Supporting Information: Mining Chromatographic Enantioseparation Data using Matched Molecular Pair Analysis

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1. SMILES for All the Compounds in Set 1

COMPOUND_NAME SMILES
71 O(c1c(OCC=C)cccc1)C[C@H](CNC(C)C)O
73 c12c(OC[C@H](CNC(C)C)O)cccc1cccc2
74 c12c([nH]cc2)cccc1OC[C@H](CNC(C)C)O
105 n1c(Oc2ccc(F)cc2)cccc1[C@@H](O)C
106 n1c(Oc2ccc(Cl)cc2)cccc1[C@@H](O)C
107 n1c(Oc2ccc(Br)cc2)cccc1[C@@H](O)C
108 n1c(Oc2ccc(I)cc2)cccc1[C@@H](O)C
110 n1c(Oc2ccc(cc2)OC)cccc1[C@@H](O)C
111 n1c(Oc2ccc(C#C)cc2)cccc1[C@@H](O)C
112 n1c(Oc2ccc(C=C)cc2)cccc1[C@@H](O)C
113 n1c(Oc2ccccc2)cccc1[C@@H](O)C
114 n1c(Oc2ccccc2)cccc1[C@H](OC(=O)C)C
115 n1c(Oc2ccc(F)cc2)cccc1[C@@H](OC(=O)C)C
116 n1c(Oc2ccc(Cl)cc2)cccc1[C@@H](OC(=O)C)C
117 n1c(Oc2ccc(Br)cc2)cccc1[C@@H](OC(=O)C)C
118 n1c(Oc2ccc(I)cc2)cccc1[C@@H](OC(=O)C)C
120 n1c(Oc2ccc(cc2)OC)cccc1[C@@H](OC(=O)C)C
121 n1c(Oc2ccc(C#C)cc2)cccc1[C@@H](OC(=O)C)C
122 n1c(Oc2ccc(C=C)cc2)cccc1[C@@H](OC(=O)C)C
159 C1[C@@H](c2ccccc2)CCCC1=O
161 C1(OCC[C@@H](C1)c1ccccc1)=O
163 O1[C@@H](c2ccccc2)COCC1
164 O1C[C@H](c2ccccc2)CCC1
165 C1(O[C@H](c2ccccc2)CCO1)=O
1390 N1(C([C@](c2ccccc2)(CC)C(NC1=O)=O)=O)C
1782 C1([C@@H](c2ccccc2)CCCC1)=O
2077 C([C@H](Oc1ccccc1)C)(=O)O
2089 C(N[C@H](C(=O)O)c1ccccc1)(=O)OCc1ccccc1
2091 C(N[C@H](C(=O)O)C(C)C)(=O)OCc1ccccc1
3751 C(O[C@H](c1ccccc1)C)(=O)c1ccccc1
4564 C(N[C@H](C(=O)OCC)C)(=O)OCc1ccccc1
4631 C(N[C@H](C(=O)OCC)CC)(=O)OCc1ccccc1
4632 C(N[C@H](C(OCc1ccccc1)=O)CC)(=O)OCc1ccccc1
4647 C(N[C@H](C(=O)OCC)CO)(=O)OCc1ccccc1

4648 C(N[C@@H](C(OCc1ccccc1)=O)CO)(=O)OCc1ccccc1
4674 C(N[C@H](C(=O)OCC)CC)(=O)OCc1ccccc1
4676 C(N[C@H](C(=O)OCC)C(C)C)(=O)OCc1ccccc1
4678 C(N[C@H](C(=O)OCC)CCC)(=O)OCc1ccccc1
4682 C(N[C@H](C(=O)OCC)CCCC)(=O)OCc1ccccc1
5312 O1[C@](c2c3c(ccc(c3)C)cc(c2)C)(c2c(cccc2)C1=O)C
7444 C([C@@H](c1ccccc1)N)(=O)O
7928 C(c1ccccc1)[C@H](N)C
7979 c1([C@@H](N)CO)ccccc1
8937 N1=C(c2c(ccc(c2)Cl)NC([C@H]1C)=O)c1ccccc1
8940 N1=C(c2c(ccc(c2)Cl)NC([C@H]1C(C)C)=O)c1ccccc1
8944 N1=C(c2c(ccc(c2)Cl)NC(C1Cc1ccccc1)=O)c1ccccc1
8949 N1=C(c2c(ccc(c2)Cl)N(C([C@H]1C)=O)C)c1ccccc1
8950 N1=C(c2c(ccc(c2)Cl)N(C([C@H]1C(C)C)=O)C)c1ccccc1
8964 N1=C(c2c(ccc(c2)Cl)NC([C@H]1OC(=O)c1ccccc1)=O)c1ccccc1
9103 C([C@H](Nc1cc2ccccc2cc1)C)(=O)OCC
9104 C([C@H](Nc1cc2ccccc2cc1)CC)(=O)OCC
9105 C([C@H](Nc1cc2ccccc2cc1)CCC)(=O)OCC
9115 C([C@H](Nc1cc2ccccc2cc1)CCCCC)(=O)OCC
9116 C([C@H](Nc1cc2ccccc2cc1)CCCCCC)(=O)OCC
9117 C([C@H](Nc1cc2ccccc2cc1)CCCCCCC)(=O)OCC
10688 C(#C[C@H](\C=C\c1ccccc1)O)c1ccccc1
11565 [nH]1c2c(c(OC[C@H](CNC(C)C)O)ccc2)c2c1cccc2
12253 C([C@H](Oc1ccc(cc1)Cl)C)(=O)OC
12258 C([C@H](Oc1ccccc1)C)(=O)OC
12355 O1[C@](c2c(c(cc3c2cccc3)C)C)(c2c(cccc2)C1=O)C
12553 C([C@@H](Oc1c(C)cccc1)C)(=O)O
12554 O(c1c(C)cccc1)[C@@H](C(=O)OC)C
12555 O(c1c(C)cccc1)[C@H](C(=O)OCC)C
12558 C([C@@H](Oc1cc(C)ccc1)C)(=O)O
12562 C([C@@H](Oc1ccc(C)cc1)C)(=O)O
12564 O(c1c(Cl)cccc1)[C@@H](C(=O)OC)C
14161 N=1[C@@H](C(N(C)c2c(C1c1ccccc1)cc(cc2)Cl)=O)OC(=O)c1ccccc1
16609 O(c1c(cc(cc1)Cl)Cl)[C@H](C(=O)OC)C
18625 N1=C(c2c(ccc(c2)Cl)NC([C@H]1OC(N(C)C)=O)=O)c1ccccc1
18630 N=1[C@H](C(N(C)c2c(C1c1ccccc1)cc(cc2)Cl)=O)OC(N(C)C)=O
20048 C=1([C@@H](C(C(=O)OC)=C(NC1C)C)c1c(c(Cl)ccc1)Cl)C(=O)OCC
22008 O1C(=O)CCC[C@@H]1c1ccccc1
22016 N(C[C@H](COc1ccccc1)O)C(C)C
22017 C(O[C@H](CNC(C)C)COc1ccccc1)(=O)C
22256 c12c(c(O)ccc1OC[C@H](CNC(C)C)O)cccc2
24136 C(C[C@@H](\C=C\c1ccccc1)O)(=O)c1ccccc1
24647 C(N[C@H](C(=O)OC)CC)(=O)OCc1ccccc1

24648 C(N[C@H](C(=O)OC)CCC)(=O)OCc1ccccc1
24708 C(N[C@H](CC(=O)OC)c1ccccc1)(=O)OCc1ccccc1
24709 C(N[C@H](CC(=O)OC)c1occc1)(=O)OCc1ccccc1
24710 C(N[C@H](CC(=O)OC)c1sccc1)(=O)OCc1ccccc1
25319 N=1[C@H](C(N(C)c2c(C1c1ccccc1)cc(cc2)Cl)=O)OC(=O)NC
25320 N1=C(c2c(ccc(c2)Cl)NC([C@@H]1OC(=O)NC)=O)c1ccccc1
25321 N=1[C@@H](C(N(C)c2c(C1c1ccccc1)cc(cc2)Cl)=O)OC(N(CO)C)=O
25322 N1=C(c2c(ccc(c2)Cl)NC([C@H]1OC(N(CO)C)=O)=O)c1ccccc1
25323 N=1[C@H](C(N(C)c2c(C1c1ccccc1)cc(cc2)Cl)=O)OC(=O)N
25324 N1=C(c2c(ccc(c2)Cl)NC([C@@H]1OC(=O)N)=O)c1ccccc1
25325 N=1[C@H](C(N(C)c2c(C1c1ccccc1)cc(cc2)Cl)=O)OC(NCO)=O
25326 N1=C(c2c(ccc(c2)Cl)NC([C@@H]1OC(NCO)=O)=O)c1ccccc1
25327 N=1[C@H](C(N(C)c2c(C1c1ccccc1)cc(cc2)Cl)=O)OC(N(CO)CO)=O
25328 N1=C(c2c(ccc(c2)Cl)NC([C@@H]1OC(N(CO)CO)=O)=O)c1ccccc1
26214 c1(oc2ccccc2c1)[C@H](n1cncc1)c1ccc(cc1)Cl
26955 c1([S@](Cc2ccccc2)=O)c(C)cccc1
27472 N(C[C@@H](COc1ccc(cc1)O)O)C(C)C
27987 C([C@H](c1ccccc1)O)(=O)N
29317 C([C@H](Oc1ccccc1)CC)(=O)O
31206 c1([C@H](c2ccccc2)O)c(OC)cccc1
31208 c1([C@H](c2ccccc2)O)c(F)cccc1
31209 c1([C@H](c2ccccc2)O)c(C)cccc1
31515 C1(Oc2ccccc2C1)(C(=O)O)CC
31518 O1[C@](C(=O)OC)(Cc2ccccc12)CC
31521 O1[C@](C(=O)N)(Cc2ccccc12)CC
37727 C([C@@H](Cc1cnccc1)N)(=O)O
40459 C([C@H](Oc1ccc(cc1)CC)C)(=O)OC
40461 c1(O[C@@H](C(=O)OC)C)c(c(C)ccc1)C
40462 c1(O[C@@H](C(=O)O)C)c(c(C)ccc1)C
40464 O(c1c(cc(cc1)C)C)[C@@H](C(=O)OC)C
40466 O(c1c(cc(cc1)C)C)[C@@H](C(=O)O)C
40472 C([C@H](Oc1cc(C)c(cc1)C)C)(=O)O
41899 C1(=C(NC(=O)N[C@@H]1c1ccccc1)C)C(=O)OCC
41900 C1(=C(NC(=O)N[C@@H]1c1ccccc1)C)C(=O)OCC
41905 C1(=C(N(C(=O)N[C@@H]1c1ccccc1)C)C)C(=O)OCC
41906 C1(=C(N(C(=O)N[C@@H]1c1ccccc1)C)C)C(=O)OCC
41911 C1(=C(NC(=O)N([C@@H]1c1ccccc1)C)C)C(=O)OCC
41912 C1(=C(NC(=O)N([C@@H]1c1ccccc1)C)C)C(=O)OCC
41917 C1(=C(N(C(=O)N([C@@H]1c1ccccc1)C)C)C)C(=O)OCC
41918 C1(=C(N(C(=O)N([C@@H]1c1ccccc1)C)C)C)C(=O)OCC
41923 N1(C(NC(C)=C([C@H]1c1ccccc1)C(=O)OCC)=O)C=O
41924 N1(C(NC(C)=C([C@H]1c1ccccc1)C(=O)OCC)=O)C=O
41929 N1(C(N(C(C)=C([C@H]1c1ccccc1)C(=O)OCC)C)=O)C=O

