

NN	Compound	Smiles	Class
1	5-Hydroxymethyl Tolterodine	<chem>Oc1ccc(cc1[C@@H](c1ccccc1)CCN(C(C)C)C(C)C)CO</chem>	1
2	Acebutolol	<chem>O=C(Nc1ccc(OCC(O)CNC(C)C)c(c1)C(=O)C)CCC</chem>	1
3	Alprazolam	<chem>Cc1nnc2n1c1ccc(cc1C(=NC2)c1ccccc1)Cl</chem>	2
4	Alprenolol	<chem>CC(C)NCC(COc1ccccc1CC=C)O</chem>	2
5	Amisulpride	<chem>CCN1CCCC1CNC(=O)c1cc(c(cc1OC)N)S(=O)(=O)CC</chem>	1
6	Amitriptyline	<chem>c1cc2c(/C(=C\CCN(C)C)c3c(cccc3)CC2)cc1</chem>	2
7	Apomorphine	<chem>CN1CCc2cccc3c2[C@H]1Cc1c3c(c(cc1)O)O</chem>	1
8	Aprepitant	<chem>C[C@H](c1cc(cc(c1)C(F)(F)F)C(F)(F)F)O[C@@H]1[C@@H](N(CCO1)Cc1[nH]c(=O)[nH]n1)c1ccc(cc1)F</chem>	1
9	Atomoxetine	<chem>Cc1ccccc1O[C@H](CCNC)c1ccccc1</chem>	1
10	Biperiden	<chem>c1ccc(cc1)C(CCN1CCCC1)(C1CC2CC1C=C2)O</chem>	2
11	Bromazepam	<chem>c1ccnc(c1)C1=NCC(=O)Nc2c1cc(cc2)Br</chem>	2
12	Cabergoline	<chem>CCNC(=O)N(CCCN(C)C)C(=O)[C@@H]1C[C@@H]2c3cccc4c3c(c[nH]4)C[C@H]2N(C1)CC=C</chem>	1
13	Ciprofloxacin	<chem>c1c2c(cc(c1F)N1CCNCC1)n(cc(c2=O)C(=O)O)C1CC1</chem>	2
14	Clemastine	<chem>Clc1ccc(cc1)[C@](OCC[C@@H]1N(C)CCC1)(c1ccccc1)C</chem>	2
15	Clomipramine	<chem>CN(C)CCCN1c2ccccc2CCc2c1cc(cc2)Cl</chem>	1
16	Clonazepam	<chem>c1ccc(c(c1)C1=NCC(=O)Nc2c1cc(cc2)N(=O)=O)Cl</chem>	2

17	Clonidine	<chem>c1cc(c(c1)Cl)NC1=NCCN1)Cl</chem>	2
18	Clozapine	<chem>CN1CCN(CC1)C1=Nc2cc(ccc2Nc2c1cc</chem> <chem>cc2)Cl</chem>	1
19	Coumarinic Acid based cyclic DADLE	<chem>CC(C)CC1NC(=O)[C@H](Cc2ccccc2)N</chem> <chem>C(=O)CNC(=O)[C@@H](C)NC(=O)[C@</chem> <chem>H](Cc2ccc(O)cc2)NC(=O)C=Cc2c(OC1</chem> <chem>=O)cccc2</chem>	1
20	Darifenacin	<chem>O=C(N)C(c1ccccc1)(c1ccccc1)[C@H]1</chem> <chem>CN(CC1)CCc1cc2c(OCC2)cc1</chem>	1
21	Desloratadine	<chem>c1cc2c(nc1)/C=C1/CCNCC1)c1ccc(cc</chem> <chem>1CC2)Cl</chem>	1
22	Diazepam	<chem>CN1c2ccc(cc2C(=NCC1=O)c1ccccc1)C</chem> <chem>I</chem>	2
23	Donepezil	<chem>COc1cc2c(cc1OC)C(=O)C(C2)CC1CCN(</chem> <chem>CC1)Cc1ccccc1</chem>	2
24	Doxepin	<chem>CN(C)CC/C=C1\c2ccccc2COc2c1cccc2</chem>	2
25	Duloxetine	<chem>O(c1cccc2c1cccc2)[C@H](c1sccc1)CC</chem> <chem>NC</chem>	2
26	Enoxacin	<chem>CCn1cc(c(=O)c2c1nc(c(c2)F)N1CCNC</chem> <chem>C1)C(=O)O</chem>	2
27	Escitalopram	<chem>CN(C)CCC[C@@]1(c2ccc(cc2CO1)C#</chem> <chem>N)c1ccc(cc1)F</chem>	1
28	Famciclovir	<chem>CC(=O)OCC(CCN1cnc2c1nc(nc2)N)CO</chem> <chem>C(=O)C</chem>	1
29	Galantamine	<chem>CN1CC[C@@]23C=C[C@@H](C[C@</chem> <chem>@H]2Oc2c3c(ccc2OC)C1)O</chem>	2
30	Hydroxyzine	<chem>Clc1ccc(cc1)C(c1ccccc1)N1CCN(CC1)</chem> <chem>CCOCCO</chem>	2
31	Imipramine	<chem>CN(C)CCCN1c2ccccc2CCc2c1cccc2</chem>	2
32	Ketamine	<chem>CNC1(CCCCC1=O)c1ccccc1Cl</chem>	2
33	Labetalol	<chem>O=C(c1cc(ccc1O)C(O)CNC(C)CCc1ccc</chem> <chem>cc1)N</chem>	1

