

Supplementary Data for

Identifying p56^{lck} SH2 Domain Inhibitors Using Molecular Docking and In Silico Scaffold Hopping

Priyanka Samanta ¹ and Robert J. Doerksen ^{1,2,*}

¹ Department of BioMolecular Sciences, School of Pharmacy, University of Mississippi, Oxford, MS 38677-1848, USA; psamanta@go.olemiss.edu

² Research Institute of Pharmaceutical Sciences, School of Pharmacy, University of Mississippi, Oxford, MS 38677-1848, USA

* Correspondence: rjd@olemiss.edu; Tel.: +1-622-915-7052

Hypotheses	Survival score	Site score	Vector score	Volume score	BEDROC score	Phase hypo score
DHRRR_1	6.143	0.909	0.824	0.824	0.997	1.365
AHRRR_2	6.014	0.915	0.821	0.821	1.000	1.361
ADHRR_2	5.998	0.905	0.823	0.823	1.000	1.360
AHRRR_1	6.018	0.919	0.830	0.830	0.998	1.359
ADHRR_5	5.971	0.910	0.814	0.814	1.000	1.358
ADHRR_4	5.977	0.894	0.822	0.822	0.999	1.358
ADHRR_1	6.000	0.872	0.797	0.797	0.998	1.358
AHRRR_3	5.982	0.906	0.827	0.827	0.999	1.358
ADHRR_6	5.931	0.870	0.799	0.799	0.999	1.355

ADHRR_3	5.992	0.885	0.789	0.789	0.993	1.353
AHRR_2	5.557	0.921	0.816	0.816	1.000	1.333
DHRR_1	5.647	0.918	0.816	0.816	0.994	1.333
HRRR_1	5.612	0.926	0.828	0.828	0.996	1.333
DHRR_3	5.579	0.940	0.810	0.810	0.997	1.332
DRRR_1	5.527	0.946	0.823	0.823	1.000	1.332
DHRR_2	5.647	0.906	0.823	0.823	0.993	1.331
AHRR_1	5.563	0.914	0.829	0.829	0.997	1.331
AHRR_3	5.552	0.924	0.815	0.815	0.997	1.330
AHRR_4	5.548	0.941	0.824	0.824	0.973	1.306
AHRR_5	5.546	0.924	0.828	0.828	0.961	1.294

Table S1. The generated e-pharmacophore models and their features. The hypothesis shown in bold is the top ligand-based e-pharmacophore that is used for further studies in this work.

