SUPPLEMENTARY MATERIAL

Blood Brain Barrier and Alzheimer's Disease: Similarity and Dissimilarity of Molecular Alerts

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IMPORTANT

Distribution into the training (+), invisible training (-), calibration (#), and validation (*) sets is done via the first symbol in each line of the input file. Table S1 contains the first split for gamma secretase inhibitors. Table S2 contains the first split for substances with blood brain barrier permeation (logBB).

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Table S1. The ID and SMILES used to represent 233 gamma-secretase inhibitors which are potential agents for treatment Alzheimer's disease together with their binding affinity.

-CHEMBL370107 OC1CCC(CC1)(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 6.700
+CHEMBL370729 Fc1ccc(F)c(c1)C1(CC2CCC(C2)C1)S(=O)(=O)c1ccc(Cl)cc1 7.280
-CHEMBL191195 Clc1ccc(cc1)S(=O)(=O)C1(CCCCC1)c1ccccc1 6.340
+CHEMBL191246 Fc1ccccc1C1(CCCCC1)S(=O)(=O)c1ccc(Cl)cc1 7.260
-CHEMBL191301 CC(C)N(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 6.770
#CHEMBL191302 C[C@H](CO)N(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 7.570
#CHEMBL191887 CC(C)C(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 7.150
#CHEMBL192356 CC(CCO)C(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 7.460
+CHEMBL192393 COC(=O)C(C)C(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 6.600
-CHEMBL193111 CC(CO)C(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 6.520
-CHEMBL194820 Fc1ccc(F)c(CS(=O)(=O)c2ccc(Cl)cc2)c1 5.360
#CHEMBL195105 CC(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 5.610
#CHEMBL195200 Fc1cccc(c1)C1(CCCCC1)S(=O)(=O)c1ccc(Cl)cc1 6.600
+CHEMBL363802 Fc1ccc(F)c(c1)C1(CCCCC1)S(=O)(=O)c1ccccc1 7.010
*CHEMBL364042 CN(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 5.720
#CHEMBL366006 COC(=O)C1CC(CCC1=O)(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 6.980
*CHEMBL366022 Fc1ccc(F)c(c1)C1(CCC(=O)CC1)S(=O)(=O)c1ccc(Cl)cc1 7.660
-CHEMBL425566 Fc1ccc(F)c(c1)C1(CCCCC1)S(=O)(=O)c1ccc(Cl)cc1 8.520
+CHEMBL209384 CC(N(c1ccccc1)S(=O)(=O)c1ccc(Br)cc1)c1ccccc1OCCCN1CCCC1 5.720
+CHEMBL209739 CC(N(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1)c1ccccc1OCCCN1CCCCC1 5.680
+CHEMBL211428 CC(N(c1ccccc1)S(=O)(=O)c1ccccc1)c1ccccc1OCCCN1CCCC1 6.160
+CHEMBL211955 CC(N(c1ccccc1C(=O)c1ccccc1)S(=O)(=O)c1ccc(Cl)cc1)c1ccccc1OCCCN1CCCC1 5.920
+CHEMBL212926 CC(N(c1ccc(cc1)C(=O)c1ccccc1)S(=O)(=O)c1ccc(Cl)cc1)c1ccccc1OCCCN1CCCC1 5.490
-CHEMBL213231 CC(N(c1ccccc1)S(=O)(=O)c1ccc(Cl)cc1)c1ccccc1OCCCN1CCCC1 8.000
#CHEMBL213557 CC(N(c1ccc(Cl)cc1)S(=O)(=O)c1ccc(Cl)cc1)c1ccccc1OCCCN1CCCC1 5.890
+CHEMBL213628 CC(N(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1)c1ccccc1OCCCN1CCOCC1 5.360
+CHEMBL213729 CC(N(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1)c1ccccc1OCCCN1CCCC1 5.700
+CHEMBL214301 CC(N(c1ccccc1)S(=O)(=O)c1ccc(Cl)cc1)c1ccc(cc1OCCCN1CCCC1)C(=O)c1ccccc1 4.770
+CHEMBL214405 CC(N(c1cccc(Cl)c1)S(=O)(=O)c1ccc(Cl)cc1)c1ccccc1OCCCN1CCCC1 6.280
-CHEMBL373983 CC(N(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1)c1ccc(cc1OCCCN1CCCC1)C(=O)c1ccccc1 6.890
-CHEMBL378664 CC(N(c1cccc(c1)C(=O)c1ccccc1)S(=O)(=O)c1ccc(Cl)cc1)c1ccccc1OCCCN1CCCC1 5.520
#CHEMBL378971 COc1ccc(cc1)N(C(C)c1ccccc1OCCCN1CCCC1)S(=O)(=O)c1ccc(Cl)cc1 5.960
-CHEMBL379428 CCN(CC)CCCOc1ccccc1C(C)N(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 6.000
#CHEMBL384963 CC(N(c1ccccc1)S(=O)(=O)c1ccc(F)cc1)c1ccccc1OCCCN1CCCC1 6.460
#CHEMBL385166 CC(N(c1ccccc1)S(=O)(=O)c1ccc(cc1)C(F)(F)F)c1ccccc1OCCCN1CCCC1 6.400
*CHEMBL386866 COc1ccccc1N(C(C)c1ccccc1OCCCN1CCCC1)S(=O)(=O)c1ccc(Cl)cc1 6.330
*CHEMBL387000 CC(N(c1ccccc1Cl)S(=O)(=O)c1ccc(Cl)cc1)c1ccccc1OCCCN1CCCC1 6.310
-CHEMBL425063 COc1cccc(c1)N(C(C)c1ccccc1OCCCN1CCCC1)S(=O)(=O)c1ccc(Cl)cc1 6.280
#CHEMBL180209 Clc1ccc(s1)S(=O)(=O)NC1C2CCC1Cc1cc(/C=C/CN3CCOCC3)ccc1C2 6.970
-CHEMBL183326 O=S(=O)(NC1C2CCC1Cc1ccccc1C2)c1ccccc1 6.720
#CHEMBL183777 Clc1ccc(s1)S(=O)(=O)NC1C2CCC1Cc1ccccc1C2 7.210
+CHEMBL179060 CN1CCN(C/C=C/c2ccc3CC4CCC(Cc3c2)C4NS(=O)(=O)c2ccc(Cl)s2)CC1 7.410
-CHEMBL179519 Clc1ccc(s1)S(=O)(=O)NC1C2CCC1Cc1cc(/C=C/Cn3ccnc3)ccc1C2 7.820
