APPENDICES

Appendix I. Dataset A (HIA data) used in Chapter 2.

ID	Name	SMILES	HIA (%)	Class
1	Arbekacin	O1C(CO)C(O)C(N)C(O)C1OC1C(O)C(OC2OC(CCC2N)CN)C(N)CC1NC(=O)C(O)CCN	0	low
2	Azlocillin	S1C2N(C(C(O)=O)C1(C)C)C(=O)C2NC(=O)C(NC(=O)N1CCNC1=O)c1ccccc1	0	low
3	Cefodizime	s1c(CC(O)=O)c(nc1SCC=1CSC2N(C(=O)C2NC(=O)\C(=N/OC)\c2nc(sc2)N)C=1C(O)=O)C	0	low
4	Gentamicin_C1	O1C(OC2C(O)C(OC3OCC(O)(C)C(NC)C3O)C(N)CC2N)C(N)CCC1C(NC)C	0	low
5	Gentamicin_C1a	O1C(OC2C(O)C(OC3OCC(O)(C)C(NC)C3O)C(N)CC2N)C(N)CCC1CC	0	low
6	Lucifer_Yellow_CH	S(O)(=O)(=O)c1cc2c3c(cc(S(O)(=O)=O)cc3c1N)C(=O)N(NNC(=O)NN)C2=O	0	low
7	Meropenem	S(C=1C(C2N(C(=O)C2C(O)C)C=1C(O)=O)C)C1NC(CC1)C(=O)N(C)C	0	low
8	Mezlocillin	S1C2N(C(C(O)=O)C1(C)C)C(=O)C2NC(=O)C(NC(=O)N1CCN(S(=O)(=O)C)C1=O)c1ccccc1	0	low
9	Netilmicin	O1C(=CC(N)CC1OC1C(O)C(OC2OCC(O)(C)C(NC)C2O)C(NCC)CC1N)CN	0	low
10	Pentamidine	O(CCCCCOc1ccc(cc1)C(N)=N)c1ccc(cc1)C(N)=N	0	low
11	Raffinose	O1C(OC2OC(COC3OC(CO)C(O)C(O)C3O)C(O)C(O)C2O)(CO)C(O)C(O)C1CO	0	low
12	Streptozocin	O1C(CO)C(O)C(O)C(NC(=O)N(N=O)C)C1O	0	low
13	Tobramycin	O1C(CO)C(O)C(N)C(O)C1OC1C(O)C(OC2OC(CN)C(O)CC2N)C(N)CC1N	0	low
14	Vancomycin	Clc1c2Oc3cc4C(NC(=O)C(NC(=O)C(NC(=O)C(NC)CC(C)C)C(O)c(c1)cc2)CC(=O)N)C(=O)NC1c2cc(-c5c(cc(O)cc5O)C(NC(=O)C(NC1=O)C(O)c1cc(Cl)c(Oc(c4)c3OC3OC(CO)C(O)C(O)C3OC3OC(C)C(O)C(N)(C3)C)cc1)C(O)=O)c(O)cc2	0	low
15	Amikacin	O1C(CN)C(O)C(O)C(O)C1OC1C(O)C(OC2OC(CO)C(O)C(N)C2O)C(NC(=O)C(O)CCN)CC1N	0	low
16	Moxalactam	S(CC=1COC2N(C(=O)C2(OC)NC(=O)C(C(O)=O)c2ccc(O)cc2)C=1C(O)=O)c1nnnn1C	0	low
17	Alendronic_acid	P(O)(O)(=O)C(P(O)(O)=O)(O)CCCN	1	low
18	Aztreonam	s1cc(nc1N)/C(=N/OC(C(O)=O)(C)C)/C(=O)NC1C(N(S(O)(=O)=O)C1=O)C	1	low
19	Ceftriaxone	s1cc(nc1N)/C(=N/OC)/C(=O)NC1C2SCC(CSC3=NC(=O)C(O)=NN3C)=C(N2C1=O)C(O)=O	1	low
20	Lactulose	O1C(O)(CO)C(O)C(OC2OC(CO)C(O)C(O)C2O)C1CO	1	low
21	Risedronic_acid	P(O)(O)(=O)C(P(O)(O)=O)(O)Cc1cccnc1	1	low

22	Streptomycin	O1C(CO)C(O)C(O)C(NC)C1OC1C(O)(C=O)C(OC1OC1C(NC(N)=N)C(O)C(NC(N)=N)C(O)C1O)C	1	low
23	Kanamycin	O1C(CNC(=O)C)C(O)C(O)C(O)C1OC1C(O)C(OC2OC(CO)C(O)C(N)C2O)C(N)CC1N	1	low
24	Acarbose	O1C(C)C(NC2C=C(CO)C(O)C(O)C2O)C(O)C(O)C1OC1C(O)C(O)C(OC1CO)OC1C(O)C(O)C(OC1CO)O	2	low
25	Zanamivir	O1C(C(O)C(O)CO)C(NC(=O)C)C(NC(N)=N)C=C1C(O)=O	2	low
26	Amphotericin_B	O1C(C)C(O)C(N)C(O)C1OC1(O)\C=C\C=C\C=C/C=C/C=C\C=C\C=C\C(C)C(O)C(C)C(OC(=O)CC(O)CC(O)CCC(O)C(O)CC(O)CC2(OC(C1)C(C(O)=O)C(O)C2)O)C	3	low
27	Clodronate	ClC(Cl)(P(O)(O)=O)P(O)(O)=O	3	low
28	Nedocromil	O1c2c(cc3c(N(CC)C(=CC3=O)C(O)=O)c2CCC)C(=O)C=C1C(O)=O	3	low
29	Neomycin	O1C(COC2C(O)C(OC2CO)OC2C(OC3OC(CN)C(O)C(O)C3N)C(N)CC(N)C2O)C(N)C(O)C(O)C1CN	3	low
30	Amygdalin	O1C(COC2OC(CO)C(O)C(O)C2O)C(O)C(O)C(O)C1OC(C#N)c1ccccc1	5	low
31	Cefotaxime	s1cc(nc1N)/C(=N\OC)/C(NC1C2SCC(COC(=O)C)=C(N2C1=O)C(O)=O)=C	5	low
32	Chlorhexidine	Clc1ccc(NC(NC(NCCCCNC(NC(Nc2ccc(Cl)cc2)=N)=N)=N)=N)cc1	5	low
33	Diatrizoate	Ic1c(C(O)=O)c(I)c(NC(=O)C)c(I)c1NC(=O)C	5	low
34	Edetic_acid	OC(=O)CN(CCN(CC(O)=O)CC(O)=O)CC(O)=O	5	low
35	Etidronate	P(O)(O)(=O)C(P(O)(O)=O)(O)C	5	low
36	Imipenem	S(CC\N=C\N)C=1CC2N(C(=O)C2C(O)C)C=1C(O)=O	5	low
37	Iohexol	Ic1c(C(=O)NCC(O)CO)c(I)c(N(C(=O)C)CC(O)CO)c(I)c1C(=O)NCC(O)CO	5	low
38	Iotroxic_acid	Ic1c(C(O)=O)c(I)cc(I)c1NC(=O)COCCOCCOCC(=O)Nc1c(I)c(C(O)=O)c(I)cc1I	5	low
39	Mitoxantrone	Oc1c2c(C(=O)c3c(C2=O)c(NCCNCCO)ccc3NCCNCCO)c(O)cc1	5	low
40	Moexipril_diacid	O(C)c1cc2CC(N(Cc2cc1OC)C(=O)C(NC(CCc1ccccc1)C(O)=O)C)C(O)=O	5	low
41	Pamidronic_acid	P(O)(O)(=O)C(P(O)(O)=O)(O)CCN	5	low
42	Phthalylsulfathiazole	s1ccnc1NS(=O)(=O)c1ccc(NC(=O)c2ccccc2C(O)=O)cc1	5	low
43	Succinylsulfathiazole	s1ccnc1NS(=O)(=O)c1ccc(NC(=O)CCC(O)=O)cc1	5	low
44	Sulbactam	S1(=O)(=O)C2N(C(C(O)=O)C1(C)C)C(=O)C2	5	low
45	Ticarcillin	S1C2N(C(C(O)=O)C1(C)C)C(=O)C2NC(=O)C(C(O)=O)c1ccsc1	5	low
46	Tiludronic_acid	Clc1ccc(cc1)CC(P(O)(O)=O)P(O)(O)=O	6	low
47	Cefmetazole	S1C2N(C(=O)C2(OC)NC(=O)CSCC#N)C(C(O)=O)=C(C1)CSc1nnnn1C	10	low
48	Acamprosate	S(O)(=O)(=O)CCCNC(=O)C	11	low
49	Cilazaprilat	O=C1N2N(CCCC1NC(CCc1ccccc1)C(O)=O)CCCC2C(O)=O	20	low

50	Lincomycin	S(C)C1OC(C(NC(=O)C2N(CC(C2)CCC)C)C(O)C)C(O)C(O)C1O	28	low
51	Netivudine	O1C(CO)C(O)C(O)C1N1C=C(C#CC)C(=O)NC1=O	28	low
52	Fosmidomycin	P(O)(O)(=O)CCCN(O)C=O	30	low
53	AAFC	FC1=CN2C3OC(CO)C(O)C3OC2=NC1=N	32	high
54	Nadolol	O(CC(O)CNC(C)(C)C)c1c2CC(O)C(O)Cc2ccc1	32	high
55	Dihydroergotamine	O1C(NC(=O)C2CC3C(N(C2)C)Cc2c4c3cccc4[nH]c2)(C)C(=O)N2C(Cc3ccccc3)C(=O)N3C(CCC3)C12O	35	high
56	Erythromycin	O1C(CC)C(O)(C)C(O)C(C)C(=O)C(CC(O)(C)C(OC2OC(CC(N(C)C)C2O)C)C(C)C(OC2OC(C)C(O)C(OC)(C2)C)C(C)C1=O)C	35	high
57	Sulpiride	CCN1CCCC1CNC(=O)c2cc(ccc2OC)S(=O)(=O)N	40	high
58	Famotidine	s1cc(nc1\N=C(\N)/N)CSCC/C(=N/S(=O)(=O)N)/N	41	high
59	Metaproterenol	Oc1cc(cc(O)c1)C(O)CNC(C)C	43	high
60	Cymarin	O1CC(=CC1=O)[C@H]1CC[C@]2(O)[C@H]3[C@H](CC[C@]12C)[C@]1(CC[C@H](O[C@@H]2O[C@H](C)[C@@H](O)[C@@H](OC)C2)C[C@@]1(O)CC3)C=O	47	high
61	Rimiterol	Oc1cc(ccc1O)C(O)C1NCCCC1	48	high
62	Atenolol	O(CC(O)CNC(C)C)c1ccc(cc1)CC(=O)N	50	high
63	Cefpodoxime_proxetil	s1cc(nc1N)/C(=N\OC)/C(=O)NC1C2SCC(COC)=C(N2C1=O)C(OC(OC(OC(C)C)=O)C)=O	50	high
64	Guanoxan	O1c2c(OCC1CNC(N)=N)cccc2	50	high
65	Trandolapril	O(C(=O)C(NC(C(=O)N1C2C(CC1C(O)=O)CCCC2)C)CCc1ccccc1)CC	50	high
66	Metformin	N(C(NC(N)=N)=N)(C)C	54	high
67	Eflornithine	FC(F)C(N)(CCCN)C(O)=O	55	high
68	Valsartan	OC(=O)C(N(Cc1ccc(cc1)-c1ccccc1-c1[nH]nnn1)C(=O)CCCC)C(C)C	55	high
69	Tranexamic_acid	OC(=O)C1CCC(CC1)CN	55	high
70	Dipyridamole	OCCN(CCO)c1nc(N2CCCCC2)c2nc(nc(N3CCCCC3)c2n1)N(CCO)CCO	58	high
71	Oxytetracycline	OC12C(C(N(C)C)C(O)=C(C(=O)N)C1=O)C(O)C1C(C2=O)=C(O)c2c(cccc2O)C1(O)C	58	high
72	Cilazapril	O=C1N2N(CCCC1NC(CCc1ccccc1)C(OCC)=O)CCCC2C(O)=O	59	high
73	Fenoterol	Oc1cc(cc(O)c1)CC(O)NC(Cc1ccc(O)cc1)C	60	high
74	Ivermectin	O1C(C)C(O)C(OC)CC1OC1C(OC(OC2/C(=C\CC3OC4(OC5C(C4)C(C)C5C(CC)C)CC(OC(=O)C4C=C(C)C(O)C5OC\C(=C/C=C/C2C)\C45O)C3)/C)CC1OC)C	60	high
75	Oxycodone	O1C2C34CCN(C(Cc5c3c1c(OC)cc5)C4(O)CCC2=O)C	60	high
76	Pirbuterol	Oc1ccc(nc1CO)C(O)CNC(C)(C)C	60	high
77	Ramipril	O(C(=O)C(NC(C(=O)N1C2C(CC1C(O)=O)CCC2)C)CCc1ccccc1)CC	60	high

78	Ziprasidone	Clc1cc2NC(=O)Cc2cc1CCN1CCN(CC1)c1nsc2c1cccc2	60	high
79	Reproterol	Oc1cc(cc(O)c1)C(O)CNCCCn1c2c(nc1)N(C)C(=O)N(C)C2=O	60	high
80	Furosemide	Clc1cc(NCc2occc2)c(C(O)=O)c(S(=O)(=O)N)c1	61	high
81	Sulfasalazine	S(=O)(=O)(Nc1ncccc1)c1ccc(N=Nc2cc(C(O)=O)c(O)cc2)cc1	62	high
82	Terbutaline	Oc1cc(cc(O)c1)C(O)CNC(C)(C)C	63	high
83	Metolazone	Clc1cc2NC(N(c3ccccc3C)C(=O)c2cc1S(=O)(=O)N)C	64	high
84	Chlorthalidone	Clc1ccc(cc1S(=O)(=O)N)C1(O)NC(=O)c2c1cccc2	65	high
85	Tolrestat	S=C(N(CC(O)=O)C)c1c2c(cc(OC)cc2)c(cc1)C(F)(F)F	66	high
86	Hydroflumethiazide	S(=O)(=O)(N)c1cc2S(=O)(=O)NCNc2cc1C(F)(F)F	67	high
87	Sumatriptan	S(=O)(=O)(NC)Cc1cc2c([nH]cc2CCN(C)C)cc1	67	high
88	Hydrochlorothiazide	Clc1cc2NCNS(=O)(=O)c2cc1S(=O)(=O)N	68	high
89	Mibefradil	Fc1cc2c(cc1)C(C(C)C)C(OC(=O)CC)(CC2)CCN(CCCc1[nH]c2c(n1)cccc2)C	69	high
90	Anagrelide	Clc1c2CN3CC(=O)NC3=Nc2ccc1Cl	70	high
91	Benserazide	Oc1c(O)c(O)ccc1CNNC(=O)C(N)CO	70	high
92	Bromhexine	Brc1cc(Br)cc(CN(C)C2CCCCC2)c1N	70	high
93	Etodolac	O1CCC2C(Nc3c2cccc3CC)C1(CC(O)=O)CC(O)=O	70	high
94	Famciclovir	O(C(=O)C)CC(CCn1c2nc(ncc2nc1)N)COC(=O)C	70	high
95	Isocarboxazid	o1nc(cc1C)C(=O)NNCc1ccccc1	70	high
96	Mianserin	N12C(c3c(Cc4c1cccc4)cccc3)CN(CC2)C	70	high
97	Moxisylyte	O(C(=O)C)c1cc(C(C)C)c(OCCN(C)C)cc1C	70	high
98	Pimozide	Fc1ccc(cc1)C(CCN1CCC(N2c3c(NC2=O)cccc3)CC1)c1ccc(F)cc1	70	high
99	Naratriptan	S(=O)(=O)(NC)CCc1cc2cc([nH]c2cc1)C1CCN(CC1)C	70	high
100	Recainam	O=C(Nc1c(cccc1C)C)NCCCNC(C)C	71	high
101	Ceftizoxime	s1cc(nc1N)/C(=N/OC)/C(=O)NC1C2SCC=C(N2C1=O)C(O)=O	72	high
102	Cycloserine	O1NC(=O)C(N)C1	72	high
103	Desogestrel	OC1(CCC2C3C(C4C(CC3)=CCCC4)C(CC12CC)=C)C#C	72	high
104	Benzbromarone	Brc1cc(cc(Br)c1O)C(=O)c1c2c(oc1CC)cccc2	73	high
105	Quetiapine	S1c2c(cccc2)C(=Nc2c1cccc2)N1CCN(CC1)CCOCCO	73	high
106	Almotriptan	S(=O)(=O)(N1CCCC1)Cc1cc2c([nH]cc2CCN(C)C)cc1	75	high
107	Clavulanic_acid	C1[C@@H]2N(C1=O)[C@H](/C(=C/CO)/O2)C(=O)O	75	high
108	Ketoconazole	Clc1cc(Cl)ccc1C1(OC(CO1)COc1ccc(N2CCN(CC2)C(=O)C)cc1)Cn1ccnc1	75	high
109	Mesna	S(O)(=O)(=O)CCS	75	high
110	Oseltamivir	O(C(CC)CC)C1C=C(CC(N)C1NC(=O)C)C(OCC)=O	75	high
111	Primidone	O=C1NCNC(=O)C1(CC)c1ccccc1	75	high

112	Estramustine	ClCCN(CCCl)C(Oc1cc2CCC3C4CCC(O)C4(CCC3c2cc1)C)=O	75	high
113	Propylthiouracil	S=C1NC(=CC(=O)N1)CCC	76	high
114	Ethylmorphine	O1C2C34C5C1=C(O)C=CC5CC(N(CC3)CC)C4C=CC2O	77	high
115	Pantoprazole	S(=O)(Cc1nccc(OC)c1OC)c1[nH]c2c(n1)cc(OC(F)F)cc2	77	high
116	Sibutramine	Clc1ccc(cc1)C1(CCC1)C(N(C)C)CC(C)C	77	high
117	Tolterodine	Oc1ccc(cc1C(CCN(C(C)C)C(C)C)c1ccccc1)C	77	high
118	Guanabenz	Clc1cccc(Cl)c1\C=N\NC(N)=N	78	high
119	Mefloquine	FC(F)(F)c1c2nc(cc(c2ccc1)C(O)C1NCCCC1)C(F)(F)F	78	high
120	Urapidil	O(C)c1ccccc1N1CCN(CC1)CCCNC=1N(C)C(=O)N(C)C(=O)C=1	78	high
121	Ethambutol	OCC(NCCNC(CC)CO)CC	78	high
122	Zatebradin	O(C)c1cc(ccc1OC)CCN(CCCN1CCc2cc(OC)c(OC)cc2CC1=O)C	79	high
123	Acetohexamide	S(=O)(=O)(\N=C(/O)\NC1CCCCC1)c1ccc(cc1)C(=O)C	80	high
124	Allopurinol	O=C1NC=Nc2[nH]ncc12	80	high
125	Carvedilol	O(CCNCC(OCc1c2c3c([nH]c2ccc1)cccc3)O)c1ccccc1OC	80	high
126	Chlorpheniramine	Clc1ccc(cc1)C(c2ncccc2)CCN(C)C	80	high
127	Clonazepam	Clc1ccccc1C1=NCC(=O)Nc2c1cc([N+](=O)[O-])cc2	80	high
128	Dantrolene	o1c(ccc1\C=N\N1CC(=O)NC1=O)-c1ccc([N+](=O)[O-])cc1	80	high
129	Enoximone	S(C)c1ccc(cc1)C(=O)C=1NC(=O)NC=1C	80	high
130	Floxacillin	Clc1cccc(F)c1-c1noc(C)c1C(=O)NC1C2SC(C)(C)C(N2C1=O)C(O)=O	80	high
131	Flunarizine	Fc1ccc(cc1)C(N1CCN(CC1)CCCc1ccccc1)c1ccc(F)cc1	80	high
132	Fluoxetine	FC(F)(F)c1ccc(OC(CCNC)c2ccccc2)cc1	80	high
133	Guanadrel	O1C(COC12CCCCC2)CNC(N)=N	80	high
134	Isoniazid	O=C(NN)c1ccncc1	80	high
135	Itraconazole	Clc1cc(Cl)ccc1C1(OC(CO1)COc1ccc(N2CCN(CC2)c2ccc(N3C=NN(C(CC)C)C3=O)cc2)cc1)Cn1ncnc1	80	high
136	Mesalamine	Oc1ccc(N)cc1C(O)=O	80	high
137	Methadone	O=C(C(CC(N(C)C)C)(c1ccccc1)c1ccccc1)CC	80	high
138	Methoxyamphetamine	O(C)c1cc(ccc1)CC(N)C	80	high
139	Methylphenidate	O(C(=O)C(C1NCCCC1)c1ccccc1)C	80	high
140	Modafinil	S(=O)(C(c1ccccc1)c1ccccc1)CC(=O)N	80	high
141	Nabumetone	O(C)c1cc2c(cc(cc2)CCC(=O)C)cc1	80	high
142	Omeprazole	S(=O)(Cc1ncc(C)c(OC)c1C)c1[nH]c2c(n1)cc(OC)cc2	80	high
143	Oxamniquine	OCc1cc2CCC(Nc2cc1[N+](=O)[O-])CNC(C)C	80	high
144	Pramipexole	s1c2CC(NCCC)CCc2nc1N	80	high

145	Quinidine	O(C)c1cc2c(nccc2C(O)C2N3CC(C(C2)CC3)C=C)cc1	80	high
146	Riboflavin	O=C1NC(=O)N=C2N(c3cc(C)c(cc3N=C12)C)CC(O)C(O)C(O)CO	80	high
147	Terbinafine	N(Cc1c2c(ccc1)cccc2)(C\C=C\C#CC(C)(C)C)C	80	high
148	Ticlopidine	Clc1ccccc1CN1CCc2sccc2C1	80	high
149	Trimeprazine	S1c2c(N(c3c1cccc3)CC(CN(C)C)C)cccc2	80	high
150	Trimipramine	N(CC(CN1c2c(CCc3c1cccc3)cccc2)C)(C)C	80	high
151	Vitamin_A	OC\C=C(\C=C\C=C(\C=C\C=1C(CCCC=1C)(C)C)/C)/C	80	high
152	Cyproheptadine	N1(CCC(CC1)=C1c2c(C=Cc3c1cccc3)cccc2)C	80	high
153	Flunisolide	FC1C2=CC(=O)C=CC2(C2C(C3CC4OC(OC4(C(=O)CO)C3(CC2O)C)(C)C)C1)C	80	high
154	Losartan	Clc1nc(n(Cc2ccc(cc2)-c2ccccc2-c2[nH]nnn2)c1CO)CCCC	80	high
155	Metyrapone	O=C(C(C)(C)c1cccnc1)c1cccnc1	80	high
156	Pizotyline	CN1CCC(=C2c3ccccc3CCc4c2ccs4)CC1	80	high
157	Flecainide	FC(F)(F)COc1ccc(OCC(F)(F)F)cc1C(=O)NCC1NCCCC1	81	high
158	Piroximone	O=C1NC(C(=O)c2ccncc2)=C(N1)CC	81	high
159	Aspirin	O(C(=O)C)c1ccccc1C(O)=O	82	high
160	Ibutilide	S(=O)(=O)(Nc1ccc(cc1)C(O)CCCN(CCCCCCC)CC)C	82	high
161	Methylprednisolone	OC1(CCC2C3C(C4(C(=CC(=O)C=C4)C(C3)C)C)C(O)CC12C)C(=O)CO	82	high
162	Mifobate	Clc1ccc(cc1)C(P(OC)(OC)=O)CP(OC)(OC)=O	82	high
163	Sorivudine	Br\C=C\C1CN(C2OC(CO)C(O)C2O)C(=O)NC1=O	82	high
164	Albuterol	Oc1ccc(cc1C(O)=O)C(O)CNC(C)(C)C	83	high
165	Milrinone	O=C1NC(C)=C(C=C1C#N)c1ccncc1	83	high
166	Nateglinide	OC(=O)C(NC(=O)C1CCC(CC1)C(C)C)Cc1ccccc1	83	high
167	Bromazepam	Brc1cc2c(NC(=O)CN=C2c2ncccc2)cc1	84	high
168	Propiverine	O(C(=O)C(OCCC)(c1ccccc1)c1ccccc1)C1CCN(CC1)C	84	high
169	Acebutolol	O(CC(O)CNC(C)C)c1ccc(NC(=O)CCC)cc1C(=O)C	85	high
170	Acetaminophen	Oc1ccc(NC(=O)C)cc1	85	high
171	Chlorguanide	Clc1ccc(NC(NC(NC(C)C)=N)=N)cc1	85	high
172	Dolasetron	O(C(=O)c1c2c([nH]c1)cccc2)C1CC2N3CC(=O)C(C2)CC3C1	85	high
173	Isoproterenol	Oc1cc(ccc1O)C(O)NC(C)C	85	high
174	Lansoprazole	S(=O)(Cc1ncc(C)c(OCC(F)(F)F)c1)c1[nH]c2c(n1)cccc2	85	high
175	Oxyfedrine	O(C)c1cc(ccc1)C(=O)CCNC(C(O)c1ccccc1)C	85	high
176	Piretanide	S(=O)(=O)(N)c1cc(cc(N2CCCC2)c1Oc1ccccc1)C(O)=O	85	high
177	Sulfamethizole	s1c(nnc1NS(=O)(=O)c1ccc(N)cc1)C	85	high
178	Triazolam	Clc1ccccc1C1=NC=C2N(c3c1cc(Cl)cc3)C(=NN2)C	85	high
179	Zalcitabine	O1C(CCC1N1C=CC(=NC1=O)N)CO	85	high

180	Fenoprofen	O(c1cc(ccc1)C(C(O)=O)C)c1ccccc1	85	high
181	Lamivudine	S1CC(OC1CO)N1CCC(=NC1=O)N	86	high
182	Topiramate	S(OCC12OC(OC1C1OC(OC1CO2)(C)C)(C)C)(=O)(=O)N	86	high
183	Benzydamine	O(CCCN(C)C)c1nn(c2c1cccc2)Cc1ccccc1	87	high
184	Bupropion	CC(C(=O)c1cccc(c1)Cl)NC(C)(C)C	87	high
185	Cimetidine	S(Cc1nc[nH]c1C)CCN\C(=N\C)\NC#N	87	high
186	Clindamycin	ClC(C(NC(=O)C1N(CC(C1)CCC)C)C1OC(SC)C(O)C(O)C1O)C	87	high
187	Clobazam	Clc1cc2N(C(=O)CC(=O)N(c2cc1)C)c1ccccc1	87	high
188	Acrivastine	OC(=O)\C=C\c1nc(ccc1)/C(=C/CN1CCCC1)/c1ccc(cc1)C	88	high
189	Disulfiram	S(SC(=S)N(CC)CC)C(=S)N(CC)CC	88	high
190	Metoclopramide	Clc1cc(C(=O)NCCN(CC)CC)c(OC)cc1N	88	high
191	Misoprostol	OC1CC(=O)C(CCCCCCC(OC)=O)C1\C=C\CC(O)(CCCC)C	88	high
192	Moricizine	S1c2c(N(c3c1cccc3)C(=O)CCN1CCOCC1)cc(NC(OCC)=O)cc2	88	high
193	Moxonidine	Clc1nc(nc(OC)c1NC=1NCCN=1)C	88	high
194	Nitrendipine	O(C(=O)C=1C(C(C(OC)=O)=C(NC=1C)C)c1cc([N+](=O)[O-])ccc1)CC	88	high
195	Trovafloxacin	Fc1cc(F)ccc1N1C=C(C(O)=O)C(=O)c2cc(F)c(nc12)N1CC2C(C1)C2N	88	high
196	Moclobemide	Clc1ccc(cc1)C(=O)NCCN1CCOCC1	88	high
197	Dihydrocodeine	O1C2C34C(C(N(CC3)C)Cc3c4c1c(OC)cc3)CCC2O	89	high
198	Sultopride	S(=O)(=O)(CC)c1cc(C(=O)NCC2N(CCC2)CC)c(OC)cc1	89	high
199	Tenidap	Clc1cc2c(N(C(=O)N)C(=O)C2C(=O)c2sccc2)cc1	89	high
200	Chloramphenicol	ClC(Cl)C(=O)NC(C(O)c1ccc([N+](=O)[O-])cc1)CO	89	high
201	Almitrine	Fc1ccc(cc1)C(N1CCN(CC1)c1nc(nc(n1)NCC=C)NCC=C)c1ccc(F)cc1	90	high
202	Amantadine	NC12CC3CC(C1)CC(C2)C3	90	high
203	Amphetamine	NC(Cc1ccccc1)C	90	high
204	Azatadine	CN1CCC(=C2c3ccccc3CCc4c2nccc4)CC1	90	high
205	Betaxolol	O(CC(O)CNC(C)C)c1ccc(cc1)CCOCC1CC1	90	high
206	Bisoprolol	O(CC(O)CNC(C)C)c1ccc(cc1)COCCOC(C)C	90	high
207	Chlorzoxazone	Clc1cc2NC(Oc2cc1)=O	90	high
208	Dapsone	S(=O)(=O)(c1ccc(N)cc1)c1ccc(O)cc1	90	high
209	Dexamethasone	FC12C(C3CC(C)C(O)(C(=O)CO)C3(CC1O)C)CCC1=CC(=O)C=CC12C	90	high
210	Diethylstilbestrol	Oc1ccc(cc1)/C(=C(/CC)\c1ccc(O)cc1)/CC	90	high
211	Diflunisal	Fc1cc(F)ccc1-c1cc(C(O)=O)c(O)cc1	90	high
212	Diloxanide	ClC(Cl)C(=O)N(C)c1ccc(O)cc1	90	high
213	Ethacrynic_acid	Clc1c(Cl)c(OCC(O)=O)ccc1C(=O)C(=O)CC	90	high
214	Felbamate	O(CC(COC(=O)N)c1ccccc1)C(=O)N	90	high

