Supporting Information

Can easy chemistry produce complex, diverse and novel molecules?

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Content

Table S1. Listing the coupling reactions making up the random set of 10k compounds according to https://www.nextmovesoftware.com/namerxn.html

Count	Class Number	Class Name	Class Sub Name
1	1.1.3	N-substitution with alkyl-X	Iodo N-methylation
2	1.1.4	N-substitution with alkyl-X	N-methylation
3	1.1.5	N-substitution with alkyl-X	Bromo Menshutkin reaction
4	1.1.6	N-substitution with alkyl-X	Chloro Menshutkin reaction
5	1.1.7	N-substitution with alkyl-X	Iodo Menshutkin reaction
6	1.2.1	Reductive amination	Aldehyde reductive amination
7	1.2.10	Reductive amination	Formaldehyde reductive amination
8	1.2.12	Reductive amination	Dimethyl acetal reductive amination
9	1.2.13	Reductive amination	Aziridine + amine coupling
10	1.2.14	Reductive amination	Epoxide + amine coupling
11	1.2.2	Reductive amination	Aldehyde reductive imination
12	1.2.3	Reductive amination	Alkylimino-de-oxo-bisubsitution
13	1.2.4	Reductive amination	Eschweiler-Clarke methylation
14	1.2.5	Reductive amination	Ketone reductive amination
15	1.2.6	Reductive amination	Ketone reductive imination
16	1.2.9	Reductive amination	Alcohol + amine condensation
17	1.3.1	N-arylation with Ar-X	Bromo Buchwald-Hartwig amination
18	1.3.10	N-arylation with Ar-X	Triflyloxy N-arylation
19	1.3.12	N-arylation with Ar-X	Mesyl N-arylation
20	1.3.2	N-arylation with Ar-X	Chloro Buchwald-Hartwig amination
21	1.3.5	N-arylation with Ar-X	Chan-Lam arylamine coupling
22	1.3.6	N-arylation with Ar-X	Bromo N-arylation
23	1.3.7	N-arylation with Ar-X	Chloro N-arylation
24	1.3.8	N-arylation with Ar-X	Fluoro N-arylation
25	1.3.9	N-arylation with Ar-X	Iodo N-arylation
26	1.6.12	Heteroaryl N-alkylation	Tosyloxy N-alkylation
27	1.6.2	Heteroaryl N-alkylation	Bromo N-alkylation
28	1.6.4	Heteroaryl N-alkylation	Chloro N-alkylation
29	1.6.8	Heteroaryl N-alkylation	Iodo N-alkylation
30	1.6.9	Heteroaryl N-alkylation	Mesyloxy N-alkylation
31	1.7.1	O-substitution	Chan-Lam ether coupling
32	1.7.11	O-substitution	SNAr ether synthesis
33	1.7.12	O-substitution	Alkene ether synthesis
34	1.7.13	O-substitution	Ether synthesis
35	1.7.17	O-substitution	Epoxide + alcohol coupling
36	1.7.18	O-substitution	Pinner reaction
37	1.7.3	O-substitution	Ethyl esterification
38	1.7.4	O-substitution	Hydroxy to methoxy
39	1.7.5	O-substitution	Hydroxy to triflyloxy
40	1.7.6	O-substitution	Methyl esterification
41	1.7.7	O-substitution	Mitsunobu aryl ether synthesis