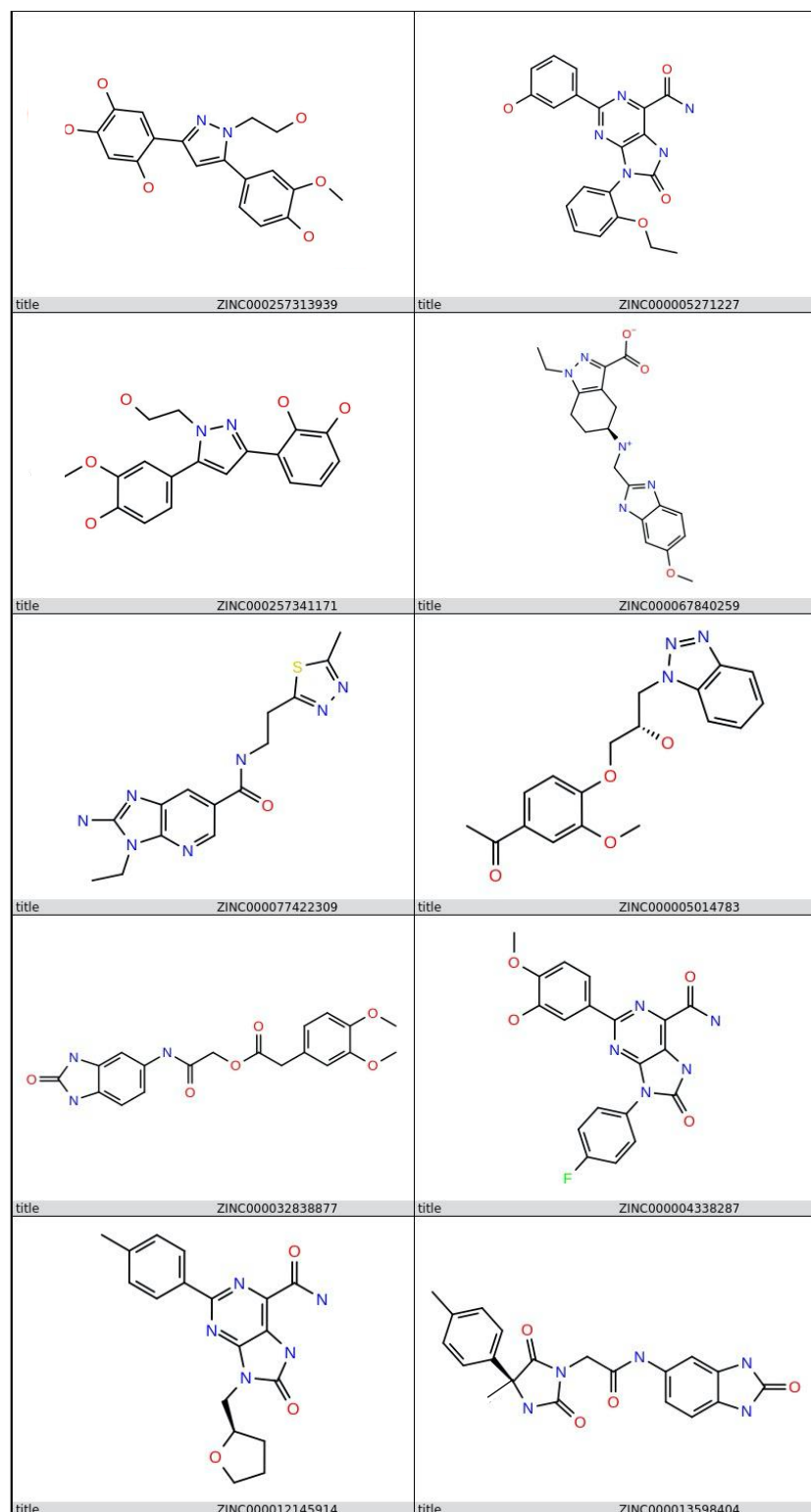


Figure S1. 2D-structures of the top 10 hits from the pool of 202 ligands that were obtained from the virtual screening docking protocol adopted in this study.

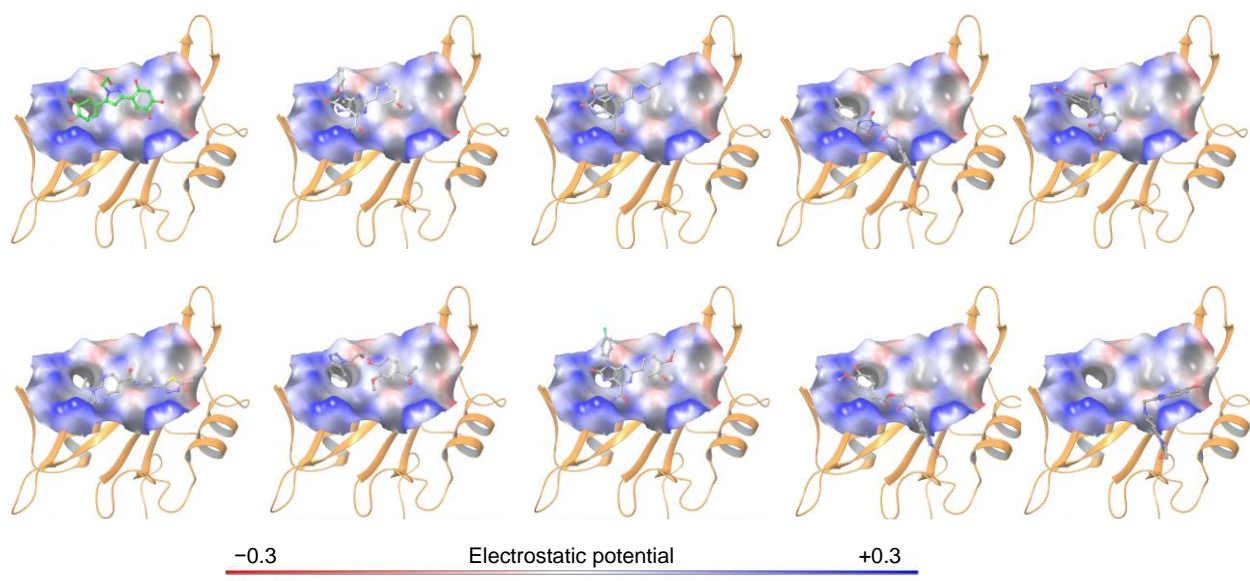


Figure S2. Docked structures of the top 10 hits from the pool of 202 ligands that were obtained from the virtual screening docking protocol adopted in this study. The ligand binding pocket is shown in surface representation. The ligands are shown in gray licorice. The best hit is shown in the first panel in green licorice.

