{"CHEMBL1087421": "COC1=C(C=C2C(=C1)CCN=C2C3=CC(=C(C=C3)Cl)Cl)Cl", "CHEMBL1088633": "COC1=C(C=C2C(=C1)CCN=C2C3=CC(=CC=C3)Cl)Cl", "CHEMBL1090360": "C1COCCN1C2=CC(=CC=C2)NC3=NC=CC(=N3)C4=C(N=C5N4C=CS5)C6=CC(=CC=C6)NC(=O)CC7=CC=CC=C7", "CHEMBL1688215": "C1=CC2=C(C=C1C3=NC(=NC=C3)N)NN=C2N", "CHEMBL1765781": "CNC1=NC(=CN=C1)C2=CNC(=O)C(=C2)NC(=O)C3=CC=C(C=C3)N4CCCC4CN5CCCC5", "CHEMBL1788116": "C1=CC=C2C(=C1)NC(=C(C#N)C3=NC(=NC=C3)NCCC4=CN=CC=C4)S2.C(=O)(C(F)(F)F)O.C(=O)(C(F)(F)F)O", "CHEMBL1929238": "CC(C)(C)C1=CC(=C(S1)NC(=O)NC2=C(C(=CC=C2)Cl)Cl)C(=O)N3CCC(=O)N(CC3)CCN(C)C", "CHEMBL1933552": "CC1CCC(CN1)N2CCC3(C2)CN(C4=CC=CC=C34)C(=O)C5=CC6=C(N5)C=C(C=C6)F", "CHEMBL202930": "COC1=C(C=CC(=C1)C2=CC3=C(C=C2)C(=CC4=CC=CN4)C(=O)N3)O", "CHEMBL204420": "CN1CCN(C(C1)C(=O)N)CC2=C(C=C3C(=C2)C(=NC=N3)NC4=C(C(=CC=C4)Cl)F)OC", "CHEMBL206783": "COC1=C(C=C2C(=C1)N=CN=C2NC3=C(C(=CC=C3)Cl)F)CN4CCCCC4C(=O)N", "CHEMBL206955": "COC1=C(C=C2C(=C1)N=CN=C2NC3=CC(=C(C=C3)F)Cl)CN4CCCC4C(=O)N", "CHEMBL207037": "COC1=C(C=C2C(=C1)N=CN=C2NC3=C(C(=CC=C3)Cl)F)CN4CC(C4)C(=O)N", "CHEMBL207130": "CN1CCC(CC1)(C(=O)N)N(C)CC2=C(C=C3C(=C2)C(=NC=N3)NC4=C(C(=CC=C4)Cl)F)OC", "CHEMBL207235": "COC1CC(N(C1)CC2=C(C=C3C(=C2)C(=NC=N3)NC4=C(C(=CC=C4)Cl)F)OC)C(=O)N", "CHEMBL207246": "COC1=C(C=C2C(=C1)N=CN=C2NC3=C(C(=CC=C3)Cl)F)CN4CCC4C(=O)N", "CHEMBL207445": "CN(CC1=C(C=C2C(=C1)C(=NC=N2)NC3=C(C(=CC=C3)Cl)F)OC)C(CCOC)C(=O)N", "CHEMBL207584": "COC1=C(C=C2C(=C1)N=CN=C2NC3=C(C(=CC=C3)Cl)F)CN4CCCC4C(=O)N", "CHEMBL207674": "COC1=C(C=C2C(=C1)N=CN=C2NC3=C(C(=CC=C3)Cl)F)CN4CCOCC4C(=O)N", "CHEMBL207687": "CC(C(=O)N)N(C)CC1=C(C=C2C(=C1)C(=NC=N2)NC3=C(C(=CC=C3)Cl)F)OC", "CHEMBL207718": "CN1CC(C1)(C(=O)N)N(C)CC2=C(C=C3C(=C2)C(=NC=N3)NC4=C(C(=CC=C4)Cl)F)OC", "CHEMBL207815": "CN(CC1=C(C=C2C(=C1)C(=NC=N2)NC3=C(C(=CC=C3)Cl)F)OC)C4(CN(C4)CCOC)C(=O)N", "CHEMBL208048": "CC(C)N(CC1=C(C=C2C(=C1)C(=NC=N2)NC3=C(C(=CC=C3)Cl)F)OC)C(C)C(=O)N", "CHEMBL208118": "CC(C(=O)N)N(C)CC1=C(C=C2C(=C1)C(=NC=N2)NC3=C(C(=CC=C3)Cl)F)OC", "CHEMBL208286": "CN(CC1=C(C=C2C(=C1)C(=NC=N2)NC3=C(C(=CC=C3)Cl)F)OC)C(CO)C(=O)N", "CHEMBL208292": "COC1=C(C=C2C(=C1)N=CN=C2NC3=C(C(=CC=C3)Cl)F)CN4CCCC4C(=O)N", "CHEMBL208637": "CCOC1=C(C(=CC(=N1)NC(=O)C)N)C#N", "CHEMBL210032": "CC(=O)NC1=NC(=C(C(=C1)N)C#N)C2=CC=CC=C2", "CHEMBL210618": "CCOC1=C(C(=CC(=N1)NC(=O)CC2=C(C=CC(=C2)OC)OC)N)C#N", "CHEMBL210928": "CCOC1=C(C(=CC(=N1)NC(=O)CC2=CC(=C(C=C2OC)S(=O)(=O)C)OC)N)Cl", "CHEMBL210963": "CCOC1=C(C(=CC(=N1)NC(=O)CC2=CC(=C(C=C2OC)S(=O)(=O)C)OC)N)C#N", "CHEMBL211003": "CC(C(=O)NC)N(C)CC1=C(C=C2C(=C1)C(=NC=N2)NC3=C(C(=CC=C3)Cl)F)OC", "CHEMBL212382": "CC(C)(C)C1=NN=C2N1C=C(C=C2)C3=C(N=CO3)C4=C(C=C(C=C4)F)F", "CHEMBL212968": "CC(C)(C)C1=NN=C2N1C=C(C=C2)C3=C(N=CO3)C4=CC(=C(C=C4F)F)F", "CHEMBL213423": "CC(C)C1=NN=C2N1C=C(C=C2)C3=C(N=CO3)C4=CC(=C(C=C4F)F)F", "CHEMBL213451": "CCNC1=NN=C2N1C=C(C=C2)C3=C(N=CO3)C4=CC=C(C=C4)F", "CHEMBL214198": "CC(C)C1=NN=C2N1C=C(C=C2)C3=C(NN=C3)C4=C(C=CC(=C4)F)F", "CHEMBL215652": "CC(C)C1=NN=C2N1C=C(C=C2)C3=C(N=CO3)C4=C(C=C(C=C4)F)Cl", "CHEMBL215803": "CC1CC2CN1CCN3C(=O)C4=C(N3)C(=CC=C4)C5=NC6=C(C=CC=C6O2)NC5=O", "CHEMBL2205426": "CC(C)(C)NC1=C(C(=O)C1=O)NC2=NC(=NC=C2)NC3=CC=C(C=C3)C4=CC=NC=C4", "CHEMBL223367": "C1CCOC2=C(C=C(C(=C2)CCCO)Cl)NC(=O)NC3=CN=C(C(=N3)OCC1)C#N", "CHEMBL223460": "CS(=O)(=O)NC1=C(C=C2C(=C1)OCCCCCOC3=NC(=CN=C3C#N)NC(=O)N2)Cl", "CHEMBL2312290": "COC1=C(C=C(C=C1)CCNC2=NC=C(C(=N2)NC3CCCC3)C(=O)NCCCN4CCCC4=O)OC", "CHEMBL2312301": "COC1=CC=CC=C1CNC2=NC=C(C(=N2)NC3CCCC3)C(=O)NCCCN4CCCC4=O", "CHEMBL2312303": "C1CCC(C1)NC2=NC(=NC=C2C(=O)NCCCN3CCCC3=O)NCC4=C(C=CC(=C4)Cl)Cl", "CHEMBL2312304": "C1CCC(C1)NC2=NC(=NC=C2C(=O)NCCCN3CCOC3=O)NCC4=C(C=CC(=C4)Cl)Cl", "CHEMBL2333365": "CC1=C(C=CC(=C1F)S(=O)(=O)C)C(=O)N2CCOC3=C(C2)C=C(C=C3)C4=CN=C(C=C4)N", "CHEMBL235157": "CC1=C(C=CC2=C3C4=CC(=C(C=C4N=CC3=C(N=C12)N)OC)OC)N", "CHEMBL242753": "C1C2=C(C=CC(=C2)C(=O)NCC3=CC=NC=C3)C4=C1C(=C5C=CC(=C6C=CC(=O)C=C6)C=C5)NN4", "CHEMBL248757": "C1CCOC2=NC(=CN=C2C#N)NC(=O)NC3=CC(=C(C=C3OC1)NCC4=CN=CS4)Cl", "CHEMBL281957": "CCN(CC)CC=CC1=C(C2=C(C3=C(C=C2)N=C(N3C)NC4=C(C=CC=C4Cl)Cl)C(=O)N1)C", "CHEMBL373598": "C1CCOC2=CC(=C(C=C2NC(=O)NC3=CN=C(C(=N3)OCC1)C#N)Cl)OCCCO", "CHEMBL376967": "CC(C(=O)N)N(CCN(C)C)CC1=C(C=C2C(=C1)C(=NC=N2)NC3=C(C(=CC=C3)Cl)F)OC", "CHEMBL377383": "CCOC1=C(C(=CC(=N1)C(=O)NCC2=CC=C(C=C2)S(=O)(=O)C)N)Cl", "CHEMBL377772": "COC1=C(C=C2C(=C1)N=CN=C2NC3=C(C(=CC=C3)Cl)F)CN4CCCC4CC(=O)N", "CHEMBL378370": "CN(CC1=C(C=C2C(=C1)C(=NC=N2)NC3=C(C(=CC=C3)Cl)F)OC)C4CCNC4=O", "CHEMBL378627": "CC(C)OC1=C(C(=CC(=N1)NC(=O)CC2=CC(=C(C=C2OC)S(=O)(=O)C)OC)N)C#N", "CHEMBL379601": "CN(CC1=C(C=C2C(=C1)C(=NC=N2)NC3=C(C(=CC=C3)Cl)F)OC)CC(=O)N", "CHEMBL379905": "CN(CC1=C(C=C2C(=C1)C(=NC=N2)NC3=C(C(=CC=C3)Cl)F)OC)C(COC)C(=O)N", "CHEMBL379929": "CC(C)C1=NN=C2N1C=C(C=C2)C3=C(N=CO3)C4=CC=CC=C4", "CHEMBL380006": "CC(C(=O)N(C)C)N(C)CC1=C(C=C2C(=C1)C(=NC=N2)NC3=C(C(=CC=C3)Cl)F)OC", "CHEMBL380386": "CC(C(=O)N)NCC1=C(C=C2C(=C1)C(=NC=N2)NC3=C(C(=CC=C3)Cl)F)OC", "CHEMBL380454": "COC1=C(C=C2C(=C1)N=CN=C2NC3=C(C(=CC=C3)Cl)F)CN4CCC(C4)C(=O)N", "CHEMBL380889": "CN(C)CC(C(=O)N)N(C)CC1=C(C=C2C(=C1)C(=NC=N2)NC3=C(C(=CC=C3)Cl)F)OC", "CHEMBL382638": "COC1=C(C=C2C(=C1)N=CN=C2NC3=CC(=C(C=C3)F)Cl)CN4CCCC4C(=O)N", "CHEMBL382822": "CN(C)C(=O)C1CCCN1CC2=C(C=C3C(=C2)C(=NC=N3)NC4=C(C(=CC=C4)Cl)F)OC", "CHEMBL382823": "CC(C(=O)N)N(CCOC)CC1=C(C=C2C(=C1)C(=NC=N2)NC3=C(C(=CC=C3)Cl)F)OC", "CHEMBL383246": "CC(C)N1CCC(CC1)(C(=O)N)N(C)CC2=C(C=C3C(=C2)C(=NC=N3)NC4=C(C(=CC=C4)Cl)F)OC", "CHEMBL383760": "CNC(=O)C1CCCN1CC2=C(C=C3C(=C2)C(=NC=N3)NC4=C(C(=CC=C4)Cl)F)OC", "CHEMBL389745": "CC(C)(C1=CC2=C(C=C1)NC3=C(C=CC(=C3)C4=CC(=C(C=C4)N)OC)C(=O)N2)C(=O)NC5=CC=C(C=C5)N6CCOCC6", "CHEMBL395080": "COC1=C(C=CC(=C1)C2=CC3=C(C=C2)C(=O)NC4=C(N3)C=CC(=C4)CC(=O)NC5=CC=C(C=C5)N6CCOCC6)N", "CHEMBL398606": "CC(C)NCC1=CC=C(C=C1)NC2=CC(=C3C=CC(=C4C=CC(=O)C=C4O)C=C3)NN2", "CHEMBL425601": "CC(C)N1CC(C1)(C(=O)N)N(C)CC2=C(C=C3C(=C2)C(=NC=N3)NC4=C(C(=CC=C4)Cl)F)OC", "CHEMBL437885": "COC1=C(C=C2C(=C1)N=CN=C2NC3=C(C(=CC=C3)Cl)F)CN4CCCC4", "CHEMBL438485": "C1CC(CCC1NC(=O)C2=CC3=C(C=C2)C4=C(C3)C(=C5C=CC(=C6C=CC(=O)C=C6)C=C5)NN4)O", "CHEMBL478649": "CC1=C(C=C(C=C1)C(=O)NC2CC2)C3=CC=C(C=C3)C(=O)NCC4CC4", "CHEMBL485285": "CC1=C(C=C(C=C1)C(=O)NC2=CC=CC(=C2)N3CCOCC3)C4=CC5=C(C=C4)C(=NO5)C6CCNCC6", "CHEMBL485286": "CC1=C(C=C(C=C1)NC(=O)C2=CC(=NC=C2)N3CCCC3)C4=CC5=C(C=C4)C(=NO5)C6CCNCC6", "CHEMBL495729": "CC1=C(C=C(C=C1)NC(=O)C2=CC(=NC=C2)N3CCCC3)C4=C(C=C(C=C4)C5=NN=C(O5)C)C", "CHEMBL497563": "CC1=C(C=C(C=C1)C(=O)NC2CC2)C3=CC4=C(C=C3)C(=NO4)C5CCNCC5", "CHEMBL522579": "CC1=C(C=C(C=C1)C(=O)NC2CC2)C3=C(C=C(C=C3)C4=NN=C(O4)C)C", "CHEMBL523559": "CC1=C(C=C(C=C1)C(=O)NC2=CC=CC(=C2)N3CCOCC3)C4=C(C=C(C=C4)C5=NN=C(O5)C)C", "CHEMBL583042": "CC1=CN=C(N=C1C2=CNC(=C2)C(=O)NC(CO)C3=CC(=CC=C3)Cl)NC4=C(C=C(C=C4)F)Cl", "CHEMBL590109": "C1=CC=C2C(=C1)C=C(S2)C3=C4C(=CC(=C3)C5=CN(C6=CN=C(N=C65)N)CCN)C=NN4", "CHEMBL606964": "COC1=CC=C(C=C1)N2CC3=CN=C(N=C3N(C2=O)C4CCC(C4)O)NC5=CC=C(C=C5)F", "CHEMBL1082440": "CC1CNCCCN1S(=O)(=O)C2=CC=CC3=CN=CC(=C32)C", "CHEMBL1084546": "CN(C1=C(C=CC=N1)CNC2=NC(=NC=C2C(F)(F)F)NC3=CC4=C(C=C3)NC(=O)C4)S(=O)(=O)C", "CHEMBL1090356": "C1COCCN1C2=CC=C(C=C2)NC3=NC=CC(=N3)C4=C(N=C5N4C=CS5)C6=CC(=CC=C6)NC(=O)CC7=CC=CC=C7", "CHEMBL1094408": "CN1CCN(CC1)C2=CC(=C(C=C2)OC)NC3=NC=C4CCC5=C(C4=N3)N(N=C5C(=O)N)C", "CHEMBL115220": "C1CC1C2=CC(=NN2)NC(=O)CC3=CC4=CC=CC=C4C=C3", "CHEMBL116070": "C1=CC(=CC=C1OC2=CN=CC3=C2C=C(S3)C(=O)N)Br", "CHEMBL1164265": "CN1CCN(CC1)C2=NC=C(C=C2)C3=CC4=C(NCCN4CC5=C(C=CC(=C5Cl)F)F)N=C3", "CHEMBL117697": "COC1=CC=CC(=C1)NC2=NC=NC3=CC=CC=C32", "CHEMBL1190711": "COC1=C(C=C(C=C1)C2=CC3=NC=CN3C(=N2)NC4=C(C=CC=N4)C(=O)N)OC", "CHEMBL1230122": "CN1C2=NC(=NC=C2C=C(C1=O)OC3=C(C=C(C=C3)F)F)NC4CCOCC4", "CHEMBL1230607": "CC(C)CC(=O)NC1=NNC2=C1CN(C2(C)C)C(=O)C3CCN(CC3)C", "CHEMBL1236126": "CC(C)(C)C(=O)OC1=CC2=C(C=C1)N(C(=N2)NC(=O)C3=CC(=CC=C3)[N+](=O)[O-])CCCO", "CHEMBL1241473": 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"CHEMBL1682546": "C1=CC=C(C=C1)CNC2=NC(=CS2)C3=CC4=C(C=C3)NN=C4", "CHEMBL1682552": "C1CCC(CC1)NC2=C(N=C3N2C=CC=N3)C4=CC5=C(C=C4)NN=C5", "CHEMBL1682553": "CC(C)NC1=C(N=C2N1C=CC=N2)C3=CC4=C(C=C3)NN=C4", "CHEMBL1682554": "CCCCNC1=C(N=C2N1C=CC=N2)C3=CC4=C(C=C3)NN=C4", "CHEMBL1682558": "C1COCCN1CCN2C=NC(=C2C3=CC4=C(C=C3)NN=C4)C5=CC=C(C=C5)F", "CHEMBL17370": "CSC1=CC=C(C=C1)C2=NC(=C(N2)C3=CC=NC=C3)C4=CC=C(C=C4)F", "CHEMBL1738758": "CN1CCN(CC1)C2=CC(=C(C=C2)OC(F)(F)F)NC3=NC=C4CCC5=C(C4=N3)N(N=C5C(=O)N)CCO", "CHEMBL1825138": "CC(C1=C(C=CC(=C1Cl)F)Cl)OC2=C(N=CC(=C2)C3=CN(N=C3)C4CCNCC4)N", "CHEMBL183844": "CC1=CC(=CC=C1)NC(=O)NC2=C(C=C(C=C2)C3=C4CNC(=O)C4=CC=C3)C", "CHEMBL184847": "CC1=C(C=C(C=C1)NC(=O)NC2=CC=C(C=C2)C3=C4CNC(=O)C4=CC=C3)C", "CHEMBL185569": "CC1=CC(=CC=C1)NC(=O)NC2=CC=C(C=C2)C3=C4CNC(=O)C4=CC=C3", "CHEMBL1933576": "CN1CCN(CC1)C2=CC(=C(C=C2)OC(F)(F)F)NC3=NC=CC(=N3)C4=CC(=CN4C)C(=O)N", "CHEMBL1933582": "CN1CCN(CC1)C2=CC(=C(C=C2)OC(F)(F)F)NC3=NC=CC(=N3)C4=CC5=C(N4C)CCNC5=O", "CHEMBL1958401": "C1CCC(CC1)NC2=NC(=O)C=C(N2)C3=CC=NC=C3", "CHEMBL196363": "CC1=CC(=CC=C1)NC(=O)NC2=CC=C(C=C2)C3=CSC4=NC=NC(=C34)N", "CHEMBL1964290": "CC1=CC=CC(=C1C)C2=C(C=C(N2)C3=NC(=NC=C3)N)C(=O)N", "CHEMBL1964413": "C1=CC2=C(C=C1C3=CN(N=N3)CC4=C(C=C(C=C4)C(F)(F)F)C(F)(F)F)C=NN2", "CHEMBL1964444": "CC1=CC2=C(C=CN=C2C=C1)NC(=O)NC3=CC=CC(=N3)C(F)(F)F", "CHEMBL1964644": "C1=CC=C(C=C1)CNC(=O)NC2=NC=C(S2)[N+](=O)[O-]", "CHEMBL1964687": "CC1=CC(=CC(=C1)NC(=O)NC2=CC3=C(C=C2)C4=C(CC3)SC5=NC=NC(=C45)N)C", "CHEMBL1964692": "CN1C2=C(C(=CN=C2)C3=CC=C(C=C3)NC(=O)NC4=CC=CC(=C4)C(F)(F)F)C(=N1)N", "CHEMBL1964777": "C1=CC(=CC(=C1)F)OC2=CN=CC3=C2C=C(S3)C(=O)N", "CHEMBL1964804": "CS(=O)(=O)NCCOC1=CN=CC(=C1)C2=CC3=C(C=C2)C=NC=C3", "CHEMBL1964937": "C1CN(CC=C1C2=CNC3=C2C=CC=N3)C(=O)NC(CO)C4=CC=CC=C4", "CHEMBL1965131": "CC1=CC=C(C=C1)C(=O)NC2=C(SC3=C2C(=C(C=C3)Cl)Cl)C(=O)N", "CHEMBL1965423": "CC(C)CN1C2=C(C=CC(=C2)C3=C(N=C4N3C=CS4)C5=CC=C(C=C5)F)N=C1N", "CHEMBL1965507": "CC1=CC(=CC=C1)NC(=O)NC2=CC=C(C=C2)NC(=O)C3=CSC4=NC=NC(=C34)N", "CHEMBL1965570": "C1=CC=C(C(=C1)NC(=O)NC2=CC=C(C=C2)C3=CSC4=C3C(=NC=C4C5=COC=C5)N)F", "CHEMBL1965589": "CC1=NC=CN2C1=NC(=C2C3=NC(=NC=C3)NCC4(CC4)O)C5=C(C=C(C=C5)F)F", "CHEMBL1965631": "CN(C)CC(=O)NC1=NNC2=C1C=C(C=C2)C3=CN(N=N3)CC4=CC=CC=C4", "CHEMBL1965660": "C1=CC(=C(C=C1Cl)Cl)C2=C(C=C(N2)C3=NC(=NC=C3)N)C(=O)N", "CHEMBL1965702": "CN(C)C1CCCC(C1)NC2=NC(=CC(=N2)Cl)C3=CNC4=C3C=CC=N4", "CHEMBL1965836": "CC1=C2C=C(C=CC2=NN1)C3=CC(=CN=C3)OCC(CC4=CC(=CC=C4)OC(F)(F)F)N", "CHEMBL1965845": "CC(C1=CC(=CC=C1)OC)NC(=O)N2CCC(=CC2)C3=CNC4=C3C=CC=N4", "CHEMBL1965988": "CC1=CC(=CC=C1)NC(=O)NC2=CC=C(C=C2)C3=CSC4=C3C(=NC=C4C#CCN)N", "CHEMBL1966040": "C1=CC(=CC(=C1)C(F)(F)F)CNC2=NC=NC(=C2)C3=CNC4=C3C=CC=N4", "CHEMBL1966204": "C1=CC=C(C=C1)CN2C=C(N=N2)C3=CC4=C(C=C3)NN=C4NC(=O)C5=CC=C(C=C5)F", "CHEMBL1966279": "C1=CC=C2C(=C1)C(=NNC2=O)C3=CC=C(C=C3)NC(=O)C4=CC(=CC=C4)S(=O)(=O)NCCCN", "CHEMBL1966343": "CC(C)CC1=NOC(=C1)C2=CC3=C(C=C2)NN=C3N", "CHEMBL1966514": "C1=CC(=CC(=C1)F)NC(=O)NC2=CC=C(C=C2)C3=CSC4=C3C(=NC=C4C5=COC=C5)N", "CHEMBL1966628": "C1CC(CCC1N)NC2=NC=CC(=N2)C3=CNC4=C3C=CC=N4", "CHEMBL1966703": "CC1=C2C(C3=C(CC(CC3=O)(C)C)N=C2NN1)C4=CC=CC=C4F", "CHEMBL1966722": "C1=CC=C(C=C1)C(C2=CC=CC=C2)(C(=O)NNC(=S)NC3=CC=C(C=C3)Cl)O", "CHEMBL1966808": "C1CCC2=C(C1)C3=C4N=C(NN4C(=O)N=C3S2)C5=CC=NC=C5", "CHEMBL1966816": "C1=CC2=C(C=CN=C2C(=C1)F)NC(=O)NC3=CC=CC(=N3)C(F)(F)F", "CHEMBL1967094": "C1=CC=C(C=C1)C2=C3C=C(SC3=NN2)C(=O)NCC4=CC=C(C=C4)Cl", "CHEMBL1967116": "CC1=CC(=CC=C1)NC(=O)NC2=CC=C(C=C2)C3=CSC4=C3C(=NC=C4C5=CN(N=C5)C)N", "CHEMBL1967302": "C1C2=C(C=CC(=C2)C3=CC(=CN=C3)OCC(CC4=CNC5=CC=CC=C54)N)NC1=O", "CHEMBL1967531": "C1=CC=C(C=C1)NC(=O)NC2=CC=C(C=C2)C3=CSC4=NC=NC(=C34)N", "CHEMBL1967544": "CN(C)C1=CC=CC2=C1C=CC=C2S(=O)(=O)N(CCN)C3=CN=CC(=C3)C4=CC5=C(C=C4)C=NC=C5", "CHEMBL1967560": "CCN1C(=O)N(C2=CN=C(N=C2N1C3CCCC3)NC4=C(C=C(C=C4)C(=O)NC5CCN(CC5)C)OC)C", "CHEMBL1967564": "CCCC(=O)NC1=NNC2=NC3=CC=CC=C3C=C21", "CHEMBL1967720": "CC(C)(C(=O)N)N1C=C(C=N1)C2=CN=C(C3=C2SC=C3C4=CC=C(C=C4)NC(=O)NC5=CC(=CC=C5)F)N", "CHEMBL1967878": "CC1=C(C=CC(=C1)NC2=NC=C(C(=N2)NC3C4CC(C3C(=O)N)C=C4)F)N5CCN(CC5)C", "CHEMBL1967887": "CC1=C2C=C(C=CC2=NN1)C3=CC(=CN=C3)OCCN", "CHEMBL1968127": "CC(C)(CNC1=NC=CC(=N1)C2=C(N=C3N2C=CO3)C4=CC=C(C=C4)F)CN(C)C", "CHEMBL1968151": "C1=CN=CC=C1C2=NC3=C4C=CSC4=NC(=O)N3N2", "CHEMBL1968380": "CCC1C(=O)N(C2=CN=C(N=C2N1C3CCCC3)NC4=C(C=C(C=C4)C(=O)NC5CCN(CC5)C)OC)C", "CHEMBL1968406": "CCC1=CC(=CC=C1)NC(=O)NC2=CC3=C(C=C2)C4=C(CC3)SC5=NC=NC(=C45)N", "CHEMBL1968459": "CCCCNC1=NC=NC(=C1)C2=CNC3=C2C=CC=N3", "CHEMBL1968590": "CC1=NC2=C(S1)C=CC(=C2)C3=CSC4=C3C(=NC=C4C=CC(=O)NC)N", "CHEMBL1968705": "CCCC(=O)NC1=CC=CC(=C1)C2=NC3=C(C=C(C=C3)OCCN4CCCC4)C(=N2)NC5=CC6=C(C=C5)NN=C6", "CHEMBL1968791": "CC1=C(C2=C(N1C3CC(C3)CN4CCCC4)N=CN=C2N)C5=CC(=CC=C5)OCC6=CC=CC=C6", "CHEMBL1968930": "CC(C)(CN)CNC1=NC(=CC(=N1)Cl)C2=CNC3=C2C=CC=N3", "CHEMBL1969042": "C1=CC(=O)C=CC1=C2C(=C(NN2)NC3=CC=C(C=C3)O)C4=CC=C(C=C4)O", "CHEMBL1969049": "CC1=C(C=CC(=C1)C(=O)NC(C)C2=CC(=CC=C2)OC)C3=CC=NC=C3", "CHEMBL1969126": "CC(C)N1C2=C(C=CC(=C2)C3=C(N=C4N3C=CO4)C5=C(C=C(C=C5)F)F)N=N1", "CHEMBL1969151": "CN(C)C1CCC(CC1)NC2=NC(=CC(=N2)Cl)C3=CNC4=C3C=CC=N4", "CHEMBL1969190": "COC1=C2C(=C(C=C1)C3=CC=C(C=C3)NC(=O)NC4=CC(=CC(=C4)F)F)C(=NO2)N", "CHEMBL1969301": "CCCCN1C2=C(C=C(C=C2)N(C)C(=O)C3CCCCC3)N=C1NC(=O)C4=CC=CC(=C4)C#N", "CHEMBL1969372": "COCCNC1=NC=CC(=N1)C2=C(N=C3N2C=CN=C3)C4=CC=C(C=C4)F", "CHEMBL1969502": "C1C(C1C(=O)NC2=CC3=C4C(=C2)C(=O)NNC=C4C=N3)C5=CC=CC=C5", "CHEMBL1969506": "CC(C)(C)OC(=O)N1C2=C(C=C(C=C2)NC3=C(C(=O)C3=O)NCC4=CC=C(C=C4)S(=O)(=O)N)C=N1", "CHEMBL1969523": "CC1=CC(=CC=C1)NC2=NC=CC(=N2)NC3=C(C(=O)C3=O)NC(C)C(C)(C)C", "CHEMBL1969537": "C1CC2=C(C1)SC3=C2C4=NNC(=S)N4C5=NNC(=S)N35", "CHEMBL1969561": "CC(C)N(C)C(=O)C1=C(N=NN1CC2=CC=CC=C2)C3=CC4=C(C=C3)NN=C4", "CHEMBL1969664": "C1COCCN1CC2=CNC(=C3C4=C(C=CC(=C4)C#N)NC3=O)C=C2", "CHEMBL1969735": "CC(C)(CNC1=NC=CC(=N1)C2=C(N=C3N2C=CN=C3Cl)C4=CC=C(C=C4)F)CO", "CHEMBL1969843": "C1COCCC1CN2C=C(N=N2)C3=CC4=C(C=C3)NN=C4", "CHEMBL1969879": "CC1CCN(CC1N(C)C2=NC=NC3=C2C=CN3)C(=O)CO", "CHEMBL1970074": "CC1=C2C(=NN1)C=CC=C2C3=CC=C(C=C3)NC(=O)NC4=CC=CC(=C4)C(F)(F)F", "CHEMBL1970104": "CC(C)(C)C1=CC2=NC(=C3C4=CC=CC=C4NN3)N=C2C=C1", "CHEMBL1970142": "CC1=CC=C(C=C1)NC(=O)NC2=CC=C(C=C2)C3=CSC4=C3C(=NC=C4C5=CN(N=C5)C(C)C(=O)NC)N", "CHEMBL1970189": "CC1=C2C(C(=C(OC2=NN1)N)C#N)C3=CC=CC=C3Cl", "CHEMBL1970203": "CC1=CC(=CC(=C1)NC(=O)NC2=CC=C(C=C2)NC(=O)C3=CSC4=NC=NC(=C34)N)C", "CHEMBL1970217": "CC1=C(C=CN=C1)C2=CC=C(C=C2)C(=O)NC(C)C3=CC(=CC=C3)OC", "CHEMBL1970314": "C1=CC(=CC(=C1)N)C2=CC(=C3C(=C2)C=CC=N3)C(=O)N", "CHEMBL1970340": "C1=CC(=CC(=C1)O)C2=C3C(=CC=C2)ON=C3N", "CHEMBL1970522": "COC1=C(C=CC(=C1)C=C2C(=O)N=C(S2)NC3=CC=CC=C3)O", "CHEMBL1970709": "C1=CC(=CC=C1CNC(=O)NC2=CC3=C(C=C2)NN=C3)Br", "CHEMBL1970903": "CC1=C2C=C(C=CC2=NN1)C3=CC(=CN=C3)OCC(CC4=CNC5=CC=CC=C54)N", "CHEMBL1970913": "CCCC(=O)NC1=NN(C2=NC3=CC=CC=C3C=C12)C(=O)CC", "CHEMBL1970950": "C1=CC=C(C(=C1)C(=O)O)NC2=NC(=NC=C2)NCC3=CC(=CC=C3)O", "CHEMBL1971021": "CC1=CC(=CC(=C1)NC(=O)NC2=CC(=C(C=C2)C3=C4CNC(=O)C4=CC=C3)C(F)(F)F)C", "CHEMBL1971029": "CC(=O)N1CCN(CC1)C2=CC(=C(C=C2)OC)NC3=NC=C(C(=N3)NC4=CC=CC=C4S(=O)(=O)NC)Br", "CHEMBL1971141": "CC1=CC(=CC=C1)NC(=O)NC2=CC=C(C=C2)C3=CC(=CC=C3)C(=O)N", "CHEMBL1971149": "CC1=NC=CN2C1=NC(=C2C3=NC(=NC=C3)NCC(C)(C)C(=O)O)C4=C(C=C(C=C4)F)F", "CHEMBL1971172": "CC(C)(CNC1=NC(=CC(=C1)C2=CNC3=C2C=CC=N3)Cl)CNS(=O)(=O)C", "CHEMBL1971186": "C1CNCCC1NC2=NC=CC(=N2)C3=C(N=C4N3C=CO4)C5=CC=C(C=C5)F", "CHEMBL1971245": "CN1CCN(CC1)C2=CC(=CC=C2)NC3=NC=CC(=N3)C4=C(N=C5N4C=CC=C5)C(=O)N", "CHEMBL1971649": "CC1=CC(=C(C=C1)F)NC(=O)NC2=CC=C(C=C2)C3=C(C4=NC=CN=C4C=C3)N", "CHEMBL1971943": "CC1=CNC2=NC=CC(=C12)OC3=C(C=C(C=C3F)NC4=CC(=NC(=N4)N)Cl)F", "CHEMBL1972119": "C1COCCN1C2=NC(=CC=C2)NC(=O)NC3=C4C=CC=C(C4=NC=C3)C(F)(F)F", "CHEMBL1972125": "C1=CC=C(C=C1)C(=O)C2=C(C=CC(=C2)C3=CC(=CN=C3)OCC(CC4=CNC5=CC=CC=C54)N)N", "CHEMBL1972142": "C1=CC=C(C=C1)CNC(=O)C2=CC=CC(=C2)C3=CN=C4C(=C3)C=CN4", "CHEMBL1972158": "C1=CC=C(C=C1)CN2C(=C(N=N2)C3=CC4=C(C=C3)NN=C4N)C5=CC=CC=C5", "CHEMBL1972221": "CCCS(=O)(=O)NC1=CC=C(C=C1)C2=CC3=C(C=C2)NN=C3NC(=O)CC", "CHEMBL1972290": "C1=CC2=C(NC=C2C3=CC(=NC(=C3)Cl)NCCN)N=C1", "CHEMBL1972339": "CC1=C2C=C(C=CC2=NN1)C3=C(N(N=N3)CC4=CC=CC=C4)C5=CC=C(C=C5)F", "CHEMBL1972576": "CC1=CC=C(C=C1)NC(=O)NC2=CC=C(C=C2)NC(=O)C3=CSC4=NC=NC(=C34)N", "CHEMBL1972584": "CC(=O)N1CCN(CC1)C2CCC(CC2)N3C4=C(C(=N3)C5=CC=C(C=C5)NC(=O)C6=CC7=CC=CC=C7N6C)C(=NC=N4)N", "CHEMBL1972659": "CC1=C2CCCC(=C2C=CC1=O)NNC(=O)CC3=CC=CC4=CC=CC=C43", "CHEMBL1972849": "CC(C)(CO)C1=NN=C2N1N=C(C=C2)C3=C(N=C4N3C=CO4)C5=C(C=C(C=C5)F)F", "CHEMBL1972937": "COC1=CC=CC(=C1)C=C2C(=O)N=C(S2)NC3=CC=CC=C3", "CHEMBL1972988": "C1=CC2=C(NC=C2C3=CC(=NC=N3)Cl)N=C1", "CHEMBL1973098": "COC1=C(C=CC(=C1)C=C2C(=O)NC(=S)S2)O", "CHEMBL1973142": "CC(=O)NC1=C(SC2=C1C(=C(C=C2)Cl)Cl)C(=O)N", "CHEMBL1973145": "CC1=CC(=CC=C1)NC(=O)NC2=CC=C(C=C2)C3=CSC4=NC(=NC(=C34)N)N", "CHEMBL1973211": "CC1=CC(=CC=C1)NC(=O)NC2=CC=C(C=C2)C3=CSC4=C3C(=NC=C4C#CCN5CCCC5)N", "CHEMBL1973348": "C1=CC=C2C(=C1)C(=CN2)CC(COC3=CN=CC(=C3)C4=CC(=C(C=C4)N)C(=O)C5=CC(=CC=C5)Cl)N", "CHEMBL1973395": "C1CN(CCC1O)C2=NC=NC3=C2C(=CN3)C4=CC=CC=C4", "CHEMBL1973483": "C1=CC(=NC(=C1)NC(=O)NC2=C3C=CC(=CC3=NC=C2)C(F)(F)F)C(F)(F)F", "CHEMBL1973540": "C1=CC=NC(=C1)NS(=O)(=O)C2=CC=C(C=C2)NC=C3C4=C(C=CC5=C4SC=N5)NC3=O", "CHEMBL1973720": "C1CC(CCC1N)NC2=NC(=CC(=N2)Cl)C3=CNC4=C3C=CC=N4", "CHEMBL1973808": "C1=CC(=CC=C1C(=O)NC2=CC3=C(C=C2)NN=C3)Cl", "CHEMBL1973860": "C1=CC2=CN=C(C=C2C=C1C3=CSC=C3)NCCO", "CHEMBL1973893": "CCCS(=O)(=O)NC1=CC=C(C=C1)C2=CC3=C(C=C2)NN=C3NC(=O)C", "CHEMBL1973937": "CC1=C2C(=C(C=C1)C3=CC=C(C=C3)NC(=O)NC4=CC(=CC=C4)Br)C(=NN2)N", "CHEMBL1973961": "CN1CCN(CC1)C2=CC(=C(C=C2)C(=O)NC3=NNC4=C3C=C(C=C4)CC5=CC(=CC(=C5)F)F)OC", "CHEMBL1974254": "CCOC1=CC=C(C=C1)NC(=O)NC2=CC=C(C=C2)C3=CSC4=C3C(=NC=C4C5=CN(N=C5)C)N", "CHEMBL1974288": "C1=CC=C(C=C1)C(CO)NC(=O)C2=CC=C(C=C2)C3=CC=NC=C3", "CHEMBL1974310": "C1=CC(=CC=C1C2=CN=CC3=C2C=C(S3)C(=O)N)F", "CHEMBL1974328": "CC1=CC(=CC=C1)NC2=NC(=CN=C2C(=O)N)NC3CCCCC3N", "CHEMBL1974416": "C1=CC=C(C=C1)C2=CNC3=NC=C(C=C23)NC(=O)C4=C(C(=CC=C4)F)F", "CHEMBL1974664": "COC1=C(C=C(C=C1)C=NNC2=NC=NC3=C2NC4=CC=CC=C43)OC", "CHEMBL1974702": "CC1=NC2=C(C(=O)O1)SC3=C(C=CC(=C23)Cl)Br", "CHEMBL1974870": "CC1=C2C=C(C=CC2=NN1)C3=CC(=CN=C3)OCC(CC4=CC(=CC=C4)Cl)N", "CHEMBL1974935": "C1=CC=C2C(=C1)C(=CN2)CC(COC3=CN=CC(=C3)C=CC4=CC=NC=C4)N", "CHEMBL1975121": "CC(C1=CC(=CC=C1)OC)NC(=O)C2=CC=C(C=C2)C3=CC=NC=C3", "CHEMBL1975128": "C1=CC=C(C=C1)CN2C(=C(N=N2)C3=CC4=C(C=C3)NN=C4N)I", "CHEMBL1975138": "C1=CC=C(C=C1)C(C2=CC=CC=C2)(C(=O)NNC(=S)NC3=CC=C(C=C3)F)O", "CHEMBL1975233": "CC1=CC(=C(C=C1Cl)NC(=O)NC2=NC=C(N=C2)C#N)OC", "CHEMBL1975256": "C1=CSC(=C1)C=NNC(=O)C2=C(N(N=N2)C3=NON=C3N)C4=CC=CS4", "CHEMBL1975490": "C1C2=C(C=C(C=C2C3=CC=C(C=C3)NC4=NC5=CC=CC=C5O4)OCCCN)C(=O)N1", "CHEMBL1975500": "CC(=O)NCCNC(=O)C1=CC2=C(C=C1)NC3=C(C=CC(=C3)C4=CC(=C(C=C4)O)OC)C(=O)N2", "CHEMBL1975534": "C1=C(C2=C(N1CC(C(CN)O)O)N=CN=C2N)I", "CHEMBL1975647": "C1=CC2=C(C=CN=C2C(=C1)F)NC(=O)NC3=NC=CN=C3", "CHEMBL1975900": "C1=CC(=C(C=C1CNC2=C(C(=O)C2=O)NC3=CC=NC=C3)Cl)Cl", "CHEMBL1976090": "C1=NC2=C(C(=N1)N)SC3=NC=NC(=C23)N", "CHEMBL1976093": "CC(C)(CNC1=NC=CC(=N1)C2=C(N=C3N2C=CN=C3)C4=CC=C(C=C4)F)CN(C)C", "CHEMBL1976134": "C1=CC2=C(C=C1C3=CN=C4C(=C3)C=CN4)NN=C2", "CHEMBL1976220": "C1=CC(=CC(=C1)Br)NC(=O)NC2=CC=C(C=C2)C3=CSC4=C3C(=NC=C4)N", "CHEMBL1976240": "COC1=CC=CC(=C1)C(CN)NC(=O)C2=CC=C(C=C2)C3=CC=NC=C3", "CHEMBL1976420": "CCC1=C(NC2=NC=CN=C12)C3=CC=C(C=C3)C(C)(C)O", "CHEMBL1976455": "C1=CC2=NC=CC(=C2C=C1C(F)(F)F)NC(=O)NC3=NC=CN=C3", "CHEMBL1976732": "CC(C)(CC1=NN=C2N1N=C(C=C2)C3=C(N=C4N3C=CO4)C5=C(C=C(C=C5)F)F)O", "CHEMBL1976936": "C1CC(CC(C1)O)NC2=CC(=NC(=N2)C3=CNC4=C3C=CC=N4)Cl", "CHEMBL1977128": "C1=CC=C(C=C1)CN2C=C(N=N2)C3=CC4=C(C=C3)NN=C4NC(=O)C5=CC=CC(=C5)C#N", "CHEMBL1977135": "C1=CC=C(C=C1)CNC(=O)C2=CC=C(C=C2)C3=CC=NC=C3", "CHEMBL1977148": "COC1=CC=C(C=C1)NC(=O)NC2=CC=C(C=C2)C3=CSC4=C3C(=NC=C4C5=CN(N=C5)CCO)N", "CHEMBL1977223": "CCCC(=O)NC1=NNC2=C1C=C(C=C2)C3=CN(N=N3)CC4=CC=CC=C4", "CHEMBL1977346": "C1=CC=C2C(=C1)NC3=NN=C(C=C3C(=O)N2)I", "CHEMBL1977681": "CNC(=O)C1=CC2=C(NN=C2S1)C3=CC=CC=C3F", "CHEMBL1978014": "CN1CCC(CC1)C(=O)N2C3=C(C=C(C=C3)C4=CN(N=N4)CC5=CC=CC=C5)C(=N2)N", "CHEMBL1978099": "CC1=C(C=C(C=C1)NC2=NC=C(C(=N2)NC3=CC=C(C=C3)OCC(=O)NC)F)S(=O)(=O)N", "CHEMBL1978200": "CC1=NC=CN2C1=NC(=C2C3=NC(=NC=C3)NCCC(C)(C)O)C4=C(C=C(C=C4)F)F", "CHEMBL1978448": "CS(=O)(=O)N(CC1=CC2=C(C=C1)NC(=O)C3=CC=CN32)C4CC4", "CHEMBL1979057": "C1C2=C(C=CC=C2C(=O)N1)C3=CC=C(C=C3)NC4=NC5=CC=CC=C5N4", "CHEMBL1979093": "CC1=C(C=CC(=C1)NC(=O)NC2=CC=C(C=C2)C3=C4C(=C(C=C3)OC)ON=C4N)F", "CHEMBL1979176": "COC1=CC2=NC=CC(=C2C=C1)NC(=O)NC3=NC=CC(=C3)C(F)(F)F", "CHEMBL1979252": "C1=CC(=CC(=C1)C(F)(F)F)CNC2=C(C(=O)C2=O)NC3=CC=NC=C3", "CHEMBL1979357": "CN1C=C(C2=CC=CC=C21)C(CN)C3=CN=CC(=C3)C=CC4=CC=NC=C4", "CHEMBL1979516": "CCNC(=O)C1=CN=C(C2=C1SC=C2C3=CC=C(C=C3)NC(=O)NC4=CC(=CC=C4)F)N", "CHEMBL1979554": "C1=CC2=C(C=C1NC3=C(C(=O)C3=O)NCC4=C(C=C(C=C4)Cl)Cl)C=NN2", "CHEMBL1979577": "CC1=CC(=CC=C1)NC(=O)NC2=CC=C(C=C2)C3=CSC4=C3C(=NC=C4C#CC(C)(C)N)N", "CHEMBL1979883": "CC1=CC(=CC=C1)NC(=O)NC2=CC=C(C=C2)C3=CSC4=C3C(=NC=C4C#CCN(C)C)N", "CHEMBL1979933": "C1=CC=C(C(=C1)C(=O)O)NC2=NC=NC(=N2)NC3=CC(=CC=C3)F", "CHEMBL1979970": "CCCC(=O)NC1=NNC2=NN=C(C=C21)C3=C(C(=CC=C3)F)F", "CHEMBL1980142": "C1=CC2=C(C=CN=C2C(=C1)C(F)(F)F)NC(=O)NC3=CC=CC(=N3)C(F)(F)F", "CHEMBL1980144": "CC1=CC=CC=C1NC(=O)NC2=CC=C(C=C2)NC(=O)C3=CSC4=NC=NC(=C34)N", "CHEMBL1980163": "C1=CC=C(C=C1)COC2=CC=C(C=C2)NC3=NC=NC4=CC=CC=C43", "CHEMBL1980178": "CC(=O)NC1CCCC(C1)NC2=NC(=CC(=N2)Cl)C3=CNC4=C3C=CC=N4", "CHEMBL1980253": "C1COCCC1NC2=NC(=CC(=N2)Cl)C3=CNC4=C3C=CC=N4", "CHEMBL1980297": "C1=CC(=CC(=C1)F)NC(=O)NC2=CC=C(C=C2)C3=CSC4=C3C(=NC=C4C5=CN(N=C5)CCO)N", "CHEMBL1980391": "CC1=C2C(=NC3=CC(=C(C=C3C(=N2)C4=CC=CC=C4Cl)F)OC)NN1", "CHEMBL1980435": "COC1=CC=CC(=C1)C(=O)NC2=NNC3=C2C=C(C=C3)C4=CN(N=N4)CC5=CC=CC=C5", "CHEMBL1980489": "C1=CC(=CC=C1CNC2=C(C(=O)C2=O)NC3=CC=NC=C3)Cl", "CHEMBL1980540": "C1=CC2=C(C=CN=C2C(=C1)Cl)NC(=O)NC3=CC=CC(=N3)C(F)(F)F", "CHEMBL1980562": "CS(=O)(=O)NC1CCC(CC1)NC2=NC(=CC(=N2)Cl)C3=CNC4=C3C=CC=N4", "CHEMBL1980592": "CC1=C(SC2=NC(=O)N3C(=C12)N=C(N3)C4=CC=NC=C4)C", "CHEMBL1980704": "CC1=CC2=NN=C(N2C3=CC=CC=C13)SCC4=CN5C=CC=CC5=N4", "CHEMBL1980896": "C1=CC(=CC(=C1)Cl)CC(=O)NC2=CC=C(C=C2)C3=C(SC4=NC=NC(=C34)N)Br", "CHEMBL1981047": "CN1CCN(CC1)C2=CC=C(C=C2)C(=O)NC3=NNC4=C3CN(C4)C(=O)C(C5=CC=CC=C5)OC", "CHEMBL1981079": "C1=CC(=C(C=C1Cl)F)C2=C(C=C(N2)C3=NC(=NC=C3)N)C(=O)N", "CHEMBL1981410": "CNC1=NC=NC2=C1N=C(CCN2)C3=CC=C(C=C3)NC(=O)NC4=CC=CC(=C4)C(F)(F)F", "CHEMBL1981511": "CC1=NC=CC(=C1)C2=CC3=C(C=C2)C(=O)NC4=CC=CC=C4N3", "CHEMBL1981720": "C1=CC=C2C(=C1)C(=CC=N2)NC(=O)NC3=NC=CN=C3", "CHEMBL1981725": "CCN1CCN(CC1)C2=CC=C(C=C2)NC3=NC=CC(=N3)C4=C(N=C5N4C=CC=C5)C6=CC(=CC=C6)C(=O)NC7=CC=CC=C7F", "CHEMBL1981782": "C1=CC(=C(C=C1CNC(=O)NC2=CC3=C(C=C2)NN=C3)Cl)Cl", "CHEMBL1982122": "C1=CC=C(C=C1)C(CCO)NC2=NC3=C(S2)C=C(C=C3)C4=CC=NC=C4", "CHEMBL1982135": "CC1=CC=CC=C1NC(=O)NC2=CC3=C(C=C2)C4=C(CC3)SC5=NC=NC(=C45)N", "CHEMBL1982271": "CN(C)CC(=O)NC1CCC(CC1)NC2=NC(=CC(=N2)Cl)C3=CNC4=C3C=CC=N4", "CHEMBL1982361": "C1=CC=C(C(=C1)CNC2=C(C(=O)C2=O)NC3=CC=NC=C3)F", "CHEMBL1982383": "CC(C)(CNC1=NC=CC(=N1)C2=C(N=C3N2C=CN=C3CCN)C4=CC=C(C=C4)F)CO", "CHEMBL1982400": "C1=CC=C(C=C1)CN2C=C(N=N2)C3=CC4=C(C=C3)NN=C4C5=CC=CC=C5", "CHEMBL1982465": "CC1=CC(=CC=C1)NC(=O)NC2=CC=C(C=C2)C3=CSC4=C3C(=NC=C4C#CCN5CCOCC5)N", "CHEMBL1982466": "CC1=CC=C(C=C1)NC(=O)NC2=CC=C(C=C2)C3=CSC4=C3C(=NC=C4C5=CN(N=C5)C)N", "CHEMBL1982506": "COC1=C(C=C2C(=C1)C=NC3=C2C(=O)NC3=O)OC", "CHEMBL1982563": "CC1=NC=CN2C1=NC(=C2C3=NC(=NC=C3)NCC(C)(C)COC)C4=CC=C(C=C4)F", "CHEMBL1982610": "C1=CC(=CC(=C1)Cl)C2=CN3C(=C(C=NC3=O)I)N2", "CHEMBL1982660": "COC1=CC2=NC=CC(=C2C=C1)NC(=O)NC3=CC=CC(=N3)C(F)(F)F", "CHEMBL1982711": "C1=CC(=CC=C1C2=CNC3=NC=CC(=C23)Cl)C(=O)N", "CHEMBL1982866": "COCCN1C=C(C(=N1)C2=CC=C(C=C2)Cl)C3=NC=NC=C3", "CHEMBL1982874": "C1CC1CN2C3=C(C=CC(=C3)C4=C(N=C5N4C=CS5)C6=CC=C(C=C6)F)N=C2N", "CHEMBL1982924": "COC1=CC=CC(=C1)C(=O)NC2=CN=C3C(=C2)C(=CN3)C4=CC=CC=C4", "CHEMBL1982957": "C1=CC=C(C=C1)C2=CNC3=NC=C(C=C23)C4=CC(=CC=C4)C(=O)N", "CHEMBL1982982": "C1=CC(=CC(=C1)F)CNC2=C(C=CC(=C2)C3=CC=NC=C3)C(=O)N", "CHEMBL1983025": "CCC(CC)(C#CC1=CN=C(C2=C1SC=C2C3=CC=C(C=C3)NC(=O)NC4=CC=CC(=C4)C)N)N", "CHEMBL1983111": "CC(=O)NCC(=O)N1C2CCC1C3=C2C=CC(=C3)NC4=NC=C(C(=N4)NC5CCC5)C(F)(F)F", "CHEMBL1983195": "CCN(CC)C(=O)NC1=CC2=C(C=C1)N=C(C(=N2)C3=CC=CO3)C4=CC=CO4", "CHEMBL1983268": "CN1CCN(CC1)C2=CC(=C(C=C2)C(=O)NC3=NNC4=C3C=C(C=C4)CC5=CC(=CC(=C5)F)F)NC6CCOCC6", "CHEMBL1983534": "C1=CC=C(C=C1)CNC2=NC3=C(S2)C=C(C=C3)C4=CC=NC=C4", "CHEMBL1983589": "C1CC(CCC1N)NC2=CC(=NC(=N2)C3=CNC4=C3C=CC=N4)Cl", "CHEMBL1983595": "C1=CC=C(C=C1)CN2C=C(N=N2)C3=CC4=C(C=C3)NN=C4NC(=O)C5=CC(=CC=C5)Cl", "CHEMBL1983923": "CC1=CC(=NN1)NC2=NC(=NC(=C2)N3CCN(CC3)C)C=CC4=CC=CC=C4", "CHEMBL1983932": "COC1=CC2=NC=CC(=C2C=C1)NC(=O)NC3=NC(=CC=C3)Br", "CHEMBL1983945": "C1=CC=C2C(=C1)C(=CN2)CC(C(=O)NC3=CN=CC(=C3)C=CC4=CC=NC=C4)N", "CHEMBL1983963": "CC1=CC(=CC=C1)NC(=O)NC2=CC=C(C=C2)C3=COC4=NC=NC(=C34)N", "CHEMBL1984038": "COC1=CC(=CC(=C1OC)OC)C2=CC3=C(C=C2)NC4=C(C=CC(=C4)C5=CC=CC=C5NS(=O)(=O)C)C(=O)N3", "CHEMBL1984162": "CC1=CC(=C2C(=C1)N=C(O2)NC3=CC=C(C=C3)C4=NN(C5=C4C(=NC=N5)N)C6CCC(CC6)OCCOC)C", "CHEMBL1984191": "C1=CC(=C(C=C1C2=C(C=NN2)C3=NC=NC=C3)Cl)Cl", "CHEMBL1984363": "CC1=C(C=CC(=C1)NC(=O)CC2=CC=C(C=C2)C3=C4C(=CC=C3)NN=C4N)F", "CHEMBL1984367": "CN(C)C1=CC=C(C=C1)CNC(=O)C2=CC3=C(NN=C3S2)C4=CC=CC=C4", "CHEMBL1984548": "CN1C=C(C=N1)NC2=NC=C(C(=N2)NC3=CC=CC=C3C(=O)N)Cl", "CHEMBL1984586": "CC1=CC=CC=C1NC(=O)NC2=CC=C(C=C2)C3=COC4=NC=NC(=C34)N", "CHEMBL1984633": "CC(C1=CC(=CC=C1)OC)NC(=O)C2=CN=C(S2)C3=CC=NC=C3", "CHEMBL1984700": "CC(C)OC1=NC=CN2C1=NC(=C2C3=NC(=NC=C3)NCC(C)(C)O)C4=C(C=C(C=C4)F)F", "CHEMBL1984711": "COC1=CC(=CC(=C1OC)OC)NC2=NC=CC(=N2)NC3=CC(=NO3)C4CCCCC4", "CHEMBL1985074": "CSC1=CC2=C(C=C1)N=C3C(=C2Cl)CCNC3=O", "CHEMBL1985092": "C1=CC(=CC(=C1)Cl)NC2=C(C(=C3C=CC(=O)C=C3)NN2)C4=CC=C(C=C4)O", "CHEMBL1985095": "C1=CC=C2C(=C1)C=C(S2)C3=C4C(=CC(=C3)C5=CN(C6=CN=C(N=C65)N)CC(=O)N)C=NN4", "CHEMBL1985153": "C1CCC(C(C1)N)NC2=NC=CC(=N2)NC3=CC=CC=C3C(=O)O", "CHEMBL1985406": "CCCC(=O)NC1=NNC2=C1C=C(C=C2)C3=C(C(=CC=C3)F)F", "CHEMBL1985723": "CC(C)(CN)CNC1=NC(=CC(=C1)C2=CNC3=C2C=CC=N3)Cl", "CHEMBL1986139": "C1=CC=C(C=C1)NC2=C3C(=CSC3=NC=N2)Cl", "CHEMBL1986186": "CC(C(C)(C)C)NC1=C(C(=O)C1=O)NC2=CC=NC=C2", "CHEMBL1986263": "CCN1C(=C(SC1=O)C2=NC(=NC=C2)NC3=CC(=CC=C3)OC)C", "CHEMBL1986328": "CN(C)C(=O)NC1=CC2=C(C=C1)N=C(C(=N2)C3=CC=CO3)C4=CC=CO4", "CHEMBL1986499": "C1=CC=C(C=C1)CN2C(=C(N=N2)C3=CC4=C(C=C3)NN=C4N)C5=CC=C(C=C5)F", "CHEMBL1986530": "C1CCC2=C(C1)C(=NNC2=O)CC3=CC(=C(C=C3)F)C(=O)N4CCN(CC4)C5=NC=CC=N5", "CHEMBL1986597": "C1COCCN1S(=O)(=O)C2=CC=CC(=C2)C(=O)NC3=CC=C(C=C3)C4=NC5=C(C=CC=C5N4)C(=O)N", "CHEMBL1986781": "CC(=O)N1CCC(CC1)NC2=NC=CC(=N2)C3=C(N=C4N3C=CO4)C5=CC=C(C=C5)F", "CHEMBL1986855": "COC1=CC=C(C=C1)CNC2=NC(=CC(=C2)C3=CNC4=C3C=CC=N4)F", "CHEMBL1986869": "CC1=CSC(=N1)NC(=O)C2=C(C3=C(S2)N=C(C=C3)C4=CC=NC=C4)N", "CHEMBL1986943": "C1CC(CCC1NC2=NC(=CC(=N2)Cl)C3=CNC4=C3C=CC=N4)O", "CHEMBL1986970": "CN(CCOC)C(=O)C1=C(N=NN1CC2=CC=CC=C2)C3=CC4=C(C=C3)NN=C4", "CHEMBL1987007": "CN1CCC(CC1)NC(=O)C2=CC3=C(NN=C3S2)C4=CC=CC=C4", "CHEMBL1987009": "COC1=CC=CC(=C1)CNC(=O)C2=CC3=C(NN=C3S2)C4=CC=CC=C4", "CHEMBL1987034": "C1=CC(=CC(=C1)S(=O)(=O)N)NC2=NC=C(C(=N2)NC3=CC=C(C=C3)OCC#N)Br", "CHEMBL1987073": "C1=CC=C(C=C1)CN2C=C(N=N2)C3=CC4=C(C=C3)NN=C4NC(=O)C5=CC=C(C=C5)Cl", "CHEMBL1987261": "CC(C)(CN)CNC1=NC(=CC(=C1)C2=CNC3=C2C=CC=N3)F", "CHEMBL1987359": "CCCCNC1=C2C=CC=C3C2=C(C=C1)C(=O)N(C3=O)CCNCCO", "CHEMBL1987448": "C1=CC2=C(NC=C2C3=CC(=NC(=C3)Cl)N)N=C1", "CHEMBL1987679": "C1=CC=C2C(=C1)C(=CN2)CC(COC3=CN=CC(=C3)C4=CC5=C(C=C4)NC(=O)O5)N", "CHEMBL1987745": "C1=CC=C2C(=C1)NC3=C(C=CC(=C3)C4=C(C=NC=C4)Cl)C(=O)N2", "CHEMBL1987793": "CC1=CC=CC=C1C2=C(N(C3=CC=CC=C32)CCCOC4=CC=CC5=CC=CC=C54)C(=O)O", "CHEMBL1987910": "C1=CC=C(C(=C1)C(F)(F)F)NC(=O)NC2=CC=C(C=C2)C3=CSC4=C3C(=NC=C4)N", "CHEMBL1987948": "CS(=O)(=O)NC1CCCC(C1)NC2=NC(=CC(=N2)Cl)C3=CNC4=C3C=CC=N4", "CHEMBL1988075": "CC1=NC=C(C=C1)C2=CN=C(C3=C2SC=C3C4=CC=C(C=C4)NC(=O)NC5=CC(=CC=C5)F)N", "CHEMBL1988153": "CC1=NN=C(O1)C2=CC3=C(S2)C=NC=C3OC4=CC=C(C=C4)C(F)(F)F", "CHEMBL1988163": "C1=CC=C(C=C1)N2C=CC3=CN=C(N=C32)NC4=CC(=CC=C4)S(=O)(=O)N", "CHEMBL1988173": "CC1=C(C=CC(=C1)Cl)NC(=S)NNC(=O)C(C2=CC=CC=C2)(C3=CC=CC=C3)O", "CHEMBL1988300": "C1=CC=C2C(=C1)NC(=N2)C=CC3=CN=C(C4=C3SC=C4C5=CC=C(C=C5)N)N", "CHEMBL1988387": "CN1C=C(C=N1)C2=CN=C(C3=C2SC=C3C4=CC=C(C=C4)NC(=O)NC5=CC=C(C=C5)OC(F)F)N", "CHEMBL1988437": "CNC(=O)C1=CC=CC=C1SC2=CC3=C(C=C2)C(=NN3)C=CC4=CC=CC=N4", "CHEMBL1988537": "COC1=CC=C(C=C1)C(=O)N2C3=CC=CC=C3SC4=C(C=NC=C42)Cl", "CHEMBL1988594": "C1=CC=C(C=C1)NC(=O)NC2=CC=C(C=C2)NC(=O)C3=CSC4=NC=NC(=C34)N", "CHEMBL1988608": "CC(=O)NC1=CC=CC(=C1)CNC2=C(C(=O)C2=O)NC3=CC4=C(C=C3)NN=C4", "CHEMBL1988717": "CN1C=C(C=N1)C2=C3N=CC(=C(N3N=C2)N)C4=CC=C(C=C4)NC(=O)NC5=CC=CC(=C5)C(F)(F)F", "CHEMBL1988838": "CC1=CN=C(N=C1NC2=CC=C(C=C2)OCC(=O)N)NC3=CC(=CC=C3)S(=O)(=O)N", "CHEMBL1989029": "CC(C)OC1=C(C(=O)NN1)C=C2C=NC3=CC=CC=C32", "CHEMBL1989646": "CC1=C(N=NN1CC2=CC=CC=C2)C3=CC4=C(C=C3)NN=C4N", "CHEMBL1989708": "CC1=CC(=CC=C1)NC(=O)NC2=CC=C(C=C2)C3=CSC4=C3C(=NC=C4C5=CN(N=C5)CC(C)O)N", "CHEMBL1989805": "C1=COC(=C1)C=C2C(=O)N3C(=C(C(C(=C3S2)C(=O)N)C4=CC=CO4)C#N)N", "CHEMBL1990162": "C1=CC=C(C=C1)CN2C=C(N=N2)C3=CC4=C(C=C3)NN=C4NC(=O)C5=CC=C(C=C5)C#N", "CHEMBL1990254": "C1=CC=C(C=C1)C(CN)NC(=O)C2=CC=C(C=C2)C3=CC=NC=C3", "CHEMBL1990288": "CC(C1=CC=CC=C1)NC2=NC=CC(=N2)C3=C(N=C4N3C=CO4)C5=CC=C(C=C5)F", "CHEMBL1990482": "C1=CC(=C2C(=C1)NC(=N2)C3=CC=NC=C3)C(=O)N", "CHEMBL1990496": "CN1C(=O)C(=C(N=C1NCC(CC2=CC=CC=C2)N)C3=CC=NC=C3)C4=CC5=CC=CC=C5C=C4", "CHEMBL1990821": "CC1=CC=CC=C1C2=CC=CC3=C2NC(=C3CCCOC4=CC(=CC(=C4C)C)C)C(=O)O", "CHEMBL1990884": "CC1=CC(=C2C(=C1)N=C(O2)NC3=C(C=C(C=C3)C4=C(C(=CC=C4)C(=O)N)N)F)C", "CHEMBL1990885": "CCN(CC)CCNC(=O)C1=C(NC(=C1C)C=C2C3=C(C=CC(=C3)F)NC2=O)C", "CHEMBL1990904": "C1CC1CNC2=NC=CC(=N2)C3=C(N=C4N3C=CN=C4)C5=CC=C(C=C5)F", "CHEMBL1990912": "C1=CC(=CN=C1)C2=CC3=CC(=NC=C3C=C2)NCCO", "CHEMBL1991063": "CC1=C2C=C(C=CC2=NN1)C3=CC(=CN=C3)OCC(CC4=CC(=C(C=C4)Cl)Cl)N", "CHEMBL1991078": "COC1=C(C=C(C=C1)C(=O)NC2=NNC3=C2C=C(C=C3)C4=CN(N=N4)CC5=CC=CC=C5)OC", "CHEMBL1991138": "C1CCN(C1)CC2CC(C2)C3=NC(=C4N3C=CN=C4N)C5=CC(=CC=C5)OCC6=CC=CC=C6", "CHEMBL1991188": "CC(C1=CC(=CC=C1)OC)NC(=O)C2=C(C=C(C=C2)C3=C(C=NC=C3)F)OC", "CHEMBL1991285": "CC1=CC(=C(C=C1Cl)NC(=O)NC2=NC=C(N=C2)C#N)OCC3CCC(C3)C(=O)O", "CHEMBL1991395": "CC(C)(CNC1=NC=CC(=N1)C2=C(N=C3N2C=CN=C3)C4=CC=C(C=C4)F)CO", "CHEMBL1991410": "C1=CC(=C(C(=C1)F)C(=O)NC2=NC(=CC(=C2)C3=CNC4=C3C=CC=N4)Cl)F", "CHEMBL1991429": "C1CC(=O)N(C1)C2=CC(=CC=C2)NC3=NC=CC(=N3)C4=C(N=C5N4C=CS5)C6=CC(=CC=C6)NC(=O)CC7=CC=CC=C7", "CHEMBL1991674": "C1CC(CCC1NC2=CC(=NC(=N2)C3=CNC4=C3C=CC=N4)Cl)O", "CHEMBL1991678": "CC1=NC=CN2C1=NC(=C2C3=NC(=NC=C3)NCC(C)(C)CO)C4=C(C=C(C=C4)F)F", "CHEMBL1991725": "CN(C)CC(=O)NC(CC1=CNC2=CC=CC=C21)COC3=CN=CC(=C3)C4=CC5=C(C=C4)C=NC=C5", "CHEMBL1991800": "CC(C)(CNC1=NC=CC(=N1)C2=C(N=C3N2C=CN=C3CC4CC4)C5=CC=C(C=C5)F)CO", "CHEMBL1992220": "CCNC(=O)NC1CCC(CC1)NC2=NC(=CC(=N2)Cl)C3=CNC4=C3C=CC=N4", "CHEMBL1992231": "C1=CC=C(C(=C1)C(=O)O)NC2=NC=NC(=N2)NC3=CC=C(C=C3)F", "CHEMBL1992242": "CC1=CC(=CC(=C1)NC(=O)NC2=CC=C(C=C2)C3=C4C=NSC4=CC=C3)C", "CHEMBL1992306": "CNC(=O)C1=NC=CC(=C1)OC2=CC=C(C=C2)NC(=O)NC3=CC=CC(=C3)C(F)(F)F", "CHEMBL1992323": "C1=CC2=C(C=C1Cl)C3=C(O2)C(=O)N=CN3", "CHEMBL1992342": "CCCS(=O)(=O)NC1=CC=C(C=C1)C2=CC3=C(C=C2)NN=C3N", "CHEMBL1992363": "CN(C)C1=CC=C(C=C1)C(=O)NC2=NNC3=C2C=C(C=C3)C4=CN(N=N4)CC5=CC=CC=C5", "CHEMBL1992536": "COC1=CC=C(C=C1)CNC2=C(C(=O)C2=O)NC3=CC4=C(C=C3)NN=C4", "CHEMBL1992634": "C1=CC=C(C=C1)C2=CNC3=NC=C(C=C23)Br", "CHEMBL1992740": "CCN1CCN(CC1)CCCC(=O)NC2=NNC3=NN=C(C=C32)C4=C(C(=CC=C4)F)F", "CHEMBL1992922": "C1=CC=C(C=C1)C2=CNC3=C2C(=NC=N3)NC(CO)CO", "CHEMBL1992937": "CC1=CN=C(C=C1)NC2=NC3=C(N2)C=C(C=C3)[N+](=O)[O-]", "CHEMBL1993243": "CNC(=O)C=CC1=CN=C(C2=C1SC=C2C3=CC4=C(C=C3)OCO4)N", "CHEMBL1993413": "C1=CC=C(C=C1)C(=O)NC2=NC(=CC(=C2)C3=CNC4=C3C=CC=N4)Cl", "CHEMBL1993424": "C1=CC=C(C=C1)CN2C=CC3=CN=C(N=C32)NC4=CC(=CC=C4)S(=O)(=O)N", "CHEMBL1993548": "CC(COC1=CN=C(C(=C1)C=CC2=CC=NC=C2)Cl)N", "CHEMBL1993584": "C1=CC=C2C(=C1)C(=CN2)CC(COC3=CN=CC(=C3)C=CC4=CC=NC=C4)O", "CHEMBL1993661": "CNS(=O)(=O)C1=CC=CC=C1NC2=NC(=NC=C2Cl)NC3=CC(=C(C(=C3)OC)OC)OC", "CHEMBL1993722": "C1=CC(=C2C(=C1)NN=C2N)C3=CC=C(C=C3)NC(=O)NC4=C(C=CC(=C4)C(=O)O)F", "CHEMBL1993781": "C1=CC=C(C=C1)COCC(COC2=CN=CC(=C2)C=CC3=CC=NC=C3)N", "CHEMBL1993941": "CCCN1C=C(C=N1)C2=CN=C(C3=C2SC=C3C4=CC=C(C=C4)NC(=O)NC5=CC(=CC=C5)F)N", "CHEMBL1994040": "CC(C)(CNC1=NC=CC(=N1)C2=C(N=C3N2C=CN=C3CC4CC4)C5=C(C=C(C=C5)F)F)O", "CHEMBL1994074": "C1=CC=C(C=C1)C2=NNC3=C2C=C(C=C3)Br", "CHEMBL1994241": "COC1=CC(=CC(=C2NC3=CC=CC=C3N2)C#N)C(=CC1=O)Br", "CHEMBL1994321": "CC1=CC(=CC=C1)NC(=O)NC2=CC=C(C=C2)C3=CSC4=C3C(=NC=C4C#CCNS(=O)(=O)C)N", "CHEMBL1994438": "C1CCC(C(C1)N)NC2=NC(=CC(=N2)Cl)C3=CNC4=C3C=CC=N4", "CHEMBL1994526": "CC(C1CCC(CC1)C(=O)NC2=CC=NC=C2)N", "CHEMBL1994538": "C1=CC2=C(C=CN=C2C(=C1)C(F)(F)F)NC(=O)NC3=NC=CN=C3", "CHEMBL1994669": "CN1C=C(C=N1)NC2=NC=C(C(=N2)NC3=CC=CC=C3C(=O)N)Br", "CHEMBL1994693": "C1CC2=C(C3=C1C=C(C=C3)NC(=O)NC4=CC=CC=C4)C5=C(N=CN=C5S2)N", "CHEMBL1994830": "C1=CC(=CC=C1OC2=CN=CC3=C2C=C(S3)C4=NN=C(O4)N)Cl", "CHEMBL1994938": "C1=CC(=CC=C1C2=CSC3=C2C(=NC=C3C=CC(=O)NCCCN4C=CN=C4)N)Br", "CHEMBL1995712": "CN(C)CC(=O)NC1CCCC(C1)NC2=NC(=CC(=N2)Cl)C3=CNC4=C3C=CC=N4", "CHEMBL1995740": "COC1=C(C=CC(=C1)C2=CC3=C(C=C2)C(=O)NC4=C(N3)C=CC(=C4)[N+](=O)[O-])O", "CHEMBL1995811": "C1=CC=C(C=C1)CN2C=C(N=N2)C3=CC4=C(C=C3)NN=C4NC(=O)C5=C(C=CC(=C5)F)F", "CHEMBL1995813": "C1CCC(C(C1)N)NC2=NC=CC(=N2)C3=CNC4=C3C=CC=N4", "CHEMBL1995832": "CC(C)(CNC1=NC=CC(=N1)C2=C(N=C3N2C=CN=C3OC)C4=C(C=C(C=C4)F)F)CO", "CHEMBL1996048": "CC1=CC=C(C=C1)C2=CC3=C(C=CC(=C3N2)C(=O)N)NCCN", "CHEMBL1996066": "C1=CC=C(C=C1)C2=CSC(=N2)N3C4=C(C=CC(=C4)C#N)N=C3N", "CHEMBL1996111": "CN(C)C(=O)C1=C(N=NN1CC2=CC=CC=C2)C3=CC4=C(C=C3)NN=C4", "CHEMBL1996234": "CC1(CC(C1)C2=NC(=C3N2C=CN=C3N)C4=CC5=C(C=C4)C=CC(=N5)C6=CC=CC=C6)O", "CHEMBL1996500": "CC1=NC=CN2C1=NC(=C2C3=NC(=NC=C3)NCC(C)(C)O)C4=C(C=C(C=C4)F)F", "CHEMBL1996587": "CC(C)(CO)C1=NN=C2N1N=C(C=C2)C3=C(N=C4N3CCC4)C5=C(C=C(C=C5)F)F", "CHEMBL1996649": "CCN(CC)CCCNC(=O)C1=CN=C(C2=C1SC=C2C3=CC=C(C=C3)NC(=O)NC4=CC(=CC=C4)F)N", "CHEMBL1996791": "C1CC(CCC1N2C3=C(C(=NC=N3)N)C(=N2)I)O", "CHEMBL1996817": "CCCCOC1=NC=NC2=C1C(=CN2)C3=CC=CC=C3", "CHEMBL1996831": "C1CCC(=C2CCC3=C(C4=CC=CC=C4N=C23)C(=O)O)C1", "CHEMBL1996931": "C1=CC(=CC=C1CC(CO)NC(=O)C2=CC=C(C=C2)C3=CC=NC=C3)Cl", "CHEMBL1996979": "C1=CC=C(C=C1)C2=CNC3=NC=C(C=C23)NC(=O)C4=C(C=CC=C4F)F", "CHEMBL1996980": "CNCC(=O)NC1CCC(CC1)NC2=NC(=CC(=N2)Cl)C3=CNC4=C3C=CC=N4", "CHEMBL1997023": "CN(C)C1=C(C=C2C=NSC2=C1)NC(=O)C(=O)O", "CHEMBL1997129": "C1CNC(=O)C2=C1NC(=C2)C3=CC(=NC=C3)C=CC4=CC=CC=C4", "CHEMBL1997340": "C1CC(CN(C1)C(=O)C2=NOC(=C2)C3=CC4=C(C=C3)NN=C4)O", "CHEMBL1997534": "CC1=C(SC(=C1)C(=O)NC(C)C2=CC(=CC=C2)OC)C3=CC4=C(NN=C4C=C3)C", "CHEMBL1997597": "CCS(=O)(=O)NC1=CC=C(C=C1)C2=CC3=C(C=C2)NN=C3N", "CHEMBL1997617": "CN1CCN(CC1)C2CCC(CC2)N3C=C(C4=C3N=CN=C4N)C5=CC=C(C=C5)OC6=CC=CC=C6", "CHEMBL1997764": "COC1=CC=C(C=C1)C(=O)NC2=CN=C3C(=C2)C(=CN3)C4=CC=CC=C4", "CHEMBL1997822": "CC1=CC2=C(N1)C=CC(=C2)C3=CSC4=C3C(=NC=C4C5=CC(=CC=C5)S(=O)(=O)C)N", "CHEMBL1997846": "C1CCC(CC1)NC2=CC(=NC(=N2)C3=CNC4=C3C=CC=N4)Cl", "CHEMBL1998112": "COC1=C(C=C(C=C1)C2=CC3=NC=CN3C(=N2)NC4=CC=CC=C4C(=O)N)OC", "CHEMBL1998121": "C1=CC(=C(C=C1C(CCN)C(=O)NC2=CC3=C(C=C2)NN=C3)Cl)Cl", "CHEMBL1998159": "CC1=C2C=C(N=CC2=NN1)C3=CC(=CN=C3)OCC(CC4=CC(=CC=C4)C(F)(F)F)N", "CHEMBL1998193": "C1=CC(=CN=C1)NC(=O)NCCCCCCNC(=O)NC2=CN=CC=C2", "CHEMBL1998432": "C1CC(CC(C1)NC2=NC(=CC(=N2)Cl)C3=CNC4=C3C=CC=N4)N", "CHEMBL1998470": "CCCC(=O)NC1=NC(=CC(=C1)C2=CNC3=C2C=CC=N3)Cl", "CHEMBL1998545": "C1=CC=C(C=C1)CC(CO)NC(=O)C2=CC=C(C=C2)C3=CC=NC=C3", "CHEMBL1998585": "C1=CC(=CC=C1C2=CSC3=NC=NC(=C23)N)NC(=O)NC4=C(C=CC(=C4)C(F)(F)F)F", "CHEMBL1998611": "C1=CC(=C2C(=C1Cl)C(=C(S2)C(=O)N)N)Br", "CHEMBL1998953": "C1CCN(CC1)C2=NC=NC3=C2C(=CN3)C4=CC=CC=C4", "CHEMBL1999112": "CCOC(=O)C1=C2N(C(=C(C1C3=CC=CO3)C#N)N)C(=O)C(=CC4=CC=CO4)S2", "CHEMBL1999321": "C1=CC=C(C=C1)OC2=CC=C(C=C2)CCNC3=C(C(=O)C3=O)NC4=CC=NC=C4", "CHEMBL1999414": "CCN(CC)CCCNC(=O)C1=CN=C(C2=C1SC=C2C3=CC=C(C=C3)NC(=O)NC4=CC=CC(=C4)C)N", "CHEMBL1999428": "CC(C1=CC=CC=C1)NC(=O)C2=CC=C(C=C2)C3=CC=NC=C3", "CHEMBL1999590": "CC1=NN(C(=C1)C2=CC=CC=C2)C3=CC(=NC=N3)NN=CC4=CC=CO4", "CHEMBL1999714": "CC1=CC2=C(C=C1)NC3=CC=CC=C3C(=O)N2", "CHEMBL1999718": "C1=CC2=C(C=CN=C2C=C1C(F)(F)F)NC(=O)NC3=NC=C(C=C3)C#N", "CHEMBL1999811": "C1=CC2=NSN=C2C(=C1)NC(=O)NNC=C3C=CC(=O)C=C3O", "CHEMBL1999931": "C1=CC=C(C=C1)CN2C=C(N=N2)C3=CC4=C(C=C3)NN=C4NC(=O)C5=CC=CC=C5", "CHEMBL2000029": "CC1=CC=CC=C1C2=C(N=NN2CC3=CC=CC=C3)C4=CC5=C(C=C4)NN=C5N", "CHEMBL2000071": "C1=CC=C(C=C1)C2=CNC3=C2C(=NC=N3)NCCCO", "CHEMBL2000114": "CSC1=CNC2=C1C(=NC=N2)NCCCO", "CHEMBL2000335": "CC1=C(C=C(C=C1)NC(=O)NC2=CC=C(C=C2)C3=CSC4=NC=NC(=C34)N)C", "CHEMBL2000345": "CC1=CC2=C(C=C1)NC(=C(C=C3C=C(C(=O)C=C3Br)OC)C#N)N2", "CHEMBL2000354": "COC1=C(C=C(C=C1)C=C2C(=O)N=C(S2)NC3=CC=CC=C3)O", "CHEMBL2000393": "C1COC2=C(C1N3C4=NC(=NC=C4NC3=O)N5C=NC6=C5C=C(C=C6)F)C=CC=C2F", "CHEMBL2000408": "CC1=CN2C(=C(N=C2C(=N1)C)C3=C(C=C(C=C3)F)F)C4=NC(=NC=C4)NCC(C)(C)CO", "CHEMBL2000429": "CC(C)OC1=NC=CN2C1=NC(=C2C3=NC(=NC=C3)NCC(C)(C)CO)C4=C(C=C(C=C4)F)F", "CHEMBL2000481": "C1=CC=C2C(=C1)C(=NNC2=O)C3=CC=C(C=C3)NC(=O)C4=CC(=CC=C4)S(=O)(=O)NCCN", "CHEMBL2000508": "C1=CC(=CC=C1C2=C(N3C=CSC3=N2)C4=CC=NC=C4)F", "CHEMBL2000568": "CC(=O)C1=CC=CC(=C1)C2=CN=C3C(=C2)C=CN3", "CHEMBL2000801": "C1=CC(=C2C=NSC2=C1)C3=CC=C(C=C3)NC(=O)NC4=CC(=C(C=C4)F)C(F)(F)F", "CHEMBL2000832": "COC1=C(C=CC(=C1)C2=CC3=C(C=C2)C(=O)NC4=C(N3)C=CC(=C4)C(=O)NCC5=CC(=CC=C5)F)O", "CHEMBL2000894": "CC1=C(C=CC(=C1)O)N2C=C(C(=O)C3=C2C=C(C=C3)C4=CC=NC=C4)C(=O)NN", "CHEMBL2001224": "CC1=CC(=C(C=C1Cl)NC(=O)NC2=NC=C(N=C2)C#N)OC3CCCC3", "CHEMBL2001239": "C1=CC(=CC=C1C2=CC(=CC(=C2O)CNC(=O)C(F)(F)F)NC3=NC=NC(=N3)N)Cl", "CHEMBL2001257": "CCN(CC)CC#CC1=CN=C(C2=C1SC=C2C3=CC=C(C=C3)NC(=O)NC4=CC=CC(=C4)C)N", "CHEMBL2001288": "C1=NC2=C(C(=N1)N)C(=NN2C3C(C(C(O3)CO)O)O)I", "CHEMBL2001477": "C1=CC=C(C=C1)CNC2=C(C=CC(=C2)C3=CC=NC=C3)C(=O)N", "CHEMBL2001485": "CC1=CC=C(C=C1)NC(=O)NC2=CC=C(C=C2)C3=CSC4=C3C(=NC=C4C5=CN(N=C5)C(C)C(=O)N(C)C)N", "CHEMBL2001547": "CCC1=NC=CN2C1=NC(=C2C3=NC(=NC=C3)NCC(C)(C)O)C4=C(C=C(C=C4)F)F", "CHEMBL2001646": "CC1=CC=CC=C1C2=C3C(=CC=C2)N(C(=C3NC4=CC=CC=C4)C(=O)O)CCCOC5=CC=CC6=CC=CC=C65", "CHEMBL2001751": "C1=CC=C2C(=C1)C(=CN2)CC(COC3=CN=CC(=C3)C4=CC5=C(C=C4)NC(=O)C5=CC6=CC=CO6)N", "CHEMBL2001920": "C1=CC2=C(C=C1Br)C(=C3C(=O)NC(=S)S3)C(=O)N2", "CHEMBL2001957": "CC(C)(CNC1=NC=CC(=N1)C2=C(N=C3N2C=CN=C3OCC(F)(F)F)C4=CC=C(C=C4)F)CO", "CHEMBL2002165": "CC(CN1C=C(C=N1)C2=CN=C(C3=C2SC=C3C4=CC=C(C=C4)NC(=O)NC5=CC(=CC=C5)F)N)O", "CHEMBL2002346": "C1=CC=C(C=C1)CNC2=NC=NC(=C2)C3=CNC4=C3C=CC=N4", "CHEMBL2002446": "CN1CCN(CC1)CC2=CC3=C(C=C2)C4=C(C3)C(=NN4)C5=CSC(=C5)C#CCOCC6CC6", "CHEMBL2002479": "C1C2=C(C=C(C=C2C3=CC=C(C=C3)NC4=NC5=C(O4)C=C(C=C5)Cl)OCCCN)C(=O)N1", "CHEMBL2002613": "COC1=CC(=CC(=C1)C(=O)NC2=NNC3=C2C=C(C=C3)C4=CN(N=N4)CC5=CC=CC=C5)OC", "CHEMBL2002649": "COC1=CC2=C(C=C1)NC(=O)C2=CC3=CN=CN3", "CHEMBL2002702": "CC1=CC(=C(N1)C=C2C3=CC=CC=C3NC2=O)C", "CHEMBL2002726": "CC1=C2C=C(C=CC2=NN1)C3=CC(=CN=C3)OCC(CC4=CC=CC=C4)N", "CHEMBL2002992": "CC(C1CCC(CC1)C(=O)NC2=C3C=CNC3=NC=C2)N", "CHEMBL2003229": "CN(C)C1=CC(=CC2=C1C(=NN2)N)C3=CC=NC=C3", "CHEMBL2003271": "C1=CC(=CC=C1C(=O)NC2=C(SC3=C2C(=C(C=C3)Cl)Cl)C(=O)N)Cl", "CHEMBL2003286": "COC1=C(C=CC(=C1)C=C2C(=O)NC(=O)S2)O", "CHEMBL2003341": "C1=CC(=CC=C1C2=CC=NC=C2)C(=O)NC(CO)C3=CC(=CC(=C3)Cl)Cl", "CHEMBL2003420": "C1=CC(=CN=C1)CNC(=O)NCCCCCCNC(=O)NCC2=CN=CC=C2", "CHEMBL2003456": "C1=CC=C(C=C1)C2=CC3=C(NC(=O)N3)N=C2", "CHEMBL2003482": "C1CC2=C(C1)NN=C2NC(=O)CC3=CC=C(C=C3)Cl", "CHEMBL2003638": "C1=CC=C(C=C1)CN2C=C(N=N2)C3=CC4=C(C=C3)NN=C4NC(=O)C5=CC(=CC=C5)F", "CHEMBL2003682": "C1=CN=CC=C1C2=CC(=O)N=C(N2)NCC3=CC(=CC(=C3)F)F", "CHEMBL2003817": "C1=CC2=C(C=CN=C2C=C1C(F)(F)F)NC(=O)NC3=NC=CN=C3", "CHEMBL2004290": "CC(C)(CN1C=C(C=N1)C2=CN=C(C3=C2SC=C3C4=CC=C(C=C4)NC(=O)NC5=CC=C(C=C5)OC)N)O", "CHEMBL2004311": "CC1=CC(=CC(=C1)NC(=O)NC2=CC(=C(C=C2)C3=C4CNC(=O)C4=CC=C3)C)C", "CHEMBL2004365": "CCOC(=O)C1=C(N2C(=C(C1C3=CC=CS3)C(=O)N)SC(=CC4=CC=CS4)C2=O)N", "CHEMBL2004419": "CC(C)CN1C2=C(C(=CC(=C2)C3=C(N=C4N3C=CS4)C5=CC=C(C=C5)F)F)N=C1N", "CHEMBL2004447": "CC(C)(C)C1=C2C(C(=C(OC2=NN1)N)C#N)C3=CC=CC=C3F", "CHEMBL2004544": "C1OC2=C(O1)C=C(C=C2)CNC3=C4C(=C(C=C3)S(=O)(=O)O)C=CC=C4O", "CHEMBL2004631": "C1CC1C2=C(N=NN2CC3=CC=CC=C3)C4=CC5=C(C=C4)NN=C5N", "CHEMBL2004716": "CCN(CC)CCNC(=O)C=CC1=CN=C(C2=C1SC=C2C3=CC=C(C=C3)NC(=O)NC4=CC=CC(=C4)C)N", "CHEMBL2004771": "C1C2=C(C=CC=C2C(=O)N1)C3=CC=C(C=C3)NC4=NC5=CC=CC=C5O4", "CHEMBL2004871": "C1=CC(=CC=C1C2=C(N(C=N2)CCCO)C3=CC=NC=C3)F", "CHEMBL2004872": "CC(C1=CC(=CC=C1)OC)NC(=O)C2=CC=C(C=C2)C3=NC=NC=C3", "CHEMBL2004892": "CS(=O)(=O)NC1=CC=C(C=C1)C2=CC3=C(C=C2)NN=C3N", "CHEMBL2004934": "CC(C1=CC(=CC=C1)OC)NC(=O)C2=CC(=C(C=C2)C3=CC=NC=C3)F", "CHEMBL2005186": "CC(C)NC(=O)COC1=CC=CC(=C1)C2=NC3=CC=CC=C3C(=N2)NC4=CC5=C(C=C4)NN=C5", "CHEMBL2005216": "CS(=O)(=O)NC1CCC(CC1)NC2=CC(=NC(=N2)C3=CNC4=C3C=CC=N4)Cl", "CHEMBL2005375": "CCC1C(=O)N(C2=CN=C(N=C2N1C3CCCC3)NC4=C(C=C(C=C4)C(=O)NC5CCCCC5)OC)C", "CHEMBL2005475": "C1CCC(CC1)CNC(=O)C2=CC3=C(NN=C3S2)C4=CC=CC=C4", "CHEMBL2005509": "CNC(=O)NC1CCC(CC1)NC2=NC(=CC(=N2)Cl)C3=CNC4=C3C=CC=N4", "CHEMBL2005528": "CCOC(=O)C1=CC2=C(C=C1)NC3=C2CCNC3=O", "CHEMBL2005631": "CC1=CC(=C(C=C1)F)NC(=O)NC2=CC=C(C=C2)C3=CSC4=C3C(=NC=C4C(=O)NC)N", "CHEMBL2005718": "CS(=O)(=O)NCCNC1=NC(=CC(=C1)C2=CNC3=C2C=CC=N3)Cl", "CHEMBL2005828": "CC1=CC=C(C=C1)NC(=O)NC2=CC=C(C=C2)C3=COC4=NC=NC(=C34)N", "CHEMBL2005886": "CC1=CC(=CC2=C1NC(=C3C(=CC=NC3=O)NCC(C4=CC(=CC=C4)Cl)O)N2)N5CCOCC5", "CHEMBL2005899": "CC(C(C)(C)C)NC1=C(C(=O)C1=O)N(C2=CC=NC=C2)C(=O)C", "CHEMBL2005936": "CCCC(=O)NC1=NNC2=C1C=C(C=C2)C3=C(N(N=N3)CC4=CC=CC=C4)C5=CC=CC=C5", "CHEMBL2006156": "CC(C)N(C(C)C)C(=O)NC1=CC2=C(C=C1)N=C(C(=N2)C3=CC=CO3)C4=CC=CO4", "CHEMBL2006188": "CC(C1=CC(=CC=C1)OC)NC(=O)C2=C(C=C(C=C2)C3=CC=NC=C3)NCCCN", "CHEMBL2006237": "CN1CCN(CC1)CCCNC2=CC=CC(=N2)C3=NC4=C(C=CC=C4N3)C(=O)N", "CHEMBL2006263": "CC1=NC2=C(C=C(C=C2)NS(=O)(=O)C3=CC=C(C=C3)N)N=C1C", "CHEMBL2006439": "C1CCC(CC1)NC2=NC(=CC(=N2)Cl)C3=CNC4=C3C=CC=N4", "CHEMBL2006450": "CCCCC(=O)NC1=NC(=CC(=C1)C2=CNC3=C2C=CC=N3)Cl", "CHEMBL2006456": "CC(C)CNC1CCC(CC1)NC2=NC(=CC(=N2)Cl)C3=CNC4=C3C=CC=N4", "CHEMBL2006715": "C1CC(=O)N(C1)C2=CC(=CC=C2)NC3=NC=CC(=N3)C4=C(N=C5N4C=CS5)C6=CC(=CC=C6)NC(=O)C7=C(C=CC=C7F)F", "CHEMBL2006778": "CC1=CC2=CC(=CC(=C2N1)F)C3=CSC4=C3C(=NC=C4C=CC(=O)NC)N", "CHEMBL2006785": "CC1=CC=C(C=C1)C(=O)NC2=C(SC3=C2C(=C(C=C3)Cl)Cl)C#N", "CHEMBL2007002": "COC1=C(C=CC(=C1)C2=CC3=C(C=C2)NN=C3C(=O)NC4=CC=CC=C4)O", "CHEMBL2007044": "CCN(CC)CC#CC1=CC2=C(CC3=C2NN=C3C4=CN=C(C=C4)C#N)C=C1", "CHEMBL2007064": "CC1=C(NC(=C1CCC(=O)O)C)C=C2C3=CC=CC=C3NC2=O", "CHEMBL2007296": "CCCOC1=CC=CC(=C1)C(C)NC(=O)C2=CC=C(C=C2)C3=CC=NC=C3", "CHEMBL2007574": "C1=CC2=C(NC=C2C3=CC(=NC(=N3)N)Cl)N=C1", "CHEMBL2007592": "C1CCC2=C(C1)C3=C4N=C(NN4C(=O)N=C3S2)C5=CC=CC=C5", "CHEMBL207400": "CN1C2=C(C(=O)C3=C(N2O)C=CC(=C3)Cl)C(=N1)C(F)(F)F", "CHEMBL210887": "C1=CC=C2C(=C1)N=C(N2CCCO)NC(=O)C3=CC(=CC=C3)[N+](=O)[O-]", "CHEMBL211378": "CC1=CC(=CC=C1)NC(=O)NC2=CC=C(C=C2)C3=NOC4=NC=NC(=C34)N", "CHEMBL213207": "C1CCC(CC1)CNC2=NC=CC(=N2)C3=CNC4=C3C=CC=N4", "CHEMBL213505": "C1=CC(=CC(=C1)NC(=O)NC2=CC=C(C=C2)C3=NOC4=NC=NC(=C34)N)C(F)(F)F", "CHEMBL2152252": "CNC(=O)C1=NC(=CN=C1N)C2=CC(=C(C=C2)Cl)S(=O)(=O)NC3=C(C(=CC=C3)F)F", "CHEMBL2152253": "CC1=C(C=CC=C1F)NS(=O)(=O)C2=C(C=CC(=C2)C3=CN=C(C(=N3)C(=O)NC)N)Cl", "CHEMBL220057": "CC1=CC(=CC=C1)NC(=O)NC2=CC=C(C=C2)C3=C4C(=CC=C3)NN=C4N", "CHEMBL220241": "CCN1C2=CC(=NC=C2N=C1C3=NON=C3N)OC4=CC=CC(=C4)NC(=O)C5=CC=C(C=C5)OCCN6CCOCC6", "CHEMBL225519": "C1CNC(=O)C2=C1NC(=C2)C3=CC=NC=C3", "CHEMBL226403": "C1CNC(=O)C2=C1NC(=C2)C3=CC(=NC=C3)C4=CC5=CC=CC=C5N=C4", "CHEMBL226471": "C1CNC(=O)C2=C1NC(=C2)C3=CC(=NC=C3)C4=CC=CC=C4F", "CHEMBL231209": "C1=CC(=CC(=C1)F)NC(=O)NC2=CC=C(C=C2)C3=CSC4=C3C(=NC=C4)N", "CHEMBL234085": "CC1CCN(CC1N(C)C2=NC=NC3=C2C=CN3)C(=O)CC#N", "CHEMBL246970": "C1CC(CCC1CN)CNC2=NC(=NC=C2[N+](=O)[O-])NCC3=CC=CC=C3Cl", "CHEMBL249282": "C1COCCN1CCOC2=CC3=C(CC4=C3NN=C4C5=CN=C(C=C5)C#N)C=C2", "CHEMBL253969": "C1CCN(C1)CCCCNC(=O)NC2=C(C(=NS2)OCC3=C(C=C(C=C3F)Br)F)C(=O)N", "CHEMBL256835": "COC1=NC=CC(=N1)C2=C(N=CN2C3CCC(CC3)O)C4=CC=C(C=C4)F", "CHEMBL259922": "CC1=C(C=C(C=C1)C(=O)NC2=NOC=C2)NC3=NC=NC4=C3C=NN4C5=CC=CC=C5", "CHEMBL260135": "C1=CC=C(C=C1)C2=C(N=NC3=NNC(=C23)N)C4=CC=CC=C4", "CHEMBL262433": "CC1=CC(=C(C=C1)F)NC(=O)NC2=CC=C(C=C2)C3=NSC4=NC=NC(=C34)N", "CHEMBL271381": "COC1=C2C(=C(C=C1)C3=CC=C(C=C3)NC(=O)NC4=CC(=CC=C4)Br)C(=NO2)N", "CHEMBL272453": "COC1=C(C=C(C=C1)NC(=O)NC2=CC=C(C=C2)C3=C4C(=CC=C3)ON=C4N)Cl", "CHEMBL274064": "C1CNCCC1N2C=NC(=C2C3=NC(=NC=C3)N)C4=CC=C(C=C4)F", "CHEMBL296586": "C1C2=C(C3=CC=CC=C3NC1=O)NC4=C2C=C(C=C4)Br", "CHEMBL306380": "CC1=CC=C(C=C1)C2=NN(C3=C2C(=NC=N3)N)C(C)(C)C", "CHEMBL316264": "C1=CC(=CC=C1C2=C(NC(=N2)C3=CC=C(C=C3)F)C4=CC=NC=C4)F", "CHEMBL340384": "C1=CC2=C(C=C1C3=CC=NC=C3)N(C=C(C2=O)C(=O)N)C4=C(C=C(C=C4)O)Cl", "CHEMBL340921": "CC1=C(C=CC(=C1)O)N2C=C(C(=O)C3=C2C=C(C=C3)C4=CC=NC=C4)C(=O)N", "CHEMBL363648": "CCC1=NC(=C(S1)C2=CC(=NC=C2)NC(=O)C3=CC=CC=C3)C4=CC(=CC=C4)C", "CHEMBL371206": "CC1=CC(=CC(=C1)NC(=O)NC2=CC=C(C=C2)C3=C(SC4=NC=NC(=C34)N)C)C", "CHEMBL377408": "CCOC1=C(C(=CC(=N1)C(=O)NCC2=CC=CC=C2S(=O)(=O)N)N)C#N", "CHEMBL385478": "C1CCC(CC1)NC2=NC=CC(=N2)C3=CNC4=C3C=CC=N4", "CHEMBL387971": "CN1CCN(CC1)CC2=CC3=C(C=C2)C4=C(C3=O)C(=NN4)C5=CSC(=C5)C#CCOCCOC", "CHEMBL392642": "CSC1=CC=CC=C1CNC2=NC=C(C(=N2)NCC3CCC(CC3)CN)[N+](=O)[O-]", "CHEMBL394619": "CC1=CC(=CC=C1)NC(=O)NC2=CC=C(C=C2)C3=CSC4=C3C(=NC=C4)N", "CHEMBL394790": "C1=CC(=CC(=C1)Cl)NC(=O)NC2=CC=C(C=C2)C3=CSC4=C3C(=NC=C4)N", "CHEMBL398951": "C1COCCN1CCCCOC2=CC3=C(CC4=C3NN=C4C5=CN=C(C=C5)C#N)C=C2", "CHEMBL402548": "CN1CCN(CC1)C2=CC=C(C=C2)C(=O)NC3=NNC4=C3CN(C4)C(=O)C(C5=CC=CC=C5)OC", "CHEMBL402846": "CC1=CC(=C(C=C1)F)NC(=O)NC2=CC=C(C=C2)C3=CN=CC4=C3C(=NN4C)N", "CHEMBL404367": "CC1=CC(=CC=C1)NC(=O)NC2=CC=C(C=C2)C3=CN=CC4=C3C(=NN4C)N", "CHEMBL411903": "C1CNC2=C(C(=NC=N2)N)N=C1C3=CC=C(C=C3)NC(=O)NC4=C(C=CC(=C4)C(F)(F)F)F", "CHEMBL412142": "CC1=CN=C(N1)C2=CN=C(N=C2C3=C(C=C(C=C3)Cl)Cl)NCCNC4=NC=C(C=C4)C#N", "CHEMBL41783": "CN(C)CCCC(=O)NC1=NNC2=NN=C(C=C21)C3=C(C(=CC=C3)F)F", "CHEMBL422897": "CN1CCC(C(C1)O)C2=C(C=C(C3=C2OC(=CC3=O)C4=CC=CC=C4Cl)O)O", "CHEMBL424872": "CCOC1=C(C(=CC(=N1)C(=O)NCC2=CC=C(C=C2)S(=O)(=O)C)N)C#N", "CHEMBL458997": "CNC(=O)C1=CC=CC=C1NC2=NC(=NC=C2Cl)NC3=C(C=C(C=C3)N4CCOCC4)OC", "CHEMBL461876": "CN(C)CC(=O)N1CCC2=CC(=C(C=C21)NC3=NC4=C(C=CN4)C(=N3)NC5=C(C(=CC=C5)F)C(=O)N)OC", "CHEMBL468280": "CCN1C2=CC(=C(C=C2C(=O)C3=C1NOC3=O)F)Cl", "CHEMBL474432": "COC1=C(C=C2C(=C1)N=CN2C3=CC(=C(S3)C(=O)O)OCC4=CC=CC=C4C(F)(F)F)OC", "CHEMBL481491": "C1=CC=C(C(=C1)COC2=C(SC(=C2)N3C=NC4=CC=CC=C43)C(=O)N)C(F)(F)F", "CHEMBL482767": "C1=CC(=CC(=C1)Cl)NC(=O)NC2=NC=C(S2)CCNC3=NC=NC4=C3SC=C4", "CHEMBL482967": "CC1=C(SC(=N1)N)C2=NC(=NC=C2)NC3=CC=C(C=C3)N4CCOCC4", "CHEMBL483158": "COC1=C(C(=CC=C1)F)C2=NCC3=CN=C(N=C3C4=C2C=C(C=C4)Cl)NC5=CC(=C(C=C5)C(=O)O)OC", "CHEMBL484390": "CCCCN1C2=C(C=C(C=C2)N(C)C(=O)C3CCCCC3)N=C1NC(=O)C4=CC=C(C=C4)C#N", "CHEMBL491758": "C1=CC=C(C=C1)NC2=NC(=NC=C2F)NC3=CC=CC=C3", "CHEMBL497151": "C1=CC(=CC=C1OC2=CN=CC3=C2C=C(S3)C4=NC(=O)ON4)I", "CHEMBL504950": "CC1=CC(=NC2=C1C3=C(S2)C(=NC=N3)N)C", "CHEMBL508928": "CC1=CC(=CC=C1)NC(=O)NC2=CC=C(C=C2)C3=C(N4C(=C(C=N4)C5=CN(N=C5)C)N=C3)N", "CHEMBL50894": "C1C2=C(C3=CC=CC=C3NC1=O)NC4=C2C=C(C=C4)[N+](=O)[O-]", "CHEMBL514499": "COC1=C(C=C2C(=C1)N=CN2C3=CC(=C(S3)C(=O)N)OCC4=CC=CC=C4C(F)(F)F)OC", "CHEMBL519697": "CN1C2=C(C=C(C=C2)N(C)C(=O)C3CCCCC3)N=C1NC(=O)C4=CC=C(C=C4)C#N", "CHEMBL524266": "C1C(C2=C(C=C(N2)C3=NC(=NC=C3)N)C(=O)N1)CCF", "CHEMBL526133": "C1=CC=C(C=C1)C2=CC(=NC(=O)N2)C3=CC4=C(C=C3)NN=C4", "CHEMBL539474": "C1CC(=O)N(C1)CC2=CC3=C(C=C2)N4C=CC=C4C(=O)N3", "CHEMBL560813": "C1=CC2=C(C=CC(=C2)NC(=O)NC3=NC=C(N=C3)C#N)C=C1C(=O)O", "CHEMBL564829": "CC1(CC2=CN=C(N=C2C3=C1C(=NN3C)C(=O)NC)NC4=CC=C(C=C4)N5CCN(CC5)C)C", "CHEMBL565612": "CN1CCN(CC1)C2=NC3=CC=CC=C3C(=N2)C4=C(C(=O)NC4=O)C5=CNC6=CC=CC=C65", "CHEMBL583144": "C1=CC(=C2C(=C1Cl)C3=C(S2)C(=O)N=CN3)Cl", "CHEMBL592030": "C1=CC=C2C(=C1)C=C(S2)C3=C4C(=CC(=C3)C5=CN(C6=CN=C(N=C65)N)CCCN)C=NN4", "CHEMBL604712": "CC1(C2=C(CN1C(=O)C(C)(C)C)C(=NN2)NC(=O)C3=CC(=CC(=C3)F)F)C", "CHEMBL7064": "C1=CC=C2C(=C1)C3=NNC4=CC=CC(=C43)C2=O", "CHEMBL95692": "COC1=NC=CC(=N1)C2=C(N=CN2C3CCNCC3)C4=CC=C(C=C4)F", "CHEMBL1081312": "C1CCC(C1)N2C3=C(C(=N2)C4=CN=C5C(=C4)C=CN5)C(=NC=N3)N", "CHEMBL1230790": "CC(C)N1C2=C(C(=N1)C3=CC(=CC=C3)O)C(=NC=N2)N", "CHEMBL1233881": "COC1=C(C=C(C=C1)C2=NN(C3=C2C(=NC=N3)N)C4CCC4)OC", "CHEMBL1233882": "CC(C)N1C2=C(C(=N1)C3=CC4=C(C=C3)N=CC=C4)C(=NC=N2)N", "CHEMBL1234815": "CN1C2=C(C(=N1)C3=CC4=CC=CC=C4C=C3)C(=NC=N2)N", "CHEMBL1240544": "CC(CN)N1C2=C(C(=N1)C3=CC(=C(C=C3)Cl)O)C(=NC=N2)N", "CHEMBL1240545": 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"C1=CC=C(C=C1)C2=C(OC=N2)CN3C4=C(C(=N3)C5=CC(=C(C=C5)F)O)C(=NC=N4)N", "CHEMBL1241483": "CC(C)N1C2=C(C(=N1)C3=CC(=C(C=C3)F)OC)C(=NC=N2)N", "CHEMBL1241484": "CC(C)N1C2=C(C(=N1)C3=CC(=C(C=C3)Cl)O)C(=NC=N2)N", "CHEMBL1241485": "CC(C)N1C2=C(C(=N1)C3=CC(=C(C=C3)N)OC)C(=NC=N2)N", "CHEMBL1241486": "CC(C)N1C2=C(C(=N1)C3=CC(=C(C=C3)NC(C)CO)OC)C(=NC=N2)N", "CHEMBL1241487": "C1CCC(C1)N2C3=C(C(=N2)C4=CC(=C(C=C4)N)O)C(=NC=N3)N", "CHEMBL1241490": "CC(C)N1C2=C(C(=N1)C3=CC4=C(C=C3)OC=C4)C(=NC=N2)N", "CHEMBL1241491": "C1CCC(C1)N2C3=C(C(=N2)C4=CC5=C(C=C4)OC=C5)C(=NC=N3)N", "CHEMBL1241492": "CC(C)N1C2=C(C(=N1)C3=CC4=NON=C4C=C3)C(=NC=N2)N", "CHEMBL1241578": "CC(C)N1C2=C(C(=N1)C3=CC(=C(C=C3)Br)O)C(=NC=N2)N", "CHEMBL1241579": "CC(CN)N1C2=C(C(=N1)C3=CC(=C(C=C3)Cl)O)C(=NC=N2)N", "CHEMBL1241580": "C1CC(C1)N2C3=C(C(=N2)C4=CC(=C(C=C4)Cl)O)C(=NC=N3)N", "CHEMBL1241581": "COC1=C(C=CC(=C1)C2=NN(C3=C2C(=NC=N3)N)C4CCCC4)N", "CHEMBL1241582": "CC(C)N1C2=C(C(=N1)C3=CC(=CC=C3)CO)C(=NC=N2)N", "CHEMBL1241583": 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"CHEMBL1241862": "CC(C)N1C2=C(C(=N1)C3=CC(=C(C=C3)C(=O)N)Cl)C(=NC=N2)N", "CHEMBL1241863": "CC(C)N1C2=C(C(=N1)C3=CC4=C(C=C3)NC(=O)C=C4)C(=NC=N2)N", "CHEMBL1241864": "C1CCC(C1)N2C3=C(C(=N2)C4=CC5=C(C=C4)NC(=O)C=C5)C(=NC=N3)N", "CHEMBL1241943": "C1CC(CNC1)CCN2C3=C(C(=N2)C4=CC(=C(C=C4)Cl)O)C(=NC=N3)N", "CHEMBL1241944": "CC(C)N1C2=C(C(=N1)C3=CC(=C(C=C3)C#N)O)C(=NC=N2)N", "CHEMBL1241945": "CC(C)N1C2=C(C(=C3C=CC(=O)C(=C3)F)N1)C(=NC=N2)N", "CHEMBL1241946": "CC(C)N1C2=C(C(=N1)C3=CC(=CC=C3)C(=O)C)C(=NC=N2)N", "CHEMBL1241947": "CC1=C(SC(=C1)C2=NN(C3=C2C(=NC=N3)N)C(C)C)C=O", "CHEMBL1241948": "CC(C)N1C2=C(C(=N1)C3=CC(=CC=C3)NS(=O)(=O)C)C(=NC=N2)N", "CHEMBL1241949": "CC(C)N1C2=C(C(=N1)C3=CC4=C(C=C3)N=C(C=C4)N)C(=NC=N2)N", "CHEMBL1241950": "CC(C)N1C2=C(C(=N1)C3=CC4=C(C=C3)N=C(C=C4)NN)C(=NC=N2)N", "CHEMBL1242024": "CC1=CC(=O)C=CC1=C2C3=C(N=CN=C3N)N(N2)C(C)C", "CHEMBL1242025": "CC1=C(C=C(C=C1)C2=C3C(=NC=NC3=NN2)N)OCC4=CC=CC=C4", "CHEMBL1242026": "CC1=C(C=C(C=C1)C2=NN(C3=C2C(=NC=N3)N)C(C)C)O", "CHEMBL1242028": "CC(C)N1C2=C(C(=C3C=C(C(=O)C=C3F)F)N1)C(=NC=N2)N", "CHEMBL1242029": "CC(C)N1C2=C(C(=N1)C3=CC(=CC=C3)OC)C(=NC=N2)N", "CHEMBL1242030": "CC(C)N1C2=C(C(=N1)C3=CC=C(C=C3)NS(=O)(=O)C)C(=NC=N2)N", "CHEMBL1242031": "CC(C)N1C2=C(C(=N1)C3=CC(=CC=C3)S(=O)(=O)N)C(=NC=N2)N", "CHEMBL1242032": "CC(C)N1C2=C(C(=N1)C3=CC=C(C=C3)S(=O)(=O)N)C(=NC=N2)N", "CHEMBL1242033": "CC(C)N1C2=C(C(=N1)C3=CC4=C(C=CN=C4C=C3)NC(=O)OC(C)(C)C)C(=NC=N2)N", "CHEMBL1242034": "CC(C)N1C2=C(C(=N1)C3=CC4=C(C=CN=C4C=C3)N)C(=NC=N2)N", "CHEMBL1242109": "CCC(C)N1C2=C(C(=N1)C3=CC(=C(C=C3)C)O)C(=NC=N2)N", "CHEMBL1242110": "CC(C)N1C2=C(C(=N1)C3=C(C(=CC=C3)O)F)C(=NC=N2)N", "CHEMBL1242111": "C1CCC(C1)N2C3=C(C(=N2)C4=C(C(=CC=C4)O)F)C(=NC=N3)N", "CHEMBL1242112": "CC(C)N1C2=C(C(=C3C=CC(=O)C(=C3)OC)N1)C(=NC=N2)N", "CHEMBL1242113": "CCN1C2=C(C(=N1)C3=CC(=C(C=C3)OC)O)C(=NC=N2)N", "CHEMBL1242114": "CC(C)N1C2=C(C(=N1)C3=CC(=C(C=C3)OC)O)C(=NC=N2)N", "CHEMBL1242115": "CC(C)N1C2=C(C(=N1)C3=CC(=CC=C3)C(=O)NC4=NCCS4)C(=NC=N2)N", "CHEMBL1242117": "CN1C2=C(C(=N1)C3=CC4=C(C=C3)OC=CC4=O)C(=NC=N2)N", "CHEMBL1242118": "CC(C)N1C2=C(C(=N1)C3=CC4=C(C=C3)OC=CC4=O)C(=NC=N2)N", "CHEMBL1242119": "C1CCC(C1)N2C3=C(C(=N2)C4=CC5=C(C=C4)OC=CC5=O)C(=NC=N3)N", "CHEMBL1242198": "CC(C)N1C2=C(C(=N1)C3=CC(=CC(=C3)F)O)C(=NC=N2)N", "CHEMBL1242199": "C1CCC(C1)N2C3=C(C(=N2)C4=CC(=CC(=C4)F)O)C(=NC=N3)N", "CHEMBL1242200": "CC(C)N1C2=C(C(=N1)C3=CC(=CC(=C3)Br)OC)C(=NC=N2)N", "CHEMBL1242201": "COC1=C(C=C(C=C1)C2=NN(C3=C2C(=NC=N3)N)C4CCCC4)O", "CHEMBL1242202": "CC1CCC(C1)N2C3=C(C(=N2)C4=CC(=C(C=C4)OC)O)C(=NC=N3)N", "CHEMBL1242203": "COC1=C(C=C(C=C1)C2=NN(C3=C2C(=NC=N3)N)C4CNC4)O", "CHEMBL1242207": "CC(C)N1C2=C(C(=N1)C3=CC4=C(C=C3)C=NC=C4)C(=NC=N2)N", "CHEMBL1242208": "CC(C)N1C2=C(C(=N1)C3=CC4=C(C=C3)C=CN=C4)C(=NC=N2)N", "CHEMBL1242209": "CC1=NC2=C(C=C1)C=CC(=C2)C3=NN(C4=C3C(=NC=N4)N)C(C)C", "CHEMBL1242285": "CC(C)N1C2=C(C(=N1)C3=CC(=CC(=C3)Br)O)C(=NC=N2)N", "CHEMBL1242286": "CC(C)N1C2=C(C(=N1)C3=CC(=C(C=C3)Br)OCOC)C(=NC=N2)N", "CHEMBL1242287": 