42	1.7.8	O-substitution	Ullmann condensation
43	1.7.9	O-substitution	Williamson ether synthesis
44	1.8.4	S-substitution	Sulfinic acid + iodide reaction
45	1.8.5	S-substitution	Thioether synthesis
46	1.8.6	S-substitution	S-methylation
47	1.9.1	Other heteroatom alkylation/arylation	Michaelis-Arbuzov reaction
48	1.9.12	Other heteroatom alkylation/arylation	Phosphorus Menshutkin reaction
49	1.9.4	Other heteroatom alkylation/arylation	Bromo stannylation
50	1.9.8	Other heteroatom alkylation/arylation	Stannylation
51	2.2.1	N-sulfonylation	Sulfinamide Schotten-Baumann
52	2.2.3	N-sulfonylation	Sulfonamide Schotten-Baumann
53	2.3.1	N-acylation to urea	Isocyanate + amine urea coupling
54	2.3.2	N-acylation to urea	Isothiocyanate + amine thiourea coupling
55	2.3.4	N-acylation to urea	Amino to ureido
56	2.3.5	N-acylation to urea	Amino to thioureido
57	2.3.6	N-acylation to urea	Urea Curtius reaction
58	2.3.7	N-acylation to urea	CDI urea synthesis
59	2.4.1	Carbamate/carbonate formation	Carbamate Curtius reaction
60	2.4.2	Carbamate/carbonate formation	Isocyanate + alcohol reaction
61	2.5.2	Amidine formation	Imidic ester + amine reaction
62	2.5.4	Amidine formation	Thioimidic ester + amine reaction
63	2.5.5	Amidine formation	Nitrile + amine reaction
64	2.6.1	O-acylation to ester	Ester Schotten-Baumann
65	2.6.2	O-acylation to ester	Esterification
66	2.6.3	O-acylation to ester	Fischer-Speier esterification
67	2.6.6	O-acylation to ester	Hydroxy to imidazolecarbonyloxy
68	2.6.9	O-acylation to ester	Steglich esterification
69	2.7.2	O-sulfonylation	Sulfonic ester Schotten-Baumann
70	2.8.3	Other acylation	Phosphonamide Schotten-Baumann
71	2.8.5	Other acylation	S-Thioester synthesis
72	3.1.1	Suzuki coupling	Bromo Suzuki coupling
73	3.1.2	Suzuki coupling	Chloro Suzuki coupling
74	3.1.3	Suzuki coupling	Iodo Suzuki coupling
75	3.1.5	Suzuki coupling	Bromo Suzuki-type coupling
76	3.1.6	Suzuki coupling	Chloro Suzuki-type coupling
77	3.1.7	Suzuki coupling	Iodo Suzuki-type coupling
78	3.1.8	Suzuki coupling	Triflyloxy Suzuki-type coupling
79	3.10.1	Friedel-Crafts reaction	Friedel-Crafts acylation
80	3.11.1	Other C-C bond formation	Aldol addition
81	3.11.10	Other C-C bond formation	Strecker aldehyde reaction

82	3.11.11	Other C-C bond formation	Strecker ketone reaction
83	3.11.13	Other C-C bond formation	Ullmann-type biaryl coupling
84	3.11.14	Other C-C bond formation	Vilsmeier-Haack reaction
85	3.11.16	Other C-C bond formation	Wurtz-Fittig coupling
86	3.11.2	Other C-C bond formation	Aldol condensation
87	3.11.3	Other C-C bond formation	Diels-Alder cycloaddition
88	3.11.31	Other C-C bond formation	Henry reaction
89	3.11.34	Other C-C bond formation	Knoevenagel condensation
90	3.11.38	Other C-C bond formation	Alkyne + aldehyde reaction
91	3.11.46	Other C-C bond formation	Baylis-Hillman reaction
92	3.11.5	Other C-C bond formation	Horner-Wadsworth-Emmons reaction
93	3.11.52	Other C-C bond formation	Cyanoalkane alkylation
94	3.11.6	Other C-C bond formation	Mannich reaction
95	3.11.74	Other C-C bond formation	Olefin hydroalkylation
96	3.11.76	Other C-C bond formation	Michael-Henry reaction
97	3.2.1	Heck reaction	Bromo Heck reaction
98	3.2.5	Heck reaction	Bromo Heck-type reaction
99	3.2.6	Heck reaction	Chloro Heck-type reaction
100	3.2.7	Heck reaction	Iodo Heck-type reaction
101	3.3.2	Sonogashira reaction	Bromo Sonogashira coupling
102	3.3.3	Sonogashira reaction	Chloro Sonogashira coupling
103	3.3.4	Sonogashira reaction	Iodo Sonogashira coupling
104	3.3.5	Sonogashira reaction	Triflyloxy Sonogashira coupling
105	3.4.3	Stille reaction	Bromo Stille reaction
106	3.4.4	Stille reaction	Chloro Stille reaction
107	3.4.5	Stille reaction	Iodo Stille reaction
108	3.5.1	Other Pd-catalyzed reactions	Hiyama coupling
109	3.5.2	Other Pd-catalyzed reactions	Kumada coupling
110	3.5.3	Other Pd-catalyzed reactions	Negishi coupling
111	3.7.10	Grignard reaction	Bromo Grignard + nitrile ketone synthesis
112	3.7.2	Grignard reaction	Bromo Grignard reaction
113	3.7.3	Grignard reaction	Chloro Grignard reaction
114	3.8.1	Wittig olefination	Wittig olefination
115	3.9.12	Other organometallic C-C bond formation	Olefin metathesis
116	3.9.13	Other organometallic C-C bond formation	Weinreb ketone synthesis
117	3.9.14	Other organometallic C-C bond formation	Weinreb bromo coupling
118	3.9.17	Other organometallic C-C bond formation	Weinreb iodo coupling
119	3.9.2	Other organometallic C-C bond formation	Bromo ketone Barbier reaction
120	3.9.23	Other organometallic C-C bond formation	Simmons-Smith reaction

