

S1 Table. Natural products that have been tested for *in-vitro* antiplasmodial activities (NAA) compiled in-house from literature, PhD and Masters Theses and public chemical databases.

| ID | Hit_Status | pIC50 | Smiles |
|-----|------------|-----------------|--|
| N78 | A | 6.15490196 | <chem>C1CC(C(CC(CN2C=Nc3ccccc3C2=O)=O)NC1)O</chem> |
| N79 | A | 5.92081875 4 | <chem>[C-]#[N+]C1C2C(CCC1(C)O)C(C)(CCC2C1(C)CCC(C(C)(C)O1)[Cl])[N+]#[C-]</chem> |
| N80 | A | 5.46852108 3 | <chem>C1CC2C(CC(CN3C=Nc4ccccc4C3=O)(O)O2)NC1</chem> |
| N81 | A | 4 | <chem>CCC(C)C(C(CC(N1CCCC1C(C(C)C(NC(Cc1ccccc1)c1nccs1)=O)OC)=O)OC)N(C)C(C(C(C)C)NC(C(C(C)C)N(C)C)=O)=O</chem> |
| N82 | A | 2.83614895 5 | <chem>CC(C)C(C)=CC(=O)OC1C2C34COC2(C(C(C3C2(C)CC(C(=C(C)C2CC4OC1=O)O)=O)O)O)C(=O)OC</chem> |
| N83 | A | 2.73880543 4 | <chem>CC1C(C(C)(CC(O1)OC1CC(C(c2c1c(c1cc(C)c3C4C5C(C6(CO6)C(C(OC)OC)(O4)O5)(OC4CC(C(C(C)O4)(C(C)=O)O)O)Oc3c1c2O)OC)=O)O)O)OC(C)=O</chem> |
| N84 | A | 2.71746942 3 | <chem>CC1C(C(C)(CC(O1)OC1CC(C(c2c1c(c1cc(C)c3C4C5C(C6(CO6)C(C(OC)OC)(O4)O5)(OC4CC(C(C(C)O4)(C(C)=O)O)O)Oc3c1c2O)OC)=O)O)O)O</chem> |
| N85 | A | 2.69897000 4 | <chem>CC(c1cc2C(c3ccccc3C(c2o1)=O)=O)=O</chem> |
| N86 | A | 2.69897000 4 | <chem>CC1C(C(C(C(O1)OC1=C(c2ccc(c(c2)O)O)Oc2cc(cc(c2C1=O)O)O)O)O)O</chem> |
| N87 | A | 2.69897000 4 | <chem>CC1C=C2C(=CC(=O)O2)C2(C)C1CC1C34COC(C4C(C(=O)O1)OC(C)=O)(C(C(C23)O)O)C(=O)OC</chem> |
| N88 | A | 2.63827216 4 | <chem>C([C@@H]1[C@H]([C@@H]([C@H]([C@H](OC2=C(c3ccc(c(c3)O)O)Oc3cc(cc(c3C2=O)O)O)O1)O)O)O</chem> |
| N89 | A | 2.53760200 2 | <chem>C[C@@H]1[C@@H]([C@H]([C@H]([C@H](OC2=C(c3ccc(c(c3)O)O)Oc3cc(cc(c3C2=O)O)O)O1)O)O)O[C@@H]1[C@@H]([C@H]([C@@H]([C@@H](CO)O1)O)O)O</chem> |
| N90 | A | 2.23932093 6 | <chem>CC(C)=CC(=O)OC1C2C34COC2(C(C(C3C2(C)CC(C(=C(C)C2CC4OC1=O)O)=O)O)O)C(=O)OC</chem> |
| N91 | A | 2.2046155 | <chem>CCC(C)C(=O)OC1C2C34COC2(C)C(C(C3C2(C)C(C4OC1=O)C(C)=CC(C2O)O)O)O</chem> |
| N92 | A | 2.20278981 5 | <chem>CCC(C)C(=O)OC1C2C34COC2(C)C(C(C3C2(C)C(C4OC1=O)C(C)=CC(C2O)=O)O)O</chem> |
| N93 | A | 2.15490196 | <chem>[H]C(=C1C(c2c(cc(cc2OC(C)=O)OC(C)=O)O1)=O)c1</chem> |

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| | | | cc(c(c(c1)OC)OC(C)=O)OC |
| N94 | A | 2.09852876 4 | CC1=CC(C(C2(C)C1CC1C34COC(C24))(C(C(=C)C3 CC(=O)O1)O)O)=O |
| N95 | A | 2.05275415 4 | CC(=CC(=O)OC1C2C34COC2(C(C(C3C2(C)CC(C(= C(C)C2CC4OC1=O)O)=O)O)C(=O)OC)C(C)(C)O |
| N96 | A | 1.97469413 5 | CC(=C)C(CC=C(C)C)Cc1c(cc(c2C(CC(c3c(cccc3O)O)Oc12)=O)O)OC |
| N97 | A | 1.97371279 6 | C1CCN2CCC3C(=CC(CCC=CC1))(C1C3(CC3C=CC CCCN13)C2)O)c1c2c(ccn1)c1cccc(c1[nH]2)O |
| N98 | A | 1.96657624 5 | CC(=C)C(CC=C(C)C)Cc1c(cc(c2C(CC(c3c(cccc3O)O)Oc12)=O)O)O |
| N99 | A | 1.96257350 2 | CC(CC=CC(C(C(CC1C(c2cc(cc(c2C(=O)O1)O)OC)O)O)O)O |
| N100 | A | 1.93930216 | CC12C(CC[Cl])C(NC1(C(C1CCCC=C1)O)C(=O)O2)= O |
| N101 | A | 1.90308998 7 | C1CCN2CCC3C(=CC(CCC=CC1))(C1C3(CC3C=CC CCCN13)C2)O)c1c2c(ccn1)c1cccc1[nH]2 |
| N102 | A | 1.89911102 4 | CCC1CN2CCc3cc(c(cc3C2CC1CC1c2c(CCN1)c1cc(ccc1[nH]2)O)OC)OC |
| N103 | A | 1.89594767 4 | CC1Cc2ccc(c3c(CO)cc(c4c(cccc34)OC)OC)c(c2C(C) N1)O |
| N104 | A | 1.85387196 4 | [C-]#[N+]C1(C)CCC2C(C)CC3CC(C)C(C)(C4CCC1C2C 34)[N+]#[C-] |
| N105 | A | 1.83923143 8 | [C-]#[N+]C1(C)CCC2C(C)CC3CC(C)C(C)(C4CCC1C2C 34)[N+]#[C-] |
| N1 | A | 1.83923143 8 | [H][C@@]12CC[C@]3([H])C([C@H](C)C[C@]4([H])C [C@H](C)[C@]([H])(CCC1=O)[C@@]2([H])[C@]34[H])=O |
| N106 | A | 1.82390874 1 | CC1=CC(C(C2(C)C1CC1C34COC(C)(C24)C(C(C3C(C(=O)O1)OC)O)O)=O |
| N107 | A | 1.76955107 9 | C[C@@]1(C)[C@H]2CC[C@@]34CC(=C)[C@@H](CC3=O)C[C@H]4[C@]2(C)CC([C@H]1O)=O |
| N108 | A | 1.72124639 9 | CC[C@@H](C)C(=O)O[C@H]1[C@H]2C(CC([C@@ H](C)CCC[C@@]1(C)O)=O)C(=C)C(=O)O2 |
| N109 | A | 1.72124639 9 | CC[C@@H](C)C(=O)O[C@H]1[C@H]2C(CC([C@@ H](C)CCC[C@@]1(C)O)=O)C(=C)C(=O)O2 |
| N110 | A | 1.72124639 9 | CC1C2C(Cc3c1cco3)C1(C)CCCC(C)(C)C1C(C2OC(C)=O)OC(C)=O |
| N111 | A | 1.72124639 9 | CCC12CCCN3CCC4(C(CC1)N(C(C)=O)c1c4ccc(c1O)OC)C23 |
| N112 | A | 1.69897000 4 | [H][C@@]12C=C(C)CC(C)(C)[C@@]2([H])[C@]([H])(c2c(CCN(C)C)c3cccc3[nH]2)n2c1c(CCN(C)C)c1ccc cc12 |

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| N114 | A | 1.69897000 4 | C[C@H]1CC=C[C@@H]([C@H])([C@H](CC=Cc2cc(c(c2C(=O)O1)O)OC)O)O |
| N113 | A | 1.69897000 4 | CC(C)=CCc1c2c(C=CC(C)(C)O2)c(c2C(C3C(C=C(C)C)O)c4cc(c(cc4C=3O)c12)O)O)=O)O |
| N115 | A | 1.67672809 4 | CC(C)CC(=O)OC1C2C34COC2(C(C(C3C2(C)CC(C(=C(C)C2CC4OC1=O)O)=O)O)O)C(=O)OC |
| N116 | A | 1.6402662 | CC1C2CC3C45COC(C5C(C(=O)O3)OC(C)=O)(C(C(C4C2(C)CC(C=1O)=O)O)O)C(=O)OC |
| N117 | A | 1.62893213 8 | CC1=CC2=CC(C=C3C2=C(C=C(C)O3)N1)=O |
| N118 | A | 1.60205999 1 | C[C@H]1CC[C@H]([C@@H](C)[C@H]2CC[C@H]3[C@@H]4CC=C5C[C@H](CC[C@]5(C)[C@H]4CC[C@]23C)N)NC1 |
| N119 | A | 1.56863623 6 | CC1C2=CC=C3[C@@]4(C)CC[C@]5(CCC(=C)C[C@H]5[C@]4(C)CC[C@@]3(C)C2=CC(C=1O)=O)C(=O)OC |
| N120 | A | 1.52287874 5 | [H]C(=C1C(c2c(cc(cc2O1)O)O)=O)c1cc([H])c(c(c1)O)C)O |
| N121 | A | 1.45076038 2 | CC1CCC2C(C)C(=O)OC3C24C1CCC(C)(O3)OO4 |
| N122 | A | 1.43713201 1 | CC1=CC(C(C2(C)C1CC1C34COC(C)(C(C(C23)O)O)C4(C(C(=O)O1)O)O)O)=O |
| N123 | A | 1.40893539 3 | CC1(C)CCC2(CCC3(C)C(=CCC4C5(C)CCC(C(C)(C)C5CCC34C)O)C2C1)C(O)=O |
| N124 | A | 1.36981573 4 | CCCCCCCc1cc(C=C2C(=CC(=C3C=CC=N3)N2)OC)[nH]c1C |
| N125 | A | 1.32790214 2 | C1CCN2CCC3C(=CC(CCC=CC1)(C1C3(CCC3C=CCCCN13)C2)O)c1c2c(ccn1)c1cccc(c1[nH]2)O |
| N126 | A | 1.32674390 9 | CC1=CC(C(C2(C)C1CC1C34C2C(CO4)(C(C2(CO2)C3(C(C(=O)O1)O)O)O)O)O)=O |
| N127 | A | 1.30102999 6 | CC(C)CC(=O)OC1C2C34COC2(C(C(C3C2(C)C(CC4OC1=O)C(C)=CC(C2O)=O)O)O)C(=O)OC |
| N128 | A | 1.30102999 6 | CCC12CCCN3CCc4c5cccc5n(C(C1)c1c(ccc5c1c1CC[N+]6(C)CC(=CC)C(CCO)CC6c1[nH]5)O)c4C23 |
| N129 | A | 1.28927646 8 | C[n+]1cc2cc(c(cc2c2ccc3cc(c(cc3c12)OC)O)OC)OC |
| N130 | A | 1.27572413 | C1CN=C2C3=C(C(c4c2c1c[nH]4)=O)NC1CC32C=C(C(CC2S1)=O)[Br] |
| N131 | A | 1.27572413 | CCCC#CC(CO)C(=O)OCCc1ccc(c2cccs2)s1 |
| N132 | A | 1.27572413 | CCCCC#CC(CO)C(=O)OCCc1ccc(c2cccs2)s1 |
| N133 | A | 1.26609352 | CC1C2=CC=C3C(C)(CCC4(C)C5CC(CCC5(C)CCC34C)CO)C2=CC(C=1O)=O |
| N134 | A | 1.25963731 1 | CCC(C)C1C(N2CCCC2C(NC(CCCCC(C)C)=O)C(NC(Cc2cn(c3cccc23)OC)C(N1)=O)=O)=O |
| N135 | A | 1.23759243 | CCC1CN2CCc3cc(c(cc3C2CC1CC1c2cc(c(cc2CCN1 |

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| | | 4 |)O)OC)OC)OC |
| N136 | A | 1.198942059 | CC1Cc2c(C(C)N1)c(cc(c2c1ccc(c2c(cc(C)cc12)OC)O)O)O |
| N137 | A | 1.148741651 | CC1=CC(C(G2(C)C1CC1C34COC(C)(C24)C(C(C3C(C(=O)O1)O)O)O)O)=O |
| N138 | A | 1.13667714 | Cc1c2cnccc2c(C)c2c1c1cccc1[nH]2 |
| N139 | A | 1.102372909 | C1C(C(c2cc(c(c(c2)O)O)O)O)c2cc(cc(c12)O)O)OC(c1cc(c(c(c1)O)O)O)=O |
| N140 | A | 1.096910013 | CC(C)=C[C@H]1C[C@@](C)(C=Cc2c(CCNC)c3cccc3[nH]2)n2c1c(CCN(C)C)c1cccc12 |
| N141 | A | 1.070581074 | C1C2C3C=C(C4CC56C7CC8C9C5N(C(CC9OCC=C8CN47)=O)c4cccc46)C(N4C3C3(CCN(CC2=CCO)C13)c1cccc14)=O |
| N142 | A | 1.068416584 | CN1CCc2cc(c3cc2C1Cc1ccc(cc1)Oc1cc(CC2c4c(CC2C)cc(c(c4O3)O)OC)ccc1OC)OC |
| N143 | A | 1.064492734 | CC1CCC(c2cc(C)ccc12)=O |
| N145 | A | 1.045757491 | CC(C)=C[C@@H]1C[C@](C)(C=Cc2c(CCN(C)C)c3cccc3[nH]2)n2c1c(CCN(C)C)c1cccc12 |
| N146 | A | 1.045757491 | CC(C)=C[C@H]1C[C@](C)(C=Cc2c(CCN(C)C)c3cccc3[nH]2)n2c1c(CCN(C)C)c1cccc12 |
| N147 | A | 1.045757491 | CC1CC(C)(C)C2C(C=1)c1c(CCN(C)c3cccc3n1C2c1c(CCN(C)c2cccc2[nH]1 |
| N148 | A | 1.026872146 | CC1C2=CC=C3[C@@]4(C)CC[C@]5(CCC(=C)C[C@@H]5[C@]4(C)CC[C@@]3(C)C2=CC(C=1O)=O)C=O |
| N149 | A | 1.022276395 | CC[C@@H]1[C@](C)([C@@H]([C@@H](C)N(C)C[C@@H](C)C[C@](C)([C@@H]([C@@H](C)[C@@H]([C@@H](C)C(=O)O1)O[C@H]1C[C@](C)([C@H]([C@H](C)O1)O)OC)O[C@H]1[C@@H]([C@H](C)[C@@H](C)O1)N(C)Cc1ccc(cc1)c1cn(CCC(C)C(C)C(=O)N)nn1)O)O)O |
| N150 | A | 1.009024851 | CC1=CC(C(G2(C)C1CC1C34COC(C23)(C(C(=C)C4(C(C(=O)O1)O)O)O)O)O)=O |
| N151 | A | 1.008773924 | [H]C12CCC3=CC4(CCC3(C2(C)CCCC1(C)CO)OO4)C(C)C |
| N152 | A | 1 | CC=C1CN2C(CC34C2CC1C1=CCC(N(C13)c1cccc14)=O)C1=CC2C3CC4C5(CCN4CC3=CCO)C2N(C1=O)c1cccc15 |
| N153 | A | 0.999559272 | CC(C)=CC(=O)OC1C2C34COC2(C)C(C(C3C2(C)C(CC4OC1=O)C(C)=CC(C2O)=O)O)O |
| N154 | A | 0.974954995 | CN1CCc2cc(c(c3c2C1Cc1ccc(cc1)Oc1cc(CC2c4cc(c(cc4CCN2)OC)O3)ccc1OC)O)OC |
| N155 | A | 0.971506569 | CN1CCc2cc(c3cc2C1Cc1ccc(cc1)Oc1cc(CC2c4c(CC2C)cc(c(c4O3)O)OC)ccc1OC)OC |

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| N156 | A | 0.95860731 5 | CCc1c[n+]2ccc3c4ccccc4[nH]c3c2cc1CCO |
| N157 | A | 0.93998315 | C[n+]1cc2cc(c(cc2c2ccc3cc4c(cc3c12)OCO4)OC)OC |
| N160 | A | 0.92081875 4 | CC(C)=CCC1=C(c2cc(c(cc2O)OC)O)Oc2cc(cc(c2C1=O)O)O |
| N161 | A | 0.89274783 8 | CC=C(C)C(=O)O[C@@H]1[C@H]2C(C)=CC([C@H]([C@]2(C)[C@H]2C3([C@@H]([C@H](C)[C@@H]4C C(=O)O[C@H]1[C@]24CO3)O)O)O)=O |
| N162 | A | 0.89273171 3 | CC1C2=CC=C3C(C)(CCC4(C)C5CC(CCC5(C)CCC3 4C)CO)C2=CC(C=1O)=O |
| N163 | A | 0.88605664 8 | C1CN=C2C3=C(C(c4c2c1c[nH]4)=O)NCCC31C=C(C (C=C1)[Br])O)[Br] |
| N164 | A | 0.87464989 8 | CN1C2C(=Cc3ccccc13)N=c1ccccc1=2 |
| N165 | A | 0.85387196 4 | [H]C1C([H])C(C)(C)C2(C(C(C3([H])C(c4ccoc4CC3([H])C2(C)C1=O)=O)O)OC(C)=O)O |
| N166 | A | 0.85387196 4 | CCC1CN2CCc3c4ccccc4[nH]c3C2CC1CC1c2c(CCN 1)c1ccccc1[nH]2 |
| N167 | A | 0.83863199 8 | CC(C1CCC(C)(C)C23CCC(C2)C(C)(C)C=13)=O |
| N168 | A | 0.82390874 1 | CC(=C)c1cc2C(c3ccccc3C(c2o1)=O)=O |
| N13 | A | 0.80489802 4 | c1cc(ccc1[C@@H]1[C@H](C(c2ccc(cc2O1)O)=O)[C @@H]1C(c2ccc(cc2O[C@H]1c1ccc(cc1)O)O)=O)O |
| N169 | A | 0.80410034 8 | [H][C@@]1(C(c2ccc(cc2O[C@@]1([H])c1ccc(cc1)O)O)=O)[C@@]1([H])C(c2ccc(cc2O[C@]1([H])c1ccc(cc1) O)O)=O |
| N170 | A | 0.79588001 7 | CC1C2=CC=C3C(C)(CCC4(C)C5CC(CCC5(C)CCC3 4C)CO)C2=CC(C=1O)=O |
| N171 | A | 0.79588001 7 | CN1CCc2cc(c(cc2C1Cc1ccc(cc1)Oc1cc(CC2c3cc(c(cc3CCN2C)OC)O)ccc1O)O)OC |
| N172 | A | 0.79342008 8 | CC1C2=CC=C3C(C)(CCC4(C)C5CC(CCC5(C)CCC3 4C)CO)C2=CC(C=1O)=O |
| N173 | A | 0.78515615 2 | [H][C@@]1(c2cccc(c2C(c2c(cc(C)c(c3c(cc(c(C(C)=O)c3O)OC)O)c12)O)=O)O)c1ccc2C(c3c(c(C)cc(c3C(c2 c1O)=O)O)c1c(cc(c(C(C)=O)c1O)OC)O)=O |
| N174 | A | 0.76955107 9 | CC(=O)OC1CC2(C)C(CC3C2(C2(C)C1C1(C)C=CC(C(C)(C)C1=C(C2=O)O)=O)O3)c1ccoc1 |
| N175 | A | 0.76955107 9 | CN1CCc2cc(c(c3c2C1Cc1ccc(c(c1)Oc1ccc(CC2c4cc (c(cc4CCN=2)OC)O3)cc1)OC)OC)OC |
| N176 | A | 0.76488824 1 | CN1CCc2cc(c3cc2C1Cc1ccc(c(c1)Oc1ccc(CC2c4c(C CN2C)cc(c(c4O3)O)OC)cc1)OC)OC |
| N177 | A | 0.76347034 1 | CN1CCc2cc3c4cc2C1Cc1ccc(c(c1)Oc1ccc(CC2c5c(CCN2)cc(c(c5O4)O3)OC)cc1)OC |
| N179 | A | 0.74472749 5 | CC(C)=CCc1c(cc(c2C(C3CC4c5c(C=3Oc12)c(cc(c5 OC4(C)C)OC)O)=O)O)O |

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| N180 | A | 0.74472749 5 | CC1CCC2C(C3=C(C)CCC13C2(C)C)=O |
| N178 | A | 0.74472749 5 | CCCCCCCCCCCCCCCC1CC(NCCCN(C)CCCN(C)CCCN1C)=O |
| N181 | A | 0.72182080 2 | CC1Cc2c(C(C)N1)c(cc(c2c1ccc(c2c(cc(C)cc12)OC)O)O)O |
| N182 | A | 0.72124639 9 | [H]C1([H])[C@@H](C)[C@]2([H])C=CC([C@@]2(C)[C@H]([C@@H]2C(=C)C(=O)O[C@H]12)OC(C(=CC)[C@@]([H])(C)O)=O)=O |
| N187 | A | 0.69897000 4 | C[C@@H]1[C@@H](C)C(c2cc(c(cc2[C@H]1c1ccc(c(c1)OC)OC)OC)OC)=O |
| N188 | A | 0.69897000 4 | C[C@@H]1[C@@H](C)C(c2cc(c(cc2[C@H]1c1ccc(c(c1)OC)OC)OC)OC)=O |
| N183 | A | 0.69897000 4 | C[n+]1cc2c(c3ccccc3[nH]2)c2ccccc12 |
| N184 | A | 0.69897000 4 | CC(=O)OC1C(C(C)(C)C2(CCC3C(Cc4c(cco4)C3=C)C2(C)C1OC(C)=O)O)OC(C)=O |
| N185 | A | 0.69897000 4 | CC=C1CN2CCC34C2CC1C1C=C(C2CC56C7CC(C(CN27)=CC)C2=CCC(N(C25)c2ccccc26)=O)C(N(C13)c1ccccc14)=O |
| N186 | A | 0.69897000 4 | CCCCCCCCCCCCCCCC1CC(NCCCN(C)CCCN(C)CCCN1)=O |
| N189 | A | 0.69080765 6 | CC1=CC(C(C2(C)C1CCC13COC4(C)C3C(=O)OC4C(C12)O)O)=O |
| N190 | A | 0.67778070 5 | CC1=CC(C(C2(C)C1CC1C34COC(C)(C24)C(C(C3C(=O)O1)O)O)O)=O |
| N191 | A | 0.67047657 4 | CN1CCc2cc(c3cc2C1Cc1ccc(c(c1)Oc1ccc(CC2c4c(CCN2C)cc(c(c4O3)OC)O)cc1)OC)OC |
| N192 | A | 0.66756154 | C(C(C(c1cnc(N)[nH]1)O)[Cl])N |
| N193 | A | 0.64474031 9 | CC1C(C2(C3C4(C)C(CC5C3(CO2)C1(C(C(=O)O5)O)O)C(C)=CC(C4O)=O)O)O |
| N194 | A | 0.63685127 | CN1CCc2cc(c3cc2C1Cc1ccc(c(c1)Oc1ccc(CC2c4c(CCN2C)cc2c(c4O3)OCO2)cc1)OC)OC |
| N195 | A | 0.63388110 9 | CC1CC2C(C)(CCC3(C)C4=CC=C5C(=CC(C(=C5C)O)=O)C4(C)CCC23C)CC=1 |
| N196 | A | 0.62482708 7 | CC1Cc2cc(c(c3c(C)cc4cccc(c4c3O)OC)c(c2C(C)N1C)OC)OC |
| N197 | A | 0.61978875 8 | [H]C1C([H])C(C)(C)C2(C(C(C3([H])C(=C([H])C(=O)O)C)c4ccoc4CC3([H])C2(C)C1=O)O)OC(C)=O)O |
| N198 | A | 0.61978875 8 | CC[C@H]1C=CCC[C@@]2(C[C@@H]3CC[C@@H]4[C@H](C(=O)O)CCCCCCCCCCCC(N(CCCN)C[C@H](CCN)O)=O)[C@]5(CCC[C@@H](C)O5)N=C(N2)N34)O1 |
| N199 | A | 0.61978875 8 | CCCCCCCCCCCCCCCC1CC(NCCCN(C)CCCN(C)CCCN1C)=O |

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| N200 | A | 0.61012980 9 | CC1Cc2cc(c(c3c(C)cc4cccc(c4c3O)OC)c(c2C(C)N1C)OC)O |
| N201 | A | 0.60797605 6 | CC1Cc2cc(c(c3c(C)cc4cccc(c4c3O)OC)c(c2C(C)=N1)OC)OC |
| N202 | A | 0.60205999 1 | CC1(C=O)C2CCC3(C)C2C=C2C(c4cc(ccc4C(C12O3)=O)O)=O |
| N205 | A | 0.58502665 2 | C[C@@H]1C(c2cc(c(cc2[C@@H])(c2ccc3c(c2)OCO3)[C@H]1C)OC)OC)=O |
| N204 | A | 0.58502665 2 | CC(=O)OC1CC(C2(C)C3Cc4c(cco4)C(C3CCC2(C1(C)C)O)=O)OC(C)=O |
| N206 | A | 0.58502665 2 | COc1ccc(cc1)C1=CC(=C)c2c(cc(c(c3cc(ccc3O)C3=C)C4c(cc(cc4O3)OC)O)=O)c2O1)OC)O |
| N203 | A | 0.58502665 2 | COc1ccc(cc1)C1=CC(c2c(cc(c(c3cc(ccc3O)C3=CC(c4c(cc(cc4O3)OC)O)=O)c2O1)OC)O)=O |
| N207 | A | 0.57682970 8 | CN1CCc2cc(c3cc2C1Cc1ccc(cc1)Oc1cc(CC2c4c(CC)N2C)cc(c(c4O3)OC)OC)ccc1OC)OC |
| N208 | A | 0.56863623 6 | [H][C@@]1(c2cccc(c2C(c2c(cc(C)c(c3c(cc(c(C(C)=O)c3O)OC)O)c12)O)=O)O)c1ccc2C(c3c(c(C)cc(c3C(c2c1O)=O)O)c1c(cc(c(C(C)=O)c1O)OC)O)=O |
| N209 | A | 0.56863623 6 | CC=C1CN2CCC34CC5C6CC7c8c(CC(C6COC5(C)O)C45C2CC1C(C(=O)OC)N5c1cccc13)N7C)c1cccc1n8C |
| N210 | A | 0.56863623 6 | CC1=CC(c2c(cccc2O)C1=O)=O |
| N211 | A | 0.56863623 6 | CN1C2C(=C(C3=C4C(=c5cccc5=N4)N(C)c4cccc34)c3cccc13)N=c1cccc1=2 |
| N212 | A | 0.56694752 3 | CC1C2=CC=C3C(C)(CCC4(C)C5CC(=C)CCC5(CCC34C)CO)C2=CC(C=1O)=O |
| N213 | A | 0.55284196 9 | CC(c1c(cc(c(c2c(C)cc(c3C(c4c(cccc4O)C(c23)=O)=O)O)c1O)OC)O)=O |
| N214 | A | 0.53760200 2 | CCCCCCCC(CCCCC1CC(NCCCN(C)CCCN(C)C)CCN1C)=O)O |
| N216 | A | 0.53711750 9 | C[C@H]1[C@@H]([C@@H](C)[C@@](C)(O)O[C@@H]1[C@H]1CC[C@H]([C@@H]2CC[C@H]([C@]3(C)[C@@H]([C@@H](C)[C@]4([C@@H](C)[C@H](C)[C@@H]([C@H]([C@](C)([C@H](C)OC)OC)O)O4)OC)O3)OC)O2)O1)O |
| N215 | A | 0.53711750 9 | CC1C(C(C)C(C)(O)OC1[C@H]1CC[C@H]([C@@H]2CC[C@H]([C@]3(C)[C@@H]([C@@H](C)C4(C(C)C)CC([C@H]([C@](C)([C@H](C)OC)OC)O)O4)OC)O3)OC)O2)O1)O |
| N217 | A | 0.52287874 5 | [H][C@@]1(CCCCCCCC(O)=O)C[C@@](C)(CC(=O)OC)OO1 |
| N218 | A | 0.52287874 5 | [H]c1ccc(c2c1C(c1c(c(c(c(CCC=C(C)C)c1O)O)OC)N2C)=O)O |
| N12 | A | 0.52287874 | c1c2C(=O)Oc3c4c(cc(c3O)O)C(=O)Oc(c24)c(c1O)O |

