Table S1. SMILES of organic chemicals, the set of each compound, their calculated and observed of pEC10 and PEC50, (training (+), invisible training (-), calibration (#) and validation (*) sets).

ID	SMILES	pEC10							pEC50						
		Split 1	Split 2	Split 3	Expr.	Prd. 1	Prd. 2	Prd. 3	Split 1	Split 2	Split 3	Expr.	Prd. 1	Prd. 2	Prd. 3
1	c1([N+](=O)[O-])ccc(cc1)N	+	*	#	3.994	4.0388	3.8463	3.5484	+	#	#	3.507	3.5349	3.0177	3.613
2	c1(ccccc1)C#N	+	+	#	3.242	2.8753	3.3681	3.3505	+	#	+	2.903	3.2193	2.7488	2.9628
3	c1(Nc2c(cccc2)Cl)nc(nc(n1)Cl)Cl	-	-	+	5.491	6.1319	5.4552	6.1869	+	#	*	5.19	5.8618	5.7377	6.0454
4	c1(Oc2ccccc2)ccc(cc1)Br	+	#	+	6.292	5.9912	5.9576	6.3602	+	*	+	5.927	5.6642	5.7642	5.6479
5	c1(Oc2ccc(cc2)Cl)ccc(cc1)N	+	#	-	5.801	5.6895	4.6564	4.9122	-	#	+	5.547	5.0397	5.1009	4.6966
6	C1(NC2CCCCC2)CCCCC1	+	+	*	5.707	5.5269	6.1507	5.2558	+	*	*	4.524	3.7892	5.6374	4.737
7	c1(Oc2ccccc2)ccccc1	-	*	+	5.398	5.3128	4.4799	5.3613	#	+	+	5.136	4.984	4.7022	4.9205
8	N(CCCC)(CCCC)CCO	#	+	+	3.734	4.9453	3.994	4.0406	#	+	#	3.289	3.5864	4.0011	4.0661
9	N(CCCC)(CCCC)CCCC	+	+	+	3.87	5.3764	4.8435	4.5192	-	+	*	3.469	4.3554	4.9119	4.3836
10	C(CCl)CCl	-	+	#	4.303	5.2676	4.7454	4.2855	*	+	+	4.1353	3.8584	5.159	4.9939
11	c1(CNC(C)C)ccccc1	-	+	#	4.812	4.5885	4.6909	4.4927	#	-	#	4.53	4.3388	3.8341	5.133
12	c1(/N=N/c2ccccc2)ccccc1	-	*	#	5.207	5.5888	5.2887	5.104	#	*	*	5.042	5.0532	5.3059	4.3227
13	C1(CO1)CCC=C	-	-	#	3.703	4.2278	3.5278	3.1948	+	-	-	3.367	3.592	3.4808	3.5683
14	c1(/C=C/COC(=O)C)ccccc1	-	*	+	4.317	4.6627	4.5551	4.4298	*	#	#	4.1321	3.7712	2.9179	3.9282
15	c1(ccccc1)N=C=S	+	-	#	5.912	5.8009	5.3661	5.5077	+	*	#	5.637	6.154	5.1604	4.675
16	c1(ccccc1)NC(=O)C	*	+	+	3.1266	3.836	3.4582	3.4798	+	*	-	2.655	3.263	2.9525	2.9216
17	c1(ccc(cc1)OC)CCC(=O)C	#	*	#	4.137	4.7437	3.6437	3.9946	+	-	+	3.642	3.7848	4.0967	3.6212
18	c1(ccc(cc1)N)CCCCCCCCCCCC	-	#	-	7.105	7.7009	7.7544	6.853	*	*	#	6.4784	6.7561	7.3284	6.6878
19	c1(ccccc1)/C=C/CO	*	+	+	3.3873	4.3169	3.716	4.0246	*	*	-	3.0983	3.6487	3.2481	2.8872
20	C(CCCC)(CC)CN	#	+	+	4.074	4.4822	3.5975	4.2491	#	#	#	3.651	4.0748	3.777	4.3097
21	c1(ccc(cc1)N)C	+	-	#	4.65	4.3847	4.0337	3.7152	-	+	+	4.439	3.9393	3.3237	3.542
22	C(=O)(CCCCC)CC	+	*	+	3.397	4.0785	4.0137	3.7168	+	*	#	3.176	3.3663	3.5031	3.4406
23	C(Cl)C	*	*	*	4.0781	4.9406	4.7388	4.4758	*	*	-	3.7533	4.3462	4.3771	3.9622
24	C(CN)C	-	#	#	3.192	3.5032	3.6524	3.7814	-	*	+	2.885	2.9593	2.7593	2.9537
25	C(=C)CN	#	-	*	2.499	3.2206	3.0244	3.1066	*	+	-	2.0948	2.7465	2.7485	2.5838
26	C(OC(=O)CCl)(C)(C)C	+	+	-	5.923	4.6472	5.3016	4.5477	+	+	+	5.506	3.4576	3.9316	4.3047
27	C(C(C)C)CN	+	*	-	3.095	3.7505	3.4948	3.6615	+	#	-	2.355	3.0462	3.0873	3.1794
28	C(C(=O)C)CC	-	*	+	1.99	3.2846	2.6241	3.0374	*	*	*	1.6587	2.5812	2.4361	2.127
29	C(C(=O)O)CN	*	+	-	4.1574	2.624	2.4076	2.9092	+	+	+	2.977	1.9929	2.0001	1.5597
30	C(OC(C)(C)Cl)(C)(C)Cl	-	-	+	3.15	3.0327	2.7241	3.6517	-	#	-	2.889	1.9832	1.3338	3.2065
31	C(CC)CN	*	-	+	3.5631	3.5456	3.102	3.578	*	+	*	3.0381	2.9574	2.7204	3.1214
32	C(CC)C#N	-	#	#	2.089	2.558	2.4417	2.6932	*	-	+	1.7223	1.8187	1.9283	1.7756
33	C(=O)(/C=C/C(=O)O)O	-	-	-	3.474	3.5218	2.7223	2.9495	-	*	*	1.989	1.6717	1.9336	1.3106
34	C(CCN)CN	#	*	-	3.389	3.9222	3.6148	3.5231	-	*	*	2.23	3.038	2.8477	3.4774
35	N(CCCN(C)C)(C)C	*	+	-	3.9686	3.7642	3.5746	4.0708	-	*	*	3.583	3.7363	3.5988	3.765
36	C(CNCC(C)C)(C)C	+	+	+	4.203	4.2236	4.0449	3.3711	+	+	-	3.907	3.3219	3.3574	3.678
37	N(CCCCCCN(C)C)(C)C	#	*	-	4.838	4.5253	4.9715	5.1569	*	*	+	4.5288	4.6072	4.7358	4.8276
38	C(CCC)CCN	-	*	+	3.964	4.3651	4.9872	3.7099	#	-	#	3.607	3.4921	3.1709	3.5717
39	S(CCC)CCC	+	+	*	3.427	3.8901	3.4482	3.2529	+	*	-	3.322	3.1536	3.2952	3.3628
40	C(CCCN)CCC	#	#	*	4.493	4.73	4.2139	4.0362	+	*	-	4.313	3.9715	3.6069	4.0845
41	C(CCC=O)CCC	-	#	#	4.053	3.6922	4.281	3.5597	#	*	*	3.798	3.3729	3.1606	3.3781
42	C(CCCC)CCCN	#	-	+	5.07	4.9588	3.562	4.3742	-	-	*	4.856	4.2285	3.9701	4.2654
43	C(CCCCl)C(=O)O	*	+	*	3.615	3.3364	4.228	3.6132	+	+	+	2.785	2.9423	2.3043	2.8724