215	Feprazone	O=C1N(N(C(=O)C1C\C=C(\C)/C)c1ccccc1)c1ccccc1	90	high
216	Flutamide	FC(F)(F)c1cc(NC(=O)C(C)C)ccc1[N+](=O)[O-]	90	high
217	Fluvoxamine	FC(F)(F)c1ccc(cc1)/C(=N/OCCN)/CCCCOC	90	high
218	Hydroxyprogesterone_caproate	O(C(=O)CCCCC)C1(CCC2C3C(CCC12C)C1(C(=CC(=O)CC1)C=C3)C)C(=O)C	90	high
219	Isosorbide_dinitrate	O1C2C(OCC2O[N+](=O)[O-])C(O[N+](=O)[O-])C1	90	high
220	Isotretinoin	OC(=O)\C=C(\C=C\C=C(\C=C/C=1C(CCCC=1C)(C)C)/C)/C	90	high
221	Ketotifen	CN1CCC(=C2c3ccccc3CC(=O)c4c2ccs4)CC1	90	high
222	Loratadine	CCOC(=O)N1CCC(=C2c3ccc(cc3CCc4c2ncccc4)Cl)CC1	90	high
223	Mebeverine	O(C)c1cc(ccc1OC)C(OCCCCN(C(Cc1ccc(OC)cc1)C)CC)=O	90	high
224	Mefenamic_acid	OC(=O)c1ccccc1Nc1cccc(C)c1C	90	high
225	Meloxicam	s1c(cnc1NC(=O)C=1N(S(=O)(=O)c2c(cccc2)C=1O)C)C	90	high
226	Mifepristone	OC1(CCC2C3C(=C4C(CC(=O)CC4)CC3)C(CC12C)c1ccc(N(C)C)cc1)C#C	90	high
227	Morphine	O1C2C34C(C(N(CC3)C)Cc3c4c1c(O)cc3)C=CC2O	90	high
228	Moxifloxacin	Fc1cc2c(c(OC)c1N1CC3C(NCCC3)C1)C(NC1CC1)C=C(C(O)=O)C2=O	90	high
229	Nalidixic_acid	O=C1c2ccc(nc2N(CC1C(O)=O)CC)C	90	high
230	Nisoldipine	O(C(=O)C=1C(C(C(OC)=O)=C(NC=1C)C)c1ccccc1[N+](=O)[O-])CC(C)C	90	high
231	Papaverine	O(C)c1cc(ccc1OC)Cc1nccc2c1cc(OC)c(OC)c2	90	high
232	Phenazopyridine	n1c(N)c(N=Nc2ccccc2)ccc1N	90	high
233	Phenytoin	O=C1NC(=O)NC1(c1ccccc1)c1ccccc1	90	high
234	Protionamide	S=C(N)c1cc(ncc1)CCC	90	high
235	Quinalbarbitone	OC=1NC(=C)C(C(CCC)C)(CC=C)C(=O)N=1	90	high
236	Rabeprazole	S(=O)(Cc1nccc(OCCCOC)c1C)c1[nH]c2c(n1)cccc2	90	high
237	Riluzole	s1c2cc(OC(F)(F)F)ccc2nc1N	90	high
238	Sparfloxacin	Fc1c(N2CC(NC(C2)C)C)c(F)c2N(C=C(C(O)=O)C(=O)c2c1N)C1CC1	90	high
239	Sulfisomidine	S(=O)(=O)(Nc1nc(nc(c1)C)C)c1ccc(N)cc1	90	high
240	Sulindac	CC\1=C(C2=C(/C1=C\C3=CC=C(C=C3)S(=O)C)C=CC(=C2)F)CC(=O)O	90	high
241	Telithromycin	O1C(CC)C2(OC(=O)N(C2C(C)C(=O)C(CC(OC)(C)C(OC2OC(CC(N(C)C)C2O)C)C(C)C(=O)C(C)C1=O)C)CCCCn1cc(nc1)-c1cccnc1)C	90	high
242	Thiabendazole	s1cc(nc1)-c1[nH]c2c(n1)cccc2	90	high
243	Tiagabine	s1ccc(C)c1\C(=C\CCN1CC(CCC1)C(O)=O)\c1sccc1C	90	high
244	Tibolone	OC1(CCC2C3C(C4=C(CC3C)CC(=O)CC4)CCC12C)C#C	90	high
245	Tolazoline	N1CCN=C1Cc1ccccc1	90	high

246	Triamcinolone_acetonide	FC12C(C3CC4OC(OC4(C(=O)CO)C3(CC1O)C)(C)C)CCC=1C2C=CC(=O)C=1	90	high
247	Alprazolam	Clc1cc2c(-n3c(nnc3C)CN=C2c2ccccc2)cc1	90	high
248	Bicalutamide	S(=O)(=O)(CC(O)(C(=O)Nc1cc(C(F)(F)F)c(cc1)C#N)C)c1ccc(F)cc1	90	high
249	Diazoxide	Clc1cc2S(=O)(=O)NC(=Nc2cc1)C	90	high
250	Ethionamide	S=C(N)c1cc(ncc1)CC	90	high
251	Hydroxychloroquine	Clc1cc2nccc(NC(CCN(CCO)CC)C)c2cc1	90	high
252	Levosimendan	O=C1NN=C(C(C1)C)c1ccc(N\N=C(\C#N)/C#N)cc1	90	high
253	Mestranol	O(C)c1cc2CCC3C4CCC(O)(C#C)C4(CCC3c2cc1)C	90	high
254	Nifedipine	CC1=C(C(C(=C(N1)C)C(=O)OC)c2ccccc2[N+](=O)[O-])C(=O)OC	90	high
255	Pindolol	O(CC(O)CNC(C)C)c1c2c([nH]cc2)ccc1	90	high
256	Rizatriptan	[nH]1cc(c2cc(ccc12)Cn1ncnc1)CCN(C)C	90	high
257	Telmisartan	CCCc1nc2c(cc(cc2n1Cc3ccc(cc3)c4ccccc4C(=O)O)c5nc6ccccc6n5C)C	90	high
258	Tolbutamide	S(=O)(=O)(NC(=O)NCCCC)c1ccc(cc1)C	90	high
259	Diltiazem	CC(=O)O[C@@H]1[C@@H](Sc2ccccc2N(C1=O)CCN(C)C)c3ccc(cc3)OC	91	high
260	Hydrocortisone	OC1(CCC2C3C(C4(C(=CC(=O)CC4)CC3)C)C(O)CC12C)C(=O)CO	91	high
261	Naloxone	O1C2C34CCN(C(Cc5c3c1c(O)cc5)C4(O)CCC2=O)CC=C	91	high
262	Terazosin	O1CCCC1C(=O)N1CCN(CC1)c1nc(N)c2cc(OC)c(OC)cc2n1	91	high
263	Saccharin	S1(=O)(=O)NC(=O)c2c1cccc2	91	high
264	Isradipine	o1nc2c(n1)cccc2C1C(C(OC(C)C)=O)=C(NC(C)=C1C(OC)=O)C	92	high
265	Alprenolol	O(CC(O)CNC(C)C)c1ccccc1CC=C	93	high
266	Amrinone	O=C1NC=C(C=C1N)c1ccncc1	93	high
267	Scopolamine	O1C2C3N(C(CC(OC(=O)C(CO)c4ccccc4)C3)C12)C	93	high
268	Tetrahydrocannabinol	O1c2c(C3C(CCC(=C3)C)C1(C)C)c(O)cc(c2)CCCCC	93	high
269	Codeine	O1C2C34C(C(N(CC3)C)Cc3c4c1c(OC)cc3)C=CC2O	93	high
270	Atropine	O(C(=O)C(CO)c1ccccc1)C1CC2N(C(C1)CC2)C	94	high
271	Clozapine	Clc1cc2N=C(N3CCN(CC3)C)c3c(Nc2cc1)cccc3	94	high
272	Felodipine	Clc1c(cccc1Cl)C1C(C(OCC)=O)=C(NC(C)=C1C(OC)=O)C	94	high
273	Fluconazole	Fc1cc(F)ccc1C(O)(Cn1ncnc1)Cn1ncnc1	94	high
274	Nicotinic_acid	OC(=O)c1cccnc1	94	high
275	Dienogest	OC1(CCC2C3C(=C4C(=CC(=O)CC4)CC3)CCC12C)CC#N	94	high
276	Acipimox	OC(=O)c1ncc([n+]([O-])c1)C	95	high
277	Amitriptyline	CN(C)CCC=C1c2ccccc2CCc3c1cccc3	95	high
278	Amobarbital	OC1=NC(O)=NC(=O)C1(CCC(C)C)CC	95	high
279	Amoxapine	Clc1cc2c(Oc3c(N=C2N2CCNCC2)cccc3)cc1	95	high

280	Baclofen	Clc1ccc(cc1)C(N)CCC(O)=O	95	high
281	Carbimazole	S=C1N(C=CN1C)C(OCC)=O	95	high
282	Carteolol	O(CC(O)CNC(C)(C)C)c1c2CCC(=O)Nc2ccc1	95	high
283	Cephradine	S1C2N(C(=O)C2NC(=O)C(N)C=2CC=CCC=2)C(C(O)=O)=C(C1)C	95	high
284	Chorpropamide	Clc1ccc(S(=O)(=O)NC(=O)NCCC)cc1	95	high
285	Clomethiazole	ClCCc1scnc1C	95	high
286	Clomipramine	Clc1cc2N(c3c(CCc2cc1)cccc3)CCCN(C)C	95	high
287	Clonidine	c1cc(c(c(c1)Cl)NC2=NCCN2)Cl	95	high
288	Clopenthixol	c1ccc2c(c1)C(=CCCN3CCN(CC3)CCO)c4cc(ccc4S2)Cl	95	high
289	Diethylpropion	O=C(C(N(CC)CC)C)c1ccccc1	95	high
290	Disopyramide	O=C(N)C(CCN(C(C)C)C(C)C)(c1ccccc1)c1cccnc1	95	high
291	Domperidone	Clc1cc2NC(=O)N(NC3CCN(CC3)CCCN3c4c(NC3=O)cccc4)c2cc1	95	high
292	Dothiepin	S1Cc2c(cccc2)\C(\c2c1cccc2)=C/CCN(C)C	95	high
293	Fludrocortisone_acetate	FC12C(C3CCC(O)(C(=O)COC(=O)C)C3(CC1O)C)CCC1=CC(=O)CCC12C	95	high
294	Flumazenil	Fc1cc2c(-n3c(CN(C)C2=O)c(nc3)C(OCC)=O)cc1	95	high
295	Flurbiprofen	Fc1cc(ccc1)-c1ccc(cc1)C(C(O)=O)C	95	high
296	Galantamine	O1c2c3C4(C1CC(O)C=C4)CCN(Cc3ccc2OC)C	95	high
297	Glymidine	S(=O)(=O)(Nc1ncc(OCCOC)cn1)c1ccccc1	95	high
298	Hexobarbital	OC1=NC(=O)C(C)(C=2CCCCC=2)C(=O)N1C	95	high
299	Ketoprofen	OC(=O)C(C)c1cc(ccc1)C(=O)c1ccccc1	95	high
300	Ketorolac	OC(=O)C1CCn2c1ccc2C(=O)c1ccccc1	95	high
301	Levamisole	S1CCN2CC(N=C12)c1ccccc1	95	high
302	Lorazepam	Clc1ccccc1C1=NC(O)C(=O)Nc2c1cc(Cl)cc2	95	high
303	Methimazole	S=C1NC=CN1C	95	high
304	Metronidazole	OCCn1c(ncc1[N+](=O)[O-])C	95	high
305	Nicardipine	O(C(=O)c1c(C2C=C(NC(=C2)C)C)c(C(OC)=O)c(cc1[N+](=O)[O-])C)CCN(Cc1ccccc1)C	95	high
306	Nitrazepam	O=C1Nc2c(cc([N+](=O)[O-])cc2)C(=NC1)c1ccccc1	95	high
307	Nitrofurantoin	o1c(ccc1[N+](=O)[O-])\C=N\N1CC(=O)NC1=O	95	high
308	Nizatidine	s1cc(nc1CN(C)C)CSCCN\C(\NC)=C\[N+](=O)[O-]	95	high
309	Pefloxacin	Fc1cc2c(N(C=C(C(O)=O)C2=O)CC)cc1N1CCN(CC1)C	95	high
310	Pentazocine	Oc1cc2c(CC3N(CCC2(C)C3C)C\C=C(\C)/C)cc1	95	high
311	Pentoxifylline	O=C1N(CCCCC(=O)C)C(=O)N(c2ncn(c12)C)C	95	high
312	Perindopril	O(C(=O)C(NC(C(=O)N1C2C(CC1C(O)=O)CCCC2)C)CCC)CC	95	high
313	Phenylpropanolamine	OC(C(N)C)c1ccccc1	95	high
314	Practolol	CC(C)NCC(COc1ccc(cc1)NC(=O)C)O	95	high
315	Promethazine	S1c2c(N(c3c1cccc3)CC(N(C)C)C)cccc2	95	high
316	Propafenone	O(CC(O)CNCCC)c1ccccc1C(=O)CCc1ccccc1	95	high
317	Propranolol	CC(C)NCC(COc1cccc2c1cccc2)O	95	high
318	Protriptyline	N(CCCC1c2c(C=Cc3c1cccc3)cccc2)C	95	high
319	Ritodrine	Oc1ccc(cc1)C(O)C(NCCc1ccc(O)cc1)C	95	high

320	Sotalol	CC(C)NCC(c1ccc(cc1)NS(=O)(=O)C)O	95	high
321	Sulfisoxazole	Cc1c(noc1NS(=O)(=O)c2ccc(cc2)N)C	95	high
322	Tacrine	n1c2c(CCCC2)c(N)c2c1cccc2	95	high
323	Temazepam	Clc1cc2c(N(C)C(=O)C(O)N=C2c2ccccc2)cc1	95	high
324	Timolol	s1nc(N2CCOCC2)c(OCC(O)CNC(C)(C)C)n1	95	high
325	Tropisetron	O(C(=O)c1c2c(n(c1)C)cccc2)C1CC2N(C(C1)CC2)C	95	high
326	Venlafaxine	O(C)c1ccc(cc1)C(CN(C)C)C1(O)CCCCC1	95	high
327	Zolpidem	O=C(N(CCC)CCC)Cc1n2C=C(C=Cc2nc1-c1ccc(cc1)C)C	95	high
328	Acitretin	O(C)c1cc(C)c(\C=C\C(=C\C=C\C(=C/C(O)=O)\C)\C)c(C)c1C	95	high
329	Bifemelane	O(CCCCNC)c1ccccc1Cc1ccccc1	95	high
330	Cinoxacin	O1c2c(OC1)cc1N(N=C(C(O)=O)C(=O)c1c2)CC	95	high
331	Delmopinol	O1CC(N(CC1)CCO)CCCC(CCC)CCC	95	high
332	Fenfluramine	FC(F)(F)c1cc(ccc1)C(CNCC)C	95	high
333	Gliquidone	S(=O)(=O)(NC(=O)NC1CCCCC1)c1ccc(cc1)CCN1C(=O)C(c2c(cc(OC)cc2)C1=O)(C)C	95	high
334	Labetalol	Oc1ccc(cc1C(=O)N)C(O)CNC(CCc1ccccc1)C	95	high
335	Naltrexone	O1C2C34CCN(C(Cc5c3c1c(O)cc5)C4(O)CCC2=O)CC1CC1	95	high
336	Oxprenolol	O(CC(O)CNC(C)C)c1ccccc1OCC=C	95	high
337	Phenprocoumon	O1c2c(cccc2)C(O)=C(C(CC)c2ccccc2)C1=O	95	high
338	Propoxyphene	O(C(Cc1ccccc1)(C(CN(C)C)C)c1ccccc1)C(=O)CC	95	high
339	Sulfamethazine	S(=O)(=O)(Nc1nc(cc(n1)C)C)c1ccc(N)cc1	95	high
340	Tramadol	O(C)c1cc(ccc1)C1(O)CCCCC1CN(C)C	95	high
341	Bumetanide	S(=O)(=O)(N)c1cc(cc(NCCCC)c1Oc1ccccc1)C(O)=O	96	high
342	Clofibrate	Clc1ccc(OC(C(OCC)=O)(C)C)cc1	96	high
343	Gatifloxacin	Fc1cc2c(N(C=C(C(O)=O)C2=O)C2CC2)c(OC)c1N1CC(NCC1)C	96	high
344	Metoprolol	O(CC(O)CNC(C)C)c1ccc(cc1)CCOC	96	high
345	Minoxidil	[O-][n+]1ccc(nc1N)N1CCCCC1	96	high
346	Progesterone	O=C1CCC2(C3C(C4CCC(C(=O)C)C4(CC3)C)CCC2=C1)C	96	high
347	Torsemide	S(=O)(=O)(NC(=O)NC(C)C)c1cnccc1Nc1cc(ccc1)C	96	high
348	Trapidil	n12ncnc1N=C(C=C2N(CC)CC)C	96	high
349	Capecitabine	FC1=CN(C2OC(C)C(O)C2O)C(=O)N=C1NC(OCCCCC)=O	96	high
350	Praziquantel	O=C1N2C(c3c(CC2)cccc3)CN(C1)C(=O)C1CCCCC1	96	high
351	Cotinine	O=C1N(C)C(CC1)c1cccnc1	97	high
352	Gallopamil	O(C)c1c(OC)cc(cc1OC)C(C(C)C)(CCCN(CCc1cc(OC)c(OC)cc1)C)C#N	97	high
353	Gliclazide	S(=O)(=O)(NC(=O)NN1CC2C(CCC2)C1)c1ccc(cc1)C	97	high
354	Oxazepam	Clc1cc2c(NC(=O)C(O)N=C2c2ccccc2)cc1	97	high

355	Risperidone	Fc1cc2onc(c2cc1)C1CCN(CC1)CCC=1C(=O)N2C(=NC=1C)CCCC2	97	high
356	Diclofenac	Clc1cc(Cl)ccc1Nc1ccccc1CC(O)=O	97	high
357	Trimethoprim	O(C)c1c(OC)cc(cc1OC)Cc1cnc(nc1N)N	97	high
358	Antipyrine	O=C1N(N(C)C(=C1)C)c1ccccc1	98	high
359	Chlorpromazine	Clc1cc2N(c3c(Sc2cc1)cccc3)CCCN(C)C	98	high
360	Cisapride	Clc1cc(C(=O)NC2CCN(CC2OC)CCCOc2ccc(F)cc2)c(OC)cc1N	98	high
361	Cyproterone_acetate	ClC=1C2=CC(=O)C3C(C3)C2(C2C(C3CCC(OC(=O)C)(C(=O)C)C3(CC2)C)C=1)C	98	high
362	Glibornuride	S(=O)(=O)(NC(=O)NC1C2CCC(C)(C1O)C2(C)C)c1ccc(cc1)C	98	high
363	Glyburide	Clc1cc(C(=O)NCCc2ccc(S(=O)(=O)NC(=O)NC3CCCCC3)cc2)c(OC)cc1	98	high
364	Ibuprofen	OC(=O)C(C)c1ccc(cc1)CC(C)C	98	high
365	Imatinib	O=C(Nc1cc(Nc2nc(ccn2)-c2cccnc2)c(cc1)C)c1ccc(cc1)CN1CCN(CC1)C	98	high
366	Isoxepac	O1Cc2c(cccc2)C(=O)c2cc(ccc12)CC(O)=O	98	high
367	Lacidipine	O(C(=O)C=1C(C(C(OCC)=O)=C(NC=1C)C)c1ccccc1\C=C\C(OC(C)(C)C)=O)CC	98	high
368	Lamotrigine	Clc1c(cccc1Cl)-c1nnc(nc1N)N	98	high
369	Lidocaine	O=C(Nc1c(cccc1C)C)CN(CC)CC	98	high
370	Mexiletine	O(CC(N)C)c1c(cccc1C)C	98	high
371	Nefopam	O1CCN(Cc2c(cccc2)C1c1ccccc1)C	98	high
372	Oxaprozin	o1c(c(nc1CCC(O)=O)-c1ccccc1)-c1ccccc1	98	high
373	Pelrinone	O=C1NC(=NC(NCc2cccnc2)=C1C#N)C	98	high
374	Rivastigmine	O(C(=O)N(CC)C)c1cc(ccc1)C(N(C)C)C	98	high
375	Ropinirole	O=C1Nc2c(C1)c(ccc2)CC(NCCC)NCCC	98	high
376	Tolmesoxide	S(=O)(C)c1cc(OC)c(OC)cc1C	98	high
377	Valproic_acid	OC(=O)C(CCC)CCC	98	high
378	Zopiclone	Clc1ccc(nc1)N1C(OC(=O)N2CCN(CC2)C)c2nccnc2C1=O	98	high
379	Desipramine	N(CCCN1c2c(CCc3c1cccc3)cccc2)C	98	high
380	Imipramine	N(CCCN1c2c(CCc3c1cccc3)cccc2)(C)C	98	high
381	Maprotiline	N(CCCC12CCC(c3c1cccc3)c1c2cccc1)C	98	high
382	Phenylbutazone	O=C1C(N(N(C1=O)c1ccccc1)c1ccccc1)CCCC	98	high
383	Ximoprofen	OC(=O)C(C)c1ccc(cc1)C1C\C(=N\O)\CCC1	98	high
384	Caffeine	O=C1N(C)C(=O)N(c2ncn(c12)C)C	99	high
385	Chlordiazepoxide	Clc1cc2c(N=C(NC)C[N+]([O-])=C2c2ccccc2)cc1	99	high
386	Ciprofibrate	ClC1(Cl)CC1c1ccc(OC(C(O)=O)(C)C)cc1	99	high
387	Diazepam	Clc1cc2c(N(C)C(=O)CN=C2c2ccccc2)cc1	99	high
388	Fluorescein	O1C2(c3c(cccc3)C1=O)c1c(Oc3c2ccc(O)c3)cc(O)cc1	99	high
389	Lomefloxacin	Fc1c2N(C=C(C(O)=O)C(=O)c2cc(F)c1N1CC(NCC1)C)CC	99	high
390	Miconazole	Clc1cc(Cl)ccc1C(OCc1ccc(Cl)cc1Cl)Cn1ccnc1	99	high
391	Pheniramine	n1ccccc1C(CCN(C)C)c1ccccc1	99	high

392	Prednisolone	OC1(CCC2C3C(C4(C(=CC(=O)C=C4)CC3)C)C(O)CC12C)C(=O)CO	99	high
393	Tiacrilast	S(C)c1cc2c(N=CN(\C=C\C(O)=O)C2=O)cc1	99	high
394	Tianeptine	Clc1cc2S(=O)(=O)N(c3c(N(c2cc1)CCCCCCC(O)=O)cccc3)C	99	high
395	Viloxazine	O1CC(NCC1)COc1ccccc1OCC	99	high
396	Desmethyldiazepam	Clc1cc2c(NC(=O)CN=C2c2ccccc2)cc1	99	high
397	Naproxen	O(C)c1cc2c(cc(cc2)C(C(O)=O)C)cc1	99	high
398	Tolmetin	OC(=O)Cc1n(C)c(cc1)C(=O)c1ccc(cc1)C	99	high
399	Acetanilide	O=C(Nc1ccccc1)C	100	high
400	Acetazolamide	s1c(nnc1S(=O)(=O)N)NC(=O)C	100	high
401	Alfacalcidol	C[C@H](CCCC(C)C)[C@H]1CC[C@@H]\2[C@@]1(CCC/C2=C\C=C/3\C[C@H](C[C@@H](C3=C)O)O)C	100	high
402	Aminopyrine	N(C)(C)C=1C(=N)N(N(C)C=1C)c1ccccc1	100	high
403	Amosulalol	S(=O)(=O)(N)c1cc(ccc1C(O)CNCCOc1ccccc1OC)C	100	high
404	Anastrozole	n1cn(nc1)Cc1cc(cc(c1)C(C#N)(C)C)C(C#N)(C)C	100	high
405	Astemizole	Fc1ccc(cc1)Cn1c2c(nc1NC1CCN(CC1)CCc1ccc(OC)cc1)cccc2	100	high
406	Azimilide	Clc1ccc(cc1)-c1oc(cc1)\C=N\N1CC(=O)N(CCCCN2CCN(CC2)C)C1=O	100	high
407	Bendroflumethiazide	S(=O)(=O)(N)c1cc2S(=O)(=O)NC(Nc2cc1C(F)(F)F)Cc1ccccc1	100	high
408	Benorylate	O(C(=O)C)c1ccccc1C(Oc1ccc(NC(=O)C)cc1)=O	100	high
409	Bepridil	O(CC(C)C)CC(N(Cc1ccccc1)c1ccccc1)CN1CCCC1	100	high
410	Bezafibrate	O(C(C(O)=O)(C)C)c1ccc(cc1)CCNC(=O)c1ccccc1	100	high
411	Biperiden	OC(CCN1CCCCC1)(C1C2CC(C1)C=C2)c1ccccc1	100	high
412	Bornaprine	O(C(=O)C1(C2CC(C1)CC2)c1ccccc1)CCCN(CC)CC	100	high
413	Budesonide	O1C2(C(OC1CCC)CC1C3C(C4(C(=CC(=O)C=C4)CC3)C)C(O)CC12C)C(=O)CO	100	high
414	Camazepam	Clc1cc2c(N(C)C(=O)C(OC(=O)N(C)C)N=C2c2ccccc2)cc1	100	high
415	Carbamazepine	O=C(N)N1c2c(C=Cc3c1cccc3)cccc2	100	high
416	Carmustine	ClCCN(N=O)C(=O)NCCCl	100	high
417	Chloral_hydrate	ClC(Cl)(Cl)C(O)O	100	high
418	Chloroquine	Clc1cc2nccc(c2cc1)NC(C)CCCN(CC)CC	100	high
419	Chlorphenesin	Clc1ccc(OCC(O)CO)cc1	100	high
420	Cicaprost	OC1CC2C(C\C(\C2)=C/COCC(O)=O)C1C#CC(O)C(CC#CCC)C	100	high
421	Cilomilast	O(c1cc(ccc1OC)C1(CCC(CC1)C(O)=O)C#N)C1CCCC1	100	high
422	Citalopram	Fc1ccc(cc1)C1(OCc2c1ccc(c2)C#N)CCCN(C)C	100	high
423	Corticosterone	OC1C2C(C3CCC(C(=O)CO)C3(C1)C)CCC1=CC(=O)CCC12C	100	high
424	Coumarin	O1c2c(C=CC1=O)cccc2	100	high

425	Cyclopenthiazide	Clc1cc2NC(NS(=O)(=O)c2cc1S(=O)(=O)N)CN1CCCC1	100	high
426	Diacetylmorphine	O1C2C34C(C(N(CCC3)C)Cc3c4c1c(OC(=O)C)cc3)C=CC2OC(=O)C	100	high
427	Dicyclomine	O(C(=O)C1(CCCCC1)C1CCCCC1)CCN(CC)CC	100	high
428	Dofetilide	S(=O)(=O)(Nc1ccc(cc1)CCN(CCOc1ccc(NS(=O)(=O)C)cc1)C)C	100	high
429	Doxazosin	O1c2c(OCC1C(=O)N1CCN(CC1)c1nc(N)c3cc(OC)c(OC)cc3n1)cccc2	100	high
430	Ergotamine	O1C(NC(=O)C2C=C3C(N(C2)C)Cc2c4c3cccc4[nH]c2)(C)C(=O)N2C(Cc3ccccc3)C(=O)N3C(CCC3)C12O	100	high
431	Ethinyl_Estradiol	OC1(CCC2C3C(CCC12C)c1c(cc(O)cc1)CC3)C#C	100	high
432	Ethyl_alcohol	OCC	100	high
433	Ethynodiol_diacetate	O(C(=O)C)C1(CCC2C3C(C4C(=CC(OC(=O)C)CC4)CC3)CCC12C)C#C	100	high
434	Fenclofenac	Clc1cc(Cl)ccc1Oc1ccccc1CC(O)=O	100	high
435	Finasteride	O=C1NC2CCC3C4CCC(C(=O)NC(C)(C)C)C4(CCC3C2(C=C1)C)C	100	high
436	Flucytosine	FC1=CNC(=O)N=C1N	100	high
437	Flupentixol	S1c2c(cc(cc2)C(F)(F)F)\C(\c2c1cccc2)=C\CCN1CCN(CC1)CCO	100	high
438	Fluvastatin	Fc1ccc(cc1)-c1c2c(n(C(C)C)c1\C=C\C(O)CC(O)CC(O)=O)cccc2	100	high
439	Fusidic_acid	C[C@H]1[C@@H]2CC[C@]3([C@H]([C@]2(CC[C@H]1O)C)[C@@H](C[C@@H]\4[C@@]3(C[C@@H](/C4=C(/CCC=C(C)C)\C(=O)O)OC(=O)C)O)C	100	high
440	Gemfibrozil	O(CCCC(C(O)=O)(C)C)c1cc(ccc1C)C	100	high
441	Genaconazole	S(=O)(=O)(C(C(O)(Cn1ncnc1)c1ccc(F)cc1F)C)C	100	high
442	Glimepiride	S(=O)(=O)(NC(=O)NC1CCC(CC1)C)c1ccc(cc1)CCNC(=O)N1CC(C)=C(CC)C1=O	100	high
443	Glipizide	S(=O)(=O)(NC(=O)NC1CCCCC1)c1ccc(cc1)CCNC(=O)c1ncc(nc1)C	100	high
444	Granisetron	O=C(NC1CC2N(C(C1)CCC2)C)c1nn(c2c1cccc2)C	100	high
445	Haloperidol	Clc1cc(ccc1)C1(O)CCN(CC1)CCCC(=O)c1ccc(F)cc1	100	high
446	Hydralazine	n1ncc2c(cccc2)c1NN	100	high
447	Indobufen	O=C1N(Cc2c1cccc2)c1ccc(cc1)C(CC)C(O)=O	100	high
448	Indomethacin	Cc1c(c2cc(ccc2n1C(=O)c3ccc(cc3)Cl)OC)CC(=O)O	100	high
449	Irbesartan	O=C1N(Cc2ccc(cc2)-c2ccccc2-c2nn[nH]n2)C(=NC12CCCC2)CCCC	100	high
450	Isosorbide-2-mononitrate	O1C2C(OCC2O)C(O[N+](=O)[O-])C1	100	high
451	Isoxicam	CC1=CC(=NO1)NC(=O)C2=C(C3=CC=CC=C3S(=O)(=O)N2C)O	100	high
452	Ketanserin	Fc1ccc(cc1)C(=O)C1CCN(CC1)CCN1C(=O)c2c(NC1=O)cccc2	100	high

