Supplementary Materials

Predicting value of binding constants of organic ligands to beta-cyclodextrin: application of MARSplines and descriptors encoded in SMILES string

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Table. S1 Experimental and calculated LnK values.

No.	Chemical name	SMILES	lnK^{exp*}	lnK^{est}	Set (ext. validation)
1	Acetonitrile	CC#N	-1.474	-1.278	test
2	Methanol	CO	-1.128	-1.235	training
3	Acetaldehyde	CC=O	-0.622	-0.225	training
4	1,2-Ethanediol	C(CO)O	-0.437	0.828	training
5	Ethanol	CCO	-0.069	0.504	training
6	2-Methoxyethanol	COCCO	0.507	0.711	test
7	Acetone	CC(=O)C	0.967	0.619	training
8	1-Propanol	CCCO	1.312	1.410	training
9	2-Propanol	CC(C)O	1.451	1.988	training
10	1,4-Butanediol	C(CCO)CO	1.474	2.177	training
11	1,3-Propanediol	C(CO)CO	1.543	1.512	test
12	Cyclobutanol	C1CC(C1)O	2.717	3.234	training
13	2-Butanol	CCC(C)O	2.740	2.849	training
14	1-Butanol	CCCCO	2.809	2.739	training
15	1,5-Pentanediol	C(CCO)CCO	2.809	2.860	training

No.	Chemical name	SMILES	lnK^{exp*}	lnK^{est}	Set (ext. validation)
16	3-Pentanol	CCC(CC)O	3.108	4.305	test
17	Diethylamine	CCNCC	3.132	2.355	training
18	Chloroform	C(Cl)(Cl)Cl	3.293	3.119	training
19	Tetrahydrofuran	C1CCOC1	3.385	2.874	training
20	Griseofulvin	C[C@@H]1CC(=O)C=C([C@]12C(=O)C3=C(O2)C(=C(C=C3OC)OC)Cl)OC	3.385	3.929	training
21	2-Pentanol	CCCC(C)O	3.431	4.916	training
22	3-Cyanophenylacetate	CC(=O)OC1=CC=CC(=C1)C#N	3.431	4.202	test
23	Aniline	C1=CC=C(C=C1)N	3.684	3.937	training
24	2-Methyl-1-propanol	CC(C)CO	3.730	2.938	training
25	2-Methyl-2-propanol	CC(C)(C)O	3.868	2.891	training
26	1,6-Hexanediol	C(CCCO)CCO	3.891	3.788	training
27	3-Fluorophenol	C1=CC(=CC(=C1)F)O	3.914	4.439	test
28	Benzyl alcohol	C1=CC=C(C=C1)CO	3.937	4.467	training
29	4-Fluorophenol	C1=CC(=CC=C1O)F	3.983	4.370	training
30	Nimetazepam	CN1C(=O)CN=C(C2=C1C=CC(=C2)[N+](=O)[O-])C3=CC=CC=C3	3.983	4.651	training
31	4-Hydroxybenzaldehyde	C1=CC(=CC=C1C=O)O	4.030	4.119	training
32	Hydrochlorothiazide	C1NC2=CC(=C(C=C2S(=O)(=O)N1)S(=O)(=O)N)Cl	4.053	4.665	test
33	Benzaldehyde	C1=CC=C(C=C1)C=O	4.099	4.366	training
34	Barbital	CCC1(C(=O)NC(=O)NC1=O)CC	4.099	5.759	training
35	Furosemide	C1=COC(=C1)CNC2=CC(=C(C=C2C(=O)O)S(=O)(=O)N)Cl	4.099	4.404	training
36	1-Pentanol	CCCCCO	4.145	3.903	training

No.	Chemical name	SMILES	lnK^{exp*}	lnK^{est}	Set (ext. validation)
37	Bendroflumethiazide	C1=CC=C(C=C1)CC2NC3=C(C=C(C(=C3)C(F)(F)F)S(=O)(=O)N)S(=O)(=O)N2	4.375	4.994	training
38	2-Methyl-2-butanol	CCC(C)(C)O	4.398	4.887	training
39	3-Fluorophenyl acetate	CC(=O)OC1=CC(=CC=C1)F	4.398	4.001	test
40	3-Methyl-2-butanol	CC(C)C(C)O	4.421	4.161	training
41	Fluorobenzene	C1=CC=C(C=C1)F	4.513	4.404	training
42	Nitrazepam	C1C(=O)NC2=C(C=C(C=C2)[N+](=O)[O-])C(=N1)C3=CC=CC=C3	4.536	4.445	training
43	Sulfamerazine	CC1=NC(=NC=C1)NS(=O)(=O)C2=CC=C(C=C2)N	4.536	5.337	training
44	Phenol	C1=CC=C(C=C1)O	4.559	5.248	training
45	2-Hexanol	CCCCC(C)O	4.559	5.650	training
46	m-Cresol	CC1=CC(=CC=C1)O	4.559	6.091	training
47	Allobarbital	C=CCC1(C(=O)NC(=O)NC1=O)CC=C	4.559	4.739	test
48	2-Methyl-2-pentanol	CCCC(C)(C)O	4.582	5.199	training
49	Nitrobenzene	C1=CC=C(C=C1)[N+](=O)[O-]	4.697	4.528	training
50	4-Methyl-2-pentanol	CC(C)CC(C)O	4.697	5.274	test
51	Hydroquinone	C1=CC(=CC=C1O)O	4.720	3.530	training
52	Cyclopentanol	C1CCC(C1)O	4.743	4.742	training
53	3-Hydroxyacetophenone	CC(=O)C1=CC(=CC=C1)O	4.743	4.938	training
54	3,5-Dichlorophenol	C1=C(C=C(C=C1Cl)Cl)O	4.766	6.262	training
55	2-Methyl-1-butanol	CCC(C)CO	4.789	4.017	training
56	Toluene	CC1=CC=CC=C1	4.812	5.559	test
57	Phenyl acetate	CC(=O)OC1=CC=CC=C1	4.835	5.236	training

No.	Chemical name	SMILES	lnK^{exp*}	lnK^{est}	Set (ext. validation)
58	Sulfisomidine	CC1=CC(=NC(=N1)C)NS(=O)(=O)C2=CC=C(C=C2)N	4.835	5.117	training
59	3-Methoxyphenol	COC1=CC=CC(=C1)O	4.858	5.009	training
60	4-Fluorophenyl acetate	CC(=O)OC1=CC=C(C=C1)F	4.858	4.841	training
61	(R)-(+)-3-Benzyloxy-1,2-propanediol	C1=CC=C(C=C1)COC[C@@H](CO)O	4.858	5.395	training
62	Benzoic acid	C1=CC=C(C=C1)C(=O)O	4.881	4.910	training
63	N-Methylaniline	CNC1=CC=CC=C1	4.881	5.028	training
64	Quinoline	C1=CC=C2C(=C1)C=CC=N2	4.881	4.759	test
65	4-Nitrophenyl acetate	CC(=O)OC1=CC=C(C=C1)[N+](=O)[O-]	4.905	5.767	test
66	1-Chloro-4-nitrobenzene	C1=CC(=CC=C1[N+](=O)[O-])Cl	4.951	5.323	training
67	3-Methyl-3-pentanol	CCC(C)(CC)O	4.951	5.740	training
68	2-Phenylethanol	C1=CC=C(C=C1)CCO	4.951	5.623	test
69	4-Hydroxybenzyl alcohol	C1=CC(=CC=C1CO)O	4.974	3.849	training
70	4-Hydroxyacetophenone	CC(=O)C1=CC=C(C=C1)O	5.020	4.955	test
71	1-Butylimidazole	CCCCN1C=CN=C1	5.043	5.579	training
72	Carbon tetrachloride	C(Cl)(Cl)(Cl)Cl	5.066	3.675	training
73	4-Hydroxybenzoic acid	C1=CC(=CC=C1C(=O)O)O	5.066	4.556	training
74	Acetoanilide	CC(=O)NC1=CC=CC=C1	5.066	4.164	test
75	4-Methoxyphenol	COC1=CC=C(C=C1)O	5.089	4.910	training
76	3-Methylphenyl acetate	CC1=CC(=CC=C1)OC(=O)C	5.089	6.271	training
77	Benzene	C1=CC=CC=C1	5.135	4.746	training
78	Benzonitrile	C1=CC=C(C=C1)C#N	5.135	4.184	training
79	3-Methyl-1-butanol	CC(C)CCO	5.181	4.480	test