*CHEMBL179524 OC1CCN(CCOc2ccc3CC4CCC(Cc3c2)C4NS(=O)(=O)c2ccc(Cl)s2)C1 6.680
-CHEMBL179982 CC1CCCCN1CCOc1ccc2CC3CCC(Cc2c1)C3NS(=O)(=O)c1ccc(Cl)s1 6.640
+CHEMBL180062 Clc1ccc(s1)S(=O)(=O)NC1C2CCC1Cc1cc(/C=C/CN3CCN(CC3)c3ccccc3)ccc1C2 7.680
#CHEMBL180118 CC1CCCN1CCOc1ccc2CC3CCC(Cc2c1)C3NS(=O)(=O)c1ccc(Cl)s1 6.470
*CHEMBL180132 Clc1ccc(cc1)S(=O)(=O)NC1C2CCC1Cc1ccccc1C2 6.330
-CHEMBL180326 OC1CCN(CCOc2ccc3CC4CCC(Cc3c2)C4NS(=O)(=O)c2ccc(Cl)s2)CC1 6.210
*CHEMBL180384 Clc1ccc(s1)S(=O)(=O)NC1C2CCC1Cc1cc(NC(=O)CN3CCCCC3)ccc1C2 8.220
-CHEMBL180784 Clc1ccc(s1)S(=O)(=O)NC1C2CCC1Cc1cc(NC(=O)OCc3ccccc3)ccc1C2 7.640
-CHEMBL181213 Fc1cccc(c1)S(=O)(=O)NC1C2CCC1Cc1ccccc1C2 6.490
*CHEMBL181306 Clc1ccc(s1)S(=O)(=O)NC1C2CCC1Cc1c(Cl)cccc1C2 6.760
-CHEMBL181519 CN(CC(=O)Nc1ccc2CC3CCC(Cc2c1)C3NS(=O)(=O)c1ccc(Cl)s1)Cc1ccccc1 6.650
*CHEMBL182327 Fc1cccc2CC3CCC(Cc12)C3NS(=O)(=O)c1ccc(Cl)s1 7.470
#CHEMBL182349 CCN(CC)CC(=O)Nc1ccc2CC3CCC(Cc2c1)C3NS(=O)(=O)c1ccc(Cl)s1 7.390
-CHEMBL182416 Fc1ccc(cc1)S(=O)(=O)NC1C2CCC1Cc1ccccc1C2 6.890
-CHEMBL182463 O=C(Nc1ccc2CC3CCC(Cc2c1)C3NS(=O)(=O)c1ccccc1)OCc1ccccc1 7.130
-CHEMBL182487 Clc1ccc(s1)S(=O)(=O)NC1C2CCC1Cc1cc(NC(=O)CNCc3ccccc3)ccc1C2 5.460
-CHEMBL182638 CCCCS(=O)(=O)NC1C2CCC1Cc1ccccc1C2 6.210
-CHEMBL182833 Clc1ccc2CC3CCC(Cc2c1)C3NS(=O)(=O)c1ccc(Cl)s1 6.840
-CHEMBL183043 Clc1ccc(COC(=O)Nc2ccc3CC4CCC(Cc3c2)C4NS(=O)(=O)c2ccccc2)cc1 7.800
*CHEMBL183137 Clc1ccccc1COC(=O)Nc1ccc2CC3CCC(Cc2c1)C3NS(=O)(=O)c1ccccc1 6.820
-CHEMBL183351 Clc1ccc(s1)S(=O)(=O)NC1C2CCC1Cc1cc(NC(=O)CN3CCN(CC3)c3ccccc3)ccc1C2 8.300
-CHEMBL183449 Fc1ccc2CC3CCC(Cc2c1)C3NS(=O)(=O)c1ccccc1 7.150
+CHEMBL183549 CC(C)CCCC(=O)Nc1ccc2CC3CCC(Cc2c1)C3NS(=O)(=O)c1ccccc1 6.270
*CHEMBL183558 Clc1ccc(s1)S(=O)(=O)NC1C2CCC1Cc1cc(NC(=O)CN3CCCC3)ccc1C2 8.150
*CHEMBL183585 O=C(Nc1ccc2CC3CCC(Cc2c1)C3NS(=O)(=O)c1ccccc1)c1cccn1 7.120
+CHEMBL183654 O=S(=O)(NC1C2CCC1Cc1ccccc1C2)c1cccs1 7.300
-CHEMBL183724 Fc1ccccc1S(=O)(=O)NC1C2CCC1Cc1ccccc1C2 6.620
+CHEMBL183764 Clc1ccc(s1)S(=O)(=O)NC1C2CCC1Cc1cc(NC(=O)c3ccccn3)ccc1C2 7.920
-CHEMBL183774 Clc1ccc(s1)S(=O)(=O)NC1C2CCC1Cc1cc(NC(=O)CN3CCOCC3)ccc1C2 8.150
#CHEMBL359693 Clc1ccc(s1)S(=O)(=O)NC1C2CCC1Cc1cc(OCCN3CCCCC3)ccc1C2 7.140
*CHEMBL360069 Clc1ccc(s1)S(=O)(=O)NC1C2CCC1Cc1cc(/C=C/CN3CCCCC3)ccc1C2 6.820
#CHEMBL360119 Clc1cccc(COC(=O)Nc2ccc3CC4CCC(Cc3c2)C4NS(=O)(=O)c2ccccc2)c1 6.390
#CHEMBL360239 CCCS(=O)(=O)NC1C2CCC1Cc1ccccc1C2 6.140
#CHEMBL360679 Cc1ccc(cc1)S(=O)(=O)NC1C2CCC1Cc1ccccc1C2 6.190
-CHEMBL361143 Nc1ccc2CC3CCC(Cc2c1)C3NS(=O)(=O)c1ccccc1 5.220
-CHEMBL361408 COc1ccc2CC3CCC(Cc2c1)C3NS(=O)(=O)c1ccc(Cl)s1 6.310
#CHEMBL362216 Fc1ccc2CC3CCC(Cc2c1)C3NS(=O)(=O)c1ccc(Cl)s1 7.540
#CHEMBL362644 CN1CCN(CC(=O)Nc2ccc3CC4CCC(Cc3c2)C4NS(=O)(=O)c2ccc(Cl)s2)CC1 7.160

#CHEMBL369557 Clc1ccc(s1)S(=O)(=O)NC1C2CCC1Cc1cc(OCCN3CCOCC3)ccc1C2 8.300
*CHEMBL427509 Oc1ccc2CC3CCC(Cc2c1)C3NS(=O)(=O)c1ccc(Cl)s1 6.570
#CHEMBL51505 CN1C(=O)[C@@H](NC(=O)C(Cc2ccc(Cl)c(Cl)c2)c2ccncc2)N=C(c2ccccc2)c2ccccc12 6.110
-CHEMBL52685 CC(C)C(Cc1ccc(Cl)c(Cl)c1)C(=O)N[C@@H]1N=C(c2ccccc2)c2ccccc2N(C)C1=O 6.470
-CHEMBL130093 C[C@@H](Cc1ccc(F)c(F)c1)C(=O)NC1N=C(c2ccc(cc2)C(=O)N)c2ccccc2N(C)C1=O 9.310
#CHEMBL132670 C[C@@H](Cc1ccc(F)c(F)c1)C(=O)N[C@@H]1N=C(c2ccc3C(=O)CCCc3c2)c2ccccc2N(C)C1=O 8.660
-CHEMBL132900 C[C@@H](Cc1ccc(F)c(F)c1)C(=O)N[C@@H]1N=C(c2ccc3C(=O)N(C)CCc3c2)c2ccccc2N(C)C1=O 5.720
#CHEMBL133235 C[C@@H](Cc1ccc(F)c(F)c1)C(=O)N[C@@H]1N=C(c2ccc3OC(F)(F)Oc3c2)c2ccccc2N(C)C1=O 7.550
-CHEMBL133237 C[C@@H](Cc1ccc(F)c(F)c1)C(=O)N[C@@H]1N=C(c2ccc3c(=O)ccoc3c2)c2ccccc2N(C)C1=O 8.920
*CHEMBL133746 C[C@@H](Cc1ccc(F)c(F)c1)C(=O)N[C@@H]1N=C(c2ccc3OCOc3c2)c2ccccc2N(C)C1=O 7.880
-CHEMBL133820 C[C@@H](Cc1ccc(F)c(F)c1)C(=O)N[C@@H]1N=C(c2ccc3C(=O)NCCc3c2)c2ccccc2N(C)C1=O 9.520
+CHEMBL133857 C[C@@H](Cc1ccc(F)c(F)c1)C(=O)N[C@@H]1N=C(c2ccc3c(O)nccc3c2)c2ccccc2N(C)C1=O 9.700
*CHEMBL134124 C[C@@H](Cc1ccc(F)c(F)c1)C(=O)N[C@@H]1N=C(c2ccc3OCOc3c2)c2ccccc2N(CC(=O)N(C)C)C1=O 8.260
+CHEMBL263980 CN1C(=O)C(NC(=O)CCc2ccc(F)cc2)N=C(c2ccc(cc2)C(=O)N)c2ccccc12 6.960
#CHEMBL291322 CN1C(=O)C(NC(=O)CCc2ccc(F)c(F)c2)N=C(c2ccc(cc2)C(=O)N)c2ccccc12 7.540
*CHEMBL292693 CN1C(=O)C(NC(=O)CCc2cc(F)cc(F)c2)N=C(c2ccc(cc2)C(=O)N)c2ccccc12 6.960
