Bioisosteric-replacement-driven optimization of 4-methoxynaphthalene-N-acylhydrazones with anti-*Paracoccidioides* activity

Amanda Alves de Oliveira[1]†*, Lívia do Carmo Silva[2]†*, Andrew Matheus Frederico Rozada[3], Vinícius Alexandre Fiaia Costa [4], Célia Maria de Almeida Soares[2], Flavio Augusto Vicente Seixas [5], Bruno Junior Neves[4], Gisele Freitas Gauze[3], Maristela Pereira[2]

[1] Institute of Tropical Pathology and Public Health, Federal University of Goiás, CEP: 74605-050, Goiânia, Goiás, Brazil.

[2] Laboratory for Molecular Biology, Institute of Biological Sciences, Federal University of Goiás, CEP: 74690-900, Goiânia, Goiás, Brazil.

[3] Chemistry Department, State University of Maringá, 87020-900, Maringá, Paraná, Brazil.

[4] LabChem – Laboratory of Cheminformatics, Faculty of Pharmacy, Federal University of Goiás, 74605-170, Goiânia, Goiás, Brazil.

[5] Department of Technology, State University of Maringá, 87506-370, Umuarama, Paraná, Brazil

† These authors contributed equally to this work

Corresponding author

* Laboratory for Molecular Biology, Federal University of Goiás, Avenida Esperança, s/n, ICB2, Sala 206, Goiânia, GO, 74690-900, Brazil; Telephone: +55 62 3521-1110; E-mail: liviacarmo.bio@gmail.com; o.amanda.alves@gmail.com.

Table S1. The vROC analysis result. The statistics of the shape-based model using three scoring functions (RefTverskyCombo, TanimotoCombo, and FitTverskyCombo)

ROCS Rank	SMILES	ROCS Tanimoto Combo	ROCS Shape Tanimoto	ROCS Color Tanimoto	ROCS Ref Tversky	ROCS Ref Color Tversky	ROCS RefTversky Combo	ROCS FitTversky	ROCS FitColor Tversky	ROCS FitTversky Combo	ROCS Scaled Color	ROCS Combo Score	ROCS Color Score	ROCS Overlap
1	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cc(cc(c3O)F)F	1.808	0.808	1.000	0.714	1.000	1.714	1.195	1.000	2.195	1.000	1.808	-9.006	1.487.297
2	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cc(cc(c3N)Cl)Cl	1.799	0.800	0.999	0.705	1.000	1.705	1.202	1.000	2.202	1.000	1.800	-9.004	1.467.565
3	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cccc(c3O)F	1.794	0.794	1.000	0.698	1.000	1.698	1.210	1.000	2.210	1.000	1.794	-9.006	1.452.219
4	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(cc3N)F	1.792	0.793	0.999	0.697	1.000	1.696	1.211	1.000	2.211	1.000	1.793	-9.004	1.449.161
5	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3c(cccc3F)N	1.792	0.793	0.999	0.697	1.000	1.697	1.210	1.000	2.209	1.000	1.792	-9.003	1.449.891
6	Cc1ccc(c(c1)/C=N\NC(=O)c2ccc(c3c2cccc3)OC)O	1.792	0.792	1.000	0.695	1.000	1.695	1.212	1.000	2.212	1.000	1.792	-9.006	1.446.425

7	Cc1ccc(c(c1)O)/C=N\NC(=O)c2ccc(c3c2cccc3)OC	1.791	0.791	1.000	0.695	1.000	1.695	1.212	1.000	2.212	1.000	1.791	-9.006	1.446.114
8	Cc1ccc(c(c1)N)/C=N\NC(=O)c2ccc(c3c2cccc3)OC	1.791	0.791	0.999	0.695	1.000	1.695	1.213	1.000	2.212	1.000	1.791	-9.004	1.445.481
9	Cc1cccc(c1/C=N\NC(=O)c2ccc(c3c2cccc3)OC)N	1.791	0.792	0.999	0.695	1.000	1.695	1.212	1.000	2.211	1.000	1.791	-9.003	1.446.276
10	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cc(ccc3O)Cl	1.789	0.789	1.000	0.693	1.000	1.693	1.213	1.000	2.213	1.000	1.789	-9.006	1.440.966
11	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(cc3O)Cl	1.789	0.789	1.000	0.693	1.000	1.693	1.213	1.000	2.213	1.000	1.789	-9.006	1.440.764
12	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(cc3N)Cl	1.788	0.789	0.999	0.692	1.000	1.692	1.214	1.000	2.214	1.000	1.789	-9.004	1.440.051
13	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3c(cccc3Cl)O	1.788	0.789	0.999	0.693	0.999	1.693	1.213	0.999	2.212	0.999	1.789	-9.001	1.442.019
14	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccccc3O	1.779	0.779	1.000	0.681	1.000	1.681	1.227	1.000	2.227	1.000	1.779	-9.006	1.414.887
15	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccccc3N	1.778	0.779	0.999	0.681	1.000	1.680	1.228	1.000	2.228	1.000	1.779	-9.003	1.414.319
16	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cc(ccc3O)C(F)(F)F	1.762	0.762	1.000	0.709	1.000	1.709	1.109	1.000	2.109	1.000	1.762	-9.006	1.480.253
17	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cc(ccc3OC)F	1.694	0.805	0.889	0.712	0.894	1.605	1.196	0.994	2.189	0.889	1.694	-8.006	1.481.889
18	Cc1ccc(c(c1)/C=N\NC(=O)c2ccc(c3c2cccc3)OC)OC	1.693	0.804	0.889	0.710	0.894	1.604	1.197	0.994	2.191	0.889	1.693	-8.006	1.478.234
19	COc1cccc(c1/C=N\NC(=O)c2ccc(c3c2cccc3)OC)Cl	1.690	0.802	0.888	0.708	0.893	1.601	1.198	0.993	2.192	0.889	1.690	-8.002	1.473.642
20	COc1cccc(c1O)/C=N\NC(=O)c2ccc(c3c2cccc3)OC	1.688	0.788	0.900	0.703	0.994	1.697	1.180	0.905	2.085	1.000	1.788	-9.006	1.464.016
21	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cc(ccc3O)Br	1.687	0.787	0.900	0.691	0.994	1.686	1.214	0.905	2.118	1.000	1.787	-9.006	1.437.114

22	COc1ccc(c(c1)O)/C=N\NC(=O)c2ccc(c3c2cccc3)OC	1.686	0.786	0.900	0.702	0.994	1.696	1.180	0.905	2.085	1.000	1.786	-9.006	1.461.704
23	COc1ccc(c(c1)/[CH:1]=N\NC(=O)c2ccc(c3c2cccc3)OC)N	1.685	0.786	0.899	0.701	0.994	1.696	1.181	0.904	2.085	1.000	1.786	-9.003	1.460.769
24	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cccc(c3O)C#N	1.684	0.784	0.900	0.701	0.994	1.696	1.177	0.904	2.082	1.000	1.784	-9.006	1.460.220
25	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(cc3O)C#N	1.682	0.782	0.900	0.700	0.994	1.694	1.177	0.905	2.081	1.000	1.782	-9.006	1.457.275
26	COc1ccccc1/[CH:1]=N\NC(=O)c2ccc(c3c2cccc3)OC	1.680	0.791	0.889	0.696	0.894	1.589	1.211	0.994	2.205	0.889	1.680	-8.006	1.446.876
27	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc4ccccc4c3O	1.680	0.780	0.900	0.721	0.994	1.715	1.118	0.904	2.023	1.000	1.780	-9.007	1.505.089
28	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3c4ccccc4ccc3O	1.679	0.782	0.897	0.722	0.993	1.715	1.119	0.903	2.022	0.999	1.781	-8.995	1.507.083
29	CNc1ccccc1/C=N\NC(=O)c2ccc(c3c2cccc3)OC	1.679	0.790	0.889	0.694	0.894	1.588	1.212	0.994	2.206	0.889	1.679	-8.004	1.444.119
30	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cnccc3N	1.677	0.778	0.899	0.681	0.994	1.675	1.224	0.904	2.128	0.999	1.777	-9.000	1.415.080
31	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3c(cccn3)O	1.677	0.778	0.899	0.682	0.994	1.676	1.222	0.904	2.126	1.000	1.777	-9.002	1.416.367
32	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cccc(c3O)CC=C	1.673	0.773	0.900	0.702	0.994	1.697	1.150	0.905	2.055	1.000	1.773	-9.006	1.463.787
33	CCOc1ccc(c(c1)O)/C=N\NC(=O)c2ccc(c3c2cccc3)OC	1.671	0.771	0.900	0.702	0.994	1.696	1.147	0.905	2.051	1.000	1.771	-9.006	1.463.022
34	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccccc3OC(F)F	1.664	0.775	0.889	0.706	0.894	1.599	1.146	0.994	2.139	0.889	1.664	-8.006	1.470.955
35	c1ccc2c(c1)c(ccc2O)C(=O)N/N=C\c3c(cccc3F)O	1.646	0.746	0.900	0.666	0.994	1.660	1.192	0.905	2.097	1.000	1.746	-9.006	1.383.449
36	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(cc3N)c4cccs4	1.637	0.737	0.900	0.701	0.994	1.696	1.074	0.904	1.978	1.000	1.737	-9.004	1.465.373

37	c1ccc(c(c1)/C=N\NC(=O)c2ccc(c3c2cccc3)O)O	1.632	0.732	0.900	0.649	0.994	1.644	1.210	0.905	2.115	1.000	1.732	-9.006	1.347.464
38	c1ccc(c(c1)/C=N\NC(=O)c2c3ccccc3c(cc2Cl)Cl)O	1.629	0.742	0.888	0.659	0.893	1.552	1.204	0.993	2.197	0.888	1.630	-8.000	1.368.459
39	Cc1cc(c(cc1O)O)/C=N\NC(=O)c2ccc(c3c2cccc3)OC	1.623	0.804	0.818	0.711	0.989	1.700	1.195	0.826	2.021	1.000	1.804	-9.006	1.480.724
40	c1ccc(c(c1)/C=N\NC(=O)c2ccc(c3c2cccc3)Cl)O	1.622	0.733	0.889	0.648	0.894	1.542	1.219	0.994	2.213	0.889	1.622	-8.006	1.344.099
41	Cc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccccc3O	1.621	0.733	0.889	0.649	0.894	1.543	1.214	0.994	2.208	0.889	1.622	-8.006	1.346.547
42	CCc1cc(c(c(c1O)/[CH:1]=N\NC(=O)c2ccc(c3c2cccc3)OC)OC)Cl	1.618	0.801	0.818	0.733	0.989	1.722	1.131	0.825	1.956	1.000	1.800	-9.003	1.530.718
43	COc1ccc(c2c1cccc2)C(=O)N/N=[CH:1]\c3c(ccc(c3O)Br)OC	1.613	0.796	0.818	0.713	0.989	1.702	1.170	0.825	1.995	1.000	1.795	-9.002	1.486.771
44	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3c(ccc(c3OC)Br)O	1.612	0.794	0.818	0.712	0.989	1.701	1.168	0.826	1.994	1.000	1.794	-9.004	1.484.785
45	COc1ccc(c2c1cccc2)C(=O)N/N=[CH:1]\c3ccc(cc3O)O	1.611	0.793	0.818	0.697	0.989	1.686	1.210	0.826	2.036	1.000	1.793	-9.006	1.449.284
46	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3c(c(c(c(c3F)F)F)F)F	1.610	0.832	0.778	0.746	0.787	1.533	1.161	0.986	2.146	0.778	1.610	-7.006	1.558.436
47	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(cc3N)N	1.610	0.792	0.818	0.696	0.989	1.685	1.212	0.826	2.037	1.000	1.792	-9.004	1.447.386
48	COc1ccc(c2c1cccc2)C(=O)N/N=[CH:1]\c3cc(c(cc3O)[N+](=O)[O-])Cl	1.603	0.786	0.817	0.719	0.989	1.708	1.134	0.825	1.958	1.000	1.786	-9.006	1.500.936

49	c1ccc(c(c1)/C=N\NC(=O)c2cccc3c2cccc3Cl)O	1.601	0.712	0.889	0.637	0.894	1.531	1.199	0.994	2.193	0.889	1.601	-8.006	1.321.349
50	Cc1ccc2cccc(c2c1)C(=O)N/N=C\c3ccccc3O	1.601	0.712	0.889	0.638	0.894	1.532	1.195	0.994	2.188	0.889	1.601	-8.006	1.323.911
51	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cnc4ccccc4c3O	1.600	0.782	0.818	0.723	0.989	1.712	1.117	0.826	1.943	1.000	1.783	-9.009	1.509.773
52	Cc1ccc2ccccc2c1C(=O)N/N=C\c3ccccc3O	1.600	0.712	0.888	0.638	0.894	1.532	1.194	0.994	2.187	0.889	1.600	-8.004	1.324.082
53	COc1ccc(c2c1cccc2)C(=O)N/N=[CH:1]\c3cc(ccc3OC)Br	1.600	0.800	0.800	0.706	0.889	1.595	1.199	0.889	2.088	0.889	1.688	-8.006	1.469.215
54	COc1cccc(c1/C=N\NC(=O)c2ccc(c3c2cccc3)OC)OC	1.599	0.799	0.800	0.717	0.889	1.606	1.167	0.889	2.056	0.889	1.688	-8.005	1.495.062
55	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3c(cccc3O)[N+](=O)[O-]	1.596	0.780	0.816	0.710	0.988	1.698	1.145	0.824	1.970	1.000	1.780	-9.002	1.479.914
56	c1ccc(c(c1)/C=N\NC(=O)c2ccc(c3c2cccc3)C#N)O	1.594	0.752	0.843	0.667	0.915	1.582	1.201	0.915	2.116	0.915	1.666	-8.239	1.386.865
57	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cc(ccc3O)C(=O)N	1.594	0.776	0.818	0.706	0.989	1.695	1.146	0.826	1.972	1.000	1.776	-9.006	1.471.798
58	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(cc3O)[N+](=O)[O-]	1.593	0.776	0.817	0.707	0.989	1.696	1.143	0.825	1.968	1.000	1.776	-9.006	1.475.087
59	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(cc3N)[N+](=O)[O-]	1.593	0.776	0.817	0.707	0.989	1.696	1.144	0.824	1.968	1.000	1.776	-9.004	1.474.464
60	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cc(ccc3N)[N+](=O)[O	1.592	0.775	0.817	0.707	0.989	1.695	1.143	0.824	1.968	1.000	1.775	-9.003	1.473.673

	-]													
61	c1ccc2c(c1)cccc2C(=O)N/N=C\c3ccccc3O	1.588	0.699	0.889	0.623	0.894	1.517	1.210	0.994	2.204	0.889	1.588	-8.006	1.292.258
62	CC(C)c1ccc(c(c1)/C=N\NC(=O)c2ccc(c3c2cccc3)OC)OC	1.586	0.786	0.800	0.717	0.889	1.606	1.140	0.889	2.029	0.889	1.675	-8.006	1.495.164
63	Cc1ccc2cccc(c2n1)/C=N\NC(=O)c3ccc(c4c3cccc4)OC	1.586	0.786	0.800	0.724	0.889	1.613	1.122	0.889	2.011	0.889	1.675	-8.008	1.511.991
64	c1ccc(c(c1)/C=N\NC(=O)c2cccc3c2CCCC3)O	1.585	0.697	0.888	0.619	0.894	1.513	1.220	0.994	2.214	0.889	1.586	-8.003	1.283.106
65	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(c(c3F)F)F	1.585	0.807	0.778	0.714	0.787	1.501	1.192	0.986	2.178	0.778	1.585	-7.006	1.487.341
66	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3c(cc(cc3F)F)F	1.584	0.806	0.778	0.713	0.787	1.500	1.193	0.986	2.178	0.778	1.584	-7.006	1.485.822
67	Cc1cc(cc(c1/C=N\NC(=O)c2ccc(c3c2cccc3)OC)C)F	1.583	0.805	0.778	0.710	0.787	1.497	1.197	0.986	2.183	0.778	1.583	-7.006	1.479.483
68	CCc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccccc3O	1.579	0.779	0.800	0.679	0.889	1.568	1.231	0.889	2.120	0.889	1.668	-8.006	1.411.421
69	CCc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccccc3O	1.579	0.779	0.800	0.679	0.889	1.568	1.231	0.889	2.120	0.889	1.668	-8.006	1.411.406
70	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cc(cc(c3Cl)Cl)Cl	1.576	0.798	0.778	0.702	0.787	1.489	1.207	0.986	2.193	0.778	1.576	-7.006	1.461.177
71	Cc1c(cccc1F)/C=N\NC(=O)c2ccc(c3c2cccc3)OC	1.572	0.794	0.778	0.697	0.787	1.484	1.213	0.986	2.199	0.778	1.572	-7.006	1.450.234
72	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccccc3N=O	1.572	0.794	0.778	0.698	0.787	1.484	1.210	0.986	2.196	0.778	1.572	-7.006	1.451.507
73	Cc1cc(ccc1/C=N\NC(=O)c2ccc(c3c2cccc3)OC)F	1.571	0.793	0.778	0.696	0.787	1.483	1.213	0.986	2.199	0.778	1.571	-7.006	1.447.803
74	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3c(cccc3F)F	1.570	0.793	0.778	0.697	0.787	1.484	1.208	0.986	2.194	0.778	1.570	-7.006	1.451.036

75	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(cc3F)F	1.570	0.792	0.778	0.697	0.787	1.484	1.209	0.986	2.195	0.778	1.570	-7.006	1.449.876
76	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3c(cccc3Cl)F	1.569	0.792	0.778	0.695	0.787	1.481	1.214	0.986	2.200	0.778	1.569	-7.006	1.444.632
77	Cc1ccc(c(c1)C)/C=N\NC(=O)c2ccc(c3c2cccc3)OC	1.569	0.791	0.778	0.694	0.787	1.481	1.214	0.986	2.200	0.778	1.569	-7.006	1.444.083
78	Cc1cccc(c1/C=N\NC(=O)c2ccc(c3c2cccc3)OC)Cl	1.568	0.790	0.778	0.693	0.787	1.479	1.217	0.986	2.202	0.778	1.568	-7.006	1.440.541
79	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cccc(c3F)Cl	1.568	0.790	0.778	0.694	0.787	1.480	1.213	0.986	2.199	0.778	1.568	-7.006	1.442.869
80	Cc1cc(ccc1/C=N\NC(=O)c2ccc(c3c2cccc3)OC)Cl	1.567	0.789	0.778	0.692	0.787	1.478	1.216	0.986	2.202	0.778	1.567	-7.006	1.438.738
81	Cc1cc(cc(c1/C=N\NC(=O)c2ccc(c3c2cccc3)OC)C)N(C)C	1.566	0.788	0.778	0.718	0.787	1.505	1.140	0.986	2.126	0.778	1.566	-7.006	1.498.975
82	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(cc3Cl)Cl	1.566	0.788	0.778	0.690	0.787	1.477	1.219	0.986	2.205	0.778	1.566	-7.006	1.434.505
83	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cc(ccc3Cl)Cl	1.565	0.788	0.778	0.690	0.787	1.477	1.219	0.986	2.205	0.778	1.566	-7.006	1.434.495
84	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3c(cccc3Cl)Cl	1.565	0.788	0.778	0.690	0.787	1.477	1.218	0.986	2.204	0.778	1.565	-7.005	1.434.904
85	COc1ccc(c2c1cccc2)C(=O)N/N=[CH:1]\c3ccccc3OCC#N	1.564	0.764	0.800	0.698	0.889	1.587	1.141	0.889	2.030	0.889	1.653	-8.006	1.455.608
86	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccccc3N=[N+]=[N-]	1.563	0.785	0.778	0.703	0.787	1.489	1.176	0.986	2.162	0.778	1.563	-7.006	1.463.252
87	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccccc3C(F)(F)F	1.562	0.785	0.777	0.713	0.786	1.499	1.148	0.985	2.134	0.778	1.562	-7.003	1.486.099
88	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccccc3F	1.557	0.779	0.778	0.681	0.787	1.468	1.226	0.986	2.212	0.778	1.557	-7.006	1.415.115
89	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccccc3Cl	1.556	0.778	0.778	0.678	0.787	1.465	1.233	0.986	2.219	0.778	1.556	-7.006	1.408.861