44	C(CCCCCC)CCC(=O)Cl	*	+	#	4.351	6.0769	4.0968	4.8455	*	+	*	4.0763	4.782	4.4645	4.8459
45	C(=O)(C1CC1)C1CC1	+	+	+	2.635	2.5017	5.0627	2.5299	+	+	*	2.267	1.6009	3.0595	2.4146
46	C(CCCCCCCCC)CCN(C)C	*	*	+	7.4261	6.3882	2.2169	6.222	+	-	+	6.898	6.0849	6.1649	6.5443
47	C(CCCCN)CCCC	*	#	-	5.8137	5.3237	6.2003	4.7005	+	#	+	5.513	4.7079	4.4062	4.7782
48	c1(cccn1)C(=O)C	*	-	*	2.4716	3.0497	5.0609	3.5086	*	#	+	2.1658	3.12	2.9949	2.8572
49	C1(CCCCC1)N=C=S	+	+	#	5.671	5.5592	3.0442	5.7593	-	+	#	5.416	5.1829	5.8532	4.5395
50	C(CCCCC)CCCCBr	*	+	+	6.1339	6.0378	5.8036	5.9953	*	-	+	5.6681	4.9844	5.2506	5.834
51	C(CCCCC=C)CCCC(=O)O	*	+	-	5.3156	5.7089	5.9205	5.0861	*	+	*	4.7442	4.924	4.8015	5.5279
52	C(COCCCC)OCCSC#N	#	*	+	5.029	5.329	4.6824	5.1838	#	+	#	4.229	4.2405	4.8331	3.9869
53	C(CO)(Cl)(Cl)Cl	+	*	*	2.848	3.6831	6.913	3.4339	*	*	*	2.4949	1.5345	1.6778	3.449
54	C(C(=O)C(Cl)(Cl)Cl)(Cl)(Cl)Cl	+	#	+	4.77	5.3335	3.3273	5.1813	*	-	+	3.4272	2.5489	3.8863	3.4862
55	C(=O)(C(Cl)Cl)OC	+	#	#	5.114	4.167	5.7693	4.0892	#	+	*	3.979	3.7879	3.635	3.0401
56	c1(c(c(cc(c1Cl)Cl)Cl)Cl)[N+](=O)[O-]	-	-	+	5.964	6.1029	3.8372	6.2366	+	+	-	5.467	5.8341	6.0523	5.997

57	c12c(C(=O)C(=C(C1=O)Cl)Cl)ccc c2	*	+	*	6.5637	6.5474	6.216	5.8015	+	+	*	6.034	6.2107	5.8084	5.0275
58	OC[C@@H]1[C@@H](O)[C@ @H](O)[C@@H](O1)n1cnc2c(= O)[nH]c(N)nc12	+	+	*	2.751	2.6404	7.1069	3.9418	+	-	-	2.044	2.6533	2.0677	2.3575
59	c12c(cccc1NCC)cccc2	*	+	+	4.7022	5.5123	2.6541	4.583	*	#	*	4.3703	4.5462	4.6268	4.6125
60	C1(=O)C(=C(C(=O)C(=C1Cl)Cl) Cl)Cl	-	+	#	5.504	5.6835	4.8663	5.89	*	*	+	5.0483	3.8833	3.9555	4.9546
61	c1(C(C(=O)c2ccc(cc2)OC)O)ccc(cc1)OC	+	+	-	4.802	4.8842	4.3521	5.2458	-	+	+	4.134	4.2654	4.4207	3.8311
62	c1(c2cc(c(cc2)N)OC)cc(c(cc1)N) OC	#	#	#	4.869	5.6019	5.1542	5.5197	+	+	-	4.274	4.7893	5.0685	4.7768
63	c1(C(=O)OCC)ccc(cc1)O	+	-	+	5.859	4.2689	4.4809	4.6894	-	#	+	5.619	3.8987	4.3344	4.4341
64	N(C(C)C)(C(C)C)CCN	-	+	-	3.045	4.459	4.6093	3.9837	*	+	+	2.5714	3.8041	3.3438	2.8449
65	1(ccc(cc1)OCCOCC[N+](Cc1ccc cc1)(C)C)C(CC(C)(C)C)(C)C^[Cl -]	#	*	*	6.809	7.8903	3.3587	7.5405	+	#	+	6.369	5.3466	5.6365	6.5027
66	c1(ccccc1)N(C)C	+	-	+	3.578	4.5133	6.2358	4.2376	#	+	#	3.298	4.6235	3.4688	4.1098
67	C(SP(=S)(OC)OC)(CC(=O)OCC) C(=O)OCC	#	#	+	4.59	4.5347	3.7834	4.5531	#	*	*	4.139	4.5165	4.3523	4.6858
68	c1(cc(c(cc1)N)Cl)[N+](=O)[O-]	-	#	*	4.705	5.639	4.6006	5.0554	*	*	+	4.0609	4.8127	4.8716	4.9684
69	c1(nc(nc(n1)Cl)NCC)NCC	#	*	-	6.305	6.7671	5.8757	6.718	-	*	*	5.681	5.3975	5.8139	4.0386
70	c1(Nc2ccccc2)ccccc1	+	*	+	5.359	5.3582	6.306	5.4007	-	+	-	4.95	4.8569	4.7154	4.1935
71	c1(C(=O)C(=O)c2ccc(cc2)OC)cc c(cc1)OC	*	+	*	5.2783	5.0033	4.7339	5.6758	*	*	-	4.4587	4.0013	4.6278	3.6911
72	C(CCCC)(CC)C=O	-	*	+	3.78	3.9296	5.3798	3.866	+	+	+	3.541	3.3468	3.2503	3.7296
73	c1(ccc(cc1)OC)C=O	#	-	*	3.603	3.6709	3.308	4.0385	-	-	+	3.143	3.7731	3.4207	2.7517
74	C(=O)(CCC)CCC	#	*	*	2.986	3.7694	3.9833	3.3301	#	+	+	2.727	3.3077	3.2894	2.6059
75	C(CC)C=O	#	#	+	3.579	3.1259	3.4222	3.1232	-	*	-	3.139	2.4695	1.9972	3.8712
76	C(CCCC)C(C)N	#	-	*	3.982	4.4746	2.8757	3.5007	*	+	*	3.4281	3.2567	3.4857	5.3596
77	C(CCCCCCCCCCCCCC)C[N+](CC)(C)C^[Br-]	-	+	*	6.938	7.2432	4.0049	6.7005	+	*	+	6.699	6.3217	6.5922	4.4084
78	C(NCCCN)CCCN	#	+	-	3.685	5.6053	6.3135	4.6272	-	#	*	3.391	4.1703	4.2352	5.6528
79	C(CCCCCC)CCCCCN	*	+	*	6.6887	6.1461	4.8803	5.7029	+	#	-	6.518	5.7013	5.5687	4.3626
80	C(=C(Cl)Cl)(Cl)Cl	-	#	*	4.497	5.214	5.7876	4.0652	*	-	+	4.224	4.0448	3.7643	5.8159
81	c1(ccc(cc1)CSC#N)[N+](=O)[O-]	+	*	+	6.635	6.3954	3.3226	6.3454	*	-	+	6.4018	5.231	5.2726	7.2581
82	c1(cc(c(cc1)Br)Cl)NC(=O)N(OC) C	*	#	#	7.3537	7.4743	5.622	7.5363	#	+	+	6.824	6.7904	7.3359	3.2523
83	c12c(NC(NS2(=O)=O)C(Cl)Cl)cc (c(c1)S(=O)(=O)N)Cl	+	*	+	3.52	4.0988	8.1615	3.8288	+	+	#	2.796	3.5218	3.7741	5.686
84	c12c(Oc3c(N1)cccc3)cccc2	*	+	#	5.5469	5.457	4.218	5.26	*	+	-	5.1168	4.1417	5.0956	5.1205
85	c1(c(nc(cc1)N)N)/N=N/c1ccccc1 ^Cl	*	+	+	5.9203	6.1132	5.471	5.1973	-	-	*	5.578	4.8647	5.1611	6.3982
86	c1(nc(nc(n1)Cl)NC(C)C)NC(C)C	*	+	-	6.282	6.4405	5.6595	6.0058	+	#	*	5.781	6.213	5.9329	5.0804