SMILES strings and unique ZINC IDs of the 202 molecules mentioned in the report

COc1cc(ccc1O)-c2cc(nn2CCO)-c3cc(O)c(O)cc3O ZINC000257313939
CCOc1cccc1-n(c(=O)[nH]2)c(c23)nc(nc3C(=O)N)-c4cccc(O)c4 ZINC000005271227
COc1cc(ccc1O)-c2cc(nn2CCO)-c3cccc(O)c3O ZINC000257341171
O=C([O-])c1nn(CC)c(c12)CC[C@@H](C2)[NH2+]Cc(n3)[nH]c(c34)cc(cc4)OC
ZINC000067840259
CCn(c(n1)N)c(c12)ncc(c2)C(=O)NCCc3nnc(s3)C ZINC000077422309
COc1cc(C(=O)C)ccc1OC[C@@H](O)Cn(nn2)c(c23)cccc3 ZINC000005014783
COc1ccc(cc1OC)CC(=O)OCC(=O)Nc(cc2)cc(c23)[nH]c(=O)[nH]3 ZINC000032838877
COc1ccc(cc1O)-c(nc2C(=O)N)nc(c23)n(c(=O)[nH]3)-c4ccc(F)cc4 ZINC000004338287
Cc1ccc(cc1)-c(nc2C(=O)N)nc(c23)n(c(=O)[nH]3)C[C@@H]4CCCCO4 ZINC000012145914
Cc1ccc(cc1)[C@]2(C)NC(=O)N(C2=O)CC(=O)Nc(cc3)cc(c34)[nH]c(=O)[nH]4
ZINC000013598404
CCn(c(n1)N)c(c12)ncc(c2)C(=O)NCCn(nc3)c(=O)c(c34)cccc4 ZINC000077487240
Cc1ccc(cc1C)-n(c(=O)[nH]2)c(c23)nc(nc3C(=O)N)-c4cccc4O ZINC000005143559
COc1cccc1-n(c(=O)[nH]2)c(c23)nc(nc3C(=O)N)-c4cccc(O)c4 ZINC000004338344
CCn(c(n1)N)c(c12)ncc(c2)C(=O)NCCc(c3)nc(n34)sc(n4)C ZINC000077339322
COc1cccc(c1)-c(nc2C(=O)N)nc(c23)n(c(=O)[nH]3)-c4cccc4OC ZINC000004338385
OCCNc1nc(-c2cccc2)cc(n1)Nc3cc(Cl)ccc3O ZINC000329031305
Cn1c(=O)[nH]c(=O)c(c12)n(c(n2)SCCO)Cc3ccc(Cl)cc3 ZINC000013590323
CCOC(=O)c1ccc(cc1)OC[C@@H](O)Cn(c(=O)cn2)c(c23)cccc3 ZINC000031560648
COc1cccc1-n(c(=O)[nH]2)c(c23)nc(nc3C(=O)N)-c4cccc4O ZINC000004338395
CCOc1cc(ccc1O)-c2cc(nn2CCO)-c3cc(O)c(O)cc3O ZINC000257269878
CCn(c(n1)N)c(c12)ncc(c2)C(=O)NCCn(c[nH]c3=O)c(c34)cccc4 ZINC000077539896
OC[C@@H](C)Nc1nc(-c2cccc2)cc(n1)Nc3cc(Cl)ccc3O ZINC000329040195
COc1ccc(cc1O)-c(nc2C(=O)N)nc(c23)n(c(=O)[nH]3)-c4ccc(C)cc4 ZINC000005151752
Cc1nc(C)c(c(=O)[nH]1)CCC(=O)Nc(cc2)cc(c23)[nH]c(=O)[nH]3 ZINC000012751973
[nH]1c(=O)[nH]c(c12)cc(cc2)NC(=O)Cn3cc(Br)ccc3=O ZINC000006879289
c1cccc1[C@@]2(CC)NC(=O)N(C2=O)CC(=O)Nc(cc3)cc(c34)[nH]c(=O)[nH]4
ZINC000012974894
OC[C@H](C)Nc1nc(-c2ccnc2)cc(n1)Nc3cc(Cl)ccc3O ZINC000328967501
COc1cccc(c1)-c2[nH]ncc2C(=O)NCCNc3nc(C)cc(=O)[nH]3 ZINC000091997939
CCOc1cccc1-n(c(=O)[nH]2)c(c23)nc(nc3C(=O)N)-c4ccc(O)cc4 ZINC000005271228
COc1cccc(c1)-n(c(=O)[nH]2)c(c23)nc(nc3C(=O)N)-c4cccc(O)c4 ZINC000005271192
CC(C)Oc1cc(O)cc(c1)C(=O)NCCc2n[nH]c(c23)necc3 ZINC001772700531
Cc1cc(=O)[nH]c(n1)NCCNC(=O)Cn2ccnc2-c3cccc3 ZINC000221231786
c1cc(Cl)ccc1-n(c(=O)[n-]2)c(=O)c(c23)n(C)cc3C(=O)NC4CCCC4 ZINC000017149002
CCn(en1)c(c12)nc(NCCO)nc2Nc3ccc(OC)cc3 ZINC000026533017
COc1cccc(c1)OC[C@@H](O)CNC(=O)c(cc2)cc(c23)nc([nH]3)CO ZINC000097814854
COc1cccc(c1O)-c(nc2C(=O)N)nc(c23)n(c(=O)[nH]3)-c4ccc(F)cc4 ZINC000004338236
[nH]1c(=O)oc(c12)cc(cc2)NC(=O)NCCc3n(c34)CCCCC4 ZINC000096141670
COc1cc(OC)cc(c12)cc([nH]2)C(=O)OCCc3nc(N)nc(n3)N(C)C ZINC000022835003
Cc1ccc(cc1)C(=O)NCC(=O)OCC(=O)Nc(cc2)cc(c23)[nH]c(=O)[nH]3 ZINC000012940511
CC(C)n(c(=O)[nH]1)c(c12)nc(nc2C(=O)N)-c3ccc(Cl)cc3 ZINC000012145938
c1cc(F)ccc1OC[C@@H](O)Cn(cn2)c(c23)ncnc3N4CCOCC4 ZINC000095397138

