1[nH]cnc1C</chem>	C12H10Cl2FN5OS	-7.6	56.77	-28.188	-1.3
283	<chem>S=C(Nc1c(F)cc(cc1Cl)Cl)NNC(=O)c1[nH]ccc1</chem>	C12H9Cl2FN4OS	-6.8	53.31	-29.622	11.7
284	<chem>S=C(Nc1c(F)cc(cc1Cl)Cl)NNC(=O)C1CCCC1</chem>	C13H14Cl2FN3OS	-6.9	54.20	-26.044	-17.0
285	<chem>S=C1N=NC(=N1)C(=O)NNC(=S)Nc1c(F)cc(cc1Cl)Cl</chem>	C10H5Cl2FN6OS2	-7.7	52.58	-32.417	1.6
286	<chem>S=C(Nc1c(F)cc(cc1Cl)Br)NNC(=O)c1ccoc1C</chem>	C13H10BrClFN3O2S	-7.7	58.39	-25.172	-29.8
287	<chem>S=C(Nc1c(F)cc(cc1Cl)Br)NNC(=O)c1[nH]cnc1C</chem>	C12H10BrClFN5OS	-7.4	58.99	-27.326	1.5
288	<chem>S=C(Nc1c(F)cc(cc1Cl)Br)NNC(=O)c1[nH]ccc1</chem>	C12H9BrClFN4OS	-6.8	53.23	-29.561	12.3
289	<chem>S=C(Nc1c(F)cc(cc1Cl)Br)NNC(=O)C1CCCC1</chem>	C13H14BrClFN3OS	-7.1	55.50	-26.637	-7.3
290	<chem>S=C1N=NC(=N1)C(=O)NNC(=S)Nc1c(F)cc(cc1Cl)Br</chem>	C10H5BrClFN6OS2	-6.9	45.94	-33.113	-3.0
291	<chem>S=C(Nc1c(F)cc(cc1Cl)I)NNC(=O)c1ccoc1C</chem>	C13H10ClFIN3O2S	-7.6	58.58	-25.854	-0.4
292	<chem>S=C(Nc1c(F)cc(cc1Cl)I)NNC(=O)c1[nH]cnc1C</chem>	C12H10ClFIN5OS	-7.4	57.20	-27.397	-13.9
293	<chem>S=C(Nc1c(F)cc(cc1Cl)I)NNC(=O)c1[nH]ccc1</chem>	C12H9ClFIN4OS	-6.8	51.26	-29.475	12.8
294	<chem>S=C(Nc1c(F)cc(cc1Cl)I)NNC(=O)C1CCCC1</chem>	C13H14ClFIN3OS	-6.9	53.44	-26.046	-17.8
295	<chem>S=C1N=NC(=N1)C(=O)NNC(=S)Nc1c(F)cc(cc1Cl)I</chem>	C10H5ClFIN6OS2	-6.9	57.84	-33.171	-2.2
296	<chem>S=C(Nc1c(F)cc(cc1Br)F)NNC(=O)c1ccoc1C</chem>	C13H10BrF2N3O2S	-7.9	62.26	-25.848	-27.7
297	<chem>S=C(Nc1c(F)cc(cc1Br)F)NNC(=O)c1[nH]cnc1C</chem>	C12H10BrF2N5OS	-7.4	60.46	-29.608	-7.5
298	<chem>S=C(Nc1c(F)cc(cc1Br)F)NNC(=O)c1[nH]ccc1</chem>	C12H9BrF2N4OS	-6.7	52.29	-29.622	-7.3
299	<chem>S=C(Nc1c(F)cc(cc1Br)F)NNC(=O)C1CCCC1</chem>	C13H14BrF2N3OS	-7.0	53.70	-26.179	-4.9
300	<chem>S=C1N=NC(=N1)C(=O)NNC(=S)Nc1c(F)cc(cc1Br)F</chem>	C10H5BrF2N6OS2	-7.0	53.67	-31.995	-5.0
301	<chem>S=C(Nc1c(F)cc(cc1Br)Cl)NNC(=O)c1ccoc1C</chem>	C13H10BrClFN3O2S	-7.8	60.97	-25.896	-28.8
302	<chem>S=C(Nc1c(F)cc(cc1Br)Cl)NNC(=O)c1[nH]cnc1C</chem>	C12H10BrClFN5OS	-7.3	57.98	-28.077	-0.1
303	<chem>S=C(Nc1c(F)cc(cc1Br)Cl)NNC(=O)c1[nH]ccc1</chem>	C12H9BrClFN4OS	-7.1	50.88	-29.165	11.0
304	<chem>S=C(Nc1c(F)cc(cc1Br)Cl)NNC(=O)C1CCCC1</chem>	C13H14BrClFN3OS	-6.8	55.00	-26.297	-15.5
305	<chem>S=C1N=NC(=N1)C(=O)NNC(=S)Nc1c(F)cc(cc1Br)Cl</chem>	C10H5BrClFN6OS2	-7.3	55.13	-32.007	-3.5
306	<chem>S=C(Nc1c(F)cc(cc1Br)Br)NNC(=O)c1ccoc1C</chem>	C13H10Br2FN3O2S	-7.7	58.32	-26.559	-0.9
307	<chem>S=C(Nc1c(F)cc(cc1Br)Br)NNC(=O)c1[nH]cnc1C</chem>	C12H10Br2FN5OS	-7.3	59.02	-27.531	1.4

308	<chem>S=C(Nc1c(F)cc(cc1Br)Br)NNC(=O)c1[nH]ccc1</chem>	C12H9Br2FN4OS	-6.6	53.25	-29.109	11.4
309	<chem>S=C(Nc1c(F)cc(cc1Br)Br)NNC(=O)C1CCCC1</chem>	C13H14Br2FN3OS	-6.9	53.93	-26.369	-14.8
310	<chem>S=C1N=NC(=N1)C(=O)NNC(=S)Nc1c(F)cc(cc1Br)Br</chem>	C10H5Br2FN6OS2	-7.2	41.07	-32.381	-4.4
311	<chem>S=C(Nc1c(F)cc(cc1Br)I)NNC(=O)c1ccoc1C</chem>	C13H10BrFIN3O2S	-7.1	59.76	-26.046	-3.1
312	<chem>S=C(Nc1c(F)cc(cc1Br)I)NNC(=O)c1[nH]cnc1C</chem>	C12H10BrFIN5OS	-6.7	53.04	-27.402	-0.2
313	<chem>S=C(Nc1c(F)cc(cc1Br)I)NNC(=O)c1[nH]ccc1</chem>	C12H9BrFIN4OS	-6.6	52.47	-29.017	12.2
314	<chem>S=C(Nc1c(F)cc(cc1Br)I)NNC(=O)C1CCCC1</chem>	C13H14BrFIN3OS	-6.8	54.66	-26.286	-17.9
315	<chem>S=C1N=NC(=N1)C(=O)NNC(=S)Nc1c(F)cc(cc1Br)I</chem>	C10H5BrFIN6OS2	-6.9	40.06	-32.079	-1.3
316	<chem>S=C(Nc1c(F)cc(cc1I)F)NNC(=O)c1ccoc1C</chem>	C13H10F2IN3O2S	-7.2	61.88	-25.905	-27.7
317	<chem>S=C(Nc1c(F)cc(cc1I)F)NNC(=O)c1[nH]cnc1C</chem>	C12H10F2IN5OS	-7.4	53.51	-29.54	7.4
318	<chem>S=C(Nc1c(F)cc(cc1I)F)NNC(=O)c1[nH]ccc1</chem>	C12H9F2IN4OS	-6.7	55.69	-29.181	1.9
319	<chem>S=C(Nc1c(F)cc(cc1I)F)NNC(=O)C1CCCC1</chem>	C13H14F2IN3OS	-7.0	55.37	-26.447	-12.3
320	<chem>S=C1N=NC(=N1)C(=O)NNC(=S)Nc1c(F)cc(cc1I)F</chem>	C10H5F2IN6OS2	-7.3	40.46	-31.953	-3.7
321	<chem>S=C(Nc1c(F)cc(cc1I)Cl)NNC(=O)c1ccoc1C</chem>	C13H10ClFIN3O2S	-7.1	53.87	-25.959	-28.3
322	<chem>S=C(Nc1c(F)cc(cc1I)Cl)NNC(=O)c1[nH]cnc1C</chem>	C12H10ClFIN5OS	-7.3	56.91	-28.721	-14.0
323	<chem>S=C(Nc1c(F)cc(cc1I)Cl)NNC(=O)c1[nH]ccc1</chem>	C12H9ClFIN4OS	-6.7	54.38	-28.711	10.6
324	<chem>S=C(Nc1c(F)cc(cc1I)Cl)NNC(=O)C1CCCC1</chem>	C13H14ClFIN3OS	-6.9	54.77	-26.538	-17.5
325	<chem>S=C1N=NC(=N1)C(=O)NNC(=S)Nc1c(F)cc(cc1I)Cl</chem>	C10H5ClFIN6OS2	-7.0	57.64	-31.995	-0.4
326	<chem>S=C(Nc1c(F)cc(cc1I)Br)NNC(=O)c1ccoc1C</chem>	C13H10BrFIN3O2S	-7.4	60.32	-26.549	-6.4
327	<chem>S=C(Nc1c(F)cc(cc1I)Br)NNC(=O)c1[nH]cnc1C</chem>	C12H10BrFIN5OS	-7.3	58.84	-27.864	-0.7
328	<chem>S=C(Nc1c(F)cc(cc1I)Br)NNC(=O)c1[nH]ccc1</chem>	C12H9BrFIN4OS	-6.6	51.60	-28.671	11.0
329	<chem>S=C(Nc1c(F)cc(cc1I)Br)NNC(=O)C1CCCC1</chem>	C13H14BrFIN3OS	-6.8	53.29	-26.593	-18.4
330	<chem>S=C1N=NC(=N1)C(=O)NNC(=S)Nc1c(F)cc(cc1I)Br</chem>	C10H5BrFIN6OS2	-7.2	45.12	-32.443	-2.1
331	<chem>S=C(Nc1c(F)cc(cc1I)I)NNC(=O)c1ccoc1C</chem>	C13H10FI2N3O2S	-7.4	59.82	-26.08	-6.6
332	<chem>S=C(Nc1c(F)cc(cc1I)I)NNC(=O)c1[nH]cnc1C</chem>	C12H10FI2N5OS	-7.3	56.40	-27.326	-3.7
333	<chem>S=C(Nc1c(F)cc(cc1I)I)NNC(=O)c1[nH]ccc1</chem>	C12H9FI2N4OS	-6.6	54.57	-28.579	11.9
334	<chem>S=C(Nc1c(F)cc(cc1I)I)NNC(=O)C1CCCC1</chem>	C13H14FI2N3OS	-6.7	54.94	-26.148	-6.8
335	<chem>S=C1N=NC(=N1)C(=O)NNC(=S)Nc1c(F)cc(cc1I)I</chem>	C10H5FI2N6OS2	-6.8	38.80	-32.485	-2.8
336	<chem>S=C(Nc1c(Cl)cc(cc1Cl)F)NNC(=O)c1ccoc1C</chem>	C13H10Cl2FN3O2S	-7.2	60.49	-24.555	-8.9
337	<chem>S=C(Nc1c(Cl)cc(cc1Cl)F)NNC(=O)c1[nH]cnc1C</chem>	C12H10Cl2FN5OS	-7.2	56.78	-26.152	-23.9
338	<chem>S=C(Nc1c(Cl)cc(cc1Cl)F)NNC(=O)c1ccc[nH]1</chem>	C12H9Cl2FN4OS	-6.7	51.49	-27.948	-1.8

339	<chem>S=C(Nc1c(Cl)cc(cc1Cl)F)NNC(=O)C1CCCC1</chem>	<chem>C13H14Cl2FN3OS</chem>	-7.0	55.05	-26.208	-7.8
340	<chem>S=C(Nc1c(Cl)cc(cc1Cl)F)NNC(=O)C1=NC(=S)N=N1</chem>	<chem>C10H5Cl2FN6OS2</chem>	-6.6	40.59	-30.601	-0.9
341	<chem>S=C(Nc1c(Cl)cc(cc1Cl)Cl)NNC(=O)c1ccoc1C</chem>	<chem>C13H10Cl3N3O2S</chem>	-7.4	55.86	-25.357	-11.9
342	<chem>S=C(Nc1c(Cl)cc(cc1Cl)Cl)NNC(=O)c1[nH]cnc1C</chem>	<chem>C12H10Cl3N5OS</chem>	-7.3	40.44	-25.822	-2.8
343	<chem>S=C(Nc1c(Cl)cc(cc1Cl)Cl)NNC(=O)c1ccc[nH]1</chem>	<chem>C12H9Cl3N4OS</chem>	-6.6	53.31	-25.931	-19.7
344	<chem>S=C(Nc1c(Cl)cc(cc1Cl)Cl)NNC(=O)C1CCCC1</chem>	<chem>C13H14Cl3N3OS</chem>	-7.1	55.32	-24.864	-28.4
345	<chem>S=C(Nc1c(Cl)cc(cc1Cl)Cl)NNC(=O)C1=NC(=S)N=N1</chem>	<chem>C10H5Cl3N6OS2</chem>	-6.6	52.27	-30.357	-5.0
346	<chem>S=C(Nc1c(Cl)cc(cc1Cl)Br)NNC(=O)c1ccoc1C</chem>	<chem>C13H10BrCl2N3O2</chem>	-7.5	58.34	-25.365	-9.0
347	<chem>S=C(Nc1c(Cl)cc(cc1Cl)Br)NNC(=O)c1[nH]cnc1C</chem>	<chem>C12H10BrCl2N5OS</chem>	-7.2	56.64	-25.834	-7.4
348	<chem>S=C(Nc1c(Cl)cc(cc1Cl)Br)NNC(=O)c1ccc[nH]1</chem>	<chem>C12H9BrCl2N4OS</chem>	-6.6	54.76	-27.342	6.5
349	<chem>S=C(Nc1c(Cl)cc(cc1Cl)Br)NNC(=O)C1CCCC1</chem>	<chem>C13H14BrCl2N3OS</chem>	-6.8	55.66	-24.869	-29.5
350	<chem>S=C(Nc1c(Cl)cc(cc1Cl)Br)NNC(=O)C1=NC(=S)N=N1</chem>	<chem>C10H5BrCl2N6OS2</chem>	-7.3	45.19	-30.46	-3.4
351	<chem>S=C(NC1=[C]([Cl])C=C(C=C1Cl)I)NNC(=O)c1ccoc1C</chem>	<chem>C13H10Cl2IN3O2S</chem>	-7.4	52.74	-22.7885	34.0
352	<chem>S=C(Nc1c(Cl)cc(cc1Cl)I)NNC(=O)c1[nH]cnc1C</chem>	<chem>C12H10Cl2IN5OS</chem>	-7.2	57.92	-26.544	28.8
353	<chem>S=C(Nc1c(Cl)cc(cc1Cl)I)NNC(=O)c1ccc[nH]1</chem>	<chem>C12H9Cl2IN4OS</chem>	-6.7	50.99	-24.548	-0.5
354	<chem>S=C(Nc1c(Cl)cc(cc1Cl)I)NNC(=O)C1CCCC1</chem>	<chem>C13H14Cl2IN3OS</chem>	-6.8	41.77	-25.78	-7.2
355	<chem>S=C(Nc1c(Cl)cc(cc1Cl)I)NNC(=O)C1=NC(=S)N=N1</chem>	<chem>C10H5Cl2IN6OS2</chem>	-6.7	43.04	-30.551	-1.7
356	<chem>S=C(Nc1c(Cl)cc(cc1Br)F)NNC(=O)c1ccoc1C</chem>	<chem>C13H10BrClFN3O2</chem>	-7.3	61.25	-24.072	-14.6
357	<chem>S=C(Nc1c(Cl)cc(cc1Br)F)NNC(=O)c1[nH]cnc1C</chem>	<chem>C12H10BrClFN5OS</chem>	-7.2	54.73	-25.877	10.1
358	<chem>S=C(Nc1c(Cl)cc(cc1Br)F)NNC(=O)c1[nH]ccc1</chem>	<chem>C12H9BrClFN4OS</chem>	-6.6	53.20	-26.04	9.6
359	<chem>S=C(Nc1c(Cl)cc(cc1Br)F)NNC(=O)C1CCCC1</chem>	<chem>C13H14BrClFN3OS</chem>	-6.7	55.36	-26.469	-7.9
360	<chem>S=C1N=NC(=N1)C(=O)NNC(=S)Nc1c(Cl)cc(cc1Br)F</chem>	<chem>C10H5BrClFN6OS2</chem>	-7.4	58.12	-31.414	-1.4
361	<chem>S=C(Nc1c(Cl)cc(cc1Br)Cl)NNC(=O)c1ccoc1C</chem>	<chem>C13H10BrCl2N3O2</chem>	-7.3	58.04	-24.57	-11.9
362	<chem>S=C(Nc1c(Cl)cc(cc1Br)Cl)NNC(=O)c1[nH]cnc1C</chem>	<chem>C12H10BrCl2N5OS</chem>	-7.2	53.49	-26.129	6.3
363	<chem>S=C(Nc1c(Cl)cc(cc1Br)Cl)NNC(=O)c1[nH]ccc1</chem>	<chem>C12H9BrCl2N4OS</chem>	-6.5	53.00	-27.304	-5.8
364	<chem>S=C(Nc1c(Cl)cc(cc1Br)Cl)NNC(=O)C1CCCC1</chem>	<chem>C13H14BrCl2N3OS</chem>	-6.8	52.79	-25.266	-29.0
365	<chem>S=C1N=NC(=N1)C(=O)NNC(=S)Nc1c(Cl)cc(cc1Br)Cl</chem>	<chem>C10H5BrCl2N6OS2</chem>	-6.7	51.20	-30.775	-22.7
366	<chem>S=C(Nc1c(Cl)cc(cc1Br)Br)NNC(=O)c1ccoc1C</chem>	<chem>C13H10Br2ClN3O2</chem>	-7.2	59.71	-24.985	0.8
367	<chem>S=C(Nc1c(Cl)cc(cc1Br)Br)NNC(=O)c1[nH]cnc1C</chem>	<chem>C12H10Br2ClN5OS</chem>	-7.2	58.12	-26.107	6.1
368	<chem>S=C(Nc1c(Cl)cc(cc1Br)Br)NNC(=O)c1[nH]ccc1</chem>	<chem>C12H9Br2ClN4OS</chem>	-6.4	48.46	-26.699	-7.9
369	<chem>S=C(Nc1c(Cl)cc(cc1Br)Br)NNC(=O)C1CCCC1</chem>	<chem>C13H14Br2ClN3OS</chem>	-6.9	55.63	-25.217	-29.6

370	<chem>S=C1N=NC(=N1)C(=O)NNC(=S)Nc1c(Cl)cc(cc1Br)Br</chem>	<chem>C10H5Br2ClN6OS2</chem>	-6.9	38.49	-30.763	2.4
371	<chem>S=C(Nc1c(Cl)cc(cc1Br)I)NNC(=O)c1ccoc1C</chem>	<chem>C13H10BrClIN3O2S</chem>	-7.2	60.27	-25.038	-9.2
372	<chem>S=C(Nc1c(Cl)cc(cc1Br)I)NNC(=O)c1[nH]cnc1C</chem>	<chem>C12H10BrClIN5OS</chem>	-6.3	48.83	-26.932	12.0
373	<chem>S=C(Nc1c(Cl)cc(cc1Br)I)NNC(=O)c1[nH]ccc1</chem>	<chem>C12H9BrClIN4OS</chem>	-6.4	54.03	-26.736	19.9
374	<chem>S=C(Nc1c(Cl)cc(cc1Br)I)NNC(=O)C1CCCC1</chem>	<chem>C13H14BrClIN3OS</chem>	-6.9	55.66	-24.648	-29.2
375	<chem>S=C1N=NC(=N1)C(=O)NNC(=S)Nc1c(Cl)cc(cc1Br)I</chem>	<chem>C10H5BrClIN6OS2</chem>	-6.8	37.51	-30.913	1.6
376	<chem>S=C(Nc1c(Cl)cc(cc1I)F)NNC(=O)c1ccoc1C</chem>	<chem>C13H10ClFIN3O2S</chem>	-6.5	55.34	-23.747	10.9
377	<chem>S=C(Nc1c(Cl)cc(cc1I)F)NNC(=O)c1[nH]cnc1C</chem>	<chem>C12H10ClFIN5OS</chem>	-6.7	52.06	-25.914	-4.0
378	<chem>S=C(Nc1c(Cl)cc(cc1I)F)NNC(=O)c1[nH]ccc1</chem>	<chem>C12H9ClFIN4OS</chem>	-6.7	55.80	-26.663	-3.5
379	<chem>S=C(Nc1c(Cl)cc(cc1I)F)NNC(=O)C1CCCC1</chem>	<chem>C13H14ClFIN3OS</chem>	-6.7	54.87	-26.561	-8.3
380	<chem>S=C1N=NC(=N1)C(=O)NNC(=S)Nc1c(Cl)cc(cc1I)F</chem>	<chem>C10H5ClFIN6OS2</chem>	-6.3	39.44	-30.214	-1.4
381	<chem>S=C(Nc1c(Cl)cc(cc1I)Cl)NNC(=O)c1ccoc1C</chem>	<chem>C13H10Cl2IN3O2S</chem>	-7.3	60.26	-27.105	-2.3
382	<chem>S=C(Nc1c(Cl)cc(cc1I)Cl)NNC(=O)c1[nH]cnc1C</chem>	<chem>C12H10Cl2IN5OS</chem>	-7.3	55.23	-26.842	-9.3
383	<chem>S=C(Nc1c(Cl)cc(cc1I)Cl)NNC(=O)c1[nH]ccc1</chem>	<chem>C12H9Cl2IN4OS</chem>	-6.5	43.90	-27.165	-0.7
384	<chem>S=C(Nc1c(Cl)cc(cc1I)Cl)NNC(=O)C1CCCC1</chem>	<chem>C13H14Cl2IN3OS</chem>	-6.6	55.16	-25.152	-30.7
385	<chem>S=C1N=NC(=N1)C(=O)NNC(=S)Nc1c(Cl)cc(cc1I)Cl</chem>	<chem>C10H5Cl2IN6OS2</chem>	-7.0	56.43	-30.404	-3.0
386	<chem>S=C(Nc1c(Cl)cc(cc1I)Br)NNC(=O)c1ccoc1C</chem>	<chem>C13H10BrClIN3O2S</chem>	-7.1	59.97	-23.689	-0.3
387	<chem>S=C(Nc1c(Cl)cc(cc1I)Br)NNC(=O)c1[nH]cnc1C</chem>	<chem>C12H10BrClIN5OS</chem>	-7.3	50.81	-25.816	24.7
388	<chem>S=C(Nc1c(Cl)cc(cc1I)Br)NNC(=O)c1[nH]ccc1</chem>	<chem>C12H9BrClIN4OS</chem>	-6.7	50.84	-26.812	-3.4
389	<chem>S=C(Nc1c(Cl)cc(cc1I)Br)NNC(=O)C1CCCC1</chem>	<chem>C13H14BrClIN3OS</chem>	-6.6	55.70	-26.617	-7.7
390	<chem>S=C1N=NC(=N1)C(=O)NNC(=S)Nc1c(Cl)cc(cc1I)Br</chem>	<chem>C10H5BrClIN6OS2</chem>	-6.9	52.15	-30.451	0.2
391	<chem>S=C(Nc1c(Cl)cc(cc1I)I)NNC(=O)c1ccoc1C</chem>	<chem>C13H10ClI2N3O2S</chem>	-7.0	58.06	-24.033	30.5
392	<chem>S=C(Nc1c(Cl)cc(cc1I)I)NNC(=O)c1[nH]cnc1C</chem>	<chem>C12H10ClI2N5OS</chem>	-6.9	51.89	-26.058	-5.1
393	<chem>S=C(Nc1c(Cl)cc(cc1I)I)NNC(=O)c1[nH]ccc1</chem>	<chem>C12H9ClI2N4OS</chem>	-6.6	54.03	-25.864	-8.1
394	<chem>S=C(Nc1c(Cl)cc(cc1I)I)NNC(=O)C1CCCC1</chem>	<chem>C13H14ClI2N3OS</chem>	-6.4	53.75	-22.812	6.1
395	<chem>S=C1N=NC(=N1)C(=O)NNC(=S)Nc1c(Cl)cc(cc1I)I</chem>	<chem>C10H5ClI2N6OS2</chem>	-6.4	56.76	-30.544	-4.1
396	<chem>S=C(Nc1c(Br)cc(cc1Br)F)NNC(=O)c1ccoc1C</chem>	<chem>C13H10Br2FN3O2S</chem>	-7.1	60.49	-24.262	3.3
397	<chem>S=C(Nc1c(Br)cc(cc1Br)F)NNC(=O)c1[nH]cnc1C</chem>	<chem>C12H10Br2FN5OS</chem>	-7.0	59.38	-26.376	28.9
398	<chem>S=C(Nc1c(Br)cc(cc1Br)F)NNC(=O)c1ccc[nH]1</chem>	<chem>C12H9Br2FN4OS</chem>	-6.6	52.43	-26.442	-3.2
399	<chem>S=C(Nc1c(Br)cc(cc1Br)F)NNC(=O)C1CCCC1</chem>	<chem>C13H14Br2FN3OS</chem>	-7.0	53.85	-25.717	-12.5
400	<chem>S=C(Nc1c(Br)cc(cc1Br)F)NNC(=O)C1=NC(=S)N=N1</chem>	<chem>C10H5Br2FN6OS2</chem>	-7.1	41.07	-30.167	9.8

401	<chem>S=C(Nc1c(Br)cc(cc1Br)Cl)NNC(=O)c1ccoc1C</chem>	C13H10Br2ClN3O2	-7.1	58.61	-23.061	-1.3
402	<chem>S=C(Nc1c(Br)cc(cc1Br)Cl)NNC(=O)c1[nH]cnc1C</chem>	C12H10Br2ClN5OS	-7.2	59.94	-26.485	27.8
403	<chem>S=C(Nc1c(Br)cc(cc1Br)Cl)NNC(=O)c1ccc[nH]1</chem>	C12H9Br2ClN4OS	-6.6	48.73	-26.731	-3.9
404	<chem>S=C(Nc1c(Br)cc(cc1Br)Cl)NNC(=O)C1CCCC1</chem>	C13H14Br2ClN3OS	-6.8	53.43	-26.027	-11.4
405	<chem>S=C(Nc1c(Br)cc(cc1Br)Cl)NNC(=O)C1=NC(=S)N=N1</chem>	C10H5Br2ClN6OS2	-7.2	36.16	-29.516	1.8
406	<chem>S=C(Nc1c(Br)cc(cc1Br)Br)NNC(=O)c1ccoc1C</chem>	C13H10Br3N3O2S	-7.3	54.00	-26.826	-3.9
407	<chem>S=C(Nc1c(Br)cc(cc1Br)Br)NNC(=O)c1[nH]cnc1C</chem>	C12H10Br3N5OS	-7.1	55.64	-26.456	27.6
408	<chem>S=C(Nc1c(Br)cc(cc1Br)Br)NNC(=O)c1ccc[nH]1</chem>	C12H9Br3N4OS	-6.6	52.93	-26.689	30.0
409	<chem>S=C(Nc1c(Br)cc(cc1Br)Br)NNC(=O)C1CCCC1</chem>	C13H14Br3N3OS	-6.7	55.22	-25.13	-30.2
410	<chem>S=C(Nc1c(Br)cc(cc1Br)Br)NNC(=O)C1=NC(=S)N=N1</chem>	C10H5Br3N6OS2	-6.7	55.00	-29.534	5.1
411	<chem>S=C(Nc1c(Br)cc(cc1Br)I)NNC(=O)c1ccoc1C</chem>	C13H10Br2IN3O2S	-7.0	59.02	-22.554	26.6
412	<chem>S=C(Nc1c(Br)cc(cc1Br)I)NNC(=O)c1[nH]cnc1C</chem>	C12H10Br2IN5OS	-7.1	57.38	-26.33	20.4
413	<chem>S=C(Nc1c(Br)cc(cc1Br)I)NNC(=O)c1ccc[nH]1</chem>	C12H9Br2IN4OS	-6.6	53.45	-26.707	31.0
414	<chem>S=C(Nc1c(Br)cc(cc1Br)I)NNC(=O)C1CCCC1</chem>	C13H14Br2IN3OS	-6.6	54.14	-24.547	-30.4
415	<chem>S=C(Nc1c(Br)cc(cc1Br)I)NNC(=O)C1=NC(=S)N=N1</chem>	C10H5Br2IN6OS2	-7.0	48.23	-29.685	2.1
416	<chem>S=C(Nc1c(Br)cc(cc1I)F)NNC(=O)c1ccoc1C</chem>	C13H10BrFIN3O2S	-7.0	61.22	-23.731	10.2
417	<chem>S=C(Nc1c(Br)cc(cc1I)F)NNC(=O)c1[nH]cnc1C</chem>	C12H10BrFIN5OS	-7.2	59.98	-27.209	33.6
418	<chem>S=C(Nc1c(Br)cc(cc1I)F)NNC(=O)c1[nH]ccc1</chem>	C12H9BrFIN4OS	-6.5	51.36	-27.445	30.3
419	<chem>S=C(Nc1c(Br)cc(cc1I)F)NNC(=O)C1CCCC1</chem>	C13H14BrFIN3OS	-6.5	55.67	-25.731	-7.6
420	<chem>S=C1N=NC(=N1)C(=O)NNC(=S)Nc1c(Br)cc(cc1I)F</chem>	C10H5BrFIN6OS2	-6.3	41.57	-30.211	8.9
421	<chem>S=C(Nc1c(Br)cc(cc1I)Cl)NNC(=O)c1ccoc1C</chem>	C13H10BrClIN3O2S	-7.1	54.18	-24.578	-3.7
422	<chem>S=C(Nc1c(Br)cc(cc1I)Cl)NNC(=O)c1[nH]cnc1C</chem>	C12H10BrClIN5OS	-7.2	54.03	-25.013	42.4
423	<chem>S=C(Nc1c(Br)cc(cc1I)Cl)NNC(=O)C1CCCC1</chem>	C13H14BrClIN3OS	-6.6	55.96	-25.826	-7.0
424	<chem>S=C(Nc1c(Br)cc(cc1I)Cl)NNC(=O)c1[nH]ccc1</chem>	C12H9BrClIN4OS	-6.2	50.76	-26.785	29.2
425	<chem>S=C1N=NC(=N1)C(=O)NNC(=S)Nc1c(Br)cc(cc1I)Cl</chem>	C10H5BrClIN6OS2	-6.5	42.60	-29.53	1.0
426	<chem>S=C(Nc1c(Br)cc(cc1I)Br)NNC(=O)c1ccoc1C</chem>	C13H10Br2IN3O2S	-7.0	58.75	-22.196	-2.4
427	<chem>S=C(Nc1c(Br)cc(cc1I)Br)NNC(=O)c1[nH]cnc1C</chem>	C12H10Br2IN5OS	-6.9	57.57	-25.851	32.0
428	<chem>S=C(Nc1c(Br)cc(cc1I)Br)NNC(=O)c1[nH]ccc1</chem>	C12H9Br2IN4OS	-6.4	43.74	-26.644	4.3
429	<chem>S=C(Nc1c(Br)cc(cc1I)Br)NNC(=O)C1CCCC1</chem>	C13H14Br2IN3OS	-6.5	53.27	-25.111	-30.1
430	<chem>S=C1N=NC(=N1)C(=O)NNC(=S)Nc1c(Br)cc(cc1I)Br</chem>	C10H5Br2IN6OS2	-6.5	42.45	-29.324	-18.7
431	<chem>S=C(Nc1c(Br)cc(cc1I)I)NNC(=O)c1ccoc1C</chem>	C13H10BrI2N3O2S	-6.9	60.66	-22.563	27.3