453	Letrozole	n1cn(nc1)C(c1ccc(cc1)C#N)c1ccc(cc1)C#N	100	high
454	Levetiracetam	O=C1N(CCC1)C(CC)C(=O)N	100	high
455	Levobunolol	O(CC(O)CNC(C)(C)C)c1c2c(ccc1)C(=O)CCC2	100	high
456	Levonorgestrel	OC1(CCC2C3C(C4C(=CC(=O)CC4)CC3)CCC12CC)C#C	100	high
457	Lisuride	O=C(NC1C=C2C(N(C1)C)Cc1c3c2cccc3[nH]c1)N(CC)CC	100	high
458	Lormetazepam	Clc1ccccc1C1=NC(O)C(=O)N(c2c1cc(Cl)cc2)C	100	high
459	Lornoxicam	Clc1sc2c(S(=O)(=O)N(C)C(C(=O)Nc3ncccc3)=C2O)c1	100	high
460	Lynestrenol	OC1(CCC2C3C(C4C(CC3)=CCCC4)CCC12C)C#C	100	high
461	Meclofenamic_acid	Clc1c(Nc2ccccc2C(O)=O)c(Cl)ccc1C	100	high
462	Megestrol_acetate	O(C(=O)C)C1(CCC2C3C(CCC12C)C1(C(=CC(=O)CC1)C(=C3)C)C)C(=O)C	100	high
463	Meperidine	O(C(=O)C1(CCN(CC1)C)c1ccccc1)CC	100	high
464	Meptazinol	Oc1cc(ccc1)C1(CCCCN(C1)C)CC	100	high
465	Methsuximide	O=C1N(C)C(=O)CC1(C)c1ccccc1	100	high
466	Methylergonovine	OCC(NC(=O)C1C=C2C(N(C1)C)Cc1c3c2cccc3[nH]c1)CC	100	high
467	Methysergide	OCC(NC(=O)C1C=C2C(N(C1)C)Cc1c3c2cccc3n(c1)C)CC	100	high
468	Midazolam	Clc1cc2c(-n3c(CN=C2c2ccccc2F)cnc3C)cc1	100	high
469	Nalbuphine	O1C2C34CCN(C(Cc5c3c1c(O)cc5)C4(O)CCC2O)CC1CCC1	100	high
470	Nefazodone	Clc1cc(N2CCN(CC2)CCCN2N=C(N(CCOc3ccccc3)C2=O)CC)ccc1	100	high
471	Nicorandil	O([N+](=O)[O-])CCNC(=O)c1cccnc1	100	high
472	Nicotine	n1cc(ccc1)C1N(CCC1)C	100	high
473	Nilvadipine	O(C(=O)C=1C(C(C(OC)=O)=C(NC=1C)C#N)c1cc([N+](=O)[O-])ccc1)C(C)C	100	high
474	Nitroxoline	Oc1c2ncccc2c([N+](=O)[O-])cc1	100	high
475	Norethindrone	OC1(CCC2C3C(C4C(=CC(=O)CC4)CC3)CCC12C)C#C	100	high
476	Norgestimate	O(C(=O)C)C1(CCC2C3C(C4C(=C/C(=N/O)/CC4)CC3)CCC12CC)C#C	100	high
477	Nortriptyline	CNCCC=C1c2ccccc2CCc3c1cccc3	100	high
478	Ofloxacin	Fc1cc2c3N(C=C(C(O)=O)C2=O)C(COc3c1N1CCN(CC1)C)C	100	high
479	Ondansetron	O=C1c2c(n(c3c2cccc3)C)CCC1Cn1ccnc1C	100	high
480	Orphenadrine	O(C(c1ccccc1C)c1ccccc1)CCN(C)C	100	high
481	Oxcarbazepine	O=C(N)N1c2c(cccc2)C(=N)Cc2c1cccc2	100	high
482	Oxybutynin	O(C(=O)C(O)(C1CCCCC1)c1ccccc1)CC#CCN(CC)CC	100	high
483	Oxyphenbutazone	Oc1ccc(N2N(C(=O)C(CCCC)C2=O)c2ccccc2)cc1	100	high
484	Paroxetine	Fc1ccc(cc1)C1CCNCC1COc1cc2OCOc2cc1	100	high
485	Pentobarbital	O=C1NC(=O)NC(=O)C1(C(CCC)C)CC	100	high
486	Perphenazine	Clc1cc2N(c3c(Sc2cc1)cccc3)CCCN1CCN(CC1)CCO	100	high
487	Phenglutarimide	O=C1NC(=O)CCC1(CCN(CC)CC)c1ccccc1	100	high

488	Phenindione	O=C1c2c(cccc2)C(=O)C1c1ccccc1	100	high
489	Piroxicam	S1(=O)(=O)N(C)C(C(=O)Nc2ncccc2)=C(O)c2c1ccccc2	100	high
490	Polythiazide	Clc1cc2NC(N(S(=O)(=O)c2cc1S(=O)(=O)N)C)CSCC(F)(F)F	100	high
491	Probenecid	S(=O)(=O)(N(CCC)CCC)c1ccc(cc1)C(O)=O	100	high
492	Procarbazine	O=C(NC(C)C)c1ccc(cc1)CNNC	100	high
493	Propofol	Oc1c(cccc1C(C)C)C(C)C	100	high
494	Proxyphylline	O=C1N(C)C(=O)N(c2ncn(c12)CC(O)C)C	100	high
495	Pseudoephedrine	OC(C(NC)C)c1ccccc1	100	high
496	Pyrazinamide	O=C(N)c1nccnc1	100	high
497	Remoxipride	Brc1ccc(OC)c(C(=O)NCC2N(CCC2)CC)c1OC	100	high
498	Repaglinide	O(CC)c1cc(ccc1C(O)=O)CC(=O)NC(CC(C)C)c1ccccc1N1CCCCC1	100	high
499	Salsalate	O(C(=O)c1ccccc1O)c1ccccc1C(O)=O	100	high
500	Selegiline	N(C(Cc1ccccc1)C)(CC#C)C	100	high
501	Sudoxicam	s1ccnc1NC(=O)C=1N(S(=O)(=O)c2c(cccc2)C=1O)C	100	high
502	Sulfamethoxazole	S(=O)(=O)(Nc1noc(c1)C)c1ccc(N)cc1	100	high
503	Sulfinpyrazone	S(=O)(CCC1C(=O)N(N(C1=O)c1ccccc1)c1ccccc1)c1ccccc1	100	high
504	Tamoxifen	O(CCN(C)C)c1ccc(cc1)\C(=C(\CC)/c1ccccc1)\c1ccccc1	100	high
505	Tenoxicam	s1c2C=C(N(S(=O)(=O)c2cc1)C)C(=O)Nc1ncccc1	100	high
506	Terfenadine	OC(C1CCN(CC1)CCCC(O)c1ccc(cc1)C(C)(C)C)(c1ccccc1)c1ccccc1	100	high
507	Tesaglitazar	S(Oc1ccc(cc1)CCOc1ccc(cc1)CC(OCC)C(O)=O)(=O)(=O)C	100	high
508	Testosterone	OC1CCC2C3C(CCC12C)C1(C(=CC(=O)CC1)CC3)C	100	high
509	Tilidine	O=C(CCC)C1(CCC=CC1N(C)C)c1ccccc1	100	high
510	Tinidazole	S(=O)(=O)(CCn1c(ncc1[N+](=O)[O-])C)CC	100	high
511	Tocainide	O=C(Nc1c(cccc1C)C)C(N)C	100	high
512	Toremifene	ClCC\C(=C(\c1ccc(OCCN(C)C)cc1)/c1ccccc1)\c1ccccc1	100	high
513	Triamcinolone	FC12C(C3CC(O)C(O)(C(=O)CO)C3(CC1O)C)CCC1=CC(=O)C=CC12C	100	high
514	Trifluoperazine	S1c2c(N(c3c1cccc3)CCCN1CCN(CC1)C)cc(cc2)C(F)(F)F	100	high
515	Trihexyphenidyl	OC(CCN1CCCCC1)(C1CCCCC1)c1ccccc1	100	high
516	Trofosfamide	ClCCN1P(OCCC1)(=O)N(CCCl)CCCl	100	high
517	Zileuton	s1c2c(cc1C(N(O)C(=O)N)C)cccc2	100	high
518	Zomepirac	Clc1ccc(cc1)C(=O)c1n(C)c(cc1C)CC(O)=O	100	high
519	Zonisamide	S(=O)(=O)(N)Cc1noc2c1cccc2	100	high
520	Zotepine	Clc1cc2c(Sc3c(C=C2OCCN(C)C)cccc3)cc1	100	high
521	Aminoglutethimide	O=C1NC(=O)CCC1(CC)c1ccc(N)cc1	100	high
522	Azelastine	Clc1ccc(cc1)CC1NN(C2CCCN(CC2)C)C(=O)c2c1ccccc2	100	high
523	Betahistine	n1ccccc1CCNC	100	high

524	Buspirone	O=C1N(CCCCN2CCN(CC2)c2ncccn2)C(=O)CC2(C1)CCCC2	100	high
525	Chlorambucil	ClCCN(CCCl)c1ccc(cc1)CCCC(O)=O	100	high
526	Cinchonine	OC(C1N2CC(C(C1)CC2)C=C)c1c2c(ncc1)cccc2	100	high
527	Dextromoramide	O1CCN(CC1)CC(C(C(=O)N1CCCC1)(c1ccccc1)c1ccccc1)C	100	high
528	Doxepin	O1Cc2c(cccc2)C(c2c1cccc2)CCCN(C)C	100	high
529	Etoricoxib	Clc1cc(c([n+]([O-])c1)-c1ccc(nc1)C)-c1ccc(S(=O)(=O)C)cc1	100	high
530	Flurazepam	Clc1cc2c(N(CCN(CC)CC)C(=O)CN=C2c2ccccc2F)cc1	100	high
531	Gestodene	OC1(C=CC2C3C(C4C(=CC(=O)CC4)CC3)CCC12CC)C#C	100	high
532	Guanfacine	Clc1cccc(Cl)c1CC(=O)\N=C(\N)/N	100	high
533	Indoprofen	O=C1N(Cc2c1cccc2)c1ccc(cc1)C(C(O)=O)C	100	high
534	Ketazolam	Clc1cc2c(N(C)C(=O)CN3C2(OC(=CC3=O)C)c2ccccc2)cc1	100	high
535	Linezolid	Fc1cc(N2CC(OC2=O)CNC(=O)C)ccc1N1CCOCC1	100	high
536	Mebendazole	O(C(=O)Nc1[nH]c2cc(ccc2n1)C(=O)c1ccccc1)C	100	high
537	Methocarbamol	O(CC(O)COC(=O)N)c1ccccc1OC	100	high
538	Nafronyl	O1CCCC1CC(Cc1cc2c(cc1)cccc2)C(OCCN(CC)CC)=O	100	high
539	Nilutamide	FC(F)(F)c1cc(N2C(=O)C(NC2=O)(C)C)ccc1[N+](=O)[O-]	100	high
540	Norgestrel	OC1(CCC2C3C(C4C(=CC(=O)CC4)CC3)C=CC12CC)C#C	100	high
541	Oxatomide	O=C1Nc2c(N1CCCN1CCN(CC1)C(c1ccccc1)c1ccccc1)cccc2	100	high
542	Penbutolol	O(CC(O)CNC(C)(C)C)c1ccccc1C1CCCC1	100	high
543	Phenobarbital	O=C1NC(=O)NC(=O)C1(CC)c1ccccc1	100	high
544	Procyclidine	OC(CCN1CCCC1)(C1CCCCC1)c1ccccc1	100	high
545	Quinagolide	S(=O)(=O)(NC1CC2C(N(C1)CCC)Cc1c(C2)c(O)ccc1)N(CC)CC	100	high
546	Stavudine	O1C(C=CC1N1C=C(C)C(=NC1=O)N)CO	100	high
547	Tamsulosin	S(=O)(=O)(N)c1cc(ccc1OC)CC(NCCOc1ccccc1OCC)C	100	high
548	Tetrabenazine	O(C)c1cc2C3N(CC(CC(C)C)C(=O)C3)CCc2cc1OC	100	high
549	Trazodone	Clc1cc(N2CCN(CC2)CCCN2N=C3N(C=CC=C3)C2=O)ccc1	100	high
550	Zaleplon	O=C(N(CC)c1cc(ccc1)C=1n2ncc(c2N=CC=1)C#N)C	100	high

Appendix II. Dataset B (Caco-2 data) used in Chapter 2.

ID	Name	SMILES	LogPapp (cm/s)
1	5-5-Aminolevulinic Acid	C(CC(=O)O)C(=O)CN	-5.34
2	Acebutolol	CCCC(=O)Nc1ccc(c(c1)C(=O)C)OCC(CNC(C)C)O	-6.1
3	Aceclofenac	c1ccc(c(c1)CC(=O)OCC(=O)O)Nc2c(cccc2Cl)Cl	-4.41
4	Acetaminophen	Oc1ccc(NC(=O)C)cc1	-4.44
5	Acetyl Salicylic Acid	CC(=O)Oc1ccccc1C(=O)O	-5.62
6	Acrivastine	CC1=CC=C(C=C1)/C(=C\CN2CCCC2)/C3=CC=CC(=N3)/C=C/C(=O)O	-6.35
7	Acyclovir	O=C1N=C(Nc2n(cnc12)COCCO)N	-6.07
8	Alanine	C[C@@H](C(=O)O)N	-5.63
9	Alfa-Methyldopa (Alpha Methyldopa)	C[C@](Cc1ccc(c(c1)O)O)(C(=O)O)N	-6.63
10	Alfentanil	CCC(=O)N(c1ccccc1)C2(CCN(CC2)CCn3c(=O)n(nn3)CC)COC	-4.26
11	Alminoprofen	CC(c1ccc(cc1)NCC(=C)C)C(=O)O	-5.53
12	Alprenolol	CC(C)NCC(COc1ccccc1CC=C)O	-4.57
13	Amfenac	c1ccc(cc1)C(=O)c2cccc(c2N)CC(=O)O	-4.29
14	Amiloride	Clc1nc(C(=O)\N=C(\N)/N)c(nc1N)N	-6.46
15	Aminopyrine	O=C1N(N(C)C(C)=C1N(C)C)c1ccccc1	-4.44
16	Amisulpride	CCN1CCCC1CNC(=O)c2cc(c(cc2OC)N)S(=O)(=O)CC	-5.66
17	Amoxicillin	CC1([C@@H](N2[C@H](S1)[C@@H](C2=O)NC(=O)[C@@H](c3ccc(cc3)O)N)C(=O)O)C	-6.31
18	Ampicillin	CC1([C@@H](N2[C@H](S1)[C@@H](C2=O)NC(=O)[C@@H](c3ccccc3)N)C(=O)O)C	-5.70
19	Antipyrine	O=C1N(N(C)C(=C1)C)c1ccccc1	-4.47
20	Argipressin	c1ccc(cc1)CC2C(=O)NC(C(=O)NC(C(=O)NC(CSSCC(C(=O)NC(C(=O)N2)Cc3ccc(cc3)O)N)C(=O)N4CCCC4C(=O)NC(CCCNC(=N)N)C(=O)NCC(=O)N)CC(=O)N)CCC(=O)N	-6.85
21	Artemisinin	O1[C@@H]2O[C@@]3(OO[C@]24[C@@H](CC[C@H]([C@@H]4CC3)C)[C@@H](C)C1=O)C	-4.52
22	Artesunate	C[C@@H]1CC[C@H]2[C@H]([C@@H](O[C@H]3[C@@]24[C@H]1CCC(O3)(OO4)C)OC(=O)CCC(=O)O)C	-5.40
23	Atenolol	CC(C)NCC(COc1ccc(cc1)CC(=O)N)O	-6.34
24	Azithromycin	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)C)O)(C)O	-6.37
25	Benzoic Acid	c1ccc(cc1)C(=O)O	-4.15
26	Benzyl Penicillin	CC1([C@@H](N2[C@H](S1)[C@@H](C2=O)NC(=O)Cc3ccccc3)C(=O)O)C	-6.08
27	Betaxolol	CC(C)NCC(COc1ccc(cc1)CCOCC2CC2)O	-4.91
28	Bosentan	S(=O)(=O)(Nc1nc(nc(OCCO)c1Oc1ccccc1OC)-c1ncccn1)c1ccc(cc1)C(C)(C)C	-6.19
29	Bremazocine	CCC12CCN(C(C1(C)C)Cc3c2cc(cc3)O)CC4(CC4)O	-4.82

30	Bromocriptine	CC(C)C[C@H]1C(=O)N2CCC[C@H]2[C@]3(N1C(=O)[C@](O3)(C(C)C)NC(=O)[C@H]4CN([C@@H]5Cc6c7c(cccc7[nH]c6Br)C5=C4)C)O	-5.91
31	Budesonide	O1[C@@]2([C@H](OC1CCC)C[C@H]1[C@H]3[C@@H]([C@@]4(C(=CC(=O)C=C4)CC3)C)[C@@H](O)C[C@@]12C)C(=O)CO	-4.89
32	Bupropion	Clc1ccc(cc1)C(=O)C(NC(C)(C)C)C	-4.24
33	Caffeine	O=C1N(C)C(=O)N(c2ncn(c12)C)C	-4.48
34	Caftaric Acid	C1=CC(=C(C=C1/C=C/C(=O)O[C@H]([C@H](C(=O)O)O)C(=O)O)O)O	-5.41
35	Camptothecin	O1CC2=C(C=C3N(Cc4c3nc3c(c4)cccc3)C2=O)[C@@](O)(CC)C1=O	-4.11
36	Carbamazepine	O=C(N)N1c2c(C=Cc3c1cccc3)cccc2	-4.37
37	Catechin	O1c2c(C[C@H](O)[C@H]1c1cc(O)c(O)cc1)c(O)cc(O)c2	-6.82
38	cefatrizine	c1cc(ccc1C(C(=O)NC2C3N(C2=O)C(=C(CS3)CSc4cn[nH]n4)C(=O)O)N)O	-6.12
39	Cefazolin	Cc1nnc(s1)SCC2=C(N3[C@@H]([C@@H](C3=O)NC(=O)Cn4cnnn4)SC2)C(=O)O	-6.23
40	Cefcapene	CC/C=C(/C1=CSC(=N1)N)\C(=O)N[C@H]2[C@@H]3N(C2=O)C(=C(CS3)COC(=O)N)C(=O)O	-6.94
41	Cefcapene Pivoxil	s1cc(nc1N)/C(=C/CC)/C(=O)N[C@H]1[C@H]2SCC(COC(=O)N)=C(N2C1=O)C(OCOC(=O)C(C)(C)C)=O	-5.11
42	Ceftriaxone	CN1C(=NC(=O)C(=O)N1)SCC2=C(N3[C@@H]([C@@H](C3=O)NC(=O)/C(=N\OC)/C4=CSC(=N4)N)SC2)C(=O)O	-6.65
43	Cefuroxime	CO/N=C(/C1=CC=CO1)\C(=O)N[C@H]2[C@@H]3N(C2=O)C(=C(CS3)COC(=O)N)C(=O)O	-6.79
44	Cephalexin	CC1=C(N2[C@@H]([C@@H](C2=O)NC(=O)[C@@H](c3ccccc3)N)SC1)C(=O)O	-6.42
45	Cephradine	CC1=C(N2[C@@H]([C@@H](C2=O)NC(=O)[C@@H](C3=CCC=CC3)N)SC1)C(=O)O	-5.69
46	Chloramphenicol	ClC(Cl)C(=O)N[C@@H]([C@H](O)c1ccc([N+](=O)[O-])cc1)CO	-4.96
47	Chlorothiazide	Clc1cc2NC=NS(=O)(=O)c2cc1S(=O)(=O)N	-6.72
48	Chlorpromazine	CN(C)CCCN1c2ccccc2Sc3c1cc(cc3)Cl	-4.70
49	Cichoric Acid	C1=CC(=C(C=C1/C=C/C(=O)O[C@@H](C(=O)O)[C@@H](OC(=O)/C=C/C2=CC(=C(C=C2)O)O)C(=O)O)O)O	-5.13
50	Cimetidine	S(Cc1nc[nH]c1C)CCN\C(=N\C)\NC#N	-5.90
51	Cinnamic Acid	c1ccc(cc1)/C=C/C(=O)O	-3.64
52	Ciprofloxacin	c1c2c(cc(c1F)N3CCNCC3)n(cc(c2=O)C(=O)O)C4CC4	-5.90
53	Clonidine	c1cc(c(c(c1)Cl)NC2=NCCN2)Cl	-4.58
54	Clozapine	CN1CCN(CC1)C2=NC3=C(C=CC(=C3)Cl)NC4=CC=CC=C42	-4.51
55	Corticosterone	O=C1CC[C@@]2([C@@H]3[C@H]([C@@H]4CC[C@H](C(=O)CO)[C@]4(C[C@@H]3O)C)CCC2=C1)C	-4.50
56	Cortisona	O=C1CC[C@@]2([C@@H]3[C@H]([C@@H]4CC[C@](O)(C(=O)CO)[C@]4(CC3=O)C)CCC2=C1)C	-4.69
57	Coumarin	O1c2c(C=CC1=O)cccc2	-4.25
58	CP-X	O=C1N(CCC)C(=O)N(c2nc([nH]c12)C1CCCC1)CCC	-4.47
59	Creatinine	O=C1NC(=N)N(C1)C	-5.95

60	Cromolina	c1cc2c(c(c1)OCC(COc3cccc4c3c(=O)cc(o4)C(=O)O)O)c(=O)cc(o2)C(=O)O	-6.89
61	Cymarin	O1CC(=CC1=O)[C@H]1CC[C@]2(O)[C@H]3[C@H](CC[C@]12C)[C@]1(CC[C@H](O[C@@H]2O[C@H](C)[C@@H](O)[C@@H](OC)C2)C[C@@]1(O)CC3)C=O	-5.70
62	Danazol	o1ncc2C[C@@]3([C@@H]4[C@H]([C@@H]5CC[C@@](O)(C#C)[C@]5(CC4)C)CCC3=Cc12)C	-4.84
63	Desipramine	CNCCCN1c2ccccc2CCc3c1cccc3	-4.97
64	Desmopressin	C1C[C@H](N(C1)C(=O)[C@@H]2CSSCCC(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N2)CC(=O)N)CCC(=O)N)CC3=CC=CC=C3)CC4=CC=C(C=C4)O)C(=O)N[C@@H](CCCNC(=N)N)C(=O)NCC(=O)N	-6.49
65	Dexamethasone	F[C@@]12[C@H]([C@@H]3C[C@@H](C)[C@](O)(C(=O)CO)[C@]3(C[C@@H]1O)C)CCC1=CC(=O)C=C[C@@]12C	-4.91
66	D-Glucose	OC[C@@H](O)[C@@H](O)[C@H](O)[C@@H](O)C=O	-4.67
67	Diazepam	Clc1cc2c(N(C)C(=O)CN=C2c2ccccc2)cc1	-4.45
68	Diclofenac	Clc1cc(Cl)ccc1Nc1ccccc1CC(O)=O	-4.75
69	Digoxin	O1CC(=CC1=O)[C@H]1CC[C@]2(O)[C@H]3[C@H](C[C@@H](O)[C@]12C)[C@@]1([C@@H](C[C@@H](O[C@@H]2O[C@H](C)[C@@H](O[C@@H]4O[C@H](C)[C@@H](O[C@@H]5O[C@H](C)[C@@H](O)[C@@H](O)C5)[C@@H](O)C4)[C@@H](O)C2)CC1)CC3)C	-5.58
70	Diltiazem	CC(=O)O[C@@H]1[C@@H](Sc2ccccc2N(C1=O)CCN(C)C)c3ccc(cc3)OC	-4.53
71	DMP 581	O=Cc1n(Cc2ccc(cc2)-c2ccccc2-c2n[n-]nn2)c(nc1CC)CCC	-5.48
72	DMP 728	CC[C@@H]1C(=O)N([C@@H](C(=O)NCC(=O)N[C@H](C(=O)NCc2cccc(c2)C(=O)N1)C(=O)O)CCCN=C(N)N)C	-6.58
73	DMP 811	CCCc1nc(c(n1Cc2ccc(cc2)c3ccccc3c4n[nH]nn4)C(=O)O)CC	-7.82
74	DMXAA	Cc1ccc2c(=O)c3cccc(c3oc2c1C)CC(=O)O	-4.60
75	Dopamine	c1cc(c(cc1CCN)O)O	-5.03
76	Doxorubicin	C[C@H]1[C@H]([C@H](C[C@@H](O1)O[C@H]2C[C@@](Cc3c2c(c4c(c3O)C(=O)c5cccc(c5C4=O)OC)O)(C(=O)CO)O)N)O	-6.48
77	Doxycycline	C[C@@H]1[C@H]2[C@@H]([C@H]3[C@@H](C(=C(C(=O)[C@]3(C(=C2C(=O)C4=C1C=CC=C4O)O)O)C(=O)N)O)N(C)C)O	-4.95
78	DuP 532	CCCc1nc(c(n1Cc2ccc(cc2)c3ccccc3c4n[nH]nn4)C(=O)O)C(C(F)(F)F)(F)F	-8.20
79	DuP 996	O=C1N(c2c(cccc2)C1(Cc1ccncc1)Cc1ccncc1)c1ccccc1	-4.62
80	Echinacoside	O1[C@@H](C)[C@H](O)[C@@H](O)[C@@H](O)[C@@H]1O[C@H]1[C@H](OC(=O)\C=C\c2cc(O)c(O)cc2)[C@H](O[C@@H](OCCc2cc(O)c(O)cc2)[C@@H]1O)CO[C@@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1O	-6.65
81	Elarofiban	c1cc(cnc1)[C@H](CC(=O)O)NC(=O)[C@@H]2CCCN(C2)C(=O)CCC3CCNCC3	-6.21
82	Enalapril	CCOC(=O)[C@H](CCC1=CC=CC=C1)N[C@@H](C)C(=O)N2CCC[C@H]2C(=O)O	-6.21
83	Enalaprilat	C[C@@H](C(=O)N1CCC[C@H]1C(=O)O)N[C@@H](CCC2=CC=CC=C2)C(=O)O	-6.59

84	Ephedrine	CC(C(c1ccccc1)O)NC	-4.97
85	Epicatechin	O1c2c(C[C@@H](O)[C@H]1c1cc(O)c(O)cc1)c(O)cc(O)c2	-6.82
86	Epicatechin-3-Gallate	O1c2c(C[C@H](OC(=O)c3cc(O)c(O)c(O)c3)[C@@H]1c1cc(O)c(O)cc1)c(O)cc(O)c2	-6.84
87	Epinephrine	CNC[C@@H](c1ccc(c(c1)O)O)O	-6.23
88	Erythritol	OC[C@@H](O)[C@@H](O)CO	-6.16
89	Erythromycin	CC[C@@H]1[C@@]([C@@H]([C@H](C(=O)[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	-5.78
90	Estradiol	Oc1cc2CC[C@H]3[C@@H]4CC[C@H](O)[C@]4(CC[C@@H]3c2cc1)C	-4.69
91	Etoposide	O1C[C@H]2[C@@H]([C@@H](c3c(cc4OCOc4c3)[C@H]2O[C@@H]2O[C@H]3[C@@H](O[C@@H](OC3)C)[C@H](O)[C@H]2O)c2cc(OC)c(O)c(OC)c2)C1=O	-5.81
92	EXP3174	CCCCc1nc(c(n1Cc2ccc(cc2)c3ccccc3c4[nH]nnn4)C(=O)O)Cl	-6.74
93	Famotidine	c1c(nc(s1)N=C(N)N)CSCC/C(=N/S(=O)(=O)N)/N	-6.16
94	Felodipine	Clc1c(cccc1Cl)C1C(C(OCC)=O)=C(NC(C)=C1C(OC)=O)C	-4.64
95	Fenoprofen	CC(c1cccc(c1)Oc2ccccc2)C(=O)O	-5.11
96	Fexofenadine	CC(C)(c1ccc(cc1)C(CCCN2CCC(CC2)C(c3ccccc3)(c4ccccc4)O)O)C(=O)O	-6.51
97	Flavone	O1c2c(cccc2)C(=O)C=C1c1ccccc1	-3.33
98	Fleroxacin	CN1CCN(CC1)c2c(F)c3c(cc2F)C(=O)C(CN3CCF)C(O)=O	-4.98
99	Fluconazole	Fc1cc(F)ccc1C(O)(Cn1ncnc1)Cn1ncnc1	-4.82
100	Fluparoxan	Fc2c1OC3C(Oc1ccc2)CNC3	-4.10
101	Flurbiprofen	CC(c1ccc(c(c1)F)c2ccccc2)C(=O)O	-4.47
102	Fluvastatin	CC(C)n1c2ccccc2c(c1/C=C/[C@H](C[C@H](CC(=O)O)O)O)c3ccc(cc3)F	-4.22
103	Formoterol	C[C@H](Cc1ccc(cc1)OC)NC[C@@H](c2ccc(c(c2)NC=O)O)O	-5.63
104	foscarnet	C(=O)(O)P(=O)(O)O	-7.47
105	Furosemide	Clc1cc(NCc2occc2)c(C(O)=O)c(S(=O)(=O)N)c1	-6.62
106	Gabapentin	C1CCC(CC1)(CC(=O)O)CN	-8.16
107	Ganciclovir	O=C1N=C(Nc2n(cnc12)COC(CO)CO)N	-6.37
108	Glipizide	Cc1cnc(cn1)C(=O)NCCc2ccc(cc2)S(=O)(=O)NC(=O)NC3CCCCC3	-5.97
109	Glycine	C(C(=O)O)N	-4.36
110	Glycine-Valine acyclovir	CC(C)C(C(=O)OCCOCN1C=NC2=C1NC(=NC2=O)N)NC(=O)CN	-5.28
111	Griseofulvin	Clc1c2O[C@]3([C@@H](CC(=O)C=C3OC)C)C(=O)c2c(OC)cc1OC	-4.36
112	Guanabenz	C1=CC(=C(C(=C1)Cl)/C=N/N=C(N)N)Cl	-4.97
113	Guanoxan	c1ccc2c(c1)OCC(O2)CNC(=N)N	-4.87
114	Harmaline	O(C)C=1C=CC2=C3C(N=C2C=1)=C(NCC3)C	-6.07
115	Harmalol	Oc1cc2[nH]c3c(CCN=C3C)c2cc1	-6.37
116	Harmane	[nH]1c2c(c3c1cccc3)ccnc2C	-6.13
117	Harmine	O(C)c1cc2[nH]c3c(c2cc1)ccnc3C	-6.13