Cc1cc(C)c(c(=O)[nH]1)CNC(=O)Cc(n[nH]c2=O)c(c23)cccc3 ZINC000010457650
CCn(c1=O)c(=O)n(C)c(c12)nc(NC[C@@H](C)O)n2Cc3ccc(C)cc3 ZINC000036693339
C1CCC1c([nH]n2)nc2NC(=O)CCc(n3)[nH]c(=O)c(c34)cccc4 ZINC000253623955
Cc1cc(=O)c(c[nH]1)OCC(=O)Nc(cc2)cc(c23)[nH]c(n3)CO ZINC000524735625
c1cc(Cl)ccc1[C@H](O)C(=O)NCCc(cc2)cc(c23)[nH]c(=O)[nH]3 ZINC000215855213
COc1cccc(c1O)-c(nc2C(=O)N)nc(c23)n(c(=O)[nH]3)-c4cccc4 ZINC000004176074
CCn(c(n1)N)c(c12)ncc(c2)C(=O)NCCc(n3)[nH]c(c34)cccc4 ZINC000077438835
COc1cccc1CCC(=O)OCC(=O)Nc(cc2)cc(c23)[nH]c(=O)[nH]3 ZINC000008328449
c1cccc(c12)c(C(=O)N)cn2CC(=O)NCCc(cc(F)c3)c(c34)OCOC4 ZINC000048286011
c1cc(F)ccc1-n(c(=O)[n-]2)c(=O)c(c23)n(C)cc3C(=O)NCCc4cccc4 ZINC000009659632
NC(=O)COc1c(Cl)cc(cc1OC)CNc(cc2)cc(c23)[nH]c(=O)[nH]3 ZINC000010315371
COc1ccc(cc1OC)-c(co2)c(=O)c(c23)ccc(O)c3C[NH2+]CCO ZINC000032501413
[nH]1c(=O)[nH]c(c12)cc(cc2)NC(=O)COc(cc3)cc(c34)CCC(=O)N4 ZINC000025457413
Oc1cccc1-c(n2)nc(C(=O)N)c(c23)[nH]c(=O)n3-c4cccc(Cl)c4 ZINC000005151508
c1cccc(c12)nc(n(c2=O)CC(=O)N)COc3ccc(Cl)cc3C(=O)N ZINC000011115668
c1cc(C)cc(c12)N(CCO2)C(=O)CSc([nH]3)nc(=O)c(c34)[nH]cn4 ZINC000033324835
CSc1ccc(cc1)[C@@H](O)CNS(=O)(=O)c(cc2)cc(c23)n(c(o3)=O)C ZINC000096103232
Cc1cc(=O)[nH]c(n1)SCC(=O)Nc(cc2)cc(c23)[nH]c(=O)[nH]3 ZINC000408541063
COc1ccc(cc1)CCC(=O)OCC(=O)Nc(cc2)cc(c23)[nH]c(=O)[nH]3 ZINC000023080685
c1c(C)cc(C)c(c12)[nH]c(C)c2CC(=O)NCC3nc(N)nc(n3)N(C)C ZINC000092022345
O[C@H]1COC[C@@H]1N(C)C(=O)c2cccc(c2)-c(cc3)cc(c34)c(=O)[nH]cn4
ZINC000426503514
COc1cccc(c1)CCNC(=O)c2c(C)n(nc2)-c3nc(C)cc(=O)[nH]3 ZINC000035598411
Cc1cc(=O)[nH]c(n1)S[C@@H](C)C(=O)N(C)Cc(n2)[nH]c(=O)c(c23)cccc3
ZINC000095378040
c1cccc(c12)[C@@H](CCO2)NC(=O)Cc(n[nH]c3=O)c(c34)cccc4 ZINC000032722163
Cc1ccc(o1)CNC(=O)Cn2c(=O)c(CCO)c(C)nc2-c3cccc3 ZINC000067300400
CC(C)(C)c(c1)[nH]nc1CN(C)Cc(cc2=O)[nH]c(c23)ccc(c3)C(=O)N ZINC000091818690
c1cc(F)ccc1-n(c(=O)[n-]2)c(=O)c(c23)n(C)cc3C(=O)NC4CCCC4 ZINC000009659627
Cc([nH]1)nc(c12)cc(cc2)CNC(=O)CCc3c(C)[nH]c(=O)nc3C ZINC000216982593
c1cccc1[C@H](O)c(nc2C3(C(=O)N)CC3)nn2-c4cccc(F)c4 ZINC000095520060
[nH]1c(=O)[nH]c(c12)cc(cc2)NC(=O)[C@@H](C)OC(=O)c3ccc(F)cc3N ZINC000018750619
COc1cccc(c1)-n(c(=O)[nH]2)c(c23)nc(nc3C(=O)N)-c4ccc(C)cc4 ZINC000004940452
NC(=O)COc1ccc(cc1Cl)/C=N/n(c(=O)[nH]2)c(=O)c(c23)cccc3 ZINC000409358485
O=C([O-])c1nn(CC=C)c(c12)CC[C@@H](C2)[NH2+]Cc(n3)[nH]c(=O)c(c34)cccc4
ZINC000067849895
Cc1cccc(C)c1N2C(=O)C[C@@H](C2=O)Nc(cc3)cc(c34)[nH]c(=O)[nH]4 ZINC000085877582
Cc1cn(nc1)CC(=O)N[C@H](c2cc(=O)[nH]c(n2)C)Cc(c[nH]3)c(c34)cccc4 ZINC000019239929
Clc1ccc(cc1N)C(=O)OCC(=O)Nc(cc2)cc(c23)[nH]c(=O)[nH]3 ZINC000012794208
O=c([nH]1)c(C)c(C)nc1-n(nc2C)c(c2)NC(=O)Cc3ccc(F)cc3 ZINC000007421322
Cc1ccc(o1)-c(nc2C(=O)N)nc(c23)n(c(=O)[nH]3)CCc4cccc4 ZINC000012145945
Cc1ccc(o1)-c2nn(-c3cccc(F)c3)cc2C[NH+](CCO)CCO ZINC000072478875
COc1ccc(cc1O)-c(nc2C(=O)N)nc(c23)n(c(=O)[nH]3)-c4cccc(C)c4 ZINC000005151653
c1nnn1N[C@@H](c(c(O)c2)ccc2O)c3cc(Cl)ccc3[O-] ZINC000006321276
O=C([O-])c1nn(C)c(c12)CC[N@@H+](C2)Cc3ccc(o3)-c4[nH]ncc4 ZINC000215432618
COc1ccc(c(c1)OC)-n(c(=O)[nH]2)c(c23)nc(nc3C(=O)N)-c4ccnc4 ZINC000004518782