*CHEMBL297723 CN1C(=O)C(NC(=O)CCc2cccc(Cl)c2Cl)N=C(c2ccc(cc2)C(=O)N)c2ccccc12 7.660
-CHEMBL298360 CN1C(=O)C(NC(=O)CCc2ccc(C)cc2)N=C(c2ccc(cc2)C(=O)N)c2ccccc12 6.740
+CHEMBL298549 CN1C(=O)[C@@H](NC(=O)C(Cc2ccc(Cl)c(Cl)c2)c2ccsc2)N=C(c2ccccc2)c2ccccc12 7.000
*CHEMBL299078 CN1C(=O)C(NC(=O)CCc2cc(Cl)cc(Cl)c2)N=C(c2ccc(cc2)C(=O)N)c2ccccc12 7.400
*CHEMBL299403 CN1C(=O)C(NC(=O)CCc2c(Cl)cccc2Cl)N=C(c2ccc(cc2)C(=O)N)c2ccccc12 5.490
-CHEMBL299976 COc1ccccc1CCC(=O)NC1N=C(c2ccc(cc2)C(=O)N)c2ccccc2N(C)C1=O 5.290
*CHEMBL300420 CN1C(=O)[C@@H](NC(=O)[C@H](Cc2ccc(Cl)c(Cl)c2)NC(=O)OC(C)(C)C)N=C(c2ccccc2)c2ccccc12 6.120
-CHEMBL300590 CN1C(=O)C(NC(=O)CCc2cccc(O)c2)N=C(c2ccc(cc2)C(=O)N)c2ccccc12 5.170
*CHEMBL301084 C[C@@H](Cc1ccc(Cl)cc1Cl)C(=O)N[C@@H]1N=C(c2ccccc2)c2ccccc2N(C)C1=O 6.090
#CHEMBL301521 COc1ccc(CCC(=O)NC2N=C(c3ccc(cc3)C(=O)N)c3ccccc3N(C)C2=O)cc1 5.870
+CHEMBL306273 CN1C(=O)[C@@H](NC(=O)[C@H](C(O)c2ccc(Cl)c(Cl)c2)c2ccc(F)cc2)N=C(c2ccccc2)c2ccccc12 8.920
+CHEMBL306536 CO[C@@H]([C@H](C)C(=O)N[C@@H]1N=C(c2ccccc2)c2ccccc2N(C)C1=O)c1ccc(Cl)c(Cl)c1 7.230
+CHEMBL307208 C[C@@H]([C@H](OCC(=O)N)c1ccc(Cl)c(Cl)c1)C(=O)N[C@@H]1N=C(c2ccccc2)c2ccccc2N(C)C1=O 5.320
+CHEMBL307243 CC[C@H]([C@@H](C(=O)N[C@@H]1N=C(c2ccccc2)c2ccccc2N(C)C1=O)c1ccc(F)cc1)c1ccc(F)c(F)c1 6.670
*CHEMBL307445 C[C@@H]([C@H](OC(=O)N)c1ccc(Cl)c(Cl)c1)C(=O)N[C@@H]1N=C(c2ccccc2)c2ccccc2N(C)C1=O 5.610
*CHEMBL307843 C[C@H]([C@@H](C(=O)N[C@@H]1N=C(c2ccccc2)c2ccccc2N(C)C1=O)c1ccc(F)cc1)c1ccc(F)c(F)c1 8.820
*CHEMBL308095 OCC[C@H]([C@@H](C(=O)N[C@@H]1N=C(c2ccccc2)c2ccccc2NC1=O)c1ccc(F)cc1)c1ccc(F)c(F)c1 7.460
-CHEMBL311153 CN1C(=O)[C@@H](NC(=O)[C@H]([C@H](CO)c2ccc(F)c(F)c2)c2ccc(F)cc2)N=C(c2ccccc2)c2ccccc12 10.150
*CHEMBL334594 C[C@@H](Cc1ccc(F)c(F)c1)C(=O)N[C@@H]1N=C(c2ccc3OCOc3c2)c2ccccc2N(CC(=O)N)C1=O 7.880
#CHEMBL335184 C[C@@H](Cc1ccc(F)c(F)c1)C(=O)N[C@@H]1N=C(c2ccc3OCOc3c2)c2ccccc2N(CCC(=O)C)C1=O 8.430
+CHEMBL335994 COC(=O)CN1C(=O)[C@@H](NC(=O)[C@@H](C)Cc2ccc(F)c(F)c2)N=C(c2ccc3OCOc3c2)c2ccccc12 7.900
-CHEMBL336071 C[C@@H](Cc1ccc(F)c(F)c1)C(=O)N[C@@H]1N=C(c2ccc3OCOc3c2)c2ccccc2NC1=O 8.740
+CHEMBL336813 C[C@@H](Cc1ccc(F)c(F)c1)C(=O)N[C@@H]1N=C(c2ccc3OCOc3c2)c2ccccc2N(CCO)C1=O 9.050
-CHEMBL337670 C[C@H](Cc1ccc(F)c(F)c1)C(=O)N[C@@H]1N=C(c2ccc3NC(=O)CCc3c2)c2ccccc2N(C)C1=O 7.000
+CHEMBL341256 CNC(=O)CN1C(=O)[C@@H](NC(=O)[C@@H](C)Cc2ccc(F)c(F)c2)N=C(c2ccc3OCOc3c2)c2ccccc12 8.740
-CHEMBL341257 C[C@H](Cc1ccc(F)c(F)c1)C(=O)N[C@@H]1N=C(c2ccc3OCCOc3c2)c2ccccc2N(C)C1=O 8.330
+CHEMBL416116 COc1cccc(CCC(=O)NC2N=C(c3ccc(cc3)C(=O)N)c3ccccc3N(C)C2=O)c1 5.800
#CHEMBL416121 CC(Cc1ccc(Cl)cc1Cl)C(=O)NC1N=C(c2ccc(cc2)C(=O)N)c2ccccc2N(C)C1=O 8.100
-CHEMBL418090 CN1C(=O)[C@@H](NC(=O)[C@H](Cc2ccc(F)c(F)c2)c2ccc(F)cc2)N=C(c2ccccc2)c2ccccc12 8.420
-CHEMBL420563 CN1C(=O)[C@@H](NC(=O)[C@H]([C@H](C=C)c2ccc(F)c(F)c2)c2ccc(F)cc2)N=C(c2ccccc2)c2ccccc12 7.000
-CHEMBL421310 CN1C(=O)[C@@H](NC(=O)[C@H]([C@H](CBr)c2ccc(F)c(F)c2)c2ccc(F)cc2)N=C(c2ccccc2)c2ccccc12 8.170
*CHEMBL423533 C[C@@H](Cc1ccc(F)c(F)c1)C(=O)N[C@@H]1N=C(c2ccc3C(=O)CCc3c2)c2ccccc2N(C)C1=O 8.440
*CHEMBL51698 CN1C(=O)C(NC(=O)CCc2ccc(Cl)cc2)N=C(c2ccc(cc2)C(=O)N)c2ccccc12 7.820
#CHEMBL51699 CN1C(=O)C(NC(=O)CCc2cccc(Cl)c2)N=C(c2ccc(cc2)C(=O)N)c2ccccc12 7.030
+CHEMBL51809 CN1C(=O)C(NC(=O)CCCc2ccccc2)N=C(c2ccc(cc2)C(=O)N)c2ccccc12 5.300
*CHEMBL52078 CN1C(=O)C(NC(=O)CCc2ccc(Cl)cc2Cl)N=C(c2ccc(cc2)C(=O)N)c2ccccc12 7.480
-CHEMBL52512 CN1C(=O)C(NC(=O)CCc2ccc(Cl)c(Cl)c2)N=C(c2ccc(cc2)C(=O)N)c2ccccc12 7.920
-CHEMBL52950 CN1C(=O)C(NC(=O)C(C)(C)Cc2ccc(Cl)cc2Cl)N=C(c2ccc(cc2)C(=O)N)c2ccccc12 6.400
#CHEMBL53095 CN1C(=O)C(NC(=O)CCc2cccc2)N=C(c2ccc(cc2)C(=O)N)c2ccccc12 6.470
+CHEMBL53177 C[C@@H](Cc1ccc(F)c(F)c1)C(=O)N[C@@H]1N=C(c2ccccc2)c2ccccc2N(C)C1=O 6.660
+CHEMBL53198 CN1C(=O)[C@@H](NC(=O)C(Cc2ccc(Cl)c(Cl)c2)c2cccs2)N=C(c2ccccc2)c2ccccc12 7.430
+CHEMBL53371 CN1C(=O)C(NC(=O)/C=C/c2ccc(Cl)cc2Cl)N=C(c2ccc(cc2)C(=O)N)c2ccccc12 5.330
+CHEMBL53381 CN1C(=O)[C@@H](NC(=O)C(Cc2ccc(Cl)c(Cl)c2)c2csc(C)[nH]2)N=C(c2ccccc2)c2ccccc12 6.190
*CHEMBL53383 CN1C(=O)[C@@H](NC(=O)[C@H](Cc2ccc(Cl)c(Cl)c2)c2ccc(Br)cc2)N=C(c2ccccc2)c2ccccc12 7.000
+CHEMBL53419 CN1C(=O)C(NC(=O)CCc2ccccc2Cl)N=C(c2ccc(cc2)C(=O)N)c2ccccc12 6.520
+CHEMBL53928 CN1C(=O)C(NC(=O)CCc2cc(Cl)ccc2Cl)N=C(c2ccc(cc2)C(=O)N)c2ccccc12 7.220
