Comparative Analysis of QSAR Models for Predicting pK_a of Organic Oxygen Acids and Nitrogen Bases from Molecular Structure

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Supporting Information

Experimental and calculated pK_a values for 1143 organic oxygen acids and nitrogen bases

Num	SMILES	Exp p*K*a	QC	*r*-QC	SPARC	ACD
1	NCCc1ccc(O)cc1	9.77	9.88	9.79	9.58	9.51
2	Cc1c(Cl)ccc(O)c1	9.20	9.31	9.36	9.45	9.63
3	CC(Cc1ccc(O)cc1)(C)C	10.43	10.09	10.05	10.25	10.21
4	c1(cc(O)ccc1[N+](=O)[O-])C(F)(F)F	6.07	6.18	6.13	6.31	6.07
5	c1(Cl)c(C)cc(cc1C)O	9.70	9.47	9.47	9.60	9.76
6	c1(ccc(cc1)O)c2ccccc2	9.55	9.73	9.74	9.45	9.82
7	C(OCCCC)(=O)c1ccc(cc1)O	8.47	8.58	8.57	7.89	8.22

8	c1(Cl)c(Cl)ccc(O)c1	8.63	8.63	8.62	8.44	8.56
9	c1(C)cc(O)ccc1C	10.36	10.14	10.16	10.40	10.38
10	C(C)(C)(C)c1ccc(cc1)O	10.39	10.09	10.11	10.25	10.13
11	C(F)(F)(F)c1cccc(O)c1	8.95	8.48	8.46	8.85	8.96
12	C(C)(=O)c1ccc(cc1)O	8.05	8.74	8.73	8.09	8.12
13	c1(C(C)C)ccc(cc1)O	10.24	10.04	10.05	10.25	10.19
14	O=Cc1cccc(O)c1	8.98	9.00	9.05	9.35	9.24
15	[N+](=O)([O-])c1ccc(cc1)O	7.15	7.17	7.14	6.66	7.23
16	C(C)(=O)Nc1ccc(cc1)O	9.38	9.20	10.16	9.49	9.86
17	c1(ccc(cc1)O)Cl	9.41	9.15	9.21	9.30	9.47
18	c1(O)ccc(cc1)C	10.26	10.04	10.05	10.25	10.21
19	c1(ccc(cc1)O)Br	9.17	8.94	8.94	9.27	9.34
20	c1(ccccc1)O	9.99	9.93	9.95	9.91	9.86
21	c1(O)cc(C)cc(C)c1	10.19	10.14	10.16	10.21	10.19
22	c1c(cccc1Cl)O	9.12	9.15	9.21	9.06	9.00
23	c1c(C)cccc1O	10.09	10.04	10.05	10.06	10.07
24	C(OCC)(=O)c1ccc(cc1)O	8.34	8.58	8.57	7.89	8.31
25	c1(cccc(O)c1)C(C)=O	9.25	9.36	9.36	9.28	9.14
26	c1(ccc(cc1)O)N	10.45	10.51	10.53	10.52	10.17
27	O=Cc1ccc(cc1)O	7.61	8.58	8.57	7.80	7.72
28	c1(O)ccc(cc1)CC	10.00	10.04	10.05	10.25	10.26
29	c1(O)ccc(cc1)OC	10.10	10.14	9.89	10.18	10.40
30	c1c(cccc1O)OC	9.65	9.78	9.79	9.67	9.58
31	c1(ccc(cc1)O)F	9.91	9.26	9.26	9.41	9.92
32	c1c(cccc1F)O	9.21	9.05	9.05	9.19	8.97
33	C(F)(F)(F)c1ccc(cc1)O	8.68	8.11	8.09	8.05	8.51
34	c1(O)cc(OC)cc(OC)c1	9.34	9.41	9.42	9.43	9.21
35	c1(ccc(cc1)O)I	9.21	8.94	8.94	9.22	9.30
36	[N+](=O)([O-])c1cccc(O)c1	8.36	7.80	7.78	8.23	8.34
37	c1(cc(O)ccc1[N+](=O)[O-])[N+](=O)[O-]	5.42	5.66	5.66	5.18	5.42
38	c1(cccc(O)c1)c2ccccc2	9.64	9.88	9.89	9.91	9.74
39	c1(cccc(O)c1)C(C)(C)C	10.12	10.14	10.16	10.06	10.08

40	[N+](=O)([O-])c1cc(O)cc(c1)[N+](=O)[O-]	6.69	6.08	6.03	6.55	6.71
41	c1(Cl)cc(O)cc(Cl)c1	8.18	8.53	8.52	8.20	8.04
42	c1c(cccc1N)O	9.86	10.09	10.11	10.02	10.01
43	c1c(cccc1Br)O	9.03	9.15	9.15	9.04	9.00
44	c1(Cl)c(Cl)cc(cc1Cl)O	7.84	8.11	8.09	7.59	7.61
45	c1(cccc(O)c1)C(C)C	10.16	10.09	10.11	10.06	10.03
46	c1c(CC)cccc1O	9.90	10.04	10.05	10.06	10.06
47	c1c(cccc1O)OCC	9.65	9.83	9.84	9.66	9.63
48	c1(O)ccc(cc1)OCC	10.13	10.25	10.27	10.17	10.44
49	c1(Br)cc(O)cc(Br)c1	8.06	8.48	8.46	8.17	8.04
50	c1c(cccc1I)O	9.03	9.15	9.21	9.00	9.11
51	c1(O)ccc(cc1)CCC	10.34	10.04	10.05	10.25	9.99
52	c1(O)cc(CC)cc(C)c1	10.10	10.14	10.21	10.21	10.18
53	N#Cc1ccc(cc1)O	7.97	8.32	8.30	7.71	7.79
54	N#Cc1cccc(O)c1	8.61	8.68	8.68	8.49	8.58
55	c1(O)ccc(cc1)CS	9.53	9.57	9.58	10.02	9.78
56	c12CCCc1ccc(O)c2	10.32	10.19	10.16	10.40	10.37
57	[N+](=O)([O-])c1c(C)ccc(O)c1	8.62	8.06	8.04	8.60	8.66
58	C(C)(=O)c1ccc(cc1)O	8.05	8.74	8.73	8.09	8.12
59	O=C(OC(c1cccc2)(c(ccc(O)c3)c3)c(ccc(O)c4)c4)c12	9.70	9.38	9.36	9.54	9.23
60	c1cc(O)ccc1C(c2ccc(O)cc2)c3ccccc3CO	9.65	9.71	9.74	9.94	9.86
61	Oc(cccc1O)c1	9.32	9.58	9.58	9.43	9.45
62	Oc(cc(O)cc1O)c1	8.45	9.13	9.10	9.08	9.06
63	Oc(ccc(O)c1)c1	10.85	9.96	9.95	9.79	10.33
64	Oc(ccc(c1ccc2)c2)c1	9.51	9.89	9.89	9.31	9.57
65	OCc1cccc(O)c1	9.83	9.59	9.58	9.86	9.74
66	OCc1ccc(O)cc1	9.82	9.99	10.00	10.56	9.7
67	Oc1cc2CCCCc2cc1	10.48	10.19	10.21	10.41	10.42
68	Oc1ccc(cc1)CCCCCCCCC	10.25	10.02	10.05	10.25	10.15
69	Oc1ccc(cc1)C(C)CC(C)CC(C)C	11.06	10.05	10.05	10.25	10.15
70	Oc(cc(C)c1N(=O)=O)cc1C	8.25	7.61	7.56	7.48	7.6
71	S(=O)(=O)(C)c(ccc1)cc1O	9.33	8.50	8.46	8.36	8.51

72	Ic(cc(I)c1)cc1O	8.10	8.55	8.52	8.09	8.27
73	Oc(cc(c1)OCC)cc1OCC	9.37	9.55	9.58	9.42	9.29
74	O=Nc(ccc(O)c1)c1	6.48	8.23	8.20	6.69	6.48
75	O=S(=O)(c1ccc(O)cc1)C	7.83	7.50	7.46	7.62	7.52
76	O=S(=O)(c1c(cc(O)cc1C)C)C	8.13	7.86	7.83	8.38	7.81
77	Oc1cc(cc(c1)C(C)(C)C)C(C)(C)C	10.29	10.35	10.37	10.21	10.21
78	c1(ccccc1O)C(N)=O	6.49	6.87	6.82	5.97	6.32
79	Oc(cc(c(c1C)C)C)c1	10.25	10.27	10.27	10.55	10.51
80	c1(ccccc1O)C(N)=O	8.89	9.10	9.13	9.54	8.37
81	C(=O)(Nc1ccccc1)c2ccccc2O	7.40	8.19	8.36	8.99	7.1
82	c1(ccccc1O)C(OC)=O	9.87	7.74	7.91	10.13	9.76
83	c1(O)c(cccc1C=O)OC	7.91	6.83	7.03	7.58	8.18
84	c1(cc(cc(Cl)c1O)Cl)C(=O)Nc2ccc(cc2)Cl	4.70	5.25	5.48	6.83	6.19
85	C(=O)(Nc1ccccc1Cl)c2ccccc2O	7.31	7.85	8.03	8.96	8.23
86	c1(c(O)ccc(c1)N(=O)=O)C(=O)Nc2ccccc2	3.03	2.76	3.04	5.87	3.9
87	C(=O)(Nc1ccc(cc1)Br)c2ccccc2O	7.31	7.40	7.58	8.96	8.27
88	c1(cc(ccc1O)Br)C(=O)Nc2ccc(cc2)Cl	6.00	5.81	6.03	8.33	7.57
89	C(=O)(Nc1ccc(cc1)Cl)c2ccccc2O	7.30	7.51	7.69	8.96	8.27
90	c1(cc(cc(Cl)c1O)Cl)C(=O)Nc2ccccc2	4.70	5.70	5.92	6.84	5.20
91	c1(cc(ccc1O)Cl)C(=O)Nc2ccccc2	6.17	6.72	6.92	8.38	6.66
92	c1(cc(ccc1O)Cl)C(=O)Nc2ccccc2C	6.60	6.83	7.03	8.28	7.76
93	C(=O)(Nc1ccc(Cl)cc1Cl)c2ccccc2O	7.14	7.29	7.47	8.93	8.16
94	N(=O)(=O)c1ccccc1NC(=O)c2ccccc2O	6.91	7.06	7.36	9.13	8.18
95	c1(cc(ccc1NC(=O)c2ccccc2O)Cl)N(=O)=O	6.74	6.61	6.70	9.11	8.11
96	c1(ccc(Br)c(C)c1O)C(NC)=O	7.52	7.40	8.25	9.06	7.74
97	c1(cc(cc(Cl)c1O)Cl)C(=O)Nc2ccc(cc2)F	4.80	5.25	5.48	6.81	6.23
98	c1(cc(cc(Br)c1O)Br)C(=O)Nc2ccc(Cl)cc2N(=O)=O	4.11	3.66	3.93	6.99	5.84
99	C(=O)(Nc1ccc(Cl)cc1C)c2ccccc2O	7.43	7.63	7.80	8.86	8.27
100	c1(cc(ccc1O)F)C(=O)Nc2ccc(Br)cc2C	7.10	6.27	6.47	8.38	8.15
101	c1(cc(ccc1O)F)C(=O)Nc2ccc(Cl)cc2C	7.30	6.49	6.70	8.37	8.15
102	c1(cc(cc(Br)c1O)Br)C(=O)Nc2ccc(F)cc2F	4.77	4.34	4.59	6.82	5.91
103	c1(cc(cc(Cl)c1O)Cl)C(=O)Nc2ccc(F)cc2F	4.77	5.02	5.26	6.8	6.1

104	c1(cc(cc(Cl)c1O)Cl)C(=O)Nc2ccc(Cl)cc2N(=O)=O	4.11	4.34	4.59	6.96	6.03
105	c1(cc(cc(Cl)c1O)Cl)C(=O)Nc2ccc(cc2C)N(=O)=O	4.41	5.25	4.04	6.77	6.06
106	O=Cc(c(O)ccc1)c1	8.34	5.61	5.81	8.18	8.18
107	O=C(c(c(O)ccc1)c1)C	9.19	8.63	8.80	10.24	10.17
108	Clc1ccc2oc(nc2c1)c1cc(N)ccc1O	9.81	8.07	8.25	10.71	8.68
109	c1(c(O)ccc(c1)[N+](=O)[O-])[N+](=O)[O-]	4.09	3.30	3.18	4.06	4.04
110	c1(Cl)c(O)c(Cl)cc(Cl)c1Cl	5.22	6.56	6.49	5.3	5.64
111	c1(c(cccc1N(=O)=O)O)N(=O)=O	4.96	4.28	4.18	5.68	5.01
112	c1(Cl)c(Cl)c(O)c(c(Cl)c1Cl)Cl	4.70	6.03	5.95	4.45	4.68
113	c1(O)c(cccc1Cl)Cl	6.79	7.99	7.95	6.76	7.02
114	c1(O)c(C)cccc1Cl	8.69	9.05	9.03	8.76	8.84
115	c1(cc(cc([N+](=O)[O-])c1O)[N+](=O)[O-])[N+](=O)[O-]	0.38	0.80	0.65	0.54	0.62
116	c1(cc(Cl)cc([N+](=O)[O-])c1O)[N+](=O)[O-]	2.96	3.00	2.88	2.78	2.51
117	c1(cc(cc(C(C)CC)c1O)[N+](=O)[O-])[N+](=O)[O-]	4.62	3.83	3.65	5.54	4.08
118	[N+](=O)([O-])c1ccccc1O	7.23	6.63	6.57	7.1	7.14
119	c1(ccccc1O)C(C)C	10.47	10.26	10.26	10.76	10.49
120	c1(ccccc1O)C(C)(C)C	10.28	10.11	10.11	11.09	11.34
121	c1(O)c(Cl)cc(cc1Cl)Cl	6.23	7.09	7.03	6.15	6.59
122	c1(O)cc(C)ccc1C(C)C	10.62	10.49	10.41	10.91	10.59
123	c1(C(C)C)c(O)cc(c(Cl)c1)C	9.98	9.43	9.41	10.3	10.16
124	[N+](=O)([O-])c1c(O)ccc(Cl)c1	6.46	5.80	5.72	6.48	6.32
125	c1(ccccc1O)c2ccccc2	9.92	10.11	10.11	10.6	10
126	c1(ccccc1OC)O	9.98	10.72	10.72	9.85	9.97
127	c1(ccccc1CC)O	10.20	10.19	10.18	10.53	10.27
128	c1(OC)cc(C)ccc1O	10.28	10.87	10.88	10.19	10.27
129	c1(ccccc1OCC)O	10.11	10.79	10.80	9.89	10.1
130	c1c(Cl)c(O)cc(Cl)c1Cl	7.40	7.16	7.11	6.86	7.1
131	c1(O)cc(C)ccc1C	10.41	10.26	10.26	10.47	10.42
132	c1(ccccc1O)Cl	8.56	8.83	8.80	8.32	8.5
133	c1(ccccc1O)Br	8.45	8.67	8.65	8.35	8.43
134	c1(ccccc1O)N	9.75	11.32	11.34	9.85	9.76
135	c1(ccccc1C)O	10.28	10.04	10.03	10.32	10.32