121	3.9.25	Other organometallic C-C bond formation	Bouveault aldehyde synthesis
122	3.9.26	Other organometallic C-C bond formation	Grignard Bouveault aldehyde synthesis
123	3.9.27	Other organometallic C-C bond formation	Lithium Bouveault aldehyde synthesis
124	3.9.41	Other organometallic C-C bond formation	Decarboxylative coupling
125	3.9.44	Other organometallic C-C bond formation	Minisci reaction
126	3.9.60	Other organometallic C-C bond formation	Negishi-type coupling
127	3.9.61	Other organometallic C-C bond formation	Blaise ketone synthesis
128	3.9.67	Other organometallic C-C bond formation	Kulinkovich-Szymoniak reaction

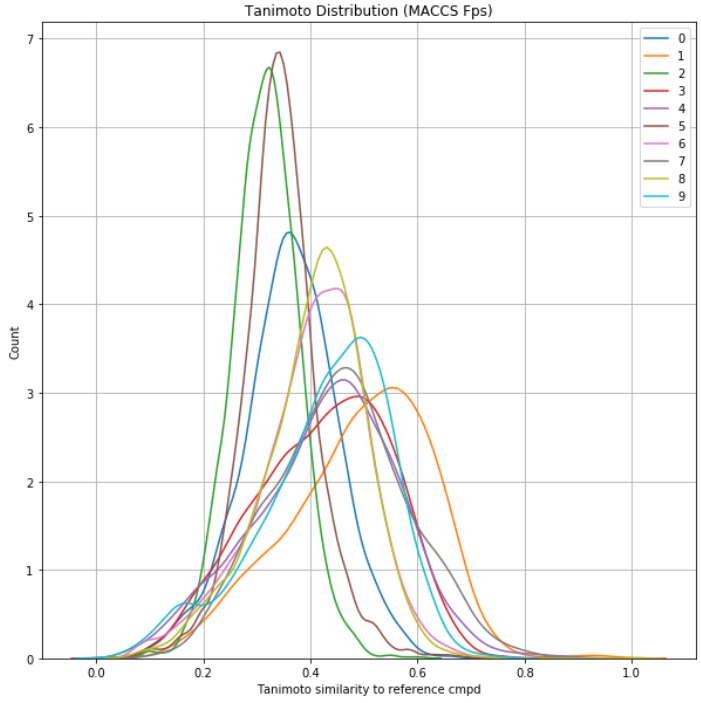
Table S2. Listing of 50 FDA approved drugs, and their corresponding reagents (amines and acids/acid chlorides)