118	Harmol	OC=1C=CC2=C3C(N=C2C=1)=C(NC=C3)C	-6.37
119	Hydralazine	n1ncc2c(cccc2)c1NN	-5.17
120	Hydrochlorothiazide	Clc1cc2NCNS(=O)(=O)c2cc1S(=O)(=O)N	-6.06
121	Hydrocortisone	O=C1CC[C@@]2([C@@H]3[C@H]([C@@H]4CC[C@](O)(C(=O)CO)[C@]4(C[C@@H]3O)C)CCC2=C1)C	-4.82
122	Ibuprofen	CC(C)Cc1ccc(cc1)C(C)C(=O)O	-4.58
123	Ibuproxam	CC(C)Cc1ccc(cc1)C(C)C(=O)NO	-4.63
124	Imipramine	CN(C)CCCN1c2ccccc2CCc3c1cccc3	-5.17
125	Indobufen	CCC(c1ccc(cc1)N2Cc3ccccc3C2=O)C(=O)O	-4.39
126	Indomethacin	Cc1c(c2cc(ccc2n1C(=O)c3ccc(cc3)Cl)OC)CC(=O)O	-4.89
127	Inuline	CCN1C[C@@]2(CC[C@@H]([C@@]34[C@@H]2[C@@H]([C@@](C31)([C@]5(C[C@@H]([C@H]6C[C@@H]4[C@@H]5[C@H]6OC)OC)O)O)OC)OC)COC(=O)c7ccccc7N	-6.25
128	Isoxicam	CC1=CC(=NO1)NC(=O)C2=C(C3=CC=CC=C3S(=O)(=O)N2C)O	-5.61
129	Ketoconazole	Clc1cc(Cl)ccc1[C@@]1(O[C@H](CO1)COc1ccc(N2CCN(CC2)C(=O)C)cc1)Cn1ccnc1	-4.93
130	Ketoprofen	CC(c1cccc(c1)C(=O)c2ccccc2)C(=O)O	-4.48
131	Ketorolac	c1ccc(cc1)C(=O)c2ccc3n2CCC3C(=O)O	-5.08
132	Labetalol	CC(CCc1ccccc1)NCC(c2ccc(c(c2)C(=O)N)O)O	-4.82
133	Lactic Acid	CC(C(=O)O)O	-6.19
134	Lactulose	O1[C@](O)(CO)[C@@H](O)[C@H](O[C@@H]2O[C@H](CO)[C@H](O)[C@H](O)[C@H]2O)[C@H]1CO	-6.81
135	Lamotrigine	Clc1c(cccc1Cl)-c1nnc(nc1N)N	-4.39
136	l-DOPA	c1cc(c(cc1C[C@@H](C(=O)O)N)O)O	-6.05
137	Lidocaine	CCN(CC)CC(=O)Nc1c(cccc1C)C	-4.36
138	Lisinopril	C1C[C@H](N(C1)C(=O)[C@H](CCCCN)N[C@@H](CCC2=CC=CC=C2)C(=O)O)C(=O)O	-7.39
139	Loracarbef	C1CC(=C(N2[C@H]1[C@@H](C2=O)NC(=O)[C@@H](C3=CC=CC=C3)N)C(=O)O)Cl	-7.34
140	Losartan	Clc1nc(n(Cc2ccc(cc2)-c2ccccc2-c2[nH]nnn2)c1CO)CCCC	-6.05
141	Loxoprofen	CC(c1ccc(cc1)CC2CCCC2=O)C(=O)O	-4.35
142	L-phenylalanine	c1ccc(cc1)CC(CC(=O)O)N	-5.00
143	Mannitol	OC[C@@H](O)[C@@H](O)[C@H](O)[C@H](O)CO	-6.48
144	Meloxicam	CC1=CN=C(S1)NC(=O)C2=C(C3=CC=CC=C3S(=O)(=O)N2C)O	-4.71
145	Metaproterenol	CC(C)NCC(c1cc(cc(c1)O)O)O	-6.42
146	Metformin	CN(C)C(=N)NC(=N)N	-6.2
147	Methanol	OC	-4.40
148	Methotrexate	CN(Cc1cnc2c(n1)c(nc(n2)N)N)c3ccc(cc3)C(=O)N[C@@H](CCC(=O)O)C(=O)O	-6.10
149	Methyl gallate	Oc1c(O)cc(cc1O)C(OC)=O	-5.39
150	Methyl Scopolamine	O1[C@H]2[C@H]3[N+]([C@@H]([C@@H]12)CC(OC(=O)[C@H](CO)c1ccccc1)C3)(C)C	-6.23
151	Methylprednisolone	O=C1C=C2[C@@]([C@@H]3[C@H]([C@@H]4CC[C@](O)(C(=O)CO)[C@]4(C[C@@H]3O)C)C[C@@H]2C)(C=C1)C	-4.93
152	metolazone	Clc1cc2NC(N(c3ccccc3C)C(=O)c2cc1S(=O)(=O)N)C	-5.21
153	Metoprolol	CC(C)NCC(COc1ccc(cc1)CCOC)O	-4.60

154	Mibefradil	CC(C)[C@H]1c2ccc(cc2CC[C@@]1(CCN(C)CCCc3[nH]c4ccccc4n3)OC(=O)COC)F	-5.04
155	Morphine	CN1CC[C@]23[C@@H]4[C@H]1CC5=C2C(=C(C=C5)O)O[C@H]3[C@H](C=C4)O	-5.45
156	Nadolol	CC(C)(C)NCC(COc1cccc2c1C[C@@H]([C@@H](C2)O)O)O	-6.14
157	Naloxone	C=CCN1CC[C@]23[C@@H]4C(=O)CC[C@]2([C@H]1CC5=C3C(=C(C=C5)O)O4)O	-4.67
158	Naproxen	C[C@@H](c1ccc2cc(ccc2c1)OC)C(=O)O	-4.66
159	Naringenin	O1c2c(C(=O)C[C@H]1c1ccc(O)cc1)c(O)cc(O)c2	-4.41
160	Naringin	O1[C@H](CO)[C@@H](O)[C@H](O)[C@@H](O[C@H]2O[C@H](C)[C@H](O)[C@H](O)[C@H]2O)[C@@H]1Oc1cc(O)c2c(O[C@@H](CC2=O)c2ccc(O)cc2)c1	-6.82
161	N-desmethylclozapine	C1CN(CCN1)C2=NC3=C(C=CC(=C3)Cl)NC4=CC=CC=C42	-4.68
162	Netivudine	O1[C@H](CO)[C@@H](O)[C@H](O)[C@@H]1N1C=C(C#CC)C(=O)NC1=O	-6.84
163	Nevirapine	O=C1Nc2c(nccc2C)N(c2ncccc12)C1CC1	-4.52
164	Nicotine	CN1CCC[C@H]1c2cccnc2	-4.71
165	Nitrendipine	O(C(=O)C=1C(C(C(OC)=O)=C(NC=1C)C)c1cc([N+](=O)[O-])ccc1)CC	-4.93
166	Nordazepan	Clc1cc2c(NC(=O)CN=C2c2ccccc2)cc1	-4.2
167	Norfloxacin	CCn1cc(c(=O)c2c1cc(c(c2)F)N3CCNCC3)C(=O)O	-6.70
168	Octyl gallate	Oc1c(O)cc(cc1O)C(OCCCCCCCC)=O	-6.82
169	Olopatadine	CN(C)CC/C=C\1/C2=CC=CC=C2COC3=C1C=C(C=C3)CC(=O)O	-5.01
170	Olsalazine	C1=CC(=C(C=C1/N=N/C2=CC(=C(C=C2)O)C(=O)O)C(=O)O)O	-7.80
171	Ondansetron	O=C1c2c(n(c3c2cccc3)C)CCC1Cn1ccnc1C	-4.34
172	Ouabain	O1CC(=CC1=O)[C@H]1CC[C@]2(O)[C@H]3[C@@H]([C@]4(CO)[C@@](O)(C[C@@H](O[C@@H]5O[C@@H](C)[C@H](O)[C@@H](O)[C@H]5O)C[C@H]4O)CC3)[C@H](O)C[C@]12C	-7.23
173	Oxacillin	Cc1c(c(no1)c2ccccc2Cl)C(=O)N[C@H]3[C@@H]4N(C3=O)[C@H](C(S4)(C)C)C(=O)O	-5.58
174	Oxazepam	Clc1cc2c(NC(=O)C(O)N=C2c2ccccc2)cc1	-4.22
175	Oxprenolol	CC(C)NCC(COc1ccccc1OCC=C)O	-4.76
176	Paclitaxel	O1[C@@H]2C[C@H](O)[C@@]3([C@H]([C@H](OC(=O)c4ccccc4)[C@]4(O)C[C@H](OC(=O)[C@H](O)[C@@H](NC(=O)c5ccccc5)c5ccccc5)C(=C([C@@H](OC(=O)C)C3=O)C4(C)C)C)[C@]2(OC(=O)C)C1)C	-7.30
177	Penicillin V	CC1([C@@H](N2[C@H](S1)[C@@H](C2=O)NC(=O)COc3ccccc3)C(=O)O)C	-7.51
178	Phencyclidine	c1ccc(cc1)C2(CCCCC2)N3CCCCC3	-4.61
179	Phenytoin	O=C1NC(=O)NC1(c1ccccc1)c1ccccc1	-4.49
180	pindolol	CC(C)NCC(COc1cccc2c1cc[nH]2)O	-4.71
181	Pirenzepine	CN1CCN(CC1)CC(=O)N2c3ccccc3C(=O)Nc4c2nccc4	-6.36
182	piroxicam	S1(=O)(=O)N(C)C(/C(/O)=N/c2ncccc2)=C(O)c2c1cccc2	-4.33
183	Pivampicillin	CC1([C@@H](N2[C@H](S1)[C@@H](C2=O)NC(=O)[C@@H](c3ccccc3)N)C(=O)OCOC(=O)C(C)(C)C)C	-4.49

184	Practolol	CC(C)NCC(COc1ccc(cc1)NC(=O)C)O	-6.02
185	Pranoprofen	CC(c1ccc2c(c1)Cc3cccnc3O2)C(=O)O	-4.39
186	Pravastatin	CC[C@H](C)C(=O)O[C@H]1C[C@@H](C=C2[C@H]1[C@H]([C@H](C=C2)C)CC[C@H](C[C@H](CC(=O)O)O)O)O	-5.84
187	Prazosin	o1cccc1C(=O)N1CCN(CC1)c1nc(N)c2cc(OC)c(OC)cc2n1	-5.26
188	Prednisolone	O=C1C=C2CC[C@@H]3[C@@H]([C@]2(C=C1)C)[C@@H](O)C[C@]1([C@H]3CC[C@]1(O)C(=O)CO)C	-4.72
189	Progesterone	O=C1CC[C@@]2([C@@H]3[C@H]([C@@H]4CC[C@H](C(=O)C)[C@]4(CC3)C)CCC2=C1)C	-4.64
190	Propofol	Oc1c(cccc1C(C)C)C(C)C	-4.77
191	Propranolol	CC(C)NCC(COc1cccc2c1cccc2)O	-4.63
192	Propyl gallate	Oc1c(O)cc(cc1O)C(OCCC)=O	-6.82
193	Propylthiouracil	S=C1NC(=CC(=O)N1)CCC	-4.46
194	Proscillaridin	O1C=C(C=CC1=O)[C@H]1CC[C@]2(O)[C@H]3[C@H](CC[C@]12C)[C@@]1(C(=C[C@@H](O[C@@H]2O[C@@H](C)[C@H](O)[C@@H](O)[C@H]2O)CC1)CC3)C	-6.41
195	Quercertin	O1c2c(C(=O)C(O)=C1c1cc(O)c(O)cc1)c(O)cc(O)c2	-6.82
196	Quinidine	COc1ccc2c(c1)c(ccn2)[C@@H]([C@H]3C[C@@H]4CC[N@]3C[C@@H]4C=C)O	-4.94
197	Raffinose	O1[C@](O[C@H]2O[C@H](CO[C@H]3O[C@H](CO)[C@H](O)[C@H](O)[C@H]3O)[C@@H](O)[C@H](O)[C@H]2O)(CO)[C@@H](O)[C@H](O)[C@H]1CO	-7.62
198	Ranitidine	S(Cc1oc(cc1)C[NH+](C)C)CCN\C(\NC)=C/[N+](=O)[O-]	-6.31
199	Rapamycin	O1[C@@H](CC(=O)[C@@H](\C=C(/C)\[C@@H](O)[C@@H](OC)C(=O)[C@@H](C[C@@H](\C=C\C=C\C=C(/C)\[C@@H](OC)C[C@H]2O[C@](O)([C@@H](CC2)C)C(=O)C(=O)N2[C@@H](CCCC2)C1=O)C)C)[C@@H](C[C@H]1C[C@@H](OC)[C@H](O)CC1)C	-4.96
200	remikiren	S(=O)(=O)(C(C)(C)C)C[C@@H](Cc1ccccc1)C(=O)N[C@@H](Cc1[nH]cnc1)C(=O)N[C@H]([C@@H](O)[C@@H](O)C1CC1)CC1CCCCC1	-6.34
201	Roxithromycin	O1[C@H](CC)[C@](O)(C)[C@H](O)[C@@H](C)\C(=N\OCOCCOC)\[C@@H](C[C@](O)(C)[C@H](O[C@@H]2O[C@@H](C[C@H]([NH+](C)C)[C@H]2O)C)[C@@H](C)[C@H](O[C@@H]2O[C@@H](C)[C@H](O)[C@](OC)(C2)C)[C@@H](C)C1=O)C	-6.91
202	Salicyclic acid	Oc1ccccc1C(OCc1ccccc1)=O	-4.82
203	Saquinavir	CC(C)(C)NC(=O)[C@@H]1C[C@@H]2CCCC[C@@H]2CN1C[C@H]([C@H](Cc3ccccc3)NC(=O)[C@H](CC(=O)N)NC(=O)c4ccc5ccccc5n4)O	-6.48
204	SB209670	CCCOc1ccc2c(c1)[C@H]([C@@H]([C@H]2c3ccc4c(c3)OCO4)C(=O)O)c5ccc(cc5OCC(=O)O)OC	-5.23
205	Scolopamine	CN1[C@@H]2C[C@H](C[C@H]1[C@H]3[C@@H]2O3)OC(=O)[C@H](CO)C4=CC=CC=C4	-4.93
206	SDZ-RAD	O1[C@@H](CC(=O)[C@@H](\C=C(/C)\[C@@H](O)[C@@H](OC)C(=O)[C@@H](C[C@@H](\C=C\C=C\C=C(/C)\[C@@H](OC)C[C@H]2O[C@](O)([C@@H](CC2)C)C(=O)C(=O)N2[C@@H](CCCC2)C1=O)C)C)[C@H](C[C@H]1C[C@@H](OC)[C@H](OCCO)CC1)C	-4.63
207	Serotonin	c1cc2c(cc1O)c(c[nH]2)CCN	-4.86

208	sildenafil	CCCc1c2c(c(=O)[nH]c(n2)c3cc(ccc3OCC)S(=O)(=O)N4CC N(CC4)C)n(n1)C	-4.51
209	Sotalol	CC(C)NCC(c1ccc(cc1)NS(=O)(=O)C)O	-5.76
210	Sucrose	O1[C@](O[C@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C @H]2O)(CO)[C@@H](O)[C@H](O)[C@H]1CO	-5.77
211	Sulfadiazine	S(=O)(=O)(Nc1ncccn1)c1ccc(N)cc1	-4.75
212	Sulfamethoxazole	Cc1cc(no1)NS(=O)(=O)c2ccc(cc2)N	-4.88
213	Sulfanilamide	S(=O)(=O)(N)c1ccc(N)cc1	-5.26
214	Sulfapyridine	S(=O)(=O)(Nc1ncccc1)c1ccc(N)cc1	-5.00
215	Sulfasalazine	C1=CC=NC(=C1)NS(=O)(=O)C2=CC=C(C=C2)N=NC3=CC(= C(C=C3)O)C(=O)O	-6.89
216	Sulfisoxazole	Cc1c(noc1NS(=O)(=O)c2ccc(cc2)N)C	-4.92
217	Sulindac	CC\1=C(c2cc(ccc2/C1=C\c3ccc(cc3)S(=O)C)F)CC(=O)O	-5.24
218	Sulpiride	CCN1CCCC1CNC(=O)c2cc(ccc2OC)S(=O)(=O)N	-6.65
219	Sumatriptan	CNS(=O)(=O)Cc1ccc2c(c1)c(c[nH]2)CCN(C)C	-5.80
220	Talinolol	CC(C)(C)NCC(COc1ccc(cc1)NC(=O)NC2CCCCC2)O	-6.11
221	TAPP	O=C(N)C(NC(=O)C(NC(=O)C(NC(=O)C(N)Cc1ccc(O)cc1)C) Cc2ccccc2)Cc3ccccc3	-7.73
222	Tartaric Acid	C(C(C(=O)O)O)(C(=O)O)O	-6.65
223	Taurocholic acid	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	-4.75
224	Telithromycin	CC[C@@H]1[C@@]2([C@@H]([C@H](C(=O)[C@@H](C[C@@]([C@@H]([C@H](C(=O)[C@H](C(=O)O1)C)C)O[C @H]3[C@@H]([C@H](C[C@H](O3)C)N(C)C)O)(C)OC)C)C)N(C(=O)O2)CCCCn4cc(nc4)c5cccnc5)C	-6.65
225	Telmisartan	CCCc1nc2c(cc(cc2n1Cc3ccc(cc3)c4ccccc4C(=O)O)c5nc6c cccc6n5C)C	-4.82
226	Tenidap	Clc1cc2c(N(C(=O)N)C(=O)C2C(=O)c2sccc2)cc1	-4.57
227	Terbutaline	CC(C)(C)NCC(c1cc(cc(c1)O)O)O	-6.16
228	Testosterone	O=C1CC[C@@]2([C@@H]3[C@H]([C@@H]4CC[C@H](O)[C@]4(CC3)C)CCC2=C1)C	-4.43
229	Tetracycline	C[C@@]1([C@H]2C[C@H]3[C@@H](C(=C(C(=O)[C@]3(C(=C2C(=O)C4=C1C=CC=C4O)O)O)C(=O)N)O)N(C)C)O	-5.70
230	Theophylline	O=C1N(C)C(=O)N(c2nc[nH]c12)C	-4.61
231	Tiacrilast	CSC1=CC2=C(C=C1)N=CN(C2=O)/C=C/C(=O)O	-5.07
232	Tiaprofenic Acid	CC(c1ccc(s1)C(=O)c2ccccc2)C(=O)O	-4.41
233	Timolol	CC(C)(C)NC[C@@H](COc1c(nsn1)N2CCOCC2)O	-4.92
234	Tiotidine	C/N=C(/NCCSCc1csc(n1)N=C(N)N)\NC#N	-5.88
235	Tolbutamide	CCCCNC(=O)NS(=O)(=O)c1ccc(cc1)C	-4.28
236	Topiramate	S(OC[C@]12OC(O[C@H]1[C@@H]1OC(O[C@@H]1CO2) (C)C)(C)C)(=O)(=O)N	-4.54
237	Tranexamic Acid	C1[C@@H](CC[C@H](C1)C(=O)O)CN	-6.28
238	Trimethoprim	O(C)c1c(OC)cc(cc1OC)Cc1cnc(nc1N)N	-4.50
239	Trovafloxacin	C1[C@@H]2[C@@H]([C@H]2N)CN1C3=C(C=C4C(=O)C(= CN(C4=N3)C5=C(C=C(C=C5)F)F)C(=O)O)F	-4.81
240	Uracil	O=C1NC(=O)NC=C1	-5.37
241	Urea	O=C(N)N	-5.34

242	Valacyclovir	CC(C)[C@@H](C(=O)OCCOCn1cnc2c1nc([nH]c2=O)N)N	-5.20
243	Valproic Acid	CCCC(CCC)C(=O)O	-4.60
244	Verapamil	CC(C)C(CCCN(C)CCc1ccc(c(c1)OC)OC)(C#N)c2ccc(c(c2)OC)OC	-4.81
245	Vinblastine	CC[C@@]1(C[C@H]2C[C@@](c3c(c4ccccc4[nH]3)CCN(C2)C1)(c5cc6c(cc5OC)N([C@@H]7[C@]68CCN9[C@H]8[C@@](C=CC9)([C@H]([C@@]7(C(=O)OC)O)OC(=O)C)CC)C)C(=O)OC)O	-5.48
246	Warfarin	CC(=O)CC(C1=CC=CC=C1)C2=C(C3=CC=CC=C3OC2=O)O	-4.63
247	Zaltoprofen	CC(c1ccc2c(c1)CC(=O)c3ccccc3S2)C(=O)O	-4.40
248	Zidovudine	O1[C@H](CO)[C@@H](N=[N+]=[N-])C[C@@H]1N1C=C(C)C(=O)NC1=O	-5.06
249	Ziprasidone	c1ccc2c(c1)c(ns2)N3CCN(CC3)CCc4cc5c(cc4Cl)NC(=O)C5	-5.23
250	Zomepirac	Cc1cc(n(c1C(=O)c2ccc(cc2)Cl)C)CC(=O)O	-5.61

Appendix III. Dataset C (PAMPA data) used in Chapter 2.

ID	Name	SMILES	Log PAMPA Permeability (pH5.5) (cm/s)	Log PAMPA Permeability (pH7.4) (cms)
1	Acebutolol	O=C(Nc1ccc(OCC(O)CNC(C)C)c(c1)C(=O)C)CCC	-0.70	0.52
2	Acetaminophen	CC(=O)Nc1ccc(cc1)O	0.36	0.54
3	Acetylsalicylic acid	CC(=O)Oc1ccccc1C(=O)O	0.51	0.58
4	Actinomycin D	C[C@@H]1[C@@H](C(=O)N[C@@H](C(=O)N2CCC[C@H]2C(=O)N(CC(=O)N([C@H](C(=O)O1)C(C)C)C)C)C(C)C)NC(=O)C3=C4C(=C(C=C3)C)OC5=C(C(=O)C(=C(C5=N4)C(=O)N[C@H]6[C@H](OC(=O)[C@@H](N(C(=O)CN(C(=O)[C@@H]7CCCN7C(=O)[C@H](NC6=O)C(C)C)C)C)C(C)C)N)C	-	-1.74
5	Acyiclovir	O=C2/N=C(\Nc1n(cnc12)COCCO)N	0.00	0.00
6	Alprenolol	O(c1ccccc1C\C=C)CC(O)CNC(C)C	0.15	1.18
7	Amoxicillin	O=C(O)[C@@H]2N3C(=O)[C@@H](NC(=O)[C@@H](c1ccc(O)cc1)N)[C@H]3SC2(C)C	-	-0.66
8	Antipyrine	O=C2\C=C(/N(N2c1ccccc1)C)C	1.30	1.12
9	Atenolol	CC(C)NCC(COc1ccc(cc1)CC(=O)N)O	-1.00	-
10	Bromocriptine	CC(C)C[C@H]1C(=O)N2CCC[C@H]2[C@]3(N1C(=O)[C@](O3)(C(C)C)NC(=O)[C@H]4CN([C@@H]5Cc6c7c(cccc7[nH]c6Br)C5=C4)C)O	0.11	-
11	Bumetanide	O=S(=O)(c2cc(cc(NCCCC)c2Oc1ccccc1)C(=O)O)N	0.66	-0.52
12	Bupropion	O=C(c1cc(Cl)ccc1)C(NC(C)(C)C)C	1.68	1.15
13	Caffeine	Cn1cnc2c1c(=O)n(c(=O)n2C)C	1.31	1.03
14	Captopril	O=C(O)[C@H]1N(C(=O)[C@H](C)CS)CCC1	0.64	1.28
15	Carbamazepine	c1ccc2c(c1)C=Cc3ccccc3N2C(=O)N	1.08	1.05
16	Ceftriaxone	O=C2N1/C(=C(\CS[C@@H]1[C@@H]2NC(=O)C(=N\OC)/c3nc(sc3)N)CS\C4=N\C(=O)C(=O)NN4C)C(=O)O	-1.00	-
17	Chloramphenicol	c1cc(ccc1[C@H]([C@@H](CO)NC(=O)C(Cl)Cl)O)[N+](=O)[O-]	0.83	0.23
18	Chlorothiazide	O=S(=O)(c1c(Cl)cc2c(c1)S(=O)(=O)/N=C\N2)N	-0.70	0.11
19	Chlorpheniramine	Clc1ccc(cc1)C(c2ncccc2)CCN(C)C	-	1.08
20	Chlorpromazine	CN(C)CCCN1c2ccccc2Sc3c1cc(cc3)Cl	1.07	0.60
21	Chloroquine	Clc1cc2nccc(c2cc1)NC(C)CCCN(CC)CC	-	0.30
22	Cimetidine	N#CN\C(=N/C)NCCSCc1ncnc1C	-	0.00
23	Colchicine	CC(=O)N[C@H]1CCc2cc(c(c(c2-c3c1cc(=O)c(cc3)OC)OC)OC)OC	-	-1.60
24	Clofibrate	Clc1ccc(OC(C(=O)OCC)(C)C)cc1	-0.40	-0.52
25	Clonidine	Clc1c(c(Cl)ccc1)N/C2=N/CCN2	1.30	1.15
26	Clozapine	CN1CCN(CC1)C2=Nc3cc(ccc3Nc4c2cccc4)Cl	1.35	1.45

27	Corticosterone	O=C4\C=C2/[C@]([C@H]1[C@@H](O)C[C@@]3([C@@H](C(=O)CO)CC[C@H]3[C@@H]1CC2)C)(C)CC4	1.59	1.34
28	Coumarin	c1ccc2c(c1)ccc(=O)o2	1.36	1.34
29	Cyclosporine	O=C1N(C)[C@H](C(=O)N[C@H](C(=O)N(C)CC(=O)N(C)[C@H](C(=O)N[C@H](C(=O)N(C)[C@H](C(=O)N[C@H](C(=O)N[C@@H](C(=O)N([C@H](C(=O)N(C)[C@H](C(=O)N(C)[C@H]1C(C)C)CC(C)C)CC(C)C)C)C)C)CC(C)C)CC)[C@H](O)[C@H](C)C/C=C/C	-1.00	-0.52
30	Desipramine	c1cc3c(cc1)CCc2c(cccc2)N3CCCNC	0.97	1.16
31	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	0.83	0.91
32	Diclofenac	c1ccc(c(c1)CC(=O)O)Nc2c(cccc2Cl)Cl	1.03	1.10
33	Diltiazem	O=C2N(c3c(S[C@@H](c1ccc(OC)cc1)[C@H]2OC(=O)C)cccc3)CCN(C)C	1.03	1.27
34	Dipyridamole	n3c(nc2c(nc(nc2N1CCCCC1)N(CCO)CCO)c3N4CCCCC4)N(CCO)CCO	-	0.54
35	Doxorubicin	C[C@H]1[C@H]([C@H](C[C@@H](O1)O[C@H]2C[C@@](Cc3c2c(c4c(c3O)C(=O)c5cccc(c5C4=O)OC)O)(C(=O)CO)O)N)O	-0.52	-0.30
36	Emetine	O(c1cc2c(cc1OC)[C@H](NCC2)C[C@H]5C[C@H]4c3c(cc(OC)c(OC)c3)CCN4C[C@@H]5CC)C	-	0.81
37	Enalapril	O=C(O)[C@H]2N(C(=O)[C@@H](N[C@H](C(=O)OCC)CCc1ccccc1)C)CCC2	0.53	-1.00
38	Erythromycin	CC[C@@H]1[C@@]([C@@H]([C@H](C(=O)[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)O)(C)O	-1.00	-1.00
39	Etoposide	C[C@@H]1OC[C@@H]2[C@@H](O1)[C@@H]([C@H]([C@@H](O2)O[C@@H]3c4cc5c(cc4[C@H]([C@@H]6[C@@H]3COC6=O)c7cc(c(c(c7)OC)O)OC)OCO5)O)O	-0.15	-0.40
40	Flumazenil	Fc2cc1C(=O)N(C)Cc3c(ncn3c1cc2)C(=O)OCC	0.68	0.78
41	Fluoxetine	CNCCC(c1ccccc1)Oc2ccc(cc2)C(F)(F)F	0.87	1.15
42	Furosemide	c1cc(oc1)CNc2cc(c(cc2C(=O)O)S(=O)(=O)N)Cl	-0.22	-0.22
43	Gabapentin	O=C(O)CC1(CN)CCCCC1	0.08	0.08
44	Griseofulvin	O=C2c3c(O[C@@]21C(/OC)=C\C(=O)C[C@H]1C)c(Cl)c(OC)cc3OC	0.89	0.72
45	Guanabenz	Clc1cccc(Cl)c1\C=N\N=C(/N)N	0.20	1.24
46	Hydrochlorothiazide	O=S(=O)(c1c(Cl)cc2c(c1)S(=O)(=O)NCN2)N	-1.00	-
47	Hydrocortisone	O=C4\C=C2/[C@]([C@H]1[C@@H](O)C[C@@]3([C@@](O)(C(=O)CO)CC[C@H]3[C@@H]1CC2)C)(C)CC4	0.49	0.53
48	Ibuprofen	CC(C)Cc1ccc(cc1)C(C)C(=O)O	1.03	0.83

