

## Supplementary Material

### Discovery of non-sulfonamides Carbonic Anhydrase IX Inhibitors through Structure-Based Virtual Screening

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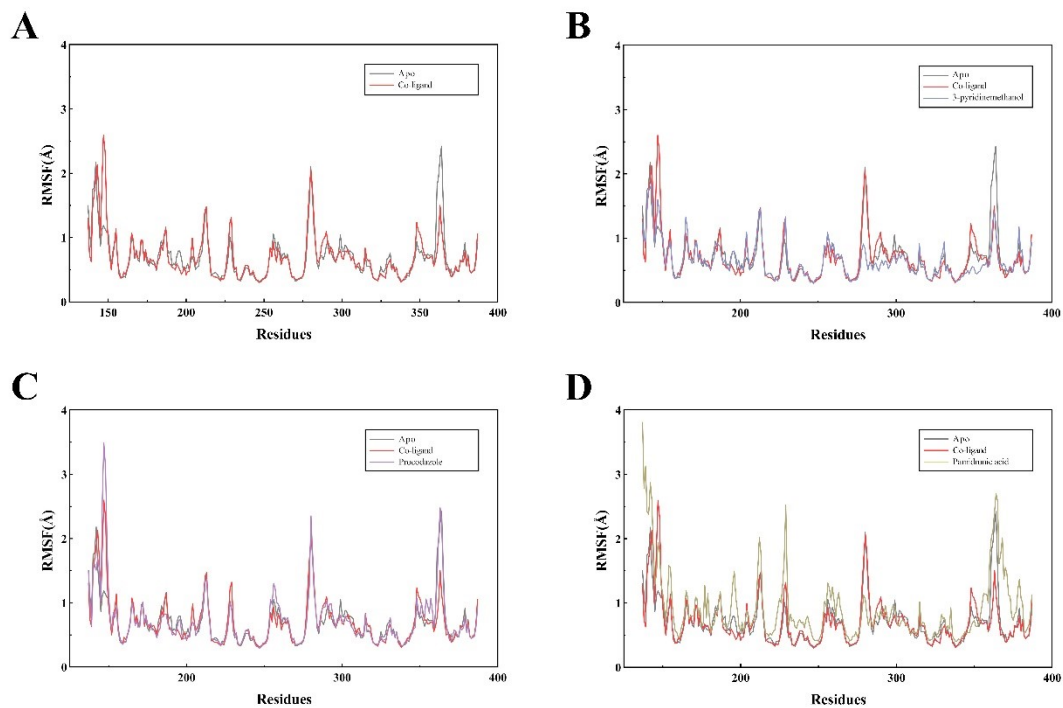
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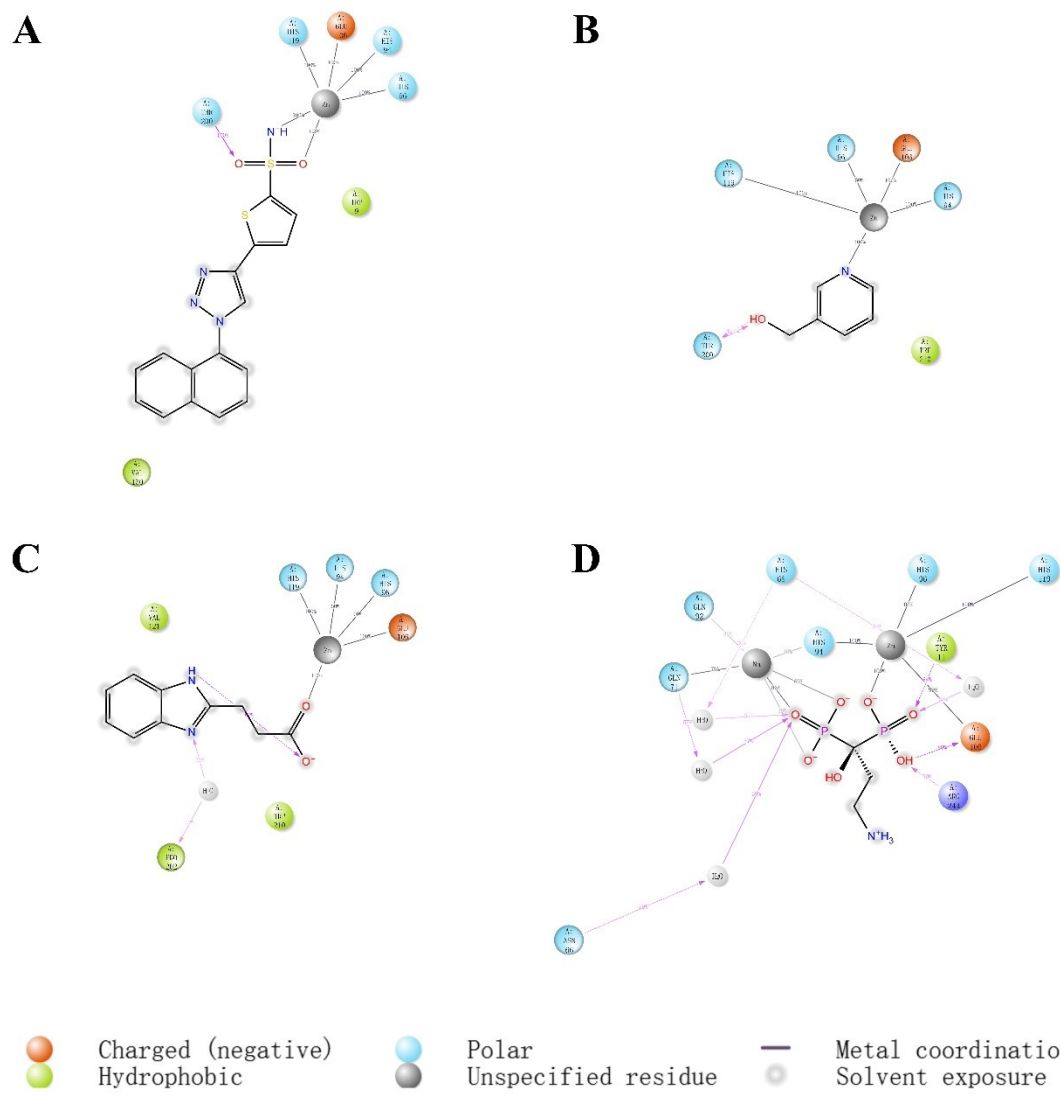
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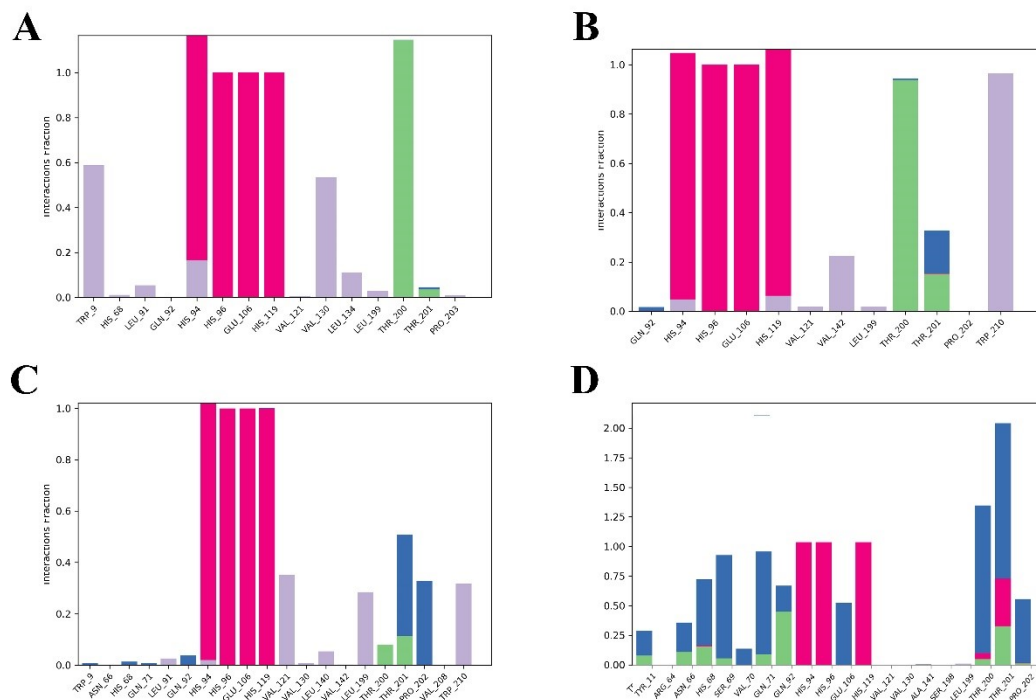
E-mail addresses: mscheng@syphu.edu.cn (Maosheng Cheng).