No.	Chemical name	SMILES	lnK^{exp*}	lnK^{est}	Set (ext. validation)
80	Sulfadimethoxine	COC1=NC(=NC(=C1)NS(=O)(=O)C2=CC=C(C=C2)N)OC	5.204	5.354	training
81	Acetophenone	CC(=O)C1=CC=CC=C1	5.227	4.853	training
82	Menadion	CC1=CC(=O)C2=CC=CC=C2C1=O	5.227	5.015	training
83	3-Chlorophenol	C1=CC(=CC(=C1)Cl)O	5.250	5.471	training
84	Carbutamide	CCCCNC(=O)NS(=O)(=O)C1=CC=C(C=C1)N	5.273	5.191	training
85	Anisole	COC1=CC=CC=C1	5.342	4.821	training
86	Sulfisoxazole	CC1=C(ON=C1C)NS(=O)(=O)C2=CC=C(C=C2)N	5.342	5.827	training
87	1-Hexanol	CCCCCCO	5.365	6.089	training
88	4-Ethoxyphenol	CCOC1=CC=C(C=C1)O	5.365	5.190	training
89	Sulfamethomidine	CC1=NC(=CC(=N1)OC)NS(=O)(=O)C2=CC=C(C=C2)N	5.365	5.771	training
90	Acridine	C1=CC=C2C(=C1)C=C3C=CC=CC3=N2	5.365	4.636	training
91	Fludiazepam	CN1C(=O)CN=C(C2=C1C=CC(=C2)Cl)C3=CC=CC=C3F	5.365	5.475	training
92	Diazepam	CN1C(=O)CN=C(C2=C1C=CC(=C2)Cl)C3=CC=CC=C3	5.365	5.149	test
93	4-Nitrobenzoic acid	C1=CC(=CC=C1C(=O)O)[N+](=O)[O-]	5.388	5.869	training
94	3,5-Dimethoxyphenol	COC1=CC(=CC(=C1)O)OC	5.388	5.161	test
95	N-ethylaniline	CCNC1=CC=CC=C1	5.388	5.205	test
96	3-Ethoxyphenol	CCOC1=CC=CC(=C1)O	5.411	6.129	training
97	Sulfaphenazole	C1=CC=C(C=C1)N2C(=CC=N2)NS(=O)(=O)C3=CC=C(C=C3)N	5.411	5.984	training
98	Phenylacetylene	C#CC1=CC=CC=C1	5.434	5.494	training
99	N,N-dimethylaniline	CN(C)C1=CC=CC=C1	5.434	5.617	test

No.	Chemical name	SMILES	lnK^{exp*}	lnK^{est}	Set (ext. validation)
100	Benzothiazole	C1=CC=C2C(=C1)N=CS2	5.480	5.573	training
101	p-Xylene	CC1=CC=C(C=C1)C	5.480	6.433	training
102	4-Nitrophenol	C1=CC(=CC=C1[N+](=O)[O-])O	5.503	5.036	training
103	p-Cresol	CC1=CC=C(C=C1)O	5.526	5.666	training
104	Medazepam	CN1CCN=C(C2=C1C=CC(=C2)Cl)C3=CC=CC=C3	5.526	6.613	test
105	Phenazine	C1=CC=C2C(=C1)N=C3C=CC=CC3=N2	5.549	5.109	training
106	3-Chlorophenyl acetate	CC(=O)OC1=CC(=CC=C1)Cl	5.618	6.813	training
107	Carbazole	C1=CC=C2C(=C1)C3=CC=CC=C3N2	5.618	6.127	test
108	Benzyl chloride	C1=CC=C(C=C1)CCl	5.641	5.671	training
109	4-Methoxyphenyl acetate	CC(=O)C1=CC(=C(C=C1)OC(=O)C)OC	5.641	5.401	test
110	4-Nitroaniline	C1=CC(=CC=C1N)[N+](=O)[O-]	5.710	4.632	training
111	Sulfamonomethoxine	COC1=NC=NC(=C1)NS(=O)(=O)C2=CC=C(C=C2)N	5.710	5.330	training
112	Phenetole	CCOC1=CC=CC=C1	5.733	6.048	training
113	p-Tolyl acetate	CC1=CC=C(C=C1)OC(=O)C	5.733	6.193	training
114	3-Ethoxyphenyl acetate	CCOC1=CC=CC(=C1)C(=O)C	5.733	5.963	training
115	Mefenamic acid	CC1=C(C(=CC=C1)NC2=CC=CC=C2C(=O)O)C	5.733	7.185	test
116	Bromobenzene	C1=CC=C(C=C1)Br	5.756	5.487	training
117	4-Chlorophenyl acetate	C1=CC(=CC=C1CC(=O)O)Cl	5.756	5.793	training
118	Methyl benzoate	COC(=O)C1=CC=CC=C1	5.756	5.085	training
119	3-Bromophenol	C1=CC(=CC(=C1)Br)O	5.779	6.133	training
120	Sulfadiazine	C1=CN=C(N=C1)NS(=O)(=O)C2=CC=C(C=C2)N	5.803	5.376	training
121	Progabide	C1=CC(=CC=C1C(=NCCCC(=O)N)C2=C(C=CC(=C2)F)O)Cl	5.826	4.451	training
122	4-Ethoxyphenyl acetate	CCOC1=CC=C(C=C1)CCO	5.849	6.046	training

No.	Chemical name	SMILES	lnK^{exp*}	lnK^{est}	Set (ext. validation)
123	3,5-Dibromophenol	C1=C(C=C(C=C1Br)Br)O	5.895	4.911	training
124	3-Hydroxycinnamic acid	C1=CC(=CC(=C1)O)/C=C/C(=O)O	5.895	6.914	test
125	Phenanthridine	C1=CC=C2C(=C1)C=NC3=CC=CC=C23	5.918	6.417	training
126	Ethylbenzene	CCC1=CC=CC=C1	5.964	6.646	training
127	3-Ethylphenol	CCC1=CC(=CC=C1)O	5.987	6.786	training
128	4-Chlorophenol	C1=CC(=CC=C1O)Cl	6.010	5.278	training
129	3′-Hydroxypropiophenone	CCC(=O)C1=CC(=CC=C1)O	6.010	6.014	training
130	1-Benzylimidazole	C1=CC=C(C=C1)CN2C=CN=C2	6.010	5.992	training
131	4′-Hydroxypropiophenone	CCC(=O)C1=CC=C(C=C1)O	6.056	5.998	training
132	Fenbufen	C1=CC=C(C=C1)C2=CC=C(C=C2)C(=O)CCC(=O)O	6.056	6.859	training
133	4-Bromophenol	C1=CC(=CC=C1O)Br	6.102	7.168	training
134	4-Methylcinnamic acid	CC1=CC=C(C=C1)/C=C/C(=O)O	6.102	6.083	test
135	Triflumizole	CCCOCC(=NC1=C(C=C(C=C1)Cl)C(F)(F)F)N2C=CN=C2	6.125	5.430	training
136	Cyclohexanol	C1CCC(CC1)O	6.148	5.930	training
137	3-Bromophenyl acetate	CC(=O)OC1=CC(=CC=C1)Br	6.148	6.378	training
138	Meclofenamic acid	C1=CC=C(C(=C1)C(=O)O)NC2=CC=CC(=C2)C(F)(F)F	6.148	7.067	training
139	4-Bromophenyl acetate	C1=CC(=CC=C1CC(=O)O)Br	6.171	6.190	training
140	3-Ethylphenyl acetate	CCC1=CC(=CC=C1)OC(=O)C	6.171	6.982	test
141	4-Ethylphenol	CCC1=CC=C(C=C1)O	6.194	6.824	training
142	Phenoxazine	C1=CC=C2C(=C1)NC3=CC=CC=C3O2	6.194	5.616	training
143	Ethyl4-aminobenzoate	CCOC(=O)C1=CC=C(C=C1)N	6.194	6.345	test
144	Sulfapyridine	C1=CC=NC(=C1)NS(=O)(=O)C2=CC=C(C=C2)N	6.217	5.326	training