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| N220 | A | 0.52287874 5 | COc1ccc(cc1c1c(cc(c2C(=C)C=C(c3ccc(cc3)O)Oc12)O)O)C1=CC(c2c(cc(cc2O1)O)O)=O |
| N219 | A | 0.52287874 5 | COc1ccc(cc1c1c(cc(c2C(C=C(c3ccc(cc3)O)Oc12)=O)O)O)C1=CC(c2c(cc(cc2O1)O)O)=O |
| N221 | A | 0.52094784 2 | CCC1CN2CCc3cc(c(cc3C2CC1CC1=C2C=C(C(C=C2CCN1)=O)OC)OC)OC |
| N222 | A | 0.50850574 8 | [H]C12CCC34C[C@@H](CCC3(C2(C)CCCC1(C)CO)OO4)C(C)C |
| N223 | A | 0.49485002 2 | C[C@@H]1C(c2cc(c(cc2[C@@H](c2ccc(c(c2)OC)OC)[C@H]1C)OC)OC)=O |
| N224 | A | 0.49485002 2 | C[C@@H]1C(c2cc(c(cc2[C@@H](c2ccc(c(c2)OC)OC)[C@H]1C)OC)OC)=O |
| N225 | A | 0.48248923 9 | [H][C@@]12C[C@@H](C)CC[C@]2([H])C(C)(C)Oc2cc(C=Cc3ccccc3O)cc(c12)O |
| N226 | A | 0.48148606 | CCCCCCCC(CCCCC1CC(NCCCN(C)CCCCN(C)CCCN1)=O)O |
| N227 | A | 0.47156403 2 | CC1C2=CC=C3C(C)(CCC4(C)C5CC(=C)CCC5(CCC34C)CO)C2=CC(C=1O)=O |
| N228 | A | 0.47154856 9 | CCC1CC2CC3(C1N(CCCc1c4cc(c(cc4[nH]c13)C1CC3C(C(Cc4c5ccccc5[nH]c14)N(C)CC3=CC)C(=O)OC)OC)C)C2)C(=O)OC |
| N229 | A | 0.46777671 | CN1CCc2c(cc(c(c2O)OC)OC)C1Cc1ccc(cc1)Oc1c2CC3c4c(CCN3C)c(c(c(c4c2cc(c1OC)OC)OC)OC)O |
| N230 | A | 0.46400177 3 | CC1Cc2c(C(C)N1C)c(cc(c2c1ccc(c2c(cc(C)cc12)OC)O)OC)O |
| N231 | A | 0.46344155 7 | [H][C@@]12CCC3=C[C@]4(CC[C@@]3([C@@]1(C)CCC[C@@]2(C)CO)OO4)C(C)C |
| N232 | A | 0.46218090 5 | CC1CCC2C(CC2(C)C)C(=C)CCC=1 |
| N233 | A | 0.45593195 6 | CN1CCc2cc(c3cc2C1Cc1ccc(cc1)Oc1cc(CC2c4c(CC2)cc(c(c4O3)OC)OC)ccc1OC)OC |
| N234 | A | 0.45222529 5 | CN1CCc2cc(c3cc2C1Cc1ccc(cc1)Oc1c2C(Cc4ccc(c(c4)O3)O)N(C)CCc2cc(c1O)OC)OC |
| N235 | A | 0.44873582 8 | CC1Cc2c(C(C)N1C)c(cc(c2c1ccc(c2c(cc(C)cc12)OC)OC)OC)O |
| N236 | A | 0.44769941 8 | CC=C1CN2CCc3c4ccccc4[nH]c3C2CC1Cc1c2c(ccn1)c1cc(ccc1[nH]2)O |
| N237 | A | 0.44608515 2 | C[C@@]12C[C@H]3[C@]4([C@@]5(C)C(C=C[C@@]6(C)CO[C@H]([C@H]56)[C@H]([C@@]4(C)C1=C[C@H]2C1=CC(O)OC1=O)OC(c1ccccc1)=O)=O)O3 |
| N238 | A | 0.44369749 9 | CC=C1CN2CCC3c4ccccc4N4C(C1CC2C34C=CC1=COCC2C1CC1c3c(CC2N1C)c1ccccc1n3C)C(=O)OC |
| N239 | A | 0.44369749 9 | CN1CCc2cc3c(c4c5ccccc5cc1c24)OCO3 |

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| N240 | A | 0.43179827 6 | CC1=CC(C(=CC2=C1CC1CC(C3(C)C(CC4C(C)=CC(C(=CC=4O3)O)=O)CC(C)(C)C=CCC1(C)O2)O)O)=O |
| N241 | A | 0.43070167 2 | CN1CCc2cc(c3cc2C1Cc1ccc(c(c1)Oc1ccc(CC2c4c(CCN2C)cc(c(c4O3)OC)OC)cc1)OC)OC |
| N242 | A | 0.42909894 8 | CN1C(C(c2ccnc3c4cc(ccc4c(c1c23)OC)OC)=O)=O |
| N243 | A | 0.41103722 7 | CC1CCC2C(C)(C)C(CCC2(C)C12Cc1c(cc(C=O)c(C=O)c1O2)O)O |
| N244 | A | 0.39794000 9 | [H]C1C[C@@H]([C@]2(C)[C@@]3([H])Cc4c(cco4)[C@]([H])(C)C3([H])[C@H](C([H])[C@]2(C1(C)C)O)O)C(C)=O |
| N245 | A | 0.39794000 9 | CCC=CC(CC)CC1(C)CC(CC)C(CC(=O)OC)OO1 |
| N246 | A | 0.39636189 2 | CC1C2=CC=C3C(C)(CCC4(C)C5CC(C)(CCC5(C)CC C34C)C(O)=O)C2=CC(C=1O)=O |
| N247 | A | 0.38744609 9 | CC1C2=CC=C3C(C)(CCC4(C)C5CC(C)(CCC5(C)CC C34C)C(=O)OC)C2=CC(C=1O)=O |
| N248 | A | 0.38721614 3 | [H]C1([H])C(C)C2([H])C=CC([C@@]2(C)C([C@@H]2 C(C)C(=O)O[C@H]12)OC(C=C)[C@@]([H])(C)O)=O)=O |
| N249 | A | 0.38404994 8 | CC1CCC2C(C)C3C(CC4C5CC=C6CC(CCC6(C)C5C CC34C)OC3C(C(C(CO)O3)O)OC3C(C(C(CO)O 3)O)O)OC3C(C(C(C(CO)O3)O)O)O)N2C1 |
| N250 | A | 0.37655999 7 | CC1C2=CC=C3C(C)(CCC4(C)C5CC(=C)CCC5(C)C CC34C)C2=CC(C=1O)=O |
| N251 | A | 0.33292451 1 | COC1CC2C3(CCN2Cc2cc4c(cc23)OCO4)C2C1O2 |
| N252 | A | 0.32909644 1 | CC1Cc2c(C(C)N1C)c(cc(c2c1ccc(c2c(cc(C)cc12)OC) O)OC)O |
| N253 | A | 0.32392857 7 | CCCCC=CC(=O)OC1CC2C(CCCCC(CCC)O)CCC C2NC1C |
| N254 | A | 0.32388080 9 | Cc1cc(c2c(ccc(c3c(cc(c4c3C[C@@H](C)N[C@@H]4 C)O)O)c2c1)O)OC |
| N255 | A | 0.31875876 3 | C1=C(c2ccc(cc2)Oc2c(cc(c3C(C=C(c4ccc(cc4)O)Oc 23)=O)O)O)Oc2cc(cc(c2C1=O)O)O |
| N256 | A | 0.31875876 3 | C1=C(c2ccc(cc2)Oc2c(cc(c3C(C=C(c4ccc(cc4)O)Oc 23)=O)O)O)Oc2cc(cc(c2C1=O)O)O |
| N257 | A | 0.30102999 6 | [H]c1c(C)cc(c2C(c3c(ccc(c3O)[C@@]3([H])c4cccc(c4 C(c4c3cc(C)cc4O)=O)O)C(c12)=O)=O)O |
| N7 | A | 0.30102999 6 | C[C@@]12CCC[C@]3(C)c4cc5C(C6=C(C(c5cc4C([C@]([C@H]23)(O)OC1)=O)=O)S(CCN6)(=O)=O)=O |
| N258 | A | 0.30102999 6 | c1c2C(=O)Oc3c4c(cc(c3O)O)C(=O)Oc(c24)c(c1O)O |
| N259 | A | 0.30102999 6 | CC1CC2C(Cc3c[nH]c4cccc2c34)N(C)C1 |
| N260 | A | 0.30102999 | CCC(C)C1C(C)C[C@H](C)C(C2=C(C(=CN(C2=O)O) |

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| | | 6 | c2cccc2)O)O1 |
| N261 | A | 0.30102999 6 | CCN(CC)C(NC1CC2C(Cc3c[nH]c4cccc2c34)N(C)C1)=O |
| N262 | A | 0.30102999 6 | CN1CCCC1c1c(ccc2c3CC[n+]4cc(C=C)c(CC5c6c(CCN5C)c5cccc5[nH]6)c(c4c3[nH]c12)O)O |
| N263 | A | 0.29499204 1 | CN1CCCC1c1c(ccc2c3CC[n+]4cc(C=C)c(CC5c6c(CCN5C)c5cccc5[nH]6)c(c4c3[nH]c12)O)O |
| N265 | A | 0.29305823 2 | CN1CCc2cc(c3cc2C1Cc1ccc(c(c1)Oc1ccc(CC2c4c(CCN2C)cc(c(c4O3)OC)O)cc1)OC)OC |
| N264 | A | 0.29305823 2 | CN1CCc2cc(c3cc2C1Cc1ccc(c(c1)Oc1ccc(CC2c4c(CCN2C)cc(c(c4O3)OC)OC)cc1)O)OC |
| N266 | A | 0.27685433 9 | CC1Cc2c(c3ccc(c4c(cc(C)cc34)O)OC)c(cc(c2C(C)N1)OC)O |
| N267 | A | 0.25963731 1 | CC(C)=CCc1c2c(C=CC(C)(C)O2)c(c2C(C3CC4c5c(C=3Oc12)c(cc(c5OC4(C)C)O)O)=O)O |
| N268 | A | 0.25181197 3 | C[C@@]12CC[C@@H]3[C@@]4(C)C(C=C[C@@]5(C)CO[C@H]([C@H]45)[C@H]([C@@]3(C)C1=CC[C@H]2c1ccoc1)O)=O |
| N269 | A | 0.25054112 6 | COc1ccc2CC3c4cc5c(cc4CCN=3)Oc3c(cc4CCN[C@@H](Cc6ccc(cc6)Oc1c2)c4c3O5)OC |
| N270 | A | 0.24948666 1 | C[n+]1ccc2c3cc(ccc3[nH]c2c1)[Cl] |
| N272 | A | 0.24055880 3 | CC1CCC2(C(C)C3C(CC4C5CC=C6CC(CCC6(C)C5CCC34)OC3C(C(C(CO)O3)O)OC3C(C(C(CO)O3)O)O)OC3C(C(C(C(CO3)O)O)O)O2)NC1 |
| N274 | A | 0.23574927 9 | CC1C2=CC=C3C(C)(CCC4(C)C5CC(C)(CCC5(C)CC C34C)C(=O)OC)C2=CC(C=1O)=O |
| N276 | A | 0.22184875 | C[C@@]12CC[C@@H]3[C@@]4(C)C(C=C[C@@]5(C)CO[C@H]([C@H]45)[C@H]([C@@]3(C)C1=CC[C@H]2c1ccoc1)O)=O |
| N277 | A | 0.22184875 | CC(C)CC(=O)O[C@H]1C(=O)O[C@@H]2C[C@H]3C(C)=CC([C@H]([C@]3(C)[C@H]3[C@H]([C@@H]([C@@]4(C(O)=O)[C@H]1[C@]23CO4)O)O)O)=O |
| N279 | A | 0.20760831 1 | CC(C)CC(=O)O[C@@H]1[C@H]([C@H]2C(=C)C(=O)O)[C@@H]2C[C@@H](C)C=CC([C@@]1(C)O)=O)O |
| N278 | A | 0.20760831 1 | CC(C)CC(=O)O[C@H]1[C@H]2C(=C)C(=O)O[C@@H]2C[C@@H](C)C=CC([C@](C)([C@@H]1O)O)=O |
| N280 | A | 0.20760831 1 | CC(C)CC(=O)OC1C2C(CC(C)C=CC(C(C)C1OC(C)=O)O)=O)OC(C2=C)=O |
| N281 | A | 0.20760831 1 | CCC(C)C(=O)OC1CC2C(C)(CC=C(C)C=C)C(C)CC(C23C(OC(C3=C1)OC(C)=O)OC(C)=O)O |
| N282 | A | 0.20065945 1 | C[C@@H]1C(c2cc(c(cc2[C@@H](c2ccc(c(c2)OC)OC)[C@@H]1C)OC)OC)=O |
| N283 | A | 0.19983820 9 | CC1=CC(C(C2(C)C1CC(C13COC4(C)C3C(=O)OC4C(C12)O)O)O)=O |

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| N284 | A | 0.19382002 6 | CC(C)[C@@H]1CCC2(C)C3C1C2C(C=C3C)=O |
| N285 | A | 0.19382002 6 | COc1cc2c(CC[n+] ³ cc4cc(c(cc4cc23)OC)OC)cc1O |
| N286 | A | 0.19362501 7 | CC(C)C=Cc1c(cc(C=Cc2ccc(cc2O)O)cc1O)O |
| N23 | A | 0.19362500 2 | CC(C)C=Cc1c(cc(C=Cc2ccc(cc2O)O)cc1O)O |
| N287 | A | 0.18782222 6 | CC1CCC2(C(C)C3C(CC4C5CC=C6CC(CCC6(C)C5 CCC34C)OC3C(C(C(C(CO)O3)OC3C(C(C(C(CO)O3) O)O)O)OC3C(C(C(C(CO)O3)O)O)O)O2)NC1 |
| N288 | A | 0.18708664 3 | [H][C@]12[C@H](C[C@@]3([H])C(C)(C)[C@H](CC[C@]3(C)[C@@]2([H])CC=C(C=C)[C@@H]1C)O)O |
| N289 | A | 0.18708664 3 | [H]C1C([H])C(C)(C)C2(C(C([H])C3([H])C(=C([H])C(= O)OC)c4ccoc4CC3([H])C2(C)C1=O)OC(C)=O)O |
| N290 | A | 0.18541948 4 | CC1CCC2(C(C)C3C(CC4C5CCC6CC(CCC6(C)C5C CC34C)OC3C(C(C(C(CO)O3)OC3C(C(C(C(CO)O3) O)OC3C(C(C(CO3)O)O)O)OC3C(C(C(C(CO)O3)O)O O)O)O)O2)NC1 |
| N291 | A | 0.18045606 5 | CC(C)=CCC1=C(c2cc(c(cc2OC)OC)O)Oc2cc(cc(c2C 1=O)O)O |
| N292 | A | 0.17849378 5 | C[C@]12C(C=C[C@@]3(C)COC(=C[C@]4(C)[C@@]25[C@H](C[C@@]2(C)[C@@H](C[C@@H]6[C@@] 24O6)C2=CC(O)OC2=O)O5)[C@H]13)=O |
| N293 | A | 0.17392519 7 | CC(C)=CCCC(C)=CCCC(C)(C=C)c1ccc(c(c1)O)O |
| N294 | A | 0.17392519 7 | CC(C)=CCCC(C)=CCCC(C)(C=C)c1ccc(c(c1)O)O |
| N295 | A | 0.15490196 | CC(C)=CCc1c(cc2c(C(c3c4C=CC(C)(C)Oc4c(c(CC= C(C)C)c3O2)O)=O)c1O)O |
| N296 | A | 0.15490196 | CCC(C)C1C2=NC(C(C)O2)C(NCc2nc(cs2)C(NC(C(C)CC)c2nc(cs2)C(N1)=O)=O)=O |
| N297 | A | 0.15251871 6 | CC(c1c(cc(c2c(C)cc(c3C(c4c(ccc4O)C(c23)=O)=O)O)c1O)O)[C@H]1[C@@H]([C@H]([C@@H]([C@ @H](CO)O1)O)O)O)=O |
| N298 | A | 0.14874165 1 | CN1CCc2cc(c(c3c2C1CC31CCC2(C(C1)OC)c1c(CC N2)c2cc(c(cc2[nH]1)OC)OC)O)OC |
| N299 | A | 0.14642345 6 | CC1CCC2C(C)C3C(CC4C5CC=C6CC(CCC6(C)C5C CC34C)OC3C(C(C(C(CO)O3)OC3C(C(C(C(CO)O3)O O)O)O)OC3C(C(C(C(CO)O3)O)O)O)N2C1 |
| N300 | A | 0.12861476 2 | C1CCN2CCC3C(=CC(CCC=CC1)(C1C3(CC3C=CC CCCN13)C2)O)c1c2c(ccn1)c1cc(ccc1[nH]2)O |
| N302 | A | 0.09988240 3 | COc1cc2CC[n+] ³ cc4c(ccc(c4OC)OC)cc3c2cc1OC |
| N303 | A | 0.09691001 3 | [H]C1CC(C)(C)C2(C(C3C4([H])C(C(=O)O3)c3ccoc3C C4([H])C2(C)C1=C([H])OC(C)=O)OC(C)=O)O |

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| N305 | A | 0.09691001 3 | C(C(=O)O[C@H]1[C@@H]([C@@H](COC(CC2(C=C C(C=C2)=O)O)=O)O[C@H]([C@@H]1OC(Cc1cccc(cc 1)O)=O)OC(CC1(C=CC(C=C1)=O)O)=O)O)c1cccc1 |
| N304 | A | 0.09691001 3 | C(C(=O)O[C@H]1[C@@H]([C@@H](COC(CC2(C=C C(C=C2)=O)O)=O)O[C@H]([C@@H]1OC(Cc1cccc 1)=O)OC(CC1(C=CC(C=C1)=O)O)=O)O)c1ccc(cc1) O |
| N306 | A | 0.09691001 3 | C1CCN[C@H]2[C@@]3(CCC=CCCCCN4CC[C@@ H](C(=C3)[C@@H]3c5c(CCN3CCc3c6c(ccn3)c3cccc c3[nH]6)c3cccc3[nH]5)[C@]2(CCC=CC1)C4)O |
| N308 | A | 0.09691001 3 | CC(=O)OC1CC(C)(C)C2(CCC3C(Cc4c(cco4)C3=O) C2(C)C1OC(C)=O)O |
| N309 | A | 0.09691001 3 | CC(=O)OC1CCC(C)(C)C2(CC3C4C(C(=O)O3)c3cco c3CC4C12C)O |
| N307 | A | 0.09691001 3 | CC(C)=CCc1cc(C(C=Cc2ccc(cc2)O)=O)c(c(CC=C(C) C)c1O)O |
| N310 | A | 0.09691001 3 | CC=C(C)C(=O)OC1CC2(C)C(C=C(C(CO)=CC3C1C(=C)C(=O)O3)O2)=O |
| N311 | A | 0.09691001 3 | CC1CC2C(C)(CCC3(C)C4=CC=C5C(=CC(C(=C5C) O)=O)C4(C)CCC23C)C(C1=O)O |
| N313 | A | 0.09691001 3 | CN1C2=CC(c3cccc3NC2c2cccc12)=O |
| N312 | A | 0.09691001 3 | CN1C2C(=C(c3cccc13)n1c3cccc3c3c1cc1cccc1n 3)c1cccc1N=2 |
| N314 | A | 0.04963514 6 | CN1CCc2cc(c(c3c2C1Cc1ccc(cc1)O)c1c2C(Cc4ccc(c c4)O3)N(C)CCc2cc(c1O)OC)O)OC |
| N315 | A | 0.04575749 1 | C[C@@]12CCC[C@]3(C)c4cc5C(C6=C(C(c5cc4C([C@]([C@H]23)(O)OC1)=O)=O)S(CCN6)(=O)=O)=O |
| N316 | A | 0.04575749 1 | COc1cc2c(CC[n+]3cc4cc(c(cc4cc23)OC)OC)cc1O |
| N317 | A | 0.03621217 3 | CC(C)CC(=O)O[C@@H]1C[C@@](C)(C(C=C[C@H] (C)C[C@@H]2[C@@H]1C(=C)C(=O)O2)=O)O |
| N318 | A | 0.02355206 5 | CC(C)C(=O)OC1CC(C)(C=CC(C(C)=CC2C1C(=C)C(=O)O2)=O)O |
| N319 | A | 0.02289858 2 | CCCCC=CC(=O)OC1CC2C(CCCCC(CCC)O)CCC C2NC1C |
| N320 | A | 0.01772876 7 | [H][C@]1(C(c2c(cc(cc2O[C@@H]1c1ccc(cc1)O)O) =O)[C@@]1([H])C(c2c(cc(cc2O[C@@H]1c1ccc(cc1) OC)O)O)=O |
| N321 | A | 0.01322826 6 | CC(C)=CCC(=O)OC1CC2C(CC=C3CC(CCC23C)N(C)C)C2CCC3CN(C)CC123 |
| N322 | A | 0.01308409 8 | COc1ccc(cc1)C1C(C2C(c3ccc(cc3)O)Oc3cc(cc(c3C2 =O)O)O)C(c2c(cc(cc2O1)O)O)=O |
| N323 | A | 0.00877392 4 | [H][C@]12CC[C@]3(C)[C@]([H])(CC[C@]4([H])[C@ @]5([H])[C@@H](CC[C@@]5(CC[C@@]34C)C(O)= O)C(C)=C)[C@@]2(C)CC[C@@H](C1(C)C)OC(C)C= |

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| | | | Cc1ccc(c(c1)O)O |
| N335 | A | 0 | [C-]#[N+]C(C)(C)C[C@H]1CC(C)C2CCC(C)C3(CCC(=C)C1[C@H]23)[N+]#[C-] |
| N326 | A | 0 | [H][C@@]1(C(c2c(cc(cc2O[C@@H]1c1ccc(cc1)O)O O)=O)[C@@]1([H])C(c2c(cc(cc2O[C@@H]1c1ccc(cc 1)OC)O)O)=O |
| N327 | A | 0 | [H]C1C([H])C(C)(C)C2(C(C(C3([H])C(=C([H])C(=O)O C)c4ccoc4CC3([H])C2(C)C1=O)OC(C)=O)OC(C)=O) O |
| N328 | A | 0 | [H]C1C([H])C(C)(C)C2(C(C(C3([H])C(c4ccoc4CC3([H])C2(C)C1=O)=O)OC(C)=O)OC(C)=O)O |
| N331 | A | 0 | C(C(=O)O[C@@H]1[C@H]([C@@H]([C@@H](COC(CC2(C=CC(C=C2)=O)O)=O)O[C@H]1OC(CC1(C=C C(C=C1)=O)O)=O)O)c1cccc1 |
| N332 | A | 0 | C1=C(c2c[nH]c3ccc(cc23)O)NC(C1=C1C(Nc2cccc1 2)=O)=O |
| N333 | A | 0 | C1C(C(c2ccc(c(c2)OC(c2cc(c(c(c2)O)O)O)=O)O)Oc2 cc(cc(c12)O)O)O |
| N329 | A | 0 | CC(=C)C[C@@H]1C[C@H](C)[C@H]2CC[C@](C)(C #N)[C@H]3CCC(=C)[C@@H]1[C@H]23 |
| N330 | A | 0 | CC(C)=CC1C[C@H](C)[C@H]2CC[C@H](C)[C@]3(CC[C@H](C)C=1[C@H]23)C#N |
| N334 | A | 0 | CC1=CC(C(C2(C)C1CC1C34COC(C23))(C(C(=C)C4(C(C(=O)O1)O)O)O)O)OC(C1C(C(C(C(O1)OC1(C O)C(C(C(CO)O1)O)O)O)O)O |
| N336 | A | 0.002710169 | - COc1ccc(cc1)C1C(C2C(c3ccc(cc3)O)Oc3cc(cc(c3C2 =O)O)O)C(c2c(cc(cc2O1)O)O)=O |
| N337 | A | 0.012281092 | - CC1C2CC3C45COC(C5C(C(=O)O3)O)(C(C(C4C2(C)CC(C=1O)=O)O)O)C(=O)OC |
| N338 | A | 0.01466708 | - COc1cc2c(CC[n+]3cc4c(ccc(c4OC)OC)cc23)cc1O |
| N339 | A | 0.015046813 | - CCCC(=O)O[C@H]1[C@H]2c3cc4c(cc3CN3CCC(=C [C@@H]1O)[C@H]23)OCO4 |
| N340 | A | 0.017033339 | - CC(C)=CCC1=C(c2cc(c(cc2O)O)O)Oc2c(CC=C(C)C) c3c(C=CC(C)(C)O3)c(c2C1=O)O |
| N341 | A | 0.017033339 | - CC1C2CCC3C4CC=C5CC(CCC5(C)C4CCC23CN1C)N(C)C |
| N342 | A | 0.028421338 | - COc1cnc2c3cccc3C(c3c2c1ccn3)=O |