34	Lopinavir	<chem>Cc1cccc(c1OCC(=O)N[C@@H](Cc1ccc cc1)[C@H](C[C@H](Cc1ccccc1)NC(=O )[C@H](C(C)C)N1CCCNC1=O)O)C</chem>	1
35	Lorazepam	<chem>c1ccc(c(c1)C1=NC(C(=O)Nc2c1cc(cc2) Cl)O)Cl</chem>	2
36	Lovastatin acid	<chem>O=C(O)C[C@H](O)C[C@H](O)CC[C@ H]1[C@H](C=CC2=C[C@@H](C[C@H] (OC(=O)[C@@H](C)CC)[C@H]12)C)C</chem>	1
37	Maprotiline	<chem>CNCCCC12CCC(c3c1cccc3)c1c2cccc1</chem>	2
38	Meprobamate	<chem>CCCC(C)(COC(=O)N)COC(=O)N</chem>	2
39	Methylprednisolone	<chem>C[C@H]1C[C@H]2[C@@H]3CC[C@@ ]([C@]3(C[C@@H]([C@@H]2[C@@] 2(C1=CC(=O)C=C2)C)O)C)(C(=O)CO)O</chem>	1
40	Metoclopramide	<chem>CCN(CC)CCNC(=O)c1cc(c(cc1OC)N)Cl</chem>	2
41	Metoprolol	<chem>CC(C)NCC(COc1ccc(cc1)CCOC)O</chem>	2
42	Mexilitene	<chem>O(c1c(cccc1C)C)CC(N)C</chem>	2
43	Mirtazapine	<chem>CN1CCN2c3c(cccn3)Cc3ccccc3C2C1</chem>	2
44	Nalmefene	<chem>Oc1c2O[C@H]3C(=C)CC[C@@]4(O)[C @@H]5N(CC[C@]34c2c(cc1)C5)CC1C C1</chem>	2
45	Nimodipine	<chem>CC1=C(C(C(=C(N1)C)C(=O)OC(C)C)c1c ccc(c1)N(=O)=O)C(=O)OCCOC</chem>	2
46	Nitrazepam	<chem>c1ccc(cc1)C1=NCC(=O)Nc2c1cc(cc2)N (=O)=O</chem>	2
47	Nordazepam	<chem>c1ccc(cc1)C1=NCC(=O)Nc2c1cc(cc2)C  </chem>	2
48	Olanzapine	<chem>Cc1cc2c(s1)Nc1ccccc1N=C2N1CCN(C C1)C</chem>	1

49	Oxcarbazepine	<chem>c1ccc2c(c1)CC(=O)c1ccccc1N2C(=O)N</chem>	2
50	Oxprenolol	<chem>CC(C)NCC(COc1ccccc1OCC=C)O</chem>	2
51	Oxybutynin	<chem>O=C(OCC#CCN(CC)CC)C(O)(c1ccccc1)C1CCCC1</chem>	2
52	Oxycodone	<chem>CN1CC[C@]23c4c5ccc(c4O[C@H]2C(=O)CC[C@]3([C@H]1C5)O)OC</chem>	2
53	Oxymethyl Modified Coumarinic Acid based cyclic DADLE	<chem>CC(C)CC1NC(=O)[C@H](Cc2ccccc2)NC(=O)CNC(=O)[C@@H](C)NC(=O)[C@H](Cc2ccc(O)cc2)NC(=O)C=Cc2c(OCOC1=O)cccc2</chem>	1
54	Paliperidone	<chem>Cc1c(c(=O)n2CCCC(c2n1)O)CCN1CCC(CC1)c1noc2c1ccc(c2)F</chem>	1
55	Practolol	<chem>O=C(Nc1ccc(OCC(O)CNC(C)C)cc1)C</chem>	2
56	Pravastatin acid	<chem>O=C(O)C[C@H](O)C[C@H](O)CC[C@H]1[C@H](C=CC2=C[C@@H](O)C[C@H](OC(=O)[C@@H](C)CC)[C@H]12)C</chem>	2
57	Prednisolone	<chem>C[C@]12C[C@@H]([C@H]3[C@H]([C@@H]1CC[C@@]2(C(=O)CO)O)CCC1=CC(=O)C=C[C@]31C)O</chem>	1
58	Prednisone	<chem>C[C@]12CC(=O)[C@H]3[C@H]([C@@H]1CC[C@@]2(C(=O)CO)O)CCC1=CC(=O)C=C[C@]31C</chem>	1
59	Promazine	<chem>CN(C)CCCN1c2ccccc2Sc2c1cccc2</chem>	2
60	Promethazine	<chem>CC(CN1c2ccccc2Sc2c1cccc2)N(C)C</chem>	2
61	Pyridostigmine	<chem>C[n+]1cccc(c1)OC(=O)N(C)C</chem>	2
62	Quetiapine	<chem>N1=C(c2c(Sc3c1cccc3)cccc2)N1CCN(CCOCCO)CC1</chem>	2
63	Ramelteon	<chem>CCC(=O)NCC[C@@H]1CCc2c1c1c(cc2)OCC1</chem>	2
64	Reboxetine	<chem>CCOc1ccccc1O[C@H](c1ccccc1)[C@H]1CNCCO1</chem>	2