432	<chem>S=C(Nc1c(Br)cc(cc1I)I)NNC(=O)c1[nH]cnc1C</chem>	C12H10BrI2N5OS	-7.2	45.87	-25.006	42.0
433	<chem>S=C(Nc1c(Br)cc(cc1I)I)NNC(=O)c1[nH]ccc1</chem>	C12H9BrI2N4OS	-6.5	51.26	-25.811	9.7
434	<chem>S=C(Nc1c(Br)cc(cc1I)I)NNC(=O)C1CCCC1</chem>	C13H14BrI2N3OS	-6.6	54.50	-24.64	-30.2
435	<chem>S=C1N=NC(=N1)C(=O)NNC(=S)Nc1c(Br)cc(cc1I)I</chem>	C10H5BrI2N6OS2	-6.5	54.79	-28.969	-6.5
436	<chem>S=C(Nc1c(I)cc(cc1I)F)NNC(=O)c1ccoc1C</chem>	C13H10FI2N3O2S	-7.1	59.30	-26.615	-10.4
437	<chem>S=C(Nc1c(I)cc(cc1I)F)NNC(=O)c1[nH]cnc1C</chem>	C12H10FI2N5OS	-6.9	50.95	-26.909	8.6
438	<chem>S=C(Nc1c(I)cc(cc1I)F)NNC(=O)c1ccc[nH]1</chem>	C12H9FI2N4OS	-6.4	53.54	-28.139	-0.7
439	<chem>S=C(Nc1c(I)cc(cc1I)F)NNC(=O)C1CCCC1</chem>	C13H14FI2N3OS	-6.3	53.92	-25.114	-11.0
440	<chem>S=C(Nc1c(I)cc(cc1I)F)NNC(=O)C1=NC(=S)N=N1</chem>	C10H5FI2N6OS2	-6.7	58.32	-28.436	15.7
441	<chem>S=C(Nc1c(I)cc(cc1I)Cl)NNC(=O)c1ccoc1C</chem>	C13H10ClI2N3O2S	-7.1	60.02	-26.643	-5.1
442	<chem>S=C(Nc1c(I)cc(cc1I)Cl)NNC(=O)c1[nH]cnc1C</chem>	C12H10ClI2N5OS	-7.0	57.89	-26.426	-3.1
443	<chem>S=C(Nc1c(I)cc(cc1I)Cl)NNC(=O)c1ccc[nH]1</chem>	C12H9ClI2N4OS	-6.4	54.54	-28.284	26.9
444	<chem>S=C(Nc1c(I)cc(cc1I)Cl)NNC(=O)C1CCCC1</chem>	C13H14ClI2N3OS	-6.3	53.86	-25.089	-11.8
445	<chem>S=C(Nc1c(I)cc(cc1I)Cl)NNC(=O)C1=NC(=S)N=N1</chem>	C10H5ClI2N6OS2	-6.5	57.32	-28.888	0.2
446	<chem>S=C(Nc1c(I)cc(cc1I)Br)NNC(=O)c1ccoc1C</chem>	C13H10BrI2N3O2S	-6.9	58.05	-26.843	-7.1
447	<chem>S=C(Nc1c(I)cc(cc1I)Br)NNC(=O)c1[nH]cnc1C</chem>	C12H10BrI2N5OS	-6.9	57.17	-27.089	-2.6
448	<chem>S=C(Nc1c(I)cc(cc1I)Br)NNC(=O)c1ccc[nH]1</chem>	C12H9BrI2N4OS	-6.3	51.47	-28.154	-2.2
449	<chem>S=C(Nc1c(I)cc(cc1I)Br)NNC(=O)C1CCCC1</chem>	C13H14BrI2N3OS	-6.6	55.27	-25.071	-11.8
450	<chem>S=C(Nc1c(I)cc(cc1I)Br)NNC(=O)C1=NC(=S)N=N1</chem>	C10H5BrI2N6OS2	-6.7	38.97	-30.082	18.9
451	<chem>S=C(Nc1c(I)cc(cc1I)I)NNC(=O)c1ccoc1C</chem>	C13H10I3N3O2S	-6.7	60.51	-26.993	-5.3
452	<chem>S=C(Nc1c(I)cc(cc1I)I)NNC(=O)c1[nH]cnc1C</chem>	C12H10I3N5OS	-6.9	53.65	-26.038	2.5
453	<chem>S=C(Nc1c(I)cc(cc1I)I)NNC(=O)c1ccc[nH]1</chem>	C12H9I3N4OS	-6.2	51.25	-27.998	5.9
454	<chem>S=C(Nc1c(I)cc(cc1I)I)NNC(=O)C1CCCC1</chem>	C13H14I3N3OS	-6.6	54.44	-24.942	-10.5
455	<chem>S=C(Nc1c(I)cc(cc1I)I)NNC(=O)C1=NC(=S)N=N1</chem>	C10H5I3N6OS2	-6.2	42.68	-29.746	11.2
456	<chem>Brc1cc(Br)cc(c1)n1c(=S)[nH]nc1C1CCCC1</chem>	C13H13Br2N3S	-6.1	36.73	-12.781	-3.3
457	<chem>Brc1cc(I)cc(c1)n1c(=S)[nH]nc1C1CCCC1</chem>	C13H13BrIN3S	-6.1	39.67	-10.722	-3.8
458	<chem>Brc1ccc(c(c1)Br)n1c(=S)[nH]nc1C1CCCC1</chem>	C13H13Br2N3S	-5.8	37.27	-9.871	-8.4
459	<chem>lc1ccc(c(c1)Br)n1c(=S)[nH]nc1C1CCCC1</chem>	C13H13BrIN3S	-5.4	39.48	-9.632	-5.4
460	<chem>Brc1ccc(c(c1)I)n1c(=S)[nH]nc1C1CCCC1</chem>	C13H13BrIN3S	-5.8	37.95	-9.946	6.1
461	<chem>Brc1cc(Br)c(c(c1)Br)n1c(=S)[nH]nc1C1CCCC1</chem>	C13H12Br3N3S	-5.6	40.18	-10.756	9.6
462	<chem>Brc1cc(F)c(c(c1)Br)n1c(=S)[nH]nc1C1CCCC1</chem>	C13H12Br2FN3S	-5.8	38.72	-10.553	10.5

463	Brc1cc(Br)c(c(c1)I)n1c(=S)[nH]nc1C1CCCC1	C13H12Br2IN3S	-5.6	34.97	-10.127	9.2
464	Clc1cc(Br)c(c(c1)Br)n1c(=S)[nH]nc1C1CCCC1	C13H12Br2ClN3S	-5.7	39.87	-10.628	9.8
465	Clc1cc(F)c(c(c1)Br)n1c(=S)[nH]nc1C1CCCC1	C13H12BrClFN3S	-5.8	38.61	-10.54	11.0
466	Clc1cc(Br)c(c(c1)I)n1c(=S)[nH]nc1C1CCCC1	C13H12BrClIN3S	-5.7	39.33	-11.072	-3.0
467	Fc1cc(Br)c(c(c1)Br)n1c(=S)[nH]nc1C1CCCC1	C13H12Br2FN3S	-5.9	38.84	-10.679	-0.9
468	Fc1cc(F)c(c(c1)Br)n1c(=S)[nH]nc1C1CCCC1	C13H12BrF2N3S	-5.8	39.26	-11.295	-4.8
469	Fc1cc(Br)c(c(c1)I)n1c(=S)[nH]nc1C1CCCC1	C13H12BrFIN3S	-5.9	39.87	-11.04	-7.4
470	lc1cc(Br)c(c(c1)Br)n1c(=S)[nH]nc1C1CCCC1	C13H12Br2IN3S	-5.5	40.42	-11.008	9.3
471	lc1cc(F)c(c(c1)Br)n1c(=S)[nH]nc1C1CCCC1	C13H12BrFIN3S	-5.8	38.85	-10.714	7.5
472	lc1cc(Br)c(c(c1)I)n1c(=S)[nH]nc1C1CCCC1	C13H12BrI2N3S	-5.5	40.29	-10.374	9.0
473	Brc1cccc(c1)n1c(=S)[nH]nc1C1CCCC1	C13H14BrN3S	-5.8	37.36	-11.17	-7.5
474	Brc1cccc1n1c(=S)[nH]nc1C1CCCC1	C13H14BrN3S	-5.3	36.66	-10.056	5.4
475	Brc1ccc(cc1)n1c(n[nH]c1=S)C1CCCC1	C13H14BrN3S	-5.6	38.59	-11.861	-8.6
476	Clc1cc(Br)cc(c1)n1c(=S)[nH]nc1C1CCCC1	C13H13BrClN3S	-6.1	36.77	-11.628	4.4
477	Clc1cc(Cl)cc(c1)n1c(=S)[nH]nc1C1CCCC1	C13H13Cl2N3S	-6.1	38.71	-12.349	-6.1
478	Clc1cc(I)cc(c1)n1c(=S)[nH]nc1C1CCCC1	C13H13ClIN3S	-6.1	36.63	-11.337	-3.1
479	Brc1ccc(c(c1)Cl)n1c(=S)[nH]nc1C1CCCC1	C13H13BrClN3S	-5.7	39.62	-11.368	5.0
480	Clc1ccc(c(c1)Cl)n1c(=S)[nH]nc1C1CCCC1	C13H13Cl2N3S	-5.9	39.43	-11.033	6.0
481	lc1ccc(c(c1)Cl)n1c(=S)[nH]nc1C1CCCC1	C13H13ClIN3S	-5.5	34.54	-11.81	7.1
482	Clc1ccc(c(c1)Br)n1c(=S)[nH]nc1C1CCCC1	C13H13BrClN3S	-6.0	39.22	-10.012	-7.6
483	Clc1ccc(c(c1)I)n1c(=S)[nH]nc1C1CCCC1	C13H13ClIN3S	-6.0	39.02	-8.761	-5.4
484	Brc1cc(Cl)c(c(c1)Br)n1c(=S)[nH]nc1C1CCCC1	C13H12Br2ClN3S	-5.6	39.44	-10.268	3.7
485	Brc1cc(Cl)c(c(c1)Cl)n1c(=S)[nH]nc1C1CCCC1	C13H12BrCl2N3S	-5.6	39.74	-10.539	1.9
486	Brc1cc(F)c(c(c1)Cl)n1c(=S)[nH]nc1C1CCCC1	C13H12BrClFN3S	-5.8	37.5	-11.272	-3.8
487	Brc1cc(Cl)c(c(c1)I)n1c(=S)[nH]nc1C1CCCC1	C13H12BrClIN3S	-5.6	37.61	-10.317	-3.0
488	Clc1cc(Cl)c(c(c1)Br)n1c(=S)[nH]nc1C1CCCC1	C13H12BrCl2N3S	-5.7	39.23	-10.357	6.7
489	Clc1cc(Cl)c(c(c1)Cl)n1c(=S)[nH]nc1C1CCCC1	C13H12Cl3N3S	-5.7	37.55	-10.401	3.0
490	Clc1cc(F)c(c(c1)Cl)n1c(=S)[nH]nc1C1CCCC1	C13H12Cl2FN3S	-5.8	37.94	-11.527	9.6
491	Clc1cc(Cl)c(c(c1)I)n1c(=S)[nH]nc1C1CCCC1	C13H12Cl2IN3S	-5.7	34.27	-10.314	-2.2
492	Fc1cc(Cl)c(c(c1)Br)n1c(=S)[nH]nc1C1CCCC1	C13H12BrClFN3S	-6.0	37.8	-10.451	2.7
493	Fc1cc(Cl)c(c(c1)Cl)n1c(=S)[nH]nc1C1CCCC1	C13H12Cl2FN3S	-6.0	37.34	-10.723	-3.9

494	Fc1cc(F)c(c(c1)Cl)n1c(=S)[nH]nc1C1CCCC1	C13H12ClF2N3S	-6.0	37.93	-11.361	-4.4
495	Fc1cc(Cl)c(c(c1)I)n1c(=S)[nH]nc1C1CCCC1	C13H12ClFIN3S	-6.0	39.37	-10.31	-1.7
496	Ic1cc(Cl)c(c(c1)Br)n1c(=S)[nH]nc1C1CCCC1	C13H12BrClIN3S	-5.6	37.03	-10.352	2.6
497	Ic1cc(Cl)c(c(c1)Cl)n1c(=S)[nH]nc1C1CCCC1	C13H12Cl2IN3S	-5.7	39.54	-11.215	-1.1
498	Ic1cc(F)c(c(c1)Cl)n1c(=S)[nH]nc1C1CCCC1	C13H12ClFIN3S	-5.7	37.6	-10.949	-0.1
499	Ic1cc(Cl)c(c(c1)I)n1c(=S)[nH]nc1C1CCCC1	C13H12ClI2N3S	-5.5	34.87	-10.29	-0.1
500	Clc1cccc(c1)n1c(=S)[nH]nc1C1CCCC1	C13H14ClN3S	-5.7	36.86	-10.795	2.2
501	Clc1cccc1n1c(=S)[nH]nc1C1CCCC1	C13H14ClN3S	-5.4	32.68	-10.076	-3.6
502	Clc1ccc(cc1)n1c(n[nH]c1=S)C1CCCC1	C13H14ClN3S	-5.6	38.3	-10.649	-2.6
503	Fc1cc(Br)cc(c1)n1c(=S)[nH]nc1C1CCCC1	C13H13BrFN3S	-6.1	38.76	-11.428	7.4
504	Fc1cc(Cl)cc(c1)n1c(=S)[nH]nc1C1CCCC1	C13H13ClFN3S	-6.1	37.53	-11.654	3.3
505	Fc1cc(F)cc(c1)n1c(=S)[nH]nc1C1CCCC1	C13H13F2N3S	-6.1	37.33	-11.665	-7.2
506	Fc1cc(I)cc(c1)n1c(=S)[nH]nc1C1CCCC1	C13H13FIN3S	-6.2	37.68	-11.279	5.7
507	BrC1ccc(c(c1)F)n1c(=S)[nH]nc1C1CCCC1	C13H13BrFN3S	-5.6	39.59	-10.296	6.5
508	Clc1ccc(c(c1)F)n1c(=S)[nH]nc1C1CCCC1	C13H13ClFN3S	-5.9	40.1	-10.304	5.9
509	Fc1ccc(c(c1)F)n1c(=S)[nH]nc1C1CCCC1	C13H13F2N3S	-6.0	39.99	-11.554	-4.9
510	Ic1ccc(c(c1)F)n1c(=S)[nH]nc1C1CCCC1	C13H13FIN3S	-5.5	35.76	-10.279	6.4
511	Fc1ccc(c(c1)Br)n1c(=S)[nH]nc1C1CCCC1	C13H13BrFN3S	-6.1	39.28	-11.813	9.3
512	Fc1ccc(c(c1)Cl)n1c(=S)[nH]nc1C1CCCC1	C13H13ClFN3S	-6.1	39.46	-10.818	10.7
513	Fc1ccc(c(c1)I)n1c(=S)[nH]nc1C1CCCC1	C13H13FIN3S	-6.2	41.54	-10.098	7.3
514	BrC1cc(F)c(c(c1)F)n1c(=S)[nH]nc1C1CCCC1	C13H12BrF2N3S	-5.8	36.69	-11.634	6.5
515	BrC1cc(F)c(c(c1)I)n1c(=S)[nH]nc1C1CCCC1	C13H12BrFIN3S	-5.7	39.42	-10.366	7.5
516	Clc1cc(F)c(c(c1)F)n1c(=S)[nH]nc1C1CCCC1	C13H12ClF2N3S	-5.8	38.49	-11.824	4.6
517	Clc1cc(F)c(c(c1)I)n1c(=S)[nH]nc1C1CCCC1	C13H12ClFIN3S	-5.6	38.29	-10.3	9.5
518	Fc1cc(F)c(c(c1)F)n1c(=S)[nH]nc1C1CCCC1	C13H12F3N3S	-5.9	37.6	-11.21	0.8
519	Fc1cc(F)c(c(c1)I)n1c(=S)[nH]nc1C1CCCC1	C13H12F2IN3S	-5.8	35.19	-10.378	-3.2
520	Ic1cc(F)c(c(c1)F)n1c(=S)[nH]nc1C1CCCC1	C13H12F2IN3S	-5.8	34.91	-11.317	10.6
521	Ic1cc(F)c(c(c1)I)n1c(=S)[nH]nc1C1CCCC1	C13H12FI2N3S	-5.7	39.79	-10.485	12.7
522	Fc1cccc(c1)n1c(=S)[nH]nc1C1CCCC1	C13H14FN3S	-5.7	37.26	-13.357	-2.2
523	Fc1cccc1n1c(=S)[nH]nc1C1CCCC1	C13H14FN3S	-5.9	36.77	-11.278	3.5
524	Fc1ccc(cc1)n1c(n[nH]c1=S)C1CCCC1	C13H14FN3S	-5.6	38.14	-11.794	-9.3

525	S=c1[nH]nc(n1c1cccc1)C1CCCC1	C13H15N3S	-5.9	37	-11.298	0.4
526	lc1cc(l)cc(c1)n1c(=S)[nH]nc1C1CCCC1	C13H13I2N3S	-6.1	36.71	-12.859	-7.3
527	lc1ccc(c(c1)l)n1c(=S)[nH]nc1C1CCCC1	C13H13I2N3S	-5.7	39.37	-9.928	5.4
528	Br1cc(l)c(c(c1)l)n1c(=S)[nH]nc1C1CCCC1	C13H12BrI2N3S	-5.5	34.29	-12.748	1.4
529	Cl1cc(l)c(c(c1)l)n1c(=S)[nH]nc1C1CCCC1	C13H12ClI2N3S	-5.6	40.36	-10.565	-2.0
530	Fc1cc(l)c(c(c1)l)n1c(=S)[nH]nc1C1CCCC1	C13H12FI2N3S	-5.6	40.21	-10.633	-3.2
531	lc1cc(l)c(c(c1)l)n1c(=S)[nH]nc1C1CCCC1	C13H12I3N3S	-5.5	34.13	-13.063	0.0
532	lc1cccc(c1)n1c(=S)[nH]nc1C1CCCC1	C13H14IN3S	-5.9	37.5	-10.764	-6.8
533	lc1cccc1n1c(=S)[nH]nc1C1CCCC1	C13H14IN3S	-5.6	34.68	-9.917	9.4
534	lc1ccc(cc1)n1c(n[nH]c1=S)C1CCCC1	C13H14IN3S	-5.6	38.37	-12.612	-7.0
535	Cc1cccc(c1)n1c(=S)[nH]nc1C1CCCC1	C14H17N3S	-5.8	37.48	-11.327	-9.0
536	Cc1cccc1n1c(=S)[nH]nc1C1CCCC1	C14H17N3S	-5.4	37.74	-10.989	12.5
537	Cc1ccc(cc1)n1c(n[nH]c1=S)C1CCCC1	C14H17N3S	-5.5	36.95	-11.744	-9.0
538	O=N(=O)c1cccc(c1)n1c(=S)[nH]nc1C1CCCC1	C13H14N4O2S	-6.1	45.65	-19.941	3.7
539	O=N(=O)c1cccc1n1c(=S)[nH]nc1C1CCCC1	C13H14N4O2S	-6.4	39.51	-20.247	21.1
540	S=c1[nH]nc(n1c1ccc(cc1)N(=O)=O)C1CCCC1	C13H14N4O2S	-6.1	43.35	-17.112	-3.5
541	Oc1cccc(c1)n1c(=S)[nH]nc1C1CCCC1	C13H15N3OS	-5.7	39.13	-14.8	-10.2
542	Oc1cccc1n1c(=S)[nH]nc1C1CCCC1	C13H15N3OS	-5.7	38.24	-15.481	1.0
543	Oc1ccc(cc1)n1c(n[nH]c1=S)C1CCCC1	C13H15N3OS	-5.5	39.24	-13.584	-11.7
544	COc1cccc(c1)n1c(=S)[nH]nc1C1CCCC1	C14H17N3OS	-5.7	39.42	-16.695	-9.9
545	COc1cccc1n1c(=S)[nH]nc1C1CCCC1	C14H17N3OS	-5.8	37.25	-12.224	-2.0
546	COc1ccc(cc1)n1c(n[nH]c1=S)C1CCCC1	C14H17N3OS	-5.6	39.34	-12.554	-6.9
547	Br1cc(Br)cc(c1)n1c(=S)[nH]nc1c1ccoc1C	C13H9Br2N3OS	-6.3	44.01	-16.772	-6.4
548	Br1cc(l)cc(c1)n1c(=S)[nH]nc1c1ccoc1C	C13H9BrIN3OS	-6.4	44.31	-16.322	-6.2
549	Br1ccc(c(c1)Br)n1c(=S)[nH]nc1c1ccoc1C	C13H9Br2N3OS	-5.8	42	-15.728	-7.5
550	Br1cc(Br)c(c(c1)Br)n1c(=S)[nH]nc1c1ccoc1C	C13H8Br3N3OS	-6.0	38.47	-12.913	-8.2
551	Br1cc(Cl)c(c(c1)Br)n1c(=S)[nH]nc1c1ccoc1C	C13H8Br2ClN3OS	-6.1	39.25	-12.925	-7.2
552	Br1cc(Br)c(c(c1)l)n1c(=S)[nH]nc1c1ccoc1C	C13H8Br2IN3OS	-6.0	38.45	-12.589	-7.5
553	Cl1cc(Cl)c(c(c1)Br)n1c(=S)[nH]nc1c1ccoc1C	C13H8BrCl2N3OS	-6.1	38.95	-13.239	-4.6
554	Cl1cc(Br)c(c(c1)Br)n1c(=S)[nH]nc1c1ccoc1C	C13H8Br2ClN3OS	-5.9	38.54	-13.196	-7.6
555	Fc1cc(Br)c(c(c1)Br)n1c(=S)[nH]nc1c1ccoc1C	C13H8Br2FN3OS	-6.0	37.9	-14.408	-8.5

556	<chem>Fc1cc(Cl)c(c(c1)Br)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H8BrClFN3OS</chem>	-6.1	38.12	-13.936	-8.3
557	<chem>lc1ccc(c(c1)Br)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H9BrIN3OS</chem>	-5.8	41.32	-15.659	-7.1
558	<chem>lc1cc(Br)c(c(c1)Br)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H8Br2IN3OS</chem>	-5.9	38.88	-12.288	-10.1
559	<chem>lc1cc(Cl)c(c(c1)Br)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H8BrClIN3OS</chem>	-6.0	39.15	-12.605	0.5
560	<chem>Brc1ccc(c(c1)I)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H9BrIN3OS</chem>	-5.8	41.33	-15.723	-14.0
561	<chem>Brc1cccc(c1)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H10BrN3OS</chem>	-6.0	42.51	-16.09	-2.2
562	<chem>Cc1occc1c1n[nH]c(=S)n1c1cccc1Br</chem>	<chem>C13H10BrN3OS</chem>	-5.7	39.57	-17.359	-0.4
563	<chem>Brc1ccc(cc1)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H10BrN3OS</chem>	-5.6	41.36	-15.639	-14.2
564	<chem>Clc1cc(Br)cc(c1)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H9BrClN3OS</chem>	-6.3	43.94	-16.591	-5.1
565	<chem>Clc1cc(Cl)cc(c1)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H9Cl2N3OS</chem>	-6.4	45.33	-15.398	-9.6
566	<chem>Clc1cc(I)cc(c1)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H9ClIN3OS</chem>	-6.4	43.62	-16.205	-4.2
567	<chem>Brc1ccc(c(c1)Cl)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H9BrClN3OS</chem>	-6.0	36.91	-16.008	2.9
568	<chem>Brc1cc(Cl)c(c(c1)Cl)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H8BrCl2N3OS</chem>	-6.1	38.25	-13.401	1.7
569	<chem>Clc1ccc(c(c1)Cl)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H9Cl2N3OS</chem>	-5.9	39.74	-15.71	-1.7
570	<chem>Clc1cc(Cl)c(c(c1)Cl)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H8Cl3N3OS</chem>	-6.1	38.47	-14.126	-2.9
571	<chem>Clc1cc(F)c(c(c1)Cl)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H8Cl2FN3OS</chem>	-6.1	38.62	-14.836	3.8
572	<chem>Clc1cc(Cl)c(c(c1)I)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H8Cl2IN3OS</chem>	-6.1	38.65	-13.46	-7.5
573	<chem>Fc1cc(Cl)c(c(c1)Cl)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H8Cl2FN3OS</chem>	-6.0	38.68	-13.91	2.6
574	<chem>Fc1cc(F)c(c(c1)Cl)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H8ClF2N3OS</chem>	-6.1	38.82	-15.258	9.1
575	<chem>lc1ccc(c(c1)Cl)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H9ClIN3OS</chem>	-5.9	40.63	-16.255	-2.3
576	<chem>lc1cc(Cl)c(c(c1)Cl)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H8Cl2IN3OS</chem>	-6.1	39.13	-13.084	1.4
577	<chem>Clc1ccc(c(c1)Br)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H9BrClN3OS</chem>	-5.7	40.35	-15.565	0.8
578	<chem>Clc1ccc(c(c1)I)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H9ClIN3OS</chem>	-5.7	41.18	-15.621	-1.1
579	<chem>Clc1cccc(c1)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H10ClN3OS</chem>	-5.9	41.53	-15.955	-2.8
580	<chem>Cc1occc1c1n[nH]c(=S)n1c1cccc1Cl</chem>	<chem>C13H10ClN3OS</chem>	-5.7	39.65	-17.373	1.4
581	<chem>Clc1ccc(cc1)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H10ClN3OS</chem>	-5.6	40.55	-15.797	-13.2
582	<chem>Fc1cc(Br)cc(c1)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H9BrFN3OS</chem>	-6.2	43.29	-15.983	-0.6
583	<chem>Fc1cc(Cl)cc(c1)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H9ClFN3OS</chem>	-6.1	43.44	-15.837	0.8
584	<chem>Fc1cc(F)cc(c1)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H9F2N3OS</chem>	-6.0	43.26	-17.315	-1.3
585	<chem>Fc1cc(I)cc(c1)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H9FIN3OS</chem>	-6.3	44.03	-16.11	0.8
586	<chem>Brc1cc(F)c(c(c1)Br)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H8Br2FN3OS</chem>	-6.0	39.74	-14.185	2.7

587	<chem>Brc1cc(F)c(c(c1)Cl)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H8BrClFN3OS</chem>	-6.1	38.97	-14.676	3.4
588	<chem>Brc1cc(F)c(c(c1)F)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H8BrF2N3OS</chem>	-6.1	39.64	-15.623	0.8
589	<chem>Clc1cc(F)c(c(c1)Br)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H8BrClFN3OS</chem>	-5.9	38.34	-14.338	3.0
590	<chem>Clc1cc(F)c(c(c1)F)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H8ClF2N3OS</chem>	-6.0	37.88	-15.71	0.8
591	<chem>Fc1cc(F)c(c(c1)Br)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H8BrF2N3OS</chem>	-6.0	38.6	-14.622	3.5
592	<chem>Fc1cc(F)c(c(c1)F)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H8F3N3OS</chem>	-6.2	38.4	-16.113	1.5
593	<chem>Fc1cc(F)c(c(c1)I)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H8F2IN3OS</chem>	-6.0	38.75	-14.395	-7.0
594	<chem>lc1cc(F)c(c(c1)Br)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H8BrFIN3OS</chem>	-6.0	39.06	-14.273	-14.5
595	<chem>lc1cc(F)c(c(c1)Cl)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H8ClFIN3OS</chem>	-6.0	40.3	-14.733	9.0
596	<chem>lc1cc(F)c(c(c1)F)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H8F2IN3OS</chem>	-5.9	39.14	-15.688	-0.8
597	<chem>lc1cc(F)c(c(c1)I)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H8FI2N3OS</chem>	-6.0	39.03	-13.175	0.3
598	<chem>Fc1ccc(c(c1)Br)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H9BrFN3OS</chem>	-5.7	42.36	-15.769	-12.8
599	<chem>Fc1ccc(c(c1)Cl)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H9ClFN3OS</chem>	-5.9	42.17	-16.11	2.3
600	<chem>Fc1ccc(c(c1)I)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H9FIN3OS</chem>	-5.7	41.99	-15.794	-12.3
601	<chem>Fc1cccc(c1)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H10FN3OS</chem>	-5.6	42.49	-15.418	-3.2
602	<chem>Brc1ccc(c(c1)F)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H9BrFN3OS</chem>	-6.0	40.17	-15.499	-3.8
603	<chem>Clc1ccc(c(c1)F)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H9ClFN3OS</chem>	-6.0	38.65	-15.352	-2.7
604	<chem>Fc1ccc(c(c1)F)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H9F2N3OS</chem>	-6.0	40.12	-17.602	-1.6
605	<chem>lc1ccc(c(c1)F)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H9FIN3OS</chem>	-5.9	40.75	-15.698	-1.6
606	<chem>Cc1occc1c1n[nH]c(=S)n1c1cccc1F</chem>	<chem>C13H10FN3OS</chem>	-5.9	39.24	-17.375	1.4
607	<chem>Fc1ccc(cc1)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H10FN3OS</chem>	-5.8	40.68	-15.917	-12.9
608	<chem>Cc1occc1c1n[nH]c(=S)n1c1cccc1</chem>	<chem>C13H11N3OS</chem>	-5.8	44.82	-17.519	-3.0
609	<chem>Brc1cc(Cl)c(c(c1)I)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H8BrClIN3OS</chem>	-6.1	38.51	-12.877	-7.4
610	<chem>Brc1cc(F)c(c(c1)I)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H8BrFIN3OS</chem>	-6.0	39.68	-13.495	0.6
611	<chem>Brc1cc(I)c(c(c1)I)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H8BrI2N3OS</chem>	-5.8	39.15	-13.794	-11.7
612	<chem>Clc1cc(Br)c(c(c1)I)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H8BrClIN3OS</chem>	-6.0	37.68	-12.895	-7.6
613	<chem>Clc1cc(F)c(c(c1)I)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H8ClFIN3OS</chem>	-6.0	39.21	-13.704	-5.9
614	<chem>Clc1cc(I)c(c(c1)I)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H8ClI2N3OS</chem>	-5.8	39.04	-13.057	-3.5
615	<chem>Fc1cc(Br)c(c(c1)I)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H8BrFIN3OS</chem>	-6.0	38.68	-13.584	-7.3
616	<chem>Fc1cc(Cl)c(c(c1)I)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H8ClFIN3OS</chem>	-6.1	38.05	-13.886	-3.2
617	<chem>Fc1cc(I)c(c(c1)I)n1c(=S)[nH]nc1c1ccoc1C</chem>	<chem>C13H8FI2N3OS</chem>	-5.7	38.36	-14.136	-10.6