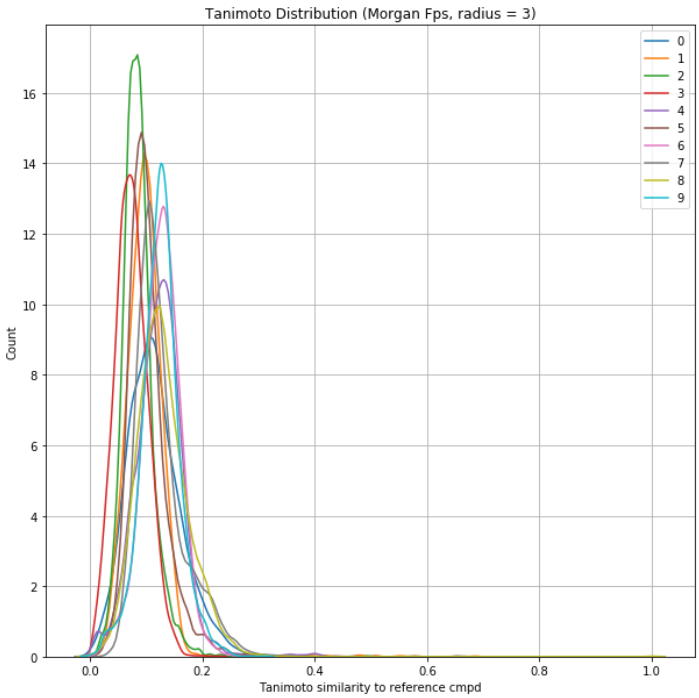
#	SMILES	Drug Name	Amine reactant	Identifier (amine)	acid/acid chloride/ester reactant	Identifier
1	COC(=O)Nc1[nH]c2ccc(cc2n1)C(=O)c3ccccc3	Mebendazole	c1ccc(cc1)C(=O)c2ccc3c(c2)nc([nH]3)N	MFCD01529678	COC(=O)Cl	MFCD00000639
2	CCCS(=O)c1ccc2c(c1)[nH]c(n2)NC(=O)OC	Albendazole Sulfoxide	CCCS(=O)c1ccc2c(c1)[nH]c(n2)N	MFCD29924114	COC(=O)Cl	MFCD00000639
3	c1ccc(cc1)C(=O)NCCC(=O)O	Betamipron	C(CN)C(=O)O	MFCD00008200	c1ccc(cc1)C(=O)Cl	MFCD00000653
4	c1ccc(cc1)C(=O)NC2CCN(CC2)CCc3c[nH]c4c3cccc4	Indoramin	c1ccc2c(c1)c(c[nH]2)CCN3CCC(CC3)N	MFCD00277757	c1ccc(cc1)C(=O)Cl	MFCD00000653
5	c1cc(ccc1C(=O)NCCN2CCOCC2)Cl	Moclobemide	C1COCCN1CCN	MFCD00006182	c1cc(ccc1C(=O)Cl)Cl	MFCD00000686
6	CC(=O)NCCCS(=O)(=O)O	AcamprosaicAcid	C(CN)CS(=O)(=O)O	MFCD00008225	CC(=O)Cl	MFCD00000719
7	CC(=O)Nc1nnc(s1)S(=O)(=O)N	Acetazolamide	c1(nnc(s1)S(=O)(=O)N)N	MFCD03425417	CC(=O)Cl	MFCD00000719
8	CC(=O)NC[C@H]1CN(C(=O)O1)c2ccc(c(c2)F)N3CCOCC3	Linezolid	c1cc(c(cc1N2C[C@@H](OC2=O)CN)F)N3CCOCC3	MFCD18379308	CC(=O)Cl	MFCD00000719
9	CCOc1ccc(cc1)NC(=O)C	Phenacetin	CCOc1ccc(cc1)N	MFCD00007865	CC(=O)Cl	MFCD00000719
10	CC(=O)N[C@H](COC)C(=O)NCc1ccccc1	Lacosamide	COC[C@H](C(=O)NCc1ccccc1)N	MFCD14708219	CC(=O)Cl	MFCD00000719
11	CC(=O)NCCc1c[nH]c2c1cc(cc2)OC	Melatonin	COc1ccc2c(c1)c(c[nH]2)CCN	MFCD00005662	CC(=O)Cl	MFCD00000719
12	CC(=O)N[C@H]1CCc2cc(c(c(c2-c3c1cc(=O)c(cc3)OC)OC)OC)OC	Colchicine	COc1ccc-2c(cc1=O)[C@H](CCc3c2c(c(c(c3)OC)OC)OC)N	MFCD00278752	CC(=O)Cl	MFCD00000719
13	Cc1ccc(cc1)S(=O)(=O)NC(=O)NC2C3CCC(C2O)(C3(C)C)C	Glibornuride	C[C@@]12CC[C@@H](C1(C)C)[C@@H]([C@@H]2O)N	MFCD09952489	Cc1ccc(cc1)S(=O)(=O)NC(=O)OC	MFCD00453717
14	C[C@]12CC[C@H]3[C@H]([C@@H]1CC[C@@H]2C(=O)Nc4cc(ccc4C(F)(F)F)C(F)(F)F)CC[C@@H]5[C@@]3(C=CC(=O)N5)C	Dutasteride	c1cc(c(cc1C(F)(F)F)N)C(F)(F)F	MFCD00074940	C[C@]12CC[C@H]3[C@H]([C@@H]1CC[C@@H]2C(=O)O)CC[C@@H]4[C@@]3(C=CC(=O)N4)C	MFCD08063794