-CHEMBL54673 CN1C(=O)C(NC(=O)CCc2cc(cc(c2)C(F)(F)F)C(F)(F)F)N=C(c2ccc(cc2)C(=O)N)c2ccccc12 6.400
-CHEMBL72016 CN1C(=O)[C@@H](NC(=O)[C@@H]([C@@H](O)c2ccc(F)c(F)c2)c2ccc(F)cc2)N=C(c2ccccc2)c2ccccc12 8.020
#CHEMBL72138 CN1C(=O)[C@@H](NC(=O)[C@H](C(O)c2ccc(F)c(F)c2)c2ccc(F)cc2)N=C(c2ccccc2)c2ccccc12 9.100
#CHEMBL73347 CC(C(=O)N[C@@H]1N=C(c2ccccc2)c2ccccc2N(C)C1=O)C(=O)c1ccc(Cl)c(Cl)c1 6.030
-CHEMBL73362 C[C@@H]([C@H](OS(=O)(=O)N)c1ccc(Cl)c(Cl)c1)C(=O)N[C@@H]1N=C(c2ccccc2)c2ccccc2N(C)C1=O 6.350
-CHEMBL73484 CC(C(=O)N[C@@H]1N=C(c2ccccc2)c2ccccc2N(C)C1=O)/C(=N\O)/c1ccc(Cl)c(Cl)c1 7.460
+CHEMBL73841 CC(C(CO)c1ccc(F)c(F)c1)C(=O)N[C@@H]1N=C(c2ccccc2)c2ccccc2N(C)C1=O 8.160
#CHEMBL74566 OC[C@H]([C@@H](C(=O)N[C@@H]1CN(c2ccccc2)c2ccccc2NC1=O)c1ccc(F)cc1)c1ccc(F)c(F)c1 10.150
*CHEMBL74568 CN1C(=O)[C@@H](NC(=O)[C@@H]([C@@H](O)c2ccc(Cl)c(Cl)c2)c2ccc(F)cc2)N=C(c2ccccc2)c2ccccc12 7.170
+CHEMBL75375 OC[C@H]([C@@H](C(=O)N[C@@H]1N=C(c2ccccc2)c2ccccc2NC1=O)c1ccc(F)cc1)c1ccc(F)c(F)c1 10.220
#CHEMBL115852 CC(C)N1N(C)C(=O)C(NC(=O)[C@H](C)NC(=O)Cc2cccc(F)c2)c2ccccc2C1=O 7.240
-CHEMBL117056 C[C@H](NC(=O)Cc1cc(F)cc(F)c1)C(=O)NC1N=C(c2ccccc2)c2ccccc2N(C)C1=O 6.680
-CHEMBL117978 C[C@H](NC(=O)Cc1cc(F)cc(F)c1)C(=O)NC1C(=O)N(C)N(C)C(=O)c2ccccc12 8.300
#CHEMBL118450 CC(C)N1N(C)C(=O)C(NC(=O)[C@H](C)NC(=O)Cc2cc(F)cc(F)c2)c2ccccc2C1=O 7.330
#CHEMBL118469 CC(C)C[C@H](NC(=O)Cc1cc(F)cc(F)c1)C(=O)NC1C(=O)N(C)N(C(C)C)C(=O)c2ccccc12 7.430
#CHEMBL119657 CC(C)N1N(C)C(=O)C(NC(=O)[C@H](C)NC(=O)Cc2occc2)c2ccccc2C1=O 7.070
*CHEMBL119731 CC(C)[C@H](NC(=O)Cc1cc(F)cc(F)c1)C(=O)NC1C(=O)N(C)N(C(C)C)C(=O)c2ccccc12 6.720
+CHEMBL332885 CC(C)N1N(C)C(=O)C(NC(=O)[C@H](C)NC(=O)Cc2cocc2)c2ccccc2C1=O 7.420
*CHEMBL333710 CC(C)N1N(C)C(=O)C(NC(=O)[C@H](C)NC(=O)Cc2ccsc2)c2ccccc2C1=O 7.850
-CHEMBL406322 CC(C)C[C@H](NC(=O)Cc1ccsc1)C(=O)NC1C(=O)N(C)N(C(C)C)C(=O)c2ccccc12 8.400
-CHEMBL421236 C[C@H](NC(=O)Cc1cc(F)cc(F)c1)C(=O)NC1C(=O)N(C)c2ccccc2c2ccccc12 7.120

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-CHEMBL431679 CC(C)N1N(C)C(=O)C(NC(=O)[C@H](C)NC(=O)[C@@H](O)c2cc(F)cc(F)c2)c2ccccc2C1=O 8.300
#CHEMBL194680 CCCNS(=O)(=O)NC1[C@H]2CC[C@H]1Cc1ccccc1C2 6.880
+CHEMBL193527 FC(F)(F)CN1C[C@]2(NS1(=O)=O)[C@H]1CC[C@H]2Cc2ccc(/C=C/CN3CCCCC3)cc2C1 6.600
+CHEMBL194084 CC1CCN(C/C=C/c2ccc3C[C@@H]4CCC(Cc3c2)[C@]24CN(CC(F)(F)F)S(=O)(=O)N2)CC1 7.740
-CHEMBL194328 CN1CCN(C/C=C/c2ccc3C[C@@H]4CCC(Cc3c2)[C@]24CN(CC(F)(F)F)S(=O)(=O)N2)CC1=O 7.680
-CHEMBL194422 FC(F)(F)N1C[C@]2(NS1(=O)=O)[C@H]1CC[C@H]2Cc2ccccc2C1 7.770
-CHEMBL194788 Clc1ccc(s1)S(=O)(=O)N[C@H]1[C@H]2CC[C@H]1Cc1ccc(/C=C/CN3CCOCC3)cc1C2 9.000
+CHEMBL194887 FC(F)(F)NS(=O)(=O)NC1[C@H]2CC[C@H]1Cc1ccccc1C2 6.870
*CHEMBL195551 CC(=O)N1CCN(C/C=C/c2ccc3C[C@@H]4CCC(Cc3c2)[C@]24CN(CC(F)(F)F)S(=O)(=O)N2)CC1 8.400
+CHEMBL196153 CCNS(=O)(=O)NC1[C@H]2CC[C@H]1Cc1ccccc1C2 6.400
-CHEMBL196192 CCN1C[C@]2(NS1(=O)=O)[C@H]1CC[C@H]2Cc2ccccc2C1 6.370
+CHEMBL196215 FC(F)(F)CN1C[C@]2(NS1(=O)=O)[C@H]1CC[C@H]2Cc2ccc(/C=C/CN3CCC(CC3)C(F)(F)F)cc2C1 9.300
*CHEMBL196523 CCCN1C[C@]2(NS1(=O)=O)[C@H]1CC[C@H]2Cc2ccc(/C=C/CN3CCOCC3)cc2C1 7.720
*CHEMBL196795 CCCN1C[C@]2(NS1(=O)=O)[C@H]1CC[C@H]2Cc2ccccc2C1 6.860
+CHEMBL198301 CCCN1C[C@]2(NS1(=O)=O)[C@H]1CC[C@H]2Cc2ccc(/C=C/CN3CCC(CC3)C(F)(F)F)cc2C1 8.700
-CHEMBL198302 FC(F)(F)CN1C[C@]2(NS1(=O)=O)[C@H]1CC[C@H]2Cc2ccc(/C=C/CN3CCOCC3)cc2C1 8.470
+CHEMBL198761 CCCCN1C[C@]2(NS1(=O)=O)[C@H]1CC[C@H]2Cc2ccccc2C1 6.910
#CHEMBL365186 CCCCNS(=O)(=O)NC1[C@H]2CC[C@H]1Cc1ccccc1C2 6.120
*CHEMBL210178 COC(=O)N1CC=CC(=O)C1Cc1ccccc1 5.070
-CHEMBL211945 CO[C@H]1[C@H](CC=CC1=O)OCc1ccccc1 4.520
#CHEMBL212055 CO[C@H]1CC=CC(=O)[C@@H]1OCc1ccccc1 5.070
-CHEMBL212569 O=C(OCc1ccccc1)N1CC=CC(=O)C1Cc1ccccc1 5.220
+CHEMBL212678 CO[C@H]1CCCC(=O)[C@@H]1OCc1ccccc1 5.030
#CHEMBL377810 OC1C=CC(=O)C(Cc2ccccc2)N1C(=O)OCc1ccccc1 6.220
-CHEMBL378672 O=C1C=CC[C@@H](OCc2ccccc2)[C@H]1OCc1ccccc1 5.870
*CHEMBL379434 O=C(N1CC=CC(=O)C1Cc1ccccc1)c1ccccc1 5.800
*CHEMBL379714 O=C1C=CCN(C1Cc1ccccc1)S(=O)(=O)c1ccccc1 5.040
+CHEMBL199570 NC(=O)O[C@H]1CC[C@](CC1)(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 8.720
*CHEMBL199912 CN(C)S(=O)(=O)C[C@H]1CC[C@](CC1)(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 8.960