65	Rhodamine 123	<chem>COC(=O)c1cccc1c1c2ccc(=[NH2+])cc2oc2c1ccc(c2)N</chem>	1
66	Riluzole	<chem>c1cc2c(cc1OC(F)(F)F)sc(n2)N</chem>	2
67	Rivastigmine	<chem>CCN(C)C(=O)Oc1cccc(c1)[C@H](C)N(C)C</chem>	2
68	Ropinirole	<chem>CCCN(CCC)CCc1cccc2c1CC(=O)N2</chem>	2
69	Ropivacaine	<chem>CCCN1CCCC[C@H]1C(=O)Nc1c(cccc1)C</chem>	2
70	Simvastatin acid	<chem>O=C(O)C[C@H](O)C[C@H](O)CC[C@H]1[C@H](C=CC2=C[C@@H](C[C@H](OC(=O)C(C)(C)CC)[C@H]12)C)C</chem>	1
71	Solifenacin	<chem>O=C(O[C@@H]1C2CCN(CC2)C1)N1[C@@H](c2cccc2)c2cccc2CC1</chem>	2
72	Sulpiride	<chem>CCN1CCCC1CNC(=O)c1cc(ccc1OC)S(=O)(=O)N</chem>	2
73	Talinolol	<chem>CC(C)(C)NCC(COc1ccc(cc1)NC(=O)NC1CCCC1)O</chem>	1
74	Thiopental	<chem>CCCC(C)C1(C(=O)NC(=S)NC1=O)CC</chem>	2
75	Tiagabine	<chem>O=C(O)[C@H]1CN(CCC1)CC/C=C/c1sccc1C)c1sccc1C</chem>	2
76	Tolterodine	<chem>Cc1ccc(c(c1)[C@H](CCN(C(C)C)C(C)C)c1cccc1)O</chem>	2
77	Topiramate	<chem>CC1(O[C@@H]2CO[C@@]3([C@H](C@@H]2O1)OC(O3)(C)C)COS(=O)(=O)N)C</chem>	2
78	Trimipramine	<chem>c1cc2c(cc1)CCc1c(cccc1)N2CC(C)N(C)C</chem>	2
79	Tropisetron	<chem>CN1[C@H]2CC[C@@H]1C[C@@H](C2)OC(=O)c1c[nH]c2c1cccc2</chem>	2
80	Trospium	<chem>O=C(OC1CC2[N+]3(C(C1)CC2)CCCC3)C(O)(c1cccc1)c1cccc1</chem>	1

