Supporting Information

Identification of novel substrates and structure activity relationship of cellular uptake mediated by the human organic cation transporters 1 and 2 (hOCT1 and hOCT2)

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Table S1. Experimental data of uptake in HEK293 cells transfected by hOCT1, hOCT2 or empty vector and log $D_{7.4}$. Data points are average of triplicates, ND=not determined.

Cmpd ID	**Project/ Reference**	**hOCT1 total uptake** (pmol/mg protein)	**hOCT1 ratio total/ passive**	**hOCT1 active uptake** (pmol/mg protein)	**hOCT2 total uptake** (pmol/mg protein)	**hOCT2 ratio total/ passive**	**hOCT2 active uptake** (pmol/mg protein)	**Passive uptake** (pmol/mg protein)	**Log$D_{7.4}$** (measured)
1	Trimethoprim	363	1.9	173	255	1.4	71	187	0.55
2	Propanolol	2371	1.1	168	1960	0.9	0	2181	ND
3	Iressa	418	1.2	76	1453	1.1	86	855	ND
4	Oxyphenonium	667	25.2	640	242	14.3	225	22	ND
5	Clozapine	2232	1.0	58	2416	1.1	242	2174	3.10
6	Amiloride	1448	75.7	1429	1684	73.9	1661	21	ND
7	Mepenzolate	624	76.2	615	ND	ND	ND	8	-1.95
8	Azithromycin	269	1.1	31	197	0.8	0	238	ND
9	Haloperidol	2583	1.2	387	2473	1.1	277	2196	2.73
10	Verapamil	1802	1.2	257	1849	1.2	305	1544	2.60
11	Imatinib	301	1.1	31	1209	1.1	129	675	2.50
12	Metoclopramide	1021	1.8	457	736	1.3	175	563	0.36
13	Disopyramide	254	1.7	107	215	0.9	0	195	-0.54
14	Albuterol	69	6.5	58	291	14.6	271	15	-1.81
15	Imipramine	2219	1.1	221	2384	1.2	314	2033	2.49
16	Sulfaphenazole	47	1.1	3	42	0.8	0	48	0.12
17	Amiodarone	226	1.2	30	276	1.4	80	196	ND
18	Fenoterol	151	17.5	142	119	11.8	109	9	-0.06
19	Diltiazem	1463	1.3	357	1587	1.1	136	1279	2.01
20	Loperamide	1287	1.1	77	2536	0.9	0	1958	3.38
21	Procainamide	275	2.5	167	316	1.6	114	155	ND
22	Benzamil	1117	1.8	510	840	1.3	200	623	0.91
23	Quinidine	1801	1.2	237	1541	1.1	183	1460	2.19
24	Ranitidine	632	18.1	597	63	1.6	22	38	-0.95
25	Sumatriptan	667	14.6	621	134	3.3	94	43	ND
26	Clidinium	703	56.5	691	ND	ND	ND	12	-1.81
27	Terazosin	316	1.3	66	347	1.3	85	256	0.94
28	Mibefradil	2031	1.1	154	1939	1.1	164	1826	3.52
29	Camostat	63	1.7	26	37	1.0	0	37	ND
30	Formoterol	507	3.0	337	195	1.1	21	172	0.34
31	Project A	2091	1.0	16	ND	ND	ND	2075	2.84
32	Project A	281	4.5	219	ND	ND	ND	63	2.38
33	Project AA	1374	1.1	125	ND	ND	ND	1248	1.80
34	Xamoterol (chiral R)	152	38.5	148	17	1.7	7	7	-0.36

Cmpd ID	Project/ Reference	hOCT1 total	hOCT1 ratio	hOCT1 active	hOCT2 total	hOCT2 ratio	hOCT2 active	Passive	LogD7.4
35	Xamoterol (chiral S)	321	46.8	314	11	1.4	3	7	-0.63
36	Atenolol (chiral S)	96	4.7	75	66	2.5	40	23	ND
37	Atropine	460	1.7	189	467	1.7	195	272	-0.66
38	Atropine	469	1.6	171	467	1.4	131	316	-0.09
39	Project T	169	1.2	30				138	2.00
40	Atenolol (chiral R)	66	4.6	51	41	2.7	26	15	ND
41	Glycopyrrolate	652	59.1	641	837	93.0	828	10	ND
42	Indacaterol	713	1.4	190	386	0.9	0	468	2.74
43	Project A	1089	25.9	1047	79	1.9	38	41	0.01
44	Project Z	1134	1.0	5	ND	ND	ND	1129	1.40
45	Nizatidine	88	3.1	60	39	1.1	2	32	-0.49
46	Tiotropium	789	65.5	777	345	39.2	336	10	ND
47	Scopolamine	340	1.1	36	ND	ND	ND	304	ND
48	Vesamicol	972	1.0	27	ND	ND	ND	945	ND
49	Procaterol	150	10.7	136	29	1.9	14	15	ND
50	Project A	1696	38.6	1653	61	1.6	22	42	0.13
51	Project A	702	11.4	641	116	2.2	63	57	0.00
52	Project A	1425	1.1	270	1210	1.0	0	1279	1.17
53	Project A	804	13.9	746	217	2.7	137	69	0.24
54	Project A	1372	68.0	1352	56	1.6	21	28	-0.20
55	Project A	1559	69.1	1537	31	1.3	7	23	-0.22
56	Project T	86	1.3	20	ND	ND	ND	65	ND
57	Project A	280	6.5	237	ND	ND	ND	43	-0.10
58	Project A	148	3.1	101	ND	ND	ND	47	0.09
59	Project A	250	2.9	163	ND	ND	ND	87	0.65
60	Project A	273	5.3	221	ND	ND	ND	52	-0.47
61	Project A	482	14.6	449	ND	ND	ND	33	-0.29
62	Project X	1508	1.1	135	ND	ND	ND	1372	ND
63	Project X	790	1.2	117	ND	ND	ND	672	ND
64	Project A	920	52.7	903	60	4.3	46	16	-1.40
65	Project A	1280	21.5	1221	ND	ND	ND	59	0.31
66	Project A	389	23.5	372	ND	ND	ND	17	-1.20
67	Project A	1270	1.0	30	ND	ND	ND	1240	3.60
68	Project A	396	1.4	108	ND	ND	ND	288	1.70
69	Project A	495	3.5	353	ND	ND	ND	141	1.70
70	Project A	864	12.7	796	160	1.3	40	94	0.50
71	Project A	625	1.9	288	ND	ND	ND	336	1.70
72	Project A	197	1.4	53	ND	ND	ND	144	1.10

Cmpd ID	Project/ Reference	hOCT1 total	hOCT1 ratio	hOCT1 active	hOCT2 total	hOCT2 ratio	hOCT2 active	Passive	LogD7.4
73	Project A	732	11.3	667	ND	ND	ND	65	0.10
74	Project A	466	12.6	429	162	5.4	132	33	-0.90
75	Project A	87	10.7	79	ND	ND	ND	8	0.83
76	Project A	796	13.9	739	69	1.5	23	52	-0.40
77	Project T	294	1.3	71	ND	ND	ND	224	1.10
78	Project A	57	3.7	42	41	1.9	19	18	-0.70
79	Project T	91	1.2	18	ND	ND	ND	73	0.60
80	Project X	115	1.1	8	ND	ND	ND	107	1.39
81	Project X	103	1.1	6	ND	ND	ND	97	1.81
82	Project A	432	14.8	402	74	2.5	45	29	-0.50
83	Project A	639	23.4	612	197	7.2	169	27	-0.70
84	Varenicline	470	1.6	184	655	1.6	245	348	ND
85	Project A	260	13.4	240	ND	ND	ND	19	1.50
86	Project A	354	1.4	106	ND	ND	ND	248	1.60
87	Project A	494	6.7	421	ND	ND	ND	74	2.10
88	Project A	222	1.4	58	ND	ND	ND	164	1.66
89	Project A	1324	1.1	80	ND	ND	ND	1244	ND
90	Project A	150	3.0	100	ND	ND	ND	50	ND
91	Project A	850	16.7	799	ND	ND	ND	51	-0.50
92	Project A	1828	1.1	137	ND	ND	ND	1691	ND
93	Project A	372	6.6	315	ND	ND	ND	57	ND
94	Project A	588	3.0	392	ND	ND	ND	196	1.00
95	Project A	305	5.2	246	ND	ND	ND	58	0.20
96	Project A	1084	9.1	964	ND	ND	ND	119	1.28
97	Project W	16	1.0	0	12	0.8	0	16	ND
98	Project A	117	6.6	99	ND	ND	ND	18	ND
99	Project A	1660	1.0	50	1774	1.1	164	1610	3.60
100	Project A	233	1.2	30	204	1.0	2	203	2.30
101	Project A	112	2.0	57	76	1.4	21	55	1.30
102	Project X	1409	1.1	94	1518	1.2	244	1295	2.77
103	Project T	32	1.0	0	37	1.2	5	32	1.25
104	Project A	1735	1.1	131	ND	ND	ND	1604	3.92
105	Project A	716	20.6	681	65	1.9	30	35	-0.97
106	Project A	353	1.9	171	ND	ND	ND	182	1.61
107	Project A	211	2.5	126	ND	ND	ND	84	1.07
108	Project W	46	1.0	1	57	1.3	12	45	2.02
109	Atenolol racemate	90	8.1	79	67	4.9	53	12	ND
110	Clonidine	570	1.2	90	420	1.0	1	449	ND
111	Oxyprenolol	990	1.1	110	ND	ND	ND	880	0.20
112	Triamterene	225	1.5	72	269	1.6	96	163	1.17

Cmpd ID	Project/ Reference	hOCT1 total	hOCT1 ratio	hOCT1 active	hOCT2 total	hOCT2 ratio	hOCT2 active	Passive	LogD7.4
113	Perphenazine	4113	1.8	1840	1419	1.2	268	1712	3.60
114	Ketamine	383	1.1	26	404	1.1	47	357	ND
115	Terbutaline	77	7.3	67	51	6.9	43	9	-1.53
116	Project A	2979	1.2	446	ND	ND	ND	2533	ND
117	Project A	806	11.3	735	ND	ND	ND	71	1.07
118	Cimetidine	87	4.0	65	290	14.7	271	21	0.29
119	Propafenone	1964	1.1	185	1924	1.1	146	1779	1.72
120	Buflomedil	544	1.0	10	ND	ND	ND	533	ND
121	Salmeterol	1316	1.0	48	1025	0.8	0	1244	2.01
122	Project A	1067	1.1	84	ND	ND	ND	983	2.29
123	Project A	2206	1.0	62	ND	ND	ND	2144	ND
124	Ipratropium	377	41.9	368	63	8.3	56	8	-0.19
125	Pindolol	797	1.2	152	581	1.3	122	552	-0.47
126	Selegiline	545	1.1	56	943	1.9	440	496	ND
127	Anisomycin racemate	432	1.0	4	612	0.8	0	588	ND
128	Project A	627	15.5	586	59	1.1	7	46	0.33
129	Project A	873	17.0	821	79	1.8	35	48	-0.27
130	Project A	253	8.4	223	52	1.7	22	30	1.55
131	Project A	632	6.8	540	69	1.4	20	71	-0.34
132	Project A	127	5.1	102	33	1.3	9	25	0.92
133	Project A	339	5.3	276	164	2.1	86	71	ND
134	Project A	1513	73.1	1493	30	1.4	9	21	-0.08
135	Project A	337	2.7	214	177	1.2	35	132	1.67
136	Project A	258	16.1	242	13	1.0	0	15	1.28
137	Project A	131	6.5	111	ND	ND	ND	20	ND
138	Project A	198	3.6	142	ND	ND	ND	56	0.51
139	Project A	223	7.2	192	ND	ND	ND	31	-0.27
140	Project A	104	1.4	29	56	1.1	3	64	1.00
141	Project A	268	7.8	233	35	0.9	0	37	ND
142	Project A	218	4.5	170	52	1.1	5	47	0.30
143	Project A	566	1.9	274	297	0.9	0	309	ND
144	Project A	1285	1.1	115	ND	ND	ND	1171	ND
145	Project A	695	12.5	640	ND	ND	ND	56	ND
146	Project A	686	11.3	625	ND	ND	ND	60	-0.40
147	Project A	348	3.4	245	ND	ND	ND	103	ND
148	Project A	1910	4.6	1495	ND	ND	ND	415	0.50
149	Project A	1348	33.7	1308	ND	ND	ND	40	0.40
150	Project A	1260	37.0	1225	ND	ND	ND	34	0.40
151	Project A	802	10.0	722	ND	ND	ND	80	0.20