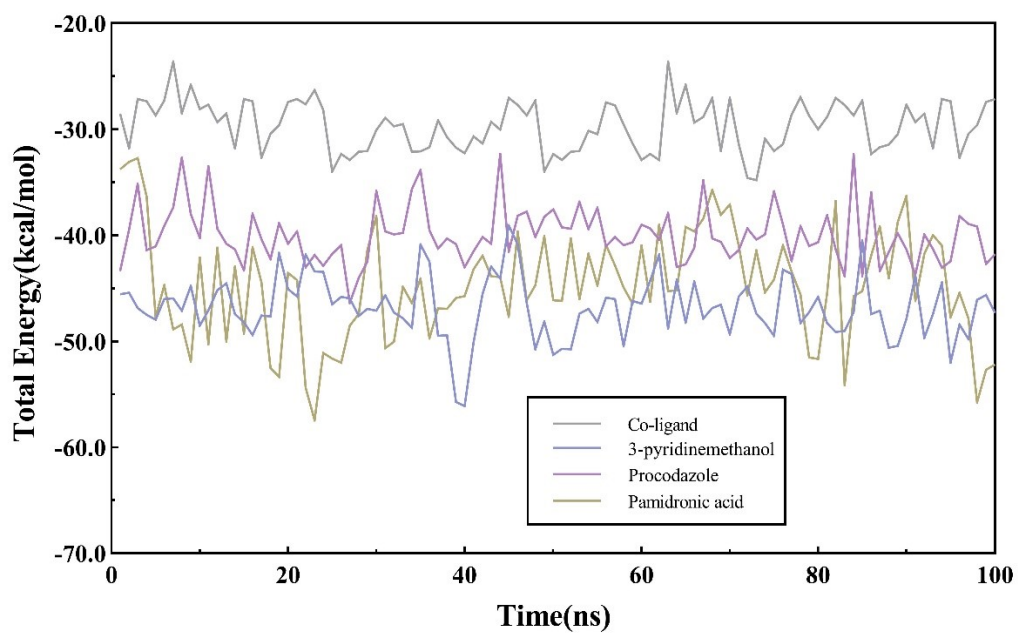
**Figure S1.** The RMSF monitored by desmond. **(A-D)** The RMSF of protein C $\alpha$  of apo state of the CA IX **(A)**, and CA IX complexed with co-ligand overlapped with **(B)** 3-pyridinemethanol, **(C)** Procodazole, **(D)** Pamidronic acid. in the same frame, respectively.