136	c1(c(O)ccc(C(C)(C)C)c1)C(C)(C)C	11.72	10.34	10.34	11.43	11.56
137	c1(OC)cc(ccc1O)C=CC	9.88	10.64	10.65	9.77	10.1
138	c1(OC)cc(CC=C)ccc1O	10.19	10.72	10.72	9.98	10.29
139	c1(ccc(c(Cl)c1)O)C(C)(C)C	8.58	9.13	9.11	8.66	8.71
140	c1(ccc(c(C)c1)O)C(C)(C)C	10.59	10.26	10.26	10.66	10.53
141	[N+](=O)([O-])c1ccc(c(N)c1)O	7.60	6.56	6.49	6.62	6.82
142	[N+](=O)([O-])c1cc(Br)c(c(Br)c1)O	3.39	4.13	4.11	3.63	3.67
143	c1(C)cc(C)ccc1O	10.60	10.19	10.26	10.66	10.61
144	c1(O)c(Br)cc(cc1Br)Br	6.80	6.48	6.41	6.19	6.34
145	N(=O)(=O)c1c(O)ccc(N)c1	7.81	7.62	7.57	7.71	7.9
146	[N+](=O)([O-])c1cc(C)ccc1O	7.40	6.86	6.80	7.44	7.45
147	c1(Cl)c(O)ccc(Cl)c1	7.89	7.84	7.80	7.71	8.05
148	c1(OC)cc(ccc1O)C=O	7.40	8.67	8.65	7.78	7.78
149	c1(O)c(cccc1C(C)(C)C)C(C)(C)C	11.70	11.10	11.11	11.91	12.16
150	c1(O)c(cc(cc1C(C)(C)C)C)C(C)(C)C	12.23	11.25	11.26	12.25	12.76
151	c2(cc(cc(C1CCCCC1)c2O)[N+](=O)[O-])[N+](=O)[O-]	4.52	3.83	3.72	5.29	4.08
152	[N+](=O)([O-])c1ccc(cc1O)[N+](=O)[O-]	5.21	4.13	4.03	5.29	5.35
153	c1(ccccc1O)F	8.70	8.83	8.72	8.55	8.71
154	[N+](=O)([O-])c1ccc(cc1O)F	6.07	5.65	5.57	6.38	6.18
155	c1(O)c(C)cc(c(C)c1)C	10.57	10.42	10.41	10.47	10.74
156	c1(C)c(C)cccc1O	10.54	10.26	10.26	10.48	10.42
157	c1(O)c(C)cc(cc1C)C	10.86	10.42	10.41	10.99	10.97
158	c1(ccccc1O)I	8.51	8.52	8.49	8.33	8.52
159	c1(c(O)c(C)cc(c1)[N+](=O)[O-])[N+](=O)[O-]	4.31	3.53	3.41	4.56	4.42
160	c1(O)c(O)ccc(CCN)c1C	9.54	10.64	10.34	9.01	9.52
161	[N+](=O)([O-])c1cccc(c1O)[N+](=O)[O-]	3.97	3.60	3.41	3.39	3.49
162	c1(O)c(C)cccc1C	10.62	10.19	10.18	10.65	10.66
163	c1(Cl)c(cccc1Cl)O	7.70	7.99	7.95	7.48	7.53
164	c1(O)c(Cl)ccc(Cl)c1	7.51	7.92	7.88	7.47	7.53
165	[N+](=O)([O-])c1cccc(Cl)c1O	5.48	5.95	5.88	5.57	5.43
166	c1(Br)c(Br)c(O)c(c(Br)c1Br)Br	4.62	5.57	5.49	4.49	4.43
167	c1(O)c(cccc1Br)Br	6.67	7.62	7.57	6.83	6.89

168	c1(cc(C)cc([N+](=O)[O-])c1O)[N+](=O)[O-]	4.23	3.83	3.72	3.73	4.03
169	N#Cc1ccccc1O	6.86	7.54	7.41	6.95	7.17
170	[N+](=O)([O-])c1ccc(cc1O)Cl	6.05	5.87	5.80	6.24	6.08
171	c1(Br)c(O)ccc(Br)c1	7.79	7.39	7.34	7.72	7.86
172	[N+](=O)([O-])c1cc(Cl)c(c(Cl)c1)O	3.55	4.44	4.34	3.54	3.81
173	[N+](=O)([O-])c1ccc(c(Cl)c1)O	5.45	5.12	5.03	5.09	5.43
174	c1(O)cc(ccc1OC)C=O	8.89	9.43	9.41	9.15	9.25
175	c1(ccccc1CCC)O	10.47	10.19	10.18	10.62	10.49
176	c1(O)cc(C)cc(C)c1C	10.67	10.42	10.41	10.63	10.53
177	c1(C)cc(c([N+]([O-])=O)cc1)O	7.41	6.86	6.80	7.25	7.28
178	c2(cc(cc(c1ccccc1)c2O)[N+](=O)[O-])[N+](=O)[O-]	3.85	3.75	3.65	5.1	4.07
179	c1(C(C)(C)C)cc(C(C)(C)C)cc(C(C)(C)C)c1O	12.19	11.32	11.34	12.25	12.61
180	c1(F)c(F)c(O)c(c(F)c1F)F	5.53	4.81	4.72	5.28	5.5
181	[N+](=O)([O-])c2c(O)ccc(c1ccccc1)c2	6.73	6.63	6.57	6.72	6.97
182	c1(Cl)c(Cl)ccc(Cl)c1O	5.80	7.24	7.18	5.91	6.06
183	c1(O)c(Cl)c(Cl)cc(Cl)c1Cl	5.14	6.56	6.49	5.07	5.09
184	c1(cc(cc(Cl)c1O)[N+](=O)[O-])[N+](=O)[O-]	2.10	2.77	2.65	2.55	2.42
185	[N+](=O)([O-])c1c(O)ccc(OC)c1	7.31	7.24	7.11	7.37	7.33
186	c1(C)cc(Cl)ccc1O	9.71	8.98	8.95	9.7	9.87
187	c1(O)c(Br)cc(cc1Br)C#N	3.86	5.65	5.57	4.67	4.78
188	c1(cc(C)cc(C)c1O)C(C)(C)C	12.04	10.57	10.57	11.67	12
189	c1(O)c(cccc1C(C)C)C(C)C	11.10	10.57	10.57	11.42	11
190	c1(cc(C)ccc1O)C(C)(C)C	11.72	10.26	10.26	11.43	11.64
191	[N+](=O)([O-])c1cc(C)c(c(C)c1)O	7.07	6.33	6.26	7.45	7.81
192	c1(O)c(Cl)cc(cc1Cl)C	7.19	8.22	8.18	7.1	7.34
193	c1(O)c(Cl)cc(cc1Cl)Br	6.21	6.86	6.80	6.13	6.46
194	[N+](=O)([O-])c1c(O)ccc(C(C)CC)c1	7.59	6.93	6.88	7.44	7.3
195	C(O)(=O)c1ccc(O)c(Cl)c1	7.52	6.71	6.65	6.35	4.2
196	c1(Cl)c(Cl)c(O)cc(Cl)c1Cl	6.35	6.56	6.49	6.01	6.15
197	N(=O)(=O)c1ccc(c(O)c1)C	8.59	7.01	6.95	8.64	8.68
198	Cl-c(cc(c1)C)c(c1)O	8.74	8.98	9.03	8.66	8.79
199	c2(c(ON=Cc1cc(Br)c(c(Br)c1)O)ccc(c2)N(=O)=O)N(=O)=O	5.46	5.87	5.11	5.89	6.44

200	Oc(c(c(c(c1)Cl)Cl)Cc(c(c(cc2Cl)Cl)Cl)c2O)c1Cl	4.95	7.54	7.49	7.3	6.49
201	OCc(c(O)ccc1)c1	9.84	9.56	9.57	10.26	9.93
202	Oc(c(c(ccc1)cc2)c1)c2	9.34	9.70	9.72	9.32	9.4
203	Oc(c(cc(c1)Cl)Cc(c(O)ccc2Cl)c2)c1	7.60	8.76	8.72	9.57	9.15
204	Oc(c(O)ccc1)c1	9.45	8.98	8.95	9.08	9.5
205	c1c(O)c2CCCCc2cc1	10.28	10.34	10.34	10.51	10.58
206	Oc(c(c(c(O)c1)ccc2)c2)c1	9.58	10.00	10.03	9.32	10.26
207	Oc(c(c(c(c1)Cl)ccc2)c2)c1	8.86	8.80	8.80	8.73	9.11
208	Oc1ccccc1C	10.22	10.05	10.03	10.31	10.32
209	Oc1c(I)cc(C#N)cc1I	3.96	5.54	5.49	4.69	4.95
210	Oc1ccccc1CCCC	10.58	10.22	10.18	10.65	10.57
211	c1c(O)c(CO)cc(C)c1	10.15	9.23	9.18	10.61	10.23
212	Oc(c(c(c(c1)C)C)C)c1	10.59	10.53	10.49	10.82	10.74
213	Oc(c(c(O)cc1)C)c1	10.05	9.43	9.41	10.14	9.8
214	Oc1cccc2c1CCC2	10.32	10.03	10.03	10.47	10.38
215	Oc(c(ccc1)CC=C)c1	10.28	10.05	10.03	9.92	10.3
216	Oc(c(cc(c1)Cl)Cc(c(O)c(cc2Cl)Cl)c2)c1Cl	5.60	7.69	7.65	8.02	7.57
217	Oc1ccc(Cl)c(Cl)c1Cl	6.5	7.25	7.18	6.89	7.1
218	Oc1cccc(O)c1O	9.01	8.71	8.72	8.58	9.28
219	Oc1cc(Cl)c(O)c(Cl)c1	7.38	8.18	8.11	6.99	7.75
220	N#Cc1cc(C)c(O)c(C)c1	8.27	7.97	7.95	8.48	8.55
221	[O-][N+](=O)c1cc(c(O)c(c1)C(C)(C)C)C(C)(C)C	6.62	7.23	7.18	8.92	7.17
222	Brc1ccc(O)c(Cl)c1	7.64	7.58	7.57	7.71	7.92
223	Oc1ccc(cc1Cl)c1ccccc1	8.07	8.65	8.65	7.89	8.40
224	Oc(c(cc1CCC)CCC)c(c1)CCC	11.47	10.45	10.49	11.58	11.09
225	C(O)(=O)c1ccc(c(Cl)c1)Cl	3.64	3.79	3.77	3.33	3.6
226	c1(cc(Cl)cc(Cl)c1)C(O)=O	3.54	3.75	3.73	3.18	3.46
227	S(=O)(=O)(N(CCC)CCC)c1ccc(cc1)C(O)=O	3.40	3.65	3.63	3.39	3.69
228	[N+](=O)([O-])c1ccc(cc1)C(O)=O	3.44	3.33	3.29	3.22	3.42
229	C(O)(c1ccccc1)=O	4.19	4.21	4.21	4.02	4.2
230	C(O)(=O)c1ccc(cc1)Cl	3.98	3.99	3.98	3.75	3.97
231	C(O)(=O)c2ccc1c(cccc1)c2	4.17	4.23	4.23	4.06	4.2

232	C(O)(=O)c1ccc(c(OC)c1)OC	4.36	4.30	4.32	4.26	4.35
233	C(O)(=O)c1ccc(cc1)C(C)(C)C	4.40	4.32	4.34	4.19	4.4
234	C(O)(=O)c1ccc(cc1)O	4.54	4.28	4.30	4.17	4.57
235	C(O)(=O)c1ccc(cc1)C	4.37	4.30	4.32	4.2	4.37
236	C(O)(=O)c1ccc(c(O)c1)O	4.48	4.15	4.17	4.08	4.45
237	[N+](=O)([O-])c1cc(cc(c1)[N+](=O)[O-])C(O)=O	2.82	2.81	2.75	2.38	2.77
238	c1(cc(O)cc(O)c1)C(O)=O	4.04	3.97	3.86	3.85	3.96
239	C(O)(=O)c1cccc(N)c1	4.74	4.28	4.30	4.87	4.75
240	C(O)(=O)c1cccc(C)c1	4.27	4.25	4.25	4.1	4.27
241	C(O)(=O)c1ccc(cc1)OC	4.47	4.36	4.38	4.41	4.47
242	[N+](=O)([O-])c1cccc(c1)C(O)=O	3.46	3.43	3.40	3.2	3.48
243	C(O)(=O)c1ccc(c(OC)c1)O	4.51	4.23	4.23	4.04	4.45
244	c1(O)c(O)cc(cc1O)C(O)=O	4.21	3.93	3.92	3.99	4.33
245	C(O)(=O)c1ccc(cc1)N	4.85	4.62	4.80	4.78	4.86
246	C(O)(=O)c1cccc(F)c1	3.86	3.91	3.90	3.67	3.86
247	C(O)(=O)c1ccc(cc1)F	4.14	4.01	4.00	3.79	4.14
248	c1(cc(ccc1[N+](=O)[O-])C(O)=O)[N+](=O)[O-]	2.82	2.77	2.71	2.46	2.81
249	c1(O)c(OC)cc(cc1OC)C(O)=O	4.34	4.15	4.13	3.9	4.33
250	C(O)(=O)c1cccc(Cl)c1	3.81	3.97	3.96	3.6	3.83
251	C(O)(=O)c1ccc(cc1)C(C)C	4.35	4.30	4.32	4.19	4.35
252	C(O)(=O)c1cccc(Br)c1	3.81	3.95	3.94	3.59	3.81
253	C(O)(=O)c1ccc(cc1)C(C)=O	3.70	3.87	3.88	3.86	3.7
254	C(O)(=O)c1ccc(cc1)Br	4.00	3.93	3.92	3.76	3.97
255	C(O)(=O)c1cccc(OC)c1	4.09	4.19	4.19	3.9	4.08
256	C(O)(=O)c1cccc(I)c1	3.85	3.97	3.94	3.57	3.85
257	C(O)(=O)c1ccc(cc1)OCC	4.45	4.40	4.42	4.4	4.49
258	c(cc(c1)C(=O)O)c(c1)C=O	3.77	3.85	3.79	3.85	3.78
259	N#Cc1ccc(cc1)C(O)=O	3.55	3.71	3.69	3.36	3.54
260	C(O)(=O)c1ccc(cc1)CC	4.35	4.28	4.30	4.2	4.35
261	C(O)(=O)c1ccc(cc1)I	4.00	3.91	3.92	3.74	4.02
262	C(O)(=O)c1cccc(c1)C=O	3.84	3.85	3.84	3.75	3.85
263	c1(cc(OC)cc(OC)c1)C(O)=O	3.97	4.19	4.19	3.79	3.96