Cc1ccc(cc1[N+](=O)[O-])C(=O)OCC(=O)Nc(cc2)cc(c23)[nH]c(=O)[nH]3 ZINC000013637947
 c1[nH+]ccn1C[C@H](C(C)(C)C)NC(=O)c(cc2)cc(c23)ncn3CCO ZINC000097575015
 [nH]1c(=O)[nH]c(c12)cc(cc2)NC(=O)[C@H](C)OC(=O)c3ccc(F)cc3N ZINC000007377395
 CCn(c(n1)N)c(c12)ncc(c2)C(=O)NCc([nH]3)nc(c34)ccc(c4)OC ZINC000077541512
 c1cccc(c12)[nH]c(n2)CNC(=O)c3ccenc3O[C@@H]4CCOC4 ZINC000240002221
 COc1ccc(Cl)cc1NC(=O)CSc(n2)[nH]c(c23)nc(N)[nH]c3=O ZINC000005639895
 Cc1ccc(C)c(c1)NC(=O)CSc([n-]c2=O)nc(c23)n[nH]c3 ZINC000013116786
 O=c([nH]1)[nH]c(c12)cc(cc2)NS(=O)(=O)c3ccc(F)c(Cl)c3 ZINC000006623468
 CCOc1cccc1-n(c(=O)[nH]2)c(c23)nc(nc3C(=O)N)-c4cccc4O ZINC000005271226
 COc1cccc1-n(c(=O)[nH]2)c(c23)nc(nc3C(=O)N)-c4ccc(F)c(F)c4 ZINC000004338368
 CCn(c(n1)N)c(c12)ncc(c2)C(=O)NCCNC(=O)c3ccc(F)cc3 ZINC000077408327
 CCn1ncnc1[C@@H](C)NC(=O)Nc(c2)c(OC)cc(c23)[nH]c(=O)[nH]3 ZINC000096164615
 CCOc1cccc1-n(c(=O)[nH]2)c(c23)nc(nc3C(=O)N)-c4ccenc4 ZINC000005271244
 CCn(c(n1)N)c(c12)ncc(c2)C(=O)N(C)CCn3cc[nH+]c3C ZINC000077357956
 COc1cccc(c1)NC(=O)CSc([nH]2)nc(=O)c(c23)[nH]cn3 ZINC000033027571
 CCOc1cccc1-n(c(=O)[nH]2)c(c23)nc(nc3C(=O)N)-c4cccc(F)c4 ZINC000004940465
 Cc1cccc(c1)-c(nc2C(=O)N)nc(c23)n(c(=O)[nH]3)C[C@@H]4CCCO4 ZINC000012145911
 COCCOC(=O)c1c(C)[nH]c(c1C)C(=O)Nc(cc2)cc(c23)[nH]c(=O)[nH]3 ZINC000036391272
 N1CC(=O)Nc(c12)cc(cc2)-c3nc(nn3CCO)[C@@H](O)c4cccc4 ZINC000096150054
 s1cc(C)n(c12)c(=O)cc(n2)CSc3nnc(C4CC4)n3CCC(=O)N ZINC000028908392
 CC(C)(C)c1ncc(c(=O)[nH]1)C(=O)NCCc(n2)[nH]c(=O)c(c23)cccc3 ZINC000082083937
 COc1ccc(C)cc1-n(c2=O)c(SCC(=O)N)nc(c23)cccc3 ZINC000003492505
 C1CCCc(c12)n(C)nc2CNS(=O)(=O)c(cc3)cc(c34)[nH]c(o4)=O ZINC000096099197