Cmpd ID	Project/ Reference	hOCT1 total	hOCT1 ratio	hOCT1 active	hOCT2 total	hOCT2 ratio	hOCT2 active	Passive	LogD7.4
152	Project A	856	8.6	756	ND	ND	ND	100	0.70
153	Project A	627	3.4	442	ND	ND	ND	185	1.20
154	Project A	893	8.0	781	ND	ND	ND	111	0.00
155	Project A	589	1.1	64	ND	ND	ND	525	ND
156	Project A	128	7.1	110	43	2.4	25	18	0.99
157	Metformin	13	> 1.7	5	115	> 15.5	107	< 7	ND
158	Phenformin	586	> 39.3	571	467	> 35.1	454	< 14	ND
159	Tiotropium	877	> 125.3	870	607	39.1	591	< 11	ND
160	Project K	112	1.4	33	98	1.2	18	80	0.40
161	Project K	899	1.1	93	908	1.1	102	806	ND
162	Project K	187	1.2	30	214	1.4	57	157	ND
163	Project K	2413	1.0	46	2101	0.9	0	2367	3.50
164	Project K	653	1.1	73	633	1.1	54	580	2.40
165	Project N	864	1.2	122	937	1.3	196	741	0.80
166	Project K	39	1.5	13	27	1.0	1	27	ND
167	Project K	2338	1.1	273	2148	1.0	83	2065	ND
168	Project K	1000	5.9	832	245	1.5	76	168	-0.10
169	Project C	425	1.4	129	ND	ND	ND	296	2.62
170	Project M	2278	1.1	137	ND	ND	ND	2141	1.11
171	Project P	17	1.0	1	ND	ND	ND	17	ND
172	Project B	1490	1.1	166	1059	0.8	0	1308	0.88
173	Project S	35	2.7	22	ND	ND	ND	13	0.40
174	Project B	252	1.0	5	243	1.0	0	247	2.50
175	Project D	1048	41.7	1023	132	3.7	97	30	1.75
176	Project D	1508	37.7	1468	144	4.0	108	38	ND
177	Project C	250	1.3	58	150	0.8	0	188	2.46
178	Project E	1510	1.1	66	ND	ND	ND	1443	3.44
179	Project D	2675	1.1	211	1714	1.1	114	2032	3.03
180	Project C	347	2.1	182	163	1.0	0	166	0.98
181	Project D	1041	70.9	1027	479	46.5	468	12	ND
182	Project C	185	5.0	148	53	0.9	0	49	-0.39
183	Project A	1132	7.6	983	192	1.3	40	151	1.03
184	Project D	1080	63.2	1063	424	20.6	403	19	ND
185	Project D	900	30.0	869	82	2.9	54	29	ND
186	Project C	84	1.1	10	55	0.9	0	67	0.64
187	Project E	1355	1.1	81	ND	ND	ND	1274	3.93
188	Project E	1139	1.2	171	ND	ND	ND	969	ND
189	Project E	1423	1.1	132	ND	ND	ND	1291	4.37
190	Project D	1645	25.7	1581	420	7.2	362	61	ND
191	Project D	1594	28.0	1537	343	8.8	304	48	ND

Cmpd ID	Project/ Reference	hOCT1 total	hOCT1 ratio	hOCT1 active	hOCT2 total	hOCT2 ratio	hOCT2 active	Passive	LogD7.4
192	Project D	422	1.2	68	519	1.4	159	358	ND
193	Project I	567	0.8	0	719	1.0	26	693	1.70
194	Project D	807	21.7	770	48	1.4	14	36	ND
195	Project B	212	4.1	161	70	1.3	18	52	-0.61
196	Project R	86	0.9	0	91	1.0	1	91	0.01
197	Project E	595	1.1	29	ND	ND	ND	566	1.24
198	Project E	171	1.3	36	ND	ND	ND	135	ND
199	Project G	173	1.2	32	ND	ND	ND	141	0.44
200	Project I	360	0.9	0	411	1.0	0	413	1.70
201	Project I	781	0.8	0	1117	1.1	116	1002	2.28
202	Project I	17	1.2	3	22	1.6	8	14	0.98
203	Project I	882	0.9	0	980	1.0	35	945	2.29
204	Project G	572	11.2	521	ND	ND	ND	51	0.03
205	Project I	751	0.9	0	772	1.0	0	806	1.79
206	Project G	117	5.2	94	ND	ND	ND	22	0.52
207	Project G	894	1.2	173	ND	ND	ND	720	1.16
208	Project G	449	1.9	215	ND	ND	ND	234	1.02
209	Project B	137	1.6	51	111	1.3	25	87	-0.40
210	Project I	726	1.1	58	728	1.1	61	668	2.40
211	Project V	ND	ND	ND	1761	0.9	161	2018	1.24
212	Project F	32	0.8	0	31	0.7	0	42	1.41
213	Project A	233	4.7	183	77	1.6	29	49	0.75
214	Project A	65	1.3	14	ND	ND	ND	51	0.80
215	Project A	152	2.2	82	74	1.2	10	66	1.06
216	Project I	1247	1.0	0	1602	1.2	290	1312	3.70
217	Project I	1385	1.0	0	1651	1.1	200	1451	2.90
218	Project A	1158	17.3	1091	ND	ND	ND	67	0.50
219	Project A	42	3.3	29	ND	ND	ND	13	ND
220	Project A	678	4.7	533	ND	ND	ND	145	1.60
221	Project A	403	2.5	243	ND	ND	ND	161	1.40
222	Project A	1109	8.9	984	ND	ND	ND	125	1.10
223	Project A	47	1.7	20	ND	ND	ND	27	0.01
224	Project A	142	1.5	45	ND	ND	ND	97	0.90
225	Project A	304	5.6	250	ND	ND	ND	54	1.10
226	Project A	336	1.7	139	ND	ND	ND	197	1.40
227	Project A	66	1.4	18	ND	ND	ND	48	0.57
228	Project A	99	1.1	8	ND	ND	ND	91	-0.79
229	Project A	199	11.8	182	ND	ND	ND	17	-1.40
230	Project A	105	1.5	33	ND	ND	ND	72	0.50
231	Project A	223	5.7	184	ND	ND	ND	39	0.10

Cmpd ID	Project/ Reference	hOCT1 total	hOCT1 ratio	hOCT1 active	hOCT2 total	hOCT2 ratio	hOCT2 active	Passive	LogD7.4
232	Project A	299	1.3	74	ND	ND	ND	225	1.70
233	Project A	1400	14.5	1304	ND	ND	ND	97	0.70
234	Project A	5	2.1	3	ND	ND	ND	2	ND
235	Project A	444	23.5	425	ND	ND	ND	19	-0.90
236	Project A	604	6.3	508	ND	ND	ND	96	0.60
237	Project J	1437	1.2	244	1378	1.2	185	1193	1.08
238	Project I	1162	1.1	80	1119	1.0	37	1082	2.60
239	Project A	132	2.4	77	65	1.4	20	50	0.57
240	Project A	418	3.0	279	ND	ND	ND	139	-0.99
241	Project A	56	1.7	23	ND	ND	ND	33	1.10
242	Project A	237	1.9	115	ND	ND	ND	122	1.80
243	Project J	1387	1.2	248	1362	1.2	223	1139	0.60
244	Project A	500	7.0	429	ND	ND	ND	72	0.45
245	Project A	320	3.0	212	ND	ND	ND	108	1.25
246	Project V	ND	ND	ND	199	0.9	20	211	1.75
247	Project J	686	1.2	108	581	1.0	3	579	-1.01
248	Project J	1540	1.0	0	1647	1.0	39	1608	1.56
249	Project I	1683	1.1	137	1745	1.1	198	1547	2.40
250	Project J	1917	1.2	257	1800	1.1	139	1660	1.44
251	Project A	1413	8.0	1236	ND	ND	ND	177	0.40
252	Project H	1728	0.9	156	ND	ND	ND	1884	2.60
253	Project H	998	0.9	131	ND	ND	ND	1129	1.80
254	Project H	1742	0.9	311	ND	ND	ND	2053	3.30
255	Project H	133	0.3	408	ND	ND	ND	541	3.30
256	Project F	ND	ND	ND	123	0.9	0	131	0.60
257	Project H	1274	0.8	329	ND	ND	ND	1604	ND
258	Project L	2000	1.1	117	2049	1.1	166	1883	1.45
259	Project F	ND	ND	ND	13	1.3	3	10	-0.55
260	Project H	1918	0.9	288	ND	ND	ND	2206	3.10
261	Project O	208	1.0	0	186	0.9	0	217	1.95
262	Project H	1943	0.8	431	ND	ND	ND	2374	2.80
263	Project H	1750	1.0	24	ND	ND	ND	1774	3.90
264	Project H	787	0.9	124	ND	ND	ND	910	3.80
265	Project O	287	1.0	0	264	0.9	0	288	2.08
266	Project F	ND	ND	ND	102	1.0	0	107	0.00
267	Project H	1523	1.0	10	ND	ND	ND	1533	1.40
268	Project H	1221	0.9	74	ND	ND	ND	1295	1.60
269	Project B	291	2.4	167	163	1.0	6	140	-0.03
270	Project F	ND	ND	ND	28	1.2	4	24	1.01
271	Project F	ND	ND	ND	287	1.1	14	273	0.81