90	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3c(ccc(c3O)Br)O	1.551	0.802	0.750	0.708	0.983	1.691	1.198	0.759	1.957	1.000	1.801	-9.003	1.473.928
91	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3c(c4ccccc4o3)O	1.550	0.784	0.766	0.715	0.954	1.670	1.139	0.795	1.935	0.965	1.749	-8.691	1.492.429
92	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cc(c(cc3O)O)Br	1.550	0.800	0.750	0.707	0.984	1.690	1.198	0.760	1.957	1.000	1.800	-9.006	1.471.314
93	COc1ccc(c2c1cccc2)C(=O)N/N=C\[C@H](c3ccccc3)O	1.546	0.745	0.802	0.671	0.890	1.561	1.174	0.890	2.064	0.890	1.635	-8.015	1.395.109
94	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3c(c4ccccc4o3)N	1.545	0.784	0.761	0.715	0.950	1.666	1.140	0.792	1.932	0.961	1.745	-8.654	1.492.425
95	Cc1cc(cc(c1/C=N\NC(=O)c2ccc(c3c2cccc3)OC)OC)O	1.544	0.817	0.727	0.726	0.884	1.610	1.182	0.804	1.986	0.889	1.706	-8.005	1.513.272
96	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cc(ccc3F)C(F)(F)F	1.540	0.762	0.778	0.709	0.787	1.496	1.109	0.986	2.095	0.778	1.540	-7.006	1.480.886
97	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(c(c3)CN=O)F	1.540	0.762	0.778	0.697	0.787	1.484	1.138	0.986	2.124	0.778	1.540	-7.006	1.453.575
98	c1ccc(c(c1)/C=N\NC(=O)c2ccc(cc2)OC(F)(F)F)O	1.539	0.655	0.884	0.606	0.891	1.497	1.140	0.991	2.130	0.886	1.541	-7.978	1.258.597
99	COc1ccc(c2c1cccc2)C(=O)N/N=C\[C@H](c3ccc(cc3)F)O	1.538	0.736	0.802	0.675	0.890	1.565	1.140	0.890	2.030	0.890	1.626	-8.015	1.405.934
100	Cc1ccc(c(c1/C=N\NC(=O)c2ccc(c3c2cccc3)OC)OC)O	1.537	0.810	0.727	0.723	0.884	1.607	1.176	0.804	1.980	0.889	1.699	-8.005	1.506.821
101	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccccc3C#N	1.537	0.788	0.749	0.694	0.814	1.507	1.208	0.905	2.112	0.809	1.597	-7.288	1.442.824
102	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cc(cc(c3O)Br)[N+](=O)[O-]	1.534	0.785	0.749	0.718	0.983	1.702	1.134	0.759	1.893	1.000	1.785	-9.005	1.498.929
103	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccccc3C=O	1.533	0.788	0.745	0.694	0.811	1.505	1.208	0.902	2.109	0.807	1.594	-7.266	1.443.097

104	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3c(ccc(c3OC)Br)OC	1.533	0.805	0.727	0.726	0.884	1.610	1.156	0.804	1.960	0.889	1.694	-8.005	1.515.673
105	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cc(c(cc3OC)OC)OC	1.532	0.805	0.727	0.738	0.884	1.622	1.128	0.804	1.932	0.889	1.694	-8.006	1.540.909
106	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3c(ccs3)Cl	1.529	0.754	0.775	0.654	0.785	1.439	1.253	0.984	2.236	0.776	1.530	-6.991	1.357.469
107	CN(C)c1ccccc1/C=N\NC(=O)c2ccc(c3c2cccc3)OC	1.528	0.751	0.778	0.683	0.786	1.469	1.153	0.986	2.139	0.778	1.529	-7.004	1.421.844
108	COc1ccc(c2c1cccc2)C(=O)N/N=C\C3=CCCCC3	1.528	0.750	0.778	0.654	0.787	1.441	1.243	0.986	2.228	0.778	1.528	-7.006	1.357.867
109	c1ccc(c(c1)/C=N\NC(=O)c2ccnc3c2cccc3)O	1.528	0.698	0.829	0.624	0.907	1.531	1.205	0.907	2.112	0.907	1.605	-8.166	1.294.307
110	c1ccc(c(c1)/C=N\NC(=O)c2ccnc3c2cccc3)O	1.527	0.698	0.829	0.624	0.907	1.531	1.205	0.907	2.112	0.907	1.605	-8.166	1.294.200
111	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cccc4c3OCO4	1.527	0.801	0.726	0.715	0.884	1.599	1.177	0.802	1.979	0.889	1.690	-8.007	1.490.079
112	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(cc3O)C(=O)O	1.525	0.775	0.749	0.706	0.984	1.690	1.145	0.759	1.904	1.000	1.775	-9.006	1.472.222
113	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cc(ccc3OC)CO	1.525	0.797	0.727	0.715	0.884	1.599	1.169	0.804	1.973	0.889	1.686	-8.006	1.490.107
114	Cn1cccc1/C=N\NC(=O)c2ccc(c3c2cccc3)OC	1.521	0.750	0.772	0.658	0.783	1.441	1.228	0.981	2.209	0.774	1.524	-6.974	1.366.569
115	Cc1cc2cccc(c2nc1)C(=O)N/N=C\c3ccccc3O	1.510	0.711	0.799	0.639	0.888	1.527	1.190	0.888	2.078	0.888	1.600	-8.000	1.326.223
116	COc1ccc2cccc(c2c1)C(=O)N/N=C\c3ccccc3O	1.510	0.710	0.800	0.646	0.889	1.535	1.163	0.889	2.052	0.889	1.599	-8.006	1.341.661
117	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cccc4c3OCCCO4	1.509	0.785	0.724	0.722	0.882	1.604	1.124	0.802	1.926	0.887	1.672	-7.987	1.507.753
118	COc1ccc2c(c1)cccc2C(=O)N/N=C\c3ccccc3O	1.508	0.708	0.800	0.645	0.889	1.533	1.161	0.889	2.050	0.889	1.597	-8.006	1.339.324

119	COc1ccc2ccccc2c1C(=O)N/N=C\c3ccccc3O	1.508	0.708	0.800	0.645	0.889	1.534	1.160	0.889	2.049	0.889	1.597	-8.005	1.340.329
120	COc1ccc2ccccc2c1C(=O)N/N=C\c3ccccc3O	1.508	0.708	0.800	0.645	0.889	1.534	1.160	0.889	2.049	0.889	1.597	-8.005	1.340.317
121	CCc1ccc2cccc(c2c1)C(=O)N/N=C\c3ccccc3O	1.507	0.707	0.800	0.642	0.889	1.531	1.165	0.889	2.054	0.889	1.596	-8.006	1.334.563
122	Cc1ccc2ccccc2c1/C=N\NC(=O)c3ccc(c4c3cccc4)OC	1.506	0.806	0.700	0.733	0.782	1.516	1.141	0.869	2.010	0.778	1.584	-7.008	1.530.882
123	COCc1ccccc1/C=N\NC(=O)c2ccc(c3c2cccc3)OC	1.502	0.780	0.722	0.697	0.796	1.494	1.180	0.885	2.065	0.792	1.572	-7.131	1.451.900
124	Cc1cccnc1/C=N\NC(=O)c2ccc(c3c2cccc3)OC	1.501	0.764	0.737	0.674	0.806	1.480	1.212	0.896	2.108	0.801	1.565	-7.218	1.400.353
125	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccccc3[N+](=O)[O-]	1.499	0.798	0.702	0.709	0.825	1.535	1.186	0.824	2.010	0.825	1.623	-7.434	1.477.195
126	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3c(cccn3)Cl	1.499	0.762	0.737	0.671	0.806	1.477	1.215	0.896	2.110	0.801	1.563	-7.218	1.395.101
127	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cccs3	1.499	0.724	0.775	0.633	0.785	1.417	1.249	0.984	2.233	0.776	1.500	-6.990	1.310.932
128	c1ccc(c(c1)/C=N\NC(=O)c2cccc3c2ccnc3)O	1.498	0.698	0.800	0.623	0.889	1.512	1.206	0.889	2.095	0.889	1.587	-8.006	1.292.711
129	c1ccc(c(c1)/C=N\NC(=O)c2cccc3c2cccn3)O	1.498	0.697	0.800	0.624	0.889	1.513	1.204	0.889	2.093	0.889	1.586	-8.006	1.293.304
130	c1ccc2c(c1)ccnc2C(=O)N/N=C\c3ccccc3O	1.498	0.698	0.800	0.624	0.889	1.512	1.205	0.889	2.094	0.889	1.587	-8.004	1.293.367
131	Cc1cc(cc(c1/C=N\NC(=O)c2ccc(c3c2cccc3)OC)C)NC	1.497	0.796	0.700	0.714	0.782	1.496	1.169	0.870	2.039	0.778	1.574	-7.006	1.488.278
132	c1ccc(c(c1)/C=N\NC(=O)c2cccc3c2nccc3)O	1.496	0.697	0.799	0.624	0.888	1.512	1.203	0.888	2.092	0.888	1.585	-8.000	1.293.437
133	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccccc3[S@@](=O)C	1.491	0.777	0.714	0.692	0.791	1.483	1.189	0.880	2.068	0.787	1.564	-7.087	1.439.947

134	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccccc3C(=O)N	1.489	0.797	0.692	0.707	0.818	1.525	1.189	0.818	2.006	0.818	1.615	-7.366	1.473.286
135	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cc(ccc3F)Br	1.487	0.787	0.700	0.691	0.782	1.473	1.213	0.870	2.083	0.778	1.565	-7.006	1.437.379
136	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccccn3	1.484	0.747	0.737	0.657	0.806	1.463	1.225	0.896	2.121	0.801	1.549	-7.217	1.364.286
137	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cc(ccc3O)c4cc[nH]n4	1.483	0.733	0.750	0.705	0.984	1.688	1.058	0.760	1.817	1.000	1.733	-9.006	1.473.554
138	CCNc1cc(c(c(c1)C)/C=N\NC(=O)c2ccc(c3c2cccc3)OC)C	1.483	0.783	0.700	0.715	0.782	1.497	1.138	0.870	2.008	0.778	1.561	-7.005	1.491.369
139	Cc1cccc(c1/C=N\NC(=O)c2ccc(c3c2cccc3)OC)CO	1.482	0.795	0.687	0.705	0.815	1.519	1.191	0.815	2.006	0.815	1.609	-7.337	1.467.187
140	Cc1c(c(n(n1)C)C)/C=N\NC(=O)c2ccc(c3c2cccc3)OC	1.482	0.786	0.696	0.694	0.779	1.473	1.204	0.866	2.071	0.775	1.561	-6.980	1.443.010
141	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cc(ccc3O)c4c[nH]nc4	1.481	0.731	0.750	0.703	0.984	1.687	1.056	0.760	1.816	1.000	1.731	-9.006	1.470.218
142	Cc1c(cccn1)/C=N\NC(=O)c2ccc(c3c2cccc3)OC	1.479	0.779	0.701	0.681	0.783	1.463	1.226	0.870	2.096	0.778	1.557	-7.010	1.414.695
143	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cc(c(c(c3)Cl)OC)Cl	1.479	0.779	0.700	0.703	0.782	1.485	1.161	0.870	2.031	0.778	1.557	-7.006	1.464.697
144	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3c(cc(cc3OC)O)OC	1.479	0.812	0.667	0.733	0.879	1.612	1.154	0.734	1.888	0.889	1.701	-8.005	1.529.063
145	Cc1cnccc1/C=N\NC(=O)c2ccc(c3c2cccc3)OC	1.478	0.778	0.700	0.681	0.782	1.463	1.226	0.870	2.096	0.778	1.556	-7.006	1.414.279
146	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccncc3Cl	1.477	0.777	0.700	0.679	0.782	1.461	1.230	0.870	2.099	0.778	1.555	-7.006	1.410.213
147	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cnccc3Cl	1.477	0.777	0.700	0.679	0.782	1.461	1.230	0.870	2.099	0.778	1.555	-7.005	1.410.168
148	COc1ccc(c2c1cccc2)C(=O)N/N=[CH:1]\c3ccccc3SC	1.477	0.777	0.700	0.684	0.782	1.466	1.213	0.870	2.082	0.778	1.555	-7.006	1.421.385

149	COc1ccc(c(c1)OC)C(=O)N/N=C\c2ccccc2O	1.476	0.678	0.798	0.609	0.888	1.497	1.201	0.888	2.089	0.887	1.566	-7.993	1.262.233
150	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccccc3Br	1.476	0.776	0.700	0.677	0.782	1.459	1.234	0.870	2.104	0.778	1.554	-7.006	1.405.404
151	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cc4c(cc3OC)OCO4	1.475	0.809	0.667	0.736	0.880	1.617	1.138	0.733	1.871	0.890	1.699	-8.019	1.537.759
152	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(c(c3)F)OC	1.475	0.775	0.700	0.697	0.782	1.479	1.171	0.870	2.040	0.778	1.553	-7.006	1.450.468
153	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3c(c4ccccc4s3)Cl	1.472	0.773	0.699	0.702	0.782	1.484	1.151	0.868	2.018	0.777	1.551	-7.001	1.463.324
154	C[C@@H](c1ccccc1/C=N\NC(=O)c2ccc(c3c2cccc3)OC)O	1.471	0.792	0.680	0.703	0.809	1.512	1.190	0.809	1.999	0.809	1.601	-7.289	1.463.403
155	COc1ccc(cc1)C(=O)N/N=C\c2ccccc2O	1.469	0.585	0.883	0.541	0.891	1.432	1.164	0.991	2.154	0.886	1.471	-7.977	1.118.397
156	CCn1c(c(cn1)/C=N\NC(=O)c2ccc(c3c2cccc3)OC)C	1.468	0.772	0.696	0.686	0.779	1.465	1.194	0.866	2.061	0.775	1.547	-6.980	1.427.163
157	CCn1cc(c(n1)C)/C=N\NC(=O)c2ccc(c3c2cccc3)OC	1.466	0.770	0.696	0.685	0.779	1.464	1.193	0.866	2.059	0.775	1.545	-6.980	1.424.344
158	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cnc(nc3OC)OC	1.466	0.800	0.665	0.720	0.879	1.599	1.163	0.732	1.895	0.889	1.690	-8.007	1.500.578
159	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc4c(c3)ccs4	1.465	0.764	0.700	0.691	0.783	1.474	1.161	0.869	2.030	0.779	1.543	-7.012	1.439.127
160	Cc1c(c(on1)C)/C=N\NC(=O)c2ccc(c3c2cccc3)OC	1.463	0.767	0.696	0.675	0.779	1.455	1.215	0.867	2.082	0.775	1.542	-6.981	1.403.541
161	COc1ccc(c(c1OC)OC)C(=O)N/N=C\c2ccccc2O	1.459	0.733	0.726	0.655	0.883	1.538	1.194	0.803	1.997	0.888	1.620	-7.995	1.359.871
162	c1ccc(c(c1)/C=N\NC(=O)c2cccc3c2cco3)O	1.455	0.664	0.791	0.598	0.884	1.482	1.199	0.883	2.082	0.884	1.548	-7.961	1.239.091
163	Cc1cc(c(c(c1/C=N\NC(=O)c2ccc(c3c2cccc3)OC)C)O)C	1.454	0.817	0.637	0.725	0.778	1.503	1.183	0.778	1.962	0.778	1.595	-7.007	1.511.933

164	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cc(ccc3O)S(=O)(=O)O	1.451	0.760	0.692	0.702	0.978	1.680	1.121	0.703	1.824	1.000	1.759	-9.006	1.464.338
165	c1ccc(c(c1)/C=N\NC(=O)c2cccc3c2occ3)O	1.451	0.664	0.787	0.598	0.882	1.480	1.197	0.880	2.078	0.882	1.545	-7.941	1.239.215
166	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3c(=O)[nH]c4ccccc4n3	1.446	0.782	0.663	0.723	0.877	1.600	1.118	0.732	1.849	0.887	1.669	-7.985	1.509.566
167	Cc1c(cc(cc1O)F)/C=N\NC(=O)c2ccc(c3c2cccc3)OC	1.444	0.808	0.637	0.713	0.778	1.491	1.198	0.778	1.976	0.778	1.586	-7.007	1.484.317
168	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cc4ccccc4s3	1.443	0.745	0.698	0.681	0.781	1.462	1.146	0.868	2.013	0.777	1.522	-7.000	1.417.221
169	c1ccc(c(c1)/C=N\NC(=O)c2cccc3c2cccc3O)O	1.443	0.716	0.728	0.641	0.884	1.525	1.195	0.804	1.999	0.889	1.605	-8.008	1.330.135
170	Cc1ccc(c(c1/C=N\NC(=O)c2ccc(c3c2cccc3)OC)C)O	1.442	0.806	0.637	0.711	0.778	1.489	1.198	0.778	1.976	0.778	1.584	-7.007	1.480.833
171	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3c(cc(cc3F)O)F	1.442	0.806	0.636	0.713	0.778	1.491	1.193	0.778	1.971	0.778	1.584	-7.006	1.485.208
172	Cc1ccc(c(c1O)C)/C=N\NC(=O)c2ccc(c3c2cccc3)OC	1.442	0.806	0.637	0.711	0.778	1.489	1.198	0.778	1.976	0.778	1.584	-7.007	1.480.591
173	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cc(c(cc3F)O)F	1.442	0.806	0.637	0.713	0.778	1.491	1.193	0.778	1.971	0.778	1.584	-7.006	1.484.718
174	COc1cc(c(cc1OC)OC)C(=O)N/N=C\c2ccccc2O	1.442	0.717	0.725	0.646	0.882	1.528	1.181	0.803	1.984	0.887	1.604	-7.992	1.341.110
175	Cc1cc(cc(c1/C=N\NC(=O)c2ccc(c3c2cccc3)OC)C)O	1.441	0.805	0.636	0.710	0.778	1.488	1.198	0.778	1.975	0.778	1.582	-7.006	1.478.985
176	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccccc3S(=O)(=O)C	1.441	0.780	0.661	0.703	0.796	1.499	1.162	0.796	1.958	0.796	1.576	-7.172	1.465.202
177	COc1ccc(c2c1cccc2)C(=O)N/N=[CH:1]\c3ccc(cc3C(=O)O)	1.441	0.807	0.634	0.723	0.815	1.537	1.169	0.740	1.910	0.819	1.626	-7.379	1.506.684