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| N343 | A | 0.04139268 5 | - [H]N1CCS(C2=C1C(c1cc3c(cc1C2=O)C(c1c2c(co1)C(CC[C@]23C)=O)=O)=O)(=O)=O |
| N344 | A | 0.04139268 5 | - CC(C)=CCc1c(c2C(c3ccc(c(c3Oc2c(c1O)C(C)(C)C=C)O)O)=O)O |
| N346 | A | 0.04139268 5 | - CC12CCc3coc(C(c4cc5C(C=CC(c5cc14)=O)=O)=O)c23 |
| N345 | A | 0.04139268 5 | - CCC=C(C)C=CCCC1(C[C@H](C)[C@H](C(C)C(=O)OC)OO)OC |
| N347 | A | 0.04139268 5 | - CN1CCc2cc3c4cc2C1Cc1ccc(c(c1)Oc1ccc(CC2c5c(CCN2C)cc(c(c5O4)O3)OC)cc1)O |
| N348 | A | 0.04921802 3 | - CC(C)=CCCC1=C(c2cc(c(cc2O)O)O)Oc2c(cc(CCC=C(C)C)c(c2CCC=C(C)C)O)C1=O |
| N349 | A | 0.05307844 4 | - CC(C)=CCC(=O)OC1CC2C(CC=C3CC(CCC23C)N(C)C)C2CCC3CN(C)CC123 |
| N350 | A | 0.05690485 1 | - CN1CCc2cc(c3cc2C1Cc1ccc(c(c1)c1cc(CC2c4c(CC N2C)cc(c(c4O3)OC)OC)ccc1OC)O)OC |
| N351 | A | -0.0651105 | - COc1ccc2c3ccnc(CCC(O)=O)c3[nH]c2c1 |
| N352 | A | 0.07918124 6 | - C1C([C@@H](c2ccc(c(c2)O)O)Oc2cc(cc(c12)OC(c1cc(c(c1)O)O)O)=O)O)O |
| N353 | A | 0.07918124 6 | - CC(C)(C=C)c1c2c(C=CC(C)(C)O2)c(c2C(c3ccc(c(c3Oc12)O)O)=O)O |
| N354 | A | 0.07918124 6 | - CC(C)CC(=O)O[C@H]1C(=O)O[C@@H]2C[C@H]3C(C)=CC([C@H]([C@]3(C)[C@H]3[C@H]([C@@H]([C@]4(C(=O)OC)[C@H]1[C@]23CO4)O)O)O)=O |
| N355 | A | 0.07918124 6 | - COc1ccc(cc1O)C1=COc2cc(ccc2C1=O)O |
| N19 | A | 0.08278537 | - CC(=O)OC1CC2C(C)(C)C(C=CC2(C)C2CCC3(C)C(CC=C3C12C)c1ccoc1)=O |
| N356 | A | 0.10587353 5 | - CC1Cc2c(C(C)N1)c(cc(c2c1ccc(c2c(cc(C)cc12)OC)O)OC)OC |
| N357 | A | 0.10720997 | - [H][C@]1(Cc2cc(C)c(c(c2)Oc2ccc(C[C@]3([H])c4cc(c(cc4CCN3C)OC)O)cc2)OC)c2cc(c(cc2CCN1C)OC)O |
| N358 | A | 0.11394335 | - [H][C@@]12c3c(cc(c(c3O)O)O)C(=O)O[C@@]1([H])[C@@H]([C@H]([C@H](CO)O2)O)OC(c1cc(c(c1)O |

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| | | 2 | C)O)O)=O |
| N362 | A | 0.11394335 2 | CC(C)=CCc1c(c(CC=C(C)C)c2c(C(c3cc(c(c3O2)O)OC)OC)=O)c1O)O |
| N359 | A | 0.11394335 2 | CC(C)=CCc1c(cc2c(C(C3=C(C=C(C(C3(CC=C(C)C)CC=C(C)C)=O)O)O2)=O)c1O)O |
| N360 | A | 0.11394335 2 | CC(C)=CCCC(C)=CCc1c(cc(c2C(c3cc(ccc3O)c12)O)=O)O)O |
| N361 | A | 0.11394335 2 | Cc1cc(c2c(ccc(c3ccc4cc(C)nc(C)c4c3O)c2c1)OC)OC |
| N363 | A | 0.11727129 6 | CC(C)=CCc1c(cc(c2C(CC(c3c(cc(cc3OC)OC)OC)OC)Oc12)=O)O)O |
| N364 | A | 0.11727129 6 | CC(C)=CCCC(C)=CCc1c2c(C=CC(C)(C)O2)c(c2C(C3CC4c5c(C=3Oc12)c(cc(c5OC4(C)C)O)O)=O)O |
| N365 | A | 0.11864191 5 | CC(C)(C=C)C1=Cc2c(c3C=CC(C)(C)Oc3c(c2OC1=O)C(C)(C)C=C)O |
| N366 | A | 0.11920247 3 | CN1CCc2cc(c(cc2C1Cc1ccc(cc1)Oc1c2CC3c4c(CC N3C)c(c(c4c2cc(c1O)OC)OC)OC)OC)OC)O |
| N367 | A | 0.11997616 7 | CC1CC(C=C(C)C)OC12CCC1(C)CC3C(C(=CCC12)C=O)C(CC3(C)O)=O |
| N368 | A | 0.12065246 7 | CC1Cc2c(c3ccc(c4c(cc(C)cc34)O)OC)c(cc(c2C(C)N1C)OC)O |
| N369 | A | 0.12595190 7 | CC=C1CN(C)C2Cc3c4cccc4[nH]c3C(CC1C2C(=O)OC)=O |
| N370 | A | 0.13159557 2 | CCC=CC(CC)CCCC1(CC)CC(CC)C(CC(=O)OC)OO1 |
| N371 | A | 0.13672056 7 | CC(C)=CCCC(C)=CCCC(C)=CCc1cc(ccc1O)O |
| N373 | A | 0.14612803 6 | C=CC12CC(C3C(C2C(=C)C(=O)OC1)OC(C3=C)=O)OC(C(=C)CO)=O |
| N372 | A | 0.14612803 6 | CC(C)=CCc1c(c2C(c3ccc(c(c3Oc2c2c1O[C@@H](C)C2(C)C)O)O)=O)O |

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| N374 | A | 0.14612803 6 | - CC(C)c1cc2C(CC3C(C)(C)CCCC3(C)c2cc1O)=O |
| N375 | A | 0.14612803 6 | - CCCCCCCCC(C#CC#CC(C=C)OC(C)=O)O |
| N376 | A | 0.14612803 6 | - CCCCCCCCC(C#CC#CC(C=C)OC(C)=O)O |
| N377 | A | 0.14612803 6 | - CNCCc1cc(c(c(c1)[Br])OCCNC(C1CC2(CC(=C(C(=CO2)[Br])OC)[Br])ON=1)=O)[Br] |
| N378 | A | 0.14612803 6 | - COc1ccc(cc1)C1=CC(c2c(cc(c(c3cc(ccc3OC)C3=CC(c4c(cc(cc4O3)OC)O)=O)c2O1)O)O)=O |
| N379 | A | 0.14894373 7 | - CC1CC(C)OC(CC(c2ccc(cc2)O)NC(C(Cc2c3cccc3[nH]c2[Br])N(C)C(C(C)NC(C(C)CC(C)=C1)=O)=O)=O)=O |
| N380 | A | 0.15031529 9 | - CC=C1CN2C3CC1C(COC(c1cc(c(c(c1)OC)OC)OC)=O)(C(=O)OC)C14CC2OC34N(C)c2cc(c(cc12)OC)OC |
| N381 | A | 0.16774337 | - CCC1CC2CC3(C1N(CCc1c4cccc4[nH]c13)C2)C(=O)OC |
| N382 | A | 0.17377635 3 | - CC(=O)OC1CC2C(C)(C)C(C=CC2(C)C2CCC3(C)C(c4ccoc4)OC(C4C3(C12C)O4)=O)=O |
| N384 | A | 0.17609125 9 | - C(C(=O)O[C@@H]1[C@@H]([C@@H](COC(CC2(C=C(C(C=C2)=O)O)=O)O[C@@H]([C@@H]1OC(Cc1cccc1)=O)OC(CC1(C=CC(C=C1)=O)O)=O)O)c1cccc1 |
| N383 | A | 0.17609125 9 | - C[C@@H]1C[C@@H]2C[C@@H](C)[C@@](C)(C#N)[C@@H]3CC[C@@H]4[C@@H]([C@@H]23)[C@@H]1CC[C@@]4(C)NC=O |
| N395 | A | 0.17609125 9 | - CC(=C)C1CCC2(CCC3(C)C(C)(CCC4C3(C)CCC3C(C)(C)C(C[C@@]34C)O)OC(C=Cc3ccc(cc3)O)=O)C12)C(O)=O |
| N396 | A | 0.17609125 9 | - CC(C)[C@]12CC[C@](C)(C3=C([C@H](C)CC3=O)[C@H]1O)OO2 |
| N394 | A | 0.17609125 9 | - CC(C)=CCc1c(cc2cc3CC(C)(CC(c3c(c2c1O)O)=O)O)OC |
| N387 | A | 0.17609125 9 | - Cc1c2c(ccn1)c1cccc1[nH]2 |
| N386 | A | 0.17609125 | - CC1CCC(C(=C)CC2C(C(C=1)O)C(=C)C(=O)O2)O |

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| N385 | A | 0.17609125 9 | CC1CCC(C(C)=CC2C(C(C=1)O)C(=C)C(=O)O2)O |
| N391 | A | 0.17609125 9 | CN1CCc2cc(c(c3c2C1Cc1ccc(cc1)Oc1c2C(Cc4ccc(c c4)O3)N(C)CCc2cc(c1OC)OC)OC)OC |
| N388 | A | 0.17609125 9 | CN1CCc2cc(c(cc2C1Cc1ccc(c(c1)O)OC)Oc1cc(c(cc1 CC1c2cc(c(cc2CCN1C)OC)O)OC)OC)OC |
| N389 | A | 0.17609125 9 | CN1CCc2cc(c(cc2C1Cc1ccc(cc1)Oc1cc(CC2c3cc(c(cc3CCN2C)OC)OC)ccc1OC)O)OC |
| N392 | A | 0.17609125 9 | CN1CCc2cc(c3c(c2C1Cc1ccc(c(c1)Oc1cc2c(ccnc2C c2ccc(CO3)cc2)cc1OC)O)O)OC |
| N393 | A | 0.17609125 9 | CN1CCc2cc(c3c(c2C1Cc1ccc(c(c1)Oc1cc2c(ccnc2C c2ccc(CO3)cc2)cc1OC)OC)O)OC |
| N390 | A | 0.17609125 9 | CN1CCc2cc(c3cc2C1Cc1ccc(c(c1)Oc1ccc(CC2c4c(C CN2C)cc(c(c4O3)OC)OC)cc1)O)OC |
| N9 | A | 0.17831804 7 | C[C@H]([C@H]1[C@H](C=C[C@H]2[C@H]([C@@H](C=C)O)O2)O1)O |
| N397 | A | 0.18184358 8 | COc1ccc2CC3c4cc5c(cc4CCN=3)Oc3c(cc4CCN[C@ @H](Cc6ccc(cc6)Oc1c2)c4c3O5)OC |
| N398 | A | 0.18523809 4 | CC(C)(C=C)c1c2c(C=CC(=O)O2)c(c2C=CC(C)(C)Oc 12)OC |
| N399 | A | 0.18752072 1 | CC(C)[C@@H]1CCC(C)=CCC[C@](C)(C=C1)O |
| N400 | A | 0.18819006 5 | CC(c1c(cc(c2c(C)cc(c3C(c4c(ccc4O)C(c23)=O)=O)O)c1O)O)OC)=O |
| N401 | A | 0.19324602 4 | CCC(CC1(CC)C=C(CC)C(=CC(=O)OC)O1)C=CC(C) =O |
| N402 | A | 0.19514863 6 | CCCC(=O)O[C@H]1C=C2CCN3Cc4cc5c(cc4[C@@ H]([C@@H]23)[C@@H]1OC(CCC)=O)OCO5 |
| N403 | A | 0.19527436 5 | C[C@@]12CC[C@@]3(C[C@@]2(CCC2[C@@]14C CC[C@@]2(C)C(=O)O4)C(C3=C)=O)OC |

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| N404 | A | 0.20116272 2 | - CC1C(CC2C=1C1(C)C(CC(O)=O)C3(C)C(C(C1O2)O))C(C)(C=CC3=O)C(=O)OC)c1ccoc1 |
| N405 | A | 0.20411998 3 | - [H][C@@]12C3CCC1=C[C@@H]([C@H]([C@@]2([H])c1cc2c(cc1C3)OCO2)OC(C[C@H](C)O)=O)O |
| N406 | A | 0.20411998 3 | - CC(=O)OC(C)(C)C=CC(C(C)(C1C(CC2(C)C3CC=C4 C(CC(C(C4(C)C)=O)O)C3(C)C(CC12C)=O)O)O)=O |
| N407 | A | 0.20411998 3 | - CC(=O)OC1C2C(C(=O)OC)c3ccoc3CC2C2(C)C(CC C(C)(C)C2(C1O)O)=O |
| N409 | A | 0.20411998 3 | - CC1(CC(c2c(C1)cc1cc(c3C=CC(C)(C)Oc3c1c2O)OC)=O)O |
| N408 | A | 0.20411998 3 | - COc1cc2C3Cc4cc(c(cc4CN3CCc2cc1O)OC)OC |
| N410 | A | 0.20597729 9 | - C[C@@H](CC(=O)O)[C@H]1[C@H]2c3cc4c(cc3CN3 CCC(=C[C@@H]1O)[C@H]23)OCO4)O |
| N411 | A | 0.21218760 4 | - CC(C)[C@@H]1CCC(=C)[C@@H](CC[C@@](C)(C=C C1)O)O |
| N412 | A | 0.21218760 4 | - CN1CCc2cc(c3c4c2C1Cc1ccc(cc1)Oc1cc(CC2c5cc(c (cc5CCN=2)O3)O4)ccc1O)OC |
| N17 | A | 0.21748394 4 | - C(c1c2c(cc[nH]2)c2cccc2n1)n1cnc2c(N)ncnc12 |
| N413 | A | 0.21757767 5 | - CC(=O)OC1CC2C(C)(C)C(C=CC2(C)C2CCC3(C)C(C(C4C3(C12C)O4)=O)c1ccoc1)=O |
| N414 | A | 0.22021773 8 | - C[C@@H](CC(=O)O)[C@H]1[C@H]2c3cc4c(cc3CN3 CCC(=C[C@@H]1O)[C@H]23)OCO4)O |
| N415 | A | 0.22027095 3 | - CC1Cc2cc(c(c3c(C)cc4cccc(c4c3O)OC)c(c2C(C)N1C)OC)OC |
| N416 | A | 0.22530928 2 | - CCC=C(C)CCC=C(C)Oc1cc2Cc3cc(C)cc(c3C(c2c(c1)O)=O)O |
| N417 | A | 0.23044892 1 | - [H]C1C([H])[C@]2(C(C)(C)C([H])[C@H](CC(C)=O)C(=C([H])OC(C)=O)[C@]2(C)[C@@]2([H])Cc3c(cco3)C (=C)C12[H])O |
| N420 | A | - | - CC(C)=CCCC(C)=CCc1c(cc2cc3CC(C)(CC(c3c(c2c1 |

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| | | 0.23044892 1 | O)O)=O)O)OC |
| N418 | A | - 0.23044892 1 | CCC(C)C(=O)OC1(c2cccc(c2C(c2c1cc(c(C(=O)OC)c2C)O)=O)O)c1ccc2C(c3cc(c(C(=O)OC)c(C)c3C(c2c1O)=O)O)=O |
| N419 | A | - 0.23044892 1 | COc1cc(ccc1O)C1C(CO)Oc2ccc(cc2O1)C1=C(C(c2c(cc(cc2O1)O)O)=O)O |
| N421 | A | - 0.23496823 1 | CC1Cc2cc(c(c3c(C)cc4cccc(c4c3O)OC)c(c2C(C)N1C)OC)O |
| N422 | A | - 0.23597600 9 | [H]c1cccc1C=Cc1cc(c2c(c1)OC(C)(C)[C@@]1([H])CC[C@H](C)C[C@@]12[H])O |
| N423 | A | - 0.23712198 3 | CC1Cc2cc(c(c3c(C)cc4cccc(c4c3O)OC)c(c2C(C)=N1)OC)OC |
| N20 | A | - 0.24054924 8 | CC(=O)OC1CC(C(C)(C)C2CC(C3(C)C(CCC4(C)C(C)C=C34)C3CC(O)OC3)C12C)OC(C)=O)=O |
| N424 | A | - 0.24211405 3 | [H][C@@]1(C[C@@H](C)CC[C@]1([H])C(C)C)c1c(c(C=Cc2cccc2O)cc1O)O |
| N425 | A | - 0.24667323 6 | CC(=CCO)C1CC2C(C)(C)C(C=CC2(C)OO1)=O |
| N426 | A | - 0.25527250 5 | [H][C@](CO)(C#CC#CC#CC#CC#CC)O |
| N427 | A | - 0.25527250 5 | C1CCN2CCC3C(=CC(CCC=CC1)(C1C3(CC3C=CCCCN13)C2)O)c1c2c(ccn1)c1cccc1[nH]2 |
| N428 | A | - 0.25527250 5 | CC(C)=CCC1=C(C(CC=C(C)C)(CC=C(C)C)c2cc3c(c(C)cc(c3c(c2C1=O)O)O)O)O |
| N429 | A | - 0.25731821 4 | c1ccc2c(c1)C(c1c3c(ccn1)ccnc23)=O |
| N430 | A | - 0.26481782 3 | CC1=C(C(C=C(C1=O)OC)=O)[Cl] |
| N431 | A | - 0.26520097 3 | C[C@@H]1CC[C@@]2(CC[C@]3(C)C(=CC[C@@H]4[C@@]5(C)C[C@H]([C@@H](C(C)(C)[C@@H]5CC[C@@]34C)O)[C@@H]2[C@]1(C)O)C(O)=O |
| N432 | A | - 0.27067883 | C[C@]12CC[C@H]3C(=C)C(=O)O[C@@H]3[C@H]2C(=C)C(C=C1)=O |

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|------|---|-----------------|--|
| | | 6 | |
| N434 | A | 0.28647836 2 | CC(=O)OC1CC2C(C)(C)C(C=CC2(C)C2CCC3(C)C(CC=C3C12C)C1CC(C2C(C)(C)O2)OC1OC(C)=O)=O |
| N435 | A | 0.29666519 | CC(C)=CCOc1cc2Cc3cc(C)cc(c3C(c2c(c1)O)=O)O |
| N3 | A | 0.30102999 6 | C[C@@]12C[C@H]3[C@H](C[C@H]4[C@@](C)(CC[C@H]1O2)O4)C(=C)C(=O)O3 |
| N436 | A | 0.30102999 6 | C1=C(C(c2c(cc(cc2O1)O)O)=O)c1ccc(cc1)O |
| N437 | A | 0.30102999 6 | C1CN=C2C3=C(C(c4c2c1c[nH]4)=O)NCCC31C=C(C(C(=C1)[Br])=O)[Br] |
| N438 | A | 0.30102999 6 | CC(=O)O[C@H]1[C@H](C(C)(C)[C@@]2(CC[C@H]3C(c4ccoc4C[C@@H]3[C@@]2(C)[C@H]1OC(C)=O)=O)O)OC(C)=O |
| N439 | A | 0.30102999 6 | CC1=CC(C(C2(C)C1CC1C34COC(C23)(C(C(=C)C4(C(C(=O)O1)O)O)O)O)O)O |
| N443 | A | 0.30102999 6 | CC12CCC(C)(CC2C2(C)CCC3=C(CCC4C(C)(C)C(CC34C)O)C2(C)CC1)C(O)=O |
| N442 | A | 0.30102999 6 | Cc1cc(c2c(ccc(c3c(cc4C[C@H](C)N(C)[C@H](C)c4c3OC)OC)c2c1)OC)OC |
| N440 | A | 0.30102999 6 | CCCCC(C)CC(C)C(N1CCCC1C(=O)OC(C(C)CC)C(=O)OC(C(C)CC)C(O)=O)=O |
| N441 | A | 0.30102999 6 | COc1cc(c2C(C=C(c3ccc(c(c3)c3c(cc(c4C(C=C(c5ccc(cc5)O)Oc34)=O)O)O)OC)Oc2c1)=O)O |
| N444 | A | 0.30338390 1 | COC(c1cc(c(c(c1)O)O)O)=O |
| N445 | A | 0.30701110 6 | C[C@@]12CC[C@@]3(C[C@@]2(CCC2[C@@]14CC[C@@]2(C)C(=O)O4)C(C3=C)=O)O |
| N446 | A | 0.30963016 7 | COc1ccc(cc1OC)C(CNC(C=Cc1cccc1)=O)OC(C=Cc1cccc1)=O |
| N447 | A | 0.30983229 4 | CC(C)C1C(N(C)C(Cc2cccc2)C(=O)OC(C(C)C)C(N(C)C(Cc2cccc2)C(=O)OC(C(C)C)C(N(C)C(Cc2cccc2)C(=O)O1)=O)=O)=O |
| N448 | A | - | CC(C)=CCCC(C)=CCc1c(CC=C(C)C)c2C(c3c(cc(cc3 |

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|------|---|----------------------|---|
| | | 0.31523866 6 | Oc2c(c1O)O)O)=O |
| N449 | A | - 0.31979978 3 | C1CN2Cc3cc4c(cc3C3C2C1=CC(C3O)O)OCO4 |
| N450 | A | - 0.32221929 5 | [H]C1CC([H])[C@]2(C)[C@@]3([H])Cc4c(cco4)[C@]([H])(C)C3([H])[C@H](C([H])[C@]2(C1(C)C)O)O |
| N452 | A | - 0.32221929 5 | CC(=C)C(CC=C(C)C)Cc1c(cc(c2C(C=C(c3ccc(cc3O)C)O)Oc12)=O)O)O |
| N451 | A | - 0.32221929 5 | CC(=C)C(CC=C(C)C)Cc1c(cc(c2C(CC(c3ccc(cc3OC)O)Oc12)=O)O)O |
| N453 | A | - 0.32221929 5 | COc1cc(ccc1O)[C@@H]([C@H](CO)Oc1c(cc(CCCO)cc1OC)OC)O[C@H]1[C@@H]([C@@H](C(C(CO)O)1)O)O)O |
| N454 | A | - 0.32837960 3 | C[C@H]1[C@H]([C@H](C(C(Oc2cc3c(C(CC(c4ccc(c(c4)O)O)O3)=O)c(c2O)O)O1)O)O)O |
| N455 | A | - 0.33645973 4 | CCCCCCCCC(C#CC#CC(C=C)OC(C)=O)O |
| N15 | A | - 0.33683431 2 | C1C(O)OCC2=C1C(c1cccc1C2=O)=O |
| N456 | A | - 0.34242268 1 | CC(=C)C(Cc1cc(C(C=Cc2ccc(c(CC=C(C)C)c2)O)=O)c(cc1O)O)O |
| N459 | A | - 0.34242268 1 | CC(=O)OCCCCCCCCCCC(C#CC#CC(C=C)OC(C)=O)O |
| N458 | A | - 0.34242268 1 | CC(C)(CCCCCCCCCCC(C#CC#CC(C=C)OC(C)=O)O)=O |
| N457 | A | - 0.34242268 1 | CC(C)=CCC1CC23CC(CC=C(C)C)C(C)(C)OC2=C(C(c2ccc(c(c2)O)O)=O)C(C(CC=C(C)C)(C3=O)C1(C)C)=O |
| N460 | A | - 0.34242268 1 | CC(C)C[C@@H]([C@@H]1Cc2cccc(c2C(=O)O1)O)NC([C@H]([C@@H]1[C@@H]2CC(N[C@](C)([C@@](C)(O)O1)N2)=O)O)=O |
| N461 | A | - 0.34830486 3 | [H]C(=C)C1=CCCC(CO)=C[C@H]2[C@H](C(=C)C(=O)O2)[C@H](CC(C(C)CC)=O)[C@@H]1OC(C)=O |
| N462 | A | - 0.35554216 | CC1Cc2c(c3ccc(c4c(cc(C)cc34)O)OC)c(cc(c2C(C)N1C)OC)O |

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| | | 3 | |
| N463 | A | 0.35823564 2 | CC=C1CN2CCC34C(C2CC1C4(COC(C)=O)C(=O)O C)=Nc1cccc13 |
| N464 | A | 0.36172783 6 | CC1CC2=CC(C=C3C2=C(C=C(C)O3)O1)=O |
| N465 | A | 0.36172783 6 | CCC(C)C1c2nc(cs2)C(NC(C)C2=NC(C(C)O2)C(NC(C(C)C)c2nc(co2)C(N1)=O)=O)=O |
| N466 | A | 0.36604549 3 | COC1CC2C3(C=C1)C(CN2Cc1cc2c(cc13)OCO2)O |
| N467 | A | 0.37166461 9 | CC=C1CN2CCC34c5cc(ccc5N(C)C45C2CC1C3(CO 5)C(=O)OC)O |
| N468 | A | 0.37474834 6 | C1Oc2cc3ccnc4C(c5cccc5c(c2O1)c34)=O |
| N470 | A | 0.38021124 2 | CC(=C)C(CC=C(C)C)Cc1c(cc(c2C(C=C(c3ccc(cc3O C)O)Oc12)=O)OC)O |
| N469 | A | 0.38021124 2 | CC(=C)C(CC=C(C)C)Cc1c(cc(c2C(CC(c3ccc(cc3OC O)Oc12)=O)OC)O |
| N472 | A | 0.38021124 2 | CC(C1CCC2C3CCC4CC(CCC4(C)C3CCC12C)N(C) C)N(C)C |
| N471 | A | 0.38021124 2 | COc1cc(c(C=Cc2cccc2)=O)c(c1OC)O)O |
| N473 | A | 0.39748274 7 | [H]C(C1CCC(COC(C)=O)=C[C@H]2C(C(=C)C(=O)O 2)[C@H](CC=1)O)=O |
| N475 | A | 0.39794000 9 | CC1C=C(C2C(C=CC=C2O)C=1c1c(cc(c2c1C[C@H](C)N[C@H]2C)OC)O)OC |
| N476 | A | 0.40015858 3 | CC(C)c1c2CC[C@H]3C(C)(C)CCC[C@]3(C)c2cc(c1 O)O |
| N477 | A | 0.40312052 1 | CCC=C(C)CCC=C(C)c1c(cc2C(=C3c4cc(C)cc(c4C(c 4c3cc(c(C(C)=CCCC(C)=CCC)c4O)O)=O)O)c3cc(C) cc(c3C(c2c1O)=O)O)O |
| N478 | A | 0.40717350 9 | CC=C1CN2C3CC1C(CO)(C2Cc1c2cccc2[nH]c13)C(=O)OC |

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| N479 | A | 0.40717350 9 | - CC1C2CN3CCc4c5ccccc5[nH]c4C3CC2C(=CO1)C(=O)OC |
| N480 | A | 0.41217059 6 | - CC1C2CN3C=CC4C(=C3CC2C(=CO1)C(=O)OC)N=c1ccccc1=4 |
| N481 | A | 0.41497334 8 | - [H]c1c2c(C(c3c(CCC=C(C)C)ccc(c3N2C)O)=O)c(c(CCC=C(C)C)c1O)O |
| N483 | A | 0.41497334 8 | - CC(=C)C(CC=C(C)C)Cc1c(cc(c2C(C=C(c3ccc(cc3O)O)Oc12)=O)O)O |
| N482 | A | 0.41497334 8 | - CC(=C)C(CC=C(C)C)Cc1c(cc(c2C(CC(c3ccc(cc3O)O)Oc12)=O)O)O |
| N484 | A | 0.41497334 8 | - CN1C2C(=Cc3ccccc13)c1ccccc1N=2 |
| N485 | A | 0.42223655 1 | - Cc1c(cc2CCc3c(ccc(c3O)OC)C3CC(C)(C)Oc1c23)O |
| N486 | A | 0.42434997 | - CC=C(C)C(=O)OC1(C)C(CC2C(C3C4(C)C=CC13OO4)OC(C2=C)=O)O |
| N488 | A | 0.43136376 4 | - CC(C)=CCc1c(C)cc(c2c(c3C(=CC(C(CC=C(C)C)(CC=C(C)C)c3cc12)=O)O)O)O |
| N487 | A | 0.43136376 4 | - CC(C)=CCOc1c2C=CC(=O)Oc2cc2c1cco2 |
| N489 | A | 0.44404479 6 | - CN1CCc2cc3c(cc2C(Cc2ccc4c(c2C1)OCO4)=O)OC O3 |
| N490 | A | 0.44584629 1 | - CC=C1CN2CCC34C2CC1C(=C3Nc1ccccc14)C(=O)OC |
| N491 | A | 0.46239799 8 | - [H]C(C1C[C@@H](CC(C)C)C(=O)[C@H]2C(=C)C(=O)O[C@H]2C=C(CCC=1)COC(C)=O)=O |
| N492 | A | 0.46239799 8 | - [H]C1C([H])C(C)(C)C2(C(C(C3([H])C(=C)c4ccoc4CC3([H])C2(C)C1=O)OC(C)=O)OC(C)=O)O |
| N493 | A | 0.46239799 8 | - CC(=O)OC(C)(C)C=CC(C)(C1C(CC2(C)C3CC=C4C(CC(C(C4(C)C)=O)O)C3(C)C(CC12C)=O)O)O)=O |
| N494 | A | 0.46239799 | - CC(=O)OC(C)(C)C=CC(C)(C1C(CC2(C)C3CC=C4C(CC(C(C4(C)C)=O)O)C3(C)C(CC12C)=O)O)O)=O |

