

Table S1. The experimental compounds in this paper

N O.	Compounds	Experimental pKa	Predicted value	Set
1	nizatidine	6.59	6.120085934	Training
2	Benzocaine	2.5	2.366315561	Training
3	Thenyldiamine	8.9	9.0979836	Training
4	Tetracaine	8.52	8.099960067	Training
5	iso-Propylamine	10.6	10.86074354	Training
6	4-Methylpyridine	6	6.48831189	Training
7	tolterodine	9.8	9.317040813	Training
8	nadolol	9.67	10.00358564	Training
9	Prazosin	7	7.038356685	Training
10	Hydroquinine	9.1	9.327727352	Training
11	Chloroquine	10.6	10.79803548	Training
12	neo-Pentylamine	10.21	10.16416564	Training
13	alprenolol	9.6	9.114841045	Training
14	Alphaprodine	8.7	8.44958465	Training
15	oxycodone	8.53	8.275543384	Training
16	Thenyldiamine	8.9	9.366983616	Training
17	Trimipramine	9.4	9.724920331	Training
18	Codeine	8.1	8.247258918	Training
19	ranitidine	8.47	8.009762811	Training
20	Morphine	8.2	7.86320014	Training
21	Alprenolol	9.55	9.407277776	Training
22	Histamine	9.7	9.323388837	Training
23	Atenolol	9.6	9.225603291	Training
24	Dimethyl-sec-butylamine	10.4	10.84269492	Training

25	trimipramine	9.24	9.246298648	Trainin g
26	clomipramine	9.38	9.71405201	Trainin g
27	Ethylamine	10.9	11.32834788	Trainin g
28	Acyclovir	2.2	1.802964981	Trainin g
29	Niacine-	4.8	4.936141249	Trainin g
30	Cyclohexylamine	10.6	11.07925925	Trainin g
31	Lidocaine	7.92	8.312245133	Trainin g
32	n-Butylamine	10.8	10.70137758	Trainin g
33	di-iso-Propylamine	11.1	10.94549528	Trainin g
34	nicotine	8.1	8.37598679	Trainin g
35	Dimethyl-n-butylamine	10.02	9.766578946	Trainin g
36	Nafronyl	9.08	8.819472308	Trainin g
37	Triethylamine	11	11.49237478	Trainin g
38	n-Octylamine	10.7	10.29050288	Trainin g
39	Mechlorethamine	6.4	6.306773365	Trainin g
40	Hydroxyimidazo[2,3-a]isoindole	8.6	8.677161029	Trainin g
41	di-n-Butylamine	11.4	10.91955687	Trainin g
42	promethazine	9.1	9.572361149	Trainin g
43	Sotalol	9.3	9.309039671	Trainin g
44	Maprotiline	10.3	10.08650994	Trainin g
45	Clozapine+	3.9	3.778745	Trainin g
46	Triallylamine	8.31	8.470837793	Trainin g
47	p-Cl-amphetamine	9.9	9.546485177	Trainin g
48	tri-n-Butylamine	10.89	10.92575892	Trainin g
49	acebutolol	9.67	9.590940191	Trainin g
50	Histamine	9.7	9.360477429	Trainin g

51	quinidine	8.05	7.753187799	Trainin g
52	atenolol	9.6	9.140437593	Trainin g
53	Labetalol	7.32	7.209246051	Trainin g
54	Phenylalanine-	8.9	9.08746508	Trainin g
55	labetalol	9.4	9.512022076	Trainin g
56	sufentanil	7.85	7.483078905	Trainin g
57	fentanyl	8.43	8.338254926	Trainin g
58	Methylguanidine	13.4	13.54924866	Trainin g
59	sumatriptan	9.5	9.181140695	Trainin g
60	remoxipride	8.9	8.760906135	Trainin g
61	propafenone	9.27	9.023265927	Trainin g
62	sec-Butylamine	10.56	11.0499904	Trainin g
63	Sotalol	9.31	8.850471696	Trainin g
64	azithromycin	8.74	8.735656245	Trainin g
65	Hydroquinine	4.06	4.414330368	Trainin g
66	2,5-Diazahehexane	10.4	10.17268837	Trainin g
67	4-Methoxyaniline	5.2	5.278058211	Trainin g
68	Metaproterenol	9.9	9.855246678	Trainin g
69	sotalol	9.76	10.08122272	Trainin g
70	tacrine	9.8	9.969584538	Trainin g
71	Acyclovir	2.18	2.620120189	Trainin g
72	Desipramine	10.34	9.931594463	Trainin g
73	Betahistine+	3.9	3.513390303	Trainin g
74	Maprotiline	10.29	10.2012957	Trainin g
75	Tolazoline	10.3	9.854250699	Trainin g
76	p-Toluidine	5.1	5.432850487	Trainin g