-CHEMBL200176 Fc1ccc(F)c(c1)[C@]1(CC[C@@H](CN2C(=O)CCC2=O)CC1)S(=O)(=O)c1ccc(Cl)cc1 9.000
#CHEMBL200190 Fc1ccc(F)c(c1)[C@]1(CC[C@H](CC1)NS(=O)(=O)c1ccccn1)S(=O)(=O)c1ccc(Cl)cc1 9.180
#CHEMBL200502 CNC(=O)OC[C@H]1CC[C@](CC1)(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 9.290
+CHEMBL200503 CC(=O)NC[C@H]1CC[C@](CC1)(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 8.890
*CHEMBL200594 NC[C@H]1CC[C@](CC1)(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 6.830
+CHEMBL200664 CS(=O)(=O)N[C@H]1CC[C@](CC1)(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 8.380
#CHEMBL200741 COC(=O)NC[C@H]1CC[C@](CC1)(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 8.660
#CHEMBL200761 Fc1ccc(F)c(c1)[C@]1(CC[C@@H](CI)CC1)S(=O)(=O)c1ccc(Cl)cc1 7.840
+CHEMBL200790 Fc1ccc(F)c(c1)[C@]1(CC[C@@H](CS(=O)(=O)C2CC2)CC1)S(=O)(=O)c1ccc(Cl)cc1 8.850
-CHEMBL200864 NS(=O)(=O)C[C@H]1CC[C@](CC1)(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 8.380
*CHEMBL200905 Fc1ccc(F)c(c1)[C@]1(CC[C@H](CC1)NS(=O)(=O)c1cccs1)S(=O)(=O)c1ccc(Cl)cc1 9.600
+CHEMBL200912 Fc1ccc(F)c(c1)[C@]1(CC[C@@H](CS(=O)(=O)N2CCC2)CC1)S(=O)(=O)c1ccc(Cl)cc1 9.440
#CHEMBL200913 O[C@H]1CC[C@](CC1)(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 7.970
+CHEMBL200928 COc1ccccc1S(=O)(=O)C[C@H]1CC[C@](CC1)(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 9.290
-CHEMBL371754 CCCS(=O)(=O)N[C@H]1CC[C@](CC1)(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 9.090
+CHEMBL372085 Fc1ccc(F)c(c1)[C@]1(CC[C@H](CC1)NS(=O)(=O)N1CCC1)S(=O)(=O)c1ccc(Cl)cc1 9.820
-CHEMBL372142 N[C@H]1CC[C@](CC1)(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 6.290
#CHEMBL372156 CC(=O)N[C@H]1CC[C@](CC1)(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 7.460
-CHEMBL372199 Fc1ccc(F)c(c1)[C@]1(CC[C@H](CC1)NS(=O)(=O)C(F)(F)F)S(=O)(=O)c1ccc(Cl)cc1 9.190
*CHEMBL372299 Oc1ccccc1S(=O)(=O)C[C@H]1CC[C@](CC1)(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 9.190
-CHEMBL372828 Fc1ccc(F)c(c1)[C@]1(CC[C@@H](CS(=O)(=O)c2ccccn2)CC1)S(=O)(=O)c1ccc(Cl)cc1 8.680
-CHEMBL380608 Fc1ccc(F)c(c1)[C@]1(CC[C@@H](CS(=O)(=O)C(F)(F)F)CC1)S(=O)(=O)c1ccc(Cl)cc1 7.670
+CHEMBL380776 CCNS(=O)(=O)NC[C@H]1CC[C@](CC1)(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 8.770
#CHEMBL380819 Fc1ccc(F)c(c1)[C@]1(CC[C@@H](CS(=O)(=O)c2ccccc2)CC1)S(=O)(=O)c1ccc(Cl)cc1 8.060
+CHEMBL382060 NC(=O)NC[C@H]1CC[C@](CC1)(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 9.000
+CHEMBL383826 OC[C@H]1CC[C@](CC1)(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 8.330
#CHEMBL425220 OC(=O)C[C@H]1CC[C@](CC1)(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 7.670
*CHEMBL207353 CCN1C[C@@H]2C[C@](CC[C@@H]2NS1(=O)=O)(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 9.400
#CHEMBL207454 CC(C)N1C[C@@H]2C[C@](CC[C@@H]2NS1(=O)=O)(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 9.390
#CHEMBL208089 CC(C)(C)N1C[C@@H]2C[C@](CC[C@@H]2NS1(=O)=O)(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 8.860
#CHEMBL209888 Fc1ccc(F)c(c1)[C@@]1(CCC2[C@H](CNS(=O)(=O)N2C2CC2)C1)S(=O)(=O)c1ccc(Cl)cc1 10.400
#CHEMBL210279 Fc1ccc(F)c(c1)[C@@]1(CC[C@@H]2NS(=O)(=O)NC[C@@H]2C1)S(=O)(=O)c1ccc(Cl)cc1 8.210
*CHEMBL210587 Fc1ccc(F)c(c1)[C@@]1(CC[C@@H]2NS(=O)(=O)N(C[C@@H]2C1)C1CC1)S(=O)(=O)c1ccc(Cl)cc1 9.720
*CHEMBL377264 CCC1C[C@@H]2C[C@](CC[C@@H]2CS1(=O)=O)(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 9.120
*CHEMBL377367 CCCN1C[C@@H]2C[C@](CC[C@@H]2NS1(=O)=O)(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 8.930
+CHEMBL377691 CCC1C[C@@H]2C[C@](CC[C@@H]2NS1(=O)=O)(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 10.220
*CHEMBL378502 Fc1ccc(F)c(c1)[C@@]1(CC[C@@H]2NS(=O)(=O)N(C[C@@H]2C1)C1CCC1)S(=O)(=O)c1ccc(Cl)cc1 9.590
*CHEMBL379089 CC1C[C@@H]2C[C@](CC[C@@H]2NS1(=O)=O)(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 10.100
+CHEMBL384207 CN1C[C@@H]2C[C@](CC[C@@H]2NS1(=O)=O)(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 9.050
+CHEMBL427397 CCCC1C[C@@H]2C[C@](CC[C@@H]2NS1(=O)=O)(c1cc(F)ccc1F)S(=O)(=O)c1ccc(Cl)cc1 9.620

Table S2. The ID and SMILES used to represent substances together with numerical data on blood brain barrier permeation (logBB).