41930 N1(C(N(C(C)=C([C@H]1c1ccccc1)C(=O)OCC)C)=O)C=O
41935 N1(C(NC(C)=C(C1c1ccccc1)C(=O)OCC)=O)C(=O)C
41941 C1(=C(NC(=S)N[C@@H]1c1ccccc1)C)C(=O)OCC
41942 C1(=C(NC(=S)N[C@@H]1c1ccccc1)C)C(=O)OCC
41947 C1(=C(N(C(=S)N[C@@H]1c1ccccc1)C)C)C(=O)OCC
41948 C1(=C(N(C(=S)N[C@@H]1c1ccccc1)C)C)C(=O)OCC
41953 N1(C(NC(C)=C([C@H]1c1ccccc1)C(=O)OCC)=S)C(=O)C
41959 C1(=C(NC(=O)N[C@@H]1c1ccccc1)C)C(=O)OC
42013 C1(=C(NC(=O)N[C@@H]1c1ccccc1)C)C(=O)N
42339 C(N[C@H](C(=O)O)C)(=O)c1ccccc1
42341 C(N[C@@H](C(=O)O)CC(C)C)(=O)c1ccccc1
42347 N(C(=O)c1ccccc1)[C@@H](C(=O)O)C(C)C
42444 C([C@H](c1ccccc1)O)(=O)O
43515 C(N1[C@@H](CCC1)C)(c1c2c(cccc2)ccc1)=O
43517 C(N1C[C@@H](C)CC1)(c1c2c(cccc2)ccc1)=O
43521 C(N1[C@H](C)CCCC1)(c1c2c(cccc2)ccc1)=O
43522 C(N1[C@H](CC)CCCC1)(c1c2c(cccc2)ccc1)=O
43524 C(N1C[C@H](C)CCC1)(c1c2c(cccc2)ccc1)=O
44997 n1c[nH]c(c1)C[C@@H](C(=O)O)N
48059 C(N[C@H](C(=O)O)C)(=O)OCc1ccccc1
48071 C(N[C@H](C(=O)O)C(C)C)(=O)OCc1ccccc1
48090 C(N[C@@H](C(=O)O)[C@H](CC)C)(=O)OCc1ccccc1
48095 C(N[C@@H](C(=O)O)[C@H](CC)C)(=O)OCc1ccccc1
48509 C(=O)(c1ccccc1)[C@@H](N)C
48885 C([C@H](c1ccccc1)O)(=O)OC
49043 N1(C([C@@](C2=CCCCC2)(C)C(NC1=O)=O)=O)C
49045 N1(C([C@](c2ccccc2)(CC)C(NC1=O)=O)=O)C
52324 c12c(OC[C@@H](O)CNCCCC)cccc1cccc2
52326 c12c(OC[C@@H](O)CNCCC)cccc1cccc2
57323 C([C@H](C(=O)C)CCC)(N1CCN(c2ncccn2)CC1)=O
57325 C([C@H](C(=O)C)CCCC)(N1CCN(c2ncccn2)CC1)=O
57327 C([C@H](C(=O)C)CCCCC)(N1CCN(c2ncccn2)CC1)=O
57329 C([C@H](C(=O)C)CCCCCC)(N1CCN(c2ncccn2)CC1)=O
57331 C([C@H](C(=O)C)CCCCCCC)(N1CCN(c2ncccn2)CC1)=O
57775 N(=C(/c1ccccc1)c1ccccc1)\[C@H](C(=O)OCC)C
57776 N(=C(/c1ccccc1)c1ccccc1)\[C@H](C(=O)OCC)C(C)C
57787 N(=C(/c1ccccc1)c1ccccc1)\[C@H](C(=O)NCCCC)CC(C)C
57788 N(\[C@H](C(N(CC)CC)=O)CC(C)C)=C(\c1ccccc1)c1ccccc1
57790 N(=C(/c1ccccc1)c1ccccc1)\[C@H](C(=O)NCCCC)C(C)C
57791 N(\[C@H](C(N(CC)CC)=O)C(C)C)=C(/c1ccccc1)c1ccccc1
57792 N(=C(/c1ccccc1)c1ccccc1)\[C@H](C(=O)OC)C
57793 N(=C(/c1ccccc1)c1ccccc1)\[C@H](C(=O)OC)C(C)C
58834 C(=C\c1ccccc1)\[C@H](c1ccccc1)O

58927 C(N[C@H](C(=O)O)Cc1ccccc1)(OC(C)(C)C)=O
58930 C(N[C@H](C(=O)O)C(C)C)(=O)OCc1ccccc1
58931 C(N[C@H](C(=O)O)CC(C)C)(=O)OCc1ccccc1
58933 C(N[C@H](C(=O)O)c1ccccc1)(=O)OCc1ccccc1
59588 C([C@@H](Oc1ccc(CC)cc1)C)(=O)OCC
59590 c1(O[C@H](C(=O)OCC)C)c(c(C)ccc1)C
59591 O(c1c(cc(cc1)C)C)[C@H](C(=O)OCC)C
59602 C([C@@H](Oc1ccc(cc1)Cl)C)(=O)OCC
59618 C([C@@H](Oc1ccccc1)C)(=O)OCC
61170 C(N[C@@H](C(=O)NC)Cc1ccccc1)(OC(C)(C)C)=O
61172 C([C@@H](NC(OC(C)(C)C)=O)Cc1ccccc1)(N(C)C)=O
61174 C(N[C@H](C(=O)NCC)Cc1ccccc1)(OC(C)(C)C)=O
61176 C([C@@H](NC(OC(C)(C)C)=O)Cc1ccccc1)(N(CC)CC)=O
61178 C(N[C@H](C(NC(C)C)=O)Cc1ccccc1)(OC(C)(C)C)=O
61180 C([C@@H](NC(OC(C)(C)C)=O)Cc1ccccc1)(N(C(C)C)C(C)C)=O
64228 N1=C(c2c(cc3c(c2)OCO3)C[C@H](N1)C)c1ccc(N)cc1
64252 N=1N(C(=O)NC)[C@@H](Cc2c(C1c1ccc(N)cc1)cc1c(OCO1)c2)C
66799 C([C@H](Cc1ccccc1)O)(=O)O
67293 C(O[C@H](c1ccccc1)CO)(=O)c1ccccc1
67346 c1([C@@](c2ccccc2)(O)C)ccc(cc1)Br
67546 C(C(=O)OC)[C@@H](c1ccccc1)O
69233 C([C@@H](Cc1cc(O)c(cc1)O)N)(=O)O
69328 c1(c[nH]c2c1cccc2)C[C@@H](C(=O)O)N
70299 c12cc(OC[C@@H](O)CNCCC)ccc1cccc2
70302 c12cc(OC[C@@H](O)CNCCCC)ccc1cccc2
70311 O(C[C@@H](O)CNCCC)c1ccccc1
70314 O(C[C@@H](O)CNCCCC)c1ccccc1
70318 N(C(C)(C)C)C[C@@H](COc1ccccc1)O
71392 C=12[C@H](NC(NC1CCCC2=O)=S)c1c(Cl)cccc1
71395 C=12[C@H](NC(NC1CCCC2=O)=S)c1c(Br)cccc1
71398 C=12[C@H](NC(NC1CCCC2=O)=S)c1c(C)cccc1
71404 C=12[C@H](NC(NC1CCCC2=O)=S)c1c(OCC)cccc1
72053 N(C[C@H](COc1ccc(C=O)cc1)O)C(C)C
72075 O(c1c(CCC)cccc1)C[C@@H](CNC(C)C)O
72081 c1(c(OC[C@@H](CNC(C)C)O)cccc1)C=O
76324 C1([C@@H](Cc2ccccc2)CCCC1)=O
78051 C(C(C)(C)C)(O[C@H](CCc1ccccc1)C)=O
78057 C(C(C)(C)C)(O[C@H](\C=C\c1ccccc1)C)=O
78058 C(O[C@H](\C=C\c1ccc(cc1)C)C)(=O)C
78059 [N+](c1ccc(\C=C\[C@@H](OC(=O)C)C)cc1)([O–])=O
78063 C(N[C@H](C(=O)O)CCC)(=O)OCc1ccccc1
79426 C([C@H](c1ccccc1)O)(=O)O
80260 c1(oc2ccccc2c1)[C@@H](n1cncc1)c1ccccc1

80281 N1(C(OC(C)(C)C)=O)[C@H](C(=O)OC1)Cc1ccccc1
81748 c1(c([S@](Cc2ccccc2)=O)cccc1)C(=O)N
83141 n12c(=NC(CC)=C([C@H]1c1c(C)cccc1)C(=O)OC)sc(\c2=O)=C\c1ccccc1
83144 n12c(=NC(CC)=C([C@H]1c1cc(C)ccc1)C(=O)OC)sc(\c2=O)=C\c1ccccc1
83146 n12c(=NC(CC)=C([C@H]1c1cc(C)ccc1)C(=O)OC)sc(\c2=O)=C\c1ccc(cc1)Cl
83149 n12c(=NC(CC)=C([C@H]1c1cc(OC)ccc1)C(=O)OC)sc(\c2=O)=C\c1ccccc1
83150 n12c(=NC(CC)=C([C@H]1c1cc(OC)ccc1)C(=O)OC)sc(\c2=O)=C\c1ccc(cc1)Cl
83647 C([C@@H](c1ccccc1)N)(=O)O
83711 N1(C([C@](c2ccccc2)(CC)C(NC1=S)=O)=O)C
84685 c1(oc2ccccc2c1)[C@@H](n1nnnc1)c1ccccc1
84689 c1(oc2ccccc2c1)[C@@H](n1nnnc1)c1ccc(cc1)Cl
85512 C([C@@H](Cc1ccccc1)N)(=O)O
85528 C([C@@H](Cc1ccc(O)cc1)N)(=O)O
85608 C([C@@H](Cc1ccc(cc1)F)N)(=O)O
85624 C([C@@H](Cc1ccc(cc1)Cl)N)(=O)O
85640 C([C@H](Cc1ccc(cc1)Br)N)(=O)O
86406 C([C@@](c1ccccc1)(O)C)(=O)O
88157 n12c(=NC(C)=C([C@H]2c2ccccc2)C(=O)OC)sc(\c1=O)=C\c1ccccc1
88158 n12c(=NC(C)=C([C@H]2c2ccccc2)C(=O)OC)sc(\c1=O)=C\c1ccc(C)cc1
88159 n12c(=NC(C)=C([C@H]2c2ccccc2)C(=O)OC)sc(\c1=O)=C\c1ccc(OC)cc1
88160 n12c(=NC(C)=C([C@H]2c2ccccc2)C(=O)OC)sc(\c1=O)=C\c1ccc(cc1)Cl
88162 n12c(=NC(C)=C([C@H]1c1c([N+]([O–])=O)cccc1)C(=O)OC)sc(\c2=O)=C\c1ccc(C)cc1
88164 n12c(=NC(C)=C([C@H]1c1c([N+]([O–])=O)cccc1)C(=O)OC)sc(\c2=O)=C\c1ccc(OC)cc1
88167 n12c(=NC(C)=C([C@H]1c1cc([N+]([O–])=O)ccc1)C(=O)OC)sc(\c2=O)=C\c1ccccc1
88168 n12c(=NC(C)=C([C@H]1c1cc([N+]([O–])=O)ccc1)C(=O)OC)sc(\c2=O)=C\c1ccc(C)cc1
88169 n12c(=NC(C)=C([C@H]1c1cc([N+]([O–])=O)ccc1)C(=O)OC)sc(\c2=O)=C\c1ccc(OC)cc1
88170 n12c(=NC(C)=C([C@H]1c1cc([N+]([O–])=O)ccc1)C(=O)OC)sc(\c2=O)=C\c1ccc(cc1)Cl
88179 n12c(=NC(C)=C([C@H]1c1cc(Cl)ccc1)C(=O)OC)sc(\c2=O)=C\c1ccccc1
88180 n12c(=NC(C)=C([C@H]1c1cc(Cl)ccc1)C(=O)OC)sc(\c2=O)=C\c1ccc(C)cc1
88181 n12c(=NC(C)=C([C@H]1c1cc(Cl)ccc1)C(=O)OC)sc(\c2=O)=C\c1ccc(OC)cc1
88182 n12c(=NC(C)=C([C@H]1c1cc(Cl)ccc1)C(=O)OC)sc(\c2=O)=C\c1ccc(cc1)Cl
88183 n12c(=NC(C)=C(C1c1c(OC)cccc1)C(=O)OC)sc(\c2=O)=C\c1ccccc1
88184 n12c(=NC(C)=C(C1c1c(OC)cccc1)C(=O)OC)sc(\c2=O)=C\c1ccc(C)cc1
88188 n12c(=NC(C)=C([C@H]1c1cc(OC)ccc1)C(=O)OC)sc(\c2=O)=C\c1ccccc1
88192 n12c(=NC(C)=C([C@H]1c1cc(OC)ccc1)C(=O)OC)sc(\c2=O)=C\c1ccc(cc1)Cl
88193 n12c(=NC(C)=C([C@H]1c1c(C)cccc1)C(=O)OC)sc(\c2=O)=C\c1ccccc1
88194 n12c(=NC(C)=C([C@H]1c1c(C)cccc1)C(=O)OC)sc(\c2=O)=C\c1ccc(C)cc1
88197 n12c(=NC(C)=C([C@H]1c1cc(C)ccc1)C(=O)OC)sc(\c2=O)=C\c1ccccc1
88198 n12c(=NC(C)=C([C@H]1c1cc(C)ccc1)C(=O)OC)sc(\c2=O)=C\c1ccc(C)cc1
88199 n12c(=NC(C)=C([C@H]1c1cc(C)ccc1)C(=O)OC)sc(\c2=O)=C\c1ccc(OC)cc1
88200 n12c(=NC(C)=C([C@H]1c1cc(C)ccc1)C(=O)OC)sc(\c2=O)=C\c1ccc(cc1)Cl
88863 C([S@](=O)c1ccccc1)C(=O)O
89680 C1(N(c2ccccc2[C@@]1(c1ccccc1)C)C)=O