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| | | 8 | |
| N495 | A | 0.46834733 | <chem>CC(C)=CCCC(C)=CCc1c(cc2C(C3c4cc(C)cc(c4C(c4c3cc(cc4O)OCC=C(C)C)=O)O)c3cc(C)cc(c3C(c2c1O)=O)O)O</chem> |
| N496 | A | 0.47129171 | <chem>CC(c1cc2C(c3ccc(c(c3C(c2o1)=O)OC)OC)=O)=O</chem> |
| N500 | A | 0.47712125 | <chem>[H][C@@]1(C(=C)C(C)=O)[C@@H]2[C@H](C(=C)C(=O)O2)[C@H](C[C@@]1(COC(C)=O)C=C)OC(C(=C)CO)=O</chem> |
| N498 | A | 0.47712125 | <chem>[H][C@@]1(CCCCCCCCCCCCCCCC)C[C@@](C)(C(C(=O)OC)OO1</chem> |
| N499 | A | 0.47712125 | <chem>[H][C@@]12C(=C)C(=O)OC[C@]2(C[C@@H]([C@@H](C(=C)C(=O)OC)[C@@H]1O)OC(C(=C)CO)=O)C=C</chem> |
| N503 | A | 0.47712125 | <chem>C=CC12CC(C3C(C2C(=C)C(=O)OC1)OC(C3=C)=O)OC(C(=C)CO)=O</chem> |
| N505 | A | 0.47712125 | <chem>CC(=O)OCC1C[C@@H]([C@H]2C(=C)C(=O)O[C@@H]2C=C(CCC=1)C=O)OC(C(=C)CO)=O</chem> |
| N506 | A | 0.47712125 | <chem>CC(C(=C)C1[C@@H]2C(C(=C)C(=O)O2)[C@H](C[C@@]1(COC(C)=O)C=C)OC(C(=C)CO)=O)=O</chem> |
| N513 | A | 0.47712125 | <chem>CC(C)=CCc1c2c(c(c3c1c(c1ccoc1n3)OC)O)OCO2</chem> |
| N514 | A | 0.47712125 | <chem>CC(C)=CCc1c2c(c(c3c1c(c1ccoc1n3)OC)O)OCO2</chem> |
| N508 | A | 0.47712125 | <chem>CC(C)=CCCC(C)=CCc1c(cc(c2C(c3c(ccc(c3O)c12)O)O)=O)O)O</chem> |
| N504 | A | 0.47712125 | <chem>CC(C)=CCCC(C)=CCc1c(cc2c(C(c3c(ccc(c3O2)O)O)=O)c1O)O</chem> |
| N509 | A | 0.47712125 | <chem>CC(C)=CCCC1(C)C=Cc2c(cc3c(C(c4c(ccc(c4O3)O)O)=O)c2O)O1</chem> |
| N507 | A | 0.47712125 | <chem>CC(C1CCC=C(C[C@@H]([C@H]2C(=C)C(=O)O[C@@H]2C=1)OC(C(=C)CO)=O)COC(C)=O)=O</chem> |
| N501 | A | 0.47712125 | <chem>CC1(C)[C@H](Cc2c(cc(c3C(c4c(ccc(c4O)c23)O)O)=O)O)OC)[C@@]2(C)CC[C@@H]1O2</chem> |

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| N510 | A | 0.47712125 5 | - CC12CCc3coc(C(c4cc5C(C=CC(c5cc14)=O)=O)=O) c23 |
| N502 | A | 0.47712125 5 | - Cn1ccc2cc3c(cc2c1Cc1ccc(cc1)O)OCO3 |
| N511 | A | 0.47712125 5 | - COc1cc2c(c3ccoc3nc2cc1OC)OC |
| N515 | A | 0.48234602 7 | - CC(=O)O[C@H]1[C@H]2c3cc4c(cc3CN3CCC(=C[C@H]1O)[C@H]23)OCO4 |
| N516 | A | 0.48855071 7 | - COc1cc2CCNC3Cc4ccc(c(c4c(c23)c1O)OC)OC |
| N518 | A | 0.49136169 4 | - [H]C1C([H])C(C)(C)[C@@]2(C([H])[C@@H](C3([H])C(c4ccoc4C[C@]3([H])[C@@]2(C)C1=C([H])OC(C)=O)=O)OC(C)=O)O |
| N520 | A | 0.49136169 4 | - CC(C)=CC(c1c(cc2c(c1C)OC(c1c(C)cc(c(C=O)c1O2)O)=O)OC)=O |
| N519 | A | 0.49136169 4 | - CC1(C)C2CC(C3(C)C(CCC4(C)C(c5ccoc5)OC(C5C34O5)=O)C2(C)C=CC1=O)O |
| N521 | A | 0.49136169 4 | - COC1C(C(CC23CCNC(C(c4ccc(c(c34)O)OC)O)C=12)O)O |
| N522 | A | 0.50514997 8 | - CC(C)=CCCC1(C)C(CC=C(C)C)CC2(CC=C(C)C)C(C(=C(c3ccc(c(c3)O)O)O)C(C1(CC=C(C)C)C2=O)=O)=O |
| N523 | A | 0.50514997 8 | - COc1cc(cc(c1OC)OC)OC1C(C(C(C(COC(c2cc(c(c(c2)O)O)O)=O)O1)O)O)O |
| N524 | A | 0.50988689 2 | - CC(C)=CCCC(C)=CCc1c2C(c3c(cc(c(CC=C(C)CO)c3O)O)Oc2cc(c1OC)O)=O |
| N525 | A | 0.51054501 | - CC(C)=CCc1ccc2c(C(CC(c3ccc(cc3)O)O2)=O)c1O |
| N526 | A | 0.51607503 7 | - CC[C@H](CCC(C)C1CCC2C3CC=C4CC(CC[C@]4(C)C3CC[C@]12C)[C@H]1C(C([C@@H](C(CO)O1)O)O)C(C)C |
| N527 | A | 0.51688904 6 | - CN1CCc2c3cc(c(c2Oc2cc4c(CCN(C)[C@H]4Cc4ccc(c(c4)Oc4ccc(CC13)cc4)O)c(c2OC)OC)OC)OC |
| N528 | A | 0.51851394 | - C(CNC(c1cc(c[nH]1)[Br])=O)C=C1C(NC(N)=N1)=O |

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| N529 | A | - 0.51851394 | CC(=C)C(=O)OC1CC2(C)C(C=C(C(CO)=CC3C1C(=C)C(=O)O3)O2)=O |
| N530 | A | - 0.51851394 | CC[C@@H]1[C@](C)([C@@H]([C@@H](C)N(C)C[C@@H](C)C[C@](C)([C@@H]([C@@H](C)[C@@H]([C@@H](C)C(=O)O1)O[C@H]1C[C@](C)([C@H]([C@H](C)O1)O)OC)O[C@H]1[C@@H]([C@H](C[C@@H](C)O1)N(C)Cc1ccc(cc1)c1cn(CCCCCCCCCC(NO)=O)nn1)O)O)O |
| N531 | A | - 0.51851394 | CC[C@@H]1C[C@]2(CC)[C@@H]3[C@H]1[C@@H](CC)OO[C@]3(CC)C(=O)O2 |
| N532 | A | - 0.51934499 1 | CC(C)c1c2CC[C@H]3C(C)(C)CCC[C@]3(C)c2cc(c1O)O |
| N533 | A | - 0.52067235 3 | CC(C)c1cc2CCC3C(C)(C)CCCC3(C)c2cc1O |
| N534 | A | - 0.53019969 8 | CC1C2CCC3C4CC=C5C[C@H](CCC5(C)C4CCC23CN1C)NC |
| N535 | A | - 0.53147891 7 | C1=CN2C(c3c1c1cccc1[nH]3)=Nc1cccc1C2=O |
| N536 | A | - 0.53147891 7 | C1CNC(c2c(C1=C1C(NC(N)N1)=O)c(c[nH]2)[Br])=O |
| N537 | A | - 0.53147891 7 | CC(=O)O[C@H]1CCC(C)(C)[C@@]2([C@H]([C@@H]([C@H]3C(=C)c4ccoc4C[C@@H]3[C@@]12C)OC(C)=O)OC(C)=O)O |
| N538 | A | - 0.53147891 7 | CC=C(C)C(NC1CCC2(C)C3CCC4(C)C(CCC4C(C)NC)C3CCC2C1OC(C)=O)=O |
| N540 | A | - 0.53147891 7 | CC1(C)C=Cc2c(cc3c(C(C(=C(c4ccc(cc4)O)O3)OC)=O)c2O)O1 |
| N539 | A | - 0.53147891 7 | CC1(C)C=Cc2c(ccc(C(C=Cc3ccc(cc3)O)=O)c2O)O1 |
| N541 | A | - 0.54294874 9 | CC(C)c1cc2CC[C@H]3C(C)(C)CCC[C@]3(C)c2cc1O |
| N546 | A | - 0.54406804 4 | CC(=C)C(=O)O[C@H]1C[C@]23C(O)OCC(CC[C@H]2O3)=C[C@@H]2[C@@H]1C(=C)C(=O)O2 |
| N547 | A | - 0.54406804 4 | CC(C)=CCc1c2c(C=CC(C)(C)O2)c(c2C(c3cc(c(c3O)c12)O)OC)OC)=O)O |

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| N543 | A | 0.54406804 4 | - 4 | CC(C1CCC2C3CCC4C(C(=CCC4(C)C3CCC12C)NC=O)=O)N(C)C |
| N544 | A | 0.54406804 4 | - 4 | CCCCCCCCCCCCCCCCOC1C(C(C(C(COC(C)=O)O1)O)O)OC1C(C(C(C(C)O1)OC(C)=O)OC(C)=O)OC(C)=O |
| N545 | A | 0.54406804 4 | - 4 | COc1ccc(cc1)C1=CC(c2c(cc(c(c3cc(ccc3OC)C3=CC(c4c(cc(cc4O3)O)O)=O)c2O1)O)O)=O |
| N548 | A | 0.54817891 5 | - 5 | CC1(C)C(CC[C@@]2(C)[C@H]1CC[C@]1(C)[C@@H]2CC[C@@H]2[C@H]3[C@@H](CC[C@]3(C)CC[C@@]12C)C(=C)C=O)=O |
| N550 | A | 0.55630250 1 | - 1 | [H]C(C(=C)[C@@H]1CC[C@]2(C)CC[C@]3(C)[C@](H))(CC[C@]4([H])[C@@]5(C)CCC(C(C)(C)[C@]5([H]))CC[C@@]34C)(O)O)[C@@]12[H])=O |
| N551 | A | 0.55630250 1 | - 1 | CC12CCCC3(C=[N+](CCO)C1)C2CCC12CCC(CC13)C(=C)C2O.[Cl-] |
| N552 | A | 0.55630250 1 | - 1 | CCCC(=O)OC1CC2C(C)(CC=C(C)C=C)C(C)C(C(C23C(OC(C3=C1)OC(C)=O)OC(C)=O)O)OC(C=Cc1ccc(cc1)O)=O |
| N554 | A | 0.55630250 1 | - 1 | COc1cc(cc(c1O)OC)C1=CC(c2c(cc(c(c2OC)OC)OC)O1)=O |
| N553 | A | 0.55630250 1 | - 1 | COc1ccc2c(CC3c4c(CCN3)c(c3c(c24)OCO3)OC)c1OC |
| N555 | A | 0.56282079 9 | - 9 | CC(C)=CCCC(C)=CCc1c(cc2c(C(c3cc(c(cc3O2)O)O)C)=O)c1O)O |
| N556 | A | 0.56585704 6 | - 6 | CC=C1CC2C3CC1C(CO)N2Cc1c2cccc2n(C)c13 |
| N557 | A | 0.56820172 4 | - 4 | [H][C@@]1(C)C[C@@H](C2C(C[C@@]3(C)CC[C@]1(O)O3)OC(C=2COC(C)=O)=O)OC(C(=C)CO)=O |
| N558 | A | 0.56820172 4 | - 4 | [H][C@]12CCC3=C(CC[C@]4(C)[C@]3(C)CC[C@@]3(C)CC[C@@](C)(C[C@]34[H])C(O)=O)[C@@]2(C)CCC(C1(C)C)=O |
| N559 | A | 0.56820172 4 | - 4 | [H]C1=C(C([H])(CC=C(C)C)c2cc3c(CC=C(C)C)c(C)c(CC=C(C)C)c(c3c(c2C1=O)O)O)O |
| N563 | A | 0.56820172 4 | - 4 | CC(C)=CCc1c(cc(c2C(c3c(Cc12)c(CC=C(C)C)c(C)c(CC=C(C)C)c3O)=O)O)O |
| N560 | A | - | - | CC(C)=CCCC(C)=CCCC(C)=CCCC(C)=CCO |

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| | | 0.56820172 4 | |
| N561 | A | - 0.56820172 4 | CC(C)CNC(C=CC=CCCCCCC=Cc1ccc2c(c1)OCO2)=O |
| N562 | A | - 0.56820172 4 | CC1(C)C=Cc2c(cc(c3C(C4CC5c6c(C=4Oc23)c(cc(c6OC5(C)C)O)O)=O)O)O1 |
| N564 | A | - 0.56820172 4 | CCOC(C1=C2C(=c3ccccc3=N2)N(C)c2ccccc12)=O |
| N565 | A | - 0.57167628 2 | CC1C(CC2C=1C1(C)C(CC(=O)OC)C3(C)C4C(C1O2)OC(C4(C)C=CC3=O)=O)c1ccoc1 |
| N566 | A | - 0.57457537 8 | CC(C)C1CCC2(C)CC3C(=CC(C12OO3)O)C=O |
| N567 | A | - 0.57863921 | CC(=O)OCCCCCCCCCCC(C#CC#CC(C=C)OC(C)=O)O |
| N568 | A | - 0.57978359 7 | CC(=O)OC1CCC(C)(C)C2(C(C(C3C(Cc4c(cco4)C3=C)C12C)O)OC(C)=O)O |
| N569 | A | - 0.58459938 3 | COC1=C(C(C(=CC1=O)C1Cc2cc(c(c(c2OC1)OC)OC)OC)=O)OC |
| N570 | A | - 0.58459938 3 | COC1=C(C(C(=CC1=O)C1Cc2cc(c(c(c2OC1)OC)OC)OC)=O)OC |
| N571 | A | - 0.59106460 7 | [H][C@@]1(C)C[C@@H](C2C(C[C@@]3(C)CC[C@]1(O)O3)OC(C=2COC(C)=O)=O)OC(C(C)=CC)=O |
| N572 | A | - 0.59106460 7 | C[C@]12CCC(c3coc(C(c4cc5C(C6=C(C(c5cc14)=O)S(CCN6)(=O)=O)=O)=O)c23)=O |
| N573 | A | - 0.59106460 7 | CC(C)=CCc1c(c(CC=C(C)C)c2c(C(CC(c3ccc(cc3)O)O2)=O)c1O)O |
| N574 | A | - 0.59106460 7 | CC(C)=CCc1c(c(CC=C(C)C)c2c(C(CC(c3ccc(cc3)O)O2)=O)c1O)O |
| N575 | A | - 0.59106460 7 | CC(C)=CCc1c(c2C(c3cc(c(c(c3Oc2c2C=CC(C)(C)Oc12)O)OC)OC)=O)O |
| N576 | A | - 0.59372842 7 | CC(C)=CCCC(C)=CCCC(C)=CCCC1(C)C(CCCO)C(CCC1(C)O)=C(C)C=O |

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| N577 | A | 0.59988307 2 | - COc1cc(c2C(C=C(c3ccccc3)Oc2c1)=O)O |
| N578 | A | 0.60205999 1 | - [H]C12Cc3ccc(c(c3c3c1c(CCN2([H])[H])cc(c3OC)OC)O)OC |
| N579 | A | 0.60205999 1 | - [H]CC1(C)C2=C[C@@H]([C@]3([H])[C@@](C)(C[C@H]([C@]4(C)[C@H](CC[C@@]34C)[C@H](C)CC=CC(C)(C)O)O)[C@]2([H])CC[C@@H]1O)O |
| N584 | A | 0.60205999 1 | - CC(=O)OC1CC(C2(C)c3cc4c(cco4)c(C)c3CCC2(C1(C)C)O)OC(C)=O |
| N581 | A | 0.60205999 1 | - CC(=O)OC1CC2C(C)(C=CC(=O)OC2(C)C)C2CCC3(C)C(c4ccoc4)OC(C4C3(C12C)O4)=O |
| N580 | A | 0.60205999 1 | - CC1(C)C2=CC[C@H]3[C@]4(C)C[C@H]([C@@H]([C@@]4(C)CC([C@@]3(C)[C@@H]2C[C@@H](C1=O)O)=O)[C@](C)(C(C=CC(C)(C)O)=O)O)O |
| N582 | A | 0.60205999 1 | - Cc1c2C(c3c(ccc(c3O)C3(c4cccc(c4C(c4c3cc(c(C(=O)OC)c4C)O)=O)O)O)C(c2cc(c1C(=O)OC)O)=O)=O |
| N583 | A | 0.60205999 1 | - Cc1c2C(c3c(cccc3O)C(c2cc(c1C(=O)OC)O)=O)=O |
| N585 | A | 0.60205999 1 | - Cc1cc2C(c3cc(cc(c3C(c2c(c1)O)=O)O)O)=O |
| N586 | A | 0.60205999 1 | - CCCCCCCCCCCCCCCC[C@]1(C)C[C@@](C)(CC(=O)OC)O1 |
| N588 | A | 0.61278385 7 | - [H]C([H])=C1[C@@]23C([H])([H])C(=O)O[C@@]([H])(C4=C([H])[C@]([H])O[H])OC4=O)[C@]2(C([H])([H])[H])C([H])([H])C([H])([H])[C@]1([H])[C@@]1(C([H])([H])[H])[C@]([H])C([H])([H])C(C(C([H])([H])[H])(C([H])([H])[H])[C@]1([H])[C@@]([H])(C(=O)OC([H])([H])[H])OC(C([H])([H])[H])=O)=O)O3 |
| N589 | A | 0.61278385 7 | - CC(C)=CCc1c(cc2c(C(c3c(cc(c3CC=C(C)C)OC)O)O2)=O)c1O)O |
| N590 | A | 0.61278385 7 | - CC=CC(c1c(cc2cc(cc(c2c1OC)OC)OC)OC)OC)=O |
| N591 | A | 0.61278385 7 | - CC1(C)C2CC(C3(C)C(CCC4(C)C(c5ccoc5)OC(C5C34O5)=O)C2(C)C=CC1=O)=O |
| N592 | A | - | - CCCC[C@@H](CCCCCCCC[C@H](CC(O)=O)O)OC |

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|------|---|----------------------|--|
| | | 0.61278385 7 | 1[C@@H]([C@H]([C@@H]([C@@H](CO[C@@H]2[C@H]([C@H]([C@@H](C(C)O)O)O)O)O)O)O)[C@@H]1C([C@@H]([C@H]([C@@H](CO)O)O)O)O C1[C@@H]([C@@H]([C@@H](C(C)O)O)O)O |
| N593 | A | - 0.62013605 5 | CC(C)C1CC2C(C)(CC=1)C(CCC2(C)O)O |
| N596 | A | - 0.62324929 | CC(=O)OC1[C@H](C2C(C)(C)C(C=C[C@]2(C)C2CC[C@]3(C)C(CC=C3[C@]12C)c1ccoc1)=O)OC(C)=O |
| N594 | A | - 0.62324929 | CC=C(C)C(=O)O[C@H]1[C@H]2C(=C)C(=O)O[C@@H]1[C@]1(C)[C@H](CC[C@@](C)([C@H]1[C@H]2OC(C(C)C)=O)O)O |
| N595 | A | - 0.62324929 | COc1cc2C3Cc4cc(c(cc4C[N+]3(CCc2cc1O)[O-])OC)OC |
| N597 | A | - 0.63245729 2 | CN1CCc2cc3c(cc2C(Cc2ccc4c(c2C1)OCO4)=O)OC O3 |
| N598 | A | - 0.63245729 2 | COc1cc2CCN3Cc4c(CC3c2cc1O)ccc1c4OCO1 |
| N599 | A | - 0.63245729 2 | COc1cc2CCN3Cc4c(CC3c2cc1O)ccc1c4OCO1 |
| N600 | A | - 0.63346845 6 | CC(CCCCC#C)CC(C)C(N(C)C(Cc1cccc1)C(NC(C)C(N(C)C(C)C(N(C)C(Cc1ccc(cc1)OC)C(N)=O)=O)=O)=O)=O |
| N601 | A | - 0.63346845 6 | CC1(C)[C@H](CC[C@]2(C)C3CC[C@@]4(C)[C@@H]5C[C@](C)(CC[C@]5(C)CC[C@]4(C)C=3CC[C@@H]12)C(O)=O)O |
| N602 | A | - 0.64345267 7 | CC(=C)C(=O)OC1CC2(C)C(C=C(C(=C)C(C3C1C(=C)C(=O)O3)O)O2)=O |
| N603 | A | - 0.64345267 7 | CC1C2=CC([C@@](C)(C[C@@H]([C@H]3C(=C)C(=O)O[C@@H]3[C@H]1O)OC(C(C)=C)=O)O2)=O |
| N604 | A | - 0.64345267 7 | CC1c2c(cc(c(c3ccc(c4c(cc(C)cc34)OC)OC)c2C[C@H](C)N=1)O)OC |
| N605 | A | - 0.64345267 7 | CC1c2c(cc(c(c3ccc(c4c(cc(C)cc34)OC)OC)c2C[C@H](C)N1C)OC)OC |
| N606 | A | - 0.64738297 | CC(C)C(=O)O[C@H]1C[C@@H]2[C@@](C)(CC=C(C)C=C)[C@@H](C)C[C@H]([C@]23C(=C1)[C@@H](OC(C)=O)O[C@H]3OC(C)=O)OC(c1cccc1)=O |
| N607 | A | - 0.65062037 | CC(=C)C(=O)O[C@H]1C[C@H](C)C2=CC([C@](C)(C=C3C1=C(COC(C)=O)C(=O)O3)O2)=O |

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| N608 | A | 0.65127801 4 | - CC=C1CN2CCC34C2CC1C1=CN2C5C(=CN(C13)c1cccc14)C1CC3C5(CCN3CC1=CC)c1cccc12 |
| N609 | A | 0.65147074 5 | - [H][C@]12Cc3ccc(cc3)Oc3cc(C[C@@]4([H])c5c(CC N4C)cc(c(c5Oc4c(CCN2C)c1cc(c4OC)OC)OC)O)ccc3O |
| N614 | A | 0.65321251 4 | - [H][C@]12CC[C@@]3([H])[C@@H](C(=O)OCCCC CCCC[C@@H]4C(=C5CCCN5C(=N)N4)C(=O)OCCC CNC(N)=N)[C@@H](C)NC(N[C@H](CCCCCCCC) C1)=N23 |
| N610 | A | 0.65321251 4 | - [H][C@]12CC[C@]3([H])C[C@H](C)NC(=NC(CCCCC CCC(C)OC([C@H]4[C@@H](C)N=C5N[C@H](CCC CCCCC)C[C@]6([H])CN[C@]4([H])N56)=O)C1)N23 |
| N611 | A | 0.65321251 4 | - [H][C@]12CC[C@]3([H])C[C@H](C)NC(=NC(CCCCC CCC(C)OC([C@H]4[C@@H](C)N=C5N[C@H](CCC CCCCC)C[C@]6([H])CN[C@]4([H])N56)=O)C1)N23 |
| N613 | A | 0.65321251 4 | - [H][C@]12CCc3c(C(=O)OCCCCNC(N)=N)c(CCCCC) nc(NC(CCCCCCCCC)C1)n23 |
| N612 | A | 0.65321251 4 | - [H][C@]12CCc3c(C(O)=O)c(C)nc(N[C@H](CCCCC C)C1)n23 |
| N616 | A | 0.65321251 4 | - C[C@H]1Cc2c(c3ccc(c4c(cccc34)OC)OC)c(cc(c2[C @@H](C)N1C)OC)OC |
| N615 | A | 0.65321251 4 | - CC(=C)C(=O)O[C@H]1C[C@H](C)[C@@]2(CC[C@] (C)(CC3C1=C(COC(C)=O)C(=O)O3)O2)O |
| N617 | A | 0.65321251 4 | - CC(C)=CCC1=C(c2ccc(cc2O)O)Oc2c3C=CC(C)(C)O c3cc(c2C1=O)O |
| N621 | A | 0.65321251 4 | - CC[C@H]1C=CCC[C@@]2(C[C@@H]3CC[C@@H] 4[C@H](C(=O)OCCCCCCCCCCCCCCC(N(CCCC N)CCCN)=O)[C@]5(CCC[C@@H](C)O5)N=C(N2)N3 4)O1 |
| N618 | A | 0.65321251 4 | - CCCCCCC[C@@H]1C[C@@H]2CC[C@H]3[C@@H](C(=O)OCCCCCCCC[C@@H]4C(=C5CCCN5C(= N)N4)C(=O)OCCCCNC(N)=N)[C@@H](C)N=C(N1)N 23 |
| N619 | A | 0.65321251 4 | - CCCCCCC[C@@H]1C[C@@H]2CC[C@H]3[C@@ H](C(=O)OCCCCCCCC[C@@H]4C(=C5CCCN5C(=N)N4)C(=O)OCCCCNC(N)=N)[C@@H](C)N=C(N1) N23 |
| N622 | A | 0.65321251 4 | - CCCCCCCCCCCCCCCCCCCC(=O)OC(COC(CCCC CCCCCCCCC)=O)CO[C@H]1[C@@H]([C@H]([C @@H]([C@@H](CN)O1)O)O)O |

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| N620 | A | 0.65321251 4 | - COC1C(C(CC23CCNC(Cc4ccc(c(c34)O)OC)C=12)O) O |
| N623 | A | 0.65609820 2 | - CC1CCC(C2(C)CCC(CC12O)C(C)=C)=O |
| N625 | A | 0.66275783 2 | - [H]C12C(C(C=O)C3=C(C(C(=C(C(C)C)C3=O)O)=O) C2(C)CCCC1(C)C)O |
| N626 | A | 0.66275783 2 | - CC(=O)OC1C(Cc2ccc(cc2)OC)NCC1O |
| N627 | A | 0.66275783 2 | - CC1C(C(C(C(O1)OC1C(c2ccc(c(c2)O)O)Oc2cc(cc(c 2C1=O)O)O)OC(C=Cc1cccc1)=O)O |
| N628 | A | 0.66707230 9 | - CC(C)=CCCc1c(c2C(C3CC4c5c(C=3Oc2c2C=CC(C) (C)Oc12)c(cc(c5OC4(C)C)O)O)=O)O |
| N629 | A | 0.66838591 7 | - [H][C@@]12C[C@@H](C=C3C(OC([C@@]13[C@H] (C[C@@H](C)[C@@]2(C)CC=C(C)C=C)OC(c1cccc 1)=O)OC(C)=O)OC(C)=O)OC(C(C)CC)=O |
| N631 | A | 0.67209785 8 | - CC(C)C1=CC(c2c(cc3c(CCCC3(C)C)c2C)C1=O)=O |
| N632 | A | 0.67209785 8 | - CC(C)C1=CC(c2c(cc3c(CCCC3(C)C)c2C)C1=O)=O |
| N630 | A | 0.67209785 8 | - CC(C)C1=CC2=CC=C3C(C)(C)CC(CC(C)c4ccc(c(c4) O)O)CC3(C)C2=C(C1=O)O |
| N633 | A | 0.67209785 8 | - CC1=CC2=CC(C=C3C2=C(C=C(C)O3)O1)=O |
| N634 | A | 0.67209785 8 | - CCCCCCC=CCCCCCCC(C[C@]1(C[C@@H](C=C C1=O)O)O)O |
| N635 | A | 0.67209785 8 | - CCCCCCC=CCCCCCCC1C[C@]2(C[C@@H](C=C C2(O)O1)O)O |
| N636 | A | 0.67209785 8 | - CCCCCCCCCCCCCCCCOC1C(C(C(C(COC(C)=O) O1)O)OC(C)=O)OC1C(C(C(C(C)O1)OC(C)=O)OC(C) =O)OC(C)=O |
| N637 | A | 0.67424483 7 | - CC(C)C1=CC(c2c(cc3c(CCCC3(C)C)c2C)C1=O)=O |
| N638 | A | - | - CC1Cc2c(C(C)=N1)c(cc(c2c1c(C)cc(c2c(cccc12)OC) |