264	C(O)(=O)c1cccc(c1)C#N	3.60	3.75	3.73	3.32	3.64
265	C(O)(=O)c1ccc(cc1)Oc2ccccc2	4.52	4.28	4.30	4.15	4.28
266	C(O)(=O)c2cccc(Oc1ccccc1)c2	3.92	4.09	4.07	3.65	3.95
267	S(C)(=O)(=O)c1ccc(cc1)C(O)=O	3.64	3.49	3.46	3.38	3.5
268	C(O)(=O)c1ccc(cc1)OCCC	4.46	4.40	4.42	4.4	4.48
269	O=C(O)c(cccc1O)c1	4.30	4.08	4.04	3.94	4.08
270	O=C(O)c(ccc(c1)C(=O)O)c1	3.51	3.74	3.71	3.43	3.49
271	O=C(O)c(cccc1C(=O)O)c1	3.70	3.87	3.86	3.42	3.53
272	OC(C1=CC(F)=CC(F)=C1)=O	3.59	3.61	3.61	3.32	3.52
273	OC(=O)c1cc(c(cc1)F)F	3.83	3.71	3.69	3.44	3.8
274	O=C(O)c(cc(cc1C(=O)O)C(=O)O)c1	3.12	3.54	3.52	2.94	2.98
275	OC(=O)c1cc(c(c(c1)F)F)F	3.54	3.42	3.40	3.09	3.46
276	c(cc(c1)S(=O)(=O)C)cc1C(=O)O	3.52	3.65	3.65	3.26	3.6
277	OC(=O)c1ccc(CN)cc1	3.59	4.31	4.27	3.67	3.75
278	OC(=O)c1ccc(S(=O)(=O)N)cc1	3.47	3.59	3.58	3.37	3.6
279	O=C(O)c(cc(cc1C)C)c1	4.30	4.34	4.30	4.17	4.34
280	O=C(Nc(ccc(c1)C(=O)O)c1)C	4.28	4.49	4.46	4.05	4.27
281	OC(=O)c1cc(NC(=O)C)ccc1	4.07	4.39	4.36	3.75	3.99
282	O=C(O)c(ccc(c1C)C)c1	4.41	4.38	4.36	4.27	4.44
283	O=C(Oc(ccc(c1)C(=O)O)c1)C	4.38	4.26	4.23	4.08	4.05
284	O=C(O)c1cccc(c1)C(C)(C)C	4.20	4.33	4.30	4.1	4.3
285	O=C(O)c(ccc(OC)c1N(=O)=O)c1	3.72	3.66	3.65	3.65	3.85
286	O=C(O)c(ccc(c1N(=O)=O)C)c1	3.62	3.54	3.52	3.39	3.66
287	O=C(O)c(ccc(c1N(=O)=O)Cl)c1	3.29	3.28	3.27	2.94	3.35
288	OC(=O)c1cccc(c1)C(F)(F)F	3.75	3.69	3.67	3.5	3.77
289	OC(=O)c1ccc(N(C)C)cc1	5.03	4.78	4.73	4.7	4.91
290	O=C(O)c(ccc(N(=O)=O)c1C)c1	3.65	3.36	3.35	3.33	3.49
291	COc1ccc(cc1C)C(O)=O	4.35	4.45	4.42	4.47	4.54
292	O=C(O)c1cc(OC)c(cc1)C	4.13	4.26	4.23	4.08	4.25
293	OC(=O)c1cc(Br)c(C)cc1	3.29	4.07	4.04	3.77	3.98
294	Cc1cc(ccc1Cl)C(O)=O	4.07	4.06	4.04	3.82	4.04
295	c1(ccc(cc1O)C)C(O)=O	3.40	3.21	3.25	3.25	3.17

296	c1(ccc(cc1Cl)Cl)C(O)=O	2.68	2.85	2.77	2.84	2.68
297	c1(cc(Cl)ccc1Cl)C(O)=O	2.47	2.82	2.74	2.7	2.51
298	c1(ccccc1OC(C)=O)C(O)=O	3.49	3.31	3.51	3.64	3.48
299	c1(c(Cl)ccc(Cl)c1Cl)C(O)=O	1.50	2.33	2.45	1.84	1.25
300	c1(c(cccc1Cl)Cl)C(O)=O	1.59	2.64	2.74	2.27	1.69
301	c1(ccc(cc1OCC)N)C(O)=O	5.09	4.96	5.05	4.68	4.87
302	c1(ccccc1Nc2cccc(C)c2C)C(O)=O	4.20	3.87	3.83	4.49	3.73
303	c1(ccc(cc1O)N)C(O)=O	3.66	3.84	3.83	3.97	3.58
304	c1(ccccc1O)C(O)=O	2.97	3.07	3.13	3.08	3.01
305	c1(cccc(C)c1O)C(O)=O	2.95	3.10	3.16	3.15	3.06
306	c1(ccccc1I)C(O)=O	2.93	2.68	2.77	3.12	2.86
307	c1(ccccc1Br)C(O)=O	2.88	3.10	2.84	3.16	2.85
308	c1(ccc(cc1O)O)C(O)=O	3.11	3.21	3.19	3.22	3.32
309	c1(cc(C)ccc1O)C(O)=O	3.15	3.14	3.19	3.15	3.3
310	O=C(O)c(c(O)ccc1Br)c1	2.66	2.19	2.65	2.18	2.53
311	c1(ccccc1NC(C)=O)C(O)=O	3.40	3.00	3.25	3.44	3.49
312	c1(ccc(cc1OC)OC)C(O)=O	4.36	4.40	4.34	4.37	4.36
313	c1(ccccc1Nc2ccccc2)C(O)=O	3.99	3.77	3.77	4.59	3.43
314	c2(C(O)=O)c(O)cc1ccccc1c2	2.79	2.82	2.90	2.96	3.02
315	[N+](=O)([O-])c1ccc(c(C(O)=O)c1)O	2.12	1.70	1.88	2.24	2.28
316	[N+](=O)([O-])c1ccc(c(Cl)c1)C(O)=O	2.14	1.73	1.91	2.34	2.04
317	c1(ccccc1N)C(O)=O	4.95	4.08	4.06	5.04	4.94
318	c1(ccccc1Cl)C(O)=O	2.89	3.21	3.09	3.15	2.97
319	C(O)(=O)c1ccccc1C	3.98	3.63	3.64	3.98	3.95
320	c1(cc(I)ccc1O)C(O)=O	2.62	2.61	2.71	2.62	2.67
321	c1(C(O)=O)c(cc(cc1[N+](=O)[O-])[N+](=O)[O-])[N+](=O)[O-]	0.65	0.75	1.01	0.35	0.42
322	c1(cc(I)cc(I)c1O)C(O)=O	2.30	2.22	2.36	2.16	2.07
323	c1(cc(Cl)cc(N)c1Cl)C(O)=O	3.40	2.78	2.87	2.78	2.75
324	c1(cccc(O)c1O)C(O)=O	2.91	2.71	2.81	2.98	2.96
325	c1(c(cccc1O)O)C(O)=O	1.05	2.50	2.61	2.71	1.3
326	c1(cc(Cl)ccc1O)C(O)=O	2.65	2.64	2.74	2.65	2.64
327	c1(ccccc1F)C(O)=O	3.27	3.28	3.29	3.26	3.27

328	c1(cc(O)ccc1O)C(O)=O	2.95	2.89	2.87	2.99	3.01
329	[N+](=O)([O-])c1ccccc1C(O)=O	2.17	2.26	2.49	2.6	2.19
330	c1(ccccc1C(C)=O)C(O)=O	4.13	3.00	2.97	4.4	4.13
331	c1(ccccc1OC)C(O)=O	3.90	4.15	4.12	4.02	4.09
332	c1(cc(cc(C(O)=O)c1O)N(=O)=O)N(=O)=O	0.70	0.60	1.72	1.41	1.57
333	c1(cc(ccc1C(O)=O)[N+](=O)[O-])[N+](=O)[O-]	1.42	1.09	1.33	1.8	1.43
334	C(O)(=O)c1c(C)cccc1C	3.35	3.59	3.64	3.92	3.56
335	c1(C(O)=O)c(F)c(F)c(c(F)c1F)C	2.00	2.33	2.45	1.95	1.83
336	c1(ccccc1c2ccccc2)C(O)=O	3.46	3.21	3.16	3.93	3.46
337	c1(c(cccc1OC)OC)C(O)=O	3.44	4.19	4.15	3.58	3.98
338	c1(cccc(OC)c1OC)C(O)=O	3.98	3.52	3.54	3.84	3.97
339	c1(c(Cl)ccc(Cl)c1OC)C(O)=O	1.97	2.64	2.81	2.61	2.4
340	c1(ccccc1Oc2ccccc2)C(O)=O	3.53	3.84	3.93	3.61	3.53
341	c1(ccccc1C(C)C)C(O)=O	3.63	3.42	3.48	3.92	3.64
342	[N+](=O)([O-])c1ccc(c(C(O)=O)c1)Cl	2.17	1.80	2.10	2.3	2.22
343	[N+](=O)([O-])c1cccc(C(O)=O)c1Cl	2.02	1.77	1.94	2.31	1.93
344	c2c(NC(c1c(C(O)=O)cccc1)=O)cccc2	2.50	2.12	2.26	3.56	3.52
345	N(=O)(=O)c1cccc(Cl)c1C(O)=O	1.34	2.26	2.39	1.68	1.62
346	c1(c(C)cccc1Cl)C(O)=O	2.75	2.96	2.97	3.06	2.63
347	c1(ccccc1NCC(N)=O)C(O)=O	4.20	4.05	4.02	4.74	3.74
348	O=C(O)c(c(c(ccc1)cc2)c1)c2	3.60	3.43	3.45	4.01	3.49
349	O=C(O)c(c(ccc1)C(=O)O)c1	2.76	2.96	3.03	3.05	2.95
350	O=C(O)c(c(cc(c1C(=O)O)C(=O)O)C(=O)O)c1	1.87	1.86	2.01	2.16	1.87
351	OC(=O)c1c(F)cccc1F	2.85	3.15	3.19	2.44	2.34
352	OC(C1=C(C=C(C(F)=C1)F)F)=O	3.28	2.42	2.52	2.65	2.87
353	O=C(O)c(c(F)c(F)c(F)c1F)c1F	2.72	1.84	2.01	1.50	1.60
354	OC(=O)c1c(c(cc(c1F)F)F)F	2.71	2.15	2.29	1.73	1.66
355	O=C(O)c(c(c(ccc1)cc2cccc3)c1)c23	3.65	3.27	3.29	4.16	3.49
356	OC(=O)c1c(c(c(c(c1)F)F)F)F	3.08	1.94	2.10	2.30	2.53
357	OC(=O)c1c(F)cc(F)cc1	3.58	2.91	2.97	3.01	3.21
358	OC(=O)c1c(c(ccc1F)F)F	2.82	2.64	2.74	2.09	2.00
359	OC(=O)c1c(F)ccc(F)c1	3.30	2.75	2.84	2.88	2.93

360	OC(=O)c1c(c(ccc1)F)F	3.29	2.75	2.84	2.88	2.93
361	OC(=O)c1c(c(c(cc1)F)F)F	3.30	2.41	2.52	2.65	2.87
362	c(cc(N(=O)=O)c1N(=O)=O)cc1C(=O)O	1.85	0.99	1.24	1.81	1.12
363	Brc(ccc1)c(c1N(=O)=O)C(=O)O	1.37	2.24	2.36	1.68	1.62
364	c(cc(O)c1C(=O)O)cc1N(=O)=O	2.24	2.01	2.17	1.52	2.00
365	O=C(O)c(c(O)cc(O)c1)c1O	1.68	2.64	2.74	2.84	1.62
366	OC(=O)c1c(O)c(N(=O)=O)ccc1	1.87	1.71	1.88	2.24	2.01
367	O=C(O)c(c(ccc1)C(=O)c(cccc2)c2)c1	3.54	3.22	3.25	4.49	3.54
368	O=C(O)c(c(cc(c1)C)C)c1C	3.45	3.75	3.74	4.10	3.85
369	c(cc(O)c1C(=O)O)cc1C	3.32	3.27	3.29	3.00	2.91
370	c(cc(N(=O)=O)c1C(=O)O)cc1N(=O)=O	1.14	1.86	2.01	1.06	1.29
371	Cc1cccc(C(O)=O)c1C	3.77	3.69	3.67	4.05	4.02
372	O=C(O)c(c(N(=O)(=O))ccc1N(=O)(=O))c1	1.62	1.10	1.33	1.78	1.55
373	O=C(O)c(c(ccc1C)C)c1	3.99	3.70	3.70	4.05	3.99
374	O=C(O)c(c(cc(c1)C)C)c1	4.22	3.77	3.77	4.16	4.18
375	CCC1=CC=CC=C1C(=O)O	3.79	3.55	3.57	3.95	3.79
376	O=C(c1c(cc(cc1Br)Br)Br)O	1.41	2.19	2.33	1.91	1.27
377	c12c(C(=O)O)c(C)ccc1cccc2	3.11	3.23	3.25	4.03	3.50
378	OC(=O)c1c(C)c(C)cc(C)c1C	3.42	3.39	3.41	4.07	3.74
379	N(=O)(=O)c1c(C(=O)O)c(C)ccc1	1.87	2.52	2.61	2.55	2.41
380	Clc(ccc1Cl)c(c1C(=O)O)C(=O)O	1.46	2.22	2.36	1.70	1.26
381	O=C(O)c(c(c(N(=O)=O)cc1N(=O)=O)C)c1	2.97	1.04	1.27	2.35	2.41
382	c(cc(C)c1C(=O)O)cc1OC	3.46	3.70	3.70	3.92	3.74
383	O=Cc(c(ccc1)C(=O)O)c1	4.55	2.54	2.65	4.27	4.57
384	OC(=O)c1c(O)ccc(F)c1	2.70	2.55	2.65	2.71	2.68
385	C(O)(C(C)O)=O	3.86	3.89	3.71	3.87	3.91
386	n3(C(=O)c1ccc(cc1)Cl)c2ccc(cc2c(CC(O)=O)c3C)OC	4.50	4.70	4.72	4.66	3.96
387	C(=O)(c1ccc(cc1)N)NCC(O)=O	3.80	3.78	4.19	4.14	3.61
388	N13C(C(O)=O)C(SC1C(NC(c2ccccc2)=O)C3=O)(C)C	2.74	2.52	3.05	3.57	2.45
389	N13C(C(O)=O)C(SC1C(NC(=O)c2c(cccc2OC)OC)C3=O)(C)C	2.77	3.14	3.18	3.6	2.44
390	OC(Cl)=O	3.15	3.17	3.36	2.95	3.18
391	C(C)(O)=O	4.76	4.43	4.41	4.77	4.79