90245 C(N[C@H](C(=O)OC)CCC)(=O)OCc1ccccc1
92149 c1(c(cc(cc1)Cl)Cl)[C@H](Cn1cncc1)OCC=C
93217 c12n(\C=C3\C[C@@H]3CO)cnc1c(Cl)nc(n2)N
93218 c12n(\C=C3\C[C@@H]3CO)cnc1c(N)nc(n2)N
93220 c12n(\C=C3\C[C@H]3CO)cnc1c(OC)nc(n2)N
95834 C([C@H](Cc1ccccc1)N)(=O)OC
95836 C([C@H](Cc1ccc(Cl)cc1)N)(=O)OC
95838 C([C@H](Cc1ccc(Cl)cc1)N)(=O)OCC
95840 C([C@@H](Cc1ccc(cc1)O)N)(=O)OC
96670 C=1([C@@H](C(C(=O)OC)=C(NC1C)C)c1c(c(Cl)ccc1)Cl)C(OCOC(=O)CCC)=O
97616 C([S@](=O)c1ccccc1)C(=O)C
97706 C([S@](=O)c1ccccc1)C(=O)OCC
98605 C([C@@H](c1ccccc1)N)(=O)N
98697 C([C@@H](Cc1c(cc(cc1)O)C)N)(=O)O
99891 C(N[C@H](C(=O)O)C)(c1ccc(Br)cc1)=O
99893 C(N[C@H](C(=O)O)C)(c1cc(Cl)ccc1)=O
99894 C(N[C@H](C(=O)O)C)(c1ccc(Cl)cc1)=O
99896 C(N[C@H](C(=O)O)C)(c1ccc(F)cc1)=O
99902 N(C(c1ccc(Br)cc1)=O)[C@@H](C(=O)O)C(C)C
99904 N(C(c1cc(Cl)ccc1)=O)[C@@H](C(=O)O)C(C)C
99919 C(N[C@@H](C(=O)O)CC(C)C)(c1ccc(cc1)Br)=O
100088 C(N[C@H](C(=O)O)CC)(c1cc(Cl)ccc1)=O
101714 C1([C@](c2ccccc2)(COC)CCCC1)=O
104139 C([C@@H](C[N+]([O–])=O)c1ccccc1)(C(=O)OCC)C(=O)OCC
104143 C([C@H](c1sccc1)C[N+]([O–])=O)(C(=O)OCC)C(=O)OCC
104857 c1([C@H](C(=O)O)N)c(C)cccc1
104868 C([C@@H](c1c(C)cccc1)N)(=O)N
105119 c1([C@H](c2ccccc2)O)ccc(OC)cc1
105466 c1([C@H](NC(=O)OCc2ccccc2)C(=O)O)sccc1
105468 c1([C@H](NC(=O)OCc2ccccc2)C(=O)O)occc1
105755 C([C@@H](Cc1ccccc1)N)(=O)OCC
106221 N1(C(N[C@](C1=O)(c1ccccc1)CC)=O)C
106386 [N+](c1ccc(NC([C@H](NC(=O)C)Cc2ccccc2)=O)cc1)([O–])=O
106389 [N+](c1ccc(OC([C@H](NC(=O)C)Cc2ccccc2)=O)cc1)([O–])=O
106392 C([C@H](NC(=O)C)Cc1ccccc1)(Oc1cc2ccccc2cc1)=O
106437 C(N[C@@H](C(=O)OC)CO)(=O)OCc1ccccc1
106615 C([C@@H](Cc1ccc(cc1)O)N)(=O)OCC
106617 C([C@H](Cc1ccc(cc1)O)N)(=O)OCCC
106619 C([C@@H](Cc1ccc(cc1)O)N)(=O)OCCCC
106631 C([C@@H](Cc1ccc(Cl)cc1)N)(=O)OCCC
106633 C([C@@H](Cc1ccc(Cl)cc1)N)(=O)OCCCC
107356 N1(N=C(c2ccc(cc2)O)C[C@H]1c1c(OC)cccc1)C(=O)C
107364 N1(N=C(c2ccc(cc2)O)C[C@H]1c1c(OC)cccc1)C(=O)C

107369 N1(N=C(c2c(cc(cc2)O)O)C[C@H]1c1c(OC)cccc1)C(=O)C
107377 N1(N=C(c2c(cc(cc2)O)O)C[C@H]1c1c(OC)cccc1)C(=O)C
107382 N1(N=C(c2ccc(cc2)O)C[C@H]1c1ccc(OC)cc1)C(=O)C
107390 N1(N=C(c2ccc(cc2)O)C[C@H]1c1ccc(OC)cc1)C(=O)C
107394 N1(N=C(c2c(cc(cc2)O)O)C[C@H]1c1ccc(cc1)OC)C(=O)C
107406 N1(N=C(c2ccc(cc2)O)C[C@H]1c1c(cc(cc1)OC)OC)C(=O)C
107418 N1(N=C(c2c(cc(cc2)O)O)C[C@H]1c1c(cc(cc1)OC)OC)C(=O)C
107426 N1(N=C(c2c(cc(cc2)O)O)C[C@H]1c1c(cc(cc1)OC)OC)C(=O)C
107430 N1(N=C(c2ccc(cc2)O)C[C@H]1c1ccc(C)cc1)C(=O)C
107438 N1(N=C(c2ccc(cc2)O)C[C@H]1c1ccc(C)cc1)C(=O)C
107442 N1(N=C(c2c(cc(cc2)O)O)C[C@H]1c1ccc(cc1)C)C(=O)C
107450 N1(N=C(c2c(cc(cc2)O)O)C[C@H]1c1ccc(cc1)C)C(=O)C
107896 c1(c(cc(cc1C)C)C)[C@H](c1ccccc1)O
107898 c1([C@@H](OC(=O)C)c2ccccc2)c(cc(cc1C)C)C
107899 c1(c(cc(cc1C)C)C)[C@H](c1ccc(C)cc1)O
107901 c1([C@@H](OC(=O)C)c2ccc(C)cc2)c(cc(cc1C)C)C
107902 c1(c(cc(cc1C)C)C)[C@H](c1ccc(OC)cc1)O
107904 c1([C@@H](OC(=O)C)c2ccc(OC)cc2)c(cc(cc1C)C)C
107905 [N+](c1ccc([C@@H](c2c(cc(C)cc2C)C)O)cc1)([O–])=O
107907 [N+](c1ccc([C@@H](c2c(cc(C)cc2C)C)OC(=O)C)cc1)([O–])=O
108066 C(\[C@](c1ccccc1)(O)C)=C\c1ccccc1
110306 C([C@@H](C(=O)OCC)CCCCCC)(N1CCN(c2ncccn2)CC1)=O
110308 C([C@@H](C(=O)OCC)CCCCC)(N1CCN(c2ncccn2)CC1)=O
110310 C([C@@H](C(=O)OCC)CCC)(N1CCN(c2ncccn2)CC1)=O
110322 C([C@@H](C(=O)OCC)CCCC)(N1CCN(c2ncccn2)CC1)=O
110340 C([C@@H](C(=O)OCC)CCCCCCC)(N1CCN(c2ncccn2)CC1)=O
111538 C(#Cc1ccccc1)[C@@H](c1ccccc1)O
111546 C(#Cc1ccccc1)[C@H](c1cc(OC)ccc1)O
111547 C(#Cc1ccccc1)[C@@H](c1ccc(cc1)OC)O
111548 C(#Cc1ccccc1)[C@H](c1ccc(cc1)F)O
111549 C(#Cc1ccccc1)[C@H](c1cc(C)ccc1)O
111551 C(#Cc1ccccc1)[C@@H](c1ccc(cc1)Br)O
111552 C(#Cc1ccccc1)[C@@H](c1ccc(cc1)C)O
111553 C(#Cc1ccccc1)[C@H](c1c2c(cccc2)ccc1)O
111714 C([C@@H](Cc1ccccc1)C)(=O)OC
111822 N1(C(c2c3c(cccc3)ccc2)=O)[C@@H](CC(C1)(C)C)CC
111823 N1(C(c2c3c(cccc3)ccc2)=O)[C@@H](CC(C1)(C)C)CCC
111824 N1(C(c2c3c(cccc3)ccc2)=O)CC(CC[C@H]1CC)(C)C
112965 N1(C(c2c3c(cccc3)ccc2)=O)[C@@H](CC(C1)(C)C)C
112968 C(N1[C@@H](CCC1)CCC)(c1c2c(cccc2)ccc1)=O
112969 N1(C(c2c3c(cccc3)ccc2)=O)CC(C)(C)CC[C@H]1C
112970 C(N1[C@H](CCC)CCCC1)(c1c2c(cccc2)ccc1)=O
113038 N([C@H](c1occc1)C#N)C(c1ccccc1)c1ccccc1

113169 C(#Cc1ccccc1)[C@](c1ccc(cc1)F)(O)C
113170 C(#Cc1ccccc1)[C@](c1ccc(cc1)Cl)(O)C
113641 C(c1ccc(O[C@H](c2ccccc2)CCNC)cc1)(F)(F)F
113665 n1cn(CC[C@H](Oc2c(cc(cc2)Cl)Cl)c2ccccc2)cc1
113681 C(c1ccc(O[C@@H](CCn2cncc2)c2ccccc2)cc1)(F)(F)F
113705 n1cn(CC[C@H](Oc2ccc(Cl)cc2)c2ccccc2)cc1
113713 n1cn(CC[C@H](Oc2c(cc(cc2)Cl)Cl)c2ccc(cc2)Cl)cc1
114061 C([C@H](C[N+]([O–])=O)c1ccccc1)(C(=O)OC)C(=O)OC
114734 C([C@H](c1ccc(O)cc1)N)(=O)O
115000 C1(O[C@H](COC(=O)c2ccccc2)c2c1cccc2)=O
115395 C(N[C@@H](Cc1ccccc1)COCc1ccccc1)(OC(C)(C)C)=O
115396 c1([C@H](NC(OC(C)(C)C)=O)COCc2ccccc2)nccs1
115521 [N+](c1c([C@@H](CC(=O)C)O)cccc1)([O–])=O
115853 c1(c(cc(cc1)Cl)Cl)[C@H](Cn1cncc1)O
115858 c1(c(cc(cc1)Cl)Cl)[C@H](Cn1cncc1)O
115979 N1(C([C@](c2ccccc2)(CC)C(NC1=O)=O)=O)C
116056 C(N[C@H](C(=O)O)CCC)(=O)OCc1ccccc1
116281 C([C@H](C[N+]([O–])=O)c1ccc(F)cc1)(C(=O)OC)C(=O)OC
116286 C([C@H](C[N+]([O–])=O)c1ccc(OC)cc1)(C(=O)OC)C(=O)OC
116292 C([C@@H](c1sccc1)C[N+]([O–])=O)(C(=O)OC)C(=O)OC
117044 C(N[C@H](C(=O)O)CC(C)C)(=O)OC
117157 N1(N=C(c2ccc(cc2)F)C[C@H]1c1ccc(cc1)Cl)C(=S)N
117174 N1(N=C(c2ccc(cc2)F)C[C@H]1c1ccc(cc1)C)C(=S)N
117191 N1(N=C(c2ccc(cc2)F)C[C@H]1c1occc1)C(=S)N
117918 C1(c2c(cccc2)CC[C@@H]1ONc1ccccc1)=O
117952 C(#Cc1ccccc1)[C@@](c1cc(OC)ccc1)(O)C
118245 C(#Cc1ccccc1)[C@@H](c1ccc(cc1)Cl)O
118705 N1c2c(CC[C@H]1c1ccccc1)cccc2
119568 C([C@H](Cc1ccc(cc1)F)O)(=O)O
119569 C([C@H](Cc1ccc(cc1)Cl)O)(=O)O
119570 C([C@H](Cc1ccc(cc1)Br)O)(=O)O
119571 C([C@@H](Cc1ccc(O)cc1)O)(=O)O
121326 C(C(OC(C)C)=O)(C(OC(C)C)=O)[C@@H](C[N+]([O–])=O)c1ccccc1
121348 C([C@@H](C[N+]([O–])=O)c1ccc(F)cc1)(C(=O)OCC)C(=O)OCC
123961 C([C@H](C[N+]([O–])=O)c1ccc(Cl)cc1)(C(=O)OC)C(=O)OC
123962 C([C@H](C[N+]([O–])=O)c1ccc(Br)cc1)(C(=O)OC)C(=O)OC
124149 C(N[C@H](C(=O)O)CCC)(=S)NCCC
124150 C(N[C@H](C(=O)O)CCC)(=S)NCCCC
124159 C(NC(C(=O)O)CCCC)(=S)NCCC
124160 C(N[C@H](C(=O)O)CCCC)(=S)NCCCC
124197 C(NC(C(=O)O)CCc1ccccc1)(=S)NC
124198 C(NC(C(=O)O)CCc1ccccc1)(=S)NCC
124199 C(NC(C(=O)O)CCc1ccccc1)(=S)NCCC

