

Supplementary Material

Computational Prediction of Blood-Brain Barrier Permeability Using Decision Tree Induction

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Appendix Table 1. Dataset (n = 153) of SMILES structural descriptors, blood-brain barrier LogPS values, classification and references.

Number	SMILES	LogPS	Classification	Reference [PMID]
1	<chem>C[C@H]1[C@H]([C@H](C[C@@H](O1)O[C@H]2C[C@@](CC3=C(C4=C(C(=C23)O)C(=O)C5=C(C4=O)C=CC=C5OC)O)(C(=O)CO)O)N)O</chem>	-5.7	CNSp-	18481317
2	<chem>C([C@@H]1[C@H]([C@@H]([C@H]([C@H](O1)O[C@]2([C@H]([C@@H]([C@H](O2)CO)O)CO)O)O)O)O</chem>	-5.3	CNSp-	9466345
3	<chem>C([C@H]([C@H]([C@@H]([C@@H](CO)O)O)O)O)O</chem>	-5.0	CNSp-	9466345
4	<chem>CC1=C2[C@H](C(=O)[C@@]3([C@H](C[C@@H]4[C@]([C@H]3[C@@H]([C@@](C2(C)C)(C[C@@H]1OC(=O)[C@H]([C@H](C5=CC=CC=C5)NC(=O)C6=CC=CC=C6)O)OC(=O)C7=CC=CC=C7)(CO4)OC(=O)C)O)C)OC(=O)COC1=CC(=CC(=C1OC)OC)[C@H]2[C@@H]3[C@H](COC3=O)[C@@H](C4=CC5=C(C=C24)OCO5)O</chem>	-4.7	CNSp-	18481317
5	<chem>CNS(=O)(=O)CC1=CC2=C(C=C1)NC=C2CCN(C)C</chem>	-4.6	CNSp-	17405866
7	<chem>C([C@H]([C@H](CO)O)O)O</chem>	-4.6	CNSp-	9466345
8	<chem>CN1CC(=O)N=C1N</chem>	-4.6	CNSp-	7392035
9	<chem>C1C[C@@H](O[C@@H]1CO)N2C=NC3=C2NC=NC3=O</chem>	-4.5	CNSp-	18481317
10	<chem>C1=CC(=C(C(=C1)O)N)C(=O)CC(C(=O)O)N</chem>	-4.5	CNSp-	19591936
11	<chem>CC(C)[C@@H](C(=O)O)N</chem>	-4.4	CNSp-	3468857

Appendix Table 1. Cont.