49	Imipramine	c1cc3c(cc1)CCc2c(cccc2)N3CCCN(C)C	1.11	0.92
50	Indomethacin	Cc1c(c2cc(ccc2n1C(=O)c3ccc(cc3)Cl)OC)CC(=O)O	0.80	0.38
51	Ketoconazole	O=C(N5CCN(c4ccc(OC[C@@H]1O[C@](OC1)(c2ccc(Cl)cc2Cl)Cn3ccnc3)cc4)CC5)C	0.52	0.08
52	Ketoprofen	CC(c1cccc(c1)C(=O)c2ccccc2)C(=O)O	1.28	1.22
53	Ketorolac	O=C(c1ccc2n1CCC2C(=O)O)c3ccccc3	0.71	0.15
54	Labetalol	O=C(c1cc(ccc1O)C(O)CNC(C)CCc2ccccc2)N	-1.00	0.65
55	Loperamide	Clc1ccc(cc1)C4(O)CCN(CCC(c2ccccc2)(c3ccccc3)C(=O)N(C)C)CC4	-	0.76
56	Loratadine	O=C(OCC)N4CC/C(=C2/c1ccc(Cl)cc1CCc3cccnc23)CC4	-	0.48
57	Mebendazole	O=C(c2cc1c(nc(n1)NC(=O)OC)cc2)c3ccccc3	-	0.98
58	Melphalan	c1cc(ccc1C[C@@H](C(=O)O)N)N(CCCl)CCCl	1.01	0.76
59	Methotrexate	O=C(O)[C@@H](NC(=O)c1ccc(cc1)N(C)Cc2nc3c(nc2)nc(nc3N)N)CCC(=O)O	-0.70	-1.00
60	Methylprednisolone	C[C@H]1C[C@H]2[C@@H]3CC[C@@]([C@]3(C[C@@H]([C@@H]2[C@@]4(C1=CC(=O)C=C4)C)O)C)(C(=O)CO)O	0.41	0.77
61	Metoprolol	O(c1ccc(cc1)CCOC)CC(O)CNC(C)C	0.08	0.54
62	Miconazole	c1cc(c(cc1Cl)Cl)COC(Cn2ccnc2)c3ccc(cc3Cl)Cl	-0.15	-
63	Midazolam	Cc1ncc2n1-c3ccc(cc3C(=NC2)c4ccccc4F)Cl	-	1.04
64	Mitoxantrone	O=C2c1c(c(NCCNCCO)ccc1NCCNCCO)C(=O)c3c2c(O)ccc3O	-	-0.15
65	Naproxen	C[C@@H](c1ccc2cc(ccc2c1)OC)C(=O)O	1.36	1.03
66	Neostigmine	O=C(Oc1cccc(c1)[N+](C)(C)C)N(C)C	-	0.04
67	Nicardipine	O=C(OCCN(Cc1ccccc1)C)\C2=C(\N/C(=C(/C(=O)OC)C2c3cccc([N+]([O-])=O)c3)C)C	-	1.11
68	Nifedipine	CC1=C(C(C(=C(N1)C)C(=O)OC)c2ccccc2[N+](=O)[O-])C(=O)OC	-	1.04
69	Nicotine	n1cc(ccc1)[C@H]2N(C)CCC2	1.17	1.33
70	Norfloxacine	O=C(O)\C2=C\N(c1cc(c(F)cc1C2=O)N3CCNCC3)CC	-0.30	-0.05
71	Penicillin-V	O=C(O)[C@@H]2N3C(=O)[C@@H](NC(=O)COc1ccccc1)[C@H]3SC2(C)C	0.20	-1.00
72	Phenytoin	O=C2NC(=O)NC2(c1ccccc1)c3ccccc3	0.88	0.71
73	Pindolol	OC(CNC(C)C)COc1cccc2c1ccn2	1.12	0.69
74	Piroxicam	CN1C(=C(c2ccccc2S1(=O)=O)O)/C(=N/c3ccccn3)/O	0.92	0.91
75	Practolol	O=C(Nc1ccc(OCC(O)CNC(C)C)cc1)C	-	-2.00
76	Prazosin	O=C(N3CCN(c2nc1cc(OC)c(OC)cc1c(n2)N)CC3)c4occc4	0.40	1.13
77	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	0.34	0.76
78	Probenecid	O=S(=O)(N(CCC)CCC)c1ccc(C(=O)O)cc1	0.60	0.38

79	Progesterone	O=C4\C=C2/[C@]([C@H]1CC[C@@]3([C@@H](C(=O)C)CC[C@H]3[C@@H]1CC2)C)(C)CC4	-0.10	0.60
80	Propranolol	CC(C)NCC(COc1cccc2c1cccc2)O	1.23	1.37
81	Puromycin	O=C(N[C@@H]3[C@H](O[C@@H](n2cnc1c2ncnc1N(C)C)[C@@H]3O)CO)[C@@H](N)Cc4ccc(OC)cc4	-	-1.00
82	Pyridostigmine	O=C(Oc1ccc[n+](c1)C)N(C)C	-	-0.85
83	Quinidine	O(c4cc1c(nccc1[C@H](O)[C@@H]2N3CC[C@@H](C2)[C@@H](/C=C)C3)cc4)C	0.78	1.04
84	Ranitidine	[O-][N+](=O)\C=C(\NC)NCCSCc1oc(cc1)CN(C)C	-	-1.47
85	Reserpine	O=C(OC)[C@H]6[C@H]4C[C@@H]3c2nc1cc(OC)ccc1c2CCN3C[C@H]4C[C@@H](OC(=O)c5cc(OC)c(OC)c(OC)c5)[C@@H]6OC	-	0.79
86	Saccharin	O=C2c1ccccc1S(=O)(=O)N2	0.85	-
87	Salicylic acid	c1ccc(c(c1)C(=O)O)O	1.33	0.52
88	Sotalol	O=S(=O)(Nc1ccc(cc1)C(O)CNC(C)C)C	0.46	0.04
89	Sulfasalazine	O=S(=O)(Nc1ccccn1)c3ccc(/N=N/c2cc(C(O)=O)c(O)cc2)cc3	-0.52	-1.00
90	Sulpiride	O=S(=O)(N)c1cc(c(OC)cc1)C(=O)NCC2N(CC)CCC2	-0.70	-1.00
91	Sumatriptan	O=S(=O)(NC)Cc1cc2c(cc1)ncc2CCN(C)C	-	-0.77
92	Taxol	CC1=C2[C@@]([C@]([C@H]([C@@H]3[C@]4([C@H](OC4)C[C@@H]([C@]3(C(=O)[C@@H]2OC(=O)C)C)O)OC(=O)C)OC(=O)c5ccccc5)(C[C@@H]1OC(=O)[C@H](O)[C@@H](NC(=O)c6ccccc6)c7ccccc7)O)(C)C	-	0.00
93	Terazosine	O=C(N3CCN(c2nc1cc(OC)c(OC)cc1c(n2)N)CC3)C4OCCC4	0.23	0.94
94	Testosterone	O=C4\C=C2/[C@]([C@H]1CC[C@@]3([C@@H](O)CC[C@H]3[C@@H]1CC2)C)(C)CC4	-	1.26
95	Theophylline	Cn1c2c(c(=O)n(c1=O)C)[nH]cn2	-	-1.37
96	Timolol	O[C@H](COc1nsnc1N2CCOCC2)CNC(C)(C)C	0.23	0.71
97	Tranexamic Acid	NC[C@@H]1CC[C@H](CC1)C(O)=O	0.00	0.00
98	Trimethoprim	COc1cc(cc(c1OC)OC)Cc2cnc(nc2N)N	0.43	0.70
99	Triamterene	n1c3c(nc(c1c2ccccc2)N)nc(nc3N)N	-	-0.80
100	Verapamil	N#CC(c1cc(OC)c(OC)cc1)(CCCN(CCc2ccc(OC)c(OC)c2)C)C(C)C	0.99	0.87
101	Vinblastine	O=C(OC)[C@]4(c2c(c1ccccc1n2)CCN3C[C@](O)(CC)C[C@H](C3)C4)c5c(OC)cc6c(c5)[C@@]89[C@@H](N6C)[C@@](O)(C(=O)OC)[C@H](OC(=O)C)[C@@]7(/C=C\CN([C@@H]78)CC9)CC	-	0.61
102	Warfarin	CC(=O)CC(C1=CC=CC=C1)C2=C(C3=CC=CC=C3OC2=O)O	1.02	1.09
103	Yohimbine	O=C(OC)[C@@H]5[C@H]4C[C@H]3c2nc1ccccc1c2CCN3C[C@@H]4CC[C@@H]5O	-	0.69
104	Zidovudine (AZT)	Cc1cn(c(=O)[nH]c1=O)[C@H]2C[C@@H]([C@H](O2)CO)N=[N+]=[N-]	-0.22	0.69

105	Zopiclone	O=C(OC3c1nccnc1C(=O)N3c2ncc(Cl)cc2)N4CCN(C)CC4	0.51	0.95

Appendix IV. Dataset D (Bioavailability data) used in Chapter 2.

ID	Name	SMILES	Human Oral F (%)
1	Acetaminophen	Oc1ccc(NC(=O)C)cc1	85
2	Albuterol	Oc1ccc(cc1C(O)=O)C(O)CNC(C)(C)C	51
3	Allopurinol	O=C1NC=Nc2[nH]ncc12	66
4	Alprazolam	Clc1cc2c(-n3c(nnc3C)CN=C2c2ccccc2)cc1	90
5	Amantadine	NC12CC3CC(C1)CC(C2)C3	90
6	Atropine	O(C(=O)C(CO)c1ccccc1)C1CC2N(C(C1)CC2)C	50
7	Betaxolol	O(CC(O)CNC(C)C)c1ccc(cc1)CCOCC1CC1	85
8	Bumetanide	S(=O)(=O)(N)c1cc(cc(NCCCC)c1Oc1ccccc1)C(O)=O	90
9	Bupropion	CC(C(=O)c1cccc(c1)Cl)NC(C)(C)C	70
10	Carbamazepine	O=C(N)N1c2c(C=Cc3c1cccc3)cccc2	70
11	Ceftriaxone	s1cc(nc1N)/C(=N/OC)/C(=O)NC1C2SCC(CSC3=NC(=O)C(O)=NN3C)=C(N2C1=O)C(O)=O	0
12	Chlorpromazine	Clc1cc2N(c3c(Sc2cc1)cccc3)CCCN(C)C	25
13	Cimetidine	S(Cc1nc[nH]c1C)CCN\C(=N\C)\NC#N	60
14	Cisapride	Clc1cc(C(=O)NC2CCN(CC2OC)CCCOc2ccc(F)cc2)c(OC)cc1N	40
15	Clofibrate	Clc1ccc(OC(C(OCC)=O)(C)C)cc1	5
16	Clonazepam	Clc1ccccc1C1=NCC(=O)Nc2c1cc([N+](=O)[O-])cc2	90
17	Clonidine	c1cc(c(c(c1)Cl)NC2=NCCN2)Cl	97
18	Codeine	O1C2C34C(C(N(CC3)C)Cc3c4c1c(OC)cc3)C=CC2O	50
19	Diazepam	Clc1cc2c(N(C)C(=O)CN=C2c2ccccc2)cc1	95
20	Diclofenac	Clc1cc(Cl)ccc1Nc1ccccc1CC(O)=O	54
21	Diltiazem	CC(=O)O[C@@H]1[C@@H](Sc2ccccc2N(C1=O)CCN(C)C)c3ccc(cc3)OC	44
22	Dofetilide	S(=O)(=O)(Nc1ccc(cc1)CCN(CCOc1ccc(NS(=O)(=O)C)cc1)C)C	98
23	Ethambutol	OCC(NCCNC(CC)CO)CC	77
24	Felbamate	O(CC(COC(=O)N)c1ccccc1)C(=O)N	90
25	Felodipine	Clc1c(cccc1Cl)C1C(C(OCC)=O)=C(NC(C)=C1C(OC)=O)C	15
26	Flecainide	FC(F)(F)COc1ccc(OCC(F)(F)F)cc1C(=O)NCC1NCCCC1	85
27	Fluconazole	Fc1cc(F)ccc1C(O)(Cn1ncnc1)Cn1ncnc1	95
28	Flumazenil	Fc1cc2c(-n3c(CN(C)C2=O)c(nc3)C(OCC)=O)cc1	21
29	Fluoxetine	FC(F)(F)c1ccc(OC(CCNC)c2ccccc2)cc1	60
30	Fluvastatin	Fc1ccc(cc1)-c1c2c(n(C(C)C)c1\C=C\C(O)CC(O)CC(O)=O)cccc2	24
31	Furosemide	Clc1cc(NCc2occc2)c(C(O)=O)c(S(=O)(=O)N)c1	66
32	Gatifloxacin	Fc1cc2c(N(C=C(C(O)=O)C2=O)C2CC2)c(OC)c1N1CC(NCC1)C	96
33	Gentamicin_C1	O1C(OC2C(O)C(OC3OCC(O)(C)C(NC)C3O)C(N)CC2N)C(N)CCC1C(NC)C	0
34	Glipizide	S(=O)(=O)(NC(=O)NC1CCCCC1)c1ccc(cc1)CCNC(=O)c1ncc(nc1)C	95

35	Glyburide	Clc1cc(C(=O)NCCc2ccc(S(=O)(=O)NC(=O)NC3CCCCC3)cc2)c(OC)cc1	77
36	Granisetron	O=C(NC1CC2N(C(C1)CCC2)C)c1nn(c2c1cccc2)C	60
37	Haloperidol	Clc1cc(ccc1)C1(O)CCN(CC1)CCCC(=O)c1ccc(F)cc1	60
38	Hydrochlorothiazide	Clc1cc2NCNS(=O)(=O)c2cc1S(=O)(=O)N	71
39	Ibuprofen	OC(=O)C(C)c1ccc(cc1)CC(C)C	85
40	Imipramine	N(CCCN1c2c(CCc3c1cccc3)cccc2)(C)C	45
41	Indomethacin	Cc1c(c2cc(ccc2n1C(=O)c3ccc(cc3)Cl)OC)CC(=O)O	99
42	Isoniazid	O=C(NN)c1ccncc1	80
43	Isradipine	o1nc2c(n1)cccc2C1C(C(OC(C)C)=O)=C(NC(C)=C1C(OC)=O)C	19
44	Ketorolac	OC(=O)C1CCn2c1ccc2C(=O)c1ccccc1	95
45	Lamivudine	S1CC(OC1CO)N1CCC(=NC1=O)N	85
46	Lamotrigine	Clc1c(cccc1Cl)-c1nnc(nc1N)N	98
47	Lansoprazole	S(=O)(Cc1ncc(C)c(OCC(F)(F)F)c1)c1[nH]c2c(n1)cccc2	83
48	Losartan	Clc1nc(n(Cc2ccc(cc2)-c2ccccc2-c2[nH]nnn2)c1CO)CCCC	33
49	Metformin	N(C(NC(N)=N)=N)(C)C	53
50	Methadone	O=C(C(CC(N(C)C)C)(c1ccccc1)c1ccccc1)CC	80
51	Methylprednisolone	OC1(CCC2C3C(C4(C(=CC(=O)C=C4)C(C3)C)C)C(O)CC12C)C(=O)CO	85
52	Metoclopramide	Clc1cc(C(=O)NCCN(CC)CC)c(OC)cc1N	50
53	Metoprolol	O(CC(O)CNC(C)C)c1ccc(cc1)CCOC	44
54	Mexiletine	O(CC(N)C)c1c(cccc1C)C	87
55	Morphine	O1C2C34C(C(N(CC3)C)Cc3c4c1c(O)cc3)C=CC2O	24
56	Moxifloxacin	Fc1cc2c(c(OC)c1N1CC3C(NCCC3)C1)C(NC1CC1)C=C(C(O)=O)C2=O	91
57	Naloxone	O1C2C34CCN(C(Cc5c3c1c(O)cc5)C4(O)CCC2=O)CC=C	2
58	Naproxen	O(C)c1cc2c(cc(cc2)C(C(O)=O)C)cc1	95
59	Nicotine	n1cc(ccc1)C1N(CCC1)C	30
60	Nitrofurantoin	o1c(ccc1[N+](=O)[O-])\C=N\N1CC(=O)NC1=O	91
61	Omeprazole	S(=O)(Cc1ncc(C)c(OC)c1C)c1[nH]c2c(n1)cc(OC)cc2	47
62	Ondansetron	O=C1c2c(n(c3c2cccc3)C)CCC1Cn1ccnc1C	60
63	Phenytoin	O=C1NC(=O)NC1(c1ccccc1)c1ccccc1	90
64	Propranolol	CC(C)NCC(COc1cccc2c1cccc2)O	30
65	Rivastigmine	O(C(=O)N(CC)C)c1cc(ccc1)C(N(C)C)C	40
66	Ropinirole	O=C1Nc2c(C1)c(ccc2)CC(NCCC)NCCC	50
67	Stavudine	O1C(C=CC1N1C=C(C)C(=NC1=O)N)CO	82
68	Sulfamethoxazole	S(=O)(=O)(Nc1noc(c1)C)c1ccc(N)cc1	100
69	Sulfasalazine	S(=O)(=O)(Nc1ncccc1)c1ccc(N=Nc2cc(C(O)=O)c(O)cc2)cc1	25
70	Sumatriptan	S(=O)(=O)(NC)Cc1cc2c([nH]cc2CCN(C)C)cc1	14
71	Timolol	s1nc(N2CCOCC2)c(OCC(O)CNC(C)(C)C)n1	62
72	Tolbutamide	S(=O)(=O)(NC(=O)NCCCC)c1ccc(cc1)C	89
73	Topiramate	S(OCC12OC(OC1C1OC(OC1CO2)(C)C)(C)C)(=O)(=O)N	88
74	Toremifene	ClCC\C(=C(\c1ccc(OCCN(C)C)cc1)/c1ccccc1)\c1ccccc1	100
75	Tramadol	O(C)c1cc(ccc1)C1(O)CCCCC1CN(C)C	70
76	Trimethoprim	O(C)c1c(OC)cc(cc1OC)Cc1cnc(nc1N)N	98

77	Valproic_acid	OC(=O)C(CCC)CCC	97
78	Valsartan	OC(=O)C(N(Cc1ccc(cc1)-c1ccccc1-c1[nH]nnn1)C(=O)CCCC)C(C)C	23
79	Venlafaxine	O(C)c1ccc(cc1)C(CN(C)C)C1(O)CCCCC1	27
80	Zolpidem	O=C(N(CCC)CCC)Cc1n2C=C(C=Cc2nc1-c1ccc(cc1)C)C	70

Appendix V. List of references that were used to obtain *in vivo* metabolites for the 59 drugs considered in Chapter 3.

########## NSAIDs DATASET ##########

1.Alclofenac
Roncucci R, Simon MJ, Lambelin G. Gas chromatographic determination of 4-allyloxy-3-chlorophenylacetic acid (alclofenac) and its metabolites. *Journal of Chromatography* 62(1):135-7.

Brown LM, Ford-Hutchinson AW (1982). The destruction of cytochrome P-450 by alclofenac: possible involvement of an epoxide metabolite. *Biochemical Pharmacology* 31(2):195-9.

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Hutt AJ, Caldwell J, Smith RL (1986). The metabolism of aspirin in man: a population study. *Xenobiotica* 16(3):239-49.

Grootveld M, Halliwell B (1988). 2,3-Dihydroxybenzoic acid is a product of human aspirin metabolism. *Biochemical Pharmacology* 37(2):271-80.

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Jones CJ (1976). The pharmacology and pharmacokinetics of azapropazone - a review. *Current Medical Research and Opinion* 4(1):3-16.

Rainsford KD (1985). Distribution of azapropazone and its principal 8-hydroxy-metabolite in plasma, urine and gastrointestinal mucosa determined by HPLC. *Journal of Pharmacy and Pharmacology* 37(5):341-5.

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Osman M, Chandrasekaran A, Chan K, Scatina J, Ermer J, Cevallos W, Sisenwine SF (1998). Metabolic disposition of 14C-bromfenac in healthy male volunteers. *The Journal of Clinical Pharmacology* 38(8):744-52.

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Rubio F, Seawall S, Pocelinko R, DeBarbieri B, Benz W, Berger L, Morgan L, Pao J, Williams TH, Koechlin B (1980). Metabolism of carprofen, a nonsteroid anti-inflammatory agent, in rats, dogs, and humans. *Journal of Pharmaceutical Sciences* 69(11):1245-53.

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Stierlin H, Faigle JW (1979). Biotransformation of diclofenac sodium (Voltaren) in animals and in man. II. Quantitative determination of the unchanged drug and principal phenolic metabolites, in urine and bile. *Xenobiotica* 9(10):611-21.

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Tuschl G, Lauer B, Mueller SO (2008). Primary hepatocytes as a model to analyze species-specific toxicity and drug metabolism. *Expert Opinion on Drug Metabolism and Toxicology* 4(7):855-70.

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Verbeeck R, Tjandramaga TB, Mullie A, Verbesselt R, Verberckmoes R, de Schepper PJ (1979). Biotransformation of diflunisal and renal excretion of its glucuronides in renal insufficiency. *British Journal of Clinical Pharmacology* 7(3):273-82.

Loewen GR, McKay G, Verbeeck RK (1986). Isolation and identification of a new major metabolite of diflunisal in man. The sulfate conjugate. *Drug Metabolism and Disposition* 14(1):127-31.

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Cuisinaud G, Legheand J, Belkahia C, Sassard J (1978). Gas chromatographic determination of 3-(4-biphenylylcarbonyl)propionic acid (fenbufen) and two metabolites in human plasma. *Journal of Chromatography* 148(2):509-13.

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Greenslade D, Havler ME, Humphrey MJ, Jordan BJ, Rance MJ (1980). Species differences in the metabolism and excretion of fenclofenac. *Xenobiotica* 10(10):753-60.

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Volland C, Sun H, Benet LZ (1990). Stereoselective analysis of fenoprofen and its metabolites. *Journal of Chromatography* 534:127-38.

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Gaetani M, Yamaguchi H, Vidi A, Hashimoto Y, Donetti A (1979). Species differences in the metabolism of feprazone, an antiinflammatory drug. *Pharmacological Research Communications* 11(8):719-30.

Berry D, Parke DV (1988). The disposition of feprazone and its hydroxylated metabolite in human volunteers. *Xenobiotica* 18(7):857-68.

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Pettersen JE, Ulsaker GA, Jellum E (1978). Studies on the metabolism of 2,4'-isobutylphenylpropionic acid (ibuprofen) by gas chromatography and mass spectrometry. Dialysis fluid, a convenient medium for studies on drug metabolism. *Journal of Chromatography* 145(3):413-20.

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Sato J, Kudo N, Owada E, Ito K, Niida Y, Umetsu M, Kikuta T, Ito K (1997). Urinary excretion of mefenamic acid and its metabolites including their esterglucuronides in preterm infants undergoing mefenamic acid therapy *Biological & Pharmaceutical Bulletin* 20(4):443-5.

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Picard N, Cresteil T, Djebli N, Marquet P (2005). In vitro metabolism study of buprenorphine: evidence for new metabolic pathways. *Drug Metabolism and Disposition* 33(5):689-95.

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Tiseo PJ, Perdomo CA, Friedhoff LT (1998). Metabolism and elimination of 14C-donepezil in healthy volunteers: a single-dose study. *British Journal of Clinical Pharmacology* 46 Suppl 1:19-24.

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Kosoglou T, Statkevich P, Johnson-Levonas AO, Paolini JF, Bergman AJ, Alton KB (2005). Ezetimibe: a review of its metabolism, pharmacokinetics and drug interactions. *Clinical Pharmacokinetics* 44(5):467-94.

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Harding SM (1990). The human pharmacology of fluticasone propionate. *Respiratory Medicine* 84 Suppl A:25-9.

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Lyrica:EPAR Product Information. Online source:
http://www.ema.europa.eu/docs/en_GB/document_library/EPAR_-_Product_Information/human/000546/WC500046602.pdf (30/01/2012 last update)

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Vincent SH, Reed JR, Bergman AJ, Elmore CS, Zhu B, Xu S, Ebel D, Larson P, Zeng W, Chen L, Dilzer S, Lasseter K, Gottesdiener K, Wagner JA, Herman GA (2007). Metabolism and excretion of the dipeptidyl peptidase 4 inhibitor [14C]sitagliptin in humans. *Drug Metabolism and Disposition* 35(4):533-8. Epub 2007 Jan 12.

29.Valsartan

Waldmeier F, Flesch G, Müller P, Winkler T, Kriemler HP, Bühlmayer P, De Gasparo M (1997). Pharmacokinetics, disposition and biotransformation of [14C]-radiolabelled valsartan in healthy male volunteers after a single oral dose. *Xenobiotica* 27(1):59-71.

30.Venlafaxine
Howell SR, Husbands GE, Scatina JA, Sisenwine SF (1993). Metabolic disposition of 14C-venlafaxine in mouse, rat, dog, rhesus monkey and man. *Xenobiotica* 23(4):349-59.

Caccia S (1988). Metabolism of the newer antidepressants. An overview of the pharmacological and pharmacokinetic implications. *Clinical Pharmacokinetics* 34(4):281-302.

Appendix VI. List of known metabolites for 29 NSAIDs discussed in Chapter 3.

No	Parent Name	Parent SMILES	M1	M2	M3	M4	M5	M6
1	Alclofenac	C=CCOc1ccc(CC(=O)O)cc1Cl	OCC(O)COc1ccc(CC(O)=O)cc1Cl	OC(=O)Cc1ccc(O)c(Cl)c1	OC(=O)Cc1ccc(OCC2CO2)c(Cl)c1			
2	Aspirin	CC(=O)Oc1ccccc1C(=O)O	OC(=O)c1ccccc1O	OC(=O)c1cc(O)ccc1O	OC(=O)c1cccc(O)c1O			
3	Azapropazone	N12C([C@@H](C(N1C(=Nc1c2cc(C)cc1)N(C)C)=O)CCC)=O	CCC[C@@H]1C(=O)N2N(C1=O)c1cc(C)c(O)cc1N=C2N(C)C	CCC[C@@H](C(O)=O)C(=O)N1Nc2cc(C)ccc2N=C1N(C)C				
4	Bromfenac	Nc1c(CC(O)=O)cccc1C(=O)c1ccc(Br)cc1	OC1C(=O)NC2=C1C=CC=C2C(=O)C1=CC=C(Br)C=C1	OC1C(=O)NC2=C1C=CC=C2C(O)C1=CC=C(Br)C=C1	BrC1=CC=C(C=C1)C(=O)C1=CC=CC2=C1NC(=O)C2			
5	Carprofen	CC(C(O)=O)c1ccc-2c(Nc3ccc(Cl)cc-23)c1	CC(O)(C(O)=O)c1ccc-2c(Nc3ccc(Cl)cc-23)c1	CC(C(O)=O)c1ccc-2c(Nc3c(O)cc(Cl)cc-23)c1	CC(C(O)=O)c1ccc-2c(Nc3cc(O)c(Cl)cc-23)c1			
6	Diclofenac	OC(=O)Cc1ccccc1Nc1c(Cl)cccc1Cl	OC(=O)Cc1ccccc1Nc1c(Cl)cc(O)cc1Cl	OC(=O)Cc1cc(O)ccc1Nc1c(Cl)cccc1Cl	OC(=O)Cc1ccc(O)ccc1Nc1c(Cl)cc(O)cc1Cl	OC(=O)Cc1ccccc1Nc1c(Cl)ccc(O)c1Cl	COc1cc(Cl)c(Nc2ccccc2CC(O)=O)c(Cl)c1O	COc1c(O)cc(Cl)c(Nc2ccccc2CC(O)=O)c1Cl
7	Diflunisal	O=C(O)c1cc(ccc1O)c2ccc(F)cc2F	OC(=O)c1cc(cc(O)c1O)-c1ccc(F)cc1F					
8	Fenbufen	O=C(O)CCC(=O)c2ccc(c1ccccc1)cc2	OC(CCC(O)=O)c1ccc(cc1)-c1ccc(O)cc1	OC(=O)Cc1ccc(cc1)-c1ccc(O)cc1	OC(CCC(O)=O)c1ccc(cc1)-c1ccccc1	OC(=O)Cc1ccc(cc1)-c1ccccc1		
9	Fenclofenac	Clc2cc(Cl)ccc2Oc1ccccc1CC(=O)O	OC(=O)Cc1cc(O)ccc1Oc1ccc(Cl)cc1Cl					

10	Fenoprofen	O=C(O)C(c2cc(Oc1ccccc1)ccc2)C	CC(C(O)=O)c1cccc(Oc2ccc(O)cc2)c1					
11	Feprazone	O=C2N(c1ccccc1)N(C(=O)C2C\C=C(/C)C)c3ccccc3	C\C(CO)=C/CC1C(=O)N(N(C1=O)c1ccccc1)c1ccccc1					
12	Flufenamic acid	FC(F)(F)c1cc(ccc1)Nc2ccccc2C(=O)O	OC(=O)c1ccccc1Nc1ccc(O)c(c1)C(F)(F)F	OC(=O)c1cc(O)ccc1Nc1cccc(c1)C(F)(F)F	OC(=O)c1cc(O)ccc1Nc1ccc(O)c(c1)C(F)(F)F			
13	Flurbiprofen	CC(C(O)=O)c1ccc(c(F)c1)-c1ccccc1	CC(C(O)=O)c1ccc(c(F)c1)-c1ccc(O)cc1	CC(C(O)=O)c1ccc(c(F)c1)-c1ccc(O)c(O)c1	COc1ccc(cc1O)-c1ccc(cc1F)C(C)C(O)=O			
14	Ibuprofen	CC(C)Cc1ccc(cc1)C(C)C(O)=O	CC(CO)Cc1ccc(cc1)C(C)C(O)=O	CC(C)C(O)c1ccc(cc1)C(C)C(O)=O	CC(Cc1ccc(cc1)C(C)C(O)=O)C(O)=O	CC(C(O)=O)c1ccc(CC(C)(C)O)cc1		
15	Indomethacin	COc1ccc2n(C(=O)c3ccc(Cl)cc3)c(C)c(CC(O)=O)c2c1	Cc1c(CC(O)=O)c2cc(O)ccc2n1C(=O)c1ccc(Cl)cc1	COC1=CC=C2NC(C)=C(CC(O)=O)C2=C1	CC1=C(CC(O)=O)C2=CC(O)=CC=C2N1			
16	Ketoprofen	CC(C(O)=O)c1cccc(c1)C(=O)c1ccccc1	CC(C(O)=O)c1cccc(c1)C(=O)c1ccc(O)cc1	CC(C(O)=O)c1cccc(c1)C(=O)c1ccc(O)c1	CC(C(O)=O)c1cccc(c1)C(O)c1ccccc1			
17	Ketorolac	O=C(c1ccc2n1CCC2C(=O)O)c3ccccc3	OC(=O)C1CCN2C1=CC=C2C(=O)C1=CC=C(O)C=C1					
18	Mefenamic acid	O=C(O)c2c(Nc1cccc(c1C)C)cccc2	Cc1c(CO)ccccc1Nc1cccc1C(O)=O	Cc1c(Nc2ccccc2C(O)=O)cccc1C(O)=O				
19	Nabumetone	CC(=O)CCC1=CC2=C(C=C1)C=C(C=C2)OC	COC1=CC2=C(C=C1)C=C(CCC(O)=O)C=C2	OC(=O)CCC1=CC2=C(C=C1)C=C(O)C=C2	CC(=O)CCC1=CC2=C(C=C1)C=C(O)C=C2	COC1=CC2=C(C=C1)C=C(CCC(C)O)C=C2	CC(O)CCC1=CC2=C(C=C1)C=C(O)C=C2	
20	Naproxen	COc1ccc2cc(ccc2c1)C(C)C(O)=O	CC(C(O)=O)c1ccc2cc(O)ccc2c1					

21	Paracetamol	CC(=O)Nc1ccc(cc1)O	CC(=O)\N=C1/C=CC(=O)C=C/1	CC(=O)Nc1ccc(O)c(O)c1	COc1cc(NC(C)=O)ccc1O			
22	Phenylbutazone	O=C2N(c1ccccc1)N(C(=O)C2CCCC)c3ccccc3	CC(O)CCC1C(=O)N(N(C1=O)c1ccccc1)c1ccccc1	CC(O)CCC1C(=O)N(N(C1=O)c1ccc(O)cc1)c1ccccc1	CCCCC1C(=O)N(N(C1=O)c1ccc(O)cc1)c1ccccc1			
23	Piroxicam	OC=2c1ccccc1S(=O)(=O)N(C)C=2C(=O)Nc3ccccn3	CN1C(C(=O)Nc2ccc(O)cn2)=C(O)c2ccccc2S1(=O)=O					
24	Pirprofen	CC(C(O)=O)c1ccc(N2CC=CC2)c(Cl)c1	CC(C(O)=O)c1ccc(N2C=CC=C2)c(Cl)c1	CC(C(O)=O)c1ccc(N)c(Cl)c1	CC(C(O)=O)c1ccc(NC(C)=O)c(Cl)c1	CC(C(O)=O)c1ccc(N2CC3OC3C2)c(Cl)c1	CC(C(O)=O)c1ccc(N2CC(O)C(O)C2)c(Cl)c1	
25	Sulindac	O=S(c1ccc(cc1)\C=C/3\c2ccc(F)cc2\C(=C\3C)CC(=O)O)C	CC1=C(CC(O)=O)c2cc(F)ccc2C\1=C\c1ccc(cc1)S(C)(=O)=O	CSc1ccc(cc1)\C=C1/C(C)=C(CC(O)=O)c2cc(F)ccc12				
26	Suprofen	CC(C(O)=O)c1ccc(cc1)C(=O)c1cccs1	CC(C(O)=O)c1ccc(cc1)C(O)c1cccs1	CC(C(O)=O)c1ccc(cc1)C(=O)c1ccc(O)s1	CC(C(O)=O)c1ccc(cc1)C(O)=O	OCC(C(O)=O)c1ccc(cc1)C(=O)c1cccs1	OC(=O)C(C(O)=O)c1ccc(cc1)C(=O)c1cccs1	
27	Tiaprofenic acid	CC(C(O)=O)c1ccc(s1)C(=O)c1ccccc1	CC(C(O)=O)c1ccc(s1)C(O)c1ccccc1	CC(C(O)=O)c1ccc(s1)C(=O)c1ccc(O)cc1				
28	Tolmetin	O=C(c1ccc(n1C)CC(=O)O)c2ccc(cc2)C	Cn1c(CC(O)=O)ccc1C(=O)c1ccc(cc1)C(O)=O	Cn1c(CC(O)=O)ccc1C(=O)c1ccc(CO)cc1				
29	Zomepirac	O=C(c1c(cc(n1C)CC(=O)O)C)c2ccc(Cl)cc2	Cn1c(CC(O)=O)cc(CO)c1C(=O)c1ccc(Cl)cc1	OC(=O)c1ccc(Cl)cc1				

Appendix VII. List of known metabolites for 30 top selling drugs discussed in Chapter 3.