	F													
178	Cc1cc(cc(c1/C=N\NC(=O)c2ccc(c3c2cccc3)OC)C)N	1.440	0.804	0.637	0.710	0.778	1.488	1.198	0.778	1.976	0.778	1.582	-7.006	1.477.683
179	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3c4ccccc4on3	1.439	0.767	0.672	0.698	0.805	1.503	1.149	0.803	1.952	0.805	1.572	-7.248	1.454.353
180	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3c(ccc(c3Cl)O)Cl	1.439	0.802	0.637	0.706	0.778	1.484	1.203	0.778	1.981	0.778	1.580	-7.007	1.470.608
181	CN1CCN(CC1)C(=O)/C=N\NC(=O)c2ccc(c3c2cccc3)OC	1.439	0.753	0.686	0.682	0.814	1.496	1.159	0.814	1.973	0.814	1.566	-7.327	1.420.500
182	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3nccs3	1.438	0.718	0.720	0.631	0.795	1.426	1.238	0.884	2.122	0.791	1.509	-7.122	1.307.725
183	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cc(c(cc3Cl)Cl)O	1.437	0.801	0.637	0.706	0.778	1.483	1.203	0.778	1.980	0.778	1.579	-7.006	1.468.755
184	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3c(cc(cc3Cl)O)Cl	1.437	0.801	0.637	0.706	0.778	1.484	1.202	0.778	1.980	0.778	1.579	-7.006	1.468.901
185	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccccc3c4ncco4	1.437	0.768	0.669	0.716	0.802	1.518	1.105	0.802	1.907	0.802	1.570	-7.222	1.494.688
186	Cc1cc(ccc1/C=N\NC(=O)c2ccc(c3c2cccc3)OC)CCN(C)C	1.437	0.737	0.700	0.697	0.782	1.479	1.083	0.870	1.953	0.778	1.515	-7.006	1.455.791
187	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cc(ccc3C(=O)O)Cl	1.435	0.802	0.634	0.718	0.815	1.532	1.171	0.740	1.911	0.819	1.621	-7.379	1.496.055
188	CCOC(=O)c1cc(ccc1Cl)/C=N\NC(=O)c2ccc(c3c2cccc3)OC	1.434	0.734	0.700	0.697	0.782	1.480	1.077	0.870	1.947	0.778	1.512	-7.006	1.456.484
189	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cccc4c3cccn4	1.433	0.796	0.637	0.721	0.778	1.499	1.151	0.778	1.929	0.778	1.575	-7.009	1.503.615
190	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccnc4c3cccc4	1.432	0.796	0.637	0.721	0.778	1.499	1.151	0.778	1.929	0.778	1.574	-7.008	1.503.289
191	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccco3	1.432	0.716	0.717	0.633	0.793	1.426	1.223	0.882	2.104	0.789	1.504	-7.103	1.312.957

192	Cn1cc(cn1)/C=N\NC(=O)c2ccc(c3c2cccc3)OC	1.432	0.737	0.696	0.652	0.779	1.432	1.213	0.866	2.080	0.775	1.512	-6.980	1.354.039
193	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cc(c(c(c3)F)O)F	1.431	0.795	0.637	0.707	0.778	1.485	1.184	0.778	1.962	0.778	1.572	-7.006	1.473.226
194	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc[nH]3	1.431	0.716	0.715	0.633	0.792	1.425	1.224	0.880	2.105	0.787	1.503	-7.092	1.312.479
195	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(s3)Br	1.430	0.733	0.697	0.643	0.780	1.423	1.236	0.868	2.104	0.776	1.509	-6.990	1.333.346
196	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccccc3C(=O)O	1.430	0.796	0.634	0.708	0.815	1.523	1.185	0.740	1.926	0.819	1.615	-7.379	1.474.199
197	Cc1ccc(cc1/C=N\NC(=O)c2ccc(c3c2cccc3)OC)O	1.429	0.793	0.637	0.696	0.778	1.474	1.213	0.778	1.991	0.778	1.571	-7.006	1.447.598
198	CC(=O)Oc1ccc(cc1)/C=N\NC(=O)c2ccc(c3c2cccc3)OC	1.429	0.729	0.700	0.680	0.782	1.463	1.108	0.870	1.978	0.778	1.507	-7.006	1.418.433
199	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(cc3F)O	1.429	0.792	0.637	0.697	0.778	1.475	1.209	0.778	1.987	0.778	1.570	-7.006	1.449.350
200	Cc1cc(ccc1/C=N\NC(=O)c2ccc(c3c2cccc3)OC)N	1.429	0.792	0.637	0.695	0.778	1.473	1.214	0.778	1.991	0.778	1.570	-7.006	1.446.042
201	Cc1cc(cc(c1O)C)/C=N\NC(=O)c2ccc(c3c2cccc3)OC	1.428	0.792	0.637	0.704	0.778	1.482	1.187	0.778	1.965	0.778	1.570	-7.006	1.465.614
202	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cc(ccc3Cl)N	1.428	0.791	0.637	0.693	0.778	1.471	1.217	0.778	1.995	0.778	1.569	-7.006	1.441.928
203	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(cc3Cl)N	1.427	0.791	0.637	0.693	0.778	1.471	1.217	0.778	1.995	0.778	1.569	-7.006	1.441.847
204	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(cc3)OC4CC4	1.427	0.727	0.700	0.679	0.782	1.462	1.106	0.870	1.975	0.778	1.505	-7.006	1.416.487
205	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3c4ccccc4n[nH]3	1.422	0.765	0.657	0.696	0.833	1.530	1.148	0.756	1.904	0.838	1.603	-7.549	1.450.865
206	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(c(c3)CO)F	1.421	0.783	0.639	0.699	0.779	1.479	1.179	0.779	1.959	0.779	1.562	-7.020	1.456.474

207	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccns3	1.420	0.723	0.698	0.632	0.781	1.413	1.246	0.868	2.114	0.776	1.499	-6.991	1.310.684
208	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3c(cccc3Br)Br	1.420	0.784	0.636	0.687	0.778	1.464	1.220	0.778	1.998	0.778	1.562	-7.006	1.427.273
209	COc1ccc(cc1OC)C(=O)N/N=C\c2ccccc2O	1.420	0.625	0.795	0.579	0.886	1.465	1.145	0.886	2.031	0.886	1.511	-7.978	1.199.834
210	C[C@H]1CCCC[C@@H]1/C=N\NC(=O)c2ccc(c3c2cccc3)OC	1.420	0.702	0.717	0.636	0.751	1.387	1.173	0.941	2.115	0.743	1.445	-6.689	1.321.000
211	Cc1c(c2ccccc2[nH]1)/C=N\NC(=O)c3ccc(c4c3cccc4)OC	1.420	0.787	0.633	0.715	0.776	1.491	1.146	0.775	1.920	0.776	1.563	-6.989	1.491.627
212	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(cc3)OC(F)(F)F	1.417	0.717	0.7000	0.685	0.782	1.467	1.070	0.870	1.939	0.778	1.494	-7.006	1.429.070
213	Cc1ccc(cc1O)/C=N\NC(=O)c2ccc(c3c2cccc3)OC	1.416	0.780	0.637	0.689	0.778	1.467	1.202	0.778	1.980	0.778	1.558	-7.008	1.433.976
214	c1ccc(c(c1)/C=N\NC(=O)c2ccc3c(c2)CCCO3)O	1.415	0.616	0.799	0.576	0.888	1.464	1.127	0.888	2.015	0.888	1.504	-7.998	1.194.391
215	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cnccn3	1.414	0.746	0.668	0.657	0.801	1.459	1.221	0.801	2.022	0.801	1.547	-7.215	1.364.852
216	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(c(c3)O)Cl	1.414	0.777	0.637	0.687	0.778	1.465	1.204	0.778	1.982	0.778	1.555	-7.008	1.428.494
217	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccncn3	1.414	0.747	0.667	0.658	0.801	1.458	1.221	0.800	2.022	0.801	1.547	-7.211	1.365.329
218	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccccc3OCC(=O)O	1.414	0.748	0.666	0.699	0.879	1.578	1.104	0.733	1.837	0.889	1.637	-8.007	1.457.914
219	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3nccccn3	1.414	0.746	0.667	0.658	0.801	1.458	1.221	0.800	2.021	0.801	1.547	-7.213	1.365.172
220	COc1cc(c(c(c1)OC)C(=O)N/N=C\c2ccccc2O)OC	1.411	0.686	0.725	0.629	0.882	1.511	1.152	0.803	1.955	0.887	1.573	-7.987	1.307.011

221	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(c(c3)CN)F	1.411	0.774	0.637	0.695	0.778	1.473	1.173	0.778	1.951	0.778	1.552	-7.006	1.447.085
222	COc1ccc(c2c1cccc2)C(=O)N/N=[CH:1]\c3ccc(cc3)n4cccc4	1.410	0.710	0.700	0.683	0.782	1.465	1.059	0.870	1.929	0.778	1.488	-7.006	1.426.071
223	Cc1cccc(c1C)C(=O)N/N=C\c2ccccc2O	1.409	0.631	0.778	0.566	0.786	1.352	1.221	0.986	2.207	0.778	1.408	-7.003	1.170.594
224	c1ccc(c(c1)/C=N\N[C:1](=O)c2c[nH]c3c2cccc3)O	1.408	0.657	0.750	0.594	0.858	1.452	1.194	0.857	2.051	0.858	1.515	-7.727	1.230.275
225	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc4c(c3)CCO4	1.407	0.770	0.637	0.697	0.779	1.476	1.157	0.777	1.934	0.779	1.549	-7.017	1.452.674
226	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3nc4ccccc4o3	1.407	0.757	0.649	0.694	0.788	1.482	1.138	0.787	1.924	0.789	1.546	-7.102	1.445.700
227	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(c(c3)Br)OC	1.406	0.770	0.637	0.690	0.778	1.468	1.175	0.778	1.953	0.778	1.547	-7.006	1.436.995
228	Cc1cc(ccc1/C=N\NC(=O)c2ccc(c3c2cccc3)OC)CCO	1.405	0.768	0.637	0.698	0.778	1.476	1.149	0.778	1.927	0.778	1.546	-7.006	1.455.565
229	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3c[nH]c4c3cccc4	1.404	0.771	0.633	0.699	0.776	1.475	1.154	0.774	1.929	0.776	1.547	-6.989	1.457.394
230	c1ccc(c(c1)/C=N\NC(=O)c2ccc3c(c2)cccn3)O	1.403	0.606	0.797	0.573	0.887	1.460	1.107	0.887	1.994	0.887	1.493	-7.990	1.187.522
231	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3nc4ccccc4s3	1.402	0.747	0.655	0.684	0.792	1.476	1.143	0.791	1.934	0.792	1.540	-7.135	1.423.647
232	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cc4ccccc4[nH]3	1.402	0.751	0.651	0.688	0.789	1.478	1.137	0.788	1.925	0.790	1.540	-7.111	1.434.513
233	CCc1cc(cc(c1/C=N\NC(=O)c2ccc(c3c2cccc3)OC)C)O	1.399	0.815	0.584	0.723	0.774	1.497	1.185	0.704	1.888	0.778	1.593	-7.006	1.507.241
234	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(c(c3)C(F)(F)F)O	1.396	0.760	0.636	0.708	0.778	1.486	1.106	0.778	1.884	0.778	1.537	-7.006	1.477.925
235	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cccnn3	1.396	0.746	0.649	0.657	0.800	1.457	1.223	0.776	1.998	0.801	1.548	-7.217	1.364.035

236	COc1ccc(c2c1cccc2)C(=O)N/N=C\C=C(\C=[N])/OC	1.395	0.696	0.699	0.625	0.781	1.407	1.194	0.869	2.063	0.777	1.473	-6.999	1.297.546
237	c1ccc(c(c1)/C=N\NC(=O)c2ccc3c(c2)CCO3)O	1.392	0.594	0.798	0.557	0.889	1.445	1.126	0.887	2.013	0.889	1.483	-8.004	1.153.423
238	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccccc3S(=O)(=O)N	1.391	0.781	0.610	0.704	0.796	1.500	1.162	0.723	1.885	0.800	1.581	-7.206	1.467.139
239	c1ccc(c(c1)/C=N\NC(=O)c2cccc3c2nsn3)O	1.388	0.670	0.719	0.597	0.879	1.476	1.221	0.798	2.019	0.884	1.553	-7.958	1.236.505
240	c1ccc(c(c1)/C=N\NC(=O)c2ccc(cc2)C(F)(F)F)O	1.385	0.608	0.777	0.571	0.786	1.357	1.120	0.986	2.105	0.777	1.385	-7.000	1.183.356
241	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3c(cccn3)C(=O)O	1.380	0.796	0.584	0.709	0.811	1.520	1.183	0.676	1.859	0.820	1.616	-7.382	1.476.791
242	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cc(c(c(c3)Cl)O)OC	1.377	0.793	0.584	0.713	0.774	1.486	1.167	0.704	1.870	0.778	1.571	-7.007	1.485.314
243	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(s3)c4ccccc4	1.377	0.679	0.697	0.660	0.780	1.441	1.045	0.868	1.913	0.776	1.456	-6.990	1.377.417
244	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cc(cc(c3Br)OC)OC	1.376	0.792	0.584	0.719	0.774	1.493	1.147	0.704	1.851	0.778	1.570	-7.006	1.500.696
245	COc1ccc(c2c1cccc2)C(=O)N/N=C\Cc3ccccn3	1.374	0.729	0.645	0.654	0.745	1.399	1.185	0.828	2.013	0.741	1.469	-6.669	1.359.693
246	COc1ccc(c2c1cccc2)C(=O)N/N=C\N3CCC[C@H]3C(=O)OC	1.373	0.752	0.621	0.683	0.728	1.411	1.154	0.809	1.963	0.724	1.475	-6.517	1.422.881
247	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(cc3Br)N	1.373	0.789	0.583	0.692	0.774	1.465	1.218	0.704	1.921	0.778	1.567	-7.006	1.438.414
248	c1ccc(c(c1)/C=N\NC(=O)c2ccccc2Cl)O	1.372	0.595	0.777	0.537	0.786	1.323	1.219	0.986	2.205	0.777	1.372	-7.000	1.109.984
249	COc1cc(cc(c1OC)OC)C(=O)N/N=C\c2ccccc2O	1.370	0.645	0.725	0.606	0.882	1.488	1.111	0.802	1.913	0.887	1.532	-7.987	1.258.790

250	COc1ccc(c2c1cccc2)C(=O)N/N=[CH:1]\c3ccc(c(c3)OC)N	1.368	0.784	0.584	0.700	0.774	1.474	1.180	0.704	1.884	0.778	1.562	-7.007	1.458.232
251	c1ccc(c(c1)/C=N\NC(=O)c2ccccc2C3CCCC3)O	1.367	0.652	0.715	0.602	0.792	1.394	1.147	0.881	2.028	0.787	1.439	-7.091	1.248.437
252	c1ccc(c(c1)/C=N\NC(=O)c2ccc3c(c2)OCCCO3)O	1.365	0.639	0.727	0.598	0.883	1.481	1.120	0.804	1.924	0.888	1.527	-8.001	1.240.413
253	Cc1nnc(o1)/C=N\NC(=O)c2ccc(c3c2cccc3)OC	1.364	0.736	0.628	0.653	0.783	1.436	1.208	0.760	1.969	0.784	1.520	-7.062	1.355.725
254	COc1ccc2cc(ccc2c1)/C=N\NC(=O)c3ccc(c4c3cccc4)OC	1.360	0.725	0.636	0.698	0.777	1.476	1.055	0.777	1.832	0.778	1.502	-7.002	1.459.156
255	Cc1ccc(c(c1O)C(=O)O)/C=N\NC(=O)c2ccc(c3c2cccc3)OC	1.359	0.819	0.541	0.737	0.806	1.543	1.157	0.622	1.779	0.819	1.638	-7.379	1.538.203
256	Cc1ccc(c(c1O)C(=O)O)/[CH:1]=N\NC(=O)c2ccc(c3c2cccc3)OC	1.359	0.819	0.541	0.737	0.806	1.543	1.157	0.622	1.778	0.819	1.638	-7.378	1.538.122
257	CCc1cc(ccc1O)/C=N\NC(=O)c2ccc(c3c2cccc3)OC	1.358	0.774	0.584	0.694	0.774	1.468	1.175	0.704	1.879	0.778	1.552	-7.006	1.445.577
258	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(cc3Cl)C(=O)O	1.357	0.774	0.583	0.703	0.774	1.477	1.150	0.703	1.853	0.778	1.552	-7.006	1.465.921
259	c1ccc(c(c1)/C=N\NC(=O)c2cc(c(c(c2)Cl)Cl)Cl)O	1.356	0.579	0.777	0.540	0.786	1.326	1.142	0.986	2.128	0.777	1.356	-7.001	1.117.206
260	c1ccc(c(c1)/C=N\NC(=O)c2ccc(cc2)O)O	1.356	0.561	0.795	0.519	0.886	1.405	1.166	0.886	2.052	0.886	1.446	-7.978	1.072.622
261	c1ccc(c(c1)/C=N\NC(=O)c2ccc(c(c2)F)F)O	1.355	0.578	0.777	0.537	0.786	1.324	1.149	0.986	2.135	0.777	1.355	-7.001	1.111.449
262	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3conc3c4ccccc4	1.355	0.722	0.633	0.690	0.775	1.465	1.069	0.775	1.844	0.775	1.497	-6.981	1.440.509
263	Cc1c2cc(ccc2sc1C(=O)N/N=C\c3ccccc3O)Cl	1.354	0.656	0.698	0.603	0.781	1.384	1.157	0.868	2.025	0.777	1.433	-6.998	1.250.044