Number	SMILES	LogPS	Classification	Reference [PMID]
12	<chem>C[C@@H]1[C@H]([C@H](C[C@@H](O1)O[C@@H]2[C@H](O[C@H](C[C@@H]2O)O[C@@H]3[C@H](O[C@H](C[C@@H]3O)O[C@H]4CC[C@]5([C@@H](C4)CC[C@@H]6[C@@H]5C[C@H]([C@]7([C@@]6(CC[C@@H]7C8=CC(=O)OC8)O)C)O)C)C)O)O</chem>	-4.3	CNSp-	14709630
13	<chem>C[C@@]1(C(=O)N2[C@H](C(=O)N3CC[C@H]3[C@@]2(O1)O)CC4=CC=CC=C4)NC(=O)[C@@H]5C[C@H]6[C@@H](CC7=CNC8=CC=CC6=C78)N(C5)C</chem>	-4.2	CNSp-	18481317
14	<chem>C1=CC=C(C(=C1)C(=O)C[C@@H](C(=O)O)N)N</chem>	-4.2	CNSp-	3819731
15	<chem>CC1=C(N=CN1)CSCCNC(=NC)NC#N</chem>	-4.1	CNSp-	10993764
16	<chem>C[C@H](CCC(=O)NCCS(=O)(=O)O)[C@@H]1CC[C@@H]2[C@@]1([C@H](C[C@H]3[C@H]2[C@@H](C[C@H]4[C@@]3(CC[C@H](C4)O)C)O)O)C</chem>	-4.1	CNSp-	14709630
17	<chem>CC(C)C[C@@H](C(=O)O)N</chem>	-4.1	CNSp-	3468857
18	<chem>C1CCC(CC1)(C(=O)O)N</chem>	-4.0	CNSp-	18481317
19	<chem>CC1=CN(C(=O)NC1=O)[C@H]2C[C@@H]([C@H](O2)CO)N=[N+]=[N-]</chem>	-4.0	CNSp-	9593963
20	<chem>C[N+](C)(C)CCO</chem>	-4.0	CNSp-	18481317
21	<chem>C1[C@H]2[C@@H]([C@@H](S1)CCC(CC(=O)O)NC(=O)N2</chem>	-4.0	CNSp-	18481317
22	<chem>C1=NC2=C(N1)C(=S)N=CN2</chem>	-4.0	CNSp-	18481317
23	<chem>CN(CC1=CN=C2C(=N1)C(=NC(=N2)N)N)C3=CC=C(C=C3)C(=O)N[C@@H](CC(=O)O)C(=O)O</chem>	-3.9	CNSp-	14709630
24	<chem>CCCN(CCC)S(=O)(=O)C1=CC=C(C=C1)C(=O)O</chem>	-3.9	CNSp-	18481317
25	<chem>CC1=CN(C(=O)NC1=O)[C@H]2C[C@@H]([C@H](O2)CO)O</chem>	-3.8	CNSp-	9593963
26	<chem>C1=NC2=C(N1)C(=O)NC(=O)N2</chem>	-3.8	CNSp-	14709630
27	<chem>C(C(=O)O)I</chem>	-3.8	CNSp-	18481317
28	<chem>CC1=C(C(=C(C2=C1N(C=C(C2=O)C(=O)O)C3CC3)N)F)N4C[C@H](C5(C4)CC5)N</chem>	-3.8	CNSp-	18481317
29	<chem>C(CC(=O)N)C(C(=O)O)N</chem>	-3.8	CNSp-	18481317
30	<chem>C(=O)(N)N</chem>	-3.8	CNSp-	9466345
31	<chem>CN(C)CCC1=CNC2=C1C=C(C=C2)CN3C=NC=N3</chem>	-3.8	CNSp-	17405866

Appendix Table 1. Cont.