No.	Chemical name	SMILES	lnK^{exp*}	lnK^{est}	Set (ext. validation)
145	2,2-Dimethyl-1-propanol	CC(C)(C)CO	6.240	5.128	training
146	Cyclobarbital	CCC1(C(=O)NC(=O)NC1=O)C2=CCCCC2	6.240	6.552	training
147	Xanthene	C1C2=CC=CC=C2OC3=CC=CC=C31	6.240	5.952	training
148	Ethyl benzoate	CCOC(=O)C1=CC=CC=C1	6.286	6.306	test
149	Phenothiazine	C1=CC=C2C(=C1)NC3=CC=CC=C3S2	6.286	6.494	test
150	3,3-Dimethyl-2-butanol	CC(C(C)(C)C)O	6.332	6.724	training
151	Sulfanilamide	C1=CC(=CC=C1N)S(=O)(=O)N	6.355	5.358	training
152	4-Hydroxycinnamicacid	C1=CC(=CC=C1/C=C\C(=O)O)O	6.516	5.034	training
153	4-Ethylphenyl acetate	CCC1=CC=C(C=C1)OC(=O)C	6.516	6.839	training
154	1-Heptanol	CCCCCCCO	6.562	6.321	training
155	Ketoprofen	CC(C1=CC=CC(=C1)C(=O)C2=CC=CC=C2)C(=O)O	6.562	6.065	training
156	4-Isopropoxyphenol	CC(C)OC1=CC=C(C=C1)O	6.585	6.789	test
157	4-Isopropylphenyl acetate	CC(C)C1=CC=C(C=C1)OC(=O)C	6.631	7.483	training
158	N-Phenylanthranilic acid	C1=CC=C(C=C1)NC2=CC=CC=C2C(=O)O	6.654	6.796	test
159	Iodobenzene	C1=CC=C(C=C1)I	6.747	6.005	training
160	3-Iodophenol	C1=CC(=CC(=C1)I)O	6.747	6.740	training
161	m-Methylcinnamicacid	CC1=CC=CC(=C1)/C=C/C(=O)O	6.747	6.822	training
162	Acetohexamide	CC(=O)C1=CC=C(C=C1)S(=O)(=O)NC(=O)NC2CCCCC2	6.770	6.505	training
163	Prostacyclin	CCCCC[C@@H](/C=C/[C@H]1[C@@H](C[C@H]2[C@@H]1C/C(=C/CCCC(=O)O)/O2)O)O	6.770	6.846	training
164	1,4-Dibromobenzene	C1=CC(=CC=C1Br)Br	6.839	6.423	training
165	Dibenzofuran	C1=CC=C2C(=C1)C3=CC=CC=C3O2	6.839	6.530	test
166	4-Iodophenol	C1=CC(=CC=C1O)I	6.862	6.647	training

No.	Chemical name	SMILES	lnK^{exp*}	lnK^{est}	Set (ext. validation)
167	4-Iodophenyl acetate	CC(=O)OC1=CC=C(C=C1)I	6.908	6.818	training
168	Pentobarbital	CCCC(C)C1(C(=O)NC(=O)NC1=O)CC	6.931	7.118	training
169	Ethyl4-hydroxybenzoate	CCOC(=O)C1=CC=C(C=C1)O	6.931	6.449	training
170	3-Iodophenyl acetate	C1=CC=C2C(=C1)C(C(=O)N2)O	7.069	6.668	training
171	Amobarbital	CCC1(C(=O)NC(=O)NC1=O)CCC(C)C	7.069	7.288	test
172	Hexobarbital	CC1(C(=O)NC(=O)N(C1=O)C)C2=CCCCC2	7.092	7.641	training
173	Prostaglandine E2	CCCCC[C@@H](/C=C/[C@H]1[C@@H](CC(=O)[C@@H]1C/C=C\CCCC(=O)O)O)O	7.115	6.904	training
174	Flufenamic acid	C1=CC=C(C(=C1)C(=O)O)NC2=CC=CC(=C2)C(F)(F)F	7.138	7.036	training
175	2-Octanol	CCCCCCC(C)O	7.207	7.083	training
176	4-n-Propylphenyl acetate	CCCC1=CC=C(C=C1)OC(=O)C	7.253	7.593	test
177	Mephobarbital	CCC1(C(=O)NC(=O)N(C1=O)C)C2=CC=CC=C2	7.276	7.225	training
178	1,4-Diiodobenzene	C1=CC(=CC=C1I)I	7.299	8.045	test
179	1-Octanol	CCCCCCCCO	7.299	6.956	test
180	Butyl 4-aminobenzoate	CCCCOC(=O)C1=CC=C(C=C1)N	7.345	6.394	training
181	Phenobarbital	CCC1(C(=O)NC(=O)NC1=O)C2=CC=CC=C2	7.414	5.754	training
182	Thianaphthene	C1=CC=C2C(=C1)C=CS2	7.437	6.547	training
183	Hydrocortisone-17-butyrate	CCCC(=O)O[C@@]1(CC[C@@H]2[C@@]1(C[C@@H]([C@H]3[C@H]2CCC4=CC(=O)CC[C@]34C)O)C)C(=O)CO	7.437	8.484	training
184	Cycloheptanol	C1CCCC(CC1)O	7.437	7.042	training
185	3-Propylphenol	CCCC1=CC(=CC=C1)O	7.552	8.084	training
186	3-n-Propylphenyl acetate	CCCC1=CC=CC(=C1)C(=O)C	7.552	7.528	training

No.	Chemical name	SMILES	lnK^{exp*}	lnK^{est}	Set (ext. validation)
187	Thiopental	CCCC(C)C1(C(=O)NC(=S)NC1=O)CC	7.552	7.994	test
188	Cyclooctanol	C1CCCC(CCC1)O	7.599	7.524	training
189	Cortisone	C[C@]12CCC(=O)C=C1CC[C@@H]3[C@@H]2C(=O)C[C@]4([C@H]3CC[C@@]4(C(=O)CO)O)C	7.714	7.551	training
190	Benzidine	C1=CC(=CC=C1C2=CC=C(C=C2)N)N	7.714	6.055	training
191	3-Isopropylphenyl acetate	CC(C)C1=CC(=CC=C1)OC(=O)C	7.737	7.512	training
192	Triamcinolone	C[C@]12C[C@@H]([C@]3([C@H]([C@@H]1C[C@H]([C@@]2(C(=O)CO)O)O)CCC4=CC(=O)C=C[C@@]43C)F)O	7.760	8.109	training
193	Dehydrocholic acid	C[C@H](CCC(=O)O)[C@H]1CC[C@@H]2[C@@]1(C(=O)C[C@H]3[C@H]2C(=O)C[C@H]4[C@@]3(CCC(=O)C4)C)C	7.783	7.557	training
194	Butyl 4-hydroxybenzoate	CCCCOC(=O)C1=CC=C(C=C1)O	7.806	7.379	test
195	Paramethasone	C[C@@H]1C[C@H]2[C@@H]3C[C@@H](C4=CC(=O)C=C[C@@]4([C@H]3[C@H](C[C@@]2([C@]1(C(=O)CO)O)C)O)C)F	7.829	7.612	training
196	3-Isopropylphenol	CC(C)C1=CC(=CC=C1)O	7.921	7.807	training
197	Dibenzothiophene	C1=CC=C2C(=C1)C3=CC=CC=C3S2	8.013	7.875	training
198	Fluocinoloneacetonide	C[C@]12C[C@@H]([C@]3([C@H]([C@@H]1C[C@@H]4[C@]2(OC(O4)(C)C)C(=O)CO)C[C@@H](C5=CC(=O)C=C[C@@]53C)F)F)O	8.013	8.052	training
199	Cholic acid	C[C@H](CCC(=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	8.059	8.506	training

No.	Chemical name	SMILES	lnK^{exp*}	lnK^{est}	Set (ext. validation)
200	Hydrocortisone-21-acetate	CC(=O)OCC(=O)C1(CCC2C1(CC(C3C2CCC4=CC(=O)CCC34C)O)C)O	8.082	8.612	training
201	Triamcinolone acetonide	C[C@]12C[C@@H]([C@]3([C@H]([C@@H]1C[C@@H]4[C@]2(OC(O4)(C)C)C(=O)CO)CCC5=CC(=O)C=C[C@@]53C)F)O	8.082	8.199	test
202	4-Propylphenol	CCCC1=CC=C(C=C1)O	8.174	8.132	training
203	Prednisolone	C[C@]12C[C@@H]([C@H]3[C@H]([C@@H]1CC[C@@]2(C(=O)CO)O)CCC4=CC(=O)C=C[C@]34C)O	8.197	7.986	training
204	Thianthrene	C1=CC=C2C(=C1)SC3=CC=CC=C3S2	8.220	8.314	training
205	4-Isopropylphenol	CC(C)C1=CC=C(C=C1)O	8.243	7.921	training
206	2-Norbornaneacetate	C1CC2CC1CC2CC(=O)O	8.266	7.779	training
207	Hydrocortisone	C[C@]12CCC(=O)C=C1CC[C@@H]3[C@@H]2[C@H](C[C@]4([C@H]3CC[C@@]4(C(=O)CO)O)C)O	8.289	7.807	training
208	4-n-Butylphenylacetate	CCCCC1=CC=C(C=C1)CC(=O)O	8.335	7.282	training
209	Cortisone-21-acetate	CC(=O)OCC(=O)[C@]1(CC[C@@H]2[C@@]1(CC(=O)[C@H]3[C@H]2CCC4=CC(=O)CC[C@]34C)C)O	8.335	7.831	test
210	Cinnarizine	C1CN(CCN1C/C=C/C2=CC=CC=C2)C(C3=CC=CC=C3)C4=CC=CC=C4	8.381	7.674	training
211	Dexamethasone	C[C@@H]1C[C@H]2[C@@H]3CCC4=CC(=O)C=C[C@@]4([C@]3([C@H](C[C@@]2([C@]1(C(=O)CO)O)C)O)F)C	8.404	7.998	training
212	3-n-Butylphenyl acetate	CCCCC1=CC(=CC=C1)OC(=O)C	8.427	8.047	training
213	Flurbiprofen	CC(C1=CC(=C(C=C1)C2=CC=CC=C2)F)C(=O)O	8.497	7.589	test