Cmpd ID	Project/ Reference	hOCT1 total	hOCT1 ratio	hOCT1 active	hOCT2 total	hOCT2 ratio	hOCT2 active	Passive	LogD7.4
272	Project F	ND	ND	ND	33	1.4	10	24	0.16
273	Project B	734	2.4	434	284	1.0	0	300	0.07
274	Project Q	1041	1.1	75	934	1.0	0	966	0.57
275	Project B	270	1.8	119	156	1.0	6	151	0.17
276	Project B	352	2.8	226	113	1.0	4	117	0.52
277	Project B	1984	1.0	0	ND	ND	ND	2014	1.40
278	Project B	2850	1.1	200	ND	ND	ND	2650	1.70
279	Project A	1527	62.0	1503	ND	ND	ND	25	ND
280	Project B	328	10.5	297	35	1.3	8	29	-0.47
281	Project B	1287	1.1	113	1165	0.9	0	1217	1.17
282	Project B	440	1.5	147	ND	ND	ND	293	0.70
283	Project B	571	1.2	109	472	0.9	0	499	2.89
284	Project B	1764	1.1	200	ND	ND	ND	1565	1.16
285	Project A	872	32.7	846	ND	ND	ND	27	-1.09
286	Project B	15	1.4	4	ND	ND	ND	11	0.10
287	Project B	322	9.0	286	46	1.3	10	36	-0.46
288	Project A	967	5.5	790	ND	ND	ND	177	1.53
289	Project U	302	0.8	0	394	1.1	28	366	3.06
290	Project B	99	2.6	61	51	1.4	13	38	-0.19
291	Project B	184	3.0	122	66	1.1	4	62	0.60
292	Project A	509	4.9	406	ND	ND	ND	103	1.13
293	Project B	19	1.3	4	15	1.1	1	15	0.41
294	Project A	478	1.8	207	ND	ND	ND	271	2.27
295	Project A	1258	1.2	208	ND	ND	ND	1050	2.69
296	Project B	176	2.9	116	73	1.2	12	60	0.99
297	Project B	165	1.5	56	133	1.2	24	109	0.26
298	Project A	349	2.4	203	ND	ND	ND	146	ND
299	Project A	456	1.6	172	ND	ND	ND	284	2.03
300	Project B	174	1.2	33	156	1.1	15	141	0.77
301	Project A	299	2.0	149	ND	ND	ND	150	1.45
302	Project B	137	3.2	94	43	1.0	1	43	-0.47
303	Project B	75	1.7	30	72	1.6	27	45	ND
304	Project A	617	10.3	557	ND	ND	ND	60	0.75
305	Project B	113	0.9	0	131	1.1	11	119	ND
306	Project A	251	11.2	229	ND	ND	ND	22	-0.66
307	Project A	195	9.9	175	ND	ND	ND	20	0.07
308	Project A	721	2.7	454	ND	ND	ND	267	1.57
309	Project A	675	4.9	537	ND	ND	ND	138	1.37
310	Project B	523	8.1	459	74	1.1	9	64	-0.47
311	Project B	1745	1.1	132	1728	1.1	114	1613	1.87

Cmpd ID	Project/ Reference	hOCT1 total	hOCT1 ratio	hOCT1 active	hOCT2 total	hOCT2 ratio	hOCT2 active	Passive	LogD7.4
312	Project B	130	1.2	25	141	1.3	36	105	-0.03
313	Prochlorperazine	1367	0.8	0	1429	0.9	0	1657	3.62
314	Promethazine	3762	0.9	0	3983	1.0	0	4081	2.81
315	Desipramine	2365	0.8	286	2973	1.2	396	2856	1.24
316	Fluphenazine	3126	0.9	0	2694	0.7	0	3679	3.79
317	Memantine	2072	1.1	92	2154	1.0	57	2039	0.06
318	Clomipramine	1626	0.8	0	2338	1.2	325	2013	3.35
319	Bupivacain	673	0.8	0	1232	1.4	343	889	2.58
320	Apomorphine	640	0.5	0	1584	1.7	655	1072	2.65
321	Prazosin	600	0.9	3	739	1.3	187	599	1.89
322	Zidovudine	26	0.9	0	16	0.7	0	27	0.09
323	Bupropion	977	0.9	0	1474	1.4	413	1061	2.12
324	Methoctramine	242	0.9	0	317	1.2	48	269	ND
325	Phenamil	1239	1.0	0	1562	1.4	446	1195	1.89
326	Lappaconitine	262	0.8	0	404	1.3	83	321	1.56
327	Ibutamoren	712	0.8	0	830	1.0	0	852	1.55
328	Puromycin	53	1.0	0	60	1.1	7	53	0.83
329	Chlorprothixene	465	0.3	0	1615	1.7	669	1369	ND
330	Anisomycin (chiral)	540	0.8	-8	1106	1.0	0	908	0.65
331	Project T	ND	ND	ND	108	1.1	9	99	1.74
332	Project E	98	1.4	27	ND	ND	ND	71	ND
333	Project E	78	1.1	6	ND	ND	ND	72	ND
334	Project E	182	1.1	13	ND	ND	ND	170	ND
335	Capromorelin	397	0.8	0	542	1.1	39	503	1.35
336	Project X	1726	1.0	0	ND	ND	ND	1762	2.65
337	Project T	16	0.7	0	26	1.0	0	24	ND
338	Project X	ND	ND	ND	1439	0.9	266	1640	2.38
339	Project Y	1256	0.9	0	1430	1.0	40	1391	1.47
340	Project A	1128	1.0	0	ND	ND	ND	1163	3.15
341	Project W	14	1.2	3	19	1.3	5	13	ND
342	Project A	10	0.7	0	5	0.4	0	13	ND
343	Project W	9	0.9	0	9	0.9	0	10	ND
344	Project W	10	0.8	0	7	0.6	0	13	-0.83
345	Project W	9	1.2	1	9	1.2	2	7	ND
346	Project W	18	1.6	7	15	1.3	4	12	ND
347	Project X	1007	1.0	0	1090	1.1	73	1017	2.63
348	Project L	ND	ND	ND	668	1.0	75	661	1.93
349	Project T	60	0.9	0	93	1.3	24	69	1.50
350	Project W	34	0.8	0	36	0.8	0	44	ND
351	Project BB	80	1.2	12	75	1.1	8	67	ND

Cmpd ID	Project/ Reference	hOCT1 total	hOCT1 ratio	hOCT1 active	hOCT2 total	hOCT2 ratio	hOCT2 active	Passive	LogD7.4
352	Project BB	33	1.0	0	40	1.2	7	33	-1.46
353	Project B	323	65.8	318	46	9.3	41	5	ND
354	Project B	169	1.9	78	113	1.2	22	91	0.04

Table S2. Calculated physicochemical parameters used for SAR analysis.

Cmpd ID	Ion Class	pKa Base 1	pKa Base 2	$LogD_{6.5}$	$LogD_{7.4}$	LogP	AREA	MW	NPSA	PSA	VOL
1	Base	7.2		0.041	0.472	0.594	339.4	290.3	236.2	103.1	246.4
2	Base	9.1		-0.101	0.796	2.9	327.9	259.3	281.6	46.24	237.9
3	Base	7.3	4.3	2.072	2.561	2.702	471.8	446.9	409.2	62.63	359.7
4	Quater			-0.659	-0.659	-0.659	479.2	348.5	429.5	49.62	321.6
5	Base	7.1	5.3	2.706	3.523	3.939	350.3	326.8	324.7	25.63	270.5
6	Base			1.22	1.22	1.22	237.3	229.6	77.64	159.6	172.2
7	Quater			-0.479	-0.479	-0.479	425.9	340.4	376.3	49.62	301.3
8	Base	8.6	8.2	-1.179	0.537	2.582	973.4	749	787.2	186.2	655.5
9	Base	8.3		2.209	3.031	3.757	422.8	375.9	380.8	42.01	312.6
10	Base	9		1.553	2.443	4.024	597.2	454.6	540.9	56.29	414.5
11	Base	8	3	1.764	2.481	2.887	567.9	493.6	488.3	79.59	428.9
12	Base	9.7		-0.452	0.44	2.161	371.1	299.8	300.3	70.79	256.5
13	Base	10.1	3.7	-1.132	-0.23	2.333	452.6	339.5	395	57.66	310.1
14	Base	9.2		-2.386	-1.49	0.692	318.3	239.3	235.7	82.56	218
15	Base	9.5		1.412	2.309	4.355	357.3	280.4	355.5	1.747	260.6
16	Acid			1.264	0.833	1.386	325.3	314.4	232.4	92.88	251.5
17	Base	9.4		4.941	5.837	7.815	557.6	645.3	519.6	37.97	408.6
18	Base	8.9		-1.136	-0.254	1.332	365	303.4	259.3	105.7	265
19	Base	8.9		2.288	3.177	4.727	478.2	414.5	421.7	56.49	351
20	Base	8.1		2.861	3.627	4.146	566.6	477	523.4	43.18	405.5
21	Base	9.9		-1.306	-0.413	1.317	320.2	235.3	258.5	61.69	219.9
22	Base	4		3.222	3.223	3.223	342.8	319.8	196.6	146.3	252.1
23	Base	9.3	4.8	0.018	0.921	2.823	377.4	324.4	334.3	43.08	284.1
24	Base	8.4		-1.936	-1.075	-0.068	389.3	314.4	305.1	84.19	273.9
25	Base	9.5		-2.367	-1.472	0.436	348.3	295.4	281.1	67.24	253.9
26	Quater			-0.334	-0.334	-0.334	422.5	352.5	372.9	49.62	308.6
27	Neutral	6.5		0.484	0.743	0.797	430.4	387.4	334.9	95.48	327.1
28	Base	9.3	6	3.279	4.247	6.213	598.3	495.6	537	61.25	433.1
29	Base	9.1		-2.236	-1.344	0.359	461.9	398.4	322.7	139.1	337.6
30	Base	8.9		-0.4	0.48	2.029	419.1	344.4	317.5	101.7	300.9
31	Neutral	6.6	3.3	3.236	3.526	3.59	311.7	322.8	244.7	67	253.4
32	Neutral			2.03	2.03	2.03	364.5	353.4	221	143.5	277
33	Zwitterion	8.7	7.1	0.751	1.79	3.603	559.1	496.4	456.3	102.8	406.4
34	Base	9.3		-3.373	-2.48	-0.701	408.7	339.4	296.8	111.9	294.7
35	Base	9.3		-3.373	-2.48	-0.701	408.7	339.4	296.8	111.9	294.7
36	Base	9.2		-2.596	-1.699	0.335	347.9	266.3	255.4	92.48	241.5
37	Base	10		-2.101	-1.202	1.38	347.7	289.4	296.9	50.8	256.4