32	<chem>CC1=C2[C@H](C(=O)[C@@]3([C@H](C[C@@H]4[C@]([C@H]3[C@@H]([C@@](C2(C)C)(C[C@@H]1OC(=O)[C@H]([C@H](C5=CC=CC=C5)NC(=O)C6=CC=CC=C6)O)OC(=O)C7=CC=CC=C7)(CO4)OC(=O)C)O)OC(=O)CCC(=O)O</chem>	−3.7	CNSp−	18481317
33	<chem>CC1CN(CCN1)C2=C(C(=C3C(=C2)N(C=C(C3=O)C(=O)O)C4CC4)C)F</chem>	−3.7	CNSp−	10991972
34	<chem>CC1([C@H](C(=O)NCC(=O)N[C@H](C(=O)N[C@H](C(SS1)(C)C)C(=O)O)CC2=CC=CC=C2)NC(=O)[C@H](CC3=CC=C(C=C3)O)N)C</chem>	−3.6	CNSp−	14709630
35	<chem>C(=N)(N)N</chem>	−3.6	CNSp−	18481317
36	<chem>CC[C@@]1(C[C@@H]2C[C@@](C3=C(CCN(C2)C1)C4=CC=CC=C4N3)(C5=C(C=C6C(=C5)[C@]78CCN9[C@H]7[C@@](C=CC9)([C@H]([C@@]([C@@H]8N6C)(C(=O)OC)O)OC(=O)C)CC)OC)C(=O)OC)O</chem>	−3.5	CNSp−	10993764
37	<chem>C1=CC(=C(C=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O)O)O</chem>	−3.5	CNSp−	14980703
38	<chem>C(C(=O)O)N</chem>	−3.5	CNSp−	14709630
39	<chem>C1=NC2=C(N1)C(=O)N=CN2</chem>	−3.5	CNSp−	14709630
40	<chem>C(C(=O)O)C(=O)O</chem>	−3.5	CNSp−	18481317
41	<chem>C1=CC=C(C=C1)C2C(=O)N=C(O2)N</chem>	−3.5	CNSp−	17405866
42	<chem>CC(C(=O)O)N</chem>	−3.4	CNSp−	10993764
43	<chem>COC1=CC2=C(C=CN=C2C=C1)[C@@H]([C@H]3CC4CCN3C[C@@H]4C=C)O</chem>	−3.4	CNSp−	14709630
44	<chem>C1=CC=C(C(=C1)C(=O)O)O</chem>	−3.4	CNSp−	14709630
45	<chem>C(=S)(N)N</chem>	−3.4	CNSp−	9466345
46	<chem>CC(=O)N[C@H]1CCC2=CC(=C(C(=C2C3=CC=C(C(=O)C=C13)OC)OC)OC)OC</chem>	−3.3	CNSp−	14709630
47	<chem>C1=CC(=CC=C1C[C@@H](C(=O)O)N)N(CCC1)CCC1</chem>	−3.3	CNSp−	3815357
48	<chem>C(CS(=O)(=O)O)N</chem>	−3.2	CNSp−	18481317
49	<chem>C1CCC(CC1)(CC(=O)O)CN</chem>	−3.2	CNSp−	18481317
50	<chem>CC[C@@]1(C[C@@H]2C[C@@](C3=C(CCN(C2)C1)C4=CC=CC=C4N3)(C5=C(C=C6C(=C5)[C@]78CCN9[C@H]7[C@@](C=CC9)([C@H]([C@@]([C@@H]8N6C(=O)(C(=O)OC)O)OC(=O)C)CC)OC)C(=O)OC)O</chem>	−3.1	CNSp−	18481317

Appendix Table 1. Cont.