 c1cccc(c12)nc(-c(n3)ccn3C)cc2C(=O)Nc4nc(es4)CC(=O)N ZINC000019716381
 Ce1c(C)sc(c12)nc([nH]c2=O)CCNc3ncnc(c34)[nH]cn4 ZINC001506404029
 c1nn(C)c(c12)nc(NCCO)nc2NCc3cccc(Cl)c3 ZINC000021930242
 c1cccc1[C@@H](C)NC(=O)COC(=O)CCc(n2)[nH]c(=O)c(c23)cccc3 ZINC000017949935
 n1c[nH]c(=O)c(c12)[nH]c(n2)N/N=C/c3ccc(Br)cc3O ZINC000006161162
 NC(=O)c1ncn(c12)c(C)c(c(n2)C)CCC(=O)Nc(cc3)cc(c34)[nH]c(=O)[nH]4 ZINC000012525618
 COc1ccc(cc1OC)-c(n2)cc(n23)c(ncc3)N4CCC(C(=O)N)CC4 ZINC000067263486
 n1cccn1[C@H](CC)c2nc(CC(=O)N)nn2Cc3ccc(C)cc3 ZINC000096136632
 COc1cccc(c1)CNC(=O)CSc(n2)n(N)c(=O)c(c23)cccc3 ZINC000071327505
 Ce1n[nH]c(C)c1Cc2nc(nn2CCO)Cc3cccc(Cl)c3 ZINC000828778500
 C1CCCN(c12)c(=O)n(n2)CCCNc(n3)[nH]c(=O)c(c34)cccc4 ZINC000097995083
 Ce1cc(=O)[nH]c(n1)S[C@H](C)C(=O)NCc2cccc2-n3ccnc3 ZINC000221421197
 c1cccc(c12)c(=O)n(c(n2)SCC(=O)N)-c3ccc(F)cc3F ZINC000003464360
 O=c([nH]1)[nH]c(=O)c(c1C)CCC(=O)NCCc(c[nH]2)c(c23)ccc(F)c3 ZINC000050766460
 C1CCCc(c12)nn(c(=O)c2)CCNS(=O)(=O)c3cccc(c34)cccc4 ZINC000575617879
 COc1cccc(c1O)-c(nc2C(=O)N)nc(c23)n(c(=O)[nH]3)C4CCCCC4 ZINC000005151373
 n1cccc1-c(n2)nc(c(c23)c(C)nn3C)NCCc4nc(C)cc(=O)[nH]4 ZINC000072468826
 COc1ccc(C)cc1NC(=O)CSc([nH]2)nc(=O)c(c23)[nH]cn3 ZINC000033027551
 CC(C)(C)c1nc(=O)[nH]c(c1)C(=O)NCc(cc2)cc(c23)[nH]c(=O)[nH]3 ZINC000216043967
 Ce1nc(C)c(c(=O)[nH]1)CC(=O)NCc(cc2)cc(c23)[nH]c(=O)[nH]3 ZINC000345094490
 n1cccn1[C@@H](CC)c2nc(CC(=O)N)nn2Cc3ccc(C)cc3 ZINC000096136631
 Ce1cccc(n1)-n(c2=O)c(S[C@H](C)C(=O)N)nc(c23)cccc3 ZINC000009368719
 n1c[nH]c(=O)c(c12)[nH]c(n2)N/N=C/c3cc(Br)ccc3O ZINC000006382830