81	Varenicline	<chem>n1c2cc3c(cc2ncc1)[C@@H]1CNC[C@H]3C1</chem>	2
82	Warfarin	<chem>CC(=O)CC(c1ccccc1)c1c(c2ccccc2oc1=O)O</chem>	2
83	Ximelagatran	<chem>O=C(NCc1ccc(/C(=N/O)N)cc1)[C@H]1N(C(=O)[C@H](NCC(=O)OCC)C2CCC(CC2)CC1</chem>	1
84	Zaleplon	<chem>CCN(c1cccc(c1)c1ccnc2n1ncc2C#N)C(=O)C</chem>	2
85	Ziprasidone	<chem>O=C1Nc2c(cc(c(Cl)c2)CCN2CCN(c3nsc4cccc34)CC2)C1</chem>	1
86	Zolmitriptan	<chem>CN(C)CCc1c[nH]c2c1cc(cc2)C[C@H]1COC(=O)N1</chem>	1
87	Zonisamide	<chem>c1ccc2c(c1)c(no2)CS(=O)(=O)N</chem>	2
88	Bromocriptine	<chem>CC(C)C[C@H]1C(=O)N2CCC[C@H]2[C@@]2(N1C(=O)[C@](O2)(C(C)C)NC(=O)[C@H]1CN([C@@H]2Cc3c4c(cccc4[nH]c3Br)C2=C1)CO</chem>	1
89	Methysergide	<chem>O=C(N[C@@H](CC)CO)[C@@H]1C=C2c3cccc4c3c(cn4C)C[C@H]2N(C1)C</chem>	1
90	Morphine	<chem>CN1CC[C@]23c4c5ccc(c4O[C@H]2[C@@H](C=C[C@H]3[C@H]1C5)O)O</chem>	2
91	Nalbuphine	<chem>O[C@@H]1[C@@H]2Oc3c4c(ccc3O)C[C@H]3N(CC[C@@]24[C@@]3(O)C1)CC1CCC1</chem>	2
92	Paroxetine	<chem>c1cc(ccc1[C@@H]1CCNC[C@H]1COc1ccc2c(c1)OCO2)F</chem>	1
93	Cyclobenzaprine	<chem>CN(C)CC/C=C1\c2ccccc2C=Cc2c1cccc2</chem>	2

94	Doxorubicin	<chem>C[C@H]1[C@H]([C@H](C[C@@H](O1)O[C@H]1C[C@@](Cc2c1c(c1c(c2O)C(=O)c2cccc(c2C1=O)OC)O)(C(=O)CO)N)O</chem>	1
95	Fluvoxamine	<chem>COCCCC/C(=N\OCCN)c1ccc(cc1)C(F)F</chem>	2
96	Loratadine	<chem>CCOC(=O)N1CC/C(=C2/c3ccc(cc3CCc3c2nccc3)Cl)CC1</chem>	2
97	Neostigmine	<chem>CN(C)C(=O)Oc1cccc(c1)[N+](C)(C)C</chem>	1
98	Ranitidine	<chem>[O-][N+](=O)/C=C(/NC)NCCSCc1oc(cc1)CN(C)C</chem>	1
99	Risperidone	<chem>Cc1c(c(=O)n2c(n1)CCCC2)CCN1CCC(C1)c1c2ccc(cc2on1)F</chem>	2
100	Trimethoprim	<chem>COc1cc(cc(c1OC)OC)Cc1cnc(nc1N)N</chem>	1
101	Fluoxetine	<chem>CNCCC(c1ccccc1)Oc1ccc(cc1)C(F)(F)F</chem>	2
102	Chlorpromazine	<chem>CN(C)CCCN1c2ccccc2Sc2c1cc(cc2)Cl</chem>	1
103	Verapamil	<chem>N#CC(c1cc(OC)c(OC)cc1)(CCCN(CCC1ccc(OC)c(OC)c1)C)C(C)C</chem>	1
104	Acyloxyalcoxy based cyclic DADLE	<chem>CC(C)CC1NC(=O)[C@H](Cc2ccccc2)NC(=O)CNC(=O)[C@@H](C)NC(=O)[C@H](Cc2ccc(O)cc2)NC(=O)OCOC1=O</chem>	1
105	Antipyrine	<chem>O=c1cc(n(n1c1ccccc1)C)C</chem>	2
106	Astemizole	<chem>COc1ccc(cc1)CCN1CCC(CC1)Nc1nc2ccccc2n1Cc1ccc(cc1)F</chem>	1
107	Atenolol	<chem>CC(C)NCC(COc1ccc(cc1)CC(=O)N)O</chem>	2
108	Caffeine	<chem>Cn1cnc2c1c(=O)n(c(=O)n2C)C</chem>	2
109	Cetirizine	<chem>c1ccc(cc1)C(c1ccc(cc1)Cl)N1CCN(CC1)CCOCC(=O)O</chem>	1