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"C1CCC(C1)N2C3=C(C(=N2)C4=CC5=C(C=C4)C=NN5)C(=NC=N3)N", "CHEMBL1242573": "CC(C)N1C2=C(C(=N1)C3=CC4=C(C=NN4)C(=C3)F)C(=NC=N2)N", "CHEMBL1242574": "CC(C)N1C2=C(C(=N1)C3=CC4=C(C=C3)C=CN4)C(=NC=N2)N", "CHEMBL1242656": "CC1CCC(C1)N2C3=C(C(=N2)C4=CC(=C(C=C4)F)O)C(=NC=N3)N", "CHEMBL1242657": "C1CNCC1N2C3=C(C(=N2)C4=CC(=C(C=C4)F)O)C(=NC=N3)N", "CHEMBL1242658": "C1CNCC1N2C3=C(C(=N2)C4=CC(=C(C=C4)F)O)C(=NC=N3)N", "CHEMBL1242659": "CCOC1=C(C=C(C=C1)C2=NN(C3=C2C(=NC=N3)N)C4CCCCC4)OC", "CHEMBL1242660": "CC(C)N1C2=C(C(=N1)C3=CC(=C(C(=C3)OC)OC)OC)C(=NC=N2)N", "CHEMBL1242661": "CCOC1=CC2=C(C=C1)C=C(C=C2)C3=NN(C4=C3C(=NC=N4)N)C", "CHEMBL1242662": "CC(C)N1C2=C(C(=C3C=CC4=CC(=O)C=CC4=C3)N1)C(=NC=N2)N", "CHEMBL1242663": "CC(C)N1C2=C(C(=N1)C3=CC4=CC=CC=C4N=C3Cl)C(=NC=N2)N", "CHEMBL1242664": "C1CCC(C1)N2C3=C(C(=N2)C4=CC5=C(C=C4)C=CN5)C(=NC=N3)N", "CHEMBL1242665": "CC(C)N1C2=C(C(=N1)C3=CC4=NC=CN4C=C3)C(=NC=N2)N", "CHEMBL1242666": "CC(C)N1C2=C(C(=N1)C3=CC4=C(C=C3)C(=CN4)C=O)C(=NC=N2)N", "CHEMBL1242748": "C1COCC1N2C3=C(C(=N2)C4=CC(=C(C=C4)F)O)C(=NC=N3)N", "CHEMBL1242749": "C1COCC1N2C3=C(C(=N2)C4=CC(=C(C=C4)F)O)C(=NC=N3)N", "CHEMBL1242750": "C1CCCC(CC1)N2C3=C(C(=N2)C4=CC(=C(C=C4)F)O)C(=NC=N3)N", "CHEMBL1242751": "CC(C)N1C2=C(C(=N1)C3=C(C(=CC=C3)OC)OC)C(=NC=N2)N", "CHEMBL1242752": "CCOC1=C(C=CC(=C1)C2=NN(C3=C2C(=NC=N3)N)C(C)C)OC", "CHEMBL1242753": "CCOC1=C(C=CC(=C1)C2=NN(C3=C2C(=NC=N3)N)CCO)OC", "CHEMBL1242754": "CC(C)N1C2=C(C(=N1)C3=CC4=CC=CC=C4N=C3)C(=NC=N2)N", "CHEMBL1242755": "C1CCC(C1)N2C3=C(C(=N2)C4=CC5=CC=CC=C5N=C4)C(=NC=N3)N", "CHEMBL1242756": "CN1C2=C(C(=N1)C3=CC4=C(C=C3)N=CC=C4)C(=NC=N2)N", "CHEMBL1242757": "CC(C)N1C2=C(C(=N1)C3=C4C=CNC4=CC=C3)C(=NC=N2)N", "CHEMBL1242758": "C1CCC(C1)N2C3=C(C(=N2)C4=C5C=CNC5=CC=C4)C(=NC=N3)N", "CHEMBL1242844": "C1CNCCC1CN2C3=C(C(=N2)C4=CC(=C(C=C4)F)O)C(=NC=N3)N", "CHEMBL1242845": "CC1=NN(N=C1CN2C3=C(C(=N2)C4=CC(=C(C=C4)F)O)C(=NC=N3)N)C5=CC=CC=C5", "CHEMBL1242846": "CC(C)N1C2=C(C(=N1)C3=CN=C(N=C3OC)OC)C(=NC=N2)N", "CHEMBL1242847": "CC(C)N1C2=C(C(=N1)C3=CC=C(C=C3)OC)C(=NC=N2)N", "CHEMBL1242848": "CC(C)N1C2=C(C(=N1)C3=CC(=C(C=C3)N)O)C(=NC=N2)N", "CHEMBL1242852": "CC(C)N1C2=C(C(=N1)C3=CC4=C(C=C3)N(C=C4)C(=O)OC(C)(C)C)C(=NC=N2)N", "CHEMBL1242853": "CC(C)(C)OC(=O)N1C=CC2=C1C=CC(=C2)C3=NN(C4=C3C(=NC=N4)N)C5CCCC5", "CHEMBL1834657": "CCN1CCN(CC1)C2=CC=C(C=C2)NC3=CC(=NC=N3)N(C)C(=O)NC4=C(C(=CC(=C4Cl)OC)OC)Cl", "CHEMBL1879463": "CC(C)(C#N)C1=CC=C(C=C1)N2C3=C4C=C(C=CC4=NC=C3N(C2=O)C)C5=CC6=CC=CC=C6N=C5", "CHEMBL1945559": "CN1C2=C(C=CC(=C2Cl)Cl)C3=C1C(=O)NC4(C3C#N)CCNCC4", "CHEMBL1986603": "CC1=CC(=NO1)NC(=O)CCNC(=O)NC2=NC(=C(S2)C3=CC=C(C=C3)N4C=CC=N4)C", "CHEMBL2205766": "CC(C)(C)NS(=O)(=O)C1=CN=CC(=C1)C2=CC3=NC(=NN3C=C2)N", "CHEMBL410643": "CC(=O)OC1CC2(C(CCC2O)C3=C1C4(C(OC(=O)C(=CN(C)CCCN(C)C)C4=C(C3=O)O)COC)C)C", "CHEMBL98350": "C1COCCN1C2=CC(=O)C3=C(O2)C(=CC=C3)C4=CC=CC=C4", "CHEMBL1461728": "C1=CC(=CC(=C1)F)C(=O)NC2=CC3=C(C=C2)NN=C3", "CHEMBL1727312": "C1=CC=C2C(=C1)C(=O)NC3=CC=CC=C3N2", "CHEMBL1966035": "CC(C1=CC=CC=C1)NC2=C(C(=O)C2=O)NC3=CC=NC=C3", "CHEMBL1966087": "C1CNCC1OC2=CN=CC(=C2)C=CC3=CC=NC=C3", "CHEMBL1968926": "C1=CC=C(C=C1)CSC2=NNC(=N2)C3=CC=NC=C3", "CHEMBL1969755": "C1=CC=C(C=C1)CC(CO)NC(=O)C2=C(C=C(C=C2)C3=CC=NC=C3)F", "CHEMBL1970735": "CCCOC1=C(C(=CC(=N1)NC(=O)C)N)C#N", "CHEMBL1970806": "C1CCC2=C(C1)C3=C4N=C(NN4C(=O)N=C3S2)C5=CN=CC=C5", "CHEMBL1971430": "CC1=CC=CC(=C1)C2=C(N=C(N(C2=O)C)NCC(CC3=CC=CC=C3)N)C4=CC=NC=C4", "CHEMBL1971694": "CCCCNC1=NS(=O)N=C1NC2=CC=C(C=C2)F", "CHEMBL1972258": "C1=CN=CC=C1C=CC2=CC(=CN=C2)OCCCN", "CHEMBL1972276": "CCN(CC)CCCNC1=CC=CC(=N1)C2=NC3=C(C=CC=C3N2)C(=O)N", "CHEMBL1972489": "C1=CC(=CC=C1C(=O)NC2=CC3=C(C=C2)C=NN3)Cl", "CHEMBL1974157": "C1=CC=C(C=C1)CNC(=O)C(=CC2=CC(=C(C=C2)O)O)C#N", "CHEMBL1974803": "C1=CC(=C(C=C1Cl)C2=C(C(=O)NC3=CC(=CC(=C32)Cl)Cl)O)O", "CHEMBL1977374": "CC(C)C1=NN=C2N1N=C(C=C2)C3=C(N=C4N3CCC4)C5=C(C=C(C=C5)F)F", "CHEMBL1979318": "CC1=C2C(C(=C(OC2=NN1)N)C#N)C3=CC=CC=C3I", "CHEMBL1980995": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)CNC6=O)NC)OC", "CHEMBL1982992": "C1=CC(=CC(=C1)O)NC2=C3C(=CSC3=NC=N2)Cl", "CHEMBL1983449": "CC1=C(C=C(C=C1)CNC2=C(C(=O)C2=O)NC3=CC=NC=C3)C", "CHEMBL1984039": "CC1=C(C(=NN1C)C)C2=CC=CC3=C2NC(=C3CCCOC4=CC=CC5=CC=CC=C54)C(=O)O", "CHEMBL1987533": "C1=CC=C(C(=C1)CC(=O)NC2=CC3=C(C=C2)C=NN3)Cl", "CHEMBL1988995": "CC(C)C1=NN=C2N1N=C(C=C2)C3=C(N=C4N3C=CO4)C5=C(C=C(C=C5)F)F", "CHEMBL1989265": "CC1CSC2=C(C(=O)C3=CC(=C(C=C3N12)N4CCC(C4)N)F)C(=O)O", "CHEMBL1989474": "CN1C=C(C(=N1)C2=CC=C(C=C2)F)C3=NC=NC=C3", "CHEMBL1989518": "C1=CN=CC=C1C=CC2=CC(=CN=C2)OCCN", "CHEMBL1990415": "C1=CC=C2C(=C1)C=C3C(=N2)NN=C3NC(=O)C4=CC=NC=C4", "CHEMBL1991356": "COC1=CC=CC(=C1)C2=CN3C4=CC=CC=C4NC(=O)C3=C2", "CHEMBL1991434": "COC1=C(C=C(C=C1)C=C2C(=NOC2=O)C3=CC=C(C=C3)Br)OC", "CHEMBL1992555": "C1=CC=C2C(=C1)NC(=N2)SC3=CC=C(O3)C=NNC(=O)C4=CC(=CC=C4)[N+](=O)[O-]", "CHEMBL1994864": "CC1=CC=C(C=C1)CNC2=C(C(=O)C2=O)NC3=CC=NC=C3", "CHEMBL1995172": "C1C2=C(C=C(C=C2)Br)C3=C1C=NN3", "CHEMBL1995736": "CCOC(=O)C1=C2C(=CC=C1)NC(=N2)C3=CC=C(C=C3)N4CCC(C4)N", "CHEMBL1996923": "C1=C(C(=CC2=NNN=C21)Cl)Cl", "CHEMBL1997025": "C1CC(CNC1)C2=CC(=C(C=C2)C3=NC4=C(C=CC=C4N3)C(=O)N)F", "CHEMBL1997349": "CC1=C(C2=NC3=CC=CC=C3N2C(=O)C1=CC4=C(NN(C4=O)C5=CC(=C(C=C5)Cl)Cl)C)C#N", "CHEMBL1997872": "C1COCCN1C(=O)C2=CC=CC(=C2)C3=CN=C4C(=C3)C=CN4", "CHEMBL1998414": "CC1=C2C=C(SC2=NN1)C(=O)NCCC3=CC=C(C=C3)Cl", "CHEMBL1998829": "C1=CC=C(C=C1)C2=CNC3=NC=C(C=C23)NC(=O)C4=CC=C(C=C4)Cl", "CHEMBL1999496": "CC1=CC=CC(=C1)C2(CC2C(=O)NC3=CC=NC=C3)C4=CC(=CC=C4)C", "CHEMBL2002373": "C1=CC=C(C=C1)C2=C(N(C=N2)CCCO)C3=CC=NC=C3", "CHEMBL2004615": "CSC1=NN(C(=C1C(=O)N)N)C2=CC=CC=N2", "CHEMBL2004692": "C1=CC=C(C=C1)C2=C(N=NN2C3=NON=C3N)C(=O)NN=CC4=CC=CS4", "CHEMBL2005112": "CC1=C(C2=NC3=CC=CC=C3N2C(=O)C1=CC4=C(NN(C4=O)C5=CC(=CC=C5)Br)C)C#N", "CHEMBL2006276": "COC1=CC=CC2=C1NC3=C(C=CC(=C3)NC4=CC=NC=C4)C(=O)N2", "CHEMBL2006493": "C1CC2=C(C(=O)C1)C(=O)C3=C(O2)C=C(C=C3)C(F)(F)F", "CHEMBL2006580": "C1=CC(=CC=C1NC2=C3C(=CSC3=NC=N2)Cl)O", "CHEMBL2006836": "CC1=C(C2=NC3=CC=CC=C3N2C(=O)C1=CC4=C(NN(C4=O)C5=CC=C(C=C5)C(=O)O)C)C#N", "CHEMBL2007372": "CC(C)(CNC1=NC=CC(=N1)C2=C(N=C3N2C=CN=C3NC)C4=CC=C(C=C4)F)CO", "CHEMBL379835": "CC1=NN(C2=C1C(=O)C3=C(N2O)C=CC(=C3)Cl)C4=CC=CC=C4", "CHEMBL443962": "COC1=CC=C(C=C1)C2=CN3C(=C(C=N3)Br)N=C2", "CHEMBL462120": "C1=CC=C(C=C1)C2=C(C(=O)NC3=C2C=C(C=C3)Cl)N", "CHEMBL52387": "CCC(CO)NC1=NC2=C(C(=N1)NCC3=CC=CC=C3)N=CN2C(C)C", "CHEMBL535331": "C1=CC=C2C(=C1)C(=CNNC3=NC4=CC=CC=C4N3)C=N2", "CHEMBL597754": "CNC(=O)C1=NN(C2=C1CCC3=CN=C(N=C32)NC4CCN(CC4)C(=O)C5CCN(CC5)S(=O)(=O)C)C", "CHEMBL599224": "CC(=O)N1CCC(CC1)NC2=NC=C3CCC4=C(C3=N2)N(N=C4C(=O)N)C", "CHEMBL599428": "CN1C2=C(CCC3=CN=C(N=C32)NC4CCN(CC4)C(=O)C5=CC=CC=C5)C(=N1)C(=O)N", "CHEMBL1082152": "CN1C=C(C2=C1C=CC(=C2)F)C3=C(C(=O)NC3=O)C4=CC(=CC=C4)NCC(CO)O", "CHEMBL127898": "CN1C=NC=C1C(C2=CC=C(C=C2)C#N)OCC3=C(C=C(C(=O)N3C)C#N)C4=CC=C(C=C4)OC(F)(F)F", "CHEMBL1288582": "COC1=CC2=NC(=C3C4=C(C=CC=N4)NN3)C=C2C=C1", "CHEMBL1381197": "C1=CC=C(C=C1)C2=NN=C3N2N=C(C=C3)NCC4=CC=C(C=C4)Cl", "CHEMBL1419458": "C1=CC=C(C=C1)C2=C(N=NN2C3=NON=C3N)C(=O)NN=CC4=CC=NC=C4", "CHEMBL143703": "C1=CC=C(C=C1)NC(=O)NC2=CC=CC=N2", "CHEMBL1472492": "CCCCCCCCCCCCCCCCN1C=C[N+](=C1C)CC2=CC=CC=C2", "CHEMBL1682345": "C1=CC=C(C=C1)CN2C=C(N=N2)C3=CC4=C(C=C3)NN=C4", "CHEMBL1682357": "C1=CC=C(C=C1)CC2=NOC(=C2)C3=CC4=C(C=C3)NN=C4", "CHEMBL1957190": "CC(C)N1C2=C(C(=O)CCC2)C3=C1C4=CC=CC=C4C3=O", "CHEMBL1964307": "CC1=CC(=CC=C1)NC(=O)CC2=CC=C(C=C2)C3=C4C(=CC=C3)NN=C4N", "CHEMBL1964399": "CC(C(C)(C)C)NC1=C(C(=O)C1=O)NC2=NC(=NC=C2)NC3=CC(=C(C=C3)OC)OC", "CHEMBL1965495": "CC1=C2C(=C(C=NC2=NN1)C#N)C3=CC=CC=C3", "CHEMBL1965910": "C1CCN(C1)C2CCC(CC2)N3C=C(C4=C3N=CN=C4N)C5=CC(=CC=C5)OCC6=CC=CC=C6", "CHEMBL1966425": "CN(C)CCCOC1=CC2=C(CNC2=O)C(=C1)C3=CC=C(C=C3)NC4=NC5=CC=CC=C5O4", "CHEMBL1966524": "C1=CC=C2C(=C1)C(=CN2)CC(COC3=CN=CC(=C3)C4=CC5=C(S4)C=NC=C5)N", "CHEMBL1967538": "CC1=NN(C2=C1C3=C(S2)C(=O)N=CN3)C", "CHEMBL1968070": "C1=CC(=C2C(=C1)NC(=O)C3=CC(=NN=C3N2)Cl)C(=O)N", "CHEMBL1968245": "C1=CC=C2C(=C1)C(=CN2)CC(COC3=C(N=CC(=C3)C=CC4=CC=NC=C4)Cl)N", "CHEMBL1968850": "C1=CC=C2C(=C1)NC3=NN=C(C=C3C(=O)N2)Cl", "CHEMBL1969102": "CC1=CC(=CC=C1)NC(=O)NC2=CC=C(C=C2)C3=CSC4=C3C(=NC=C4C5=CNN=C5)N", "CHEMBL1969156": "C1=CC=C(C=C1)C2=NC=C3N2C(=NC=C3)N", "CHEMBL1969264": "CC(C)(C)NC(=O)C1=CC2=C(C=C1)N=C3C(=N2)C4=CC=CC=C4N3", "CHEMBL1969588": "C1=CC=C(C=C1)CNC2=NC(=CC(=C2)C3=CNC4=C3C=CC=N4)Cl", "CHEMBL1970083": "C1=CC(=CC=C1C2=CSC3=C2C(=NC=C3C4=CC=NC=C4)N)NC(=O)NC5=C(C=CC(=C5)C(F)(F)F)F", "CHEMBL1970317": "CN1C=C(C=N1)C2=CN=C(C3=C2SC=C3C4=CC=C(C=C4)NC(=O)NC5=CC(=CC=C5)F)N", "CHEMBL1970369": "C1CC(CN(C1)C(=O)C2=NOC(=C2)C3=CC4=C(C=C3)NN=C4)C(=O)N", "CHEMBL1970873": "CC1=CC2=C(C=C1)NC3=CC=CC=C3NC2=O", "CHEMBL1970879": "CC(=O)N1CCN(CC1)C2CCC(CC2)N3C4=C(C(=N3)C5=CC(=C(C=C5)NC(=O)C6=CC7=CC=CC=C7N6C)OC)C(=NC=N4)N", "CHEMBL1971017": "C1=CC(=CC(=C1)F)C2=CN=CC3=C2C=C(S3)C(=O)N", "CHEMBL1971801": "C1=CC=C2C(=C1)NC3=C(C=CN=N3)C(=O)N2", "CHEMBL1971947": "CC1=CC(=CC=C1)NC(=O)NC2=CC=C(C=C2)C3=CSC4=C3C(=NC=C4C#CC5=CN=CC=C5)N", "CHEMBL1972152": "C1C2=C(CS1)N=C3C=C(NN3C2=O)C4=CC=CO4", "CHEMBL1972183": "CN1CCCC1COC2=CN=CC(=C2)CCC3=CC=CC=C3", "CHEMBL1972250": "COC1=CC2=C(CC3=C2NN=C3C4=CN=C(C=C4)C#N)C=C1C#C", "CHEMBL1972365": "C1=CC=C(C=C1)C2=CN3C=NC(=CC3=N2)N", "CHEMBL1972568": "COC1=CN=CC(=C1)C=CC2=CC=NC=C2", "CHEMBL1972820": "C1=CC=C2C(=C1)C(=O)N(C2=O)C3=CC(=C(C=C3)C(=O)O)O", "CHEMBL1972840": "C1=CC=C2C(=C1)C(=CN2)CC(COC3=CN=CC(=C3)C4=CC5=C(S4)C=CN=C5)N", "CHEMBL1973711": "C1=CC2=C(C=C1Cl)C3=C(C(=O)NC(=O)C3=C(O2)N)C#N", "CHEMBL1974457": "C1=CC(=CC(=C1)F)C2=CN=CC3=C2C=C(S3)C(=O)O", "CHEMBL1975208": "CC1=C2C(=O)C(=CNC2=NC(=C1F)N3CCC(C3)NC(=O)C)C(=O)O", "CHEMBL1975787": "C1=CC(=C(C=C1F)F)C2=CN=CC3=C2C=C(S3)C(=O)N", "CHEMBL1976328": "CC1=CC(=CC(=C1)NC(=O)NC2=CC=C(C=C2)C3=C4C(=CC=C3)SN=C4N)C", "CHEMBL1976872": "CC(=O)NC1=NN2C=CC=CC2=C1", "CHEMBL1977041": "CC1=C(C(=C2N1N=CN=C2N)C3=CC=C(C=C3)NC(=O)NC4=CC=CC=C4)C(=O)OC", "CHEMBL1977619": "C1=CSC(=C1)C2=CC(=NC3=CC=NN32)C(=O)O", "CHEMBL1977814": "CC1=NN(C2=C1C(=O)C3=C(N2OCC(C)C)C=CC(=C3)Cl)C", "CHEMBL1979718": "CC1=C(N(C2=C1C=C(C=C2)C(=O)NC3=NC=NN3)CC4=CC=CC=C4)C", "CHEMBL1979855": "CC(C)(C)C1=NN(C(=C1)NC(=O)NC2=CC=CC3=CC=CC=C32)C4=CC=CC(=C4)C(=O)NCC#N", "CHEMBL1980161": "C1=CC2=C(C(=C1)Cl)NN=C2N", "CHEMBL1980715": "CCCCCCCCCCCCOC1=C(C=C(C=C1)N=C(N)N)N=C(N)N", "CHEMBL1980802": "C1C(C(COC2=NC(=CN=C2C#N)NC(=O)NC3=C(O1)C=CC(=C3)Cl)O)O", "CHEMBL1981045": "COC1=C(C=CC(=C1)C2=CC3=C(C=C2)C(=O)NC4=C(N3)C=CC(=C4)CCOC5=CC=C(C=C5)N6CCOCC6)OCC(CO)O", "CHEMBL1982167": "COC1=CC(=C(C=C1)OC)NC(=O)C2=C3N=CC=C(N3N=C2)C4=CC=CC=C4", "CHEMBL1982476": "CNC(=O)C1=CN=C(C2=C1SC=C2C3=CC=C(C=C3)NC(=O)NC4=CC(=CC=C4)Cl)N", "CHEMBL1983006": "COC1=C(C=C(C(=C1)C(=O)O)Cl)NC(=O)NC2=NC=C(N=C2)C#N", "CHEMBL1984206": "CCOC1=C(C(=CC(=N1)C(=O)NCC2=CC=NC=C2)N)C#N", "CHEMBL1984432": "CC1=CC(=C(C=C1)CN2C=C(N=N2)C3=CC4=C(C=C3)NN=C4)C", "CHEMBL1984788": "C1CC(CNC1)C2=CC(=C(C=C2)C3=NC4=C(N3)C=C(C=C4C(=O)N)Cl)F", "CHEMBL1985311": "C1=CC(=C2C(=C1)NN=C2N)C3=CC=C(C=C3)NC(=O)NC4=C(C=CC(=C4)CO)F", "CHEMBL1985566": "COC1=C(C=CC(=C1)C2=CC3=C(C=C2)C(=O)NC4=C(N3)C=CC(=C4)CCOC5=CC=C(C=C5)N6CCOCC6)CC#N", "CHEMBL1985580": "C1=CC=C2C(=C1)C=CC=C2CC(C(=O)NC3=CN=CC(=C3)C=CC4=CC=NC=C4)N", "CHEMBL1986588": "CC1=NN(C2=C1C=C(S2)C(=O)N)C", "CHEMBL1987054": "CC1=CC2=C(C(=C1)Cl)OC(=N2)NC3=CC=C(C=C3)C4=NN(C5=C4C(=NC=N5)N)C6CCC(CC6)OCCOC", "CHEMBL1987143": "C1=CC=C(C=C1)C2=CN3C(=NN=C3N)C=C2", "CHEMBL1987756": "C1=CC2=C(C=CN=C2)C(=C1)S(=O)(=O)NCCNCC=CC3=CC=C(C=C3)Br", "CHEMBL1988370": "C1CCN(C1)CC2CC(C2)N3C=C(C4=C3N=CN=C4N)C5=CC(=CC=C5)OCC6=CC=CC=C6", "CHEMBL1989423": "C1C2=CC=CC=C2C3=C1C=NN3", "CHEMBL1989834": "C1=CC=C(C=C1)C2=C3C(=CC=C2)NNC3=O", "CHEMBL1989856": "CC1=C(C(=O)N2C3=CC=CC=C3NC2=C1C#N)C=O", "CHEMBL1990346": "C1=CC(=C2C(=C1)NN=C2N)C3=CC=C(C=C3)Br", "CHEMBL1990583": "C1=CC(=CC(=C1)F)NC(=O)NC2=CC=C(C=C2)NC(=O)C3=C4C(=NC=NN4C=C3)N", "CHEMBL1991143": "CC1=CC=C(C=C1)N2C3=C(C(=N2)C)C(=O)C4=C(N3O)C=CC(=C4)Cl", "CHEMBL1991180": "CC(=C1C=CC(=O)C=C1O)NNC(=O)C2=C(N=NN2C3=NON=C3N)COC", "CHEMBL1991577": "CC(C1CCCCC1)NC2=C(C(=O)C2=O)NC3=CC=NC=C3", "CHEMBL1991640": "C1CC1N2C3=C(C(=C(C=C3C(=O)C4=C2SNC4=O)F)NCC5=CC=CC=C5)F", "CHEMBL1991728": "CC(=NN=C(N)N)C1=CC(=CC(=C1)NC(=O)NCCCCCCNC(=O)NC2=CC(=CC(=C2)C(=NN=C(N)N)C)C(=NN=C(N)N)C)C(=NN=C(N)N)C", "CHEMBL1991846": "C1=CC=C(C=C1)CC(COC2=CN=CC(=C2)C=CC3=CC=NC=C3)N", "CHEMBL1992645": "C1=CC(=CC=C1C2=CC=C(C=C2)F)C(=O)NS(=O)(=O)C3=CC(=C(C=C3)NCCSC4=CC=C(C=C4)O)[N+](=O)[O-]", "CHEMBL1992732": "CCOC1=CC=CC=C1C=NNC(=O)C2=C(N(N=N2)C3=NON=C3N)N4CCCC4", "CHEMBL1992796": "C1C(NNC1=C2C(=C3C=C(C=CC3=NC2=O)Cl)C4=CC=CC=C4)C5=CC=CC=C5", "CHEMBL1993166": "CC(=NN=C(N)N)C1=CC(=CC(=C1)NC(=O)NCCCN(C)CCCNC(=O)NC2=CC(=CC(=C2)C(=NN=C(N)N)C)C(=NN=C(N)N)C)C(=NN=C(N)N)C", "CHEMBL1995592": "CC1=C(C=CC(=C1)O)N2C3=C(C=CC(=C3)Cl)C(=O)C4=C2N=C(N=C4N)N", "CHEMBL1996155": "CN1CCC1COC2=CN=CC(=C2)CCC3=CC=NC=C3", "CHEMBL1996208": "C1COCCN1C2=CC(=NC(=N2)OCCC3=CC=CC=N3)NN", "CHEMBL1996390": "C1=CC=C(C=C1)C2=CN=CC3=C2C=C(S3)C(=O)O", "CHEMBL1996543": "C1=CC=C2C(=C1)C(=CN2)CC(COC3=CN=CC(=C3)C4=CC=C(C=C4)F)N", "CHEMBL1996780": "CCOC(=O)C1=CN(C2=C(C1=O)C=CC(=C2)C3=CC=NC=C3)C4=C(C=C(C=C4)O)C", "CHEMBL1996837": "CC1=NN(C2=C1C(=C(S2)C(=O)N)N)C", "CHEMBL1997503": "CC(C)OC1=C(C=C(C=C1)C2=NOC(=N2)C3=CC=C(C=C3)NC4CCC(C4)C(=O)O)Cl", "CHEMBL1997623": "C1=CC(=CC(=C1)NC(=O)NC2=CC=C(C=C2)C3=CC4=C(C=C3)C(=NN4)N)C(F)(F)F", "CHEMBL1997759": "COC1=CC=CC(=C1)NC(=O)C2=C3N=CC=C(N3N=C2)C4=CC=CC=C4", "CHEMBL1999556": "C1=CC=C(C=C1)C2=CN=CC3=C2C=C(S3)C(=O)N", "CHEMBL1999749": "COC1=C(C=CC(=C1)NC2=NC=NC3=C2C=C(C=C3)C4=CC=C(C=C4)CN5CC6C(C5)C6CO)OC7=CC=CC=C7", "CHEMBL1999774": "CC1=C2C(=O)C(=CNC2=NC(=C1Cl)N3CCC(C3)CN)C(=O)O", "CHEMBL1999918": "C1=CC(=C(C(=C1C2=CN=CC3=C2C=C(S3)C(=O)N)F)F)Br", "CHEMBL2000104": "CCS(=O)(=O)C1=CC=C(C=C1)C2=CN=CC3=C2C=C(S3)C(=O)N", "CHEMBL2000271": "CC1=C2C=C(C=CC2=NN1)C3=CC(=CN=C3)OCC(CC4=CC=CC=C4)CN", "CHEMBL2000685": "CC(=NN=C(N)N)C1=CC(=CC(=C1)NC(=O)C2=CC(=CC=C2)C(=O)NC3=CC(=CC(=C3)C(=NN=C(N)N)C)C(=NN=C(N)N)C)C(=NN=C(N)N)C", "CHEMBL2001539": "C1CC2=C(C=CS2)C3=C1C=NN3", "CHEMBL2001923": "C1COCCN1C2=CC=C(C=C2)OCCC3=CC4=C(C=C3)NC5=C(C=CC(=C5)C6=CN(C7=C6C=CN=C7)CC8=CC(=C(C(=C8)F)F)F)C(=O)N4", "CHEMBL2001998": "CNC(=O)N1CCN(CC1)CCCOC2=CC3=C(CC4=C3NN=C4C5=CN=C(C=C5)C#N)C=C2", "CHEMBL2002322": "C1=C(C=C(C=C1C(F)(F)F)C(F)(F)F)C2=CN=CC3=C2C=C(S3)C(=O)N", "CHEMBL2002323": "CC1=CC(=C(C=C1)F)C2=CN3C(=NN=C3N)C=C2", "CHEMBL2002407": "COC1=CC(=CC(=C2C(=C(NN2)N)C#N)C#N)C=CC1=O", "CHEMBL2003524": "CCC1=NC2=C(C3=CC(=C(C=C31)OC)OC)C(=O)NC2=O", "CHEMBL2003657": "CC(C)S(=O)(=O)N1C2=C(C=CC(=C2)C3=C(N=C4N3C=CS4)C5=CC=C(C=C5)F)N=C1N", "CHEMBL2004355": "CCOC1=C(C(=CC(=N1)C(=O)NCC2=CC=C(C=C2)S(=O)(=O)N)N)C#N", "CHEMBL2004438": "C1=CC(=CC(=C1)NC(=O)NC2=CC=C(C=C2)C3=C(C4=NC=CN=C4C=C3)N)C(F)(F)F", "CHEMBL2006010": "C1=CC(=NC(=C1)NC(=O)NC2=C3C=CC(=C(C3=NC=C2)Cl)Cl)C(F)(F)F", "CHEMBL2006567": "CC(=O)NC1=NC(=C(C(=C1)N)C#N)C2=CSC=C2", "CHEMBL2006581": "CCOC1=C(C(=CC(=N1)C(=O)NCC2=CC=CC=C2S(=O)(=O)N)N)Cl", "CHEMBL2006933": "CSC1=CNC2=C(C1=O)C=CC3=C2C=CN=C3", "CHEMBL2007151": "CC1=C(C2=C(N1C3CCC(CC3)N4CCCC4)N=CN=C2N)C5=CC(=CC=C5)OCC6=CC=CC=C6", "CHEMBL201511": "COC1=CC(=CC(=C1OC)OC)C2=C(C(=O)NC2=O)C3=CNC4=CC=CC=C43", "CHEMBL207995": "COC1=C(C=C(C(=C1)C=O)Cl)NC(=O)NC2=NC=C(N=C2)C#N", "CHEMBL209534": "CCOC1=C(C(=CC(=N1)C(=O)NCC2=CN=CC=C2)N)C#N", "CHEMBL219722": "C1=CC=C(C=C1)NC(=O)NC2=CC=C(C=C2)C3=C4C(=CC=C3)NN=C4N", "CHEMBL223257": "C1CCOC2=CC(=C(C=C2NC(=O)NC3=CN=C(C(=N3)OCC1)C#N)Cl)OCC(CO)O", "CHEMBL243088": "C1=CC=C(C(=C1)C(=O)O)NC2=NC(=NC=C2)NC3=CC(=CC=C3)O", "CHEMBL244378": "C1=CC=C(C(=C1)C(=O)O)NC2=NC(=NC=C2)NC3=CC4=C(C=C3)C=NN4", "CHEMBL259850": "COC1=CC=C(C=C1)CNC(=O)NC2=NC=C(S2)[N+](=O)[O-]", "CHEMBL260092": "C1CNC2=C(C(=NC=N2)N)N=C1C3=CC=C(C=C3)NC(=O)NC4=CC=CC(=C4)C(F)(F)F", "CHEMBL289959": "C1=CC=C(C=C1)NC2=NC=NC3=CC=CC=C32", "CHEMBL302449": "CN1C2=CC=CC=C2C3=C4C(=C5C6=CC=CC=C6N(C5=C31)CCC#N)CNC4=O", "CHEMBL326282": "C1C(CC(=O)C2=C1NC3=C(C2=O)C=CC(=C3)Cl)C4=C(C=C(C=C4)Cl)Cl", "CHEMBL336961": "C1C2=C(C3=C(C=CC=N3)NC1=O)NC4=C2C=C(C=C4)Br", "CHEMBL354676": "C1=CC=C(C=C1)NC(=O)NC2=CC=CC=C2", "CHEMBL375284": "CC1=CC(=CC=C1)NC(=O)NC2=CC=C(C=C2)C3=C4C=NNC4=CC=C3", "CHEMBL38380": "C1CNCCN(C1)S(=O)(=O)C2=CC=CC3=C2C=CN=C3", "CHEMBL396523": "C1=CC=C(C(=C1)C(=O)O)NC2=NC(=NC=C2)NC3=CC4=C(C=C3)NN=C4", "CHEMBL408995": "CC1=CC(=O)C(C12C3=CC(=CC(=C3C(=O)O2)O)OC)O", "CHEMBL413779": "C1CCOC2=CC(=C(C=C2NC(=O)NC3=CN=C(C(=N3)OCC1)C#N)Cl)OCCO", "CHEMBL437747": "CCCN1C(=NC(=C1C2=NC(=NC=C2)NC3CCCCC3)C4=CC(=C(C=C4)Cl)Cl)C5CCNCC5", "CHEMBL451401": "C1=CC2=C(C(=C1)C(=O)N)NN=C2", "CHEMBL463054": "CC1=C(C=C2C(=C1)C(=O)C3=CC(=CC(=C3C2=O)O)OC)O", "CHEMBL483525": "CC1=CC(=CC2=C1C3=CC(=CC(=C3C(=O)O2)O)OS(=O)(=O)O)O", "CHEMBL483526": "CC1=CC(=CC2=C1C3=CC(=CC(=C3C(=O)O2)O)OC)O", "CHEMBL483531": "CC1=CC(=C(C=C1C2=CC(=CC(=C2C(=O)O)O)OC)O)O", "CHEMBL483532": "CC1=CC(=C(C=C1C2=CC(=CC(=C2C(=O)O)O)O)O)O", "CHEMBL485556": "CN(C1=CC2=C(C=C1)N(C(=N2)NC(=O)C3=CC=C(C=C3)C#N)CCC(=O)N)C(=O)C4CCCCC4", "CHEMBL488646": "CC(C)(C)OCN1C=C(C2=CC=CC=C21)C3=C(C(=O)NC3)C4=CC(=C(C(=C4)OC)OC)OC", "CHEMBL488811": "COC1=CC(=CC(=C1OC)OC)C2=C(CNC2=O)C3=CN(C4=CC=CC=C43)COC5=CC=CC=C5", "CHEMBL505637": "C1=CC(=C(C=C1CCNC(=O)C(=NO)CC2=CC(=C(C(=C2)C3=CC(=CC(=C3O)Br)CC(=NO)C(=O)NCCC4=CC(=C(C=C4)O)Br)O)Br)Br)O", "CHEMBL507058": "COC1=CC(=C2C(=C1)C3=CC(=C(C=C3COC2=O)O)O)O", "CHEMBL507936": "CC1=CC(=CC=C1)NC(=O)NC2=CC=C(C=C2)C3=C(C4=NC=CN=C4C=C3)N", "CHEMBL509435": "CN1C=C(C2=CC=CC=C21)C3=C(CNC3=O)C4=CC(=C(C(=C4)OC)OC)OC", "CHEMBL512054": "CC1(C(C(C2=C(C1O)C(=O)C3=CC(=CC(=C3C2=O)O)OC)O)O)O", "CHEMBL513846": "CC1=C(N2C=CC=CC2=N1)C3=CSC(=N3)NC4=CC=C(C=C4)O", "CHEMBL519395": "CC1=C(C(=O)C(C1)O)C2=CC(=CC(=C2C(=O)O)O)OC", "CHEMBL519982": "CC1=CC(=CC2=C1C3=CC(=CC(=C3C(=O)O2)O)O)O", "CHEMBL520144": "CC1=CC(=C(C2=C1C3=CC(=CC(=C3C(=O)O2)O)OC)O)O", "CHEMBL521470": "C1CC2(C3C(CC(=O)C4=C(C=CC(=C34)C5=C2C(=C(C=C5)O)C1=O)O)O)O", "CHEMBL529663": "COC1=CC(=CC(=C1OC)OC)C2=C(CNC2=O)C3=CNC4=CC=CC=C43", "CHEMBL554993": "CC1=C(C=C2C(=C1)C(=O)C3=CC(=C(C(=C3C2=O)O)C4=C5C(=C(C=C4OC)O)C(=O)C6=C(C5=O)C(C(C(C6O)O)(C)O)O)OC)O", "CHEMBL556684": "CC1=C(C(=C2C(=C1)C(=O)C3=CC(=CC(=C3C2=O)O)OC)O)O", "CHEMBL562488": "C1=CC2=C(C=C1Br)C(=O)N=CN2", "CHEMBL6246": "C1=C2C3=C(C(=C1O)O)OC(=O)C4=CC(=C(C(=C43)OC2=O)O)O", "CHEMBL101311": "CN(C)CC(COC1=CC=C(C=C1)NC2=NC=CC(=N2)NC3=C(C=CC(=C3)Cl)Cl)O", "CHEMBL1080994": "CC1=C(C=CC2=C1C=CN2)NC3=C(C=NC=C3C#N)C=CC4=CC(=CC=C4)S(=O)(=O)N5CCN(CC5)C", "CHEMBL1080995": "CC1=C(C=CC2=C1C=CN2)NC3=C(C(=NC=C3C#N)C)C=CC4=CC(=CC=C4)S(=O)(=O)N5CCN(CC5)C", "CHEMBL1087650": "CN1CC2CC1CN2C3=CC=C(C=C3)C4=CC=NC5=C(C(=NN45)C6=CC=NC=C6)C7=CC(=CC=C7)O", "CHEMBL1089082": "C1=CC(=CC(=C1)NC(=O)C2=CC(=CC=C2)C(F)(F)F)C3=CC=NC4=CC(=NN34)C5=CC=NC=C5", "CHEMBL1091356": "CC(C)N1CCN(CC1)C(=O)C2=CC=C(C=C2)NC(=O)NC3=CC=C(C=C3)C4=NC(=NC(=N4)N5C6CCC5COC6)C7CCOCC7", "CHEMBL1095626": "COC(=O)N1CCC(CC1)N2C3=C(C=N2)C(=NC(=N3)C4=CC=C(C=C4)N)N5CCOCC5", "CHEMBL1095627": "CC(C)(C)OC(=O)N1CCC(CC1)N2C3=C(C=N2)C(=NC(=N3)C4=CC=C(C=C4)N)N5CCOCC5", "CHEMBL1164180": "CN1CCN(CC1)C2=NC=C(C=C2)C3=CC4=C(NCCN4CC5=C(C=CC(=C5)Cl)C(F)(F)F)N=C3", "CHEMBL1173055": "CNCC1=CC=C(C=C1)C2=C3CCNC(=O)C4=CC(=CC(=C34)N2)F", "CHEMBL1178727": "C1C2=CC=CC=C2C3=C1SC(=N3)N", "CHEMBL1270399": "CC1CN(CC(O1)C)C(C)C2=NSC(=C2)NC3=NC(=CN4C3=NC=C4C5=CNN=C5)C", "CHEMBL1270795": "CC1=NSC(=C1)NC2=NC(=CN3C2=NC=C3C4=CNN=C4)SC", "CHEMBL1421720": "C1=CC=C2C(=C1)N=C(S2)NC(=O)CC3=CC=CS3", "CHEMBL150894": "CC(C)OCC1=CC2=C(C=C1)N(C3=C4CC5=CC=CC=C5C4=C6C(=C23)CNC6=O)CCCO", "CHEMBL1650533": "CCN(CC1=NSC(=C1)NC2=NC(=CN3C2=NC=C3C4=CNN=C4)C)C(C)(C)CO.Cl", "CHEMBL1650545": "CC1=CN2C(=CN=C2C(=N1)NC3=CC(=NS3)CN4CCC(C4)(F)F)C5=CNN=C5", "CHEMBL1650551": "CC1=CN2C(=CN=C2C(=N1)NC3=CC(=NS3)CN4CCC(C4)(F)F)C5=CNN=C5.Cl", "CHEMBL1682359": "CCCC1=NOC(=C1)C2=CC3=C(C=C2)NN=C3", "CHEMBL1682360": "C1CCN(CC1)CC2=NOC(=C2)C3=CC4=C(C=C3)NN=C4", "CHEMBL178737": "C1CN2C=C(C3=C2C(=CC=C3)CN1C(=O)N4CCOCC4)C5=C(C(=O)NC5=O)C6=CN=C7N6C=CC=C7", "CHEMBL1890036": "CC(=NNC(=O)C1=C(N(N=N1)C2=NON=C2N)C3=CC=CC=C3)C4=CC=CO4", "CHEMBL189963": "CC1=C(C(=O)N(C2=NC(=NC=C12)NC3=NC=C(C=C3)N4CCNCC4)C5CCCC5)C(=O)C", "CHEMBL1916359": "C1=CC(=C(C(=C1)Cl)C2=[N+](C=CC3=C(C=CN=C32)C4=C(C=C(C=C4)F)Cl)[O-])Cl", "CHEMBL1933538": "C1CC(CNC1)N2CCC3(C2)CN(C4=CC=CC=C34)C(=O)C5=CC6=C(N5)C=CC(=C6)F", "CHEMBL1933550": "C1CNCC1N2CCC3(C2)CN(C4=CC=CC=C34)C(=O)C5=CC6=C(N5)C=C(C=C6)F", "CHEMBL1933551": "CC1CCC(CN1)N2CCC3(C2)CN(C4=CC=CC=C34)C(=O)C5=CC6=CC=CC=C6N5", "CHEMBL1938680": "C1CN(CCN1)C2=CC=C(C=C2)NC(=O)C3=CC=C(O3)C4=CC=C(C=C4)Cl", "CHEMBL1964382": "CC(C)(C1=CC(=C(C(=C1)I)O)Br)C2=CC(=C(C(=C2)I)O)Br", "CHEMBL1964441": "CC1=CC(=CC=C1)NC(=O)NC2=CC=C(C=C2)C3=CSC4=C3C(=NC=C4C#CCNC)N", "CHEMBL1964718": "CC1=CN2CC(=O)NN=C2C=C1", "CHEMBL1964902": "CC(C)(C)C1=NN(C(=C1)NC(=O)C(=O)C2=CC=CC3=CC=CC=C32)C4=CC(=CC=C4)OCC(=O)O", "CHEMBL1965033": "CC1=CC(=O)NN=C1C2=CC=C(C=C2)NC(=O)NC3=C(C=CC(=C3)C(F)(F)F)F", "CHEMBL1965169": "CC1=CC=C(C=C1)C2=CC3=NC(=CN=C3N2)Br", "CHEMBL1965170": "COC1=CC=C(C=C1)NC(=O)NC2=CC=C(C=C2)C3=CSC4=C3C(=NC=C4C5=CN(N=C5)CC(CO)O)N", "CHEMBL1965351": "CC1=CC=CC(=C1)C=NNC2=NC(=NC(=C2)N3CCOCC3)OCCC4=CC=CC=N4", "CHEMBL1965387": "C1=CN(C=C1)CCCOC2=C3C(=C(C=C2)C4=CC=C(C=C4)NC(=O)NC5=CC(=CC=C5)Cl)C(=NN3)N", "CHEMBL1966069": "C1=CC=C2C(=C1)N=NN2CC3=CN(N=N3)C4=CC5=C(C=C4)NN=C5", "CHEMBL1967252": "CC1=C2C=C(C=CC2=