87	c1(ccc(cc1)C(=O)CCl)NC(=O)C	*	*	+	6.2464	6.238	6.2909	6.4928	+	+	-	5.794	4.5208	5.2753	7.0067
88	c1(N(C(=O)COc2sc(nn2)C(F)(F) F)C(C)C)ccc(cc1)F	+	#	#	9.069	8.9197	6.2155	8.621	-	#	#	7.356	6.9867	7.4023	5.4977
89	C(=O)(c1ccc(cc1)N)OCCCCCCC C	+	-	-	6.457	6.6699	8.6172	6.5488	#	-	+	5.958	5.1843	5.9209	5.8055
90	C(CCCCC)CCCCS	-	#	*	6.27	6.4579	6.5018	5.6291	*	-	-	5.6867	5.8304	5.5418	5.5118
91	N(CCCCCC)CCCCCC	+	+	*	5.43	5.7031	6.2651	5.2204	#	#	+	5.271	5.4899	5.7874	7.0402
92	C(CCCCCCCC)CCCCCCCN	+	+	+	6.92	7.3333	5.9424	7.0315	+	-	-	6.815	7.1741	7.1672	3.7335
93	c1(ccc(cc1)C#N)C(=O)C	#	+	#	3.499	4.2406	7.3473	3.8363	*	-	*	3.1841	4.2791	4.0439	2.7475
94	c1(S(=O)(=O)Nc2ccccn2)ccc(cc1)N	+	+	-	5.402	5.411	4.2279	5.07	*	-	#	3.1157	3.1598	3.2213	2.2196
95	c1(C(=O)O)ccc(cc1)N	#	#	*	2.757	3.2844	4.5471	3.2764	+	+	-	2.221	3.3148	2.8756	3.2437
96	c1(ccc(cc1)N)CCCC(=O)O	*	#	+	2.9746	5.2637	3.4531	3.7358	+	+	+	2.566	3.2285	3.5288	6.3413
97	c1(nc(NC(C)C)nc(n1)OC)NC(C) C	-	+	+	6.143	5.9162	3.8462	5.7284	+	+	*	5.83	5.7079	4.9708	3.0233
98	C(=O)(N=C=S)OCC	+	+	*	4.626	5.1073	5.7771	5.5179	#	-	+	3.516	4.6217	4.5955	1.3213
99	c12c(cc(cc2)S(=O)(=O)[O-])ccc(c1)S(=O)(=O)[O-]^[Na+]^[Na+]	+	*	+	2.84	1.7959	4.5842	2.019	-	*	#	1.612	1.0902	0.8584	7.0645
100	c1(C(=O)CCCCCCCCCCC)ccccc 1	*	-	*	7.8313	6.5786	2.0057	6.6692	*	*	-	7.1604	6.3811	6.5788	5.4658
101	c1(NC(=O)N(OC)C)ccc(cc1)Cl	#	*	-	6.493	5.4759	7.3336	6.2812	+	-	+	5.764	5.6929	4.706	3.0299
102	C(CCC)(C(=O)O)(Cl)Cl	#	+	-	3.382	3.873	6.3674	3.3915	-	-	-	2.704	2.7279	1.9167	5.4382

103	c1(/C=C/C(=O)OCC=C)ccccc1	+	-	*	5.302	5.8365	3.3084	5.9814	-	*	+	5.161	4.9817	4.9765	5.2169
104	n1(c2c(nc1)c(ncn2)NC)[C@@H]1O[C@@H]([C@H]([C@H]1O)O)CO	-	+	-	5.449	5.6275	5.4474	5.1467	#	+	*	5.107	3.6484	4.7373	5.126
105	c1(c(cc(cc1[N+](=O)[O-])S(=O)(=O)N)[N+](=O)[O-])N(CCC)CCC	+	+	+	7.284	7.0434	5.5937	7.2978	+	-	#	6.021	5.4969	5.5555	5.7773
106	c1(nc(nc(n1)Cl)NCC)NC(C)C	*	*	#	6.6617	6.9772	6.3245	6.3168	*	#	-	6.1297	5.7861	5.8817	5.7102
107	c1(c(c(cc(c1)C#N)[N+](=O)[O-])Cl)[N+](=O)[O-]	-	+	+	5.826	6.2342	6.2196	6.2278	+	#	+	5.482	6.0941	5.47	3.766
108	[C@@]12([n+]3ccccc3)C[C@H]3C[C@@H](C1)C[C@@H](C2)C3^[Br-]	+	#	-	4.806	4.455	6.5621	4.5183	-	+	#	3.977	3.3803	3.9966	4.0976
109	c1(c(cccc1Cl)Cl)C(=O)N	*	+	+	3.8475	4.3776	4.445	4.5746	*	-	-	3.6161	4.6947	4.4696	6.4625
110	C(CCCCCCCCCCCCCC)N	-	*	-	7.763	6.5111	5.4167	6.205	-	+	+	7.444	6.5504	6.739	4.9591
111	C(CCCCC)CCCCN	*	#	#	6.6725	5.5524	7.2872	5.0386	-	-	-	6.279	4.9649	4.7694	6.2184
112	c1(Oc2ccc(cc2)Br)ccc(cc1)Br	+	-	+	6.34	6.91	5.0078	6.6148	-	+	+	6.136	5.8248	5.9022	5.8907
113	c12c(c(cc(c1O)Cl)Cl)cccc2	+	+	+	6.705	5.9	6.4333	5.749	*	-	+	6.1824	5.8559	5.5531	6.4577
114	c1(c(=O)n(c(nn1)SC)N)C(C)(C)C	-	-	-	7.331	6.8757	5.7316	6.0708	+	+	+	6.787	6.1947	6.025	4.4169
115	S(SCC=C)CC=C	-	-	+	4.625	5.1518	6.628	5.29	-	#	#	4.36	4.3725	4.4985	6.25
116	c1(c(cc(cc1Cl)Cl)Cl)N=C=S	#	+	-	6.632	6.8669	4.5333	6.7081	*	#	*	6.3131	7.5414	6.872	3.8846
117	N(=C=S)C(C)C	-	*	*	5.552	5.4679	7.7057	4.7494	+	#	*	5.138	5.2244	4.3454	6.7879
118	c1(nc(nc(n1)SC)NCC)NC(C(C)C)C	+	+	+	7.849	7.7773	5.4339	8.4381	-	+	*	7.519	7.0036	7.5803	8.2702
119	c1(N(COCCCC)C(=O)CCl)c(ccc c1CC)CC	+	+	-	8.523	8.6758	7.79	8.1328	*	+	*	7.7501	7.7757	8.2776	5.1414
120	[N+](Cc1ccccc1)(CCCC)(CCCC)CCCC^[Cl-]	#	*	-	5.938	4.9094	9.0827	5.0692	*	*	+	4.8606	4.7718	4.4754	4.141
121	C(=O)(OCCN(C)C)C=C	+	#	+	5.709	4.3717	5.5159	4.5906	-	+	-	4.952	3.4738	3.9704	2.9996
122	C(=O)(/N=N/C(=O)OC(C)C)OC(C)C	#	-	-	3.607	4.0463	4.2513	3.9866	+	+	+	2.971	3.8025	3.266	4.9621
123	c1(c(c(C(C)C)ccc1)N)C(C)C	#	-	-	4.929	5.826	4.0547	5.197	-	-	-	3.987	4.8724	5.0619	4.8376
124	c1(ccc(cc1)CCCCCCCCCCCC)S(=O)(=O)[O-]^[Na+]	+	*	*	4.501	5.7465	6.5609	5.7345	+	+	+	3.919	4.9632	5.5567	3.8246
125	c1(CCC(=O)C)ccccc1	-	#	+	3.809	4.3391	5.9376	3.8169	*	+	*	3.6146	3.6092	3.6631	6.8592
126	C(CCCCCCCN)CCCCCCC	+	*	*	7.609	7.1046	3.6771	6.6935	+	+	+	7.412	6.9171	6.8039	2.8446
127	C(C(=O)O)CCBr	-	#	-	2.953	3.7251	7.4003	3.4211	-	#	*	2.602	2.6346	2.0501	5.6668