No.	Chemical name	SMILES	lnK^{exp*}	lnK^{est}	Set (ext. validation)
214	Betamethasone	C[C@H]1C[C@H]2[C@@H]3CCC4=CC(=O)C=C[C@@]4([C@]3([C@H](C[C@@]2([C@]1(C(=O)CO)O)C)O)F)C	8.589	8.022	training
215	3-n-Butylphenol	CCCCC1=CC(=CC=C1)O	8.658	8.834	training
216	Prednisolone-21-acetate	CC(=O)OCC(=O)[C@]1(CC[C@@H]2[C@@]1(C[C@@H]([C@H]3[C@H]2CCC4=CC(=O)C=C[C@]34C)O)C)O	8.658	8.749	test
217	4-n-Amylphenyl acetate	CCCCCC1=CC=C(C=C1)OC(=O)C	8.750	8.871	training
218	3-Isobutylphenyl acetate	CC(C)CC1=CC(=CC=C1)OC(=O)C	8.819	8.136	training
219	Tolnaftate	CC1=CC(=CC=C1)N(C)C(=S)OC2=CC3=CC=CC=C3C=C2	8.819	8.693	test
220	4-tert-Butylphenyl acetate	CC(=O)OC1=CC=C(C=C1)C(C)(C)C	8.865	9.295	training
221	Corticosterone	C[C@]12CCC(=O)C=C1CC[C@@H]3[C@@H]2[C@H](C[C@]4([C@H]3CC[C@@H]4C(=O)CO)C)O	8.865	9.069	training
222	4-n-Butylphenol	CCCCC1=CC=C(C=C1)O	9.141	8.746	training
223	3-sec-Butylphenol	CC(C)(C)C1=C(C=C(C(=C1)O)C=O)Cl	9.348	8.105	training
224	4-sec-Butylphenol	CCC(C)C1=CC=C(C=C1)O	9.625	8.612	training
225	4-n-Amylphenol	CCCCCC1=CC=C(C=C1)O	9.648	9.372	training
226	3-Isobutylphenol	CC(C)CC1=CC(=CC=C1)O	9.694	8.728	training
227	1-Adamantaneacetate	C1C2CC3CC1CC(C2)(C3)CC(=O)O	9.947	10.330	training
228	Chenodeoxycholic acid	C[C@H](CCC(=O)O)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2[C@@H](C[C@H]4[C@@]3(CC[C@H](C4)O)C)O)C	10.039	10.547	training
229	3-tert-Butylphenol	CC(C)(C)C1=CC(=CC=C1)O	10.154	9.859	test

No.	Chemical name	SMILES	lnK^{exp*}	lnK^{est}	Set (ext. validation)
230	Spironolactone	CC(=O)S[C@@H]1CC2=CC(=O)CC[C@@]2([C@@H]3[C@@H]1[C@@H]4CC[C@]5([C@]4(CC3)C)CCC(=O)O5)C	10.223	9.236	training
231	Ursodeoxycholic acid	C[C@H](CCC(=O)O)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2[C@H](C[C@H]4[C@@]3(CC[C@H](C4)O)C)O)C	10.385	10.361	training
232	4-tert-Butylphenol	CC(C)(C)C1=CC=C(C=C1)O	10.500	9.885	training
233	4-tert-Amylphenol	CCC(C)(C)C1=CC=C(C=C1)O	10.822	10.447	training

*Source: a) Suzuki, T. A Nonlinear Group Contribution Method for Predicting the Free Energies of Inclusion Complexation of Organic Molecules with α- and β-Cyclodextrins. J. Chem. Inf. Comput. Sci. 2001, 41 b) Mirrahimi, F.; Salahinejad, M.; Ghasemi, J.B. QSPR approaches to elucidate the stability constants between β-cyclodextrin and some organic compounds: Docking based 3D conformer. J. Mol. Liq. 2016, 219, 1036–1043

Table. S2 LnK values predicted for compounds belonging to different classes according to Biopharmaceutical Classification System (BCS).

No.	API	SMILES	LnK^{est}	BCS*
1	alfacalcidol	CC(C)CCCC(C)C1CCC2C1(CCCC2=CC=C3CC(CC(C3=C)O)O)C	14.343	Class I
2	alprazolam	CC1=NN=C2N1C3=C(C=C(C=C3)Cl)C(=NC2)C4=CC=CC=C4	8.767	Class I
3	azulene sulfonate sodium	CC1=C2C(=CC(=C2C=C(C=C1)C(C)C)C)S(=O)(=O)[O-].[Na+]	9.039	Class I
4	beraprost sodium	CC#CCC(C)C(C=CC1C(CC2C1C3=C(O2)C(=CC=C3)CCCC(=O)[O-])O)O.[Na+]	7.171	Class I
5	bisoprolol fumarate	CC(C)NCC(COC1=CC=C(C=C1)COCCOC(C)C)O.C(=CC(=O)O)C(=O)O	5.832	Class I
6	brotizolam	CC1=NN=C2N1C3=C(C=C(S3)Br)C(=NC2)C4=CC=CC=C4Cl	5.955	Class I
7	cabergoline	CCNC(=O)N(CCCN(C)C)C(=O)C1CC2C(CC3=CNC4=CC=CC2=C34)N(C1)CC=C	7.982	Class I
8	chlorpheniramine maleate	CN(C)CCC(C1=CC=C(C=C1)Cl)C2=CC=CC=N2.C(=CC(=O)O)C(=O)O	8.132	Class I
9	clomiphene citrate	CCN(CC)CCOC1=CC=C(C=C1)C(=C(C2=CC=CC=C2)Cl)C3=CC=CC=C3.C(C(=O)O)C(CC(=O)O)(C(=O)O)O	13.098	Class I
10	desloratadine	C1CC2=C(C=CC(=C2)Cl)C(=C3CCNCC3)C4=C1C=CC=N4	8.016	Class I
11	dexamethasone	CC1CC2C3CCC4=CC(=O)C=CC4(C3(C(CC2(C1(C(=O)CO)O)C)O)F)C	8.679	Class I
12	diclofenac sodium	C1=CC=C(C(=C1)CC(=O)[O-])NC2=C(C=CC=C2Cl)Cl.[Na+]	6.802	Class I
13	ergocalciferol	CC(C)C(C)C=CC(C)C1CCC2C1(CCCC2=CC=C3CC(CCC3=C)O)C	14.937	Class I
14	escitalopram oxalate	CN(C)CCCC1(C2=C(CO1)C=C(C=C2)C#N)C3=CC=C(C=C3)F.C(=O)(C(=O)O)O	7.266	Class I
15	ethinyl estradiol	CC12CCC3C(C1CCC2(C#C)O)CCC4=C3C=CC(=C4)O	10.099	Class I
16	etizolam	CCC1=CC2=C(S1)N3C(=NN=C3CN=C2C4=CC=CC=C4Cl)C	6.964	Class I

No.	API	SMILES	LnK^{est}	BCS*
17	finasteride	CC12CCC3C(C1CCC2C(=O)NC(C)(C)C)CCC4C3(C=CC(=O)N4)C	11.766	Class I
18	fluvastatin sodium	CC(C)N1C2=CC=CC=C2C(=C1C=CC(CC(CC(=O)[O-])O)O)C3=CC=C(C=C3)F.[Na+]	8.943	Class I
19	fluvoxamine maleate	COCCCCC(=NOCCN)C1=CC=C(C=C1)C(F)(F)F.C(=CC(=O)O)C(=O)O	9.480	Class I
20	indapamide	CC1CC2=CC=CC=C2N1NC(=O)C3=CC(=C(C=C3)Cl)S(=O)(=O)N	7.833	Class I
21	levonorgestrel	CCC12CCC3C(C1CCC2(C#C)O)CCC4=CC(=O)CCC34	10.595	Class I
22	levothyroxine sodium	C1=C(C=C(C(=C1I)OC2=CC(=C(C(=C2)I)O)I)I)CC(C(=O)[O-])N.[Na+]	6.143	Class I
23	lorazepam	C1=CC=C(C(=C1)C2=NC(C(=O)NC3=C2C=C(C=C3)Cl)O)Cl	5.091	Class I
24	losartan potassium	CCCCC1=NC(=C(N1CC2=CC=C(C=C2)C3=CC=CC=C3C4=NN=N[N-]4)CO)Cl.[K+]	19.588	Class I
25	loxoprofen sodium	CC(C1=CC=C(C=C1)CC2CCCC2=O)C(=O)[O-].[Na+]	7.685	Class I
26	metoprolol tartrate	CC(C)NCC(COC1=CC=C(C=C1)CCOC)O.CC(C)NCC(COC1=CC=C(C=C1)CCOC)O.C(C(C(=O)O)O)(C(=O)O)O	3.656	Class I
27	mirtazapine	CN1CCN2C(C1)C3=CC=CC=C3CC4=C2N=CC=C4	8.189	Class I
28	norethindrone (norethisterone)	CC12CCC3C(C1CCC2(C#C)O)CCC4=CC(=O)CCC34	10.123	Class I
29	norgestimate	CCC12CCC3C(C1CCC2(C#C)OC(=O)C)CCC4=CC(=NO)CCC34	10.172	Class I
30	phendimetrazine tartrate	CC1C(OCCN1C)C2=CC=CC=C2.C(C(C(=O)O)O)(C(=O)O)O	7.415	Class I
31	pravastatin sodium	CCC(C)C(=O)OC1CC(C=C2C1C(C(C=C2)C)CCC(CC(CC(=O)[O-])O)O)O.[Na+]	6.859	Class I