51	<chem>C1CC(OC1)N2C=C(C(=O)NC2=O)F</chem>	−3.1	CNSp−	18481317
52	<chem>CCCC(C)(COC(=O)N)COC(=O)N</chem>	−3.1	CNSp−	17405866
53	<chem>CN1C=NC2=C1C(=O)NC(=O)N2C</chem>	−3.0	CNSp−	14709630
54	<chem>C1C2CC3CC1CC(C2)(C3)N</chem>	−3.0	CNSp−	18481317
55	<chem>CC1=C(SC=[N+])1CC2=CN=C(N=C2N)C)CCO</chem>	−3.0	CNSp−	18481317
56	<chem>C(CO)O</chem>	−2.9	exempt	9466345
57	<chem>COC1=CC=CC2=C1NC3=C(C2=O)CCC</chem>	−2.9	exempt	18481317
58	<chem>CC3</chem>	−2.9	exempt	18481317
59	<chem>COCC(CN1C=CN=C1[N+])(=O)[O-])O</chem>	−2.9	exempt	18481317
60	<chem>CN(CC[C@H](C1=CC=C(C=C1)F)OC2=</chem>	−2.9	exempt	14709630
61	<chem>CC=C(C=C2)C3=CC=CC=C3)CC(=O)O</chem>	−2.9	exempt	14709630
62	<chem>CN1C2=C(C(=O)N(C1=O)C)NC=N2</chem>	−2.9	exempt	14709630
63	<chem>CCCCC[C@@H](/C=C/[C@H]1[C@@H</chem>	−2.9	exempt	18481317
64	<chem>](C[C@@H])([C@@H]1C/C=C\CCCC(=</chem>	−2.9	exempt	18481317
65	<chem>O)O)O)O)O</chem>	−2.8	exempt	18481317
66	<chem>CCCCNC(=O)NS(=O)(=O)C1=CC=C(C=</chem>	−2.8	exempt	18481317
67	<chem>C1)C</chem>	−2.8	exempt	18481317
68	<chem>C1CC(=O)NC(=O)C1NC(=O)N(CCCl)N</chem>	−2.8	exempt	18481317
69	<chem>=O</chem>	−2.8	exempt	18481317
70	<chem>COC1=C(C=C(C=C1)Cl)C(=O)NCCC2=</chem>	−2.8	exempt	10993764
71	<chem>CC=C(C=C2)S(=O)(=O)NC(=O)NC3CC</chem>	−2.8	exempt	10993764
72	<chem>CCC3</chem>	−2.8	exempt	18481317
73	<chem>CO[C@H]1[C@@H]([C@H](OC([C@@</chem>	−2.8	exempt	18481317
74	<chem>H]1O)O)CO)O</chem>	−2.8	exempt	18481317
75	<chem>C[C@@H]1[C@H]2CC3=C([C@@]1(C</chem>	−2.8	exempt	18481317
76	<chem>CN2CC=C(C)C)C=C(C=C3)O</chem>	−2.7	exempt	18481317
77	<chem>CC1=NC=C(N1CCO)[N+](=O)[O-]</chem>	−2.7	exempt	18481317
78	<chem>C[C@H]1[C@H]([C@H](C[C@@H](O1</chem>	−2.7	exempt	14709630
79	<chem>)O[C@H]2C[C@@](CC3=C(C4=C(C(=C</chem>	−2.7	exempt	14709630
80	<chem>23)O)C(=O)C5=C(C4=O)C=CC=C5OC)</chem>	−2.7	exempt	14709630
81	<chem>O)(C(=O)C)O)N)O</chem>	−2.7	exempt	14709630
82	<chem>CN1CC[C@]23[C@@H]4[C@H]1CC5=</chem>	−2.7	exempt	14709630
83	<chem>C2C(=C(C=C5)O)O[C@H]3[C@H](C=C</chem>	−2.7	exempt	14709630
84	<chem>4)O</chem>	−2.7	exempt	17405866
85	<chem>C1=CC(=C(C(=C1)Cl)Cl)C2=C(N=C(N=</chem>	−2.7	exempt	17405866
86	<chem>N2)N)N</chem>	−2.7	exempt	17405866
87	<chem>CCN(CC)CCNC(=O)C1=CC(=C(C=C1O</chem>	−2.7	exempt	17405866
88	<chem>C)N)Cl</chem>	−2.7	exempt	17405866
89	<chem>C1=CC=C(C=C1)CCNN</chem>	−2.7	exempt	17405866
90	<chem>C1C(OC2=CC(=CC(=C2C1=O)O)O)C3=</chem>	−2.6	exempt	14980703
91	<chem>CC=C(C=C3)O</chem>	−2.6	exempt	14980703
92	<chem>CCCC(CCC)C(=O)O</chem>	−2.5	exempt	14709630
93	<chem>CN1C=C(C2=CC=CC=C21)C(=O)[C@</chem>	−2.5	exempt	18481317
94	<chem>@H]3CCC4=C(C3)NC=N4</chem>	−2.5	exempt	18481317

Appendix Table 1. Cont.