15	C[C@]12CC[C@H]3[C@H]([C@@H]1CC[C@@H]2C(=O)NC(C)(C)C)CC[C@@H]4[C@@]3(C=CC(=O)N4)C	Finasteride	CC(C)(C)N	MFCD00008050	C[C@]12CC[C@H]3[C@H]([C@@H]1CC[C@@H]2C(=O)O)CC[C@@H]4[C@@]3(C=CC(=O)N4)C	MFCD08063794
16	CCCNC(=O)NS(=O)(=O)c1ccc(cc1)Cl	Chlorpropamide	CCCN	MFCD00008205	C(=O)Cl	MFCD17013587
17	CC1=C(N2[C@@H]([C@@H](C2=O)NC(=O)[C@@H](C3=CCC=CC3)N)SC1)C(=O)O	Cephradine	CC1=C(N2[C@@H]([C@@H](C2=O)N)SC1)C(=O)O	MFCD09750368	C1C=CCC(=C1)[C@H](C(=O)O)N	MFCD00137746
18	c1cc(c(cc1[N+](=O)[O-])Cl)NC(=O)c2cc(ccc2O)Cl	Niclosamide	c1cc(c(cc1[N+](=O)[O-])Cl)N	MFCD00007665	CCOC(=O)NS(=O)(=O)c1ccc(cc1)Cl	MFCD00454650
19	Cc1nnc(n1C2C[C@H]3CC[C@@H](C2)N3CC[C@@H](c4ccccc4)NC(=O)C5CCC(CC5)(F)F)C(C)C	Maraviroc	Cc1nnc(n1C2C[C@H]3CC[C@@H](C2)N3CC[C@@H](c4ccccc4)N)C(C)C	MFCD18381982	C1CC(CCC1C(=O)Cl)(F)F	MFCD13173983
20	c1cc(cnc1)C(=O)NCCO[N+](=O)[O-]	Nicorandil	C(CO[N+](=O)[O-])N	MFCD00868298	c1cc(cnc1)C(=O)Cl	MFCD00464814
21	CN(CCCNC(=O)C1CCCO1)c2nc3cc(c(cc3c(n2)N)OC)OC	Alfuzosin	CN(CCCN)c1nc2cc(c(cc2c(n1)N)OC)OC	MFCD14155925	C1CC(OC1)C(=O)Cl	MFCD09897727
22	CC1([C@@H](N2[C@H](S1)[C@@H](C2=O)NC(=O)Cc3ccccc3)C(=O)O)C	PenicillinG	CC1([C@@H](N2[C@H](S1)[C@@H](C2=O)N)C(=O)O)C	MFCD00005176	c1ccc(cc1)CC(=O)Cl	MFCD00000729
23	CCNC(=O)CCC/C=C\C[C@H]1[C@H](C[C@H]([C@@H]1/C=C/[C@H](CCc2ccccc2)O)O)O	Bimatoprost	CCN	MFCD00008160	c1ccc(cc1)CC[C@@H](/C=C/[C@H]2[C@@H](C[C@@H]([C@@H]2C/C=C\CCCC(=O)O)O)O)O	MFCD00135254
24	Cc1nnc(s1)SCC2=C(N3[C@@H]([C@@H](C3=O)NC(=O)Cn4cnnn4)SC2)C(=O)O	Cefazolin	Cc1nnc(s1)SCC2=C(N3[C@@H]([C@@H](C3=O)N)SC2)C(=O)O	MFCD29913098	c1nnnn1CC(=O)Cl	MFCD02094027
25	CCN(CC)CCNC(=O)c1ccc(cc1)NC(=O)C	Acecainide	CCN(CC)CCN	MFCD00008176	CC(=O)Nc1ccc(cc1)C(=O)Cl	MFCD02094022
26	CC(C)/C=C/CCCCC(=O)NCc1ccc(c(c1)OC)O	Capsaicin	COc1cc(ccc1O)CN	MFCD00044577	CC(C)/C=C/CCCCC(=O)Cl	MFCD06797318
27	CC(C)C(=O)Nc1ccc(c(c1)C(F)(F)F)[N+](=O)[O-]	Flutamide	c1cc(c(cc1N)C(F)(F)F)[N+](=O)[O-]	MFCD00014717	CC(C)C(=O)Cl	MFCD00000717