-6 [N][N] 0.030
-7 [N-]=[N+]=O 0.030
+8 [H]C([H])([H])[H] 0.030
#9 CCCCC 0.632
*10 CCCCCC 0.680
-11 CCCCCCC 0.442
*12 CCCCCCCC 0.689
+13 CCCCCCCCC 0.520
#14 CCCCCCCCCC 0.665
#15 CC(C)CCC 0.970
#16 CC(C)CCCC 0.860
#17 CC(C)CCCCC 0.980
-18 CC(C)CCCCCC 1.050
*19 CCC(C)CC 1.013
-20 CCCC(C)CC 0.899
+21 CCC(C)(C)C 1.037
+22 C1CC1 0.110
*23 CC1CCCC1 0.933
*24 C1CCCCC1 1.110
+25 CC1CCCCC1 0.960
-26 C1CC(C)C(C)CC1 1.070
-27 CC(C1CCCCC1)(C)C 0.610
-28 C1C(C)C(C)CC(C)C1 1.020
*29 ClCCl -0.342
-30 ClC(Cl)Cl 0.151
*31 ClC(Cl)C -0.280
+32 ClCCCl -0.140
#33 CC(Cl)(Cl)Cl 0.289
-34 ClC(Cl)CCl -0.100
+35 ClC(Cl)(Cl)CCl 0.330
+36 ClCC(F)(F)F 0.115
*37 BrCCC 0.270
-38 CC(Br)C 0.560
#39 FC(Br)C(F)(F)F 0.267
-40 FC(F)(F)C(Cl)Br 0.142
*41 FS(F)(F)(F)(F)F 0.390
-42 C=C 0.305
+43 Cl/C=C/Cl 0.040
+44 Cl/C=C\Cl -0.130
*45 Cl/C(Cl)=C(Cl)\Cl 0.370
+46 CC=C -0.060
+47 CCCCCCC=C 0.740
#48 CCCCCCCC=C 0.860
-49 CCCCCCCCC=C 0.960
-50 C=CC=C -0.166
-51 ClC=C(Cl)Cl 0.105
-52 ClC=C(F)F -0.020
-53 S=C=S 0.600
+54 CO 0.020
-55 CCO -0.124
*56 CCCO -0.082
-57 CCCCO -0.023
*58 CCCCCO 0.203
#59 CC(C)O -0.113
+60 CC(C)CO -0.140
#61 CCC(C)CO 0.038
*62 CC(C)(C)O 0.110
*63 CCC(C)(C)O 0.070
*64 CCOCC -0.010
-65 CC(OCC)(C)C 0.220
#66 CC(OC)(C)C 0.360
#67 CCC(C)(C)OC 0.170
-68 COC(F)(F)C(Cl)Cl 0.119
+69 FC(F)OC(Cl)C(F)(F)F 0.190
-70 FC(F)OC(F)(F)C(F)Cl 0.140
-71 FCOC(C(F)(F)F)C(F)(F)F 0.300
+72 C1CO1 0.010
+73 FC(F)(F)COC=C 0.140
*74 C=COC=C 0.130
#75 CC(C)=O -0.170
#76 CC(=O)CC -0.170
-77 CCCC(C)=O -0.010
+78 COC(C)=O -0.134
+79 CCOC(C)=O 0.003
+80 CC(OCCC)=O 0.120
+81 CCCCOC(C)=O 0.277
#82 CC(OCCCCC)=O 0.400
+83 CC(C)OC(C)=O 0.399
+84 CC(C)COC(=O)C 0.450

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-85 CC(OCCC(C)C)=O 0.554
#86 C1=CC=CC=C1 0.198
-87 CC1=CC=CC=C1 0.271
#88 CC1=CC=CC=C1C 0.410
-89 CC1=CC(C)=CC=C1 0.220
*90 CC1=CC=C(C)C=C1 0.380
+91 CCC1=CC=CC=C1 0.260
#92 C=CC1=CC=CC=C1 0.450
*93 CC(C1=CC=CC=C1)(C)C 0.430
#94 CC1=CC(C)=C(C)C=C1 0.160
*95 FC(F)(C1=CC=C(Cl)C=C1)F 0.170
-96 OCC#C -0.230
-97 C=CC#N -0.400
+98 FCCCN1C=CN=C1N(=O)=O -0.240
-99 FCCCCCCCCN1C(N(=O)=O)=NC=C1 -0.170
-100 OC1=CC4=C(C3CCC(C(C(CC2C3CC4)F)O)2C)C=C1 -0.301
-101 IC1=CC=C(N2CCN(CC2)CCCCCC)C=C1 1.010
#102 OCC3=NC=C4CN=C(C2=C(N34)C=CC(Cl)=C2)C1=C(F)C=CC=C1 -0.070
+103 IC1=CC=C(N2CCN(CC2)C(CC)C)C=C1 1.380
+104 FC1=C(C)N(C)N(C2=CC=CC=C2)C1=O -0.050
#105 CC3=NC=C4C(N=C(C2=C(N34)C=CC(Cl)=C2)C1=C(F)C=CC=C1)O -0.030
+106 IC3=C(C=C(C=C3)CN2CCCCC2)CN1CCCCC1 0.980
-107 CC2=C(C(N(N2C)C1=CC=CC=C1)=O)I -0.100
+108 IC1=C(C=C(C=C1)NC(CC)C)NC(CC)C 0.640
#109 O=C1C(CC)(C(NC(N1)=O)=O)CCCC 0.188
*110 O=C1C(CC)(C(NC(N1)=O)=O)CCCCCCC 0.017
+111 O=C1C(CC)(C(NC(N1)=O)=O)CCCCCC 0.364
*112 O=C1C(CC)(C(NC(N1)=O)=O)C -0.222
*113 O=C1C(CC)(C(NC(N1)=O)=O)CCCCCCCC 0.241
+114 O=C1C(CC)(C(NC(N1)=O)=O)CCCCC 0.086
-115 O=C1C(CC)(C(NC(N1)=O)=O)CCC 0.086
#116 O=C2N1CCCC(O)C1=NC(C)=C2CCN3CCC(C4=NOC5=C4C=CC(F)=C5)CC3 -0.670
+117 FCCC2=CC(N)=C(C=C2)SC1=CC=CC=C1N(C)C 0.548
+118 CC1N(C3=C(C)C(C)=NC(NC4=CC=C(C=C4)F)=N3)CCC2=CC=CC=C12 0.675
+119 CC1N(C3=C(C)C(C)=NC(NC4=CC=C(F)C=C4)=N3)CCC2=CC=CC=C12 -0.260
-120 CC2=CN(C([NH]C2=O)=O)C1CC(C(O1)CO)F -0.590
+121 [O-]/[N+](C(C)(C)C)=C/C1=CC=[N+]([O-])C=C1 -0.380
+122 CC3=NN=C4CN=C(C2=CC(Cl)=CC=C2N34)C1=CC=CC=C1 0.000
-124 CN(C2=C(N(N(C2=O)C1=CC=CC=C1)C)C)C 0.000
#125 CCC(C(NC(NC1=O)=O)=O)1CCC(C)C 0.040
#126 CC2=CC(N(N2C)C1=CC=CC=C1)=O -0.160
-128 CC(NCC(COC1=CC=C(C=C1)CC(N)=O)O)C -0.699
+129 CCC(C(NC(NC1=O)=O)=O)1CC -0.137
+130 CN4CC3C1=CC=CC(C)=C1OC2=CC=CC=C2C(CC4)3O 0.820
+131 CCN3CN(C4=CC=C(Br)C=C4)C2(C3=O)CCN(CC2)CCCC(C1=CC=C(C=C1)F)=O -0.430
-132 CNCCC1=NC=CC=C1 -0.300
*133 OC(C2=CC=CC=C2)(C3C4CC(C=C4)C3)CCN1CCCCC1 0.845
-134 CC(C1=CC=C(O)C=C1)(C2=CC=C(C=C2)O)C -0.120
+135 BrC1=CC=C(N4C3(C(N(C)C4)=O)CCN(CC3)CCCC(C2=CC=C(F)C=C2)=O)C=C1 -0.550
#136 CCCN3CN(C4=CC=C(Br)C=C4)C2(C3=O)CCN(CC2)CCCC(C1=CC=C(C=C1)F)=O -0.010
+137 CC(C)(OC(C1=C(C2CCCN2C(C4=C3C=CC(Br)=C4)=O)N3C=N1)=O)C -0.090
+138 BrC1=CC=C(N4C3(C(NC4)=O)CCN(CC3)CCCC(C2=CC=C(C=C2)F)=O)C=C1 0.070
*139 CCCCOC(C1=CC=C(C=C1)N)=O 0.420
+140 CN1C=NC(N(C(N2C)=O)C)=C1C2=O 0.030
*142 NC(N2C1=C(C=CC3=C2C=CC=C3)C=CC=C1)=O 0.000
-143 ClCCNC(N(N=O)CCCl)=O -0.520