264	COc1ccc(c2c1cccc2)C(=O)NCCc3ccccc3O	1.354	0.675	0.679	0.624	0.768	1.392	1.137	0.854	1.991	0.764	1.439	-6.878	1.296.978
265	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cccc(c3)c4cnco4	1.354	0.717	0.637	0.687	0.778	1.465	1.064	0.778	1.842	0.778	1.495	-7.006	1.435.287
266	c1ccc(c(c1)/C=N\NC(=O)c2ccc(c(c2)Cl)Cl)O	1.353	0.576	0.777	0.532	0.786	1.318	1.165	0.986	2.151	0.777	1.353	-7.002	1.100.096
267	COc1ccc(c2c1cccc2)C(=O)N/N=[CH:1]\c3ccc(c(c3)CN)OC	1.352	0.769	0.584	0.700	0.774	1.474	1.146	0.704	1.849	0.778	1.546	-7.006	1.459.316
268	CCOC[C@@H]1CCCN1/[CH:1]=N\NC(=O)c2ccc(c3c2cccc3)OC	1.350	0.731	0.619	0.669	0.727	1.395	1.145	0.808	1.953	0.723	1.453	-6.507	1.391.771
269	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(cc3)c4nccs4	1.349	0.713	0.637	0.680	0.778	1.458	1.071	0.778	1.849	0.778	1.491	-7.006	1.419.990
270	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccccc3S(=O)(=O)O	1.346	0.782	0.563	0.705	0.792	1.498	1.162	0.661	1.823	0.801	1.584	-7.216	1.469.915
271	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cc(nc(n3)OC)OC	1.344	0.782	0.562	0.710	0.792	1.502	1.148	0.660	1.807	0.801	1.583	-7.214	1.481.035
272	c1ccc(c(c1)/C=N\NC(=O)c2ccc3c(c2)OCCO3)O	1.344	0.618	0.726	0.579	0.883	1.462	1.123	0.803	1.926	0.888	1.506	-7.998	1.200.329
273	c1ccc(c(c1)/C=N\NC(=O)c2ccc(cc2)Cl)O	1.340	0.562	0.777	0.518	0.786	1.305	1.176	0.986	2.162	0.777	1.340	-7.001	1.070.681
274	c1ccc(c(c1)/C=N\NC(=O)c2ccc(cc2)Cl)O	1.340	0.562	0.777	0.518	0.786	1.305	1.176	0.986	2.162	0.777	1.340	-7.001	1.070.663
275	c1ccc(c(c1)/C=N\NC(=O)c2ccc(cc2)F)O	1.339	0.562	0.777	0.520	0.786	1.306	1.167	0.986	2.153	0.777	1.339	-7.001	1.074.632
276	c1ccc(c(c1)/C=N\NC(=O)c2ccc(cc2)C3CCCC3)O	1.339	0.639	0.700	0.594	0.782	1.376	1.133	0.870	2.003	0.777	1.416	-7.001	1.232.784
277	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc4c(c3)oc(=O)[nH]4	1.338	0.754	0.584	0.700	0.775	1.475	1.113	0.703	1.816	0.779	1.533	-7.018	1.460.932

278	COc1ccc(c2c1cccc2)C(=O)N/N=C\[C@H]3C=CN=N3	1.337	0.656	0.681	0.602	0.729	1.330	1.161	0.913	2.074	0.720	1.377	-6.488	1.247.621
279	COc1ccc(c2c1cccc2)C(=O)N/N=C\C3CCOCC3	1.337	0.693	0.643	0.625	0.744	1.369	1.186	0.827	2.013	0.740	1.433	-6.661	1.297.376
280	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(c(c3)O)C(=O)OC	1.333	0.749	0.584	0.701	0.774	1.474	1.102	0.704	1.805	0.778	1.527	-7.007	1.462.043
281	COc1ccc(c2c1cccc2)C(=O)N/N=[CH:1]\N3CCCCC3	1.332	0.738	0.594	0.648	0.670	1.318	1.230	0.840	2.069	0.663	1.400	-5.967	1.345.437
282	COc1cc(ccc1O)C(=O)N/N=C\c2ccccc2O	1.331	0.607	0.724	0.562	0.881	1.443	1.155	0.802	1.957	0.886	1.493	-7.981	1.162.653
283	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cc(c(c(c3)OC)O)OC	1.330	0.791	0.539	0.722	0.769	1.492	1.138	0.642	1.780	0.778	1.569	-7.007	1.507.115
284	COc1ccccc1C(=O)N/N=C\c2ccccc2O	1.330	0.630	0.700	0.567	0.782	1.349	1.214	0.870	2.084	0.777	1.407	-7.001	1.172.637
285	COc1ccc(c2c1cccc2)C(=O)N/N=C\[C@@H]3CCCc4c3cccc4	1.329	0.699	0.630	0.664	0.735	1.399	1.081	0.816	1.897	0.730	1.430	-6.579	1.385.154
286	CN(C)Cc1cc(ccc1O)/C=N\NC(=O)c2ccc(c3c2cccc3)OC	1.328	0.745	0.584	0.696	0.774	1.469	1.105	0.704	1.808	0.778	1.523	-7.006	1.451.168
287	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3c4ccc(cc4on3)O	1.328	0.761	0.567	0.703	0.796	1.499	1.120	0.663	1.784	0.805	1.566	-7.248	1.467.506
288	c1ccc(c(c1)/C=N\NC(=O)c2cccc(c2)Cl)O	1.324	0.546	0.777	0.509	0.786	1.295	1.155	0.986	2.141	0.777	1.324	-7.001	1.050.993
289	c1ccc(c(c1)/C=N\NC(=O)c2cccc(c2)Cl)O	1.324	0.546	0.777	0.509	0.786	1.295	1.155	0.986	2.141	0.777	1.324	-7.001	1.050.984
290	c1ccc(c(c1)/C=N\NC(=O)c2ccc(cc2)C#N)O	1.322	0.580	0.741	0.538	0.808	1.346	1.157	0.899	2.057	0.804	1.384	-7.240	1.112.588
291	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(c(c3)O)N	1.319	0.780	0.539	0.690	0.770	1.460	1.201	0.642	1.844	0.778	1.559	-7.008	1.435.939

292	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(c(c3)N)O	1.319	0.780	0.539	0.690	0.769	1.460	1.201	0.642	1.843	0.778	1.558	-7.007	1.435.883
293	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(c(c3)N)N	1.319	0.780	0.539	0.690	0.769	1.459	1.202	0.642	1.844	0.778	1.558	-7.007	1.434.699
294	c1ccc(c(c1)/C=N\NC(=O)c2ccc3c(c2)OCO3)O	1.317	0.598	0.719	0.561	0.879	1.440	1.125	0.798	1.923	0.884	1.482	-7.963	1.162.090
295	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(s3)C(=O)O	1.317	0.736	0.581	0.664	0.772	1.436	1.172	0.701	1.873	0.776	1.512	-6.990	1.381.260
296	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(cc3Cl)n4ccnc4	1.315	0.732	0.584	0.702	0.774	1.476	1.060	0.704	1.764	0.778	1.509	-7.006	1.468.310
297	CC(C)c1ccc(cc1)C(=O)N/N=C\c2ccccc2O	1.313	0.613	0.700	0.562	0.782	1.344	1.173	0.869	2.042	0.777	1.391	-7.001	1.163.980
298	c1ccc(cc1)c2ccccc2C(=O)N/N=C\c3ccccc3O	1.312	0.612	0.700	0.589	0.782	1.372	1.066	0.870	1.936	0.778	1.390	-7.005	1.224.510
299	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(c(c3)[N+](=O)[O-])O	1.312	0.773	0.538	0.706	0.770	1.476	1.141	0.642	1.783	0.778	1.552	-7.010	1.471.729
300	c1ccc(c(c1)/C=N\NC(=O)c2ccc3c(c2)CCCC3)O	1.310	0.610	0.700	0.571	0.782	1.353	1.127	0.870	1.996	0.778	1.388	-7.005	1.182.974
301	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cnc[nH]3	1.309	0.715	0.595	0.633	0.783	1.416	1.220	0.712	1.932	0.787	1.502	-7.091	1.312.652
302	c1ccc(cc1)C(=O)N/N=C\c2ccccc2O	1.308	0.531	0.777	0.494	0.786	1.280	1.163	0.986	2.149	0.777	1.308	-7.002	1.019.274
303	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3[nH]ccn3	1.307	0.715	0.592	0.633	0.781	1.414	1.220	0.710	1.930	0.785	1.500	-7.072	1.313.109
304	c1ccc(c(c1)/C=N\NC(=O)c2ccc(cc2)[N+](=O)[O-])O	1.305	0.599	0.706	0.558	0.828	1.386	1.140	0.827	1.967	0.828	1.427	-7.460	1.154.808
305	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3[nH]c4ccccc4n3	1.305	0.754	0.551	0.692	0.781	1.473	1.136	0.651	1.787	0.790	1.544	-7.114	1.441.578

306	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(s3)CN4CCCC4	1.304	0.670	0.634	0.652	0.776	1.428	1.043	0.776	1.819	0.776	1.446	-6.990	1.360.227
307	c1ccc2cc(ccc2c1)C(=O)N/N=C\c3ccccc3O	1.303	0.605	0.698	0.571	0.781	1.352	1.110	0.868	1.978	0.777	1.382	-6.995	1.183.690
308	c1ccc(c(c1)/C=N\NC(=O)c2cccs2)O	1.300	0.526	0.774	0.481	0.784	1.266	1.213	0.984	2.197	0.776	1.301	-6.987	991.573
309	Cc1ccc2ccc(cc2c1)C(=O)N/N=C\c3ccccc3O	1.295	0.595	0.700	0.572	0.782	1.354	1.072	0.870	1.942	0.778	1.373	-7.006	1.186.821
310	c1ccc(c(c1)/C=N\NC(=O)C2CCCCC2)O	1.294	0.545	0.750	0.499	0.770	1.269	1.201	0.966	2.167	0.762	1.306	-6.859	1.029.485
311	c1ccc(c(c1)/C=N\NC(=O)c2ccc3c(c2)ccs3)O	1.294	0.594	0.700	0.554	0.783	1.337	1.138	0.870	2.007	0.778	1.372	-7.010	1.147.041
312	COc1ccc(c2c1cccc2)C(=O)N/N=C\[C@H]3CCCNC3	1.294	0.699	0.595	0.628	0.746	1.374	1.194	0.746	1.940	0.746	1.445	-6.719	1.302.384
313	c1ccc(cc1)c2ccc(cc2)C(=O)N/N=C\c3ccccc3O	1.293	0.594	0.699	0.579	0.781	1.360	1.047	0.869	1.916	0.777	1.371	-6.999	1.201.970
314	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(cc3)n4ccnc4	1.292	0.709	0.584	0.683	0.774	1.456	1.056	0.704	1.760	0.778	1.486	-7.006	1.425.947
315	COc1ccc(c2c1cccc2)C(=O)N/N=C\[C@H]3CCCC[C@@H]3O	1.289	0.702	0.587	0.637	0.740	1.377	1.170	0.740	1.910	0.740	1.442	-6.663	1.322.583
316	COc1ccc2c(c1)nc(o2)/C=N\NC(=O)c3ccc(c4c3cccc4)OC	1.288	0.702	0.586	0.680	0.776	1.456	1.048	0.705	1.753	0.781	1.483	-7.031	1.420.574
317	c1ccc(cc1)CC(=O)N/N=C\c2ccccc2O	1.285	0.556	0.729	0.515	0.758	1.272	1.168	0.950	2.118	0.749	1.305	-6.749	1.062.875
318	COc1ccc(c(c1)C(=O)N/N=C\c2ccccc2O)OC	1.283	0.647	0.636	0.592	0.777	1.369	1.169	0.778	1.947	0.777	1.425	-7.002	1.226.715
319	CS(=O)(=O)c1ccc(cc1)C(=O)N/N=C\c2ccccc2O	1.282	0.620	0.662	0.572	0.797	1.369	1.157	0.797	1.953	0.797	1.417	-7.174	1.184.633

320	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cc(c(c(c3)OC)O)[N+](=O)[O-]	1.282	0.782	0.500	0.728	0.765	1.493	1.106	0.590	1.696	0.778	1.560	-7.007	1.520.528
321	c1ccc(c(c1)/C=N\NC(=O)c2ccsc2)O	1.280	0.506	0.773	0.470	0.784	1.254	1.182	0.983	2.165	0.775	1.282	-6.981	967.961
322	COc1cc(cc2c1cccc2)C(=O)N/N=C\c3ccccc3O	1.278	0.642	0.636	0.608	0.777	1.385	1.096	0.777	1.874	0.777	1.420	-7.001	1.263.401
323	c1ccc(c(c1)CC(=O)N/N=C\c2ccccc2O)Cl	1.278	0.557	0.721	0.521	0.753	1.274	1.139	0.944	2.084	0.745	1.301	-6.707	1.077.441
324	c1ccc(c(c1)/C=N\NC(=O)c2c[nH]c(=O)[nH]c2=O)O	1.278	0.619	0.658	0.563	0.872	1.435	1.193	0.728	1.921	0.882	1.501	-7.945	1.164.401
325	COc1ccc(c2c1cccc2)C(=O)N/N=[CH:1]\N3CCOCC3	1.277	0.737	0.540	0.649	0.666	1.316	1.224	0.741	1.965	0.663	1.400	-5.968	1.347.851
326	COc1ccc(c2c1cccc2)C(=O)N/N=[CH:1]\CCC3CCCC3	1.273	0.672	0.601	0.619	0.675	1.294	1.146	0.846	1.991	0.667	1.339	-6.010	1.285.425
327	COc1ccc(c2c1cccc2)C(=O)N/N=[CH:1]\CCC3CCCCC3	1.271	0.666	0.605	0.622	0.678	1.300	1.117	0.850	1.966	0.670	1.336	-6.037	1.293.378
328	COc1ccc(c2c1cccc2)C(=O)N/N=C\C=C\c3ccccc3Cl	1.267	0.667	0.600	0.634	0.674	1.309	1.083	0.845	1.928	0.667	1.333	-6.005	1.320.104
329	COc1ccc(c2c1cccc2)C(=O)N/N=C\Cc3ccccc3O	1.266	0.690	0.576	0.642	0.731	1.373	1.123	0.731	1.854	0.731	1.421	-6.584	1.334.892
330	CN(/C=N\NC(=O)c1ccc(c2c1cccc2)OC)c3ccccc3	1.264	0.722	0.543	0.659	0.632	1.292	1.150	0.793	1.943	0.625	1.347	-5.633	1.371.539
331	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cc(c(c(c3)O)O)O	1.261	0.794	0.467	0.707	0.761	1.468	1.184	0.547	1.731	0.778	1.572	-7.008	1.472.174
332	c1ccc(c(c1)/C=N\NC(=O)c2ccc(cc2)Br)O	1.261	0.561	0.700	0.517	0.782	1.299	1.179	0.870	2.048	0.777	1.339	-7.001	1.068.361
333	c1ccc(c(c1)/C=N\NC(=O)c2ccncc2)O	1.261	0.532	0.728	0.496	0.800	1.296	1.162	0.890	2.052	0.796	1.328	-7.167	1.022.584

334	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3nc(on3)c4ccccc4	1.250	0.667	0.583	0.660	0.774	1.433	1.018	0.703	1.721	0.778	1.445	-7.007	1.377.409
335	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3csc(n3)N4CCOCC4	1.246	0.658	0.588	0.648	0.777	1.425	1.025	0.707	1.731	0.781	1.440	-7.037	1.352.518
336	c1ccc(cc1)c2cccc(c2)C(=O)N/N=C\c3ccccc3O	1.242	0.634	0.608	0.602	0.718	1.321	1.090	0.799	1.889	0.714	1.348	-6.433	1.251.169
337	COc1ccc(c2c1cccc2)C(=O)N/N=C\C(=O)O	1.242	0.612	0.630	0.558	0.774	1.331	1.188	0.773	1.961	0.774	1.385	-6.968	1.153.282
338	c1ccc(c(c1)/C=N\NC(=O)c2ccc3ccncc3c2)O	1.240	0.603	0.637	0.571	0.778	1.349	1.103	0.778	1.881	0.778	1.381	-7.007	1.183.480
339	c1ccc(c(c1)/C=N\NC(=O)c2ccc(cc2)C(=O)O)O	1.235	0.599	0.637	0.557	0.817	1.374	1.143	0.743	1.886	0.821	1.420	-7.398	1.153.000
340	Cc1nc2cc(ccc2c(n1)N)/C=N\NC(=O)c3ccc(c4c3cccc4)OC	1.235	0.735	0.500	0.706	0.765	1.471	1.059	0.590	1.649	0.778	1.513	-7.009	1.476.062
341	COc1ccccc1CC(=O)N/N=C\c2ccccc2O	1.234	0.581	0.652	0.545	0.750	1.295	1.130	0.834	1.964	0.746	1.327	-6.715	1.127.465
342	CC[C@H](CC#N)/C=N\NC(=O)c1ccc(c2c1cccc2)OC	1.233	0.688	0.546	0.618	0.671	1.289	1.196	0.745	1.941	0.667	1.354	-6.006	1.281.539
343	COc1ccc(c2c1cccc2)C(=O)N/N=C\C=C\c3ccoc3	1.233	0.687	0.546	0.632	0.671	1.303	1.144	0.746	1.889	0.667	1.354	-6.007	1.313.838
344	c1ccc(c(c1)/C=N\NC(=O)c2cccc(c2)[N+](=O)[O-])O	1.232	0.633	0.600	0.577	0.750	1.327	1.179	0.749	1.929	0.750	1.383	-6.756	1.194.840
345	c1ccc(c(c1)/C=N\NC(=O)c2ccc3ccc(=O)oc3c2)O	1.231	0.597	0.635	0.574	0.777	1.351	1.070	0.777	1.847	0.777	1.373	-6.994	1.191.975
346	CC(C)c1cccc(c1/C=N\NC(=O)c2ccc(c3c2cccc3)OC)C(C)C	1.228	0.713	0.516	0.684	0.680	1.364	1.063	0.680	1.743	0.680	1.393	-6.128	1.427.901
347	Cc1ccccc1OC/C=N\NC(=O)c2ccc(c3c2cccc3)OC	1.225	0.677	0.548	0.643	0.672	1.315	1.085	0.747	1.832	0.669	1.346	-6.022	1.339.003
348	COc1ccc2ccc(cc2c1)C(=O)N/N=C\c3ccccc3O	1.222	0.587	0.635	0.575	0.777	1.351	1.037	0.777	1.814	0.777	1.364	-6.994	1.194.559