618	<chem>Ic1cc(Br)c(c(c1)I)n1c(=S)[nH]nc1c1ccoc1C</chem>	C13H8BrI2N3OS	-5.9	38.51	-12.131	-7.7
619	<chem>Ic1cc(Cl)c(c(c1)I)n1c(=S)[nH]nc1c1ccoc1C</chem>	C13H8ClI2N3OS	-6.0	39.08	-12.468	-7.8
620	<chem>Ic1cc(I)c(c(c1)I)n1c(=S)[nH]nc1c1ccoc1C</chem>	C13H8I3N3OS	-5.7	39.35	-13.662	-11.8
621	<chem>Ic1cccc(c1)n1c(=S)[nH]nc1c1ccoc1C</chem>	C13H10IN3OS	-6.1	42.36	-16.3	-2.8
622	<chem>Cc1occc1c1n[nH]c(=S)n1c1cccc1I</chem>	C13H10IN3OS	-5.7	40.08	-17.399	-2.0
623	<chem>Ic1ccc(cc1)n1c(=S)[nH]nc1c1ccoc1C</chem>	C13H10IN3OS	-5.7	41.52	-16.937	1.5
624	<chem>Ic1cc(I)cc(c1)n1c(=S)[nH]nc1c1ccoc1C</chem>	C13H9I2N3OS	-6.5	43.89	-14.351	-2.1
625	<chem>Ic1ccc(c(c1)I)n1c(=S)[nH]nc1c1ccoc1C</chem>	C13H9I2N3OS	-5.8	41.74	-15.156	-13.8
626	<chem>Cc1cccc(c1)n1c(=S)[nH]nc1c1ccoc1C</chem>	C14H13N3OS	-6.0	42.46	-17.549	-3.4
627	<chem>Cc1occc1c1n[nH]c(=S)n1c1cccc1C</chem>	C14H13N3OS	-5.8	42.32	-17.014	-4.3
628	<chem>Cc1ccc(cc1)n1c(=S)[nH]nc1c1ccoc1C</chem>	C14H13N3OS	-5.8	42.04	-17.455	-1.9
629	<chem>O=N(=O)c1cccc(c1)n1c(=S)[nH]nc1c1ccoc1C</chem>	C13H10N4O3S	-6.2	48.48	-24.497	13.7
630	<chem>Cc1occc1c1n[nH]c(=S)n1c1cccc1N(=O)=O</chem>	C13H10N4O3S	-6.2	43.4	-22.705	3.4
631	<chem>O=N(=O)c1ccc(cc1)n1c(=S)[nH]nc1c1ccoc1C</chem>	C13H10N4O3S	-6.5	45.55	-23.079	-0.3
632	<chem>Oc1cccc(c1)n1c(=S)[nH]nc1c1ccoc1C</chem>	C13H11N3O2S	-5.8	43.18	-21.659	-10.9
633	<chem>Cc1occc1c1n[nH]c(=S)n1c1cccc1O</chem>	C13H11N3O2S	-6.1	42.29	-18.063	-0.7
634	<chem>Oc1ccc(cc1)n1c(=S)[nH]nc1c1ccoc1C</chem>	C13H11N3O2S	-5.9	43.7	-18.156	-6.1
635	<chem>COc1cccc(c1)n1c(=S)[nH]nc1c1ccoc1C</chem>	C14H13N3O2S	-5.8	43.21	-20.136	4.6
636	<chem>COc1cccc1n1c(=S)[nH]nc1c1ccoc1C</chem>	C14H13N3O2S	-5.6	40.33	-15.809	-5.2
637	<chem>COc1ccc(cc1)n1c(=S)[nH]nc1c1ccoc1C</chem>	C14H13N3O2S	-5.8	45.32	-18.792	-13.3
638	<chem>Brc1cc(Br)cc(c1)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H9Br2N5S	-6.4	41.35	-17.821	9.0
639	<chem>Brc1cc(I)cc(c1)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H9BrIN5S	-6.4	41.54	-18.591	16.8
640	<chem>Brc1ccc(c(c1)Br)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H9Br2N5S	-5.9	37.5	-18.408	8.4
641	<chem>Ic1ccc(c(c1)Br)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H9BrIN5S	-5.9	38.05	-18.996	10.4
642	<chem>Brc1ccc(c(c1)I)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H9BrIN5S	-5.9	37.73	-18.324	10.6
643	<chem>Brc1cc(Br)c(c(c1)Br)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8Br3N5S	-6.0	36.9	-21.471	11.0
644	<chem>Brc1cc(F)c(c(c1)Br)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8Br2FN5S	-6.0	36.1	-19.126	1.3
645	<chem>Brc1cc(Br)c(c(c1)I)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8Br2IN5S	-6.0	35.94	-20.997	3.6
646	<chem>Clc1cc(Br)c(c(c1)Br)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8Br2ClN5S	-5.9	35.35	-21.862	8.0
647	<chem>Clc1cc(F)c(c(c1)Br)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8BrClFN5S	-6.0	36.79	-19.642	1.2
648	<chem>Clc1cc(Br)c(c(c1)I)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8BrClIN5S	-6.0	36.08	-21.316	10.3

649	<chem>Fc1cc(Br)c(c(c1)Br)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8Br2FN5S	-5.9	38.41	-22.471	1.3
650	<chem>Fc1cc(F)c(c(c1)Br)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8BrF2N5S	-6.1	37.81	-20.806	0.9
651	<chem>Fc1cc(Br)c(c(c1)I)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8BrFIN5S	-5.9	36.51	-21.971	6.3
652	<chem>lc1cc(Br)c(c(c1)Br)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8Br2IN5S	-5.9	35.77	-20.791	14.8
653	<chem>lc1cc(F)c(c(c1)Br)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8BrFIN5S	-6.0	37.6	-19.035	10.0
654	<chem>lc1cc(Br)c(c(c1)I)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8BrI2N5S	-5.9	35.44	-19.822	3.9
655	<chem>Brc1cccc(c1)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H10BrN5S	-6.2	40.48	-19.233	-5.4
656	<chem>Brc1cccc1n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H10BrN5S	-5.6	37.67	-18.682	8.6
657	<chem>Brc1ccc(cc1)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H10BrN5S	-5.6	38.41	-18.942	3.3
658	<chem>Clc1cc(Br)cc(c1)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H9BrClN5S	-6.4	41.37	-18.963	6.3
659	<chem>Clc1cc(Cl)cc(c1)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H9Cl2N5S	-6.3	39.54	-17.893	10.5
660	<chem>Clc1cc(I)cc(c1)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H9ClIN5S	-6.4	41.7	-18.522	3.9
661	<chem>Brc1ccc(c(c1)Cl)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H9BrClN5S	-5.9	38.63	-20.315	12.2
662	<chem>Clc1ccc(c(c1)Cl)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H9Cl2N5S	-6.0	36.91	-20.803	9.8
663	<chem>lc1ccc(c(c1)Cl)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H9ClIN5S	-5.8	38.26	-19.59	19.1
664	<chem>Clc1ccc(c(c1)Br)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H9BrClN5S	-6.0	37.9	-18.939	7.3
665	<chem>Clc1ccc(c(c1)I)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H9ClIN5S	-5.9	39.71	-18.451	7.5
666	<chem>Brc1cc(Cl)c(c(c1)Br)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8Br2ClN5S	-6.0	36.01	-18.572	7.4
667	<chem>Brc1cc(Cl)c(c(c1)Cl)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8BrCl2N5S	-6.1	36.73	-19.285	7.9
668	<chem>Brc1cc(F)c(c(c1)Cl)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8BrClFN5S	-6.0	38.12	-19.2	8.8
669	<chem>Brc1cc(Cl)c(c(c1)I)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8BrClIN5S	-6.1	36.05	-20.067	8.7
670	<chem>Clc1cc(Cl)c(c(c1)Br)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8BrCl2N5S	-6.0	37.76	-18.716	5.0
671	<chem>Clc1cc(Cl)c(c(c1)Cl)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8Cl3N5S	-6.2	38.76	-18.57	1.9
672	<chem>Clc1cc(F)c(c(c1)Cl)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8Cl2FN5S	-5.9	38.94	-19.506	8.3
673	<chem>Clc1cc(Cl)c(c(c1)I)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8Cl2IN5S	-5.8	33.07	-20.491	8.3
674	<chem>Fc1cc(Cl)c(c(c1)Br)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8BrClFN5S	-5.8	38.94	-18.786	4.5
675	<chem>Fc1cc(Cl)c(c(c1)Cl)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8Cl2FN5S	-6.5	42.58	-18.684	3.7
676	<chem>Fc1cc(F)c(c(c1)Cl)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8ClF2N5S	-6.1	38.54	-20.674	-1.4
677	<chem>Fc1cc(Cl)c(c(c1)I)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8ClFIN5S	-5.9	36.09	-18.68	-5.0
678	<chem>lc1cc(Cl)c(c(c1)Br)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8BrClIN5S	-5.9	36.72	-19.102	9.7
679	<chem>lc1cc(Cl)c(c(c1)Cl)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8Cl2IN5S	-6.1	37.71	-19.043	8.6

680	<chem>Ic1cc(F)c(c(c1)Cl)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8ClFIN5S	-6.0	38.27	-19.025	9.0
681	<chem>Ic1cc(Cl)c(c(c1)I)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8ClI2N5S	-5.8	36.04	-19.194	13.9
682	<chem>Clc1cccc(c1)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H10ClN5S	-6.2	40.27	-19.169	3.3
683	<chem>Clc1cccc1n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H10ClN5S	-5.9	38.04	-18.584	1.9
684	<chem>Clc1ccc(cc1)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H10ClN5S	-5.6	38.38	-19.027	8.1
685	<chem>Fc1cc(Br)cc(c1)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H9BrFN5S	-6.3	40.76	-18.951	7.9
686	<chem>Fc1cc(Cl)cc(c1)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H9ClFN5S	-6.3	38.22	-18.985	4.2
687	<chem>Fc1cc(F)cc(c1)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H9F2N5S	-6.0	38.45	-18.999	3.1
688	<chem>Fc1cc(I)cc(c1)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H9FIN5S	-6.4	40.42	-18.902	-8.8
689	<chem>Brc1ccc(c(c1)F)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H9BrFN5S	-6.0	40.2	-18.547	9.2
690	<chem>Clc1ccc(c(c1)F)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H9ClFN5S	-6.1	37.19	-19.677	8.1
691	<chem>Fc1ccc(c(c1)F)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H9F2N5S	-6.2	42.53	-18.534	4.3
692	<chem>Ic1ccc(c(c1)F)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H9FIN5S	-5.9	40.89	-18.344	12.1
693	<chem>Fc1ccc(c(c1)Br)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H9BrFN5S	-6.0	42.17	-22.1	4.8
694	<chem>Fc1ccc(c(c1)Cl)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H9ClFN5S	-6.2	40.26	-21.855	5.3
695	<chem>Fc1ccc(c(c1)I)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H9FIN5S	-6.0	37.49	-22.221	4.1
696	<chem>Brc1cc(F)c(c(c1)F)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8BrF2N5S	-6.0	38.96	-18.527	8.2
697	<chem>Brc1cc(F)c(c(c1)I)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8BrFIN5S	-5.9	36.33	-21.058	-1.9
698	<chem>Clc1cc(F)c(c(c1)F)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8ClF2N5S	-5.9	39.17	-18.677	-4.0
699	<chem>Clc1cc(F)c(c(c1)I)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8ClFIN5S	-5.9	35.94	-21.377	6.5
700	<chem>Fc1cc(F)c(c(c1)F)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8F3N5S	-6.0	38.55	-18.068	14.5
701	<chem>Fc1cc(F)c(c(c1)I)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8F2IN5S	-5.9	37.42	-18.737	7.5
702	<chem>Ic1cc(F)c(c(c1)F)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8F2IN5S	-6.0	38.7	-18.359	8.5
703	<chem>Ic1cc(F)c(c(c1)I)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8FI2N5S	-5.8	35.3	-20.302	10.5
704	<chem>Fc1cccc(c1)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H10FN5S	-6.2	40.71	-19.104	1.2
705	<chem>Fc1cccc1n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H10FN5S	-6.0	41.69	-18.331	2.7
706	<chem>Fc1ccc(cc1)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H10FN5S	-6.0	38.3	-18.62	4.9
707	<chem>Cc1nc[nH]c1c1n[nH]c(=S)n1c1cccc1</chem>	C12H11N5S	-5.8	42.69	-18.137	6.9
708	<chem>Ic1cc(I)cc(c1)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H9I2N5S	-6.4	41	-18.006	-5.4
709	<chem>Ic1ccc(c(c1)I)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H9I2N5S	-5.9	35.07	-18.212	12.5
710	<chem>Brc1cc(I)c(c(c1)I)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8BrI2N5S	-5.8	36.42	-22.589	12.6

711	<chem>Clc1cc(I)c(c(c1)I)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8ClI2N5S	-5.7	35.09	-22.926	7.5
712	<chem>Fc1cc(I)c(c(c1)I)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8FI2N5S	-5.6	37.23	-23.039	13.5
713	<chem>Ic1cc(I)c(c(c1)I)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H8I3N5S	-5.7	34.93	-22.254	10.9
714	<chem>Ic1cccc(c1)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H10IN5S	-6.2	40.7	-19.113	3.3
715	<chem>Ic1ccccc1n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H10IN5S	-5.6	39.54	-18.606	3.7
716	<chem>Ic1ccc(cc1)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H10IN5S	-6.2	41.37	-18.247	14.5
717	<chem>Cc1cccc(c1)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C13H13N5S	-6.1	39.44	-20.24	2.7
718	<chem>Cc1ccccc1n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C13H13N5S	-5.8	40.22	-18.761	4.8
719	<chem>Cc1ccc(cc1)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C13H13N5S	-6.2	38.02	-18.459	-11.2
720	<chem>O=N(=O)c1cccc(c1)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H10N6O2S	-6.3	47.58	-24.381	12.6
721	<chem>O=N(=O)c1ccccc1n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H10N6O2S	-6.4	44.65	-26.791	9.3
722	<chem>O=N(=O)c1ccc(cc1)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H10N6O2S	-6.5	40.8	-22.292	4.4
723	<chem>Oc1cccc(c1)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H11N5OS	-5.9	39.92	-24.409	0.4
724	<chem>Oc1ccccc1n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H11N5OS	-5.8	40.72	-21.65	-5.3
725	<chem>Oc1ccc(cc1)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C12H11N5OS	-6.0	42.09	-20.567	3.6
726	<chem>COc1cccc(c1)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C13H13N5OS	-6.0	40.95	-21.332	10.7
727	<chem>COc1ccccc1n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C13H13N5OS	-5.8	38.91	-19.884	3.2
728	<chem>COc1ccc(cc1)n1c(=S)[nH]nc1c1[nH]cnc1C</chem>	C13H13N5OS	-5.8	40.32	-20.727	-2.3
729	<chem>BrC1cc(Br)cc(c1)n1c(=S)[nH]nc1C1=NC(=S)N=N1</chem>	C10H4Br2N6S2	-6.2	39.4	-19.3	-3.4
730	<chem>S=C1N=NC(=N1)c1n[nH]c(=S)n1c1cc(Br)cc(c1)I</chem>	C10H4BrIN6S2	-6.1	36.23	-18.484	2.1
731	<chem>BrC1ccc(c(c1)Br)n1c(=S)[nH]nc1C1=NC(=S)N=N1</chem>	C10H4Br2N6S2	-5.7	35.5	-19.373	0.8
732	<chem>Ic1ccc(c(c1)Br)n1c(=S)[nH]nc1C1=NC(=S)N=N1</chem>	C10H4BrIN6S2	-5.8	35.47	-19.499	3.3
733	<chem>BrC1ccc(c(c1)I)n1c(=S)[nH]nc1C1=NC(=S)N=N1</chem>	C10H4BrIN6S2	-5.5	34.93	-20.021	0.1
734	<chem>BrC1cc(Br)c(c(c1)Br)n1c(=S)[nH]nc1C1=NC(=S)N=N1</chem>	C10H3Br3N6S2	-5.7	38.37	-17.974	8.9
735	<chem>S=C1N=NC(=N1)c1n[nH]c(=S)n1c1c(F)cc(cc1Br)Br</chem>	C10H3Br2FN6S2	-6.0	37	-18.692	5.1
736	<chem>S=C1N=NC(=N1)c1n[nH]c(=S)n1c1c(Br)cc(cc1I)Br</chem>	C10H3Br2IN6S2	-5.8	37.82	-18.176	8.5
737	<chem>Clc1cc(Br)c(c(c1)Br)n1c(=S)[nH]nc1C1=NC(=S)N=N1</chem>	C10H3Br2ClN6S2	-5.8	37.9	-17.92	9.4
738	<chem>S=C1N=NC(=N1)c1n[nH]c(=S)n1c1c(F)cc(cc1Br)Cl</chem>	C10H3BrClFN6S2	-6.0	36.15	-18.634	4.6
739	<chem>S=C1N=NC(=N1)c1n[nH]c(=S)n1c1c(Br)cc(cc1I)Cl</chem>	C10H3BrClIN6S2	-5.8	38.05	-18.112	8.3
740	<chem>Fc1cc(Br)c(c(c1)Br)n1c(=S)[nH]nc1C1=NC(=S)N=N1</chem>	C10H3Br2FN6S2	-5.8	38.5	-17.913	9.1
741	<chem>S=C1N=NC(=N1)c1n[nH]c(=S)n1c1c(F)cc(cc1Br)F</chem>	C10H3BrF2N6S2	-6.2	38.21	-18.791	-2.7

742	<chem>S=C1N=NC(=N1)c1n[nH]c(=S)n1c1c(Br)cc(cc1I)F</chem>	C10H3BrFIN6S2	-5.8	37.49	-18.107	8.7
743	<chem>Ic1cc(Br)c(c(c1)Br)n1c(=S)[nH]nc1C1=NC(=S)N=N1</chem>	C10H3Br2IN6S2	-5.7	38.35	-18.747	17.9
744	<chem>S=C1N=NC(=N1)c1n[nH]c(=S)n1c1c(F)cc(cc1Br)I</chem>	C10H3BrFIN6S2	-6.0	36.1	-19.363	5.2
745	<chem>S=C1N=NC(=N1)c1n[nH]c(=S)n1c1c(Br)cc(cc1I)I</chem>	C10H3BrI2N6S2	-5.7	38.71	-18.289	9.6
746	<chem>Brc1cccc(c1)n1c(=S)[nH]nc1C1=NC(=S)N=N1</chem>	C10H5BrN6S2	-5.8	39.58	-20.822	-2.3
747	<chem>S=C1N=NC(=N1)c1n[nH]c(=S)n1c1cccc1Br</chem>	C10H5BrN6S2	-5.6	37.58	-20.289	-0.3
748	<chem>Brc1ccc(cc1)n1c(=S)[nH]nc1C1=NC(=S)N=N1</chem>	C10H5BrN6S2	-6.1	35.21	-19.708	5.3
749	<chem>S=C1N=NC(=N1)c1n[nH]c(=S)n1c1cc(Cl)cc(c1)Br</chem>	C10H4BrClN6S2	-6.3	35.33	-17.437	-2.5
750	<chem>Clc1cc(Cl)cc(c1)n1c(=S)[nH]nc1C1=NC(=S)N=N1</chem>	C10H4Cl2N6S2	-6.3	36.09	-17.413	-2.1
751	<chem>S=C1N=NC(=N1)c1n[nH]c(=S)n1c1cc(Cl)cc(c1)I</chem>	C10H4ClIN6S2	-6.4	37.41	-17.667	-2.2
752	<chem>Brc1ccc(c(c1)Cl)n1c(=S)[nH]nc1C1=NC(=S)N=N1</chem>	C10H4BrClN6S2	-6.1	35.41	-20.655	0.5
753	<chem>Clc1ccc(c(c1)Cl)n1c(=S)[nH]nc1C1=NC(=S)N=N1</chem>	C10H4Cl2N6S2	-6.1	39.49	-20.275	-0.4
754	<chem>Ic1ccc(c(c1)Cl)n1c(=S)[nH]nc1C1=NC(=S)N=N1</chem>	C10H4ClIN6S2	-5.9	37.25	-19.505	2.0
755	<chem>Clc1ccc(c(c1)Br)n1c(=S)[nH]nc1C1=NC(=S)N=N1</chem>	C10H4BrClN6S2	-6.1	35.1	-19.309	0.5
756	<chem>Clc1ccc(c(c1)I)n1c(=S)[nH]nc1C1=NC(=S)N=N1</chem>	C10H4ClIN6S2	-5.9	39.67	-19.275	5.2
757	<chem>S=C1N=NC(=N1)c1n[nH]c(=S)n1c1c(Cl)cc(cc1Br)Br</chem>	C10H3Br2ClN6S2	-5.7	37.41	-18.324	8.1
758	<chem>Brc1cc(Cl)c(c(c1)Cl)n1c(=S)[nH]nc1C1=NC(=S)N=N1</chem>	C10H3BrCl2N6S2	-6.5	39.55	-18.624	2.0
759	<chem>S=C1N=NC(=N1)c1n[nH]c(=S)n1c1c(F)cc(cc1Cl)Br</chem>	C10H3BrClFN6S2	-6.3	37.92	-19.059	8.4
760	<chem>S=C1N=NC(=N1)c1n[nH]c(=S)n1c1c(Cl)cc(cc1I)Br</chem>	C10H3BrClIN6S2	-5.7	39.02	-18.565	14.0
761	<chem>S=C1N=NC(=N1)c1n[nH]c(=S)n1c1c(Cl)cc(cc1Br)Cl</chem>	C10H3BrCl2N6S2	-5.8	39.06	-18.262	9.1
762	<chem>Clc1cc(Cl)c(c(c1)Cl)n1c(=S)[nH]nc1C1=NC(=S)N=N1</chem>	C10H3Cl3N6S2	-6.6	39.59	-18.9617	1.0
763	<chem>S=C1N=NC(=N1)c1n[nH]c(=S)n1c1c(F)cc(cc1Cl)Cl</chem>	C10H3Cl2FN6S2	-6.2	37.11	-18.573	1.2
764	<chem>S=C1N=NC(=N1)c1n[nH]c(=S)n1c1c(Cl)cc(cc1I)Cl</chem>	C10H3Cl2IN6S2	-5.7	37.72	-18.496	8.6
765	<chem>S=C1N=NC(=N1)c1n[nH]c(=S)n1c1c(Cl)cc(cc1Br)F</chem>	C10H3BrClFN6S2	-5.7	37.57	-18.259	10.0
766	<chem>Fc1cc(Cl)c(c(c1)Cl)n1c(=S)[nH]nc1C1=NC(=S)N=N1</chem>	C10H3Cl2FN6S2	-6.7	37.46	-18.8296	-1.0
767	<chem>S=C1N=NC(=N1)c1n[nH]c(=S)n1c1c(F)cc(cc1Cl)F</chem>	C10H3ClF2N6S2	-6.1	37.27	-18.968	16.6
768	<chem>S=C1N=NC(=N1)c1n[nH]c(=S)n1c1c(Cl)cc(cc1I)F</chem>	C10H3ClFIN6S2	-5.7	38.39	-18.492	7.1
769	<chem>S=C1N=NC(=N1)c1n[nH]c(=S)n1c1c(Cl)cc(cc1Br)I</chem>	C10H3BrClIN6S2	-5.7	38.9	-18.964	15.3
770	<chem>Ic1cc(Cl)c(c(c1)Cl)n1c(=S)[nH]nc1C1=NC(=S)N=N1</chem>	C10H3Cl2IN6S2	-5.9	38.56	-18.716	4.3
771	<chem>S=C1N=NC(=N1)c1n[nH]c(=S)n1c1c(F)cc(cc1Cl)I</chem>	C10H3ClFIN6S2	-6.2	36.04	-19.142	4.0
772	<chem>S=C1N=NC(=N1)c1n[nH]c(=S)n1c1c(Cl)cc(cc1I)I</chem>	C10H3ClI2N6S2	-5.7	39.09	-18.67	14.7

773	Clc1cccc(c1)n1c(=S)[nH]nc1C1=NC(=S)N=N1	C10H5ClN6S2	-6.1	36.99	-20.752	-4.4
774	S=C1N=NC(=N1)c1n[nH]c(=S)n1c1cccc1Cl	C10H5ClN6S2	-5.9	38.97	-20.151	-2.8
775	Clc1ccc(cc1)n1c(=S)[nH]nc1C1=NC(=S)N=N1	C10H5ClN6S2	-6.1	38.22	-19.716	2.8
776	S=C1N=NC(=N1)c1n[nH]c(=S)n1c1cc(F)cc(c1)Br	C10H4BrFN6S2	-6.3	35.8	-18.719	2.8
777	S=C1N=NC(=N1)c1n[nH]c(=S)n1c1cc(F)cc(c1)Cl	C10H4ClFN6S2	-6.0	37.82	-18.702	1.0
778	Fc1cc(F)cc(c1)n1c(=S)[nH]nc1C1=NC(=S)N=N1	C10H4F2N6S2	-6.2	38.4	-19.049	-2.3
779	S=C1N=NC(=N1)c1n[nH]c(=S)n1c1cc(F)cc(c1)I	C10H4FIN6S2	-6.0	38.63	-18.679	-0.9
780	Brc1ccc(c(c1)F)n1c(=S)[nH]nc1C1=NC(=S)N=N1	C10H4BrFN6S2	-6.3	35.55	-20.264	-1.3
781	Clc1ccc(c(c1)F)n1c(=S)[nH]nc1C1=NC(=S)N=N1	C10H4ClFN6S2	-6.3	36.61	-20.261	-1.8
782	Fc1ccc(c(c1)F)n1c(=S)[nH]nc1C1=NC(=S)N=N1	C10H4F2N6S2	-6.2	41.28	-20.396	10.8
783	lc1ccc(c(c1)F)n1c(=S)[nH]nc1C1=NC(=S)N=N1	C10H4FIN6S2	-6.3	35.14	-19.182	2.2
784	Fc1ccc(c(c1)Br)n1c(=S)[nH]nc1C1=NC(=S)N=N1	C10H4BrFN6S2	-6.1	39.45	-19.763	1.0
785	Fc1ccc(c(c1)Cl)n1c(=S)[nH]nc1C1=NC(=S)N=N1	C10H4ClFN6S2	-6.1	35.82	-20.47	8.3
786	Fc1ccc(c(c1)I)n1c(=S)[nH]nc1C1=NC(=S)N=N1	C10H4FIN6S2	-5.9	41.59	-19.822	0.8
787	Brc1cc(F)c(c(c1)F)n1c(=S)[nH]nc1C1=NC(=S)N=N1	C10H3BrF2N6S2	-6.4	37.85	-20.528	-1.4
788	S=C1N=NC(=N1)c1n[nH]c(=S)n1c1c(F)cc(cc1l)Br	C10H3BrFIN6S2	-5.8	36.91	-19.892	3.4
789	Clc1cc(F)c(c(c1)F)n1c(=S)[nH]nc1C1=NC(=S)N=N1	C10H3ClF2N6S2	-6.4	37.2	-20.527	-1.6
790	S=C1N=NC(=N1)c1n[nH]c(=S)n1c1c(F)cc(cc1l)Cl	C10H3ClFIN6S2	-5.8	38.47	-19.898	2.3
791	Fc1cc(F)c(c(c1)F)n1c(=S)[nH]nc1C1=NC(=S)N=N1	C10H3F3N6S2	-6.4	37.79	-20.476	1.5
792	S=C1N=NC(=N1)c1n[nH]c(=S)n1c1c(F)cc(cc1l)F	C10H3F2IN6S2	-5.9	38.96	-19.611	4.0
793	lc1cc(F)c(c(c1)F)n1c(=S)[nH]nc1C1=NC(=S)N=N1	C10H3F2IN6S2	-6.4	37.16	-20.528	-0.2
794	S=C1N=NC(=N1)c1n[nH]c(=S)n1c1c(F)cc(cc1l)I	C10H3FI2N6S2	-5.7	36.76	-19.966	5.9
795	Fc1cccc(c1)n1c(=S)[nH]nc1C1=NC(=S)N=N1	C10H5FN6S2	-6.0	42.95	-22.084	15.2
796	S=C1N=NC(=N1)c1n[nH]c(=S)n1c1cccc1F	C10H5FN6S2	-6.0	40.93	-19.623	-0.9
797	Fc1ccc(cc1)n1c(=S)[nH]nc1C1=NC(=S)N=N1	C10H5FN6S2	-6.0	37.88	-19.464	0.8
798	S=C1N=NC(=N1)c1n[nH]c(=S)n1c1cccc1	C10H6N6S2	-5.8	38.75	-20.613	20.4
799	lc1cc(l)cc(c1)n1c(=S)[nH]nc1C1=NC(=S)N=N1	C10H4I2N6S2	-6.1	35.9	-19.444	-4.6
800	lc1ccc(c(c1)l)n1c(=S)[nH]nc1C1=NC(=S)N=N1	C10H4I2N6S2	-5.6	34.91	-20.176	7.8
801	Brc1cc(l)c(c(c1)l)n1c(=S)[nH]nc1C1=NC(=S)N=N1	C10H3BrI2N6S2	-5.7	38.03	-17.787	11.5
802	Clc1cc(l)c(c(c1)l)n1c(=S)[nH]nc1C1=NC(=S)N=N1	C10H3ClI2N6S2	-5.7	37.96	-17.789	9.5
803	Fc1cc(l)c(c(c1)l)n1c(=S)[nH]nc1C1=NC(=S)N=N1	C10H3FI2N6S2	-5.7	38.28	-17.789	9.8

804	<chem>Ic1cc(I)c(c(c1)I)n1c(=S)[nH]nc1C1=NC(=S)N=N1</chem>	C10H3I3N6S2	-5.7	37.75	-17.911	10.7
805	<chem>Ic1cccc(c1)n1c(=S)[nH]nc1C1=NC(=S)N=N1</chem>	C10H5IN6S2	-6.1	34.27	-20.598	-3.8
806	<chem>S=C1N=NC(=N1)c1n[nH]c(=S)n1c1cccc1I</chem>	C10H5IN6S2	-5.4	37.64	-20.491	-1.8
807	<chem>Ic1ccc(cc1)n1c(=S)[nH]nc1C1=NC(=S)N=N1</chem>	C10H5IN6S2	-6.1	36.12	-19.703	6.7
808	<chem>Cc1cccc(c1)n1c(=S)[nH]nc1C1=NC(=S)N=N1</chem>	C11H8N6S2	-6.1	40.02	-19.46	0.0
809	<chem>S=C1N=NC(=N1)c1n[nH]c(=S)n1c1cccc1C</chem>	C11H8N6S2	-5.7	37.4	-20.346	1.7
810	<chem>Cc1ccc(cc1)n1c(=S)[nH]nc1C1=NC(=S)N=N1</chem>	C11H8N6S2	-6.1	35.63	-19.207	-1.1
811	<chem>S=C1N=NC(=N1)c1n[nH]c(=S)n1c1cccc(c1)N(=O)=O</chem>	C10H5N7O2S2	-6.6	43.43	-24.709	-0.7
812	<chem>S=C1N=NC(=N1)c1n[nH]c(=S)n1c1cccc1N(=O)=O</chem>	C10H5N7O2S2	-6.5	40.89	-27.288	8.1
813	<chem>S=C1N=NC(=N1)c1n[nH]c(=S)n1c1ccc(cc1)N(=O)=O</chem>	C10H5N7O2S2	-6.4	40.7	-22.498	9.3
814	<chem>Oc1cccc(c1)n1c(=S)[nH]nc1C1=NC(=S)N=N1</chem>	C10H6N6OS2	-5.7	43.88	-22.711	30.7
815	<chem>S=C1N=NC(=N1)c1n[nH]c(=S)n1c1cccc1O</chem>	C10H6N6OS2	-6.0	43.51	-21.457	4.1
816	<chem>Oc1ccc(cc1)n1c(=S)[nH]nc1C1=NC(=S)N=N1</chem>	C10H6N6OS2	-5.9	39.06	-22.246	7.8
817	<chem>COc1cccc(c1)n1c(=S)[nH]nc1C1=NC(=S)N=N1</chem>	C11H8N6OS2	-6.0	39.08	-21.701	7.5
818	<chem>COc1cccc1n1c(=S)[nH]nc1C1=NC(=S)N=N1</chem>	C11H8N6OS2	-6.1	36.66	-21.191	-1.2
819	<chem>COc1ccc(cc1)n1c(=S)[nH]nc1C1=NC(=S)N=N1</chem>	C11H8N6OS2	-6.1	38.84	-21.085	0.6
820	<chem>Brc1cc(Br)cc(c1)N1CNN=C1c1ccc[nH]1</chem>	C12H10Br2N4	-6.2	41.23	-23.462	-15.9
821	<chem>Brc1cc(I)cc(c1)N1CNN=C1c1[nH]ccc1</chem>	C12H10BrIN4	-6.2	40.51	-23.519	-15.3
822	<chem>Brc1ccc(c(c1)Br)N1CNN=C1c1ccc[nH]1</chem>	C12H10Br2N4	-6.1	41.93	-25.131	-10.0
823	<chem>Ic1ccc(c(c1)Br)N1CNN=C1c1ccc[nH]1</chem>	C12H10BrIN4	-6.1	40.77	-24.875	-7.9
824	<chem>Brc1ccc(c(c1)I)N1CNN=C1c1ccc[nH]1</chem>	C12H10BrIN4	-6.2	42.33	-25.088	-10.5
825	<chem>Brc1cc(Br)c(c(c1)Br)n1c(=S)[nH]nc1c1ccc[nH]1</chem>	C12H7Br3N4S	-5.8	40.23	-24.365	-3.8
826	<chem>Brc1cc(F)c(c(c1)Br)n1c(=S)[nH]nc1c1[nH]ccc1</chem>	C12H7Br2FN4S	-5.7	38.89	-20.902	-9.3
827	<chem>Brc1cc(Br)c(c(c1)I)n1c(=S)[nH]nc1c1[nH]ccc1</chem>	C12H7Br2IN4S	-5.8	40.48	-24.218	-8.2
828	<chem>Clc1cc(Br)c(c(c1)Br)n1c(=S)[nH]nc1c1ccc[nH]1</chem>	C12H7Br2ClN4S	-5.9	39.8	-24.627	-5.3
829	<chem>Clc1cc(F)c(c(c1)Br)n1c(=S)[nH]nc1c1[nH]ccc1</chem>	C12H7BrClFN4S	-6.3	39.04	-20.842	-10.1
830	<chem>Clc1cc(Br)c(c(c1)I)n1c(=S)[nH]nc1c1[nH]ccc1</chem>	C12H7BrClIN4S	-5.9	40.46	-24.507	-8.3
831	<chem>Fc1cc(Br)c(c(c1)Br)n1c(=S)[nH]nc1c1ccc[nH]1</chem>	C12H7Br2FN4S	-5.9	39.19	-24.698	-11.4
832	<chem>Fc1cc(F)c(c(c1)Br)n1c(=S)[nH]nc1c1[nH]ccc1</chem>	C12H7BrF2N4S	-6.5	40.47	-21.439	-14.6
833	<chem>Fc1cc(Br)c(c(c1)I)n1c(=S)[nH]nc1c1[nH]ccc1</chem>	C12H7BrFIN4S	-5.9	39.25	-24.671	-11.7
834	<chem>Ic1cc(Br)c(c(c1)Br)n1c(=S)[nH]nc1c1ccc[nH]1</chem>	C12H7Br2IN4S	-5.7	41.06	-24.478	-7.6