No	Parent Name	Parent SMILES	M1	M2	M3	M4	M5	M6	M7	M8	M9	M10	M11
1	Aripiprazole	Clc4cccc(N3CCN(CCCCOc2ccc1c(NC(=O)CC1)c2)CC3)c4Cl	ClC1=CC=CC(N2CCN(CCCCOC3=CC=C4C=CC(=O)NC4=C3)CC2)=C1Cl	OCCCCOC1=CC=C2CCC(=O)NC2=C1	ClC1=CC=CC(N2CCNCC2)=C1Cl	OC1=C(Cl)C(Cl)=C(C=C1)N1CCN(CCCCOC2=CC=C3CCC(=O)NC3=C2)CC1	OC1CC(=O)NC2=CC(OCCCCN3CCN(CC3)C3=C(Cl)C(Cl)=CC=C3)=CC=C12						
2	Atorvastatin	CC(C)c1c(c(c(n1CC[C@H](C[C@H](CC(=O)O)O)O)c2ccc(cc2)F)c3ccccc3)C(=O)Nc4ccccc4	CC(C)c1c(C(=O)Nc2ccccc2O)c(-c2ccccc2)c(-c2ccc(F)cc2)n1CCC(O)CC(O)CC(O)=O	CC(C)c1c(C(=O)Nc2ccccc2O)c(-c2ccccc2)c(-c2ccc(F)cc2)n1CCC1CC(O)CC(=O)O1	CC(C)c1c(C(=O)Nc2ccc(O)cc2)c(-c2ccccc2)c(-c2ccc(F)cc2)n1CCC(O)CC(O)CC(O)=O	CC(C)c1c(C(=O)Nc2ccc(O)cc2)c(-c2ccccc2)c(-c2ccc(F)cc2)n1CCC1CC(O)CC(=O)O1	CC(C)c1c(C(=O)Nc2ccccc2)c(-c2ccccc2)c(-c2ccc(F)cc2)n1CCC1CC(O)CC(=O)O1						
3	Buprenorphine	CO[C@]12CC[C@@]3(C[C@@H]1[C@](C)(O)C(C)(C)C)[C@H]1Cc4ccc(O)c5O[C@@H]2[C@]3(CCN1CC1CC1)c45	CO[C@]12CC[C@@]3(C[C@@H]1C(C)(O)C(C)(C)C)[C@H]1CC4=C5C(O[C@@H]2[C@]35CCN1)=C(O)C=C4										
4	Celecoxib	O=S(=O)(c3ccc(n1nc(cc1c2ccc(cc2)C(F)(F)F)cc3)N	NS(=O)(=O)C1=CC=C(C=C1)N1N=C(C=C1C1=CC=C(CO)C=C1)C(F)(F)F	NS(=O)(=O)C1=CC=C(C=C1)N1N=C(C=C1C1=CC=C(C=C1)C(O)=O)C(F)(F)F									
5	Clopidogrel	COC(=O)[C@H](N1CCc2sccc2C1)c1ccccc1Cl	OC(=O)C(N1CCC2=C(C1)C=CS2)C1=CC=CC=C1Cl	COC(=O)C(N1CCC2SC(=O)C=C2C1)C1=CC=CC=C1Cl	OC(=O)C(N1CCC2SC(=O)C=C2C1)C1=CC=CC=C1Cl	COC(=O)C(N1CCC(S)\C(C1)=C/C(C)=O)C1=CC=CC=C1Cl							
6	Donepezil	O=C2c1cc(OC)c(OC)cc1CC2CC4CCN(Cc3ccccc3)CC4	COC1=C(O)C=C2C(=O)C(CC3CCN(CC3)CC3=CC=CC=C3)CC2=C1	COC1=C(O)C=C2CC(CC3CCN(CC3)CC3=CC=CC=C3)C(=O)C2=C1	COC1=CC2=C(C=C1OC)C(=O)C(CC1CC[N+](O-])(CC1)CC1=CC=CC=C1)C2	COC1=CC2=C(C=C1OC)C(=O)C(CC1CCNCC1)C2							
7	Duloxetine	O(c1cccc2c1cccc2)[C@H](c3sccc3)CCNC	CNCCC(OC1=CC=C(O)C2=C1C=CC=C2)C1=CC=CS1	CNCCC(Oc1ccc(cc)c2cc(O)ccc12)c1cccs1	CNCCC(Oc1ccccc2c(O)cccc12)c1cccs1	CNCCC(Oc1ccccc2cc(O)ccc12)c1cccs1	CNCCC(Oc1ccccc2c(O)c(O)ccc12)c1cccs1	CNCCC(O)c1ccc2c(O)c(OC)ccc12)c1ccs1	CNCCC(Oc1ccccc2c(OC)c(O)ccc12)c1cccs1	CNCCC(Oc1ccccc2C3OC3C=Cc12)c1ccs1	CNCCC(Oc1ccccc2C(O)C(O)C=Cc12)c1ccs1	NCCC(OC1=CC=CC2=C1C=CC=C2)C1=CC=CS1	CNCCC(O)c1cccs1
8	Efavirenz	FC(F)(F)[C@]1(OC(=O)Nc2ccc(Cl)cc12)C#CC1CC1	OC1=C2NC(=O)O[C@@](C#CC3CC3)(C	OC1=C(Cl)C=C2C(NC(=O)O[C@]2(C#CC2CC2	OC1=C2NC(=O)O[C@@](C#CC3(O)CC3)(C2=CC(Cl)=C1)C(F)(F)F								

			2=CC(Cl)=C1)C(F)(F)F	)C(F)(F)F)=C1									
9	Emtricitabine	FC=1\C(=N/C(=O)N(C=1)[C@H]2O[C@H](SC2)CO)\N	CNCCCC1(OCC2=CC(=CC=C12)C#N)C1=CC=C(F)C=C1										
10	Escitalopram	Fc1ccc(cc1)[C@@]3(OCc2cc(C#N)ccc23)CCCN(C)C	CNCCCC1(OCC2=CC(=CC=C12)C#N)C1=CC=C(F)C=C1	NCCCC1(OCC2=CC(=CC=C12)C#N)C1=CC=C(F)C=C1	C[N+](C)([O-])CCCC1(OCC2=CC(=CC=C12)C#N)C1=CC=C(F)C=C1	OC(=O)CCC1(OCC2=CC(=CC=C12)C#N)C1=CC=C(F)C=C1	FC1=CC=C(C=C1)C1(CCC=O)OCC2=CC(=CC=C12)C#N						
11	Esomeprazole	COc1ccc2nc(nc2c1)S(=O)Cc1ncc(C)c(OC)c1C	COC1=CC=C2NC(=NC2=C1)S(=O)CC1=NC=C(CO)C(OC)=C1C	COC1=CC=C2NC(=NC2=C1)S(=O)CC1=NC=C(C(O)=O)C(OC)=C1C	COC1=CC=C2NC(=NC2=C1)S(=O)(=O)CC1=NC=C(C)C(OC)=C1C	COC1=CC=C2NC(=NC2=C1)S(=O)(=O)CC1=NC=C(C)C(OC)=C1C	COC1=CC=C2NC(=NC2=C1)S(=O)(=O)CC1=[N+]([O-])C=C(C)C(OC)=C1C	COC1=C(C)C(CS(=O)C2=NC3=CC(O)=CC=C3N2)=NC=C1C	COC1=CC=C2NC(=NC2=C1)S(=O)CC1=NC=C(C)C(OC)=C1CO				
12	Ezetimibe	Fc1ccc(cc1)[C@@H](O)CC[C@H]4C(=O)N(c2ccc(F)cc2)[C@@H]4c3ccc(O)cc3	OC1=CC=C(C=C1)[C@@H]1[C@@H](CCC(=O)C2=CC=C(F)C=C2)C(=O)N1C1=CC=C(F)C=C1										
13	Fenofibrate	CC(C)OC(=O)C(C)(C)Oc1ccc(cc1)C(=O)c1ccc(Cl)cc1	CC(C)(OC1=CC=C(C=C1)C(=O)C1=CC=C(Cl)C=C1)C(=O)=O	CC(C)(OC1=CC=C(C=C1)C(O)C1=CC=C(Cl)C=C1)C(O)=O									
14	Fluticasone propionate	O=C(SCF)[C@]3(OC(=O)CC)[C@]2(C[C@H](O)[C@]4(F)[C@@]/1(\C(=C/C(=O)\C=C\1)[C@@H](F)C[C@H]4[C@@H]2C[C@H]3C)C)C	CCC(=O)OC1(C(C)CC2C3CC(F)C4=CC(=O)C=CC4(C)C3(F)C(O)CC12)C(O)=O										
15	Levofloxacin	C[C@H]1COc2c(N3CCN(C)CC3)c(F)cc3c2n1cc(C(O)=O)c3=O	CC1COC2=C3N1C=C(C(O)=O)C(=O)C3=CC(F)=C2N1CCNCC1	CC1COC2=C3N1C=C(C(O)=O)C(=O)C3=CC(F)=C2N1CC[N+](C)([O-])CC1									
16	Methylphenidate	COC(=O)C(C1CCCCN1)c1ccccc1	OC(=O)C(C1CCCCN1)C1=CC=CC=C1	COC(=O)C(C1CCC(=O)N1)C1=CC=CC=C1	COC(=O)C(C1CCCCN1)C1=CC=C(O)C=C1	OC(=O)C(C1CCCC(=O)N1)C1=CC=CC=C1	OC(=O)C(C1CCCCN1)C1=CC=C(O)C=C1	CCOC(=O)C(C1CCCCN1)C1=CC=CC=C1					
17	Modafinil	O=S(C(c1ccccc1)c2ccccc2)CC(=O)N	OC(=O)CS(=O)C(c1ccccc1)c1ccccc1	NC(=O)CS(=O)(=O)C(c1ccccc1)c1ccccc1									
18	Montelukast	O=C(O)CC1(CC1)CS[C@@H](c2cccc(c2)\C=C\c3nc4cc(Cl)ccc4	CC(C)(O)C1=CC=CC=C1CCC(C1=C	CC(C)(O)C1=CC(O)=CC=C1CCC(SCC1(C	CC(O)(CO)C1=CC=CC=C1CCC(SCC1(CC1)CC(O)=O)C1=CC=CC(\C=	CC(O)(C(O)=O)C1=CC=CC=C1CCC(SCC1(CC1)CC(O)=O)C1=CC=CC(	CC(C)(O)C1=CC=CC=C1C(O)CC(SCC1(CC1)CC(O)=O)C1=CC=CC(\C					

		cc3)CCc5ccc c5C(O)(C)C	C=CC(\C=C\C2=NC3=C(C=CC(Cl)=C3)C=C2)=C1)S(=O)CC1(CC1)CC(O)=O	C1)CC(O)=O)C1=CC=CC(\C=C\C2=NC3=CC(Cl)=CC=C3C=C2)=C1	C\C2=NC3=CC(Cl)=CC=C3C=C2)=C1	\C=C\C2=NC3=CC(Cl)=CC=C3C=C2)=C1	=C\C2=NC3=CC(Cl)=CC=C3C=C2)=C1						
19	Naloxone	O=C4[C@@H]5Oc1c2c(ccc1O)C[C@H]3N(CC[C@]25[C@@]3(O)CC4)C\C=C	OC1=CC=C2C[C@H]3NCC[C@@]45[C@@H](OC1=C24)C(=O)CC[C@@]35O	CC(C)(O)C1=CC=CC=C1C(O)CC(SCC1(CC1)CC(O)=O)C1=CC=CC(\C=C\C2=NC3=CC(Cl)=CC=C3C=C2)=C1									
20	Olanzapine	CN1CCN(CC1)C/2=N/c4ccccc4Nc3sc(C)cc\23	CC1=CC2=C(NC3=CC=CC=C3N=C2N2CCNCC2)S1	CN1CCN(CC1)C1=NC2=CC=CC=C2NC2=C1C=C(S2)C(O)=O	CN1CCN(CC1)C1=NC2=CC=CC=C2NC2=C1C=C(S2)C(O)=O	OC(=O)C1=CC2=C(NC3=CC=CC=C3N=C2N2CCNCC2)S1	CC1=CC2=C(NC3=CC=CC=C3N=C2N2CC[N+](C)([O-])CC2)S1	OCC1=CC2=C(NC3=CC=CC=C3N=C2N2CCNCC2)S1					
21	Oxycodone	O=C4[C@@H]5Oc1c2c(ccc1OC)C[C@H]3N(CC[C@]25[C@@]3(O)CC4)C	CN1CC[C@@]23[C@H]4OC5=C2C(C[C@@H]1[C@]3(O)CCC4=O)=CC=C5O	COC1=CC=C2C[C@H]3NCC[C@@]45[C@@H](OC1=C24)C(=O)CC[C@@]35O	OC1=CC=C2C[C@H]3NCC[C@@]45[C@@H](OC1=C24)C(=O)CC[C@@]35O								
22	Pioglitazone	O=C1NC(=O)SC1Cc3ccc(OCCc2ncc(cc2)CC)cc3	CCC1=CN=C(C=C1)C(O)COC1=CC=C(CC2SC(=O)NC2=O)C=C1	CC(O)C1=CN=C(CCOC2=CC=C(CC3SC(=O)NC3=O)C=C2)C=C1	CC(=O)C1=CN=C(CCOC2=CC=C(CC3SC(=O)NC3=O)C=C2)C=C1	OC(=O)CC1=CN=C(CCOC2=CC=C(CC3SC(=O)NC3=O)C=C2)C=C1	OC(=O)C1=CN=C(CCOC2=CC=C(CC3SC(=O)NC3=O)C=C2)C=C1	OC1=CC=C(CC2SC(=O)NC2=O)C=C1					
23	Pregabalin	O=C(O)C[C@H](CC(C)C)CN	CNC[C@@H](CC(C)C)CC(O)=O										
24	Quetiapine	N\1=C(\c3c(Sc2c/1cccc2)cccc3)N4CCN(CCOCCO)CC4	OCCOCCN1CCN(CC1)C1=NC2=C(C=CC=C2)S(=O)C2=C1C=CC=C2	OC(=O)COCCN1CCN(CC1)C1=NC2=C(SC3=C1C=CC=C3)C=CC=C2	OCCOCCN1CCN(CC1)C1=NC2=C(SC3=C1C=CC=C3)C=C(O)C=C2	OCCN1CCN(CC1)C1=NC2=C(SC3=C1C=CC=C3)C=CC=C2	C1CN(CCN1)C1=NC2=C(SC3=C1C=CC=C3)C=CC=C2						
25	Rosuvastatin	O=S(=O)(N(c1nc(c(c(n1)C(C)C)/C=C/[C@@H](O)C[C@@H](O)CC(=O)O)c2ccc(F)cc2)C)C	CC(C)C1=NC(NS(C)(=O)=O)=NC(C2=CC=C(F)C=C2)=C1\C=C\C(O)CC(O)CC(O)=O	CC(C)C1=NC(=NC(C2=CC=C(F)C=C2)=C1\C=C\C1CC(O)CC(=O)O1)N(C)S(C)(=O)=O									
26	Salmeterol	OCc1cc(ccc1O)C(O)CNCCCCCCOCCCCc2ccccc2	OCC1=CC(=CC=C1O)C(O)CNCCCCCCOCCCCC(O)C1=CC=CC=C1	OCC1=CC(=CC=C1O)C(O)CNCCCCCC(O)=O									

27	Sildenafil	O=S(=O)(N1CCN(C)CC1)c4cc(C\2=N\C(=O)c3c(N/2)c(nn3C)CCC)c(OCC)cc4	CCOC1=C(C=C(C=C1)S(=O)(=O)N1CCN(C)CC1)C1=NC2=C(N(C)N=C2CCCO)C(=O)N1	CCCC1=NN(C)C2=C1N=C(NC2=O)C1=C(OCC)C=CC(=C1)S(=O)(=O)NCCNC	CCCC1=NN(C)C2=C1N=C(NC2=O)C1=C(OCC)C=CC(=C1)S(=O)(=O)N1CCNCC1	CCCC1=NN(C)C2=C1N=C(NC2=O)C1=C(OCC)C=CC(=C1)S(=O)(=O)NCCN							
28	Sitagliptin	Fc1cc(c(F)cc1F)C[C@@H](N)CC(=O)N3Cc2nnc(n2CC3)C(F)(F)F	[H][C@]1(CC(=O)N2CCN3C(=NN=C3C(F)(F)F)[C@]2([H])N1)CC1=C(F)C=C(F)C(F)=C1										
29	Valsartan	O=C(O)[C@@H](N(C(=O)CCCC)Cc3ccc(c1ccccc1c2nnnn2)cc3)C(C)C	CC(O)CCC(=O)N(CC1=CC=C(C=C1)C1=CC=CC=C1C1=NN=NN1)C(C(C)C)C(O)=O										
30	Venlafaxine	OC2(C(c1ccc(OC)cc1)CN(C)C)CCCCC2	CN(C)CC(C1=CC=C(O)C=C1)C1(O)CCCCC1	CNCC(C1=CC=C(OC)C=C1)C1(O)CCCCC1	CNCC(C1=CC=C(O)C=C1)C1(O)CCCCC1	NCC(C1=CC=C(O)C=C1)C1(O)CCCCC1							

Appendix VIII. H_244 dataset used in Chapter 4.

ID	Name	SMILES	pIC50	Class
1	(2R)-N-(4-tert-butylphenyl)-N'-cyano-4-(3-fluoropyridin-2-yl)-2-methylpiperazine-1-carboximidamide	N#C/N=C(/N1CCN(C[C@H]1C)c1ncccc1F)\Nc1ccc(cc1)C(C)(C)C	6.00	Active
2	(4R)-4-(4-fluorophenyl)-8-[1-(4-fluorophenyl)cyclohexyl]-2,8-diazaspiro[4.5]decan-1-one	Fc1ccc(cc1)[C@H]1CNC(=O)C21CCN(CC2)C1(CCCCC1)c1ccc(cc1)F	5.89	Active
3	(5aR,9R)-2,9-dimethyl-5,5a,6,7,8,9-hexahydropyrido[3',2':4,5]pyrrolo[1,2-a]pyrazine	Cc1ccc2c(n1)N1[C@H](C)CNC[C@H]1C2	4.68	Inactive
4	1,4-Dihydroindeno[1,2-c]pyrazol_50	COCCOCC#Cc1scc(c1)c1n[nH]c2c1C(=O)c1c2ccc(c1)CN1CCN(CC1)C	5.28	Active
5	1,4-Dihydroindeno[1,2-c]pyrazol_77	CN1CCN(C(=O)C1)Cc1ccc2c(c1)Cc1c2[nH]nc1c1csc(c1)C#CCOc1ccccc1	4.28	Inactive
6	1,4-Dihydroindeno[1,2-c]pyrazol_85	c1ccc(cc1)OCC#Cc1scc(c1)c1n[nH]c2c1Cc1c2ccc(c1)Cn1cncn1	5.77	Active
7	1,4-Dihydroindeno[1,2-c]pyrazol_90	COCCOCC#Cc1scc(c1)c1n[nH]c2c1Cc1c2cc(cc1)Cn1cncn1	4.94	Inactive
8	1-{4-[({4-[(4-bromo-2-fluorophenyl)amino]-6-methoxyquinazolin-7-yl}oxy)methyl]piperidin-1-yl}-2-(dimethylamino)ethanone	COc1cc2c(ncnc2cc1OCC1CCN(CC1)C(=O)CN(C)C)Nc1ccc(cc1F)Br	5.82	Active
9	1-{4-[2-({4-[(2,3-dimethyl-1H-indol-5-yl)oxy]-6-methoxyquinazolin-7-yl}oxy)ethyl]piperazin-1-yl}propan-2-one	COc1cc2c(ncnc2cc1OCCN1CCN(CC1)CC(=O)C)Oc1ccc2c(c1)c(C)c([nH]2)C	5.00	Inactive
10	1-bis(4-fluorophenyl)methyl_piperazine	Fc1ccc(cc1)C(c1ccc(cc1)F)N1CCNCC1	5.80	Active
11	2-Amino-N-pyrimidin-4-ylacetamide-1	CN1CCN(CC1)CC(=O)Nc1nc(nc(c1)n1nccc1C)c1ccc(o1)C	6.02	Active
12	2-Amino-N-pyrimidin-4-ylacetamide-2	CN1CCCN(CC1)CC(=O)Nc1nc(nc(c1)n1nccc1C)c1ccc(o1)C	6.55	Active
13	2-Amino-N-pyrimidin-4-ylacetamide-3	CN(C[C@@H]1CCN(CC1)CC(=O)Nc1nc(nc(c1)n1nccc1C)c1ccc(o1)C)C	5.78	Active
14	2-Amino-N-pyrimidin-4-ylacetamide-4	CN1CCC(CC1)CC(=O)Nc1nc(nc(c1)n1nccc1C)c1ccc(o1)C	5.38	Active
15	2-Amino-N-pyrimidin-4-ylacetamide-5	CN(CCC(=O)Nc1nc(nc(c1)n1nccc1C)c1ccc(o1)C)C	6.19	Active

16	2-ethylidene-1,5-dimethyl-3,3-diphenylpyrrolidine_(EDDP)_(Racemate)	CC=C1N(C)C(CC1(c1ccccc1)c1ccccc1)C	4.00	Inactive
17	2-hydroxymethyl_olanzapine	OCc1sc2c(c1)C(=Nc1c(N2)cccc1)N1CCN(CC1)C	4.93	Inactive
18	4,4-difluorobenzhydrol	OC(c1ccc(cc1)F)c1ccc(cc1)F	4.00	Inactive
19	4,4-difluorobenzophenone	O=C(c1ccc(cc1)F)c1ccc(cc1)F	4.14	Inactive
20	4-Aminopyridine	Nc1ccncc1	2.37	Inactive
21	5-chloro-N-(2,4-dimethoxybenzyl)-1-benzofuran-2-carboxamide	COc1cc(OC)ccc1CNC(=O)c1cc2c(o1)ccc(c2)Cl	4.78	Inactive
22	5-chloro-N-[3-(10,11-dihydro-5H-dibenzo[b,f]azepin-5-yl)propyl]-N-methyl-1-benzofuran-2-carboxamide	Clc1ccc2c(c1)cc(o2)C(=O)N(CCCN1c2ccccc2CCc2c1cccc2)C	4.70	Inactive
23	6-(4-chlorophenyl)-3-{4-[(3S)-3-hydroxypyrrolidin-1-yl]-3-methoxyphenyl}thieno[3,2-d]pyrimidin-4(3H)-one	COc1cc(ccc1N1CC[C@@H](C1)O)n1cnc2c(c1=O)sc(c2)c1ccc(cc1)Cl	5.18	Active
24	9-hydroxyrisperidone	OC1CCc2n(C1)c(=O)c(c(n2)C)CCN1CCC(CC1)c1noc2c1ccc(c2)F	5.95	Active
25	AF_3013_(NM-394)	Fc1cc2c(cc1N1CCNCC1)n1C(C)Sc1c(c2=O)C(=O)O	3.00	Inactive
26	Ajmaline	CCC1C2CC3N(C1O)C1C2C(O)C2(C3N(C)c3c2cccc3)C1	5.98	Active
27	Alfuzosin	COc1cc2nc(nc(c2cc1OC)N)N(CCCNC(=O)C1CCCO1)C	4.08	Inactive
28	Alosetron	O=C1N(CCc2c1c1ccccc1n2C)Cc1[nH]cnc1C	5.50	Active
29	Aminomethyl-tetrahydronaphthalene-ketopiperazine_1	CCN(Cc1ccc2c(c1)CC[C@@H](C2)N1CCN(CC1=O)CCc1ccc(cc1)F)CC	5.09	Active
30	Aminomethyl-tetrahydronaphthalene-ketopiperazine_2a	CCN(Cc1ccc2c(c1)CC[C@@H](C2)N1CCN(CC1=O)CCc1ccc(cc1)Cl)CC	5.48	Active
31	Aminomethyl-tetrahydronaphthalene-ketopiperazine_2b	CCN(Cc1ccc2c(c1)CC[C@@H](C2)N1CCN(CC1=O)CCc1cc(N)cc(c1)C(F)(F)F)CC	5.77	Active
32	Aminomethyl-tetrahydronaphthalene-ketopiperazine_2c	CCN(Cc1ccc2c(c1)CC[C@@H](C2)N1CCN(CC1=O)CCC1CCCCC1)CC	5.48	Active
33	Aminomethyl-tetrahydronaphthalene-ketopiperazine_2d	CCN(Cc1ccc2c(c1)CC[C@@H](C2)N1CCN(CC1=O)Cc1cscc1)CC	5.92	Active
34	Aminomethyl-tetrahydronaphthalene-ketopiperazine_4a	Fc1ccc(cc1)CCN1CCN(C(=O)C1)[C@H]1CCc2c(C1)ccc(c2)CN1CCC(CC1)C(F)(F)F	5.70	Active
35	Aminomethyl-tetrahydronaphthalene-ketopiperazine_4b	Fc1ccc(cc1)CCN1CCN(C(=O)C1)[C@H]1CCc2c(C1)ccc(c2)Cn1cncc1	5.40	Active