124200 C(NC(C(=O)O)CCc1ccccc1)(=S)NCCCC
124227 c1(c[nH]c2c1cccc2)C[C@H](NC(=S)NC)C(=O)O
124228 c1(c[nH]c2c1cccc2)C[C@H](NC(=S)NCC)C(=O)O
124229 c1(c[nH]c2c1cccc2)C[C@H](NC(=S)NCCC)C(=O)O
124230 c1(c[nH]c2c1cccc2)C[C@H](NC(=S)NCCCC)C(=O)O
124278 N1(C(=S)NCCC)[C@@H](C(=O)O)CCCC1
124279 N1(C(=S)NCCCC)[C@@H](C(=O)O)CCCC1
124297 C(N[C@H](C(=O)O)CCC(=O)O)(=S)NCCC
124298 C(N[C@H](C(=O)O)CCC(=O)O)(=S)NCCCC
125998 c1([C@H](CC(=O)c2ccccc2)O)c2c(cccc2)ccc1
126051 C(C(OC(C)(C)C)=O)(C(OC(C)(C)C)=O)[C@H](C[N+]([O–])=O)c1ccccc1
126055 C([C@H](C[N+]([O–])=O)c1ccc(C)cc1)(C(=O)OCC)C(=O)OCC
126056 C([C@@H](C[N+]([O–])=O)c1ccc(OC)cc1)(C(=O)OCC)C(=O)OCC
126057 C([C@H](C[N+]([O–])=O)c1ccc(Br)cc1)(C(=O)OCC)C(=O)OCC
126058 C([C@@H](c1c(Cl)cccc1)C[N+]([O–])=O)(C(=O)OCC)C(=O)OCC
126062 C([C@@H](c1occc1)C[N+]([O–])=O)(C(=O)OCC)C(=O)OCC
126248 C(#Cc1ccccc1)[C@](c1ccccc1)(O)C
126252 C(#Cc1ccccc1)[C@](c1cc(Cl)ccc1)(O)C
128036 C([C@H](CC(=O)C)c1ccccc1)(C(=O)OC)C(=O)OC
128037 C([C@H](CC(=O)C)c1ccccc1)(C(=O)OCC)C(=O)OCC
128038 C(C(OC(C)C)=O)(C(OC(C)C)=O)[C@H](CC(=O)C)c1ccccc1
128043 C([C@@H](c1c(C(F)(F)F)cccc1)CC(=O)C)(C(=O)OCC)C(=O)OCC
128044 C([C@@H](c1occc1)CC(=O)C)(C(=O)OCC)C(=O)OCC
128661 c1(c[nH]c2c1cccc2)C[C@@H](C(=O)OC)N
128667 c1(c[nH]c2c1cccc2)C[C@H](C(=O)OCC)N
128685 c1(c[nH]c2c1cccc2)C[C@H](N)CO
128806 C([C@H](c1ccccc1)O)(=O)OC
128915 C(N[C@H](C(=O)O)C(C)C)(=O)N
128921 C(N[C@H](C(=O)O)CO)(=O)N
129823 N1(N[C@H](c2cc3OCOc3cc2CC1=O)c1ccc(cc1)N)C(=O)NC
129829 N1(N[C@H](c2cc3OCOc3cc2CC1=O)c1ccc(cc1)N)C(=O)NCC
129835 N1(N[C@H](c2cc3OCOc3cc2CC1=O)c1ccc(cc1)N)C(=O)NCCC
130406 C(N[C@H](C(=O)O)CCC)(Nc1cc(cc(c1)Cl)Cl)=S
130463 C(N[C@H](C(=O)O)CO)(Nc1c(c(Cl)ccc1)Cl)=S
130464 C(N[C@H](C(=O)O)CO)(Nc1cc(cc(c1)Cl)Cl)=S
130484 C(N[C@H](C(=O)O)Cc1ccccc1)(Nc1c(cc(cc1)F)F)=S
130487 C(N[C@H](C(=O)O)Cc1ccccc1)(Nc1c(cc(cc1)F)F)=O
130522 c1(c[nH]c2c1cccc2)C[C@H](NC(Nc1c(cc(cc1)F)F)=S)C(=O)O
130525 c1(c[nH]c2c1cccc2)C[C@H](NC(Nc1c(cc(cc1)F)F)=O)C(=O)O
130531 c1(c2c(ccc(c2)C)[nH]c1)C[C@H](NC(Nc1c(cc(cc1)F)F)=S)C(=O)O
130533 c1(c2c(ccc(c2)C)[nH]c1)C[C@H](NC(Nc1c(cc(cc1)F)F)=O)C(=O)O
130538 C(N[C@H](C(=O)O)Cc1ccc(O)cc1)(Nc1c(cc(cc1)F)F)=S
130541 C(N[C@H](C(=O)O)Cc1ccc(O)cc1)(Nc1c(cc(cc1)F)F)=O

130547 C(N[C@H](C(=O)O)Cc1cc(O)ccc1)(Nc1c(cc(cc1)F)F)=S
130549 C(N[C@H](C(=O)O)Cc1cc(O)ccc1)(Nc1c(cc(cc1)F)F)=O
130553 C(N[C@H](CC(=O)O)c1ccccc1)(Nc1c(cc(cc1)F)F)=S
130555 C(NC(CC(=O)O)c1ccccc1)(Nc1c(cc(cc1)F)F)=O
130561 C(Nc1c(cc(cc1)F)F)(N[C@H](C(=O)O)CC)=S
130590 C(N[C@@H](C(=O)O)CC=C)(Nc1cc(cc(c1)Cl)Cl)=S
130592 C(N1[C@H](C(=O)O)CCC1)(Nc1c(cc(cc1)F)F)=S
130593 C(N1[C@H](C(=O)O)CCC1)(Nc1c(c(Cl)ccc1)Cl)=S
130594 C(N1[C@H](C(=O)O)CCC1)(Nc1cc(Cl)cc(c1)Cl)=S
130596 C(N1C[C@@H](C(=O)O)CCC1)(Nc1c(cc(cc1)F)F)=S
130598 C(N1[C@@H](C(=O)O)CCCC1)(Nc1c(cc(cc1)F)F)=S
130613 C(Nc1c(c(Cl)ccc1)Cl)(N[C@@H](CC(=O)O)C(=O)O)=S
130614 C(N[C@@H](CC(=O)O)C(=O)O)(Nc1cc(cc(c1)Cl)Cl)=S
135510 C([C@@H](NC(=O)C)CC(C)C)(=O)O
136160 C([C@H](Oc1ccc(C)cc1)CC)(=O)O
136218 C(#Cc1ccccc1)[C@](c1ccc(cc1)Br)(O)C
136221 C(#Cc1ccccc1)[C@@](c1cc(C)ccc1)(O)C
136224 C(#Cc1ccccc1)[C@@](c1ccc(cc1)C)(O)C
136758 N1(C([C@@](c2ccccc2)(C)C(NC1=O)=O)=O)C
136773 N1(C([C@@](c2ccccc2)(CCC)C(NC1=O)=O)=O)C
136779 N1(C([C@@](c2ccccc2)(CCC)C(NC1=O)=O)=O)C
136786 N1(C([C@@](C2=CCCCC2)(CC)C(NC1=O)=O)=O)C
136787 N1(C([C@@](c2ccccc2)(CCCC)C(NC1=O)=O)=O)C
136793 N1(C([C@@](c2ccccc2)(CCCC)C(NC1=O)=O)=O)C
136807 N1(C([C@@](C2=CCCCC2)(C)C(NC1=O)=O)=O)CC
136814 N1(C([C@](C2=CCCCC2)(C)C(NC1=O)=O)=O)CCC
136938 N=1C(C(Nc2c(C1c1ccccc1)cc(Cl)cc2)=O)(Cc1ccccc1)CO
136942 N1=C(c2c(ccc(c2)Cl)NC([C@H]1CO)=O)c1ccccc1
139143 C(#Cc1ccccc1)[C@@H](c1cc2ccccc2cc1)O
139147 C(#Cc1ccccc1)[C@@](c1ccc(cc1)OC)(O)C
139706 C12=C(NC(=O)N[C@@H]1c1ccccc1)CC(CC2=O)(C)C
139714 C12=C(NC(=O)N[C@@H]1c1c(Cl)cccc1)CC(CC2=O)(C)C
139722 C12=C(NC(=O)N[C@@H]1c1cc(Cl)ccc1)CC(CC2=O)(C)C
139730 C12=C(NC(=O)N[C@@H]1c1ccc(Cl)cc1)CC(CC2=O)(C)C
139738 C12=C(NC(=O)N[C@@H]1c1c(Br)cccc1)CC(CC2=O)(C)C
139746 C12=C(NC(=O)N[C@@H]1c1cc(Br)ccc1)CC(CC2=O)(C)C
139754 C12=C(NC(=O)N[C@@H]1c1ccc(Br)cc1)CC(CC2=O)(C)C
139762 C12=C(NC(=O)N[C@@H]1c1c(C)cccc1)CC(CC2=O)(C)C
139770 C12=C(NC(=O)N[C@@H]1c1cc(C)ccc1)CC(CC2=O)(C)C
139778 C12=C(NC(=O)N[C@@H]1c1ccc(C)cc1)CC(CC2=O)(C)C
139788 C12=C(NC(=O)N[C@@H]1c1c(OC)cccc1)CC(CC2=O)(C)C
139796 C12=C(NC(=O)N[C@@H]1c1cc(OC)ccc1)CC(CC2=O)(C)C
139810 C12=C(N(C(=O)N[C@@H]1c1ccccc1)C)CC(CC2=O)(C)C