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|------|---|-----------------|---|
| | | 0.67828482 1 | OC)OC)OC |
| N639 | A | 0.68124123 7 | CC(C)=CCc1c(c2C(C3CC4c5c(C=3Oc2c2C=CC(C)(C)Oc12)c(cc(c5OC4(C)C)O)O)=O)O |
| N640 | A | 0.68124123 7 | Cc1cc(c2c(cccc2c1c1c(cc2C[C@H](C)N[C@H](C)c2c1OC)O)OC)OC |
| N641 | A | 0.68394713 1 | CC(=C)C(=O)OC1CC2C(C)(C(C3C4C(C)(CO3)C=C(C(C24C)=O)O)C2=CCC(c3ccoc3)C12C |
| N642 | A | 0.68841982 2 | CC(C)=CCC1=C(c2ccccc2C(C1=O)=O)O |
| N643 | A | 0.69019608 | [H]C12C=C(C)C(C(CC(C(C)(C)CC=C(C)C(C2(C(C(C)C1OC(c1cccc1)=O)OC(C)=O)OC(C)=O)OC(C)=O)OC(C)=O)OC(C)=O)=O |
| N644 | A | 0.69019608 | CC(C)c1cc2CCC3C(C)(C)CCCC3(C)c2cc1O |
| N645 | A | 0.69019608 | CN1Cc2cc(c(cc2c2ccc3cc4c(cc3c12)OCO4)OC)OC |
| N646 | A | 0.69090018 7 | CC1Cc2c(c(cc(c2C(C)N1)OC)O)c1c(C)cc(c2c(cccc12)OC)OC |
| N647 | A | 0.69127724 2 | CCC1CC2CC3(C1N(CCc1c4cc(ccc4[nH]c13)OC)C2)C(=O)OC |
| N648 | A | 0.69292509 | CCCCC1cc2c(c3cc(C)ccc3C(C)(C)O2)c(c1C(=C)CC1(CCC(C)=CC1)C(C)C)O |
| N649 | A | 0.69635638 9 | CC1(C)CCC[C@@]2(C)C1CC[C@@]1(CO1)[C@@H]2CC=C(C1CO1)C(=O)OC |
| N650 | A | 0.69635638 9 | CC1(C)CCC[C@@]2(C)C1CC[C@@]1(CO1)[C@@H]2CC=C(C1CO1)C(=O)OC |
| N657 | A | 0.69897000 4 | CC(=O)OC1CC(C)(C)C2(CCc3c(cc(c(C=O)c3C)O)C2(C)C1OC(C)=O)O |
| N653 | A | 0.69897000 4 | CC(=O)OCC[C@H]1C[C@H]2c3c(CCN2C[C@@H]1C=C)c1cc(ccc1[nH]3)O |
| N654 | A | 0.69897000 4 | CC(C)=CC[C@@H]1C[C@]23C[C@H](C=CC(C)(C)O)C(C)(C)OC2=C(C(c2ccc(c(c2)O)O)=O)C([C@@](C=C(C)C)(C3=O)C1(C)C)=O |
| N655 | A | 0.69897000 | CC(C)=CC[C@@H]1C[C@]23C[C@H](CCC(C)(C)O)C(C)(C)OC2=C(C(c2ccc(c(c2)O)O)=O)C([C@@](CC |

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|------|---|-----------------|---|
| | | 4 | =C(C)C)(C3=O)C1(C)C)=O |
| N652 | A | 0.69897000 4 | - CC(C)=CC[C@@H]1C[C@@]23CC4CCC(C)(C)C[C@@ @]4(C)OC2=C(C(c2ccc(c(c2)O)O)=O)C([C@@](CC= C(C)C)(C3=O)C1(C)C)=O |
| N656 | A | 0.69897000 4 | - CC(C)=CC[C@H]1C[C@@]23C[C@@H](CC(C(C)(C)O)O)C(C)(C)[C@@](CC=C(C)C)(C(C(=C2OC1(C)C) C(c1ccc(c(c1)O)O)=O)=O)C3=O |
| N651 | A | 0.69897000 4 | - CC(C)=CC[C@H]1C[C@@]23C[C@@H](CC=C(C)C)C(C)(C)[C@@](CC=C(C)C)(C(C(=C2OC1(C)C)C(c1 ccc(c(c1)O)O)=O)=O)C3=O |
| N658 | A | 0.69897000 4 | - CC(C)=CCc1c(C)cc2cc3c(C(=CC(C3(CC=C(C)C)CC =C(C)C)=O)O)c(c2c1O)O |
| N662 | A | 0.69897000 4 | - Cc1cc(c2c(ccc(c3c(cc4C[C@H](C)N(C)[C@H](C)c4c 3OC)O)c2c1)OC)OC |
| N659 | A | 0.69897000 4 | - CC1CC(CCCC(C=C(C)C(C)O)O)(OC)OOC1CC(=O) OC |
| N660 | A | 0.69897000 4 | - CC1CC(CCCC=CC(C)=O)(OC)OOC1CC(=O)OC |
| N661 | A | 0.69897000 4 | - CCC(C)C(=O)OC1(c2cccc(c2C(c2c1cc(c(C(=O)OC)c 2C)O)=O)O)c1ccc2c(C(c3c(cc(c(C(=O)OC)c3C)O)C2 (c2ccc3C(c4cc(c(C(=O)OC)c(C)c4C(c3c2O)=O)O)=O)OC(C(C)CC)=O)=O)c1O |
| N663 | A | 0.70415051 7 | - CC12COC3C2C(C)(C2CCC4(C)C(CC=C4C2(C)C3O)C2=CCOC2=O)C(C=C1)=O |
| N664 | A | 0.70492263 9 | - [H][C@]12C=C(C)C([C@@H]([C@@H](C(C)(C)CC= C(C)[C@H]([C@]2([C@H]([C@H](C)[C@@H]1O)c1cc ccc1)OC(C)=O)OC(C)=O)OC(C)=O)OC(C)=O)OC(C) =O)=O |
| N665 | A | 0.70611230 6 | - Cc1cc(c2c(ccc(c3c(cc(c4c3C[C@@H](C)N[C@@H]4 C)OC)O)c2c1)OC)O |
| N666 | A | 0.70757017 6 | - [H]C1(C(=C)C(CC)=O)[C@@]2(C)C=C(C)C[C@]1(C) C=C(C)[C@@H]2C(C)=C[C@H]1CC(C=C1)=O |
| N670 | A | 0.70757017 6 | - CC(C)C=Cc1cc(C=CC(c2cc(C=CC(C)C)c(cc2O)O)= O)ccc1O |
| N667 | A | 0.70757017 6 | - Cc1cc2C(C3C(C(C(C(O3)OC(c3cccc3)=O)O)O)O)c 3cccc(c3C(c2c(c1)O)=O)O |
| N668 | A | - | - Cc1cc2C(C3C(C(C(C(O3)OC(c3cccc3)=O)O)O)O)c |

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|------|---|----------------------|---|
| | | 0.70757017 6 | 3cccc(c3C(c2c(c1)O)=O)O |
| N669 | A | - 0.70757017 6 | CCCCCCCCC=CC(N[C@H]1C[C@]2(C(C=C[C@H])[C@@H]2O[C@H]1O)[C!])=O)O)=O |
| N674 | A | - 0.71600334 4 | CC(=O)O[C@H]1[C@H]2[C@H]3[C@H](C(=O)O2)c2 ccoc2C[C@@H]3[C@@]2(C)[C@H](CCC(C)(C)[C@] 12O)O |
| N672 | A | - 0.71600334 4 | CC(C)=CCC1=C(c2ccc(cc2O)O)Oc2cc3c(C=CC(C)(C)O3)c(c2C1=O)O |
| N671 | A | - 0.71600334 4 | CC(C)=CCc1c(cc(c(c1CC=C(C)C)O)O)C1CC(c2c(cc(cc2O1)O)O)=O |
| N673 | A | - 0.71600334 4 | CC(C)CC(=O)OC1CC2C(C)(CC=C(C)C=C)C(C)C(C(C23C(OC(C3=C1)OC(C)=O)OC(C)=O)O)OC(C)=O |
| N675 | A | - 0.71798846 6 | CC(C)=CCc1c(cc2c(C(c3c(CC=C(C)C)c(c(c(CC=C(C)C)c3O2)O)OC)=O)c1O)O |
| N676 | A | - 0.72427587 | CC(C)=CCc1cc(cc(CC=C(C)C)c1O)C1CC(c2c(cc(c(C C=C(C)C)c2O1)O)O)=O |
| N677 | A | - 0.72427587 | CC(C)C1=CC2=CC=C3C(C)(C)CC(CC3(C)C2=C(C1 =O)O)OC(c1ccc(cc1)O)=O |
| N678 | A | - 0.72754125 7 | CCC=C(C)CCC=C(C)c1c(cc2C(c3cc(C)cc(c3C(c2c1 O)=O)O)=O)O |
| N679 | A | - 0.73239376 | C(C[C@@H]1c2c(CCN1)c1ccc(cc1[nH]2)[Br])CNC(N)=N |
| N18 | A | - 0.73239376 | C(CC1c2c(CCN1)c1ccc(cc1[nH]2)[Br])CN=C(N)N |
| N681 | A | - 0.73239376 | CC1c2c(cc(c(c3ccc(c4c(cc(C)cc34)OC)O)c2C[C@H](C)N=1)O)OC |
| N680 | A | - 0.73239376 | CCCCCCC(CO)C=C(C)[C@H]([C@@H](C)C(=O)O[C@@H]1CC[C@H](C)[C@@]2(C)CC3C(=C[C@]12 O)OC(C=3C)=O)O |
| N682 | A | - 0.73458915 2 | CC(=O)OC1CC2C(C)(C)C(CCC2(C)C2CCC3(C)C(c4 ccoc4)OC(C4C3(C12C)O4)=O)=O |
| N683 | A | - 0.73579392 4 | CC(C)C=Cc1c(cc(C=Cc2ccc(cc2O)O)cc1O)O |
| N684 | A | - 0.73877630 6 | CC(COC(C)=O)=CC(=O)O[C@H]1C[C@H](C)C2=C C([C@](C)(C=C3C1=C(COC(C)=O)C(=O)O3)O2)=O |
| N686 | A | - | CC(C)CC(=O)OC1CC2C(C)(CCC(=C)C=C)C(C)CC(|

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|------|---|-------------|--|
| N699 | A | 0.755874856 | - CC(CC1c2c(ccc(c2OC)OC)c2ccc3cc4c(cc3c2N1C)OCO4)=O |
| N701 | A | 0.759883191 | - CC(=O)OC1CC2(C)C(c3ccoc3)OC(C3C2(C2(C)C1C1(C)C=CC(C(C)(C)C1CC2OC(C)=O)=O)O3)=O |
| N702 | A | 0.762678564 | - CC1=CC(c2c(ccc(c2C1=O)O)O)=O |
| N703 | A | 0.763427994 | - [H]C12C(C(C)=C(C(CC(C(C)(C)CC=C(C)C(C2(C(C)C)C1OC(c1cccc1)=O)OC(C)=O)OC(C)=O)OC(C)=O)OC(C)=O)OC(C)=O)OC(C)=O)O |
| N704 | A | 0.763427994 | - CC(=C)C1CCC2(CCC3(C)C(CCC4C5(C)C(C(C(C)C)C)C5CCC34C)OC(c3ccc(c(c3)OC)O)=O)C(O)=O)C12)C(O)=O |
| N705 | A | 0.763427994 | - CC(=O)OC1C2C(Cc3c(cco3)C2=C)C2(C)C(CCC(C)C)C2(C1O)O)=O |
| N706 | A | 0.763427994 | - CCC(C)C(C(NC(C(C)C)C(NC(C(C)C)C(N(C)C(C(C)C)C(=O)OC(C(C)CC)C(N1CCCC1C(=O)OC)=O)=O)=O)=O)N(C)C(CCCC(CCCC#C)OC)=O |
| N707 | A | 0.763427994 | - COC1=CC(C(=CC1=O)C(C=C)c1cccc1)=O |
| N708 | A | 0.763427994 | - COC1=CC(C(=CC1=O)C(C=C)c1cccc1)=O |
| N709 | A | 0.763427994 | - COC1=CC(C2=C(CCCc3cccc3O2)C1=O)=O |
| N710 | A | 0.770817478 | - CCC1C(=O)OC2(C)CC(C3C(C4C(C)(CCC12O)O4)OC(C=3COC(C)=O)=O)OC(C(=C)CO)=O |
| N711 | A | 0.770852012 | - [H]C12C=C(C)C(C(C)CC(C(C)(C)C=CC(C)(C(C2(C)C(C)C1OC(c1cccc1)=O)O)OC(C)=O)O)OC(C)=O)OC(c1cccc1)=O |
| N712 | A | 0.770852012 | - CCC(C)C(C(NC(C(C)C)C(N1CCC2C1C(N1CCCC1C(NC=Cc1cc(ccc1OC)O2)=O)=O)=O)=O)N(C)C |
| N713 | A | 0.775974331 | - CC(C)(C=C)c1cc(C=CC(c2ccc(cc2)O)=O)c(cc1O)OC |
| N716 | A | 0.77815125 | - [H][C@@]12C[C@@H](C=C3[C@@H](OC([C@@]23[C@@H](C[C@H](C)[C@]1(C)CC=C(C)C=C)O)OC(C)=O)OC(C)=O)OC(C(C)CC)=O |
| N715 | A | - | - [H][C@]12C[C@]3(C)[C@@H](C)CC[C@H]([C@@]3 |

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|------|---|----------------------|---|
| | | 0.77815125 | 4[C@@H]([C@]2(O)OCC1=C)O4)OC([C@H](C)[C@@H](C(C)=CC(CCCCC)CO)O)=O |
| N717 | A | - 0.77815125 | [H]C12C(C(C)=C(C(C(C(C)(C)CC=C(C)C(C2(C(C(C)C1OC(c1cccc1)=O)O)OC(C)=O)OC(C)=O)OC(C)=O)OC(C)=O)OC(C)=O)OC(C)=O)O |
| N721 | A | - 0.77815125 | CC(=O)OC(C1C(C)(C)C(C=CC1(C)C1CCC2(C)C(c3ccoc3)OC(CC2(C1=C)O)=O)=O)C(=O)OC |
| N730 | A | - 0.77815125 | CC(C)=CCc1c(cc2c(C(c3c(cc(c(c3CC=C(C)C)OC)O)O2)=O)c1O)O |
| N722 | A | - 0.77815125 | CC(C)=CCc1c(cc2c(C(c3c(CC=C(C)C)c(c(c(CC=C(C)C)c3O2)O)O)=O)c1O)O |
| N723 | A | - 0.77815125 | CC(C)=CCc1c(cc2c(C(c3c4C=CC(C)(C)Oc4c(c(CC=C(C)C)c3O2)O)=O)c1O)O |
| N718 | A | - 0.77815125 | CC(C)=CCc1c(cc2c(C(c3c4CC(C(C)(C)Oc4c(c(CC=C(C)C)c3O2)O)O)=O)c1O)O |
| N719 | A | - 0.77815125 | CC(C)=CCc1c2C(c3c(cc4c(C=CC(C)(C)O4)c3O)Oc2c(CC=C(C)C)c(c1O)O)=O |
| N731 | A | - 0.77815125 | CC(C)=CCc1c2C(c3c(cc4c(C=CC(C)(C)O4)c3O)Oc2cc(c1OC)O)=O |
| N732 | A | - 0.77815125 | CC(C)=CCc1c2C(c3c(cc4c(CCC(C)(C)O4)c3O)Oc2cc(c1OC)O)=O |
| N720 | A | - 0.77815125 | CC(C)=CCCC(C)=CCc1c(cc2c(C(c3c(cc(c(c3CC=C(C)C)OC)O)O2)=O)c1O)O |
| N729 | A | - 0.77815125 | CC(C)=CCCC(C)=CCc1c2C(c3c(cc(cc3Oc2cc(c1OC)O)O)O)=O |
| N724 | A | - 0.77815125 | CC(C)C1=CC2=CC=C3C(C)(CCCC3(C)C2=C(C1=O)O)COC(C(C)C)=O |
| N725 | A | - 0.77815125 | CC(CCCCC#C)C(N(C)C(Cc1cccc1)C(NC(C)C(N(C)C(C)C(N(C)C(Cc1ccc(cc1)OC)C(N)=O)=O)=O)=O)=O |
| N726 | A | - 0.77815125 | CC(CCCCC#C)C(N(C)C(Cc1cccc1)C(NC(C)C(N(C)C(C)C(N(C)C(Cc1ccc(cc1)OC)C(N)=O)=O)=O)=O)=O |
| N727 | A | - 0.77815125 | CC=C(C)C=CCCC1(CC(C)C(CC(=O)OC)OO1)OC |
| N728 | A | - 0.77815125 | CC1(C)C2CC(C3(C)C(CCC4(C)C(c5ccoc5)OC(C5C34O5)=O)C2(C)C=CC1=O)=O |
| N734 | A | - 0.77815125 | COc1ccc(cc1)[C@@H]1CC(c2c(cc(c(c2O1)[C@@H]1C(c2c(cc(cc2O[C@H]1c1ccc(cc1)O)O)O)=O)O)=O)O)=O |
| N733 | A | - 0.77815125 | COc1ccc(cc1)C1CC(c2c(cc(c(C3=C(c4ccc(cc4)O)Oc4cc(cc(c4C3=O)O)OC)c2O1)O)O)=O |
| N735 | A | - 0.78103693 9 | CCC(C)C(=O)O[C@@H]1C[C@@H]2[C@](C=O)(C(=C1)C=O)[C@H](C[C@@H](C)[C@@]2(C)CC=C(C)C=C)OC |
| N736 | A | - | CC(=O)OC(C1C(C)(C)C(C=CC1(C)C1CCC2(C)C(c3c |

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| | | 0.782030428 | coc3)OC(CC2(C1=C)O)=O)=O)C(=O)OC |
| N737 | A | 0.785329835 | CC(C)=CCc1cc(cc(CC=C(C)C)c1O)C1CC(c2c(cc(cc2O1)O)O)=O |
| N738 | A | 0.785329835 | CN1c2c(cccc2O)C(c2c1c(c(c2O)OC)OC)OC)=O |
| N740 | A | 0.785329835 | COc1cc(c2c(C=O)c(c3ccc(c(c3OC)O)OC)oc2c1)O |
| N739 | A | 0.785329835 | COc1ccc(cc1OC)C(CNC(C=Cc1cccc1)=O)OC(C=Cc1cccc1)=O |
| N741 | A | 0.787298101 | Cc1c(cc2CCc3c(ccc(c3O)O)C3CC(C)(C)Oc1c23)O |
| N742 | A | 0.79239169 | CC1c2c(cc(c(c3ccc(c4c(cc(C)cc34)O)OC)c2C[C@H](C)N1C)OC)OC |
| N743 | A | 0.79716974 | CC(C)=CCCC(C)=CCc1c2C(c3c(cc(c(CC=C(C)C)c3O)O)Oc2cc(c1OC)O)=O |
| N744 | A | 0.797959644 | [H][C@]12CC[C@H]([C@H](C)C=C[C@H](C)C(C)C)[C@@]2(C)CC[C@@]2([H])[C@]13C=C[C@]1(C[C@H](CC[C@@]12C)O)OO3 |
| N745 | A | 0.79934055 | CC(C)=CC[C@]12C([C@]3(C[C@@H](C(C)(C)O2)[C@]12C(=C3)C(c1c(cccc1O2)O)=O)OC)=O |
| N748 | A | 0.79934055 | CC(C)=CCc1ccc(C2=COc3cc(cc(c3C2=O)O)O)c(c1OC)O |
| N746 | A | 0.79934055 | CC(C)=CCCC(C)=CCc1c2C(c3c(cc(c(CC=C(C)C)c3O)O)Oc2cc(c1O)O)=O |
| N747 | A | 0.79934055 | CC1C2C(NCc3nc(cs3)C(NC(CCSC)C3=NC(CS3)C(NC(Cc3cccc3)C(=N2)O1)=O)=O)=O |
| N752 | A | 0.806179974 | C[C@H]1CC[C@@]2(C)[C@@H](CC=C3C(=O)O[C@H]([C@]23O)O)C1=C |
| N750 | A | 0.806179974 | CC(=O)OC1CC2C(C)(C)C(C=CC2(C)C2CCC3(C)C(C(C=C3C12C)=O)c1ccoc1)=O |
| N749 | A | 0.806179974 | CC(C)=CCC1=C(c2cc(c(cc2O)O)O)Oc2c3C=CC(C)(C)Oc3cc(c2C1=O)O |
| N751 | A | 0.806179974 | CCC(C)C(C(NC(CC(C)C)C(N1CCC2C1C(N1CCCC1C(NC=Cc1cc(ccc1OC)O2)=O)=O)=O)N(C)C |
| N753 | A | 0.80888586 | CC=C1CN2CCc3c4cccc4n4C(C1CC2c34)C(=O)OC |

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|------|---|-----------------|---|
| | | 7 | |
| N754 | A | 0.81291335 7 | [H]C1CC(C2(C)C3([H])Cc4c(cco4)C([H])(C(=O)OC)C3([H])C([H])C(C2(C1(C)C)O)OC(C)=O)OC(C)=O |
| N755 | A | 0.81291335 7 | [H]C1Cc2c(cc3c(cco3)c2C)C2(C)C(C(C(C(C)(C)C12O)OC(C)=O)OC(C)=O)OC(C)=O |
| N756 | A | 0.81291335 7 | CC(C)=CCc1cc2C3C(COc2cc1O)c1ccc(c(CC=C(C)C)c1O3)O |
| N757 | A | 0.81291335 7 | CC(c1ccccc1)O[C@@H]1CC2C(C=C3C[C@H](CC[C@]23C)O[C@H]2[C@@H]([C@@H]([C@@H]([C@@H](CO)O2)O[C@H]2[C@@H]([C@@H]([C@@H]([C@@H](CO)O2)O[C@H]2[C@@H]([C@@H]([C@@H]([C@@H](CO)O2)O)OC)O)OC)O)O)[C@]2(CC[C@H](C(C)OC(C)=O)[C@@]12C)O |
| N758 | A | 0.81954393 6 | CC(=C)C1CCC2(CCC3(C)C(CCC4C5(C)C(CCC34C)C(C)(C)C=C5C=O)C12)C(O)=O |
| N759 | A | 0.81954393 6 | CC(C)=CCc1c(cc(cc1O)O)C1=CC(c2c(cc(c(CC=C(C)C)c2O1)O)O)=O |
| N760 | A | 0.81954393 6 | CC(C1CCC2C3CCC4CC(CCC4(C)C3CCC12C)N(C)C(c1ccccc1)=O)NC |
| N761 | A | 0.81954393 6 | CC1(C)C=Cc2c(ccc3C4C(COc23)c2ccc(cc2O4)O)O1 |
| N762 | A | 0.81954393 6 | CC1CCC2=C(CCCC2(C)C)C1(C)CCC(C)=CCn1c[n+](C)c2c1c(N)ncn2.[Cl-] |
| N763 | A | 0.81954393 6 | COc1c(cc2c(C(C=C(c3ccc(c(c3)O)O)O2)=O)c1O)O |
| N764 | A | 0.82477646 3 | CC1=CC(c2c3cc(c(c(C)c3oc2C1=O)O)OC)=O |
| N765 | A | 0.82477646 3 | CC1=CC(c2c3cc(c(c(C)c3oc2C1=O)O)OC)=O |
| N766 | A | 0.82607480 3 | CC(C)=CCc1c(cc2c(C(C=C(c3ccc(cc3)O)O2)=O)c1O)O |
| N768 | A | 0.82607480 3 | COc1cc2c(cc1O)C1CC(CC3CCCN13)OC(C=Cc1cc(c2c1)O)=O |

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| N769 | A | 0.826074803 | - COc1ccc(cc1)[C@@H]1CC(c2c(cc(c2O1)[C@@H]1C(c2c(cc(cc2O[C@H]1c1ccc(cc1)O)O)O)=O)O)O)=O |
| N767 | A | 0.826074803 | - COc1ccc(cc1c1c(cc(c2C(C=C(c3ccc(cc3)O)Oc12)=O)O)O)C1=CC(c2c(cc(cc2O1)O)O)=O |
| N770 | A | 0.832508913 | - CCC=C(C)C=CCCC1(CC(C)C(CC(=O)OC)OO1)OC |
| N771 | A | 0.832508913 | - COc1cc(ccc1O)C1=COc2cc(ccc2C1=O)O |
| N772 | A | 0.838849091 | - CC(=C)C1CC2=C(c3c(cc(c(c13)O)O)O)Oc1c3C=CC(C)(C)Oc3cc(c1C2=O)O |
| N773 | A | 0.838849091 | - CC(C)C=Cc1c(cc2c(C(C(CC=C(C)C)=C(c3ccc(cc3O)O)O2)=O)c1O)OC |
| N774 | A | 0.838849091 | - COc1cc(c(C(C=Cc2cc(c(c2)OC)OC)OC)=O)c(c1)OC)O |
| N775 | A | 0.84509804 | - [H]C(CC(=CCCC(C)=CCCC(C)=CCc1cc(cc(c1O)O)C(O)=O)C(O)=O)C=C(C)C |
| N776 | A | 0.84509804 | - [H]C1C[C@@H]([C@]2(C)[C@@]3([H])Cc4c(cco4)[C@@]([H])(C(=O)O[H])C3([H])[C@H](C([C@]2(C1(C)C)O)OC(C)=O)O)OC(C)=O |
| N782 | A | 0.84509804 | - C[C@H]1CC=C[C@H]([C@H]([C@H](CC=Cc2cc(cc(c2C(=O)O1)O)OC)O)O)O |
| N779 | A | 0.84509804 | - CC(C)=CC(c1c(cc2c(c1C)OC(c1c(C)cc(c(C=O)c1O2)O)=O)O)=O |
| N778 | A | 0.84509804 | - CC(CCC=C(C)CC[C@@H](C(C)(C)O)O)=CCCC=C(C)CCC=C(C)CC[C@H]([C@](C)(CO)O)O |
| N777 | A | 0.84509804 | - CC(CCC=C(C)CC[C@H](C(C)(C)O)O)=CCCC=C(C)CCC=C(C)CC[C@H]([C@](C)(CO)O)O |
| N780 | A | 0.84509804 | - CC1CC=CC(C(C(CC2C(c3cc(cc(c3C(=O)O1)O)OC)O2)O)O)O |
| N781 | A | 0.84509804 | - CCCCC1=CC(C(CC=C(C)CCC=C(C)C)=C(C1=O)OC(C)=O)=O |
| N14 | A | 0.847008951 | - C(c1cc2C(c3ccccc3C(c2c(c1)O)=O)O)=O)O |
| N783 | A | 0.849113248 | - CC=C1CN2C3CC1C(CO)(C2Cc1c2ccccc2n(C)c13)C(=O)OC |
| N784 | A | 0.84925765 | - CC(C)=CCc1c(cc2c(C(c3c(cc(c(c3CC=C(C)C)OC)O)O2)=O)c1O)OC |