128	N(CCCN=C=S)(CC)CC	+	+	+	5.668	6.3644	3.3382	6.3786	*	-	+	5.5642	6.292	5.6974	4.4435
129	C(/C=C/c1ccccc1)Cl	+	#	#	4.466	4.9654	5.7042	4.0545	*	#	#	3.9653	4.5748	3.9573	5.1686
130	c1(Oc2ccccc2)c(cccc1)N	+	+	#	4.724	5.6213	4.87	5.6057	*	+	*	4.3539	4.1767	4.684	3.968
131	C1(CC(CC(C1)N)(C)C)(CN)C	*	-	-	5.1898	5.1734	4.7387	4.0725	*	#	*	4.9759	2.7312	2.8343	1.8262
132	C(=O)([C@@H](C)Cl)O	*	-	*	2.6394	3.0412	3.858	3.5455	#	-	+	1.482	2.4213	2.8554	6.1655
133	C(CCCCCCN)CCCCCC	-	-	*	6.855	6.5109	2.943	6.0292	+	-	-	6.568	6.1807	6.0047	2.7872
134	c1ncncn1	-	#	#	2.913	3.2303	6.6205	1.471	-	-	+	2.531	2.352	2.9649	5.0161
135	C(=O)(OCC=C)CCl	+	-	*	6.025	5.1707	2.5204	5.5319	+	+	+	5.597	4.2391	4.5528	2.5732
136	[N+](CC1CO1)(C)(C)C^[Cl-]	-	+	*	3.08	2.4795	5.1559	2.601	*	*	#	2.928	2.0145	1.3787	2.4615
137	[C@@H](Cc1c[nH]cn1)(NC(=O)CCN)C(=O)O	-	#	+	3.836	3.8464	2.4339	3.6223	+	-	-	3.622	2.9317	3.1843	5.5841
138	c1(NC(=O)N(OC)C)ccc(cc1)Br	+	+	-	6.209	5.8907	3.2351	6.2881	-	*	#	5.621	5.2956	4.8549	3.8003
139	[N+](CCCC)(CCCC)(CCCC)CCCC^[I-]	+	*	#	5.289	5.7049	6.591	4.5965	#	*	-	5.011	4.9732	5.9162	3.6826
140	c1(ccc(o1)C)C(CC=O)C	*	*	+	4.0684	3.9183	7.0622	3.9309	#	*	+	3.881	3.133	3.0347	4.1732
141	C1(CCCCC1)CN	+	-	*	4.441	3.6212	3.6031	4.487	-	-	-	3.94	3.3869	4.2337	3.8211
142	C(Oc1ccc(cc1)C(=O)O)(F)(F)F	+	+	*	3.952	3.7154	4.466	4.4683	+	+	-	3.469	3.7517	4.2925	4.6067
143	c1(ccc(cc1)N)CCCCCC	#	-	#	5.579	5.92	3.6062	4.8601	-	*	*	5.416	4.5469	4.9307	5.8558
144	N(C(=O)CCCCCCCCCCC)(CC)CC	-	#	+	6.453	6.2656	5.4149	6.2124	-	-	#	6.321	5.3012	5.5717	4.9456
145	c1(c(cc(cc1)OC)OC)N=C=S	*	*	+	6.1145	5.0058	6.096	5.6389	#	+	-	5.711	5.9436	5.7936	3.4122
146	C1(=CCCCC1)CCN	+	*	*	3.721	4.3127	5.3534	3.7684	*	*	-	3.3373	3.3765	5.1123	5.1535
147	c1(ccc(cc1)C(C)C)NC(=O)N(C)C	*	+	-	6.8673	5.697	3.7906	5.529	#	+	*	6.273	4.9478	5.3253	6.9095
148	c1(N(C(=O)CCl)COCC)c(cccc1C)CC	#	#	+	9.033	7.3529	5.2064	7.3998	+	-	+	7.477	6.7128	6.5089	1.2522
149	S(=O)(=O)(c1c(cc(cc1C)C)C)O	+	+	-	2.089	2.1751	9.2576	2.6119	#	*	+	1.784	2.3126	2.413	5.1004
150	c1(c(c(cc(c1Cl)Cl)Cl)Cl)N	+	*	-	5.601	5.2268	1.991	4.9801	-	+	*	5.317	4.9205	4.8113	5.8199
151	c1(c(cnc(n1)Cl)Br)Cl	-	+	+	5.96	5.7496	4.9866	5.774	+	+	+	5.801	5.6197	5.0814	4.5043
152	c1(cc(sc1Cl)Cl)C(=O)C	*	-	*	4.6566	4.166	4.4752	4.4545	*	+	-	4.464	3.8255	4.4018	2.0485
153	C(CCNC(=O)N)[C@@H](C(=O)	-	-	-	2.567	3.6761	4.3336	3.0781	-	-	*	1.403	2.172	1.8659	2.9038

	O)N														
154	C(C(CO)(F)F)(C(F)(F)F)(F)F	+	-	#	3.034	3.1058	2.4981	4.1061	+	+	+	2.713	2.4213	2.6744	2.981
155	C(C(C(=O)O)(F)F)(C(F)(F)F)(F)F	-	#	#	3.54	3.9674	4.0188	4.6355	+	#	*	2.068	2.7819	3.4573	4.9536
156	c1(ccc(cc1)N)CCCCCCC	+	+	*	6.009	6.2168	3.8092	5.1922	*	-	*	5.7365	4.9151	5.3303	5.9941
157	c1(ccc(cc1)N)CCCCCCCCCC	*	*	*	7.1209	7.1073	5.8048	6.1887	-	*	+	6.598	6.0197	6.5292	5.5964
158	C(c1ccc(cc1)Oc1ccc(cc1)O)(F)(F)F	*	+	+	5.3614	5.8519	6.9746	5.9743	*	#	*	5.1651	5.4229	5.3082	4.9319
159	c1(ccc(cc1)N)OCCCCCC	-	#	-	5.576	5.9269	5.6198	5.2464	#	-	+	4.934	4.5627	5.0776	5.9422
160	c1(c(c(c(cc1[N+](=O)[O-])C)C)[N+](=O)[O-])NC(CC)CC	*	#	-	7.3021	6.106	5.5565	7.0816	*	#	+	6.3851	5.7887	6.0166	2.5325
161	C(=O)(C(C)Cl)C	+	-	+	5.119	3.4114	6.7905	4.214	-	+	*	4.772	3.35	3.6216	7.5529
162	C(CCCCCCCCN)CCCCCCCC	*	-	#	6.7172	7.6982	4.1901	7.3578	+	-	*	6.608	7.6535	7.6032	3.7459
163	C(CC(=O)O)CCCBr	#	+	#	4.583	4.4013	8.1802	3.918	*	#	-	3.5193	2.8649	2.3771	2.9324
164	C(C(F)(F)F)(C(=O)O)(F)F	+	-	+	5.069	3.7046	3.7551	3.8878	+	+	+	3.784	2.6992	3.4015	7.8052
165	c1(c(ccc(c1)Oc1c(cc(cc1)Cl)Cl)[N+](=O)[O-])C(=O)OC	+	-	+	9.225	7.8427	3.802	8.519	-	-	*	9.113	8.1608	7.4345	3.8041
166	P(=O)(Oc1ccc(cc1)[N+](=O)[O-])([O-])[O-]^[Na+]^[Na+]	+	+	#	3.852	3.5212	7.8797	3.6742	+	*	*	2.238	2.1417	2.3461	5.5512
167	[N+](CCCCC)(CCCCC)(CCCCC)CCCCC^[Cl-]	+	-	+	5.842	5.9517	3.9033	5.0742	-	*	+	4.427	4.3478	6.3997	4.0623
168	c1(c(ncnc1Cl)Cl)[N+](=O)[O-]	+	+	+	4.796	5.1653	5.1953	4.6173	+	+	#	4.443	4.4827	4.6409	3.1533
169	c1(c(c(c(c(c1F)F)F)F)F)C(F)(F)F	+	*	-	4.356	4.9153	5.5145	4.6933	+	#	+	3.921	4.2819	3.2574	4.0288