392	C(CS)(O)=O	3.55	3.62	3.45	3.75	3.73
393	C(C)(Cl)(Cl)C(O)=O	1.79	1.89	2.48	1.38	1.68
394	C(O)(=O)C(C)(C)C	5.03	4.60	4.63	4.69	4.94
395	C(O)(c1ccccc1)(c2ccccc2)C(O)=O	3.05	3.94	4.02	3.33	3.34
396	C(F)(F)(F)C(O)=O	0.52	0.04	0.07	1.12	0.05
397	C(Cl)(Cl)(Cl)C(O)=O	0.51	1.01	1.38	0.63	0.09
398	C125C=CC(C(C(=O)O1)(C)C2C(C34CC(C(C3)(O)CCC45)=C)C(O)=O)O	4.00	3.76	3.45	3.9	4.06
399	C(O)(=O)C(Cl)Cl	1.26	1.68	2.04	1.4	1.37
400	C(O)(C(C)C)=O	4.84	4.54	4.54	4.72	4.85
401	C(CO)(O)=O	3.83	3.72	3.53	3.9	3.74
402	C(CCl)(O)=O	2.87	2.84	3.18	2.97	2.65
403	C(CC)(O)=O	4.88	4.46	4.54	4.75	4.79
404	C(CBr)(O)=O	2.89	2.81	3.18	2.96	2.73
405	C14(C)C(C(C)CCC(O)=O)CCC1C3C(C2(C)CCC(CC2CC3O)O)CC4O	4.98	4.74	5.29	4.73	4.76
406	c1(c(Cl)ccc(Cl)c1Cl)CC(O)=O	3.70	3.85	3.93	3.82	3.63
407	c1(cccc2ccccc12)CC(O)=O	4.23	4.18	4.23	4.28	4.30
408	c2(CC(O)=O)c1ccccc1[nH]c2	4.75	4.87	4.85	4.66	4.49
409	N13C(C(O)=O)C(SC1C(NC(COc2ccccc2)=O)C3=O)(C)C	2.79	2.73	2.87	3.55	2.44
410	C(O)(C(CC)CC)=O	4.71	4.72	4.67	4.72	4.80
411	C(O)(=O)C(O)c1ccccc1	3.41	3.70	3.84	3.56	3.41
412	c1c(Cl)c(Cl)cc(Cl)c1OCC(O)=O	2.83	3.11	2.61	3.49	2.88
413	c1(c(Cl)cc(c(Cl)c1)Cl)OC(C)C(O)=O	2.84	3.10	3.36	3.47	2.93
414	c1(Cl)c(OCCCC(O)=O)ccc(Cl)c1	4.95	3.84	3.84	4.49	4.56
415	c1(Cl)c(ccc(Cl)c1)OCC(O)=O	2.73	3.32	2.79	3.55	2.98
416	c1(C)cc(Cl)ccc1OCC(O)=O	3.13	3.42	3.53	3.61	3.14
417	C(O)(C(C)CCC)=O	4.79	4.57	4.63	4.72	4.82
418	C(O)(C1CCCCC1)=O	4.90	4.57	4.63	4.82	4.91
419	C(O)(C(CCC)CCC)=O	4.60	4.69	4.67	4.72	4.82
420	c1(O)cc(ccc1O)CC(O)=O	4.25	4.31	4.23	4.52	4.42
421	C(O)(Cc1ccccc1)=O	4.31	4.44	4.45	4.43	4.30
422	N(=O)(=O)c1ccc(cc1)CC(O)=O	3.85	3.08	3.22	4.01	3.86
423	C(O)(Cc1ccc(cc1)OC)=O	4.36	4.56	4.58	4.58	4.45

424	C(O)(=O)CCCl	3.99	3.77	3.79	4.02	4.00
425	C(CCC)(O)=O	4.82	4.48	4.54	4.75	4.76
426	C(O)(C(C)CC)=O	4.81	4.57	4.58	4.72	4.80
427	C(O)(=O)C(c1ccccc1)c2ccccc2	3.94	4.51	4.54	4.21	4.72
428	O(C(C)C(O)=O)c1ccc(cc1Cl)Cl	3.10	3.27	3.53	3.53	3.03
429	C(O)(COc1ccc(cc1)Cl)=O	3.10	2.83	3.01	3.65	3.09
430	C(O)(COc1ccccc1)=O	3.17	3.06	3.27	3.7	3.17
431	C(O)(CCC(C)=O)=O	4.64	4.33	4.32	4.4	4.78
432	C(C(O)=O)C(O)=O	2.85	2.74	3.05	2.67	2.92
433	C(O)(=O)CCI	4.09	3.85	3.88	3.99	4.12
434	C(CF)(O)=O	2.59	2.78	2.96	3.16	2.62
435	CC(CC(O)=O)O	4.41	4.33	4.67	4.32	4.36
436	C(CCCc1ccc(cc1)N(CCCl)CCCl)(O)=O	5.75	4.39	4.41	4.71	4.82
437	c1(OC)cc(ccc1O)CC(O)=O	4.41	4.43	4.32	4.51	4.39
438	C2(O)(C(O)=O)CC(OC(=O)C=Cc1ccc(O)c(O)c1)C(O)C(O)C2	2.66	3.38	3.31	3.24	3.90
439	C(O)(Cc1cccc(F)c1)=O	4.13	4.09	3.93	4.3	4.10
440	C(O)(COc1ccccc1F)=O	3.08	3.49	3.18	3.61	3.10
441	N#CCC(O)=O	2.45	2.59	2.70	2.45	2.47
442	F-c(ccc1)cc1OCC(=O)O	3.13	3.61	3.01	3.65	3.09
443	C(O)(COc1ccc(cc1)F)=O	3.13	3.61	3.01	3.66	3.13
444	C(O)(Cc1ccc(cc1)F)=O	4.24	4.15	4.01	4.33	4.26
445	C(N)(=O)NCC(O)=O	3.89	2.94	3.92	3.84	3.88
446	OCC(C(O)=O)O	3.55	3.35	3.44	3.54	3.42
447	C(O)(CCc1ccccc1)=O	4.66	4.40	4.45	4.59	4.65
448	C(O)(CC(C)C)=O	4.77	4.57	4.58	4.75	4.78
449	OCCC(O)=O	4.51	3.99	4.15	4.32	4.39
450	C(C)(O)(c1ccccc1)C(O)=O	3.53	3.94	3.79	3.52	3.53
451	C(C)(C(O)=O)C(O)=O	3.12	2.86	3.18	2.64	2.97
452	OC(CCCCCC1SCC(=O)N1)=O	5.10	4.17	4.23	4.71	4.76
453	C(O)(Cc2ccc1c(cccc1)c2)=O	4.25	4.38	4.19	4.37	4.30
454	C(O)(COc1cccc(Cl)c1)=O	3.07	2.92	3.27	3.64	3.08
455	c1(Cl)c(Cl)ccc(OCC(O)=O)c1	2.92	2.65	2.87	3.6	2.99

456	C(O)(=O)C(C)(C)O	3.61	4.07	3.71	3.83	4.01
457	C(C)(C)(C(O)=O)C(O)=O	3.15	3.22	3.10	2.9	3.16
458	C(O)(=O)C(C)(C)CC	5.03	4.66	4.63	4.69	4.97
459	C(O)(C(C)Cl)=O	2.80	3.17	3.36	2.94	2.96
460	C(O)(C(C)Br)=O	2.97	3.17	3.36	2.94	3.00
461	C(CC)(C(O)=O)C(O)=O	2.96	3.33	3.31	2.64	2.97
462	C(O)(COc1ccccc1Cl)=O	3.05	3.55	3.14	3.6	3.07
463	C(CCC)(C(O)=O)C(O)=O	2.99	3.22	3.27	2.64	3.32
464	C(O)(C(CCC)O)=O	3.89	3.95	3.75	3.87	3.85
465	c(cc(c1)CC(=O)O)c(c1)C	4.37	4.49	4.54	4.56	4.39
466	C(O)(CCC(C)C)=O	4.84	4.54	4.54	4.75	4.78
467	OC(CN(C=O)O)=O	3.50	3.32	3.13	3.73	3.85
468	C(O)(COc1ccc(cc1)C)=O	3.21	3.86	4.01	3.79	3.22
469	C(O)(COc1cccc(C)c1)=O	3.20	3.08	4.01	3.74	3.19
470	C1(CC1)C(O)=O	4.83	4.63	4.67	4.72	4.78
471	C(O)(COc1cccc(Br)c1)=O	3.09	3.57	3.01	3.64	3.08
472	N(=O)(=O)c1ccc(cc1)OCC(O)=O	2.89	2.16	2.35	3.36	2.92
473	C(O)(Cc1ccc(cc1)I)=O	4.18	4.06	3.97	4.28	4.20
474	C(CCCc1ccccc1)(O)=O	4.76	4.39	4.45	4.62	4.76
475	C(O)(COc1ccc(cc1)OC)=O	3.21	3.89	3.31	3.84	3.24
476	N(=O)(=O)c1cccc(CC(O)=O)c1	3.97	3.56	3.35	4.14	4.04
477	C(O)(COc1ccc(cc1)I)=O	3.16	2.74	2.96	3.64	3.08
478	C(O)(COc1cccc(I)c1)=O	3.13	3.57	3.01	3.63	3.10
479	C(O)(COc1ccccc1I)=O	3.17	3.42	3.01	3.61	3.07
480	C(O)(COc1ccc(cc1)Br)=O	3.13	2.69	2.96	3.65	3.09
481	N(=O)(=O)c1cccc(OCC(O)=O)c1	2.95	3.05	2.35	3.54	3.01
482	[N+](=O)([O-])c1ccccc1OCC(O)=O	2.90	3.01	3.14	3.57	2.91
483	C(O)(COc1ccccc1OC)=O	3.23	4.01	3.53	3.57	3.21
484	N#Cc1ccc(cc1)OCC(O)=O	2.93	2.54	2.74	3.52	2.96
485	C(O)(Cc1cccc(I)c1)=O	4.16	4.12	4.01	4.27	4.15
486	C(O)(Cc1ccc(cc1)Br)=O	4.19	4.06	3.97	4.29	4.17
487	C(O)(Cc1ccc(cc1)Cl)=O	4.19	4.12	4.06	4.3	4.17

488	C(O)(Cc1cccc(Cl)c1)=O	4.14	4.15	4.06	4.28	4.12
489	C(O)(COc1ccccc1C)=O	3.23	3.67	3.80	3.66	3.22
490	N#Cc1cccc(c1)OCC(O)=O	3.03	3.41	2.79	3.57	3.03
491	C(O)(COc1ccccc1Br)=O	3.13	3.52	3.27	3.6	3.07
492	C(O)(COc1cccc(OC)c1)=O	3.14	3.05	3.31	3.74	3.14
493	C(CCCCc1ccccc1)(O)=O	4.88	4.43	4.50	4.63	4.74
494	C(O)(COc1cccc2ccccc12)=O	3.20	3.00	3.14	3.68	3.18
495	N2(CC(O)=O)c1c(cccc1SC2=O)Cl	3.04	3.50	3.58	3.59	3.50
496	C(O)(CC1CCCCC1)=O	4.80	4.57	4.58	4.75	4.80
497	C(O)(COc1ccccc1O)=O	3.02	3.58	3.44	3.6	3.24
498	C(O)(=O)C(O)c1ccc(cc1)OC	3.42	3.79	4.10	3.71	3.43
499	C(O)(Cc1ccc(cc1)CC)=O	4.37	4.49	4.41	4.56	4.38
500	N(c1ccccc1CC(O)=O)c2c(cccc2Cl)Cl	4.15	4.16	4.49	4.12	4.18
501	c(cc(c1)C(C(=O)O)C)c(c1)CC(C)C	4.45	4.61	4.54	4.53	4.41
502	OC(C(C)Oc1ccc(Cl)cc1C)=O	3.68	3.53	3.66	3.59	3.19
503	c(ccc1c(c2)OCCC(=O)O)cc1cc2	4.00	3.95	3.88	4.21	4.19
504	n2c(c1ccc(cc1)Cl)c(sc2c3ccccc3)CC(O)=O	3.60	4.02	3.84	3.82	3.89
505	C(O)(=O)Cc1ccccc1I	4.04	4.24	4.28	4.2	4.09
506	C(O)(C(CCC)CC)=O	4.71	4.66	4.67	4.72	4.82
507	C(c1ccccc1)(=O)c2cccc(C(C)C(O)=O)c2	4.45	4.38	4.23	4.35	4.23
508	c1(Cl)cc(ccc1OCC=C)CC(O)=O	4.29	4.30	4.32	4.4	4.26
509	c2(ccc1c(ccc(OC)c1)c2)C(C)C(O)=O	4.15	4.52	4.50	4.5	4.84
510	CC(c2cc(Oc1ccccc1)ccc2)C(O)=O	4.50	4.38	4.32	4.17	4.20
511	C(O)(Cc1ccc(cc1)C(C)(C)C)=O	4.42	4.52	4.45	4.56	4.41
512	C(CCC(O)=O)(=O)c1ccc(cc1)c2ccccc2	4.51	4.42	4.41	4.56	4.55
513	C3(=Cc1ccc(cc1)S(C)=O)c2ccc(cc2C(CC(O)=O)=C3C)F	4.70	4.30	4.10	4.22	4.26
514	CC(c2ccc(C(c1sccc1)=O)cc2)C(O)=O	3.91	4.11	4.10	4.26	4.07
515	C(O)(=O)C(C)Oc1ccc(cc1)Oc2ccc(cc2Cl)Cl	3.43	2.96	3.23	3.73	3.19
516	OC(Cc3c(c1ccc(Cl)cc1)nn(c2ccccc2)c3)=O	4.30	4.27	4.15	4.25	4.04
517	n1c(Cl)c(Cl)cc(Cl)c1OCC(O)=O	2.68	2.83	3.01	3.22	2.26
518	C2(=O)c1ccccc1CSc3ccc(CC(O)=O)cc23	3.71	4.20	3.88	4.20	4.12
519	Cl-c(c(F)cc1)cc1N(C(=O)-c(ccc2)cc2)C(C(=O)O)C	3.72	3.55	4.01	3.69	3.53

520	n2c(Oc1ccc(OC(C(O)=O)C)cc1)ccc(C(F)(F)F)c2	3.12	3.66	3.23	3.7	3.17
521	CC(C(O)=O)Oc2ccc(Oc1c(Cl)cc(C(F)(F)F)cn1)cc2	2.90	2.90	3.14	3.7	3.12
522	OC(C3c2ccc(C(c1ccccc1)=O)n2CC3)=O	3.49	3.84	3.75	4.06	4.29
523	N(=O)(=O)c1c(Cl)ccc(OCC(O)=O)c1	2.96	2.77	2.17	3.5	2.92
524	OC(C2CC(=O)C(=C(C1CC1)O)C(=O)C2)=O	5.32	3.79	3.84	4.31	3.63
525	O=C(O-c(cc(c1)OC(OC(C2O)C(=O)O)C(O)C2O)c3c1)C=C3C	2.82	2.75	2.79	3.2	2.76
526	O=C(O)CCCCCN	4.43	4.52	4.45	4.55	4.68
527	O=C(O)CCCCCCCCC=CCC=CCCCCC	4.77	4.58	4.54	4.74	4.78
528	O=C(O)C=C	4.26	4.62	4.67	4	4.25
529	O=C(O)C(O)C	3.79	3.75	3.71	3.86	3.91
530	O=C(O)C(=C)C	4.65	4.65	4.67	4.03	4.58
531	O=C(O)C(=CC)C	4.96	4.98	4.89	4.34	5.04
532	O=C(O)C(O)C(O)C(=O)O	3.06	2.74	2.78	2.86	3.07
533	O=C(O)C(Oc(c(cc(c1)Cl)C)c1)C	3.10	3.66	3.66	3.61	3.19
534	O=C(O)C=CC	4.17	4.97	4.89	4.31	4.8
535	O=C(O)CCCC	4.84	4.60	4.54	4.75	4.78
536	O=C(O)CCC(=O)O	4.21	3.82	3.75	3.97	4.24
537	O=C(O)C=CC(=O)O	3.03	3.12	3.18	3.17	3.15
538	O=C(O)CCCC(=O)O	4.34	4.00	3.97	4.21	4.33
539	O=C(O)CCCCCC	4.80	4.59	4.54	4.75	4.78
540	O=C(O)CCCCCC(=O)O	4.51	4.32	4.32	4.41	4.43
541	O=C(O)CCSCCC(=O)O	4.11	3.97	3.97	4.05	4.03
542	O=C(O)CCCCCCCC	4.95	4.59	4.54	4.75	4.78
543	O=C(O)CCCCCCCC(=O)O	4.55	4.44	4.41	4.44	4.47
544	O=C(O)CCCCC(=O)O	4.44	4.25	4.19	4.35	4.39
545	O=C(O)CCCCCCC	4.89	4.59	4.54	4.75	4.78
546	O=C(O)C(=O)C	2.45	2.93	2.96	3.67	2.65
547	O=C(O)C=Cc(cccc1)c1	4.44	4.91	4.85	4.1	4.34
548	O=C(O)CCCCC	4.88	4.60	4.54	4.75	4.78
549	O=C(O)CCCCCCCCCCC	5.30	4.59	4.54	4.75	4.78
550	O=C(O)C(=O)O	1.25	1.08	1.12	1.3	1.38
551	O=C(O)C(C(C(=O)O)C(O1)CC2)C12	3.40	4.16	4.10	3.64	3.62