835	<chem>Ic1cc(F)c(c(c1)Br)n1c(=S)[nH]nc1c1[nH]ccc1</chem>	C12H7BrFIN4S	-5.7	38.45	-20.77	-8.5
836	<chem>Ic1cc(Br)c(c(c1)I)n1c(=S)[nH]nc1c1[nH]ccc1</chem>	C12H7BrI2N4S	-5.7	39.7	-24.4	-7.7
837	<chem>Brc1cccc(c1)n1c(=S)[nH]nc1c1ccc[nH]1</chem>	C12H9BrN4S	-5.8	37.2	-23.527	-16.9
838	<chem>S=c1[nH]nc(n1c1cccc1Br)c1[nH]ccc1</chem>	C12H9BrN4S	-6.0	38.81	-22.405	-14.7
839	<chem>Brc1ccc(cc1)n1c(=S)[nH]nc1c1ccc[nH]1</chem>	C12H9BrN4S	-6.0	37.49	-21.47	-8.9
840	<chem>Clc1cc(Br)cc(c1)N1CNN=C1c1[nH]ccc1</chem>	C12H10BrClN4	-6.2	40.39	-23.447	-15.5
841	<chem>Clc1cc(Cl)cc(c1)N1CNN=C1c1ccc[nH]1</chem>	C12H10Cl2N4	-6.0	40.57	-20.161	-11.5
842	<chem>Clc1cc(I)cc(c1)N1CNN=C1c1[nH]ccc1</chem>	C12H10ClIN4	-6.2	41.44	-23.771	-12.3
843	<chem>Brc1ccc(c(c1)Cl)N1CNN=C1c1ccc[nH]1</chem>	C12H10BrClN4	-6.1	41.53	-22.393	-7.9
844	<chem>Clc1ccc(c(c1)Cl)N1CNN=C1c1ccc[nH]1</chem>	C12H10Cl2N4	-6.2	40.95	-21.395	-9.2
845	<chem>Ic1ccc(c(c1)Cl)N1CNN=C1c1ccc[nH]1</chem>	C12H10ClIN4	-6.1	40.8	-24.558	-7.6
846	<chem>Clc1ccc(c(c1)Br)N1CNN=C1c1ccc[nH]1</chem>	C12H10BrClN4	-6.2	42.38	-22.357	-9.5
847	<chem>Clc1ccc(c(c1)I)N1CNN=C1c1ccc[nH]1</chem>	C12H10ClIN4	-6.1	41.53	-25.119	-11.9
848	<chem>Brc1cc(Cl)c(c(c1)Br)n1c(=S)[nH]nc1c1[nH]ccc1</chem>	C12H7Br2ClN4S	-5.7	39.09	-24.37	-10.0
849	<chem>Brc1cc(Cl)c(c(c1)Cl)n1c(=S)[nH]nc1c1ccc[nH]1</chem>	C12H7BrCl2N4S	-6.2	45.08	-24.41	-8.6
850	<chem>Brc1cc(F)c(c(c1)Cl)n1c(=S)[nH]nc1c1[nH]ccc1</chem>	C12H7BrClFN4S	-5.8	39.57	-21.302	-10.6
851	<chem>Brc1cc(Cl)c(c(c1)I)n1c(=S)[nH]nc1c1[nH]ccc1</chem>	C12H7BrClIN4S	-5.7	40.33	-24.341	-9.2
852	<chem>Clc1cc(Cl)c(c(c1)Br)n1c(=S)[nH]nc1c1[nH]ccc1</chem>	C12H7BrCl2N4S	-5.9	39.52	-24.66	-11.0
853	<chem>Clc1cc(Cl)c(c(c1)Cl)n1c(=S)[nH]nc1c1ccc[nH]1</chem>	C12H7Cl3N4S	-6.3	39.29	-23.3452	-8.0
854	<chem>Clc1cc(F)c(c(c1)Cl)n1c(=S)[nH]nc1c1[nH]ccc1</chem>	C12H7Cl2FN4S	-6.4	38.84	-21.187	-10.1
855	<chem>Clc1cc(Cl)c(c(c1)I)n1c(=S)[nH]nc1c1[nH]ccc1</chem>	C12H7Cl2IN4S	-5.8	39.89	-24.814	-8.3
856	<chem>Fc1cc(Cl)c(c(c1)Br)n1c(=S)[nH]nc1c1[nH]ccc1</chem>	C12H7BrClFN4S	-6.0	38.49	-24.824	-12.5
857	<chem>Fc1cc(Cl)c(c(c1)Cl)n1c(=S)[nH]nc1c1ccc[nH]1</chem>	C12H7Cl2FN4S	-6.6	40.54	-22.1748	-13.0
858	<chem>Fc1cc(F)c(c(c1)Cl)n1c(=S)[nH]nc1c1[nH]ccc1</chem>	C12H7ClF2N4S	-6.5	38.91	-21.486	-15.7
859	<chem>Fc1cc(Cl)c(c(c1)I)n1c(=S)[nH]nc1c1[nH]ccc1</chem>	C12H7ClFIN4S	-5.9	40.26	-24.797	-10.9
860	<chem>Ic1cc(Cl)c(c(c1)Br)n1c(=S)[nH]nc1c1[nH]ccc1</chem>	C12H7BrClIN4S	-5.6	40.67	-24.544	-7.1
861	<chem>Ic1cc(Cl)c(c(c1)Cl)n1c(=S)[nH]nc1c1ccc[nH]1</chem>	C12H7Cl2IN4S	-5.9	42.81	-22.179	-0.5
862	<chem>Ic1cc(F)c(c(c1)Cl)n1c(=S)[nH]nc1c1[nH]ccc1</chem>	C12H7ClFIN4S	-5.8	41.03	-21.746	-8.9
863	<chem>Ic1cc(Cl)c(c(c1)I)n1c(=S)[nH]nc1c1[nH]ccc1</chem>	C12H7ClI2N4S	-5.7	38.94	-24.468	-7.4
864	<chem>Clc1cccc(c1)n1c(=S)[nH]nc1c1ccc[nH]1</chem>	C12H9ClN4S	-6.1	37.97	-23.241	-15.9
865	<chem>S=c1[nH]nc(n1c1cccc1Cl)c1[nH]ccc1</chem>	C12H9ClN4S	-6.0	36.68	-23.233	-14.3

866	Clc1ccc(cc1)n1c(=S)[nH]nc1c1ccc[nH]1	C12H9ClN4S	-6.1	36.74	-22.165	-10.1
867	Fc1cc(Br)cc(c1)n1c(=S)[nH]nc1c1[nH]ccc1	C12H8BrFN4S	-6.0	39.22	-23.514	-15.2
868	Fc1cc(Cl)cc(c1)n1c(=S)[nH]nc1c1[nH]ccc1	C12H8ClFN4S	-5.9	39.86	-23.592	-16.7
869	Fc1cc(F)cc(c1)n1c(=S)[nH]nc1c1ccc[nH]1	C12H8F2N4S	-6.1	37.44	-23.176	-13.9
870	Fc1cc(I)cc(c1)n1c(=S)[nH]nc1c1[nH]ccc1	C12H8FIN4S	-6.0	39.04	-23.391	-17.7
871	Brc1ccc(c(c1)F)n1c(=S)[nH]nc1c1ccc[nH]1	C12H8BrFN4S	-6.0	37.71	-22.325	-4.5
872	Clc1ccc(c(c1)F)n1c(=S)[nH]nc1c1ccc[nH]1	C12H8ClFN4S	-6.3	37.82	-23.054	-6.1
873	Fc1ccc(c(c1)F)n1c(=S)[nH]nc1c1ccc[nH]1	C12H8F2N4S	-6.1	40.2	-24.1814	-9.0
874	Ic1ccc(c(c1)F)n1c(=S)[nH]nc1c1ccc[nH]1	C12H8FIN4S	-5.5	40.78	-21.599	-0.3
875	Fc1ccc(c(c1)Br)n1c(=S)[nH]nc1c1ccc[nH]1	C12H8BrFN4S	-6.2	38.53	-24.724	-15.2
876	Fc1ccc(c(c1)Cl)n1c(=S)[nH]nc1c1ccc[nH]1	C12H8ClFN4S	-6.2	39.06	-24.608	-11.6
877	Fc1ccc(c(c1)I)n1c(=S)[nH]nc1c1ccc[nH]1	C12H8FIN4S	-5.7	38.63	-24.113	-14.7
878	Brc1cc(F)c(c(c1)F)n1c(=S)[nH]nc1c1ccc[nH]1	C12H7BrF2N4S	-6.1	39.9	-21.204	-8.9
879	Brc1cc(F)c(c(c1)I)n1c(=S)[nH]nc1c1[nH]ccc1	C12H7BrFIN4S	-5.6	40.34	-24.865	-4.5
880	Clc1cc(F)c(c(c1)F)n1c(=S)[nH]nc1c1ccc[nH]1	C12H7ClF2N4S	-6.4	39.9	-21.764	-11.5
881	Clc1cc(F)c(c(c1)I)n1c(=S)[nH]nc1c1[nH]ccc1	C12H7ClFIN4S	-6.3	39.42	-20.327	-9.7
882	Fc1cc(F)c(c(c1)F)n1c(=S)[nH]nc1c1ccc[nH]1	C12H7F3N4S	-6.5	34.03	-22.757	-12.8
883	Fc1cc(F)c(c(c1)I)n1c(=S)[nH]nc1c1[nH]ccc1	C12H7F2IN4S	-6.5	38.92	-20.689	-8.1
884	Ic1cc(F)c(c(c1)F)n1c(=S)[nH]nc1c1ccc[nH]1	C12H7F2IN4S	-5.7	41.7	-21.61	-8.0
885	Ic1cc(F)c(c(c1)I)n1c(=S)[nH]nc1c1[nH]ccc1	C12H7FI2N4S	-5.5	39.51	-24.597	-2.7
886	Fc1cccc(c1)n1c(=S)[nH]nc1c1ccc[nH]1	C12H9FN4S	-6.0	39.98	-21.085	-12.3
887	S=c1[nH]nc(n1c1ccccc1F)c1[nH]ccc1	C12H9FN4S	-5.7	38.46	-20.767	-13.3
888	Fc1ccc(cc1)n1c(=S)[nH]nc1c1ccc[nH]1	C12H9FN4S	-5.6	40.56	-20.793	-11.4
889	S=c1[nH]nc(n1c1ccccc1)c1ccc[nH]1	C12H10N4S	-5.5	34.34	-20.53	-12.5
890	Ic1cc(I)cc(c1)N1CNN=C1c1ccc[nH]1	C12H10I2N4	-6.1	41.13	-22.571	-13.4
891	Ic1ccc(c(c1)I)N1CNN=C1c1ccc[nH]1	C12H10I2N4	-6.1	41.3	-24.814	-8.4
892	Brc1cc(I)c(c(c1)I)n1c(=S)[nH]nc1c1ccc[nH]1	C12H7BrI2N4S	-5.9	39.93	-24.451	-3.7
893	Clc1cc(I)c(c(c1)I)n1c(=S)[nH]nc1c1ccc[nH]1	C12H7ClI2N4S	-5.9	40.26	-24.738	-8.0
894	Fc1cc(I)c(c(c1)I)n1c(=S)[nH]nc1c1ccc[nH]1	C12H7FI2N4S	-5.8	40.17	-24.905	-10.1
895	Ic1cc(I)c(c(c1)I)n1c(=S)[nH]nc1c1ccc[nH]1	C12H7I3N4S	-5.8	39.68	-24.362	-4.4
896	Ic1cccc(c1)n1c(=S)[nH]nc1c1ccc[nH]1	C12H9IN4S	-5.9	39.58	-23.41	-18.0

897	<chem>S=c1[nH]nc(n1c1ccccc1l)c1[nH]ccc1</chem>	C12H9IN4S	-6.0	35.93	-22.292	-14.1
898	<chem>lc1ccc(cc1)n1c(=S)[nH]nc1c1ccc[nH]1</chem>	C12H9IN4S	-5.4	37.88	-20.742	-2.6
899	<chem>Cc1cccc(c1)n1c(=S)[nH]nc1c1ccc[nH]1</chem>	C13H12N4S	-6.0	36.27	-24.717	-15.8
900	<chem>S=c1[nH]nc(n1c1ccccc1C)c1[nH]ccc1</chem>	C13H12N4S	-6.1	39.05	-24.376	-0.6
901	<chem>Cc1ccc(cc1)n1c(=S)[nH]nc1c1ccc[nH]1</chem>	C13H12N4S	-6.2	39.42	-22.406	-11.0
902	<chem>O=N(=O)c1cccc(c1)n1c(=S)[nH]nc1c1ccc[nH]1</chem>	C12H9N5O2S	-6.2	43.27	-26.725	-3.1
903	<chem>S=c1[nH]nc(n1c1ccccc1N(=O)=O)c1[nH]ccc1</chem>	C12H9N5O2S	-6.2	43.91	-28.57	-5.7
904	<chem>O=N(=O)c1ccc(cc1)n1c(=S)[nH]nc1c1ccc[nH]1</chem>	C12H9N5O2S	-6.3	47.25	-22.961	-11.9
905	<chem>Oc1cccc(c1)n1c(=S)[nH]nc1c1ccc[nH]1</chem>	C12H10N4OS	-6.0	36.76	-22.238	-11.9
906	<chem>S=c1[nH]nc(n1c1ccccc1O)c1[nH]ccc1</chem>	C12H10N4OS	-6.0	44.86	-24.878	-10.4
907	<chem>Oc1ccc(cc1)n1c(=S)[nH]nc1c1ccc[nH]1</chem>	C12H10N4OS	-5.8	39.99	-22.405	-4.3
908	<chem>COc1cccc(c1)n1c(=S)[nH]nc1c1ccc[nH]1</chem>	C13H12N4OS	-5.9	38.43	-25.012	-15.1
909	<chem>COc1ccccc1n1c(=S)[nH]nc1c1[nH]ccc1</chem>	C13H12N4OS	-5.7	35.71	-23.096	-8.9
910	<chem>COc1ccc(cc1)n1c(=S)[nH]nc1c1ccc[nH]1</chem>	C13H12N4OS	-6.0	40.82	-20.992	-9.4
911	<chem>Brc1cccc(c1)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H14BrN3S	-6.9	46.66	-14.918	18.2
912	<chem>Brc1cc(cc(c1)Br)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H13Br2N3S	-7.1	44.39	-12.047	21.1
913	<chem>Brc1cc(Sc2[nH]nc(n2)C2CCCC2)cc(c1)I</chem>	C13H13BrIN3S	-7.2	48.12	-11.816	4.3
914	<chem>Brc1ccccc1Sc1[nH]nc(n1)C1CCCC1</chem>	C13H14BrN3S	-6.6	48.37	-16.485	-0.4
915	<chem>Brc1cc(Br)c(c(c1)Br)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H12Br3N3S	-6.4	43.74	-14.178	26.1
916	<chem>Clc1cc(Br)c(c(c1)Br)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H12Br2ClN3S	-6.4	50.92	-14.328	26.4
917	<chem>Fc1cc(Br)c(c(c1)Br)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H12Br2FN3S	-6.5	45.25	-14.251	27.1
918	<chem>lc1cc(Br)c(c(c1)Br)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H12Br2IN3S	-6.3	42.74	-13.647	26.1
919	<chem>Brc1ccc(c(c1)Br)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H13Br2N3S	-6.8	51.53	-14.866	5.7
920	<chem>Brc1cc(F)c(c(c1)Br)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H12Br2FN3S	-6.6	42.72	-16.007	28.1
921	<chem>Clc1cc(F)c(c(c1)Br)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H12BrClFN3S	-6.6	43.91	-16.207	28.0
922	<chem>Fc1cc(F)c(c(c1)Br)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H12BrF2N3S	-6.5	43.81	-16.297	28.7
923	<chem>lc1cc(F)c(c(c1)Br)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H12BrFIN3S	-6.6	43.2	-15.747	26.1
924	<chem>Brc1cc(Br)c(c(c1)I)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H12Br2IN3S	-6.4	42.47	-13.139	27.0
925	<chem>Clc1cc(Br)c(c(c1)I)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H12BrClIN3S	-6.4	41.99	-13.33	27.0
926	<chem>Fc1cc(Br)c(c(c1)I)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H12BrFIN3S	-6.4	44.03	-13.364	27.9
927	<chem>lc1cc(Br)c(c(c1)I)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H12BrI2N3S	-6.5	42.44	-13.187	-0.9

928	<chem>Ic1ccc(c(c1)Br)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H13BrIN3S	-6.6	46	-14.933	23.7
929	<chem>Brc1ccc(cc1)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H14BrN3S	-6.9	51.53	-15.483	15.5
930	<chem>Brc1ccc(c(c1)I)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H13BrIN3S	-6.2	50.98	-14.551	5.2
931	<chem>Clc1cccc(c1)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H14ClN3S	-6.9	46.92	-15.065	18.9
932	<chem>Clc1cc(Sc2[nH]nc(n2)C2CCCC2)cc(c1)Br</chem>	C13H13BrClN3S	-7.1	46.38	-12.812	-3.6
933	<chem>Clc1cc(cc(c1)Cl)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H13Cl2N3S	-7.1	48.16	-12.93	2.0
934	<chem>Clc1cc(Sc2[nH]nc(n2)C2CCCC2)cc(c1)I</chem>	C13H13ClIN3S	-7.1	44.48	-12.315	16.3
935	<chem>Clc1cccc1Sc1[nH]nc(n1)C1CCCC1</chem>	C13H14ClN3S	-6.8	48.3	-17.148	17.6
936	<chem>Brc1cc(Cl)c(c(c1)Br)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H12Br2ClN3S	-6.7	42.07	-13.445	5.7
937	<chem>Clc1cc(Cl)c(c(c1)Br)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H12BrCl2N3S	-6.8	42.27	-15.564	7.5
938	<chem>Fc1cc(Cl)c(c(c1)Br)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H12BrClFN3S	-6.5	42.53	-14.476	3.6
939	<chem>Ic1cc(Cl)c(c(c1)Br)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H12BrClIN3S	-6.5	43.16	-14.534	25.5
940	<chem>Brc1ccc(c(c1)Cl)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H13BrClN3S	-6.9	50.91	-15.413	7.4
941	<chem>Brc1cc(Cl)c(c(c1)Cl)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H12BrCl2N3S	-6.9	43.99	-15.534	6.5
942	<chem>Clc1cc(Cl)c(c(c1)Cl)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H12Cl3N3S	-6.4	45.34	-15.326	10.2
943	<chem>Fc1cc(Cl)c(c(c1)Cl)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H12Cl2FN3S	-6.9	41.42	-15.039	-3.9
944	<chem>Ic1cc(Cl)c(c(c1)Cl)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H12Cl2IN3S	-6.6	42.03	-13.951	9.2
945	<chem>Clc1ccc(c(c1)Cl)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H13Cl2N3S	-6.8	51.51	-15.138	5.7
946	<chem>Brc1cc(F)c(c(c1)Cl)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H12BrClFN3S	-6.9	42.82	-15.713	8.0
947	<chem>Clc1cc(F)c(c(c1)Cl)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H12Cl2FN3S	-6.9	43.23	-16.064	9.3
948	<chem>Fc1cc(F)c(c(c1)Cl)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H12ClF2N3S	-6.9	51.19	-16.338	11.8
949	<chem>Ic1cc(F)c(c(c1)Cl)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H12ClFIN3S	-6.8	43.1	-15.512	26.9
950	<chem>Brc1cc(Cl)c(c(c1)I)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H12BrClIN3S	-6.4	43.46	-14.343	16.8
951	<chem>Clc1cc(Cl)c(c(c1)I)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H12Cl2IN3S	-6.5	42.61	-14.554	16.9
952	<chem>Fc1cc(Cl)c(c(c1)I)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H12ClFIN3S	-6.7	44.42	-13.121	26.2
953	<chem>Ic1cc(Cl)c(c(c1)I)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H12ClI2N3S	-6.4	42.96	-14.076	15.9
954	<chem>Ic1ccc(c(c1)Cl)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H13ClIN3S	-6.6	50.05	-15.277	6.8
955	<chem>Clc1ccc(cc1)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H14ClN3S	-6.8	54.88	-15.921	15.2
956	<chem>Clc1ccc(c(c1)Br)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H13BrClN3S	-6.8	48.71	-14.975	6.0
957	<chem>Clc1ccc(c(c1)I)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H13ClIN3S	-6.8	45.77	-14.671	5.5
958	<chem>Fc1cccc(c1)Sc1[nH]nc(n1)C1CCCC1</chem>	C13H14FN3S	-6.9	48.23	-15.81	19.0

959	Fc1cc(Sc2[nH]nc(n2)C2CCCC2)cc(c1)Br	C13H13BrFN3S	-6.5	50.14	-15.477	5.0
960	Fc1cc(Sc2[nH]nc(n2)C2CCCC2)cc(c1)Cl	C13H13ClFN3S	-7.1	49.44	-15.585	-1.6
961	Fc1cc(cc(c1)F)Sc1[nH]nc(n1)C1CCCC1	C13H13F2N3S	-6.5	48.28	-14.777	-3.5
962	Fc1cc(Sc2[nH]nc(n2)C2CCCC2)cc(c1)I	C13H13FIN3S	-7.0	48.35	-15.413	-0.5
963	Fc1cccc1Sc1[nH]nc(n1)C1CCCC1	C13H14FN3S	-7.1	51.95	-17.63	17.3
964	Brc1ccc(c(c1)F)Sc1[nH]nc(n1)C1CCCC1	C13H13BrFN3S	-6.5	49.29	-14.843	12.7
965	Clc1ccc(c(c1)F)Sc1[nH]nc(n1)C1CCCC1	C13H13ClFN3S	-6.7	52.78	-15.648	4.5
966	Brc1cc(F)c(c(c1)F)Sc1[nH]nc(n1)C1CCCC1	C13H12BrF2N3S	-6.8	41.79	-14.402	13.1
967	Clc1cc(F)c(c(c1)F)Sc1[nH]nc(n1)C1CCCC1	C13H12ClF2N3S	-6.9	42.32	-14.649	13.2
968	Fc1cc(F)c(c(c1)F)Sc1[nH]nc(n1)C1CCCC1	C13H12F3N3S	-6.9	45.93	-15.535	5.8
969	Ic1cc(F)c(c(c1)F)Sc1[nH]nc(n1)C1CCCC1	C13H12F2IN3S	-6.8	42.51	-15.274	28.3
970	Fc1ccc(c(c1)F)Sc1[nH]nc(n1)C1CCCC1	C13H13F2N3S	-6.7	52.57	-15.758	14.0
971	Brc1cc(F)c(c(c1)I)Sc1[nH]nc(n1)C1CCCC1	C13H12BrFIN3S	-6.7	43.11	-13.641	11.4
972	Clc1cc(F)c(c(c1)I)Sc1[nH]nc(n1)C1CCCC1	C13H12ClFIN3S	-6.6	43.86	-14.235	7.2
973	Fc1cc(F)c(c(c1)I)Sc1[nH]nc(n1)C1CCCC1	C13H12F2IN3S	-6.6	44.69	-14.402	7.9
974	Ic1cc(F)c(c(c1)I)Sc1[nH]nc(n1)C1CCCC1	C13H12FI2N3S	-6.7	42.13	-14.123	7.0
975	Ic1ccc(c(c1)F)Sc1[nH]nc(n1)C1CCCC1	C13H13FIN3S	-6.7	50.12	-14.121	2.8
976	Fc1ccc(cc1)Sc1[nH]nc(n1)C1CCCC1	C13H14FN3S	-6.8	54.32	-16.542	17.1
977	Fc1ccc(c(c1)Br)Sc1[nH]nc(n1)C1CCCC1	C13H13BrFN3S	-6.8	52.9	-15.06	12.4
978	Fc1ccc(c(c1)Cl)Sc1[nH]nc(n1)C1CCCC1	C13H13ClFN3S	-6.8	48.45	-15.87	12.8
979	Fc1ccc(c(c1)I)Sc1[nH]nc(n1)C1CCCC1	C13H13FIN3S	-6.8	52.27	-14.714	6.9
980	C1CCC(C1)c1n[nH]c(n1)Sc1cccc1	C13H15N3S	-6.8	46.93	-17.611	1.1
981	Ic1cccc(c1)Sc1[nH]nc(n1)C1CCCC1	C13H14IN3S	-6.9	47.1	-14.8	17.5
982	Ic1cc(cc(c1)I)Sc1[nH]nc(n1)C1CCCC1	C13H13I2N3S	-6.1	45.73	-11.832	1.0
983	Ic1cccc1Sc1[nH]nc(n1)C1CCCC1	C13H14IN3S	-6.3	47.6	-16.98	-0.1
984	Brc1cc(I)c(c(c1)I)Sc1[nH]nc(n1)C1CCCC1	C13H12BrI2N3S	-6.2	42.71	-13.285	20.1
985	Clc1cc(I)c(c(c1)I)Sc1[nH]nc(n1)C1CCCC1	C13H12ClI2N3S	-6.3	43.15	-13.492	20.3
986	Fc1cc(I)c(c(c1)I)Sc1[nH]nc(n1)C1CCCC1	C13H12FI2N3S	-6.3	45.05	-12.855	-4.0
987	Ic1cc(I)c(c(c1)I)Sc1[nH]nc(n1)C1CCCC1	C13H12I3N3S	-6.1	42.09	-12.183	-0.6
988	Ic1ccc(c(c1)I)Sc1[nH]nc(n1)C1CCCC1	C13H13I2N3S	-6.5	48.64	-14.435	4.7
989	Ic1ccc(cc1)Sc1[nH]nc(n1)C1CCCC1	C13H14IN3S	-6.7	53.9	-14.898	14.9

990	Cc1cccc(c1)Sc1[nH]nc(n1)C1CCCC1	C14H17N3S	-6.9	46.57	-15.904	16.3
991	Cc1cccc1Sc1[nH]nc(n1)C1CCCC1	C14H17N3S	-6.7	51.12	-16.669	19.7
992	Cc1ccc(cc1)Sc1[nH]nc(n1)C1CCCC1	C14H17N3S	-6.9	57	-16.969	11.3
993	O=N(=O)c1cccc(c1)Sc1[nH]nc(n1)C1CCCC1	C13H14N4O2S	-7.2	51.57	-28.603	14.0
994	O=N(=O)c1cccc1Sc1[nH]nc(n1)C1CCCC1	C13H14N4O2S	-7.5	52.33	-22.285	23.0
995	O=N(=O)c1ccc(cc1)Sc1[nH]nc(n1)C1CCCC1	C13H14N4O2S	-7.1	50.7	-20.436	43.5
996	Oc1cccc(c1)Sc1[nH]nc(n1)C1CCCC1	C13H15N3OS	-7.3	49.5	-18.657	31.0
997	Oc1cccc1Sc1[nH]nc(n1)C1CCCC1	C13H15N3OS	-6.6	53.05	-21.698	8.8
998	Oc1ccc(cc1)Sc1[nH]nc(n1)C1CCCC1	C13H15N3OS	-6.8	52.47	-21.793	15.6
999	COc1cccc(c1)Sc1[nH]nc(n1)C1CCCC1	C14H17N3OS	-6.4	47.24	-20.869	-11.9
1000	COc1cccc1Sc1[nH]nc(n1)C1CCCC1	C14H17N3OS	-7.0	47.18	-25.491	6.4
1001	COc1ccc(cc1)Sc1[nH]nc(n1)C1CCCC1	C14H17N3OS	-6.7	44.82	-19.072	20.6
1002	Brc1cccc(c1)Sc1[nH]nc(n1)c1ccoc1C	C13H10BrN3OS	-6.8	50.63	-16.303	-5.4
1003	Brc1cc(cc(c1)Br)Sc1[nH]nc(n1)c1ccoc1C	C13H9Br2N3OS	-6.8	47.48	-17.071	-7.5
1004	Brc1cc(Sc2[nH]nc(n2)c2ccoc2C)cc(c1)I	C13H9BrIN3OS	-6.7	47.73	-16.439	-7.6
1005	Brc1cccc1Sc1[nH]nc(n1)c1ccoc1C	C13H10BrN3OS	-6.2	48.71	-17.209	-10.0
1006	Brc1cc(Br)c(c(c1)Br)Sc1[nH]nc(n1)c1ccoc1C	C13H8Br3N3OS	-5.9	50.03	-15.566	9.1
1007	Clc1cc(Br)c(c(c1)Br)Sc1[nH]nc(n1)c1ccoc1C	C13H8Br2ClN3OS	-6.4	44.08	-15.816	8.8
1008	Fc1cc(Br)c(c(c1)Br)Sc1[nH]nc(n1)c1ccoc1C	C13H8Br2FN3OS	-6.2	43.05	-15.998	9.6
1009	Ic1cc(Br)c(c(c1)Br)Sc1[nH]nc(n1)c1ccoc1C	C13H8Br2IN3OS	-5.9	45.38	-15.353	8.4
1010	Brc1ccc(c(c1)Br)Sc1[nH]nc(n1)c1ccoc1C	C13H9Br2N3OS	-6.0	49.3	-15.871	3.6
1011	Brc1cc(F)c(c(c1)Br)Sc1[nH]nc(n1)c1ccoc1C	C13H8Br2FN3OS	-6.3	47.9	-15.969	4.2
1012	Clc1cc(F)c(c(c1)Br)Sc1[nH]nc(n1)c1ccoc1C	C13H8BrClFN3OS	-6.5	45.36	-16.024	4.3
1013	Fc1cc(F)c(c(c1)Br)Sc1[nH]nc(n1)c1ccoc1C	C13H8BrF2N3OS	-6.8	43.84	-16.531	-1.7
1014	Ic1cc(F)c(c(c1)Br)Sc1[nH]nc(n1)c1ccoc1C	C13H8BrFIN3OS	-6.1	44.71	-15.901	3.5
1015	Brc1cc(Br)c(c(c1)I)Sc1[nH]nc(n1)c1ccoc1C	C13H8Br2IN3OS	-5.9	42.96	-15.596	10.0
1016	Clc1cc(Br)c(c(c1)I)Sc1[nH]nc(n1)c1ccoc1C	C13H8BrClIN3OS	-6.0	42.88	-15.753	10.3
1017	Fc1cc(Br)c(c(c1)I)Sc1[nH]nc(n1)c1ccoc1C	C13H8BrFIN3OS	-6.2	42.82	-15.433	-7.6
1018	Ic1cc(Br)c(c(c1)I)Sc1[nH]nc(n1)c1ccoc1C	C13H8BrI2N3OS	-5.7	43.17	-15.305	9.4
1019	Ic1ccc(c(c1)Br)Sc1[nH]nc(n1)c1ccoc1C	C13H9BrIN3OS	-7.3	42.91	-15.864	3.3
1020	Brc1ccc(cc1)Sc1[nH]nc(n1)c1ccoc1C	C13H10BrN3OS	-6.3	52.6	-14.998	22.7