+144 CC(C)(NCC(COC1=CC=CC(N2)=C1CCC2=O)O)C -0.400
+145 CN(CCCN2C1=C(SC3=C2C=C(Cl)C=C3)C=CC=C1)C 1.060
-148 CN2C(CC(N(C3=C2C=CC(Cl)=C3)C1=CC=CC=C1)=O)=O 0.350
+149 ClC1=CC=CC(Cl)=C1/N=C2NCCN\2 0.110
+150 COC(C1C(OC(C3=CC=CC=C3)=O)CC2CCC1N2C)=O 0.600
+151 OC1C4C2(CCN5C)C(C5CC3=C2C(O4)=C(OC)C=C3)C=C1 -0.220
+152 CN1C(C2=CN=CC=C2)CCC1=O -0.348
-154 OC1=CC=C(C3=COC2=C(C3=O)C=CC(O)=C2)C=C1 -0.150
-155 CNCCCN2C1=C(CCC3=C2C=CC=C3)C=CC=C1 1.000
*156 NCCCN1C(C=CC=C3)=C3CCC2=C1C=CC=C2 1.060
-157 ClC3=CC(N(C(C2)=O)C1=CC=CC=C1)=C(C=C3)NC2=O 0.360
*158 ClC(C=CC=C1N2)=C1C(C3=CC=CC=C3)=NCC2=O 0.500
*159 CNCCCN1C(C=CC=C3)=C3SC2=C1C=CC=C2 0.590
#160 CN2C(CN=C(C3=C2C=CC(Cl)=C3)C1=CC=CC=C1)=O 0.275
+162 OCC1CCC(N2C=NC3=C2N=C[NH]C3=O)O1 -1.300
-163 CN(CCOC(C2=CC=CC=C2)C1=CC=CC=C1)C 1.260
-164 ClC5=CC=C4N(C([NH]C4=C5)=O)C3CCN(CC3)CCCN1C([NH]C2=CC=CC=C12)=O -0.925
+165 CN(CCOC(C1=CC=CC=C1)(C2=CC=CC=N2)C)C 0.640
-166 CCOC1=CC=CC=C1C(N)=O -0.046
-167 CCOC(C1=CC=C(N)C=C1)=O 0.270
+168 CCC(N(C3=CC=CC=C3)C1CCN(CCC2=CC=CC=C2)CC1)=O 0.578
+170 FC1=CC3=C(N2C=NC(C(OC(C)F)=O)=C2CN(C3=O)C)C=C1 -0.095
+171 CCOC(C1=C(CN(C(C3=C2C=CC(F)=C3)=O)C)N2C=N1)=O -0.290
-172 CN2C(CN=C(C3=C2C=CC(N(=O)=O)=C3)C1=C(F)C=CC=C1)=O 0.060
-173 CCOC(C1=C(CN(C(C3=C2C=CC(F)=C3)=O)CCF)N2C=N1)=O -0.140
+174 O=N(C1=NC=CN1CC(COCF)O)=O -0.010
+175 CNCCC(C2=CC=CC=C2)OC1=CC=C(C(F)(F)F)C=C1 0.360
-176 CC(C(CCC(C1CCC(C2C(C=C5C3CC(CCC(CCC45C)3C)(C(O)=O)C)=O)4C)2C)O)1C -1.398
+177 OC(CC)(CC(N)=O)C1=CC=CC=C1 0.040

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-178 CN2C(NC(C(C1=CCCCC1)(C2=O)C)=O)=O    0.073
+180 OCCOCCN1CCN(C(C3=CC=C(C=C3)Cl)C2=CC=CC=C2)CC1    0.390
+181 IC1=CC(C(CCCN4CCC2(CC4)C(N(CN2C3=CC=CC=C3)C)=O)=O)=CS1   -0.254
-182 I/C=C/CN1CCC(COC2=CC=C(C#N)C=C2)CC1    1.134
-183 CC(CC1=CC=C(C(C(O)=O)C)C=C1)C   -0.180
*184 CN(CCCN2C1=C(CCC3=C2C=CC=C3)C=CC=C1)C    0.830
-185 CC(C)(NC(C1CN(CC5=CN=CC=C5)CCN1CC(CC(C(NC3C(CC4=CC=CC=C34)O)=O)CC2=CC=CC=C2)O)=O)C   -0.745
-186 COC1=CC3=C(N(C(C)=C3CC(O)=O)C(C2=CC=C(C=C2)Cl)=O)C=C1   -1.260
-188 NC1=NC(N)=C(C2=C(Cl)C(Cl)=CC=C2)N=N1    0.480
#189 CCN(CC(NC1=C(C=CC=C1C)C)=O)CC    0.340
#190 OC3N=C(C2=CC(Cl)=CC=C2NC3=O)C1=CC=CC=C1Cl    0.440
-192 CN(CC3=CC=C(O3)CSCC[NH]C1=NC(C(CC2=CN=C(C)C=C2)=C[NH]1)=O)C   -1.060
#193 OCC(C(C(C(CO)O)O)O)O   -1.600
-194 OC(C2=CC(C(F)(F)F)=NC3=C2C=CC=C3C(F)(F)F)C1CCCCN1    0.630
-195 CNC(CC1=CC=CC=C1)C    0.900
+196 CCC#CC(C(C(NC(N(C1=O)C)=O)=O)1CC=C)C   -0.060
#197 CN1CCN3C(C2=CC=CC=C2CC4=CC=CC=C34)C1    0.990
-198 CC3=NC=C4CN=C(C2=C(N34)C=CC(Cl)=C2)C1=C(F)C=CC=C1    0.426
+201 CON1C=C(C(C3=C1C=C2OCOC2=C3)=O)C(O)=O   -0.921
-202 CN1CCN3C(C2=CC=CC=C2CC4=CC=CN=C34)C1    0.530
-203 OC(CN1C=CN=C1N(=O)=O)COCF   -0.010
-204 OC4=C(O5)C2=C(C=C4)CC3C1C=CC(O)C5C12CCN3C   -0.648
-205 CN3CN(C4=CC=CC=C4)C2(C3=O)CCN(CC2)CCCC(C1=CC=C(C=C1)F)=O    0.460
-206 CCN1C=C(C(C2=C1N=C(C)C=C2)=O)C(O)=O   -0.658
-207 CC1=CC=NC(N(C4=C3C=CC=N4)C2CC2)=C1NC3=O    0.000
#208 CN1CCCC1C2=CC=CN=C2    0.236
+209 CSC4=CC2=C(C=C4)SC1=CC=CC=C1N2CCC3CCCNC3    0.750
-210 CN1CCN(C3=NC2=CC=CC=C2NC4=C3C=C(C)S4)CC1    0.780
-211 O=C1N(CCCCN2CCN(C3=CC(C(F)(F)F)=CC=N3)CC2)CCC1    0.160
-212 ClC4=CC1=C(C=C4)OC3=C(C=CC=C3)C2C1CNC2    0.390
-213 OC12C4=C(C=CC=C4)OC3=C(C=CC=C3C)C1CNCC2    0.520
+214 C=CCC(N)C(C=CC=C3)=C3C1=NOC2=C1C=CC=C2    0.000
-215 CN1CC3C(C2=C(OC4=C3C=CC=C4)C=CC(Cl)=C2)C1    1.030
+216 OC3N=C(C2=CC(Cl)=CC=C2NC3=O)C1=CC=CC=C1    0.580
#218 CC(NC1=CC=C(O)C=C1)=O   -0.340
-219 O=C1N(C(NC2=C1N(C)C=N2)=O)C    0.060
+220 OC1=CC2=C(CC3C(C)C(C)2CCN3C/C=C(C)\C)C=C1    0.544
#222 CCCC(C(C(NC(NC1=O)=O)=O)1CC)C    0.140
+224 C12=NN=NN1CCCCC2   -0.030
+226 N1(C2(C3=CC=CC=C3)CCCCC2)CCCCC1    0.440
-227 CCCCC1C(N(C3=CC=CC=C3)N(C2=CC=CC=C2)C1=O)=O   -0.520
+228 [O-]/[N+](C(C)(C)C)=C/C1=CC=CC=C1    0.050
+229 O=C1NC(C(C2=CC=CC=C2)(C3=CC=CC=C3)N1)=O   -0.100
-231 CNC(OC3=CC=C2N(C1N(CCC(C2=C3)1C)C)C)=O    0.080
+232 CC([NH]CC(COC1=CC=CC2=C1C=C[NH]2)O)C   -0.135
-234 CCC(N(C(C2=CC1=CC=CC=C1C(C3=C(Cl)C=CC=C3)=N2)=O)C)C    0.480
+235 OC(C1=CC=C(C2=CC=CC=C2)C=C1)=O   -1.260
+236 CCN(CCOC(C1=CC=C(C=C1)N)=O)CC    0.050
+237 CN(CCCN2C1=CC=CC=C1SC3=CC=CC=C23)C    0.950
+239 CC(C1=CC=CC(C(C)C)=C1O)C    0.697