77	Azetidine	11.3	11.333975	Trainin g
78	Quinine	8.5	8.689438648	Trainin g
79	clozapine	7.63	7.152286738	Trainin g
80	Nefopam	8.5	8.694999394	Trainin g
81	Imidazo[2,3-b]thioxazole	8	8.489021964	Trainin g
82	codeine	8.2	8.203630158	Trainin g
83	Dimethyl-iso-propylamine	10.3	10.51028986	Trainin g
84	4-Aminopyridine	9.23	9.364127387	Trainin g
85	Alphaprodine	8.7	9.0870573	Trainin g
86	mirtazapine	7.3	6.907096406	Trainin g
87	Clomipramine	9.4	9.127863469	Trainin g
88	Acebutolol	9.5	9.068828431	Trainin g
89	Dimethyl-iso-butylamine	9.91	9.921690329	Trainin g
90	Clozapine	3.85	3.867800534	Trainin g
91	amitriptyline	9.4	9.732196648	Trainin g
92	haloperidol	8.65	8.947201431	Trainin g
93	Pyrazine	0.7	0.696615832	Trainin g
94	bisoprolol	9.57	9.178494263	Trainin g
95	2-Methylimidazole	8	7.635312355	Trainin g
96	Piroxicam	5.25	5.061091669	Trainin g
97	nortriptyline	10.1	10.02847124	Trainin g
98	2-Aminoethanol	9.5	9.652918496	Trainin g
99	desipramine	10.23	10.59095782	Trainin g
100	Tryptophan-	9.1	9.145330482	Trainin g
101	Dimethylamine	10.7	10.20731844	Trainin g
102	risperidone	8.3	8.550791092	Trainin g

103	Sparteine	12	11.55961121	Trainin g
104	diphenhydramine	9.1	8.910158363	Trainin g
105	Cimetidine	6.8	6.52426336	Trainin g
106	1-Allylpiperidine	9.7	9.388773896	Trainin g
107	Dimethylethylamine	10.2	10.31050722	Trainin g
108	Desipramine	10.3	10.49829283	Trainin g
109	Niacine	1.61	1.659472654	Trainin g
110	2-Aminothiazole	5.4	5.674858561	Trainin g
111	2-Methylbenzylamine	9.44	9.598862281	Trainin g
112	Metaproterenol	9.91	10.02187883	Trainin g
113	Morphine	9.3	9.072697763	Trainin g
114	di-sec-Butylamine	11.01	10.69902101	Trainin g
115	Dimethyl-n-propylamine	9.99	10.42709294	Trainin g
116	Nikethamide	3.5	3.814268405	Trainin g
117	4-Chloroaniline	4	3.54571264	Trainin g
118	Aniline	4.6	4.228167719	Trainin g
119	Quinoline	4.8	4.430787315	Trainin g
120	Phenacaine	9.3	9.629936555	Trainin g
121	ergotamine	6.3	5.837484689	Trainin g
122	diltiazem	8.06	8.120602629	Trainin g
123	2-Aminopyridine	6.71	6.681428668	Trainin g
124	Clotrimazole	5.75	6.079250061	Trainin g
125	Nicotine	8.07	8.048352005	Trainin g
126	Trazodone	6.78	7.112764529	Trainin g
127	domperidone	7.9	7.522258487	Trainin g
128	2-Aminopyridine	6.71	6.426793161	Trainin g