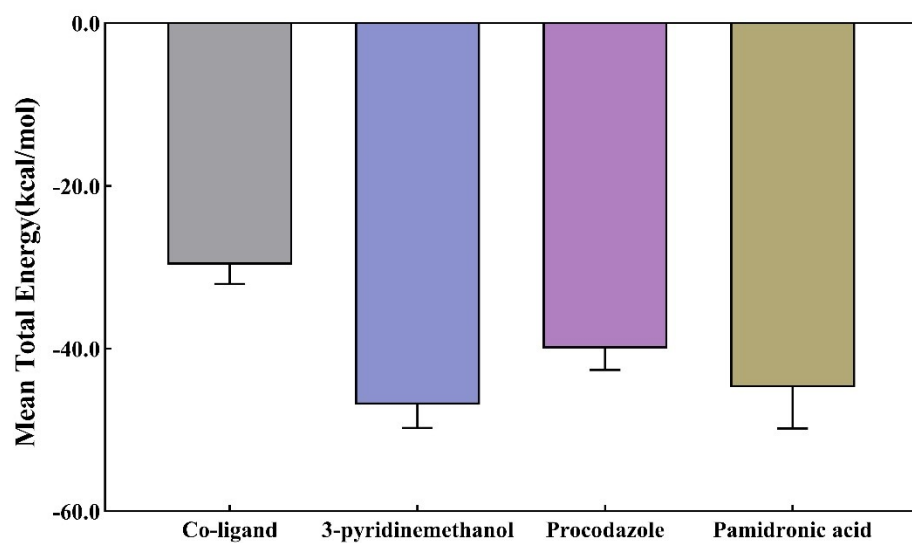
**Figure S2.** 2D interaction diagrams of the complexes of CA IX with co-ligand, 3-pyridinemethanol, procodazole and pamidronic acid after 100 ns' MD simulations. **(A)** Co-ligand, **(B)** 3-pyridinemethanol, **(C)** Procodazole, **(D)** Pamidronic acid.



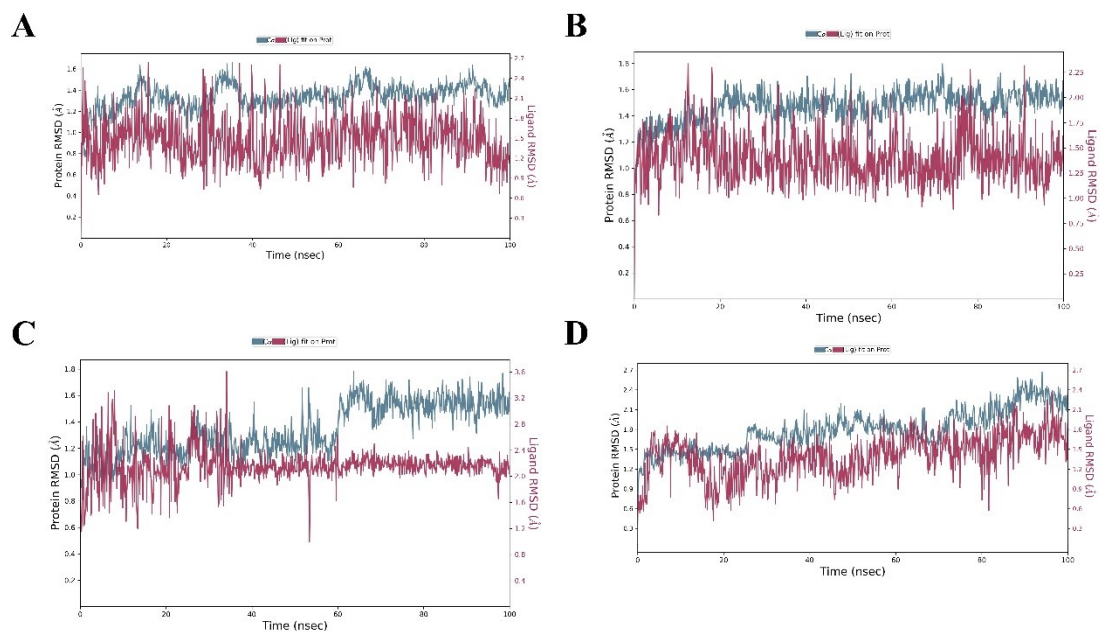
**Figure S3.** The interactions between protein and the ligand were monitored across the MD simulation, which are categorized into four types: hydrogen bonds (green), hydrophobic (purple), ionic (red) and water bridges (Blue) and normalized into stacked bar charts over the course of the trajectory. The normalized stacked bar chart of CA IX with co-ligand, 3-pyridinemethanol, procodazole and pamidronic acid after 100 ns' MD simulations. (A) Co-ligand, (B) 3-pyridinemethanol, (C) Procodazole, (D) Pamidronic acid.