1021	Brc1ccc(c(c1)I)Sc1[nH]nc(n1)c1ccoc1C	C13H9BrIN3OS	-6.0	48.96	-15.654	1.9
1022	Clc1cccc(c1)Sc1[nH]nc(n1)c1ccoc1C	C13H10ClIN3OS	-6.9	50.55	-16.248	6.8
1023	Clc1cc(Sc2[nH]nc(n2)c2ccoc2C)cc(c1)Br	C13H9BrClIN3OS	-6.5	46.49	-17.102	-10.0
1024	Clc1cc(cc(c1)Cl)Sc1[nH]nc(n1)c1ccoc1C	C13H9Cl2N3OS	-6.8	50.71	-17.303	-0.1
1025	Clc1cc(Sc2[nH]nc(n2)c2ccoc2C)cc(c1)I	C13H9ClIN3OS	-7.0	51.32	-16.444	-0.5
1026	Clc1ccccc1Sc1[nH]nc(n1)c1ccoc1C	C13H10ClIN3OS	-6.2	45.9	-15.874	-2.1
1027	Brc1cc(Cl)c(c(c1)Br)Sc1[nH]nc(n1)c1ccoc1C	C13H8Br2ClIN3OS	-6.3	49.15	-16.331	6.5
1028	Clc1cc(Cl)c(c(c1)Br)Sc1[nH]nc(n1)c1ccoc1C	C13H8BrCl2N3OS	-6.1	43.82	-16.473	6.9
1029	Fc1cc(Cl)c(c(c1)Br)Sc1[nH]nc(n1)c1ccoc1C	C13H8BrClFN3OS	-6.6	45.1	-16.469	9.8
1030	Ic1cc(Cl)c(c(c1)Br)Sc1[nH]nc(n1)c1ccoc1C	C13H8BrClIN3OS	-6.0	48.4	-16.059	6.4
1031	Brc1ccc(c(c1)Cl)Sc1[nH]nc(n1)c1ccoc1C	C13H9BrClIN3OS	-6.2	46.17	-15.109	7.0
1032	Brc1cc(Cl)c(c(c1)Cl)Sc1[nH]nc(n1)c1ccoc1C	C13H8BrCl2N3OS	-6.5	43.27	-15.449	16.2
1033	Clc1cc(Cl)c(c(c1)Cl)Sc1[nH]nc(n1)c1ccoc1C	C13H8Cl3N3OS	-6.9	46.68	-16.395	-8.3
1034	Fc1cc(Cl)c(c(c1)Cl)Sc1[nH]nc(n1)c1ccoc1C	C13H8Cl2FN3OS	-6.7	51.84	-15.827	16.0
1035	Ic1cc(Cl)c(c(c1)Cl)Sc1[nH]nc(n1)c1ccoc1C	C13H8Cl2IN3OS	-6.1	50.66	-16.661	5.8
1036	Clc1ccc(c(c1)Cl)Sc1[nH]nc(n1)c1ccoc1C	C13H9Cl2N3OS	-6.3	49.03	-15.478	-25.7
1037	Brc1cc(F)c(c(c1)Cl)Sc1[nH]nc(n1)c1ccoc1C	C13H8BrClFN3OS	-6.7	46.79	-17.286	-7.6
1038	Clc1cc(F)c(c(c1)Cl)Sc1[nH]nc(n1)c1ccoc1C	C13H8Cl2FN3OS	-6.6	48.78	-17.562	-8.2
1039	Fc1cc(F)c(c(c1)Cl)Sc1[nH]nc(n1)c1ccoc1C	C13H8ClF2N3OS	-6.9	48.94	-16.549	17.1
1040	Ic1cc(F)c(c(c1)Cl)Sc1[nH]nc(n1)c1ccoc1C	C13H8ClFIN3OS	-6.8	47.82	-16.94	-8.1
1041	Brc1cc(Cl)c(c(c1)I)Sc1[nH]nc(n1)c1ccoc1C	C13H8BrClIN3OS	-6.1	41.98	-16.056	9.9
1042	Clc1cc(Cl)c(c(c1)I)Sc1[nH]nc(n1)c1ccoc1C	C13H8Cl2IN3OS	-6.1	49.31	-16.447	8.0
1043	Fc1cc(Cl)c(c(c1)I)Sc1[nH]nc(n1)c1ccoc1C	C13H8ClFIN3OS	-6.4	43.62	-16.449	11.1
1044	Ic1cc(Cl)c(c(c1)I)Sc1[nH]nc(n1)c1ccoc1C	C13H8ClI2N3OS	-6.1	47.42	-15.825	9.4
1045	Ic1ccc(c(c1)Cl)Sc1[nH]nc(n1)c1ccoc1C	C13H9ClIN3OS	-6.1	44.55	-15.664	4.6
1046	Clc1ccc(cc1)Sc1[nH]nc(n1)c1ccoc1C	C13H10ClIN3OS	-6.3	52.07	-15.435	15.3
1047	Clc1ccc(c(c1)Br)Sc1[nH]nc(n1)c1ccoc1C	C13H9BrClIN3OS	-6.4	51.89	-15.422	13.1
1048	Clc1ccc(c(c1)I)Sc1[nH]nc(n1)c1ccoc1C	C13H9ClIN3OS	-6.2	44.35	-15.136	-26.4
1049	Fc1cccc(c1)Sc1[nH]nc(n1)c1ccoc1C	C13H10FN3OS	-7.4	50.14	-16.377	-8.5
1050	Fc1cc(Sc2[nH]nc(n2)c2ccoc2C)cc(c1)Br	C13H9BrFN3OS	-7.3	48.55	-17.151	-8.9
1051	Fc1cc(Sc2[nH]nc(n2)c2ccoc2C)cc(c1)Cl	C13H9ClFN3OS	-6.5	47.05	-17.303	-5.1

1052	Fc1cc(cc(c1)F)Sc1[nH]nc(n1)c1ccoc1C	C13H9F2N3OS	-7.1	53.43	-16.368	-3.0
1053	Fc1cc(Sc2[nH]nc(n2)c2ccoc2C)cc(c1)I	C13H9FIN3OS	-7.3	53.57	-16.547	-12.0
1054	Fc1cccc1Sc1[nH]nc(n1)c1ccoc1C	C13H10FN3OS	-7.4	50.94	-16.999	18.5
1055	Brc1ccc(c(c1)F)Sc1[nH]nc(n1)c1ccoc1C	C13H9BrFN3OS	-6.0	51.23	-15.989	20.5
1056	Clc1ccc(c(c1)F)Sc1[nH]nc(n1)c1ccoc1C	C13H9ClFN3OS	-6.5	51.08	-16.751	17.1
1057	Brc1cc(F)c(c(c1)F)Sc1[nH]nc(n1)c1ccoc1C	C13H8BrF2N3OS	-6.5	44.18	-16.432	11.2
1058	Clc1cc(F)c(c(c1)F)Sc1[nH]nc(n1)c1ccoc1C	C13H8ClF2N3OS	-6.3	43.34	-16.964	5.7
1059	Fc1cc(F)c(c(c1)F)Sc1[nH]nc(n1)c1ccoc1C	C13H8F3N3OS	-6.8	44.82	-16.353	-5.8
1060	lc1cc(F)c(c(c1)F)Sc1[nH]nc(n1)c1ccoc1C	C13H8F2IN3OS	-6.2	43.3	-15.697	6.4
1061	Fc1ccc(c(c1)F)Sc1[nH]nc(n1)c1ccoc1C	C13H9F2N3OS	-7.5	57.13	-18.138	17.9
1062	Brc1cc(F)c(c(c1)I)Sc1[nH]nc(n1)c1ccoc1C	C13H8BrFIN3OS	-6.0	44.91	-15.512	-4.0
1063	Clc1cc(F)c(c(c1)I)Sc1[nH]nc(n1)c1ccoc1C	C13H8ClFIN3OS	-6.5	45.28	-15.824	-3.1
1064	Fc1cc(F)c(c(c1)I)Sc1[nH]nc(n1)c1ccoc1C	C13H8F2IN3OS	-6.7	44.84	-16.187	-6.2
1065	lc1cc(F)c(c(c1)I)Sc1[nH]nc(n1)c1ccoc1C	C13H8FI2N3OS	-6.0	43.36	-15.165	3.2
1066	lc1ccc(c(c1)F)Sc1[nH]nc(n1)c1ccoc1C	C13H9FIN3OS	-7.2	46.11	-15.857	20.0
1067	Fc1ccc(cc1)Sc1[nH]nc(n1)c1ccoc1C	C13H10FN3OS	-6.7	52.47	-16.63	-6.1
1068	Fc1ccc(c(c1)Br)Sc1[nH]nc(n1)c1ccoc1C	C13H9BrFN3OS	-6.6	44.64	-15.639	-7.2
1069	Fc1ccc(c(c1)Cl)Sc1[nH]nc(n1)c1ccoc1C	C13H9ClFN3OS	-6.7	46.72	-15.883	16.0
1070	Fc1ccc(c(c1)I)Sc1[nH]nc(n1)c1ccoc1C	C13H9FIN3OS	-6.4	51.37	-15.947	-8.3
1071	Cc1occc1c1n[nH]c(n1)Sc1cccc1	C13H11N3OS	-6.7	54.19	-17.408	-1.0
1072	lc1cccc(c1)Sc1[nH]nc(n1)c1ccoc1C	C13H10IN3OS	-7.1	50.09	-16.335	5.3
1073	lc1cc(cc(c1)I)Sc1[nH]nc(n1)c1ccoc1C	C13H9I2N3OS	-6.3	47.83	-16.592	19.4
1074	lc1cccc1Sc1[nH]nc(n1)c1ccoc1C	C13H10IN3OS	-6.1	46.32	-17.268	14.2
1075	Brc1cc(I)c(c(c1)I)Sc1[nH]nc(n1)c1ccoc1C	C13H8BrI2N3OS	-5.7	42.96	-15.207	10.5
1076	Clc1cc(I)c(c(c1)I)Sc1[nH]nc(n1)c1ccoc1C	C13H8ClI2N3OS	-6.3	44.28	-15.439	10.9
1077	Fc1cc(I)c(c(c1)I)Sc1[nH]nc(n1)c1ccoc1C	C13H8FI2N3OS	-5.8	44.2	-15.611	12.0
1078	lc1cc(I)c(c(c1)I)Sc1[nH]nc(n1)c1ccoc1C	C13H8I3N3OS	-5.7	43.43	-14.984	10.1
1079	lc1ccc(c(c1)I)Sc1[nH]nc(n1)c1ccoc1C	C13H9I2N3OS	-6.8	45.9	-15.652	3.5
1080	lc1ccc(cc1)Sc1[nH]nc(n1)c1ccoc1C	C13H10IN3OS	-5.8	52.95	-14.709	17.1
1081	Cc1cccc(c1)Sc1[nH]nc(n1)c1ccoc1C	C14H13N3OS	-7.2	47.01	-16.136	8.4
1082	Cc1cccc1Sc1[nH]nc(n1)c1ccoc1C	C14H13N3OS	-6.3	47.66	-17.358	9.5

1083	Cc1ccc(cc1)Sc1[nH]nc(n1)c1ccoc1C	C14H13N3OS	-6.9	53.42	-16.799	-8.3
1084	O=N(=O)c1cccc(c1)Sc1[nH]nc(n1)c1ccoc1C	C13H10N4O3S	-7.7	48.71	-29.517	12.1
1085	Cc1occc1c1n[nH]c(n1)Sc1cccc1N(=O)=O	C13H10N4O3S	-6.8	49.36	-25.931	17.6
1086	O=N(=O)c1ccc(cc1)Sc1[nH]nc(n1)c1ccoc1C	C13H10N4O3S	-6.8	51.72	-22.282	42.7
1087	Oc1cccc(c1)Sc1[nH]nc(n1)c1ccoc1C	C13H11N3O2S	-7.4	51.86	-19.875	25.6
1088	Oc1ccccc1Sc1[nH]nc(n1)c1ccoc1C	C13H11N3O2S	-6.5	55.27	-20.073	-18.0
1089	Oc1ccc(cc1)Sc1[nH]nc(n1)c1ccoc1C	C13H11N3O2S	-6.7	48.51	-21.684	-24.2
1090	COc1cccc(c1)Sc1[nH]nc(n1)c1ccoc1C	C14H13N3O2S	-7.0	48.94	-22.129	12.1
1091	COc1ccccc1Sc1[nH]nc(n1)c1ccoc1C	C14H13N3O2S	-6.5	49.69	-24.818	4.3
1092	COc1ccc(cc1)Sc1[nH]nc(n1)c1ccoc1C	C14H13N3O2S	-6.7	54.12	-18.82	21.2
1093	Brc1cccc(c1)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H10BrN5S	-7.0	47.85	-20.582	3.9
1094	Brc1cc(cc(c1)Br)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H9Br2N5S	-6.6	45.02	-18.578	19.0
1095	Brc1cc(Sc2[nH]nc(n2)c2[nH]cnc2C)cc(c1)I	C12H9BrIN5S	-7.0	48.71	-17.644	-0.6
1096	Brc1ccccc1Sc1[nH]nc(n1)c1[nH]cnc1C	C12H10BrN5S	-7.2	45.95	-23.821	7.4
1097	Brc1cc(Br)c(c(c1)Br)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8Br3N5S	-6.8	44.68	-20.609	13.0
1098	Clc1cc(Br)c(c(c1)Br)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8Br2ClN5S	-6.8	44.75	-20.852	13.4
1099	Fc1cc(Br)c(c(c1)Br)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8Br2FN5S	-6.7	45.23	-20.551	-0.1
1100	Ic1cc(Br)c(c(c1)Br)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8Br2IN5S	-6.9	44.42	-20.104	22.3
1101	Brc1ccc(c(c1)Br)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H9Br2N5S	-6.0	46.87	-22.129	3.9
1102	Brc1cc(F)c(c(c1)Br)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8Br2FN5S	-6.8	44.61	-21.411	-3.7
1103	Clc1cc(F)c(c(c1)Br)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8BrClFN5S	-6.6	45.03	-21.053	-3.2
1104	Fc1cc(F)c(c(c1)Br)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8BrF2N5S	-7.0	45.61	-21.171	-2.5
1105	Ic1cc(F)c(c(c1)Br)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8BrFIN5S	-6.8	45.1	-21.328	-4.2
1106	Brc1cc(Br)c(c(c1)I)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8Br2IN5S	-6.8	44.78	-19.436	-0.8
1107	Clc1cc(Br)c(c(c1)I)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8BrClIN5S	-6.1	42.96	-19.49	-0.5
1108	Fc1cc(Br)c(c(c1)I)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8BrFIN5S	-6.8	40.04	-20.159	-0.3
1109	Ic1cc(Br)c(c(c1)I)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8BrI2N5S	-6.8	44.66	-19.574	-3.2
1110	Ic1ccc(c(c1)Br)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H9BrIN5S	-6.7	42.71	-20.933	-3.6
1111	Brc1ccc(cc1)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H10BrN5S	-6.8	52.25	-20.12	6.3
1112	Brc1ccc(c(c1)I)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H9BrIN5S	-6.6	44.08	-20.848	-3.6
1113	Clc1cccc(c1)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H10ClN5S	-6.2	47.7	-21.294	4.2

1114	Clc1cc(Sc2[nH]nc(n2)c2[nH]cnc2C)cc(c1)Br	C12H9BrClN5S	-7.0	46.73	-18.24	1.1
1115	Clc1cc(cc(c1)Cl)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H9Cl2N5S	-6.9	41.55	-18.311	2.9
1116	Clc1cc(Sc2[nH]nc(n2)c2[nH]cnc2C)cc(c1)I	C12H9ClIN5S	-6.4	42.95	-18.261	6.1
1117	Clc1cccc1Sc1[nH]nc(n1)c1[nH]cnc1C	C12H10ClN5S	-6.0	51.27	-22.923	7.4
1118	Brc1cc(Cl)c(c(c1)Br)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8Br2ClN5S	-6.9	48.6	-20.314	-2.0
1119	Clc1cc(Cl)c(c(c1)Br)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8BrCl2N5S	-6.8	42.6	-20.301	-1.6
1120	Fc1cc(Cl)c(c(c1)Br)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8BrClFN5S	-6.4	43.33	-22.789	8.4
1121	lc1cc(Cl)c(c(c1)Br)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8BrClIN5S	-6.9	44.21	-20.062	-1.8
1122	Brc1ccc(c(c1)Cl)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H9BrClN5S	-6.6	43.8	-20.404	-3.4
1123	Brc1cc(Cl)c(c(c1)Cl)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8BrCl2N5S	-7.5	43.43	-22.43	25.6
1124	Clc1cc(Cl)c(c(c1)Cl)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8Cl3N5S	-7.7	52.66	-22.95	10.1
1125	Fc1cc(Cl)c(c(c1)Cl)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8Cl2FN5S	-7.2	42.58	-21.525	-0.2
1126	lc1cc(Cl)c(c(c1)Cl)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8Cl2IN5S	-6.1	41.54	-20.955	-0.9
1127	Clc1ccc(c(c1)Cl)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H9Cl2N5S	-6.8	44.38	-20.461	-3.2
1128	Brc1cc(F)c(c(c1)Cl)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8BrClFN5S	-6.3	41.94	-21.03	-3.5
1129	Clc1cc(F)c(c(c1)Cl)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8Cl2FN5S	-6.9	47.8	-24.114	27.0
1130	Fc1cc(F)c(c(c1)Cl)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8ClF2N5S	-6.6	45.29	-21.322	-2.6
1131	lc1cc(F)c(c(c1)Cl)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8ClFIN5S	-6.9	44.55	-20.882	-3.6
1132	Brc1cc(Cl)c(c(c1)I)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8BrClIN5S	-6.8	44.12	-19.757	-2.1
1133	Clc1cc(Cl)c(c(c1)I)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8Cl2IN5S	-6.8	42.49	-19.908	-3.9
1134	Fc1cc(Cl)c(c(c1)I)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8ClFIN5S	-6.2	44.7	-22.038	7.6
1135	lc1cc(Cl)c(c(c1)I)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8ClI2N5S	-6.1	45.08	-20.06	12.9
1136	lc1ccc(c(c1)Cl)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H9ClIN5S	-6.2	42.02	-20.641	-2.5
1137	Clc1ccc(cc1)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H10ClN5S	-6.9	47.28	-20.446	6.9
1138	Clc1ccc(c(c1)Br)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H9BrClN5S	-6.6	44.43	-21.255	-2.2
1139	Clc1ccc(c(c1)I)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H9ClIN5S	-6.2	43.9	-21.57	4.2
1140	Fc1cccc(c1)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H10FN5S	-7.4	46.97	-21.754	5.2
1141	Fc1cc(Sc2[nH]nc(n2)c2[nH]cnc2C)cc(c1)Br	C12H9BrFN5S	-7.4	49.89	-18.842	14.8
1142	Fc1cc(Sc2[nH]nc(n2)c2[nH]cnc2C)cc(c1)Cl	C12H9ClFN5S	-7.3	50.06	-19.362	15.2
1143	Fc1cc(cc(c1)F)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H9F2N5S	-7.4	49.19	-20.753	18.8
1144	Fc1cc(Sc2[nH]nc(n2)c2[nH]cnc2C)cc(c1)I	C12H9FIN5S	-7.0	45	-18.62	6.4

1145	Fc1ccccc1Sc1[nH]nc(n1)c1[nH]cnc1C	C12H10FN5S	-7.5	46.71	-22.973	7.0
1146	Brc1ccc(c(c1)F)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H9BrFN5S	-7.1	45.27	-22.005	9.0
1147	Clc1ccc(c(c1)F)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H9ClFN5S	-7.0	46.22	-22.066	6.2
1148	Brc1cc(F)c(c(c1)F)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8BrF2N5S	-6.9	44.56	-20.961	-0.5
1149	Clc1cc(F)c(c(c1)F)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8ClF2N5S	-6.5	44.64	-21.002	-0.3
1150	Fc1cc(F)c(c(c1)F)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8F3N5S	-7.2	41.99	-21.14	0.0
1151	lc1cc(F)c(c(c1)F)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8F2IN5S	-6.2	43.38	-20.888	-1.1
1152	Fc1ccc(c(c1)F)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H9F2N5S	-7.6	59.04	-21.519	7.2
1153	Brc1cc(F)c(c(c1)I)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8BrFIN5S	-6.5	40.95	-21.357	-4.6
1154	Clc1cc(F)c(c(c1)I)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8ClFIN5S	-6.8	44.6	-21.373	-4.5
1155	Fc1cc(F)c(c(c1)I)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8F2IN5S	-6.8	43.51	-21.518	-3.9
1156	lc1cc(F)c(c(c1)I)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8FI2N5S	-6.2	45.2	-21.297	-5.2
1157	lc1ccc(c(c1)F)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H9FIN5S	-6.1	47.07	-21.336	16.2
1158	Fc1ccc(cc1)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H10FN5S	-7.2	51.26	-21.058	7.7
1159	Fc1ccc(c(c1)Br)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H9BrFN5S	-6.9	46.32	-20.72	-3.5
1160	Fc1ccc(c(c1)Cl)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H9ClFN5S	-6.5	47.1	-22.659	15.9
1161	Fc1ccc(c(c1)I)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H9FIN5S	-6.7	45.81	-20.922	-4.8
1162	Cc1nc[nH]c1c1n[nH]c(n1)Sc1ccccc1	C12H11N5S	-6.8	50.64	-22.489	15.5
1163	lc1cccc(c1)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H10IN5S	-6.8	48.09	-19.43	3.1
1164	lc1cc(cc(c1)I)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H9I2N5S	-6.6	44.45	-17.962	5.0
1165	lc1ccccc1Sc1[nH]nc(n1)c1[nH]cnc1C	C12H10IN5S	-6.5	44.79	-23.548	7.2
1166	Brc1cc(I)c(c(c1)I)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8BrI2N5S	-6.9	44.14	-20.561	15.6
1167	Clc1cc(I)c(c(c1)I)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8ClI2N5S	-6.9	43.67	-20.782	15.1
1168	Fc1cc(I)c(c(c1)I)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8FI2N5S	-6.0	45.59	-21.611	15.9
1169	lc1cc(I)c(c(c1)I)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H8I3N5S	-5.7	44.55	-20.724	-1.3
1170	lc1ccc(c(c1)I)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H9I2N5S	-6.0	44.28	-20.977	5.9
1171	lc1ccc(cc1)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H10IN5S	-6.9	46.51	-19.909	3.0
1172	Cc1cccc(c1)Sc1[nH]nc(n1)c1[nH]cnc1C	C13H13N5S	-7.3	44.77	-20.896	4.1
1173	Cc1ccccc1Sc1[nH]nc(n1)c1[nH]cnc1C	C13H13N5S	-6.9	48.05	-20.558	0.1
1174	Cc1ccc(cc1)Sc1[nH]nc(n1)c1[nH]cnc1C	C13H13N5S	-7.1	44.24	-20.692	6.5
1175	O=N(=O)c1cccc(c1)Sc1[nH]nc(n1)c1[nH]cnc1C	C12H10N6O2S	-7.8	48.31	-30.51	13.2

1176	<chem>O=N(=O)c1ccccc1Sc1[nH]nc(n1)c1[nH]cnc1C</chem>	C12H10N6O2S	-7.7	48.45	-28.122	0.2
1177	<chem>O=N(=O)c1ccc(cc1)Sc1[nH]nc(n1)c1[nH]cnc1C</chem>	C12H10N6O2S	-7.0	50.69	-24.876	22.2
1178	<chem>Oc1cccc(c1)Sc1[nH]nc(n1)c1[nH]cnc1C</chem>	C12H11N5OS	-7.1	50.25	-25.018	36.6
1179	<chem>Oc1ccccc1Sc1[nH]nc(n1)c1[nH]cnc1C</chem>	C12H11N5OS	-6.3	50.46	-24.539	1.8
1180	<chem>Oc1ccc(cc1)Sc1[nH]nc(n1)c1[nH]cnc1C</chem>	C12H11N5OS	-7.2	49.25	-24.707	20.9
1181	<chem>COc1cccc(c1)Sc1[nH]nc(n1)c1[nH]cnc1C</chem>	C13H13N5OS	-7.5	51	-25.182	-0.3
1182	<chem>COc1ccccc1Sc1[nH]nc(n1)c1[nH]cnc1C</chem>	C13H13N5OS	-6.4	49.54	-27.092	-5.4
1183	<chem>COc1ccc(cc1)Sc1[nH]nc(n1)c1[nH]cnc1C</chem>	C13H13N5OS	-6.8	48.32	-24.266	10.9
1184	<chem>Brc1cccc(c1)Sc1[nH]nc(n1)C1=NC(=S)N=N1</chem>	C10H5BrN6S2	-6.7	49.2	-19.995	28.5
1185	<chem>Brc1cc(cc(c1)Br)Sc1[nH]nc(n1)C1=NC(=S)N=N1</chem>	C10H4Br2N6S2	-7.0	44.05	-18.11	-1.7
1186	<chem>S=C1N=NC(=N1)c1n[nH]c(n1)Sc1cc(Br)cc(c1)I</chem>	C10H4BrIN6S2	-7.0	46.08	-18.223	7.1
1187	<chem>S=C1N=NC(=N1)c1n[nH]c(n1)Sc1ccccc1Br</chem>	C10H5BrN6S2	-6.6	44.3	-20.258	47.8
1188	<chem>Brc1cc(Br)c(c(c1)Br)Sc1[nH]nc(n1)C1=NC(=S)N=N1</chem>	C10H3Br3N6S2	-6.7	41.79	-17.432	-13.9
1189	<chem>Clc1cc(Br)c(c(c1)Br)Sc1[nH]nc(n1)C1=NC(=S)N=N1</chem>	C10H3Br2ClN6S2	-6.6	35.82	-16.781	-12.3
1190	<chem>Fc1cc(Br)c(c(c1)Br)Sc1[nH]nc(n1)C1=NC(=S)N=N1</chem>	C10H3Br2FN6S2	-6.6	41.28	-18.265	-12.6
1191	<chem>Ic1cc(Br)c(c(c1)Br)Sc1[nH]nc(n1)C1=NC(=S)N=N1</chem>	C10H3Br2IN6S2	-6.7	41.82	-17.1	-13.4
1192	<chem>Brc1ccc(c(c1)Br)Sc1[nH]nc(n1)C1=NC(=S)N=N1</chem>	C10H4Br2N6S2	-6.5	40.33	-18.834	-2.9
1193	<chem>S=C1N=NC(=N1)c1n[nH]c(n1)Sc1c(F)cc(cc1Br)Br</chem>	C10H3Br2FN6S2	-6.7	44.11	-19.004	11.6
1194	<chem>S=C1N=NC(=N1)c1n[nH]c(n1)Sc1c(F)cc(cc1Br)Cl</chem>	C10H3BrClFN6S2	-6.8	42.33	-20.515	41.8
1195	<chem>S=C1N=NC(=N1)c1n[nH]c(n1)Sc1c(F)cc(cc1Br)F</chem>	C10H3BrF2N6S2	-6.8	49.58	-19.197	12.5
1196	<chem>S=C1N=NC(=N1)c1n[nH]c(n1)Sc1c(F)cc(cc1Br)I</chem>	C10H3BrFIN6S2	-6.7	43.24	-21.036	37.8
1197	<chem>S=C1N=NC(=N1)c1n[nH]c(n1)Sc1c(Br)cc(cc1I)Br</chem>	C10H3Br2IN6S2	-6.7	42.94	-17.957	-4.5
1198	<chem>S=C1N=NC(=N1)c1n[nH]c(n1)Sc1c(Br)cc(cc1I)Cl</chem>	C10H3BrClIN6S2	-6.6	41.65	-17.476	-13.3
1199	<chem>S=C1N=NC(=N1)c1n[nH]c(n1)Sc1c(Br)cc(cc1I)F</chem>	C10H3BrFIN6S2	-6.3	49.27	-17.984	-12.5
1200	<chem>S=C1N=NC(=N1)c1n[nH]c(n1)Sc1c(Br)cc(cc1I)I</chem>	C10H3BrI2N6S2	-6.7	42.11	-16.828	-13.0
1201	<chem>Ic1ccc(c(c1)Br)Sc1[nH]nc(n1)C1=NC(=S)N=N1</chem>	C10H4BrIN6S2	-6.6	43.99	-18.914	-5.3
1202	<chem>Brc1ccc(cc1)Sc1[nH]nc(n1)C1=NC(=S)N=N1</chem>	C10H5BrN6S2	-7.0	46.55	-21.656	57.7
1203	<chem>Brc1ccc(c(c1)I)Sc1[nH]nc(n1)C1=NC(=S)N=N1</chem>	C10H4BrIN6S2	-6.5	41.41	-18.984	40.5
1204	<chem>Clc1cccc(c1)Sc1[nH]nc(n1)C1=NC(=S)N=N1</chem>	C10H5ClN6S2	-6.7	42.16	-20.367	28.9
1205	<chem>S=C1N=NC(=N1)c1n[nH]c(n1)Sc1cc(Cl)cc(c1)Br</chem>	C10H4BrClN6S2	-7.0	44.98	-18.945	7.7
1206	<chem>Clc1cc(cc(c1)Cl)Sc1[nH]nc(n1)C1=NC(=S)N=N1</chem>	C10H4Cl2N6S2	-6.9	40.88	-18.875	8.7

1207	<chem>S=C1N=NC(=N1)c1n[nH]c(n1)Sc1cc(Cl)cc(c1)I</chem>	C10H4ClIN6S2	-7.0	47.79	-18.884	7.3
1208	<chem>S=C1N=NC(=N1)c1n[nH]c(n1)Sc1cccc1Cl</chem>	C10H5ClN6S2	-6.6	48.03	-21.331	17.5
1209	<chem>S=C1N=NC(=N1)c1n[nH]c(n1)Sc1c(Cl)cc(cc1Br)Br</chem>	C10H3Br2ClN6S2	-6.7	44.46	-18.373	-14.6
1210	<chem>S=C1N=NC(=N1)c1n[nH]c(n1)Sc1c(Cl)cc(cc1Br)Cl</chem>	C10H3BrCl2N6S2	-6.6	44.11	-18.01	-13.3
1211	<chem>S=C1N=NC(=N1)c1n[nH]c(n1)Sc1c(Cl)cc(cc1Br)F</chem>	C10H3BrClFN6S2	-6.8	41.39	-18.481	-4.3
1212	<chem>S=C1N=NC(=N1)c1n[nH]c(n1)Sc1c(Cl)cc(cc1Br)I</chem>	C10H3BrClIN6S2	-6.7	43.99	-18.351	22.2
1213	<chem>Brc1ccc(c(c1)Cl)Sc1[nH]nc(n1)C1=NC(=S)N=N1</chem>	C10H4BrClN6S2	-6.5	42.86	-18.979	13.2
1214	<chem>Brc1cc(Cl)c(c(c1)Cl)Sc1[nH]nc(n1)C1=NC(=S)N=N1</chem>	C10H3BrCl2N6S2	-6.8	44.47	-17.568	11.5
1215	<chem>Clc1cc(Cl)c(c(c1)Cl)Sc1[nH]nc(n1)C1=NC(=S)N=N1</chem>	C10H3Cl3N6S2	-6.9	48.98	-18.788	26.0
1216	<chem>Fc1cc(Cl)c(c(c1)Cl)Sc1[nH]nc(n1)C1=NC(=S)N=N1</chem>	C10H3Cl2FN6S2	-6.9	44.39	-20.391	27.1
1217	<chem>lc1cc(Cl)c(c(c1)Cl)Sc1[nH]nc(n1)C1=NC(=S)N=N1</chem>	C10H3Cl2IN6S2	-6.6	47.89	-17.814	-14.3
1218	<chem>Clc1ccc(c(c1)Cl)Sc1[nH]nc(n1)C1=NC(=S)N=N1</chem>	C10H4Cl2N6S2	-6.5	39.14	-19.364	4.1
1219	<chem>S=C1N=NC(=N1)c1n[nH]c(n1)Sc1c(F)cc(cc1Cl)Br</chem>	C10H3BrClFN6S2	-6.9	48.17	-20.555	38.6
1220	<chem>S=C1N=NC(=N1)c1n[nH]c(n1)Sc1c(F)cc(cc1Cl)Cl</chem>	C10H3Cl2FN6S2	-6.8	40.25	-20.452	39.3
1221	<chem>S=C1N=NC(=N1)c1n[nH]c(n1)Sc1c(F)cc(cc1Cl)F</chem>	C10H3ClF2N6S2	-6.9	45.62	-19.757	12.6
1222	<chem>S=C1N=NC(=N1)c1n[nH]c(n1)Sc1c(F)cc(cc1Cl)I</chem>	C10H3ClFIN6S2	-6.8	43.01	-20.255	40.7
1223	<chem>S=C1N=NC(=N1)c1n[nH]c(n1)Sc1c(Cl)cc(cc1I)Br</chem>	C10H3BrClIN6S2	-6.7	49.73	-17.545	-12.9
1224	<chem>S=C1N=NC(=N1)c1n[nH]c(n1)Sc1c(Cl)cc(cc1I)Cl</chem>	C10H3Cl2IN6S2	-6.7	49.21	-17.863	-9.5
1225	<chem>S=C1N=NC(=N1)c1n[nH]c(n1)Sc1c(Cl)cc(cc1I)F</chem>	C10H3ClFIN6S2	-6.6	41.43	-18.366	-12.6
1226	<chem>S=C1N=NC(=N1)c1n[nH]c(n1)Sc1c(Cl)cc(cc1I)I</chem>	C10H3ClI2N6S2	-6.7	42.77	-17.263	-13.7
1227	<chem>lc1ccc(c(c1)Cl)Sc1[nH]nc(n1)C1=NC(=S)N=N1</chem>	C10H4ClIN6S2	-6.5	41.29	-19.027	-0.1
1228	<chem>Clc1ccc(cc1)Sc1[nH]nc(n1)C1=NC(=S)N=N1</chem>	C10H5ClN6S2	-6.8	51.14	-21.699	57.8
1229	<chem>Clc1ccc(c(c1)Br)Sc1[nH]nc(n1)C1=NC(=S)N=N1</chem>	C10H4BrClN6S2	-6.5	44.78	-18.792	-4.9
1230	<chem>Clc1ccc(c(c1)I)Sc1[nH]nc(n1)C1=NC(=S)N=N1</chem>	C10H4ClIN6S2	-6.4	46.77	-18.796	-4.3
1231	<chem>Fc1cccc(c1)Sc1[nH]nc(n1)C1=NC(=S)N=N1</chem>	C10H5FN6S2	-6.8	44.98	-20.971	29.9
1232	<chem>S=C1N=NC(=N1)c1n[nH]c(n1)Sc1cc(F)cc(c1)Br</chem>	C10H4BrFN6S2	-6.9	47.67	-20.062	6.0
1233	<chem>S=C1N=NC(=N1)c1n[nH]c(n1)Sc1cc(F)cc(c1)Cl</chem>	C10H4ClFN6S2	-6.9	50.21	-19.815	9.4
1234	<chem>Fc1cc(cc(c1)F)Sc1[nH]nc(n1)C1=NC(=S)N=N1</chem>	C10H4F2N6S2	-6.6	46.73	-20.615	13.8
1235	<chem>S=C1N=NC(=N1)c1n[nH]c(n1)Sc1cc(F)cc(c1)I</chem>	C10H4FIN6S2	-6.8	44.67	-19.373	13.8
1236	<chem>S=C1N=NC(=N1)c1n[nH]c(n1)Sc1cccc1F</chem>	C10H5FN6S2	-6.6	45.35	-21.013	16.4
1237	<chem>Brc1ccc(c(c1)F)Sc1[nH]nc(n1)C1=NC(=S)N=N1</chem>	C10H4BrFN6S2	-7.1	45.74	-20.832	8.7