139812 C12=C(N(C(=O)N[C@@H]1c1c(Cl)cccc1)C)CC(CC2=O)(C)C
139814 C12=C(N(C(=O)N[C@@H]1c1cc(Cl)ccc1)C)CC(CC2=O)(C)C
139816 C12=C(N(C(=O)N[C@@H]1c1ccc(Cl)cc1)C)CC(CC2=O)(C)C
139818 C12=C(N(C(=O)N[C@@H]1c1c(Br)cccc1)C)CC(CC2=O)(C)C
139820 C12=C(N(C(=O)N[C@@H]1c1cc(Br)ccc1)C)CC(CC2=O)(C)C
139822 C12=C(N(C(=O)N[C@@H]1c1ccc(Br)cc1)C)CC(CC2=O)(C)C
139824 C12=C(N(C(=O)N[C@@H]1c1c(C)cccc1)C)CC(CC2=O)(C)C
139826 C12=C(N(C(=O)N[C@@H]1c1cc(C)ccc1)C)CC(CC2=O)(C)C
139828 C12=C(N(C(=O)N[C@@H]1c1ccc(C)cc1)C)CC(CC2=O)(C)C
139830 C12=C(N(C(=O)N[C@@H]1c1c(OC)cccc1)C)CC(CC2=O)(C)C
139832 C12=C(N(C(=O)N[C@@H]1c1cc(OC)ccc1)C)CC(CC2=O)(C)C
141244 c1([C@H](CC(=O)C)O)c(Br)cccc1
141368 C([C@@H](Cc1ccccc1)C)(=O)O
142694 N([C@](C(OC(C)(C)C)=O)(C#N)c1ccccc1)(C(=O)OC)NC(=O)OC
142697 N([C@](C(OC(C)(C)C)=O)(C#N)c1ccc(OC)cc1)(C(=O)OC)NC(=O)OC
142698 N([C@](C(OC(C)(C)C)=O)(C#N)c1ccc(Cl)cc1)(C(=O)OC)NC(=O)OC
142699 N([C@](C(OC(C)(C)C)=O)(C#N)c1ccc(C)cc1)(C(=O)OC)NC(=O)OC
142955 C(N[C@@H](C(OC(C)C)=O)Cc1ccccc1)(OC(C)(C)C)=O
143387 C1([C@@](Cc2ccccc2)(O)CCCC1)=O
143517 C(#Cc1ccccc1)[C@@H](c1cc(Cl)ccc1)O
143703 C1(=C(N(C=C[C@H]1c1ccc([N+]([O–])=O)cc1)c1ccc(OC)cc1)C)C(=O)OCC
143704 C1(=C(N(C=C[C@H]1c1ccc([N+]([O–])=O)cc1)c1cc(OC)ccc1)C)C(=O)OCC
143710 C1(=C(N(C=C[C@H]1c1ccc([N+]([O–])=O)cc1)c1ccc(OC)cc1)C)C(=O)OC
143713 C1(=C(N(C=C[C@H]1c1ccc([N+]([O–])=O)cc1)c1cc(OC)ccc1)C)C(=O)OC
143719 C1(=C(N(C=C[C@H]1c1c([N+]([O–])=O)cccc1)c1ccc(cc1)OC)C)C(=O)OCC
143720 C1(=C(N(C=C[C@H]1c1c([N+]([O–])=O)cccc1)c1cc(OC)ccc1)C)C(=O)OCC
143721 C1(=C(N(C=C[C@H]1c1c([N+]([O–])=O)cccc1)c1ccc(cc1)OC)C)C(=O)OC
143722 C1(=C(N(C=C[C@H]1c1c([N+]([O–])=O)cccc1)c1cc(OC)ccc1)C)C(=O)OC
145713 [N+](c1c([C@H](CC(=O)CC)O)cccc1)([O–])=O
146171 P(C[C@@H]1C(=O)CCC1)(=O)(OCC)OCC
146173 P(C[C@@H]1C(=O)COC1)(=O)(OCC)OCC
147344 C([C@H](NC(=O)CN)CO)(=O)O
147350 C([C@H](NC(=O)CN)C(C)C)(=O)O
148538 C(Nc1c(OCCCCCCC)cccc1)(O[C@@H](CN1CCN(C)CC1)COC)=O
148568 C(Nc1ccc(OCCC)cc1)(O[C@@H](CN1CCN(C)CC1)COC)=O
148574 C(Nc1ccc(OCCCC)cc1)(O[C@@H](CN1CCN(C)CC1)COC)=O
151693 C(C(=O)c1ccccc1)[C@@H](c1cc2ccccc2cc1)O
152426 N1C(c2ccccc2N[C@@H]1c1ccccc1)=O
152820 C(N[C@H](C(=O)OC)c1ccccc1)(=O)OCc1ccccc1
158126 C([C@@H](c1ccc(Cl)cc1)CC(=O)C)(C(=O)OCC)C(=O)OCC
158127 C([C@@H](c1ccc(Br)cc1)CC(=O)C)(C(=O)OCC)C(=O)OCC
158131 C([C@@H](c1ccc(C)cc1)CC(=O)C)(C(=O)OCC)C(=O)OCC
158134 C([C@@H](c1ccc(OC)cc1)CC(=O)C)(C(=O)OCC)C(=O)OCC

158137 C([C@@H](c1sccc1)CC(=O)C)(C(=O)OCC)C(=O)OCC
158258 c1([C@@H]2CC(=O)CC2)ccc(cc1)OC
162728 C([C@@H](C[N+]([O–])=O)c1ccccc1)(C(=O)OCC)(C(=O)OCC)F
164148 N(C(c1ccccc1)c1ccccc1)[C@@H](C#N)c1ccc(OC)cc1
164151 N([C@@H](c1sccc1)C#N)C(c1ccccc1)c1ccccc1
164295 C1(=C(NC=2CC(C)(C)CC(C2[C@H]1c1ccccc1)=O)C)C(=O)OCC
164296 C1(=C(NC=2CC(C)(C)CC(C2[C@H]1c1ccc(cc1)Br)=O)C)C(=O)OCC
164304 C1(=C(NC=2CC(C)(C)CC(C2[C@H]1c1ccc(C#N)cc1)=O)C)C(=O)OCC
164386 c1([C@@H]2CC(=O)CC2)cc(Br)ccc1
164387 c1([C@H]2CC(=O)CC2)ccc(cc1)F
164494 C1([C@](c2ccccc2N1)(c1ccc(cc1)C)C)=O
164495 C1([C@](c2ccccc2N1)(c1ccc(cc1)C)CC)=O
164732 C(C(OC(C)(C)C)=O)(C(OC(C)(C)C)=O)[C@@H](c1cc(OC)c(cc1)OC)C[N+]([O–])=O
164736 C([C@@H](c1occc1)C[N+]([O–])=O)(C(OC(C)(C)C)=O)C(OC(C)(C)C)=O
165840 C([C@H](c1c(Cl)cccc1)C[N+]([O–])=O)(C(=O)OC)C(=O)OC
166222 C([C@@H](C[N+]([O–])=O)c1ccc(Cl)cc1)(C(=O)OCC)C(=O)OCC
166223 C([C@H](c1c(C(F)(F)F)cccc1)C[N+]([O–])=O)(C(=O)OCC)C(=O)OCC
166224 C([C@H](c1c(cc(cc1)Cl)Cl)C[N+]([O–])=O)(C(=O)OCC)C(=O)OCC
168178 c1(n(c2ccc(C([C@@H](N3CCN(c4cc(C(F)(F)F)ccc4)CC3)C)=O)cc2o1)C)=O
168190 c1(n(c2ccc(C([C@@H](N3CCN(CC3)c3ccc(cc3)F)C)=O)cc2o1)C)=O
168195 c1([nH]c2ccc(C([C@@H](N3CCN(c4cc(C(F)(F)F)ccc4)CC3)C)=O)cc2o1)=O
168206 c1([nH]c2ccc(C([C@@H](N3CCN(CC3)c3ccc(cc3)F)C)=O)cc2o1)=O
168470 C(N[C@@H](C(=O)O)CC(C)C)(OC(C)(C)C)=O
168530 C(N[C@H](C(=O)OCC)CC(C)C)(OC(C)(C)C)=O
168788 N1(c2c(OC)cccc2)CCN(CC1)C[C@@H](COc1c2c(cccc2)ccc1)O
168797 N1(c2ccc(cc2)O)CCN(CC1)C[C@@H](COc1c2c(cccc2)ccc1)O
168805 N1(c2ccc(cc2)OC)CCN(CC1)C[C@@H](COc1c2c(cccc2)ccc1)O
168813 N1(c2ccc(cc2)OCC)CCN(CC1)C[C@@H](COc1c2c(cccc2)ccc1)O
168829 N1(c2ccc(cc2)Cl)CCN(CC1)C[C@@H](COc1c2c(cccc2)ccc1)O
168845 N1(c2cc(OC)ccc2)CCN(C[C@@H](COc2c3c(cccc3)ccc2)O)CC1
168853 N1(c2cc(OCC)ccc2)CCN(C[C@@H](COc2c3c(cccc3)ccc2)O)CC1
168861 N1(c2cc(Cl)ccc2)CCN(C[C@@H](COc2c3c(cccc3)ccc2)O)CC1
169507 C1(S(=O)(=O)c2ccccc2)(S(=O)(=O)c2ccccc2)CC(=C)[C@H](C1)C(OC)(C)C
169508 C1(S(=O)(=O)c2ccccc2)(S(=O)(=O)c2ccccc2)C\C(=C\c2ccccc2)[C@H](C1)C(OC)(C)C
171775 c12c([nH]cc2)cccc1OC[C@H](CNC(C)C)O
176561 n1c(Nc2cc(OC(C)C)[nH]n2)c(Cl)cnc1N[C@H](c1ncc(cn1)F)C
180115 C(c1cc(C(F)(F)F)cc(NNC([C@H](N2CCN(CC2)C)c2c(F)cccc2)=O)c1)(F)(F)F
180120 c1([C@H](C(NNc2cc(C(F)(F)F)cc(C(F)(F)F)c2)=O)N2CCN(C)CC2)c(c(F)ccc1)F
180122 c1([C@H](C(NNc2cc(C(F)(F)F)cc(C(F)(F)F)c2)=O)N2CCN(CC2)C)c(F)cccc1F
181223 C(C(OC(C)(C)C)=O)(c1n(ccc1)CC)C(C(=O)OCC)C(=O)OCC
181229 C([C@H](c1c(cc[nH]1)C)C(C(=O)OCC)C(=O)OCC)(OC(C)(C)C)=O
181297 C([C@@H](c1cc(Cl)c(cc1)Cl)C[N+]([O–])=O)(C(=O)OCC)C(=O)OCC
181530 C(C(=O)OCC)[C@@H](c1ccccc1)O