Cmpd ID	Ion Class	pKa Base 1	pKa Base 2	$LogD_{6.5}$	$LogD_{7.4}$	LogP	AREA	MW	NPSA	PSA	VOL
38	Base	10		-2.101	-1.202	1.38	347.7	289.4	296.9	50.8	256.4
39	Base	7.5		0.583	0.928	1.012	609.5	577.6	511.4	98.11	459.4
40	Base	9.2		-2.596	-1.699	0.335	347.9	266.3	255.4	92.48	241.5
41	Quater			-0.962	-0.962	-0.962	408.1	318.4	358.5	49.62	287.2
42	Base	9		1.803	2.67	4.088	457	392.5	364.8	92.24	346
43	Base	9.7		-0.639	0.256	2.131	369.7	346.4	239.3	130.4	284
44	Base	9.2	5.8	0.829	1.786	3.569	519.1	434.6	451.4	67.64	385.2
45	Base	7.3		-1.241	-0.688	-0.486	394	331.5	309	85.02	282.3
46	Quater			-1.121	-1.121	-1.121	403.5	392.5	345.1	58.42	317.4
47	Base	8		-0.829	-0.012	0.693	333.1	303.4	273.5	59.59	261.7
48	Base	9		0.868	1.759	3.395	333.2	259.4	309.5	23.73	243
49	Base	9.5		-1.117	-0.237	1.737	355.8	290.4	263.6	92.24	256.7
50	Base	9.6		-0.978	-0.084	1.703	392.1	371.4	243	149.1	303.7
51	Base	9.4		-1.641	-0.745	1.191	347.2	332.4	216.7	130.4	269.7
52	Base	10.1	3.5	-2.639	-1.885	0.209	426.9	395.5	328.8	98.13	337.7
53	Base	8.4		-0.868	-0.004	1.033	349.7	320.4	205.9	143.8	262.1
54	Base	9.8		-0.758	0.137	2.049	369.7	346.4	239.3	130.4	283.9
55	Base	8.5		-0.784	0.082	1.148	349.7	320.4	205.9	143.8	262
56	Base	9.7		1.14	2.037	4.184	500.3	478.5	411.4	88.87	388
57	Base	8.4		-0.503	0.359	1.386	440	394.5	264.4	175.6	325.4
58	Base	9.1		-0.379	0.518	2.534	451.7	392.5	298.7	153	330.5
59	Base	9.5		-0.324	0.572	2.589	448.3	404.5	295.3	153	338.4
60	Base	8.1		-0.776	0.049	0.79	383.1	350.4	216.7	166.4	286.2
61	Base	9.1		-1.084	-0.189	1.671	406.6	364.4	253.6	153	300.9
62	Base	7.8		3.133	3.938	4.584	579.5	517.7	497.5	81.95	437.4
63	Base	6.5		6.104	6.363	6.417	690.3	631.8	585.8	104.5	528.2
64	Quater			-0.75	-0.75	-0.75	428.9	375.5	313	115.9	313.9
65	Base	9.6		-0.828	0.066	1.889	365.7	347.4	225	140.7	282.1
66	Quater			-2.23	-2.23	-2.23	465.7	393.5	327.3	138.4	329.3
67	Neutral	4.7	4.6	5.473	5.498	5.502	571.4	521.6	452	119.5	440.1
68	Base	7.8		0.412	1.251	2.077	450.4	404.5	297.4	153	339.4
69	Base	7.8		0.439	1.272	2.062	425.7	390.5	272.7	153	325.5
70	Base	8.3		-1.026	-0.17	0.792	345.6	321.4	191.6	154.1	260.2
71	Base	8.2		0.223	1.07	1.947	449.7	404.5	323.8	125.8	338.4
72	Acid	5.4	4.6	2.396	1.548	5.327	548.4	507.6	415.1	133.2	424.7
73	Base	9.7	5.2	-1.311	-0.4	1.464	367.3	354.4	259.5	107.8	294
74	Quater			0.169	0.805	0.487	473.9	393.5	385.3	88.59	350.2
75	Neutral			1.853	1.853	1.853	318.6	286.3	154.4	164.1	229
76	Base	9.5		-1.241	-0.344	1.747	368.2	335.4	214.1	154.1	275.4
77	Base	9.4		0.755	1.651	3.667	594.2	548.6	509.5	84.68	451.4

Cmpd ID	Ion Class	pKa Base 1	pKa Base 2	$LogD_{6.5}$	$LogD_{7.4}$	LogP	AREA	MW	NPSA	PSA	VOL
78	Quater	3		-3.741	-3.005	-3.162	486.1	424.5	402.5	83.55	366.6
79	Base	10.3		0.286	1.185	4.088	615.9	562.6	517.8	98.07	466.3
80	Base	10.3	7.4	0.165	1.308	4.255	771.7	734.8	642.1	129.6	606.2
81	Base	9.4	3.4	0.843	1.733	3.367	726.6	706.8	596.9	129.6	576.1
82	Quater			0.169	0.805	0.487	473.9	393.5	385.3	88.59	350.2
83	Quater			0.169	0.805	0.487	473.9	393.5	385.3	88.59	350.2
84	Base	9.6		-1.994	-1.097	1.011	222.6	211.3	187.5	35.06	183.8
85	Neutral			1.263	1.239	1.266	299.1	293.3	146.6	152.5	229.9
86	Neutral			1.488	1.481	1.49	287.8	277.3	158.1	129.6	220.4
87	Neutral			2.094	2.071	2.097	322.2	307.3	183.4	138.7	244.7
88	Base	7.6		1.778	2.251	2.396	429.4	404.4	271.9	157.5	328.5
89	Neutral			3.805	3.805	3.805	522.6	460.6	378.5	144.1	386.5
90	Neutral			2.067	2.067	2.067	444.9	390.5	309.6	135.3	324
91	Base	10.7		-1.319	-0.42	2.203	392.3	360.4	261.9	130.4	299
92	Neutral			2.496	2.496	2.496	349.5	359.3	233.6	115.9	267.8
93	Neutral			2.241	2.183	2.25	347.4	335.3	190.7	156.7	264.9
94	Base	9.5		0.11	1.002	2.687	399.5	443.3	269	130.4	308.5
95	Base	9		-0.846	0.049	1.924	403.1	376.4	250.1	153	307.9
96	Base	9.6		0.166	1.06	2.829	386.2	380.9	255.8	130.4	299.2
97	Base	10	6.2	-3.182	-2.274	0.308	529.5	470.5	341.5	188	399.5
98	Neutral			-0.141	-0.141	-0.141	358	344.4	212.6	145.5	268.5
99	Base	6.7	4.2	2.28	2.634	2.721	505.3	470	419.1	86.17	386.3
100	Neutral			-0.763	-0.763	-0.763	436	425.5	267.3	168.8	332.2
101	Base	7.9		1.369	2.177	2.837	458.7	417.5	308.8	149.9	344.5
102	Zwitterion	9	7.2	3.37	4.485	6.202	879.1	764.9	745.2	133.9	662.2
103	Base	10.3		-1.801	-0.901	1.98	478.7	478.4	353.8	124.9	375.4
104	Base	6.7	4.4	3.36	3.715	3.802	561.7	514	466.8	94.96	422.6
105	Base	11.9	10.4	-4.403	-3.503	-0.495	433.1	375.9	286.8	146.3	309.7
106	Base	8.5		0.583	1.456	2.619	397.7	378.4	267.2	130.4	304.8
107	Base	9		-0.106	0.779	2.175	426.2	390.5	287	139.2	323.5
108	Neutral	6.3	5.2	1.535	1.731	1.768	637.3	556.6	433.4	204	470.1
109	Base	9.2		-2.596	-1.699	0.335	347.9	266.3	255.4	92.48	241.5
110	Base	7.7		-0.01	0.81	1.524	225	230.1	186.5	38.46	172.9
111	Base	9.2		-0.789	0.108	2.151	354.7	265.4	299.3	55.34	245.7
112	Neutral	6.3		0.909	1.121	1.162	264.9	253.3	140.9	124	208.1
113	Base	6.9	3.4	2.912	3.595	3.942	445.1	404	419.6	25.48	339.4
114	Base	6.5		2.732	2.965	3.012	278.9	237.7	246.1	32.84	198.5
115	Base	9.3		-2.366	-1.475	0.696	296.2	225.3	213.4	82.87	203.6
116	Neutral			3.466	3.466	3.466	292.9	295.7	186.1	106.8	226.6
117	Base	9.3		-0.868	0.028	1.924	373.2	334.4	242.7	130.4	276.9

Cmpd ID	Ion Class	pKa Base 1	pKa Base 2	$LogD_{6.5}$	$LogD_{7.4}$	LogP	AREA	MW	NPSA	PSA	VOL
118	Base	7.1		-1.001	-0.357	-0.065	309.5	252.3	227.8	81.67	220.5
119	Base	9.3		0.543	1.439	3.351	436.2	341.4	371.7	64.51	312.8
120	Base	10.2		-0.524	0.375	3.131	387	307.4	340.2	46.76	275.8
121	Base	9.3		0.965	1.858	3.714	545	415.6	453.6	91.35	386.4
122	Base	7.8		1.376	2.141	2.655	433.6	374.5	316.6	117	316.5
123	Base	9.8		1.391	2.018	3.855	414.7	364.4	311.6	103.2	321.7
124	Quater			-3.712	-3.712	-3.712	428.5	332.5	378.9	49.62	297.9
125	Base	9.2		-1.397	-0.5	1.68	309.5	248.3	249.3	60.21	225.5
126	Base	7.5		1.611	2.309	2.682	268.2	187.3	267	1.175	182.7
127	Base	8.3		-0.464	0.416	1.684	316.9	265.3	243.6	73.3	231.8
128	Base	9.7		-0.639	0.256	2.131	369.7	346.4	239.3	130.4	284
129	Base	10.1		-0.12	0.778	3.071	392.3	360.4	261.9	130.4	298.2
130	Neutral			2.088	2.088	2.088	375.4	348.4	213.3	162.1	281
131	Base	9.5		-1.038	-0.141	1.988	372.2	334.4	228.4	143.8	277.2
132	Base	8.4		0.202	1.066	2.105	485.6	422.5	323.8	161.8	355.8
133	Base	10.7		-0.773	0.126	2.659	414.8	374.5	284.4	130.4	313.2
134	Base	9.8		-0.542	0.353	2.245	369.7	346.4	239.3	130.4	283.9
135	Base	7.8		0.439	1.272	2.062	425.7	390.5	272.7	153	325.5
136	Neutral			1.849	1.849	1.849	352.8	334.4	190.7	162.1	266.5
137	Neutral			1.653	1.653	1.653	352.8	334.4	190.7	162.1	266.5
138	Base	9.3		0.131	1.027	3.043	474.2	406.5	321.2	153	345.2
139	Base	9.1		-0.653	0.242	2.18	429.1	378.5	276.1	153	315.9
140	Neutral			0.433	0.433	0.433	290.1	273.3	131.8	158.3	213.4
141	Base	8.4		-0.503	0.359	1.386	440	394.5	264.4	175.6	325.4
142	Base	9.1		-0.379	0.518	2.534	451.7	392.5	298.7	153	330.5
143	Base	8.2		0.223	1.07	1.947	449.7	404.5	323.8	125.8	338.4
144	Neutral			3.805	3.805	3.805	522.6	460.6	378.5	144.1	386.5
145	Base	10.3		-0.649	0.251	3.163	414.8	374.5	284.4	130.4	310.4
146	Base	10.7		-1.319	-0.42	2.203	392.3	360.4	261.9	130.4	299
147	Neutral			2.92	2.92	2.92	469.3	440.5	298.1	171.2	357.4
148	Base	10		-0.876	0.023	2.567	415.8	374.5	298.7	117	313.5
149	Base	9.7		-0.117	0.777	2.656	392.3	360.4	261.9	130.4	297.9
150	Base	9.7		-0.117	0.777	2.656	392.3	360.4	261.9	130.4	297.9
151	Base	9.6		-0.475	0.419	2.247	374.6	364.4	244.2	130.4	290
152	Base	8.5		-0.556	0.311	1.387	372.2	334.4	228.4	143.8	276.4
153	Base	9.4		0.526	1.419	3.141	440.8	376.5	310.4	130.4	321
154	Base	10.3		-0.907	-0.008	2.925	413.9	374.5	270.1	143.8	312.7
155	Neutral			1.472	1.472	1.472	421.5	366.4	286.5	135	304.8
156	Neutral			0.368	0.368	0.368	380.6	358.4	235.1	145.5	283
157	Base	13.1		-5.438	-4.538	-1.016	182.8	129.2	93.08	89.74	117.5