349	COc1ccc(c2c1cccc2)C(=O)N/N=C\[C@@H]3CCNC3	1.221	0.658	0.562	0.599	0.720	1.319	1.177	0.720	1.897	0.720	1.378	-6.483	1.241.637
350	c1ccc(c(c1)/C=N\NC(=O)c2nccs2)O	1.220	0.526	0.694	0.482	0.778	1.260	1.209	0.866	2.074	0.774	1.300	-6.969	993.487
351	COc1ccc(c2c1cccc2)C(=O)N/N=C\[C@H]3C=NC=N3	1.217	0.655	0.562	0.601	0.720	1.321	1.159	0.720	1.879	0.720	1.375	-6.483	1.246.279
352	c1ccc(c(c1)/C=N\NC(=O)c2ccno2)O	1.215	0.521	0.694	0.482	0.778	1.260	1.181	0.865	2.046	0.773	1.294	-6.965	994.702
353	COc1cccc(c1)CC(=O)N/N=C\c2ccccc2O	1.212	0.554	0.658	0.528	0.754	1.282	1.098	0.838	1.936	0.749	1.304	-6.749	1.092.902
354	COc1cc(cc(c1)OC)C(=O)N/N=C\c2ccccc2O	1.202	0.566	0.636	0.544	0.777	1.321	1.078	0.778	1.856	0.777	1.344	-7.001	1.127.565
355	c1ccc(c(c1)/C=N\NC(=O)c2ccoc2)O	1.201	0.504	0.697	0.472	0.780	1.252	1.159	0.868	2.026	0.776	1.280	-6.985	972.817
356	COc1ccc(c2c1cccc2)C(=O)NCc3ccccc3O	1.187	0.576	0.611	0.560	0.721	1.281	1.052	0.801	1.854	0.717	1.293	-6.454	1.161.988
357	c1ccc(c(c1)/C=N\N[C:1](=O)c2cccc(c2)O)O	1.184	0.548	0.636	0.511	0.777	1.289	1.148	0.778	1.926	0.777	1.325	-7.002	1.056.575
358	COc1ccc(c2c1cccc2)C(=O)N/N=C\COCc3ccccc3	1.173	0.627	0.546	0.612	0.671	1.283	1.040	0.746	1.785	0.667	1.294	-6.006	1.274.826
359	COc1ccc(c2c1cccc2)C(=O)N/N=C\C=C\c3ccccc3O	1.169	0.668	0.501	0.637	0.667	1.304	1.078	0.667	1.746	0.667	1.335	-6.008	1.326.565
360	COc1ccc(c2c1cccc2)C(=O)NN3[C@@H](SCC3=O)c4ccccc4O	1.167	0.608	0.559	0.618	0.753	1.371	0.974	0.685	1.659	0.757	1.365	-6.818	1.290.122
361	COc1ccc(c2c1cccc2)C(=O)NN3[C@@H](SCC3=O)[c:2]4ccccc4O	1.166	0.607	0.559	0.618	0.753	1.370	0.973	0.685	1.658	0.757	1.364	-6.817	1.289.163

362	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3cccc(c3)c4[nH]nnn4	1.163	0.716	0.447	0.687	0.758	1.445	1.062	0.522	1.584	0.778	1.494	-7.007	1.434.572
363	COc1ccc(c2c1cccc2)C(=O)N/N=C\c3ccc(cc3)c4[nH]nnn4	1.154	0.706	0.447	0.682	0.758	1.440	1.054	0.522	1.576	0.778	1.484	-7.006	1.423.474
364	COc1ccc(c2c1cccc2)C(=O)OCc3ccccc3O	1.152	0.658	0.493	0.609	0.594	1.203	1.141	0.744	1.886	0.587	1.246	-5.290	1.263.453
365	Cc1c([nH]cn1)C(=O)N/N=C\c2ccccc2O	1.139	0.558	0.581	0.512	0.771	1.283	1.194	0.702	1.896	0.775	1.334	-6.984	1.056.421
366	COc1ccc(c2c1cccc2)C(=O)N/N=C\[C@@H](COc3ccccc3)O	1.128	0.659	0.469	0.639	0.671	1.310	1.048	0.610	1.658	0.674	1.333	-6.073	1.332.691
367	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3ccccc3CC(=O)N	1.115	0.503	0.612	0.539	0.759	1.298	0.884	0.759	1.643	0.759	1.262	-6.837	1.123.794
368	COc1ccc(c2c1cccc2)C(=O)[C@@H](c3c(cccn3)N)N=C	1.098	0.650	0.448	0.612	0.619	1.231	1.105	0.619	1.724	0.619	1.269	-5.572	1.271.899
369	Cc1ccsc1/C=N/NC(=O)c2ccc(c3c2cccc3)OC	1.097	0.496	0.600	0.506	0.674	1.180	0.965	0.845	1.810	0.667	1.163	-6.006	1.048.796
370	B(c1ccccc1/C=N/NC(=O)c2ccc(c3c2cccc3)OC)(O)O	1.088	0.488	0.600	0.521	0.674	1.195	0.884	0.845	1.730	0.667	1.155	-6.006	1.084.902
371	C/C(=C(\CNNC(=O)c1ccc(c2c1cccc2)OC)/C=C)/O	1.084	0.649	0.435	0.598	0.585	1.183	1.152	0.630	1.782	0.583	1.231	-5.247	1.239.648
372	CCN(CC)c1ccccc1/C=N/NC(=O)c2ccc(c3c2cccc3)OC	1.084	0.483	0.600	0.530	0.674	1.204	0.846	0.845	1.691	0.667	1.150	-6.006	1.105.567
373	COc1ccc(c2c1cccc2)C(=O)N/N=C/Cc3ccccc3Cl	1.083	0.483	0.600	0.510	0.674	1.184	0.901	0.845	1.746	0.667	1.150	-6.005	1.059.929
374	COc1ccc(c2c1cccc2)/C(=N/CC[c:2]3ccccc3O)/N	1.082	0.664	0.418	0.618	0.560	1.178	1.127	0.622	1.750	0.557	1.221	-5.014	1.284.076
375	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3cc(ccc3F)Cl	1.079	0.479	0.600	0.509	0.674	1.183	0.892	0.845	1.738	0.667	1.146	-6.006	1.057.684

376	COc1ccc(c2c1cccc2)C(=O)N/N=C/Cc3ccccc3F	1.079	0.479	0.600	0.509	0.674	1.183	0.890	0.845	1.736	0.667	1.145	-6.005	1.057.688
377	CNS(=O)(=O)Cc1ccccc1/C=N/NC(=O)c2ccc(c3c2cccc3)OC	1.078	0.507	0.571	0.551	0.763	1.314	0.864	0.694	1.558	0.767	1.275	-6.912	1.150.779
378	COc1ccc(c2c1cccc2)c3n[nH]c(=S)n3c4ccccc4O	1.069	0.652	0.417	0.625	0.618	1.243	1.069	0.562	1.631	0.621	1.273	-5.597	1.301.807
379	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3c(ccc(c3F)F)F	1.069	0.469	0.600	0.510	0.674	1.184	0.852	0.845	1.697	0.667	1.135	-6.003	1.062.885
380	COc1ccc(c2c1cccc2)C(=O)N/N=[CH:1]/C=C/c3ccccc3	1.068	0.468	0.600	0.500	0.674	1.175	0.880	0.845	1.725	0.667	1.135	-6.005	1.040.319
381	CC(=O)NCc1ccccc1/[CH:1]=N/NC(=O)c2ccc(c3c2cccc3)OC	1.066	0.542	0.524	0.573	0.687	1.260	0.911	0.687	1.598	0.687	1.230	-6.191	1.194.887
382	COc1ccc(c2c1cccc2)c3n[nH]c(=S)n3[c:2]4ccccc4O	1.058	0.639	0.419	0.618	0.620	1.238	1.056	0.564	1.620	0.623	1.262	-5.614	1.285.837
383	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3cc(ccc3Cl)C(F)(F)F	1.050	0.450	0.600	0.506	0.674	1.181	0.800	0.845	1.645	0.667	1.116	-6.006	1.056.799
384	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3cncs3	1.049	0.504	0.545	0.505	0.670	1.175	0.996	0.745	1.741	0.667	1.170	-6.004	1.046.027
385	CCCCc1ccccc1/C=N/NC(=O)c2ccc(c3c2cccc3)OC	1.048	0.502	0.546	0.536	0.671	1.206	0.889	0.745	1.634	0.667	1.169	-6.005	1.115.962
386	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3ccccc3C(=O)C(F)(F)F	1.047	0.502	0.546	0.554	0.670	1.225	0.842	0.745	1.587	0.667	1.169	-6.005	1.157.985
387	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3cnco3	1.047	0.501	0.546	0.507	0.671	1.177	0.979	0.745	1.724	0.667	1.168	-6.005	1.050.452
388	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3ccccc3OCCCF	1.043	0.498	0.546	0.540	0.671	1.211	0.863	0.745	1.608	0.667	1.164	-6.006	1.127.014

389	CC(=O)c1ccccc1/C=N/NC(=O)c2ccc(c3c2cccc3)OC	1.040	0.482	0.558	0.518	0.680	1.198	0.875	0.756	1.631	0.676	1.159	-6.092	1.078.759
390	Cc1ccoc1/C=N/NC(=O)c2ccc(c3c2cccc3)OC	1.039	0.494	0.546	0.507	0.671	1.178	0.948	0.745	1.694	0.667	1.160	-6.006	1.052.917
391	Cc1c(ocn1)/C=N/NC(=O)c2ccc(c3c2cccc3)OC	1.038	0.492	0.546	0.507	0.671	1.177	0.944	0.745	1.689	0.667	1.159	-6.006	1.052.262
392	COc1ccc(c2c1cccc2)S(=O)(=O)N/N=C/[c:2]3ccccc3O	1.037	0.493	0.544	0.516	0.740	1.255	0.919	0.673	1.591	0.744	1.237	-6.699	1.072.203
393	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3ccccc3C=C	1.036	0.490	0.546	0.517	0.671	1.188	0.905	0.745	1.650	0.667	1.157	-6.006	1.075.293
394	Cc1ccncc1/C=N/NC(=O)c2ccc(c3c2cccc3)OC	1.032	0.487	0.546	0.509	0.671	1.179	0.919	0.745	1.664	0.667	1.154	-6.006	1.056.725
395	CN(CC[c:2]1ccccc1O)C(=O)c2ccc(c3c2cccc3)OC	1.031	0.645	0.386	0.615	0.501	1.116	1.081	0.628	1.709	0.495	1.141	-4.463	1.279.533
396	COc1ccc(c2c1cccc2)C(=O)N/N=C/C(=O)N3CCCCC3	1.030	0.485	0.546	0.511	0.671	1.182	0.903	0.745	1.649	0.667	1.152	-6.006	1.063.124
397	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3cccc(c3C#N)Cl	1.030	0.479	0.551	0.514	0.675	1.190	0.873	0.751	1.624	0.671	1.150	-6.047	1.070.886
398	COc1ccccc1/C=N/NC(=O)c2ccc(c3c2cccc3)OC	1.029	0.484	0.546	0.513	0.671	1.183	0.895	0.746	1.641	0.667	1.150	-6.007	1.066.345
399	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3cccc(n3)F	1.028	0.482	0.546	0.506	0.671	1.177	0.910	0.745	1.655	0.667	1.149	-6.006	1.051.834
400	COc1ccccc1C/C=N/NC(=O)c2ccc(c3c2cccc3)OC	1.027	0.476	0.551	0.513	0.675	1.187	0.869	0.750	1.619	0.671	1.147	-6.043	1.067.031
401	COc1ccc(c2c1cccc2)c3[nH]c(nn3)[c:2]4ccccc4O	1.026	0.552	0.474	0.558	0.684	1.243	0.981	0.606	1.587	0.689	1.242	-6.208	1.161.167
402	CCOc1ccc(cc1/C=N/NC(=O)c2ccc(c3c2cccc3)OC)Cl	1.025	0.479	0.546	0.520	0.671	1.191	0.859	0.745	1.604	0.667	1.146	-6.006	1.083.985
403	Cc1c(c(ccn1)/C=N/NC(=O)c2ccc(c3c2cccc3)OC)Cl	1.025	0.479	0.546	0.508	0.671	1.179	0.892	0.745	1.637	0.667	1.146	-6.006	1.057.279

404	CCOc1cc(ccc1/C=N/NC(=O)c2ccc(c3c2cccc3)OC)C	1.023	0.478	0.546	0.520	0.671	1.191	0.855	0.745	1.600	0.667	1.145	-6.006	1.083.894
405	CC(=O)Oc1ccccc1/C=N/NC(=O)c2ccc(c3c2cccc3)OC	1.022	0.476	0.546	0.521	0.671	1.191	0.849	0.745	1.594	0.667	1.143	-6.006	1.085.341
406	COCCOc1ccccc1/C=N/NC(=O)c2ccc(c3c2cccc3)OC	1.018	0.516	0.502	0.554	0.668	1.222	0.883	0.668	1.552	0.668	1.184	-6.021	1.155.168
407	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3ccccc3NS(=O)(=O)C	1.017	0.513	0.504	0.550	0.704	1.254	0.885	0.640	1.525	0.707	1.221	-6.372	1.147.252
408	CC(=O)Oc1ccc(cc1/C=N/NC(=O)c2ccc(c3c2cccc3)OC)Cl	1.015	0.469	0.546	0.520	0.671	1.191	0.827	0.745	1.572	0.667	1.136	-6.006	1.085.504
409	C/C(=N\NC(=O)c1ccc(c2c1cccc2)OC)/c3ccccc3O	1.013	0.513	0.500	0.534	0.667	1.201	0.930	0.667	1.597	0.667	1.180	-6.008	1.109.908
410	COc1cccc(c1F)/C=N/NC(=O)c2ccc(c3c2cccc3)OC	1.013	0.468	0.546	0.508	0.671	1.179	0.855	0.745	1.600	0.667	1.134	-6.006	1.057.983
411	CN(C)C(=O)c1ccccc1/C=N/NC(=O)c2ccc(c3c2cccc3)OC	1.012	0.464	0.548	0.517	0.672	1.190	0.820	0.747	1.567	0.669	1.133	-6.021	1.079.521
412	CNC(=O)c1ccccc1/C=N/NC(=O)c2ccc(c3c2cccc3)OC	1.010	0.492	0.518	0.532	0.682	1.214	0.869	0.682	1.551	0.682	1.175	-6.145	1.108.640
413	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3ccccc3OS(=O)(=O)C	1.008	0.479	0.529	0.526	0.692	1.218	0.844	0.691	1.535	0.692	1.171	-6.229	1.097.412
414	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3ccccc3OCCBr	1.004	0.504	0.500	0.537	0.667	1.204	0.891	0.667	1.557	0.667	1.171	-6.005	1.119.245
415	CC(=O)Oc1cccc(c1)/C=N/NC(=O)c2ccc(c3c2cccc3)OC	1.000	0.456	0.544	0.505	0.669	1.175	0.825	0.744	1.569	0.666	1.122	-5.996	1.053.236
416	COc1ccc(c2c1cccc2)C(=O)N/N=[CH:1]/c3ccccc3CCO	0.999	0.487	0.513	0.520	0.678	1.198	0.884	0.678	1.562	0.678	1.165	-6.106	1.081.997
417	COc1ccc(c2c1cccc2)C(=O)N/N=[CH:1]/c3c(cccn3)C(=O)OC	0.995	0.475	0.520	0.520	0.685	1.205	0.845	0.685	1.529	0.685	1.159	-6.166	1.084.497

418	Cn1cc(c2c1cccc2)/C=N/NC(=O)c3ccc(c4c3cccc4)OC	0.995	0.450	0.545	0.504	0.670	1.175	0.809	0.744	1.552	0.667	1.117	-6.006	1.051.282
419	Cn1ccnc1/C=N/NC(=O)c2ccc(c3c2cccc3)OC	0.995	0.495	0.500	0.509	0.667	1.175	0.947	0.667	1.614	0.667	1.161	-6.004	1.056.349
420	COc1ccc(c2c1cccc2)C(=O)N/N=C/Cc3cccc4c3cccc4	0.994	0.449	0.545	0.508	0.670	1.178	0.795	0.745	1.540	0.667	1.115	-6.005	1.059.431
421	CC(C)COc1ccccc1/C=N/NC(=O)c2ccc(c3c2cccc3)OC	0.993	0.493	0.500	0.536	0.667	1.203	0.858	0.667	1.525	0.667	1.160	-6.007	1.119.072
422	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3cc(ccc3OC)C(F)(F)F	0.991	0.445	0.546	0.510	0.671	1.181	0.777	0.746	1.522	0.667	1.112	-6.007	1.065.975
423	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3cccc(c3)OC(F)(F)F	0.989	0.444	0.545	0.504	0.670	1.174	0.789	0.745	1.534	0.667	1.111	-6.003	1.052.089
424	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3cccc(n3)Br	0.986	0.486	0.500	0.506	0.667	1.173	0.922	0.667	1.589	0.667	1.152	-6.006	1.051.852
425	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3ccc(cc3)C4CCCCC4	0.985	0.441	0.544	0.504	0.670	1.174	0.779	0.744	1.523	0.666	1.107	-5.996	1.052.879
426	CC(C)(C)Oc1ccccc1/C=N/NC(=O)c2ccc(c3c2cccc3)OC	0.985	0.485	0.500	0.533	0.667	1.199	0.845	0.667	1.511	0.667	1.152	-6.005	1.111.451
427	COc1ccc(c2c1cccc2)C(=O)N/N=[CH:1]/c3ccccc3OCCO	0.985	0.468	0.517	0.513	0.715	1.228	0.843	0.651	1.494	0.719	1.188	-6.479	1.069.227
428	CC(C)(C)COc1ccccc1/C=N/NC(=O)c2ccc(c3c2cccc3)OC	0.983	0.483	0.500	0.536	0.667	1.203	0.831	0.667	1.498	0.667	1.150	-6.007	1.118.426
429	COCOc1ccccc1/[CH:1]=N/NC(=O)c2ccc(c3c2cccc3)OC	0.983	0.483	0.500	0.524	0.667	1.191	0.860	0.666	1.526	0.667	1.150	-6.006	1.092.378
430	Cc1cccc(c1N)/C=N/NC(=O)c2ccc(c3c2cccc3)OC	0.980	0.478	0.502	0.509	0.668	1.177	0.889	0.668	1.557	0.668	1.147	-6.020	1.057.889
431	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3cccc(c3Cl)N	0.980	0.480	0.500	0.509	0.667	1.175	0.894	0.667	1.561	0.667	1.147	-6.006	1.057.716
432	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3cccc(c3Cl)O	0.979	0.479	0.500	0.508	0.667	1.175	0.892	0.667	1.559	0.667	1.146	-6.006	1.057.179