28	CC(C)C1CCC(CC1)C(=O)N[C@H](Cc2ccccc2)C(=O)O	Nateglinide	c1ccc(cc1)C[C@H](C(=O)O)N	MFCD00004270	CC(C)C1CCC(CC1)C(=O)Cl	MFCD25954097
29	Cc1cccc(c1)Nc2ccncc2S(=O)(=O)NC(=O)NC(C)C	Torsemide	Cc1cccc(c1)Nc2ccncc2S(=O)(=O)N	MFCD00661332	CC(C)NC(=O)Cl	MFCD19217025
30	CCN(CC)CCNC(=O)c1c(c([nH]c1C)/C=C\2/c3cc(ccc3NC2=O)F)C	Sunitinib Malate	CCN(CC)CCN	MFCD00008176	Cc1c([nH]c(c1C(=O)O)C)/C=C\2/c3cc(ccc3NC2=O)F	MFCD11521323
31	Cc1c(c(no1)c2c(cccc2Cl)Cl)C(=O)N[C@H]3[C@@H]4N(C3=O)[C@H](C(S4)(C)C)C(=O)O	Dicloxacillin	CC1([C@@H](N2[C@H](S1)[C@@H](C2=O)N)C(=O)O)C	MFCD00005176	Cc1c(c(no1)c2c(cccc2Cl)Cl)C(=O)Cl	MFCD00052556
32	Cc1c(cno1)C(=O)Nc2ccc(cc2)C(F)(F)F	Leflunomide	c1cc(ccc1C(F)(F)F)N	MFCD00064396	Cc1c(cno1)C(=O)Cl	MFCD03411599
33	Cc1ccc(cc1Nc2nccc(n2)c3cccnc3)C(=O)Nc4cc(cc(c4)n5cc(nc5)C)C(F)(F)F	Nilotinib	Cc1cn(cn1)c2cc(cc(c2)N)C(F)(F)F	MFCD11846236	Cc1ccc(cc1Nc2nccc(n2)c3cccnc3)C(=O)O	MFCD11521324
34	Cc1cccc(c1OCC(=O)N[C@@H](Cc2ccccc2)[C@H](C[C@H](Cc3ccccc3)NC(=O)[C@H](C(C)C)N4CCCNC4=O)O)C	Lopinavir	CC(C)[C@@H](C(=O)N[C@@H](Cc1ccccc1)C[C@@H]([C@H](Cc2ccccc2)N)O)N3CCCNC3=O	MFCD09952131	Cc1cccc(c1OCC(=O)Cl)C	MFCD09753506
35	Cc1cnc(cn1)C(=O)NCCc2ccc(cc2)S(=O)(=O)NC(=O)NC3CCCCC3	Glipizide	c1cc(ccc1CCN)S(=O)(=O)NC(=O)NC2CCCCC2	MFCD01631095	Cc1cnc(cn1)C(=O)Cl	MFCD13173590
36	CCC(=O)NCC[C@@H]1CCc2c1c3c(cc2)OCC3	Ramelteon	c1cc2c(c3c1CC[C@H]3CCN)CCO2	MFCD12911899	CCC(=O)Cl	MFCD00000745
37	CCCCCOC(=O)Nc1c(cn(c(=O)n1)[C@H]2[C@@H]([C@@H]([C@H](O2)C)O)O)F	Capecitabine	C[C@@H]1[C@H]([C@H]([C@@H](O1)n2cc(c(nc2=O)N)F)O)O	MFCD07369278	CCCCCOC(=O)Cl	MFCD00058933
38	CCCCN1CCCCC1C(=O)Nc2c(cccc2C)C	Bupivacaine	Cc1cccc(c1N)C	MFCD00007747	CCCCN1CCCCC1C(=O)O	MFCD09026200
39	CCN(CC)CC(=O)Nc1c(cccc1C)C	Lidocaine	Cc1cccc(c1N)C	MFCD00007747	CCN(CC)CC(=O)Cl	MFCD25965185
40	CCN(CC(C)O)c1ccc(nn1)NNC(=O)OCC	Cadralazine	CCN(CC(C)O)c1ccc(nn1)NN	MFCD00874858	CCOC(=O)Cl	MFCD00000644