183380 c12nc(n3c(ncc3)c3ccccc3)ncc1N(C(=O)[C@@]1(N2CCCC1)CC)C
183381 c12nc(n3c(ncc3)c3cc(F)ccc3)ncc1N(C(=O)[C@@]1(N2CCCC1)CC)C
183384 c12nc(n3cncc3)ncc1N(C(=O)[C@@]1(N2CCCC1)CC)C
188645 c1([C@H](OC(=O)C)Cn2cncc2)c(cc(cc1)Cl)Cl
189350 n1c(Nc2n[nH]c(c2)C)c(Cl)cnc1N[C@H](c1ncc(cn1)F)C
197212 C(O[C@H](C#N)c1ccccc1)(=O)c1ccccc1
197558 c1(C([C@H](OCc2cc3ccccc3cc2)Cc2ccccc2)=O)n(ccn1)C
197564 c1(C([C@H](OCc2cc3ccccc3cc2)Cc2ccc(C(C)(C)C)cc2)=O)n(ccn1)C
197567 C([C@@H](OCc1cc2ccccc2cc1)Cc1ccccc1)(=O)OC
197568 C([C@@H](OCc1cc2ccccc2cc1)Cc1ccc(C(C)(C)C)cc1)(=O)OC
198803 c1([C@](c2ccccc2)(O)C)c(C)cccc1
198809 c1([C@@](c2ccccc2)(O)C)c(OC)cccc1
198811 c1([C@@](c2ccccc2)(O)C)ccc(cc1)OC
199352 [N+](c1c([C@@H](CC(=O)CO)O)cccc1)([O–])=O
200523 C(N[C@@H](C(C#N)C#N)c1c(C)cccc1)(OC(C)(C)C)=O
200524 C(N[C@@H](C(C#N)C#N)c1ccc(cc1)C)(OC(C)(C)C)=O
200685 c1([C@@]2(C(Nc3c2cccc3)=O)Cc2ccccc2)c(oc(c1)c1ccccc1)c1ccccc1
200686 c1([C@@]2(C(Nc3c2cccc3)=O)Cc2ccccc2)c(oc(c1)c1ccc(cc1)F)c1ccc(F)cc1
200687 c1([C@@]2(C(Nc3c2cccc3)=O)Cc2ccccc2)c(oc(c1)c1ccc(cc1)Cl)c1ccc(Cl)cc1
200688 c1([C@@]2(C(Nc3c2cccc3)=O)Cc2ccccc2)c(oc(c1)c1ccc(cc1)Br)c1ccc(Br)cc1
200689 c1([C@@]2(C(Nc3c2cccc3)=O)Cc2ccccc2)c(oc(c1)c1cc(Cl)ccc1)c1cc(Cl)ccc1
200691 c1([C@@]2(C(Nc3c2cccc3)=O)Cc2ccccc2)c(oc(c1)c1cc(OC)ccc1)c1cc(OC)ccc1
200692 c1([C@@]2(C(Nc3c2cccc3)=O)Cc2ccccc2)c(oc(c1)c1cc2ccccc2cc1)c1cc2ccccc2cc1
200694 c1([C@@]2(C(Nc3c2cccc3)=O)Cc2cc(F)ccc2)c(oc(c1)c1ccccc1)c1ccccc1
200695 c1([C@@]2(C(Nc3c2cccc3)=O)Cc2c(F)cccc2)c(oc(c1)c1ccccc1)c1ccccc1
200696 c1([C@@]2(C(Nc3c2cccc3)=O)Cc2cc(C)ccc2)c(oc(c1)c1ccccc1)c1ccccc1
200697 c1([C@@]2(C(Nc3c2cccc3)=O)Cc2c(OC)cccc2)c(oc(c1)c1ccccc1)c1ccccc1
200698 c1([C@@]2(C(Nc3c2cccc3)=O)Cc2ccc(cc2)OC)c(oc(c1)c1ccccc1)c1ccccc1
200705 c1([C@@]2(C(Nc3c2cccc3)=O)Cc2ccccc2)c([nH]c(c1)c1ccccc1)c1ccccc1
200706 c1([C@@]2(C(Nc3c2cccc3)=O)Cc2ccccc2)c([nH]c(c1)c1ccc(cc1)F)c1ccc(F)cc1
200707 c1([C@@]2(C(Nc3c2cccc3)=O)Cc2ccccc2)c([nH]c(c1)c1ccc(cc1)Cl)c1ccc(Cl)cc1
200708 c1([C@@]2(C(Nc3c2cccc3)=O)Cc2ccccc2)c([nH]c(c1)c1ccc(cc1)Br)c1ccc(Br)cc1
200709 c1([C@@]2(C(Nc3c2cccc3)=O)Cc2ccccc2)c([nH]c(c1)c1cc(Cl)ccc1)c1cc(Cl)ccc1
200710 c1([C@@]2(C(Nc3c2cccc3)=O)Cc2ccccc2)c([nH]c(c1)c1cc(OC)ccc1)c1cc(OC)ccc1
200711 c1([C@@]2(C(Nc3c2cccc3)=O)Cc2ccccc2)c([nH]c(c1)c1cc2ccccc2cc1)c1cc2ccccc2cc1
200712 c1([C@@]2(C(Nc3c2cccc3)=O)Cc2cc(F)ccc2)c([nH]c(c1)c1ccccc1)c1ccccc1
200714 c1([C@@]2(C(Nc3c2cccc3)=O)Cc2cc(C)ccc2)c([nH]c(c1)c1ccccc1)c1ccccc1
200715 c1([C@@]2(C(Nc3c2cccc3)=O)Cc2c(OC)cccc2)c([nH]c(c1)c1ccccc1)c1ccccc1
200716 c1([C@@]2(C(Nc3c2cccc3)=O)Cc2ccc(cc2)OC)c([nH]c(c1)c1ccccc1)c1ccccc1
200718 c1([C@@]2(C(Nc3c2cccc3)=O)Cc2c3c(cccc3)ccc2)c([nH]c(c1)c1ccccc1)c1ccccc1
200720 c1([C@@]2(C(Nc3c2cccc3)=O)C)c([nH]c(c1)c1ccccc1)c1ccccc1
200721 c1([C@@]2(C(Nc3c2cccc3)=O)CCCC)c([nH]c(c1)c1ccccc1)c1ccccc1
200723 c1([C@@]2(C(Nc3c2cccc3)=O)Cc2c(F)cccc2)c([nH]c(c1)c1ccccc1)c1ccccc1

200749 C(N[C@@H](C(=O)OCC)Cc1ccccc1)(OC(C)(C)C)=O
200900 c12c(c3ccccc3[nH]1)CC[N@@]([C@H]2c1ccc(Br)cc1)Cc1c2c(cccc2)ccc1
200913 c12c(c3ccccc3[nH]1)CC[N@@]([C@H]2c1ccccc1)Cc1c2c(cccc2)ccc1
200914 c12c(c3ccccc3[nH]1)CC[N@@]([C@H]2c1ccc(OC)cc1)Cc1c2c(cccc2)ccc1
200966 C([C@@H](CC(=O)OC)c1ccccc1)(C(=O)OC)C(=O)OC
200977 C([C@@H](CC(=O)OC)c1ccccc1)(C(=O)OCC)C(=O)OCC
201588 N1([C@H](c2ccccc2CC1)Cc1ccccc1)C(=O)OC
202955 C1([C@@](c2ccccc2)(O)CCCC1)=O
204377 C=1([C@]2(C(Nc3c2cccc3OC)=O)C(OC1C)=O)[Si](C(C)C)(C(C)C)C(C)C
204378 C=1([C@]2(C(Nc3c2cc(cc3)Br)=O)C(OC1C)=O)[Si](C(C)C)(C(C)C)C(C)C
205423 C1([C@](c2ccccc2)(CO)CCCC1)=O
206419 C([C@H]1[N@@](NC(=O)c2ccccc2)CCc2ccccc12)#Cc1ccccc1
206421 C([C@H]1[N@@](NC(=O)c2ccccc2)CCc2cc(C)ccc12)#Cc1ccccc1
206424 C([C@H]1[N@@](NC(=O)c2ccccc2)CCc2cc(Br)ccc12)#Cc1ccccc1
206426 C([C@H]1[N@@](NC(=O)c2ccccc2)CCc2cc(OC)ccc12)#Cc1ccccc1
206428 C([C@H]1[N@@](NC(=O)c2ccccc2)CCc2ccccc12)#Cc1c(C)cccc1
206429 C([C@H]1[N@@](NC(=O)c2ccccc2)CCc2ccccc12)#Cc1cc(C)ccc1
206430 C([C@H]1[N@@](NC(=O)c2ccccc2)CCc2ccccc12)#Cc1ccc(C)cc1
206432 C([C@H]1[N@@](NC(=O)c2ccccc2)CCc2ccccc12)#Cc1ccc(OC)cc1
206433 C([C@H]1[N@@](NC(=O)c2ccccc2)CCc2ccccc12)#CC1=CCCCC1
206435 C([C@H]1[N@@](NC(=O)c2ccccc2)CCc2ccccc12)#CC1CC1
206436 C([C@H]1[N@@](NC(=O)c2ccccc2)CCc2ccccc12)#CC1CCCC1
206438 C([C@]1([N@@](NC(=O)c2ccccc2)CCc2c1cccc2)C)#Cc1ccccc1
206439 C([C@]1([N@@](NC(=O)c2ccccc2)CCc2c1cccc2)C)#Cc1ccc(C)cc1
206441 C([C@]1([N@@](NC(=O)c2ccccc2)CCc2c1cccc2)C)#Cc1ccc(OC)cc1
206442 C([C@]1([N@@](NC(=O)c2ccccc2)CCc2c1cccc2)C)#CC1=CCCCC1
206443 C([C@]1([N@@](NC(=O)c2ccccc2)CCc2c1cccc2)C)#CC1CC1
206444 C([C@]1([N@@](NC(=O)c2ccccc2)CCc2c1cccc2)C)#CC1CCCC1
206707 c1([C@H]2CC(=O)CC2)ccc(cc1)Br
206709 c1([C@H]2CC(=O)CC2)ccc(C(=O)C)cc1
208360 C(\[C@@](C(OC(C)(C)C)=O)(C#N)c1ccccc1)(=C\C(=O)OC)C(=O)OC
208361 C(\[C@@](C(OC(C)(C)C)=O)(C#N)c1ccc(OC)cc1)(=C\C(=O)OC)C(=O)OC
208362 C(\[C@@](C(OC(C)(C)C)=O)(C#N)c1ccc(C)cc1)(=C\C(=O)OC)C(=O)OC
208363 C(\[C@@](C(OC(C)(C)C)=O)(C#N)c1ccc(Cl)cc1)(=C\C(=O)OC)C(=O)OC
209489
C(C(Oc1ccccc1)=O)(C(Oc1ccccc1)=O)[C@@H](c1cc(C(C)(C)C)c(c(c1)C(C)(C)C)O)c1ccc([N+]([O–])=O)cc1
209491 C(C(Oc1ccccc1)=O)(C(Oc1ccccc1)=O)[C@@H](c1cc(c(O)c(c1)C(C)(C)C)C(C)(C)C)c1cc(Br)ccc1
209494
C(C(Oc1ccccc1)=O)(C(Oc1ccccc1)=O)[C@@H](c1cc(c(O)c(c1)C(C)(C)C)C(C)(C)C)c1cc(OC)c(cc1)OC
209495
C([C@@H](c1cc(c(O)c(c1)C(C)(C)C)C(C)(C)C)c1c2c(cccc2)ccc1)(C(Oc1ccccc1)=O)C(Oc1ccccc1)=O
209498 C(C(Oc1ccccc1)=O)(C(Oc1ccccc1)=O)[C@@H](c1cc(C(C)(C)C)c(c(c1)C(C)(C)C)O)C(C)(C)C

209806 O1c2c(CC[C@H]1c1ccccc1)cccc2
210534 c1(NC[C@@H](c2ccccc2)OC)c(cc(F)cc1F)F
210535 c1(c(c(F)c(c(c1F)F)F)F)NC[C@@H](c1ccccc1)OC
210536 c1(NC[C@@H](c2ccccc2)O)c(cc(F)cc1F)F
210688 c12[C@@H](NCCc2cc(c(c1)OC)OC)c1ccccc1
210695 c12[C@@H](c3c(C)cccc3)NCCc2cc(c(c1)OC)OC
210696 c12[C@@H](c3c(OC)cccc3)NCCc2cc(c(c1)OC)OC
210698 c12[C@@H](c3c(cc(cc3)OC)OC)NCCc2cc(c(c1)OC)OC
210701 c12[C@@H](c3c(Cl)cccc3)NCCc2cc(c(c1)OC)OC
210702 c12[C@@H](c3c(Br)cccc3)NCCc2cc(c(c1)OC)OC
210706 c1([C@@H]2c3c(cccc3)CCN2)c(Cl)cccc1
210709 c12[C@@H](c3c(Cl)cccc3)NCCc1cc(cc2)OC
210710 c12[C@@H](c3c(C)cccc3)NCCc1ccc(c2)OC
210711 c12[C@@H](c3c(OC)cccc3)NCCc1ccc(c2)OC
210712 c12[C@@H](c3c(Cl)cccc3)NCCc1ccc(c2)OC
210713 c12[C@@H](c3c(Br)cccc3)NCCc1ccc(c2)OC
211297 N1([C@@H](Cc2c(C1)cccc2)c1c(C)cccc1)C(=O)C
211972 C1(N(c2ccccc2[C@@]1(c1ccccc1)CC)C)=O
212400 C1([C@](c2cc3ccccc3cc2)(\C=C/C(=O)OCC)c2c(cccc2)N1)=O
212411 C1([C@@](C#CC(=O)OCC)(c2cc3ccccc3cc2)c2c(cccc2)N1)=O
216325 [nH]1c2c(c(OC[C@H](CNC(C)C)O)ccc2)c2c1cccc2
216463 c12c(c3c(cc(OC)cc3)oc1ccc(C(N[C@H](CC(C)C)CO)=O)c2)=O
216479 c12c(c3c(cc(OC)cc3)oc1ccc(C(N[C@H](C(C)C)CO)=O)c2)=O
216493 c12c(c3ccc(cc3oc1ccc(C(N[C@@H](CO)C)=O)c2)OC)=O
216502 c12c(c3ccc(cc3oc1ccc(C(NC[C@H](O)C)=O)c2)OC)=O