1238	Clc1ccc(c(c1)F)Sc1[nH]nc(n1)C1=NC(=S)N=N1	C10H4CIFN6S2	-7.3	54.05	-20.41	5.4
1239	Brcc1cc(F)c(c(c1)F)Sc1[nH]nc(n1)C1=NC(=S)N=N1	C10H3BrF2N6S2	-6.7	41.64	-20.71	35.5
1240	Clc1cc(F)c(c(c1)F)Sc1[nH]nc(n1)C1=NC(=S)N=N1	C10H3CIF2N6S2	-6.9	39.06	-20.951	35.6
1241	Fc1cc(F)c(c(c1)F)Sc1[nH]nc(n1)C1=NC(=S)N=N1	C10H3F3N6S2	-6.9	41.52	-21.259	36.4
1242	lc1cc(F)c(c(c1)F)Sc1[nH]nc(n1)C1=NC(=S)N=N1	C10H3F2IN6S2	-6.8	44.91	-21.426	22.3
1243	Fc1ccc(c(c1)F)Sc1[nH]nc(n1)C1=NC(=S)N=N1	C10H4F2N6S2	-7.1	52.04	-20.857	15.1
1244	S=C1N=NC(=N1)c1n[nH]c(n1)Sc1c(F)cc(cc1I)Br	C10H3BrFIN6S2	-6.7	40.59	-18.874	-0.3
1245	S=C1N=NC(=N1)c1n[nH]c(n1)Sc1c(F)cc(cc1I)Cl	C10H3CIFIN6S2	-6.7	43.82	-18.595	-7.6
1246	S=C1N=NC(=N1)c1n[nH]c(n1)Sc1c(F)cc(cc1I)F	C10H3F2IN6S2	-6.7	43.17	-18.501	-10.2
1247	S=C1N=NC(=N1)c1n[nH]c(n1)Sc1c(F)cc(cc1I)I	C10H3FI2N6S2	-6.7	40.32	-21.514	38.7
1248	lc1ccc(c(c1)F)Sc1[nH]nc(n1)C1=NC(=S)N=N1	C10H4FIN6S2	-6.6	47.42	-20.685	9.3
1249	Fc1ccc(cc1)Sc1[nH]nc(n1)C1=NC(=S)N=N1	C10H5FN6S2	-6.7	47.45	-21.013	26.9
1250	Fc1ccc(c(c1)Br)Sc1[nH]nc(n1)C1=NC(=S)N=N1	C10H4BrFN6S2	-6.7	41.91	-20.281	4.9
1251	Fc1ccc(c(c1)Cl)Sc1[nH]nc(n1)C1=NC(=S)N=N1	C10H4CIFN6S2	-6.8	42.82	-20.26	12.5
1252	Fc1ccc(c(c1)I)Sc1[nH]nc(n1)C1=NC(=S)N=N1	C10H4FIN6S2	-6.5	42.28	-19.693	2.8
1253	S=C1N=NC(=N1)c1n[nH]c(n1)Sc1cccc1	C10H6N6S2	-6.4	46.28	-20.389	13.0
1254	lc1cccc(c1)Sc1[nH]nc(n1)C1=NC(=S)N=N1	C10H5IN6S2	-6.7	44.67	-19.145	27.9
1255	lc1cc(cc(c1)I)Sc1[nH]nc(n1)C1=NC(=S)N=N1	C10H4I2N6S2	-7.1	43.67	-16.917	-0.8
1256	S=C1N=NC(=N1)c1n[nH]c(n1)Sc1cccc1I	C10H5IN6S2	-6.5	49.66	-20.15	47.3
1257	Brcc1cc(I)c(c(c1)I)Sc1[nH]nc(n1)C1=NC(=S)N=N1	C10H3BrI2N6S2	-6.7	43.45	-16.825	-8.9
1258	Clc1cc(I)c(c(c1)I)Sc1[nH]nc(n1)C1=NC(=S)N=N1	C10H3ClI2N6S2	-6.6	45.24	-18.677	-10.6
1259	Fc1cc(I)c(c(c1)I)Sc1[nH]nc(n1)C1=NC(=S)N=N1	C10H3FI2N6S2	-6.6	49.8	-17.654	-11.6
1260	lc1cc(I)c(c(c1)I)Sc1[nH]nc(n1)C1=NC(=S)N=N1	C10H3I3N6S2	-6.7	42.96	-17.939	-11.5
1261	lc1ccc(c(c1)I)Sc1[nH]nc(n1)C1=NC(=S)N=N1	C10H4I2N6S2	-6.5	40.15	-19.114	40.1
1262	lc1ccc(cc1)Sc1[nH]nc(n1)C1=NC(=S)N=N1	C10H5IN6S2	-6.4	51.31	-21.617	57.4
1263	Cc1cccc(c1)Sc1[nH]nc(n1)C1=NC(=S)N=N1	C11H8N6S2	-6.7	49.52	-20.752	9.6
1264	S=C1N=NC(=N1)c1n[nH]c(n1)Sc1cccc1C	C11H8N6S2	-6.6	47.56	-20.35	33.0
1265	Cc1ccc(cc1)Sc1[nH]nc(n1)C1=NC(=S)N=N1	C11H8N6S2	-6.7	49.36	-21.552	16.3
1266	S=C1N=NC(=N1)c1n[nH]c(n1)Sc1cccc(c1)N(=O)=O	C10H5N7O2S2	-7.0	52.97	-30.862	19.6
1267	S=C1N=NC(=N1)c1n[nH]c(n1)Sc1cccc1N(=O)=O	C10H5N7O2S2	-7.1	54.66	-28.155	-10.7
1268	S=C1N=NC(=N1)c1n[nH]c(n1)Sc1ccc(cc1)N(=O)=O	C10H5N7O2S2	-7.0	47.51	-25.406	18.1

1269	Oc1cccc(c1)Sc1[nH]nc(n1)C1=NC(=S)N=N1	C10H6N6OS2	-6.8	46.33	-24.224	39.1
1270	S=C1N=NC(=N1)c1n[nH]c(n1)Sc1cccc1O	C10H6N6OS2	-6.8	46.34	-24.678	20.0
1271	Oc1ccc(cc1)Sc1[nH]nc(n1)C1=NC(=S)N=N1	C10H6N6OS2	-6.7	47.5	-26.093	14.9
1272	COc1cccc(c1)Sc1[nH]nc(n1)C1=NC(=S)N=N1	C11H8N6OS2	-6.6	46.95	-23.941	26.6
1273	COc1cccc1Sc1[nH]nc(n1)C1=NC(=S)N=N1	C11H8N6OS2	-6.6	40.13	-26.428	16.2
1274	COc1ccc(cc1)Sc1[nH]nc(n1)C1=NC(=S)N=N1	C11H8N6OS2	-6.3	47.58	-24.337	27.3
1275	Brc1cccc(c1)Sc1[nH]nc(n1)c1ccc[nH]1	C12H9BrN4S	-6.2	46.22	-20.831	4.0
1276	Brc1cc(cc(c1)Br)Sc1[nH]nc(n1)c1ccc[nH]1	C12H8Br2N4S	-6.7	47.32	-20.837	23.1
1277	Brc1cc(Sc2[nH]nc(n2)c2[nH]ccc2)cc(c1)I	C12H8BrIN4S	-6.7	45.58	-21.758	18.9
1278	Brc1cccc1Sc1[nH]nc(n1)c1[nH]ccc1	C12H9BrN4S	-6.6	46.06	-23.289	9.3
1279	Brc1cc(Br)c(c(c1)Br)Sc1[nH]nc(n1)c1ccc[nH]1	C12H7Br3N4S	-6.4	43.06	-20.34	-5.9
1280	Clc1cc(Br)c(c(c1)Br)Sc1[nH]nc(n1)c1ccc[nH]1	C12H7Br2ClN4S	-6.5	44.72	-22.155	2.8
1281	Fc1cc(Br)c(c(c1)Br)Sc1[nH]nc(n1)c1ccc[nH]1	C12H7Br2FN4S	-6.5	43.05	-22.648	4.3
1282	Ic1cc(Br)c(c(c1)Br)Sc1[nH]nc(n1)c1ccc[nH]1	C12H7Br2IN4S	-6.5	41.07	-20.238	-6.3
1283	Brc1ccc(c(c1)Br)Sc1[nH]nc(n1)c1ccc[nH]1	C12H8Br2N4S	-6.2	48.05	-20.03	9.6
1284	Brc1cc(F)c(c(c1)Br)Sc1[nH]nc(n1)c1[nH]ccc1	C12H7Br2FN4S	-6.4	41.25	-21.193	-7.5
1285	Clc1cc(F)c(c(c1)Br)Sc1[nH]nc(n1)c1[nH]ccc1	C12H7BrClFN4S	-6.5	42.77	-21.231	-7.2
1286	Fc1cc(F)c(c(c1)Br)Sc1[nH]nc(n1)c1[nH]ccc1	C12H7BrF2N4S	-6.5	43.08	-21.457	-6.9
1287	Fc1cc(F)c(c(c1)F)Sc1[nH]nc(n1)c1ccc[nH]1	C12H7F3N4S	-6.7	48.53	-21.836	5.1
1288	Brc1cc(Br)c(c(c1)I)Sc1[nH]nc(n1)c1[nH]ccc1	C12H7Br2IN4S	-6.5	43.4	-20.437	-7.1
1289	Clc1cc(Br)c(c(c1)I)Sc1[nH]nc(n1)c1[nH]ccc1	C12H7BrClIN4S	-6.4	43.84	-20.99	27.3
1290	Fc1cc(Br)c(c(c1)I)Sc1[nH]nc(n1)c1[nH]ccc1	C12H7BrFIN4S	-6.5	42.82	-20.606	-6.4
1291	Ic1cc(Br)c(c(c1)I)Sc1[nH]nc(n1)c1[nH]ccc1	C12H7BrI2N4S	-6.5	40.39	-22.021	2.8
1292	Ic1ccc(c(c1)Br)Sc1[nH]nc(n1)c1ccc[nH]1	C12H8BrIN4S	-6.2	47.58	-19.563	-6.4
1293	Brc1ccc(cc1)Sc1[nH]nc(n1)c1ccc[nH]1	C12H9BrN4S	-6.2	50.98	-20.664	-17.8
1294	Brc1ccc(c(c1)I)Sc1[nH]nc(n1)c1ccc[nH]1	C12H8BrIN4S	-6.3	47.78	-19.418	-20.1
1295	Clc1cccc(c1)Sc1[nH]nc(n1)c1ccc[nH]1	C12H9ClN4S	-6.3	45.56	-21.06	4.5
1296	Clc1cc(Sc2[nH]nc(n2)c2[nH]ccc2)cc(c1)Br	C12H8BrClN4S	-6.8	51.07	-20.874	23.2
1297	Clc1cc(cc(c1)Cl)Sc1[nH]nc(n1)c1ccc[nH]1	C12H8Cl2N4S	-6.7	50.39	-20.367	23.1
1298	Clc1cc(Sc2[nH]nc(n2)c2[nH]ccc2)cc(c1)I	C12H8ClIN4S	-6.8	47.52	-22.288	17.4
1299	Clc1cccc1Sc1[nH]nc(n1)c1[nH]ccc1	C12H9ClN4S	-6.6	49.08	-23.486	9.3

1300	Brc1cc(Cl)c(c(c1)Br)Sc1[nH]nc(n1)c1[nH]ccc1	C12H7Br2ClN4S	-6.4	42.48	-22.19	10.9
1301	Clc1cc(Cl)c(c(c1)Br)Sc1[nH]nc(n1)c1[nH]ccc1	C12H7BrCl2N4S	-6.5	42.23	-20.891	7.1
1302	Fc1cc(Cl)c(c(c1)Br)Sc1[nH]nc(n1)c1[nH]ccc1	C12H7BrClFN4S	-6.5	42.72	-20.728	-6.1
1303	lc1cc(Cl)c(c(c1)Br)Sc1[nH]nc(n1)c1[nH]ccc1	C12H7BrClIN4S	-6.5	41.82	-20.863	7.2
1304	Brc1ccc(c(c1)Cl)Sc1[nH]nc(n1)c1ccc[nH]1	C12H8BrClN4S	-6.2	47.41	-21.17	11.4
1305	Brc1cc(Cl)c(c(c1)Cl)Sc1[nH]nc(n1)c1ccc[nH]1	C12H7BrCl2N4S	-6.6	42.7	-21.185	10.6
1306	Clc1cc(Cl)c(c(c1)Cl)Sc1[nH]nc(n1)c1ccc[nH]1	C12H7Cl3N4S	-7.1	48.15	-20.87	-13.7
1307	Fc1cc(Cl)c(c(c1)Cl)Sc1[nH]nc(n1)c1ccc[nH]1	C12H7Cl2FN4S	-6.8	46.83	-21.847	-3.4
1308	lc1cc(Cl)c(c(c1)Cl)Sc1[nH]nc(n1)c1ccc[nH]1	C12H7Cl2IN4S	-6.4	42.95	-20.682	10.6
1309	Clc1ccc(c(c1)Cl)Sc1[nH]nc(n1)c1ccc[nH]1	C12H8Cl2N4S	-6.4	48.31	-20.328	23.0
1310	Brc1cc(F)c(c(c1)Cl)Sc1[nH]nc(n1)c1[nH]ccc1	C12H7BrClFN4S	-6.5	43.2	-21.18	-6.5
1311	Clc1cc(F)c(c(c1)Cl)Sc1[nH]nc(n1)c1[nH]ccc1	C12H7Cl2FN4S	-6.5	43.41	-21.092	20.2
1312	Fc1cc(F)c(c(c1)Cl)Sc1[nH]nc(n1)c1[nH]ccc1	C12H7ClF2N4S	-6.6	46	-21.876	25.6
1313	lc1cc(F)c(c(c1)Cl)Sc1[nH]nc(n1)c1[nH]ccc1	C12H7ClFIN4S	-6.5	43.85	-21.022	-7.3
1314	Brc1cc(Cl)c(c(c1)I)Sc1[nH]nc(n1)c1[nH]ccc1	C12H7BrClIN4S	-6.4	41.84	-20.711	-8.1
1315	Clc1cc(Cl)c(c(c1)I)Sc1[nH]nc(n1)c1[nH]ccc1	C12H7Cl2IN4S	-6.4	44.83	-20.797	-7.8
1316	Fc1cc(Cl)c(c(c1)I)Sc1[nH]nc(n1)c1[nH]ccc1	C12H7ClFIN4S	-6.5	42.84	-20.891	-7.3
1317	lc1cc(Cl)c(c(c1)I)Sc1[nH]nc(n1)c1[nH]ccc1	C12H7ClI2N4S	-6.5	45.57	-20.616	-8.6
1318	lc1ccc(c(c1)Cl)Sc1[nH]nc(n1)c1ccc[nH]1	C12H8ClIN4S	-6.3	43.36	-19.915	-6.7
1319	Clc1ccc(cc1)Sc1[nH]nc(n1)c1ccc[nH]1	C12H9ClN4S	-6.3	52.03	-21.018	22.1
1320	Clc1ccc(c(c1)Br)Sc1[nH]nc(n1)c1ccc[nH]1	C12H8BrClN4S	-6.7	46.32	-20.619	8.3
1321	Clc1ccc(c(c1)I)Sc1[nH]nc(n1)c1ccc[nH]1	C12H8ClIN4S	-6.2	44.65	-18.743	3.5
1322	Fc1cccc(c1)Sc1[nH]nc(n1)c1ccc[nH]1	C12H9FN4S	-6.7	46.58	-21.934	9.8
1323	Fc1cc(Sc2[nH]nc(n2)c2[nH]ccc2)cc(c1)Br	C12H8BrFN4S	-6.6	49.37	-22.757	19.2
1324	Fc1cc(Sc2[nH]nc(n2)c2[nH]ccc2)cc(c1)Cl	C12H8ClFN4S	-6.7	49.55	-22.812	19.9
1325	Fc1cc(cc(c1)F)Sc1[nH]nc(n1)c1ccc[nH]1	C12H8F2N4S	-6.6	47.24	-21.965	22.8
1326	Fc1cc(Sc2[nH]nc(n2)c2[nH]ccc2)cc(c1)I	C12H8FIN4S	-6.7	48.27	-22.973	18.8
1327	Fc1ccccc1Sc1[nH]nc(n1)c1[nH]ccc1	C12H9FN4S	-6.8	49.64	-23.129	7.7
1328	Brc1ccc(c(c1)F)Sc1[nH]nc(n1)c1ccc[nH]1	C12H8BrFN4S	-6.3	48.97	-20.405	11.0
1329	Clc1ccc(c(c1)F)Sc1[nH]nc(n1)c1ccc[nH]1	C12H8ClFN4S	-6.4	48.72	-21.514	31.2
1330	Brc1cc(F)c(c(c1)F)Sc1[nH]nc(n1)c1ccc[nH]1	C12H7BrF2N4S	-6.4	41.83	-21.082	22.1

1331	Clc1cc(F)c(c(c1)F)Sc1[nH]nc(n1)c1ccc[nH]1	C12H7ClF2N4S	-6.6	44.4	-23.601	28.0
1332	Fc1cc(F)c(c(c1)F)Sc1[nH]nc(n1)c1ccc[nH]1	C12H7F3N4S	-6.7	43.35	-21.836	5.1
1333	lc1cc(F)c(c(c1)F)Sc1[nH]nc(n1)c1ccc[nH]1	C12H7F2IN4S	-6.4	42.28	-20.827	22.0
1334	Fc1ccc(c(c1)F)Sc1[nH]nc(n1)c1ccc[nH]1	C12H8F2N4S	-6.6	48.98	-22.364	19.6
1335	Brc1cc(F)c(c(c1)I)Sc1[nH]nc(n1)c1[nH]ccc1	C12H7BrFIN4S	-6.4	46.72	-21.972	20.3
1336	Clc1cc(F)c(c(c1)I)Sc1[nH]nc(n1)c1[nH]ccc1	C12H7ClFIN4S	-6.3	44.69	-20.262	18.4
1337	Fc1cc(F)c(c(c1)I)Sc1[nH]nc(n1)c1[nH]ccc1	C12H7F2IN4S	-6.4	43.88	-20.062	19.7
1338	lc1cc(F)c(c(c1)I)Sc1[nH]nc(n1)c1[nH]ccc1	C12H7FI2N4S	-6.5	44.73	-20.111	18.1
1339	lc1ccc(c(c1)F)Sc1[nH]nc(n1)c1ccc[nH]1	C12H8FIN4S	-6.3	49.11	-20.264	10.7
1340	Fc1ccc(cc1)Sc1[nH]nc(n1)c1ccc[nH]1	C12H9FN4S	-6.3	50.83	-21.66	24.2
1341	Fc1ccc(c(c1)Br)Sc1[nH]nc(n1)c1ccc[nH]1	C12H8BrFN4S	-6.4	48.13	-21.076	-6.8
1342	Fc1ccc(c(c1)Cl)Sc1[nH]nc(n1)c1ccc[nH]1	C12H8ClFN4S	-6.5	53.48	-21.107	21.8
1343	Fc1ccc(c(c1)I)Sc1[nH]nc(n1)c1ccc[nH]1	C12H8FIN4S	-6.4	41.76	-21.158	-7.4
1344	c1ccc(cc1)Sc1[nH]nc(n1)c1ccc[nH]1	C12H10N4S	-6.6	46.41	-21.975	9.5
1345	lc1cccc(c1)Sc1[nH]nc(n1)c1ccc[nH]1	C12H9IN4S	-6.5	45.22	-20.202	-17.5
1346	lc1cc(cc(c1)I)Sc1[nH]nc(n1)c1ccc[nH]1	C12H8I2N4S	-6.6	44.39	-21.093	22.2
1347	lc1ccccc1Sc1[nH]nc(n1)c1[nH]ccc1	C12H9IN4S	-6.3	46.37	-19.552	-5.8
1348	Brc1cc(I)c(c(c1)I)Sc1[nH]nc(n1)c1ccc[nH]1	C12H7BrI2N4S	-6.5	43.13	-21.532	-0.9
1349	Clc1cc(I)c(c(c1)I)Sc1[nH]nc(n1)c1ccc[nH]1	C12H7ClI2N4S	-6.4	43.56	-21.62	-0.6
1350	Fc1cc(I)c(c(c1)I)Sc1[nH]nc(n1)c1ccc[nH]1	C12H7FI2N4S	-6.3	43.69	-21.555	0.4
1351	lc1cc(I)c(c(c1)I)Sc1[nH]nc(n1)c1ccc[nH]1	C12H7I3N4S	-6.6	43.38	-21.183	-1.5
1352	lc1ccc(c(c1)I)Sc1[nH]nc(n1)c1ccc[nH]1	C12H8I2N4S	-6.3	43.75	-19.512	0.4
1353	lc1ccc(cc1)Sc1[nH]nc(n1)c1ccc[nH]1	C12H9IN4S	-6.1	48.81	-20.337	-20.0
1354	Cc1cccc(c1)Sc1[nH]nc(n1)c1ccc[nH]1	C13H12N4S	-6.5	46.59	-20.999	4.6
1355	Cc1ccccc1Sc1[nH]nc(n1)c1[nH]ccc1	C13H12N4S	-6.3	49.8	-23.563	6.3
1356	Cc1ccc(cc1)Sc1[nH]nc(n1)c1ccc[nH]1	C13H12N4S	-6.3	51.57	-21.075	15.9
1357	O=N(=O)c1cccc(c1)Sc1[nH]nc(n1)c1ccc[nH]1	C12H9N5O2S	-7.5	49.46	-30.888	10.9
1358	O=N(=O)c1ccccc1Sc1[nH]nc(n1)c1[nH]ccc1	C12H9N5O2S	-6.9	54.19	-29.335	-11.5
1359	O=N(=O)c1ccc(cc1)Sc1[nH]nc(n1)c1ccc[nH]1	C12H9N5O2S	-6.7	50.7	-26.321	12.4
1360	Oc1cccc(c1)Sc1[nH]nc(n1)c1ccc[nH]1	C12H10N4OS	-6.8	48.23	-24.388	41.7
1361	Oc1ccccc1Sc1[nH]nc(n1)c1[nH]ccc1	C12H10N4OS	-7.1	50.93	-24.209	5.7

1362	<chem>Oc1ccc(cc1)Sc1[nH]nc(n1)c1ccc[nH]1</chem>	C12H10N4OS	-6.9	49.24	-27.441	8.1
1363	<chem>COC1cccc(c1)Sc1[nH]nc(n1)c1ccc[nH]1</chem>	C13H12N4OS	-6.9	50.66	-27.67	19.1
1364	<chem>COC1cccccc1Sc1[nH]nc(n1)c1[nH]ccc1</chem>	C13H12N4OS	-6.8	49.04	-29.368	3.7
1365	<chem>COC1ccc(cc1)Sc1[nH]nc(n1)c1ccc[nH]1</chem>	C13H12N4OS	-6.2	50.39	-23.79	25.6
1366	<chem>COC1ccc(cc1)Nc1nnc(s1)c1ccc[nH]1</chem>	C13H12N4OS	-7.2	51.19	-26.9	21.7
1367	<chem>Oc1ccc(cc1)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H10N4OS	-7.1	52.72	-26.65	-10.0
1368	<chem>[O-][N](=O)c1ccc(cc1)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H9N5O2S	-7.6	54.11	-31.633	25.8
1369	<chem>Cc1ccc(cc1)Nc1nnc(s1)c1ccc[nH]1</chem>	C13H12N4S	-6.9	48.62	-26.802	26.7
1370	<chem>lc1ccc(cc1)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H9IN4S	-6.3	50.59	-25.247	10.0
1371	<chem>Fc1ccc(cc1)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H9FN4S	-6.9	50.38	-27.313	30.0
1372	<chem>Clc1ccc(cc1)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H9ClN4S	-6.8	56.67	-26.373	23.6
1373	<chem>Brc1ccc(cc1)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H9BrN4S	-6.6	58.06	-25.894	24.4
1374	<chem>COC1cccccc1Nc1nnc(s1)c1[nH]ccc1</chem>	C13H12N4OS	-6.5	54.28	-28.735	32.8
1375	<chem>Oc1cccccc1Nc1nnc(s1)c1[nH]ccc1</chem>	C12H10N4OS	-7.5	56.06	-32.207	1.5
1376	<chem>[O-][N](=O)c1cccccc1Nc1nnc(s1)c1[nH]ccc1</chem>	C12H9N5O2S	-7.2	56.37	-38.356	36.9
1377	<chem>Cc1cccccc1Nc1nnc(s1)c1[nH]ccc1</chem>	C13H12N4S	-6.4	50.14	-27.477	30.7
1378	<chem>lc1cccccc1Nc1nnc(s1)c1[nH]ccc1</chem>	C12H9IN4S	-6.2	51.13	-25.842	30.2
1379	<chem>Fc1cccccc1Nc1nnc(s1)c1[nH]ccc1</chem>	C12H9FN4S	-7.3	51.77	-28.416	31.2
1380	<chem>Clc1cccccc1Nc1nnc(s1)c1[nH]ccc1</chem>	C12H9ClN4S	-6.6	52.16	-27.707	30.8
1381	<chem>Brc1cccccc1Nc1nnc(s1)c1[nH]ccc1</chem>	C12H9BrN4S	-6.3	52.67	-26.977	30.4
1382	<chem>COC1cccc(c1)Nc1nnc(s1)c1ccc[nH]1</chem>	C13H12N4OS	-6.8	60.56	-30.01	23.5
1383	<chem>Oc1cccc(c1)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H10N4OS	-7.3	53.31	-32.152	23.5
1384	<chem>[O-][N](=O)c1cccc(c1)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H9N5O2S	-7.5	53.21	-35.267	-8.5
1385	<chem>Cc1cccc(c1)Nc1nnc(s1)c1ccc[nH]1</chem>	C13H12N4S	-7.1	53.23	-29.958	22.5
1386	<chem>lc1cccc(c1)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H9IN4S	-6.4	50.52	-27.668	22.7
1387	<chem>Fc1cccc(c1)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H9FN4S	-7.1	55.31	-27.528	29.6
1388	<chem>Clc1cccc(c1)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H9ClN4S	-7.1	49.86	-27.305	22.3
1389	<chem>Brc1cccc(c1)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H9BrN4S	-6.8	55.18	-27.665	21.7
1390	<chem>c1ccc(cc1)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H10N4S	-6.8	51.14	-27.801	22.5
1391	<chem>COC1ccc(cc1)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C11H8N6OS2	-7.5	53.25	-32.799	24.5
1392	<chem>Oc1ccc(cc1)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C10H6N6OS2	-7.3	48.61	-29.487	20.6

1393	<chem>S=C1N=NC(=N1)c1nnc(s1)Nc1ccc(cc1)[N](=O)[O-]</chem>	C10H5N7O2S2	-7.7	47.86	-37.045	49.4
1394	<chem>Cc1ccc(cc1)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C11H8N6S2	-7.4	44.59	-30.388	37.3
1395	<chem>lc1ccc(cc1)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C10H5IN6S2	-6.8	48.14	-27.036	27.0
1396	<chem>Fc1ccc(cc1)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C10H5FN6S2	-7.3	58.04	-30.584	29.7
1397	<chem>Clc1ccc(cc1)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C10H5ClN6S2	-6.9	55.29	-28.668	31.1
1398	<chem>Brc1ccc(cc1)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C10H5BrN6S2	-7.2	56.34	-27.877	33.4
1399	<chem>COc1ccccc1Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C11H8N6OS2	-6.6	51.54	-31.042	13.9
1400	<chem>S=C1N=NC(=N1)c1nnc(s1)Nc1ccccc1O</chem>	C10H6N6OS2	-7.5	62.14	-31.829	24.0
1401	<chem>S=C1N=NC(=N1)c1nnc(s1)Nc1ccccc1[N](=O)[O-]</chem>	C10H5N7O2S2	-7.2	48.79	-36.419	-1.3
1402	<chem>S=C1N=NC(=N1)c1nnc(s1)Nc1ccccc1C</chem>	C11H8N6S2	-7.1	44.89	-28.668	18.8
1403	<chem>S=C1N=NC(=N1)c1nnc(s1)Nc1ccccc1I</chem>	C10H5IN6S2	-6.3	58.52	-33.171	14.9
1404	<chem>S=C1N=NC(=N1)c1nnc(s1)Nc1ccccc1F</chem>	C10H5FN6S2	-7.3	58.63	-33.135	20.6
1405	<chem>S=C1N=NC(=N1)c1nnc(s1)Nc1ccccc1Cl</chem>	C10H5ClN6S2	-7	44.62	-33.606	29.0
1406	<chem>S=C1N=NC(=N1)c1nnc(s1)Nc1ccccc1Br</chem>	C10H5BrN6S2	-6.9	42.94	-34.334	12.3
1407	<chem>COc1cccc(c1)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C11H8N6OS2	-6.9	57.67	-36.987	5.9
1408	<chem>Oc1cccc(c1)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C10H6N6OS2	-7.2	52.01	-32.28	24.9
1409	<chem>S=C1N=NC(=N1)c1nnc(s1)Nc1cccc(c1)[N](=O)[O-]</chem>	C10H5N7O2S2	-7.5	59.72	-38.01	22.3
1410	<chem>Cc1cccc(c1)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C11H8N6S2	-7.5	59.25	-31.341	14.8
1411	<chem>lc1cccc(c1)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C10H5IN6S2	-6.7	50.4	-30.204	17.6
1412	<chem>Fc1cccc(c1)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C10H5FN6S2	-7.1	53.1	-31.728	18.0
1413	<chem>Clc1cccc(c1)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C10H5ClN6S2	-7.3	57.77	-31.362	24.6
1414	<chem>Brc1cccc(c1)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C10H5BrN6S2	-6.7	50.98	-31.048	23.5
1415	<chem>S=C1N=NC(=N1)c1nnc(s1)Nc1ccccc1</chem>	C10H6N6S2	-6.9	58.38	-27.563	24.1
1416	<chem>COc1ccc(cc1)Nc1nnc(s1)c1[nH]cnc1C</chem>	C13H13N5OS	-7.3	57.7	-28.004	19.4
1417	<chem>Oc1ccc(cc1)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H11N5OS	-7.5	55.27	-24.812	7.8
1418	<chem>[O-][N](=O)c1ccc(cc1)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H10N6O2S	-7.8	54.47	-33.955	35.7
1419	<chem>Cc1ccc(cc1)Nc1nnc(s1)c1[nH]cnc1C</chem>	C13H13N5S	-7.1	56.38	-26.223	24.9
1420	<chem>lc1ccc(cc1)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H10IN5S	-5.8	55.36	-24.576	14.7
1421	<chem>Fc1ccc(cc1)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H10FN5S	-7.3	58.4	-24.495	27.1
1422	<chem>Clc1ccc(cc1)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H10ClN5S	-7	56.82	-25.22	21.7
1423	<chem>Brc1ccc(cc1)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H10BrN5S	-6.8	56.87	-24.463	33.7