110	Chloroquine	<chem>CCN(CC)CCCC(C)Nc1ccnc2c1ccc(c2)Cl</chem>	1
111	Citalopram	<chem>CN(C)CCCC1(c2ccc(cc2CO1)C#N)c1cc</chem> <chem>c(cc1)F</chem>	2
112	Clarithromycin	<chem>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]1C[C@@]([C@H]([C@@H](O1)C)O)(C)OC)C)O[C@H]1[C@@H]([C@H](C[C@H](O1)C)N(C)C)O)(C)OC)C)O)(C)O</chem>	1
113	Daunorubicin	<chem>C[C@H]1[C@H]([C@H](C[C@@H](O1)O[C@H]1C[C@@](Cc2c1c(c1c(c2O)C(=O)c2ccc(c2C1=O)OC)O)(C(=O)C)O)N)O</chem>	1
114	Desipramine	<chem>CNCCCN1c2cccc2CCc2c1cccc2</chem>	2
115	Dexamethasone	<chem>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</chem>	1
116	Diphenhydramine	<chem>CN(C)CCOC(c1ccccc1)c1ccccc1</chem>	2
117	Dipyridamole	<chem>C1CCN(CC1)c1c2c(c(nc(n2)N(CCO)CCO)N2CCCC2)nc(n1)N(CCO)CCO</chem>	1
118	Domperidone	<chem>c1ccc2c(c1)[nH]c(=O)n2CCCN1CCC(C1)n1c2ccc(cc2[nH]c1=O)Cl</chem>	1
119	Ethosuximide	<chem>CCC1(CC(=O)NC1=O)C</chem>	2
120	Flumazenil	<chem>CCOC(=O)c1c2n(cn1)c1ccc(cc1C(=O)N(C2)C)F</chem>	2
121	Hydrocodone	<chem>CN1CC[C@]23c4c5ccc(c4O[C@H]2C(=O)CC[C@H]3[C@H]1C5)OC</chem>	2
122	Indomethacin	<chem>Cc1c(c2cc(ccc2n1C(=O)c1ccc(cc1)Cl)OC)CC(=O)O</chem>	2



123	Itraconazole	<chem>CCC(C)n1c(=O)n(cn1)c1ccc(cc1)N1CCN(CC1)c1ccc(cc1)OCC1COC(O1)(Cn1cncn1)c1ccc(cc1)Cl</chem>	2
124	Ketoconazole	<chem>CC(=O)N1CCN(CC1)c1ccc(cc1)OC[C@H]1CO[C@](O1)(Cn1ccnc1)c1ccc(cc1)Cl</chem>	2
125	Lamotrigine	<chem>c1cc(c(c1)Cl)Cl)c1c(nc(nn1)N)N</chem>	2
126	Methotrexate	<chem>CN(Cc1cnc2c(n1)c(nc(n2)N)N)c1ccc(c1)C(=O)N[C@@H](CCC(=O)O)C(=O)O</chem>	2
127	Methylphenidate	<chem>COC(=O)C(c1ccccc1)C1CCCN1</chem>	2
128	Mitoxantrone	<chem>c1cc(c2c(c1NCCNCCO)C(=O)c1c(ccc(c1C2=O)O)O)NCCNCCO</chem>	1
129	Naloxone	<chem>C=CCN1CC[C@]23c4c5ccc(c4O[C@H]2C(=O)CC[C@]3([C@H]1C5)O)O</chem>	2
130	Nicardipine	<chem>CC1=C(C(C(=C(N1)C)C(=O)OCCN(C)Cc1ccccc1)c1ccc(c1)N(=O)=O)C(=O)OC</chem>	2
131	Nifedipine	<chem>CC1=C(C(C(=C(N1)C)C(=O)OC)c1ccccc1N(=O)=O)C(=O)OC</chem>	2
132	Nitrendipine	<chem>CCOC(=O)C1=C(NC(=C(C1c1cccc(c1)N(=O)=O)C(=O)OC)C)C</chem>	2
133	Nortriptyline	<chem>CNCC/C=C1\c2ccccc2CCc2c1cccc2</chem>	2
134	Reserpine	<chem>COc1ccc2c(c1)[nH]c1c2CCN2[C@@H]1C[C@H]1[C@@H](C2)C[C@H]([C@@H]([C@H]1C(=O)OC)OC)OC(=O)c1cc(c(c1)OC)OC)OC</chem>	1
135	Rosuvastatin	<chem>O=S(=O)(N(c1nc(c(c1)C(C)C)/C=C/[C@@H](O)C[C@@H](O)CC(=O)O)c1cc(F)cc1)C</chem>	2
136	Scopolamine	<chem>CN1[C@H]2C[C@@H](C[C@@H]1[C@@H]1[C@H]2O1)OC(=O)[C@H](CO)c1ccccc1</chem>	2