NN1)C3=CN=CC=C3", "CHEMBL1967612": "C1=CC2=C(C=C1Cl)C(=O)NS2(=O)=O", "CHEMBL1967992": "C1=CC=C(C=C1)CNC2=C(C=CC(=C2)C3=CC=NC=C3)C#N", "CHEMBL1968130": "C1=C(N2C(=NN=C2N)C=N1)Cl", "CHEMBL1969942": "C1=CC(=CC(=C1)F)NC(=O)NC2=CC=C(C=C2)C3=CC4=C(C=C3)C=NN4", "CHEMBL1970006": "CN(C1=CC=CC=C1CNC2=NC(=NC3=C2C=CN3)N)S(=O)(=O)C", "CHEMBL1970352": "CCOC(=O)C1=C(N(C2=C1C=C(C3=CC=CC=C32)O)C4=CC=C(C=C4)I)C", "CHEMBL1971227": "C1=CC(=CC=C1C2=CC=C(C=C2)S(=O)(=O)CC(C3=CC=C(C=C3)O)N(C=O)O)C(F)(F)F", "CHEMBL1971289": "CCOC1=CC(=C(C=C1)C=C2C(=O)N=C(S2)N)O", "CHEMBL1971534": "C1=CN=CC2=C1C=C(S2)C(=O)N", "CHEMBL1972220": "C1=CC(=CC=C1C2=CSC3=C2C(=NC=C3C4=CN(N=C4)CCO)N)NC(=O)NC5=CC=C(C=C5)OC(F)F", "CHEMBL1972355": "CC1=CC(=O)C2=C(C(=C3NC4=CC=CC=C4N3)C(=O)C=C2O1)OC", "CHEMBL1972362": "CS(=O)(=O)C1=CC=C(C=C1)C2=CN=CC3=C2C=C(S3)C(=O)N", "CHEMBL1972454": "CC(=O)N1C2=C(C=C(C=C2)N)C=N1", "CHEMBL1972462": "CCCCC#CC1=CC=C(C=C1)CN2CC(C2)C(=O)O", "CHEMBL1972934": "C1=CSC2=NC=NC(=C21)N", "CHEMBL1973013": "CC1=CN=C(S1)NC2=NC(=NC=C2Br)NC(C)C", "CHEMBL1973016": "CS(=O)(=O)C1=CC=CC(=C1)C(=O)NC2=NC3=CC=CC=C3N2CCCO", "CHEMBL1973138": "CC1=C(C=CC=C1NC(=O)C2=CC=C(C=C2)C(C)(C)C)C3=CN(C(=O)C(=C3)NC4=NC=C(C=C4)C(=O)N5CCOCC5)C", "CHEMBL1973359": "C1=CC2=NC(=CN2C=C1C(=O)N)C3=CC=C(O3)[N+](=O)[O-]", "CHEMBL1973363": "COC1=CC=CC(=C1)NC(=O)N2CCC(CC2)C3=NC4=C(C=CC=C4N3)C(=O)N", "CHEMBL1973399": "C1CNC2=C(C1=O)SC=C2C(=O)N", "CHEMBL1973793": "C1=CC=C2C(=C1)C3=C(C2=NO)C=C(C=C3)NS(=O)(=O)C4=CC(=CC=C4)Br", "CHEMBL1973868": "C1=CC2=NC=C(C=C2C=C1C3=CC=NC=C3)O", "CHEMBL1974574": "C1=CC=C(C=C1)N2C(=C3C=CC(=CC3=N2)N)C(=O)O", "CHEMBL1974617": "C1=CC2=C(C=C1C3=CC(=NO3)CO)C=NN2", "CHEMBL1974875": "C1CNC(=O)C2=C(N1)C(=CS2)C(=O)O", "CHEMBL1975357": "CC(C)(C)OC(=O)N1C=C(C2=CC=CC=C21)C3=CN=CN3C4CCCCC4", "CHEMBL1975418": "C1CC1C2=C(N=NN2CC3=CC=CC=C3)C4=CC5=C(C=C4)NN=C5", "CHEMBL1975503": "C1=CN2C(=NNC2=O)C(=C1)C3=CC=C(C=C3)N", "CHEMBL1975903": "COC1=CC=CC=C1C2=NC(=NC=C2)NC3=CC(=CC=C3)S(=O)(=O)C", "CHEMBL1975923": "CC(CCC(=O)O)(C1=CC(=C(C=C1)O)N)C2=CC(=C(C=C2)O)N", "CHEMBL1976040": "CC(C)(C1=NC(=CC=C1)N2C3=NC(=NC=C3C(=O)N2CC=C)NC4=CC=C(C=C4)N5CCN(CC5)C)O", "CHEMBL1976158": "C1=CC2=C(C(=C1)Br)C(=O)N3C4=C(C=C(C=C4)[N+](=O)[O-])C(=O)C3=N2", "CHEMBL1976196": "C1CN(CC2=C1NC3=C(C=C(C=C23)Cl)Cl)C(=O)NC4=CC=C(C=C4)[N+](=O)[O-]", "CHEMBL1976376": "C1COCC1N2C=C(C3=C2N=CN=C3N)C4=CC=C(C=C4)OC5=CC=C(C=C5)CO", "CHEMBL1977134": "C1OC2=C(O1)C=C(C=C2)C3=C4N=CC(=C(N4N=C3)N)C5=CC=C(C=C5)NC(=O)NC6=CC=CC(=C6)C(F)(F)F", "CHEMBL1977138": "CC(C1=CC=CC=C1F)NC2=NC(=CN=C2)N3C=NC4=C3C=C(C=C4)C#N", "CHEMBL1977634": "CC(C)(C)C1=NN(C(=C1)NC(=O)C(=O)C2=CC=CC3=CC=CC=C32)C4=CC=C(C=C4)OCC(=O)N", "CHEMBL1977713": "C1=CC2=C(C=NN2)C(=C1)NC(=O)NCC3=CC=C(C=C3)Cl", "CHEMBL1977749": "C=CCC1=CC=CC2=C1OC(=CC2=NO)C3=CC=CC=C3", "CHEMBL1978166": "CC1=CC(=CC=C1)NC(=O)NC2=CC=C(C=C2)C3=CSC4=C3C(=NC=C4C#CCCCCCCCCN)N", "CHEMBL1978167": "CN1C=C(C2=CC=CC=C21)C3=CC4=NC(=CN=C4N3)Br", "CHEMBL1978195": "C1=CC(=CC=C1C2=CN=CC3=C2C=C(S3)C(=O)N)Br", "CHEMBL1978371": "C1C(C(C(=O)C(=C1C2=CC=CC=C2)C#N)C(=O)C3=CC=CC=C3)C4=CC=C(C=C4)Cl", "CHEMBL1978562": "CN1C=C(C2=C1C=CC(=C2)C#N)C3=CC4=NC(=CN=C4N3)Br", "CHEMBL1978567": "CC1=C(SC(=N1)C2=CC=NC=C2)C(=O)NC(C)C3=CC(=CC=C3)OC", "CHEMBL1978656": "CC1=C(C=CC=C1O)NC(=O)C2=C3N=CC=C(N3N=C2)C4=CC=CC=C4", "CHEMBL1979690": "CN1CCN(CC1)C2=CC=C(C=C2)NC3=NC=C(C(=N3)NC4=CC5=C(C=C4)NN=C5)Cl", "CHEMBL1980167": "CN(C)C1=CC=C(C=C1)C2=CC(=NC(=N2)NS(=O)(=O)C3=CC=C(C=C3)N)C4=CC=C(C=C4)[N+](=O)[O-]", "CHEMBL1980246": "C1=CC=C(C=C1)C2=NC(=NC=N2)NC3=CC(=C(C=C3)O)CN", "CHEMBL1980329": "C1=CNC(=C1)C=C2C3=C(C=C(C=C3)C4=CC=C(C=C4)O)NC2=O", "CHEMBL1980376": "CC1=CC=CC(=C1)C2=C3C(=CC=C2)ON=C3N", "CHEMBL1980407": "C1=CC=C(C=C1)CC(COC2=CN=CC(=C2)C3=CC4=C(C=C3)NC(=O)C4=CC5=CC=CN5)N", "CHEMBL1980763": "CC(C)CC1=C2C=CNC2=NC(=N1)NC3=CC(=C(C=C3)N4CCOCC4)Cl", "CHEMBL1981107": "CN1C2=C(C=N1)C(=O)CCC2", "CHEMBL1981215": "C1=CC(=NC(=C1)NC(=O)NC2=C3C=CC(=CC3=NC=C2)OC(F)F)C(F)(F)F", "CHEMBL1981671": "CCOC(=O)CC1=NC2=C(N1)C=CC=C2N", "CHEMBL1982413": "CN(CC1=CC(=C(C2=C1C=CC=N2)O)Cl)C3CCCCC3", "CHEMBL1982541": "CC(C)OC1=C(C(=CC(=N1)C(=O)NCC2=C(C=CC(=C2)OC)OC)N)C#N", "CHEMBL1982700": "CCCCNC(=O)C1=CN(C(=O)C2=CC(=C(C=C21)OC)OC)C(CC)CC", "CHEMBL1982880": "COC1=CC(=C(C=C1)OC)NC2=NN3C(=NN=C3C4=CC=CC=C4)C=C2", "CHEMBL1982980": "CC(=C(C)C1=CC=CC2=C1NC(=C2CCCOC3=C(C(=CC=C3)Cl)Cl)C(=O)O)C", "CHEMBL1983309": "COC1=CC(=C(C=C1)C(=O)NC2=NC3=C(S2)C=C(C=C3)Cl)OC", "CHEMBL1983348": "CCCCN(CCC#N)C(=O)C1=CC2=NC(=C3C4=CC=CC=C4NN3)N=C2C=C1", "CHEMBL1983393": "C1=CC(=CC(=C1)NC(=O)NC2=CC(=CC=C2)F)C3=CC4=C(C=C3)C=NN4", "CHEMBL1983575": "C1=CC=C(C=C1)NC(=O)NNC=C2C=C(C(=O)C(=C2)Br)Br", "CHEMBL1983630": "C1C2=C(NC1=O)N=CC(=C2)C3=CC=CC=C3", "CHEMBL1983640": "CC1=CC(=C(C=C1)F)NC(=O)NC2=CC=C(C=C2)C3=COC4=C3C(=NC=C4C#CCN5CCOCC5)N", "CHEMBL1983715": "CCNC1=NC(=C(S1)C2=NC(=NC=C2)NC3=CC=C(C=C3)N4CCN(CC4)C(=O)C)C", "CHEMBL1983980": "C1CN(CC2=C(C=CC=C21)C(=O)NC3=NC4=CC=CC=C4S3)C5=NC(=C(S5)C6=CC=C(C=C6)CO)C(=O)O", "CHEMBL1984044": "CCN(CC)CCOC1=CC=C(C=C1)C2=NC3=C(C=CC=C3N2)C(=O)N", "CHEMBL1984236": "CN(C)C1=CC=C(C=C1)NC2=NNC(=C2)C3=CSC(=C3)Br", "CHEMBL1984274": "C1=CC=C(C=C1)C2=C(C(=O)N(N2)C3=CC=CC=C3)NNC4=CC=CC5=C4C(=O)N=NC5=O", "CHEMBL1984296": "CC1=CC(=C(C=C1)C)NC(=O)C2=CC(=NC3=CC=CC=C32)C4=CC=CO4", "CHEMBL1984500": "C1C2=C(C=CC=C2Br)C(=O)N1", "CHEMBL1984686": "C1=CC2=CN=C(C=C2C=C1Br)NC3=NC=NC=C3", "CHEMBL1984760": "CCCNC(=O)C1=CC=C(C=C1)NC2=NC(=C3C=CNC3=N2)CCC(F)(F)F", "CHEMBL1984842": "CC(C)COC1=NC=CN2C1=NC(=C2C3=NC(=NC=C3)NCC(C)(C)CO)C4=CC=C(C=C4)F", "CHEMBL1985206": "COCC#CC1=C2CC3=C(NN=C3C2=CC=C1)C4=CC=CS4", "CHEMBL1985367": "CC1=CC(=NC=C1)NC2=NC(=NC(=C2)C)C3=CC=CC=C3", "CHEMBL1985681": "C1CC(C2=C(C1)N=C(C=C2)C3C4=C(C=CC(=C4)C#N)NC3=O)O", "CHEMBL1986143": "C1=CC=C(C=C1)C(CCO)NC(=O)C2=CC=C(C=C2)C3=CC=NC=C3", "CHEMBL1986177": "C1=CC(=CC(=C1)Cl)NC(=O)NC2=NC(=CS2)CCNC3=NC=NC4=C3SC=C4", "CHEMBL1986265": "C1C(CN1CC2=C(C=C(C=C2)OCC3=CC(=CC=C3)C(F)(F)F)Cl)C(=O)O", "CHEMBL1986503": "C1=CC2=C(C=C1Cl)N=NC3=NN=NN23", "CHEMBL1986590": "C1=CC=C2C(=C1)C(=CN2)C=C3C4=CC=CC=C4NC3=O", "CHEMBL1986899": "CC1=CC=C(C=C1)NCC2=CN=C(C=C2)C3=CC=C(C=C3)F", "CHEMBL1987430": "CCCC1=CC2=C(C=CN=C2C=C1)NC(=O)NC3=CC=CC(=N3)C(F)(F)F", "CHEMBL1987535": "C1CN(CC=C1C2=CNC3=C2C=CC=N3)C(=O)NCCC4=CC=CS4", "CHEMBL1987648": "CC1=NC=CN2C1=NC(=C2C3=NC(=NC=C3)NCC(C)(C)CO)C4=CC=C(C=C4)F", "CHEMBL1987982": "C1CNCC=C1C2=CNC3=C2C=C(C=C3)C4=CC=C(C=C4)OC(F)(F)F", "CHEMBL1987998": "C1C(CN1CC2=C(C=C(C=C2)OCC3=CC=CC=C3)Cl)C(=O)O", "CHEMBL1988141": "CCC(=O)NC1=CC(=C(C=C1)C(=O)N2CCNCC2)O", "CHEMBL1988581": "CC1=CC(=O)N2C=CC(=C(C2=N1)O)CN(C)C", "CHEMBL1988692": "CC(C)NC1=C(C(=O)NN1)C=C2C=C3C=CC=CC3=N2", "CHEMBL1988805": "C1=CC2=C(C=C1C#N)N(C(=N2)N)C3=NC=CS3", "CHEMBL1988872": "CS(=O)(=O)NC1=CC=C(C=C1)NC2=CC3=C(C=C2)NN=C3N", "CHEMBL1989043": "CN1CCN(CC1)C2=CC=C(C=C2)NC3=NC(=C(S3)C(=O)C4=C(C=CC=C4Cl)Cl)N", "CHEMBL1989267": "CN1C2=CC=CC=C2C=C1C(=O)NC3=C(C=C(C=C3)C4=CSC5=C4C(=NC=C5C=CC(=O)NCCN(C)C)N)OC", "CHEMBL1989471": "CC1=C2C(=O)C3=C(C=C(C=C3)C(C)C)NC2=NC=C1", "CHEMBL1989957": "C1=CC=C(C=C1)C2=CC3=CC(=NC=C3C=C2)NCCO", "CHEMBL1990212": "COC1=CC(=C(C=C1NC2=NN3C(=NN=C3C4=CC=CC=C4)C=C2)Cl)OC", "CHEMBL1990223": "CC1=C(C=CC(=C1)OCC2=CC(=C(C=C2)Cl)Cl)CN3CC(C3)C(=O)O", "CHEMBL1991734": "CN1C2=C(C=C(C=C2)N)C(C3=C1C=CC(=C3)N)C4=CC=CC=C4", "CHEMBL1991782": "C1C2=C(C=CC=C2C(=O)N1)C3=CC=CS3", "CHEMBL1991818": "CCN1C2=C(C=CC(=C2)N)C3=C(C1(C4=CC=CC=C4)O)C=C(C=C3)N", "CHEMBL1992042": "C1C=CC2C1C(NC3=C2C4=CC=CC=C4C=C3)C5=CC(=CC=C5)NC(=O)C6=CC=C(C=C6)F", "CHEMBL1992371": "C1=CC(=NC(=O)NC2=CNC=CN2)C3=CC=CC(=O)C3=C1", "CHEMBL1992581": "C1=CC(=CN=C1)C2=CC=C(C=C2)CC(=O)NC3=CC=C(C=C3)SC(F)F", "CHEMBL1992607": "C1CNC(=O)C2=C(N1)N=CN=C2N", "CHEMBL1992644": "C1=CC=C(C=C1)C2=C(C=NN2)C3=CC=NC=C3", "CHEMBL1992673": "C1=CC2=NC(=O)N3C(=C2C=C1Cl)N=CN3", "CHEMBL1992723": "C1=CC=C(C=C1)C2=CC=CC3=NC=CN32", "CHEMBL1993335": "CN1C=C(C2=C1C=CC(=C2)F)C3=CC4=NC(=CN=C4N3)Br", "CHEMBL1993374": "CC(C)C(C)NC1=NC=C(C(=N1)NC2=NC=CS2)Cl", "CHEMBL1993877": "C#CC1=CN(C2=C1C(=NC=N2)N)C3CCCC3", "CHEMBL1993904": "C1=CC=C2C(=C1)N=C(O2)NC3=CC=C(C=C3)C4=CN=C(C5=C4C=C(S5)C(=O)N)N", "CHEMBL1994308": "C1=CC=C2C(=C1)C(=CNNC(=O)CCC(=O)NC3=C(C=CC(=C3)C(F)(F)F)Cl)C=N2", "CHEMBL1994361": "C1=CC=C2C(=C1)C(=CN2)CC(COC3=CN=CC(=C3)C4=CC(=C(C=C4)N)C(=O)C5=CC=CC=C5F)N", "CHEMBL1994555": "CCC1=C(NC2=NC=CN=C12)C3=CC=C(C=C3)C(=O)C", "CHEMBL1994724": "CC(C1=CC(=CC=C1)OC)NC(=O)C2=CC=C(S2)C3=CC=NC=C3", "CHEMBL1994808": "CC1=NC(=C(N=N1)C2=CC=CC=C2)C#N", "CHEMBL1995391": "CC(C)NC1=NNC2=C1C=C(C=C2)N", "CHEMBL1995448": "C1=CC(=CC(=C1)OCCN)NC2=NC(=NC=C2)N", "CHEMBL1995765": "C1=CC=NC(=C1)N2C(=CC(=O)N2)N", "CHEMBL1995916": "CNC(=O)C1=CC(=NN1)C2=CC=CC=C2", "CHEMBL1995927": "CCNC1=NC2=CC(=C(C=C2N=C1NCC)Cl)OC", "CHEMBL1996176": "C1=CC=C2C(=C1)C(=CC3=CC=CN3)C(=O)N2", "CHEMBL1996345": "C1CCC2=C(C1)N=C(S2)N3C4=C(C=CC(=C4)C#N)N=C3N", "CHEMBL1996576": "C1CNC2(CCN(CC2)C(=O)CC3=CC=C(C=C3)OC(F)(F)F)C4=C1C5=CC=CC=C5N4", "CHEMBL1996646": "COC1=C(C(=CC=C1)OC)CNC2=NC(=NC3=C2C=C(C=C3)Cl)NC4CCCCC4", "CHEMBL1996702": "CN(C)CCCNC(=O)C1=CC2=C(C=C1)NC3=C(C=CC(=C3)C4=CC(=C(C=C4)O)OC)C(=O)N2", "CHEMBL1996795": "C1CCC(CC1)NC2=C(C=C(C=C2)S(=O)(=O)NC(=O)C3=CC=C(C=C3)C4=CC=C(C=C4)F)N", "CHEMBL1997007": "CCCNC(=O)C1=CC=C(C=C1)NC2=NC(=C3C=CNC3=N2)CC", "CHEMBL1997193": "CC1=CC=C(S1)C2=C(C(=O)NC(=C2)C3=C(C=CC(=C3)Br)O)C#N", "CHEMBL1997197": "COC1=CC=CC=C1CN=C(N)NC2=NC=CC(=N2)C3=CC=CS3", "CHEMBL1997335": "COC1=C2C=CC=C3C2=C(C=C1)C(=NN3)C4=CC(=C(C=C4)OC)OC", "CHEMBL1997611": "CCOC(=O)C1=C(N2C3=CC(=C(C=C3NC(=O)C2=N1)[N+](=O)[O-])NC(=O)C)C", "CHEMBL1997892": "CC1=CC(=O)NN=C1C2=CC(=C(C=C2)NC(=O)NC3=C(C=CC(=C3)C(F)(F)F)F)Cl", "CHEMBL1998110": "CC1=C(SC(=N1)C2=CC=NC=C2)C(=O)NC(C)C3=CC(=CC=C3)OC", "CHEMBL1998253": "CN(C)C1=CC=C(C2=CC=CC=C21)N", "CHEMBL1998435": "C1=CC2=CN=C(C=C2C=C1C3=CC=NC=C3)NCCO", "CHEMBL1998551": "CC(C)(C1=NN=C2N1N=C(C=C2)C3=C(N=C4N3CCC4)C5=C(C=C(C=C5)F)F)O", "CHEMBL1998680": "CC(C)(C)C1=NN(C(=C1)NC(=O)C(=O)C2=CC=CC3=CC=CC=C32)C4=CC(=CC=C4)OCC(=O)NCCO", "CHEMBL1999120": "CC(C)C1=CC(=O)NC2=C1C(=O)NN2", "CHEMBL1999126": "CC1=C(C2=NC3=CC=CC=C3N2C(=O)C1=CC4=C(NN(C4=O)C5=CC=CC=C5)C)C#N", "CHEMBL1999484": "CC1=C(SC(=N1)NC)C2=NC(=NC=C2)NC3=CC=C(C=C3)N4CCNCC4", "CHEMBL2000433": "CCNNC1=CC(=C(C2=NC3=CC=CC=C3N12)C#N)C", "CHEMBL2001019": "C1=CC2=C(C=CC(=C2)CN3C4=NC(=CN=C4N=N3)C5=CN(N=C5)CCO)N=C1", "CHEMBL2001149": "C1=CC(=CC=C1C2=NC3=C(N2)C=C(C=C3)O)SC4=CC=C(C=C4)C5=NC6=C(N5)C=C(C=C6)O", "CHEMBL2001584": "CC(C)(C)C1=CC=C(C=C1)C(=O)NC2=CC=CC(=C2CO)C3=CN(C(=O)C(=C3)NC4=NC=C(C=C4)C(=O)N5CCOCC5)C", "CHEMBL2001613": "C1=CC2=C(C=C1Br)C(=O)NN2", "CHEMBL2001641": "CC(C)(C1=CN(N=N1)C2=CC3=C(C=C2)NN=C3)O", "CHEMBL2001668": "C1=CC=C(C=C1)C2=CN3C(=C(C=NC3=O)I)N2", "CHEMBL2002105": "C1=C(C=NC2=NNC(=C21)N)Br", "CHEMBL2002240": "CC(=O)NC1=NC(=C(C(=C1)N)C#N)C2=CC3=CC=CC=C3C=C2", "CHEMBL2002450": "COC1=C2C(=C(C=C1)C3=CC=C(C=C3)N)C=NO2", "CHEMBL2002553": "CC1=C2C(=O)C(=CN=C2SN1)C(=O)O", "CHEMBL2002586": "C1CC1NC2=NC(=NC3=C2SC=C3)NC4=CC(=C(C=C4)N5CCOCC5)Cl", "CHEMBL2002682": "CC1=C(C(=CC=C1)Cl)C2=CC=CC3=C2NC(=C3CCCOC4=CC=CC5=CC=CC=C54)C(=O)NCCOCCOCCN", "CHEMBL2002690": "C1=CC=C(C=C1)C2=CC=CC=C2NC(=O)NC3=NC4=C(C=CC=C4S3)O", "CHEMBL2002723": "CC(=O)NC1=CC=C(C=C1)N2N=C3C=CC(=NC3=N2)N", "CHEMBL2003514": "CC(C1=CC(=CC=C1)OC)NC(=O)C2=CN=C(N=C2)C3=CC=NC=C3", "CHEMBL2003689": "CC(C)(C)C1=NN(C(=C1)NC(=O)C(=O)C2=CC=CC3=CC=CC=C32)C4=CC=C(C=C4)OCCC(=O)O", "CHEMBL2003768": "COC1=CC(=C(C=C1)CNC2=C(C(=O)C2=O)NC3=CC=NC=C3)OC", "CHEMBL2004025": "COCOC1=C(C(=CC=C1)OCOC)C2=C(C=C(C=C2)NS(=O)(=O)C)C(=O)OC", "CHEMBL2004033": "C1=CC2=C(C(=O)NN2C=C1)Br", "CHEMBL2004072": "COC(=O)C1=CC2=C(S1)C=NC=C2C3=CC(=CC=C3)F", "CHEMBL2004118": "CCC1=C2C=CNC2=NC(=N1)NC3=CC(=C(C=C3)N4CCOCC4)Cl", "CHEMBL2004159": "COC1=CC=CC(=C1)CNC(=O)C2=CN=C(N=C2)C3=CC=NC=C3", "CHEMBL2004513": "COC(=O)C1=CC=CC=C1C2=CC3=C(C=C2)C(=O)NC4=CC=CC=C4N3", "CHEMBL2004515": "C1OC2=C(O1)C=C(C=C2)C3=C4C=CNC4=NC=N3", "CHEMBL2004647": "CC1=C2C(=O)C(=CNC2=NC(=C1Br)N3CCC(C3)NC)C(=O)O", "CHEMBL2005449": "CC1=CC(=NN1)NC2=NC(=CC(=N2)Cl)NCC3=CC=CC=C3", "CHEMBL2005478": "CN1C=C(C2=C1C=CC(=C2)OC)C3=CC4=NC(=CN=C4N3)Br", "CHEMBL2005548": "CC(C)(C)OC(=O)N1C2=C(C=C(C=C2)NC3=C(C(=O)C3=O)NCC4=C(C=C(C=C4)Cl)Cl)C=N1", "CHEMBL2005699": "CC(C)(C)C1=NN(C(=C1)NC(=O)C(=O)C2=CC=CC3=CC=CC=C32)C4=CC=C(C=C4)OCC(=O)O", "CHEMBL2005792": "CC(C)(CNC1=NC=CC(=N1)C2=C(N=C3N2C=CN=C3OC)C4=CC=C(C=C4)F)CO", "CHEMBL2006299": "COC1=CC=CC(=C1)CNC(=O)C2=CC=C(C=C2)C3=CC=NC=C3", "CHEMBL2006481": "C1CCN(CC1)C(=O)C2=NOC(=C2)C3=CC4=C(C=C3)NN=C4", "CHEMBL2006631": "CN(C)S(=O)(=O)C1=CC=CC=C1C2=CC3=C(C=C2)C(=O)NC4=CC=CC=C4N3", "CHEMBL2006674": "CCC1=C2N=C(C=C(N2N=C1)NCC3=C[N+](=CC=C3)[O-])N4CCCCC4CCO", "CHEMBL2006765": "CCCNC(=O)C1=CC=C(C=C1)NC2=NC3=C(C=CN3)C(=N2)NCC(F)(F)F", "CHEMBL2007097": "C1=CSC2=NC(=O)NC(=C21)N", "CHEMBL2007124": "C1=CC(=CC(=C1)NC(=O)NC2=CC=C(C=C2)C3=NNC(=O)C=C3)C(F)(F)F", "CHEMBL2007138": "C1=CC=C(C=C1)NC2=C(C(=O)NC2=O)Cl", "CHEMBL2007266": "CC1=CC(=C(C=C1)F)NC(=O)NC2=CC=C(C=C2)C3=C4C(=C(C=C3)OCCCN5C=CC=C5)NN=C4N", "CHEMBL2007479": "CCCCNC1=NC(=C(S1)C(=O)C2=CC=CC=C2)N", "CHEMBL2007559": "CCCNC(=O)C1=CC=C(C=C1)NC2=NC3=C(C(=N2)NCC(F)(F)F)SC=C3", "CHEMBL2017214": "CSC1=CC=CC=C1NC2=NC(=NC3=C2N=CN=C3NCC4CC4)N5CCNCC5", "CHEMBL202635": "COC1=C(C=C(C(=C1)CN2CCCCC2)Cl)NC(=O)NC3=NC=C(N=C3)C#N", "CHEMBL202721": "COC1=C(C=C2C(=C1)C(=NC=N2)NC3=CC=C(C=C3)NC(=O)C4=CC=CC=C4)OCCCN5CCOCC5", "CHEMBL2063926": "CSC1=CC=CC=C1NC2=NC(=NC3=C2N=CN=C3NCC4CC4)N5CCN(CC5)C6CCNCC6", "CHEMBL207253": "CCCON1C2=C(C=C(C=C2)Cl)C(=O)C3=C1N(N=C3C)C", "CHEMBL21156": "CC(C)(C)C1=NC2=C(N1)C3=C(C=C(C=C3)F)C4=C2C=CNC4=O", "CHEMBL214253": "C1=CC=C(C=C1)C2=CC3=C(C4=C(N3)C=CC(=C4)O)C5=C2C(=O)NC5=O", "CHEMBL2204532": "CC(C)(C#N)OC1=CC=CC(=C1Cl)C(=O)NC2=C(C=CC(=C2)N(C)C3=NC4=C(C=C3)N=C(S4)NC(=O)C5CC5)F", "CHEMBL2312645": "CN1CCC(CC1)NC(=O)C2=CN=C(N=C2NC3CCCC3)NCC4=CC=CC=C4OC", "CHEMBL2312646": "CN1CCC(CC1)NC(=O)C2=CN=C(N=C2NC3CCCC3)NCC4=C(C=CC(=C4)Cl)Cl", "CHEMBL2312649": "CN1CCC(CC1)NC(=O)C2=CN=C(N=C2NC3CCC(CC3)N(C)C)NC4=CC(=CC(=C4)Cl)Cl", "CHEMBL2312652": "CN1CCC(CC1)NC(=O)C2=CN=C(N=C2NC3COCC3O)NC4=CC(=CC(=C4)Cl)Cl", "CHEMBL2312654": "CC1=NOC(=C1)C2=CN=C(N=C2NC3CCC(CC3)N(C)C)NC4=CC(=CC(=C4)Cl)Cl", "CHEMBL2332840": "C1=CC(=CC=C1NC(=O)NC2=CC(=C(C=C2)Cl)C(F)(F)F)OC3=NC=NC4=C3C=NN4", "CHEMBL242237": "C1=CC=C(C(=C1)C(=O)N)NC2=NC(=NC=C2)NC3=CC(=CC=C3)O", "CHEMBL242865": "C1=CC=C(C(=C1)C(=O)O)NC2=NC(=NC=C2)NC3=CC=C(C=C3)[N+](=O)[O-]", "CHEMBL262623": "C1CNC2=C(C(=NC=N2)N)N=C1C3=CC=CC=C3", "CHEMBL360847": "CN(C)CC1CCN2C=C(C3=CC=CC=C32)C4=C(C5=CN(CCO1)C6=CC=CC=C65)C(=O)NC4=O", "CHEMBL361708": "C1CNC(=O)C2=C(C1=C3C(=O)N=C(N3)N)C=C(N2)Br", "CHEMBL362558": "C1CCN(CC1)C(=O)N2CCN3C=C(C4=CC(=CC(=C43)C2)F)C5=C(C(=O)NC5=O)C6=CN=C7N6C=CC=C7", "CHEMBL379975": "C1=CC=C(C(=C1)C2=CC3=C(C4=C(N3)C=CC(=C4)O)C5=C2C(=O)NC5=O)Cl", "CHEMBL383264": "C1=CC=C2C(=C1)C(=CN2)CC(COC3=CN=CC(=C3)C4=CC5=C(C=C4)C=NC=C5)N", "CHEMBL383541": "C1=CC=C2C(=C1)C(=CN2)CC(COC3=CN=CC(=C3)C=CC4=CC=NC=C4)N", "CHEMBL406845": "CC(C)(C)N1C2=C(C(=N1)C3=CC=C(C=C3)Cl)C(=NC=N2)N", "CHEMBL407391": "CN(C)C1=NC=NC2=C1NC=N2", "CHEMBL415049": "CCN(CCCOC1=CC2=C(C=C1)C(=NC=N2)NC3=NNC(=C3)CC(=O)NC4=CC(=CC=C4)F)CCOP(=O)(O)O", "CHEMBL445162": "CS(=O)(=O)C1=CC=CC(=C1)NC2=NC=CC(=N2)NC3=C(C=CC4=C3OCO4)Cl", "CHEMBL451964": "C1CC1NC2=NN3C(=NN=C3C4=CC=C(C=C4)C(F)(F)F)C=C2", "CHEMBL460989": "COC1=CC2=C(C=C1)C3=C4C(=C5C6=CC=CC=C6N(C5=C3CC2)CCO)CNC4=O", "CHEMBL460990": "CC(C)OC1=CC2=C(C=C1)C3=C4C(=C5C6=CC=CC=C6N(C5=C3CC2)CCO)CNC4=O", "CHEMBL475817": "C1=CC(=CC(=C1)C(F)(F)F)C(=O)NC2=CC(=C(C=C2)Cl)C(=O)NC3=CC(=C(N=C3)N)Cl", "CHEMBL477817": "CC1=C(C=CC2=C1C=CN2)NC3=C4C=C(SC4=NC=C3C#N)C=CC(=O)N5CCCC5", "CHEMBL523823": "CCN1C2=CC(=C(C=C2C(=O)C3=C1NOC3=O)O)Cl", "CHEMBL536151": "C1=CC(=C(C=C1Cl)C(=O)NC2=CC(=CC(=C2)C(F)(F)F)C(F)(F)F)O", "CHEMBL546797": "C1=CC=C2C(=C1)NC(=C(C3=NC4=CC=CC=C4N3)N=O)N2", "CHEMBL550418": "COC1=C(C=CC(=C1)C2=CC3=C(C=C2)C(=O)NC4=C(N3)C(=CC=C4)O)O", "CHEMBL561708": "COC(=O)NC1=CC=C(C=C1)C2=NC3=C(C=NN3C4CCN(CC4)C(=O)OC)C(=N2)N5CCOCC5", "CHEMBL574588": "CC1=CC=C(O1)C2=CC3=C(C=C2)OC=C3C4=CC=C(C=C4)S(=O)C", "CHEMBL574613": "CCS(=O)C1=CC=C(C=C1)C2=COC3=C2C=C(C=C3)C4=CC=C(O4)C", "CHEMBL574737": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)C(NC6=O)O)NC)OC", "CHEMBL576113": "CCN(CC)CCNC1=CC=C(C2=CC=CC=C21)O", "CHEMBL578061": "C1=CC=C(C=C1)NC2=NC(=NC=C2)NC3=CC=CC=C3", "CHEMBL606245": "CC1=C(C=CC2=C1C=CN2)NC3=C(C=NC=C3C#N)C=CCCN4CCCC(C4)N", "CHEMBL1087397": "CN(C)CC1=CC=C(C=C1)C2=C3N=CC=C(N3N=C2)C4=CC(=CC=C4)NC(=O)C5=CC(=CC=C5)C(F)(F)F", "CHEMBL1090143": "C1=CC(=CC(=C1)NC(=O)C2=CC(=CC=C2)C(F)(F)F)C3=C4C=C(SC4=NC=N3)C5=CC=NC=C5", "CHEMBL142425": "CC(CNC1=NC=CC(=C1)C2=C(C3=C(N2)C=CC=N3)C4=CC=C(C=C4)F)O", "CHEMBL1614725": "CC(C)(CC(=O)NCCN1C=CC2=C1C(=NC=N2)NC3=CC(=C(C=C3)OC4=CC=CC(=C4)C(F)(F)F)Cl)O", "CHEMBL1738710": "CC1=C(C=C(C=C1)C(=O)NCCO)N2C=NC(=C(C2=O)Cl)OCC3=C(C=C(C=C3)F)F", "CHEMBL1807446": "CC1=C(C=C(C=C1)C(=O)NC2CC2)NC3=NC=NN4C3=C(C(=C4)C(=O)C5=CC=CC=C5)C", "CHEMBL189338": "CC1CN(CCN1)C2=NC3=C(C=C2)N=C(C4=CN=CN43)NC5=C(C=CC=C5Cl)C", "CHEMBL1956071": "CCN1C2=C(C=NC=C2C(=O)N3CCC(C3)N)N=C1C4=NON=C4N", "CHEMBL1957085": "COC1=CC=C(C=C1)C2=C(N=CO2)C(=O)NCC3=CC=NC=C3", "CHEMBL2036343": "C1C(=CC2=CC=CC=N2)C(=O)C(=CC3=CC=CC=N3)CS1", "CHEMBL2048912": "CC(C)(C(=O)NCCN1C=CC2=C1C(=NC=N2)NC3=CC(=C(C=C3)OC4=C5C=NSC5=CC=C4)Cl)N", "CHEMBL209148": "CC1=C(C=C(C(=C1)OC)C(=O)N2CCN(CC2)C(=O)C)SC3=CN=C(S3)NC(=O)C4=CC=C(C=C4)CNC(C)C(C)(C)C", "CHEMBL2148053": "CC1=CC=C(C=C1)S(=O)(=O)O.CC(C)(C(=O)NCCN1C=CC2=C1C(=NC=N2)NC3=CC(=C(C=C3)OC4=CC(=CC=C4)Cl)Cl)S(=O)(=O)C", "CHEMBL2208034": "C1CC(NC1)C(=O)NC2=CC=C(C=C2)C3=NC(=NC=C3)NC4=CC=C(C=C4)N5CCOCC5", "CHEMBL225088": "CC1=C(C=C(C=C1)C(=O)NOC)NC2=NC(=NC(=N2)N3CCCN(CC3)C)N(C)CC(C)(C)C", "CHEMBL2312185": "CC1=C(SC(=N1)NC)C2=NC(=NC=C2C#N)NC3=CC=CC(=C3)N4CCCNCC4", "CHEMBL2338333": "CN1CC(=CC2=CC=CC=N2)C(=O)C(=CC3=CC=CC=N3)C1", "CHEMBL2338334": "CN1CC(C(=O)C(=CC2=CC=CC=N2)C1)CC3=CC=CC=N3", "CHEMBL2338335": "CN1CC(C(=O)C(=CC2=CC=CC=N2)C1)CC3=CC=CC=N3", "CHEMBL2348417": "C1CNC2=C(C=C1C(=O)NCCO)C(=NC=N2)NC3=CC(=C(C=C3)OC4=C5C=CSC5=CC=C4)Cl", "CHEMBL271190": "CC(=O)OC1CC2(C(CCC2O)C3=C1C4(C(OC(=O)C(=CN(CCO)C(C)(C)C)C4=C(C3=O)O)COC)C)C", "CHEMBL275224": "C1=CC=C2C(=C1)C3=C(N2)C=NC=C3", "CHEMBL373101": "CN1CCN(CC1)CC2=CN=C(C=C2)C3=CC4=NC=C(C(=C4S3)NC5=CC(=C(C=C5Cl)Cl)OC)C#N", "CHEMBL373751": "COC1=C(C=C2C(=C1)N=CN2C3=CC(=C(S3)C#N)OCC4=CC=CC=C4S(=O)(=O)C)OC", "CHEMBL379849": "C1C(=CC2=CC=CC=C2F)C(=O)C(=CC3=CC=CC=C3F)CN1", "CHEMBL383172": "CC1=C(C=C(C=C1)C(=O)NC2=NOC=C2)NC3=C(C(=NC=N3)NC4CCCC4)C#N", "CHEMBL410659": "C1CN(C1)CC2CC(C2)C3=NC(=C4N3C=CN=C4N)C5=CC6=C(C=C5)C=CC(=N6)C7=CC=CC=C7", "CHEMBL436817": "C1=CC(=C(C=C1NC2=C(C=NC3=C(C=C(C=C32)NCC4=CN=CN4)Cl)C#N)Cl)F", "CHEMBL482538": "C1