1424	<chem>COc1cccc1Nc1nnc(s1)c1[nH]cnc1C</chem>	C13H13N5OS	-7	56.95	-27.639	15.9
1425	<chem>Oc1cccc1Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H11N5OS	-7.8	62.5	-30.608	23.5
1426	<chem>[O-][N](=O)c1cccc1Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H10N6O2S	-7.2	62.36	-33.727	9.3
1427	<chem>Cc1cccc1Nc1nnc(s1)c1[nH]cnc1C</chem>	C13H13N5S	-7.1	58.78	-28.638	21.8
1428	<chem>lc1cccc1Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H10IN5S	-6.9	48.6	-28.598	14.3
1429	<chem>Fc1cccc1Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H10FN5S	-7.5	57.79	-28.716	18.0
1430	<chem>Clc1cccc1Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H10ClN5S	-7.2	58.34	-28.883	12.1
1431	<chem>Brc1cccc1Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H10BrN5S	-7.1	57.32	-29.814	10.9
1432	<chem>COc1cccc(c1)Nc1nnc(s1)c1[nH]cnc1C</chem>	C13H13N5OS	-7.3	59.48	-33.646	21.0
1433	<chem>Oc1cccc(c1)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H11N5OS	-7.5	59.96	-31.467	17.1
1434	<chem>[O-][N](=O)c1cccc(c1)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H10N6O2S	-7.9	59.23	-34.497	20.1
1435	<chem>Cc1cccc(c1)Nc1nnc(s1)c1[nH]cnc1C</chem>	C13H13N5S	-7.5	58.35	-29.082	20.1
1436	<chem>lc1cccc(c1)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H10IN5S	-6.8	58.42	-29.301	20.7
1437	<chem>Fc1cccc(c1)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H10FN5S	-7.5	58.38	-29.039	16.8
1438	<chem>Clc1cccc(c1)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H10ClN5S	-7.3	58.32	-30.724	10.9
1439	<chem>Brc1cccc(c1)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H10BrN5S	-7.2	57.94	-30.181	15.1
1440	<chem>Cc1nc[nH]c1c1nnc(s1)Nc1cccc1</chem>	C12H11N5S	-7.1	55.06	-28.506	20.8
1441	<chem>COc1ccc(cc1)Nc1nnc(s1)c1ccoc1C</chem>	C14H13N3O2S	-7.4	60.57	-24.808	19.4
1442	<chem>Oc1ccc(cc1)Nc1nnc(s1)c1ccoc1C</chem>	C13H11N3O2S	-7.6	58.34	-23.851	2.3
1443	<chem>[O-][N](=O)c1ccc(cc1)Nc1nnc(s1)c1ccoc1C</chem>	C13H10N4O3S	-7.5	57.43	-32.924	29.8
1444	<chem>Cc1ccc(cc1)Nc1nnc(s1)c1ccoc1C</chem>	C14H13N3OS	-7.3	59.82	-24.91	37.1
1445	<chem>lc1ccc(cc1)Nc1nnc(s1)c1ccoc1C</chem>	C13H10IN3OS	-7.6	60.3	-23.532	-5.5
1446	<chem>Fc1ccc(cc1)Nc1nnc(s1)c1ccoc1C</chem>	C13H10FN3OS	-7.2	59.99	-25.859	-3.1
1447	<chem>Clc1ccc(cc1)Nc1nnc(s1)c1ccoc1C</chem>	C13H10ClN3OS	-7.3	60.35	-23.977	7.5
1448	<chem>Brc1ccc(cc1)Nc1nnc(s1)c1ccoc1C</chem>	C13H10BrN3OS	-6.4	60.4	-23.607	-4.9
1449	<chem>COc1cccc1Nc1nnc(s1)c1ccoc1C</chem>	C14H13N3O2S	-7.3	61.33	-26.719	12.3
1450	<chem>Oc1cccc1Nc1nnc(s1)c1ccoc1C</chem>	C13H11N3O2S	-7.8	65.34	-30.31	15.9
1451	<chem>Cc1occc1c1nnc(s1)Nc1cccc1[N](=O)[O-]</chem>	C13H10N4O3S	-6.9	63.29	-33.754	-3.1
1452	<chem>Cc1cccc1Nc1nnc(s1)c1ccoc1C</chem>	C14H13N3OS	-7.6	62.32	-27.207	20.6
1453	<chem>lc1cccc1Nc1nnc(s1)c1ccoc1C</chem>	C13H10IN3OS	-6.9	61.06	-27.54	16.5
1454	<chem>Fc1cccc1Nc1nnc(s1)c1ccoc1C</chem>	C13H10FN3OS	-7.5	61.46	-27.84	21.9

1455	Clc1cccc1Nc1nnc(s1)c1ccoc1C	C13H10CIN3OS	-7.6	61.31	-27.791	7.3
1456	Brc1cccc1Nc1nnc(s1)c1ccoc1C	C13H10BrN3OS	-7.5	60.94	-27.834	15.3
1457	COc1cccc(c1)Nc1nnc(s1)c1ccoc1C	C14H13N3O2S	-7.3	62.49	-33.312	6.6
1458	Oc1cccc(c1)Nc1nnc(s1)c1ccoc1C	C13H11N3O2S	-7.5	62.11	-32.717	11.1
1459	[O-][N](=O)c1cccc(c1)Nc1nnc(s1)c1ccoc1C	C13H10N4O3S	-7.9	62.92	-33.74	27.4
1460	Cc1cccc(c1)Nc1nnc(s1)c1ccoc1C	C14H13N3OS	-7.5	61.24	-28.889	18.9
1461	lc1cccc(c1)Nc1nnc(s1)c1ccoc1C	C13H10IN3OS	-6.5	61.13	-27.866	20.8
1462	Fc1cccc(c1)Nc1nnc(s1)c1ccoc1C	C13H10FN3OS	-7.4	62.04	-28.638	21.5
1463	Clc1cccc(c1)Nc1nnc(s1)c1ccoc1C	C13H10CIN3OS	-7.4	61.31	-28.044	19.0
1464	Brc1cccc(c1)Nc1nnc(s1)c1ccoc1C	C13H10BrN3OS	-7.3	61.88	-27.705	22.9
1465	Cc1occc1c1nnc(s1)Nc1cccc1	C13H11N3OS	-7.4	60.66	-25.913	-1.1
1466	COc1ccc(cc1)Nc1nnc(s1)C1CCCC1	C14H17N3OS	-7.3	56.94	-20.696	8.3
1467	Oc1ccc(cc1)Nc1nnc(s1)C1CCCC1	C13H15N3OS	-6.9	54.39	-22.011	23.6
1468	[O-][N](=O)c1ccc(cc1)Nc1nnc(s1)C1CCCC1	C13H14N4O2S	-7.5	54.24	-27.134	-8.3
1469	Cc1ccc(cc1)Nc1nnc(s1)C1CCCC1	C14H17N3S	-6.6	50.76	-18.921	16.9
1470	lc1ccc(cc1)Nc1nnc(s1)C1CCCC1	C13H14IN3S	-6.4	51.22	-19.434	11.7
1471	Fc1ccc(cc1)Nc1nnc(s1)C1CCCC1	C13H14FN3S	-7.1	53.72	-19.298	-11.1
1472	Clc1ccc(cc1)Nc1nnc(s1)C1CCCC1	C13H14CIN3S	-6.8	51.83	-19.312	7.9
1473	Brc1ccc(cc1)Nc1nnc(s1)C1CCCC1	C13H14BrN3S	-6.6	53.29	-19.353	-13.5
1474	COc1cccc1Nc1nnc(s1)C1CCCC1	C14H17N3OS	-6.5	49.83	-21.768	35.5
1475	Oc1cccc1Nc1nnc(s1)C1CCCC1	C13H15N3OS	-7.7	57.67	-27.211	19.4
1476	[O-][N](=O)c1cccc1Nc1nnc(s1)C1CCCC1	C13H14N4O2S	-6.9	56.52	-30.28	-2.5
1477	Cc1cccc1Nc1nnc(s1)C1CCCC1	C14H17N3S	-6.9	55.13	-19.763	16.1
1478	lc1cccc1Nc1nnc(s1)C1CCCC1	C13H14IN3S	-6.2	50.69	-19.092	3.5
1479	Fc1cccc1Nc1nnc(s1)C1CCCC1	C13H14FN3S	-7.5	54.01	-20.719	22.3
1480	Clc1cccc1Nc1nnc(s1)C1CCCC1	C13H14CIN3S	-6.7	51.47	-19.753	21.5
1481	Brc1cccc1Nc1nnc(s1)C1CCCC1	C13H14BrN3S	-6.4	53.83	-19.474	13.0
1482	COc1cccc(c1)Nc1nnc(s1)C1CCCC1	C14H17N3OS	-7	62.07	-22.75	29.5
1483	Oc1cccc(c1)Nc1nnc(s1)C1CCCC1	C13H15N3OS	-7.3	55.36	-26.013	13.2
1484	[O-][N](=O)c1cccc(c1)Nc1nnc(s1)C1CCCC1	C13H14N4O2S	-6.6	53.29	-27.22	12.1
1485	Cc1cccc(c1)Nc1nnc(s1)C1CCCC1	C14H17N3S	-7.3	57.3	-21.697	21.6

1486	<chem>Ic1cccc(c1)Nc1nnc(s1)C1CCCC1</chem>	C13H14IN3S	-6.5	56.12	-25.067	18.2
1487	<chem>Fc1cccc(c1)Nc1nnc(s1)C1CCCC1</chem>	C13H14FN3S	-7.3	58.47	-21.141	21.2
1488	<chem>Clc1cccc(c1)Nc1nnc(s1)C1CCCC1</chem>	C13H14ClN3S	-6.9	53.78	-21.18	17.7
1489	<chem>Brc1cccc(c1)Nc1nnc(s1)C1CCCC1</chem>	C13H14BrN3S	-6.6	59.03	-21.355	19.8
1490	<chem>C1CCC(C1)c1nnc(s1)Nc1cccc1</chem>	C13H15N3S	-7	52.21	-20.314	26.0
1491	<chem>Ic1ccc(c(c1)I)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H8I2N4S	-5.9	51.87	-22.085	0.1
1492	<chem>Ic1ccc(c(c1)F)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H8FIN4S	-6.4	52.98	-24.009	35.3
1493	<chem>Ic1ccc(c(c1)Cl)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H8ClIN4S	-5.8	53.21	-22.413	25.5
1494	<chem>Ic1ccc(c(c1)Br)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H8BrIN4S	-6.5	53.24	-22.112	26.7
1495	<chem>Fc1ccc(c(c1)I)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H8FIN4S	-6.6	49.52	-22.591	-10.0
1496	<chem>Fc1ccc(c(c1)F)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H8F2N4S	-7.3	53.23	-25.489	22.1
1497	<chem>Fc1ccc(c(c1)Cl)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H8ClFN4S	-6.7	48.17	-23.109	16.0
1498	<chem>Fc1ccc(c(c1)Br)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H8BrFN4S	-6.6	50.56	-23.012	-10.5
1499	<chem>Clc1ccc(c(c1)I)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H8ClIN4S	-6.1	50.76	-22.118	-9.2
1500	<chem>Clc1ccc(c(c1)F)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H8ClFN4S	-6.8	53.58	-24.984	36.1
1501	<chem>Clc1ccc(c(c1)Cl)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H8Cl2N4S	-6.7	53.06	-23.361	13.2
1502	<chem>Clc1ccc(c(c1)Br)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H8BrClN4S	-6.5	52.54	-22.24	0.9
1503	<chem>Brc1ccc(c(c1)I)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H8BrIN4S	-6	44.58	-22.084	0.5
1504	<chem>Brc1ccc(c(c1)F)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H8BrFN4S	-6.8	53.3	-24.331	35.7
1505	<chem>Brc1ccc(c(c1)Cl)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H8BrClN4S	-6.7	53.45	-22.621	10.6
1506	<chem>Brc1ccc(c(c1)Br)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H8Br2N4S	-6.6	48.14	-22.237	0.4
1507	<chem>Ic1cc(cc(c1)I)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H8I2N4S	-6.4	51.78	-27.593	20.4
1508	<chem>Fc1cc(Nc2nnc(s2)c2[nH]ccc2)cc(c1)I</chem>	C12H8FIN4S	-7.2	53.78	-28.205	21.5
1509	<chem>Fc1cc(cc(c1)F)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H8F2N4S	-7.5	57.94	-25.742	22.1
1510	<chem>Fc1cc(Nc2nnc(s2)c2[nH]ccc2)cc(c1)Cl</chem>	C12H8ClFN4S	-7.3	57.24	-26.237	19.8
1511	<chem>Fc1cc(Nc2nnc(s2)c2[nH]ccc2)cc(c1)Br</chem>	C12H8BrFN4S	-7.3	56.14	-28.398	19.6
1512	<chem>Clc1cc(Nc2nnc(s2)c2[nH]ccc2)cc(c1)I</chem>	C12H8ClIN4S	-7.1	55.01	-27.927	20.9
1513	<chem>Clc1cc(cc(c1)Cl)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H8Cl2N4S	-7.3	55.06	-26.011	19.2
1514	<chem>Clc1cc(Nc2nnc(s2)c2[nH]ccc2)cc(c1)Br</chem>	C12H8BrClN4S	-7.2	57.21	-28.109	19.1
1515	<chem>Brc1cc(Nc2nnc(s2)c2[nH]ccc2)cc(c1)I</chem>	C12H8BrIN4S	-6.8	56.72	-28.789	20.7
1516	<chem>Brc1cc(cc(c1)Br)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H8Br2N4S	-6.9	56.89	-27.952	18.8

1517	<chem>Ic1ccc(c(c1)I)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C10H4I2N6S2	-6.1	41.9	-28.326	32.1
1518	<chem>Ic1ccc(c(c1)F)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C10H4FIN6S2	-6.2	57.4	-29.534	28.1
1519	<chem>Ic1ccc(c(c1)Cl)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C10H4CIIN6S2	-7	46.15	-29.811	31.7
1520	<chem>Ic1ccc(c(c1)Br)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C10H4BrIN6S2	-7.1	47.16	-29.654	30.2
1521	<chem>Fc1ccc(c(c1)I)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C10H4FIN6S2	-6.6	44.5	-31.829	16.7
1522	<chem>Fc1ccc(c(c1)F)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C10H4F2N6S2	-7.6	44.03	-32.701	18.3
1523	<chem>Fc1ccc(c(c1)Cl)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C10H4ClFN6S2	-7.3	54.9	-32.678	15.7
1524	<chem>Fc1ccc(c(c1)Br)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C10H4BrFN6S2	-6.5	42.59	-32.534	17.9
1525	<chem>Clc1ccc(c(c1)I)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C10H4CIIN6S2	-6.3	42	-30.385	23.3
1526	<chem>Clc1ccc(c(c1)F)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C10H4ClFN6S2	-7.1	47.72	-31.423	26.9
1527	<chem>Clc1ccc(c(c1)Cl)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C10H4Cl2N6S2	-7.3	41.9	-31.23	23.5
1528	<chem>Clc1ccc(c(c1)Br)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C10H4BrClN6S2	-7.2	60.09	-31.087	23.2
1529	<chem>Brc1ccc(c(c1)I)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C10H4BrIN6S2	-6.2	48.34	-29.578	24.5
1530	<chem>Brc1ccc(c(c1)F)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C10H4BrFN6S2	-7	44.69	-30.608	30.8
1531	<chem>Brc1ccc(c(c1)Cl)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C10H4BrClN6S2	-6.2	40.03	-30.876	31.0
1532	<chem>Brc1ccc(c(c1)Br)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C10H4Br2N6S2	-7.1	51.13	-30.283	18.8
1533	<chem>Ic1cc(cc(c1)I)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C10H4I2N6S2	-6.8	47.57	-30.348	17.0
1534	<chem>S=C1N=NC(=N1)c1nnc(s1)Nc1cc(F)cc(c1)I</chem>	C10H4FIN6S2	-7.4	50.85	-32.004	11.1
1535	<chem>Fc1cc(cc(c1)F)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C10H4F2N6S2	-7.6	50.6	-34.202	18.8
1536	<chem>S=C1N=NC(=N1)c1nnc(s1)Nc1cc(F)cc(c1)Cl</chem>	C10H4ClFN6S2	-7.4	61.8	-33.982	12.1
1537	<chem>S=C1N=NC(=N1)c1nnc(s1)Nc1cc(F)cc(c1)Br</chem>	C10H4BrFN6S2	-7.4	50.21	-31.998	15.7
1538	<chem>S=C1N=NC(=N1)c1nnc(s1)Nc1cc(Cl)cc(c1)I</chem>	C10H4CIIN6S2	-7.3	60.26	-31.182	11.6
1539	<chem>Clc1cc(cc(c1)Cl)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C10H4Cl2N6S2	-7.4	54.08	-32.801	13.9
1540	<chem>S=C1N=NC(=N1)c1nnc(s1)Nc1cc(Cl)cc(c1)Br</chem>	C10H4BrClN6S2	-7.3	49.68	-32.059	14.6
1541	<chem>S=C1N=NC(=N1)c1nnc(s1)Nc1cc(Br)cc(c1)I</chem>	C10H4BrIN6S2	-6.9	51.69	-31.053	27.2
1542	<chem>Brc1cc(cc(c1)Br)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C10H4Br2N6S2	-6.9	52.62	-31.919	14.1
1543	<chem>Ic1ccc(c(c1)I)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H9I2N5S	-6.9	52.1	-24.538	25.6
1544	<chem>Ic1ccc(c(c1)F)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H9FIN5S	-7.4	49.83	-25.021	28.0
1545	<chem>Ic1ccc(c(c1)Cl)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H9CIIN5S	-7.5	44.75	-25.272	21.1
1546	<chem>Ic1ccc(c(c1)Br)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H9BrIN5S	-7.5	58.1	-25.083	20.7
1547	<chem>Fc1ccc(c(c1)I)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H9FIN5S	-7.1	55.96	-27.972	9.1

1548	Fc1ccc(c(c1)F)Nc1nnc(s1)c1[nH]cnc1C	C12H9F2N5S	-7.5	58.38	-27.694	26.8
1549	Fc1ccc(c(c1)Cl)Nc1nnc(s1)c1[nH]cnc1C	C12H9ClFN5S	-7.4	50.3	-28.827	21.0
1550	Fc1ccc(c(c1)Br)Nc1nnc(s1)c1[nH]cnc1C	C12H9BrFN5S	-7.3	51.85	-28.661	12.5
1551	Clc1ccc(c(c1)I)Nc1nnc(s1)c1[nH]cnc1C	C12H9ClIN5S	-7.1	52.53	-26.515	22.6
1552	Clc1ccc(c(c1)F)Nc1nnc(s1)c1[nH]cnc1C	C12H9ClFN5S	-7.4	53.66	-26.909	22.6
1553	Clc1ccc(c(c1)Cl)Nc1nnc(s1)c1[nH]cnc1C	C12H9Cl2N5S	-6.9	59.16	-27.368	24.8
1554	Clc1ccc(c(c1)Br)Nc1nnc(s1)c1[nH]cnc1C	C12H9BrClN5S	-7.4	59.52	-27.206	24.0
1555	Brc1ccc(c(c1)I)Nc1nnc(s1)c1[nH]cnc1C	C12H9BrIN5S	-6.8	59.12	-25.66	21.0
1556	Brc1ccc(c(c1)F)Nc1nnc(s1)c1[nH]cnc1C	C12H9BrFN5S	-6.3	59.46	-26.064	5.2
1557	Brc1ccc(c(c1)Cl)Nc1nnc(s1)c1[nH]cnc1C	C12H9BrClN5S	-7.5	58.78	-26.292	26.1
1558	Brc1ccc(c(c1)Br)Nc1nnc(s1)c1[nH]cnc1C	C12H9Br2N5S	-7.5	53.05	-26.349	24.2
1559	lc1cc(cc(c1)I)Nc1nnc(s1)c1[nH]cnc1C	C12H9I2N5S	-7	54.33	-28.691	22.9
1560	Fc1cc(Nc2nnc(s2)c2[nH]cnc2C)cc(c1)I	C12H9FIN5S	-7.5	59.59	-29.014	23.8
1561	Fc1cc(cc(c1)F)Nc1nnc(s1)c1[nH]cnc1C	C12H9F2N5S	-7.8	58.11	-28.971	14.9
1562	Fc1cc(Nc2nnc(s2)c2[nH]cnc2C)cc(c1)Cl	C12H9ClFN5S	-7.5	59.1	-28.752	17.7
1563	Fc1cc(Nc2nnc(s2)c2[nH]cnc2C)cc(c1)Br	C12H9BrFN5S	-7.4	56.2	-28.995	23.1
1564	Clc1cc(Nc2nnc(s2)c2[nH]cnc2C)cc(c1)I	C12H9ClIN5S	-7.4	57.36	-28.837	23.2
1565	Clc1cc(cc(c1)Cl)Nc1nnc(s1)c1[nH]cnc1C	C12H9Cl2N5S	-7.5	54.42	-28.416	24.8
1566	Clc1cc(Nc2nnc(s2)c2[nH]cnc2C)cc(c1)Br	C12H9BrClN5S	-7.5	58.19	-28.814	22.5
1567	Brc1cc(Nc2nnc(s2)c2[nH]cnc2C)cc(c1)I	C12H9BrIN5S	-7.1	53.27	-28.711	17.6
1568	Brc1cc(cc(c1)Br)Nc1nnc(s1)c1[nH]cnc1C	C12H9Br2N5S	-7.2	59.83	-28.353	20.9
1569	lc1ccc(c(c1)I)Nc1nnc(s1)c1ccoc1C	C13H9I2N3OS	-7.2	51.16	-23.603	-7.7
1570	lc1ccc(c(c1)F)Nc1nnc(s1)c1ccoc1C	C13H9FIN3OS	-6	61.38	-23.691	15.2
1571	lc1ccc(c(c1)Cl)Nc1nnc(s1)c1ccoc1C	C13H9ClIN3OS	-7.9	47.96	-23.902	31.6
1572	lc1ccc(c(c1)Br)Nc1nnc(s1)c1ccoc1C	C13H9BrIN3OS	-7.8	62.55	-23.738	20.1
1573	Fc1ccc(c(c1)I)Nc1nnc(s1)c1ccoc1C	C13H9FIN3OS	-6.8	53.26	-26.636	10.4
1574	Fc1ccc(c(c1)F)Nc1nnc(s1)c1ccoc1C	C13H9F2N3OS	-7.7	63.03	-26.63	19.1
1575	Fc1ccc(c(c1)Cl)Nc1nnc(s1)c1ccoc1C	C13H9ClFN3OS	-6.9	62.72	-27.192	20.9
1576	Fc1ccc(c(c1)Br)Nc1nnc(s1)c1ccoc1C	C13H9BrFN3OS	-7.7	63.4	-27.078	25.3
1577	Clc1ccc(c(c1)I)Nc1nnc(s1)c1ccoc1C	C13H9ClIN3OS	-6.2	61.72	-25.119	35.7
1578	Clc1ccc(c(c1)F)Nc1nnc(s1)c1ccoc1C	C13H9ClFN3OS	-7.1	62.84	-25.479	20.5

1579	Clc1ccc(c(c1)Cl)Nc1nnc(s1)c1ccoc1C	C13H9Cl2N3OS	-6.5	62.68	-25.645	44.3
1580	Clc1ccc(c(c1)Br)Nc1nnc(s1)c1ccoc1C	C13H9BrClN3OS	-7.7	63.1	-25.542	43.7
1581	Brc1ccc(c(c1)I)Nc1nnc(s1)c1ccoc1C	C13H9BrIN3OS	-7.1	47.61	-24.45	14.5
1582	Brc1ccc(c(c1)F)Nc1nnc(s1)c1ccoc1C	C13H9BrFN3OS	-7.9	62.44	-24.66	25.5
1583	Brc1ccc(c(c1)Cl)Nc1nnc(s1)c1ccoc1C	C13H9BrClN3OS	-7.9	58.89	-24.867	21.9
1584	Brc1ccc(c(c1)Br)Nc1nnc(s1)c1ccoc1C	C13H9Br2N3OS	-7.8	62.54	-24.661	24.0
1585	Ic1cc(cc(c1)I)Nc1nnc(s1)c1ccoc1C	C13H9I2N3OS	-7.4	57.85	-26.615	25.6
1586	Fc1cc(Nc2nnc(s2)c2ccoc2C)cc(c1)I	C13H9FIN3OS	-7.4	58.11	-27.905	20.5
1587	Fc1cc(cc(c1)F)Nc1nnc(s1)c1ccoc1C	C13H9F2N3OS	-7.8	58.64	-27.277	25.1
1588	Fc1cc(Nc2nnc(s2)c2ccoc2C)cc(c1)Cl	C13H9ClFN3OS	-7.6	57	-28.62	18.1
1589	Fc1cc(Nc2nnc(s2)c2ccoc2C)cc(c1)Br	C13H9BrFN3OS	-7.4	58.34	-28.575	19.3
1590	Clc1cc(Nc2nnc(s2)c2ccoc2C)cc(c1)I	C13H9ClIN3OS	-7.4	59.56	-26.394	8.2
1591	Clc1cc(cc(c1)Cl)Nc1nnc(s1)c1ccoc1C	C13H9Cl2N3OS	-7.6	60.69	-27.196	21.9
1592	Clc1cc(Nc2nnc(s2)c2ccoc2C)cc(c1)Br	C13H9BrClN3OS	-7.5	60.37	-26.937	30.4
1593	Brc1cc(Nc2nnc(s2)c2ccoc2C)cc(c1)I	C13H9BrIN3OS	-7.4	57.25	-26.52	35.0
1594	Brc1cc(cc(c1)Br)Nc1nnc(s1)c1ccoc1C	C13H9Br2N3OS	-7.2	57.54	-27.06	23.0
1595	Ic1ccc(c(c1)I)Nc1nnc(s1)C1CCCC1	C13H13I2N3S	-6	54.74	-17.728	2.4
1596	Ic1ccc(c(c1)F)Nc1nnc(s1)C1CCCC1	C13H13FIN3S	-6.5	55	-19.952	17.8
1597	Ic1ccc(c(c1)Cl)Nc1nnc(s1)C1CCCC1	C13H13ClIN3S	-6.1	55.24	-18.003	18.4
1598	Ic1ccc(c(c1)Br)Nc1nnc(s1)C1CCCC1	C13H13BrIN3S	-6	55.18	-17.7	17.0
1599	Fc1ccc(c(c1)I)Nc1nnc(s1)C1CCCC1	C13H13FIN3S	-6	54.61	-17.729	2.1
1600	Fc1ccc(c(c1)F)Nc1nnc(s1)C1CCCC1	C13H13F2N3S	-7.5	55.32	-18.752	4.8
1601	Fc1ccc(c(c1)Cl)Nc1nnc(s1)C1CCCC1	C13H13ClFN3S	-7	52.46	-18.254	7.7
1602	Fc1ccc(c(c1)Br)Nc1nnc(s1)C1CCCC1	C13H13BrFN3S	-6.7	56.27	-18.145	17.8
1603	Clc1ccc(c(c1)I)Nc1nnc(s1)C1CCCC1	C13H13ClIN3S	-5.9	51.24	-17.729	-18.1
1604	Clc1ccc(c(c1)F)Nc1nnc(s1)C1CCCC1	C13H13ClFN3S	-6.7	56.36	-19.949	17.4
1605	Clc1ccc(c(c1)Cl)Nc1nnc(s1)C1CCCC1	C13H13Cl2N3S	-7	55.7	-17.653	5.9
1606	Clc1ccc(c(c1)Br)Nc1nnc(s1)C1CCCC1	C13H13BrClN3S	-5.9	54.17	-17.651	6.0
1607	Brc1ccc(c(c1)I)Nc1nnc(s1)C1CCCC1	C13H13BrIN3S	-5.9	51.53	-17.742	6.3
1608	Brc1ccc(c(c1)F)Nc1nnc(s1)C1CCCC1	C13H13BrFN3S	-6.7	56.04	-19.95	17.6
1609	Brc1ccc(c(c1)Cl)Nc1nnc(s1)C1CCCC1	C13H13BrClN3S	-7	55.15	-18.044	24.3

1610	Brc1ccc(c(c1)Br)Nc1nnc(s1)C1CCCC1	C13H13Br2N3S	-6.7	54.9	-17.72	5.6
1611	Ic1cc(cc(c1)I)Nc1nnc(s1)C1CCCC1	C13H13I2N3S	-6.5	60.2	-25.175	15.6
1612	Fc1cc(Nc2nnc(s2)C2CCCC2)cc(c1)I	C13H13FIN3S	-7.3	59.1	-22.286	16.1
1613	Fc1cc(cc(c1)F)Nc1nnc(s1)C1CCCC1	C13H13F2N3S	-7.8	62.87	-23.168	21.1
1614	Fc1cc(Nc2nnc(s2)C2CCCC2)cc(c1)Cl	C13H13ClFN3S	-7.7	60.1	-20.963	18.5
1615	Fc1cc(Nc2nnc(s2)C2CCCC2)cc(c1)Br	C13H13BrFN3S	-6.9	62.51	-22.51	16.2
1616	Clc1cc(Nc2nnc(s2)C2CCCC2)cc(c1)I	C13H13ClIN3S	-7.2	60.62	-22.823	17.5
1617	Clc1cc(cc(c1)Cl)Nc1nnc(s1)C1CCCC1	C13H13Cl2N3S	-7.4	59.75	-24.175	18.6
1618	Clc1cc(Nc2nnc(s2)C2CCCC2)cc(c1)Br	C13H13BrClN3S	-7.3	59.71	-23.066	17.7
1619	Brc1cc(Nc2nnc(s2)C2CCCC2)cc(c1)I	C13H13BrIN3S	-6.9	59.12	-25.23	18.2
1620	Brc1cc(cc(c1)Br)Nc1nnc(s1)C1CCCC1	C13H13Br2N3S	-6.5	58.45	-24.862	15.0
1621	Ic1cc(I)c(c(c1)I)Nc1nnc(s1)c1ccc[nH]1	C12H7I3N4S	-5.7	41.26	-22.905	-9.6
1622	Ic1cc(F)c(c(c1)I)Nc1nnc(s1)c1[nH]ccc1	C12H7FI2N4S	-6	46.01	-23.499	22.4
1623	Ic1cc(F)c(c(c1)F)Nc1nnc(s1)c1ccc[nH]1	C12H7F2IN4S	-6.5	48.46	-23.399	-10.8
1624	Ic1cc(F)c(c(c1)Cl)Nc1nnc(s1)c1[nH]ccc1	C12H7ClFIN4S	-6.5	45.59	-24.102	-11.2
1625	Ic1cc(F)c(c(c1)Br)Nc1nnc(s1)c1[nH]ccc1	C12H7BrFIN4S	-6.3	47.3	-24.171	-12.8
1626	Ic1cc(Cl)c(c(c1)I)Nc1nnc(s1)c1[nH]ccc1	C12H7ClI2N4S	-5.9	45.18	-23.411	-10.3
1627	Ic1cc(Cl)c(c(c1)Cl)Nc1nnc(s1)c1ccc[nH]1	C12H7Cl2IN4S	-6.2	41.23	-23.535	-9.2
1628	Ic1cc(Cl)c(c(c1)Br)Nc1nnc(s1)c1[nH]ccc1	C12H7BrClIN4S	-6	41.96	-23.605	-11.5
1629	Ic1cc(Br)c(c(c1)I)Nc1nnc(s1)c1[nH]ccc1	C12H7BrI2N4S	-5.8	40.33	-23.308	-7.2
1630	Ic1cc(Br)c(c(c1)Br)Nc1nnc(s1)c1ccc[nH]1	C12H7Br2IN4S	-6.1	43.35	-23.384	-12.4
1631	Fc1cc(I)c(c(c1)I)Nc1nnc(s1)c1ccc[nH]1	C12H7FI2N4S	-5.8	45.94	-24.389	-10.2
1632	Fc1cc(F)c(c(c1)I)Nc1nnc(s1)c1[nH]ccc1	C12H7F2IN4S	-6.8	47.25	-24.277	-6.7
1633	Fc1cc(F)c(c(c1)F)Nc1nnc(s1)c1ccc[nH]1	C12H7F3N4S	-6.8	48.68	-26.661	19.6
1634	Fc1cc(F)c(c(c1)Cl)Nc1nnc(s1)c1[nH]ccc1	C12H7ClF2N4S	-6.9	47.23	-25.542	33.4
1635	Fc1cc(F)c(c(c1)Br)Nc1nnc(s1)c1[nH]ccc1	C12H7BrF2N4S	-6.9	48.3	-24.185	31.0
1636	Fc1cc(Cl)c(c(c1)I)Nc1nnc(s1)c1[nH]ccc1	C12H7ClFIN4S	-6.5	47.58	-24.227	-10.0
1637	Fc1cc(Cl)c(c(c1)Cl)Nc1nnc(s1)c1ccc[nH]1	C12H7Cl2FN4S	-7	47.44	-24.03	-9.9
1638	Fc1cc(Cl)c(c(c1)Br)Nc1nnc(s1)c1[nH]ccc1	C12H7BrClFN4S	-6.3	41.69	-24.141	-12.1
1639	Fc1cc(Br)c(c(c1)I)Nc1nnc(s1)c1[nH]ccc1	C12H7BrFIN4S	-5.8	45.66	-24.196	-11.3
1640	Fc1cc(Br)c(c(c1)Br)Nc1nnc(s1)c1ccc[nH]1	C12H7Br2FN4S	-6.6	41.36	-24.311	-7.5