552	O=CC(=O)O	3.30	2.06	2.04	3.19	2.61
553	c1c(O)c(O)ccc1C=CC(=O)O	4.62	4.81	4.72	4.4	4.58
554	CCCCCCCCCC(=O)O	4.90	4.59	4.54	4.75	4.79
555	c1cc(O)ccc1C=CC(=O)O	4.64	5.00	4.89	4.32	4.65
556	CC=CC(=O)O	4.17	4.96	4.89	4.31	4.8
557	O=C(O)CCCCCCC(=O)O	4.52	4.42	4.37	4.43	4.46
558	CC(=O)CC(O)=O	3.59	3.59	3.53	4.85	3.55
559	O=C(O)CCCCCCCCCCCCC	4.90	4.59	4.54	4.75	4.78
560	O=C(O)Cc(c(N(=O)=O)cc(N(=O)=O)c1)c1	3.50	2.84	2.87	3.67	3.5
561	c1cc(N(=O)=O)ccc1C=CC(=O)O	4.05	3.65	3.66	3.72	4.07
562	NCCCCCCC(=O)O	4.52	4.55	4.50	4.65	4.72
563	O=C(O)C=Cc(ccc(OC)c1)c1	4.54	5.10	4.98	4.68	4.6
564	NCCCCCCCC(=O)O	4.59	4.56	4.50	4.74	4.76
565	COc1ccccc1C=CC(=O)O	4.46	5.38	5.29	4.47	4.47
566	O=C(O)C=Cc(ccc(O)c1OC)c1	4.58	4.93	4.85	4.42	4.58
567	OC(=O)C(Cl)=C(Cl)Cl	1.15	3.11	3.14	1.7	0.93
568	COc1ccc(C=CC(=O)(O))cc1OC	4.53	5.01	4.89	4.77	4.53
569	O=CO	3.75	2.72	2.75	3.75	3.74
570	OCCCC(O)=O	4.72	4.32	4.23	4.26	4.67
571	OC(=O)CN(=O)=O	1.48	1.20	1.25	2.2	2.07
572	O=C(O)CCCCl	4.52	4.00	3.88	4.35	4.51
573	OC(=O)Cc1ccccc1Cl	4.07	4.32	4.36	4.21	4.05
574	BrCCCC(=O)O	4.58	4.00	3.88	4.35	4.51
575	OC(=O)CC=C	4.34	4.40	4.37	4.48	4.35
576	OC(=O)CCBr	3.99	3.76	3.79	4.01	4.00
577	CCC(O)C(O)=O	3.68	3.79	3.75	3.86	3.83
578	OC(=O)C(Cl)CC	2.84	3.31	3.36	2.94	2.95
579	O=C(O)C(Br)CC	2.55	3.35	3.40	2.93	2.95
580	O=C(O)C(F)F	1.24	1.74	1.86	1.77	1.32
581	Nc1cc(C(O)=O)ccc1	3.07	3.76	3.13	3.05	3.34
582	Nc1ccc(C(O)=O)cc1	2.38	2.45	2.22	2.38	2.51
583	Nc1cc(O)c(C(O)=O)cc1	2.05	2.02	1.92	2.15	2.21

584	Nc1ccc(O)cc1	5.48	5.72	4.49	4.91	5.28
585	Nc1cc(O)ccc1	4.37	4.85	3.88	4.45	4.30
586	Nc1cc(N(=O)=O)cc(N(=O)=O)c1	0.30	-2.12	-0.95	0.29	0.24
587	Nc1cc(Cl)cc(Cl)c1	2.51	2.89	2.52	2.44	2.48
588	Nc2ccc(c1ccccc1)cc2	4.35	5.18	4.11	4.18	4.26
589	Cc1c(N(=O)=O)ccc(N)c1	1.64	0.39	0.78	1.02	1.12
590	C(c1ccccc1)(=O)c2ccc(cc2)N	2.24	3.44	2.90	2.68	2.17
591	[N+](=O)([O-])c1c(C)cc(cc1C)N	2.54	0.82	1.09	1.57	1.24
592	[N+](=O)([O-])c1c(C)ccc(N)c1	0.40	1.91	1.77	0.05	2.96
593	S(C)(=O)(=O)c1ccc(cc1)N	1.35	0.49	0.86	1.3	1.36
594	N(=O)(=O)c1c(Cl)ccc(N)c1	1.90	0.28	0.78	1.71	1.87
595	C(F)(F)(F)c1ccc(cc1)N	2.45	2.02	2.52	2.5	2.77
596	C(OC)(=O)c1ccc(cc1)N	2.47	2.89	2.98	2.37	2.47
597	C(OCCCC)(=O)c1ccc(cc1)N	2.47	3.00	3.13	2.38	2.39
598	C(OCCC)(=O)c1ccc(cc1)N	2.49	3.00	3.13	2.38	2.40
599	C(OCC)(=O)c1ccc(cc1)N	2.51	3.00	3.13	2.38	2.51
600	c1(Cl)c(Cl)ccc(N)c1	2.97	3.11	2.60	2.75	2.90
601	C(F)(F)(F)c1cccc(N)c1	3.49	2.78	2.45	3.29	3.37
602	c1c(cccc1N)Br	3.58	4.20	4.56	3.54	3.52
603	c1c(cccc1N)I	3.61	5.94	4.64	3.48	3.63
604	c1(ccc(cc1)I)N	3.78	3.76	3.13	3.77	3.81
605	c1(ccc(cc1)Br)N	3.86	3.87	3.20	3.84	3.90
606	c1(C)cc(ccc1Br)N	4.05	4.20	3.35	4.04	4.02
607	c1(ccccc1N)C(O)=O	2.14	3.76	3.13	2.22	2.11
608	c1(ccccc1O)N	4.84	4.52	3.66	5.19	4.74
609	[N+](=O)([O-])c1ccc(c(N)c1)O	3.10	2.02	1.99	3	2.62
610	c1(Br)c(N)ccc(Br)c1	2.30	3.11	2.22	1.78	1.83
611	[N+](=O)([O-])c1cc(C)ccc1N	3.03	0.71	1.01	2.96	0.46
612	c1(ccccc1N)c2ccccc2	3.83	5.94	4.64	3.87	3.81
613	[N+](=O)([O-])c1cc(Cl)c(c(Cl)c1)N	-2.55	-2.45	-1.18	-3.55	-3.18
614	[N+](=O)([O-])c1cc(C)c(c(C)c1)N	0.98	0.49	0.86	0.11	0.76
615	c1(N)c(Cl)ccc(Cl)c1	2.05	3.22	2.75	1.5	1.60

616	c1(c(N)ccc(c1)[N+](=O)[O-])[N+](=O)[O-]	-4.25	-5.49	-3.30	-4.24	-4.30
617	[N+](=O)([O-])c1c(N)ccc(Cl)c1	-1.02	-1.03	-0.20	-1.19	-1.00
618	[N+](=O)([O-])c1ccc(c(Cl)c1)N	-0.94	-1.14	-0.27	-1.51	-1.05
619	c1(N)c(F)c(F)c(c(F)c1F)F	-0.28	-0.49	-0.27	-1.32	-0.16
620	c1(N)c(cccc1Cl)Cl	0.42	3.44	2.90	0.52	0.71
621	N(=O)(=O)c1c(N)ccc(OC)c1	0.77	1.26	1.39	-0.04	0.96
622	[N+](=O)([O-])c1ccc(c(C)c1)N	1.04	0.49	0.63	0.46	0.92
623	c1(Cl)c(cccc1N)Cl	1.76	3.33	3.66	1.47	1.60
624	c1(Cl)c(N)ccc(Cl)c1	2.00	3.11	2.67	1.78	2.02
625	c1(ccccc1N)C(OCC)=O	2.18	4.42	3.58	2.03	2.20
626	c1(ccccc1N)C(OC)=O	2.23	4.20	3.43	2.03	2.19
627	[N+](=O)([O-])c1ccc(c(N)c1)C	2.35	1.69	1.69	2.36	2.34
628	c1(c(C)c(C)c(c(C)c1C)N)[N+](=O)[O-]	2.36	1.91	1.84	1.18	1.01
629	[N+](=O)([O-])c1ccc(c(N)c1)OC	2.49	2.45	3.28	2.02	2.42
630	c1(ccccc1Br)N	2.53	4.31	3.58	2.61	2.54
631	c1(ccccc1I)N	2.60	4.31	3.43	2.57	2.54
632	N(=O)(=O)c1cccc(c1N)N(=O)=O	-5.00	-4.95	-2.92	-5.17	-5.45
633	c1(N)c(Cl)cc(cc1Cl)Cl	-0.03	2.02	1.99	-0.28	0.07
634	c1c(Cl)c(Cl)cc(Cl)c1N	1.09	2.02	2.52	0.71	0.96
635	c1(N)c(OC)ccc(OC)c1	3.93	5.18	4.11	3.88	4.12
636	N(=Nc(cccc1)c1)c(ccc(N)c2)c2	2.82	3.84	3.88	2.88	3.12
637	Nc(cccc1)c1	4.60	4.50	4.56	4.66	4.61
638	O=S(=O)(c(ccc(N)c1)c1)c(ccc(N)c2)c2	2.41	1.89	1.99	1.28	1.24
639	Nc(c(c(cc1)C)C)c1	4.70	4.82	4.87	4.76	4.57
640	Nc(c(ccc1)C)c1C	3.95	4.76	4.79	4.17	4.31
641	Nc(c(cc(c1)C)C)c1C	4.38	4.89	4.87	4.62	4.74
642	N(=O)(=O)c(c(N)ccc1)c1	-0.28	0.65	0.78	-0.42	-0.23
643	O(c(c(N)ccc1)c1)C	4.53	6.70	6.68	4.22	4.54
644	c(c(ccc1N)ccc2)(c2)c1	4.16	4.18	4.26	4.03	4.32
645	Nc(ccc(c(ccc(N)c1)c1)c2)c2	4.66	4.50	4.56	5.08	4.70
646	O(c(c(N)ccc1)c1)CC	4.43	5.10	5.09	4.26	4.48
647	Nc(c(ccc1)Cl)c1	2.66	3.63	3.66	2.61	2.65

648	Nc(c(ccc1)C)c1	4.44	4.63	4.64	4.55	4.45
649	Nc(c(N)ccc1)c1	4.47	4.89	4.87	4.53	4.46
650	Nc(ccc(c1C)C)c1	5.28	4.78	4.79	5.31	5.15
651	Nc(c(cc(c1)C)C)c1	4.89	4.76	4.79	5	4.88
652	Nc(c(cc(c1)Cl)C)c1	3.85	3.52	3.58	3.76	3.81
653	Nc(ccc(c1Cl)C)c1	4.05	3.61	3.66	4.01	3.97
654	Nc(c(ccc1C)C)c1	4.53	4.78	4.79	4.75	4.57
655	Nc1cc(cc(N(=O)=O)c1O)N(=O)=O	1.00	-0.57	-0.35	0.92	0.39
656	O=S(=O)(N)c(cccc1N)c1	2.90	2.65	2.75	2.65	3.08
657	O=C(c(cccc1N)c1)C	3.56	3.61	3.66	3.86	3.41
658	N(=O)(=O)c(cccc1N)c1	2.47	2.31	2.45	2.5	2.46
659	CC(C)c1ccc(N)cc1	4.85	4.63	4.64	5.11	5.01
660	N(=O)(=O)c(ccc(N)c1)c1	1.00	0.52	0.71	0.5	1.01
661	O(c(ccc(N)c1)c1)C	5.34	4.67	4.71	5.02	5.21
662	Nc(ccc(c1)Cl)c1	3.98	3.37	3.43	3.87	3.97
663	Nc(ccc(c1)C)c1	5.10	4.63	4.64	5.11	5.04
664	Nc(ccc(N)c1)c1	6.16	5.12	5.09	5.77	6.17
665	Nc(cccc1Cl)c1	3.52	3.42	3.50	3.56	3.54
666	Nc(cccc1C)c1	4.69	4.65	4.71	4.86	4.72
667	Nc(cccc1N)c1	4.98	4.76	4.79	5	4.88
668	Nc(cc(cc1C)C)c1	4.79	4.80	4.79	5.06	4.84
669	Nc(c(cc(c(ccc(N)c1C)c1)c2)C)c2	4.50	4.67	4.71	5.08	4.59
670	c(c(c(N)cc1)ccc2)(c2)c1	3.92	4.08	4.11	4.46	4.21
671	Cc1cc(C)c(N)cc1C	5.09	4.91	4.94	5.2	5.01
672	O(c(ccc(N)c1)c1)CC	5.20	4.78	4.79	4.99	5.26
673	Fc(c(N)ccc1)c1	3.20	4.76	4.79	2.9	3.20
674	Fc(c(cc(N)c1)Cl)c1	3.66	2.54	2.67	2.92	3.60
675	Fc(ccc(N)c1)c1	4.65	3.46	3.50	4.03	4.66
676	Nc1cccc(F)c1	3.50	3.29	3.35	3.74	3.58
677	c(c(c(N)cc1)c(N)cc2)(c1)c2	4.44	4.59	4.64	4.37	4.46
678	Nc1cc(OC)ccc1	4.24	4.35	4.41	4.36	4.17
679	O=C(c(c(N)ccc1)c1)C	2.22	3.86	3.88	2.18	2.31