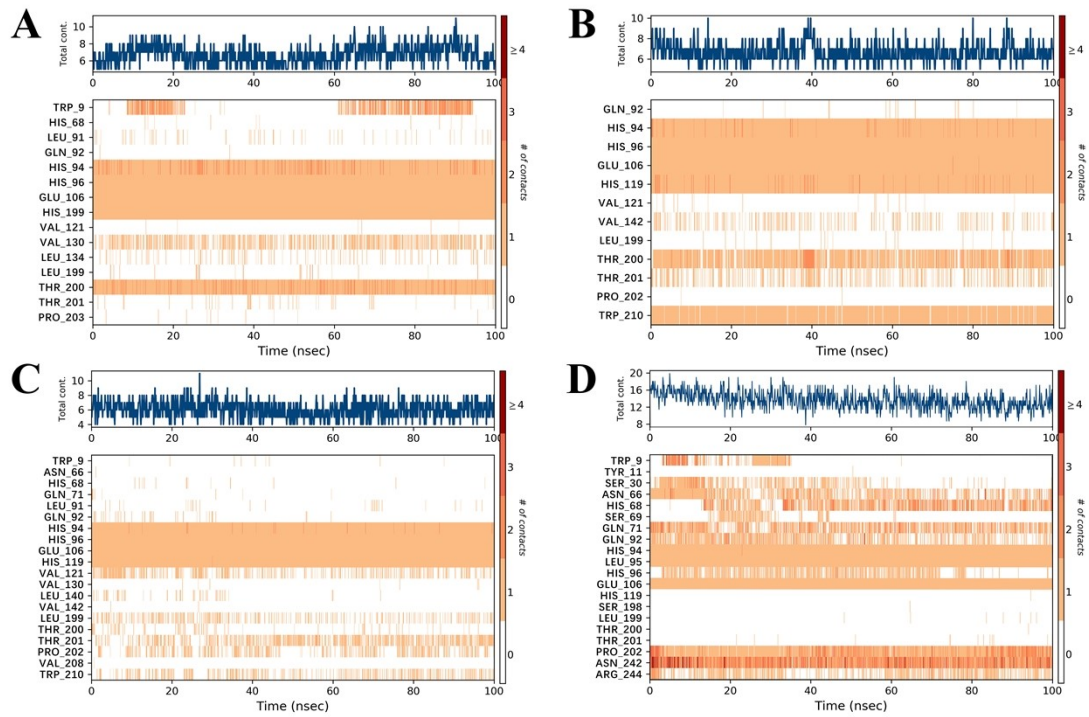
**Figure S4.** Total energy curves of the CA IX complexed with co-ligand overlapped with 3-pyridinemethanol, procodazole and pamidronic acid during 100 ns MD simulations.



**Figure S5.** The mean total energy values of CA IX complexed with co-ligand, 3-pyridinemethanol, procodazole and pamidronic acid during 100 ns MD simulations.

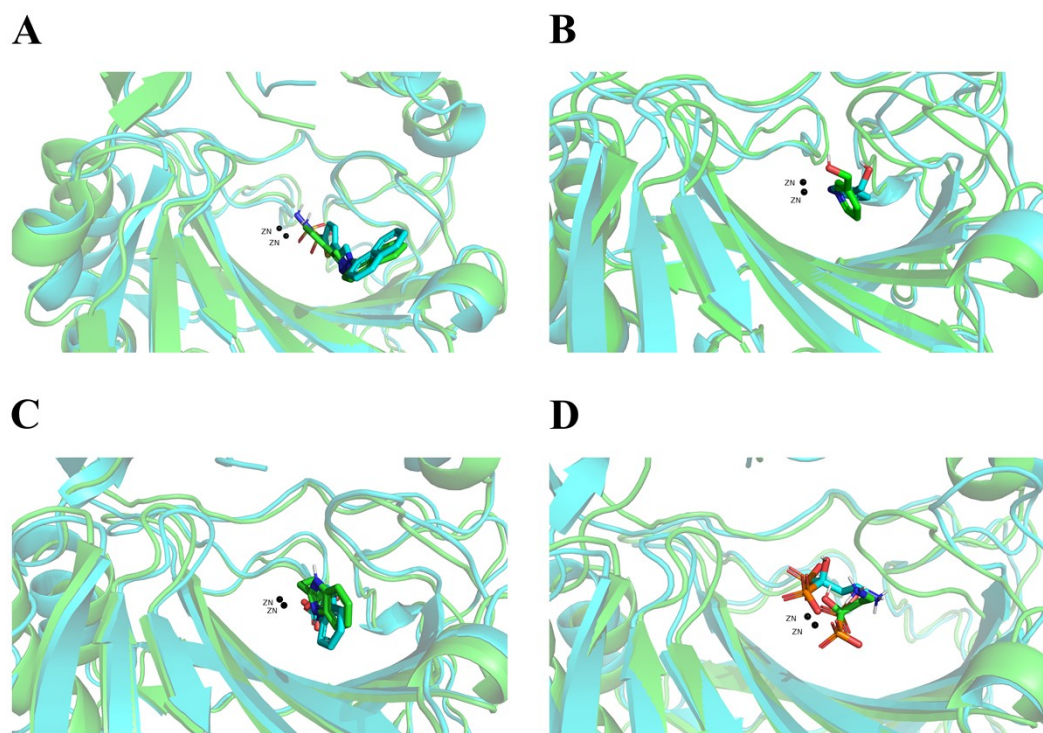


**Figure S6.** The RMSD values of ligands monitored by desmond. (A-D) The RMSD values of ligands calculated for the systems including CA IX complexed with co-ligand, 3-pyridinemethanol, procodazole and pamidronic acid during the simulation of 100 ns.