Cmpd ID	Ion Class	pKa Base 1	pKa Base 2	$LogD_{6.5}$	$LogD_{7.4}$	LogP	AREA	MW	NPSA	PSA	VOL
158	Base	12.6		-3.058	-2.158	1.158	264	205.3	160.8	103.1	184.2
159	Quater			-1.121	-1.121	-1.121	403.5	392.5	345.1	58.42	317.4
160	Base	9.2		0.01	0.907	3.012	585.6	508	360.3	225.3	414
161	Base			2.383	2.383	2.383	373.4	328.8	194.3	179.1	259.1
162	Base	7.9		0.292	1.145	2.083	434.8	360.8	307.3	127.4	301.5
163	Base	7.7		4.08	4.821	5.275	494.4	518.8	348.6	145.7	351.4
164	Base	7		3.656	3.656	3.656	358.4	342.8	215.9	142.5	268
165	Base	7.4		0.845	1.492	1.788	426.7	380.8	285.2	141.5	308.2
166	Base			1.862	1.566	1.928	617.2	636.5	311.2	306	466.5
167	Base	7.5		2.591	3.211	3.476	458.6	449.7	303.7	154.9	339.5
168	Base	12.9		0.067	0.966	4.479	424.5	408.3	291.6	132.9	319.9
169	Base	7.8		1.643	2.386	2.954	513	464.6	397.7	115.2	389.9
170	Base	11		0.753	1.653	4.763	394.8	358.8	352.5	42.38	297.8
171	Base	10.4		-2.302	-1.404	1.089	471.7	445.9	320	151.7	349.6
172	Base	7.1		1.029	1.494	1.635	357	320.8	220.3	136.6	259.4
173	Neutral	3.7		2.209	2.21	2.21	364.5	298.4	310.6	53.9	262.8
174	Neutral			2.137	2.137	2.137	330.2	346.7	211.3	118.9	249.6
175	Quater			0.341	0.341	0.341	443.4	378.5	407.5	35.86	328.8
176	Quater			-0.028	-0.028	-0.028	443.6	330.5	416.6	27.06	305.8
177	Base	9.8	9.1	-0.628	1.119	4.313	661.2	563.2	562.1	99.1	483.9
178	Base	9.2	4.6	0.079	0.972	2.537	610.9	536.7	546.7	64.25	466
179	Base	8.4		2.673	3.452	4.007	407.9	315.5	379.7	28.24	292
180	Base	9.8	8.2	-1.252	0.455	3.746	526.5	482.1	419.6	106.8	399.9
181	Quater			-1.082	-1.082	-1.082	398.5	302.4	371.4	27.06	278.6
182	Base	9.7	8.7	-2.147	-0.421	2.956	486.7	415.6	379.9	106.8	362.2
183	Base	9.6		0.386	1.28	3.095	394.6	425.3	264.1	130.4	303.5
184	Quater			-1.77	-1.77	-1.77	439.6	346.4	393.7	45.9	309.3
185	Quater			0.346	0.346	0.346	443.6	330.5	416.6	27.06	300.4
186	Base	8.9	7.5	-0.433	1.099	2.85	583.6	516	458.8	124.8	432.7
187	Base	8.6	7.7	0.009	1.425	3.055	701.7	639.8	626.9	74.79	542
188	Base	7.7	3.1	3.512	4.041	4.223	596.7	549.7	533.3	63.38	466.7
189	Base	8.6		1.859	2.745	4.193	579.2	541.7	506.4	72.75	453.5
190	Quater			-0.525	-0.525	-0.525	457.1	378.6	430	27.06	329.6
191	Quater			-0.751	-0.751	-0.751	484.8	374.5	438.9	45.9	338.8
192	Quater			3.645	3.645	3.645	579.2	462.7	543.1	36.17	413.7
193	Base	8.1	3.6	0.621	1.379	1.874	552.6	536.1	437.9	114.7	425
194	Quater			-2.065	-2.065	-2.065	529.9	453.6	488.2	41.7	398.3
195	Base	4.1		3.308	3.309	3.309	511.7	451.9	311.2	200.5	368.8
196	Base	9		-0.469	0.421	1.999	476.7	412.5	410.7	66.01	355.7
197	Base	9.3		-0.422	0.473	2.418	564.8	475.6	465.2	99.58	417

Cmpd ID	Ion Class	pKa Base 1	pKa Base 2	$LogD_{6.5}$	$LogD_{7.4}$	LogP	AREA	MW	NPSA	PSA	VOL
198	Base	9.8	6.4	-1.559	-0.288	2.307	614.1	502.7	522.4	91.65	450.6
199	Base	9.7		-1.07	-0.172	2.096	494.9	409	402.4	92.54	354.9
200	Base	8.1	3.6	0.428	1.187	1.682	645.8	621.2	521.4	124.4	497
201	Base	8.1	3.6	1.171	1.929	2.424	581.9	560.1	467.2	114.7	446.8
202	Base	8.1	5.3	-1.11	-0.331	0.168	647.9	601.8	513.2	134.6	493.9
203	Base	7.8		2.396	2.948	3.149	582.6	578.1	459.4	123.2	454.9
204	Base	10.6		-0.042	0.857	4.013	447.9	418.3	363.4	84.48	334.8
205	Base	9.9		-0.345	0.553	3.016	631.2	594.2	507.9	123.2	478.2
206	Base	9.1	6.9	0.873	1.811	3.07	491.4	476.4	373.2	118.2	375.6
207	Base	9.5	4.2	0.949	1.835	3.273	462	445.4	376.7	85.35	353.8
208	Base	9.5	3.6	1.132	2.018	3.456	460.7	464.9	362	98.75	355.5
209	Base	3.5		4.238	4.239	4.239	559.8	539.4	267.3	292.5	412.9
210	Base	7.8	4.8	1.718	2.275	2.476	573.3	542.7	448.6	124.7	443.1
211	Base	9.5	8.5	-0.133	1.579	4.413	585.5	441.6	494.8	90.67	409.4
212	Neutral			1.354	1.342	1.355	303.5	268.3	237.6	65.82	223.6
213	Base	9.8		-0.838	0.058	1.973	451.1	426.5	307	144.2	351
214	Base	9.8		-0.86	0.036	1.947	496.2	454.6	352.1	144.2	381.2
215	Base	9.7		-0.398	0.497	2.397	469.3	441.5	315.6	153.8	363.9
216	Base	8.8		1.42	2.303	3.663	630.8	606.2	507.6	123.2	482.3
217	Base	8.1		1.453	2.283	3.05	633.3	594.2	496.7	136.6	475.6
218	Base	9.8		-0.102	0.793	2.731	392.3	360.4	261.9	130.4	299
219	Base	9.7		-2.08	-1.185	0.696	493.1	447.5	334.1	159	369.4
220	Base	9.6		-0.589	0.306	2.136	408.4	414.4	277.9	130.4	316.5
221	Base	9.9	9.5	-0.288	0.602	2.37	462.2	438.5	308.9	153.3	360
222	Base	9.6		0.207	1.1	2.884	386.2	380.9	255.8	130.4	299.5
223	Base	9.7		-1.085	-0.19	1.707	503.8	445.5	353.9	149.9	372.8
224	Base	9.7		-2.217	-1.322	0.553	511.6	484.5	342.4	169.1	394.3
225	Base	9.8		-0.817	0.079	1.995	473.7	440.5	329.5	144.2	366.3
226	Base	9.5		-0.376	0.517	2.237	495.8	461.5	346.6	149.1	384.9
227	Base	9.4		-1.049	-0.159	1.453	570.3	535.6	411.6	158.7	442.4
228	Base	9.7	9.4	-2.816	-1.03	2.509	544.1	507.6	390	154.1	423.4
229	Base	9.7		-1.512	-0.617	1.265	446.1	419.5	260.4	185.8	339.5
230	Base	9.7	5.7	-1.016	-0.067	1.832	481.2	453.5	331.4	149.8	372.1
231	Base	9.7		-1.694	-0.799	1.091	442.8	424.5	291.8	150.9	345.1
232	Base	9.9	9.5	-0.106	0.785	2.553	462.2	438.5	308.9	153.3	359.5
233	Base	9.4		-0.575	0.316	1.941	379.5	382.4	249.1	130.4	296.7
234	Zwitterion	9.8		-1.118	-1.122	1.383	406.3	390.4	235	171.3	313.1
235	Base	9.8		-1.004	-0.124	1.784	381.1	362.4	227.8	153.3	293.5
236	Base	10		0.691	1.588	3.824	408.8	394.9	278.3	130.4	313.7
237	Base	8.9	3.2	-0.009	0.851	1.855	270	224.3	231.8	38.21	202.5

Cmpd ID	Ion Class	pKa Base 1	pKa Base 2	$LogD_{6.5}$	$LogD_{7.4}$	LogP	AREA	MW	NPSA	PSA	VOL
238	Base	7.8		2.294	2.847	3.047	553.6	577.1	426.6	127	440.2
239	Base	9.8		-0.888	0.007	1.918	473.7	440.5	329.5	144.2	366.2
240	Base	9.7	3.5	-0.723	0.172	2.072	431.8	429.5	291.3	140.5	345.2
241	Base	9.8	3.2	-0.439	0.457	2.37	472.8	440.5	315.2	157.6	366
242	Base	9.7	3.4	0.059	0.954	2.854	478.5	457.6	337.8	140.7	374.7
243	Base	9.6	5.8	-0.891	0.072	1.934	270	224.3	231.8	38.21	204
244	Base	9.7		-1.782	-0.887	1.017	424.2	413.5	270.5	153.8	333.5
245	Base	10.1		-0.087	0.811	3.076	430.9	428.4	300.5	130.4	330.7
246	Base	9.4	7.8	0.525	1.884	3.775	732	615.8	612.2	119.8	543.4
247	Base	8.3	4.8	-0.011	0.714	1.135	292	227.3	243.5	48.46	204.3
248	Base	8.7	4.9	0.177	1.047	2.158	300.9	244.3	262.7	38.21	213
249	Base	8.2		0.882	1.744	2.757	498	474	411.5	86.47	382.6
250	Base	8.7	4.9	0.177	1.047	2.158	300.9	244.3	262.7	38.21	213
251	Base	8.4		0.518	1.376	2.351	397.1	413.3	253.3	143.8	296.3
252	Base	9.3		2.966	3.862	5.877	477.6	445	414.5	63.11	366.9
253	Base	8.1	3.3	1.073	1.815	2.271	492.8	446.5	447.7	45.16	380.5
254	Base	8.7		2.891	3.788	5.914	474.1	457	411	63.11	376.9
255	Base	8.5		1.959	2.819	3.81	541.3	492	488.8	52.47	409.8
256	Base	8.7		-0.552	0.324	1.627	367.6	329.4	309.4	58.2	274.3
257	Base	10		1.744	2.643	5.261	500.1	459	437	63.11	381.9
258	Base	9.3		0.526	1.384	2.363	466	402.5	380.8	85.26	354.1
259	Base	10.1		-0.979	-0.086	2.217	375.1	357.4	294.4	80.7	291.7
260	Base	9.9		1.424	2.323	4.871	529.9	476	486.3	43.68	399.9
261	Base	9.2	9.1	-1.246	0.515	3.843	976.7	819.1	829.7	147	717.8
262	Base	9.9		0.547	1.446	4.075	516.5	442	472.8	43.68	378.7
263	Base	7.9		3.029	3.776	4.243	512.7	480	469.1	43.68	392
264	Base	7.6		2.17	2.904	3.345	515.3	490	462.8	52.47	404.3
265	Base	9.2	8	-0.476	1.211	3.555	944.6	837.5	797.6	147	707.2
266	Base	10.1		-0.048	0.85	3.161	379.2	356.4	308.7	70.46	294.6
267	Base	10.7		-0.779	0.12	2.724	447.9	399.9	390.8	57.08	335.7
268	Base	9.9		0.237	1.136	3.756	518.4	433.6	445.7	72.62	385.1
269	Base	12.4		0.754	1.652	4.046	509.8	452.9	348.9	160.8	372.8
270	Base	6.9		1.118	1.435	1.516	457.5	437.5	363	94.42	357.9
271	Base	10.3		-0.238	0.661	3.069	390.6	372.5	329.2	61.35	304.2
272	Base	9.5		-1.233	-0.341	1.711	395.2	383.5	327.8	67.31	312.4
273	Base	11.6	10.1	0.414	1.314	4.001	470	423.9	323.8	146.3	346.8
274	Base	8.3	4.8	0.23	0.971	1.427	314.5	241.3	266.1	48.46	219
275	Base	11.2		2.397	3.204	3.861	486.7	438.9	326.2	160.5	357.3
276	Base	12.1	10.7	-3.189	-2.289	0.99	515.1	452	368.9	146.3	376
277	Base	7.1		1.481	1.95	2.093	379.5	334.8	242.9	136.6	273.7