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| | | 8 | |
| N785 | A | 0.85125834 9 | CC1C(C(C(C(OCC2C(C(C(C(O2)OC2=C(c3ccc(c(c3)O)O)Oc3cc(cc(c3C2=O)O)O)O)O)O)O)O)O)O |
| N786 | A | 0.85308953 | CC(C)[C@@H](C)C=C[C@@H](C)[C@H]1CC[C@@]23[C@]4(C=C[C@@]56C[C@H](CC[C@]5(C)[C@]4(CC[C@]12C)OO6)O)O3 |
| N787 | A | 0.85705091 8 | CC(C)[C@@H]1CC[C@@]2(CC[C@]3(C)[C@H](CC[C@@H]4[C@@]5(C)CC[C@@H](C(C)(C)[C@@H]5CC[C@@]34C)O)[C@@H]12)CO |
| N788 | A | 0.85733249 6 | [H][C@@]12CC=C(C)[C@@H](C[C@@H](C3=CC(=O)OC3O)O)[C@]2(C)CCCC1(C)C |
| N789 | A | 0.85733249 6 | [H]C(C(=C)[C@@H]1CC[C@]2(C)CC[C@]3(C)[C@](H))(CC[C@]4([H])[C@@]5(C)CC[C@]([H])(C(C)(C)[C@]5([H])CC[C@@]34C)O)[C@@]12[H])=O |
| N792 | A | 0.85733249 6 | CC(C)=CC(c1c(C)c2c(c(c1OC)O)OC(c1c(C)c(c(C=O)c1O2)O)[Cl]=O)=O |
| N791 | A | 0.85733249 6 | CC=C(C)C(=O)OC1CC2(C)C(C=C(C(CO)=CC3C1C(=C)C(=O)O3)O2)=O |
| N793 | A | 0.85733249 6 | CC1CC2=C(C(C=C(C2=C(C)N1)OC)=O)c1c(C)cc(c2c(ccc12)O)OC |
| N794 | A | 0.86033800 7 | CC(C)=CCc1cc2C(c3c(cc(c(CC=C(C)C)c3O)OC)Oc2c(c1OC)O)=O |
| N795 | A | 0.86332286 | c1cc(ccc1C1C(C2C(c3ccc(cc3)O)Oc3cc(cc(c3C2=O)O)O)C(c2c(cc(cc2O1)O)O)=O)O |
| N796 | A | 0.86332286 | CC1Cc2cc3c(c(cc(c3c(c2C(=O)O1)O)O)O)c1c(cc(c2c(c3C(=O)OC(C)Cc3cc12)O)O)O |
| N797 | A | 0.86332286 | COC(CC1(C=CC(C=C1)=O)O)=O |
| N798 | A | 0.86359192 7 | CN1CCc2cc(c(cc2C1Cc1ccc(cc1)Oc1c2CC3c4c(CC N3C)c(c(c4c2cc(c1OC)OC)OC)OC)OC)OC)OC |
| N799 | A | 0.86923172 | [H]C1C=C2C[C@H](CC[C@]2(C)C2C[C@H]([C@]3(C)[C@H](CC[C@@]3(C12)O)C(C)OC(C)=O)OC(C)c1cccc1)O[C@H]1[C@@H]([C@@H]([C@@H]([C@@H]([C@@H](CO)O1)O[C@H]1[C@@H]([C@@H]([C@@H]([C@@H]([C@@H](CO)O1)O[C@H]1[C@@H]([C@@H]([C@@H]([C@@H]([C@@H]([C@@H](CO)O1)O)OC)O)OC)O)OC)O |
| N800 | A | 0.86923172 | CC(C)C1CC[C@H]2C(=CC[C@H]3C(C)(C)CCC[C@]23C)C=1 |
| N801 | A | - | [H][C@@]12CC=CC([C@]2(C)C=C2C(C1)=C(C)C(= |

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| | | 0.87506126 3 | O)O2)=O |
| N802 | A | 0.87506126 3 | [H]C1C=C2C[C@H](CC[C@]2(C)C2C[C@H]([C@]3(C)[C@H](CC[C@@]3(C12)O)C(C)OC(C)=O)OC(C)c1cccc1)O[C@H]1[C@@H]([C@@H]([C@@H]([C@@H]([C@@H](CO)O1)O[C@H]1[C@@H]([C@@H]([C@@H]([C@@H]([C@@H](CO)O1)O[C@H]1[C@@H]([C@@H]([C@@H]([C@@H]([C@@H]([C@@H](CO)O1)O[C@H]1[C@@H]([C@@H]([C@@H]([C@@H]([C@@H]([C@@H](CO)O1)O)O)OC)O)OC)O)OC)O |
| N803 | A | 0.87506126 3 | c1c(C(O)=O)c(c2c3C(=O)Oc4c5c(C(=O)Oc(c35)c(c2O)O)c(c2c(cc(c2O)O)O)C(O)=O)c(c4O)O)c(c(c1O)O)O |
| N804 | A | 0.87563993 7 | C=CC(CO)C1CCN2CCc3c4cccc4[nH]c3C2C1 |
| N805 | A | 0.88081359 2 | CC(C)=CC(CC(C)=CC(C1COC(C1=C)=O)O)=O |
| N806 | A | 0.88081359 2 | COc1cc(c2C(C=C(c3ccc4c(c3)OCO4)Oc2c1)=O)OC |
| N808 | A | 0.88649072 5 | CC(C)=CCc1cc(cc(CC=C(C)C)c1O)C1CC(c2ccc(cc2O1)O)=O |
| N809 | A | 0.88649072 5 | CC(C)C(C(N(C)C(C(C)C)C(N(C)C(C(C)C)C(N(C)C(Cc1cccc1)C(N)=O)=O)=O)=O)N(C)C(C(C)CCCC#C)=O |
| N813 | A | 0.88649072 5 | CC(C)C=Cc1c(cc2c(C(C3CC(C(C)(C)O)Oc4cc(ccc4C=3O2)O)=O)c1O)OC |
| N810 | A | 0.88649072 5 | CC(Cc1ccc(c(c1)O)O)C(C)Cc1ccc(c(c1)O)O |
| N811 | A | 0.88649072 5 | CC1(C)C2=CCC3C(C)(C2CC(C1=O)O)C(CC1(C)C(C(C13C)O)C(C)(C=C(C)(C)O)=O)O)=O |
| N812 | A | 0.88649072 5 | CC1C(CCC2C1(C)CCC1C2(C)CCC2(C)C3CC(C)(C)CCC3(C)CCC12C)=O |
| N814 | A | 0.88649072 5 | COc1ccc2c(c1)c(c1c3c4c(CCN3)cc3c(c4c4ccc(cc14)OC)OCO3)c1c3c(CCN1)cc1c(c23)OCO1 |
| N815 | A | 0.89209460 3 | C(=Cc1ccc(cc1)O)C(c1ccc(cc1O)O)=O |
| N816 | A | - | C1CC2C(C(C1O2)C(O)=O)C(O)=O |

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| | | 0.89209460 3 | |
| N817 | A | - 0.89209460 3 | CC1(C)C2=CCC3C(C)(C2CC(C1=O)O)C(CC1(C)C(C(C13C)O)C(C)(C(C=CC(C)(C)O)=O)O)=O |
| N819 | A | - 0.89762709 1 | CC(=C)C1CC2=C(c3c1c(c1c(C=CC(C)(C)O1)c3O)O)Oc1cc(cc(c1C2=O)O)O |
| N820 | A | - 0.89762709 1 | CC(C)C(=O)OC1(c2cccc(c2C(c2c1cc(c(C(=O)OC)c2C)O)=O)O)c1ccc2C(c3cc(c(C(=O)OC)c(C)c3C(c2c1O)=O)O)=O |
| N818 | A | - 0.89762709 1 | CC(c1c(cc(c2c(C)cc(c3C(c4c(cccc4O)C(c23)=O)=O)O)c1O)OS(O)(=O)=O)O)=O.[Na] |
| N821 | A | - 0.89762709 1 | CC1CCC23C(CC(C=C3C(OC2OC(C)=O)OC(C)=O)O)C1(C)CC=C(C)C=C |
| N822 | A | - 0.90167703 2 | C[n+] ₁ cc2c3c(ccc2c2ccc4cc5c(cc4c12)OCO5)OCO3 |
| N823 | A | - 0.90308998 7 | [H][C@@]1(C)C[C@H]([C@]([H])(C=C)C2C=C3c4c(CCN3C(=C)C1=2)c1cccc1[nH]4)OC1C(C(C(CO)O1)O)O |
| N826 | A | - 0.90308998 7 | C[C@@H]1C(c2cc3c(cc2[C@@H](c2ccc(c(c2)OC)OC)[C@@H]1C)OCO3)=O |
| N827 | A | - 0.90308998 7 | C[C@]12C[C@@H](C[C@@]3(C)C1[C@@H]([C@@H]1[C@@]4(COC(C=C24)=O)O1)OC3=O)O |
| N824 | A | - 0.90308998 7 | CC=C(C)C(=O)O[C@H]1C[C@]2(C)C(C=C(C(C)[C@@H]([C@@H]3[C@@H]1C(=C)C(=O)O3)O)O2)=O |
| N825 | A | - 0.90308998 7 | CCC(C)C(C(N(C)C(Cc1cccc1)C(NC(CC(C)C)C(Nc1cccc1C(O)=O)=O)=O)=O)N |
| N828 | A | - 0.90363251 6 | C[C@]12C[C@@H](C[C@@]3(C)C1[C@@H](C=C1COC(C=C12)=O)OC3=O)O |
| N829 | A | - 0.90363251 6 | C[C@]12C=C[C@@H]([C@@]3(C)C1[C@@H]([C@@H]1[C@@]4(COC(C=C24)=O)O1)OC3=O)O |
| N830 | A | - 0.90363251 6 | C[C@]12C=C[C@@H]([C@@]3(C)C1[C@@H](C=C1COC(C=C12)=O)OC3=O)O |
| N832 | A | - 0.90363251 | C[C@]12C=CC[C@@]3(C)C1[C@@H]([C@@H]1[C@@]4(COC(C=C24)=O)O1)OC3=O |

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| N833 | A | 0.90363251 6 | <chem>C[C@]12C=CC[C@@]3(C)C1[C@@H](C=C1COC(C=C12)=O)OC3=O</chem> |
| N831 | A | 0.90363251 6 | <chem>C[C@]12CC[C@H]([C@@]3(C)C1[C@@H](C=C1COC(C=C13)=O)OC2=O)O</chem> |
| N834 | A | 0.90363251 6 | <chem>C[C@]12CCC[C@@]3(C)C1[C@@H](C=C1COC(C=C12)=O)OC3=O</chem> |
| N835 | A | 0.90363251 6 | <chem>CC12CCCC(C)(C1C=CC1(COC(CC12)=O)O)C(O)=O</chem> |
| N836 | A | 0.90848501 9 | <chem>CCCCCCCCCCCCCCCCOC1C(C(C(C(COC(CCCC CCCCCCCCCCC)=O)O1)O)O)OC1C(C(C(C(C)O1)O C(C)=O)OC(C)=O)OC(C)=O</chem> |
| N837 | A | 0.91381385 2 | <chem>c1cc(c(cc1C1=C(C(c2ccc(cc2O1)O)=O)O)O)O</chem> |
| N838 | A | 0.91381385 2 | <chem>CC(C)=CCc1c(cc(c(C(C=Cc2ccc(cc2)O)=O)c1O)OC)O</chem> |
| N839 | A | 0.91381385 2 | <chem>CC(C)C1c2nc(cs2)C(NC(C)c2nc(C(NC(C)c3nc(cs3)C(N1)=O)=O)c(C)o2)=O</chem> |
| N840 | A | 0.91381385 2 | <chem>CC(C)C1c2nc(cs2)C(NC(C)c2nc(C(NC(C)c3nc(cs3)C(N1)=O)=O)c(C)o2)=O</chem> |
| N841 | A | 0.91907809 2 | <chem>CC1(C)C=Cc2c(ccc3C4C(COc23)c2ccc(cc2O4)O)O1</chem> |
| N842 | A | 0.91907809 2 | <chem>CC1C(C)C(c2ccc(c(c2)OC)OC)OC1c1ccc(c(c1)OC)OC</chem> |
| N843 | A | 0.91907809 2 | <chem>CC1CCC2(C)C(C)C=CCC2C1(C)CCC(C)=CCn1c[n+](C)c2c1c(N)ncn2.[Cl-]</chem> |
| N844 | A | 0.92427928 6 | <chem>[H][C@@]12c3c(cc(c(c3O)O)O)C(=O)O[C@@]1([H])[C@@H]([C@H]([C@H](CO)O2)O)OC(c1cc(c(c1)O)O)O)=O</chem> |
| N845 | A | 0.92427928 6 | <chem>CC[C@H](C)[C@H](C(=O)O[C@@H](CC(C)C)C(N[C@@H](CC(C)C)C(N[C@@H](C)C=CC(N1C(C=C([C@@H]1C)OC)=O)=O)=O)N(C)C</chem> |
| N846 | A | 0.92941892 6 | <chem>CC1(C)C=Cc2c(cc(c3C(C4CC5c6c(C=4Oc23)c(cc(c6OC5(C)C)O)O)=O)O)O)O1</chem> |

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| N847 | A | - 0.93027393 | [H]c1c(c2C(C3CC4c5c(C=3Oc2c2C=CC(C)(C)Oc12) c(cc(c5OC4(C)C)O)O)=O)O |
| N848 | A | - 0.93196611 5 | COc1cc(c2C(C(=COc2c1)c1ccc(cc1)O)=O)O |
| N849 | A | - 0.93449845 1 | C(CCCCc1cccc1)CCCC(c1c(cccc1O)O)=O |
| N851 | A | - 0.93449845 1 | CC1(C)CC[C@@]2(CC[C@]3(C)C(=CCC4[C@@]5(C)C[C@H]([C@@H](C(C)(C)C5CC[C@@]34C)O)O)C2C1)C(O)=O |
| N850 | A | - 0.93449845 1 | CC1=CC(c2c(CC(C)=O)cc(cc2O1)O)=O |
| N852 | A | - 0.93449845 1 | Cc1c2C(CC(C)(C)Oc2cc2c1OC(c1c(C)c(c(c(C=O)c1O2)O)[Cl])=O)=O |
| N853 | A | - 0.93449845 1 | Cc1cc(c2c(cccc2c1c1ccc2cc(C)nc(C)c2c1O)O)OC |
| N854 | A | - 0.93951925 3 | [H][C@@]12CC[C@@H]([C@](C)(CO)C1=C[C@@H]([C@]1([H])[C@@]2(C)CC[C@]2(C)[C@H](CC[C@@]12C)[C@H](C)C[C@H](C=C(C)C)O)O)O |
| N855 | A | - 0.93951925 3 | CC(C)=CCc1c(ccc2C3C(COc12)c1ccc(c(CC=C(C)C)c1O3)O)O |
| N858 | A | - 0.93951925 3 | CC(C)=CCc1cc(cc(c1OC)O)C1=COc2cc(cc(c2C1=O)O)O |
| N857 | A | - 0.93951925 3 | CC1C(c2ccccc2)Oc2cc(c(cc12)O)OC |
| N856 | A | - 0.93951925 3 | CCC=C[C@H](CC)CCC[C@@]1(CC)C[C@@]2(CC)[C@H](CC(=O)O2)O1 |
| N859 | A | - 0.94448267 2 | C1C2C(C3C(C(O)O2)OC(c2cc(c(c(c2c2c(cc(c(c2O)O)O)C(=O)O3)O)O)O)=O)OC(c2cc(c(c(c2c2c3C(=O)O)c4c5c(C(=O)Oc(c35)c(c2O)O)c(c2c(cc(c(c2O)O)O)C(=O)O1)c(c4O)O)O)O)=O |
| N860 | A | - 0.94448267 2 | COc1cc2c(C(C[C@@H](c3ccc(cc3)O)O2)=O)c(c1OC)O |
| N862 | A | - 0.94939000 7 | CC(C)=CCc1c2C(c3c(cccc3Oc2c(c(c1OC)O)OC)O)=O |
| N861 | A | - | CN1c2c(cccc2O)C(c2c(cc(c(c12)OC)O)O)=O |

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| | | 0.94939000 7 | |
| N863 | A | - 0.95036485 4 | CC(C1=COCC2C1CC1c3c(CC2N1C)c1cc(CC2C4CC5c6c(CC(C4COC2(C)O)N5C)c2cccc2n6C)c(cc1[nH]3)OC)=O |
| N865 | A | - 0.95424250 9 | CC(C)=CCc1cc2C3C(COc2cc1O)(c1ccc(c(CC=C(C)C)c1O3)OC)O |
| N864 | A | - 0.95424250 9 | Cc1cc(c2c(cccc2c1c1c(cc(c2c1C[C@H](C)N(C)[C@H]2C)OC)OC)OC)OC |
| N866 | A | - 0.95424250 9 | COc1ccc(CC(=C)C(=C)Cc2ccc(cc2)O)c(c1)O |
| N867 | A | - 0.95424250 9 | COc1ccc(cc1)C1=CC(c2c(cc(c(c2O)O)OC)O1)=O |
| N868 | A | - 0.95904139 2 | [H][C@]12[C@H](C(C(=C)C(=O)O2)[C@@H](C2(C)[C@@]1(C)[C@H](CC[C@]2(C)O)O)OC(C(C)=C)=O)OC(C(C)=CC)=O |
| N869 | A | - 0.95904139 2 | CC(C)=CCc1cc(ccc1O)C1CC(c2c(cc(c(CC=C(C)C)c2O1)O)O)=O |
| N871 | A | - 0.95904139 2 | CC1CC23C4C(C(C)(C=C2C1=O)OC41C(CC(C)C3=O)C1(C)C)O |
| N870 | A | - 0.95904139 2 | CCC=C(C)CCC=C(C)CCCCC(C)=CC=C(C)CCCCC CC(=O)OC |
| N872 | A | - 0.96378782 7 | CC1=CCCC2(C)C1=C(C(c1cc3C(C=CC(c3cc12)=O)=O)=O)O |
| N873 | A | - 0.96810548 5 | COC1CC2C3(C=C1)C(CN2Cc1cc2c(cc13)OCO2)O |
| N874 | A | - 0.96848294 9 | COc1ccc2c(c3ccoc3nc2c1OC)OC |
| N875 | A | - 0.96975961 7 | CC(=O)O[C@H]1C[C@H](C(C)(C)C2C[C@H]([C@]3(C)C(CC[C@@]4(C)[C@H](c5ccoc5)OC([C@@H]5[C@]34O5)=O)[C@@]12C)O)OC(C)=O |
| N876 | A | - 0.97772360 5 | [H]c1c(cc(c(C(C=Cc2cccc2)=O)c1O)OC)O |
| N878 | A | - 0.97772360 | CC1(C)C=Cc2c(ccc(C(CC(c3ccc4c(c3)OCO4)=O)=O)c2OC)O1 |

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| | | 5 | |
| N877 | A | 0.97772360 5 | <chem>Cc1c(c(C)c2c(C(CC(c3ccccc3)O2)=O)c1O)O</chem> |
| N879 | A | 0.98136550 9 | <chem>CC(C)=CCCC(C)=CCC[C@]1(C)C=Cc2cc(ccc2O1)O</chem> |
| N880 | A | 0.98227123 3 | <chem>C1CCN2CC[C@H]3C(=C[C@@](CCC=CC1)([C@H]1[C@@]3(C[C@@H]3C=CCCCN13)C2)O)[C@@H]1c2c(CCN1CCc1c3c(ccn1)c1ccccc1[nH]3)c1ccccc1[nH]2</chem> |
| N883 | A | 0.98227123 3 | <chem>CC(c1ccccc1)O[C@@H]1CC2C(C=C[C@@]3(C)C[C@H](CC[C@]23C)O[C@H]2[C@@H]([C@@H]([C@@H]([C@@H](CO)O2)O[C@H]2[C@@H]([C@@H]([C@@H]([C@@H](CO)O2)O[C@H]2[C@@H]([C@@H]([C@@H]([C@@H](CO)O2)O)O)OC)O)OC)O)OC)O)[C@]2(CC[C@H](C(C)OC(C)=O)[C@@]12C)O</chem> |
| N882 | A | 0.98227123 3 | <chem>CC1(C)C=Cc2cc(C=CC(c3ccc(cc3O)O)=O)ccc2O1</chem> |
| N884 | A | 0.98542647 4 | <chem>CC(C1=COCC2C1CC1c3c(CC2N1C)c1ccccc1n3C)=O</chem> |
| N885 | A | 0.98677173 4 | <chem>CC=C(COC1C(C(C(C(CO)O1)O)O)O)C1C=C2c3c(CCN2C(C=1CO)=O)c1ccccc1[nH]3</chem> |
| N886 | A | 0.98677173 4 | <chem>CC1CCC2C(C=C(C)C(CC=1)O)OC(C2=C)=O</chem> |
| N887 | A | 0.99122607 6 | <chem>CC1=CC(CC2C(C)(CCC3=CCOC3=O)C(CCC12C)COC(C)=O)=O</chem> |
| N888 | A | 0.99122607 6 | <chem>CC1=CCC(C2(C)CC3C(C(C12)O)C(=C)C(=O)O3)O</chem> |
| N889 | A | 0.99563519 5 | <chem>CC(=C)C1CCC2(CCC3(C)C(CCC4C5(C)CCC(C(C)(C)C5CCC34C)O)C12)C(O)=O</chem> |
| N890 | A | 0.99563519 5 | <chem>CC(C)C=Cc1c(cc2c(C(C3C(C=C(C)C)Oc4cc(ccc4C=3O2)O)=O)c1O)OC</chem> |
| N891 | A | 0.99563519 5 | <chem>CCCCCCCc1cc(cc(c1)OC(c1c(CCCCCC)cc(cc1O)O)=O)O</chem> |

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|------|---|-----------------|--|
| N898 | N | -1 | CC(C)=CCCc1c(ccc2C[C@@H](COc12)c1ccc(c(c1O C)O)OC)OC |
| N892 | N | -1 | CC[C@@H](C)C[C@]1(C)C=CC(=C2C([C@@H](CC(O)=O)OC2=O)=O)O1 |
| N893 | N | -1 | CC=CC1=CC=CC(=C2C(CNC2=O)=O)O1 |
| N894 | N | -1 | CC1(C)CC2C3=CCC4C5(C)CCC(C(C)(CO)C5CCC4(C)C3(C)CCC2(C)C(C1)O)O |
| N895 | N | -1 | CCCCCCC1C2CC3C4C(C=CC1C24)C(=CC3O)C(O)=O |
| N897 | N | -1 | COC1=CC(C(=CC12CCc1cc(ccc12)O)O)=O |
| N896 | N | -1 | COc1cc(c(cc1CCc1cccc(c1)O)OC)O |
| N899 | N | 1.00106372 | C(C=Cc1cnc(N)[nH]1)NC(c1cc(c([nH]1)[Br])[Br])=O |
| N903 | N | 1.00432137 4 | CC(C)(C=C)c1c(cc(c2C(C=C(c3ccc(cc3)OC)Oc12)=O)O)O |
| N900 | N | 1.00432137 4 | CC=CCC=CCCC(C1C(C(N)=O)O1)=O |
| N902 | N | 1.00432137 4 | CCCCCCC=CCCCCCCCc1cccc(c1C(O)=O)O |
| N901 | N | 1.00432137 4 | CCCCCCC=CCCCCCCCC1c1cccc(c1C(O)=O)O |
| N904 | N | 1.00434986 6 | CC1C(C)C(c2ccc3c(c2)OCO3)OC1c1ccc(c(c1)OC)OC |
| N905 | N | 1.00599512 3 | CC=C1CN2CCC34C2CC1C1C=C(C2CC56C7CC(C8C=CC(N(C58)c5cccc56)=O)C(CN27)=CC)C(N(C13)c1cccc14)=O |
| N906 | N | 1.00860017 2 | CC1CCC2C(C)(C)C3CC12CCC3(C)O |
| N907 | N | 1.01267209 8 | CCCCC1c1cc(c2C=CC(C)(CCC(C(C)=C)O)Oc2c1OC(C)=O)O |
| N908 | N | 1.01283722 5 | C[C@@H]([C@H]1CC[C@H]2[C@@H]3CC[C@H]4C[C@H](CC[C@]4(C)[C@H]3CC[C@]12C)N(C)C(c1cccc1)=O)N(C)C |
| N913 | N | 1.01283722 5 | CC(C(=COC)C(=O)OC)=C(C=Cc1ccc(c(c1)OC)[Cl])OC |
| N914 | N | 1.01283722 5 | CC(C(=COC)C(=O)OC)=C(C=Cc1cccc1)OC |

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| N911 | N | 1.01283722 5 | - CC(C(C=Cc1cccc1)OC)C(=COC)C(=O)OC |
| N909 | N | 1.01283722 5 | - CC(C)=CCc1cc(C=CC(c2ccc(cc2O)O)=O)cc(c1O)O |
| N915 | N | 1.01283722 5 | - CC(C)=CCO[C@H]1COc2ccc(C=CC(=C(C)C(=COC)C(=O)OC)OC)cc2OC1(C)C |
| N910 | N | 1.01283722 5 | - CC(C)C1CCC(C)=CC1c1c(cc2c(C(CC(c3cccc3)O2)=O)c1O)O |
| N912 | N | 1.01283722 5 | - COC=C(C(C(C=Cc1ccc(c(c1)OC)[Cl])OC)OC)C(O)=O |
| N916 | N | 1.01703333 9 | - CC(C)=CCCC(C)(C1CCC2(C)C1C(CC1C3(C)CCC(C)(C)C3CCC12C)O)O |
| N917 | N | 1.01703333 9 | - CC1(C)C2=CC(C=CC2=c2c(c(c(c3C=CNC1=c23)OC)OC)O)=O |
| N918 | N | 1.01703333 9 | - CC1(C)C2CC[C@]3(C)C(C[C@H]([C@@H]4[C@H](CC[C@@]34C)[C@]3(C)CC[C@H](C(C)(C)O)O3)O)[C@@]2(C)CC[C@H]1O |
| N919 | N | 1.02118929 9 | - [H]C1CC(C)(C)C2([H])CCC3=C[C@](C)(C[C@H]([C@]3([H])[C@@]2(C)[C@H]1O)O)C=C |
| N920 | N | 1.02118929 9 | - CC1=C(C(C2CCc3cc(ccc3OC=2C1=O)O)=O)OC |
| N922 | N | 1.02118929 9 | - CC1=CC(NC2=C1C(c1cccc1C2=O)=O)=O |
| N921 | N | 1.02118929 9 | - Cc1cc(c2c(cccc2c1c1ccc2cc(C)nc(C)c2c1O)OC)OC |
| N923 | N | 1.02184153 1 | - COc1ccc(cc1)C1=CC(=O)Oc2c1c(cc(c2OC)OC)OC |
| N924 | N | 1.02326863 3 | - CC(C#CC#CC#CC#CCCCCCCC(O)=O)O |
| N925 | N | 1.02517294 6 | - CC1(C)[C@H](CC[C@@]2(C)[C@H]1CC[C@]1(C)[C@@H]2CC[C@@H]2[C@H]3[C@@H](CC[C@]3(C)CC[C@@]12C)C(=C)C=O)O |
| N926 | N | - | - CN1Cc2c(ccc(c2OC)OC)c2ccc3cc4c(cc3c12)OCO4 |