**Figure S7.** Ligand-Protein contacts of CA IX with co-ligand, 3-pyridinemethanol, procodazole and pamidronic acid complexes during the simulation of 100 ns.





**Figure S8.** The Superimposition of complexes' binding poses before (green) and after (cyan) 100ns' MD simulations. The complexes consist of CA IX with (A) co-ligand, (B) 3-pyridinemethanol, (C) procodazole and (D) pamidronic acid. The pictures were produced using PyMol.

**Table S1.** The results of cross-docking study.

Receptor	Scal	%Docked	%RefDocked	AveRMSD	%RefCorrect
5FL4	0.8	100	100	0.94	100
5FL5	0.8	100	100	0.97	100
5ULN	0.8	100	100	1.31	100
6FE1	0.8	100	100	1.56	100

**Table S2.** The decoy set generated by DUDE.

Zinc ID	Smile
ZINC49871821	<chem>CCOC(=O)c1sc2c(c1C)c(=O)n(CCO)c(=O)n2CC(=O)O</chem>
ZINC43702114	<chem>C[C@@]12CCC(=O)N1[C@H](C(=O)N1CCO[C@H](C(=O)O)C1)CS2</chem>
ZINC42690308	<chem>CCN(CC(=O)O)C(=O)N1CCCN(C(C=O)CC)1</chem>
ZINC08296731	<chem>O=C(O)CCC(=O)N[C@H]1CCN2C(=O)c3cc(-c4cccs4)ccc3NC(=O)[C@H]12</chem>
ZINC50421638	<chem>C[C@@H](NC(=O)N1CSC[C@H]1C(=O)O)c1nnc1C</chem>
ZINC20548403	<chem>CCCCN1C(=O)[C@@H]2[C@H](CCC(=O)O)N[C@@]3(C(=O)Nc4c(CC)cccc43)[C@@H]2C1=O</chem>
ZINC43702646	<chem>O=C(O)[C@H]1CN(C(=O)C[C@@H]2CCS(=O)(=O)C2)CCO1</chem>
ZINC65347481	<chem>O=C(O)c1nc(O)c(-c2cc(O)cc(F)c2)c1</chem>
ZINC13019120	<chem>C[C@H](Se1nc2cc(C(=O)O)ccc2c(=O)n1C)C(=O)Nc1cc(F)ccc1F</chem>
ZINC13272312	<chem>CCNC(=O)NC(=O)[C@H](C)Sc1nc2cc(C(=O)O)ccc2c(=O)n1Cc1cccc1Cl</chem>
ZINC50376502	<chem>CO[C@H]1CCC[C@@H]1NC(=O)N1CCO[C@H](C(=O)O)C1</chem>
ZINC20588256	<chem>Nn1c(SCC(=O)O)nnc1-c1cc2c(s1)CCCC2</chem>
ZINC34002497	<chem>Nc1nc2c(nc(Sc3ccc(Cl)cc3)n2[C@@H]2O[C@@H]3CO[P@](O)(=S)O[C@H]3[C@H]2O)c(=O)[nH]1</chem>
ZINC13049550	<chem>CC(C)Cn1c(S[C@H](C)C(=O)Nc2cc(F)ccc2F)nc2cc(C(=O)O)ccc2c1=O</chem>
ZINC43414178	<chem>Cc1esc(NC(=O)NCC2(CC(=O)O)CCCC2)n1</chem>
ZINC39465523	<chem>CC(C)S(=O)(=O)c1cc2c(cc1Cc1cccc1)[C@@H]1CO[P@](=O)(O)NN1CC2</chem>
ZINC62925916	<chem>C[C@]1(C(=O)O)CCN(C(=O)NC[C@H]2COCCO2)C1</chem>
ZINC13231774	<chem>CCNC(=O)NC(=O)CSc1nc2cc(C(=O)O)ccc2c(=O)n1CC(C)C</chem>
ZINC36865857	<chem>Cn1c(SCC(=O)O)nnc1N1CCS(=O)(=O)CC1</chem>
ZINC16021948	<chem>CCCCN1C(=O)[C@@H]2[C@H](CCC(=O)O)N[C@]3(C(=O)Nc4c(CC)cccc43)[C@@H]2C1=O</chem>
ZINC03097414	<chem>O=C(O)c1nc2ncc(-n3cc([N+](=O)[O-])cn3)cn2n1</chem>
ZINC22000495	<chem>CCCCc1ncc(C(=O)O)nc1N</chem>
ZINC37030336	<chem>C[C@H](NS(=O)(=O)c1c[nH]c(C(=O)O)c1)ccc(Cl)s1</chem>
ZINC44218213	<chem>N[C@@H](CC(=O)O)c1ccc2oc(C(=O)c3ccc(Br)cc3)cc2c1</chem>
ZINC61593834	<chem>O=C(O)c1ccc(Sc2n[nH]c(=O)n2C2CC2)nn1</chem>
ZINC03911303	<chem>COc1ccc(NC(=O)C(=O)c2c(O)[nH]c3cccc23)cc1OC</chem>