Cmpd ID	Ion Class	pKa Base 1	pKa Base 2	$LogD_{6.5}$	$LogD_{7.4}$	LogP	AREA	MW	NPSA	PSA	VOL
278	Base	6.7		1.843	2.153	2.223	373.4	355.2	236.8	136.6	273.1
279	Quater			-0.15	-0.15	-0.15	451.4	389.5	335.6	115.9	328.9
280	Base	3.9		2.702	2.703	2.703	512	466.9	319.5	192.5	377.8
281	Base	4.2		4.793	4.795	4.795	486.5	458.4	340.2	146.3	362.3
282	Base	4.2		4.34	4.342	4.342	538.8	484	374.4	164.5	395
283	Base	8		2.547	3.351	3.993	557	517	378.5	178.5	418.6
284	Base	9.7		1.449	2.347	4.637	508.7	491.9	362.4	146.3	377.9
285	Quater			-0.15	-0.15	-0.15	451.4	389.5	335.6	115.9	328.9
286	Zwitterion	4.7		1.593	0.702	3.869	506.6	467.9	319.5	187.1	376.3
287	Base	3.4		2.619	2.619	2.62	529.7	503	317.9	211.7	396.5
288	Base	9.8		0.702	1.598	3.537	437.4	388.5	307	130.4	328.2
289	Neutral			1.653	1.653	1.653	538.6	532.5	436.2	102.4	412.6
290	Base	3.6		3.161	3.161	3.161	534.6	481	342.1	192.5	392.1
291	Base	3		3.078	3.077	3.079	552.2	517	340.5	211.7	410.9
292	Base	9.8		0.004	0.902	3.267	414.8	374.5	284.4	130.4	313.6
293	Zwitterion	4.4		2.043	1.147	4.327	529.1	481.9	342.1	187.1	390.6
294	Base	9.7		-0.482	0.416	2.671	430.9	428.4	300.5	130.4	331.2
295	Base	9.1		0.986	1.878	3.551	460.9	402.5	343.8	117	342.8
296	Base	7.9		1.136	1.912	2.46	521	468.9	342.5	178.5	381.9
297	Base			3.456	3.456	3.456	558.1	516	375.1	183	414.8
298	Base	9.1		0.123	1.017	2.829	448.8	404.5	309.5	139.2	338.6
299	Base	8.6		1.12	1.997	3.219	420.2	392.5	289.8	130.4	319.8
300	Base	12.3		0.419	1.319	4.549	569.1	519	394.8	174.2	424.2
301	Base	9.1		0.431	1.318	2.775	448.8	404.5	309.5	139.2	338.4
302	Base	4.5		3.12	3.124	3.124	557.1	495	364.6	192.5	406.5
303	Base	12.3	11.4	-5.685	-3.887	2.92	556.1	495	344.3	211.8	406.5
304	Base	9.7		-0.268	0.627	2.499	403	396.4	272.6	130.4	310.9
305	Base	4.2	3.6	4.072	4.073	4.074	798.8	731.6	440.6	358.2	579.8
306	Base	9.7		-1.68	-0.785	1.066	435.2	424.5	268	167.2	335.1
307	Base	9.7		-1.574	-0.676	1.601	457.8	438.5	290.6	167.2	349.9
308	Base	9.8		0.513	1.412	3.776	437.4	388.5	307	130.4	328.5
309	Base	9.8		-0.161	0.737	3.035	425.6	410.4	295.1	130.4	325.6
310	Base	10.8		-5.331	-4.431	-1.028	557.1	495	364.6	192.5	405.7
311	Base	9	8.2	-0.442	1.275	3.69	590	508.1	465.6	124.4	427.7
312	Base	12.6	8.4	-4.77	-3.003	3.218	593.7	510	404.9	188.8	425.3
313	Base	8.2	4	3.25	4.04	4.65	412	374	409	2.92	315
314	Base	9		2.51	3.39	4.89	335	284	334	1.75	249
315	Base	10.4		0.146	1.05	3.97	334	266	319	15.1	246
316	Base	6.9	3.4	2.89	3.57	3.92	467	438	442	25.5	357
317	Base	10.8		-1.29	-0.391	3	244	179	216	28	173

Cmpd ID	Ion Class	pKa Base 1	pKa Base 2	$LogD_{6.5}$	$LogD_{7.4}$	LogP	AREA	MW	NPSA	PSA	VOL
318	Base	9.5		2.02	2.92	4.94	374	315	372	1.75	273
319	Base	8.2		1.67	2.5	3.31	391	288	357	33.7	273
320	Base	7.9		0.4	1.16	1.7	291	267	244	46.9	229
321	Neutral	6.5		1.83	2.09	2.14	415	383	319	96.1	317
322	Neutral			0.052	0.052	0.052	304	267	158	145	216
323	Base	7.2		1.58	2.13	2.32	305	240	272	32.8	209
324	Base	11.1	10.5	-8.8	-5.21	6.2	824	583	748	76.5	568
325	Base			3.04	3.04	3.04	320	306	174	146	238
326	Base	5.5		1.75	1.78	1.79	657	585	525	132	491
327	Base	8.2		1.11	1.95	2.84	612	529	485	128	447
328	Base	7.5	3.9	0.302	0.973	1.3	526	472	370	156	394
329	Base	9.1		2.66	3.55	5.21	349	316	348	1.18	266
330	Base	8.3		-0.464	0.416	1.68	317	265	244	73.3	232
331	Neutral			4.27	4.27	4.27	482	478	388	93.7	378
332	Quater	4.4					624	538	561	63.1	468
333	Quater	4.4	4				647	552	584	63.1	478
334	Quater						632	565	570	62.2	481
335	Base	8.2		-0.408	0.44	1.33	604	506	483	121	438
336	Base	8.4	5.6	2.61	3.51	4.57	532	509	459	73	419
337	Quater						630	564	546	83.5	466
338	Base	9.6	4.1	1.44	2.34	4.28	736	682	630	107	572
339	Base	8.5	4.9	0.548	1.41	2.43	301	244	263	38.2	212
340	Neutral			1.86	1.86	1.86	297	265	190	107	221
341	Quater	6.2					612	514	452	160	444
342	Neutral			0.04	0.04	0.04	488	471	277	211	364
343	Neutral	6.3		-0.715	-0.541	-0.509	550	515	314	236	417
344	Neutral	6.3	6.1	-1.1	-0.906	-0.869	524	487	306	217	397
345	Quater	6.1					551	502	343	208	413
346	Quater						577	530	351	226	433
347	Base	9.7	4.3	3.68	4.58	6.6	797	682	682	115	596
348	Base	6.7		1.2	1.55	1.63	439	374	332	107	328
349	Base	10.3		-1.25	-0.355	2.53	437	435	358	78.6	346
350	Quater	5.2					665	572	470	194	486
351	Base	8.8					206	163	127	79.6	146
352	Base	8.9					297	237	185	111	209
353	Quater						403	316	294	109	265
354	Quater						658	542	531	127	461

Table S3. SMILES notation of test compounds.

Cmpd ID	SMILES
1	COc1cc(cc(c1OC)OC)Cc2cnc(nc2N)N
2	CC(C)NCC(COc1cccc2c1cccc2)O
3	COc1cc2c(cc1OCCCN3CCOCC3)c(ncn2)Nc4ccc(c(c4)Cl)F
4	CC[N+](C)(CC)CCOC(=O)C(c1ccccc1)(C2CCCCC2)O
5	CN1CCN(CC1)C2=Nc3cc(ccc3Nc4c2cccc4)Cl
6	c1(c(nc(c(n1)Cl)N)N)C(=O)NC(=N)N
7	C[N+]1(CCCC(C1)OC(=O)C(c2ccccc2)(c3ccccc3)O)C
8	CC[C@@H]1[C@@]([C@@H]([C@H](N(C[C@@H](C[C@@]([C@@H]([C@H]([C@@H]([C@H](C(=O)O1)C)O[C@H]2C[C@@]([C@H]([C@@H](O2)C)O)(C)OC)C)O[C@H]3[C@@H]([C@H](C[C@H](O3)C)N(C)C)O)(C)O)C)C)O)(C)O
9	c1cc(ccc1C(=O)CCCN2CCC(CC2)(c3ccc(cc3)Cl)O)F
10	CC(C)C(CCCN(C)CCc1ccc(c(c1)OC)OC)(C#N)c2ccc(c(c2)OC)OC
11	Cc1ccc(cc1Nc2nccc(n2)c3cccnc3)NC(=O)c4ccc(cc4)CN5CCN(CC5)C
12	CCN(CC)CCNC(=O)c1cc(c(cc1OC)N)Cl
13	CC(C)N(CCC(c1ccccc1)(c2ccccn2)C(=O)N)C(C)C
14	CC(C)(C)NCC(c1ccc(c(c1)CO)O)O
15	CN(C)CCCN1c2ccccc2CCc3c1cccc3
16	c1ccc(cc1)n2c(ccn2)NS(=O)(=O)c3ccc(cc3)N
17	CCCCc1c(c2ccccc2o1)C(=O)c3cc(c(c(c3)I)OCCN(CC)CC)I
18	CC(Cc1ccc(cc1)O)NCC(c2cc(cc(c2)O)O)O
19	CC(=O)O[C@@H]1[C@@H](Sc2ccccc2N(C1=O)CCN(C)C)c3ccc(cc3)OC
20	CN(C)C(=O)C(CCN1CCC(CC1)(c2ccc(cc2)Cl)O)(c3ccccc3)c4ccccc4
21	CCN(CC)CCNC(=O)c1ccc(cc1)N
22	c1ccc(cc1)CNC(=N)NC(=O)c2c(nc(c(n2)Cl)N)N
23	COc1ccc2c(c1)c(ccn2)[C@@H]([C@H]3C[C@@H]4CCN3C[C@@H]4C=C)O
24	CNC(=C[N+](=O)[O-])NCCSCc1ccc(o1)CN(C)C
25	CNS(=O)(=O)Cc1ccc2c(c1)c(c[nH]2)CCN(C)C
26	C[N+]12CCC(CC1)C(C2)OC(=O)C(c3ccccc3)(c4ccccc4)O
27	COc1cc2c(cc1OC)nc(nc2N)N3CCN(CC3)C(=O)C4CCCO4
28	CC(C)[C@H]1c2ccc(cc2CC[C@@]1(CCN(C)CCCc3[nH]c4ccccc4n3)OC(=O)COC)F
29	CN(C)C(=O)COC(=O)Cc1ccc(cc1)OC(=O)c2ccc(cc2)NC(=N)N
30	C[C@H](Cc1ccc(cc1)OC)NC[C@@H](c2ccc(c(c2)NC=O)O)O
31	c1cc(cnc1)C(=O)Nc2cc(cc3c2[nH]c4c3ccnc4)Cl
32	CCS(=O)(=O)c1ccc(cc1)c2cc(c(s2)NC(=O)N)C(=O)N
33	CC(=O)Nc1cc(c(cc1OC[C@](C)(CNC2CCN(CC2)Cc3ccc(cc3)Cl)O)O)Cl
34	c1cc(ccc1O)OC[C@@H](CNCCNC(=O)N2CCOCC2)O
35	c1cc(ccc1O)OC[C@H](CNCCNC(=O)N2CCOCC2)O
36	CC(C)NC[C@@H](COc1ccc(cc1)CC(=O)N)O