137	Selegiline	<chem>C#CCN([C@@H](Cc1ccccc1)C)C</chem>	2
138	Sertraline	<chem>Clc1ccc(cc1Cl)[C@H]1c2c(cccc2)[C@@H](NC)CC1</chem>	1
139	Sulfasalazine	<chem>c1ccnc(c1)NS(=O)(=O)c1ccc(cc1)/N=N/c1ccc(c(c1)C(=O)O)O</chem>	2
140	Tacrine	<chem>c1ccc2c(c1)c(c1c(n2)CCCC1)N</chem>	2
141	Testosterone	<chem>C[C@]12CC[C@H]3[C@H]([C@@H]1CC[C@@H]2O)CCC1=CC(=O)CC[C@]31C</chem>	2
142	Trazodone	<chem>C1=CC=N2C(=C1)NN(C2=O)CCCN1CCN(CC1)c1ccc(c1)Cl</chem>	2
143	Venlafaxine	<chem>OC1(C(c2ccc(OC)cc2)CN(C)C)CCCCC1</chem>	2
144	Vincristine	<chem>CC[C@@]1(C[C@@H]2C[C@@](c3cc4cccc4[nH]3)CCN(C2)C1)(c1cc2c(cc1OC)N([C@@H]1[C@@]32CCN2[C@H]3[C@@](C=CC2)([C@H]([C@@]1C(=O)OC)O)OC(=O)C)CC)C(=O)C(=O)OC)O</chem>	1
145	Vinorelbine	<chem>COC(=O)[C@H]1c2[nH]c3cccc3c2CN2CC(=C[C@H](C2)[C@@H]1c1cc2c(cc1OC)N(C)C1[C@@]32CCN2CC=CC(CC)([C@@H](OC(=O)C)[C@]1(O)C(=O)OC)[C@@H]32)CC</chem>	1
146	Amantadine	<chem>C1C2CC3CC1CC(C2)(C3)N</chem>	2
147	Carbamazepine	<chem>c1ccc2c(c1)C=Cc1ccccc1N2C(=O)N</chem>	2
148	Colchicine	<chem>CC(=O)N[C@H]1CCc2cc(c(c2c2c1cc(=O)c(cc2)OC)OC)OC)OC</chem>	1

149	Erythromycin	<chem>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]1C[C@@]([C@H]([C@@H](O1)C)O)(C)OC)C)O[C@H]1[C@@H]([C@H](C[C@H](O1)C)N(C)C)O)(C)O)C)O)C)O</chem>	1
150	Etoposide	<chem>C[C@@H]1OC[C@@H]2[C@@H](O1)[C@@H]([C@H]([C@@H](O2)O[C@@H]1c2cc3c(cc2[C@H]([C@@H]2[C@@H]1COC2=O)c1cc(c(c1)OC)O)C)OCO3)O)O</chem>	1
151	Haloperidol	<chem>c1cc(ccc1C(=O)CCCN1CCC(CC1)(c1cc(c(cc1)Cl)O)F</chem>	2
152	Hoechst 33342	<chem>CCOc1ccc(cc1)c1nc2c([nH]1)cc(cc2)c1nc2c([nH]1)cc(cc2)N1CCN(CC1)C</chem>	1
153	Indinavir	<chem>CC(C)(C)NC(=O)[C@@H]1CN(CCN1C[C@H](C[C@@H](Cc1ccccc1)C(=O)N[C@H]1c2ccccc2C[C@H]1O)O)Cc1ccnc1</chem>	1
154	Mannitol	<chem>C([C@H]([C@H]([C@@H]([C@@H](C)O)O)O)O)O</chem>	2
155	Naltrexone	<chem>c1cc(c2c3c1C[C@@H]1[C@]4([C@]3(CCN1CC1CC1)[C@@H](O2)C(=O)CC4)O)O</chem>	2
156	Nelfinavir	<chem>Cc1c(cccc1O)C(=O)N[C@@H](CSc1ccccc1)[C@@H](CN1C[C@H]2CCCC[C@H]2C[C@H]1C(=O)NC(C)(C)C)O</chem>	1