36	Aminomethyl-tetrahydronaphthalene-ketopiperazine_4e	Fc1ccc(cc1)CCN1CCN(C(=O)C1)[C@H]1CCc2c(C1)ccc(c2)CN1CCCCC1	4.96	Inactive
37	Aminomethyl-tetrahydronaphthalene-ketopiperazine_4f	Fc1ccc(cc1)CCN1CCN(C(=O)C1)[C@H]1CCc2c(C1)ccc(c2)CN1CCN(CC1)S(=O)(=O)C	4.89	Inactive
38	Aminomethyl-tetrahydronaphthalene-ketopiperazine_4g	Fc1ccc(cc1)CCN1CCN(C(=O)C1)[C@H]1CCc2c(C1)ccc(c2)CN1CCS(=O)(=O)CC1	4.62	Inactive
39	Aminomethyl-tetrahydronaphthalene-ketopiperazine_4h	Fc1ccc(cc1)CCN1CCN(C(=O)C1)[C@H]1CCc2c(C1)ccc(c2)CN1CCN(CC1)C(=O)C	4.60	Inactive
40	Aminomethyl-tetrahydronaphthalene-ketopiperazine_4i	OCC(C(=O)N(C)C)N(Cc1ccc2c(c1)CC[C@@H](C2)N1CCN(CC1=O)CCc1ccc(cc1)F)C	4.60	Inactive
41	Amitriptyline	CN(CC/C=C/1\c2ccccc2CCc2c1cccc2)C	5.00	Inactive
42	Amsacrine	COc1cc(ccc1Nc1c2ccccc2nc2c1cccc2)NS(=O)(=O)C	6.68	Active
43	Aripiprazole	O=C1CCc2c(N1)cc(cc2)OCCCCN1CCN(CC1)c1cccc(c1Cl)Cl	6.20	Active
44	Articaine	CCCNC(C(=O)Nc1c(C)csc1C(=O)OC)C	3.65	Inactive
45	Astemizole	COc1ccc(cc1)CCN1CCC(CC1)Nc1nc2c(n1Cc1ccc(cc1)F)cccc2	8.55	Active
46	Atenolol (Racemate)	OC(COc1ccc(cc1)CC(=O)N)CNC(C)C	3.00	Inactive
47	AVE-0118	COc1ccc(cc1)CC(=O)NCc1ccccc1c1ccccc1C(=O)NCCc1cccnc1	5.00	Inactive
48	Azimilide	CN1CCN(CC1)CCCCN1C(=O)CN(C1=O)/N=C/c1ccc(o1)c1ccc(cc1)Cl	6.17	Active
49	BAPTA-AM	OC(=O)CN(c1ccccc1OCCOc1ccccc1N(CC(=O)O)CC(=O)O)CC(=O)OCOC(=O)C	5.88	Active
50	BCTC	O=C(N1CCN(CC1)c1ncccc1Cl)Nc1ccc(cc1)C(C)(C)C	6.00	Active
51	Benperidol	Fc1ccc(cc1)C(=O)CCCN1CC[C@H](CC1)n1c(=O)[nH]c2c1cccc2	8.47	Active
52	Benzoylecgonine	CN1[C@H]2CC[C@@H]1[C@H]([C@H](C2)OC(=O)c1ccccc1)C(=O)O	3.21	Inactive
53	Bepridil	CC(COCC(N1CCCC1)CN(c1ccccc1)Cc1ccccc1)C	6.70	Active
54	Berberine	COc1c(OC)ccc2c1c[n+]1CCc3c(c1c2)cc1c(c3)OCO1	5.51	Active
55	Bicifadine	Cc1ccc(cc1)C12CNCC2C1	4.34	Inactive
56	Bisindolylmaleimide	O=C1NC(=O)C(=C1c1c[nH]c2c1cccc2)c1c[nH]c2c1cccc2	6.00	Active
57	BMCL_03_13_1829-1835_1	Clc1ccc2c(c1)c(cn2c1ccccc1)C1CCN(CC1)CCN1CCNC1=O	7.06	Active
58	BMCL_03_13_1829-1835_10	Fc1ccc(cc1)n1cc(c2c1cccc2)C1CCN(CC1)CCN1CCNC1=S	8.21	Active
59	BMCL_03_13_1829-1835_12	Fc1ccc(cc1)n1ccc2c1ccc(c2)C(C)(C)C	4.00	Inactive
60	BMCL_03_13_1829-1835_14	Clc1ccc2c(c1)c(cn2c1ccc(cc1)F)C1CCNCC1	6.69	Active
61	BMCL_03_13_1829-1835_15	CN(Cc1cn(c2c1cc(Cl)cc2)c1ccc(cc1)F)C	7.96	Active
62	BMCL_03_13_1829-1835_16	CCCc1cn(c2c1cc(Cl)cc2)c1ccc(cc1)F	4.59	Inactive
63	BMCL_03_13_1829-1835_17	CCC(c1cn(c2c1cc(Cl)cc2)c1ccc(cc1)F)CC	5.83	Active
64	BMCL_03_13_1829-1835_18	Fc1ccc(cc1)n1cc(c2c1ccc(c2)Cl)C(O)C	5.34	Active
65	BMCL_03_13_1829-1835_19	CCC(=O)c1cn(c2c1cc(Cl)cc2)c1ccc(cc1)F	5.71	Active
66	BMCL_03_13_1829-1835_2	Clc1ccc2c(c1)c(cn2c1ccc(cc1)F)C1=CCN(CC1)CCN1CCNC1=O	8.00	Active
67	BMCL_03_13_1829-1835_20	CCC(c1cn(c2c1cc(Cl)cc2)c1ccc(cc1)F)(CC)O	4.80	Inactive
68	BMCL_03_13_1829-1835_21	CCC(c1cn(c2c1cc(Cl)cc2)c1ccc(cc1)F)O	5.66	Active
69	BMCL_03_13_1829-1835_22	CCc1cn(c2c1cc(Cl)cc2)c1ccc(cc1)F	5.46	Active

70	BMCL_03_13_1829-1835_23	Fc1ccc(cc1)n1cc(c2c1ccc(c2)Cl)C(=O)C	4.00	Inactive
71	BMCL_03_13_1829-1835_3	Fc1ccc(cc1)n1cc(c2c1cccc2)C1CCN(CC1)CCN1CCNC1=O	8.15	Active
72	BMCL_03_13_1829-1835_4	OC(=O)Cc1ccc(cc1)n1cc(c2c1ccc(c2)Cl)C1CCN(CC1)CCN1CCNC1=O	6.24	Active
73	BMCL_03_13_1829-1835_5	Clc1ccc2c(c1)c(cn2c1ccc(cc1)C(=O)O)C1CCN(CC1)CCN1CCNC1=O	4.12	Inactive
74	BMCL_03_13_1829-1835_7	COC(=O)Cc1ccc(cc1)n1cc(c2c1ccc(c2)Cl)C1CCN(CC1)CCN1CCNC1=O	6.88	Active
75	BMCL_03_13_1829-1835_8	COC(=O)c1ccc(cc1)n1cc(c2c1ccc(c2)Cl)C1CCN(CC1)CCN1CCNC1=O	7.44	Active
76	BMCL_03_13_1829-1835_9	Fc1ccc(cc1)n1cc(c2c1ccc(c2)Cl)C(C)C	4.00	Inactive
77	BMCL_2006_1207_19	Fc1ccc(c(c1)C1CN([C@@H](C1)c1ccccc1)C(=O)[C@H](C1CC1)N)F	5.46	Active
78	BMCL131829-02	Fc1ccc(cc1)n1cc(c2c1cccc2)C1=CCN(CC1)CCN1CCNC1=O	8.00	Active
79	BMCL131829-05	O=C1NCCN1CCN1CCC(CC1)c1cn(c2c1cccc2)c1ccc(cc1)C(=O)O	5.13	Active
80	BMCL131829-16	CCCc1cn(c2c1cccc2)c1ccc(cc1)F	4.59	Inactive
81	BMCL131829-17	CCC(c1cn(c2c1cccc2)c1ccc(cc1)F)CC	5.83	Active
82	BRL-32872	COc1cc(ccc1OC)N(C(=O)c1ccc(cc1)[N+](=O)[O-])CCCN(CCc1ccc(c(c1)OC)OC)C	7.70	Active
83	Brompheniramine	CN(CCC(c1ccccn1)c1ccc(cc1)Br)C	5.76	Active
84	Buprenorphine	CO[C@]12CC[C@]3(C[C@@H]1[C@@](C(C)(C)C)(O)C)[C@@]14[C@H]2Oc2c4c(C[C@H]3N(CC1)CC1CC1)ccc2O	5.10	Active
85	Canrenoic_Acid	OC(=O)CC[C@@]1(O)CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2C=CC2=CC(=O)CC[C@]12C	3.98	Inactive
86	Carbamazepine	NC(=O)N1c2ccccc2C=Cc2c1cccc2	2.52	Inactive
87	Carvedilol	COc1ccccc1OCCNCC(COc1cccc2c1c1ccccc1[nH]2)O	6.29	Active
88	Chlorobutanol	CC(C(Cl)(Cl)Cl)(O)C	2.36	Inactive
89	Chloroquine	CCN(CCCC(Nc1ccnc2c1ccc(c2)Cl)C)CC	5.60	Active
90	Chlorpheniramine	CN(CCC(c1ccccn1)c1ccc(cc1)Cl)C	4.89	Inactive
91	Chlorpromazine	CN(CCCN1c2ccccc2Sc2c1cc(Cl)cc2)C	5.80	Active
92	Chromanolol_293B	CCS(=O)(=O)N(C1C(O)C(C)(C)Oc2c1cc(cc2)C#N)C	4.72	Inactive
93	Cibenzoline	c1ccc(cc1)C1(CC1C1=NCCN1)c1ccccc1	5.43	Active
94	Cimetidine	N#C/N=C(/NCCSCc1nc[nH]c1C)\NC	2.00	Inactive
95	Ciprofloxacin	Fc1cc2c(cc1N1CCNCC1)n(cc(c2=O)C(=O)O)C1CC1	3.02	Inactive
96	Citalopram	N#Cc1ccc2c(c1)COC2(CCCN(C)C)c1ccc(cc1)F	5.40	Active
97	CJ-033466	CC(CN1CCC(CC1)CNC(=O)c1cc(Cl)c(n2c1nc(c2)C)N)C	5.59	Active
98	Clarithromycin	CC[C@H]1OC(=O)[C@H](C)C(O[C@H]2C[C@@](C)(OC)[C@H]([C@@H](O2)C)O)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@@H]([C@H]2O)N(C)C)[C@](C[C@H](C(=O)[C@@H]([C@H]([C@]1(C)O)O)C)C)(C)OC	4.26	Inactive
99	Clebopride	COc1cc(N)c(cc1C(=O)NC1CCN(CC1)Cc1ccccc1)Cl	6.21	Active
100	Clemastine	Clc1ccc(cc1)[C@@](c1ccccc1)(OCC[C@H]1CCCN1C)C	7.92	Active
101	Clenbuterol	OC(c1cc(Cl)c(c(c1)Cl)N)CNC(C)(C)C	4.10	Inactive
102	Clomifene	CCN(CCOc1ccc(cc1)/C(=C(/c1ccccc1)\Cl)/c1ccccc1)CC	6.74	Active
103	Clozapine	CN1CCN(CC1)C1=Nc2cc(Cl)ccc2Nc2c1cccc2	6.22	Active
104	Cocaethylene	CCOC(=O)[C@H]1[C@H](C[C@H]2N([C@@H]1CC2)C)OC(=O)c1ccccc1	5.92	Active
105	Cocaine	COC(=O)[C@H]1[C@H](C[C@H]2N([C@@H]1CC2)C)OC(=O)c1ccccc1	5.36	Active
106	Codeine	COc1ccc2c3c1OC1C43CCN(C(C2)C4C=CC1O)C	3.26	Inactive
107	Cyamemazine	N#Cc1ccc2c(c1)N(CC(CN(C)C)C)c1c(S2)cccc1	6.33	Active
108	Desbutyl-lumefantrine	CCCCNCC(c1cc(Cl)cc2c1c1ccc(cc1/C/2=C/c1ccc(cc1)Cl)Cl)O	5.26	Active
109	Desipramine	CNCCCN1c2ccccc2CCc2c1cccc2	5.89	Active
110	Desmethylastemizole	Oc1ccc(cc1)CCN1CCC(CC1)Nc1nc2c(n1Cc1ccc(cc1)F)cccc2	9.00	Active

111	Desmethylolanzapine	Cc1sc2=Nc3ccccc3NC(=c2c1)N1CCNCC1	4.85	Inactive
112	Diltiazem	COc1ccc(cc1)[C@@H]1Sc2ccccc2N(C(=O)[C@@H]1OC(=O)C)CCN(C)C	4.76	Inactive
113	Diphenhydramine	CN(CCOC(c1ccccc1)c1ccccc1)C	5.59	Active
114	Disopyramide	CC(N(C(C)C)CCC(c1ccccn1)(c1ccccc1)C(=O)N)C	5.14	Active
115	Dofetilide	CN(CCc1ccc(cc1)NS(=O)(=O)C)CCOc1ccc(cc1)NS(=O)(=O)C	7.90	Active
116	Dolasetron	O=C1CN2[C@@H]3C[C@H]1C[C@H]2C[C@H](C3)OC(=O)c1c[nH]c2c1cccc2	5.15	Active
117	Domperidone	Clc1ccc2c(c1)[nH]c(=O)n2C1CCN(CC1)CCCn1c(=O)[nH]c2c1cccc2	6.79	Active
118	Doxazosin	COc1cc2nc(nc(c2cc1OC)N)N1CCN(CC1)C(=O)C1COc2c(O1)cccc2	6.23	Active
119	Doxepin	CN(CC/C=C/1\c2ccccc2OCc2c1cccc2)C	5.19	Active
120	Dronedarone	CCCCc1oc2c(c1C(=O)c1ccc(cc1)OCCCN(CCCC)CCCC)cc(cc2)NS(=O)(=O)C	7.23	Active
121	Droperidol	Fc1ccc(cc1)C(=O)CCCN1CCC(=CC1)n1c(=O)[nH]c2c1cccc2	7.49	Active
122	DW-224a	CO/N=C/1\CN(CC21CNC2)c1nc2N(CC(C(=O)c2cc1F)C(=O)O)C1CC1	3.66	Inactive
123	E-4031	Cc1cccc(n1)CCN1CCC(CC1)C(=O)c1ccc(cc1)NS(=O)(=O)C	7.70	Active
124	EDDP(Edifenphos)	CCOP(=O)(Sc1ccccc1)Sc1ccccc1	4.30	Inactive
125	EGCG	Oc1cc(O)c2c(c1)OC(C(C2)OC(=O)c1cc(O)c(c(c1)O)O)c1cc(O)c(c(c1)O)O	5.22	Active
126	Eliprodil	Fc1ccc(cc1)CC1CCN(CC1)CC(c1ccc(cc1)Cl)O	7.70	Active
127	EMD-60263	C/N=C(/N1CCCc2c1ccc(c2)C1=NNC(=O)SC1C)\c1ccc(c(c1)OC)OC	5.18	Active
128	ER-118585	N#Cc1ccc2c(c1)c(nnc2N1CCC2(CC1)CC(C2)O)NCc1ccc(c(c1)Cl)OC	7.40	Active
129	Erythromycin	CC[C@H]1OC(=O)[C@H](C)C(O[C@@H]2O[C@@H](C)[C@@H]([C@](C2)(C)OC)O)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@@H]([C@H]2O)N(C)C)[C@](C[C@H](C(=O)[C@@H]([C@H]([C@]1(C)O)O)C)C)(C)O	3.95	Inactive
130	Erythromycylamine	CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@@H]2O[C@@H](C)[C@@H]([C@](C2)(C)OC)O)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@@H]([C@H]2O)N(C)C)[C@](C[C@H]([C@@H]([C@@H]([C@H]([C@]1(C)O)O)C)N)C)(C)O	3.52	Inactive
131	Estradiol	Oc1ccc2c(c1)CCC1C2CCC2(C1CCC2O)C	4.00	Inactive
132	Famotidine	NC(=Nc1scc(n1)CSCC/C(=N/S(=O)(=O)N)/N)N	5.00	Inactive
133	Fentanyl	CCC(=O)N(c1ccccc1)C1CCN(CC1)CCc1ccccc1	5.75	Active
134	Fexofenadine	OC(=O)C(c1ccc(cc1)C(CCCN1CCC(CC1)C(c1ccccc1)(c1ccccc1)O)O)(C)C	4.66	Inactive
135	Flecainide	O=C(c1cc(OCC(F)(F)F)ccc1OCC(F)(F)F)NCC1CCCCN1	5.41	Active
136	Fluoxetine	CNCCC(c1ccccc1)Oc1ccc(cc1)C(F)(F)F	5.99	Active
137	Fluvoxamine	NCCON=C(c1ccc(cc1)C(F)(F)F)CCCCOC	5.46	Active
138	Gatifloxacin	COc1c(N2CCNC(C2)C)c(F)cc2c1n(cc(c2=O)C(=O)O)C1CC1	3.89	Inactive
139	GF109203X	CN(CCCn1cc(c2c1cccc2)C1=C(C(=O)NC1=O)c1c[nH]c2c1cccc2)C	6.00	Active
140	Grepafloxacin	CC1NCCN(C1)c1cc2c(c(c1F)C)c(=O)c(cn2C1CC1)C(=O)O	4.23	Inactive
141	Halofantrine	CCCCN(CC[C@@H](c1cc2c(Cl)cc(cc2c2c1ccc(c2)C(F)(F)F)Cl)O)CCCC	7.13	Active
142	Haloperidol	Fc1ccc(cc1)C(=O)CCCN1CCC(CC1)(O)c1ccc(cc1)Cl	7.39	Active
143	HY-2901	Fc1ccc2c(c1)COc1c(C2=C2CCN(CC2)CC(C(=O)O)(C)C)cccc1	5.00	Inactive
144	ICI_118551	CC(NC(C(COc1ccc(c2c1CCC2)C)O)C)C	5.04	Active
145	Ifenprodil	Oc1ccc(cc1)C(C(N1CCC(CC1)Cc1ccccc1)C)O	7.00	Active
146	Imipramine	CN(CCCN1c2ccccc2CCc2c1cccc2)C	5.47	Active
147	Indometacin	COc1ccc2c(c1)c(CC(=O)O)c(n2C(=O)c1ccc(cc1)Cl)C	3.52	Inactive
148	Irbesartan	CCCCC1=NC2(C(=O)N1Cc1ccc(cc1)c1ccccc1c1nnn[nH]1)CCCC2	3.71	Inactive
149	Isradipine	COC(=O)C1=C(C)NC(=C(C1c1cccc2c1non2)C(=O)OC(C)C)C	4.50	Inactive
150	Josamycin	O=CC[C@H]1C[C@@H](C)[C@@H](O)/C=C/C=C/C[C@H](OC(=O)C[C@H]([C@@H]([C@H]1O[C@@H]1O[C@H](C)[C@H]([C@@H]([C@H]1O)N(C)C)O[C@@H]1O[C@@H](C)[C@@H]([C@](C1)(C)O)OC(=O)CC(C)C)OC)OC(=O)C)C	3.99	Inactive
151	Ketanserin	Fc1ccc(cc1)C(=O)C1CCN(CC1)CCn1c(=O)[nH]c2c(c1=O)cccc2	6.97	Active
152	Ketoconazole	Clc1ccc(c(c1)Cl)[C@@]1(OC[C@H](O1)COc1ccc(cc1)N1CCN(CC1)C(=O)C)Cn1cncc1	5.64	Active

153	L-alpha-Acetylmethadol	CC[C@@H](C(c1ccccc1)(c1ccccc1)C[C@@H](N(C)C)C)OC(=O)C	5.61	Active
154	Lamotrigine	Nc1nnc(c(n1)N)c1cccc(c1Cl)Cl	3.64	Inactive
155	Levofloxacin	CN1CCN(CC1)c1c(F)cc2c3c1OC[C@@H](n3cc(c2=O)C(=O)O)C	3.06	Inactive
156	Lidoflazine	O=C(Nc1c(C)cccc1C)CN1CCN(CC1)CCCC(c1ccc(cc1)F)c1ccc(cc1)F	7.72	Active
157	Lignocaine	CCN(CC(=O)Nc1c(C)cccc1C)CC	3.58	Inactive
158	Lomefloxacin	CCn1cc(C(=O)O)c(=O)c2c1c(F)c(N1CCNC(C1)C)c(c2)F	2.62	Inactive
159	Lopinavir	O=C(N[C@H]([C@H](C[C@H](Cc1ccccc1)NC(=O)[C@@H](N1CCCNC1=O)C(C)C)O)Cc1ccccc1)COc1c(C)cccc1C	5.07	Active
160	Loratadine	CCOC(=O)N1CCC(=C2c3ccc(cc3CCc3c2ncccc3)Cl)CC1	6.25	Active
161	Lovastatine	CC[C@@H](C(=O)O[C@H]1C[C@@H](C)C=C2[C@H]1[C@@H](CC[C@@H]1C[C@@H](O)CC(=O)O1)[C@H](C=C2)C)C	5.15	Active
162	Lumefantrine	CCCCN(CC(c1cc(Cl)cc2c1c1ccc(cc1/C/2=C/c1ccc(cc1)Cl)Cl)O)CCCC	5.09	Active
163	LY-97241	CCCCCCCN(CCCCc1ccc(cc1)[N+](=O)[O-])CC	8.66	Active
164	M-43068	Oc1ccc(cc1)C(=O)NC(C(=O)O)(C)C	3.52	Inactive
165	Maraviroc	O=C(C1CCC(CC1)(F)F)N[C@H](c1ccccc1)CCN1[C@@H]2CC[C@H]1C[C@@H](C2)n1c(C)nnc1C(C)C	5.00	Inactive
166	MDL-74156	O[C@@H]1CN2[C@@H]3C[C@H]1C[C@H]2C[C@H](C3)OC(=O)c1c[nH]c2c1cccc2	5.00	Inactive
167	Mefloquine	O[C@@H](c1cc(nc2c1cccc2C(F)(F)F)C(F)(F)F)C1CCCCN1	5.42	Active
168	Meperidine	O=C(OCC)C2(c1ccccc1)CCN(C)CC2	4.13	Inactive
169	Mepivacaine	CN1CCCCC1C(=O)Nc1c(C)cccc1C	3.81	Inactive
170	Mesoridazine	CN1CCCCC1CCN1c2ccccc2Sc2c1cc(cc2)S(=O)C	6.40	Active
171	Methadone	CCC(=O)C(c1ccccc1)(c1ccccc1)CC(N(C)C)C	4.93	Inactive
172	Methylecgonidine	COC(=O)C1=CC[C@H]2N([C@@H]1CC2)C	3.76	Inactive
173	Metoclopramide	CCN(CCNC(=O)c1cc(Cl)c(cc1OC)N)CC	5.27	Active
174	Metoprolol	COCCc1ccc(cc1)OCC(CNC(C)C)O	3.84	Inactive
175	Mexiletine	CC(COc1c(C)cccc1C)N	5.00	Inactive
176	Mibefradil	COCC(=O)O[C@]1(CCN(CCCc2nc3c([nH]2)cccc3)C)CCc2c([C@@H]1C(C)C)ccc(c2)F	5.90	Active
177	Miconazole	Clc1ccc(c(c1)Cl)COC(c1ccc(cc1Cl)Cl)Cn1cncc1	5.68	Active
178	Mizolastine	Fc1ccc(cc1)Cn1c(nc2c1cccc2)N1CCC(CC1)N(c1nccc(=O)[nH]1)C	6.43	Active
179	MK-499	N#Cc1ccc2c(c1)CC[C@H](C2)N1CC[C@]2(CC1)C[C@@H](O)c1c(O2)ccc(c1)NS(=O)(=O)C	7.68	Active
180	Morphine	OC1C=CC2C34C1Oc1c4c(CC2N(CC3)C)ccc1O	3.00	Inactive
181	Mosapride	CCOc1cc(N)c(cc1C(=O)NCC1OCCN(C1)Cc1ccc(cc1)F)Cl	5.32	Active
182	Moxifloxacin	COc1c(N2C[C@@H]3[C@H](C2)CCCN3)c(F)cc2c1n(cc(c2=O)C(=O)O)C1CC1	3.98	Inactive
183	N-{(1S)-2-[(3S)-3-hydroxypyrrolidin-1-yl]-1-phenylethyl}-N-methyl-2-(4-{[(methylsulfonyl)amino]methyl}phenyl)acetamide	O[C@H]1CCN(C1)C[C@@H](N(C(=O)Cc1ccc(cc1)CNS(=O)(=O)C)C)c1ccccc1	5.00	Inactive
184	Naringenin	Oc1ccc(cc1)[C@@H]1CC(=O)c2c(O1)cc(cc2O)O	4.44	Inactive
185	N-Demethylerythromycin	CN[C@H]1C[C@@H](C)O[C@H]([C@@H]1O)O[C@@H]1[C@@H](C)[C@H](O[C@@H]2O[C@@H](C)[C@@H]([C@]2)(C)OC)O)[C@@H](C)C(=O)O[C@H](CC)[C@@]([C@@H]([C@H](C(=O)[C@@H](C[C@]1(C)O)C)C)O)(C)O	3.83	Inactive
186	N-Demethylolanzapine	Cc1sc2c(c1)C(=Nc1c(N2)cccc1)N1CCNCC1	4.85	Inactive
187	N-Desbutylhalofantrine	CCCCNCCC(c1cc2c(Cl)cc(cc2c2c1ccc(c2)C(F)(F)F)Cl)O	7.14	Active
188	N-Desmethylclozapine	Clc1ccc2c(c1)N=C(N1CCNCC1)c1c(N2)cccc1	5.35	Active
189	Nelfinavir	O[C@@H]([C@@H](NC(=O)c1cccc(c1C)O)CSc1ccccc1)CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C	4.94	Inactive

190	Nicotine	CN1CCC[C@H]1c1cccnc1	3.61	Inactive
191	Nifedipine	COC(=O)C1=C(C)NC(=C(C1c1ccccc1[N+](=O)[O-])C(=O)OC)C	4.20	Inactive
192	NIP-142	COc1ccc(cc1)CC(=O)Nc1cc2c(cc1[N+](=O)[O-])OC([C@@H]([C@H]2NC1CC1)O)(C)C	4.36	Inactive
193	Nitrendipine	CCOC(=O)C1=C(C)NC(=C(C1c1cccc(c1)[N+](=O)[O-])C(=O)OC)C	5.00	Inactive
194	Noracetylmethadol	CCC(C(c1ccccc1)(c1ccccc1)CC(NC)C)O	4.92	Inactive
195	Norastemizole	Fc1ccc(cc1)Cn1c(NC2CCNCC2)nc2c1cccc2	7.56	Active
196	Norfluoxetine	NCCC(c1ccccc1)Oc1ccc(cc1)C(F)(F)F	5.62	Active
197	Olanzapine	CN1CCN(CC1)C1=Nc2ccccc2Nc2c1cc(s2)C	6.67	Active
198	Ondansetron	O=C1C(CCc2c1c1ccccc1n2C)Cn1ccnc1C	6.09	Active
199	Orphenadrine	CN(CCOC(c1ccccc1C)c1ccccc1)C	6.07	Active
200	Oxatomide	O=c1[nH]c2c(n1CCCN1CCN(CC1)C(c1ccccc1)c1ccccc1)cccc2	6.45	Active
201	Paliperidone	Fc1ccc2c(c1)onc2C1CCN(CC1)CCc1c(C)nc2n(c1=O)CCCC2O	5.89	Active
202	Perhexiline	C1CCC(NC1)CC(C1CCCCC1)C1CCCCC1	5.11	Active
203	Perphenazine	OCCN1CCN(CC1)CCCN1c2ccccc2Sc2c1cc(Cl)cc2	6.00	Active
204	Phenobarbital	CCC1(C(=O)NC(=O)NC1=O)c1ccccc1	2.52	Inactive
205	Phenytoin	O=C1NC(=O)NC1(c1ccccc1)c1ccccc1	3.62	Inactive
206	Pilsicainide	O=C(CC12CCCN2CCC1)Nc1c(C)cccc1C	4.69	Inactive
207	Pimozide	Fc1ccc(cc1)C(c1ccc(cc1)F)CCCN1CCC(CC1)n1c(=O)[nH]c2c1cccc2	7.59	Active
208	Prazosin	COc1cc2nc(nc(c2cc1OC)N)N1CCN(CC1)C(=O)c1ccco1	5.80	Active
209	Prenylamine	CC(Cc1ccccc1)NCCC(c1ccccc1)c1ccccc1	6.23	Active
210	Procainamide	CCN(CCNC(=O)c1ccc(cc1)N)CC	3.86	Inactive
211	Propafenone	CCCNCC(COc1ccccc1C(=O)CCc1ccccc1)O	6.17	Active
212	Protriptyline	CNCCC[C@@H]1c2ccccc2C=Cc2c1cccc2	5.93	Active
213	Prucalopride	COCCCN1CCC(CC1)NC(=O)c1cc(Cl)c(c2c1OCC2)N	5.31	Active
214	Prulifloxacin	O=c1oc(c(o1)CN1CCN(CC1)c1cc2c(cc1F)c(=O)c(c1n2C(C)S1)C(=O)O)C	3.46	Inactive
215	Pyrilamine	COc1ccc(cc1)CN(c1ccccn1)CCN(C)C	5.22	Active
216	Quetiapine	OCCOCCN1CCN(CC1)C1=Nc2ccccc2Sc2c1cccc2	5.24	Active
217	Quinidine	O(c4cc1c(nccc1[C@H](O)[C@@H]2N3CC[C@@H](C2)[C@@H](/C=C)C3)cc4)C	6.30	Active
218	Renzapride	COc1cc(N)c(cc1C(=O)N[C@@H]1CCN2C[C@@H]1CCC2)Cl	5.70	Active
219	Risperidone	Fc1ccc2c(c1)onc2C1CCN(CC1)CCc1c(C)nc2n(c1=O)CCCC2	6.75	Active
220	Ritonavir	O=C(N[C@H]([C@H](C[C@H](Cc1ccccc1)NC(=O)[C@H](C(C)C)NC(=O)N(Cc1csc(n1)C(C)C)C)O)Cc1ccccc1)OCc1cncs1	5.09	Active
221	Roxithromycin	COCCOCO/N=C\1/[C@H](C)C[C@@](C)(O)[C@H](O[C@@H]2O[C@H](C)C[C@@H]([C@H]2O)N(C)C)[C@@H](C)C(O[C@@H]2O[C@@H](C)[C@@H]([C@](C2)(C)OC)O)[C@H](C(=O)O[C@@H]([C@@]([C@@H]([C@H]1C)O)(C)O)CC)C	4.44	Inactive
222	Saquinavir	NC(=O)C[C@@H](C(=O)N[C@H]([C@@H](CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)O)Cc1ccccc1)NC(=O)c1ccc2c(n1)cccc2	4.82	Inactive
223	Saxitoxin	N=C1NC2C3(N1)N(CCC3(O)O)C(=N)NC2COC(=O)N	5.89	Active
224	Sertindole	Clc1ccc2c(c1)c(cn2c1ccc(cc1)F)C1CCN(CC1)CCN1CCNC1=O	8.07	Active
225	Sildenafil	CCCc1nn(c2c1nc([nH]c2=O)c1cc(ccc1OCC)S(=O)(=O)N1CCN(CC1)C)C	4.69	Inactive
226	Sophocarpine	O=C1CCC[C@H]2N1C[C@@H]1CCCN3[C@@H]1[C@@H]2CCC3	3.70	Inactive
227	Sotalol	CC(NCC(c1ccc(cc1)NS(=O)(=O)C)O)C	3.57	Inactive
228	Sparfloxacin	C[C@@H]1N[C@H](C)CN(C1)c1c(F)c(N)c2c(c1F)n(cc(c2=O)C(=O)O)C1CC1	4.67	Inactive
229	Spironolactone	CC(=O)S[C@@H]1CC2=CC(=O)CC[C@@]2([C@@H]2C1[C@@H]1CC[C@]3([C@]1(CC2)C)CCC(=O)O3)C	4.64	Inactive
230	sulfamethoxazole	Nc1ccc(cc1)S(=O)(=O)Nc1noc(c1)C	2.00	Inactive
231	Tadalafil	O=C1N(C)CC(=O)N2[C@@H]1Cc1c([C@H]2c2ccc3c(c2)OCO3)[nH]c2c1cccc2	4.00	Inactive
232	Tamsulosin	CCOc1ccccc1OCCNC(Cc1ccc(c(c1)S(=O)(=O)N)OC)C	3.98	Inactive

233	Telithromycin	CC[C@H]1OC(=O)[C@H](C)C(=O)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@@H]([C@H]2O)N(C)C)[C@](C[C@H](C(=O)[C@@H]([C@@H]2[C@]1(C)OC(=O)N2CCCCn1cnc(c1)c1ccccnc1)C)C)(C)OC	4.28	Inactive
234	Terazosin	COc1cc2nc(nc(c2cc1OC)N)N1CCN(CC1)C(=O)C1CCCO1	4.75	Inactive
235	Terfenadine	OC(c1ccc(cc1)C(C)(C)C)CCCN1CCC(CC1)C(c1ccccc1)(c1ccccc1)O	7.25	Active
236	Thioridazine	CSc1ccc2c(c1)N(CCC1CCCCN1C)c1c(S2)cccc1	7.03	Active
237	Trazodone	Clc1cccc(c1)N1CCN(CC1)CCCn1nc2n(c1=O)cccc2	5.75	Active
238	Trifluoperazine	CN1CCN(CC1)CCCN1c2ccccc2Sc2c1cc(cc2)C(F)(F)F	5.45	Active
239	Trimetoprim	COc1cc(Cc2cnc(nc2N)N)cc(c1OC)OC	3.62	Inactive
240	Vardenafil	CCOc1ccc(cc1c1nc(=O)c2n([nH]1)c(CCC)nc2C)S(=O)(=O)N1CCN(CC1)CC	4.90	Inactive
241	Verapamil	COc1ccc(cc1OC)CCN(CCCC(c1ccc(c(c1)OC)OC)(C(C)C)C#N)C	6.68	Active
242	Vesnarinone	COc1ccc(cc1OC)C(=O)N1CCN(CC1)c1ccc2c(c1)CCC(=O)N2	5.97	Active
243	Vinpocetine	CCOC(=O)[C@@H]1C[C@]2(CC)CCCN3[C@H]2c2n1c1ccccc1c2CC3	6.89	Active
244	Ziprasidone	O=C1Nc2c(C1)cc(c(c2)Cl)CCN1CCN(CC1)c1nsc2c1cccc2	6.88	Active

Appendix IX. Descriptors used for modelling compounds from H_244 dataset.