433	CC(C)(C)Oc1ccc(cc1/C=N/NC(=O)c2ccc(c3c2cccc3)OC)Cl	0.978	0.477	0.500	0.532	0.667	1.199	0.823	0.667	1.490	0.667	1.144	-6.007	1.110.834
434	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3cc(c[nH]c3=O)Cl	0.977	0.477	0.500	0.507	0.667	1.175	0.888	0.667	1.555	0.667	1.144	-6.009	1.055.425
435	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3cc(ccc3F)O	0.977	0.477	0.500	0.508	0.667	1.175	0.885	0.667	1.552	0.667	1.144	-6.006	1.057.713
436	COc1ccc(c2c1cccc2)C(=O)Nn\3c(cs/c3=N\c4ccccc4O)O	0.977	0.555	0.422	0.592	0.652	1.244	0.898	0.545	1.443	0.660	1.214	-5.940	1.236.444
437	COc1ccc(c2c1cccc2)C(=O)Nn\3c(cs/c3=N\c4ccccc4O)O	0.977	0.555	0.422	0.592	0.652	1.244	0.898	0.545	1.443	0.660	1.214	-5.940	1.236.418
438	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3cccc(c3)CN	0.975	0.475	0.500	0.505	0.667	1.172	0.887	0.667	1.554	0.667	1.141	-6.005	1.050.592
439	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3c(ccc(c3Cl)N)Cl	0.974	0.474	0.500	0.510	0.667	1.176	0.871	0.667	1.538	0.667	1.141	-6.006	1.060.747
440	Cc1cc(c(c(c1)/C=N/NC(=O)c2ccc(c3c2cccc3)OC)O)C	0.970	0.469	0.502	0.508	0.668	1.176	0.858	0.668	1.526	0.668	1.137	-6.019	1.057.938
441	Cc1cc(c(c(c1)O)C)/C=N/NC(=O)c2ccc(c3c2cccc3)OC	0.969	0.469	0.500	0.508	0.667	1.175	0.859	0.667	1.526	0.667	1.136	-6.006	1.057.443
442	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3ccccc3NN	0.967	0.479	0.489	0.509	0.666	1.175	0.890	0.647	1.536	0.668	1.146	-6.012	1.058.353
443	CC(=O)Nc1ccccc1/C=N/NC(=O)c2ccc(c3c2cccc3)OC	0.963	0.462	0.501	0.509	0.668	1.177	0.831	0.668	1.499	0.668	1.129	-6.012	1.061.901
444	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3cc(ccc3Cl)[N+](=O)[O-]	0.958	0.459	0.499	0.507	0.667	1.174	0.828	0.666	1.494	0.667	1.126	-6.006	1.057.272
445	COc1ccc(c2c1cccc2)C(=O)N/N=[CH:1]/c3ccc4cc[nH]c4c3	0.958	0.458	0.499	0.504	0.667	1.171	0.834	0.665	1.500	0.667	1.125	-6.005	1.050.614
446	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3ccc(cc3C(=O)O)Cl	0.957	0.477	0.481	0.520	0.682	1.201	0.851	0.620	1.471	0.686	1.162	-6.175	1.083.167

447	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3cc(ccc3F)[N+](=O)[O-]	0.956	0.457	0.500	0.507	0.667	1.174	0.821	0.666	1.487	0.667	1.124	-6.006	1.057.676
448	C[C@@H]1CCCN1/C=N/NC(=O)c2ccc(c3c2cccc3)OC	0.956	0.502	0.454	0.510	0.562	1.072	0.966	0.704	1.670	0.555	1.057	-5.002	1.059.129
449	COc1ccc(c2c1cccc2)C(=O)[C@@H](c3ccc(c(c3)O)C(=O)N)N=C	0.955	0.563	0.392	0.581	0.591	1.172	0.948	0.538	1.486	0.595	1.158	-5.356	1.210.870
450	COc1ccc(c2c1cccc2)C(=O)N/N=C/N3CCCC3=O	0.955	0.500	0.455	0.511	0.562	1.073	0.959	0.705	1.664	0.556	1.056	-5.006	1.061.005
451	COc1ccc(c2c1cccc2)C(=O)[C@@H](c3ccc4c(c3)ncnc4N)N=C	0.953	0.622	0.331	0.631	0.547	1.177	0.978	0.456	1.434	0.553	1.175	-4.979	1.316.729
452	Cc1c2ccccc2oc1/C=N/NC(=O)c3ccc(c4c3cccc4)OC	0.950	0.451	0.499	0.505	0.667	1.172	0.809	0.665	1.474	0.667	1.118	-6.006	1.052.936
453	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3ccc4ccccc4n3	0.950	0.450	0.500	0.504	0.667	1.171	0.807	0.666	1.474	0.667	1.117	-6.007	1.051.819
454	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3ccc(cc3N)C(F)(F)F	0.950	0.448	0.502	0.507	0.668	1.175	0.795	0.668	1.464	0.668	1.117	-6.019	1.057.465
455	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3ccc(s3)c4cnco4	0.950	0.450	0.500	0.502	0.667	1.168	0.814	0.667	1.480	0.667	1.117	-6.004	1.045.936
456	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3ccc(cc3O)C(F)(F)F	0.950	0.448	0.502	0.507	0.668	1.175	0.794	0.668	1.463	0.668	1.116	-6.019	1.057.669
457	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3cnccc3O	0.949	0.486	0.463	0.509	0.664	1.173	0.916	0.604	1.520	0.668	1.154	-6.016	1.057.253
458	COc1ccc(c2c1cccc2)C(=O)[C@@H](c3cc(c(c(c3)O)OC)O)	0.946	0.613	0.333	0.613	0.549	1.162	1.000	0.459	1.458	0.556	1.168	-5.004	1.277.370

	N=C													
459	COc1ccc(c2c1cccc2)C(=O)NNC(=S)Nc3ccccc3O	0.944	0.574	0.370	0.579	0.602	1.181	0.984	0.490	1.474	0.610	1.184	-5.493	1.205.597
460	COCC[C@H]1CCCCN1/C=N/NC(=O)c2ccc(c3c2cccc3)OC	0.943	0.514	0.428	0.543	0.570	1.113	0.906	0.633	1.540	0.566	1.081	-5.101	1.131.539
461	COc1ccc(c2c1cccc2)C(=O)[C@@H](c3ccc(c(c3)N)C(=O)N)N=C	0.942	0.551	0.391	0.573	0.590	1.163	0.936	0.537	1.473	0.593	1.144	-5.344	1.193.721
462	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3cccc(c3Br)O	0.942	0.480	0.462	0.509	0.663	1.172	0.896	0.603	1.499	0.667	1.147	-6.006	1.057.500
463	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3ccccc3OCC(=O)N	0.941	0.480	0.462	0.529	0.663	1.192	0.838	0.603	1.441	0.667	1.147	-6.006	1.103.162
464	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3cc(ccc3OC)N	0.936	0.474	0.462	0.512	0.663	1.175	0.864	0.603	1.467	0.667	1.141	-6.007	1.066.119
465	CN(C(=O)c1ccc(c2c1cccc2)OC)/N=C/c3ccccc3O	0.933	0.552	0.381	0.560	0.524	1.084	0.976	0.582	1.559	0.521	1.073	-4.691	1.164.788
466	COc1cccc(c1N)/C=N/NC(=O)c2ccc(c3c2cccc3)OC	0.930	0.468	0.462	0.508	0.663	1.171	0.857	0.603	1.460	0.667	1.135	-6.008	1.057.691
467	COc1cc[c:1](c2c1cccc2)C(=O)NCCCNC(=O)c3ccccc3O	0.925	0.567	0.357	0.590	0.553	1.143	0.937	0.503	1.440	0.556	1.123	-5.006	1.230.648
468	CC(C)c1ccc(c(c1)/C=N/NC(=O)c2ccc(c3c2cccc3)OC)O	0.923	0.461	0.462	0.507	0.663	1.171	0.835	0.603	1.438	0.667	1.128	-6.008	1.057.198
469	COc1ccc(c2c1cccc2)C(=O)N/N=[CH:1]/c3ccccc3NC(=O)N	0.922	0.460	0.462	0.509	0.663	1.172	0.828	0.603	1.431	0.667	1.127	-6.007	1.060.885
470	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3cccc(c3)S(=O)(=O)N	0.921	0.460	0.461	0.505	0.662	1.167	0.838	0.602	1.441	0.666	1.126	-5.998	1.052.238
471	COc1ccccc1CO/C=N/NC(=O)c2ccc(c3c2cccc3)OC	0.916	0.462	0.455	0.509	0.562	1.071	0.833	0.704	1.538	0.556	1.017	-5.005	1.059.919

472	C[C@@H]1CC[C@H](N1/C=N/NC(=O)c2ccc(c3c2cccc3)OC)COC	0.915	0.498	0.417	0.526	0.559	1.085	0.901	0.621	1.522	0.556	1.053	-5.005	1.095.794
473	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3cccc(c3)NS(=O)(=O)C	0.913	0.452	0.461	0.504	0.663	1.167	0.813	0.603	1.415	0.666	1.118	-6.001	1.051.794
474	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3ccc4c(c3)OCCO4	0.911	0.450	0.461	0.503	0.663	1.166	0.808	0.603	1.411	0.667	1.117	-6.006	1.049.607
475	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3cccc(c3O)C(=O)OC	0.910	0.448	0.462	0.507	0.663	1.170	0.796	0.603	1.400	0.667	1.116	-6.008	1.057.342
476	CCOC(=O)c1ccc(c(c1)/C=N/NC(=O)c2ccc(c3c2cccc3)OC)O	0.904	0.443	0.462	0.507	0.663	1.170	0.778	0.603	1.381	0.667	1.109	-6.004	1.058.240
477	COc1cc[c:1](c2c1cccc2)SCc3cc(=O)[nH]c(n3)c4ccccc4O	0.904	0.550	0.354	0.580	0.549	1.128	0.915	0.499	1.414	0.552	1.102	-4.969	1.209.640
478	CN(C)C(=O)c1cccc(c1O)/C=N/NC(=O)c2ccc(c3c2cccc3)OC	0.904	0.442	0.462	0.506	0.663	1.170	0.776	0.603	1.379	0.667	1.109	-6.008	1.057.423
479	COc1ccc(c2c1cccc2)C(=O)N/N=[CH:1]/c3nc(no3)c4ccccc4	0.903	0.441	0.461	0.504	0.663	1.167	0.780	0.603	1.383	0.667	1.108	-6.006	1.051.928
480	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3cc(=O)[nH]c(=O)[nH]3	0.900	0.472	0.429	0.506	0.660	1.165	0.875	0.550	1.426	0.667	1.139	-6.006	1.052.223
481	COc1ccc(c2c1cccc2)SCc3cc(=O)[nH]c(n3)[c:2]4ccccc4O	0.899	0.546	0.352	0.577	0.547	1.124	0.911	0.498	1.408	0.550	1.096	-4.955	1.204.495

482	Cc1c(ccc(c1O)/C=N/NC(=O)c2ccc(c3c2cccc3)OC)O	0.898	0.467	0.430	0.508	0.661	1.169	0.854	0.552	1.406	0.668	1.136	-6.019	1.058.052
483	Cc1nc(on1)c2cccc(c2)/C=N/NC(=O)c3ccc(c4c3cccc4)OC	0.894	0.433	0.461	0.503	0.663	1.166	0.757	0.603	1.359	0.667	1.099	-6.005	1.050.644
484	COc1ccc(c2c1cccc2)C(=O)N/N=C/N3CCC[C@H]3CO	0.889	0.504	0.385	0.519	0.556	1.074	0.948	0.556	1.504	0.556	1.060	-5.005	1.077.025
485	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3c([nH]nn3)C(=O)N	0.887	0.486	0.401	0.517	0.666	1.182	0.892	0.501	1.394	0.678	1.164	-6.107	1.074.906
486	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3cccc(c3O)C(=O)N	0.887	0.458	0.429	0.507	0.660	1.167	0.824	0.551	1.375	0.667	1.125	-6.008	1.057.663
487	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3[nH]nnn3	0.885	0.503	0.382	0.508	0.652	1.160	0.980	0.480	1.460	0.665	1.168	-5.987	1.054.371
488	COc1ccc(c2c1cccc2)C(=O)NNC(=O)[c:2]3ccccc3O	0.884	0.487	0.397	0.516	0.605	1.121	0.896	0.536	1.432	0.609	1.097	-5.489	1.074.007
489	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3ccccc3c4[nH]nnn4	0.882	0.488	0.395	0.540	0.695	1.234	0.835	0.478	1.313	0.712	1.200	-6.417	1.126.707
490	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3ccc(c(c3O)C(=O)N)Cl	0.881	0.451	0.430	0.507	0.661	1.168	0.802	0.552	1.354	0.668	1.119	-6.020	1.057.958
491	COc1ccc(c2c1cccc2)C(=O)N/N=C/Oc3cccc4c3ccnc4	0.881	0.464	0.417	0.521	0.559	1.080	0.809	0.621	1.430	0.556	1.020	-5.005	1.088.446
492	CNC(=O)c1cccc(c1O)/C=N/NC(=O)c2ccc(c3c2cccc3)OC	0.878	0.449	0.429	0.507	0.660	1.166	0.798	0.551	1.349	0.667	1.116	-6.008	1.057.566
493	COc1ccc(c2c1cccc2)C(=O)N/N=C/N3CCc4ccccc4C3	0.872	0.456	0.417	0.506	0.559	1.065	0.821	0.621	1.442	0.556	1.011	-5.005	1.055.104
494	CCNC(=O)c1cccc(c1O)/C=N/NC(=O)c2ccc(c3c2cccc3)OC	0.868	0.440	0.429	0.505	0.659	1.164	0.774	0.550	1.324	0.667	1.107	-6.005	1.054.774
495	COC[C@@H]1C[C@@H](CN1/C=N/NC(=O)c2ccc(c3c2ccc3)OC)OC	0.868	0.483	0.385	0.523	0.556	1.078	0.865	0.556	1.420	0.556	1.039	-5.005	1.088.767

496	COc1ccc(c2c1cccc2)C(=O)N/N=C/c3cc(ccc3O)C(=O)O	0.859	0.461	0.397	0.510	0.653	1.163	0.829	0.504	1.332	0.664	1.125	-5.978	1.063.023
497	CC(C)Oc1ccc(cc1/C=N/NC(=O)c2cccc3c2cccc3)Cl	0.844	0.427	0.417	0.474	0.559	1.033	0.811	0.621	1.432	0.556	0.983	-5.007	986.426
498	C/C(=N\NC(=O)Cc1ccc(c2c1cccc2)OC)/[c:2]3ccccc3O	0.838	0.445	0.393	0.490	0.564	1.054	0.830	0.564	1.394	0.564	1.010	-5.084	1.019.937
499	COc1ccc(c2c1cccc2)c3nnc(s3)Nc4ccccc4O	0.825	0.445	0.379	0.486	0.585	1.071	0.844	0.519	1.362	0.589	1.035	-5.307	1.010.123
500	COc1ccc(c2c1cccc2)c3nnc(s3)Nc4ccccc4O	0.824	0.445	0.379	0.485	0.585	1.070	0.843	0.519	1.362	0.589	1.034	-5.308	1.009.294

Table S 2. Score Values for ligands screened in AutoDock Vina, Molegro Virtual Docker (MVD) and Gold docking programs based on consensual docking methodology**.**

Ligand	AutoDock Vina	MVD	Gold
AOS1	**-7.4**	**-105.68**	**25.19**
AOS2	**-7.3**	**-116.62**	**23.01**
AOS3	**-8.2**	**-122.11**	**25.93**
AOS4	**-7.6**	**-107.98**	**25.25**
AOS5	**-7.4**	**-119.32**	**24.76**
AOS6	**-7.4**	**-127.45**	**23.52**
AOS	**-7.2**	**-93.22**	**22.31**