ZINC32501315 Cc1c(C(=O)O)oc2ccc(N)cc12

ZINC63074746 CC1(C)CCCN1c1ccc(N)cc1C(=O)O

ZINC37931598 Cc1oc2nc[nH]c(=O)e2c1C(=O)N(C)CCC(=O)O

ZINC43703101 Cc1n[nH]c(C)c1S(=O)(=O)N1CCO[C@H](C(=O)O)C1

ZINC49080522 O=C(NCCn1cccn1)Nc1cc(Br)ccc1C(=O)O

ZINC13256143 C[C@H](Sc1nc2cc(C(=O)O)ccc2c(=O)n1-c1ccc(F)cc1)C(=O)Nc1cccc1F

ZINC43701077 O=C(O)[C@H]1CN(C(=O)CCN2CCSC2=O)CCO1

ZINC62832103 CC[C@H](C#N)N(C)c1ccc(N)cc1C(=O)O

ZINC12384893 CC1(C)Cc2sc3nc(SCC(=O)O)nc(N)e3c2CO1

ZINC05853788 Cc1cn([C@H]2[C@H](N=[N+]=[N-])[C@H](C(=O)O)O2)c(=O)[nH]c1=O

ZINC44931730 Cc1nnc(SCC(=O)O)n1[C@H]1(C)CCS(=O)(=O)C1

ZINC13462231 COc1cc(O)ccc1[C@H]1C=C(c2ccc(O[C@H](C)C(=O)O)cc2)Nc2nmm21

ZINC06955176 COc1cc(C(C)=N/NC(=O)CNe2c(C)cc(C)cc2C)ccc1OCC(=O)O

ZINC05734475 CC1(C)CCC(C)(C)C1C(=O)N[C@@H](O)C(=O)O

ZINC62828877 O=C(Nc1secc1C(=O)O)NC1CCCC1

ZINC43701705 Cc1nn(C)c(C)c1CC(=O)N1CCO[C@@H](C(=O)O)C1

ZINC20596650 O=C(O)c1cn(CCN2C(=O)NC3(CCCC3)C2=O)nn1

ZINC40557135 C[C@@H](CC(=O)O)NC(=O)N[C@@H]1CCC[C@@H](C)[C@H]1C

ZINC13272514 N#Cc1c(N)sc2c1CCN(c1ccc(S(=O)(=O)N3CCC(C(=O)O)CC3)cc1[N+](=O)[O-])C2

ZINC62118415 CC1(C)NC(=O)N(CC(=O)N2CC[C@H](C(=O)O)C2)C1=O

ZINC41606403 CC(C)c1ccc(-c2ccc(C(=O)O)c(=O)n2CC(N)=O)cc1

ZINC43414105 CNC(=O)NCC1(CC(=O)O)CCCCC1

ZINC62339875 Cc1cc(C)c2c(CNC(=O)[C@@H]3CCCC3)c(C(=O)O)[nH]e2c1

ZINC41073491 O=C(O)COCC(=O)N1CCC(N2CCNC2=O)CC1

ZINC63215707 O=C(CN1CSCC1=O)Nc1nccn1C(=O)O

ZINC57934824 C[C@H](C(=O)O)N1C(=O)C(C)(C)Ne2cc3c(cc21)OCO3

ZINC27531874 CCOC(=O)Cn1c(=O)n(CCO)c(=O)e2c(C)c(C(=O)O)sc21

ZINC37834521 CN(Cc1en(C)c(=O)n(C)c1=O)C(=O)[C@H]1C[C@@H]1C(=O)O

ZINC41049355 C[C@H](CC(=O)O)Sc1ncccc1N

ZINC61770464 Cc1nn(-c2nccn(C(C)C)c2=O)c(C)c1CC(=O)O

ZINC62100900 O=C(O)C[C@H]1CCCN(C(=O)N2CCNC(=O)CC2)C1

ZINC43503541 O=C(N[C@H]1(C(=O)O)CCSC1)c1ccc([N+](=O)[O-])o1

ZINC62925708 CC[C@H]1(C(=O)O)CCN(C(=O)Nc2ccn(C)n2)C1

ZINC58158061 Cc1c(C(=O)O)[nH]e2c1/C(=N/N1CC(=O)NC1=O)CC(C)(C)C2

ZINC20304047 CNC(=O)NC(=O)[C@H](C)Oe1ccc(Br)cc1C(=O)O

ZINC54054898 C[C@H](C(=O)O)N(C)c1nc2c([nH]1)c(=O)n(C)c(=O)n2C

ZINC46088389 CC1(C)Oe2ccc(NC(=O)[C@H]3CCCC[C@@H]3C(=O)O)cc2NC1=O

ZINC49850976 C[C@H](OC(=O)c1cc(F)ccc1N)C(=O)O

ZINC54054697 C[C@@H](C(=O)O)N(C)c1nc2scn2c1[N+](=O)[O-]