129	Nicotine	3.24	2.848592118	Trainin g
130	Imipramine	9.6	10.0031399	Trainin g
131	chlorpromazine	9.25	9.017683499	Trainin g
132	tert-Butylcyclohexylamine	11.23	11.30743502	Trainin g
133	procainamide	9.24	9.576729208	Trainin g
134	rivastigmine	8.99	9.045805802	Trainin g
135	1-Methylpiperidine	10.2	10.17574278	Trainin g
136	Acebutolol	9.48	9.922037815	Trainin g
137	metoprolol	9.7	9.376886901	Trainin g
138	Trimipramine	9.39	9.68239991	Trainin g
139	Debrisoquin	11.9	11.9363046	Trainin g
140	n-Hexylamine	10.6	10.43667682	Trainin g
141	DABCO	8.2	8.47914402	Trainin g
142	Cefadroxil-	7	7.308835442	Trainin g
143	amantadine	10.68	11.05880007	Trainin g
144	Dimethylbenzylamine	9	9.050014962	Trainin g
145	Tryptophan	9.1	8.91866225	Trainin g
146	Codeine	8.09	8.165839325	Trainin g
147	Cefadroxil	6.96	7.350769688	Trainin g
148	Nikethamide	3.5	3.694386452	Trainin g
149	atomoxetine	10.1	10.31752889	Trainin g
150	promazine	9.28	9.723908643	Trainin g
151	betaxolol	9.21	9.231515047	Trainin g
152	Hydroquinine+	4.1	4.153245016	Trainin g
153	Dimethylcyclohexylamine	10.7	10.41696822	Trainin g
154	Melamine	5	4.632289058	Trainin g

155	Pyrimidine	1.3	1.695031021	Trainin g
156	tert-Butylamine	10.7	10.77731937	Trainin g
157	paroxetine	9.51	9.414001035	Trainin g
158	Guanethidine	11.4	10.96312178	Trainin g
159	3-Aminopyridine	6	6.456651021	Trainin g
160	Clomipramine	9.42	9.548016159	Trainin g
161	1,2-Ethanediamine	10.7	10.47014492	Trainin g
162	Nicotine+	3.2	3.2511895	Trainin g
163	Propanolol	9.61	9.361150984	Trainin g
164	Hexamethylenetetramine	5.3	5.042370754	Trainin g
165	Hydroquinine	9.13	9.191551428	Trainin g
166	verapamil	8.92	8.599958508	Trainin g
167	3-Hydro-2-methylamine-4-oxy-5-phenyl-1,4-benzodia zepine	4.8	4.550880406	Trainin g
168	Pyridine	5.14	5.26453443	Trainin g
169	citalopram	9.38	9.724543146	Trainin g
170	Betahistine	9.97	10.39542704	Trainin g
171	Trazodone	6.8	6.694240416	Trainin g
172	1,3-Dihydro-3-hydroxy-5-phenyl-1,4-benzodiazepin-2 -one	1.7	1.653207627	Trainin g
173	flecainide	9.3	9.348614749	Trainin g
174	2,3-Dihydro-1-methyl-5-phenyl-1,4-benzodiazepine	6.2	6.445006495	Trainin g
175	Tetrahydrozoline	10.5	10.24086462	Trainin g
176	venlafaxine	9.5	9.236568483	Trainin g
177	Cysteamine	10.5	10.92438706	Trainin g
178	Betahistine	10	9.610581356	Trainin g
179	Guanidine	13.8	14.03545797	Trainin g
180	atropine	9.84	9.584098904	Trainin g

181	p-Chloroamphetamine	9.85	9.415610403	Trainin g
182	galanthamine	8.32	7.878941803	Trainin g
183	di-n-Propylamine	11	11.33139802	Trainin g
184	Atenolol	9.56	9.419741688	Trainin g
185	Labetalol	7.3	7.046567559	Trainin g
186	meperidine	8.7	8.550577544	Trainin g
187	Benzylamine	9.45	9.777337062	Trainin g
188	Procaine	9.11	8.985408246	Trainin g
189	levomepromazine	9.19	9.488904673	Validati on
190	butorphanol	8.19	8.093927365	Validati on
191	Cimetidine0	6.8	6.716743512	Validati on
192	timolol	8.8	8.53537014	Validati on
193	Tetracaine	8.5	8.642948851	Validati on
194	naloxone	7.94	8.214306586	Validati on
195	Prazosin	6.95	6.732828501	Validati on
196	Betahistine	3.9	4.086521041	Validati on
197	lidocaine	7.94	7.680925256	Validati on
198	Alprenolol	9.6	9.278406383	Validati on
199	trazodone	6.79	6.94072087	Validati on
200	1,3-Propanediamine	10.9	10.80828903	Validati on
201	Methylamine	10.62	10.72637075	Validati on
202	Clonidine	8.1	8.137667449	Validati on
203	Nafronyl	9.1	8.943271279	Validati on
204	chlorpheniramine	9.26	9.15324288	Validati on
205	Clotrimazole	5.8	5.471639648	Validati on
206	n-Heptylamine	10.7	10.58066772	Validati on