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| | | 1.02530586 5 | |
| N927 | N | 1.02632893 9 | CC1C(C(C(C(O1)OC1=C(c2ccc(cc2)O)Oc2cc(cc(c2C1=O)O)O)O)O)O |
| N928 | N | 1.02687599 6 | CC1(C)C=Cc2cc3C(C([C@@H](c4ccccc4)Oc3cc2O1)O)OC |
| N929 | N | 1.02938377 8 | CC1C(C)C(c2ccc3c(c2)OCO3)OC1c1ccc(c(c1)OC)OC |
| N930 | N | 1.02952055 7 | COC(C(=C)C1C(C2C(=C)C(=O)OCC2(CC1OC(C(=C)CO)=O)C=C)O)=O |
| N931 | N | 1.03489423 5 | CC(=C)C(CC=C(C)C)Cc1c(cc(c2C(CC(c3c(cccc3O)O)Oc12)=O)O)O |
| N932 | N | 1.03742649 8 | CCC=CCC=CCC=CCCCCCCC(=O)OC |
| N933 | N | 1.03742649 8 | CCCCCC1=CC(C=C(C1=O)OC)=O |
| N934 | N | 1.03742649 8 | COc1cc2C3CC(CC4CCCCN34)OC(C=Cc3ccc(c(c3)c2cc1OC)O)=O |
| N935 | N | 1.03782475 1 | COc1ccc(cc1)C1=COc2cc(c(cc2C1=O)OC)O |
| N936 | N | 1.04139268 5 | [H][C@]12[C@@H](C)C([C@@]34[C@H](C)C(C3=C[C@@]3(C)[C@@H]([C@@]4([H])[C@@]2(C1(C)C)O3)O)=O)=O |
| N937 | N | 1.04139268 5 | C1=C(c2ccc(c(c2)O)O)Oc2cc(cc(c2C1=O)O)O |
| N940 | N | 1.04139268 5 | C1=C(c2ccc(c(c2)O)O)Oc2cc(cc(c2C1=O)O)O |
| N938 | N | 1.04139268 5 | CCCCCCC1C2CC3C4C(C=CC1C24)C(=CC3O)C(O)=O |
| N939 | N | 1.04139268 5 | COc1cc(c(cc1OC)O)[C@@H]1COc2cc(ccc2C1=O)O |
| N941 | N | 1.05307844 | [H][C@]12[C@@H]([C@H]([C@H](COC(c3ccc(cc3)O)=O)O[C@]1([H])c1c(cc(c(c1O)O)O)C(=O)O2)O)O |

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| N942 | N | 1.05690485 1 | <chem>CC1C=CNC2C=1C(C1=CC=C(C(C1=2)=O)OC)=O</chem> |
| N943 | N | 1.05690485 1 | <chem>CCCCC1c1cc(c2C(C(CCC(C)=O)C(C)(C)Oc2c1)=O)O</chem> |
| N944 | N | 1.05695336 5 | <chem>COc1cc(C=CC(CC(C=Cc2ccc(c(c2)OC)O)=O)=O)ccc1O</chem> |
| N945 | N | 1.05897868 6 | <chem>CC1(C)C(CC(=O)OC)C2(C)C3CCC4(C)C(c5ccoc5)OC(C4(C3=C)OC2CC1=O)=O</chem> |
| N946 | N | 1.07188200 7 | <chem>CC(c1cc2C(c3ccc(c(c3C(c2o1)=O)OC)O)=O)=O</chem> |
| N947 | N | 1.07448480 5 | <chem>CC(=O)OC1C2C(C)(C)C(CC[C@]2(C)C2CCC3(C)C(CC=C3C2C1O)c1ccoc1)=O</chem> |
| N950 | N | 1.07918124 6 | <chem>C(C(O)=O)c1cc(ccc1O)O</chem> |
| N948 | N | 1.07918124 6 | <chem>C[C@H]1[C@H](C)[C@@H](c2ccc(c(c2)O)O)O[C@@H]1c1ccc(c(c1)O)O</chem> |
| N949 | N | 1.07918124 6 | <chem>C=CC(C=Cc1ccc(cc1)O)c1ccc(cc1)O</chem> |
| N951 | N | 1.07918124 6 | <chem>C1C2C(Cc3ccc4c(c3)OCO4)C3C=CC4C(C1C(C=C4C(O)=O)=O)C23</chem> |
| N952 | N | 1.07918124 6 | <chem>COc1cc(C2=Cc3ccc(cc3OC2=O)O)c(cc1O)O</chem> |
| N953 | N | 1.07918124 6 | <chem>COc1cc(ccc1O)C1C(COC(c2cccc2)=O)c2cc(C=CCOC(c3cccc3)=O)cc(c2O1)OC</chem> |
| N954 | N | 1.08635983 1 | <chem>[H]C(c1cc2c3ccc(cc3[nH]c2cc1O)OC)=O</chem> |
| N955 | N | 1.08635983 1 | <chem>CC(C)=CCc1c(cc2c(c1C)OC(c1c(C)c(c(c(C=O)c1O2)O)[Cl])=O)O</chem> |
| N956 | N | 1.08878997 4 | <chem>[H][C@]12C(C)C(C=C(C)[C@]1(C)C[C@]([H])([C@@H](C)[C@]2(C)CC[C@H](C)CC(O)=O)O)=O</chem> |

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| N957 | N | 1.08990511 1 | - Cc1cc(c(C=O)c2c1C(=O)Oc1c(cc3c(C(CC(C)(C)O3)=O)c1C)O2)O |
| N958 | N | 1.08990511 1 | - CN1c2cccc2C(c2c1cc(c(c2O)OC)OC)=O |
| N959 | N | 1.09223398 6 | - [H]C1=C(c2cc([H])c(c(c2)OC)O)Oc2c([H])c(c([H])c(c2C1=O)OC)OC |
| N960 | N | 1.09342168 5 | - [H][C@]12CCN3CCCC=CCC[C@](C=C1C1c4c(CC N=1O)c1cccc1[nH]4)([C@H]1[C@@]2(CCC=CCCC CN1)C3)O |
| N961 | N | 1.10380372 1 | - [H]c1cc(cc(CC=C(C)C)c1C)C(=O)OC |
| N964 | N | 1.10380372 1 | - C(CCCCCCCCCCCC(=O)OCC(CO)O)CCCCCCCC CCCCCO |
| N962 | N | 1.10380372 1 | - C[C@@H]1C2C3=CCC4[C@@]5(C)CC[C@@H]([C@@](C)(CO)C5CC[C@@]4(C)[C@]3(C)CC[C@]2(C C[C@H]1C)C(O)=O)O |
| N963 | N | 1.10380372 1 | - CCC1=COCC2C1CC1c3c(CC2N1C)c1cccc1n3C |
| N965 | N | 1.10720997 1 | - CC(C)=CCc1c(cc(c2C(C(COc12)(c1ccc(c(CC=C(C)C)c1OC)OC)O)=O)O)O |
| N966 | N | 1.10720997 1 | - COc1c2c(c3c4cccc4C(c4c3c1ccn4)=O)OCO2 |
| N967 | N | 1.11394335 2 | - CCCCCCC1C2CC3C=CC(C4C=CC1C2C34)C(O)=O |
| N968 | N | 1.11727129 6 | - [H]N12C=C(C(C)C)C3CC1c1c(CC2C3(C)CO)c2cccc c2n1C |
| N969 | N | 1.12057393 1 | - C(C1C(C(C(C(O1)Oc1cc(C=Cc2ccc(cc2)O)cc(c1)O) O)O)O)O |
| N970 | N | 1.12385164 1 | - CCC=CCC=CCC=CCCCCCCCCc1cccc(c1C(O)=O) O |
| N971 | N | 1.13307940 7 | - CCCCCCCC1=CC(=C(CCCCC)C(=O)O1)O |
| N972 | N | 1.13353890 8 | - CC(C)=CCc1cc(cc(c1O)OC)C1CC(c2ccc(cc2O1)O)= O |

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| N973 | N | 1.14612803 6 | - C1C2C=CC(C3C=CC4C(Cc5ccc6c(c5)OCO6)C1C4C23)C(O)=O |
| N974 | N | 1.14612803 6 | - CCCCCCCCCCCCC1CC(NCCCNCCCCNCCCN1)=O |
| N975 | N | 1.14961927 7 | - CC(=O)OC(C1C(C)(C)C(C2CC3C(CCC4(C)C(c5ccco5)OC(CC=34)=O)C1(C)C2=O)O)C(=O)OC |
| N976 | N | 1.15228834 4 | - CC=Cc1ccc(cc1)O |
| N977 | N | 1.16136800 2 | - C([C@@H]1[C@H]([C@@H]([C@@H](O)O1)O)O)O C1=C(c2ccc(c(c2)O)O)Oc2cc(cc(c2C1=O)OC(c1cc(c(c1)O)O)O)=O)O |
| N978 | N | 1.16381145 5 | - [H][C@]12CCC=C(COC(C=Cc3ccc(c(c3)O)O)=O)[C@]1(C)C[C@H]([C@@H](C)[C@]2(C)CC[C@H](C)C(C(O)=O)O |
| N979 | N | 1.16731733 5 | - CN1c2ccccc2C(c2c1c(c(c(c2O)OC)OC)OC)=O |
| N980 | N | 1.16731733 5 | - COc1cc(ccc1O)C1=C(C(c2c(cc(cc2O1)O)O)=O)O |
| N981 | N | 1.17609125 9 | - C[C@H]1C([C@@H](C[C@H]2[C@]3(C)CC[C@@]4(C)C5CC(C)(C)CC[C@@]5(CC[C@]4(C)[C@H]3CC[C@]12C)CO)O)=O |
| N982 | N | 1.17609125 9 | - C1=C(c2ccc(cc2)O)Oc2c(C3C(c4ccc(cc4)O)Oc4cc(c(c4C3=O)O)O)c(cc(c2C1=O)O)O |
| N985 | N | 1.17609125 9 | - CC(=C)C(CC=C(C)C)C[C@@]12C[C@@H](CC=C(C)C)C(C)(C)[C@@](CC=C(C)C)(C(C(=C1O)C(c1ccc(c(c1)O)O)=O)=O)C2=O |
| N983 | N | 1.17609125 9 | - CC(C)=CC(CC(=CCCC(C)=CCCC(C)=CCc1cc(cc(c1O)O)C(O)=O)C(O)=O)O |
| N984 | N | 1.17609125 9 | - CC(C)=CC[C@@H]1C[C@]2(CC3CCC(C)(C)C=C3C)C(=C(C(c3ccc(c(c3)O)O)=O)C([C@@](CC=C(C)C)(C2=O)C1(C)C)=O)O |
| N986 | N | 1.17609125 9 | - CC1C(CCC2C1(C)CCC1C2(C)CCC2(C)C3CC(C)(C)CCC3(CCC12C)C=O)=O |
| N987 | N | 1.17609125 9 | - CCCCCCCCCCCCC1CC(NCCCNCCCCNCCCN1)=O |
| N988 | N | - | - CCC(C)C1C(N(C)C(Cc2ccccc2)C(=O)OC(C(C)C)C(N |

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| | | 1.17719176 5 | (C)C(Cc2ccccc2)C(=O)OC(C(C)C)C(N(C)C(Cc2ccccc2)C(=O)O1)=O)=O)=O |
| N989 | N | - 1.18103920 6 | C1=C(C(c2c(cc(cc2O1)O)O)=O)c1ccc(cc1)O |
| N990 | N | - 1.18403466 5 | CC1CC2C(CC=C1C=CC(C)=O)C1(C(=CC3(C(C)CC4C(CC3O1)C(=C)C(=O)O4)O)C(C)=O)C(=O)O2 |
| N991 | N | - 1.18469143 1 | CC1=CC2C(CCC(=C)C(CC1O)O)C(=C)C(=O)O2 |
| N992 | N | - 1.19033169 8 | [H]C(c1cc2c3ccc([H])cc3[nH]c2cc1O)=O |
| N993 | N | - 1.19865708 7 | CN1c2ccccc2C(c2c1cc(c(c2O)OC)OC)=O |
| N994 | N | - 1.19970977 1 | CC1Cc2c(c3ccc(c4c(cc(C)cc34)O)OC)c(cc(c2C(C)N1)OC)O |
| N995 | N | - 1.20006988 2 | COc1cc2c(C(c3ccccc3N2)=O)c(c1OC)O |
| N996 | N | - 1.20139712 4 | Cc1cc(c2c(cc(cc2c1c1c(cc(c2c1C[C@H](C)N(C)[C@H]2C)OC)OC)OC)OC)OC |
| N997 | N | - 1.20311577 8 | CC(=C)[C@H](CC=C(C)C)Cc1c(cc(c2C(C[C@@H](c3c(cccc3O)O)Oc12)=O)O)OC |
| N100 2 | N | - 1.20411998 3 | C[C@@](C=C)([C@H](C=CC(=C[Cl])C([Cl])[Cl])[Cl])[Cl] |
| N998 | N | - 1.20411998 3 | CC(C)=CCc1c(c(CC=C(C)C)c2c(C(c3ccccc3O2)O)=O)c1O)O |
| N999 | N | - 1.20411998 3 | CC1C(C(CC2C1(C)CCC1C2(C)CCC2(C)C3CC(C)(C)CCC3(C)CCC12C)O)=O |
| N100 0 | N | - 1.20411998 3 | CC1C(CCC2C1(C)CCC1C2(C)CCC2(C)C3CC(C)(C)CCC3(C)CCC12C)=O |
| N100 1 | N | - 1.20411998 3 | CC1CCC2(C(C)C3C(CC4C5=CCC6=CC(C(CC6(C)C5CC(C34C)O)O)=O)O2)OC1 |
| N100 3 | N | - 1.21218760 | [H][C@@]12CCN3CCCC=CCC[C@]4([C@H]([C@]2([H])[C@@]2([H])c5c(CCN2CCc2c6c(ccn2)c2ccc |

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| | | 4 | cc2[nH]6)c2cccc2[nH]5)O4)[C@H]2[C@@]1(C[C@]1([H])C=CCCCN12)C3 |
| N1005 | N | 1.21218760 4 | C[C@@H](CC(c1c(cc2c(C=CC(C)(C)O2)c1O)OC)=O)c1cccc1 |
| N1004 | N | 1.21218760 4 | CC(C)=CCc1cc(cc(c1C)O)C(=O)OC |
| N1006 | N | 1.21748394 4 | CC(CCC=C(C)C)c1ccc(C)cc1O |
| N1007 | N | 1.21774707 3 | CC(C)CC(=O)OC1C2C(C=C(C)C3=CC(C(C)(C1O)O3)=O)OC(C2=C)=O |
| N1008 | N | 1.22788670 5 | COc1cc2c(C(C=C(c3ccc(cc3)O)O2)=O)c(c1OC)O |
| N1009 | N | 1.22840035 9 | CC1(C)C=Cc2c(ccc(C(Cc3ccc(cc3)OC)=O)c2O)O1 |
| N1010 | N | 1.23044892 1 | C[C@](C=C)([C@@H](C=CC(=C)C([Cl])[Cl])[Cl])[Cl] |
| N1011 | N | 1.23044892 1 | C1=C(c2ccc(c(c2)O)O)Oc2c(C3C(c4ccc(cc4)O)Oc4cc(cc(c4C3=O)O)O)c(cc(c2C1=O)O)O |
| N1012 | N | 1.23044892 1 | CC(=O)OC1CCG2(C)C(CCC3(C)C2CC=C2C4CC(C)(C)CCC4(CCC23C)C(Nc2ccc(C)cc2)=O)C1(C)C |
| N1013 | N | 1.23044892 1 | CC1C(CCC2C1(C)CCC1C2(C)CCC2(C)C3CC(C)(C)CCC3(CCC12C)CO)=O |
| N1014 | N | 1.23044892 1 | COc1cc2c(C(c3ccccc3N2)=O)c(c1OC)O |
| N1015 | N | 1.23051566 7 | c1cc(c2C(c3cc(ccc3Oc2c1)O)=O)O |
| N1016 | N | 1.23070431 4 | CC1(C)C=Cc2c(ccc(C(Cc3ccc(c(c3)O)O)=O)c2O)O1 |
| N1017 | N | 1.23790715 4 | CCCC(=O)OC1(C)CCC2C(C)C(=O)OC3(C)CCC(C(=C)CC4C1C2C3O4)OC(C)=O |
| N1018 | N | 1.24054924 4 | C1=C(c2ccc(cc2)O)Oc2cc(cc(c2C1=O)O)O |

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| N1019 | N | 1.247814115 | <chem>CC(=O)O[C@H]1C[C@H](C(C)(C)C2C[C@H]([C@@]3(C)C(CC[C@@]4(C)[C@H](c5ccoc5)OC([C@@H]5[C@]34O5)=O)[C@@]12C)O)OC(C)=O</chem> |
| N1020 | N | 1.252607094 | <chem>CCCCC1cc(c(CC=C(C)CCC=C(C)C)c(c1O)OC(C)=O)O</chem> |
| N1021 | N | 1.252847634 | <chem>CC(C)=CCc1c(c(C=O)cc2c3cccc3[nH]c12)O</chem> |
| N1022 | N | 1.252853031 | <chem>[H]C(c1c2c(cc(cc2oc1c1ccc(c(c1OC)O)O)OC)O)=O</chem> |
| N1025 | N | 1.255272505 | <chem>CC(C)=CCO1cc(c2C(c3c(cc(C)cc3O)c2c1)O)=O)O</chem> |
| N1024 | N | 1.255272505 | <chem>CC1(C)[C@H](Cc2cc(C[C@@]3(C(=C(C(=C)O3)O)c3ccc(cc3)O)C(=O)OC)ccc2O1)O</chem> |
| N1023 | N | 1.255272505 | <chem>CC1CCC=C2C1(C)CCC(C)C2(C)CCC(C)=CCn1c[n+](C)c2c1c(N)ncn2.[Cl-]</chem> |
| N1026 | N | 1.257678575 | <chem>C(C1[C@H](C(C([C@H](c2c(cc3c(C(c4cc(c(cc4O3)O)O)=O)c2O)O)O1)O)OC(C=Cc1ccc(cc1)O)=O)O)O</chem> |
| N1027 | N | 1.259699298 | <chem>CC(=C)C1CC2=C(c3c1c(c1c(C=CC(C)(C)O1)c3O)O)Oc1cc(cc(c1C2=O)O)O</chem> |
| N1028 | N | 1.278753601 | <chem>CC12CCCC(CO)(C1C(CC1CC(=C)C3CCC12C3)OC(c1cccc1)=O)C(O)=O</chem> |
| N1029 | N | 1.278753601 | <chem>CCCCCCCC[C@]1(CC[C@@H](C)C(=O)O[C@@](CCCCCCCC)(CC[C@@H](C)C(=O)O1)CO)CO</chem> |
| N1030 | N | 1.283301229 | <chem>CC(C)=CCc1c(C=Cc2cccc2)cc(cc1OC)O</chem> |
| N1031 | N | 1.284430734 | <chem>C1CCc2cccc2C1</chem> |
| N1032 | N | 1.295324839 | <chem>CC1CC=CC(C(CCC=Cc2cc(cc(c2C(=O)O1)O)O)O)O</chem> |
| N1033 | N | 1.29666519 | <chem>CC1(C)C2CC[C@]3(C)C(CCC4C5C(CC[C@]5(C)CC[C@@]34C)C(C)(C)O)[C@@]2(C)CC[C@H]1O</chem> |
| N103 | N | - | <chem>Cc1c(cc(c2C(C[C@@H](c3cccc3)Oc12)=O)OC)OC</chem> |

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| 4 | | 1.29666519 | |
| N1035 | N | 1.29704208 2 | CC([C@H]1CC[C@@]2(C3CC=C4C[C@H](CC[C@]4(C)C3C[C@H]([C@]12C)Oc1cccc1)OC1C(C(C(C(CO)O1)O)O)O)OC(C)=O |
| N1037 | N | 1.30102999 6 | CC1(C)C=Cc2c(cc(c3C(CC(c4cccc4)Oc23)=O)O)O1 |
| N1036 | N | 1.30102999 6 | CC1(C)C=Cc2c(ccc3C(C4C(COc5cc(c(cc45)OC)OC)Oc23)=O)O1 |
| N1038 | N | 1.30102999 6 | CC1(C)C2CC=C(C=O)C1C2 |
| N1039 | N | 1.30102999 6 | CC1(C)C2CC=C(CO)C1C2 |
| N1040 | N | 1.30102999 6 | CC1(C)C2CC1C(=C)C(C2)O |
| N1041 | N | 1.30102999 6 | CN(CCc1cc(c(c1)[Br])OCCNC(C1CC2(CC(=C(C(=CO2)[Br])OC)[Br])ON=1)=O)[Br])C(N)=O |
| N1042 | N | 1.30318174 8 | c1cc(c(cc1C1=C(C(c2c(cc(cc2O1)O)O)=O)O)O)O |
| N1043 | N | 1.31175386 1 | C=C(Cc1ccc(cc1)O)C(=C)Cc1ccc(cc1)O |
| N1044 | N | 1.32221929 5 | CC(C)=CCc1c(ccc2c3COc4cc(ccc4c3oc12)O)OC |
| N1045 | N | 1.32428245 5 | C[C@@H]1C[C@@]2(C)C(CC[C@]3(C)C2CC=C2C4CC(C)(C)CC[C@@]4(CC[C@]23C)C(O)=O)C(C)(C)[C@H]1O |
| N1046 | N | 1.32577395 9 | [H]C1=C(c2ccc(cc2)O)Oc2c(CCC=C(C)C)c(c(CCC=C(C)C)c(c2C1=O)O)O |
| N1047 | N | 1.33043619 1 | CCCC(=O)OC1(C)CCC2C(C)C(=O)OC3(C)CCC(C(=C)CC4C1C2C3O4)O |
| N1048 | N | 1.33312994 2 | C([C@@H]1[C@H]([C@@H]([C@H]([C@H](Oc2cc(c3C(C(=C(c4ccc(c4)O)O)Oc3c2)O)=O)O)O1)O)O)O |
| N1049 | N | 1.33645973 4 | CC1C(C(C(C(O1)OC1C(c2ccc(cc2)O)Oc2cc(cc(c2C1=O)O)O)O)O)O |

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| N1050 | N | 1.339025844 | - [H][C@]12C(C)C(C=C(C)[C@]1(C)CC([C@@H](C)[C@]2(C)CC[C@H](C)CC(O)=O)(O)O)=O |
| N1051 | N | 1.342422681 | - [H][C@@]12CCc3cc4c(cc3[C@]1(C(c1ccc3c(C=CC(C)(C)O3)c1O2)=O)O)OCO4 |
| N1052 | N | 1.342422681 | - CC(C)=CC(c1c(C)c2c(c(c1OC)O)OC(c1c(C)cc(c(C=O)c1O2)O)=O)=O |
| N1053 | N | 1.352182518 | - [H]c1cc(cc2c1C(C(=CO2)c1cc([H])c(c(CCC=C(C)C)c1)OC)=O)O |
| N1054 | N | 1.355920837 | - CCC=CC(CC)CC=CC1(CC)CC(CC)C(CC(=O)OC)O O1 |
| N1055 | N | 1.35836451 | - CC1C(c2cc3c(cc2c2cccc(c12)N)OCO3)=O |
| N1056 | N | 1.360418472 | - CC1C2CCC(C)(C3C2C2C(C)(CCC(C(=C)CC3O2)O)OC1=O)OC(C)=O |
| N1057 | N | 1.361727836 | - CC1CC(C2(COC(C)=O)C(CCCC23CO3)C1(C)CCC1COC(C=1)=O)OC(C)=O |
| N1058 | N | 1.36512252 | - CC(=C)C(=O)OC1CC23C(CCC(COC2O)=CC2C1C(=C)C(=O)O2)O3 |
| N1059 | N | 1.367542274 | - C[C@H]1[C@@H]([C@H]([C@H]([C@@H](O1)O[C@H]1C(c2c(cc(cc2O[C@@H]1c1ccc(c(c1)O)O)O)O)=O)O)O)O |
| N1060 | N | 1.371499665 | - [H]c1cc(C=CC(=O)OC[C@@]2(C)CCC[C@@]3(C)[C@]([H])(CC[C@H](C)CC(O)=O)C(=C)[C@@H](C[C@]23[H])O)ccc1O |
| N1061 | N | 1.374748346 | - CC(CO)=CCc1c(cc2c(C(C(CO2)c2ccc(cc2O)O)=O)c1O)O |
| N1062 | N | 1.376576957 | - C([C@@H]1[C@H]([C@@H]([C@H]([C@H](c2c(cc3c(Cc4cc(c(cc4O3)O)O)=O)c2O)O)O1)O)O)O)O |
| N1063 | N | 1.380211242 | - CCOC(CC(C=C)=CC[C@H]1C(=C)CCC2C(C)(C)CC[C@]12C)OCC |
| N1064 | N | 1.380979773 | - CCCCC=CC=CC(NCC(C)C)=O |
| N1065 | N | 1.383399246 | - CCCCC=CC=CC(NCC(C)C)=O |

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| N1066 | N | 1.389166084 | - 4 | CC(C)(C(COc1ccc2c(c3ccoc3nc2c1OC)OC)O)O |
| N1067 | N | 1.389166084 | - 4 | CC(C)(C(COc1ccc2c(c3ccoc3nc2c1OC)OC)O)O |
| N1068 | N | 1.389166084 | - 4 | CC1C(C(C(C(O1)OC1CCC2(C)C(CCC3(C)C2C=CC24C5CC(C)(C)CCC5(CO4)C(CC23C)O)C1(C)CO)O)O)C1C(C(C(C(CO)O1)O)O)OC1C(C(C(CO1)O)O)O |
| N1069 | N | 1.390935107 | - 7 | CC1(CCC2C(C1)=CCC1C(C)(C)C(CCC12C)O)C=C |
| N1070 | N | 1.391366611 | - 1 | C1CCN2C3CC4(C2C1)C(C=C3)=CC(=O)O4 |
| N1071 | N | 1.392696953 | - 3 | COc1cc(c2C(=CC(=O)Oc2c1)c1ccc(c(c1)O)OC)OC1C(C(C(C(CO)O1)O)O)O |
| N1072 | N | 1.392725984 | - 4 | COc1cc2cc3COC(c3c(c3ccc4c(c3)OCO4)c2cc1OC)=O |
| N1073 | N | 1.394451681 | - 1 | COc1cc(c(cc1C1=COc2cc(cc(c2C1=O)O)O)O)OC |
| N1074 | N | 1.397940009 | - 9 | [H]C1=C(C(C=C(CC(C)(C)O)NC1=O)=O)O |
| N1075 | N | 1.397940009 | - 9 | C(C1C(C(C(C(OCC2C(C(C(C(O2)OC2=Cc3c4c(ccn3)c3cccc3n4C2=O)O)O)O)O1)O)O)O)O |
| N1076 | N | 1.397940009 | - 9 | CC(C)(CC1=CC(C(=C(C(N1)=O)[Cl]O)=O)O |
| N1077 | N | 1.397940009 | - 9 | CC1(C)CCCC2(C)C1CCC1(CO1)C2CC=C(CC=O)C=O |
| N1078 | N | 1.401240165 | - 5 | CC(=C)C1CCC2(C)CCC(C(C)=C2C1)=O |
| N1079 | N | 1.401400541 | - 1 | [H][C@]12C[C@@]3(C)C(C=CC[C@]3([H])CC1=C(C)C(=O)O2)=O |
| N1080 | N | 1.408239965 | - 5 | CC(C)c1ccc2c(CCC3C(C)(CCCC23C)CO)c1 |
| N108 | N | - | - | CC(C)=CCc1c(ccc2C(C3(C(COc4cc5c(cc34)OCO5) |