680	Nc(c(ccc1)CC)c1	4.30	4.76	4.79	4.472	4.36
681	Nc(ccc(c1)CC)c1	5.00	4.61	4.64	5.11	5.09
682	Nc1c2cc3ccccc3cc2ccc1	4.10	3.91	3.96	3.36	4.21
683	Nc(c(ccc1)C(C)C)c1	4.42	4.82	4.87	4.55	4.42
684	c1cc(N)ccc1C(C)(C)C	4.95	4.69	4.71	5.11	4.93
685	N#Cc(ccc(N)c1)c1	1.74	2.14	2.22	2	1.73
686	S(c(cccc1N)c1)C	4.00	5.63	5.62	4	3.96
687	Nc1cccc(C#N)c1	2.75	2.63	2.75	2.81	2.79
688	Nc1cccc2c(N)cccc12	4.44	4.42	4.49	5.04	4.59
689	Nc1ccccc1SC	3.45	4.40	4.41	3.39	3.58
690	O=N(C(C=C2)=CC=C2NC1=CC=C(N)C=C1)=O	4.38	2.31	2.45	3.9	4.43
691	Nc1c2Cc3ccccc3c2ccc1	3.87	4.14	4.19	3.41	4.40
692	N(=Nc(cccc1)c1)c(ccc(N(C)C)c2)c2	2.96	2.46	2.52	3.41	3.29
693	c1ccccc1N2C(=O)C=C(C)N2C	1.40	-0.04	0.18	0.46	0.65
694	N(c(c(c(ccc1)cc2)c1)c2)(C)C	4.83	4.23	4.26	5.38	5.14
695	N(c(cccc1)c1)(CC)CC	6.57	5.25	5.24	5.67	6.69
696	N(c(ccc(c1)C)c1)(C)C	5.63	3.91	3.96	5.82	5.64
697	N(c(ccc(N(C)C)c1)c1)(C)C	6.35	4.59	4.64	6.43	5.92
698	O=N(=O)c(ccc(N(C)C)c1)c1	0.61	-0.38	-0.20	1.87	0.74
699	N(c(cccc1)c1)C	4.85	3.97	4.03	5.01	4.70
700	N(c(cccc1C)c1)CC	5.25	4.63	4.64	5.34	5.27
701	N(c(cccc1)c1)CC	5.12	4.48	4.49	5.14	5.12
702	N(c(c(c(ccc1)cc2)c1)c2)CC	4.19	4.06	4.11	5.18	5.12
703	N(c(cccc1)c1)(C)C	5.15	3.80	3.88	5.37	5.10
704	N(c(cccc1C)c1)(C)C	5.34	3.95	4.03	5.57	5.22
705	N(c(cccc1)c1)c(cccc2)c2	0.78	2.12	2.22	1.07	0.78
706	OCCNc(cccc1)c1	4.06	4.46	4.49	4.59	4.52
707	O=C(N(c(cccc1)c1)C)C	-0.50	1.16	1.31	-0.5	0.54
708	N(c(c(ccc1)C)c1)(C)C	5.94	4.76	4.79	5.86	5.65
709	N(c(c(ccc1)C)c1)C	4.62	4.12	4.19	4.93	4.72
710	O=N(=O)c(cccc1N(C)C)c1	2.63	0.77	0.93	3.21	2.60
711	N(c(ccc(c1)C)c1)C	5.36	4.10	4.11	5.46	5.26

712	N(c(cccc1C)c1)C	5.00	4.14	4.19	5.21	5.00
713	c1cc(OC)ccc1N(C)C	5.85	3.95	4.03	5.72	5.84
714	N(c(cccc1)c1)C(C)C	5.30	4.50	4.56	5.2	5.82
715	N(c(cccc1)c1)CCCC	5.12	4.48	4.49	5.21	5.05
716	CN(C)c1ccc(C#N)cc1	1.78	1.48	1.62	1.8	1.61
717	N(c(c(c(ccc1)cc2)c1)c2)C	3.67	3.59	3.66	5.05	4.85
718	c12ccccc1CCC(N)C2	9.93	9.86	10.14	9.95	10.5
719	c1(ccccc1)C(C)N	9.83	10.40	10.02	9.44	9.04
720	C(C(C)N)c1ccccc1	10.13	10.51	10.02	9.97	9.94
721	NCCC	10.71	11.06	10.36	10.41	10.66
722	NCCCC	10.78	10.95	10.31	10.41	10.69
723	NCC	10.87	11.06	10.36	10.41	10.64
724	NC1CCCCC1	10.63	10.73	10.59	10.38	10.57
725	NCc1ccccc1	9.33	10.40	9.51	9.49	9.06
726	c1(CN)ccc(cc1)C	9.36	10.51	9.63	9.81	9.21
727	c1(ccc(cc1)OC)CC(C)N	9.53	10.51	10.02	10.32	10
728	c12cc(ccc1OCO2)CC(C)N	9.67	11.17	9.80	10.45	9.94
729	NC(C)CCc1ccccc1	9.79	10.30	10.42	10.03	10.64
730	NCCCc1ccccc1	10.16	10.62	10.14	10.07	10.29
731	NCCCCc1ccccc1	10.36	10.73	10.19	10.11	10.66
732	NCC(C)C	10.68	11.17	10.42	10.41	10.72
733	c1(CN)ccco1	8.89	8.34	8.94	9.16	9.12
734	C(CN)(F)(F)F	5.7	4.74	7.07	6.13	5.47
735	c1(OC)c(OC)cc(cc1OC)CCN	9.56	9.75	9.68	10.4	9.57
736	C(CN)=C	9.7	10.51	10.02	9.7	9.53
737	NC(C)CC	10.56	10.95	10.25	10.37	10.74
738	NC	10.62	10.40	10.02	10.39	10.66
739	NC(C)C	10.63	10.84	10.25	10.39	10.68
740	C(C)(C)(C)N	10.68	11.17	10.42	10.39	10.68
741	NCCc1cnc2ccc(O)cc12	9.97	10.94	10.70	10.06	9.52
742	C1=NC=C(CCN)N1	9.8	8.86	9.23	9.54	9.26
743	NC(C)Cc(cccc1)c1	9.9	10.02	10.02	9.96	9.94

744	CC(N)C(O)c1cccc(O)c1	8.79	9.47	9.68	9.06	8.47
745	NC(=S)N	2.03	3.01	5.08	1.3	1.44
746	O=C(O)C(N)CC(c(c(N1)ccc2)c2)=C1	7.38	6.76	7.75	9.91	9.71
747	OCC(N)(CO)CO	8.069	7.41	8.21	8.15	7.78
748	OC(CN)C	9.937	9.23	9.51	9.81	9.19
749	OCC(N)CC	9.52	10.46	10.36	9.83	9.27
750	N(=O)(=O)c(ccc(NN)c1)c1	3.7	0.78	3.50	3.42	3.81
751	NCCN	9.922	9.83	9.91	10.2	9.89
752	NCCCN	10.62	10.05	10.08	10.46	10.43
753	NCCCCC	10.63	10.44	10.31	10.41	10.69
754	NCCCCN	10.8	10.19	10.14	10.68	10.68
755	NCCCCCC	10.64	10.44	10.31	10.41	10.69
756	NCCCCCCC	10.66	10.42	10.31	10.41	10.69
757	NCCCCCCCC	10.65	10.42	10.31	10.41	10.75
758	NCCCCCCCCC	10.64	10.42	10.31	10.41	10.75
759	OCC(N)(CO)C	8.801	9.52	9.68	9	8.90
760	OCC(N)(CC)CO	8.8	7.96	8.60	9	8.87
761	NC(CCCCC)C	10.58	10.37	10.31	10.36	11.04
762	NCCCCCCN	11.02	10.31	10.25	10.39	10.92
763	NCCCCCCCCCCCCC	10.63	10.42	10.31	10.41	10.67
764	NCCCCCCCCCCCCCCCCCC	10.65	10.42	10.31	10.41	10.67
765	OCC(N)(C)C	10.194	10.61	10.48	9.78	9.84
766	OCCN	9.499	8.68	9.11	9.81	9.16
767	c1ccccc1CC(N)C	10.13	10.04	10.08	9.97	9.94
768	OCCCN	9.96	9.89	9.97	10.21	9.91
769	NN	7.96	6.01	7.24	7.84	8.18
770	C12(C)C3CCC4(C)C(C(=O)C)CCC4C3CCC1CC(N)CC2	9.18	10.48	10.36	10.37	10.91
771	N#CCN	5.34	6.67	7.70	4.61	5.43
772	c1c(Br)ccc(NN)c1	5.05	2.79	4.97	4.8	4.93
773	NC(C(N)CCC1)C1	10.24	10.04	10.08	10.35	10.76
774	C(#C)CN	8.15	8.49	8.94	10.39	7.89
775	n(c(ccc1)CCN)c1	10.03	10.28	10.25	9.58	9.10

776	n1c(CN)cccc1	9.09	9.50	9.68	8.58	8.70
777	NCc1ccc(N(=O)(=O))cc1	8.5	7.06	7.98	8.39	8.36
778	OC(c(cccc1)c1)C(N)C	9.44	9.17	9.46	9.43	8.47
779	CCCCC(C)CN	11.13	10.55	10.42	10.41	10.75
780	Cc(cccc1C)c1NC(C(CC)N)=O	8.71	6.89	7.81	7.85	8.12
781	O=S(=O)(N)c(ccc(c1)C)c1	10.17	10.09	10.08	10.25	10.20
782	c1cc(NC)ccc1S(=O)(=O)N	10.77	11.29	10.93	10.27	10.21
783	c1cc(S(=O)(=O)N)ccc1SCCO	9.27	9.82	9.91	9.65	9.99
784	c1cc(S(=O)(=O)N)ccc1S(=O)(=O)CCO	9.38	7.66	8.38	8.94	9.51
785	c1cc(SCCCO)ccc1S(=O)(=O)N	10.23	10.11	10.08	9.65	10.02
786	c1cc(S(=O)(=O)N)ccc1SCCC(C)(C)O	10	10.50	10.36	9.65	10.04
787	c1cc(S(=O)(=O)N)ccc1SCCCCCO	9.25	10.17	10.14	9.66	10.03
788	NS(=O)(=O)c1ccc(S(=O)(=O)CCCO)cc1	8.98	7.57	8.32	8.96	9.53
789	c1cc(S(=O)(=O)N)ccc1S(=O)(=O)CCC(C)(C)O	9.35	7.85	8.49	8.96	9.55
790	O=N(=O)c1cc(S(=O)(=O)N)ccc1SCCO	9.42	8.27	8.83	9.03	9.38
791	O=N(=O)c1cc(S(=O)(=O)N)ccc1SCCCO	9.38	8.29	8.83	9.03	9.41
792	O=N(=O)c1cc(S(=O)(=O)N)ccc1S(=O)(=O)CCCO	8	6.03	7.24	8.38	8.92
793	Nc1cc(S(=O)(=O)N)ccc1S(=O)(=O)CCCO	9.15	7.85	8.49	9.06	9.79
794	COC(=O)c1cc(S(=O)(=O)N)ccc1SCCCO	9.3	9.58	9.74	9.29	9.7
795	COC(=O)c1cc(S(=O)(=O)N)ccc1S(=O)(=O)CCCO	8.9	7.17	8.04	8.65	9.21
796	Fc1cc(S(=O)(=O)N)ccc1SCCO	9.76	9.30	9.51	9.35	9.78
797	Clc1cc(S(=O)(=O)N)ccc1SCCCO	9.45	9.54	9.68	9.3	9.75
798	Fc1cc(S(=O)(=O)N)ccc1SCCCO	9.64	9.32	9.57	9.35	9.81
799	Fc1cc(S(=O)(=O)N)ccc1SCCCCO	9.82	9.41	9.63	9.36	9.82
800	Fc1cc(S(=O)(=O)N)ccc1S(=O)(=O)CCO	9	7.02	7.92	8.67	9.3
801	Fc1cc(S(=O)(=O)N)ccc1S(=O)(=O)CCCO	9.02	6.93	7.87	8.68	9.32
802	NS(=O)(=O)c1ccc(c(F)c1)S(=O)(=O)CCCCO	9.6	7.04	7.92	8.69	9.33
803	c1cc(OC)ccc1C(=O)C2=CSC(S(=O)(=O)N)=C2	8.2	9.74	9.85	9.02	9.57
804	c1cc(O)ccc1C(=O)C2=CSC(S(=O)(=O)N)=C2	7.9	9.54	9.68	9	7.39
805	c1cc(OC)ccc1C(=O)C2=COC(S(=O)(=O)N)=C2	9.5	8.49	8.94	9.11	9.42
806	c1cc(C)ccc1C(=O)C2=CSC(S(=O)(=O)N)=C2	9.3	9.69	9.80	8.97	9.56
807	c1cc(OC)ccc1S(=O)(=O)C2=CSC(S(=O)(=O)N)=C2	8.78	9.08	9.40	8.55	9.38

808	C1COCCN1Cc2cc3cc(S(=O)(=O)N)oc3s2	9.2	9.12	9.40	9.28	9.85
809	c1cc(C)ccc1S(=O)(=O)C2=CSC(S(=O)(=O)N)=C2	8.95	8.99	9.34	8.52	9.43
810	c1cc(C)ccc1S(=O)(=O)C2=COC(S(=O)(=O)N)=C2	8.02	7.68	8.38	8.73	9.28
811	c1cc(OC)ccc1S(=O)(=O)C2=COC(S(=O)(=O)N)=C2	6.32	7.83	8.49	8.76	9.23
812	S1C(S(=O)(=O)N)=CC=C1S(=O)(=O)CCOC(=O)C	8.65	7.59	8.32	7.86	9.37
813	S1C(S(=O)(=O)N)=CC=C1SCCCCO	9.5	10.70	10.53	9.02	9.89
814	S1C(S(=O)(=O)N)=CC=C1S(=O)(=O)CCCCO	8.67	7.83	8.49	7.94	9.4
815	c1cc(S(=O)(=O)N)ccc1SCCCCO	10.17	10.20	10.14	9.66	10.03
816	c1cc(S(=O)(=O)N)ccc1S(=O)(=O)CCCCO	9.6	7.70	8.38	8.95	9.54
817	COC(=O)c1cc(S(=O)(=O)N)ccc1S(=O)(=O)CCO	9.2	7.02	7.92	8.64	9.19
818	c1cc(CCCO)ccc1S(=O)(=O)N	10.23	10.57	10.42	10.01	10.17
819	c1cc(S(=O)(=O)N)ccc1CCCOC(=O)C	10.22	9.80	9.91	9.98	10.17
820	c1cc(S(=O)(=O)N)ccc1CCCCO	10.32	9.93	9.97	10.02	10.19
821	c1cc(S(=O)(=O)N)ccc1CCCCCO	10.28	10.04	10.08	10.02	10.19
822	c1cc(S(=O)(=O)N)ccc1CCCCCOC(=O)C	10.3	9.91	9.97	10.01	10.19
823	CC(C)(C)CN	10.21	10.70	10.53	10.41	10.78
824	N(C)CCc1ccccc1	10.08	9.32	9.77	10.42	10.35
825	N(CC)CC	11.09	10.51	11.47	10.84	10.76
826	N1CCCCC1	11.28	10.19	10.67	10.9	10.45
827	N(CCCC)CCCC	11.39	10.40	10.85	10.8	11.03
828	N1CCOCC1	8.49	7.90	8.98	8.26	8.97
829	C(CNCC=C)=C	9.29	9.42	9.70	9.45	9.02
830	N(C)Cc1ccccc1	9.54	9.21	9.51	9.88	9.75
831	N(CC)Cc1ccccc1	9.64	9.86	9.96	9.87	9.77
832	N(C)C(C)Cc1ccccc1	9.87	9.64	9.84	10.28	10.38
833	c(ccc1CC(NC)C)cc1	9.87	9.64	10.50	10.28	
834	N(C)CCCC	10.9	9.75	10.39	10.83	10.84
835	N(CCC)CCC	11	10.40	10.89	10.81	10.94
836	N1CCCCCC1	11.07	11.28	10.98	10.87	11.24
837	N(C(C)C)C(C)C	11.07	11.38	11.27	10.73	10.76
838	N1C(C)(C)CCCC1(C)C	11.72	12.04	11.68	10.82	11.19
839	N1CCCCC1C	11.08	10.73	10.91	10.86	10.63