170	c1(ccccc1)/C=C/CBr	*	-	*	4.156	4.7912	4.0011	4.0604	#	#	*	4.018	3.975	3.8684	4.5226
171	c1(ccccc1)CCS	*	-	+	5.5174	5.4477	4.2932	5.0205	+	+	+	5.099	5.1008	4.6229	4.3868
172	c12c([nH]cn2)ncnc1NC	#	#	-	3.998	4.1086	5.0626	4.2685	*	#	#	3.5109	4.3407	3.7959	3.2435
173	C1(CCCC(=O)O)CCCCC1	+	*	+	4.173	4.2242	4.6626	4.0148	*	#	*	3.5307	2.5425	4.2047	6.5468
174	N(CCCCCCCC)(CCCCCCCC)C	*	+	*	6.7946	6.6687	3.773	6.7343	+	*	#	6.504	6.9685	6.4065	5.3447
175	c1(C(=O)C(c2ccccc2)Cl)ccccc1	+	*	#	5.284	5.5641	7.3661	5.4213	*	*	#	4.6555	5.1113	4.5409	2.949
176	c1(c(ccc(c1)O)O)CC(=O)O	+	-	*	4.253	4.0001	5.1618	3.6423	-	#	*	4.05	2.937	2.991	5.0444
177	C(CCCCBr)CCCBr	+	*	+	5.861	5.5303	3.3559	5.6144	#	#	#	4.868	4.0967	4.842	3.3208
178	N(CCCC)(CC)N=O	-	+	-	4.001	4.1631	4.8892	3.9719	*	*	-	3.3986	3.5799	3.6569	4.5889
179	C(/C=C/CN(C)C)N(C)C	#	-	*	5.112	4.3015	3.3135	4.0208	#	*	*	4.51	4.4239	4.0697	2.7679
180	c1(C(=O)O)ccc(cc1)F	-	+	-	3.785	4.098	4.9164	3.7631	+	#	+	3.227	4.3038	3.6368	4.8988
181	C(C(=O)CCCCCC)CCCCC	-	-	#	5.646	5.3725	3.9149	5.2608	#	*	#	5.241	4.9248	5.0833	3.6024
182	C(CCN)CCN	-	+	+	3.231	4.6633	5.7878	3.7967	*	*	+	2.6729	3.4184	3.0588	5.4894
183	c1(/[N+](=N/c2ccccc2)/[O-])ccccc1	#	*	+	5.411	4.8585	3.6552	5.5261	-	+	-	5.17	4.6741	4.8391	5.4301
184	[C@H]12C(C[C@H](C1)C=C2)C(=O)C	*	+	-	3.3777	4.4819	5.2014	5.2392	*	-	+	5.4283	6.7071	5.7042	8.5133
185	c12c3c4ccc1c1c(cc2ccc3ccc4)cccc1	+	-	+	8.424	8.9428	6.6587	8.7289	-	+	#	8.165	7.973	8.6666	2.7745
186	C1CSCSC1	+	+	+	3.051	3.6466	8.7178	2.7441	+	+	#	2.398	2.619	3.0369	3.0911
187	C(n1cncn1)(Oc1ccc(cc1)Cl)C(=O)C(C)(C)C	-	*	*	5.126	6.1367	3.841	3.9419	-	+	*	3.117	2.9677	3.4263	1.6074
188	C1(=O)C(=O)NC(=O)NC1=O^O^O^O^O	#	-	-	2.253	2.4228	3.2811	2.3051	*	-	-	1.8669	2.9129	1.5587	3.677
189	c1(c(cccc1)OC(=O)C)C(=O)O	-	#	#	3.779	3.8812	3.1437	4.0063	+	#	#	2.874	3.4716	3.4598	6.9848
190	c1(N(C(COC)C)C(=O)CCl)c(cccc1C)CC	*	*	-	7.3069	7.6138	3.4557	7.5913	-	*	*	6.131	7.023	7.0219	7.9064
191	c1(N(CCOCCC)C(=O)CCl)c(ccc c1CC)CC	+	*	-	8.667	8.8357	9.3995	8.5678	+	#	-	7.684	7.272	8.3667	6.4447
192	n1(C2CCCCC2)c(=O)n(c(nc1=O)N(C)C)C	+	*	#	7.288	6.9614	9.0003	7.0901	+	#	+	6.883	6.4494	5.7051	7.2291
193	[N+](CCCCCCCC)(CCCCCCCC)(CCCCCCCC)C^[Cl-]	-	#	+	7.147	7.8512	7.1471	7.4301	+	#	+	6.764	8.6833	8.4426	3.7526
194	C(C(C)(C)S)(C(=O)O)N	*	*	-	4.4836	3.4372	9.0712	4.8484	+	#	*	3.794	3.0848	4.192	1.9705
195	c12c(ccc(c1)S(=O)(=O)[O-])cccc2^[Na+]	+	+	-	2.153	2.5888	4.3744	3.0671	#	+	+	1.476	1.7286	1.6675	4.9021
196	c1(cc(cc(c1O)C)[N+](=O)[O-])[N+](=O)[O-]	+	+	#	5.498	5.0584	2.465	5.7917	+	*	*	5.183	4.2295	3.6122	4.6187
197	c1(NNC(=O)/N=N/c2ccccc2)ccccc1	*	*	*	6.2668	6.1309	4.951	5.6886	+	+	*	5.79	5.3479	5.2417	4.3811
198	c12c3c(Cc1cc(cc2)NC(=O)C)cccc3	-	-	+	5.307	5.64	5.6117	5.6192	+	*	+	4.917	5.3918	4.6472	3.5272
199	C1(C(=O)c2ccccc2)CCC1	*	-	-	4.6131	4.1607	5.2113	3.6974	*	+	+	4.1627	2.5746	3.6692	3.3929
200	C([N+](C)(C)C)CCCCCCCCC[N	*	+	+	4.3662	4.4131	3.4994	4.601	*	*	+	2.8725	4.6475	3.9747	4.1283

	+](C)(C)C^[Br-]^[Br-]														
201	C(CCCC(C)N)(C)C	-	-	*	4.203	4.5916	4.4149	3.5278	#	#	+	3.769	3.3718	3.5715	4.0565
202	S(CCCC)CCCC	#	*	*	4.849	4.4837	4.0123	3.9172	*	+	-	4.3031	3.89	4.0945	6.5352
203	c12c(cccc1N=C=S)cccc2	-	#	*	7.329	7.1211	4.9937	6.042	#	*	+	6.99	6.8201	6.1819	5.0182
204	c1(c(cc(c(n1)Cl)Cl)Cl)OCC(=O)O	-	+	-	3.577	5.9434	7.1803	4.8963	-	+	+	3.106	4.0806	4.5247	7.9554
205	c1(NC(=N)NC(=N)NCCCCCCNC(=N)NC(=N)Nc2ccc(cc2)Cl)ccc(cc1)Cl	+	+	-	7.24	7.2657	4.3302	7.0877	+	+	#	7.046	6.9085	7.7432	4.2388
206	C(=C)CI	-	+	#	5.785	5.4597	7.3903	4.9499	+	-	#	5.432	5.3804	3.8568	2.7402
207	C(OCC)C=C	#	-	+	4.36	3.3596	5.0161	3.2532	#	+	*	4.111	3.2979	2.5487	4.0168
208	c1(ccc(cc1)OC)CCN	-	*	+	3.648	4.6412	2.8317	4.3666	+	+	*	3.394	4.0204	3.842	2.0055
209	C([N+](C)(C)C)CCCCC[N+](C)(C)C^[Br-]^[Br-]	-	+	*	2.828	3.2258	3.8938	3.2724	+	-	-	2.455	3.1579	2.3762	2.2911
210	c1(cc(nc(n1)N)O)N	*	#	*	2.6521	4.6389	2.8552	2.8633	+	+	*	2.388	1.5837	2.1146	1.8056