=CC=C(C=C1)C2=C3C=CNC3=NC=C2", "CHEMBL484967": "C1CNCCC1OC2=C(C=C3C=CN=CC3=C2)C4=CC=C(C=C4)CN", "CHEMBL484968": "C1CNCCC1OC2=C(C=C3C=CN=CC3=C2)C4=CC=CC=C4", "CHEMBL489058": "CCN1CCN(CC1)CCC=CC2=CC3=NC=C(C(=C3C=C2)NC4=CC(=C(C=C4)SC5=NC=CN5C)Cl)C#N", "CHEMBL504547": "C1=CC(=C(C=C1CNC=C2C3=C(C=CC(=C3)I)C(=O)NC2=O)O)C4=COC=C4", "CHEMBL507249": "C1CCC(C1)NC2=NC=CC(=N2)C3=C(NN=C3)C4CCC(CC4)O", "CHEMBL516640": "COC1=CC=C(C=C1)N2C=NC3=C2C=C(C=C3)C4=NN=C(O4)SCC5=CC=CC(=C5)C#N", "CHEMBL519693": "C1CNCCC1OC2=C(C=C3C=CN=CC3=C2)C4=CC=C(C=C4)S(=O)(=O)N", "CHEMBL568922": "CCCC1=CC(=NC2=C1C(=C(S2)C(=O)N)N)N3CCNCC3", "CHEMBL574646": "C1C(=CC2=CC=CC=N2)C(=O)C(=CC3=CC=CC=N3)CN1", "CHEMBL576887": "CCCC1=CC(=NC2=C1C(=C(S2)C(=O)N)N)N3CCC(CC3)O", "CHEMBL576989": "CCCC1=CC(=NC2=C1C(=C(S2)C(=O)N)N)N3CCCC(C3)O", "CHEMBL578601": "CCCC1=CC(=NC2=C1C(=C(S2)C(=O)N)N)N3CCC(CC3)N", "CHEMBL79004": "C1=CC(=CN=C1)C(=O)NC2=C3C(=CC(=C2)Cl)C4=C(N3)C=NC=C4", "CHEMBL1222044": "C1=C(C=C2C(=C1[N+](=O)[O-])SC(=[N+]2[O-])C(=O)N)SC(F)(F)F", "CHEMBL1233887": "CN1C=C(C2=C1C=CC(=C2)OC)C3=CC4=NC=CN=C4N3", "CHEMBL1254007": "CN1C=CC2=C1C(=NC=N2)OC3=CC(=C(C=C3)NC(=O)NC4=CC=CC(=C4)C(F)(F)F)F", "CHEMBL1290072": "COC1=CC=C(C=C1)CNC2=C3C4=CC=CC=C4OC3=NC=C2", "CHEMBL1448": "C1=CC(=C(C=C1[N+](=O)[O-])Cl)NC(=O)C2=C(C=CC(=C2)Cl)O", "CHEMBL1651521": "CC1CC=CC(=O)CC(CCCC2=CC(=CC(=C2C(=O)O1)O)OC)O", "CHEMBL1684800": "CC1=C(C=C(C=C1)NC(=O)NC2=CC(=C(C=C2)Cl)C(F)(F)F)C(=O)NC3=C(N(N=C3)CC4=CC=C(C=C4)OC)N", "CHEMBL1765740": "CC1CCC(CN1C2=NC(=NC(=C2)C3=CC4=C(C=C3)C(=NN4)N)NC)C(=O)NC5CCCCC5", "CHEMBL1779202": "CC1(C2=C(C=CC(=C2)C3CCN(CC3)C4COC4)C(=O)C5=C1NC6=C5C=CC(=C6)C#N)C", "CHEMBL1784637": "CC1=C(C=C(C=C1)C(=O)NC2=CC(=C(C=C2)CN3CCN(CC3)CCO)C(F)(F)F)C#CC4=CN=C(N4C)C(=O)NC", "CHEMBL1822792": "CN1C=C(C=N1)C2=CN=C3C=CC4=C(C=C(C=C4)NS(=O)(=O)N(C)CC5COCCO5)C(=O)C3=C2", "CHEMBL1823221": "CCC1=C(C=C2C(=C1)C(=O)C3=C(C2(C)C)NC4=C3C=CC(=C4)C#N)N5CCN(CC5)C6COC6", "CHEMBL1870106": "CCN1C2=C(C=NC=C2C(=O)N3CCC(C3)N)N=C1C4=NON=C4N", "CHEMBL1934327": "CN1CCC(CC1)COC2=CC3=C(C=C2)C(=NC=N3)NC4=CC=C(C=C4)NC(=O)NC5=CC(=CC=C5)F", "CHEMBL1949855": "C1=CC2=C(C(=C1)Cl)NC=NC2=O", "CHEMBL1964948": "CC(C)(C)C1=NN(C(=C1)NC(=O)NC2=CC=CC3=CC=CC=C32)C4=CC=CC(=C4)C(=O)N(C)CCCN(C)C", "CHEMBL1966175": "CC1CCN(CC1C2=NC=C3N2C4=C(NC=C4)N=C3)C(=O)CC#N", "CHEMBL1967211": "C1=CC(=NC=C1C2=NN3C=CN=C3C=C2)F", "CHEMBL1967336": "C1=CN=C2C(=CC(=CC2=C1NC(=O)NC3=NC=CN=C3)F)F", "CHEMBL1967513": "C1=CC(=NC(=C1)NC(=O)NC2=C3C=C(C=CC3=NC=C2)Cl)C(F)(F)F", "CHEMBL1967998": "CCN1CCN(CC1)C2=CC=C(C=C2)NC3=NC=C(C(=N3)NC4=CC5=C(C=C4)NN=C5)Cl", "CHEMBL1968394": "CC1=CC=CC(=C1)C2=CC3=C(CNC3=O)C=C2", "CHEMBL1968515": "C1C(=O)NN=C2N1C3=CC=CC=C3OC2", "CHEMBL1968868": "C1=CC(=NC(=C1)NC(=O)NC2=C3C=CC(=CC3=NC=C2)C(F)(F)F)C#N", "CHEMBL1970290": "CCN(CC)CCNC(=O)C1=CC(=CC=C1)N2C(=CC(=N2)C(C)(C)C)NC(=O)NC3=CC=CC4=CC=CC=C43", "CHEMBL1971519": "C1=CC(=C2C(=C1)NN=C2N)C3=CC=C(C=C3)F", "CHEMBL1971606": "CCCOC1=CC=CC(=C1)C(C)NC(=O)C2=CC=C(C=C2)C3=C(C=NC=C3)F", "CHEMBL1972583": "C1=CC=C(C=C1)C2=CC=NC3=C(C=NN23)C(=O)N", "CHEMBL1973516": "CCN1CCN(CC1)C2=CC=C(C=C2)NC3=NC=C(C(=N3)NC4=CC5=C(C=C4)NN=C5)C#N", "CHEMBL1973795": "C1C2=C(C=C(C=C2)C3=CC=CC=C3)C(=O)N1", "CHEMBL1975212": "C1=CC=C(C=C1)C2=CSC3=NC=NC(=C23)N", "CHEMBL1975921": "C1=C2C(=NC=C1Br)NC(=O)N2", "CHEMBL1975927": "COC1=CC=C(C=C1)N2C=CC3=CN=C(N=C32)NC4=CC(=C(C(=C4)OC)OC)OC", "CHEMBL1976290": "CC1=C(C=CC(=C1)C2=CC3=C(C=C2)C(=O)NC3)F", "CHEMBL1977931": "CC(=O)C1=CC=CC=C1C2=C3C=CNC3=NC=N2", "CHEMBL1978271": "CC(C)(C)C1=NN(C(=C1)NC(=O)NC2=CC=CC3=CC=CC=C32)C4=CC=CC(=C4)C(=O)NCCOCCO", "CHEMBL1979773": "CC(C)(C)C1=NN(C(=C1)NC(=O)NC2=CC=CC3=CC=CC=C32)C4=CC=CC(=C4)C(=O)N(C)CCN", "CHEMBL1980671": "C1=CC=C2C(=C1)NC3=C(C(=NC=N3)N)C(=O)N2", "CHEMBL1981133": "C1=CC=C2C(=C1)C(=CN2)CC(COC3=CN=CC(=C3)C4=CC5=C(C=C4)C=NC=C5)N", "CHEMBL1981492": "COC(=O)C1=C(N=C2N1C=CC=C2)N", "CHEMBL1981744": "C1=CC(=NC(=C1)NC(=O)NC2=C3C=CC(=CC3=NC=C2)Cl)C(F)(F)F", "CHEMBL1981792": "C1=CC(=NC(=C1)NC(=O)NC2=C3C=C(C(=CC3=NC=C2)F)F)C(F)(F)F", "CHEMBL1983070": "CCOC1=CC=CC=C1C2=CC(=CC=C2)C3=C4C(=CC(=O)N=C4NN3)C", "CHEMBL1983573": "C=CC1=CC=C(C=C1)C2=CC=CC3=NN=C(N32)N", "CHEMBL1984402": "CC(=O)C1=C(C(=O)N(N=C1C2=CC=CC=C2)C)N", "CHEMBL1984847": "CC(=O)OCCN1C2=NC(=O)C=C(C2=C(N1)C3=CC(=CC=C3)Br)C(F)(F)F", "CHEMBL1985042": "CC1=CC(=O)NC2=C1C(=O)N(N2)C3=CC=CC=C3", "CHEMBL1986684": "CC1=NC2=CC(=NN2C(=C1)C(=O)N)C(C)(C)C", "CHEMBL1986756": "CCC1=CC2=NC=CC(=C2C=C1)NC(=O)NC3=CC=CC(=N3)C(F)(F)F", "CHEMBL1986851": "CC1=CC(=CC=C1)NC(=O)NC2=C(C=C(C=C2)C3=CSC4=C3C(=NC=C4C5=CN(N=C5)CCO)N)F", "CHEMBL1987815": "C1=CSC(=C1)C2=CC(=NC3=CC=NN32)C(=O)N", "CHEMBL1988622": "C1=CC=C(C=C1)C=CC2=NN3C=CN=C3C=C2", "CHEMBL1990590": "CC1=CC(=O)N=C2C1=C(NN2)C3=CC=CC(=C3)C4=CC=C(C=C4)Cl", "CHEMBL1991867": "C12=C(NN=C1N=C(S2)Cl)N", "CHEMBL1992073": "CCC1CC(CC1C2=NC=C3N2C4=C(NC=C4)N=C3)NS(=O)(=O)C5CC5", "CHEMBL1992125": "CC1=CC2=C(C=C1)N(CCC2)C3=NC(=NC=N3)NC4=CC(=C(C(=C4)OC)OC)OC", "CHEMBL1994159": "CC(=O)C1=CC=CC(=C1)C2=NN3C=CN=C3C=C2", "CHEMBL1994977": "CC(C)(C)C1=NN(C(=C1)NC(=O)NC2=CC=CC3=CC=CC=C32)C4=CC=CC(=C4)C(=O)NCCCCO", "CHEMBL1995211": "CC(C)(C)NC1=NC=NC2=C1C(=CN2)C3=CC=CC=C3", "CHEMBL1996510": "C1CN(CCN1)C2=NC3=CC=CC=C3C(=N2)C4=C(C(=O)NC4=O)C5=CNC6=CC=CC=C65", "CHEMBL1997041": "CC1=C(C=CC(=C1)C2=C3C=CNC3=NC=N2)F", "CHEMBL1997119": "C1=CC=C(C=C1)C2=CC=CC3=CN=C(N32)N", "CHEMBL2000724": "CC1=CC(=O)N=C2C1=C(NN2)C3=CC=CC(=C3)C4=CC=C(C=C4)C#N", "CHEMBL2001987": "C1=CC(=NC(=C1)NC(=O)NC2=CC=NC3=C(C=CC(=C23)F)F)C(F)(F)F", "CHEMBL2002099": "C1CCC(C1)C(CC#N)N2C=C(C=N2)C3=C4C=CNC4=NC=N3", "CHEMBL2002599": "C1C2COCC2CN1C3=CC4=C(C=CN=C4C=C3)NC(=O)NC5=NC=CN=C5", "CHEMBL2003785": "C1=CC(=CC(=C1)F)CNC2=NC=NC3=C2NC=N3", "CHEMBL2004637": "CCN(CCN)C(=O)C1=CC(=CC=C1)N2C(=CC(=N2)C(C)(C)C)NC(=O)NC3=CC=CC4=CC=CC=C43", "CHEMBL2006564": "CCN(C1=CC=C(C=C1)NC2=NC3=C(C(=N2)NC4CC4)NC=N3)C(=O)C", "CHEMBL2007375": "CC#CC1=CC2=C(C=CN=C2C=C1)NC(=O)NC3=CC=CC(=N3)C(F)(F)F", "CHEMBL2007421": "CC(C)OC1=NNC(=C1)NC2=NC(=NC=C2Cl)NC(C)C3=NC=C(C=C3)F", "CHEMBL2010872": "CC(C)CN1C2=C(C=C(C=C2)NC3=NC=CC=N3)C4=C5CNC(=O)C5=C6C(=C41)CCC7=NN(C=C76)C", "CHEMBL201307": "COC1=C(C=C2C(=C1)C(=NC=N2)NC3=NC=C(S3)CC(=O)NC4=CC(=CC=C4)F)OCCCN5CCC(CC5)CO", "CHEMBL2029988": "CC(C)(C1=CC(=NO1)NC(=O)NC2=CC(=CC=C2)OC3=NC=NC4=CC(=C(C=C43)OC)OC)C(F)(F)F", "CHEMBL2031893": "CC1=C(C(=O)N(N1C)C2=CC=CC=C2)C(=O)NC3=CC(=C(C=C3)OC4=C5C=C(C(=CC5=NC=C4)OC)OC)F", "CHEMBL2035810": "C=CC(=O)NCC1=COC(=N1)C2=C(N=CN=C2NC3=CC(=C(C=C3)OCC4=CC=CC=N4)Cl)N", "CHEMBL2042135": "CC(C=CC(F)(F)F)OC1=C(C=CC(=C1)C2=C(N=CC(=C2)C3=CC(=CS3)CN(C)C)N)C(=O)N", "CHEMBL2046883": "CC1=CC=C(C=C1)NC(=O)NC2=NN=C(S2)SC3=NC=NC4=C3C=CC(=C4)OCCCN5CCOCC5", "CHEMBL2071201": "CN1C=C(C=N1)NC2=NC=C(C(=N2)NC3C4CC(C3C(=O)N)C=C4)Br", "CHEMBL214329": "CN1CCN(CC1)C2=CC=C(C=C2)NC3=NC=C4C=CN(C4=N3)C5CCCCC5", "CHEMBL215943": "CC1=C(C=C(C=C1)C(=O)NC2=CC=CC(=C2)C(F)(F)F)C3=CC4=CN=C(N=C4C=C3)NCCN5CCOCC5", "CHEMBL243518": "CC1=C(C=C(C=C1)NC2=NC=CC(=N2)NC3=CC=CC=C3C(=O)O)F", "CHEMBL298445": "CC1=C(SC(=N1)N)C2=NC(=NC=C2)NC3=CC(=CC=C3)[N+](=O)[O-]", "CHEMBL301018": "COC1=C(C=C2C(=C1)C(=NC=N2)NC3=CC(=C(C=C3)F)Cl)OC", "CHEMBL373882": "CNC1=NC=NC(=N1)C2=C(N=CC=C2)OC3=CC(=C(C=C3)F)C(=O)NC4=C(C=CC(=C4)C(F)(F)F)N(C)CCCN(C)C", "CHEMBL386661": "CC1=C(C=C(C=C1)C(=O)NC2=C(C=CC(=C2)C(F)(F)F)OC3CCN(CC3)C)C4=CC5=CN=C(N=C5C=C4)NC", "CHEMBL387385": "C1=CC(=CC(=C1)Cl)C2=CNNC2=C3C=C(N=C3)C(=O)NC(CO)C4=CC(=C(C=C4)F)Cl", "CHEMBL393929": "C1=CC2=C(C=CC(=C2)C=C3C(=O)N=C(S3)NCC4=CC=CS4)N=C1", "CHEMBL429743": "COC1=CC2=C(C=CN=C2C=C1OC)OC3=CC4=C(C=C3)C(=CC=C4)C(=O)NC5=CC=C(C=C5)Cl", "CHEMBL447602": "CN1C(=O)C(=CN=C1NC2=CC=C(C=C2)F)C3=NC=C(C=C3)OC4=C5C=C(C(=CC5=NC=C4)OCCCN6CCOCC6)OC", "CHEMBL453737": "CN1C(=O)C(=CN=C1NC2=CC=C(C=C2)F)C3=CC(=C(C=C3)OC4=C5C=C(C(=CC5=NC=C4)OCCCN6CCOCC6)OC)F", "CHEMBL460472": "CC1=C(C(=O)N(N1CC(C)(C)O)C2=CC=CC=C2)C(=O)NC3=NC=C(C=C3)OC4=C5C=CC(=CC5=NC=C4)OC", "CHEMBL461139": "C1COCCN1CC2=CC=C(C=C2)C=CC3=NC=CC(=C3)C4=CC5=C(N4)NC=NC5=O", "CHEMBL461140": "CN(C)CCOC1=CC=C(C=C1)C=CC2=NC=CC(=C2)C3=CC4=C(N3)NC=NC4=O", "CHEMBL465465": "CS(=O)(=O)C1=CC=C(C=C1)CNCC2=C(C(=C(C(=C2)C(=O)O)NC3=C(C=C(C=C3)I)F)F)F", "CHEMBL476124": "C1=C(C=C(C2=C1[N+](=C(S2)C(=O)N)[O-])[N+](=O)[O-])C(F)(F)F", "CHEMBL481968": "C1=CC(=C(C=C1I)F)NC2=C(C(=C(C=C2C(=O)O)C=NNC(=O)C3=CC=C(O3)CO)F)F", "CHEMBL481969": "C1=CC(=CC=C1S(=O)(=O)CC(=O)NN=CC2=C(C(=C(C(=C2)C(=O)O)NC3=C(C=C(C=C3)I)F)F)F)Cl", "CHEMBL490555": "C1=CC=C2C(=C1)N=C(S2)C3=CC(=CC=C3)NC4=NC=NC5=C4C=CN5", "CHEMBL49120": "CCN(CC)CCOC1=CC=C(C=C1)NC2=NC=C3C=C(C(=O)N(C3=N2)C)C4=C(C=CC=C4Cl)Cl", "CHEMBL491686": "CC1=CC(=NN1)NC2=NC(=NC=C2)NC3=CC=CC(=C3)C4=NC5=CC=CC=C5S4", "CHEMBL493169": "C1CNCCC1NC2=NN3C(=NN=C3C4=CC(=CC=C4)C(F)(F)F)C=C2", "CHEMBL495727": "C1CC1NC(=O)NC2=CNNC2=C3N=C4C=CC(=CC4=N3)CN5CCOCC5", "CHEMBL505896": "CN1C(=NC=C(C1=O)C2=CC(=C(C=C2)OC3=C4C=C(C(=CC4=NC=C3)OCCCN5CCOCC5)OC)F)CC6=CC=CC=C6", "CHEMBL514409": "CCS(=O)(=O)NC1=CC2=C(C=C1)NC(=O)C2=C(C3=CC=CC=C3)NC4=CC=C(C=C4)CN5CCCCC5", "CHEMBL517647": "C1=CC(=C(C=C1I)F)NC2=C(C(=C(C=C2C(=O)O)CNC(=O)C(CC(=O)N)N)F)F", "CHEMBL522785": "CC1=CC(=NN1)NC2=NC3=CC(=C(C=C3C(=N2)NC4=CC=CC(=C4)C5=NC6=CC=CC=C6S5)OC)OC", "CHEMBL600795": "CC(C1=C(C=CC(=C1Cl)F)Cl)OC2=CC3=C(C=C2)N=CC=C3", "CHEMBL602471": "CC(C1=C(C=CC(=C1Cl)F)Cl)OC2=CC3=CC(=CN=C3C=C2)C=CC(=O)N", "CHEMBL602472": "CC(C1=C(C=CC(=C1Cl)F)Cl)OC2=CC3=CC(=CN=C3C=C2)C4CC4C(=O)N", "CHEMBL1977604": "CC1CSC2=C(C(=O)C3=CC(=C(C(=C3N12)F)N4CCC(C4)N)F)C(=O)O", "CHEMBL1985309": "C1CCN(C1)CCNC2=CC=CC(=N2)C3=NC4=C(C=CC=C4N3)C(=O)N", "CHEMBL1996604": "COC1=C(C=C(C=C1)C=C2C(=O)N=C(S2)NC3=CC=CC=C3)OC", "CHEMBL1092754": "CN1C=C(C2=C(C=CN=C21)C3=CC=C(C=C3)C(=O)NCCO)C=C4C(=O)C5=C(O4)C=CC=C5O", "CHEMBL309265": "C1=CC=C(C=C1)S(=O)(=O)NC2=C3C(=CC(=C2)Cl)C4=C(N3)C=NC=C4", "CHEMBL309953": "C1=CNC=C2C1=C3C=C(C(=O)C(=C3N2)Cl)Cl", "CHEMBL310179": "COC1=CC=CC(=C1)C(=O)NC2=C3C(=CC(=C2)Cl)C4=C(N3)C=NC=C4", "CHEMBL310975": "COC1=C(C2=C(C=C1)NC3=C2C=CN=C3)Br", "CHEMBL311201": "C1=CC2=C(C=C1Cl)C3=C(N2)C=NC=C3", "CHEMBL311306": "C1COCCN1C(=O)NC2=C3C(=CC(=C2)Cl)C4=C(N3)C=NC=C4", "CHEMBL312170": "C1CCC(CC1)COC2=C(C=C3C4=C(C=NC=C4)NC3=C2Cl)Cl", "CHEMBL312648": "COC1=CC=CC=C1C(=O)NC2=C3C(=CC(=C2)Cl)C4=C(N3)C=NC=C4", "CHEMBL312651": "COC1=C(C=C2C3=C(C=NC=C3)NC2=C1Cl)Cl", "CHEMBL312676": "CS(=O)(=O)NC1=C2C(=CC(=C1)Cl)C3=C(N2)C=NC=C3", "CHEMBL312698": "COC(=O)NC1=C2C(=CC(=C1)Cl)C3=C(N2)C=NC=C3", "CHEMBL460702": "CCOC1=C(C(=O)N(C=C1)C2=CC=C(C=C2)F)C(=O)NC3=CC(=C(C=C3)OC4=C(C(=NC=C4)N)Cl)F", "CHEMBL466496": "CC(C1=CC=CC=C1)NC2=C(C(=O)C2=O)NC3=CC=NC=C3", "CHEMBL468125": "CC(C1=CC=CC=C1)NC2=C(C(=O)C2=O)NC3=CC(=NC=C3)C4=CC=CC=C4F", "CHEMBL481248": "CC(C1=CC=CC=C1)NC2=C(C(=O)C2=O)NC3=CC(=NC=C3)C4=CSC=C4", "CHEMBL511410": "C1=CC(=CC(=C1)O)C(C(=O)N)NC2=C(C(=O)C2=O)NC3=CC=NC=C3", "CHEMBL519113": "CC(C1=CC=CC=C1)NC2=C(C(=O)C2=O)NC3=CC(=NC=C3)C4=CC=CO4", "CHEMBL78464": "C1=CN=CC2=C1C3=CC(=CC(=C3N2)Cl)Cl", "CHEMBL78618": "C1=CC2=C(C=C1C(F)(F)F)C3=C(N2)C=NC=C3", "CHEMBL78862": "C1=CC=C(C=C1)C(=O)NC2=C3C(=CC(=C2)Cl)C4=C(N3)C=NC=C4", "CHEMBL78885": "COC1=CC=C(C=C1)C(=O)NC2=C3C(=CC(=C2)Cl)C4=C(N3)C=NC=C4", "CHEMBL78917": "C1=CC=NC(=C1)C(=O)NC2=C3C(=CC(=C2)Cl)C4=C(N3)C=NC=C4", "CHEMBL80121": "CC(=O)NC1=C2C(=CC(=C1)Cl)C3=C(N2)C=NC=C3", "CHEMBL80619": "COC1=CC2=C(C=C1)NC3=C2C=CN=C3", "CHEMBL80793": "C1=CC=C(C=C1)CNC2=C3C(=CC(=C2)Cl)C4=C(N3)C=NC=C4", "CHEMBL80843": "C1=CN=CC=C1C(=O)NC2=C3C(=CC(=C2)Cl)C4=C(N3)C=NC=C4", "CHEMBL81169": "C1=CC2=C(C=C1Br)C3=C(N2)C=NC=C3", "CHEMBL81170": "C1=CC2=C(C=C1F)C3=C(N2)C=NC=C3", "CHEMBL81214": "C1=CC2=C(C=C1C#N)C3=C(N2)C=NC=C3", "CHEMBL81229": "CCOC1=C(C=C2C3=C(C=NC=C3)NC2=C1Cl)Cl", "CHEMBL81315": "CNC(=O)NC1=C2C(=CC(=C1)Cl)C3=C(N2)C=NC=C3", "CHEMBL81603": "C1CC1COC2=C(C=C3C4=C(C=NC=C4)NC3=C2Cl)Cl", "CHEMBL81809": "C1COCCN1C(=O)OC2=C(C=C3C4=C(C=NC=C4)NC3=C2Cl)Cl", "CHEMBL81838": "C1=CN=CC2=C1C3=CC(=CC(=C3N2)[N+](=O)[O-])Cl", "CHEMBL82136": "C1=CC=NC(=C1)CC(=O)NC2=C3C(=CC(=C2)Cl)C4=C(N3)C=NC=C4", "CHEMBL82137": "C1=CN=CC2=C1C3=CC(=CC(=C3N2)NC(=O)CCCO)Cl", "CHEMBL102301": "COC1=C(C=C2C(=C1)C(=NC=N2)N3CCN(CC3)C(=S)NCC4=CC5=C(C=C4)OCO5)OC", "CHEMBL106966": "COC1=C(C=C2C(=C1)C(=NC=N2)N3CCN(CC3)C(=O)NC4=CC=C(C=C4)C#N)OC", "CHEMBL115769": "COC1=CC(=NC2=C1C(=C(N2)C3=CC=C(C=C3)F)C4=CC=NC=C4)N", "CHEMBL131577": "CC1=C(C(=CC=C1)Cl)NC(=O)C2=CN=C(S2)NC(=O)C3CC3", "CHEMBL185238": "CC1=CC=CC(=N1)C2=C(C=NN2)C3=NC4=C(C=C3)N=CC=C4", "CHEMBL186290": "CC1=CC2=C3C(=C1)C(=CN3CCN(C2)C(=O)N4CCCCC4)C5=C(C(=O)NC5=O)C6=CN=C7N6C=CC=C7", "CHEMBL197538": "C1COCCN1CCNC2=NC=C3C(=C2)C(=C(C=N3)C#N)NC4=CC(=C(C=C4)F)Cl", "CHEMBL199210": "C1COCCN1CCNC2=NC=C3C(=C2)C(=C(C=N3)C#N)NC4=CC=C(C=C4)SC5=CC=CC=C5", "CHEMBL200381": "C1=CC(=CN=C1)CNC2=NC=C3C(=C2)C(=C(C=N3)C#N)NC4=CC(=C(C=C4)F)Cl", "CHEMBL29197": "COC1=C(C=C2C(=C1)C(=NC=N2)NC3=CC(=CC=C3)Br)OC", "CHEMBL303144": "CC(C1=CC=CC=C1)NC2=NC=CC(=C2)C3=C(N=C(N3C)C4CCNCC4)C5=CC(=CC=C5)C(F)(F)F", "CHEMBL305178": 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"CHEMBL217090": "C1CCN(C1)CCCOC2=CC(=C3C(=C2)N=CN=C3NC4=C(C=CC5=C4OCO5)Cl)OC6CCOCC6", "CHEMBL217092": "CN1CCN(CC1)CCOC2=CC(=C3C(=C2)N=CN=C3NC4=C(C=CC5=C4OCO5)Cl)OC6CCOCC6", "CHEMBL281872": "COC1=C(C=C2C(=C1)C(=NC=N2)NC3=C(C=C(C=C3)Br)F)OCCN4C=CN=N4", "CHEMBL533849": "CN1CCC(CC1)COC2=C(C=C3C(=C2)N=CN=C3NC4=C(C=C(C=C4)Br)F)OC.Cl", "CHEMBL86755": "C1=CC=C2C(=C1)C(=CC3=CC=CN3)C(=O)N2", "CHEMBL148471": "C1C2=CC=CC=C2C3=C4CNC(=O)C4=C5C6=CC=CC=C6NC5=C31", "CHEMBL1966501": "CC1=C(C=CC(=C1)OCC2=CC(=CC=C2)C(F)(F)F)CN3CC(C3)C(=O)O", "CHEMBL1971132": "C1C(CN1CC2=CC=C(C=C2)OCC3=CC(=CC=C3)C(F)(F)F)C(=O)O", "CHEMBL1971223": "CC(C)C(CO)NC(=O)C1=CC(=CC=C1)N2C(=CC(=N2)C(C)(C)C)NC(=O)NC3=CC=CC4=CC=CC=C43", "CHEMBL1974998": "CC(C)(C)C1=NN(C(=C1)NC(=O)NC2=CC=CC3=CC=CC=C32)C4=CC=CC(=C4)C(=O)N(C)CCC#N", "CHEMBL1985469": "CN(C)C1=CC=C(C=C1)NC(=O)CC2C(=O)NC3=CC=CC=C3N2", "CHEMBL1986666": "C1=CC=C(C(=C1)C(=O)O)NC2=NC=NC(=N2)NC3=CC4=C(C=C3)C=NN4", "CHEMBL1991377": "CC1=CC(=O)N=C2C1=C(NN2)C3=CC(=CC=C3)C(F)(F)F", "CHEMBL1994318": "CC(C)N(CCCN)C(=O)C1=CC(=CC=C1)N2C(=CC(=N2)C(C)(C)C)NC(=O)NC3=CC=CC4=CC=CC=C43", "CHEMBL1997275": "COC1=CC2=C(C=C1)NC=C2C=C3C4=CC=CC=C4NC3=O", "CHEMBL1999506": "CC(C)(C)C1=NN(C(=C1)NC(=O)NC2=CC=CC3=CC=CC=C32)C4=CC=CC(=C4)C(=O)NCCCCC(=O)O", "CHEMBL2000879": "C1CC2=C(CC1C3=CC=CC=C3)C=NN2", "CHEMBL2001398": "CC(C)(C)CCOC1=CC(=CC2=C1C(=NN2)N)C3=CC=C(C=C3)C(=O)N", "CHEMBL2002660": "CC(C)(C)C1=NN(C(=C1)NC(=O)NC2=CC=CC3=CC=CC=C32)C4=CC=CC(=C4)C(=O)N(C)CCOC", "CHEMBL2002736": "CCOCC(C)OC1=CC=CC2=C1C(=NN2)N", "CHEMBL2007073": "CC(C)(C)C1=NN(C(=C1)NC(=O)NC2=CC=CC3=CC=CC=C32)C4=CC=CC(=C4)C(=O)NCCCO", "CHEMBL221536": "C1C2=C3C4=CC=CC=C4NC3=C5C(=C2C(=O)N1)C6=CC=CC=C6S5", "CHEMBL243298": "C1=CC=C(C(=C1)C(=O)O)NC2=NC(=NC=C2)NC3=CC(=CC=C3)F", "CHEMBL357490": "C1C2=CC=CC=C2C3=C4C(=C5C6=CC=CC=C6NC5=C31)CNC4=O", "CHEMBL374581": "C1CC2=C3C(=C4C(=C2C5=CC=CC=C51)CNC4=O)C6=CC=CC=C6N3", "CHEMBL386636": "C1CC2=C3C(=C4C(=C2C5=CC=CC=C51)C(=O)NC4=O)C6=CC=CC=C6N3", "CHEMBL416056": 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"CHEMBL494221": "C1CC(CCC1NC2=NN3C(=NN=C3C4=CC(=CC=C4)C(F)(F)F)C=C2)O", "CHEMBL104264": "C1=CC2=C(C=CN=C2)C(=C1)S(=O)(=O)NCCNCC=CC3=CC=C(C=C3)Br", "CHEMBL559147": "CC(C1CCC(CC1)C(=O)NC2=CC=NC=C2)N", "CHEMBL604087": "COC1=C(C=C(C=C1)C(=O)NCC2=CC=CC(=C2)C(=O)NC3=CC4=C(CCNC4)C=C3)OC", "CHEMBL2347053": "C1=CC=C2C(=C1)C(=CC3=C(NN=C3)C4=CC=CC=C4[N+](=O)[O-])C(=O)N2", "CHEMBL410295": "CC1=C(C(=CC=C1)C)N2C(=O)C3=CN=C(N=C3N4C2=NC5=CC=CC=C54)NC6=CC=C(C=C6)N7CCN(CC7)C", "CHEMBL583187": "C1CN(CC1O)CC2=NC(=O)C3=C(N2)C4=C(S3)C=CC(=C4)C5=CC=C(C=C5)O", "CHEMBL6291": "CN1C=C(C2=CC=CC=C21)C3=C(C(=O)NC3=O)C4=CN(C5=CC=CC=C54)CCCSC(=N)N", "CHEMBL100102": "C1=CC=C2C(=C1)C=C(N2)C3=C(C(=O)NC3=O)NCCCCCCN", "CHEMBL102346": "COC1=C(C=C2C(=C1)C(=NC=N2)N3CCN(CC3)C(=O)NC4=CC=C(C=C4)OC5=CC=CC=C5)OC", "CHEMBL104067": "CC(C)C1=CC=C(C=C1)NC(=O)N2CCN(CC2)C3=NC=NC4=CC(=C(C=C43)OC)OC", "CHEMBL111779": "C1=CC=C2C(=C1)C3=C4C(=C5C6=C(C=CC(=C6)O)N(C5=C3N2)C7C(C(C(C(O7)CO)O)O)O)C(=O)N(C4=O)NC(CO)CO", "CHEMBL111889": "C1=CC=C2C(=C1)C3=C4C(=C5C6=C(C=CC=C6O)N(C5=C3N2)C7C(C(C(C(O7)CO)O)O)O)C(=O)N(C4=O)NC(CO)CO", "CHEMBL112235": "C1=CC2=C(C=C1O)NC3=C4C(=C5C(=C23)C(=O)N(C5=O)NC(CO)CO)C6=C(N4C7C(C(C(C(O7)CO)O)O)O)C=C(C=C6)O", "CHEMBL112239": "C1=CC2=C(C=C1O)N(C3=C4C(=C5C(=C23)C(=O)N(C5=O)NC(CO)CO)C6=CC(=CC(=C6N4)O)O)C7C(C(C(C(O7)CO)O)O)O", "CHEMBL112263": "COC1=CC(=CC(=C1OC)OC)NC2=NC=CC(=N2)C3=CN=CC=C3", "CHEMBL112346": "CCC1CN(CCN1)C2=NC=C(C=C2)C3=NC(=NC=C3)NC4=CC(=C(C(=C4)OC)OC)OC", "CHEMBL112602": "C1=CC2=C(C(=C1)O)NC3=C4C(=C5C(=C23)C(=O)N(C5=O)NC(CO)CO)C6=C(N4C7C(C(C(C(O7)CO)O)O)O)C=CC(=C6)O", "CHEMBL113185": "COC1=CC(=CC(=C1OC)OC)NC2=NC=CC(=N2)C3=CN=C(C=C3)NCCN", "CHEMBL115531": "C1CC2=CC(=N)N(N=C2C3=CC=CC=C31)CCCCCCCCCCC(=O)NC4=NN=C(C=C4)C5=CC=CC=C5", "CHEMBL1159459": "C1=C(C=C(C(=C1O)O)O)C(=O)OCC2C3C(C(C(O2)OC(=O)C4=CC(=C(C(=C4)O)O)O)OC(=O)C5=CC(=C(C6=C5C(C(C(=O)O3)CC(=O)O)C(C(=O)O6)O)O)O)OC(=O)C7=CC(=C(C(=C7)O)O)O", "CHEMBL1159460": "C1=C(C=C(C(=C1O)O)O)C(=O)OCC2C3C(C(C(O2)OC(=O)C4=CC(=C(C(=C4)O)O)O)OC(=O)C5=CC(=C(C6=C5C7C(=CC(=O)C(C7(O6)O)(O)O)C(=O)O3)O)O)OC(=O)C8=CC(=C(C(=C8)O)O)O", "CHEMBL1159461": "C1=C(C=C(C(=C1O)O)O)C(=O)OC2C3C(C(C(O2)CO)OC(=O)C4=CC(=O)C(C5(C4C6=C(O5)C(=C(C=C6C(=O)O3)O)O)O)(O)O)O", "CHEMBL1159462": "C1=C(C=C(C(=C1O)O)O)C(=O)OCC2C(C(C(C(O2)OC(=O)C3=CC(=C(C(=C3)O)O)O)O)O)OC(=O)C4=CC(=C(C(=C4)O)O)O", "CHEMBL1159463": "C1=C(C=C(C(=C1O)O)O)C(=O)OCC2C(C(C(C(O2)OC(=O)C3=CC(=C(C(=C3)O)O)O)OC(=O)C4=CC(=C(C(=C4)O)O)O)OC(=O)C5=CC(=C(C(=C5)O)O)O)O", "CHEMBL1159466": "C1C2C3C(C(C(O2)OC(=O)C4=CC(=C(C(=C4)O)O)O)OC(=O)C5=CC(=C(C6=C5C7C(=CC(=O)C(C7(O6)O)(O)O)C(=O)O3)O)O)OC(=O)C8=CC(=C(C(=C8C9=C(C(=C(C=C9C(=O)O1)O)O)O)O)O)O", "CHEMBL1159467": "C1C2C3C(C(C(O2)OC(=O)C4=CC(=C(C(=C4)O)O)O)OC(=O)C5=CC(=C(C6=C5C7C(=CC(=O)C(C7(O6)O)(O)O)C(=O)O3)O)O)OC(=O)C8=CC(=C(C(=C8C9=C(C(=C(C=C9C(=O)O1)OC1=C(C(=C(C=C1C(=O)O)O)O)O)O)O)O)O)O", "CHEMBL1159468": "C1C2C(C(C(C(O2)OC(=O)C3=CC(=C(C(=C3)O)O)O)O)OC(=O)C4=CC(=C(C(=C4C5=C(C(=C(C=C5C(=O)O1)OC6=C(C(=C(C=C6C(=O)O)O)O)O)O)O)O)O)O)O", "CHEMBL116963": "C1=CC=C(C=C1)C2=NN=C(C=C2)NC(=O)CCCCCCCCCCN3C(=N)C=CC(=N3)C4=CC=CC=C4", "CHEMBL117443": "CC1=NN(C(=N)C=C1)CCCCCCCCCCC(=O)NC2=NN=C(C=C2)C3=CC=CC=C3", "CHEMBL1202927": "CN1C=C(C2=CC=CC=C21)C3=C(C(=O)NC3=O)C4=C5CC(CCN5C6=CC=CC=C64)CN(C)C.Cl", "CHEMBL1233654": "CC1CNCCN1S(=O)(=O)C2=CC=CC3=C2C=CN=C3", "CHEMBL127277": "C1=CC=C2C(=C1)C3=C4C(NC(=O)C4=C5C6=CC=CC=C6NC5=C3N2)O", "CHEMBL127929": "CCOC(=O)CSC1=CN=C(S1)NC(=O)C", "CHEMBL129946": "CCN(C)C1CC2N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N(C7=C53)C(C1OC)(O2)C)CNC6=O", "CHEMBL130049": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)CNC6=O)N(C)C(=O)OC)OC", "CHEMBL130163": "CC(=O)N(C)C1CC2N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N(C7=C53)C(C1OC)(O2)C)CNC6=O", "CHEMBL130181": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(NC(=O)C6=C7C8=CC=CC=C8N2C7=C53)O)NC)OC", "CHEMBL130208": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)CNC6=O)N(C)C(=O)C9=CC(=CC=C9)[N+](=O)[O-])OC", "CHEMBL131020": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)CNC6=O)N(C)S(=O)(=O)C)OC", "CHEMBL131193": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)CNC6=O)N(C)CC9=CC=CC=C9)OC", "CHEMBL131426": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)CNC6=O)N(C)CCC#N)OC", "CHEMBL131456": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)CN(C6=O)CC(=O)OC)N(C)C(=O)C9=CC=CC=C9)OC", "CHEMBL131590": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)CNC6=O)N(C)C(=O)C9=CC=CC=C9Cl)OC", "CHEMBL131715": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)CNC6=O)N(C)C(=O)C9=CC=C(C=C9)Cl)OC", "CHEMBL132169": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)CNC6=O)N(C)C(=O)C9=CC=C(C=C9)OC)OC", "CHEMBL132170": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)CNC6=O)N(C)C(=O)C9=CC(=CC(=C9)[N+](=O)[O-])[N+](=O)[O-])OC", "CHEMBL132348": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)CNC6=O)N(C)CC(=O)O)OC", "CHEMBL132533": "C1=CC2=C(C=C1O)NC3=C4C(=C5C(=C23)C(=O)N(C5=O)NC(CO)CO)C6=C(N4C7C(C(C(O7)CO)O)O)C=C(C=C6)O", "CHEMBL133209": "C1=CC2=C(C=C1O)NC3=C4C(=C5C(=C23)C(=O)N(C5=O)NC(CO)CO)C6=C(N4C7C(C(C(O7)CO)O)O)C=C(C=C6)O", "CHEMBL134536": "CC1C(C(C(C(O1)N2C3=C(C=CC(=C3)O)C4=C5C(=C6C7=C(C=C(C=C7)O)NC6=C42)C(=O)N(C5=O)NC(CO)CO)O)O)O", "CHEMBL135491": "C1=CC2=C(C=C1O)NC3=C4C(=C5C(=C23)C(=O)N(C5=O)NC(CO)CO)C6=C(N4C7C(C(C(O7)CO)O)O)C=C(C=C6)O", "CHEMBL135492": "C1=CC2=C(C=C1O)NC3=C4C(=C5C(=C23)C(=O)N(C5=O)NC(CO)CO)C6=C(N4C7C(C(C(O7)CO)O)O)C=C(C=C6)O", "CHEMBL135881": "C1=CC2=C(C=C1O)NC3=C4C(=C5C(=C23)C(=O)N(C5=O)NC(CO)CO)C6=C(N4C7C(C(C(O7)C(CO)O)O)O)C=C(C=C6)O", "CHEMBL135970": "C1=CC2=C(C=C1O)NC3=C4C(=C5C(=C23)C(=O)N(C5=O)NC(CO)CO)C6=C(N4C7C(C(C(O7)CO)O)O)C=C(C=C6)O", "CHEMBL139517": "C1=CC2=C(C(=C1)Cl)NC3=C4C(=C5C(=C23)C(=O)NC5=O)C6=C(N4)C(=CC=C6)Cl", "CHEMBL140600": "CC12C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)CNC6=O)(C(=O)O)O", "CHEMBL141247": "C1CC2C3=C(C=CC=C3NC(=O)NC4=CC=CC=N4)C(=O)N2C1", "CHEMBL14217": "C1=CC=C2C(=C1)C3=C(N2)C(=NC=C3)C4=C(C=CC(=C4)[N+](=O)[O-])Cl", "CHEMBL14445": "CC1=NC=CC2=C1NC3=C2C=CC(=C3)F", "CHEMBL144479": "C1CC2N(C1N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)C(=O)NC6=O)CC9=CC=CC=C9", "CHEMBL144598": "C1CC2N(C(C1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)C(=O)NC6=O)CC9=CC=CC=C9", "CHEMBL146564": "C1C2NC(CO1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)C(=O)NC6=O", "CHEMBL147986": "C1CC2NC(C1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)C(=O)NC6=O", "CHEMBL148333": "CNCCNS(=O)(=O)C1=CC=CC2=C1C=CN=C2", "CHEMBL151546": "C1=CC2=C(C(=C1)NC(=O)N)C(=O)C3=C2NN=C3C4=CSC(=C4)Cl", "CHEMBL154620": "COC1C(OC(C(C1O)O)N2C3=CC=CC=C3C4=C5C(=C6C7=CC=CC=C7NC6=C42)C(=O)N(C5=O)CCCCOC(=O)CBr)CO", "CHEMBL156776": "COC1C(OC(C(C1O)O)N2C3=C(C=CC=C3Cl)C4=C5C(=C6C7=C(C(=CC=C7)Cl)NC6=C42)C(=O)NC5=O)COC(=O)CBr", "CHEMBL160030": 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"C1=CC2=C(C=C1O)NC3=C4C(=C5C(=C23)C(=O)N(C5=O)NC(CO)CO)C6=C(N4C7C(C(C(C(O7)CO)OC8C(C(C(C(O8)CO)O)O)O)O)O)C=C(C=C6)O", "CHEMBL2311100": "C1=C(C=C(C(=C1O)O)O)C(=O)OCC2C(C(C(O2)O)(COC(=O)C3=CC(=C(C(=C3)O)O)O)O)OC(=O)C4=CC(=C(C(=C4)O)O)O", "CHEMBL263188": "CC(C(=O)NC(CO)C(=O)NC(CCCN=C(N)N)C(=O)NC(CCCN=C(N)N)C(=O)NC(CCCN=C(N)N)C(=O)NC(CCCN=C(N)N)C(=O)O)NC(=O)C(C)NS(=O)(=O)C1=CC=C(C2=CC=CC=C21)N(C)C", "CHEMBL263225": "CC(C(=O)NC(CO)C(=O)NC(CCCN=C(N)N)C(=O)NC(CCCN=C(N)N)C(=O)NC(CCCN=C(N)N)C(=O)NC(CCCN=C(N)N)C(=O)NC(CCCN=C(N)N)C(=O)NC(CCCN=C(N)N)C(=O)O)N", "CHEMBL26501": "CN1C=C(C2=CC=CC=C21)C3=C(C(=O)NC3=O)C4=C5CC(CCN5C6=CC=CC=C64)CN(C)C", "CHEMBL265315": "C1CC(N(C1)C(=O)C(CC2=CC=CC=C2)N)C(=O)NC(CCCN=C(N)N)CCl", "CHEMBL265502": "CC1=C(C=C(C=C1)C(=O)NC2=C3C(=CC(=CC3=C(C=C2)S(=O)(=O)O)S(=O)(=O)O)S(=O)(=O)O)NC(=O)C4=CC(=CC=C4)NC(=O)NC5=CC=CC(=C5)C(=O)NC6=C(C=CC(=C6)C(=O)NC7=C8C(=CC(=CC8=C(C=C7)S(=O)(=O)O)S(=O)(=O)O)S(=O)(=O)O)C", "CHEMBL265876": 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"CC1=C(N=CN1)C2=NC=CC3=C2NC4=CC=CC=C34", "CHEMBL277008": "C1=CC2=C(C(=C1)O)NC3=C4C(=C5C(=C23)C(=O)N(C5=O)NC(CO)CO)C6=C(N4C7C(C(C(C(O7)CO)O)O)O)C(=CC=C6)O", "CHEMBL27852": "C1CC(N2C1CCC(C2)(CC3=CC=CC=C3)N)C(=O)NC(CCCN=C(N)N)C(=O)C4=NC5=CC=CC=C5S4", "CHEMBL278819": "CC1=CC(=NN=C1NCCN2CCOCC2)C3=CC=CC=C3", "CHEMBL279405": "CC(C)CCOC1=C2C=NNC2=NC=C1C(=O)C3=CC=CC=C3", "CHEMBL280069": "COC1=CC2=CC(=CN=C2C=C1OC)C3=CC=NC=C3", "CHEMBL281470": "COC1=CC=C(C=C1)C2=NNC3=C2C(=O)C4=CC=CC=C43", "CHEMBL282830": "C1CN2CCC(CN2C1C(=O)NC(CCCN=C(N)N)C(=O)C3=NC4=CC=CC=C4S3)(CC5=CC=CC=C5)N", "CHEMBL284436": "C1CN2CCC(CN2C1C(=O)NC(CCCN=C(N)N)CCl)(CC3=CC=CC=C3)N", "CHEMBL28509": "CCCCCCCCCCCCCCCCCCOCC(COP(=O)([O-])OCC[N+](C)(C)C)OC", "CHEMBL28641": "CCCCCCCCCCCCCCCCCCSCC(C[N+](C)(C)CCCO)OC.[I-]", "CHEMBL28657": "CCCCCCCCCCCCCCCCOCC(C[N+](C)(C)C)OC.[Br-]", "CHEMBL288273": 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"CN1C=C(C=C1C(=O)C2=CN(C(=C2)C(=O)OC)C)C(=O)C3=CC(=CN3C)NC(=O)CCN4C5=CC=CC=C5C6=C7CNC(=O)C7=C8C9=CC=CC=C9NC8=C64", "CHEMBL334064": "C1=C(C=C2C3=C4C(=C5C6=CC(=CC(=C6N(C5=C3NC2=C1O)C7C(C(C(C(O7)CO)O)O)O)O)O)C(=O)N(C4=O)NC(CO)CO)O", "CHEMBL334337": "C1C(C(OC1N2C3=C(C=CC(=C3)O)C4=C5C(=C6C7=C(C=C(C=C7)O)NC6=C42)C(=O)N(C5=O)NC(CO)CO)CO)O", "CHEMBL334360": "C1C(C(C(O1)N2C3=C(C=CC(=C3)O)C4=C5C(=C6C7=C(C=C(C=C7)O)NC6=C42)C(=O)N(C5=O)NC(CO)CO)O)O", "CHEMBL334461": "C1C(C(C(OC1N2C3=C(C=CC(=C3)O)C4=C5C(=C6C7=C(C=C(C=C7)O)NC6=C42)C(=O)N(C5=O)NC(CO)CO)CO)O)O", "CHEMBL334869": "C1=CC2=C(C=C1O)NC3=C4C(=C5C(=C23)C(=O)N(C5=O)NC(CO)CO)C6=C(N4C7C(C(C(C(O7)CO)O)O)O)C=C(C=C6)O", "CHEMBL335012": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)CNC6=O)N(C)C(=O)C9=CN=CC=C9)OC", "CHEMBL335020": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)C(=O)NC6=O)N(C)C(=O)C9=CC=CC=C9)OC", "CHEMBL335648": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)CNC6=O)[N+](C)(C)C)OC", "CHEMBL335718": "CCCCC(CN(C)C1CC2N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N(C7=C53)C(C1OC)(O2)C)CNC6=O)O", "CHEMBL335931": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)CNC6=O)N(C)C(=O)CNC(=O)OC(C)(C)C)OC", "CHEMBL335932": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)CNC6=O)N(C)C(=O)C(F)(F)F)OC", "CHEMBL335940": "C1=CC2=C(C=C1O)NC3=C4C(=C5C(=C23)C(=O)N(C5=O)NC(CO)CO)C6=C(N4C7C(C(C(C(O7)CO)O)O)O)C=C(C=C6)O", "CHEMBL336192": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)CNC6=O)N(C)C(=O)C9=CC=C(C=C9)C(=O)OC)OC", "CHEMBL336603": "C1=CC2=C(C=C1O)NC3=C4C(=C5C(=C23)C(=O)N(C5=O)NC(CO)CO)C6=C(N4C7C(C(C(C(O7)CO)O)O)O)C=C(C=C6)O", "CHEMBL336626": "C1=CC2=C(C=C1O)NC3=C4C(=C5C(=C23)C(=O)N(C5=O)NC(CO)CO)C6=C(N4C7C(C(C(O7)C(CO)O)O)O)C=C(C=C6)O", "CHEMBL337026": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)C(=O)NC6=O)NC)OC", "CHEMBL337027": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)CNC6=O)N(C)C(=O)CCC(=O)O)OC", "CHEMBL337035": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)CNC6=O)N(C)C(=S)NC)OC", "CHEMBL337297": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)CNC6=O)N(C)C(=O)C9=NC=CN=C9)OC", "CHEMBL338049": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)C(NC6=O)O)NC)OC", "CHEMBL338155": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(NC(=O)C6=C7C8=CC=CC=C8N2C7=C53)O)NC)OC", "CHEMBL338449": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)CNC6=O)N(C)C(=O)OC(C)(C)C)OC", "CHEMBL338935": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)CNC6=O)N(C)C(=O)CN)OC", "CHEMBL338944": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)CNC6=O)N(C)C(=O)C9=CC(=CC=C9)Cl)OC", "CHEMBL338956": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)C(NC6=O)O)N(C)C(=O)C9=CC=CC=C9)OC", "CHEMBL338966": "C1=CC2=C(C=C1O)NC3=C4C(=C5C(=C23)C(=O)N(C5=O)NC(CO)CO)C6=C(N4C7C(C(C(C(O7)CO)O)O)O)C=C(C=C6)O", "CHEMBL338967": "C1C(C(C(C(O1)N2C3=C(C=CC(=C3)O)C4=C5C(=C6C7=C(C=C(C=C7)O)NC6=C42)C(=O)N(C5=O)NC(CO)CO)O)O)O", "CHEMBL339364": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)CNC6=O)N(C)C(=O)C9CCCCC9)OC", "CHEMBL339799": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)C(NC6=O)O)NC)OC", "CHEMBL340611": "CC[N+](C)(C)C1CC2N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N(C7=C53)C(C1OC)(O2)C)CNC6=O", "CHEMBL342767": "CN1C2CCCC1N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)C(=O)NC6=O", "CHEMBL344314": "C1=CC2=C(C=CN=C2)C(=C1)S(=O)(=O)NCCN", "CHEMBL345384": "COC1C(OC(C(C1O)O)N2C3=C(C=CC=C3Cl)C4=C5C(=C6C7=C(C(=CC=C7)Cl)NC6=C42)C(=O)N(C5=O)CC(=O)CCl)CO", "CHEMBL345881": "COC1C(OC(C(C1O)OC(=O)CBr)N2C3=C(C=CC=C3Cl)C4=C5C(=C6C7=C(C(=CC=C7)Cl)NC6=C42)C(=O)NC5=O)CO", "CHEMBL347195": "COC1C(OC(C(C1OC(=O)CBr)O)N2C3=CC=CC=C3C4=C5C(=C6C7=CC=CC=C7NC6=C42)C(=O)NC5=O)CO", "CHEMBL347466": "CC(=O)OC1C(C(C(OC1N2C3=C(C=CC=C3Cl)C4=C5C(=C6C7=C(C(=CC=C7)Cl)NC6=C42)C(=O)NC5=O)CO)OC)O", "CHEMBL347684": "COC1C(OC(C(C1O)OC(=O)CBr)N2C3=CC=CC=C3C4=C5C(=C6C7=CC=CC=C7NC6=C42)C(=O)NC5=O)CO", "CHEMBL348586": "CN(C)C1=C(C(=O)NC1=O)C2=C(N(C3=CC=CC=C32)CCCSC(=N)N)C4=CC5=CC=CC=C5S4", "CHEMBL348943": "C1=CC=C(C=C1)C2=CC=C(C=C2)C3=C(C4=CC=CC=C4N3CCCSC(=N)N)C5=CC(=O)NC5=O", "CHEMBL349382": "C1CN=C(N1)NCCCN2C3=CC=CC=C3C(=C2C4=CC5=CC=CC=C5S4)C6=CC(=O)NC6=O", "CHEMBL350059": "C1=CC=C2C(=C1)C=CC=C2C3=C(C4=CC=CC=C4N3CCCSC(=N)N)C5=CC(=O)NC5=O", "CHEMBL350084": "COC(=O)CCNS(=O)(=O)C1=CC=CC2=C1C=CN=C2", "CHEMBL350143": "CC(=O)C1=C(C(=O)NC1=O)C2=C(N(C3=CC=CC=C32)CCCSC(=N)N)C4=CC5=CC=CC=C5S4", "CHEMBL350375": "C1=CC=C2C(=C1)C=C(S2)C3=C(C4=CC=CC=C4N3CCCN=C(N)N)C5=C(C(=O)NC5=O)C#N", "CHEMBL351282": "COC(=O)CCNCCNS(=O)(=O)C1=CC=CC2=C1C=CN=C2", "CHEMBL351291": "C1=CC2=C(C=CN=C2)C(=C1)S(=O)(=O)NCCNC(=O)CCC(=O)O", "CHEMBL351295": "CN(C)CCCN1C2=CC=CC=C2C(=C1C3=CC4=CC=CC=C4S3)C5=CC(=O)NC5=O", "CHEMBL351380": "COC(=O)CCN1CCN(CC1)S(=O)(=O)C2=CC=CC3=C2C=CN=C3", "CHEMBL351859": "CC1(CCC(C2=C1C=CC(=C2)C3=C(C4=CC=CC=C4N3CCCSC(=N)N)C5=CC(=O)NC5=O)(C)C)C", "CHEMBL352085": "COC(=O)CCC(=O)NCCNS(=O)(=O)C1=CC=CC2=C1C=CN=C2", "CHEMBL353795": "C1=CC=C(C=C1)C(=O)C2=C(C(=O)NC2=O)C3=C(N(C4=CC=CC=C43)CCCSC(=N)N)C5=CC6=CC=CC=C6S5", "CHEMBL354246": "C1=CC=C2C(=C1)C=C(S2)C3=C(C4=CC=CC=C4N3CCCN=C(N)NC#N)C5=C(C(=O)NC5=O)C#N", "CHEMBL357602": "C1CC2NC1N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)C(=O)NC6=O", "CHEMBL357892": "C1C2N(C(CO1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)C(=O)NC6=O)CC9=CC=CC=C9", "CHEMBL358130": "COCC1CC(C2NC1N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)C(=O)NC6=O)COC", "CHEMBL358314": "COCC1CC(C2N(C1N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)C(=O)NC6=O)CC9=CC=CC=C9)COC", "CHEMBL36432": "CC1(CCC2(CCC3(C(=CCC4C3(CCC5C4(CC(C6C5(COC(=O)C7=CC(=C(C(=C7C8=C(C(=C(C=C8C(=O)O6)O)O)O)O)O)O)CO)O)C)C)C2C1)C)C(=O)O)C", "CHEMBL365598": "C1CC(C(CNC1)NC(=O)C2=CC=C(C=C2)O)OC(=O)C3=CC=C(C=C3)C(=O)C4=C(C=CC=C4O)C(=O)O", "CHEMBL36985": "C1C(C(C(CC1(C(=O)O)OC(=O)C2=CC(=C(C(=C2)O)O)O)OC(=O)C3=CC(=C(C(=C3)O)O)O)OC(=O)C4=CC(=C(C(=C4)O)O)O)OC(=O)C5=CC(=C(C(=C5)O)O)O", "CHEMBL370100": "COC1C(OC(C(C1O)O)N2C3=C(C=CC=C3Cl)C4=C5C(=C6C7=C(C(=CC=C7)Cl)NC6=C42)C(=O)NC5=O)CO", "CHEMBL370283": "CC1=NC(=O)C2=C(NN(C2=N1)C3=C(C=C(C=C3Cl)Cl)Cl)SC", "CHEMBL382408": "C1=C(C=C(C(=C1O)O)O)C(=O)OCC2C(C(C(C(O2)OC(=O)C3=CC(=C(C(=C3)O)O)O)OC(=O)C4=CC(=C(C(=C4)O)O)O)OC(=O)C5=CC(=C(C(=C5)O)O)O)OC(=O)C6=CC(=C(C(=C6)O)O)O", "CHEMBL384283": "C=C1C23CC(=O)C(C4(C2C5=C(O4)C(=C(C=C5C(=O)OC6C7C(O1)C(COC(=O)C8=CC(=C(C(=C8C9=C(C(=C(C=C9C(=O)O7)O)O)O)O)O)O)OC6OC(=O)C1=CC(=C(C(=C1)O)O)O)O)O)O)(OC31C(=O)OC2C1(OCC2O)O)O", "CHEMBL386276": "C1C(C(OC2=C1C(=CC(=C2C3C(C(OC4=C(C(=CC(=C34)O)O)C5C(C(OC6=CC(=CC(=C56)O)O)C7=CC(=C(C=C7)O)O)OC(=O)C8=CC(=C(C(=C8)O)O)O)C9=CC(=C(C=C9)O)O)OC(=O)C1=CC(=C(C(=C1)O)O)O)O)O)C1=CC(=C(C=C1)O)O)OC(=O)C1=CC(=C(C(=C1)O)O)O", "CHEMBL39413": "C1C(C(C(C=C1C(=O)O)O)O)OC(=O)C2=CC(=C(C(=C2)OC(=O)C3=CC(=C(C(=C3)O)O)O)O)O", "CHEMBL39504": "C1C(C(OC2=C1C(=CC(=C2C3C(C(OC4=CC(=CC(=C34)O)O)C5=CC(=C(C=C5)O)O)OC(=O)C6=CC(=C(C(=C6)O)O)O)O)O)C7=CC(=C(C=C7)O)O)OC(=O)C8=CC(=C(C(=C8)O)O)O", "CHEMBL39530": "C1C(C(C(CC1(C(=O)O)OC(=O)C2=CC(=C(C(=C2)O)O)O)O)OC(=O)C3=CC(=C(C(=C3)O)O)O)O", "CHEMBL39744": "C1C(C(C(CC1(C(=O)O)O)O)OC(=O)C2=CC(=C(C(=C2)O)O)O)O", "CHEMBL405405": "C1C(C(C(OC1N2C3=C(C=CC(=C3)O)C4=C5C(=C6C7=C(C=C(C=C7)O)NC6=C42)C(=O)N(C5=O)NC(CO)CO)CO)O)O", "CHEMBL406635": "C1C2C(C3C(C(O2)O)OC(=O)C4=CC(=C(C(=C4C5=C(C(=C(C=C5C(=O)O3)O)O)O)O)O)O)OC(=O)C6=CC(=C(C(=C6C7=C(C(=C8C9=C7C(=O)OC2=C(C(=C(C3=C(C(=C(C=C3C1=O)O)O)O)C(=C92)C(=O)O8)O)O)O)O)O)O)O", "CHEMBL406901": "C1=CC2=C(C=C1O)NC3=C4C(=C5C(=C23)C(=O)N(C5=O)NC(CO)CO)C6=C(N4C7C(C(C(C(O7)CO)O)O)O)C=C(C=C6)O", "CHEMBL407100": "CC(C(=O)NC(C)C(=O)NC(CO)C(=O)NC(CCCN=C(N)N)C(=O)NC(CCCN=C(N)N)C(=O)NC(CCCN=C(N)N)C(=O)NC(CCCN=C(N)N)C(=O)O)NC(=O)C(C)NC(=O)C(C)NS(=O)(=O)C1=CC=CC2=C1C=CN=C2", "CHEMBL407558": "C1C2C(C3C4C(C5=C(C(=C(C(=C5C(=O)O4)C6=C(C(=C(C(=C6C(=O)O3)C7=C(C(=C(C=C7C(=O)O2)O)O)O)O)O)O)O)O)O)O)OC(=O)C8=CC(=C(C(=C8C9=C(C(=C2C3=C9C(=O)OC4=C(C(=C(C5=C(C(=C(C=C5C(=O)O1)O)O)O)C(=C34)C(=O)O2)O)O)O)O)O)O)O", "CHEMBL407914": "C1C(C(OC2=C3C4C5C6C7C(COC(=O)C8=CC(=C(C(=C8C9=C(C(=C(C=C9C(=O)O7)O)O)O)O)O)O)OC(=O)C7=CC(=C(C(=C7C7=C(C(=C(C(=C7O)O)O)C7=C(C(=O)C4(C7C(=O)O5)OC3=CC(=C21)O)O)C(=O)O6)O)O)O)C1=CC(=C(C=C1)O)O)O", "CHEMBL409397": "C1C2C(C3C(C(O2)OC(=O)C4=CC(=C(C(=C4)OC5=C(C(=C(C6=C5C(=O)OC7C(COC(=O)C8=CC(=C(C(=C86)O)O)O)OC(C9C7OC(=O)C2=CC(=C(C(=C2C2=C(C(=C(C=C2C(=O)O9)O)O)O)O)O)O)OC(=O)C2=CC(=C(C(=C2)OC2=C(C(=C(C4=C2C(=O)OC2C(COC(=O)C5=CC(=C(C(=C54)O)O)O)OC(C4C2OC(=O)C2=CC(=C(C(=C2C2=C(C(=C(C=C2C(=O)O4)O)O)O)O)O)O)OC(=O)C2=CC(=C(C(=C2)OC2=C(C(=C(C4=C2C(=O)OC2C(COC(=O)C5=CC(=C(C(=C54)O)O)O)OC(C4C2OC(=O)C2=CC(=C(C(=C2C2=C(C(=C(C=C2C(=O)O4)O)O)O)O)O)O)OC(=O)C2=CC(=C(C(=C2)O)O)O)O)O)O)O)O)O)O)O)O)O)O)O)O)O)O)OC(=O)C2=CC(=C(C(=C2C2=C(C(=C(C=C2C(=O)O3)O)O)O)O)O)O)OC(=O)C2=CC(=C(C(=C2C2=C(C(=C(C=C2C(=O)O1)O)O)O)O)O)O", "CHEMBL410778": "CC(C(=O)NC(C)C(=O)NC(CCCN=C(N)N)C(=O)NC(CCCN=C(N)N)C(=O)NC(CCCN=C(N)N)C(=O)NC(CCCN=C(N)N)C(=O)O)NC(=O)C(C)NS(=O)(=O)C1=CC=C(C2=CC=CC=C21)N(C)C", "CHEMBL411351": "C1C(C(OC2=C1C(=CC(=C2C3C(C(OC4=C5C6C(C(OC5=CC(=C34)O)(OC7=C6C(=CC(=C7C8C(C(OC9=CC(=CC(=C89)O)O)C1=CC(=C(C=C1)O)O)O)O)O)C1=CC(=C(C=C1)O)O)O)C1=CC(=C(C=C1)O)O)O)O)O)C1=CC(=C(C=C1)O)O)O", "CHEMBL411401": "C1C(C(OC2=C1C(=CC(=C2C3C4C5C6C(COC(=O)C7=CC(=C(C(=C7C8=C(C(=C(C=C8C(=O)O6)O)O)O)O)O)O)OC(=O)C9=CC(=C(C(=C9C1=C(C(=C(C(=C1O)O)O)C1=C(C3=C(C(=C1O)O)O)C(=O)O4)C(=O)O5)O)O)O)O)O)C1=CC(=C(C=C1)O)O)O", "CHEMBL413375": "C1C2C(C(C(C(O2)OC(=O)C3=CC(=C(C(=C3)O)O)O)OC(=O)C4=CC(=C(C(=C4)O)O)O)OC(=O)C5=CC(=C(C(=C5)O)O)O)OC(=O)C6=CC(=C(C(=C6C7=C(C(=C(C=C7C(=O)O1)O)O)O)O)O)OC8=C(C(=C(C=C8C(=O)OC9C(OC(C(C9OC(=O)C1=CC(=C(C(=C1)O)O)O)OC(=O)C1=CC(=C(C(=C1)O)O)O)OC(=O)C1=CC(=C(C(=C1)O)O)O)COC(=O)C1=CC(=C(C(=C1)O)O)O)O)O)O", "CHEMBL415233": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)CN(C6=O)CC9=CC=CC=C9)N(C)C(=O)C1=CC=CC=C1)OC", "CHEMBL415414": "CC(C(=O)NC(CO)C(=O)NC(CCCN=C(N)N)C(=O)NC(CCCN=C(N)N)C(=O)NC(CCCN=C(N)N)C(=O)NC(CCCN=C(N)N)C(=O)NC(CCCN=C(N)N)C(=O)NC(CCCN=C(N)N)C(=O)O)NC(=O)C(C)NS(=O)(=O)C1=CC=CC2=C1C=CN=C2", "CHEMBL416110": "CCCCCCCCCCCCCCCCOCCC[N+](C)(C)C.[Br-]", "CHEMBL418479": "CC(C)N1C2=CC=CC=C2C3=C4C(=C5C6=CC=CC=C6NC5=C31)C(=O)NC4=O", "CHEMBL421565": "CN1C=C(C2=CC=CC=C21)C3=C(C(=O)NC3=O)C4=C5CC(CCN5C6=CC=CC=C64)CN", "CHEMBL421947": "CN1C2CCC1N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)C(=O)NC6=O", "CHEMBL423731": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)CNC6=O)O)OC", "CHEMBL424168": "COC(=O)CCCCN1CCN(CC1)S(=O)(=O)C2=CC=CC3=C2C=CN=C3", "CHEMBL428973": "CC(C(=O)NC(C)C(=O)NC(CCCN=C(N)N)C(=O)NC(CCCN=C(N)N)C(=O)NC(CCCN=C(N)N)C(=O)NC(CCCN=C(N)N)C(=O)O)NC(=O)C(C)NS(=O)(=O)C1=CC=CC2=C1C=CN=C2", "CHEMBL429225": "C1=CC=C(C=C1)CN2C3C(C(C(C2N4C5=CC=CC=C5C6=C7C(=C8C9=CC=CC=C9N3C8=C64)C(=O)NC7=O)O)O)O", "CHEMBL430440": "C1C2C(C3C(C(O2)O)OC(=O)C4=CC(=C(C(=C4C5=C(C(=C(C=C5C(=O)O3)O)O)O)O)O)O)OC(=O)C6=CC(=C(C(=C6C7=C(C(=C(C=C7C1=O)O)O)O)O)O)O", "CHEMBL431176": "C1=CC=C2C(=C1)C3=C4C(=C5C6=CC=CC=C6N(C5=C3N2)CC(F)(F)F)C(=O)NC4=O", "CHEMBL431432": "CN1CCCC1CCNC(=O)CCN2C3=CC=CC=C3C4=C5CNC(=O)C5=C6C7=CC=CC=C7NC6=C42", "CHEMBL432622": "C1=CC=C2C(=C1)C3=C4C(=C5C6=C(C(=CC=C6)O)N(C5=C3N2)C7C(C(C(C(O7)CO)O)O)O)C(=O)N(C4=O)NC(CO)CO", "CHEMBL433841": "C1=CC2=C(C=C1O)NC3=C4C(=C5C(=C23)C(=O)N(C5=O)NC(CO)CO)C6=C(N4C7C(C(C(C(O7)CO)O)O)O)C=CC(=C6)O", "CHEMBL433855": "C1=CC2=C(C=C1O)NC3=C4C(=C5C(=C23)C(=O)N(C5=O)NC(CO)CO)C6=C(N4C7C(C(C(O7)CO)O)O)C=C(C=C6)O", "CHEMBL434037": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)C(=O)NC6=O)N(C)OC(=O)C(C)(C)C)OC", "CHEMBL434237": "C1=CC2=C(C=C1O)NC3=C4C(=C5C(=C23)C(=O)N(C5=O)NC(CO)CO)C6=C(N4C7C(C(C(C(O7)CO)O)O)O)C=C(C=C6)O", "CHEMBL434415": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)CNC6=O)N(C)C9=CC=CC=C9)OC", "CHEMBL435191": "C1=CC2=C(C=C1O)NC3=C4C(=C5C(=C23)C(=O)N(C5=O)NC(CO)CO)C6=C(N4C7C(C(C(C(O7)CO)O)O)O)C=C(C=C6)O", "CHEMBL435809": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)CNC6=O)N(C)C(=O)C9=CC=C(C=C9)C(=O)O)OC", "CHEMBL435868": "C1=CC=C2C(=C1)C=C(O2)C3=C(C4=CC=CC=C4N3CCCSC(=N)N)C5=CC(=O)NC5=O", "CHEMBL436718": "C1=CC2=C(C=CN=C2)C(=C1)S(=O)(=O)NCCNCCC(=O)NC(CO)C(=O)NC(CCCN=C(N)N)C(=O)NC(CCCN=C(N)N)C(=O)NC(CCCN=C(N)N)C(=O)NC(CCCN=C(N)N)C(=O)NC(CCCN=C(N)N)C(=O)NC(CCCN=C(N)N)C(=O)O", "CHEMBL437640": "CC(C(=O)NC(C)C(=O)NC(CO)C(=O)NC(CCCN=C(N)N)C(=O)NC(CCCN=C(N)N)C(=O)NC(CCCN=C(N)N)C(=O)NC(CCCN=C(N)N)C(=O)O)NC(=O)C(C)NC(=O)C(C)NS(=O)(=O)C1=CC=C(C2=CC=CC=C21)N(C)C", "CHEMBL44137": "CN1C(=O)C2=C3C4=CC=CC=C4NC3=C5C(=C2C1=O)C6=CC=CC=C6N5C7C(C(C(C(O7)CO)OC)O)O", "CHEMBL444337": "CC12C(C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)CNC6=O)N(C)CC(=O)OC)OC", "CHEMBL444864": "C1=CC=C2C=C(C=CC2=C1)C3=C(C4=CC=CC=C4N3CCCSC(=[NH2+])N)C5=CC(=O)NC5=O.[Br-]", "CHEMBL447974": "C1=C(C=C(C(=C1O)O)O)C(=O)OCC2C(C(C(C(O2)OC(=O)C3=CC(=C(C(=C3)O)O)O)OC(=O)C4=CC(=C(C(=C4)O)O)O)O)O", "CHEMBL449392": "C1C2C(C(C(C(O2)OC(=O)C3=CC(=C(C(=C3)O)O)O)O)OC(=O)C4=CC(=C(C(=C4C5=C(C(=C(C=C5C(=O)O1)O)O)O)O)O)O)O", "CHEMBL45827": "CCN(CC)CCCCNC1=NC2=NC(=C(C=C2C=N1)C3=C(C=CC=C3Cl)Cl)NC(=O)NC(C)(C)C", "CHEMBL47243": "COC1C(OC(C(C1O)O)N2C3=CC=CC=C3C4=C5C(=C6C7=CC=CC=C7NC6=C42)C(=O)NC5=O)CO", "CHEMBL47940": "C1CCC(C1)N2C=C(C3=C2N=CN=C3N)C4=CC=C(C=C4)OC5=CC=CC=C5", "CHEMBL480283": "C1=C(C=C(C(=C1O)O)O)C(=O)OC2C(C(C(C(O2)CO)O)O)O", "CHEMBL491592": "C1=C(C=C(C(=C1O)O)O)C(=O)OCC2C(C(C(O2)O)(COC(=O)C3=CC(=C(C(=C3)O)O)O)O)O", "CHEMBL500292": "C1=C(C=C(C(=C1O)O)O)C(=O)OCC2C(C(C(C(O2)O)OC(=O)C3=CC(=C(C(=C3)O)O)O)OC(=O)C4=CC(=C(C(=C4)O)O)O)OC(=O)C5=CC(=C(C(=C5)O)O)O", "CHEMBL507308": "C1C2C(C(C(C(O2)OC(=O)C3=CC(=C(C(=C3)O)O)O)OC(=O)C4=CC(=C(C(=C4)O)O)O)OC(=O)C5=CC(=C(C(=C5C6=C(C(=C(C=C6C(=O)O1)O)O)O)O)O)O)OC(=O)C7=CC(=C(C(=C7)O)O)O", "CHEMBL50749": "CCCCCCCCCCCCCCCCCC1OCC(O1)C[N+](C)(C)CCCO.