1641	<chem>Clc1cc(I)c(c(c1)I)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H7ClI2N4S	-5.8	40.9	-23.521	-10.4
1642	<chem>Clc1cc(F)c(c(c1)I)Nc1nnc(s1)c1[nH]ccc1</chem>	C12H7ClFIN4S	-6.2	43.69	-23.398	-12.2
1643	<chem>Clc1cc(F)c(c(c1)F)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H7ClF2N4S	-6.7	45.99	-25.719	42.3
1644	<chem>Clc1cc(F)c(c(c1)Cl)Nc1nnc(s1)c1[nH]ccc1</chem>	C12H7Cl2FN4S	-6.6	47.28	-24.108	-12.6
1645	<chem>Clc1cc(F)c(c(c1)Br)Nc1nnc(s1)c1[nH]ccc1</chem>	C12H7BrClFN4S	-6.6	47.01	-23.466	-11.4
1646	<chem>Clc1cc(Cl)c(c(c1)I)Nc1nnc(s1)c1[nH]ccc1</chem>	C12H7Cl2IN4S	-5.9	46.43	-23.629	6.0
1647	<chem>Clc1cc(Cl)c(c(c1)Cl)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H7Cl3N4S	-6.4	45.44	-23.649	-12.4
1648	<chem>Clc1cc(Cl)c(c(c1)Br)Nc1nnc(s1)c1[nH]ccc1</chem>	C12H7BrCl2N4S	-6.2	40.5	-23.711	-10.9
1649	<chem>Clc1cc(Br)c(c(c1)I)Nc1nnc(s1)c1[nH]ccc1</chem>	C12H7BrClIN4S	-6	45.52	-23.529	-10.6
1650	<chem>Clc1cc(Br)c(c(c1)Br)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H7Br2ClN4S	-5.9	45.82	-23.616	-11.5
1651	<chem>Brc1cc(I)c(c(c1)I)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H7BrI2N4S	-5.8	45.49	-23.084	-6.7
1652	<chem>Brc1cc(F)c(c(c1)I)Nc1nnc(s1)c1[nH]ccc1</chem>	C12H7BrFIN4S	-6	45.62	-23.295	-11.4
1653	<chem>Brc1cc(F)c(c(c1)F)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H7BrF2N4S	-6.5	48.36	-23.71	38.2
1654	<chem>Brc1cc(F)c(c(c1)Cl)Nc1nnc(s1)c1[nH]ccc1</chem>	C12H7BrClFN4S	-6.2	47.01	-24.106	-11.2
1655	<chem>Brc1cc(F)c(c(c1)Br)Nc1nnc(s1)c1[nH]ccc1</chem>	C12H7Br2FN4S	-6.5	46.6	-24.176	1.3
1656	<chem>Brc1cc(Cl)c(c(c1)I)Nc1nnc(s1)c1[nH]ccc1</chem>	C12H7BrClIN4S	-5.9	43.49	-23.53	-10.5
1657	<chem>Brc1cc(Cl)c(c(c1)Cl)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H7BrCl2N4S	-6.3	45.25	-23.537	-12.5
1658	<chem>Brc1cc(Cl)c(c(c1)Br)Nc1nnc(s1)c1[nH]ccc1</chem>	C12H7Br2ClN4S	-6.1	45.46	-23.606	-10.8
1659	<chem>Brc1cc(Br)c(c(c1)I)Nc1nnc(s1)c1[nH]ccc1</chem>	C12H7Br2IN4S	-5.9	41.06	-23.423	-9.7
1660	<chem>Brc1cc(Br)c(c(c1)Br)Nc1nnc(s1)c1ccc[nH]1</chem>	C12H7Br3N4S	-5.9	44.47	-23.51	-11.1
1661	<chem>Ic1cc(I)c(c(c1)I)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C10H3I3N6S2	-6.1	36.69	-22.162	14.6
1662	<chem>S=C1N=NC(=N1)c1nnc(s1)Nc1c(F)cc(cc1)I</chem>	C10H3FI2N6S2	-6.4	36.87	-27.262	21.5
1663	<chem>Ic1cc(F)c(c(c1)F)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C10H3F2IN6S2	-6.6	42.92	-25.223	42.9
1664	<chem>S=C1N=NC(=N1)c1nnc(s1)Nc1c(F)cc(cc1Cl)I</chem>	C10H3ClFIN6S2	-6.4	53.01	-29.191	29.5
1665	<chem>S=C1N=NC(=N1)c1nnc(s1)Nc1c(F)cc(cc1Br)I</chem>	C10H3BrFIN6S2	-6.6	35.11	-27.788	19.6
1666	<chem>S=C1N=NC(=N1)c1nnc(s1)Nc1c(Cl)cc(cc1)I</chem>	C10H3ClI2N6S2	-6.3	42.19	-24.289	52.0
1667	<chem>Ic1cc(Cl)c(c(c1)Cl)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C10H3Cl2IN6S2	-6.5	40.93	-27.154	22.2
1668	<chem>S=C1N=NC(=N1)c1nnc(s1)Nc1c(Cl)cc(cc1Br)I</chem>	C10H3BrClIN6S2	-6.3	34.72	-25.89	22.0
1669	<chem>S=C1N=NC(=N1)c1nnc(s1)Nc1c(Br)cc(cc1)I</chem>	C10H3BrI2N6S2	-6.1	38.56	-23.356	12.1
1670	<chem>Ic1cc(Br)c(c(c1)Br)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C10H3Br2IN6S2	-6.2	38.76	-25.753	29.0
1671	<chem>Fc1cc(I)c(c(c1)I)Nc1nnc(s1)C1=NC(=S)N=N1</chem>	C10H3FI2N6S2	-6	39.99	-24.745	5.2

1672	S=C1N=NC(=N1)c1nnc(s1)Nc1c(F)cc(cc1I)F	C10H3F2IN6S2	-6.5	41.19	-31.174	18.9
1673	Fc1cc(F)c(c(c1)F)Nc1nnc(s1)C1=NC(=S)N=N1	C10H3F3N6S2	-6.9	39.93	-31.828	25.5
1674	S=C1N=NC(=N1)c1nnc(s1)Nc1c(F)cc(cc1Cl)F	C10H3ClF2N6S2	-6.6	45.78	-28.14	29.8
1675	S=C1N=NC(=N1)c1nnc(s1)Nc1c(F)cc(cc1Br)F	C10H3BrF2N6S2	-6.5	43.88	-28.92	17.5
1676	S=C1N=NC(=N1)c1nnc(s1)Nc1c(Cl)cc(cc1I)F	C10H3ClFIN6S2	-6.2	38.47	-29.565	17.0
1677	Fc1cc(Cl)c(c(c1)Cl)Nc1nnc(s1)C1=NC(=S)N=N1	C10H3Cl2FN6S2	-6.5	41.58	-31.061	40.7
1678	S=C1N=NC(=N1)c1nnc(s1)Nc1c(Cl)cc(cc1Br)F	C10H3BrClFN6S2	-6.2	41.13	-30.485	9.3
1679	S=C1N=NC(=N1)c1nnc(s1)Nc1c(Br)cc(cc1I)F	C10H3BrFIN6S2	-6.1	38	-25.843	11.9
1680	Fc1cc(Br)c(c(c1)Br)Nc1nnc(s1)C1=NC(=S)N=N1	C10H3Br2FN6S2	-6	42.23	-29.625	37.0
1681	Clc1cc(I)c(c(c1)I)Nc1nnc(s1)C1=NC(=S)N=N1	C10H3ClI2N6S2	-6	34.5	-24.04	33.5
1682	S=C1N=NC(=N1)c1nnc(s1)Nc1c(F)cc(cc1I)Cl	C10H3ClFIN6S2	-6.3	35.24	-29.465	21.2
1683	Clc1cc(F)c(c(c1)F)Nc1nnc(s1)C1=NC(=S)N=N1	C10H3ClF2N6S2	-6.7	40.1	-27.013	10.6
1684	S=C1N=NC(=N1)c1nnc(s1)Nc1c(F)cc(cc1Cl)Cl	C10H3Cl2FN6S2	-6.7	45.35	-27.35	23.6
1685	S=C1N=NC(=N1)c1nnc(s1)Nc1c(F)cc(cc1Br)Cl	C10H3BrClFN6S2	-6.7	37.96	-29.998	38.8
1686	S=C1N=NC(=N1)c1nnc(s1)Nc1c(Cl)cc(cc1I)Cl	C10H3Cl2IN6S2	-6.2	39.38	-27.895	16.3
1687	Clc1cc(Cl)c(c(c1)Cl)Nc1nnc(s1)C1=NC(=S)N=N1	C10H3Cl3N6S2	-6.4	45.86	-29.352	19.3
1688	S=C1N=NC(=N1)c1nnc(s1)Nc1c(Cl)cc(cc1Br)Cl	C10H3BrCl2N6S2	-6.2	45.6	-28.792	21.9
1689	S=C1N=NC(=N1)c1nnc(s1)Nc1c(Br)cc(cc1I)Cl	C10H3BrClIN6S2	-6.2	43.03	-25.241	8.9
1690	Clc1cc(Br)c(c(c1)Br)Nc1nnc(s1)C1=NC(=S)N=N1	C10H3Br2ClN6S2	-6.1	35.34	-27.925	19.3
1691	Brc1cc(I)c(c(c1)I)Nc1nnc(s1)C1=NC(=S)N=N1	C10H3BrI2N6S2	-6.1	37.58	-23.234	27.6
1692	S=C1N=NC(=N1)c1nnc(s1)Nc1c(F)cc(cc1I)Br	C10H3BrFIN6S2	-6.3	40.35	-28.497	24.9
1693	Brc1cc(F)c(c(c1)F)Nc1nnc(s1)C1=NC(=S)N=N1	C10H3BrF2N6S2	-6.7	37.91	-26.145	9.1
1694	S=C1N=NC(=N1)c1nnc(s1)Nc1c(F)cc(cc1Cl)Br	C10H3BrClFN6S2	-6.7	40.84	-30.241	32.3
1695	S=C1N=NC(=N1)c1nnc(s1)Nc1c(F)cc(cc1Br)Br	C10H3Br2FN6S2	-6.6	37	-26.263	31.9
1696	S=C1N=NC(=N1)c1nnc(s1)Nc1c(Cl)cc(cc1I)Br	C10H3BrClIN6S2	-6.3	39.93	-25.209	21.5
1697	Brc1cc(Cl)c(c(c1)Cl)Nc1nnc(s1)C1=NC(=S)N=N1	C10H3BrCl2N6S2	-6.4	40.59	-28.382	26.9
1698	S=C1N=NC(=N1)c1nnc(s1)Nc1c(Cl)cc(cc1Br)Br	C10H3Br2ClN6S2	-6.2	46.11	-27.798	11.2
1699	S=C1N=NC(=N1)c1nnc(s1)Nc1c(Br)cc(cc1I)Br	C10H3Br2IN6S2	-6.1	37.2	-24.414	20.3
1700	Brc1cc(Br)c(c(c1)Br)Nc1nnc(s1)C1=NC(=S)N=N1	C10H3Br3N6S2	-6.1	38.9	-27.075	23.0
1701	lc1cc(I)c(c(c1)I)Nc1nnc(s1)c1[nH]cnc1C	C12H8I3N5S	-6	42.56	-24.396	-4.4
1702	lc1cc(F)c(c(c1)I)Nc1nnc(s1)c1[nH]cnc1C	C12H8FI2N5S	-6.2	49.81	-25.285	9.2

1703	<chem>Ic1cc(F)c(c(c1)F)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H8F2IN5S	-7	53.92	-25.348	22.0
1704	<chem>Ic1cc(F)c(c(c1)Cl)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H8ClFIN5S	-7.2	52.27	-25.179	-2.5
1705	<chem>Ic1cc(F)c(c(c1)Br)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H8BrFIN5S	-6.2	44.62	-25.43	-0.3
1706	<chem>Ic1cc(Cl)c(c(c1)I)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H8ClI2N5S	-6.2	42.64	-25.335	-2.8
1707	<chem>Ic1cc(Cl)c(c(c1)Cl)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H8Cl2IN5S	-6.7	42.15	-24.831	-3.0
1708	<chem>Ic1cc(Cl)c(c(c1)Br)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H8BrClIN5S	-6.1	43.48	-25.081	-2.5
1709	<chem>Ic1cc(Br)c(c(c1)I)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H8BrI2N5S	-6	43.76	-24.308	-3.7
1710	<chem>Ic1cc(Br)c(c(c1)Br)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H8Br2IN5S	-6.1	42.29	-23.909	-2.5
1711	<chem>Fc1cc(I)c(c(c1)I)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H8FI2N5S	-5.8	49.03	-24.387	-4.5
1712	<chem>Fc1cc(F)c(c(c1)I)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H8F2IN5S	-6.7	53.19	-26.496	20.3
1713	<chem>Fc1cc(F)c(c(c1)F)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H8F3N5S	-7.2	52.94	-26.134	11.9
1714	<chem>Fc1cc(F)c(c(c1)Cl)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H8ClF2N5S	-6.8	42.86	-27.038	25.0
1715	<chem>Fc1cc(F)c(c(c1)Br)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H8BrF2N5S	-6.4	55.76	-26.784	17.8
1716	<chem>Fc1cc(Cl)c(c(c1)I)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H8ClFIN5S	-6.1	52.99	-24.616	22.4
1717	<chem>Fc1cc(Cl)c(c(c1)Cl)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H8Cl2FN5S	-6.9	47.28	-25.661	23.7
1718	<chem>Fc1cc(Cl)c(c(c1)Br)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H8BrClFN5S	-6.7	42.9	-25.409	25.6
1719	<chem>Fc1cc(Br)c(c(c1)I)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H8BrFIN5S	-6	47.09	-24.297	-3.7
1720	<chem>Fc1cc(Br)c(c(c1)Br)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H8Br2FN5S	-6.1	54.63	-24.567	12.5
1721	<chem>Clc1cc(I)c(c(c1)I)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H8ClI2N5S	-5.9	41.45	-24.396	-4.2
1722	<chem>Clc1cc(F)c(c(c1)I)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H8ClFIN5S	-6.2	54.35	-25.287	-2.0
1723	<chem>Clc1cc(F)c(c(c1)F)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H8ClF2N5S	-6.5	53.46	-25.348	22.1
1724	<chem>Clc1cc(F)c(c(c1)Cl)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H8Cl2FN5S	-7.1	52.38	-25.698	25.5
1725	<chem>Clc1cc(F)c(c(c1)Br)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H8BrClFN5S	-6.8	43.83	-25.445	25.5
1726	<chem>Clc1cc(Cl)c(c(c1)I)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H8Cl2IN5S	-6.1	55	-24.51	-2.4
1727	<chem>Clc1cc(Cl)c(c(c1)Cl)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H8Cl3N5S	-6.9	52.25	-24.831	-2.9
1728	<chem>Clc1cc(Cl)c(c(c1)Br)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H8BrCl2N5S	-6.5	44.43	-24.172	-3.0
1729	<chem>Clc1cc(Br)c(c(c1)I)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H8BrClIN5S	-6	43.25	-24.308	-4.0
1730	<chem>Clc1cc(Br)c(c(c1)Br)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H8Br2ClN5S	-6	44.43	-23.924	-2.5
1731	<chem>Brc1cc(I)c(c(c1)I)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H8BrI2N5S	-5.9	50.95	-24.393	1.8
1732	<chem>Brc1cc(F)c(c(c1)I)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H8BrFIN5S	-6.2	44.01	-25.278	-2.1
1733	<chem>Brc1cc(F)c(c(c1)F)Nc1nnc(s1)c1[nH]cnc1C</chem>	C12H8BrF2N5S	-6.3	49.91	-25.353	22.1

1734	Brc1cc(F)c(c(c1)Cl)Nc1nnc(s1)c1[nH]cnc1C	C12H8BrClFN5S	-7.1	43.4	-25.178	-2.4
1735	Brc1cc(F)c(c(c1)Br)Nc1nnc(s1)c1[nH]cnc1C	C12H8Br2FN5S	-6.9	46.02	-25.41	-2.5
1736	Brc1cc(Cl)c(c(c1)I)Nc1nnc(s1)c1[nH]cnc1C	C12H8BrClIN5S	-6.1	43.01	-24.523	-3.2
1737	Brc1cc(Cl)c(c(c1)Cl)Nc1nnc(s1)c1[nH]cnc1C	C12H8BrCl2N5S	-6.8	53.51	-24.831	-2.5
1738	Brc1cc(Cl)c(c(c1)Br)Nc1nnc(s1)c1[nH]cnc1C	C12H8Br2ClN5S	-6.5	54.58	-24.608	-2.5
1739	Brc1cc(Br)c(c(c1)I)Nc1nnc(s1)c1[nH]cnc1C	C12H8Br2IN5S	-6	43.05	-24.298	-3.3
1740	Brc1cc(Br)c(c(c1)Br)Nc1nnc(s1)c1[nH]cnc1C	C12H8Br3N5S	-6	43.52	-23.923	-2.6
1741	lc1cc(I)c(c(c1)I)Nc1nnc(s1)c1ccoc1C	C13H8I3N3OS	-5.9	45.16	-21.257	1.2
1742	lc1cc(F)c(c(c1)I)Nc1nnc(s1)c1ccoc1C	C13H8FI2N3OS	-6.6	46.94	-21.484	1.5
1743	lc1cc(F)c(c(c1)F)Nc1nnc(s1)c1ccoc1C	C13H8F2IN3OS	-7.4	53.57	-22.962	-6.8
1744	lc1cc(F)c(c(c1)Cl)Nc1nnc(s1)c1ccoc1C	C13H8ClFIN3OS	-7.2	47.33	-22.061	15.0
1745	lc1cc(F)c(c(c1)Br)Nc1nnc(s1)c1ccoc1C	C13H8BrFIN3OS	-7.1	47.37	-21.633	1.9
1746	lc1cc(Cl)c(c(c1)I)Nc1nnc(s1)c1ccoc1C	C13H8ClI2N3OS	-6	56.35	-21.349	1.3
1747	lc1cc(Cl)c(c(c1)Cl)Nc1nnc(s1)c1ccoc1C	C13H8Cl2IN3OS	-6	46.16	-20.827	-0.4
1748	lc1cc(Cl)c(c(c1)Br)Nc1nnc(s1)c1ccoc1C	C13H8BrClIN3OS	-6.6	46.22	-21.112	3.4
1749	lc1cc(Br)c(c(c1)I)Nc1nnc(s1)c1ccoc1C	C13H8BrI2N3OS	-6	45.85	-21.324	0.6
1750	lc1cc(Br)c(c(c1)Br)Nc1nnc(s1)c1ccoc1C	C13H8Br2IN3OS	-6.4	45.09	-21.08	0.7
1751	Fc1cc(I)c(c(c1)I)Nc1nnc(s1)c1ccoc1C	C13H8FI2N3OS	-5.9	52.01	-23.47	3.7
1752	Fc1cc(F)c(c(c1)I)Nc1nnc(s1)c1ccoc1C	C13H8F2IN3OS	-6.1	48.08	-24.862	18.4
1753	Fc1cc(F)c(c(c1)F)Nc1nnc(s1)c1ccoc1C	C13H8F3N3OS	-7.1	55.06	-26.734	8.3
1754	Fc1cc(F)c(c(c1)Cl)Nc1nnc(s1)c1ccoc1C	C13H8ClF2N3OS	-7.2	57.35	-24.858	19.7
1755	Fc1cc(F)c(c(c1)Br)Nc1nnc(s1)c1ccoc1C	C13H8BrF2N3OS	-7.1	48.17	-24.876	24.7
1756	Fc1cc(Cl)c(c(c1)I)Nc1nnc(s1)c1ccoc1C	C13H8ClFIN3OS	-6	46.17	-24.034	-2.4
1757	Fc1cc(Cl)c(c(c1)Cl)Nc1nnc(s1)c1ccoc1C	C13H8Cl2FN3OS	-7.2	60.92	-23.988	-3.7
1758	Fc1cc(Cl)c(c(c1)Br)Nc1nnc(s1)c1ccoc1C	C13H8BrClFN3OS	-6	51.03	-24.059	-2.2
1759	Fc1cc(Br)c(c(c1)I)Nc1nnc(s1)c1ccoc1C	C13H8BrFIN3OS	-5.9	58.94	-23.918	1.0
1760	Fc1cc(Br)c(c(c1)Br)Nc1nnc(s1)c1ccoc1C	C13H8Br2FN3OS	-6.5	48.85	-23.83	-3.2
1761	Clc1cc(I)c(c(c1)I)Nc1nnc(s1)c1ccoc1C	C13H8ClI2N3OS	-5.8	44.88	-21.285	-4.7
1762	Clc1cc(F)c(c(c1)I)Nc1nnc(s1)c1ccoc1C	C13H8ClFIN3OS	-6.2	48.08	-22.858	14.4
1763	Clc1cc(F)c(c(c1)F)Nc1nnc(s1)c1ccoc1C	C13H8ClF2N3OS	-7.4	60.42	-23.087	-4.9
1764	Clc1cc(F)c(c(c1)Cl)Nc1nnc(s1)c1ccoc1C	C13H8Cl2FN3OS	-7.2	56.62	-23.083	17.1

1765	Clc1cc(F)c(c(c1)Br)Nc1nnc(s1)c1ccoc1C	C13H8BrClFN3OS	-7.1	55.79	-22.489	27.9
1766	Clc1cc(Cl)c(c(c1)I)Nc1nnc(s1)c1ccoc1C	C13H8Cl2IN3OS	-6	50.34	-21.87	-2.4
1767	Clc1cc(Cl)c(c(c1)Cl)Nc1nnc(s1)c1ccoc1C	C13H8Cl3N3OS	-6.5	46.5	-21.988	-1.1
1768	Clc1cc(Cl)c(c(c1)Br)Nc1nnc(s1)c1ccoc1C	C13H8BrCl2N3OS	-6.3	48.87	-22.209	21.1
1769	Clc1cc(Br)c(c(c1)I)Nc1nnc(s1)c1ccoc1C	C13H8BrClIN3OS	-6	46.02	-21.733	-6.5
1770	Clc1cc(Br)c(c(c1)Br)Nc1nnc(s1)c1ccoc1C	C13H8Br2ClN3OS	-6.5	45.62	-21.643	-1.4
1771	Brc1cc(I)c(c(c1)I)Nc1nnc(s1)c1ccoc1C	C13H8BrI2N3OS	-5.9	45.18	-21.249	1.4
1772	Brc1cc(F)c(c(c1)I)Nc1nnc(s1)c1ccoc1C	C13H8BrFIN3OS	-6.1	46.93	-22.011	38.9
1773	Brc1cc(F)c(c(c1)F)Nc1nnc(s1)c1ccoc1C	C13H8BrF2N3OS	-7.5	51.35	-23.035	-4.6
1774	Brc1cc(F)c(c(c1)Cl)Nc1nnc(s1)c1ccoc1C	C13H8BrClFN3OS	-7.2	48.05	-23.13	5.4
1775	Brc1cc(F)c(c(c1)Br)Nc1nnc(s1)c1ccoc1C	C13H8Br2FN3OS	-6.2	47.65	-22.663	26.4
1776	Brc1cc(Cl)c(c(c1)I)Nc1nnc(s1)c1ccoc1C	C13H8BrClIN3OS	-6.1	46.6	-21.359	-0.6
1777	Brc1cc(Cl)c(c(c1)Cl)Nc1nnc(s1)c1ccoc1C	C13H8BrCl2N3OS	-6	45.13	-22.231	29.7
1778	Brc1cc(Cl)c(c(c1)Br)Nc1nnc(s1)c1ccoc1C	C13H8Br2ClN3OS	-6	45.53	-21.103	3.6
1779	Brc1cc(Br)c(c(c1)I)Nc1nnc(s1)c1ccoc1C	C13H8Br2IN3OS	-6	44.9	-21.333	-0.3
1780	Brc1cc(Br)c(c(c1)Br)Nc1nnc(s1)c1ccoc1C	C13H8Br3N3OS	-6	59.26	-21.082	0.0
1781	Ic1cc(I)c(c(c1)I)Nc1nnc(s1)C1CCCC1	C13H12I3N3S	-5.9	44.23	-16.11	22.2
1782	Ic1cc(F)c(c(c1)I)Nc1nnc(s1)C1CCCC1	C13H12FI2N3S	-6	44.58	-17.211	13.1
1783	Ic1cc(F)c(c(c1)F)Nc1nnc(s1)C1CCCC1	C13H12F2IN3S	-6.5	50.67	-18.644	17.7
1784	Ic1cc(F)c(c(c1)Cl)Nc1nnc(s1)C1CCCC1	C13H12ClFIN3S	-6.3	48	-18.677	8.7
1785	Ic1cc(F)c(c(c1)Br)Nc1nnc(s1)C1CCCC1	C13H12BrFIN3S	-6.1	49.73	-17.562	11.6
1786	Ic1cc(Cl)c(c(c1)I)Nc1nnc(s1)C1CCCC1	C13H12ClI2N3S	-6	44.02	-17.021	22.8
1787	Ic1cc(Cl)c(c(c1)Cl)Nc1nnc(s1)C1CCCC1	C13H12Cl2IN3S	-6	40.84	-16.181	-17.7
1788	Ic1cc(Cl)c(c(c1)Br)Nc1nnc(s1)C1CCCC1	C13H12BrClIN3S	-6	49.43	-16.82	24.3
1789	Ic1cc(Br)c(c(c1)I)Nc1nnc(s1)C1CCCC1	C13H12BrI2N3S	-5.9	43.63	-16.614	22.6
1790	Ic1cc(Br)c(c(c1)Br)Nc1nnc(s1)C1CCCC1	C13H12Br2IN3S	-5.9	47.07	-16.389	25.4
1791	Fc1cc(I)c(c(c1)I)Nc1nnc(s1)C1CCCC1	C13H12FI2N3S	-5.9	45.69	-17.053	19.6
1792	Fc1cc(F)c(c(c1)I)Nc1nnc(s1)C1CCCC1	C13H12F2IN3S	-6.4	47.69	-18.237	-0.4
1793	Fc1cc(F)c(c(c1)F)Nc1nnc(s1)C1CCCC1	C13H12F3N3S	-6.7	51.16	-20.169	23.6
1794	Fc1cc(F)c(c(c1)Cl)Nc1nnc(s1)C1CCCC1	C13H12ClF2N3S	-6.6	50.28	-18.163	32.0
1795	Fc1cc(F)c(c(c1)Br)Nc1nnc(s1)C1CCCC1	C13H12BrF2N3S	-6.4	51.35	-18.252	-2.2

1796	Fc1cc(Cl)c(c(c1)I)Nc1nnc(s1)C1CCCC1	C13H12ClFIN3S	-6.6	50.72	-17.979	20.3
1797	Fc1cc(Cl)c(c(c1)Cl)Nc1nnc(s1)C1CCCC1	C13H12Cl2FN3S	-6.5	43.42	-17.824	11.0
1798	Fc1cc(Cl)c(c(c1)Br)Nc1nnc(s1)C1CCCC1	C13H12BrClFN3S	-6.3	45.91	-17.88	21.8
1799	Fc1cc(Br)c(c(c1)I)Nc1nnc(s1)C1CCCC1	C13H12BrFIN3S	-5.9	51.41	-17.558	20.1
1800	Fc1cc(Br)c(c(c1)Br)Nc1nnc(s1)C1CCCC1	C13H12Br2FN3S	-5.9	45.54	-17.491	21.5
1801	Clc1cc(I)c(c(c1)I)Nc1nnc(s1)C1CCCC1	C13H12ClI2N3S	-5.9	44.93	-16.611	20.4
1802	Clc1cc(F)c(c(c1)I)Nc1nnc(s1)C1CCCC1	C13H12ClFIN3S	-6.2	44.8	-17.746	8.8
1803	Clc1cc(F)c(c(c1)F)Nc1nnc(s1)C1CCCC1	C13H12ClF2N3S	-6.7	52.32	-18.638	17.4
1804	Clc1cc(F)c(c(c1)Cl)Nc1nnc(s1)C1CCCC1	C13H12Cl2FN3S	-6.5	50.12	-16.985	-3.2
1805	Clc1cc(F)c(c(c1)Br)Nc1nnc(s1)C1CCCC1	C13H12BrClFN3S	-6.2	44.27	-16.835	-3.2
1806	Clc1cc(Cl)c(c(c1)I)Nc1nnc(s1)C1CCCC1	C13H12Cl2IN3S	-6	45.55	-17.517	21.1
1807	Clc1cc(Cl)c(c(c1)Cl)Nc1nnc(s1)C1CCCC1	C13H12Cl3N3S	-6.2	43.89	-16.421	-15.4
1808	Clc1cc(Cl)c(c(c1)Br)Nc1nnc(s1)C1CCCC1	C13H12BrCl2N3S	-6.2	49.8	-17.401	22.7
1809	Clc1cc(Br)c(c(c1)I)Nc1nnc(s1)C1CCCC1	C13H12BrClIN3S	-5.9	45.68	-17.108	20.9
1810	Clc1cc(Br)c(c(c1)Br)Nc1nnc(s1)C1CCCC1	C13H12Br2ClN3S	-6	45.25	-17.036	23.7
1811	Brc1cc(I)c(c(c1)I)Nc1nnc(s1)C1CCCC1	C13H12BrI2N3S	-5.9	44.4	-16.366	21.2
1812	Brc1cc(F)c(c(c1)I)Nc1nnc(s1)C1CCCC1	C13H12BrFIN3S	-6	45.67	-17.51	10.9
1813	Brc1cc(F)c(c(c1)F)Nc1nnc(s1)C1CCCC1	C13H12BrF2N3S	-6.2	50.27	-18.643	17.6
1814	Brc1cc(F)c(c(c1)Cl)Nc1nnc(s1)C1CCCC1	C13H12BrClFN3S	-6.3	49.85	-18.679	8.5
1815	Brc1cc(F)c(c(c1)Br)Nc1nnc(s1)C1CCCC1	C13H12Br2FN3S	-6	44.46	-16.836	-3.2
1816	Brc1cc(Cl)c(c(c1)I)Nc1nnc(s1)C1CCCC1	C13H12BrClIN3S	-6	45.03	-17.289	21.9
1817	Brc1cc(Cl)c(c(c1)Cl)Nc1nnc(s1)C1CCCC1	C13H12BrCl2N3S	-6.2	49.99	-16.243	-15.7
1818	Brc1cc(Cl)c(c(c1)Br)Nc1nnc(s1)C1CCCC1	C13H12Br2ClN3S	-6	47.56	-17.163	23.4
1819	Brc1cc(Br)c(c(c1)I)Nc1nnc(s1)C1CCCC1	C13H12Br2IN3S	-5.9	44.64	-16.874	21.7
1820	Brc1cc(Br)c(c(c1)Br)Nc1nnc(s1)C1CCCC1	C13H12Br3N3S	-5.9	43.15	-16.77	23.1