211	C(=O)(CCCN)O	+	+	-	3.445	3.5002	2.8796	3.2039	*	#	*	2.8065	2.22	2.2262	2.7633
212	[N+](Cc1ccccc1)(CC)(CC)CC^[Cl-]	*	*	+	2.869	3.9044	3.0737	3.7727	+	+	#	2.035	2.739	1.7333	5.7749
213	C(=C(\c1ccc(cc1)O)/CC)(/c1ccc(cc1)O)\CC	-	-	-	5.81	6.4346	2.4637	5.9718	-	+	+	5.048	4.9306	4.8484	5.8796
214	c12c3c(ccc1cc1c(c2)cccc1)cccc3	+	*	+	7.86	7.4775	6.8869	8.0202	-	#	-	5.896	5.7103	6.4861	5.3858
215	c1([C@H]([C@H](NC(=O)C(Cl)Cl)CO)O)ccc(cc1)[N+](=O)[O-]	*	+	+	6.2306	7.1073	7.5969	6.3865	+	-	+	4.897	5.2141	5.0732	6.3777
216	n1(c(nnc(c1=O)CC(C)C)SC)/N=C/C(C)C	+	#	#	6.516	6.1752	6.3277	6.5186	+	-	*	6.027	6.2649	5.9465	4.9646
217	C(N=C=S)C=C	*	+	*	6.0825	5.4525	6.1515	5.267	+	+	+	5.85	5.5633	5.041	3.3541
218	O=c1n(C)c2c(n(C)cn2)c(=O)n1C	+	*	+	3.306	3.7639	5.3127	3.4784	-	#	-	2.745	2.2785	2.1786	2.8293
219	c1(c(cnc(n1)O)C)N^Cl	-	+	-	2.121	3.6228	3.9819	2.795	+	-	#	1.623	2.3539	2.8704	4.5226
220	c1(cc(cc(c1)O)[N+](=O)[O-])[N+](=O)[O-]	*	-	+	5.4589	5.422	3.0998	4.9053	#	*	+	5.297	3.7297	3.2948	3.3596
221	n1(c2c(nc1)c(ncn2)N)[C@@H]1O[C@@H]([C@H]([C@H]1O)O)COP(=O)(OP(=O)(O)O)O	*	-	+	4.9585	4.4523	4.8131	4.6813	#	*	-	3.696	3.9901	2.8951	3.2449
222	c12c(c(cc(n1)C(=O)O)O)cccc2O	+	+	*	4.455	4.1395	4.7484	3.4322	-	*	-	3.932	3.7351	4.4111	2.1237
223	c1(ccncn1)N	+	+	+	2.352	3.1482	4.4288	2.2951	-	-	+	1.961	2.2261	1.9127	2.4523
224	C(C(=O)C)CCC	*	#	+	2.6169	3.3631	2.4367	2.8957	#	-	-	2.215	2.7355	2.6754	5.1082
225	C(CCC)N=C=S	+	-	#	5.719	5.3473	2.9298	5.1101	+	+	+	5.505	5.6508	5.1973	3.7818
226	c12c(ccc(=O)[nH]1)cccc2	*	*	*	3.406	4.3802	5.3838	3.486	+	+	+	2.571	3.0192	3.3613	3.6697
227	c12c(cc(c(c1)C(=O)O)N)cccc2	+	-	*	4.403	4.3013	3.514	4.6162	-	*	*	3.825	3.178	3.6809	2.3811
228	N1(CCOCC1)N=O	*	*	+	4.1254	3.0172	4.7473	3.8647	-	*	*	3.141	2.3929	3.4281	5.2678
229	C(COC(=O)CCC)(COC(=O)CCC)OC(=O)CCC	-	+	#	3.962	5.3773	3.9216	4.6105	+	+	-	3.431	3.9533	2.3779	2.5645
230	C(CC(=O)O)CCCN	*	*	+	2.3492	3.8229	4.4923	3.2059	-	*	+	1.17	2.6038	4.2008	3.489
231	c12c(ccc([n+]1CC)C)cccc2^[I-]	#	*	-	3.455	3.4426	2.7808	3.1066	+	*	#	3.158	3.5869	2.7788	4.86
232	N(c1ccccc1)(c1ccccc1)C=O	+	#	*	4.016	4.7578	4.0963	4.9646	*	-	-	3.7765	4.7753	4.6878	4.412
233	c1(C(=O)CCc2ccc(cc2)O)c(cc(cc1O)O)O	#	+	+	4.058	5.4146	4.3546	4.5128	+	+	+	3.907	4.2397	1.6996	1.6469
234	S(=O)(=O)(c1c(ccc(c1)C)C)O	*	-	*	1.5557	1.8818	4.3077	2.7477	+	+	-	1.04	2.471	3.7024	4.1388
235	c1(N(N=O)C)ccccc1	*	+	*	3.9036	3.6572	1.8489	4.4437	#	*	+	3.532	4.2877	3.9581	3.4502
236	c1(ccc(cc1)CCCCCCCC)S(=O)(=O)[O-]^[Na+]	-	+	-	3.813	4.5593	3.9734	4.4058	+	#	+	3.433	3.4905	3.4995	4.4648
237	c12c(nc(o1)N)cc(cc2)Cl	-	*	*	4.324	4.5014	4.378	3.5943	-	-	+	3.865	3.2912	3.5548	3.1666
238	c1(ccc(cc1)N)C(=O)OC	+	*	*	3.661	4.0928	3.7346	4.0388	+	*	-	3.235	3.751	3.7676	4.5824
239	c1(C(=O)N)ccc(cc1)[N+](=O)[O-]	+	*	*	5.208	4.8962	3.8387	5.4587	#	+	-	5.003	3.9852	4.5062	4.5009
240	C\1(=N/c2ccc(cc2)[O-])/C=C(C(=O)C(=C1)Cl)Cl^[Na+]	+	#	+	4.781	4.9622	4.4894	4.6258	+	-	-	4.14	4.3876	4.6998	4.3488
241	c1(cc(c(cc1)O)O)C(=O)CNC^Cl	#	+	-	5.192	4.0968	4.7711	4.3618	*	-	*	4.8326	4.5693	5.3696	5.4579
242	N(CCCCC)(CCCCC)CCCCC	*	+	-	5.9551	6.0798	4.911	5.487	-	+	#	4.738	4.8339	3.6184	3.6373
243	c1(C(=O)O)ccc(cc1)[N+](=O)[O-]	*	+	*	4.0769	4.0676	6.6372	4.5351	+	*	+	3.761	3.8703	4.069	3.6984
244	c1(ccc(cc1)OCC)NC(=O)C	+	-	*	3.641	4.7723	3.9142	3.9085	-	#	+	3.052	3.4688	3.0704	3.0932
245	c1(ccccc1)N	#	*	*	3.714	3.8831	4.0354	3.4444	*	-	-	3.124	4.0258	2.5705	2.2403
246	[n+]1(ccccc1)CC(=O)O^[Cl-]	-	#	+	2.422	3.2584	3.3549	2.3767	+	-	*	2.122	3.0576	1.8984	1.977
247	C(C(=O)O)CCCl	+	*	*	2.297	2.6144	2.934	2.8599	#	+	+	1.831	2.5078	4.2045	4.6538
248	C(CCCBr)CCBr	*	#	+	5.2932	5.0589	2.3053	5.63	-	-	+	4.571	3.5743	4.7989	4.9687

249	c1(c(c(ccc1N)Cl)Cl)Cl	+	+	#	5.316	4.7633	4.682	4.1911	+	+	-	4.932	4.8215	4.2947	4.4451
250	c1(c(cc(cc1Cl)N)Cl)Cl	+	*	+	5.179	5.3269	4.7964	4.9042	-	-	*	4.737	4.4273	2.9804	2.8923
251	c1(ccccc1)NC(=O)N	#	+	#	3.501	4.1306	4.7019	3.6627	*	-	+	2.9667	3.1397	3.202	4.3882
252	C(=O)(Cl)O	+	+	+	5.228	5.3478	3.4281	6.0433	-	+	-	4.57	3.8725	-0.0706	6.3928