100	<chem>C1CN(CCN1CCCN2C3=CC=CC=C3SC4=CC=C(C=C4)C(F)(F)F)CCO</chem>	−1.9	CNSp+	17405866
101	<chem>CN1CCCCC1CCN2C3=CC=CC=C3SC4=CC=C(C=C4)S(=O)C</chem>	−1.8	CNSp+	17405866
102	<chem>CC1=C(C(=O)N2CCCCC2=N1)CCN3CC(C(CC3)C4=NOC5=C4C=CC(=C5)F</chem>	−1.8	CNSp+	17405866
103	<chem>CCC1=C(C(=NC(=N1)N)N)C2=CC(=C(C=C2)Cl)Cl</chem>	−1.8	CNSp+	18481317
104	<chem>C1=CC(=C(C=C1C[C@@H](C(=O)O)N)O)O</chem>	−1.8	CNSp+	14709630
105	<chem>CCCCCCCCC(=O)O</chem>	−1.8	CNSp+	18481317
106	<chem>CC(C1=CC(=C(C=C1)C2=CC=CC=C2)F)C(=O)O</chem>	−1.8	CNSp+	16715377
107	<chem>C1=CC=C2C(=C1)C=CC3=CC=CC=C3N2C(=O)N</chem>	−1.8	CNSp+	17405866
108	<chem>C1CN(CCN1CCC2=C(C=C3C(=C2)CC(=O)N3)Cl)C4=NSC5=CC=CC=C54</chem>	−1.7	CNSp+	17405866
109	<chem>CNC(=S)NC1=CC=CC=C1</chem>	−1.7	CNSp+	18481317
110	<chem>C1CC2([C@H]3CC4=C5[C@@]2(CCN3CC6CC6)[C@@H]([C@@H]1F)OC5=C(C=C4)O)O</chem>	−1.7	CNSp+	18481317
111	<chem>COC1=C(C=C2C(=C1O)C(=O)C=C(O2)C3=CC=C(C=C3)O)O</chem>	−1.7	CNSp+	18481317
112	<chem>CC(C)O</chem>	−1.7	CNSp+	9466345
113	<chem>CC1=C(N(N=C1C(=O)NN2CCCCC2)C3=C(C=C(C=C3)Cl)Cl)C4=CC=C(C=C4)Cl</chem>	−1.6	CNSp+	14709630
114	<chem>C1=CC(=CC=C1CCCC(=O)O)N(CCCl)CCl</chem>	−1.6	CNSp+	14709630
115	<chem>CC(CC1=CC=CC=C1)(C2=CC=CC=C2)N</chem>	−1.6	CNSp+	18481317
116	<chem>CC(C)CC1=CC=C(C=C1)C(C)C(=O)O</chem>	−1.6	CNSp+	16715377
117	<chem>CCO</chem>	−1.5	CNSp+	9466345
118	<chem>CC(C(=O)C1=CC(=CC=C1)Cl)NC(C)(C)C</chem>	−1.5	CNSp+	17405866
119	<chem>CNCCC(C1=CC=CC=C1)OC2=CC=C(C=C2)C(F)(F)F</chem>	−1.5	CNSp+	14709630
120	<chem>COC1=C(C=C2C(=C1)CC(C2=O)CC3CCN(CC3)CC4=CC=CC=C4)OC</chem>	−1.5	CNSp+	17405866
121	<chem>C1CN(CCN1CCCN2C(=O)N3C=CC=CC3=N2)C4=CC(=CC=C4)Cl</chem>	−1.5	CNSp+	17405866
122	<chem>C1CN(CCC1(C2=CC=C(C=C2)Cl)O)CC(C(=O)C3=CC=C(C=C3)F</chem>	−1.5	CNSp+	17405866
123	<chem>CN1CCN(CC1)C2=NC3=CC=CC=C3OC4=C2C=C(C=C4)Cl</chem>	−1.5	CNSp+	17405866

Appendix Table 1. Cont.