No.	API	SMILES	LnK^{est}	BCS*
32	quetiapine fumarate	C1CN(CCN1CCOCCO)C2=NC3=CC=CC=C3SC4=CC=CC=C42.C1CN(CCN1CCOCCO)C2=NC3=CC=CC=C3SC4=CC=CC=C42.C(=CC(=O)O)C(=O)O	6.521	Class I
33	quinine sulfate	COC1=CC2=C(C=CN=C2C=C1)C(C3CC4CCN3CC4C=C)O.OS(=O)(=O)O	7.766	Class I
34	rabeprazole sodium	CC1=C(C=CN=C1CS(=O)C2=NC3=CC=CC=C3[N-]2)OCCCOC.[Na+]	12.421	Class I
35	ramipril	CCOC(=O)C(CCC1=CC=CC=C1)NC(C)C(=O)N2C3CCCC3CC2C(=O)O	9.084	Class I
36	reserpine	COC1C(CC2CN3CCC4=C(C3CC2C1C(=O)OC)NC5=C4C=CC(=C5)OC)OC(=O)C6=CC(=C(C(=C6)OC)OC)OC	6.174	Class I
37	rivastigmine tartrate	CCN(C)C(=O)OC1=CC=CC(=C1)C(C)N(C)C.C(C(C(=O)O)O)(C(=O)O)O	7.717	Class I
38	saquinavir mesylate	CC(C)(C)NC(=O)C1CC2CCCCC2CN1CC(C(CC3=CC=CC=C3)NC(=O)C(CC(=O)N)NC(=O)C4=NC5=CC=CC=C5C=C4)O.CS(=O)(=O)O	10.621	Class I
39	tacrolimus	CC1CC(C2C(CC(C(O2)(C(=O)C(=O)N3CCCCC3C(=O)OC(C(C(CC(=O)C(C=C(C1)C)CC=C)O)C)C(=CC4CCC(C(C4)OC)O)C)O)C)OC)OC	4.398	Class I
40	thioctic acid	C1CSSC1CCCCC(=O)O	7.057	Class I
41	toremifene citrate	CN(C)CCOC1=CC=C(C=C1)C(=C(CCCl)C2=CC=CC=C2)C3=CC=CC=C3.C(C(=O)O)C(CC(=O)O)(C(=O)O)O	12.935	Class I
42	trimebutin maleate	CCC(COC(=O)C1=CC(=C(C(=C1)OC)OC)OC)(C2=CC=CC=C2)N(C)C.C(=CC(=O)O)C(=O)O	7.435	Class I
43	valproate sodium	CCCC(CCC)C(=O)[O-].[Na+]	6.765	Class I

No.	API	SMILES	LnK^{est}	BCS*
44	zolpidem tartrate	CC1=CC=C(C=C1)C2=C(N3C=C(C=CC3=N2)C)CC(=O)N(C)C.C(C(C(=O)O)O)(C(=O)O)O	9.459	Class I
45	aceclofenac	C1=CC=C(C(=C1)CC(=O)OCC(=O)O)NC2=C(C=CC=C2Cl)Cl	6.062	Class II
46	albendazole	CCCSC1=CC2=C(C=C1)N=C(N2)NC(=O)OC	7.950	Class II
47	alibendol	COC1=C(C(=CC(=C1)CC=C)C(=O)NCCO)O	5.501	Class II
48	anastrozole	CC(C)(C#N)C1=CC(=CC(=C1)CN2C=NC=N2)C(C)(C)C#N	8.127	Class II
49	atropine sulfate	CN1C2CCC1CC(C2)OC(=O)C(CO)C3=CC=CC=C3.CN1C2CCC1CC(C2)OC(=O)C(CO)C3=CC=CC=C3.OS(=O)(=O)O	4.299	Class II
50	bicalutamide	CC(CS(=O)(=O)C1=CC=C(C=C1)F)(C(=O)NC2=CC(=C(C=C2)C#N)C(F)(F)F)O	6.174	Class II
51	bisacodyl	CC(=O)OC1=CC=C(C=C1)C(C2=CC=C(C=C2)OC(=O)C)C3=CC=CC=N3	11.166	Class II
52	camostat mesylate	CN(C)C(=O)COC(=O)CC1=CC=C(C=C1)OC(=O)C2=CC=C(C=C2)N=C(N)N.CS(=O)(=O)O	7.754	Class II
53	candesartan cilexetil	CCOC1=NC2=CC=CC(=C2N1CC3=CC=C(C=C3)C4=CC=CC=C4C5=NNN=N5)C(=O)OC(C)OC(=O)OC6CCCCC6	14.839	Class II
54	carbamazepine	C1=CC=C2C(=C1)C=CC3=CC=CC=C3N2C(=O)N	8.899	Class II
55	carvedilol	COC1=CC=CC=C1OCCNCC(COC2=CC=CC3=C2C4=CC=CC=C4N3)O	4.483	Class II
56	celecoxib	CC1=CC=C(C=C1)C2=CC(=NN2C3=CC=C(C=C3)S(=O)(=O)N)C(F)(F)F	7.388	Class II
57	cilazapril	CCOC(=O)C(CCC1=CC=CC=C1)NC2CCCN3CCCC(N3C2=O)C(=O)O	7.178	Class II
58	cilostazol	C1CCC(CC1)N2C(=NN=N2)CCCCOC3=CC4=C(C=C3)NC(=O)CC4	9.067	Class II

No.	API	SMILES	LnK^{est}	BCS*
59	clarithromycin	CCC1C(C(C(C(=O)C(CC(C(C(C(C(C(=O)O1)C)OC2CC(C(C(O2)C)O)(C)OC)C)OC3C(C(CC(O3)C)N(C)C)O)(C)OC)C)C)O)(C)O	4.294	Class II
60	clofazimine	CC(C)N=C1C=C2C(=NC3=CC=CC=C3N2C4=CC=C(C=C4)Cl)C=C1NC5=CC=C(C=C5)Cl	10.379	Class II
61	clopidogrel bisulfate	COC(=O)C(C1=CC=CC=C1Cl)N2CCC3=C(C2)C=CS3.OS(=O)(=O)O	8.383	Class II
62	clozapine	CN1CCN(CC1)C2=NC3=C(C=CC(=C3)Cl)NC4=CC=CC=C42	8.836	Class II
63	colchicine	CC(=O)NC1CCC2=CC(=C(C(=C2C3=CC=C(C(=O)C=C13)OC)OC)OC)OC	7.259	Class II
64	cyclosporin a	CCC1C(=O)N(CC(=O)N(C(C(=O)NC(C(=O)N(C(C(=O)NC(C(=O)NC(C(=O)N(C(C(=O)N(C(C(=O)N(C(C(=O)N(C(C(=O)N1)C(C(C)CC=CC)O)C)C(C)C)C)CC(C)C)C)CC(C)C)C)C)CC(C)C)C(C)C)CC(C)C)C)C	-6.361	Class II
65	cyproterone acetate	CC(=O)C1(CCC2C1(CCC3C2C=C(C4=CC(=O)C5CC5C34C)Cl)C)OC(=O)C	8.878	Class II
66	diazepam	CN1C(=O)CN=C(C2=C1C=CC(=C2)Cl)C3=CC=CC=C3	7.663	Class II
67	diethylcarbamazine citrate	CCN(CC)C(=O)N1CCN(CC1)C.C(C(=O)O)C(CC(=O)O)(C(=O)O)O	4.967	Class II
68	digoxin	CC1C(C(CC(O1)OC2C(OC(CC2O)OC3C(OC(CC3O)OC4CCC5(C(C4)CCC6C5CC(C7(C6(CCC7C8=CC(=O)OC8)O)C)O)C)C)C)O)O	6.803	Class II
69	diloxanide furoate	CN(C1=CC=C(C=C1)OC(=O)C2=CC=CO2)C(=O)C(Cl)Cl	6.826	Class II
70	ebastine	CC(C)(C)C1=CC=C(C=C1)C(=O)CCCN2CCC(CC2)OC(C3=CC=CC=C3)C4=CC=CC=C4	18.020	Class II
71	efavirenz	C1CC1C#CC2(C3=C(C=CC(=C3)Cl)NC(=O)O2)C(F)(F)F	8.514	Class II
72	epalrestat	CC(=CC1=CC=CC=C1)C=C2C(=O)N(C(=S)S2)CC(=O)O	8.714	Class II