157	Paclitaxel	<chem>CC1=C2[C@H](C(=O)[C@@]3([C@H](C[C@@H]4[C@]([C@H]3[C@@H]([C@@](C2(C)C)(C[C@@H]1OC(=O)[C@@H]([C@H](c1ccccc1)NC(=O)c1ccccc1)O)O)OC(=O)c1ccccc1)(CO4)OC(=O)C)O)C)OC(=O)C</chem>	1
158	Sumatriptan	<chem>O=S(=O)(NC)Cc1cc2c(cc1)[nH]cc2CCN(C)C</chem>	2
159	Terfenadine	<chem>CC(C)(C)c1ccc(cc1)C(CCCN1CCC(CC1)C(c1ccccc1)(c1ccccc1)O)O</chem>	1
160	Zolpidem	<chem>O=C(N(C)C)Cc1c(nc2ccc(cn12)C)c1ccc(cc1)C</chem>	2
161	Amprenavir	<chem>CC(C)CN(C[C@H]([C@H](Cc1ccccc1)NC(=O)O[C@H]1CCOC1)O)S(=O)(=O)c1ccc(cc1)N</chem>	1
162	Buspirone	<chem>c1cnc(nc1)N1CCN(CC1)CCCCN1C(=O)CC2(CCCC2)CC1=O</chem>	2
163	Chlorpheniramine	<chem>CN(C)CCC(c1ccc(cc1)Cl)c1cccn1</chem>	2
164	Cimetidine	<chem>Cc1c([nH]cn1)CSCC/N=C(\NC)NC#N</chem>	1
165	Digoxin	<chem>C[C@@H]1[C@H]([C@H](C[C@@H](O1)O[C@@H]1[C@H](O[C@@H](C[C@@H]1O)O[C@@H]1[C@H](O[C@@H](C[C@@H]1O)O[C@@H]1CC[C@]2([C@@H](C1)CC[C@@H]1[C@@H]2C[C@@H]([C@]2([C@@]1(CC[C@@H]2C1=CC(=O)OC1)O)C)O)C)C)O)O</chem>	1
166	Diltiazem	<chem>CC(=O)O[C@@H]1[C@@H](Sc2ccccc2N(C1=O)CCN(C)C)c1ccc(cc1)OC</chem>	2
167	Eletriptan	<chem>O=S(=O)(c1ccccc1)CCc1ccc2c(c(c[nH]2)C[C@@H]2N(C)CCC2)c1</chem>	1
168	Lidocaine	<chem>CCN(CC)CC(=O)Nc1c(cccc1)C</chem>	2

169	Loperamide	<chem>CCN1CCC(CC1)(c1ccc(cc1)Cl)O)(c1ccccc1)c1ccccc1</chem>	1
170	Midazolam	<chem>O=c1cc(n(n1c1ccccc1)C)C</chem>	2
171	Prazosin	<chem>COc1cc2c(cc1OC)nc(nc2N)N1CCN(CC1)C(=O)c1ccco1</chem>	1
172	Propranolol	<chem>CC(C)NCC(COc1cccc2c1cccc2)O</chem>	2
173	Ritonavir	<chem>CC(C)c1nc(cs1)CN(C)C(=O)N[C@@H](C(C)C)C(=O)N[C@@H](Cc1ccccc1)C[C@@H]([C@H](Cc1ccccc1)NC(=O)OCc1cnsc1)O</chem>	1
174	Saquinavir	<chem>O=C(N)C[C@H](NC(=O)c1nc2c(cc1)ccc2)C(=O)N[C@@H](Cc1ccccc1)[C@H](O)CN1[C@H](C(=O)NC(C)(C)C[C@@H]2CCCC[C@@H]2C1</chem>	1
175	Velban	<chem>CC[C@@]1(C[C@@H]2C[C@@])(c3cc4ccccc4[nH]3)CCN(C2)C1)(c1cc2c(cc1OC)N([C@@H]1[C@@]32CCN2[C@H]3[C@@](C=CC2)([C@H]([C@@]1(C(=O)OC)O)OC(=O)C)CC)C(=O)OC)O</chem>	1
176	Phenytoin	<chem>O=C1NC(=O)NC1(c1ccccc1)c1ccccc1</chem>	2
177	Quinidine	<chem>O(c1cc2c(nccc2[C@H](O)[C@@H]2N3CC[C@@H](C2)[C@@H](C=C)C3)cc1)C</chem>	1
178	QUININE	<chem>c1c(c(c2c(ccc(c2)OC)n1)CO)C1CC2C(C=C)C[NH+]1CC2</chem>	2
179	PROMAZINE	<chem>c1cccc2c1Sc1c(cccc1)N2CCC[NH+](C)C</chem>	2
180	LANSOPRAZOLE	<chem>c1cccc2c1nc(S(=O)Cc1c(C)c(ccn1)OC)C(F)(F)F)[nH]2</chem>	2
181	ESTRADIOL	<chem>c1c2c(C3CCC4(C(C3CC2)CCC4O)C)ccc1O</chem>	2