2. **Statistics for Each Cluster**

CSP CLUSTER ZSCORE NPAIR MEANDIFF STDEVDIFF
2966 1 4.43 2 0.64 0.04
2966 2 4.27 1 0.77 0.00
2966 3 4.21 1 0.76 0.00
2966 4 4.17 1 0.75 0.00
23735 1 11.52 12 0.43 0.23
23735 10 6.56 1 0.86 0.00
23735 11 6.54 1 0.86 0.00
23735 12 6.49 1 0.86 0.00
23735 13 6.39 1 0.84 0.00
23735 14 6.29 1 0.83 0.00
23735 15 6.21 1 0.82 0.00
23735 16 6.16 1 0.81 0.00
23735 17 6.16 1 0.81 0.00
23735 18 6.04 1 0.80 0.00
23735 19 6.03 1 0.80 0.00

23735 2 7.75 10 0.31 0.13
23735 20 5.80 1 0.76 0.00
23735 21 5.71 1 0.75 0.00
23735 22 5.71 1 0.75 0.00
23735 23 5.71 1 0.75 0.00
23735 24 5.70 1 0.75 0.00
23735 25 5.68 1 0.75 0.00
23735 26 5.62 2 0.51 0.15
23735 27 5.62 2 0.49 0.24
23735 28 5.61 2 0.49 0.27
23735 29 5.57 2 0.49 0.19
23735 3 7.20 1 0.95 0.00
23735 30 5.56 1 0.73 0.00
23735 31 5.56 1 0.73 0.00
23735 32 5.56 1 0.73 0.00
23735 33 5.55 1 0.73 0.00
23735 34 5.47 1 0.72 0.00
23735 35 5.47 2 0.48 0.08
23735 36 5.46 1 0.72 0.00
23735 37 5.45 1 0.72 0.00
23735 38 5.41 1 0.71 0.00
23735 39 5.34 1 0.70 0.00
23735 4 7.04 1 0.93 0.00
23735 40 5.33 1 0.70 0.00
23735 41 5.32 1 0.70 0.00
23735 42 5.19 1 0.68 0.00
23735 43 5.17 1 0.68 0.00
23735 44 5.14 2 0.46 0.07
23735 45 5.10 5 0.29 0.24
23735 46 5.08 2 0.45 0.24
23735 47 5.05 2 0.45 0.19
23735 48 5.05 1 0.67 0.00
23735 49 5.03 1 0.66 0.00
23735 5 6.93 6 0.35 0.03
23735 50 5.02 1 0.66 0.00
23735 51 5.00 2 0.45 0.43
23735 52 4.95 1 0.65 0.00
23735 53 4.92 1 0.65 0.00
23735 54 4.87 1 0.64 0.00
23735 55 4.86 1 0.64 0.00
23735 56 4.86 2 0.42 0.39
23735 57 4.85 1 0.64 0.00
23735 58 4.84 9 0.21 0.09

23735 59 4.83 2 0.43 0.35
23735 6 6.84 1 0.90 0.00
23735 60 4.82 4 0.31 0.30
23735 61 4.80 4 0.31 0.01
23735 62 4.79 5 0.27 0.11
23735 63 4.79 1 0.63 0.00
23735 64 4.79 2 0.43 0.35
23735 65 4.78 4 0.31 0.16
23735 7 6.81 1 0.90 0.00
23735 8 6.77 1 0.89 0.00
23735 9 6.60 1 0.87 0.00
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45167 20 5.52 1 0.68 0.00
45167 21 5.46 1 0.68 0.00
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45167 8 6.37 1 0.79 0.00
45167 9 6.31 1 0.78 0.00
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45172 6 4.52 1 0.51 0.00
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45173 16 5.86 2 0.62 0.06
45173 17 5.85 2 0.62 0.06
45173 18 5.82 2 0.62 0.06
45173 19 5.76 3 0.48 0.13
45173 2 8.29 12 0.35 0.20
45173 20 5.72 2 0.61 0.29
45173 21 5.70 2 0.61 0.32
45173 22 5.65 2 0.60 0.04
45173 23 5.61 2 0.60 0.26
45173 24 5.50 1 0.83 0.00
45173 25 5.49 2 0.58 0.46
45173 26 5.46 1 0.83 0.00
45173 27 5.43 2 0.57 0.01
45173 28 5.43 2 0.58 0.06
45173 29 5.24 3 0.43 0.13
45173 3 8.05 2 0.86 0.08
45173 30 5.23 1 0.79 0.00
45173 31 5.18 2 0.55 0.08
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45173 33 5.11 2 0.55 0.01
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45173 35 5.10 2 0.54 0.03
45173 36 5.10 2 0.55 0.11
45173 37 5.07 2 0.54 0.31
45173 38 5.06 2 0.55 0.11
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45173 4 7.33 10 0.34 0.14

45173 40 5.05 1 0.76 0.00
45173 41 5.04 3 0.42 0.24
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45173 44 4.95 3 0.41 0.08
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90220 2 4.12 1 0.64 0.00
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90589 13 4.31 2 0.47 0.02
90589 14 4.26 2 0.47 0.05
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90589 9 4.86 1 0.72 0.00
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90704 14 4.22 1 0.38 0.00
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90879 4 4.84 6 0.41 0.30
90879 5 4.76 2 0.77 0.17
90879 6 4.73 2 0.76 0.05
90879 7 4.71 1 0.98 0.00
90879 8 4.68 1 0.97 0.00
90879 9 4.67 1 0.97 0.00
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91119 2 4.42 1 0.93 0.00
91119 3 3.99 1 0.84 0.00
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91423 7 4.77 1 0.65 0.00
91423 8 4.39 1 0.60 0.00
91423 9 4.37 1 0.59 0.00

3. **Compound Membership in Each Cluster and the Citation for Each Compound**

CSP_NO CLUSTER MOLECULE COMPOUND_NAME CITATION
2966 1 1 7444 Shinbo, T.; Yamaguchi, T.; Nishimura, K.; Sugiura, M.; J. Chromatogr., 405, 145–153, 1987.
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23735 1 20 200689 Liao, Y.H.; Liu, X.L.; Wu, Z.J.; Du, X.L.; Zhang, X.M.; Yuan, W.C.; Chem. Eur. J., 18, 6679–6687, 2012.
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4. Computational Modeling

Our general approach for conformational sampling including the detailed computational workflow, has been published elsewhere [1]. A subset of the details of the computational methodology is provided here. Conformers of each structure were geometry optimized at the B3LYP/6–31G** level and stationary points were confirmed by performing frequency calculations (scaled by 0.98) [2–11]. All calculations were performed using Gaussian 09 [11]. Conformations contributing to the *in vacuo* Boltzmann distribution were calculated and used to interpret conformational differences induced by various substitution.

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5. Minimized Conformations for Nitro and Methyl ketone Analogs from MMP Shown in Figure 2 from manuscript

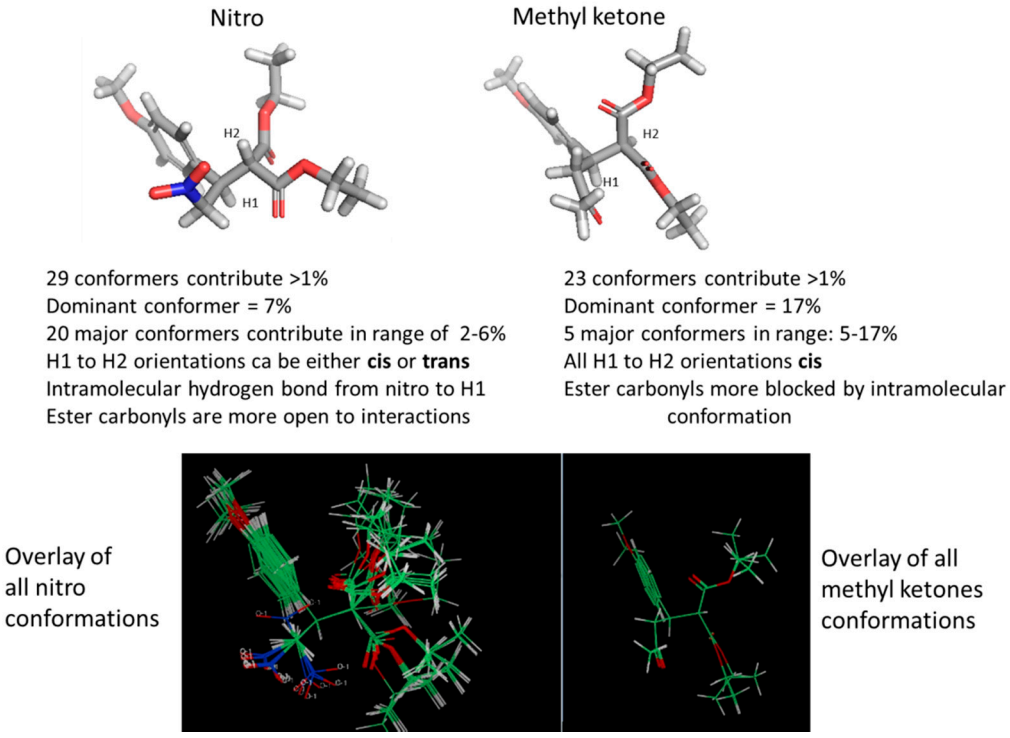

Figure S1. Minimized Conformations for Nitro and Methyl ketone Analogs from MMP.

Coordinates for lowest energy conformer of each species. All conformations for each compound available upon request.

Lowest energy nitro compound
B3LYP/6–31G** Electronic energy = –203.620229 hartrees
6 –5.48697 0.804433 0.701257
1 –5.0763 0.459098 1.65289
1 –5.25714 1.86699 0.582481
1 –6.57531 0.688973 0.733903
6 –4.92109 –0.005031 –0.453985
1 –5.32622 0.321628 –1.41396
1 –5.10999 –1.07278 –0.323911
6 –2.69203 –0.564694 0.180437
6 –1.22627 –0.191059 –0.051374
1 –1.03683 –0.260564 –1.12248
6 –1.05546 1.26601 0.387512
8 –3.48882 0.199941 –0.586279
8 –3.09146 –1.41638 0.946878
8 –1.19817 1.64275 1.53135
8 –0.730971 2.06151 –0.642229
6 –0.53763 3.46263 –0.321028
1 –1.46142 3.85005 0.11917
1 0.248745 3.54047 0.435419

6 –0.170984 4.17595 –1.60704
1 –0.014137 5.24044 –1.40753
1 0.749456 3.76597 –2.03189
1 –0.967562 4.07839 –2.3499
6 –0.244929 –1.07691 0.758556
1 –0.548879 –0.9699 1.80536
6 3.89128 0.234333 0.496072
6 3.18149 –0.063328 –0.672555
6 1.84919 –0.473795 –0.5885
6 1.19827 –0.599282 0.644036
6 1.92623 –0.28708 1.80331
6 3.25103 0.12255 1.73834
1 3.64871 0.016376 –1.64655
1 1.32244 –0.698192 –1.51098
1 1.44246 –0.361456 2.77363
1 3.81116 0.364235 2.63544
8 5.19239 0.641918 0.533455
6 5.89818 0.752076 –0.693366
1 6.90684 1.07469 –0.431847
1 5.44262 1.49742 –1.3578
1 5.9515 –0.210311 –1.21774
6 –0.377591 –2.5938 0.499353
1 0.279379 –3.14879 1.16687
1 –1.41351 –2.91019 0.624873
7 0.017223 –3.01652 –0.889572
8 0.913255 –3.84346 –1.00423
8 –0.600323 –2.51064 –1.83077

Lowest energy methyl ketone compound
B3LYP/6–31G** Electronic energy = –1151.768991hartrees
6 4.44005 –1.17952 –2.88048
1 3.7951 –2.02205 –3.1443
1 4.28571 –0.380958 –3.61193
1 5.48136 –1.50977 –2.94639
6 4.14587 –0.696321 –1.47458
1 4.7727 0.152951 –1.18751
1 4.27475 –1.48739 –0.731073
6 2.3145 0.202129 –0.272748
6 0.79866 0.394062 –0.295728
1 0.514496 0.641483 –1.32171
6 0.46189 1.60002 0.577857
8 2.75539 –0.279462 –1.44259
8 3.0175 0.416283 0.695125