840	N1CCC1	11.29	8.99	10.08	11.25	11.26
841	N1CCCC1	11.31	8.99	10.01	10.97	10.5
842	N1CCCCC1c2cccnc2	8.7	8.88	9.16	8.5	8.98
843	N1CCCC1c2ccccc2	9.4	9.21	9.41	9.34	10.13
844	N(C)C	10.73	9.21	10.21	10.83	10.73
845	N1CCCCC1CCC	11	10.84	11.01	10.82	10.63
846	C2CCC(NC1CCCCC1)CC2	10.4	11.38	11.43	10.68	11.43
847	CNCCCN2c1ccccc1CCc3ccccc23	10.4	9.22	9.65	9.48	10.40
848	c1cc2ccccc2cc1C(O)CNC(C)C	9.42	9.67	9.82	9.51	9.26
849	N(C1C)C1	8.22	6.14	8.62	9.36	8.21
850	OC(c(cccc1)c1)C(NC)C	10.252	8.51	9.34	9.7	9.38
851	N(C(CNC1C)C)C1	9.66	10.10	10.48	10.01	9.65
852	N(CCNC)C	10.16	8.96	9.93	10.35	10.54
853	N(CCNC1)C1	9.731	9.30	9.94	9.69	9.55
854	N(CC(C)C)CC(C)C	10.91	10.76	11.14	10.78	11.07
855	OC(C)CNCC(O)C	9.1	8.72	9.73	9.35	9.16
856	OCCNCCO	8.96	8.42	9.59	9.37	8.71
857	N(CCNCC)CC	11.06	9.71	10.27	10.64	11.17
858	C(#N)CCNCCC(#N)	5.26	3.89	5.82	5.52	6.13
859	N(C1)C1	8.04	5.64	8.29	9.34	8.14
860	CC(C)NCC(O)COc1cccc2ccccc12	9.42	8.39	9.80	8.98	9.50
861	O=S(=O)(O)CCCNC(CCCC1)C1	10.35	8.42	8.98	9.89	10.69
862	CCNNCC	7.71	6.26	8.14	8.4	9.20
863	N(C1)C1(C)C	8.64	6.62	8.45	9.34	8.28
864	c1ccccc1CS(=O)(=O)NC(=O)N	5.09	4.30	5.02	4.3	5.07
865	N(C(CC)C)C(CC)C	11.01	11.59	11.53	10.6	11.12
866	C1(NC(C)(C)C)CCCCC1	11.23	11.65	11.59	10.65	11.03
867	N1(CCOCC1)CC	7.67	7.68	8.43	7.48	7.66
868	c2c(CC(CN1CC(C)OC(C)C1)C)ccc(C(C)(C)C)c2	6.98	8.01	8.58	7.43	7.34
869	N(C)(C)CC	10.16	8.88	8.99	10.02	9.83
870	N(C)(C)CCCC	10.19	8.77	8.94	10.04	9.83
871	N1(C)CCOCC1	7.38	7.03	8.12	7.41	7.58

872	n1cccc(CN(C)C)c1	8	6.81	8.02	8.22	8.01
873	C(CN(CC=C)CC=C)=C	8.31	8.34	8.74	7.87	7.14
874	n1ccccc1CCN(C)C	8.75	8.77	9.04	9.23	8.96
875	n1cccc(c1)CCN(C)C	8.86	7.46	8.33	9.27	9.08
876	N(C)(C)Cc1ccccc1	8.91	8.12	8.63	9.17	8.8
877	C(c1ccccc1)(c2ccccc2)(C(CC)=O)CC(C)N(C)C	8.94	8.66	9.14	9.19	9.05
878	C(c1ccccn1)(c2ccc(cc2)Cl)CCN(C)C	9.13	8.55	8.74	9.56	9.33
879	N1(CCCC1)CCc2cccnc2	9.28	8.44	8.79	9.43	9.97
880	N1(CCCCC1)C	10.08	9.32	9.20	10.04	9.59
881	N1(CCCC1)C	10.32	9.10	9.09	10.11	10.55
882	N(CC)(CC)CC	10.78	10.40	9.71	10.15	10.62
883	N1(CCCCC1)CCC	10.41	9.86	9.45	10.13	9.84
884	CN1C(C)(C)CCCC1(C)C	11.25	11.82	10.37	10.16	11.25
885	N1(C)CCCC1c2cccnc2	8.18	7.79	8.53	7.85	8
886	CCN(CCCl)CCCl	6.57	5.94	7.61	6.36	6.48
887	C1(=CCCN(C)C1)C(OC)=O	7.16	7.03	8.12	8.15	7.84
888	c1(OCCN(C)C)cc(C)ccc1C(C)C	8.66	8.01	8.63	8.57	8.73
889	c1(C(C)C)c(OCCN(C)C)cc(c(OC(C)=O)c1)C	8.72	7.90	8.58	8.66	8.71
890	CC2N(CCCOC(c1cc(Cl)c(Cl)cc1)=O)CCCC2	8.9	8.66	8.84	9.11	9.36
891	c1(ccccc1C)C(OCCN(C)C)c2ccccc2	8.91	8.77	9.04	8.52	8.72
892	C(OCCN(C)C)(c1ccccc1)c2ccccc2	8.98	8.77	8.94	8.63	8.76
893	N(C)(C)C	9.8	8.34	8.74	9.94	9.75
894	CC(Cc1ccc(C(C)(C)C)cc1)CN2CCCCC2	10.1	9.75	9.40	10.07	9.75
895	N(CCC)(CCC)CCC	10.65	10.51	9.76	10.2	9.99
896	N(CCCC)(CCCC)CCCC	10.89	10.40	9.71	10.23	9.99
897	COC(=O)C1C(CC2CCC1N2C)OC(=O)c3ccccc3	8.61	7.24	7.87	7.56	8.97
898	CN(C)CCC=C2c1ccccc1CCc3ccccc23	9.4	9.01	8.79	9.47	9.18
899	CN(C)CCCN2c1ccccc1CCc3ccccc23	9.4	8.83	8.68	9	9.49
900	CCN(CC)CCNC(=O)c1ccc(N)cc1	9.32	10.15	9.40	9.89	9.09
901	CN1C2CC(CC1C3OC23)OC(=O)C(CO)c4ccccc4	7.75	7.35	7.92	7.24	8.01
902	O=C(OC(CC(N(C1C2)C)C2)C1)C(c(cccc3)c3)CO	9.43	7.66	8.07	8.95	9.98
903	CN(CCCl)CCCl	6.43	6.00	7.20	6.26	6.40

904	COc2ccc(CCN(C)CCCC(C#N)(C(C)C)c1ccc(OC)c(OC)c1)cc2OC	8.92	8.51	8.53	9.57	8.97
905	OC2(CCN(CCCC(=O)c1ccc(F)cc1)CC2)c3ccc(Cl)cc3	8.66	8.48	8.53	8.39	8.04
906	CCN(CC)CCCC(C)Nc1ccnc2cc(Cl)ccc12	10.1	9.57	9.09	9.86	10.47
907	CCOC(=O)C1(CCN(C)CC1)c2ccccc2	8.59	8.85	8.74	8.67	7.84
908	O=C(OCCN(CC)CC)c(ccc(N)c1)c1	8.05	9.75	9.20	8.8	9.24
909	c(ccc1c2CCN(C)C)cc1nc2	8.68	9.67	9.14	10.31	9.74
910	C1CCN(CC1)C2(CCCCC2)c3ccccc3	8.29	10.78	9.76	8.47	8.21
911	CCC(=O)OC1(CCN(C)CC1C)c2ccccc2	8.46	9.22	8.94	8.36	7.34
912	CCCCOc2cc(C(=O)NCCN(CC)CC)c1ccccc1n2	8.85	9.20	8.89	8.84	9.07
913	OCCN(CC)CC	9.87	10.52	9.60	9.57	9.79
914	N(CCC(C1)C2)(C1)C2	10.95	6.98	7.71	10.08	10.87
915	OCCN(CCO)CCO	7.762	9.14	8.89	7.91	7.77
916	OCCN(CCO)C	8.52	9.17	8.89	8.67	8.81
917	OCCN(C)C	9.31	7.58	8.07	9.44	8.88
918	N(CCN(C)C)(C)C	9.1	9.26	8.94	9.57	8.86
919	OC(C)CN(CC(O)C)CC(O)C	8.06	9.44	9.04	7.95	8.51
920	O=C(Nc(c(ccc1)C)c1C)CN(CC)CC	8.01	6.61	7.56	8.21	7.96
921	c1c(OC)c(OC)c(OC)cc1C(=O)NCc2ccc(OCCN(C)C)cc2	8.78	8.30	8.43	8.72	8.66
922	N(CCN(C1)C2)(C1)C2	8.82	4.93	6.64	9.16	8.19
923	CCN(CC)CCNC(=O)c1cc(Cl)c(N)cc1OC	9.27	10.60	9.66	9.21	9.08
924	ClCCN(CCCl)CCCl	4.64	4.99	6.69	4.42	5.05
925	CCCCN1CC1	7.86	6.08	7.25	8.52	7.88
926	O=S(=O)(O)CCCN(CCOC1)C1	7.15	6.13	7.30	6.69	7.83
927	c1ccccc1C(O)C(C)N(C)C	9.2	8.40	8.48	9.26	9.04
928	C1CCCCCCCCCCC1N2CC(C)OC(C)C2	8.08	9.86	9.25	7.48	8.56
929	OCC(N(C)C)(C)C	10.2	9.44	9.04	9.52	9.04
930	CN(O)C	5.2	0.63	4.39	5.6	5.20
931	O=P(C)(OCC)SCCN(C(C)C)C(C)C	9.12	9.44	9.04	9.12	9.78
932	CC(CC2)(C)CCC2(c3ccccc3)N1CCCCC1	8.27	11.63	10.17	8.47	8.23
933	CN1CCN(C(=O)c2ccccc2)CC1	6.78	7.61	8.07	6.94	6.73
934	C1CC(C(C)(C)C)CCC12(OCC(CN(CC)CCC)O2)	6.9	10.33	9.50	8.96	8.78
935	O1CCN(C)CC1(O)c2ccccc2	7.26	7.93	8.22	6.14	7.18

936	O1C(C)CN(C)CC1(O)c2ccccc2	7.41	7.72	8.12	6.14	7.19
937	O1CCN(C)CC1(O)c2ccc(Br)cc2	7.07	7.16	7.82	5.99	7.15
938	O1CCN(C)C(C)C1(O)c2ccccc2	7.88	8.51	8.53	6.19	7.24
939	O1C(c3ccccc3)C(C)N(C)CC1(O)c2ccccc2	7.68	7.50	8.02	5.78	7.11
940	O1CCN(C)C(c2ccccc2)C1(O)	6.02	7.80	8.17	5.1	6.56
941	O1CCN(C)CC1(O)c2cc(C(F)(F)F)ccc2	7.54	6.63	7.56	6.09	7.15
942	O1CCN(C)CC1(OCCC)c2ccccc2	7.12	8.22	8.38	5.78	7.13
943	O1CCN(C)CC1(OCC=C)c2ccccc2	7.09	8.01	8.28	5.52	7.16
944	O1CCN(C)C(C)C1(OCC)c2ccccc2	7.79	8.77	8.68	5.83	7.20
945	O1CCN(C)CC1(OCCCC)c2ccccc2	7.73	8.22	8.38	5.78	7.13
946	O1CCN(C)CC1(OCC(C)C)c2ccccc2	7.14	8.19	8.38	5.78	7.12
947	C(CCC1)N(C1)CC=C	9.7	9.73	9.20	9.34	9.16
948	N(C(CCCC1)C1)(C)C	10.7	10.28	9.45	10.03	10.72
949	CCCN(C)C	9.99	9.33	8.99	10.04	9.83
950	N(C(C)C)(C)C	10.3	9.83	9.25	10.01	9.91
951	N(CC(C)C)(C)C	9.91	9.46	9.04	10.06	9.67
952	C(C)(c1ccncc1)=O	3.59	3.24	3.18	4.47	3.57
953	n1cccc(c1)Br	2.91	3.57	3.52	3.02	2.87
954	C(OCC)(=O)c1cccnc1	3.35	3.53	3.52	3.09	3.3
955	C(OCC)(c1ccncc1)=O	3.45	2.91	2.85	3.91	3.24
956	n1ccc(cc1)Br	3.78	3.49	3.43	4.03	3.35
957	n1cccc(C=O)c1	3.8	3.53	3.52	3.73	3.43
958	n1ccc(cc1)Cl	3.84	3.93	3.93	3.85	3.18
959	n1ccc(cc1)C=O	4.77	2.93	2.85	4.37	3.3
960	n1ccc(cc1)c2ccncc2	4.82	4.19	4.18	4.9	3.27
961	C(OC)(=O)c1cccnc1	3.13	3.41	3.35	3.08	3.19
962	C(OC)(c1ccncc1)=O	3.26	2.79	2.68	3.91	3.16
963	n1cc(Cl)cc(Cl)c1	0.67	2.12	2.02	1.25	0.32
964	n1cccc(c1)Cl	2.84	3.56	3.52	3.05	2.95
965	n1cccc(c1)F	2.97	2.99	2.93	3.36	2.81
966	C(C)(=O)c1cccnc1	3.18	3.65	3.60	3.81	3.43
967	n1cccc(c1)I	3.25	3.72	3.68	2.9	3.21

968	n1cccc(CO)c1	4.9	4.49	5.27	5.01	4.74
969	n1ccc(cc1)CO	5.33	5.54	5.69	5.22	5.09
970	n1cccc(CCCO)c1	5.47	5.18	5.27	5.35	5.41
971	n1cccc(CC)c1	5.56	5.35	5.44	5.42	5.58
972	n1ccc(cc1)Cc2ccccc2	5.59	5.63	5.52	5.1	5.75
973	n1ccc(cc1)CCO	5.6	5.12	5.19	5.46	5.65
974	n1ccc(cc1)C=C	5.62	5.37	5.44	5.14	5.39
975	n1cccc(C)c1	5.63	5.30	5.35	5.42	5.52
976	n1ccc(cc1)CCCO	5.84	5.45	5.52	5.54	5.94
977	n1ccc(cc1)CC	5.87	5.65	5.77	5.61	6.08
978	n1ccc(cc1)C	5.98	5.67	5.77	5.63	5.94
979	C(C)(C)(C)c1ccncc1	5.99	5.78	5.94	5.56	5.98
980	n1ccc(cc1)CCC	6.05	5.65	5.77	5.61	6.04
981	n1cc(C)cc(C)c1	6.15	5.42	5.52	5.96	5.81
982	n1ccc(c(C)c1)C	6.46	5.78	5.94	6.17	6.19
983	n1ccc(cc1)OC	6.47	6.15	6.27	6.03	6.59
984	n1cccc(c1)CCN(C)C	4.3	5.23	5.27	4.27	3.77
985	N1CCCCC1c2cccnc2	3.21	5.50	5.83	3.2	4.19
986	N#Cc1ccncc1	1.9	2.41	2.35	2.17	1.92
987	N1(C)CCCC1c2cccnc2	3.1	5.86	6.27	3.2	3.21
988	C(=O)(N(CC)CC)c1cccnc1	3.5	3.89	3.85	3.31	4.01
989	C(=CC(O)=O)C(=O)c1cccnc1	3.82	3.00	2.85	3.13	3.28
990	n2cccc(c1ccccc1)c2	4.8	4.95	5.02	4.87	4.85
991	n1ccccc1	5.23	5.18	5.27	4.87	5.23
992	n1ccc(cc1)c2ccccc2	5.55	5.28	5.35	5.11	5.45
993	n1cccc(CN)c1	5.96	5.24	5.52	2.95	3.5
994	N(=O)(=O)c1cccnc1	1.18	0.71	0.52	0.9	1.2
995	n1cccc(O)c1	4.8	3.79	3.93	4.81	4.67
996	n1cccc(OC)c1	4.91	4.31	4.35	4.8	4.77
997	O=C(N)c(cccn1)c1	3.35	3.42	3.43	3.31	3.54
998	N#Cc(cccn1)c1	1.39	2.50	2.43	1.51	1.78
999	n(ccc(N)c1)c1	9.17	8.49	8.85	8.55	9.26