182	IMIPRAMINE	<chem>c12c(CCc3c(cccc3)N2CCC[NH+](C)C)c</chem>	2
		<chem>ccc1</chem>	
183	HYDROCORTISONE	<chem>C1=C2C(C3C(CC4(C(CCC4C3CC2)(C(=O)CO)O)C)O)(CCC1=O)C</chem>	2
184	NICARDIPINE	<chem>C1(=C(C)NC(=C(C1c1cc(ccc1)[N+](=O)[O-]))C(=O)OCC[NH+]Cc1cccc1)C(=O)OC</chem>	2
185	PIROXICAM	<chem>c1cccc2c1C(=C(C(=O)Nc1ccccn1)N(C)S2(=O)=O)O</chem>	2
186	OMEPRAZOLE	<chem>c12ccc(cc1nc(S(=O)Cc1c(C)c(c(C)cn1)OC)[nH]2)OC</chem>	2
187	LOPERAMIDE	<chem>c1c(ccc(c1)C1(CC[NH+](CC1)CCC(c1ccc1)(c1cccc1)C(=O)N(C)C)O)Cl</chem>	2
188	LOMEFLOXACIN	<chem>CC1CN(c2c(cc3c(c2F)n(CC)cc(c3=O)C(=O)O)F)CC[NH2+]1</chem>	2
189	PROGESTERONE	<chem>C1=C2C(CCC1=O)(C1C(CC2)C2C(CC1)C(CC2)C(=O)C)C</chem>	2
190	MEBENDAZOLE	<chem>c1cc(cc2c1[nH]c(NC(=O)OC)n2)C(=O)c1cccc1</chem>	2
191	TAMOXIFEN	<chem>C(COc1ccc(cc1)/C(=C(\c1cccc1)CC)c1cccc1)[NH+](C)C</chem>	2
192	VERAPAMIL	<chem>c1(c(ccc(c1)C(CCC[NH+](CCc1ccc(c(c1)OC)OC)C)(C(C)C)C#N)OC)OC</chem>	2
193	CHLORPROMAZINE	<chem>c1cccc2c1Sc1c(cc(cc1)Cl)N2CCC[NH+](C)C</chem>	2
194	CLOZAPINE	<chem>c12c(cc(cc1)Cl)N=C(c1c(cccc1)N2)N1CC[NH+](C)CC1</chem>	2
195	CLONIDINE	<chem>c1cc(c(c(c1)Cl)/N=C1\NCCN1)Cl</chem>	2
196	ASTEMIZOLE	<chem>c12cccc1nc(NC1CC[NH+](CC1)CCc1c(cc(cc1)OC)n2Cc1ccc(cc1)F</chem>	2
197	CHLOROQUINE	<chem>c1cc(cc2c1c(ccn2)NC(CCC[NH+](CC)C)C)Cl</chem>	2

198	TESTOSTERONE	<chem>C1=C2C(C3CCC4(C(C3CC2)CCC4O)C)(CCC1=O)C</chem>	2
199	DILTIAZEM	<chem>c12c(cccc1)SC(C(C(=O)N2CC[NH+])(C)C)OC(=O)C)c1ccc(cc1)OC</chem>	2
200	DESIPRAMINE	<chem>C[NH2+]CCCN1c2c(CCc3c1cccc3)cccc2</chem>	2
201	CORTICOSTERONE	<chem>C1=C2C(C3C(CC4(C(C3CC2)CCC4C(=O)CO)C)O)(CCC1=O)C</chem>	2
202	VINBLASTINE	<chem>c1c(c(cc2c1N(C1C32C2C(C(C1(C(=O)OC)O)OC(=O)C)(C=CCN2CC3)CC)C)C1(C(=O)OC)CC2C[NH+])(CCc3c1[nH]c1cccc31)CC(CC)(C2)O)OC</chem>	1
203	TENOXICAM	<chem>C1(=C(C(=O)Nc2cccn2)N(C)S(=O)(=O)c2c1scc2)O</chem>	1
204	TERFENADINE	<chem>C1C(CC[NH+])(C1)CCCC(c1ccc(cc1)C(C)(C)C)O)C(c1cccc1)(c1cccc1)O</chem>	1
205	RANITIDINE	<chem>C[NH+](C)Cc1ccc(CSCCN/C(=C\[N+](=O)[O-])NC)o1</chem>	1
206	PREDNISOLONE	<chem>C1=C2C(C3C(CC4(C(C3CC2)CCC4(C(=O)CO)O)C)O)(C=CC1=O)C</chem>	1
207	DOXORUBICIN	<chem>C1(CC(Cc2c1c(c1c(c2O)C(=O)c2c(C1=O)c(ccc2)OC)O)(C(=O)CO)O)OC1CC(C(C)O1)O)N</chem>	1
208	ENOXACIN	<chem>CCn1c2c(cc(c(n2)N2CC[NH2+]CC2)F)c(=O)c(C(=O)[O-])c1</chem>	1
209	ERYTHROMYCIN A	<chem>C1(C(=O)OC(C(C(C(=O)C(CC(C(C(C1OC1CC(C)(C(C(C)O1)O)OC)C)OC1C(C(C(C)O1)[NH+](C)C)O)(C)O)C)O)(C)O)CC)C</chem>	1
210	DIGOXIN	<chem>CC1C(C(CC(OC2C(C)OC(CC2O)OC2C(C(OC2C)OC2CC3C(C4C(C5(C(C)(C(CC5)C5=CC(=O)OC5)C(C4)O)O)CC3)(C)CC2)O)O1)O)O</chem>	1