No.	API	SMILES	LnK^{est}	BCS*
73	eprosartan mesylate	CCCCC1=NC=C(N1CC2=CC=C(C=C2)C(=O)O)C=C(CC3=CC=CS3)C(=O)O.CS(=O)(=O)O	11.444	Class II
74	erythromycin ethylsuccinate	CCC1C(C(C(C(=O)C(CC(C(C(C(C(C(=O)O1)C)OC2CC(C(C(O2)C)O)(C)OC)C)OC3C(C(CC(O3)C)N(C)C)OC(=O)CCC(=O)OCC)(C)O)C)C)O)(C)O	4.943	Class II
75	ethylicosapentate	CCC=CCC=CCC=CCC=CCC=CCCCC(=O)OCC	12.192	Class II
76	ezetimibe	C1=CC(=CC=C1C2C(C(=O)N2C3=CC=C(C=C3)F)CCC(C4=CC=C(C=C4)F)O)O	4.077	Class II
77	fenofibrate	CC(C)OC(=O)C(C)(C)OC1=CC=C(C=C1)C(=O)C2=CC=C(C=C2)Cl	9.089	Class II
78	flurbiprofen	CC(C1=CC(=C(C=C1)C2=CC=CC=C2)F)C(=O)O	10.607	Class II
79	furosemide	C1=COC(=C1)CNC2=CC(=C(C=C2C(=O)O)S(=O)(=O)N)Cl	5.463	Class II
80	fursultiamine	CC1=NC=C(C(=N1)N)CN(C=O)C(=C(CCO)SSCC2CCCO2)C	5.355	Class II
81	gefitinib	COC1=C(C=C2C(=C1)N=CN=C2NC3=CC(=C(C=C3)F)Cl)OCCCN4CCOCC4	6.112	Class II
82	glibenclamide	COC1=C(C=C(C=C1)Cl)C(=O)NCCC2=CC=C(C=C2)S(=O)(=O)NC(=O)NC3CCCCC3	8.756	Class II
83	glimepiride	CCC1=C(CN(C1=O)C(=O)NCCC2=CC=C(C=C2)S(=O)(=O)NC(=O)NC3CCC(CC3)C)C	9.320	Class II
84	glipizide	CC1=NC=C(N=C1)C(=O)NCCC2=CC=C(C=C2)S(=O)(=O)NC(=O)NC3CCCCC3	7.827	Class II
86	glyceryl trinitrate	C(C(CO[N+](=O)[O-])O[N+](=O)[O-])O[N+](=O)[O-]	5.277	Class II
87	griseofulvin	CC1CC(=O)C=C(C12C(=O)C3=C(O2)C(=C(C=C3OC)OC)Cl)OC	4.465	Class II
88	haloperidol	C1CN(CCC1(C2=CC=C(C=C2)Cl)O)CCCC(=O)C3=CC=C(C=C3)F	8.490	Class II

No.	API	SMILES	LnK^{est}	BCS*
89	ibuprofen	CC(C)CC1=CC=C(C=C1)C(C)C(=O)O	10.426	Class II
90	iopanoic acid	CCC(CC1=C(C(=C(C=C1I)I)N)I)C(=O)O	8.035	Class II
91	irbesartan	CCCCC1=NC2(CCCC2)C(=O)N1CC3=CC=C(C=C3)C4=CC=CC=C4C5=NNN=N5	11.184	Class II
92	isotretinoin	CC1=C(C(CCC1)(C)C)C=CC(=CC=CC(=CC(=O)O)C)C	12.422	Class II
93	itraconazole	CCC(C)N1C(=O)N(C=N1)C2=CC=C(C=C2)N3CCN(CC3)C4=CC=C(C=C4)OCC5COC(O5)(CN6C=NC=N6)C7=C(C=C(C=C7)Cl)Cl	0.662	Class II
94	ivermectin	CCC(C)C1C(CCC2(O1)CC3CC(O2)CC=C(C(C(C=CC=C4COC5C4(C(C=C(C5O)C)C(=O)O3)O)C)OC6CC(C(C(O6)C)OC7CC(C(C(O7)C)O)OC)OC)C)C	2.013	Class II
95	ketoprofen	CC(C1=CC=CC(=C1)C(=O)C2=CC=CC=C2)C(=O)O	8.559	Class II
96	lamotrigine	C1=CC(=C(C(=C1)Cl)Cl)C2=C(N=C(N=N2)N)N	6.406	Class II
97	letrozole	C1=CC(=CC=C1C#N)C(C2=CC=C(C=C2)C#N)N3C=NC=N3	4.313	Class II
98	lopinavir	CC1=C(C(=CC=C1)C)OCC(=O)NC(CC2=CC=CC=C2)C(CC(CC3=CC=CC=C3)NC(=O)C(C(C)C)N4CCCNC4=O)O	11.268	Class II
99	loratadine	CCOC(=O)N1CCC(=C2C3=C(CCC4=C2N=CC=C4)C=C(C=C3)Cl)CC1	6.915	Class II
100	lovastatin	CCC(C)C(=O)OC1CC(C=C2C1C(C(C=C2)C)CCC3CC(CC(=O)O3)O)C	7.600	Class II
101	mebendazole	COC(=O)NC1=NC2=C(N1)C=C(C=C2)C(=O)C3=CC=CC=C3	8.974	Class II
102	medroxyprogesterone acetate	CC1CC2C(CCC3(C2CCC3(C(=O)C)OC(=O)C)C)C4(C1=CC(=O)CC4)C	10.949	Class II
103	meloxicam	CC1=CN=C(S1)NC(=O)C2=C(C3=CC=CC=C3S(=O)(=O)N2C)O	7.164	Class II

No.	API	SMILES	LnK^{est}	BCS*
104	menatetrenone	CC1=C(C(=O)C2=CC=CC=C2C1=O)CC=C(C)CCC=C(C)CCC=C(C)CCC=C(C)C	12.348	Class II
105	metaxalone	CC1=CC(=CC(=C1)OCC2CNC(=O)O2)C	6.586	Class II
106	morphine sulfate	CN1CCC23C4C1CC5=C2C(=C(C=C5)O)OC3C(C=C4)O	7.213	Class II
107	mycophenolate mofetil	CC1=C(C(=C(C2=C1COC2=O)O)CC=C(C)CCC(=O)OCCN3CCOCC3)OC	3.767	Class II
108	nabumetone	CC(=O)CCC1=CC2=C(C=C1)C=C(C=C2)OC	8.071	Class II
109	nevirapine	CC1=C2C(=NC=C1)N(C3=C(C=CC=N3)C(=O)N2)C4CC4	6.723	Class II
110	nicergoline	CN1CC(CC2(C1CC3=CN(C4=CC=CC2=C34)C)OC)COC(=O)C5=CC(=CN=C5)Br	7.587	Class II
111	niclosamide	C1=CC(=C(C=C1[N+](=O)[O-])Cl)NC(=O)C2=C(C=CC(=C2)Cl)O	7.410	Class II
112	nifedipine	CC1=C(C(C(=C(N1)C)C(=O)OC)C2=CC=CC=C2[N+](=O)[O-])C(=O)OC	6.948	Class II
113	nimesulide	CS(=O)(=O)NC1=C(C=C(C=C1)[N+](=O)[O-])OC2=CC=CC=C2	8.133	Class II
114	olanzapine	CC1=CC2=C(S1)NC3=CC=CC=C3N=C2N4CCN(CC4)C	7.369	Class II
115	orlistat	CCCCCCCCCCCC(CC1C(C(=O)O1)CCCCCC)OC(=O)C(CC(C)C)NC=O	7.572	Class II
116	perindopril erbumine	CCCC(C(=O)OCC)NC(C)C(=O)N1C2CCCCC2CC1C(=O)O.CC(C)(C)N	7.162	Class II
117	phenytoin	C1=CC=C(C=C1)C2(C(=O)NC(=O)N2)C3=CC=CC=C3	7.552	Class II
118	phenytoin sodium	C1=CC=C(C=C1)C2(C(=O)[N-]C(=O)N2)C3=CC=CC=C3.[Na+]	8.011	Class II
119	praziquantel	C1CCC(CC1)C(=O)N2CC3C4=CC=CC=C4CCN3C(=O)C2	7.981	Class II
120	prednisolone	CC12CC(C3C(C1CCC2(C(=O)CO)O)CCC4=CC(=O)C=CC34C)O	8.617	Class II