253	[C@@H]12[C@](C(=C3C(C2)[C@](c2c(C3=O)c(ccc2Cl)O)(C)O)O)(C(=O)C(=C([C@H]1N(C)C)O)C(=O)N)O^Cl	*	+	+	7.1226	6.0079	4.95	7.2394	+	*	+	6.613	6.7862	6.1096	0.2747
254	[C@H]12[C@](C(=C3[C@H](C1)[C@](c1c(C3=O)c(ccc1)O)(C)O)O)(C(=O)C(=C([C@H]2N(C)C)O)C(=O)N)O^Cl~	+	+	#	7.104	6.979	6.6448	0.2508	+	+	+	6.0986	0.0414	6.063	5.9858
255	c1(S(=O)(=O)NC(=O)Nc2nc(nc(n2)C)OC)c(cccc1)Cl	+	-	#	7.106	7.3418	0.4685	7.6206	#	*	-	6.091	6.0543	2.6167	3.264
256	c1(c(cnc(c1O)C)CO)C=O^Cl	*	#	*	3.8175	3.5538	7.7604	5.0737	+	+	#	3.446	3.7033	3.1837	2.7221
257	n1(c2c(nc1)c(ncn2)N)[C@@H]1O[C@@H]([C@H](C1)O)COP(=O)(O)O	-	+	*	3.586	3.9634	3.482	3.8739	#	*	*	3.135	3.2474	3.0445	3.4923
258	c1(c(cccc1)O)C(=O)N	+	#	+	3.933	3.4711	3.5958	3.6743	+	*	+	3.198	2.9674	4.9929	3.593
259	c1(nc(nc(n1)N)N)NC1CC1	+	+	*	3.92	4.4345	3.8516	4.0169	#	-	-	3.549	3.2433	2.2874	1.7737
260	[nH]1c(=O)cc[nH]c1=O	#	#	-	1.618	2.6474	3.7305	2.1559	-	+	*	1.301	2.0331	2.7882	3.3126
261	C(CCC)CC=O	*	#	+	3.6785	3.7631	3.0077	3.2035	-	*	+	3.432	3.1249	3.8073	3.8713
262	c12c(cccc1C=O)cccc2	*	#	*	4.5124	4.6682	3.2807	4.3688	+	-	*	4.152	3.6301	3.7166	4.0771
263	c12c(ccc(c1)C=O)cccc2	+	*	#	4.478	4.0094	4.9271	4.4173	-	+	*	4.018	3.5906	5.7227	4.7987
264	c1(ccc(cc1)C(C)(C)C)C[C@@H](CN1CCCCC1)C	#	+	-	6.006	5.761	4.2169	5.6022	*	#	-	5.3577	4.61	4.6615	4.7239
265	c1(Oc2ccccc2)ccc(cc1)C=O	+	+	*	5.143	5.3887	6.4904	5.7376	#	+	+	4.675	4.4493	2.5056	2.6662
266	C([N+](C)(C)C)CO^[Cl-]	+	+	+	3.421	2.5013	4.8855	3.2929	*	-	-	2.9519	2.3458	1.7713	1.8101
267	C(=O)(C)C	-	-	*	1.28	2.7854	2.1244	2.3013	-	*	-	0.957	1.7206	3.2622	3.1472
268	C(Cl)(Cl)Cl	*	+	*	3.1556	4.4287	2.444	3.3719	+	+	*	2.927	2.805	0.7012	1.52
269	S(=O)(C)C	+	-	+	0.538	1.5011	3.6391	0.8717	#	+	-	0.31	1.2843	3.6001	3.1325
270	C(=O)(C(Cl)Cl)N	+	-	#	3.852	4.0856	0.7014	4.2887	-	-	+	2.454	3.4172	2.0836	2.3768
271	N(C(=O)C)(CC)CC	+	*	-	2.036	3.3138	4.0622	2.9839	+	+	#	1.687	2.37	2.9619	2.207
272	c12c(c(=O)[nH]c(=O)[nH]2)[nH]c(=O)[nH]1	*	*	-	3.1725	4.6481	2.4312	3.3108	-	*	+	3.013	2.3027	3.5455	2.6601
273	C1(=O)[C@H]2C[C@H]3C[C@@H]1C[C@@H](C2)C3	#	#	-	3.116	3.8651	3.6404	3.4555	*	#	-	2.8524	3.8167	5.6604	5.5399
274	c1(cc(c(cc1)Cl)Cl)NC(=O)CC	+	#	-	7.77	5.521	3.107	5.6739	+	-	*	6.441	5.0143	2.6192	1.8334
275	C(=O)([C@@H](N)Cc1c[nH]cn1)O	-	-	#	3.182	3.2505	6.1056	2.606	*	*	-	2.1301	1.9194	5.4435	4.1931
276	NCCCNCCCCNCCCN	-	*	-	5.625	6.6048	2.4902	5.8426	+	*	#	4.683	5.1077	1.1215	0.5441
277	[N+](CC)(CC)(CC)CC^[Br-]	+	+	+	3.108	3.7039	5.5545	3.4726	-	#	*	2.785	1.2802	7.4589	6.8535
278	c1(C[N+](CCCCCCCCCCCC)(C)C)ccccc1^[Br-]	+	*	+	6.381	6.8244	1.8996	6.9088	-	*	-	5.886	7.0646	6.4827	6.5024
279	c1(nc(NC(C)C)nc(n1)SC)NC(C)C	+	#	+	7.519	7.0829	7.5653	7.547	#	+	+	6.956	6.7271	5.2054	5.4719
280	C(CCCCCN)CCCCC	-	-	-	7.365	5.9173	7.0597	5.3648	-	*	-	6.868	5.4443	3.1163	3.2596
281	n1cnc2c(c1N)[nH]cn2	#	-	#	4.212	3.6188	5.8407	3.2876	+	-	*	3.639	3.4628	5.8294	7.2867
282	c12c(sc(n1)OCC(=O)N(c1ccccc1)C)cccc2	+	#	#	7.132	6.9451	4.0324	6.992	#	+	+	6.077	4.7181	3.4597	2.7047
283	c12c(c(=O)[nH]c(n1)N)nc[nH]2	*	-	+	4.4085	4.1308	5.8669	3.7517	*	-	+	3.4633	3.3294	6.0179	6.2015
284	c1(ccc(cc1)N=[N+]=[N-])N=C=S	*	-	-	6.4519	6.1829	4.1739	6.4789	*	#	#	6.1228	5.5769	2.7118	2.5887
285	C(Cl)Cl	+	#	*	2.863	2.6474	6.0872	3.4133	+	*	#	2.641	2.5872	2.3406	3.14
286	C(C)(C)(C)O	*	*	#	2.9109	2.954	3.0487	2.6308	+	+	#	2.718	1.7871	3.342	3.4903
287	N(CCCC)(CCCC)C=O	*	-	*	3.3515	3.9434	2.3317	3.6317	-	-	#	2.862	3.3694	2.276	2.9118
288	O(C(C)(C)C)C=O	*	*	-	1.8133	2.6257	3.9018	1.9607	+	+	-	1.64	1.7623	4.3587	3.9973
289	c12c(cc(c(c1)N)N)cccc2	#	*	+	5.12	4.7485	2.7089	4.329	-	+	-	4.546	3.8387	3.8418	3.9371
290	c1(C(=O)c2ccccc2)ccc(cc1)C[N+](C)(C)C^[Cl-]	#	*	*	4.326	4.7981	4.6703	5.6801	*	-	+	3.9583	4.4308	2.5071	2.8586
291	C(=O)(C=C)N	+	+	+	2.65	3.4911	4.7772	3.7559	-	+	*	2.341	2.3786	5.4635	5.9154
292	c1(c(S(=O)(=O)NC(=O)Nc2nc(nc(n2)C)OC)ccs1)C(=O)OC	+	#	*	6.333	6.7163	2.7261	6.2501	#	+	#	5.287	4.4407	4.3735	3.6581
293	c1(ccc(cc1)S(=O)(=O)N(N=O)C)C	+	+	#	5.252	4.4224	6.7687	5.0956	+	+	#	4.826	4.0316	6.4503	6.1595