1. NMR spectra of compounds **AOS1**, **AOS2**, **AOS3**, **AOS4**, **AOS5**, **AOS6**, **AOS1'** and **AOS6'.**

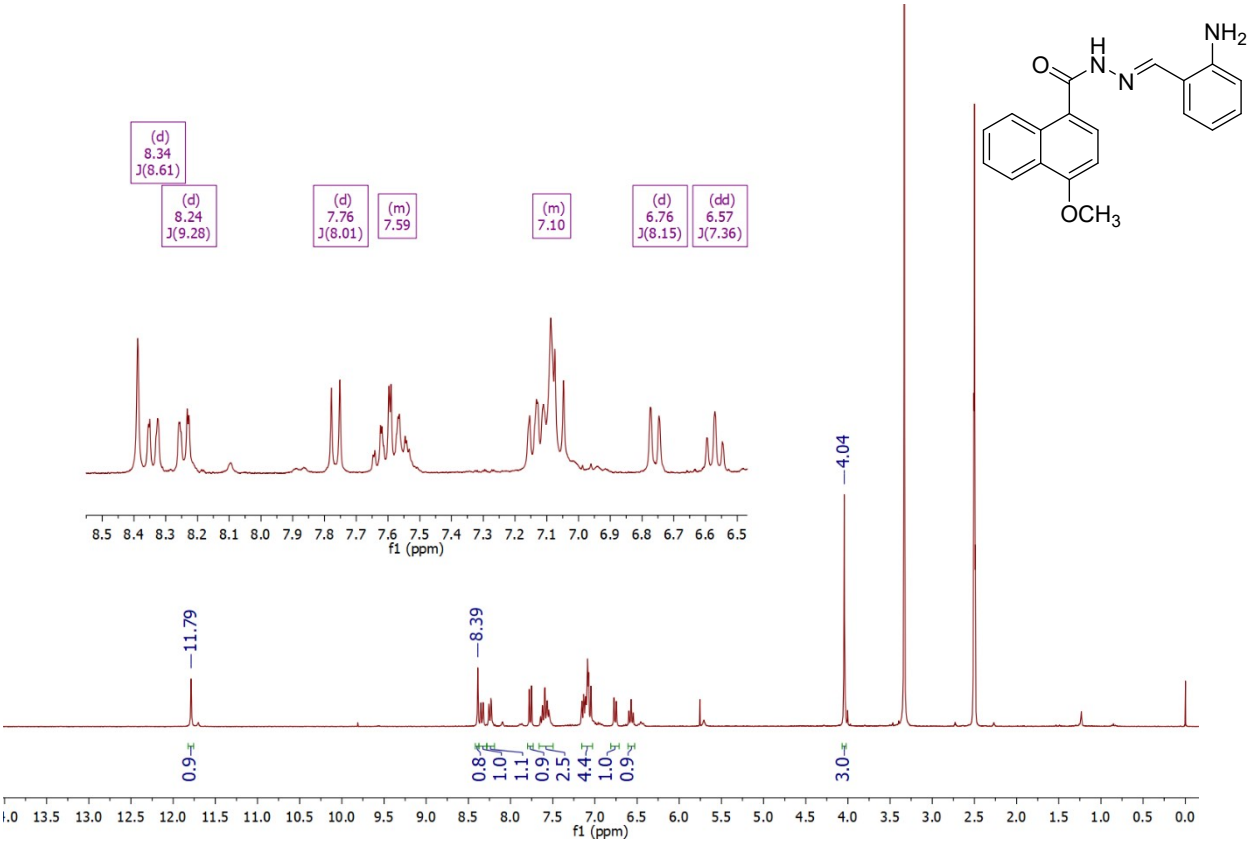


Figure S1. ^{1}H NMR spectra of **AOS1** in DMSO-d_6

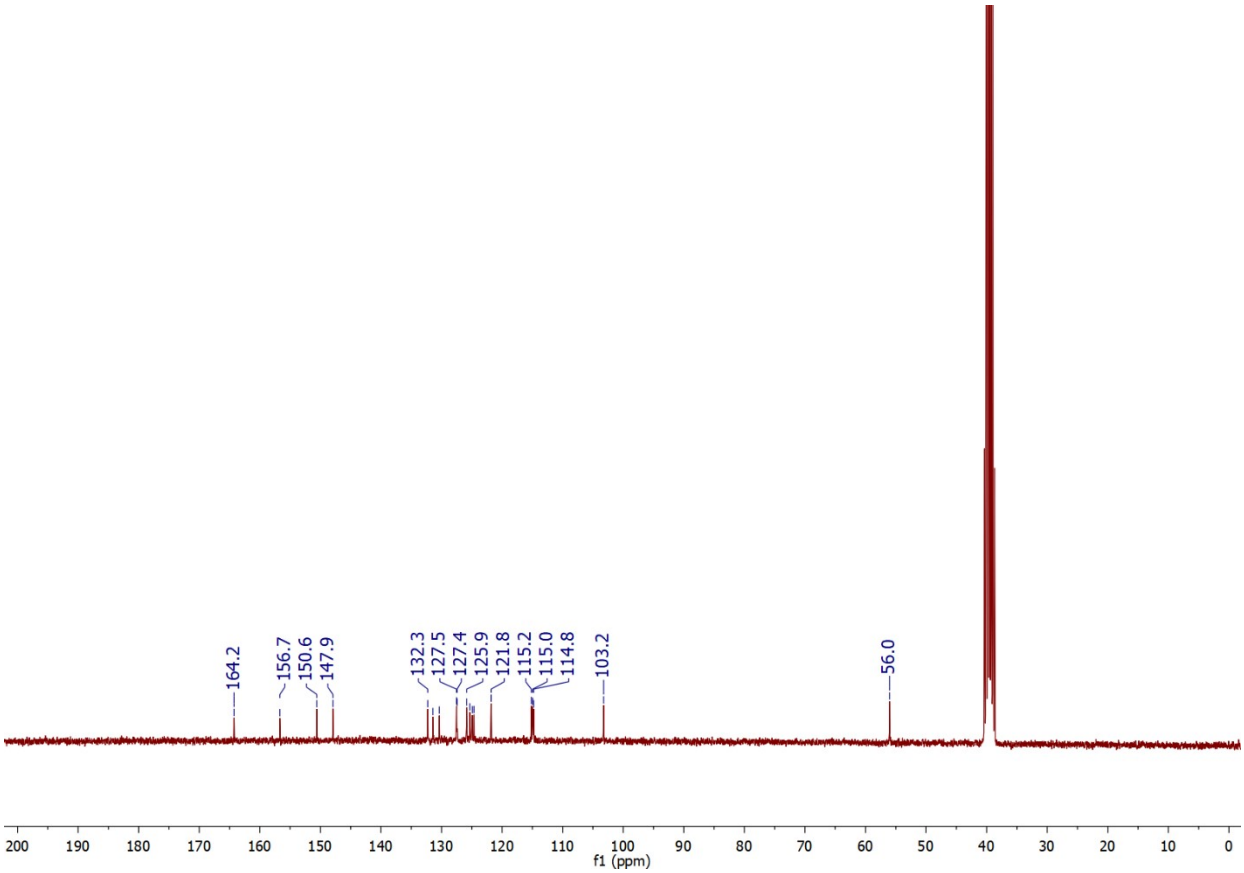


Figure S2. ^{13}C NMR spectra of **AOS1** in DMSO-d_6

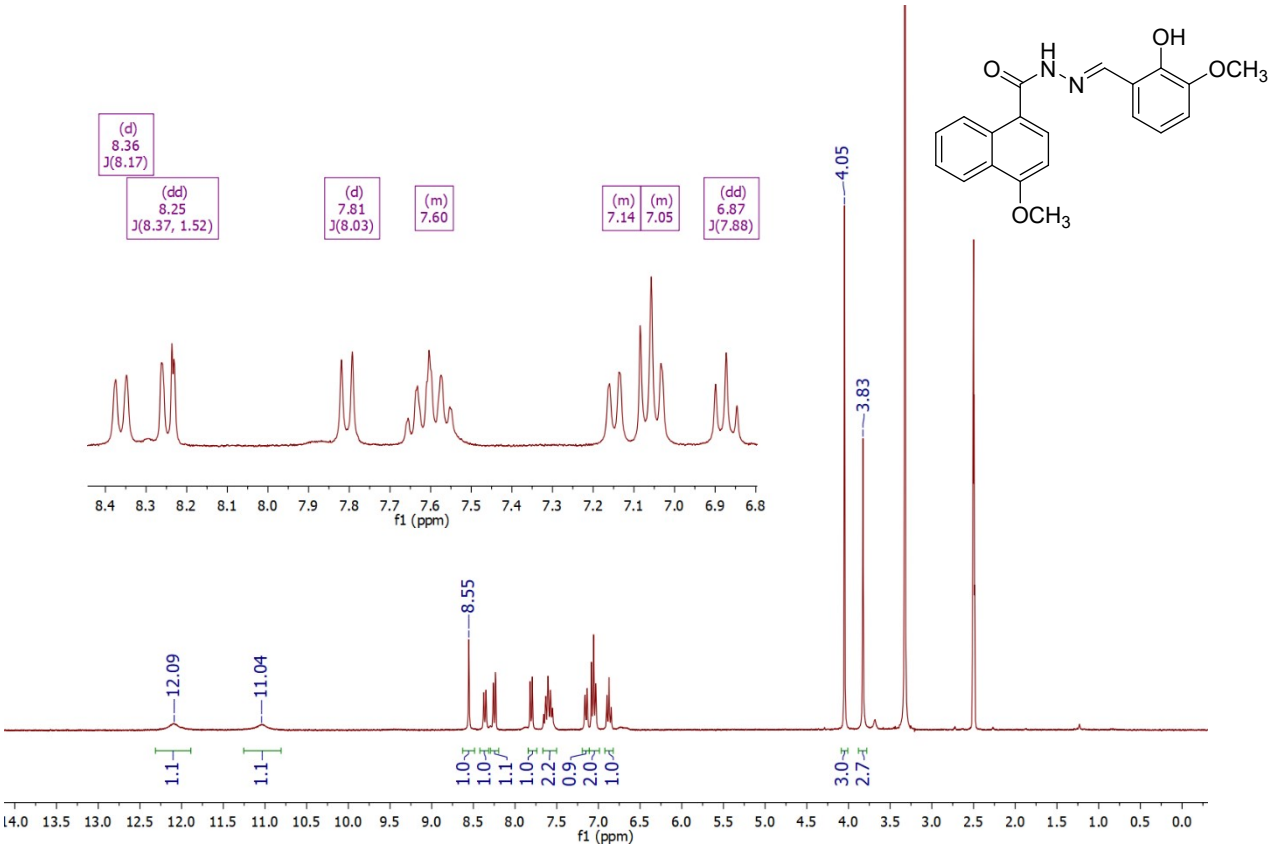


Figure S3. [1]H NMR spectra of **AOS2** in DMSO-d_6

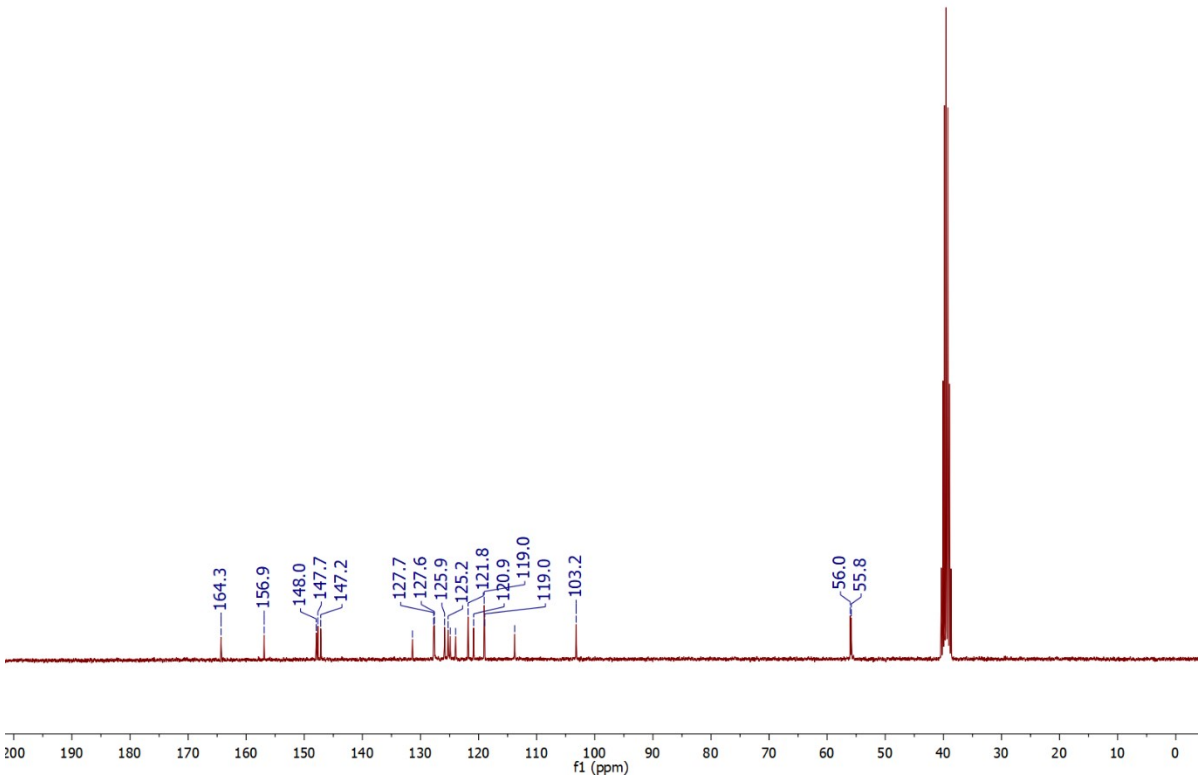
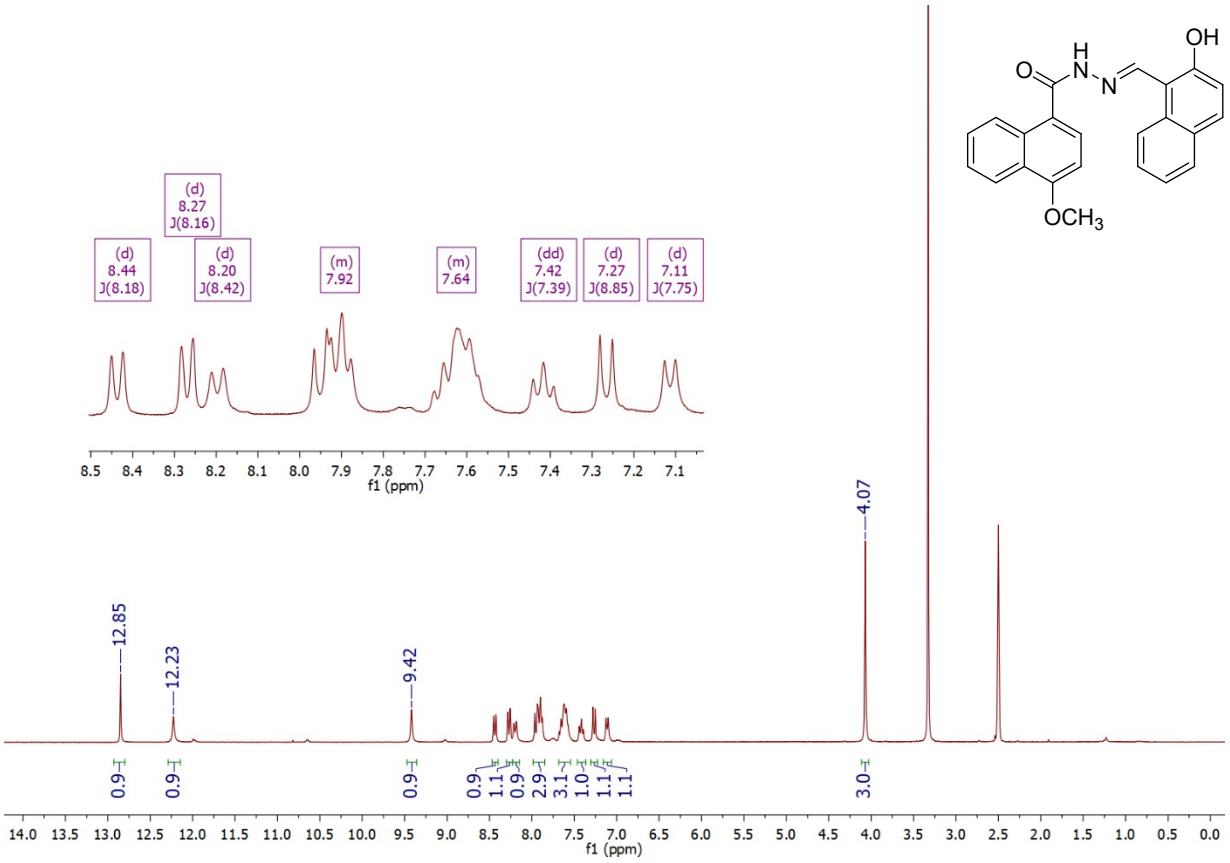