41	CCN1CCCC1CNC(=O)c2cc(c(cc2OC)N)S(=O)(=O)CC	Amisulpride	CCN1CCCC1CN	MFCD00003178	CCS(=O)(=O)c1cc(c(cc1N)OC)C(=O)O	MFCD04973619
42	Cn1c2ccccc2c(n1)C(=O)NC3C[C@H]4CCC[C@@H](C3)N4C	Granisetron	CN1[C@@H]2CCC[C@H]1CC(C2)N	MFCD06657547	Cn1c2ccccc2c(n1)C(=O)Cl	MFCD02093096
43	Cc1cccc(c1NC(=O)C2CCCCN2C)C	Mepivacaine	Cc1cccc(c1N)C	MFCD00007747	CN1CCCCC1C(=O)O	MFCD08060082
44	Cc1ccc(cc1Nc2nccc(n2)c3cccnc3)NC(=O)c4ccc(cc4)CN5CCN(CC5)C	Imatinib Mesylate	Cc1ccc(cc1Nc2nccc(n2)c3cccnc3)N	MFCD09028125	CN1CCN(CC1)Cc2ccc(cc2)C(=O)Cl	MFCD09833009
45	CCN(CC)CCNC(=O)c1cc(c(cc1OC)N)Cl	Metoclopramide	CCN(CC)CCN	MFCD00008176	COc1cc(c(cc1C(=O)Cl)Cl)N	MFCD30303709
46	COc1ccc(cc1C(=O)NCCc2ccc(cc2)S(=O)(=O)NC(=O)NC3CCCCC3)Cl	Glyburide Glibenclamide	c1cc(ccc1CCN)S(=O)(=O)NC(=O)NC2CCCCC2	MFCD01631095	COc1ccc(cc1C(=O)Cl)Cl	MFCD03208980
47	CC1([C@@H](N2[C@H](S1)[C@@H](C2=O)NC(=O)c3c(cccc3OC)OC)C(=O)O)C	Methicillin	CC1([C@@H](N2[C@H](S1)[C@@H](C2=O)N)C(=O)O)C	MFCD00005176	COc1cccc(c1C(=O)Cl)OC	MFCD00000665
48	CNC(=O)c1cc(ccn1)Oc2ccc(cc2)NC(=O)Nc3ccc(c(c3)C(F)(F)F)Cl	Sorafenib Tosylate	CN	MFCD00008104	c1cc(ccc1NC(=O)Nc2ccc(c(c2)C(F)(F)F)Cl)Oc3ccnc(c3)C(=O)O	MFCD26954590
49	C[C@@H](CO)NC(=O)[C@H]1CN([C@@H]2Cc3c[nH]c4c3c(ccc4)C2=C1)C	Ergonovine	C[C@@H](CO)N	MFCD00064412	CN1C[C@@H](C=C2[C@H]1Cc3c[nH]c4c3c2ccc4)C(=O)O	MFCD00133297
50	CC[C@@H](CO)NC(=O)[C@H]1CN([C@@H]2Cc3c[nH]c4c3c(ccc4)C2=C1)C	Methylergonovine	CC[C@@H](CO)N	MFCD00064418	CN1C[C@@H](C=C2[C@H]1Cc3c[nH]c4c3c2ccc4)C(=O)O	MFCD00133297

Figure S1. Similarity distributions used estimate appropriate Tanimoto cut-off for MACCS and Morgan FPs.




Tanimoto Distribution (Morgan Fps, radius = 3)
Count
Tanimoto similarity to reference cmpd
0
1
2
3
4
5
6
7
8
9
0
2
4
6
8
10
12
14
16
0.0
0.2
0.4
0.6
0.8
1.0