ZINC52884990 CC(C)c1ccn(-c2ccc(N)cc2C(=O)O)n1

ZINC41116141 Ne1cc(Br)ccc1SCCn1cc(C(=O)O)nn1

ZINC67588578 O=C(O)c1[nH]ncc1CN1CCC[C@@H](c2n[nH]cc2-c2ccccc2)C1

ZINC41049361 CC[C@@H](Sc1ncccc1N)C(=O)O

ZINC42696421 C[C@H](CN(C)C(=O)CN1C(=O)NC(C)(C)C1=O)C(=O)O

ZINC50019827 CCN(c1cc(C(=O)O)c(N)cc1F)C1CC1

ZINC43425967 O=C(O)c1cn(CCN2CCO[C@@H]3CCC[C@@H]32)nn1

ZINC50030070 C[C@@H]1COCCN1c1cc(C(=O)O)c(N)cc1F

ZINC37325956 Ce1nc(=O)n([C@@H]2CCS(=O)(=O)C2)c(C)c1CCC(=O)O

ZINC20319186 Cc1c([C@H](C)NC(=O)c2nn(C)cc2C(=O)O)cnn1C

ZINC49821947 Cc1ccc(C)c(-n2nc(C(=O)O)cc2N)c1

ZINC13416288 Cc1sc2nenc(SCc3nc4sc(C(=O)O)c(C)c4c(=O)[nH]3)e2c1C

ZINC13044389 CCCCn1c(SCC(=O)NC(=O)N[C@H]2CCC[C@H](C)[C@@H]2C)nc2cc(C(=O)O)ccc2c1=O

ZINC16021948 CCCCNC1C(=O)[C@@H]2[C@H](CCC(=O)O)N[C@]3(C(=O)Nc4c(CC)cccc43)[C@@H]2C1=O

ZINC41049361 CC[C@@H](Se1nccc1N)C(=O)O

ZINC04533488 O=[P@]1(O)O[C@@H]2[C@H](CO)O[C@@H](n3nc4c3nnc3cnc43)[C@@H]2O1

ZINC62872963 Cc1cc(CS(=O)(=O)N2CCC[C@](C)(C(=O)O)C2)no1

ZINC40551044 C[C@@H](CC(=O)O)NC(=O)N[C@@H]1CCCC[C@H]1C

ZINC52094205 O=C(O)CCCCC(=O)c1cc2[nH]c(=O)[nH]c2cc1Br

ZINC13263694 C[C@@@]1(e2cccc(OCC(=O)O)c2)NC(=O)c2cccc2N1

ZINC13024842 CC(C)[C@H](C(=O)O)n1c(SCC(=O)Nc2c(Cl)cccc2Cl)nc2cccc2c1=O

ZINC11617280 O=C(O)CCC(=O)N1N=C(c2c(-c3cccc3)c3cc(Cl)ccc3[nH]c2=O)C[C@H]1c1cccc1

ZINC65347480 O=C(O)c1cc(O)nc1-c1cc(O)cc(F)c1

ZINC16901242 Cc1ccc(O)c(N[C@@H]2CC(=O)N(c3ccc(CC(=O)O)cc3)C2=O)c1

ZINC13418397 Cc1c(C(=O)O)sc2nncn(CC(=O)N[C@H](C)c3cccc4cccc34)c(=O)c12

ZINC13223720 C[C@@H](Se1nc2cccc2c(=O)n1CCCCC(=O)O)C(=O)NC(=O)NC1CCCCC1

ZINC48721252 C[C@@H](Cn1ccn1)NC(=O)/C(O)=N/c1nncs1

ZINC40590007 CC[C@@H]1COCCN1C(=O)N1C[C@H](OC)C[C@@H]1C(=O)O

ZINC62874812 CC[C@]1(C(=O)O)CCCN(c2nccc3nmmn23)C1

ZINC05728860 O=C(N/N=C/C/c1cccc(Br)c1)c1c[nH][nH]c1=O

ZINC05728860 O=C(N/N=C/C/c1cccc(Br)c1)c1c[nH][nH]c1=O

ZINC13199754 Cn1c(SCC(=O)NC(=O)NC2CCCC2)nc2cc(C(=O)O)ccc2c1=O

ZINC13816333 CO[C@@H]1[C@@H]2O[P@](=O)(O)OC[C@H]2O[C@H]1n1c(Sc2ccc(Cl)cc2)nc2c(N)nene21

ZINC09218955 COc1cccc1NC(=O)Cl=C(C)N(c2cccc(C(=O)O)c2)C(=O)N[C@H]1c1ccc(C#N)cc1

ZINC62843100 CN(C)C(=O)CNC(=O)N1CCC(C)(C(=O)O)CC1

ZINC13044387 CCCCn1c(SCC(=O)NC(=O)N[C@@H]2CCC[C@H](C)[C@@H]2C)nc2cc(C(=O)O)ccc2c1=O