[Br-]", "CHEMBL51563": "CCCCCCCCCCCCCCCCOCCC[N+]1=CC=CC=C1.[Br-]", "CHEMBL522251": "C1=C(C=C(C(=C1O)O)O)C(=O)OCC2C(C(C(C(O2)OC(=O)C3=CC(=C(C(=C3)O)O)O)O)O)O", "CHEMBL525240": "C1C2C3C(C(C(O2)OC(=O)C4=CC(=C(C(=C4)O)O)O)OC(=O)C5=CC(=C(C6=C5C(C(C(=O)O3)CC(=O)O)C(C(=O)O6)O)O)O)OC(=O)C7=CC(=C(C(=C7C8=C(C(=C(C=C8C(=O)O1)O)O)O)O)O)O", "CHEMBL52850": "CCCCCCCCCCCCCCCCOCC(COCCCC[N+](C)(C)C)OCC.[Br-]", "CHEMBL53606": "CCCCCCCCCCCCCCCCOCC(COCCCCCC[N+](C)(C)C)OC.[Br-]", "CHEMBL53826": "CCCCCCCCCCCCCCCCOCC(COCCCC[N+](C)(C)C)OC.[Br-]", "CHEMBL538718": "CN1CC2CC3=C(C4=CC=CC=C4N3CC2C1)C5=C(C(=O)NC5=O)C6=CN(C7=CC=CC=C76)C", "CHEMBL540848": "CC1CNCCN1S(=O)(=O)C2=CC=CC3=C2C=CN=C3.Cl.Cl", "CHEMBL55382": "CC12C(C(CC(O1)N3C4=C(C=C(C=C4)O)C5=C6C(=C7C8=C(N2C7=C53)C=CC(=C8)O)COC6=O)NC)OC", "CHEMBL553824": "COC1=C(C=C2C(=C1)C(=NC=N2)N3CCN(CC3)C(=O)NC4=CSC=C4)OC", "CHEMBL56236": "CC1=CC(=C(C(=C1C)C2=C(N=C3C(=C2)C=NC(=N3)N)NC(=O)NC(C)(C)C)C)C", "CHEMBL56983": "CCN(CC)CCCCNC1=NC2=NC(=C(C=C2C=N1)C3=C(C=CC=C3Cl)Cl)NC(=O)NC4=CC=CC=C4", "CHEMBL57347": "CC(C)(C)NC(=O)NC1=C(C=C2C=NC(=NC2=N1)NCCCN3CCN(CC3)C)C4=C(C=CC=C4Cl)Cl", "CHEMBL57366": "CC(C)(C)NC(=O)NC1=C(C=C2C=NC(=NC2=N1)N)C3=C(C=CC=C3Cl)Cl", "CHEMBL60254": "C1CC(C(CNC1)NC(=O)C2=CC=C(C=C2)O)OC(=O)C3=CC(=C(C(=C3)O)C(=O)C4=C(C=CC=C4O)C(=O)O)O", "CHEMBL611124": "C1C2C(C3C4C(C5=C(C(=C(C(=C5C(=O)O4)C6=C(C(=C(C(=C6C(=O)O3)C7=C(C(=C(C=C7C(=O)O2)O)O)O)O)O)O)O)O)O)C8(C(C(C(O8)CO)O)O)O)OC(=O)C9=CC(=C(C(=C9C2=C(C(=C(C=C2C(=O)O1)O)O)O)O)O)O", "CHEMBL61867": "CCN1C2=CC=CC=C2C3=C4C(=C5C6=CC=CC=C6NC5=C31)C(=O)NC4=O", "CHEMBL66031": "C1=CC(=CC(=C1)Br)NC2=NC=NC3=CC4=C(C=C32)NC=N4", "CHEMBL68423": "COC1=CC2=NC=C(C=C2C(=C1)OC)C3=CC=NC=C3", "CHEMBL69129": "C1CC(CC1N2C=C(C3=C2N=CN=C3N)C4=CC=C(C=C4)OC5=CC=CC=C5)O", "CHEMBL7352": "COC1=CC=C(C=C1)NC2=C(C=C3C(=C2)C(=O)NC3=O)NC4=CC=C(C=C4)OC", "CHEMBL75773": "C1CN(CCN1)S(=O)(=O)C2=CC=CC3=C2C=CN=C3", "CHEMBL7775": "CN(C1=CC=CC=C1)C2=C(C=C3C(=C2)C(=O)NC3=O)NC4=CC=CC=C4", "CHEMBL78573": "C1C(C(OC2=CC(=CC(=C21)O)O)C3=CC(=C(C=C3)O)O)OC(=O)C4=CC(=C(C(=C4)O)O)O", "CHEMBL7914": "CC1=CC=C(C=C1)NC2=C(C=C3C(=C2)C(=O)NC3=O)NC4=CC=C(C=C4)C", "CHEMBL79244": "C1C(C(OC(=O)C2=CC(=C(C(=C2C3=C(C(=C(C=C3C(=O)O1)O)O)O)O)O)O)C4C5C(C6=C(C(=C(C(=C6C(=O)O5)C7=C(C(=C(C=C7C(=O)O4)O)O)O)O)O)O)O)OC(=O)C8=CC(=C(C(=C8)O)O)O", "CHEMBL7929": "C1=CC=C(C=C1)C2=CC=C(C=C2)NC3=C(C=C4C(=C3)C(=O)NC4=O)NC5=CC=C(C=C5)C6=CC=CC=C6", "CHEMBL7939": "C1=CC(=CC=C1NC2=C(C=C3C(=C2)C(=O)NC3=O)NC4=CC=C(C=C4)F)F", "CHEMBL8000": "C1=CC=C(C=C1)NC2=C(C=C3C(=C2)C(=O)N(C3=O)C4=CC=CC=C4)NC5=CC=CC=C5", "CHEMBL80024": "C1C2C(C(C(C(O2)O)O)O)OC(=O)C3=CC(=C(C(=C3C4=C(C(=C5C6=C4C(=O)OC7=C(C(=C(C8=C(C(=C(C=C8C1=O)O)O)O)C(=C67)C(=O)O5)O)O)O)O)O)O)O", "CHEMBL8036": "CN1C(=O)C2=CC(=C(C=C2C1=O)NC3=CC=CC=C3)NC4=CC=CC=C4", "CHEMBL8091": "COC(=O)C1=CC(=C(C=C1C(=O)OC)NC2=CC=C(C=C2)F)NC3=CC=C(C=C3)F", "CHEMBL80941": "C1C(C(OC2=CC(=CC(=C21)O)O)C3=CC(=C(C=C3)O)O)O", "CHEMBL8095": "COC1=CC=C(C=C1)NC2=C(C=C3C(=C2)C(=O)NC3=O)NC4=CC=CC=C4", "CHEMBL81478": "C1C(C(OC2=C1C(=CC(=C2C3C(C(OC4=C5C6C(C(OC7=CC(=CC(=C67)O)O)(OC5=CC(=C34)O)C8=CC(=C(C=C8)O)O)O)C9=CC(=C(C=C9)O)O)O)O)O)C1=CC(=C(C=C1)O)O)O", "CHEMBL8163": "C1=CC(=CC=C1NC2=C(C=C3C(=C2)C(=O)NC3=O)NC4=CC=C(C=C4)I)I", "CHEMBL81646": "C1C(C(OC2=C3C4C(C(OC5=CC(=CC(=C45)O)O)(OC3=CC(=C21)O)C6=CC(=C(C=C6)O)O)O)C7=CC(=C(C=C7)O)O)O", "CHEMBL81753": "C1C(C(OC2=C1C(=CC(=C2C3C(C(OC4=CC(=CC(=C34)O)O)C5=CC(=C(C=C5)O)O)O)O)O)C6=CC(=C(C=C6)O)O)O", "CHEMBL8222": "COC(=O)C1=CC(=C(C=C1C(=O)OC)NC2=CC=CC=C2)NC3=CC=CC=C3", "CHEMBL8223": "CCN(CC)C1=CC=C(C=C1)NC2=C(C=C3C(=C2)C(=O)NC3=O)NC4=CC=C(C=C4)N(CC)CC", "CHEMBL8271": "C1=CC=C(C=C1)SC2=C(C=C3C(=C2)C(=O)NC3=O)SC4=CC=CC=C4", "CHEMBL82762": "C1C2C(C(C(C(O2)OC(=O)C3=CC(=C(C(=C3)O)O)O)O)O)OC(=O)C4=CC(=C(C(=C4C5=C(C(=C(C=C5C1=O)O)O)O)O)O)O", "CHEMBL83790": "CC12C(C(CC(O1)N3C4=C(C=C(C=C4)O)C5=C6C(=C7C8=CC=CC=C8N2C7=C53)CNC6=O)NC)OC", "CHEMBL84333": "C1C(C(C(C=C1C(=O)O)OC(=O)C2=CC(=C(C(=C2)O)O)O)O)OC(=O)C3=CC(=C(C(=C3)O)O)O", "CHEMBL86664": "C1=CC(=CC2=NC=C(C=C21)C3=CC=NC=C3)Cl", "CHEMBL87084": "C1=CN=CC=C1C2=CNC3=CC(=O)C(=CC3=C2)O", "CHEMBL93559": "C1=CC=C(C=C1)CC(C(=O)NCCCCCNC2=C(C(=O)NC2=O)C3=CC4=CC=CC=C4N3)N", "CHEMBL94678": "CC12C(CC(O1)N3C4=CC=CC=C4C5=C6C(=C7C8=CC=CC=C8N2C7=C53)CNC6=O)(C(=O)OC)O", "CHEMBL95539": "CN1C=C(C=C1C(=O)OC)NC(=O)CCN2C3=CC=CC=C3C4=C5CNC(=O)C5=C6C7=CC=CC=C7NC6=C42", "CHEMBL95737": "C1=CC=C2C(=C1)C=C(N2)C3=C(C(=O)NC3=O)NCCCNCCCN", "CHEMBL95812": "C1=CC=C2C(=C1)C=C(N2)C3=C(C(=O)NC3=O)NCCCCCNC(=O)C(CCC(=O)O)N", "CHEMBL95825": "C1CCN(CC1)CCNC(=O)CCN2C3=CC=CC=C3C4=C5CNC(=O)C5=C6C7=CC=CC=C7NC6=C42", "CHEMBL97026": "C1=CC=C2C(=C1)C=C(N2)C3=C(C(=O)NC3=O)NCCN", "CHEMBL97117": "CN1C=C(C=C1C(=O)OC)C(=O)C2=CC(=CN2C)NC(=O)CCN3C4=CC=CC=C4C5=C6CNC(=O)C6=C7C8=CC=CC=C8NC7=C53", "CHEMBL97448": "C1=CC=C2C(=C1)C=C(N2)C3=C(C(=O)NC3=O)NCCCCCNCCN", "CHEMBL97768": "C1=CC=C2C(=C1)C=C(N2)C3=C(C(=O)NC3=O)NCCCCCCCN", "CHEMBL97796": "C1=CC=C2C(=C1)C=C(N2)C3=C(C(=O)NC3=O)NCCNCCN", "CHEMBL97822": "C1COCC1CNC(=O)CCN2C3=CC=CC=C3C4=C5CNC(=O)C5=C6C7=CC=CC=C7NC6=C42", "CHEMBL98721": "C1=CC=C2C(=C1)C=C(N2)C3=C(C(=O)NC3=O)NCCCCCNC(=O)C(CCCN=C(N)N)N", "CHEMBL99572": "C1=CC=C2C(=C1)C=C(N2)C3=C(C(=O)NC3=O)NCCCCCNCCNC(=O)C(CCCN=C(N)N)N", "CHEMBL1971485": "CN(C)C1=C(C=CC=C1NC(=O)CC2=CC=CC=C2)C3=C(N4C=CSC4=N3)C5=NC(=NC=C5)NC6=CC=CC(=C6)N7CCOCC7", "CHEMBL1991008": "C1=CC=C(C=C1)C2=CC=CC3=C2NN=C3N", "CHEMBL2002480": "C1=CC=C(C=C1)C2=CN3C(=NC(=N3)N)N=C2", "CHEMBL2333445": "CCC1=CC=C(C=C1)C2=CC3=C(C=C2)N(S(=O)(=O)C4=C3NN=C4)C", "CHEMBL197923": "C1=CC=C(C=C1)CCNC(=O)C2=CC3=C(NN=C3S2)C4=CC=CC=C4", "CHEMBL199383": "COC1=CC=C(C=C1)CNC(=O)C2=CC3=C(NN=C3S2)C4=CC=CC=C4", "CHEMBL199528": "CCCCN(C)C(=O)C1=CC2=C(NN=C2S1)C3=CC=CC=C3", "CHEMBL199755": "C1CCC(CC1)NC(=O)C2=CC3=C(NN=C3S2)C4=CC=CC=C4", "CHEMBL23327": "CC(C)C(CO)NC1=NC2=C(C(=N1)NC3=CC(=CC=C3)Cl)N=CN2C(C)C", "CHEMBL371239": "CN1CCN(CC1)C(=O)C2=CC3=C(NN=C3S2)C4=CC=CC=C4", "CHEMBL1986996": "CCN1C(=O)C(=CNC2=CC=CC=C2)SC1=C(C#N)C(=O)O", "CHEMBL1081198": "C1=CC(=CC(=C1)NC(=O)NC2=CC=CC(=C2)C(F)(F)F)C3=CN4C=CN=C4C(=N3)NCC5=CC=NC=C5", "CHEMBL1163016": "CC1(CC(CC(N1[O])(C)C)NC(=O)C2=CC=CC(=C2)C3=NN4C(=CC=NC4=C3)NC5=CC(=CC=C5)O)C", "CHEMBL1172957": "C1COCCN1C2=NC3=C(C(=N2)NC4=CC=C(C=C4)S(=O)(=O)N)NC=N3", "CHEMBL118258": "CN1CCC(CC1)(C2=CN(C(=N2)C3=CC(=CC=C3)C(F)(F)F)C4=NC(=NC=C4)NC5CCCC5)O", "CHEMBL120077": "COC1=C(C=C2C(=C1)CC3=C2NN=C3NC4=CC(=CC=C4)F)OC", "CHEMBL120185": "CN1CCN(CC1)C2=NC3=C(C=C2)N(C(=N3)C4=CC=C(C=C4)F)C5=NC(=NC=C5)NC6CCCC6", "CHEMBL121405": "C1CCC(CC1)NC2=NC=CC(=C2)C3=C(N=C(O3)C4(CCNCC4)O)C5=CC=C(C=C5)F", "CHEMBL1242027": "CC(C)N1C2=C(C(=N1)C3=CC(=C(C=C3F)OC)F)C(=NC=N2)N", "CHEMBL153843": "C1=CC=C(C(=C1)C(=O)NC2=CC=CC(=C2)C(F)(F)F)NCC3=CC=NC=C3", "CHEMBL1766529": "CC(=O)N1CCN(CC1)C2=CN=C3C=C(C=C(C3=C2)NCC4=CC(=CC=C4)[N+](=O)[O-])C(F)(F)F", "CHEMBL1784725": "CCOC(=O)C1=C2C3=CC=CC4=C3C(=CC=C4)C2=NC1=O", "CHEMBL1813632": "C1=CC=C(C=C1)C2=CSC3=NC=NC(=C23)OC4=C(C=C(C=C4)NC(=O)C5=CC=CN(C5=O)C6=CC=C(C=C6)F)F", "CHEMBL1835870": "C1CC(CCC1C2=CC=C(C=C2)NC3=NN(C(=N3)N)C4=CC=CC=N4)N5CCOCC5", "CHEMBL1916891": "CC1=CC=CC=C1NC2=NC3=CC(=C(C=C3N4C2=CN=C4)N(C)C(=O)C=CCN(C)C)F", "CHEMBL1949788": "COC1=C(C=C(C=C1)C(=O)NCC(CO)O)C=CC2=CC=C(C=C2)Cl", "CHEMBL1949789": "COC1=C(C=C(C=C1)C(=O)NCC(CO)O)C=CC2=CC=C(C=C2)Cl", "CHEMBL195029": "COC1=CC2=CC3=C(C(=CN=C3C=C2C=C1OCCN4CCOCC4)C#N)NC5=CC(=C(C=C5Cl)Cl)OC", "CHEMBL1966836": "CN1C2=NC=CC(=C2C(=N1)N)C3=CC=C(C=C3)NC(=O)NC4=CC(=C(C=C4)F)C(F)(F)F", "CHEMBL1973178": "COC1=C2C(=C(C=C1)C3=CC=C(C=C3)NC(=O)NC4=CC=C(C=C4)OC(F)(F)F)C(=NO2)N", "CHEMBL1980904": "C1=CC(=CC(=C1)NC(=O)NC2=C(C=C(C=C2)C3=C4C(=CC=C3)NN=C4N)F)C(F)(F)F", "CHEMBL1985491": "CC1=CC(=C(C=C1)F)NC(=O)NC2=CC=C(C=C2)C3=C4C(=CC=C3)N(N=C4N)C", "CHEMBL1985888": "CN1C2=NC=CC(=C2C(=N1)N)C3=CC=C(C=C3)NC(=O)NC4=CC=CC(=C4)C(F)(F)F", "CHEMBL1986979": "CC1=C(C=CC(=C1)NC(=O)NC2=CC(=C(C=C2)C3=C4C(=CC=C3)NN=C4N)F)F", "CHEMBL1988778": "CC1=CC(=C(C=C1)F)NC(=O)NC2=CC(=C(C=C2)C3=C4C(=CC=C3)NN=C4N)F", "CHEMBL1993996": "CC1=C(C=CC(=C1)NC(=O)NC2=CC=C(C=C2)C3=C(C=CC4=C3C(=NN4)N)F)F", "CHEMBL1994638": "CC1=CC(=CC=C1)NC(=O)NC2=CC(=C(C=C2)C3=C4C(=CC=C3)NN=C4N)F", "CHEMBL1996255": "CC1=CC(=C(C=C1)F)NC(=O)NC2=CC=C(C=C2)C3=C(C=CC4=C3C(=NN4)N)F", "CHEMBL2000652": "C1=CC(=CC(=C1)Cl)NC(=O)NC2=C(C=C(C=C2)C3=C4C(=CC=C3)NN=C4N)F", "CHEMBL2002432": "CC(C)NC1=NC=CC(=N1)NC2=NC=C(S2)C3=CC=CC=C3", "CHEMBL2071457": "CC(C1=C(C=CC(=C1Cl)F)Cl)NC(=O)C2=C(N=CC(=C2)C3=CN(N=C3)C4CCOCC4)N", "CHEMBL2111784": "CC(C1=CC=CC=C1)NC2=NC=CC(=C2)C3=C(N=C(S3)C4CCN(CC4)C)C5=CC=C(C=C5)F", "CHEMBL237570": "CC1=C(C=CC(=C1)S(=O)C)C2=NC(=C(N2C)C3=CC4=C(C=C3)C=C(C=C4)OC)C5=CC=NC=C5", "CHEMBL264406": "CC(C)(C)N1C2=C(C(=N1)C3=CC=CC4=CC=CC=C43)C(=NC=N2)N", "CHEMBL271441": "CC1=CC(=C(C=C1)F)NC(=O)NC2=CC=C(C=C2)C3=CN=CC4=C3C(=NN4)N", "CHEMBL272938": "CC1=CC(=CC=C1)NC(=O)NC2=CC=C(C=C2)C3=CN=CC4=C3C(=NN4)N", "CHEMBL273187": "CC1=C(C=CC(=C1)NC(=O)NC2=CC=C(C=C2)C3=CC=NC4=NNC(=C34)N)F", "CHEMBL276711": "CC1=CC(=C(N1)C=C2C3=CC=CC=C3NC2=O)C", "CHEMBL347537": "C1=CC=C2C(=C1)C=NC=C2C3=CC(=CC=C3)NC(=O)C4=CC=CC=C4NCC5=CC=NC=C5", "CHEMBL373798": "C1=CC(=CC(=C1)F)NC(=O)NC2=CC=C(C=C2)C3=C4C(=CC=C3)NN=C4N", "CHEMBL374044": "CC1=C(C=CC(=C1)NC(=O)NC2=CC=C(C=C2)C3=C4C(=CC=C3)NN=C4N)F", "CHEMBL403402": "C1=CC(=CC=C1C2=CC=NC3=NNC(=C23)N)NC(=O)NC4=C(C=CC(=C4)C(F)(F)F)F", "CHEMBL404366": "CN1C2=C(C(=CN=C2)C3=CC=C(C=C3)NC(=O)NC4=CC(=CC=C4)Cl)C(=N1)N", "CHEMBL406375": "C1=CC=C(C=C1)C2=NNC3=C2OC4=CC=CC=C43", "CHEMBL409349": "CC1=CC(=CC(=C1)NC(=O)NC2=CC=C(C=C2)C3=C4C(=CC=C3)ON=C4N)C", "CHEMBL436137": "CC1=C(C(=CC=C1)C)C2=CC(=C3C(=C2)N=NC(=N3)NC4=CC=C(C=C4)OCCN5CCCC5)C", "CHEMBL44": "C1=CC(=CC=C1C2=COC3=CC(=CC(=C3C2=O)O)O)O", "CHEMBL488840": "CC1=C(C(=CC=C1)C)C=CN2C=NC3=C2N=CN=C3NC4=CC=C(C=C4)P(=O)(C)C", "CHEMBL569880": "COCCOC1=C(C=C2C(=C1)N=CN=C2NC3=C(C(=C(C=C3)F)Cl)F)NC(=O)C4CCCN4C(=O)C=C", "CHEMBL571040": "COCCOC1=C(C=C2C(=C1)N=CN=C2NC3=C(C(=CC=C3)Cl)F)NC(=O)C4CCCN4C(=O)C=C", "CHEMBL57553": "C1=CC(=CC(=C1)NC2=NC=CC(=N2)C3=CN=CC=C3)N", "CHEMBL685": "COC(=O)NC1=NC2=C(N1)C=C(C=C2)C(=O)C3=CC=CC=C3", "CHEMBL75232": "C1=CC=C2C(=C1)C(=NN=C2NC3=CC=C(C=C3)Cl)CC4=CC=NC=C4.C(CC(=O)O)C(=O)O", "CHEMBL101683": "C1=CC=C(C(=C1)C(=O)NC2=CC=C(C=C2)Cl)NCC3=CC=NC=C3", "CHEMBL103055": "CCN1CCOCCN2C=C(C3=CC=CC=C32)C4=C(C5=CN(CCOCC1)C6=CC=CC=C65)C(=O)NC4=O", "CHEMBL113": "CN1C=NC2=C1C(=O)N(C(=O)N2C)C", "CHEMBL125898": "CC(C)OC1=CC=C(C=C1)NC(=O)N2CCN(CC2)C3=NC=NC4=CC(=C(C=C43)OC)OCCCN5CCOCC5", "CHEMBL129": "CC1=CN(C(=O)NC1=O)C2CC(C(O2)CO)N=[N+]=[N-]", "CHEMBL177688": "C1=CC(=CC(=C1)Cl)NC2=NC(=CN=C2)C3=CC(=CN=C3)NCCCO", "CHEMBL188386": "C1=CC(=CC(=C1)Cl)NC2=NC(=CN=C2)C3=CC(=CN=C3)NCCCCO", "CHEMBL188502": "C1=CC(=CC(=C1)Cl)NC2=NC(=CN=C2)C3=CC(=CN=C3)NCCCC4=CN=CC=C4", "CHEMBL189584": "CCN(CC)CCCCNC1=NC2=NC(=C(C=C2C=N1)C3=CC(=CC(=C3)OC)OC)NC(=O)NC(C)(C)C", "CHEMBL190984": "CN(C)CCNC1=CN=CC(=C1)C2=CN=CC(=N2)NC3=CC(=CC=C3)Cl", "CHEMBL191336": "C1=CC(=CC(=C1)Cl)NC2=NC=NC(=N2)C3=CC(=NC=C3)NCCCO", "CHEMBL194498": "CC(C)C1=C2C(=NC=NN2C=C1C3=NN=C(O3)C(F)F)NC4=C(C=C(C(=C4)C(=O)NOC)F)F", "CHEMBL195218": "CC(C)C1=C2C(=NC=NN2C=C1NC(=O)OCCCS(=O)(=O)C)NC3=C(C=C(C(=C3)C(=O)NOC)F)F", "CHEMBL195903": "CC(C)C1=C2C(=NC=NN2C=C1C3=NN=C(O3)C(F)(F)S(=O)(=O)C)NC4=C(C=C(C(=C4)C(=O)NOC)F)F", "CHEMBL2086760": "CCN1CCC(CC1)NC2=CC3=C(C=C2)NC(=O)C3=C(C4=CC=C(C=C4)Cl)C5=NC=CN5", "CHEMBL212084": "C1C2=C(C=C(C=C2)CN3C=CN=C3)C4=C1C(=NN4)C5=CSC=C5", "CHEMBL213618": "CNC1=NC=CC(=N1)C2=CC=C(S2)C(=O)NC(CC3=C(C=C(C=C3)Cl)Cl)CN", "CHEMBL213743": "CN1CCN(CC1)CC2=CC3=C(CC4=C3NN=C4C5=CSC=C5)C=C2", "CHEMBL2163772": "C1=CC=C(C=C1)C2=C3C4=C(C=CC(=C4)O)OC3=NC=C2O", "CHEMBL230232": "C1=CC(=C(C=C1NC2=C(C=NC3=C(C=C(C=C32)NCC4=NNN=C4)Br)C#N)Cl)F", "CHEMBL231568": "CNC(=O)C1=NC=CC(=C1)OC2=CC3=C(C=C2)OC(=N3)NC4=CC(=C(C=C4)Cl)OCC5CCCN5C", "CHEMBL232601": "C1CC2=C(N(C1)C(=O)C3CC3)SC(=C2C#N)NC(=O)C4=CC=CC5=CC=CC=C54", "CHEMBL233001": "C1CCC2=C(C1)C(=C(S2)NC(=O)C3=CC=CC4=CC=CC=C43)C#N", "CHEMBL245212": "C1=CC(=C(C=C1NC2=C(C=NC3=C(C=C(C=C32)NCC4=CN=CN4)F)C#N)Cl)F", "CHEMBL258805": "COC1=CC2=C(C=C1)NC(=O)C2=CC3=CN=CN3", "CHEMBL261720": "C1=CC(=C(C(=C1)F)NC(=S)N2C(=NC(=N2)NC3=CC=C(C=C3)S(=O)(=O)N)N)F", "CHEMBL280074": "CN1C=NC2=C1N=C(N=C2NCC3=CC=CC=C3)NCCO", "CHEMBL300936": "CC(C)(C)C1=CN=C(O1)CSC2=CN=C(S2)NC(=O)CC3=CC=C(C=C3)CNC(CO)CO", "CHEMBL363130": "CC1=C(SC=C1)C(=O)N2C(=NC(=N2)NC3=CC=C(C=C3)S(=O)(=O)N)N", "CHEMBL363607": "CC1=C(C(=C(C=C1)F)C(=O)N2C(=NC(=N2)NC3=CC=C(C=C3)S(=O)(=O)N)C)F", "CHEMBL365318": "CC1=NN=C(O1)C2=CN3C(=C2C(C)C)C(=NC=N3)NC4=C(C=C(C(=C4)C(=O)NOC)F)F", "CHEMBL370266": "CC(C)C1=C2C(=NC=NN2C=C1NC(=O)OCC3CCCO3)NC4=C(C=C(C(=C4)C(=O)NOC)F)F", "CHEMBL381207": "CC1=C(C2=C(N=CN=C2S1)N)C3=CC=C(C=C3)NC(=O)NC4=C(C=CC(=C4)C(F)(F)F)F", "CHEMBL395573": "C1=CC=[N+](C(=C1)CNC2=CC(=C3C(=C2)C(=C(C=N3)C#N)NC4=CC(=C(C=C4)F)Cl)Cl)[O-]", "CHEMBL425834": "CN(C)CCCN1C=C(N=N1)CNC2=CC(=C3C(=C2)C(=C(C=N3)C#N)NC4=CC(=C(C=C4)F)Cl)Br", "CHEMBL453336": "COC1=CC(=CC(=C1OC)OC)C2=C(CNC2=O)C3=CN(C4=CC=CC=C43)COCC5=CC=CC=C5", "CHEMBL459729": "CC1=C2C(=CC(=C1)C3CCN(CC3)CCCF)NC(=C4C(=CC=NC4=O)NCCN5C=C(C=N5)Cl)N2", "CHEMBL460746": "C1=CC=C2C(=C1)NC(=C3C=C(C=CC3=O)NC(=S)NC(=O)C4=CC=C(C=C4)[N+](=O)[O-])S2", "CHEMBL485745": "C1=CC2=C(C(=NN2C=C1)C3=CC=C(C=C3)F)C4=CC=NC=C4", "CHEMBL489083": "C1=CC=C2C(=C1)C=C3N2C4=C(C(=O)N(C4=O)CCCSC(=N)N)N5C=CC6=C5C3=CC=C6", "CHEMBL492251": "COC1=C(C=C(C=C1)C2=C(C(=CN=C2)C#N)NC3=CC4=C(C=C3)NC=C4)OC", "CHEMBL493937": "CN1CCCN(CC1)C2=NC(=CN=C2)C3=CC(=CC=C3)C=CC(=O)O", "CHEMBL50": "C1=CC(=C(C=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O)O)O", "CHEMBL504075": "CC1=CC=CC(=C1)C(=O)NC2=CC=CC(=C2)C(C)NC3=CN=CC(=N3)Cl", "CHEMBL523586": "C1=CC(=CC(=C1)F)CC(CN)NC(=O)C2=CC(=C(S2)C3=C4C=CNC4=NC=C3)Br", "CHEMBL76904": "C1=CC(=C(C=C1C=C(C#N)C#N)O)O", "CHEMBL2326002": "CC(C)C(C)(C1CN(CCN1)C2=C(C=C(C(=N2)C3=C4C=CC=NC4=NN3)F)Cl)O", "CHEMBL296682": "C1=CC(=C2C(=C1O)C(=CN2)C3=NC(=NC=C3)N)Br", "CHEMBL597592": "CC(C)(C)C1=NN(C(=C1)NC(=O)NC2=CC(=CC=C2)OC3=CC=CC4=C3NC(=O)N4)C5=CC=CC=C5", "CHEMBL598626": "CC(C)(C)C1=NN(C(=C1)NC(=O)C2=CC(=CC=C2)OC3=CC=CC4=C3NC(=O)N4)C5=CC=CC=C5", "CHEMBL602123": "C1=CC(=CC(=C1)OC(F)(F)F)C(=O)NC2=CC(=C(C(=C2F)F)F)OC3=CC=CC4=C3NC(=O)N4", "CHEMBL75680": "CCCCC1=C2C(=NC=CN2)NC1=C3C=CC(=O)C=C3", "CHEMBL1968606": "CC1=CC(=O)NN=C1C2=CC=C(C=C2)NC(=O)NC3=CC(=CC=C3)Cl", "CHEMBL1998477": "CS(=O)(=O)C1=CC=CC(=C1)C2=C3N=C(C=C(N3N=C2)C(=O)N)C4=CC=CC=C4", "CHEMBL2004887": "C1=CC=C(C=C1)C2=CN3C(=N2)C=CN=C3N", "CHEMBL2171124": "CN1C=C(C2=C1N=CN=C2N)C3=CC4=C(C=C3)N(CC4)C(=O)CC5=CC(=CC=C5)C(F)(F)F", "CHEMBL207544": "C#CC1=NC=C(C=C1C2=CC3=C(C=C2)C=NC=C3)OCC(CC4=CNC5=CC=CC=C54)N", "CHEMBL210390": "C1=CC=C2C(=C1)C(=CN2)CC(COC3=CN=CC(=C3)C4=CC5=CC(=NC=C5C=C4)N)N", "CHEMBL23254": "CC(C)C(CO)NC1=NC2=C(C(=N1)NC3=CC(=C(C=C3)C(=O)O)Cl)N=CN2C(C)C", "CHEMBL291975": "CN1C=C(C2=CC=CC=C21)C3=C(C(=O)NC3=O)C4=CN(C5=CC=CC=C54)C6CCN(C6)CC7=CC=CC=C7", "CHEMBL300549": "CN1C=C(C2=CC=CC=C21)C3=C(C(=O)NC3=O)C4=CN(C5=CC=CC=C54)C6CCN(CC6)CC7=CC=CC=C7", "CHEMBL301860": "CC(C)N1CCC(CC1)N2C=C(C3=CC=CC=C32)C4=C(C(=O)NC4=O)C5=CN(C6=CC=CC=C65)C", "CHEMBL332575": "C1=CC=C2C(=C1)C=CC3=C2C4=C(C5=C3NC6=CC=CC=C65)C(=O)NC4=O", "CHEMBL337642": "C1COCCOCCOCCOCCN2C=C(C3=C2N=CC=C3)C4=C(C5=CN1C6=C5C=CC=N6)C(=O)NC4=O", "CHEMBL340259": "C1COCCOCCOCCN2C=C(C3=CC=CC=C32)C4=C(C5=CN1C6=CC=CC=C65)C(=O)NC4=O", "CHEMBL340776": "C1COCCOCCOCCN2C=C(C3=C2N=CC=C3)C4=C(C5=CN1C6=C5C=CC=N6)C(=O)NC4=O", "CHEMBL340935": "C1COCCOCCOCCN2C=C(C3=C2N=CC=C3)C4=C(C5=CN1C6=CC=CC=C65)C(=O)NC4=O", "CHEMBL378963": "C1=CC=C2C(=C1)C(=CN2)CC(COC3=CN=C(C(=C3)C4=CC5=C(C=C4)C=NC=C5)Cl)N", "CHEMBL432130": "CN(C)CC1CCN2C=C(C3=CC=CC=C32)C4=C(C5=CN(CCO1)C6=CC=CC=C65)C(=O)NC4=O", "CHEMBL52654": "CN1CCC(CC1)N2C=C(C3=CC=CC=C32)C4=C(C(=O)NC4=O)C5=CNC6=CC=CC=C65", "CHEMBL53596": "CN1CCC(CC1)N2C=C(C3=CC=CC=C32)C4=C(C(=O)NC4=O)C5=CN(C6=CC=CC=C65)C", "CHEMBL54382": "CCN1CCC(CC1)N2C=C(C3=CC=CC=C32)C4=C(C(=O)NC4=O)C5=CN(C6=CC=CC=C65)C", "CHEMBL55394": "CN1C=C(C2=CC=CC=C21)C3=C(C(=O)NC3=O)C4=CN(C5=CC=CC=C54)C6CCN(CC6)CC7CC7", "CHEMBL55788": "CN1C=C(C2=CC=CC=C21)C3=C(C(=O)NC3=O)C4=CN(C5=CC=CC=C54)C6CCNCC6", "CHEMBL7463": "CN(C)CCCN1C=C(C2=CC=CC=C21)C3=C(C(=O)NC3=O)C4=CNC5=CC=CC=C54", "CHEMBL1290746": "CC1=C(C=C(C=C1)C(=O)NC2=NOC=C2)NC(=O)C3=C(N(N=C3)C4=CC=CC=C4F)N", "CHEMBL479835": "CC1=C(C=CC2=C1C=CN2)NC3=C4C=C(SC4=NC=C3C#N)C5=C(C=CC(=C5)OC)CN(C)C", "CHEMBL2206666": "C1=CC(=CC(=C1)C(F)(F)F)C(=O)NC2=CC(=CC=C2)OC3=NN4C=CN=C4C=C3", "CHEMBL371169": "C1=CC(=CC(=C1)Cl)NC2=NC(=CN=C2)C3=CC(=CN=C3)NCCCN4C=CC=N4", "CHEMBL372657": "C1=CC(=CC(=C1)Cl)NC2=NC(=CN=C2)C3=CC(=CN=C3)NCCCN4C=NC=N4", "CHEMBL1651523": "CC1CC=CC(=O)CCCCCC2=CC(=CC(=C2C(=O)O1)O)OC", "CHEMBL1993634": "CC(C)(C)C1=NN(C(=C1)NC(=O)NC2=CC=CC3=CC=CC=C32)C4=CC=CC(=C4)C(=O)N(CCN)CCO", "CHEMBL223971": "COCCOCC#CC1=CC(=CS1)C2=NNC3=C2CC4=C3C=C(C=C4)CN5C=NC=N5", "CHEMBL230761": "CN1C=C(N=C1)CNC2=CC(=C3C(=C2)C(=C(C=N3)C#N)NC4=CC(=C(C=C4)F)Cl)Br", "CHEMBL245377": "CN1CCN(CC1)CC(=O)NC2=CC=CC3=C2CC4=C3NN=C4C5=CSC(=C5)C#CCOC6=CC=CC=C6", "CHEMBL245769": "COCC(=O)NC1=CC=CC2=C1CC3=C2NN=C3C4=CSC(=C4)C#CCOC5=CC=CC=C5", "CHEMBL245968": "COCCOCC(=O)NC1=CC=CC2=C1CC3=C2NN=C3C4=CSC(=C4)C#CCOC5=CC=CC=C5", "CHEMBL246166": "COC(=O)C(=O)NC1=CC=CC2=C1CC3=C2NN=C3C4=CSC(=C4)C#CCOC5=CC=CC=C5", "CHEMBL249097": "CC1=C(C=C(C=C1)O)NC2=NC(=NC=C2)NC3=CC=CC(=C3)C(=O)N", "CHEMBL390156": "CN1CCN(CC1)CC2=CC3=C(C=C2)C4=C(C3)C(=NN4)C5=CSC(=C5)C#CCOC6=CC=CC=C6", "CHEMBL395427": "CCOC(=O)CC(=O)NC1=CC=CC2=C1CC3=C2NN=C3C4=CSC(=C4)C#CCOC5=CC=CC=C5", "CHEMBL565061": "CCOC(=O)C1=C2N=CC=C(N2N=C1)C3=CC(=CC=C3)NC(=O)C4=CC(=CC=C4)C(F)(F)F", "CHEMBL235345": "C1C(C1NC2=NC(=O)C(=CC3=CC4=C(C=C3)N=CC=C4)S2)C5=CC=CC=C5", "CHEMBL396377": "C1=CC2=C(C=CC(=C2)C=C3C(=O)N=C(S3)N)N=C1", "CHEMBL1234833": "CC(C)C1=C2N=C(C=C(N2N=C1)NCC3=CC=CC=C3)NC(CO)C(CO)O", "CHEMBL1272116": "CC(C)C1=C(C(=NN1)Cl)C2=NC(=NC=C2)NC3=NC=C(C=C3)N4CCC(CC4)N(C)C", "CHEMBL1272171": "CC(C)C1=C(C(=NN1)C(F)(F)F)C2=NC(=NC=C2)NC3=NC=C(C=C3)N4CCC(CC4)N(C)C", "CHEMBL1974363": "C1=CC=C(C=C1)C2=CC=NC3=C(C=NN23)C(=O)NC4=CC=C(C=C4)CO", "CHEMBL44541": "C1=CC2=C(C=C1Br)C(=CN2)C3=NC(=NC=C3)N", "CHEMBL44545": "C1=CN=C(N=C1C2=CNC3=CC(=CC(=C32)O)Br)N", "CHEMBL46440": "C1=CC2=C(C=C1Br)NC=C2C3=NC(=NC=C3)N", "CHEMBL86771": "C1=CC=C2C(=C1)C(=O)C3=C(C=CC(=C3C2=O)N)N", "CHEMBL2001451": "CC(C)(C)C1=NN(C(=C1)NC(=O)NC2=CC=CC3=CC=CC=C32)C4=CC=CC(=C4)C(=O)NCCCCN(C)C", "CHEMBL2002182": "C1=CC=C(C=C1)C2=CC=CN3C2=NNC3=O", "CHEMBL1668418": "CC1CC=CC(=O)CCCC=CC2=CC(=CC(=C2C(=O)O1)O)OC", "CHEMBL1668419": "CC1CC=CC(=O)CCCCCC2=CC(=CC(=C2C(=O)O1)O)OC", "CHEMBL408982": "CCN1C2=C(C=CC(=C2)OC)SC1=CC(=O)C", "CHEMBL307152": "CN1C=CC2=C1C3=C(C=C2)C4=C(C5=C(N4)C(=CC=C5)CCCNC6CCC(CC6)O)C7=C3C(=O)NC7=O", "CHEMBL230654": "CCCC1=C(NC=N1)CNC2=CC(=C3C(=C2)C(=C(C=N3)C#N)NC4=CC(=C(C=C4)F)Cl)Cl"}