207	Phenylalanine	8.86	8.666829967	Validati on
208	Nefopam	8.46	8.509525679	Validati on
209	Nicotine	8.1	7.912762291	Validati on
210	nefazodone	6.5	6.320356184	Validati on
211	Benzimidazole	5.8	5.801108436	Validati on
212	pindolol	9.54	9.61485833	Validati on
213	Chloroquine	10.6	10.76416876	Validati on
214	morphine	8.18	8.168186114	Validati on
215	Metoprolol	9.56	9.362202915	Validati on
216	1,3-Dihydro-3-hydroxy-1-methyl-5-phenyl-1,4-benzodiazepin-2-one	1.6	1.487172182	Validati on
217	Diethylbenzylamine	9.5	9.384601592	Validati on
218	Imidazole	7	6.962247874	Validati on
219	Quinine	8.48	8.228383122	Validati on
220	Trimethylamine	9.76	9.814235157	Validati on
221	4-Aminopyridine	9.23	8.906241603	Validati on
222	Miconazole	6.4	6.30729538	Validati on
223	imipramine	9.45	9.235704306	Validati on
224	Thiazole	2.8	2.762324772	Validati on
225	Benzocaine	2.5	2.393569452	Validati on
226	4-Nitroaniline	1	1.040379684	Validati on
227	Procaine	9.1	9.08249151	Validati on
228	quinacrine	10.2	10.12179838	Validati on
229	1,3-Dihydro-5-phenyl-1,4-benzodiazepin-2-one	3.5	3.644502008	Testing
230	azelastine	9.54	9.409754804	Testing
231	nebivolol	8.22	8.381397656	Testing
232	Piroxicam	5.3	5.681813605	Testing
233	Mechlorethamine	6.4	6.986728392	Testing
234	Diethylamine	10.94	10.3812128	Testing
235	propranolol	9.45	9.961578351	Testing
236	maprotiline	10.5	10.9157707	Testing

237	Clozapine	7.52	7.201693551	Testing
238	Morpholine	8.5	9.149096828	Testing
239	Piperidine	11.1	11.03561659	Testing
240	Propylamine	10.7	10.05016009	Testing
241	Pyrazole	2.5	2.438155913	Testing
242	Isoquinoline	5.4	4.757253123	Testing
243	perphenazine	8.11	7.840279134	Testing
244	Clozapine	7.5	6.989216607	Testing
245	Procaine	2.02	1.988346301	Testing
246	Procaine+	2	2.388703277	Testing
247	Tripropylamine	10.7	10.78543458	Testing
248	Pyrrolidine	11.3	10.93058874	Testing
249	Metoprolol	9.6	9.543115315	Testing
250	Propanolol	9.6	9.664149803	Testing
251	clonidine	8.05	7.700048014	Testing
252	Miconazole	6.39	6.916545728	Testing
253	Lidocaine	7.9	7.843477842	Testing
254	terbutaline	10	9.546586943	Testing
255	di-iso-Butylamine	10.5	11.05044333	Testing
256	tolamolol	7.9	7.64752115	Testing
257	Phenacaine	9.3	9.730906656	Testing
258	cocaine	8.7	8.635598058	Testing
259	Sparteine	12	11.47364193	Testing
260	Imipramine	9.56	10.02136211	Testing
261	Papaverine	6.4	6.449877696	Testing
262	n-Pentylamine	10.6	9.955601179	Testing
263	Dimethyl-tert-butylamine	10.52	10.10918683	Testing
264	Guanethidine	11.4	10.80487942	Testing
265	Papaverine	6.4	6.037542121	Testing
266	1,3-Dihydro-1-methyl-5-phenyl-1,4-benzodiazepin-2-one	3.3	3.896732424	Testing
267	mexiletine	9.15	8.902120603	Testing
268	cimetidine	6.97	7.114604361	Testing