No.	API	SMILES	LnK^{est}	BCS*
121	pyrantel embonate	CN1CCCN=C1C=CC2=CC=CS2.C1=CC=C2C(=C1)C=C(C(=C2CC3=C(C(=CC4=CC=CC=C43)C(=O)O)O)O)C(=O)O	4.535	Class II
122	pyrimethamine	CCC1=C(C(=NC(=N1)N)N)C2=CC=C(C=C2)Cl	6.646	Class II
123	rebamipide	C1=CC=C2C(=C1)C(=CC(=O)N2)CC(C(=O)O)NC(=O)C3=CC=C(C=C3)Cl	7.917	Class II
124	retinol palmitate	CCCCCCCCCCCCCCCC(=O)OCC=C(C)C=CC=C(C)C=CC1=C(CCCC1(C)C)C	21.946	Class II
125	rifampicin	CC1C=CC=C(C(=O)NC2=C(C3=C(C4=C(C(=C3O)C)OC(C4=O)(OC=CC(C(C(C(C(C(C1O)C)O)C)OC(=O)C)C)OC)C)C(=C2C=NN5CCN(CC5)C)O)O)C	3.958	Class II
126	risperidone	CC1=C(C(=O)N2CCCCC2=N1)CCN3CCC(CC3)C4=NOC5=C4C=CC(=C5)F	6.868	Class II
127	ritonavir	CC(C)C1=NC(=CS1)CN(C)C(=O)NC(C(C)C)C(=O)NC(CC2=CC=CC=C2)CC(C(CC3=CC=CC=C3)NC(=O)OCC4=CN=CS4)O	12.463	Class II
128	rofecoxib	CS(=O)(=O)C1=CC=C(C=C1)C2=C(C(=O)OC2)C3=CC=CC=C3	9.614	Class II
129	roxithromycin	CCC1C(C(C(C(=NOCOCCOC)C(CC(C(C(C(C(C(=O)O1)C)OC2CC(C(C(O2)C)O)(C)OC)C)OC3C(C(CC(O3)C)N(C)C)O)(C)O)C)C)O)(C)O	5.065	Class II
130	simvastatin	CCC(C)(C)C(=O)OC1CC(C=C2C1C(C(C=C2)C)CCC3CC(CC(=O)O3)O)C	9.364	Class II
131	spironolactone	CC(=O)SC1CC2=CC(=O)CCC2(C3C1C4CCC5(C4(CC3)C)CCC(=O)O5)C	9.911	Class II
132	sulfasalazine	C1=CC=NC(=C1)NS(=O)(=O)C2=CC=C(C=C2)N=NC3=CC(=C(C=C3)O)C(=O)O	8.413	Class II
133	tamoxifen citrate	CCC(=C(C1=CC=CC=C1)C2=CC=C(C=C2)OCCN(C)C)C3=CC=CC=C3.C(C(=O)O)C(CC(=O)O)(C(=O)O)O	13.075	Class II

No.	API	SMILES	LnK^{est}	BCS*
134	telmisartan	CCCC1=NC2=C(C=C(C=C2N1CC3=CC=C(C=C3)C4=CC=CC=C4C(=O)O)C5=NC6=CC=CC=C6N5C)C	13.148	Class II
135	teprenone	CC(=CCCC(=CCCC(=CCCC(=CCCC(=O)C)C)C)C)C	12.508	Class II
136	tocopherol nicotinate	CC1=C2C(=C(C(=C1C)OC(=O)C3=CN=CC=C3)C)CCC(O2)(C)CCCC(C)CCCC(C)CCCC(C)C	12.136	Class II
137	triflusal	CC(=O)OC1=C(C=CC(=C1)C(F)(F)F)C(=O)O	6.934	Class II
138	ursodeoxycholic acid (ursodiol)	CC(CCC(=O)O)C1CCC2C1(CCC3C2C(CC4C3(CCC(C4)O)C)O)C	12.364	Class II
139	valproic acid	CCCC(CCC)C(=O)O	7.762	Class II
140	valsartan	CCCCC(=O)N(CC1=CC=C(C=C1)C2=CC=CC=C2C3=NNN=N3)C(C(C)C)C(=O)O	11.789	Class II
141	warfarin sodium	CC(=O)CC(C1=CC=CC=C1)C2=C(C3=CC=CC=C3OC2=O)[O-].[Na+]	9.164	Class II
142	zaltoprofen	CC(C1=CC2=C(C=C1)SC3=CC=CC=C3C(=O)C2)C(=O)O	8.186	Class II
143	zolmitriptan	CN(C)CCC1=CNC2=C1C=C(C=C2)CC3COC(=O)N3	7.136	Class II
144	acarbose	CC1C(C(C(C(O1)OC2C(OC(C(C2O)O)OC3C(OC(C(C3O)O)O)CO)CO)O)O)NC4C=C(C(C(C4O)O)O)CO	4.589	Class III
145	acyclovir	C1=NC2=C(N1COCCO)N=C(NC2=O)N	5.495	Class III
146	alendronate sodium	C(CC(O)(P(=O)(O)O)P(=O)(O)[O-])CN.[Na+]	3.859	Class III
147	ascorbic acid	C(C(C1C(=C(C(=O)O1)O)O)O)O	4.571	Class III
148	atenolol	CC(C)NCC(COC1=CC=C(C=C1)CC(=O)N)O	5.606	Class III
149	benznidazole	C1=CC=C(C=C1)CNC(=O)CN2C=CN=C2[N+](=O)[O-]	6.944	Class III
150	capecitabine	CCCCCOC(=O)NC1=NC(=O)N(C=C1F)C2C(C(C(O2)C)O)O	5.546	Class III
151	captopril	CC(CS)C(=O)N1CCCC1C(=O)O	5.872	Class III
152	cefaclor	C1C(=C(N2C(S1)C(C2=O)NC(=O)C(C3=CC=CC=C3)N)C(=O)O)Cl	5.173	Class III

No.	API	SMILES	LnK^{est}	BCS*
153	cefmetazole sodium	CN1C(=NN=N1)SCC2=C(N3C(C(C3=O)(NC(=O)CSCC#N)OC)SC2)C(=O)[O-].[Na+]	4.535	Class III
154	cefroxadine	COC1=C(N2C(C(C2=O)NC(=O)C(C3=CCC=CC3)N)SC1)C(=O)O	5.218	Class III
155	chloramphenicol	C1=CC(=CC=C1C(C(CO)NC(=O)C(Cl)Cl)O)[N+](=O)[O-]	5.894	Class III
156	choline alfoscerate	C[N+](C)(C)CCOP(=O)([O-])OCC(CO)O	5.679	Class III
157	cimetidine	CC1=C(N=CN1)CSCCNC(=NC)NC#N	6.674	Class III
158	cyclophosphamide	C1CNP(=O)(OC1)N(CCCl)CCCl	5.578	Class III
159	dapsone	C1=CC(=CC=C1N)S(=O)(=O)C2=CC=C(C=C2)N	6.071	Class III
160	didanosine	C1CC(OC1CO)N2C=NC3=C2N=CNC3=O	4.995	Class III
161	dl-methionine	CSCCC(C(=O)O)N	5.157	Class III
162	doxifluridine	CC1C(C(C(O1)N2C=C(C(=O)NC2=O)F)O)O	5.152	Class III
163	enalapril maleate	CCOC(=O)C(CCC1=CC=CC=C1)NC(C)C(=O)N2CCCC2C(=O)O.C(=CC(=O)O)C(=O)O	7.075	Class III
164	ethosuximide	CCC1(CC(=O)NC1=O)C	6.022	Class III
165	famciclovir	CC(=O)OCC(CCN1C=NC2=CN=C(N=C21)N)COC(=O)C	5.305	Class III
166	famotidine	C1=C(N=C(S1)N=C(N)N)CSCCC(=NS(=O)(=O)N)N	5.233	Class III
167	fluconazole	C1=CC(=C(C=C1F)F)C(CN2C=NC=N2)(CN3C=NC=N3)O	4.650	Class III
168	gabapentin	C1CCC(CC1)(CC(=O)O)CN	7.539	Class III
169	gliclazide	CC1=CC=C(C=C1)S(=O)(=O)NC(=O)NN2CC3CCCC3C2	8.190	Class III
170	isoniazid	C1=CN=CC=C1C(=O)NN	3.637	Class III
171	isosorbide dinitrate	C1C(C2C(O1)C(CO2)O[N+](=O)[O-])O[N+](=O)[O-]	4.614	Class III
172	lamivudine	C1C(OC(S1)CO)N2C=CC(=NC2=O)N	5.141	Class III
173	levetiracetam	CCC(C(=O)N)N1CCCC1=O	5.030	Class III
174	levodopa	C1=CC(=C(C=C1CC(C(=O)O)N)O)O	4.970	Class III