37	CN1[C@@H]2CC[C@H]1C[C@H](C2)OC(=O)C(CO)c3ccccc3
38	CN1C2C[C@@H](CC1CC2)OC(=O)C(c3ccccc3)CO
39	Cc1c(cc(c(=O)n1c2cccc(c2)C(F)(F)F)C(=O)NCc3ccc(cc3)S(=O)(=O)C)C(C)N4CCOCC4
40	CC(C)NC[C@H](COc1ccc(cc1)CC(=O)N)O
41	C[N+]1(CCC(C1)OC(=O)C(c2ccccc2)(C3CCCC3)O)C
42	CCc1cc2c(cc1CC)CC(C2)NC[C@@H](c3ccc(c4c3ccc(=O)[nH]4)O)O
43	c1ccc(c(c1)c2cc(c(s2)NC(=O)N)C(=O)N)O[C@H]3CCNC3
44	CC1(Cc2c(cccc2O1)CN3CCC4(CC3)CCN(CC4)C(=O)c5ccnc(c5)N)C
45	CNC(=C[N+](=O)[O-])NCCSCc1csc(n1)CN(C)C
46	C[N+]1([C@@H]2C[C@H](C[C@H]1[C@H]3[C@@H]2O3)OC(=O)C(c4cccs4)(c5cccs5)O)C
47	CN1[C@@H]2CC(C[C@H]1[C@H]3[C@@H]2O3)OC(=O)[C@H](CO)c4ccccc4
48	c1ccc(cc1)C2CCN(CC2)[C@@H]3CCCC[C@H]3O
49	CC[C@@H]([C@@H](c1ccc(c2c1ccc(=O)[nH]2)O)O)NC(C)C
50	c1cc(c(cc1C#N)c2cc(c(s2)NC(=O)N)C(=O)N)OC3CCNC3
51	c1ccc(c(c1)c2cc(c(s2)NC(=O)N)C(=O)N)OC3CNC3
52	c1cc(c(c(c1)OCC2CC2)c3cc(c4c(n3)NC(=O)OC4)[C@@H]5CCCNC5)O
53	c1ccc(c(c1)c2cc(c(s2)NC(=O)N)C(=O)N)OCCN
54	c1cc(cc(c1)OC2CCNC2)c3cc(c(s3)NC(=O)N)C(=O)N
55	c1cc(ccc1c2cc(c(s2)NC(=O)N)C(=O)N)OCCN
56	Cc1c(nc(c(=O)n1c2cccc(c2)C(F)(F)F)CCCN)c3ccnn3c4ccc(cc4)C#N
57	c1ccc(c(c1)c2cc(c(s2)NC(=O)N)C(=O)N)OCC(CNCCO)O
58	CC(C)NCC(COc1ccccc1c2cc(c(s2)NC(=O)N)C(=O)N)O
59	c1ccc(c(c1)c2cc(c(s2)NC(=O)N)C(=O)N)OCC(CNC3CCC3)O
60	c1ccc(c(c1)c2cc(c(s2)NC(=O)N)C(=O)N)OCC(CN)O
61	CNCC(COc1ccccc1c2cc(c(s2)NC(=O)N)C(=O)N)O
62	CC1CCN(CC1)CC(=O)N[C@H]2CC[C@H](CC2)n3c(=O)n(c4ncc(cc4c3=O)F)C5CCSCC5
63	COc1ccc(cc1)C(NCc2ccccc2)C(=O)N[C@H]3CC[C@H](CC3)n4c(=O)n(c5ncc(cc5c4=O)F)C6CCSCC6
64	C[N+]1(CCC(C1)Oc2ccccc2c3cc(c(s3)NC(=O)N)C(=O)N)C
65	c1ccc(c(c1)c2nc(c(s2)NC(=O)N)C(=O)N)OC3CCNC3
66	C[N+](C)(C)CC(COc1ccccc1c2cc(c(s2)NC(=O)N)C(=O)N)O
67	CNc1nccc(n1)c2cc3cc(ccc3[nH]2)C(=O)NC(CN(c4ccccc4)c5ccccn5)C(=O)OC
68	CC(CNC1CC1)(COc2ccccc2c3cc(c(s3)NC(=O)N)C(=O)N)O
69	c1ccc(c(c1)c2cc(c(s2)NC(=O)N)C(=O)N)OC[C@H](CNC3CC3)O
70	c1ccc(c(c1)c2nc(c(s2)NC(=O)N)C(=O)N)OCCN
71	COCCN1CC[C@@H](C1)Oc2ccccc2c3cc(c(s3)NC(=O)N)C(=O)N
72	CNc1nccc(n1)c2cc3cc(ccc3[nH]2)C(=O)NC(CN(c4ccccc4)c5ccccn5)C(=O)O
73	c1ccc(c(c1)c2cc3c(s2)c(cnc3N)C(=O)N)OC4CCNC4
74	C[N+]1(CCCC(C1)c2cc(nc(c2C#N)N)c3c(cccc3OCC4CC4)O)C
75	CC(C)NC(=O)Nc1nc(c(s1)NC(=O)N)C(=O)N
76	c1ccc(c(c1)c2nc(c(s2)NC(=O)N)C(=O)N)OCCCN

77	Cc1c(cc(c(=O)n1c2cccc(c2)C(F)(F)F)C(=O)NCCCN(C)C)c3ccnn3c4ccc(cc4)C#N
78	C[N+]1(CCCC(C1)c2cc(nc3c2COC(=O)N3)c4c(cccc4OCC5CC5)O)C
79	Cc1c(cc(c(=O)n1c2cccc(c2)C(F)(F)F)C(=O)NCCCNC(C)C)c3ccnn3c4ccc(cc4)C#N
80	CNC1CCN(CC1)Cc2c(ccc(c2)O)c3cc(ccc3)n4c(=O)n(c(=O)c5c4ncc(c5)F)[C@H]6CC[C@H](CC6)NC(=O)c7nc8n(c7)cc(cc8)F
81	c1cc(cc(c1)c2c(cc(cc2)O)CN3CCNCC3)n4c(=O)n(c(=O)c5c4ncc(c5)F)[C@H]6CC[C@H](CC6)NC(=O)c7nc8n(c7)cc(cc8)F
82	C[N+]1(CCCC(C1)c2cc(nc(c2C#N)N)c3c(cccc3OCC4CC4)O)C
83	C[N+]1(CCCC(C1)c2cc(nc(c2C#N)N)c3c(cccc3OCC4CC4)O)C
84	c1cnc2cc3c(cc2n1)C4CC3CNC4
85	c1cc(c(cc1O)O)c2cc(c(s2)NC(=O)N)C(=O)N
86	c1ccc(c(c1)c2cc(c(s2)C(=O)N)NC(=O)N)O
87	COc1ccc(c(c1)O)c2cc(c(s2)NC(=O)N)C(=O)N
88	COC(=O)[C@@H]1CC(CN1)Oc2ccccc2c3cc(c(s3)NC(=O)N)C(=O)N
89	CC(C)(C)OC(=O)N1CC[C@@H](C1)COc2ccccc2c3cc(c(s3)NC(=O)N)C(=O)N
90	CCN(CC)C(=O)c1ccc(c(c1)OC)c2cc(c(s2)NC(=O)N)C(=O)N
91	c1ccc(c(c1)c2cc(c(s2)NC(=O)N)C(=O)N)OC[C@H]3CCNC3
92	COc1cc(ccc1c2cc(c(s2)NC(=O)N)C(=O)N)C(F)(F)F
93	COC(=O)c1ccc(c(c1)O)c2cc(c(s2)NC(=O)N)C(=O)N
94	c1c(cc(c(c1c2cc(c(s2)NC(=O)N)C(=O)N)O[C@H]3CCNC3)Br)F
95	c1ccc(c(c1)c2cc(c(s2)NC(=O)N)C(=O)N)O[C@H]3C[C@H](NC3)CO
96	c1cc(c(cc1Cl)c2cc(c(s2)NC(=O)N)C(=O)N)O[C@H]3CCNC3
97	CCNC(=O)[C@@H]1[C@H]([C@H]([C@@H](O1)n2cnc3c2nc(nc3N)NCCc4ccc(cc4)CCN)O)O
98	CS(=O)(=O)N1CCC(=CC1)c2cc(c(s2)NC(=O)N)C(=O)N
99	CC1(CN([C@@H](CO1)C(=O)Nc2cc(cc3c2[nH]c4c3ccnc4)Cl)CC(=O)N5CCCC5)C
100	Cc1c(c(on1)C)S(=O)(=O)N2CCC(=CC2)c3cc(c(s3)NC(=O)N)C(=O)N
101	CN(C)C(=O)[C@@H]1C[C@@H](CN1)Oc2ccccc2c3cc(c(s3)NC(=O)N)C(=O)N
102	Cc1cc(c(cc1)O)C(=O)N[C@H]2CC[C@H](CC2)NC(=O)c3c(ncc(c3)F)Oc4cc(ccc4)c5c(cc(cc5)CN6C[C@@H](N[C@@H](C6)C)C)CN7CCOCC7
103	c1cc(cc(c1)n2c(c(cc(c2=O)C(=O)N)c3ccnn3c4ccc(cc4)C#N)CN)C(F)(F)F
104	C[C@@H]1CN(C[C@@H](O1)C)C(=O)CN2CC(OC[C@H]2C(=O)Nc3cc(cc4c3[nH]c5c4ccnc5)Cl)(C)C
105	Cc1ccccc1C[C@@H](CNC(=O)c2c(nc(c(n2)Cl)N)N)NC(=N)C
106	c1ccc(c(c1)c2cc(c(s2)NC(=O)N)C(=O)N)O[C@H]3C[C@H](NC3)CF
107	COC[C@@H]1C[C@@H](CN1)Oc2ccccc2c3cc(c(s3)NC(=O)N)C(=O)N
108	CCC(CC)Nc1c2c(nc(n1)NCCNC(=O)Nc3ccncc3)n(cn2)[C@H]4[C@@H]([C@@H]([C@H](O4)C(=O)NCC)O)O
109	CC(C)NCC(COc1ccc(cc1)CC(=O)N)O
110	c1cc(c(c(c1)Cl)N=C2NCCN2)Cl
111	CC(C)NCC(COc1ccccc1OCC=C)O
112	c1ccc(cc1)c2c(nc3c(n2)c(nc(n3)N)N)N
113	c1ccc2c(c1)N(c3cc(ccc3S2)Cl)CCCN4CCN(CC4)CCO