294	[Zn]^[Mn]^C(CSC(=S)N)SC(=S)N	*	+	-	6.7473	6.6332	5.0471	6.7791	#	*	+	6.181	5.304	1.5441	2.0873
295	C1(=O)N(CCN1C)C	-	-	#	1.733	2.6898	6.3611	1.4756	*	*	+	1.4964	2.447	1.8726	1.6064
296	c1(c2c(c(S(=O)(=O)O)ccc2)ccc1)	#	+	-	1.504	1.7793	2.4944	1.4996	+	-	#	1.267	1.5706	7.0538	6.6182

	S(=O)(=O)O															
297	c12c(C(=O)c3c(C1=O)cccc3)c(cc(c2N)C)Br	+	-	+	8.059	8.2188	1.371	7.8578	-	+	#	7.485	7.1655	4.0999	3.6361
298	C1(=O)C(CCCC1)Cl	#	*	+	4.531	3.4376	9.273	4.3465	+	#	#	4.14	3.0901	4.8875	4.3216
299	c1(Nc2ccccc2)ccc(cc1)[N+](=O)[O-]	+	*	-	6.381	5.9651	4.2353	5.8788	*	-	+	5.0013	4.8094	3.9441	4.2903
300	n1(c2c(nc3c1nc(=O)[nH]c3=O)cc(c(c2)C)C)C[C@@H]([C@@H]([C@@H](CO)O)O)O	*	*	+	4.8353	3.5795	4.9949	4.9426	#	-	*	4.496	3.9698	3.8817	4.5764
301	N(c1ccccc1)(c1ccccc1)N=O	*	*	+	5.2972	5.5249	6.103	5.4803	*	*	#	3.9152	5.183	4.93	4.3585
302	c1(C(=O)Nc2ccccc2)c(cccc1)O	#	#	-	5.824	5.4481	4.6417	6.1476	*	+	+	5.2875	4.2198	1.497	1.6487
303	OC1C(O)C(O)C(O)C(O)C1O	-	+	+	1.588	1.9625	5.6599	1.7382	+	-	-	1.511	2.4428	3.5486	3.4079
304	c1(c(cccc1)N)[N+](=O)[O-]	*	#	+	3.6632	4.374	2.1564	4.0061	+	#	+	3.308	3.6123	7.368	7.8519
305	c1(c(S(=O)(=O)NC(=O)Nc2nc(cc(n2)Cl)OC)cccc1)C(=O)OCC	-	#	-	9.296	8.8497	4.1854	8.1437	+	+	*	8.363	7.1773	4.4185	4.7959
306	c12c(cccc1)cccc2	+	+	*	4.25	4.9673	8.5806	3.9611	-	-	*	4.108	4.0426	4.2221	4.061
307	c1(c(cccc1)C(=O)O)Nc1ccccc1	*	+	+	4.7056	4.3064	4.2099	5.2961	-	*	-	4.384	4.4226	3.495	3.4113
308	c1(c(ccc(c1)OC)C(=O)O)OC	-	#	#	3.102	3.6971	4.9178	4.362	*	#	+	2.7265	4.197	4.4013	4.6599
309	C1(N(CC)CC)CCCCC1	-	+	*	3.776	5.4251	3.7467	4.6197	+	*	*	3.352	3.3742	3.6338	5.1452
310	c1(N(CC)CC)ccccc1	-	+	-	4.873	5.5388	4.0834	4.4002	-	#	-	4.606	4.3114	3.3728	4.0457
311	c1(c(ccc(c1)OC)OC)C=O	#	#	*	4.044	3.4788	4.0392	4.9163	-	+	+	3.597	3.69	4.0564	4.3033
312	c12c(nc[nH]2)ncnc1N(C)C	-	-	*	4.009	4.4772	3.9711	4.6298	#	#	-	3.6	4.6033	4.3196	4.7176
313	c1(C(=O)Oc2ccccc2)ccccc1	+	+	+	5.256	5.2355	4.2866	5.511	*	*	#	4.7408	4.4078	3.982	3.4751
314	c1(C(=O)OCC)ccc(cc1)N	+	*	+	3.771	4.2977	4.5676	4.2714	*	#	#	3.3919	3.5808	6.9489	7.4315
315	c1(c(S(=O)(=O)NC(=O)Nc2nc(nc(n2)C)OC)cccc1)CCC(F)(F)F	*	-	-	7.9608	9.0307	4.0472	7.4321	-	+	+	7.191	6.7382	4.7705	5.0905
316	c1(C(=O)OCCC)ccc(cc1)O	+	*	+	6.214	4.7204	8.8223	4.8855	-	*	+	6.025	4.1378	4.5707	4.4896
317	c1(C(=O)OCCCC)ccc(cc1)N	#	+	*	4.924	4.9836	5.0074	4.7901	*	+	-	4.5379	3.9795	4.923	5.4487
318	c1(C(=O)OCCCC)ccc(cc1)O	*	-	*	6.4828	4.9548	5.5694	5.2081	+	*	#	6.293	4.2974	4.2922	4.6752
319	c1(c(cc(cc1)Cl)N)OC	+	-	+	4.629	4.5411	4.8361	5.1083	#	#	*	3.942	4.3547	3.7422	4.231
320	c1(c(cccc1)C)C	#	*	*	3.916	4.3018	5.1487	3.9728	*	+	-	3.795	4.4095	3.7246	3.995
321	c1(c(ccc(c1)C)C)C	*	*	-	4.2617	4.5811	5.3358	4.3326	+	*	*	4.086	4.4687	3.6795	4.0526
322	c1(c(ccc(c1)N)Cl)Cl	-	+	+	4.909	4.8139	4.5508	4.2584	*	+	*	4.2505	4.2454	3.255	3.2396
323	c1(c(ccc(c1)N)C)N	#	#	+	3.656	4.5105	4.3395	3.4957	#	+	#	3.004	3.6364	3.7822	4.0307
324	c1(c(cc(c(c1)C)C)C)C	-	*	*	4.697	4.6941	6.1488	4.5557	*	-	*	4.1621	4.338	4.1428	4.2395
325	C(=O)(C(=C)C)OCC=C	-	+	#	3.438	4.2898	3.194	3.8373	*	*	+	3.1187	3.5914	3.668	3.3106
326	c1(OP(=S)(OCC)OCC)c(cc(cc1)Cl)Cl	+	+	*	6.208	6.635	6.8688	6.6666	#	+	-	5.893	6.5063	5.4963	5.1838
327	C1(NC(=O)NC1=O)NC(=O)N	*	*	+	2.0498	4.2235	4.0434	2.3466	+	+	+	1.597	1.655	2.53	2.7508
328	c1(ccccc1)[N+](C)(C)C^[I-]	-	#	+	2.772	3.417	3.7426	2.8318	*	-	*	2.4535	2.749	2.3921	2.083
329	c1(ccc(cc1)CC)S(=O)(=O)O	*	*	#	3.3724	2.5146	1.6782	1.8078	*	+	+	2.7542	2.3432	3.1778	3.3844
330	c1(ccccc1)C(=O)C	-	+	-	3.08	3.5055	3.4088	3.6626	*	+	-	2.7809	3.8552	3.2693	3.0633
331	C(=O)(CCl)c1cc(c(cc1)O)O	#	#	-	5.192	5.7551	6.0965	5.1283	+	+	+	4.809	5.0112	4.7462	4.0862
332	[C@@H](CC(=O)O)(NC(=O)C)C(=O)O	-	+	-	1.642	2.5016	1.8251	2.201	*	-	-	1.4122	2.1588	1.6369	1.3315
333	c1(ccc(cc1)O)C(=O)OC	*	-	#	3.8021	3.4423	3.8171	4.1219	-	+	+	3.29	3.7122	3.3858	3.8929
334	[N+](C)(C)(C)CCCl^[Cl-]	+	-	#	1.696	2.1833	1.3488	2.259	*	-	#	1.463	1.4858	1.9162	1.496