COc1ccc(OC)c(c1)[C@@H](C)NC(=O)Cc(n[nH]c2=O)c(c23)cccc3 ZINC000018204220
CC(C)Cc1n[nH]/c([nH]1)=N\C(=O)[C@@H]2CC(=O)N(C2)c(n[nH]3)c(c34)cccc4
 ZINC000095472147
Fe(c1)cccc1-c(n2)nc(C(=O)N)c(c23)[nH]c(=O)n3-c4cccc4F ZINC000004518709
CC(C)n(c(=O)[nH]1)c(c12)nc(nc2C(=O)N)-c3cccc(Cl)c3 ZINC000012145941
OC[C@H]1COCCN1C(=O)c2cccc(c2)-c(cc3)cc(c34)c(=O)[nH]cn4 ZINC000299788375
c1cccc(c12)C(=O)N[C@@H](C2)c3nc(nn3CCO)-c(c[nH]4)c(c45)cccc5 ZINC000096133536
COc1cccc1Cc2nn(c(n2)CCC(=O)N)-c3cccc(n3)C ZINC000097495105
Cc1ccnc(c1)[C@@H](C2CC2)NC(=O)Cn([nH]3)c(=O)c(c34)cccc4 ZINC000097259282
COc1ccc(cc1OC)Cc(n2)n(CC(=O)N)c(c23)cccc3 ZINC000032497981
COc1ccc(OC)c(c1)NS(=O)(=O)c(cc2)cc(c23)[nH]c(=O)[nH]3 ZINC000004148342
Cc1ccc(s1)CN(CCO)C(=O)c(cc(=O)n2)n(c23)ccs3 ZINC000097547524
COc1cccc1-n(c(=O)[nH]2)c(c23)nc(nc3C(=O)N)-c4cccs4 ZINC000004338401
Cn1nenc1-c2nc(ncc2C)NCCc(n3)[nH]c(=O)c(c34)cccc4 ZINC000023478862
Cc1cccc(c1)C(=O)N(CCO)Cc(c2)c(=O)[nH]c(c23)cc4c(c3)OCO4 ZINC000004231128
Cc(n1)[nH]c(=O)c(c12)CCN(C2)C(=O)c3cc(n[nH]3)-c4cccc4O ZINC000071752127
c1n[nH]cc1S(=O)(=O)[N-]c(c2=O)cccn2Cc3ccc(F)cc3 ZINC000088547559
COc1ccc(cc1)CNC(nc(c23)n(C)nc3)nc2NCCCO ZINC000020744634
COc1ccc(cc1)-c(nc2C(=O)N)nc(c23)n(c(=O)[nH]3)-c4cccc4OC ZINC000004338362
Cc1cccc(c1)-n(c(=O)[nH]2)c(c23)nc(nc3C(=O)N)-c4cccc4O ZINC000005151664
Cc1ccc(c(C)c1)OC[C@H](O)Cn(nc2C(=O)N)c(=O)c(c23)cccc3 ZINC000042757594
N1CC(=O)Nc(c12)cc(cc2)-c3nc(nn3CCO)[C@H](O)c4cccc4 ZINC000096150055
[nH]1c(=O)[nH]c(c12)cc(cc2)NC(=O)CN3C(=O)CCOc(c34)cccc4 ZINC000012744985
NC(=O)COc1ccc(cc1OC)CNC(cc2)cc(c23)[nH]c(=O)[nH]3 ZINC000004413442
Fe1ccc(F)cc1NC(=O)CSc([nH]2)nc(=O)c(c23)[nH]cn3 ZINC000033324894
c1ccnc(n12)nc(c2)[C@H](CC)NC(=O)CCc(n3)c(=O)[nH]c(c34)cccc4 ZINC000091595595
Cc([nH]1)nc(c12)ncc(c2)-c3cccc(c3)C(=O)N4CCC[C@H](C4)C(=O)N ZINC000534576676
O1CCOc(c12)c(ccc2)NC(=O)Cc(n[nH]c3=O)c(c34)cccc4 ZINC000055950795
CCOc1cccc1-n(c(=O)[nH]2)c(c23)nc(nc3C(=O)N)-c4ccncc4 ZINC000005271247
N#CCCN(nc1C)c(C)c1CCC(=O)Nc(cc2)cc(c23)[nH]c(=O)[nH]3 ZINC000024049738
c1cc(F)ccc1-n(n2)c(O)c(c2C)CCC(=O)Nc(cc3)cc(c34)[nH]c(=O)[nH]4 ZINC000016260581
COc1ccc(cc1F)-c(c2)nc(n23)sc3C(=O)N[C@H](C(=O)N)[C@@H](C)O ZINC000067820619
COc1ccc(OC)c(c12)[nH]c(c2)C(=O)NCC(=O)N=c([nH]3)[nH]c(c34)cccc4 ZINC000020730073
c1cccc(c12)c(=O)[nH]c(n2)CN(CC)CC(=O)Nc(cc3)cc(c34)[nH]c(=O)[nH]4
 ZINC000025480179
CCc(n1)cc(n(c12)ncn2)N[C@H](CO)Cc(c[nH]3)c(c34)cccc4 ZINC000096429845
COc1cc(ccc1O)[C@@H](CC(=O)N2)c(c23)c(C)nn3-c(n4)ccc(n45)nnc5 ZINC000033011354
COc(cc1)cc(c12)[nH]c3c2ncn(c3=O)/N=C/c4cccc(OC)c4O ZINC000002349172
[nH]1c(=O)[nH]c(c12)cc(cc2)NC(=O)CNC(=O)C3(CCC3)c4cccc4 ZINC000039559621
Nc(n1)[nH]c(=O)c(c12)nc([nH]2)SCC(=O)Nc3c(Cl)cccc3Cl ZINC000020429052
Cc1cc(=O)oc(C)c1C(=O)O[C@@H](C)c(n2)[nH]c(=O)c(c23)cccc3 ZINC000026013054
O=c1[nH]c(=O)n(CC)c(c12)ncc(c2)C(=O)c3cc(F)ccc3O ZINC000002652841
Cc1ccc(cc1C)-c(nc2C(=O)N)nc(c23)n(c(=O)[nH]3)C[C@@H]4CCCO4 ZINC000012145915
COc(cc1)cc(c12)[nH]c(=O)c(c2)CN(CCO)C(=O)c3cccc3F ZINC000008716803
COc1cccc(c1)OC[C@H](O)CNC(=O)c(cc(=O)[nH]2)c(c23)cccc3 ZINC000097730289
CCSc1nc(N)c(Br)c(n1)Sc2nc(N)nc(c23)[nH]cn3 ZINC000008615351