Figure S4. [13]C NMR spectra of **AOS2** in DMSO-d_6



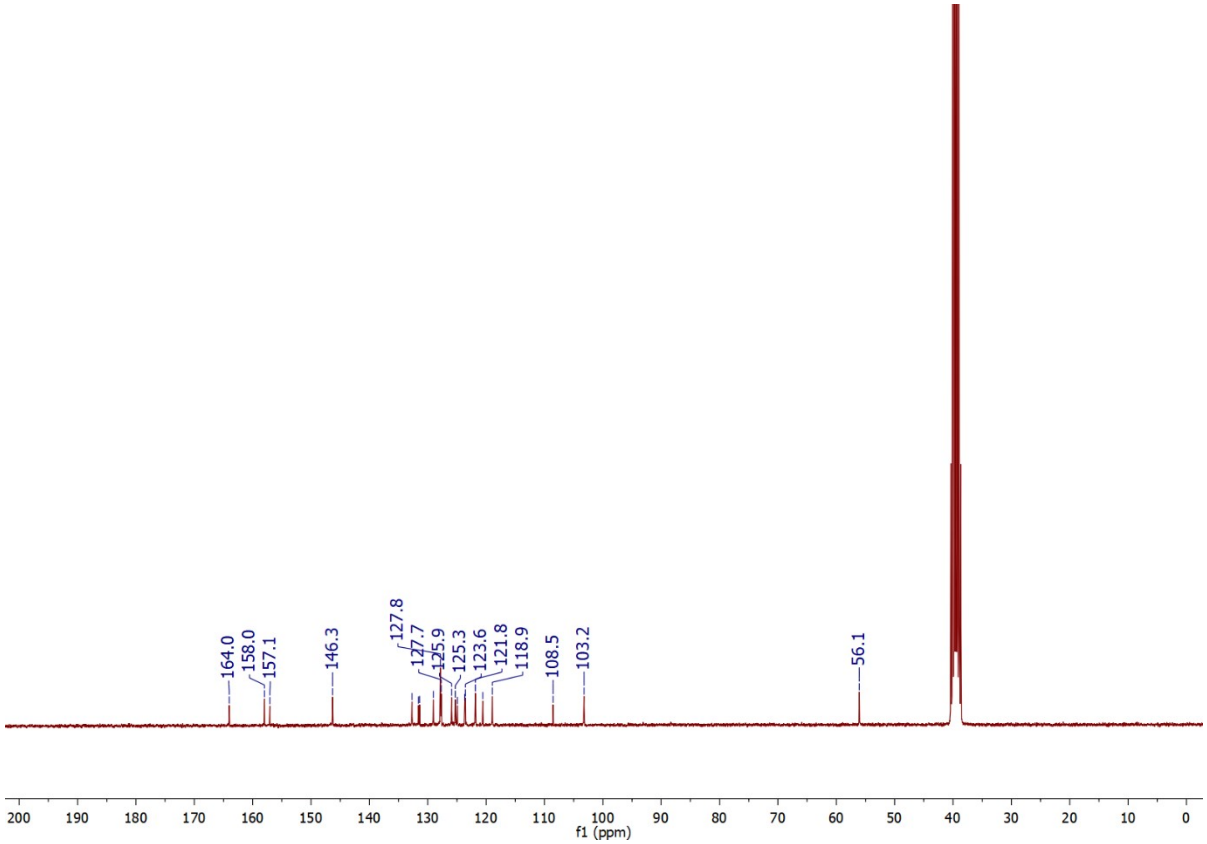


Figure S5. ^{1}H NMR spectra of **AOS3** in DMSO-d_6

Figure S6. ^{13}C NMR spectra of **AOS3** in DMSO-d_6

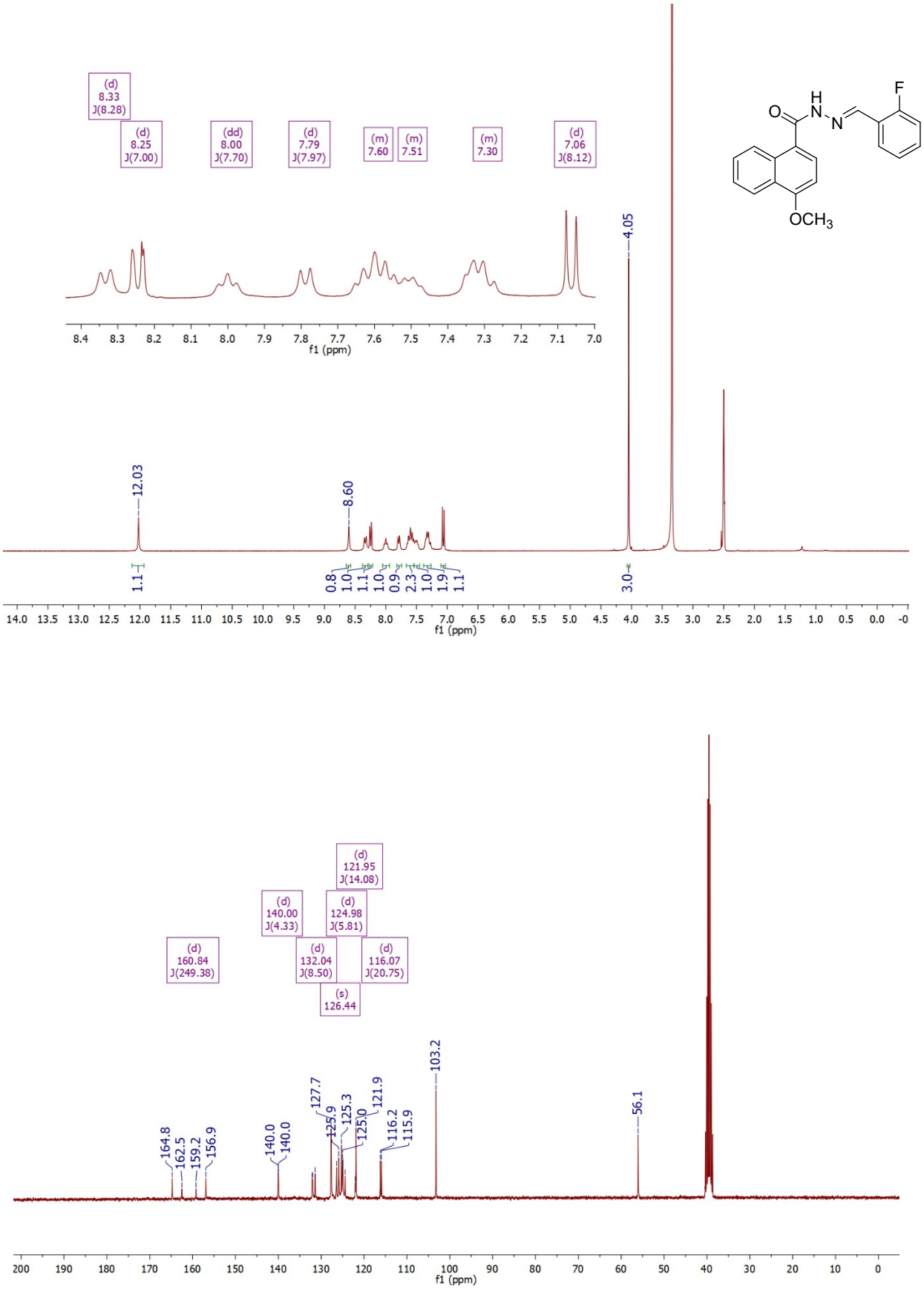


Figure S7. ^{1}H NMR spectra of **AOS4** in DMSO-d_6

Figure S8. ^{13}C NMR spectra of **AOS4** in DMSO-d_6

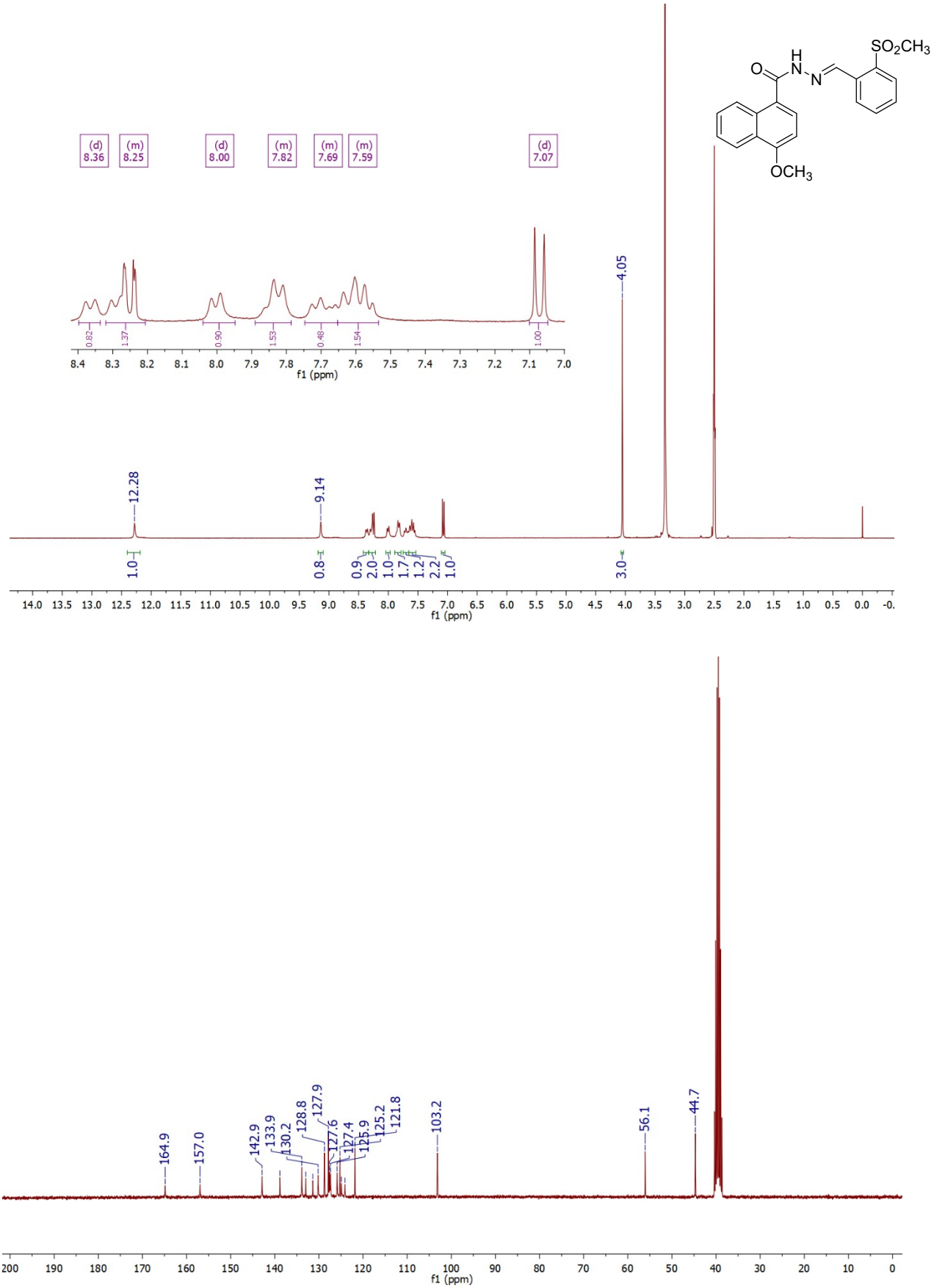


Figure S9. ^{1}H NMR spectra of **AOS5** in DMSO-d_6

Figure S10. ^{13}C NMR spectra of **AOS5** in DMSO-d_6

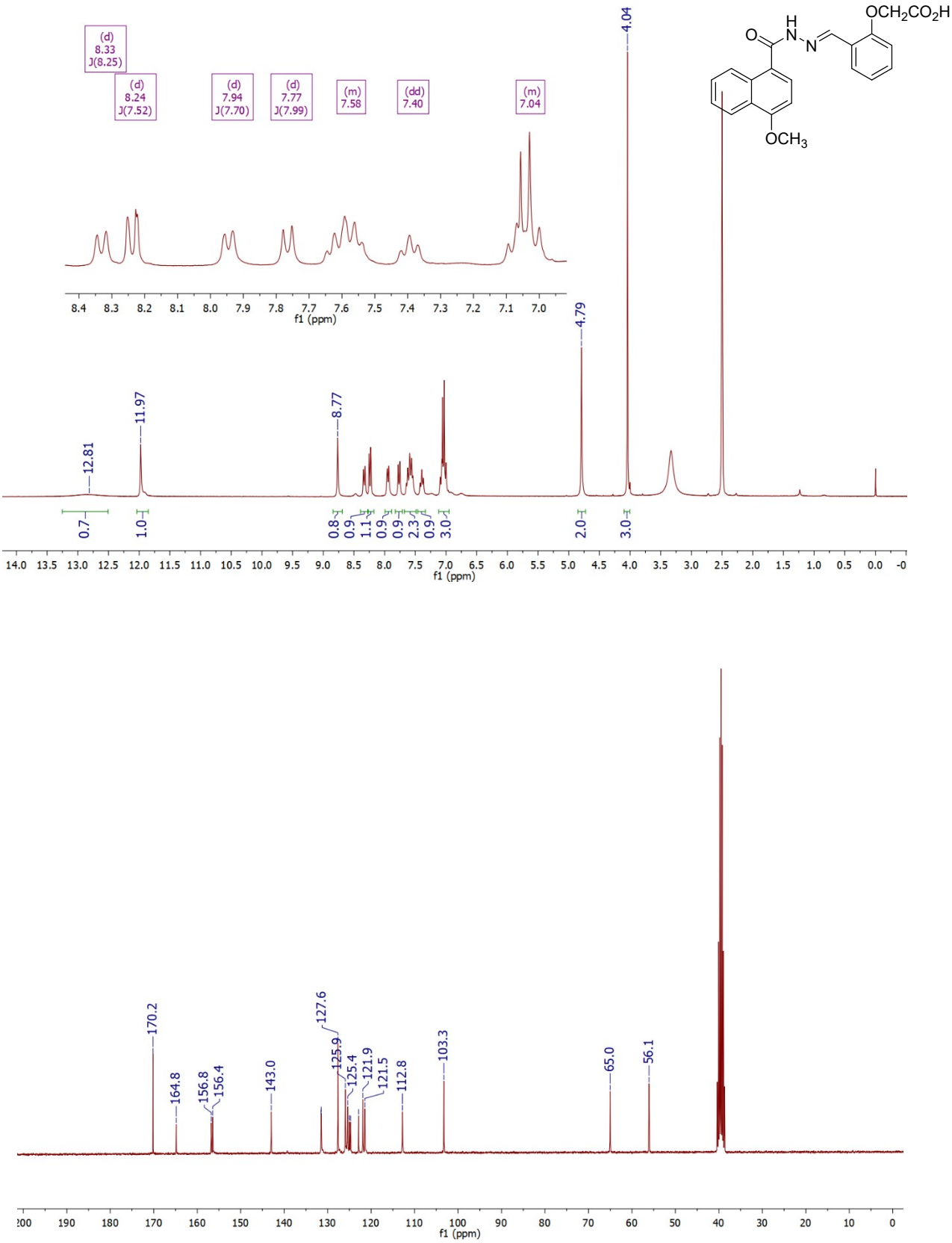


Figure S11. ^{1}H NMR spectra of **AOS6** in DMSO-d_6

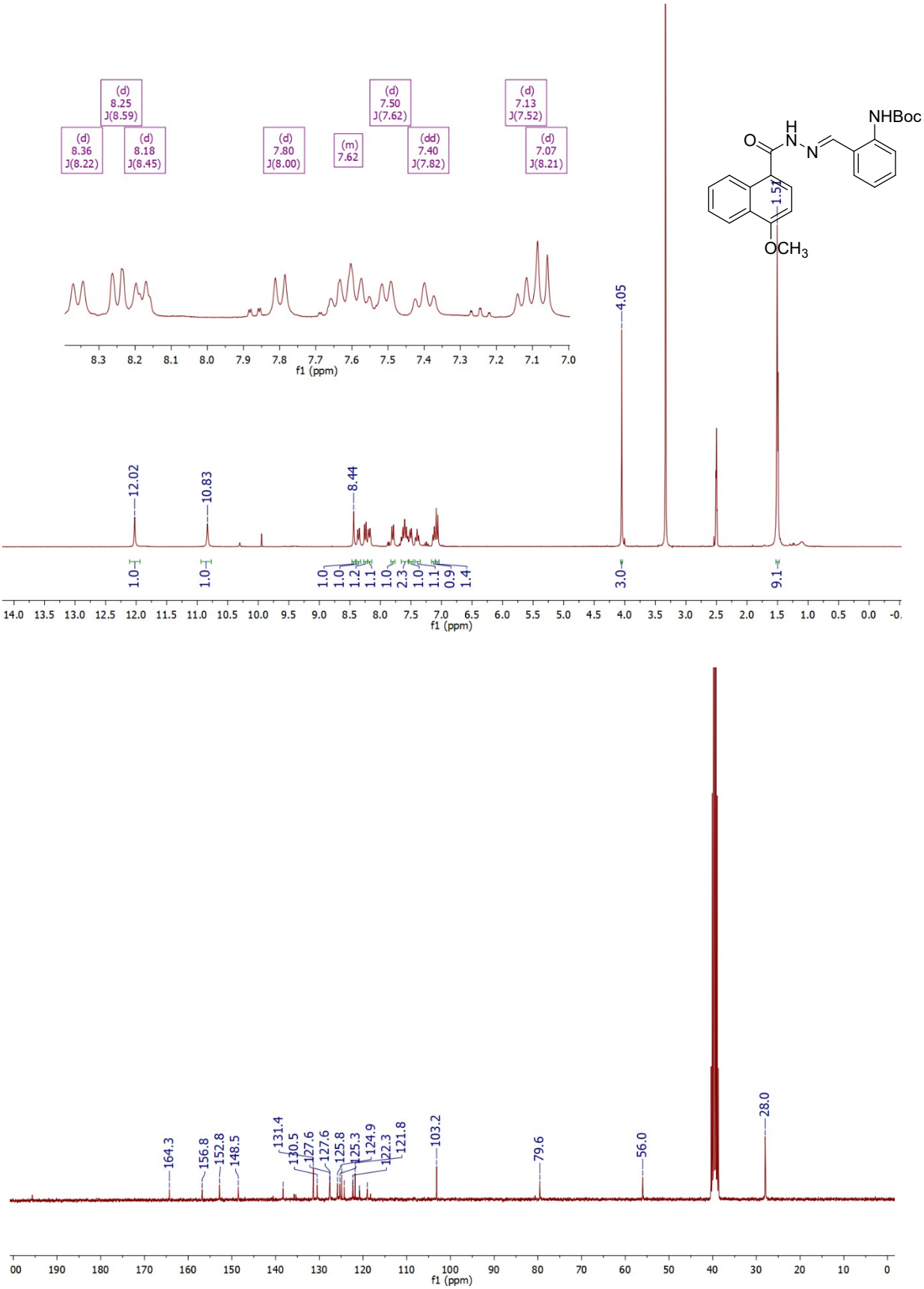


Figure S12. ^{13}C NMR spectra of **AOS6** in DMSO-d_6

Figure S13. ^{1}H NMR spectra of **AOS1'** in DMSO-d_6

Figure S14. ^{13}C NMR spectra of **AOS1'** in DMSO-d_6

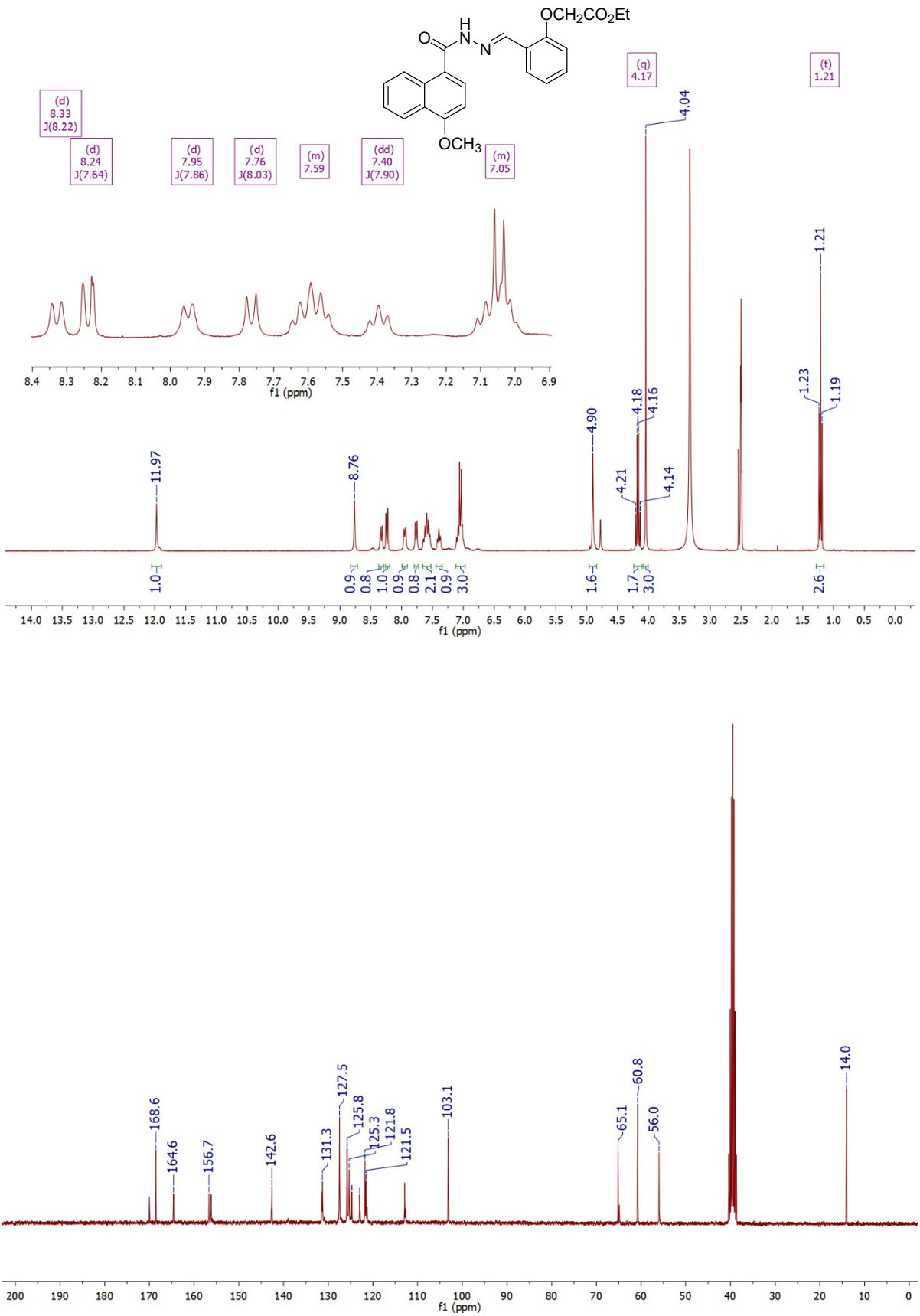


Figure S15. ^{1}H NMR spectra of **AOS6'** in DMSO-d_6

Figure S16. ^{13}C NMR spectra of **AOS6'** in DMSO-d_6

Table S3. Contact frequency (in percentage of time contact) of PbHSD residues with **AOS2** and **AOS3** ligands throughout the molecular dynamics simulation. The values in bold represent the contacts shown in Figure 5. Only contacts with a frequency greater than 5% are shown.

Residue number	AOS2	AOS3
Pro-120	-	26.3
Lys-122	-	**57.9**
Val-15	33.0	-
Ser-150	49.6	100.0
Thr-151	**49.0**	99.8
Val-152	**-**	99.1
Gly-153	11.4	95.5
Ala-154	**40.5**	**99.6**
Phe-179	**25.9**	98.6
Ser-180	-	71.9
Gly-181	**59.6**	98.8
Thr-182	**91.3**	91.6
Phe-185	6.9	4.3
Leu-214	23.8	0.1
Gly-215	**85.0**	16.3
Tyr-216	**91.1**	99.5
Thr-217	42.3	-
Glu-218	49.4	1.0
Pro-219	26.3	-
Lys-233	**26.3**	**99.3**
Ser-327	**47.1**	82.5
Asn-329	43.1	99.7
Arg-337	-	35.8
Lys-340	-	11.2
Gly-349	50.7	100.0
Ala-350	**97.7**	**97.8**
Gly-351	99.9	**98.4**
Gly-352	29.6	24.9
Val-354	33.7	-
Thr-355	94.6	90,0
NAD	100.0	57.2