124	<chem>CC1=CC=CC=C1O[C@H](CCNC)C2=C C=CC=C2</chem>	-1.4	CNSp+	17405866
125	<chem>CN1CCN2C(C1)C3=CC=CC=C3CC4=C 2N=CC=C4</chem>	-1.4	CNSp+	17405866
126	<chem>C[C@H](CC1=CC=CC=C1)N(C)CC#C</chem>	-1.4	CNSp+	17405866
127	<chem>CN1C2=C(C=C(C=C2)Cl)C(=NC(C1=O) O)C3=CC=CC=C3</chem>	-1.4	CNSp+	17405866
128	<chem>CNCCCC12CCC(C3=CC=CC=C31)C4= CC=CC=C24</chem>	-1.4	CNSp+	17405866
129	<chem>CN1CCCCC1CCN2C3=CC=CC=C3SC4 =C2C=C(C=C4)SC</chem>	-1.4	CNSp+	17405866
130	<chem>CN1C(=O)CN=C(C2=C1C=CC(=C2)Cl) C3=CC=CC=C3</chem>	-1.4	CNSp+	17405866
131	<chem>C1CN(CCN1CCOCCO)C2=NC3=CC=C C=C3SC4=CC=CC=C42</chem>	-1.3	CNSp+	17405866
132	<chem>CN(C)CC/C=C/1\C2=CC=CC=C2COC3 =CC=CC=C31</chem>	-1.3	CNSp+	17405866
133	<chem>C1=CC=C(C=C1)CC(C(=O)O)N</chem>	-1.3	CNSp+	18481317
134	<chem>CC[C@H](C)C(=O)O[C@H]1C[C@H](C=C2[C@H]1[C@H]([C@H](C=C2)C)C C[C@@H]3C[C@H](CC(=O)O3)O)C</chem>	-1.3	CNSp+	18481317
135	<chem>CC1=CC2=C(NC3=CC=CC=C3N=C2S1) N4CCN(CC4)C</chem>	-1.3	CNSp+	17405866
136	<chem>CN1CCN(CC1)C2=C3C=CC=CC3=NC4 =C(N2)C=C(C=C4)Cl</chem>	-1.3	CNSp+	17405866
137	<chem>C1CN(CCN1CCCN2C3=CC=CC=C3SC4 =C2C=C(C=C4)Cl)CCO</chem>	-1.3	CNSp+	17405866
138	<chem>CC1=CC(=NO1)C(=O)NNCC2=CC=CC =C2</chem>	-1.2	CNSp+	17405866
139	<chem>CC(C)NCC(COC1=CC=CC2=CC=CC=C 21)O</chem>	-1.2	CNSp+	14709630
140	<chem>CN(C)CCCN1C2=CC=CC=C2SC3=C1C =C(C=C3)Cl</chem>	-1.2	CNSp+	17405866
141	<chem>C1CN(CCN1)C2=NC3=CC=CC=C3OC4 =C2C=C(C=C4)Cl</chem>	-1.2	CNSp+	17405866
142	<chem>CN1CCN(CC1)CC/C=C/2\C3=CC=CC= C3SC4=C2C=C(C=C4)S(=O)(=O)N(C)C</chem>	-1.2	CNSp+	17405866
143	<chem>CC1=C(C(=O)N(N1C)C2=CC=CC=C2)I</chem>	-1.1	CNSp+	10993764
144	<chem>C[C@]12CC[C@H]3[C@H]([C@@H]1 CC[C@@H]2O)CCC4=CC(=O)CC[C@] 34C</chem>	-1.1	CNSp+	14709630
145	<chem>CN(C)CCC=C1C2=CC=CC=C2CCC3=C C=CC=C31</chem>	-1.1	CNSp+	17405866
146	<chem>CC1=NC=C2N1C3=C(C=C(C=C3)Cl)C(=NC2)C4=CC=CC=C4F</chem>	-1.0	CNSp+	18481317

Appendix Table 1. Cont.

147	<chem>C1=CC=C(C=C1)C2=NC(C(=O)NC3=C2C=C(C=C3)Cl)O</chem>	−1.0	CNSp+	18481317
148	<chem>C1C(=O)NC2=C(C=C(C=C2)Cl)C(=N1)C3=CC=CC=C3</chem>	−1.0	CNSp+	18481317
149	<chem>CCC(C)(C)C(=O)O[C@H]1C[C@H](C=C2[C@H]1[C@H]([C@H](C=C2)C)CC[C@@H]3C[C@H](CC(=O)O3)O)C</chem>	−1.0	CNSp+	18481317
150	<chem>CCCN(C(=S)NC1=CC=CC=C1)</chem>	−1.0	CNSp+	18481317
151	<chem>CCCN1C[C@@H](C[C@H]2[C@H]1CC3=CNC4=CC=CC2=C34)CSC</chem>	−1.0	CNSp+	17405866
152	<chem>C[C@]12CC[C@H]3[C@H]([C@@H]1CC[C@@H]2O)CCC4=C3C=CC(=C4)O</chem>	−0.8	CNSp+	9466345
153	<chem>CN[C@H]1CC[C@H](C2=CC=CC=C12)C3=CC(=C(C=C3)Cl)Cl</chem>	−0.7	CNSp+	17405866