No.	API	SMILES	LnK^{est}	BCS*
175	levofloxacin	CC1COC2=C3N1C=C(C(=O)C3=CC(=C2N4CCN(CC4)C)F)C(=O)O	4.391	Class III
176	lisinopril	C1CC(N(C1)C(=O)C(CCCCN)NC(CCC2=CC=CC=C2)C(=O)O)C(=O)O	5.270	Class III
177	mesalazine	C1=CC(=C(C=C1N)C(=O)O)O	4.226	Class III
178	methotrexate	CN(CC1=CN=C2C(=N1)C(=NC(=N2)N)N)C3=CC=C(C=C3)C(=O)NC(CCC(=O)O)C(=O)O	4.981	Class III
179	methyldopa	CC(CC1=CC(=C(C=C1)O)O)(C(=O)O)N	4.822	Class III
180	methylmethioninesulfonium chloride	C[S+](C)CCC(C(=O)O)N.[Cl-]	5.412	Class III
181	modafinil	C1=CC=C(C=C1)C(C2=CC=CC=C2)S(=O)CC(=O)N	7.872	Class III
182	neostigmine bromide	CN(C)C(=O)OC1=CC=CC(=C1)[N+](C)(C)C.[Br-]	6.387	Class III
183	niacin	C1=CC(=CN=C1)C(=O)O	4.504	Class III
184	nicorandil	C1=CC(=CN=C1)C(=O)NCCO[N+](=O)[O-]	5.631	Class III
185	nicotinamide	C1=CC(=CN=C1)C(=O)N	3.981	Class III
186	nifurtimox	CC1CS(=O)(=O)CCN1N=CC2=CC=C(O2)[N+](=O)[O-]	6.819	Class III
187	nilvadipine	CC1=C(C(C(=C(N1)C#N)C(=O)OC)C2=CC(=CC=C2)[N+](=O)[O-])C(=O)OC(C)C	5.349	Class III
188	nizatidine	CNC(=C[N+](=O)[O-])NCCSCC1=CSC(=N1)CN(C)C	7.075	Class III
189	nystatin	CC1C=CC=CCCC=CC=CC=CC=CC(CC2C(C(CC(O2)(CC(C(CCC(CC(CC(CC(=O)OC(C(C1O)C)C)O)O)O)O)O)O)O)O)C(=O)O)OC3C(C(C(C(O3)C)O)N)O	5.015	Class III
190	oxcarbazepine	C1C2=CC=CC=C2N(C3=CC=CC=C3C1=O)C(=O)N	6.827	Class III
191	pamidronate disodium	C(CN)C(O)(P(=O)(O)[O-])P(=O)(O)[O-].[Na+].[Na+]	0.764	Class III
192	penicillamine	CC(C)(C(C(=O)O)N)S	4.746	Class III
193	pyrazinamide	C1=CN=C(C=N1)C(=O)N	3.775	Class III
194	pyridostigmine bromide	C[N+]1=CC=CC(=C1)OC(=O)N(C)C.[Br-]	6.166	Class III

No.	API	SMILES	LnK^{est}	BCS*
195	ribavirin	C1=NC(=NN1C2C(C(C(O2)CO)O)O)C(=O)N	5.353	Class III
196	riboflavin	CC1=CC2=C(C=C1C)N(C3=NC(=O)NC(=O)C3=N2)CC(C(C(CO)O)O)O	5.035	Class III
197	risedronate sodium	C1=CC(=CN=C1)CC(O)(P(=O)(O)O)P(=O)(O)[O-].[Na+]	5.530	Class III
198	sodium iodide	[Na+].[I-]	-2.880	Class III
199	stavudine	CC1=CN(C(=O)NC1=O)C2C=CC(O2)CO	5.078	Class III
200	tegafur	C1CC(OC1)N2C=C(C(=O)NC2=O)F	4.815	Class III
201	thiamine	CC1=C(SC=[N+]1CC2=CN=C(N=C2N)C)CCO	5.457	Class III
202	topiramate	CC1(OC2COC3(C(C2O1)OC(O3)(C)C)COS(=O)(=O)N)C	4.291	Class III
203	voglibose	C1C(C(C(C(C1(CO)O)O)O)O)NC(CO)CO	4.486	Class III
204	zidovudine	CC1=CN(C(=O)NC1=O)C2CC(C(O2)CO)N=[N+]=[N-]	5.253	Class III
205	acetaminophen	CC(=O)NC1=CC=C(C=C1)O	6.040	Class IV
206	acetazolamide	CC(=O)NC1=NN=C(S1)S(=O)(=O)N	4.865	Class IV
207	acetylsalicylic acid	CC(=O)OC1=CC=CC=C1C(=O)O	6.830	Class IV
208	allopurinol	C1=NNC2=C1C(=O)NC=N2	4.146	Class IV
209	amoxicillin	CC1(C(N2C(S1)C(C2=O)NC(=O)C(C3=CC=C(C=C3)O)N)C(=O)O)C	5.050	Class IV
210	azathioprine	CN1C=NC(=C1SC2=NC=NC3=C2NC=N3)[N+](=O)[O-]	5.246	Class IV
211	cefdinir	C=CC1=C(N2C(C(C2=O)NC(=O)C(=NO)C3=CSC(=N3)N)SC1)C(=O)O	5.048	Class IV
212	cefditoren pivoxil	CC1=C(SC=N1)C=CC2=C(N3C(C(C3=O)NC(=O)C(=NOC)C4=CSC(=N4)N)SC2)C(=O)OCOC(=O)C(C)(C)C	6.371	Class IV
213	cefixime	C=CC1=C(N2C(C(C2=O)NC(=O)C(=NOCC(=O)O)C3=CSC(=N3)N)SC1)C(=O)O	4.856	Class IV
214	cefpodoxime proxetil	CC(C)OC(=O)OC(C)OC(=O)C1=C(CSC2N1C(=O)C2NC(=O)C(=NOC)C3=CSC(=N3)N)COC	4.759	Class IV

No.	API	SMILES	LnK^{est}	BCS*
215	cefuroxime axetil	CC(OC(=O)C)OC(=O)C1=C(CSC2N1C(=O)C2NC(=O)C(=NOC)C3=CC=CO3)COC(=O)N	4.297	Class IV
216	folic acid	C1=CC(=CC=C1C(=O)NC(CCC(=O)O)C(=O)O)NCC2=CN=C3C(=N2)C(=O)NC(=N3)N	5.325	Class IV
217	hydrochlorothiazide	C1NC2=CC(=C(C=C2S(=O)(=O)N1)S(=O)(=O)N)Cl	5.217	Class IV
218	l-carbocysteine	C(C(C(=O)O)N)SCC(=O)O	5.172	Class IV
219	levosulpiride	CCN1CCCC1CNC(=O)C2=C(C=CC(=C2)S(=O)(=O)N)OC	5.280	Class IV
220	linezolid	CC(=O)NCC1CN(C(=O)O1)C2=CC(=C(C=C2)N3CCOCC3)F	5.191	Class IV
221	metronidazole	CC1=NC=C(N1CCO)[N+](=O)[O-]	4.868	Class IV
222	nalidixic acid	CCN1C=C(C(=O)C2=C1N=C(C=C2)C)C(=O)O	5.563	Class IV
223	nitrofurantoin	C1C(=O)NC(=O)N1N=CC2=CC=C(O2)[N+](=O)[O-]	5.969	Class IV
224	phenobarbital	CCC1(C(=O)NC(=O)NC1=O)C2=CC=CC=C2	6.594	Class IV
225	propylthiouracil	CCCC1=CC(=O)NC(=S)N1	5.175	Class IV
226	sulfadiazine	C1=CN=C(N=C1)NS(=O)(=O)C2=CC=C(C=C2)N	6.007	Class IV
227	sulfamethoxazole	CC1=CC(=NO1)NS(=O)(=O)C2=CC=C(C=C2)N	6.720	Class IV
228	theophylline	CN1C2=C(C(=O)N(C1=O)C)NC=N2	5.675	Class IV
229	trimethoprim	COC1=CC(=CC(=C1OC)OC)CC2=CN=C(N=C2N)N	5.248	Class IV

*Source: Dahan, A.; Wolk, O.; Kim, Y.H.; Ramachandran, C.; Crippen, G.M.; Takagi, T.; Bermejo, M.; Amidon, G.L. Purely in silico BCS classification: Science based quality standards for the world's drugs. Mol. Pharm. 2013, 10, 4378–4390