Cn1c(CO)nnc1[C@@H]2CCC[N@@H+](C2)Cc([nH]c3=O)nc(c34)ccs4 ZINC000253536562
COc1ccc(O)c(c1)/C=N/n(cn2)c(=O)c(c23)[nH]c4c3cccc4 ZINC000000501417
c1cc(F)ccc1CCNC(=O)CCc(n2)[nH]c(=O)c(c23)cccc3 ZINC000009577373
Cn1cc(en1)[C@@H]([C@H]2C[C@@H](O)C2)NC(=O)c(cc(=O)[nH]3)c(c34)cccc4 ZINC000220347321
[nH]1c(=O)[nH]c(c12)cc(cc2)NC(=O)c3cccnc3O[C@@H]4CCSC4 ZINC000252571735
c1cc(Cl)ccc1NC(=O)Cn(c(=O)n(c2=O)CCO)c(c23)cccc3 ZINC000071280422
CCc1noc(n1)CN(CC)C(=O)c(en2)cc(c23)nc(N)n3CC ZINC000077515943
Fc(c1)cccc1NC(=O)CN(C)C(=O)CCc(n2)[nH]c(=O)c(c23)cccc3 ZINC000012875080
COc1ccc(cc1)CNC(=O)CCNc2nenc(c23)[nH]cn3 ZINC000012296989
c1cccc(c12)[C@H](CCO2)NC(=O)CCc(n3)[nH]c(=O)c(c34)cccc4 ZINC000006971386
CSc1nc(Cl)cc(n1)Sc2nc(N)nc(c23)[nH]cn3 ZINC000008615340
COc(cc1)cc(c12)c(C)c([nH]2)C(=O)NCCn(c(=O)c(=O)[nH]3)c(c34)cccc4 ZINC000096118493
[nH]1c(=O)c(=O)[nH]c(c12)cc(cc2)C(=O)N[C@@H](c3cccs3)[C@H]4C[C@@H](O)C4 ZINC000253534854
C1CCCc(c12)c(C)nc(n2)CCNC(=O)c(c3)c(=O)[nH]c(c34)cccc4 ZINC000215630478
COc1cccc1-c2n[nH]c(c2)C(=O)NCCc(n[nH]c3=O)c(c34)cccc4 ZINC000077099371
CCc1ccc(cc1)OCCSc([nH]2)nc(c23)c(N)nc(n3)N ZINC000005285507
COc1cc(cc(c1)OC)C(=O)NCCNC(=O)c(n2)[nH]c(=O)c(c23)cccc3 ZINC000022470444
COCCn1ennc1[C@@H](C)NC(=O)c(cc(=O)[nH]2)c(c23)ccc(F)c3 ZINC000824466137
Cc1nn(c(C)c1)CCC(=O)O[C@H](C)c(n2)[nH]c(=O)c(c23)cccc3 ZINC000011593824
c1cccc(c12)c(=O)[nH]c(n2)CN(C)CC(=O)Nc(cc3)cc(c34)[nH]c(=O)[nH]4 ZINC000023077525
c1csc(c1C)C(=O)OCC(=O)Nc(cc2)cc(c23)[nH]c(=O)[nH]3 ZINC000002636591
COc1ccc(cc1)C(=O)CNC(=O)[C@H]2CC(=O)N(C2)c(n[nH]3)c(c34)cccc4 ZINC000095477470
c1cccc(c12)nc(C)cc2NC(=O)[C@H](C)n(n3)c(=O)cc(c34)CCC4 ZINC000585150149
Cc1nn(C)c(C)c1-c2[nH]nc(c2)C(=O)NCCc(n3)[nH]c(c34)cccc4 ZINC000095478685
c1cnccc1-c2nnc(n2CC)SCC(=O)Nc(cc3)cc(c34)[nH]c(=O)[nH]4 ZINC000006586722
[nH]1c(=O)[nH]c(c12)cc(cc2)NC(=O)[C@@H]3CCCN3C(=O)c4cccs4 ZINC000008231397
C1CC1c2nnc(n2CC)S[C@@H](C)C(=O)Nc(cc3)cc(c34)[nH]c(=O)[nH]4 ZINC000007841312
COc1ccc(C(=O)N)cc1NS(=O)(=O)c(c2)c(C)cc(c23)[nH]c(=O)[nH]3 ZINC000011635243