-241 CC(NCC(COC2=C1C=CC=CC1=CC=C2)O)C    0.640
+242 CCCOC(C1=CC=C(N)C=C1)=O    0.550
-243 C13=CC=CC4=C1C2=C(C=C4)C=CC=C2C=C3    0.230
#244 COC2=CC=C(C=C2)CN(C1=CC=CC=N1)CCN(C)C    0.500
+245 OC(C3C(CC4C=C)CCC4C3)C2=C1C=C(C=CC1=NC=C2)OC    0.100
+246 CCC1=CC=CC2=C1[NH]C3=C2CCOC(CC([OH])=O)3CC   -1.423
-247 CC(N=C1CCCCN12)=C(CCN3CCC(C4=NOC5=C4C=CC(F)=C5)CC3)C2=O   -0.020
-248 COC1=C(OC2CCCC2)C=C(C3CNC(C3)=O)C=C1    0.610
*249 CCCN(CCC(C=CC=C1N2)=C1CC2=O)CCC    0.250
+250 NC(SCCF)=N   -0.275
+251 CC(C)(NCC(C1=CC=C(C(CO)=C1)O)O)C   -1.300
-252 OC(C1=CC=CC=C1O)=O   -1.161
-254 CC(C)(NC(C2CC1CCCCC1CN2CC(C(NC(C(NC(C4=NC5=C(C=CC=C5)C=C4)=O)CC(N)=O)=O)=O)CC3=CC=CC=C3)O)=O)C   -1.030
+256 BrC1=CC=CN=C1CSCC[NH]C2=C(N(=O)=O)C=C[NH]2   -0.670
#257 O=N(C1=C([NH]CCSCC2=NC=CC=C2)[NH]C=C1)=O   -0.660
-258 O=N(C1=C([NH]CCSCC3=NC=CC=C3)[NH]C=C1CC2=CC=CC=C2)=O   -0.120
+259 [NH2]/C([NH2])=N\C1=NC(C2=CC=CC=C2)=CS1   -0.180
*260 CC1=CSC(/N=C([NH2])/[NH2])=N1   -0.040
#261 N/C(N)=N\C1=NC(C2=CC=CC(N)=C2)=CS1   -1.150
*262 CC([NH]C1=CC=CC(C2=CSC(/N=C(N)\N)=N2)=C1)=O   -1.570
#263 C[NH]/C([NH]C1=CC(C2=CSC(/N=C(N)/N)=N2)=CC=C1)=N/C#N   -1.540
-264 CN(CC2=CC=C(O2)CSCC[NH]C1=C(N(=O)=O)C=C[NH]1)C   -1.120
#265 CN(CC3=CC=C(O3)CSCC[NH]C1=C(N(=O)=O)C(CC2=CC=CC=C2)=C[NH]1)C   -0.730
+266 CN(CC1=CC=C(C2=CC([NH]C3=C(N(=O)=O)C=C[NH]3)=CC=C2)O1)C   -0.270
*267 CN(CC1=CC=NC(C2=CC([NH]C3=C(N(=O)=O)C=C[NH]3)=CC=C2)=C1)C   -0.280
*268 CC([NH]CCCOC1=CC(CN2CCCCC2)=CC=C1)=O   -0.460
+269 O=C(C3=CC=CC=C3)[NH]CCCOC1=CC=CC(CN2CCCCC2)=C1   -0.240
*270 OCCCOC1=CC(CN2CCCCC2)=CC=C1   -0.020
*271 C1(NCCCOC2=CC(CN3CCCCC3)=CC=C2)=CC=CC=N1    0.690
-272 C1(NCCCOC2=CC=CC(CN3CCCCC3)=C2)=NC=CS1    0.440
+273 C(NCCCOC2=CC(CN4CCCCC4)=CC=C2)3=NC1=C(O3)C=CC=C1    0.220
+274 CCCN(CCC(C=CC(O)=C1N2)=C1CC2=O)CCC   -0.430
-275 NC(SC)=N   -0.602
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#276 FC1=CC=C(C(CCCN2CCC3(N(C4=CC=CC=C4)CNC3=O)CC2)=O)C=C1 0.260
*277 CC2=CN(C([NH]C2=O)=O)C1OC(C=C1)CO -0.482
-278 CN1CCCCC1CCN3C2=C(SC4=CC=C(S(C)(=O)=O)C=C34)C=CC=C2 0.180
+279 CN(CC2=C1C=CC=CC1=CC=C2)C/C=C/C#CC(C)(C)C 0.095
-280 CC(C)(OC(CCCC1=CC=C(N(CCCl)CCCl)C=C1)=O)C 1.000
-281 CN1C=NC(N(C([NH]2)=O)C)=C1C2=O -0.300
*282 CN2C(N(C1=C(C2=O)NC=N1)C)=O -0.345
#283 CCCC(C(C(NC(NC1=O)=S)=O)1CC)C -0.147
-285 S=C(N2CCC(C3=CNC=N3)CC2)NC1CCCCC1 -0.160
+286 CSC4=CC=C3SC1=C(N(C3=C4)CCC2CCCCN2C)C=CC=C1 0.283
+289 CC3CC1=C(C4CCC2(C(C34)CCC(C#C)2O)C)CCC(C1)=O 0.400
-290 CN/C(NCCSCC1=CSC(/N=C(N)/N)=N1)=N/C#N -0.820
*291 CC(NCC(COC1=CC(C)=CC=C1)O)C 0.280
-293 CC3=NN=C4CN=C(C2CC(CCC2N34)Cl)C1=CC=CC=C1Cl 0.570
+294 CN1CCN(CCCN3C2=C(SC4=C3C(C(F)(F)F)=CC=C4)C=CC=C2)CC1 1.440
-295 CN(CC/C=C2\C1=C(CCC3=C2C=CC=C3)C=CC=C1)C 0.890
-296 CCCC(C(O)=O)CCC -1.155
+297 COC2=CC=C(C=C2OC)CCN(CCCC(C(C)C)(C1=CC(OC)=C(OC)C=C1)C#N)C -0.469
#299 O -0.040
+300 CN(CCC1=CC=CC=N1)C -0.060
+301 NCCC1=NC=CS1 -0.420
+302 CC2=CN(C(NC2=O)=O)C1CC(C(O1)CO)N=N#N -0.720
#303 N1(CC2=CC=CC(OCCCNC4=NC3=C(S4)C=CC=C3)=C2)CCCCC1 0.140
*304 C1C3=CC=C2NC(CN=C(C2=C3)C1=CC=CC=C1)=O 0.500
+305 CN(C1=NC=CC(C2=NNC(N)=N2)=C1)C -1.170
+306 BrC1=CC=CN=C1CSCCNC2=C(C=CN2)N(=O)=O -0.670
-307 O=N(C(C=CN2)=C2NCCSCC1=NC=CC=C1)=O -0.660
-308 O=N(C(C(CC3=CC=CC=C3)=CN2)=C2NCCSCC1=NC=CC=C1)=O -0.120
+309 N/C(N)=N/C1=NC(C2=CC=CC=C2)=CS1 -0.180
+311 N/C(N)=N/C1=NC(C2=CC(NC(C)=O)=CC=C2)=CS1 -1.570
-312 N/C(N)=N\C1=NC(C2=CC(N/C(NC)=N/C#N)=CC=C2)=CS1 -1.540
*313 CN(CC1=CC=C(SCCNC2=C(C=CN2)N(=O)=O)O1)C -1.120
*314 CN(CC1=CC=C(SCCNC2=C(C(CC3=CC=CC=C3)=CN2)N(=O)=O)O1)C -0.730
+315 CN(CC1=CC=C(C2=CC=CC(NC3=C(C=CN3)N(=O)=O)=C2)O1)C -0.270
*316 CN(CC1=CC(C2=CC(NC3=C(C=CN3)N(=O)=O)=CC=C2)=NC=C1)C -0.280
+317 O=C(C)NCCCOC1=CC(CN2CCCCC2)=CC=C1 -0.460
-320 N1(CC2=CC=CC(OCCCNC3=NC=CC=C3)=C2)CCCCC1 0.690
-321 N1(CC2=CC=CC(OCCCNC3=NC=CS3)=C2)CCCCC1 0.440
+322 N1(CC2=CC(OCCCNC4=NC3=C(O4)C=CC=C3)=CC=C2)CCCCC1 0.220
-324 CCC(NC(C2=C(C(C4=CC=CC=C4)=NC3=C2C=CC=C3)C)=O)C1=CC=CC=C1 0.300
-325 NC(N3C1=CC=CC=C1C2CC2C4=CC=CC=C34)=O -0.340
+326 O=C3C1=C(N2C=NC(C4=NOC(C(C)C)=N4)=C2CN3C)C=CC=C1Cl -0.300
-327 O=C3C1=C(N2C=NC(C4=NOC(C(C)(O)C)=N4)=C2CN3C)C=CC=C1Cl -1.340
-328 O=C3C1=C(N2C=NC(C4=NOC(C(C)(O)CO)=N4)=C2CN3C)C=CC=C1Cl -1.820