8 0.018598 1.58115 1.70641
8 0.750395 2.73533 –0.08731
6 0.551597 3.96938 0.645132
1 –0.497303 4.0295 0.951065
1 1.1608 3.93762 1.55342
6 0.947138 5.11068 –0.270783
1 0.812269 6.06488 0.247834
1 1.99576 5.0266 –0.569352
1 0.330578 5.11995 –1.17404
6 0.070227 –0.938378 0.091368
1 0.451969 –1.67547 –0.62307
6 –4.20497 –0.66051 –0.658029
6 –3.69295 –0.251545 0.577658
6 –2.31968 –0.337683 0.824375
6 –1.43195 –0.830253 –0.137835
6 –1.96951 –1.23644 –1.37091
6 –3.33008 –1.15451 –1.6355
1 –4.34522 0.134565 1.35193
1 –1.93958 0.002135 1.78131
1 –1.30646 –1.63302 –2.13627
1 –3.74106 –1.47555 –2.58702
8 –5.52568 –0.622483 –1.00657
6 –6.45655 –0.13951 –0.051668
1 –7.43603 –0.198592 –0.528606
1 –6.25253 0.903352 0.223505
1 –6.46121 –0.753934 0.85793
6 0.46319 –1.46001 1.48797
1 –0.309985 –2.15768 1.84049
1 0.504483 –0.655813 2.22577
8 2.22824 –2.76746 0.500609
6 1.76771 –2.25334 1.50644
6 2.45525 –2.37562 2.84885
1 1.73883 –2.5669 3.65442
1 2.9417 –1.41668 3.06403
1 3.21094 –3.16185 2.81595

6. General Differences in Preferred Conformations for Keto and Keto Ester Analogs Shown in Figure 4e from manuscript.

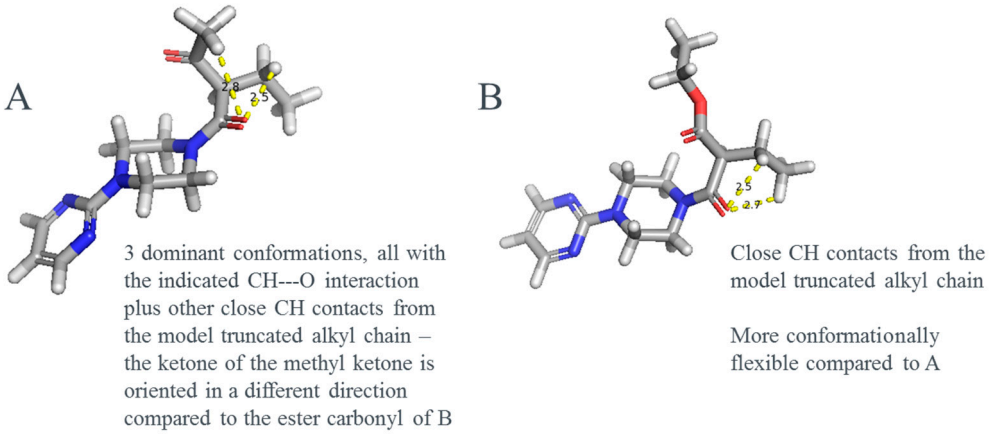

Figure S2. General Differences in Preferred Conformations for Keto and Keto Ester Analogs.

Coordinates for lowest energy conformer of each species. All conformations for each compound available upon request.

Lowest energy ketone compound A
B3LYP/6–31G** Electronic energy = –15.039736 hartrees
6 –5.26297 –0.850081 0.410776
6 –5.86033 0.1668 –0.332345
6 –4.98723 1.12362 –0.847704
7 –3.66992 1.08897 –0.657713
6 –3.19772 0.055441 0.076274
7 –3.9511 –0.924399 0.626036
7 –1.84324 –0.009194 0.272145
6 –1.21243 –1.05078 1.07485
6 –0.058282 –1.68902 0.297193
7 0.872812 –0.667809 –0.193247
6 0.233698 0.382578 –0.992048
6 –0.928608 1.01551 –0.214793
6 2.20291 –0.77912 0.116622
6 3.17723 0.273595 –0.464094
8 2.63023 –1.66754 0.852789
6 3.11716 1.51622 0.441806
6 3.83543 1.44384 1.77195
8 2.4876 2.50223 0.099116
6 4.59353 –0.320436 –0.59487
6 4.6889 –1.38822 –1.68845
1 –5.86307 –1.64271 0.856376
1 –6.93001 0.2122 –0.495499
1 –5.35982 1.95834 –1.44044
1 –1.96325 –1.79671 1.33054
1 –0.824212 –0.611786 2.00608

1 –0.461795 –2.24147 –0.56267
1 0.504692 –2.37668 0.927428
1 –0.147907 –0.057465 –1.92421
1 0.946629 1.16775 –1.23359
1 –1.48111 1.703 –0.853085
1 –0.51886 1.5806 0.635002
1 2.83839 0.60163 –1.44984
1 3.53573 2.28708 2.39534
1 4.91913 1.48369 1.61326
1 3.62274 0.493062 2.27114
1 4.88715 –0.756653 0.363126
1 5.29183 0.496072 –0.817607
1 5.71278 –1.76564 –1.77165
1 4.40199 –0.987569 –2.66741
1 4.03868 –2.23696 –1.45908

Lowest energy ester compound B
B3LYP/6–31G** Electronic energy = –1029.591846 hartrees
6 5.72826 0.162163 0.786964
6 6.24742 –0.625839 –0.239067
6 5.30449 –1.18134 –1.10257
7 3.9936 –0.985251 –0.977503
6 3.60082 –0.198666 0.0508
7 4.42589 0.38514 0.950203
7 2.25758 0.035755 0.185709
6 1.70378 0.797508 1.30049
6 0.685592 1.82033 0.790153
7 –0.326713 1.17193 –0.048243
6 0.240177 0.419989 –1.17069
6 1.26356 –0.605468 –0.667304
6 –1.6526 1.35524 0.252738
6 –2.70663 0.676432 –0.664265
8 –2.01565 2.02457 1.21446
6 –2.75106 –0.817321 –0.348132
8 –3.48742 –1.0714 0.747277
8 –2.17291 –1.67294 –0.992147
6 –4.07746 1.36112 –0.511511
6 –4.10776 2.7683 –1.11385
6 –3.58769 –2.45688 1.16573
6 –4.70631 –3.17577 0.428999
1 6.38621 0.636464 1.51439
1 7.31034 –0.798462 –0.354724
1 5.61283 –1.81506 –1.93345

1 1.20714 0.112496 2.00443
1 2.52065 1.2938 1.82205
1 0.171233 2.30606 1.61865
1 1.20463 2.58547 0.196084
1 –0.537724 –0.114256 –1.71071
1 0.736238 1.1228 –1.85546
1 0.73109 –1.38489 –0.102853
1 1.77459 –1.07583 –1.50567
1 –2.38293 0.745194 –1.7063
1 –4.32466 1.40166 0.550729
1 –4.83137 0.733229 –1.00085
1 –5.104 3.20931 –1.00965
1 –3.86246 2.755 –2.18247
1 –3.39793 3.42499 –0.60416
1 –2.62487 –2.9448 0.998008
1 –3.78524 –2.39741 2.2381
1 –4.81327 –4.19267 0.820615
1 –5.65849 –2.65457 0.563233
1 –4.48421 –3.24207 –0.638737

7. General Differences in Preferred Conformations for Urea and Thiourea Analogs Shown in Figure 4f from manuscript

Percentages are *in vacuo* Boltzmann population, where ranges cover the estimates of percent contribution determined from electronic (E) or free energies (G).

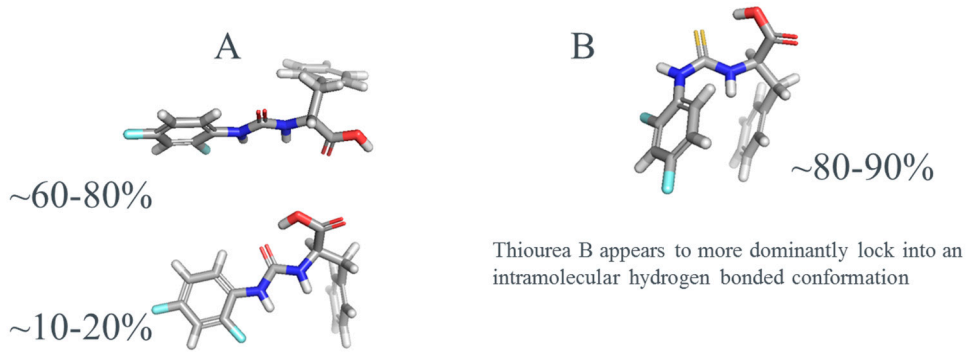

Figure S3. Preferred Conformations for Urea and Thiourea Analogs.

Coordinates for lowest energy conformer of each species. All conformations for each compound available upon request.

Lowest energy urea compound A
B3LYP/6–31G** Electronic energy = –1153.051329 hartrees
6 4.98933 0.849111 0.823067
6 3.63645 0.634741 1.01566

6 2.83144 –0.080689 0.117368
6 3.44752 –0.598797 –1.03077
6 4.81143 –0.397518 –1.2518
6 5.56111 0.31845 –0.329
7 1.47714 –0.217394 0.456271
6 0.484543 –0.83589 –0.285364
7 –0.756068 –0.77676 0.310066
6 –1.85919 –1.51723 –0.269204
6 –2.62683 –0.718725 –1.36376
8 0.665962 –1.36615 –1.37809
9 6.87944 0.511162 –0.545105
9 3.03635 1.13743 2.12817
6 –2.76441 –1.95509 0.871409
8 –3.79711 –2.70584 0.438866
8 –2.59168 –1.67728 2.03937
6 –3.3067 0.537752 –0.867251
6 –4.65714 0.520912 –0.490148
6 –5.28246 1.6732 –0.012256
6 –4.56534 2.86515 0.095676
6 –3.22175 2.89725 –0.281695
6 –2.59979 1.74392 –0.76002
1 5.57234 1.40852 1.54398
1 2.8454 –1.15144 –1.73746
1 5.29305 –0.794941 –2.1379
1 1.216 0.243988 1.31565
1 –0.851893 –0.582712 1.29941
1 –1.46768 –2.42064 –0.753601
1 –1.88355 –0.480863 –2.13
1 –3.35899 –1.39404 –1.81627
1 –4.32105 –2.93343 1.22585
1 –5.2227 –0.403087 –0.57756
1 –6.33101 1.64077 0.269951
1 –5.05123 3.76397 0.463898
1 –2.65835 3.82329 –0.209774
1 –1.55672 1.7773 –1.06072

Lowest energy thiourea compound B
B3LYP/6–31G** Electronic energy = −1475.997487 hartrees
6 –3.9684 –0.204968 0.339802
6 –2.83303 –0.632233 1.00967
6 –1.74929 –1.23303 0.353529
6 –1.84691 –1.42044 –1.03283
6 –2.96478 –0.977155 –1.73945

6 –4.00626 –0.377911 –1.04043
7 –0.652924 –1.68002 1.126
6 0.684684 –1.4666 0.925007
7 1.03851 –0.752298 –0.163949
6 2.39862 –0.283466 –0.461456
6 2.34665 1.05645 –1.21409
16 1.79458 –2.11513 2.03381
9 –5.09231 0.042242 –1.71148
9 –2.76366 –0.48917 2.34604
6 3.16462 –1.3449 –1.29375
8 3.42457 –2.49554 –0.663366
8 3.50519 –1.15082 –2.43782
6 1.58991 2.14337 –0.48011
6 0.3637 2.61375 –0.966735
6 –0.346177 3.60717 –0.287977
6 0.163941 4.14646 0.891987
6 1.3883 3.68947 1.38606
6 2.09339 2.69866 0.705465
1 –4.78964 0.25536 0.875096
1 –1.04957 –1.93705 –1.55624
1 –3.04493 –1.11456 –2.8113
1 –0.858562 –2.0897 2.02728
1 0.296808 –0.295448 –0.680909
1 2.91315 –0.164456 0.498927
1 3.38283 1.3578 –1.39576
1 1.91474 0.884537 –2.20515
1 3.08119 –2.47775 0.263882
1 –0.03309 2.21039 –1.89594
1 –1.29319 3.96061 –0.685531
1 –0.383802 4.92019 1.42155
1 1.79584 4.10823 2.30153
1 3.04773 2.35549 1.09754