1000	ON=Cc1ccncc1	4.73	4.40	4.43	4.83	4.78
1001	n(ccc(N(C)C)c1)c1	10.14	7.81	8.10	9.31	9.52
1002	n1ccc(CN)cc1	4.39	5.38	5.52	3.23	2.91
1003	n1cc(NC(=O)C)ccc1	4.36	4.46	4.52	3.64	4.63
1004	Nc1ccncc1Br	7.05	6.36	6.52	6.59	7.11
1005	c1ccncc1CC(c2ccc(Cl)cc2Cl)=NOC	4.61	5.31	5.44	4.48	4.38
1006	n(cccc1N)c1	6	5.36	5.52	5.61	6.16
1007	n1cc(CC)ccc1C	6.51	5.99	5.66	6.21	6.3
1008	n1c(C)c(C)cc(C)c1C	7.9	7.59	6.89	7.57	7.26
1009	n1ccccc1F	-0.44	1.11	1.60	-0.44	-0.43
1010	n1ccccc1Cl	0.49	2.14	2.12	1.1	0.14
1011	n1ccccc1Br	0.9	2.20	2.26	1.29	0.79
1012	n1ccccc1C=C	4.98	5.64	5.29	5.11	4.8
1013	n1ccccc1Cc2ccccc2	5.13	5.14	4.93	5.25	4.98
1014	n1ccccc1CCO	5.31	4.45	4.18	5.47	5.17
1015	n1ccccc1CCCO	5.61	5.28	4.93	5.55	5.6
1016	n1cc(ccc1C)C=C	5.67	5.26	5.17	5.62	5.58
1017	C(C)(C)(C)c1ccccn1	5.76	6.07	5.66	5.6	5.73
1018	n1ccccc1CC	5.89	5.69	5.29	5.64	5.9
1019	n1cc(C)ccc1C	6.4	5.96	5.54	6.21	6.24
1020	n1cccc(C)c1C	6.57	6.02	5.54	6.21	6.24
1021	n1c(C)cccc1C	6.6	6.89	6.26	6.46	6.67
1022	n1ccc(cc1C)C	6.99	6.31	5.77	6.42	6.62
1023	n1c(C)cc(cc1C)C	7.43	7.57	7.00	7.22	7.33
1024	n1c(cccc1Cl)Cl	-2.86	0.27	0.66	-2.67	-3.02
1025	n1c(Cl)c(Cl)c(c(Cl)c1Cl)Cl	-1	-3.60	-2.76	-7.32	-6.23
1026	c1(Cl)c(cccn1)Cl	-0.85	0.35	0.66	-0.7	-0.63
1027	n1c(Cl)c(Cl)cc(Cl)c1Cl	-0.8	-2.71	-2.02	-6.28	-5.5
1028	n1ccccc1c2ccccc2	4.48	5.22	5.06	4.73	4.44
1029	n1ccccc1C	6	5.62	5.42	5.66	5.95
1030	n1ccccc1c2ccccn2	4.33	4.35	4.45	4.32	4.4
1031	n1ccccc1CO	4.86	3.84	4.55	5.2	5.01

1032	n1cc(C)ccc1N	7.22	5.98	6.22	7.22	7.04
1033	n1ccccc1SC	3.59	4.30	4.29	3.52	3.62
1034	n1ccccc1OC	3.06	2.98	3.76	3.09	3.4
1035	n1c(cccc1OC)OC	1.6	1.31	2.70	1.56	1.57
1036	n1ccccc1C(C)=O	2.73	1.92	1.89	3.2	3
1037	n1ccccc1C=O	3.8	3.22	2.91	3.72	3.72
1038	C(OC)(=O)c1ccccn1	2.21	2.32	1.80	1.79	1.69
1039	C(#N)c(nccc1)c1	-0.26	0.48	0.81	-0.03	-0.32
1040	n(c(N)ccc1)c1	6.86	7.17	7.30	6.67	6.67
1041	n1c(C(C)(C)C)cccc1C(C)(C)C	5.02	7.71	7.12	5.66	6.23
1042	ON=Cc1ccccn1	3.59	5.08	4.47	4.12	3.57
1043	O=N(=O)c(ccc(n1)N)c1	2.78	-2.03	-0.67	2.78	2.82
1044	c1cc(Cl)ncc1CN(C)C(C)=NC#N	0.7	-0.89	-0.32	0.35	-0.44
1045	c1(Br)ncccn1	-1.63	0.59	0.31	-2.2	-1.59
1046	c1(ncccn1)C(OC)=O	-0.68	0.22	-0.08	-1.67	-1.42
1047	c1(SC)ncccn1	0.59	2.20	2.09	0.94	0.82
1048	N(=O)(=O)c1cncnc1	0.72	-0.88	-1.28	-2.59	0.59
1049	n1cccnc1	1.23	1.50	1.32	1.37	1.78
1050	c1(OCC)ncccn1	1.27	2.37	2.28	0.62	1.23
1051	n1cc(C)cnc1	1.91	1.58	1.41	2.13	2.02
1052	c1(SC)nc(C)cc(C)n1	2.12	2.98	2.95	2.47	2.38
1053	n1c(C)cc(nc1)C	2.70	2.38	2.28	2.93	3.04
1054	c1(N)ncccn1	3.45	3.31	3.29	4.07	3.76
1055	c2c(Nc1nc(C)cc(C)n1)cccc2	3.52	3.63	3.62	3.71	4.41
1056	c1(N)nc(C)cc(C)n1	4.82	4.05	4.10	5.54	5.11
1057	n1c(N)cc(nc1N)N	6.81	6.10	7.90	7.41	6.8
1058	CCc1nc(N)nc(N)c1c2ccc(Cl)cc2	7.34	4.95	5.11	7.25	7.18
1059	n1cnc(OC)cc1	2.50	1.92	2.09	3.14	3.01
1060	c1ccccc1Nc2nc(C3CC3)cc(C)n2	4.44	3.55	3.72	3.95	4.22
1061	c1(cn(cn1)C)[N+](=O)[O-]	-0.53	0.38	0.44	-0.12	0.32
1062	c1(c[nH]cn1)[N+](=O)[O-]	-0.05	-0.05	-0.01	0.04	0.49
1063	c1(cncn1C)[N+](=O)[O-]	2.13	1.82	1.86	1.56	2.13

1064	n1(ccnc1)C(C)=O	3.6	3.95	3.89	3.59	3.6
1065	n1(ccnc1)C(COCCC)=Nc2ccc(cc2C(F)(F)F)Cl	3.7	4.59	4.27	2.72	3.21
1066	c2(c1ccccc1)[nH]ccn2	6.48	6.77	6.60	6.25	6.84
1067	n1ccn(C)c1	6.95	7.01	6.82	6.62	7.01
1068	n1cc[nH]c1	6.95	6.66	6.52	6.79	7.18
1069	n1cc[nH]c1C	7.85	7.39	7.20	7.87	8.15
1070	c1(cncn1C)CC(C(=O)O)NC(=O)CCN	7.04	6.40	6.22	6.92	7.26
1071	n1(ccnc1)C(=O)N(CCC)CCOc2c(Cl)cc(cc2Cl)Cl	3.8	5.92	4.64	3.09	4.84
1072	n2(C1CC(O)C(CO)O1)cnc3C(O)CNC=Nc23	5.2	6.00	6.97	2.5	4.11
1073	n2ccn(Cc1ccccc1)c2	6.7	7.15	6.97	5.99	6.79
1074	c1(cncn1C)CC2COC(=O)C2CC	6.78	5.37	5.24	6.81	7.02
1075	c1(CSCCN=C(NC)NC#N)[nH]cnc1C	6.8	6.42	6.22	6.25	7.07
1076	n1(ccnc1)CC(OCC=C)c2ccc(cc2Cl)Cl	6.53	7.41	6.97	5.59	6.74
1077	n2c1ccccc1[nH]c2	5.53	6.00	5.84	5.6	5.26
1078	COc3ccc(Cc2[nH]c1ccc(N(=O)=O)cc1n2)cc3	4.26	3.55	3.52	4.75	3.63
1079	Clc3ccc(Cc2[nH]c1ccc(Cl)cc1n2)cc3	4.86	5.54	5.38	5.11	4.61
1080	Cc3c(c2[nH]c1ccc(N(=O)=O)cc1n2)cccc3	4.87	4.13	2.99	4.27	3.15
1081	Cc3cc(C)c(c2[nH]c1ccc(N(=O)=O)cc1n2)cc3	5.29	4.16	3.14	5	3.31
1082	Clc3cc2nc(Cc1ccc(Br)cc1)[nH]c2cc3	5.42	5.43	5.32	5.09	4.61
1083	Cc3ccc(c2[nH]c1ccccc1n2)cc3	6.9	6.80	6.60	6.24	5.17
1084	Cc3ccc(Cc2[nH]c1ccc(Cl)cc1n2)cc3	7.09	6.21	5.99	5.46	4.72
1085	COc3c(c2[nH]c1ccccc1n2)cccc3	7.17	7.28	7.50	5.96	5.05
1086	Nc3ccc(Cc2[nH]c1ccc(Cl)cc1n2)cc3	7.47	6.50	6.29	5.76	4.84
1087	c1ccccc1CC2=NCCN2	10.3	8.32	8.10	11.49	10.90
1088	c1c(C)cc2N=C(c3c(OC)cc(OC)cc3)Nc2c1	7.25	8.25	8.10	7.51	4.99
1089	Cn1ccnc1Br	3.82	4.76	4.72	2.51	3.83
1090	Cn1ccnc1F	2.3	4.97	4.87	3.23	4.26
1091	Cn1ccnc1N	8.54	7.85	7.65	8.87	8.53
1092	C1=CN(C)C(N(=O)=O)=N1	-0.48	-0.12	-0.01	-3.31	1.10
1093	Brc1ncc[nH]1	3.79	4.23	4.19	2.68	4.49
1094	Clc1ncc[nH]1	3.55	4.76	4.72	2.77	4.59
1095	CCc1ncc[nH]1	7.73	7.45	7.27	7.90	8.22

1096	C1=CN=C(N1)F	2.4	4.48	4.42	3.41	5.28
1097	N1C(N)=NC=C1	8.46	6.94	6.82	9.03	8.56
1098	N1C(N(=O)(=O))=NC=C1	-0.81	-0.75	-0.61	-3.11	-0.47
1099	CSC1=NC=CN1	5.95	7.26	7.12	5.26	5.87
1100	[O-][N+](=O)C1=CC2=C([NH]C=N2)C=C1	4.17	2.04	2.09	3.90	3.39
1101	ClC1=NC2=CC=CC=C2[NH]1	4.68	4.46	4.42	1.62	3.68
1102	C[N]1C=NC2=C1C=CC=C2	5.57	6.18	6.07	5.51	5.4
1103	CC1=CC2=C([NH]C=N2)C=C1	5.81	6.16	6.07	5.85	5.54
1104	CC1=CC2=C(C=C1C)N=C[NH]2	5.89	6.30	6.14	6.38	5.78
1105	CC1=NC2=CC=CC=C2[NH]1	6.1	6.81	6.67	6.72	6.29
1106	NC1=CC2=C([NH]C=N2)C=C1	6.11	6.77	6.60	5.95	6.1
1107	CCC1=NC2=CC=CC=C2[NH]1	6.2	6.88	6.75	6.73	5.75
1108	n2c1ccccc1nc2C(C)C	6.23	7.00	6.82	6.75	5.72
1109	n1cccc2ccccc12	4.9	5.20	5.34	4.56	4.97
1110	c12cccnc1cccc2O	5.02	4.57	5.46	4.75	5.08
1111	c12c(cccn1)ccc(OC)c2	5.03	5.07	5.21	5.69	5.26
1112	n2cccc1cc(OC)ccc12	5.03	5.12	5.27	5.14	5.02
1113	c12c(cccn1)cccc2C	5.05	5.30	5.46	4.55	5.03
1114	n2cc(C)cc1ccccc12	5.17	5.41	5.59	4.84	5.17
1115	n2cccc1cc(C)ccc12	5.34	5.40	5.59	5.07	5.21
1116	c12c(cccn1)ccc(C)c2	5.34	5.41	5.59	5.28	5.44
1117	n2cccc1cc(O)ccc12	5.15	4.77	4.89	4.96	5.22
1118	c12c(cccn1)ccc(O)c2	5.46	4.76	4.89	5.39	5.68
1119	c12ccccc1nccc2C	5.67	5.23	5.40	5.65	5.66
1120	n1c(C)ccc2ccccc12	5.71	5.50	5.72	5.67	5.91
1121	n2cc(Br)cc1ccccc12	2.69	3.54	3.48	2.76	2.53
1122	c12c(Cl)ccnc1cc(Cl)cc2	2.8	2.49	2.34	3.09	1.99
1123	c12c(cccn1)cccc2Cl	3.12	3.89	3.87	3.07	2.33
1124	c12c(cccn1)cccc2F	3.34	3.84	3.80	3.28	1.93
1125	n2cccc1cc(Cl)ccc12	3.85	3.85	3.87	3.89	4.18
1126	c12c(cccn1)ccc(Br)c2	3.87	3.63	3.61	4.02	3.36
1127	n2cccc1cc(Br)ccc12	3.87	3.59	3.55	3.86	4.18

1128	n1c(C)ccc2cc(C)ccc12	6.1	5.67	5.91	6.18	6.05
1129	n1c(C)cc(c2ccccc12)C	5.12	5.53	5.72	6.76	6.48
1130	n2cc(cc1ccccc12)O	4.28	4.80	4.89	4.16	4.23
1131	c12cccnc1c(ccc2Cl)O	3.56	3.54	3.48	3.59	3.77
1132	c12c(cccn1)cccc2OC	5.01	5.69	5.91	4.31	3.28
1133	n1c(C)ccc2cccc(O)c12	5.55	5.16	5.34	5.68	5.23
1134	c12c(cccc1c(ccn2)C)O	5.56	4.87	5.02	5.66	5.23
1135	CCCCCC(OC(COc2c1ncccc1c(Cl)cc2)=O)C	3.75	3.56	3.42	2.53	1.94
1136	COc3ccc(Cc1nccc2cc(OC)c(OC)cc12)cc3OC	8.07	4.78	4.89	7.17	6.32
1137	c1ccc2c(c1)ccc3ncccc23	4.21	4.45	4.51	4.44	5.15
1138	c1ccc2c(c1)ccc3cccnc23	4.21	4.67	4.76	4.21	4.25
1139	n(c(c(ccc1)cc2)c1N)c2	3.95	6.17	6.42	4.22	4.09
1140	c1ccc2c(N)ccnc2c1	9.13	6.68	7.00	7.95	9.00
1141	Nc2ccc1ncccc1c2	6.61	5.80	6.04	5.54	5.63
1142	n(c(c(ccc1)cc2)c1)c2N	7.3	6.53	6.87	7.22	6.72
1143	c1c(N)c2cccnc2c(O)c1	5.67	5.15	5.27	5.54	5.65