114	CNC1(CCCCC1=O)c2ccccc2Cl
115	CC(C)(C)NCC(c1cc(cc(c1)O)O)O
116	c1cc(ccc1c2cc(c(s2)NC(=O)N)C(=O)N)Cl
117	CNCCOc1ccccc1c2cc(c(s2)NC(=O)N)C(=O)N
118	Cc1c(nc[nH]1)CSCCN=C(NC)NC#N
119	CCCNCC(COc1ccccc1C(=O)CCc2ccccc2)O
120	COc1cc(c(c(c1)OC)C(=O)CCCN2CCCC2)OC
121	c1ccc(cc1)CCCCOCCCCCCNCC(c2ccc(c(c2)CO)O)O
122	CN(CCOc1ccccc1c2cc(c(s2)NC(=O)N)C(=O)N)CC=C
123	c1cc(c(c(c1)OCC2CC2)c3cc(c(c(n3)N)C#N)C4CCCNC4)O
124	CC(C)[N+]1([C@@H]2CC[C@H]1C[C@H](C2)OC(=O)C(CO)c3ccccc3)C
125	CC(C)NC[C@@H](COc1cccc2c1cc[nH]2)O
126	C[C@H](Cc1ccccc1)N(C)CC#C
127	CC(=O)O[C@H]1[C@@H](CN[C@H]1Cc2ccc(cc2)OC)O
128	c1ccc(c(c1)c2cc(c(s2)NC(=O)N)C(=O)N)O[C@@H]3CCNC3
129	c1ccc(c(c1)c2cc(c(s2)NC(=O)N)C(=O)N)OC3CCNCC3
130	CC(C(=O)N)Oc1ccccc1c2cc(c(s2)NC(=O)N)C(=O)N
131	c1ccc(c(c1)c2cc(c(s2)NC(=O)N)C(=O)N)OCCCN
132	CCOCCNCC(COc1ccccc1c2cc(c(s2)NC(=O)N)C(=O)N)O
133	c1ccc(c(c1)c2cc(c(s2)NC(=O)N)C(=O)N)OCC3CCCNC3
134	c1cc(ccc1c2cc(c(s2)NC(=O)N)C(=O)N)OC3CCNC3
135	c1ccc(c(c1)c2cc(c(s2)NC(=O)N)C(=O)N)OCC(CNC3CC3)O
136	c1cc(ccc1c2cc(c(s2)NC(=O)N)C(=O)N)OCC(=O)N
137	c1cc(cc(c1)OCC(=O)N)c2cc(c(s2)NC(=O)N)C(=O)N
138	CCC(C)NCC(COc1ccccc1c2cc(c(s2)NC(=O)N)C(=O)N)O
139	CCNCC(COc1ccccc1c2cc(c(s2)NC(=O)N)C(=O)N)O
140	CCOC(=O)Nc1nc(c(s1)NC(=O)N)C(=O)N
141	c1ccc(c(c1)c2cc(c(s2)NC(=O)N)C(=O)N)OC[C@H](CNCCO)O
142	CC(C)NC[C@@H](COc1ccccc1c2cc(c(s2)NC(=O)N)C(=O)N)O
143	COCCN1CC[C@H](C1)Oc2ccccc2c3cc(c(s3)NC(=O)N)C(=O)N
144	CC(C)(C)OC(=O)N1CC[C@H](C1)COc2ccccc2c3cc(c(s3)NC(=O)N)C(=O)N
145	c1ccc(c(c1)c2cc(c(s2)NC(=O)N)C(=O)N)OC3CCCNCC3
146	c1ccc(c(c1)c2cc(c(s2)NC(=O)N)C(=O)N)OC[C@@H]3CCNC3
147	c1ccc(cc1)COc2cc(ccc2c3cc(c(s3)NC(=O)N)C(=O)N)OCC(=O)N
148	CN1CCC(C1)COc2ccccc2c3cc(c(s3)NC(=O)N)C(=O)N
149	Cc1cccc(c1O[C@H]2CCNC2)c3cc(c(s3)NC(=O)N)C(=O)N
150	Cc1cccc(c1O[C@@H]2CCNC2)c3cc(c(s3)NC(=O)N)C(=O)N
151	c1cc(c(cc1F)c2cc(c(s2)NC(=O)N)C(=O)N)O[C@H]3CCNC3
152	C[C@H](COc1ccccc1c2cc(c(s2)NC(=O)N)C(=O)N)N
153	CC(C)NC(C)COc1ccccc1c2cc(c(s2)NC(=O)N)C(=O)N
154	c1cc(c(cc1)OC2CC[C@@H](CC2)N)c3sc(c(c3)C(=O)N)NC(=O)N

155	CC(C)(C)OC(=O)N1CCC(=CC1)c2cc(c(s2)NC(=O)N)C(=O)N
156	CCS(=O)(=O)N1CCC(=CC1)c2cc(c(s2)NC(=O)N)C(=O)N
157	CN(C)C(=N)NC(=N)N
158	c1ccc(cc1)CCNC(=N)NC(=N)N
159	C[N+]1([C@@H]2C[C@H](C[C@H]1[C@H]3[C@@H]2O3)OC(=O)C(c4cccs4)(c5cccs5)O)C
313	CN1CCN(CC1)CCCN2c3ccccc3Sc4c2cc(cc4)Cl
314	CC(CN1c2ccccc2Sc3c1cccc3)N(C)C
315	CNCCCN1c2ccccc2CCc3c1cccc3
316	c1ccc2c(c1)N(c3cc(ccc3S2)C(F)(F)F)CCCN4CCN(CC4)CCO
317	CC12CC3CC(C1)(CC(C3)(C2)N)C
318	CN(C)CCCN1c2ccccc2CCc3c1cc(cc3)Cl
319	CCCCN1CCCCC1C(=O)Nc2c(cccc2C)C
320	CN1CCc2cccc-3c2C1Cc4c3c(c(cc4)O)O
321	COc1cc2c(cc1OC)nc(nc2N)N3CCN(CC3)C(=O)c4ccco4
322	Cc1cn(c(=O)[nH]c1=O)C2CC(C(O2)CO)N=[N+]=[N-]
323	CC(C(=O)c1cccc(c1)Cl)NC(C)(C)C
324	COc1ccccc1CNCCCCCCNCCCCCCCCNCCCCCCNCc2ccccc2OC
325	c1ccc(cc1)NC(=N)NC(=O)c2c(nc(c(n2)Cl)N)N
326	CCN1C[C@@]2(CCC(C34[C@@H]1C(CC23)[C@]5(C[C@@H]([C@H]6CC4[C@@]5(C6OC)O)OC)O)OC)OC(=O)c7ccccc7NC(=O)C
327	CC(C)(C(=O)N[C@H](COCc1ccccc1)C(=O)N2CCC3(CC2)CN(c4c3cccc4)S(=O)(=O)C)N
328	CN(C)c1c2c(ncn1)n(cn2)[C@H]3[C@@H]([C@@H]([C@H](O3)CO)NC(=O)[C@H](Cc4ccc(cc4)OC)N)O
329	CN(C)CC/C=C\1/c2ccccc2Sc3c1cc(cc3)Cl
330	CC(=O)O[C@@H]1[C@H](CN[C@@H]1Cc2ccc(cc2)OC)O
331	Cc1c(nc(c(=O)n1c2cccc(c2)C(F)(F)F)C(=O)NC)c3ccnn3c4ccc(cc4)C#N
335	CC(C)(C(=O)N[C@H](COCc1ccccc1)C(=O)N2CCC3=NN(C(=O)[C@@]3(C2)Cc4ccccc4)C)N
336	c1cc2n(cc(n2)CN[C@H]3CC[C@H](CC3)n4c(=O)n(c5ncc(cc5c4=O)F)C6CCSCC6)cc1
337	Cc1c(cc(c(=O)n1c2cccc(c2)C(F)(F)F)C(=O)NCCC[N+](C)(C)C)c3ccnn3c4ccc(cc4)C#N
338	Cc1scc(n1)C(=O)N[C@H]2CC[C@H](CC2)n3c(=O)n(c4ncc(cc4c3=O)F)c5cc(ccc5)c6ccc(cc6)CCCN7CCNCC7
339	CC(C)(c1ccccn1)C(c2ccccc2F)N
340	c1c(c(sc1C2=CCCCC2)NC(=O)N)C(=O)N
341	CCNC(=O)[C@@H]1[C@H]([C@H]([C@@H](O1)n2cnc3c2nc(nc3N)NCCc4ccc(cc4)CC[N+](C)(C)C)O)O
342	CC[C@@]1(C(=O)NC(=O)N1)CS(=O)(=O)N2CCC(=CC2)c3cc(c(s3)NC(=O)N)C(=O)N
343	CCNC(=O)[C@@H]1[C@H]([C@H]([C@@H](O1)n2cnc3c2nc(nc3N)C(=O)NCCNC(=O)Nc4ccncc4)O)O
344	CCNC(=O)[C@@H]1[C@H]([C@H]([C@@H](O1)n2cnc3c2nc(nc3N)NCCNC(=O)Nc4ccncc4)O)O
345	CCNC(=O)[C@@H]1[C@H]([C@H]([C@@H](O1)n2cnc3c2nc(nc3N)NCCNC(=O)Nc4cc[n+](cc4)C)O)O

346	CCNC(=O)[C@@H]1[C@H]([C@H]([C@@H](O1)n2cnc3c2nc(nc3N)C(=O)NCCNC(=O)Nc4cc[n+](cc4)C)O)O
347	Cc1n(nc(c1)C(=O)N[C@H]2CC[C@H](CC2)NC(=O)c3c(ncc(c3)F)Oc4cc(ccc4)c5ccc(cc5)CCCN6C[C@@H](N[C@@H](C6)C)C)C
348	c1cc(ccc1C[C@@H](C#N)NC(=O)C2(CCOCC2)N)c3ccc(cc3)C#N
349	c1cc(cc(c1)n2c(=O)ccc(c2CN)c3ccnn3c4ccc(cc4)C#N)C(F)(F)F
350	CCC(CC)Nc1c2c(nc(n1)NCCNC(=O)Nc3cc[n+](cc3)C)n(cn2)[C@H]4[C@@H]([C@@H]([C@H](O4)C(=O)NCC)O)O
351	B1(c2ccccc2[C@H](O1)CN)O
352	B1(c2c(cccc2OCCCO)[C@H](O1)CN)O