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| 1 | | 1.41161970 6 | Oc12)O)=O)OC |
| N108 2 | N | 1.41329976 4 | COc1cc(c2C(=CC(=O)Oc2c1)c1ccc(c(c1)O)O)OC1C(C(C(C(CO)O1)O)O)O |
| N108 3 | N | 1.41497334 8 | C[C@@]1(C)CCC[C@]2(C)[C@@H](C3C=C(CC(O)OO3)C=O)C(=C)CC[C@@H]12 |
| N108 4 | N | 1.41915885 5 | CC(C)=CCc1c(cc(C=Cc2ccc(cc2O)O)cc1O)O |
| N108 5 | N | 1.41967192 2 | CC(C)(C=C)C1=Cc2c(c3C=CC(C)(C)Oc3c(c2OC1=O)C(C)(C)C=C)O |
| N108 6 | N | 1.42324587 4 | C(C1[C@H](C(C([C@H](c2c(cc3c(C(c4cc(c(cc4O3)O)O)=O)c2O)O)O1)O)OC(c1ccc(cc1)O)=O)O)O |
| N108 7 | N | 1.42674149 8 | [H][C@]12CC[C@@]3(C)[C@H](c4ccco4)OC([C@@H]4[C@@]3([C@]1(C)C(C[C@@]1(C)C(C)(C)O[C@@H](CC(=O)OC)[C@@]12CO)=O)O4)=O |
| N108 8 | N | 1.43136376 4 | CC1(C)C=Cc2c(ccc3C(C(=COc23)c2cc(c(cc2OC)OC)OC)=O)O1 |
| N108 9 | N | 1.43837687 | CN1CCC23C4C5C(CC2=O)C(C1)=CCOC5CC(N4c1cccc13)=O |
| N109 0 | N | 1.44404479 6 | COc1c2c3cccc3C(c3c2c(ccn3)c(c1OC)OC)=O |
| N109 1 | N | 1.44715803 1 | CC(CCCC(C)(C)O)=CCc1c2C(c3c(cc(cc3Oc2cc(c1OC)O)O)O)=O |
| N109 2 | N | 1.45045984 5 | CCC1CC2(CC)C3C1C(C(C)O)OOC3(CC)C(=CC(=O)OC)O2 |
| N109 3 | N | 1.47051402 8 | CC=C1CN2CCC34C2CC1C(CO)C3N(C(C)=O)c1cccc14 |
| N109 4 | N | 1.47421626 4 | C1=C(c2cccc2)Oc2cc(cc(c2C1=O)O)O |
| N109 5 | N | 1.47567118 8 | CN1c2c(cccc2O)C(c2c(cc(c(c12)OC)OC)O)=O |
| N109 6 | N | 1.47712125 5 | C1=C(c2ccc(cc2)O)Oc2c(C1=O)c(cc(c2c1c(cc(c2C(C=C(c3ccc(cc3)O)Oc12)=O)O)O)O)O |

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| N1097 | N | 1.477907297 | - CC1CCC2C1CC1(C)CC=C(C(C)C(C(C=C(C)C(O)=O)O)O)C1CC=C2C(O)=O |
| N1098 | N | 1.478984506 | - C=C(CO)C(=O)OC1CC23C(CCC(COC2O)=CC2C1C(=C)C(=O)O2)O3 |
| N1099 | N | 1.48128478 | - CC1(C)C=Cc2c(cc(C=Cc3ccc(cc3O)O)cc2O1)O |
| N1100 | N | 1.481442629 | - C[C@H]1CC[C@@H]2[C@@H](C)C[C@H]3[C@@H]4C(C)(C)C(C([C@]4(C)C([C@@]23C1=O)=O)=O)=O |
| N1101 | N | 1.481619031 | - CC(C)(C=Cc1c(cc(c2C=CC(=O)Oc12)OC)OC)O |
| N1102 | N | 1.486268106 | - CC(C)(C=C)c1c2c(C=CC(=O)O2)c(c2C=CC(C)(C)Oc12)OC |
| N1103 | N | 1.491361694 | - CC1(C)CCC2(C)CCC3(C)C4CC=C5C(CCC(C5(C)C)O)C4(C)CCC3(C)C2C1 |
| N1104 | N | -1.4915523 | - CCC(CC1(CC)C=C(CC)C(=CC(=O)OC)O1)C=CC(C)O |
| N1105 | N | 1.497087275 | - CC1CC2C(CC=C1CCC(C)=O)C(=C)C(=O)O2 |
| N1106 | N | 1.50242712 | - CC1C[C@@]23C(C=C(C)C([C@@]34[C@@H](C[C@H](C)[C@H]4CC[C@@H]2C)C=1)=O)O)=O |
| N1107 | N | 1.51315757 | - COc1c(C=O)c(cc2C(c3ccccc3C(c12)=O)=O)O |
| N1108 | N | -1.5132176 | - COc1cc2CCN3Cc4c(CC3c2cc1OC)ccc(c4OC)OC |
| N1109 | N | 1.51851394 | - CC1(C)CCc2c(ccc3C[C@@H](COc23)c2ccc(c(c2OC)O)OC)O1 |
| N1110 | N | 1.518714796 | - [H][C@@]12CCC(=C)[C@@]([H])(CC[C@H](C)CCOC(C=Cc3ccc(c(c3)O)O)=O)[C@]2(C)CCC[C@]1(C)C(O)=O |
| N1111 | N | 1.520964492 | - CC=C(C)C(=O)OC(C)c1cc2C=CC(C)(C)Oc2cc1OC |
| N1112 | N | 1.522444234 | - CC1(C)C=Cc2c(ccc3C(C4=C(COC5cc6c(cc45)OCO6)Oc23)=O)O1 |
| N1113 | N | 1.522444234 | - CC1(C)C=Cc2c(ccc3CC(COC23)c2ccc(c(c2OC)O)OC)O1 |
| N1114 | N | - | - CC(C)=CCc1c(cc(C=Cc2ccccc2)cc1OC)O |

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| 4 | | 1.53529412 | |
| N1115 | N | 1.556302501 | CC1CCC2(CCC3(C)C(=CCC4C5(C)CCC(C(C)(C)C5CCC34C)O)C2C1C)C(O)=O |
| N1116 | N | 1.57054294 | CC#CC#CC#Cc1ccccc1 |
| N1117 | N | 1.576248058 | Cc1c2c(ccn1)c1ccc(cc1[nH]2)OC |
| N1118 | N | 1.578595044 | CC(=O)OC1CC2C(C)(C=CC(=O)OC2(C)C)C2C(CC3(C)C(c4ccoc4)OC(C4C3(C12C)O4)=O)O |
| N1119 | N | 1.579783597 | CCC=CCC=CCC=CCCC(NCCc1ccc(cc1)O)=O |
| N1120 | N | 1.595496222 | c1ccc(cc1)C1=C(C(c2c(cc(cc2O1)O)O)=O)O |
| N1121 | N | 1.602059991 | C(C1[C@H](C(C([C@H](c2c(cc3c(C(c4cc(c(cc4O3)O)O)=O)c2O)O)O1)O)O)OC(C=Cc1ccc(cc1)O)=O |
| N1122 | N | 1.605305046 | CN1CCc2cc(c(cc2C1Cc1cc(c(cc1Oc1cc2CC3c4c(CC3C)cc(c4c2cc1OC)OC)OC)OC)OC)OC |
| N1123 | N | 1.611723308 | COc1ccc2C(C=C(c3ccccc3)Oc2c1OC)=O |
| N1124 | N | 1.612783857 | C[C@H]1C[C@H]2C[C@@H](C)[C@](C)([C@H]3CC[C@H]4[C@H]([C@H]23)[C@@H]1CC[C@]4(C)NC=O)NC=O |
| N1125 | N | 1.613841822 | CCC1CN2CCc3c4ccccc4[nH]c3C2CC1C(=COC)C(=O)OC |
| N1126 | N | 1.615950052 | CC=C1CN2CC[C@@]34C(=C(C(=O)OC)[C@H]1C[C@@H]24)Nc1ccccc13 |
| N1127 | N | 1.622707889 | [H][C@@]1(CC[C@H](C)CC(O)=O)C(=C)[C@@H](C[C@]2([H])[C@](C)(CCC[C@@]12C)COC(C=Cc1ccc(c(c1)O)O)=O)O |
| N1128 | N | 1.625089987 | CC1COC2=C1C(C(c1c2ccc2c1CCCC2(C)C)=O)=O |
| N1129 | N | 1.632659713 | CC1=CC(Nc2c1c(c1ccc(c(c1c2OC)OC)OC)OC)=O |
| N113 | N | - | CCC=CCC=CCCC=CC=CC(NCC(C)C)=O |

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| 0 | | 1.63346845 6 | |
| N113 1 | N | 1.63865929 6 | [H][C@]12C(C)C(=[H])C=C(C)[C@]1(C)C[C@]([H])([C@@H](C)[C@]2(C)CC[C@H](C)CC(O)=O)O |
| N113 2 | N | 1.64246452 | COc1c2c(cc3c1c1C(CO)Oc4cc(ccc4c1o3)O)OCO2 |
| N113 3 | N | 1.64345267 7 | C=CC1C(OC=C2C(=O)OCCC12O)OC1C(C(C(C(CO)O1)O)O)O |
| N113 4 | N | 1.64664947 7 | COc1ccc(cc1)C1=CC(c2c(cc(cc2O1)O)O)=O |
| N113 5 | N | 1.65041213 3 | CCCCCCC1=C(CC(CCCCC)OC1=O)O |
| N113 6 | N | 1.65321251 4 | CCCCCCCCC(C)CC(NCCc1ccc(cc1)O)=O |
| N113 7 | N | 1.66275783 2 | COc1cc(c2C(C=C(c3ccc(c(c3)O)O)Oc2c1)=O)O |
| N113 8 | N | 1.67329744 | COc1ccc(cc1)C1=CC(c2c(cc(c(c3cc(ccc3O)C3=CC(c4c(cc(cc4O3)OC)O)=O)c2O1)O)O)=O |
| N113 9 | N | 1.68124123 7 | C1=C(c2ccc(cc2)O)Oc2c(C3C(c4ccc(cc4)O)Oc4cc(cc4C3=O)O)O)c(cc(c2C1=O)O)O |
| N114 0 | N | 1.68124123 7 | CC1(C)CCC[C@@]2(C)C1CCC(=C)[C@@H]2CC=C(C=O)C=O |
| N114 1 | N | 1.68202718 5 | Cc1cc2C(c3ccccc3C(c2c(c1O)OC)=O)=O |
| N114 2 | N | 1.69548167 7 | COc1ccc(cc1)C1=CC(c2c(cc(c(c3cc(ccc3O)C3=CC(c4c(cc(cc4O3)O)O)=O)c2O1)O)O)=O |
| N6 | N | 1.69897000 4 | C[C@@]12CCC[C@]3(C)c4cc5C(C=C(C(c5cc4C([C@]([C@H]23)(O)OC1)=O)=O)OC)=O |
| N8 | N | 1.69897000 4 | C[C@@]12CCC[C@]3(C)c4cc5C(C=CC(c5cc4C([C@]([C@H]23)(O)OC1)=O)=O)=O |
| N114 3 | N | 1.69897000 4 | C1Cc2ccc(cc2OC1c1ccc2c(c1)OCO2)O |
| N114 | N | - | COc1cc(c2C(c3c(ccc(c3O)O)Oc2c1)=O)O |

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| 7 | | 1.69897000 4 | |
| N114 4 | N | 1.69897000 4 | <chem>COc1cc(c2C(c3c(ccc(c3O)OC)Oc2c1)=O)O</chem> |
| N114 5 | N | 1.69897000 4 | <chem>COc1cc(c2C(c3c(ccc(c3OC)OC)Oc2c1)=O)O</chem> |
| N114 6 | N | 1.69897000 4 | <chem>COc1ccc(CC(CO)(C=C)Cc2ccc(cc2)O)O)c(c1)O</chem> |
| N114 8 | N | 1.70500795 9 | <chem>C1=C(c2ccc(c(c2)c2c(cc(c3C(C=C(c4ccc(cc4)O)Oc23)=O)O)O)O)Oc2cc(cc(c2C1=O)O)O</chem> |
| N114 9 | N | 1.70880701 3 | <chem>CC(CC(C=C(C)C)c1ccc2cc[nH]c2c1)c1c[nH]c2cc(CC=C(C)C)ccc12</chem> |
| N115 0 | N | 1.71600334 4 | <chem>CC(C)=CCCC(C)=CCO</chem> |
| N115 1 | N | 1.71850168 9 | <chem>COc1cc2CC3c4cc(c(cc4CCN3Cc2cc1OC)OC)OC</chem> |
| N115 2 | N | 1.72427587 - | <chem>CN1c2cccc2C(c2c1c(c(c2OC)OC)OC)OC)=O</chem> |
| N115 3 | N | 1.73239376 - | <chem>CC1C(C)(CC(C2C(C)(C)O2)=O)C2=C(c3c(C)cccc3OC2=O)O1</chem> |
| N115 4 | N | 1.73239376 - | <chem>Cc1cccc2c1C1=C(C(=O)O2)[C@](C)(CC(C2C(C)(C)O2)=O)[C@H](C)O1</chem> |
| N115 5 | N | 1.74364609 1 | <chem>CC(C)(CCc1c(cc(c2C=CC(=O)Oc12)OC)OC)O</chem> |
| N115 6 | N | 1.75511226 6 | <chem>CN1c2cc3c(c(c2C(c2cccc(c12)OC)=O)OC)OCO3</chem> |
| N115 7 | N | 1.75815462 2 | <chem>c1c(cc(c(c1O)O)O)C1=C(C(c2c(cc(cc2O1)O)O)=O)O</chem> |
| N115 8 | N | 1.76042248 3 | <chem>COc1ccc(C2Cc3ccc4c(cco4)c3OC2)c(c1O)OC</chem> |
| N115 9 | N | 1.76267856 4 | <chem>CN1c2cc3c(c(c2C(c2ccc(c(c12)OC)OC)=O)OC)OCO3</chem> |
| N116 0 | N | 1.76342799 - | <chem>COc1ccc(c(c1O)OC)[C@H]1Cc2ccc3c(cco3)c2OC1</chem> |

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| N116 1 | N | 1.76779965 7 | <chem>CC(=C)C1CCC2(C)CCC3(C)C(CCC4C5(C)CCC(C(C)(C)C5CCC34C)O)C12</chem> |
| N116 2 | N | 1.77085201 2 | <chem>COc1c2ccccc2nc2c1cco2</chem> |
| N21 | N | 1.77815125 | <chem>CC(C)(CO)C(C(NCCCO)=O)O</chem> |
| N116 3 | N | 1.78031731 2 | <chem>CC(=O)Oc1ccc(cc1OC(C)=O)C1=CC(=O)Oc2cc(cc(c12)OC(C)=O)OC</chem> |
| N116 4 | N | 1.78145471 3 | <chem>C[C@H]1[C@H](C)[C@@H](c2ccc3c(c2)OCO3)O[C@@H]1c1ccc(c(c1)OC)O</chem> |
| N116 5 | N | 1.78175537 5 | <chem>C[C@H]1[C@H](C)[C@@H](c2ccc3c(c2)OCO3)O[C@@H]1c1ccc(c(c1)OC)O</chem> |
| N116 6 | N | 1.78946538 3 | <chem>C1=Cc2ccccc2OC1=O</chem> |
| N116 7 | N | 1.79669537 | <chem>CC1(C)C(CC[C@@]2(C)[C@H]1CC[C@]1(C)[C@@H]2CC([C@@H]2[C@@]3(C)CC[C@@]([C@H]3[C@H](C[C@@]12C)O[C@@H]1[C@H]([C@@H]([C@@H](CO1)O)O)O)(C(C)(C)O)O)O)=O</chem> |
| N116 8 | N | 1.80617997 4 | <chem>C1=C(c2ccc(c(c2)O)O)Oc2c(C1=O)c(cc(c2[C@@H]1C(c2c(cc(cc2O[C@H]1c1ccc(cc1)O)O)O)=O)O)O</chem> |
| N116 9 | N | 1.81480700 8 | <chem>CC(C)=CC(CC(C)=C[C@@H]([C@@H]1COC(C1=C)=O)OC(C)=O)=O</chem> |
| N117 0 | N | -1.8162413 | <chem>C1=C(c2ccccc2)Oc2cc(ccc2C1=O)O</chem> |
| N117 1 | N | 1.81888541 5 | <chem>C1=C(c2ccccc2)Oc2cccc(c2C1=O)O</chem> |
| N117 2 | N | 1.81954393 6 | <chem>CC(=C)C1CCC(C)=CC1</chem> |
| N117 3 | N | 1.82216807 9 | <chem>CCC1CN2CCc3c4ccccc4[nH]c3C2CC1C(=COC)C(=O)OC</chem> |
| N117 4 | N | 1.82410610 8 | <chem>CN1CCc2cc(c3cc2C1Cc1ccc(c(c1)Oc1ccc(CC2c4c(CN2C)cc(c(c4O3)O)OC)cc1)OC)OC</chem> |
| N117 | N | - | <chem>[H][C@@]12CC=CC([C@]2(C)C[C@]2(C(C1)=C(C)C</chem> |

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| 5 | | 1.82801506 4 | (=O)O2)O)=O |
| N117 6 | N | - 1.83197113 | CC1(C)C(CC[C@@]2(C)[C@H]1CC[C@]1(C)[C@@ H]2CC([C@@H]2[C@@]3(C)CC[C@@]([C@H]3[C@ H](C[C@@]12C)O[C@@H]1[C@H]([C@@H]([C@@ H](CO1)O)O)O)(C(C)(C)O)O)O)=O |
| N117 7 | N | - 1.83505610 2 | CC(C)C1CCC(C)(C2C1c1c(cc(c(CCC3cccc3)=O)c 1O2)O)OC)O |
| N117 8 | N | - 1.83671051 4 | C[C@@]1(CCC2C1[C@H](OC1C(C(C(C(COC(C=Cc 3ccc(cc3)O)=O)O1)O)O)O)[C@H](C=2C(=O)OC)O C)O |
| N117 9 | N | - 1.83695673 7 | CC=Cc1ccc(cc1)OC(C(C)C)=O |
| N118 0 | N | - 1.84509804 | CCc1ccc(cc1)OC(C=C)=O |
| N118 1 | N | - 1.86510397 5 | COC1=C(c2ccc(c(c2)OC)OC)Oc2cc(cc(c2C1=O)O)O C |
| N118 2 | N | - 1.86671228 2 | CC(=O)O[C@@H]1C(c2c(cc(cc2O[C@@H]1c1ccc(c c1)O)O)O)=O |
| N118 3 | N | - 1.86948136 4 | CC(=O)OC1CC(C2(C)c3cc4c(cc4)c(C)c3CCC2(C1(C)C)O)OC(C)=O |
| N118 4 | N | - 1.87448181 8 | COc1ccc(cc1)C1=CC(c2c(cc(c(c2O)OC)OC)O1)=O |
| N118 5 | N | - 1.87890506 4 | CC(C)=CC(CC(C)=CC(C1COC(C1=C)=O)O)=O |
| N118 6 | N | - 1.90902085 4 | COC=C(C1CC2c3c(CCN2CC1C=C)c1cccc1[nH]3)C (=O)OC |
| N118 7 | N | - 1.91009054 6 | C(C(C(O)=O)N)c1c[nH]c2cccc12 |
| N118 8 | N | - 1.91193154 9 | [H]C(C(CC(O)=O)=CC[C@H]1C(=C)CCC2C(C)(C)C CC[C@]12C)=O |
| N118 9 | N | - 1.96275207 9 2 | CC1C2CCC3C(C)(CCCC3(C)C(=O)OC)C2Cc2c1cco |
| N119 0 | N | - 1.99961911 | C1Oc2cc3cc(c4ccc(cc4O)O)oc3cc2O1 |

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| | | 4 | |
| N119 1 | N | 2.00160392 4 | <chem>CC(=O)O[C@H]1[C@H]([C@@]2(C)C3=CC[C@@H](c4ccoc4)[C@]3(C)CC[C@@H]2[C@@]2(C)C(C=C[C@@H]([C@H]12)O)=O)O</chem> |
| N119 2 | N | 2.00513873 4 | <chem>CC1CC2C(CC=C1C(CC(C)=O)OC(C)=O)C(=C)C(=O)O2</chem> |
| N119 3 | N | 2.00548081 | <chem>CC(C)C1CCC2(C)CC1c1c(cc(c(C(Cc3ccccc3)=O)c1O2)O)OC</chem> |
| N119 4 | N | 2.00860017 2 | <chem>CN1c2ccccc2C(c2c1c1ccccc1[nH]2)=O</chem> |
| N119 5 | N | 2.01577875 6 | <chem>C1=C(C(c2ccc(cc2O1)O)=O)c1ccc(cc1)O</chem> |
| N119 6 | N | 2.01845317 8 | <chem>CC(C)=CCc1ccc2CC(Nc2c1)=O</chem> |
| N4 | N | 2.02734960 8 | <chem>C[C@@]12CCC[C@@](C)(C(O)=O)[C@H]1CC[C@@]13CC(=C)[C@H](CC[C@@H]23)C1</chem> |
| N119 7 | N | 2.04296907 3 | <chem>c1cc(C2=C(C(c3c(cc(cc3O2)O)O)=O)O)c(cc1O)O</chem> |
| N119 8 | N | 2.06032002 9 | <chem>CC1=CC(CC2C(C)(CCC3=CCOC3=O)C(CCC12C)CO)=O</chem> |
| N119 9 | N | 2.06445798 9 | <chem>CC1C2=COC=CC2=C(C=O)C(=O)O1</chem> |
| N120 0 | N | 2.06872641 9 | <chem>CC1=C2C(CCN1)=c1ccc(cc1=N2)OC</chem> |
| N120 1 | N | 2.07918124 6 | <chem>COc1cc(c2C(CC(c3ccccc3)Oc2c1)=O)O</chem> |
| N120 2 | N | 2.08774617 8 | <chem>CC1(C)C2CC(C3(C)C(CCC4(C)C(C(C=C34)=O)c3ccoc3)C2(C)C=CC1=O)O</chem> |
| N120 3 | N | 2.11058971 | <chem>CC=C1CN2CCC34C2CC1C(CC=O)=C3Nc1ccccc14</chem> |
| N120 4 | N | 2.13672056 7 | <chem>CC(CCC=C(C)CCC(C(C)(C)O)O)=CCCC=C(C)CCC=C(C)CCC(C(C)(CO(C)=O)O)O</chem> |
| N120 5 | N | 2.13987908 | <chem>CC=C1CN2C3CC1C1(C2CC2(C3N(C)c3ccccc23)C1O)C(=O)OC</chem> |

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| N1206 | N | 2.149219113 | <chem>C1C(c2ccc(cc2)O)Oc2cc(cc(c2C1=O)O)O</chem> |
| N1207 | N | 2.192650338 | <chem>COc1cc(c2c(c1)c(c1ccoc1n2)OC)OC</chem> |
| N16 | N | 2.217483944 | <chem>C1C2C(c3ccc(cc3O1)O)Oc1cc3c(cc12)OCO3</chem> |
| N1208 | N | 2.221468359 | <chem>COc1ccc(cc1O)C1=COc2cc(cc(c2C1=O)O)O</chem> |
| N1209 | N | 2.242517044 | <chem>CC(=C)C(CCC(C)=O)C=CC1=C(C)C(O)OC1=O</chem> |
| N1210 | N | 2.245248936 | <chem>COc1ccc(cc1)C1=COc2cc(cc(c2C1=O)O)O</chem> |
| N1211 | N | 2.255272505 | <chem>CC(=CCO)C1CC2C(C)(C)C(C=CC2(C)OO1)=O</chem> |
| N1212 | N | 2.270407479 | <chem>COc1ccc(cc1)C1=COc2cc(ccc2C1=O)O</chem> |
| N10 | N | 2.301029996 | <chem>C=CC1C(OC=C2C1=CCOC2=O)OC1C(C(C(C(CO)O1)O)O)O</chem> |
| N1213 | N | 2.301029996 | <chem>COC(C1C2CC3c4c(CCN3CC2CCC1O)c1cccc1[nH]4)=O</chem> |
| N1214 | N | 2.342422681 | <chem>C=CC1C(OC=C2C1=CCOC2=O)OC1C(C(C(C(CO)O1)O)O)O</chem> |
| N1215 | N | 2.344392274 | <chem>C=CC1C2CCOC(C2=COC1OC1C(C(C(C(CO)O1)O)O)O)=O</chem> |
| N1216 | N | 2.359835482 | <chem>c1ccc2c(c1)cc1c(c3ccccc3[nH]1)n2</chem> |
| N1217 | N | 2.409806333 | <chem>CN1CCc2cc(c3cc2C1Cc1ccc(cc1)Oc1cc(CC2c4c(CC2C)cc(c(c4O3)OC)OC)ccc1OC)OC</chem> |
| N1218 | N | 2.468047733 | <chem>CN1(C)C[C@@H](C[C@H]1C(O)=O)OC(C=Cc1ccc(cc1)O)=O</chem> |
| N121 | N | - | <chem>CN1CCc2cc(c3cc2C1Cc1ccc(cc1)Oc1c2C(Cc4ccc(c</chem> |

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| 9 | | 2.54777470 5 | c4)O3)O)N(C)CCc2cc(c1O)OC)OC |
| N122 0 | N | - 2.76902589 | C1CO[C@H]2C=C(CO)[C@@H](CO)[C@@H]12 |
| N122 1 | N | - 2.91474979 1 | c1nc2c(C(NC(N2)=O)=O)[nH]1 |
| N122 2 | N | - 2.95036485 4 | CN1CCc2cc(c(c3c2C1Cc1ccc(cc1)Oc1c2C(Cc4ccc(c4)O3)N(C)CCc2cc(c1O)OC)O)OC |
| N122 3 | N | - 3.17048933 6 | COc1ccc2CC3c4cc(c(c4CCN3Cc2c1OC)O)OC)OC |
| N122 4 | N | - 3.24506253 9 | COc1c(cc2CCNC3Cc4cccc4c1c23)O |
| N122 5 | N | - 3.39101459 9 | COc1cc2CCN3Cc4c(CC3c2cc1OC)ccc(c4OC)O |
| N122 6 | N | - 3.71116001 4 | COc1ccc2CC3c4c(CCN3Cc2c1OC)cc(c(c4O)OC)OC |
| N122 7 | N | - 3.71636303 7 | CN1CCc2cc3c(c4c5ccc(cc5CC1c24)OC)OCO3 |
| N122 8 | N | - 3.71792837 6 | COc1cc2CC3c4c(CCN3Cc2cc1OC)cc(c(c4O)OC)OC |
| N122 9 | N | - 3.78010879 | CN1CCc2cc3c(c4c5ccc(cc5CC1c24)O)OCO3 |
| N123 0 | N | - 3.84174633 5 | CN1CCc2cc3c(c4c5cc(c(cc5CC1c24)O)OC)OCO3 |
| N123 1 | N | - 3.85500571 1 | C1CNC2Cc3cccc3c3c2c1cc1c3OCO1 |
| N123 2 | N | - 3.87584748 6 | CN1CCc2cc3c(c4c5cc(c(cc5CC1c24)OC)OC)OCO3 |
| N123 3 | N | - 3.88571464 5 | COc1ccc2c(CC3c4c(CCN3)cc3c(c24)OCO3)c1 |
| N123 4 | N | - 3.94703038 4 | CN1CCc2cc3c(c4c5cc(c(cc5CC1c24)OC)O)OCO3 |
| N123 | N | - | COc1cc2C=CC(=O)Oc2c(c1O)OC |

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| 5 | | 4.55363459 2 | |
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