Software	No	Type	Descriptors
MOE	303	*2-D:* *-physical properties* *-subdivided surface areas* *-atom counts and bond counts* *-Kier&Hall connectivity and Kappa shape indices* *-adjacency and distance matrix* *-pharmacophore Feature* *-partial charge* *3-D:* *-potential energy* *-surface area, volume and shape* *-conformation dependent charge*	*AM1_dipole, apol, ASA, ASA+, ASA-, ASA_H, ASA_P, a_acc, a_aro, a_count, a_don, a_heavy, a_hyd, a_IC, a_ICM, a_nC, a_nCl, a_nF, a_nH, a_nN, a_nO, a_nS, balabanJ, BCUT_PEOE_0, BCUT_PEOE_1, BCUT_PEOE_2, BCUT_PEOE_3, BCUT_SLOGP_0, BCUT_SLOGP_1, BCUT_SLOGP_2, BCUT_SLOGP_3, BCUT_SMR_0, BCUT_SMR_1, BCUT_SMR_2, BCUT_SMR_3, bpol, b_1rotN, b_1rotR, b_ar, b_count, b_double, b_heavy, b_rotN, b_rotR, b_single, b_triple, CASA+, CASA-, chi0, chi0v, chi0v_C, chi0_C, chi1, chi1v, chi1v_C, chi1_C, chiral, chiral_u, DASA, DCASA, dens, density, diameter, dipole, dipoleX, dipoleY, dipoleZ, E, E_ang, E_ele, E_nb, E_oop, E_rnb, E_rsol, E_sol, E_stb, E_str, E_strain, E_tor, E_vdw, FASA+, FASA-, FASA_H, FASA_P, FCASA+, FCASA-, GCUT_PEOE_0, GCUT_PEOE_1, GCUT_PEOE_2, GCUT_PEOE_3, GCUT_SLOGP_0, GCUT_SLOGP_1, GCUT_SLOGP_2, GCUT_SLOGP_3, GCUT_SMR_0, GCUT_SMR_1, GCUT_SMR_2, GCUT_SMR_3, glob, Kier1, Kier2, Kier3, KierA1, KierA2, KierA3, KierFlex, lip_acc, lip_don, lip_druglike, lip_violation, logP(o/w), logS, MNDO_dipole, mr, npr1, npr2, opr_brigid, opr_leadlike, opr_nring, opr_nrot, opr_violation, PC+, PC-, PEOE_PC+, PEOE_PC-, PEOE_RPC+, PEOE_RPC-, PEOE_VSA+0, PEOE_VSA+1, PEOE_VSA+2, PEOE_VSA+3, PEOE_VSA+4, PEOE_VSA+5, PEOE_VSA+6, PEOE_VSA-0, PEOE_VSA-1, PEOE_VSA-2, PEOE_VSA-3, PEOE_VSA-4, PEOE_VSA-5, PEOE_VSA-6, PEOE_VSA_FHYD, PEOE_VSA_FNEG, PEOE_VSA_FPNEG, PEOE_VSA_FPOL, PEOE_VSA_FPOS, PEOE_VSA_FPPOS, PEOE_VSA_HYD, PEOE_VSA_NEG, PEOE_VSA_PNEG, PEOE_VSA_POL, PEOE_VSA_POS, PEOE_VSA_PPOS, petitjean, petitjeanSC, PM3_dipole, pmi, pmi1, pmi2, pmi3, pmiX, pmiY, pmiZ, Q_PC+, Q_PC-, Q_RPC+, Q_RPC-, Q_VSA_FHYD, Q_VSA_FNEG, Q_VSA_FPNEG, Q_VSA_FPOL, Q_VSA_FPOS, Q_VSA_FPPOS, Q_VSA_HYD, Q_VSA_NEG, Q_VSA_PNEG, Q_VSA_POL, Q_VSA_POS, Q_VSA_PPOS, radius, reactive, rgyr, MAX_DIAMETER, rings, RPC+, RPC-, rsynth, SlogP, SlogP_VSA0, SlogP_VSA1, SlogP_VSA2, SlogP_VSA3, SlogP_VSA4, SlogP_VSA5, SlogP_VSA6, SlogP_VSA7, SlogP_VSA8, SlogP_VSA9, SMR, SMR_VSA0, SMR_VSA1, SMR_VSA2, SMR_VSA3, SMR_VSA4, SMR_VSA5, SMR_VSA6, SMR_VSA7, std_dim1, std_dim2, std_dim3, TPSA, VAdjEq, VAdjMa, VDistEq, VDistMa, vdw_area, vdw_vol, vol, VSA, vsa_acc, vsa_don, vsa_hyd, vsa_other, vsa_pol, vsurf_A, vsurf_CP, vsurf_CW1, vsurf_CW2, vsurf_CW3, vsurf_CW4, vsurf_CW5, vsurf_CW6, vsurf_CW7, vsurf_CW8, vsurf_D1, vsurf_D2, vsurf_D3, vsurf_D4, vsurf_D5, vsurf_D6, vsurf_D7, vsurf_D8, vsurf_DD12, vsurf_DD13, vsurf_DD23, vsurf_DW12, vsurf_DW13, vsurf_DW23, vsurf_EDmin1, vsurf_EDmin2, vsurf_EDmin3, vsurf_EWmin1, vsurf_EWmin2, vsurf_EWmin3, vsurf_G, vsurf_HB1, vsurf_HB2, vsurf_HB3, vsurf_HB4, vsurf_HB5, vsurf_HB6, vsurf_HB7, vsurf_HB8, vsurf_HL1, vsurf_HL2, vsurf_ID1, vsurf_ID2, vsurf_ID3, vsurf_ID4, vsurf_ID5, vsurf_ID6, vsurf_ID7, vsurf_ID8, vsurf_IW1, vsurf_IW2, vsurf_IW3, vsurf_IW4, vsurf_IW5, vsurf_IW6, vsurf_IW7, vsurf_IW8, vsurf_R, vsurf_S, vsurf_V, vsurf_W1, vsurf_W2, vsurf_W3, vsurf_W4, vsurf_W5, vsurf_W6, vsurf_W7, vsurf_W8, vsurf_Wp1, vsurf_Wp2, vsurf_Wp3, vsurf_Wp4, vsurf_Wp5, vsurf_Wp6, vsurf_Wp7, Weight, weinerPath, weinerPol, zagreb*
ACD	28	*-physical properties (mostly medicine chemistry type descriptors)*	*ACD_LogD_1, ACD_LogD_2, ACD_LogD_3, ACD_LogD_4, ACD_LogD_5, ACD_LogP, ACD_MW, ACD_PSA, ACD_FRB, ACD_Rule_Of_5, ACD_HDonors, ACD_HAcceptors, ACD_Molar_Refractivity_cm^3, ACD_Molar_Volume_cm^3, ACD_Parachor_cm^3, ACD_Index_of_Refraction, ACD_Surface_Tension_dyne/cm, ACD_Density_g/cm^3, ACD_Polarizability_10e-24_cm^3, ACD_C_ratio, ACD_N_ratio, ACD_NO_ratio, ACD_Hetero_ratio, ACD_Halogen_ratio, ACD_Num_Rings, ACD_Num_Aromatic_Rings, ACD_Num_Rings_5, ACD_Num_Rings_6*
HYBOT	32	*H-bond thermodynamics*	*Alpha, max(Q+), max(Q-), Sum(Q+), Sum(Q-), Sum(|Q|)], Sum(Q+)/Alpha, Sum(Q-)/Alpha, Max(Ea), Max(Ca), Max(Ca(o)), Max(Ed), Max(Cd), Max(Ea)*Max(Ed), Max(Ca)*Max(Cd), Max(Ca(o))*Max(Cd(o)), Sum(Ea), Sum(Ed), Sum(Ead), Sum(Ca), Sum(Cd), Sum(Cad), Sum(Ca(o)), Sum(Cad(o)), Sum(Ea)/Alpha, Sum(Ed)/Alpha, Sum(Ead)/Alpha, Sum(Ca)/Alpha, Sum(Cd)/Alpha, Sum(Cad)/Alpha, Sum(Ca(o))/Alpha, Sum(Cad(o))/Alpha*
MOPAC	*1*	*molecular size*	*Maximum diameter*

Appendix X. DS1 (training) and DS2 (test) discussed in Chapter 6.

ID	Name	SMILES	log(1/EC50)	Dataset
1	Acetyl salicylic acid	O(C(=O)C)c1ccccc1C(O)=O	-2.45	training
2	Acrolein	O=CC=C	-0.82	training
3	2-Aminoethanol	OCCN	-4.78	training
4	4-Aminophenol	Oc1ccc(N)cc1	-0.63	training
5	Aniline	Nc1ccccc1	-3.47	training
6	Atrazine	Clc1nc(nc(n1)NCC)NC(C)C	-2.23	training
7	Benzoic acid	OC(=O)c1ccccc1	-2.21	training
8	4-Bromoindole	Brc1c2c([nH]cc2)ccc1	-1.38	training
9	5-Bromoindole	Brc1cc2c([nH]cc2)cc1	-1.44	training
10	6-Bromoindole	Brc1cc2[nH]ccc2cc1	-1.55	training
11	2-Bromophenol	Brc1ccccc1O	-2.42	training
12	3-Bromophenol	Brc1cc(O)ccc1	-2.54	training
13	4-Bromophenol	Brc1ccc(O)cc1	-2.43	training
14	n-Butylamine	NCCCC	-2.69	training
15	sec-Butylamine	NC(CC)C	-3.11	training
16	Butyldiglycol	O(CCCC)CCOCCO	-3.90	training
17	p-tert-Butylphenol	Oc1ccc(cc1)C(C)(C)C	-1.06	training
18	Carbaryl	O(C(=O)NC)c1c2c(ccc1)cccc2	-1.37	training
19	Chloroacetaldehyde	ClCC=O	-1.63	training
20	2-Chloroaniline	Clc1ccccc1N	-2.35	training
21	3-Chloroaniline	Clc1cc(N)ccc1	-2.22	training
22	4-Chloroaniline	Clc1ccc(N)cc1	-2.22	training
23	4-Chlorophenol	Clc1ccc(O)cc1	-2.49	training
24	Colcemide	O(C)C1=CC=C2C(=CC1=O)C(NC)CCc1c2c(OC)c(OC)c(OC)c1	-0.96	training
25	Cyclohexanol	OC1CCCCC1	-4.14	training
26	Cycloheximide	O=C1C(CC(CC1C)C)C(O)CC1CC(=O)NC(=O)C1	-0.69	training
27	Cyclohexylamine	NC1CCCCC1	-2.81	training
28	n-Decylamine	NCCCCCCCCCC	-1.30	training
29	2,4-Dibromophenol	Brc1cc(Br)ccc1O	-1.50	training
30	2,6-Dibromophenol	Brc1cccc(Br)c1O	-2.22	training
31	Dibutylamine	N(CCCC)CCCC	-2.50	training
32	2,4-Dichloroaniline	Clc1cc(Cl)ccc1N	-2.12	training
33	3,4-Dichloroaniline	Clc1cc(N)ccc1Cl	-1.09	training
34	Dicyclohexylamine	N(C1CCCCC1)C1CCCCC1	-2.24	training
35	Diethylamine	N(CC)CC	-3.11	training
36	Diethylene glycol	O(CCO)CCO	-5.68	training
37	Diethylene glycol dimethylether	O(CCOC)CCOC	-4.92	training
38	N,N-Diethylmethylamine	N(CC)(CC)C	-2.90	training
39	N,N-Diisopropylethylamine	N(C(C)C)(C(C)C)CC	-2.91	training
40	Diisobutylamine	N(CC(C)C)CC(C)C	-2.56	training

41	Diisopropylamine	N(C(C)C)C(C)C	-2.96	training
42	N,N-Dimethylamine	N(C)C	-3.94	training
43	N,N-Dimethylanilin	N(C)(C)c1ccccc1	-2.65	training
44	N,N-Dimethylbutylamine	N(CCCC)(C)C	-2.70	training
45	N,N-Dimethylcyclohexylamine	N(C)(C)C1CCCCC1	-2.62	training
46	N,N-Dimethylethylamine	N(CC)(C)C	-3.05	training
47	N,N-Dimethylformamide	O=CN(C)C	-5.11	training
48	Dimethylsulfoxide	S(=O)(C)C	-5.57	training
49	4,6-Dinitro-o-cresol	Oc1c(cc([N+](=O)[O-])cc1[N+](=O)[O-])C	-0.37	training
50	2,4-Dinitrophenol	Oc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]	-0.69	training
51	Dipentylamine	N(CCCCC)CCCCC	-2.43	training
52	Dipropylamine	N(CCC)CCC	-2.49	training
53	D-Mannitol	OC(C(O)C(O)CO)C(O)CO	-2.63	training
54	Dodecyl linear alkyl benzene sulfonate	S(O)(=O)(=O)c1ccc(cc1)CCCCCCCCCCCC	-0.96	training
55	Ethanol	OCC	-5.40	training
56	Ethyl acetate	O(C(=O)C)CC	-4.32	training
57	Ethylenediamine	NCCN	-3.82	training
58	1-Ethylpiperidine	N1(CCCCC1)CC	-2.80	training
59	2-Ethylpiperidine	N1CCCCC1CC	-2.92	training
60	Formamide	O=CN	-5.31	training
61	a-D-Glucose	O1C(CO)C(O)C(O)C(O)C(O)C1O	-5.63	training
62	n-Heptylamine	NCCCCCCC	-2.39	training
63	Hexamethyleneimine	N1CCCCCC1	-3.07	training
64	2,5-Hexanedion	O=C(CCC(=O)C)C	-4.61	training
65	n-Hexylamine	NCCCCCC	-2.62	training
66	Hydroquinone	Oc1ccc(O)cc1	-1.86	training
67	Hydroxyurea	O=C(NO)N	-4.35	training
68	Isobutylamine	NCC(C)C	-3.10	training
69	Isoniazid	O=C(NN)c1ccncc1	-2.49	training
70	Isopentylamine	NCCC(C)C	-2.83	training
71	Isopropylamine	NC(C)C	-4.18	training
72	Lindane	ClC1C(Cl)C(Cl)C(Cl)C(Cl)C1Cl	-0.44	training
73	Malathion	S(P(=S)(OC)OC)C(CC(OCC)=O)C(OCC)=O	-1.32	training
74	Methanol	OC	-5.84	training
75	Methoxyacetic acid	O(CC(O)=O)C	-2.78	training
76	2-Methoxyethanol	O(CCO)C	-5.43	training
77	1-Methoxy-2-propanol	O(CC(O)C)C	-5.22	training
78	3-Methyl-1-butanol	OCCC(C)C	-4.08	training
79	N-Methylamine	NC	-4.36	training
80	N-Methylanilin	N(C)c1ccccc1	-0.59	training
81	N-Methylformamide	O=CNC	-5.44	training
82	1-Methylpiperidine	N1(CCCCC1)C	-2.84	training
83	2-Methylpiperidine	N1CCCCC1C	-3.01	training

84	4-Methylpiperidine	N1CCC(CC1)C	-2.97	training
85	Morpholine	O1CCNCC1	-3.84	training
86	2-Nitro-4'-hydroxydiphenylamine	Oc1ccc(Nc2ccccc2[N+](=O)[O-])cc1	-0.14	training
87	2-Nitroaniline	O=[N+]([O-])c1ccccc1N	-2.19	training
88	2-Nitroanisole (2-NA)	O(C)c1ccccc1[N+](=O)[O-]	-2.30	training
89	4-Nitrobenzoic acid	OC(=O)c1ccc([N+](=O)[O-])cc1	-2.25	training
90	4-Nitrophenol	Oc1ccc([N+](=O)[O-])cc1	-2.55	training
91	n-Nonylamine	NCCCCCCCCC	-1.90	training
92	1-Octanol	OCCCCCCCC	-2.08	training
93	n-Octylamine	NCCCCCCCC	-2.29	training
94	Penicillin G	S1C2N(C(C(O)=O)C1(C)C)C(=O)C2NC(=O)Cc1ccccc1	-4.18	training
95	Pentachlorophenol	Clc1c(O)c(Cl)c(Cl)c(Cl)c1Cl	-0.20	training
96	n-Pentylamine	NCCCCC	-2.55	training
97	4-tert-Pentylphenol	Oc1ccc(cc1)C(CC)(C)C	-1.33	training
98	Phenol	Oc1ccccc1	-2.97	training
99	Piperidine	N1CCCCC1	-3.11	training
100	Prochloraz	Clc1cc(Cl)cc(Cl)c1OCCN(CCC)C(=O)n1ccnc1	-0.89	training
101	2-Propanol	OC(C)C	-5.19	training
102	n-Propylamine	NCCC	-3.13	training
103	Quinone	O=C1C=CC(=O)C=C1	-0.64	training
104	Retinoic acid	OC(=O)C=C(C=CC=C(C=CC=1C(CCCC=1C)(C)C)C)C	-0.56	training
105	all-trans-Retinol	OCC=C(C=CC=C(C=CC=1C(CCCC=1C)(C)C)C)C	-0.33	training
106	Saccharin	S1(=O)(=O)N=C(O)c2c1cccc2	-5.01	training
107	Salicylic acid	Oc1ccccc1C(O)=O	-2.23	training
108	2,4,6-Tribromophenol	Brc1cc(Br)cc(Br)c1O	-1.13	training
109	Tributylamine	N(CCCC)(CCCC)CCCC	-3.21	training
110	Triclocarban	Clc1cc(NC(=O)Nc2ccc(Cl)cc2)ccc1Cl	1.08	training
111	Triclosan	Clc1cc(Cl)ccc1Oc1ccc(Cl)cc1O	-0.04	training
112	Triethylamine	N(CC)(CC)CC	-2.78	training
113	Triethylene glycol	O(CCOCCO)CCO	-5.55	training
114	Tripropylamine	N(CCC)(CCC)CCC	-3.12	training
115	Urea	O=C(N)N	-5.58	training
116	Valpromide	O=C(N)C(CCC)CCC	-3.87	training
117	Valproic acid	OC(=O)C(CCC)CCC	-2.15	training
118	1,2,4-Trichlorobenzene	Clc1cc(Cl)ccc1Cl	-2.02	test
119	1,2-Dibromoethane	BrCCBr	-2.86	test
120	1,2-Dichlorobenzene	Clc1ccccc1Cl	-1.90	test
121	1,4-Dimethoxybenzol	O(C)c1ccc(OC)cc1	-2.49	test
122	2,2,2-Trichloroethanol	ClC(Cl)(Cl)CO	-3.40	test
123	2,2'-Methylenebis(3,4,6-trichlorophenol)	Clc1c(Cc2c(O)c(Cl)cc(Cl)c2Cl)c(O)c(Cl)cc1Cl	0.74	test

124	2,2'-Methylenebis(4-chlorophenol)	Clc1cc(Cc2cc(Cl)ccc2O)c(O)cc1	-0.11	test
125	2,3,6-Trimethylphenol	Oc1c(C)c(ccc1C)C	-1.96	test
126	2,3-Dimethyl-1,3-butadiene	C(C(C)=C)(C)=C	-3.11	test
127	2,4,6-Trichloroaniline	Clc1cc(Cl)cc(Cl)c1N	-1.13	test
128	2,4,6-Trichlorophenol	Clc1cc(Cl)cc(Cl)c1O	-1.16	test
129	2,4-Dichlorophenol	Clc1cc(Cl)ccc1O	-2.10	test
130	2,4-Dimethylphenol	Oc1ccc(cc1C)C	-2.12	test
131	2-Amino-4-Methyl-3-Nitropyridine	O=[N+]([O-])c1c(ccnc1N)C	-2.41	test
132	2-Amino-5-Nitropyridine	O=[N+]([O-])c1ccc(nc1)N	-3.18	test
133	2-Chlor-4-Nitropyridin-N-oxide	Clc1[n+]([O-])ccc([N+](=O)[O-])c1	-1.60	test
134	2-Chlor-5-Nitropyridine	Clc1ncc([N+](=O)[O-])cc1	-0.23	test
135	2-Methyl-1,4-naphthoquinone	O=C1c2c(cccc2)C(=O)C=C1C	0.15	test
136	3,5-Dichloroaniline	Clc1cc(N)cc(Cl)c1	-2.08	test
137	3-Nitropyridine	O=[N+]([O-])c1cccnc1	-2.79	test
138	4-Fluoroaniline	Fc1ccc(N)cc1	-2.73	test
139	4-Nitropyridin-N-oxide	O=[N+]([O-])c1cc[n+]([O-])cc1	-2.36	test
140	4-Nitroquinoline-1-oxide	O=[N+]([O-])c1c2c([n+]([O-])cc1)cccc2	-0.75	test
141	6-Methyl-5-hepten-2-one	O=C(CCC=C(C)C)C	-3.10	test
142	Acetaldehyde	O=CC	-2.99	test
143	Allyl alcohol	OCC=C	-3.62	test
144	Azinophosmethyl	S(P(=S)(OC)OC)CN1N=Nc2c(cccc2)C1=O	-1.10	test
145	Benzhydrazide	O=C(NN)c1ccccc1	-2.70	test
146	Benzofuran	o1c2c(cccc2)cc1	-2.18	test
147	Benzylhydrazine dihydrochloride	N(N)Cc1ccccc1	-1.96	test
148	Bisphenol-A	Oc1ccc(cc1)C(C)(C)c1ccc(O)cc1	-1.42	test
149	Caffeine	O=C1N(C)C(=O)N(c2ncn(c12)C)C	-3.41	test
150	Carbamazepine	O=C(N)N1c2c(C=Cc3c1cccc3)cccc2	-2.82	test
151	Cetyl trimethyl ammonium	N(CCCCCCCCCCCCCCCC)(C)(C)C	-0.10	test
152	Chlorothalonil	Clc1c(C#N)c(Cl)c(Cl)c(Cl)c1C#N	-2.22	test
153	Chlorotoluron	Clc1cc(NC(=O)N(C)C)ccc1C	-1.46	test
154	Cyclohexane	C1CCCCC1	-4.47	test
155	Dialkyl sulphosuccinate (C7-C8)	S(O)(=O)(=O)C(CC(OCC(CCCC)CC)=O)C(OCC(CCCC)CC)=O	-1.39	test
156	Dibutyl maleate	O(CCCC)C(=O)\C=C/C(OCCCC)=O	-0.62	test
157	Dichloromethane	ClCCl	-3.95	test
158	Diclofenac	Clc1cccc(Cl)c1Nc1ccccc1CC(O)=O	-0.84	test
159	Diethyl phthalate	O(C(=O)c1ccccc1C(OCC)=O)CC	-2.24	test
160	Dimethylacetamide	O=C(N(C)C)C	-5.29	test
161	Di-n-butylorthophthalate	O(C(=O)c1ccccc1C(OCCCC)=O)CCCC	-0.93	test
162	Disulfoton	S(CCSP(=S)(OCC)OCC)CC	-1.60	test

163	Dodecyl sulfate	S(OCCCCCCCCCCCC)(O)(=O)=O	-1.28	test
164	Fatty alkyl ester sulphonate (C14)	S(O)(=O)(=O)C(CCCCCCCCCCCC)C(OC)=O	-1.24	test
165	Fluoxetine	FC(F)(F)c1ccc(OC(CCNC)c2ccccc2)cc1	-1.88	test
166	Genistein	O1C=C(C(=O)c2c1cc(O)cc2O)c1ccc(O)cc1	-1.32	test
167	Hexamethylenetetramine	N12CN3CN(C1)CN(C2)C3	-5.57	test
168	Ibuprofen	OC(=O)C(C)c1ccc(cc1)CC(C)C	-1.58	test
169	Isobutyl-ethyl-valproic acid	O(CC)c1cc(ccc1O)C=O	-3.60	test
170	Juglone	Oc1c2c(ccc1)C(=O)C=CC2=O	0.53	test
171	Lauric acid	OC(=O)CCCCCCCCCCC	-1.70	test
172	Menadione sodium bisulfite	S(O)(=O)(=O)C1(CC(=O)c2c(cccc2)C1=O)C	0.19	test
173	Merquat 100	[N+](CC=C)(CC=C)(C)C	-0.61	test
174	Methoxy acetic acid isopropylester	O(C(C)C)C(=O)COC	-1.88	test
175	Methylcarbamoyl cysteine	S(C[C@H](N)C(O)=O)C(=O)NC	-3.25	test
176	Methylcarbamoyl glutathione	S(C[C@H](NC(=O)CC[C@H](N)C(O)=O)C(=O)NCC(O)=O)C(=O)NC	-2.87	test
177	N-(Hydroxymethyl)-N-methylformamide	OCN(C=O)C	-4.17	test
178	Naphthalene	c12c(cccc1)cccc2	-1.85	test
179	Nonylphenol	[O-]c1ccccc1CCCCCCCCC	-0.96	test
180	Parathion-ethyl	S=P(Oc1ccc([N+](=O)[O-])cc1)(OCC)OCC	-1.23	test
181	Paroxetine	Fc1ccc(cc1)[C@@H]1CCNC[C@H]1COc1cc2OCOc2cc1	-1.88	test
182	Phenylhydrazine	N(N)c1ccccc1	-1.14	test
183	Propoxur	O(C(C)C)c1ccccc1OC(=O)NC	-2.13	test
184	Quinoline	n1c2c(cccc2)ccc1	-2.13	test
185	Resmethrin	o1cc(cc1Cc1ccccc1)COC(=O)C1C(C)(C)C1C=C(C)C	-2.15	test
186	Rotenone	O1c2c(C[C@@H]1C(C)=C)c1O[C@H]3[C@H](c4cc(OC)c(OC)cc4OC3)C(=O)c1cc2	0.70	test
187	Sertraline	Clc1cc(ccc1Cl)[C@@H]1CC[C@H](NC)c2c1cccc2	-0.79	test
188	Tamiflu	O(C(CC)CC)[C@@H]1C=C(C[C@H](N)[C@H]1NC(=O)C)C(OCC)=O	-2.65	test
189	Tetrabromobisphenol-A	Brc1cc(cc(Br)c1O)C(C)(C)c1cc(Br)c(O)c(Br)c1	0.14	test
190	Tetradecyl sulfate	S(OCCCCCCCCCCCCCC)(O)(=O)=O	-0.04	test
191	Thiram	S(SC(=S)N(C)C)C(=S)N(C)C	-2.67	test
192	Toluene	c1ccccc1C	-2.83	test
193	Zimelidine	Brc1ccc(cc1)\C(=C\CN(C)C)\c1cccnc1	-2.00	test