ZINC02806563 Cc1c(/C=C/C(=O)Nc2en(C)nc2C(=O)O)cnn1C

ZINC49556841 O=C(O)c1cc(S(=O)(=O)Nc2nc3c(s2)CCCC3)c[nH]1

ZINC38036662 CC(C)(C)NC(=O)N[C@H](C(=O)O)C1CCCCC1

ZINC40557561 O=C(NC[C@H]1CCCO1)Nc1cc(Br)ccc1C(=O)O

ZINC62935903 C[C@@@]1(C(=O)O)CCN(C(=O)N2CCNC(=O)CC2)C1

ZINC66134106 Ne1nc(C(=O)O)cc(-e2ccc(OC[C@H]3CCCO3)cc2)n1

ZINC22116712 CC/C=C(C(=O)O)c1csc(N)n1

ZINC45138961 CC1(C)C[C@@H]1NC(=O)NC1CCC(C(=O)O)CC1

ZINC40530751 CO[C@@H]1C[C@H](C(=O)O)N(C(=O)N2C[C@H](C)O[C@@H](C)C2)C1

ZINC62843068 C[C@H]1CN(S(=O)(=O)N2CCC(C)(C(=O)O)CC2)C[C@@H](C)O1

ZINC35023547 O=C(O)CNc1nc2c(C(=O)N3CCN(c4cccc4)CC3)ccn2c1=O

ZINC44265005 NC(=O)/C=C/c1cc(I)cc([N+](=O)[O-])c1O

ZINC07785061 CC1=C(C(=O)O)N=C2CC(C)C(C)CC(NN3CC(=O)NC3=O)=C21

ZINC40148351 COC(=O)[C@@H]1SC2=NC=NC(=O)C2=C1CC(=O)O

ZINC50123311 Ce1ccc(N)c(C)c1OCC(=O)O

ZINC05517016 C/C(=N)NC(=O)c1cccs1)c1cc2c(cc1NC(=O)CCC(=O)O)OCO2

ZINC43623542 Ce1c(N)cccc1O[C@@H](C)C(=O)O

ZINC50421552 C[C@H](NC(=O)N1CCC(C(=O)O)CC1)c1nncn1C

ZINC41049113 Ce1nc(N)sc1S[C@H](C(=O)O)C(C)C

ZINC13462239 COc1c(O)cccc1[C@H]1C=C(c2ccc(O[C@H](C)C(=O)O)cc2)Nc2mnn21

ZINC10159706 O=C(NNC(=O)[C@H]1Cc2cc(Cl)ccc2O1)c1nn(-c2cccc2)cc1O

ZINC65371303 O=C1C[C@H]([C@@H]2C=NN=C2C(=O)O)C2=C(c3ccnc3)N=N[C@@H]2N1

ZINC55156946 COc1ccc(Br)cc1N[C@@H](C)C(=O)Nc1sccc1C(N)=O

ZINC62135414 CN(C(=O)N1CC[C@H](C(=O)O)C1)[C@H]1CCS(=O)(=O)C1

ZINC13446618 CC(C)[C@@H](C(=O)O)n1c(SCC(=O)N[C@@H](c2cccs2)C(C)C)nc2cccc2c1=O

ZINC13050893 [C@@H]1CCCC[C@@H]1NC(=O)NC(=O)CSc1nc2cc(C(=O)O)ccc2c(=O)n1Cc1cccc1

ZINC37321394 O[C@H]1CCC[C@H](N[C@@H]2CCOc3c(Cl)cc(Cl)cc32)C1

ZINC41049309 C[C@H](CSc1ccc(N)cn1)C(=O)O

ZINC05847033 CC(C)[C@H]1NC(=O)N[C@@H](CC(=O)O)C1(C)C

ZINC19088505 CC(C)Cc1cc(C(=O)O)nc(N)n1

ZINC44028970 CC[C@](O)(C(=O)O)C1=CC2=Cc3nc4c(cc3CN2C(O)=C1CO)=C(CN(C)C)C(=O)C=C4

ZINC13044385 CCCCn1c(SCC(=O)NC(=O)N[C@@H]2CCC[C@@H](C)[C@@H]2C)nc2cc(C(=O)O)ccc2c1=O

ZINC64820722 Ce1noc(C)c1CCN(C)c1ccc(C(=O)O)cc1NC(=O)c1ccc(Br)cc1

ZINC67588578 O=C(O)c1[nH]ncc1CN1CCC[C@@H](c2n[nH]cc2-c2cccc2)C1

ZINC62828748 Ce1cc([C@@H](C)NC(=O)Nc2sccc2C(=O)O)c(C)o1

ZINC54501818 Cc1cc(C)n2nc(C(=O)N[C@H](C(=O)O)C3CC3)nc2n1

ZINC51021810 O=C(O)c1cn(CCSc2nnc3[nH]cnc23)nn1

ZINC13257063 COc1ccc([C@H](CC(=O)O)NC(=O)c2ccc(-c3cccc(C(F)F)c3)o2)cc1OC

ZINC01640357 O=C(NCCCC1N[C@@H]1CCC[C@H](C(=O)O)C1

ZINC04721800 Cn1c(SCCC(=O)O)nc2c1c(=O)[nH]c(=O)n2C

ZINC62339609 CCCS(=O)(=O)NCc1c(C(=O)O)[nH]c2cc(C)cc(C)c12

ZINC50223669 O=C(O)c1nnn(CCN2C(=O)CNC2=O)c1C1CC1

ZINC17098013 O=C(O)[C@H]1[C@@H]2CC[C@@H](O2)[C@H]1C(=O)Nc1sc2c(c1C(=O)N1CCCCC1)CCCC2

ZINC06074614 CC(C)(C)NC(=O)[C@@H](c1ccc2ncccc2e1)N(Cc1cccs1)C(=O)c1snc(C(N)=O)c1N

ZINC38187042 O=C1NC(S)=N/C1=C/c1cc2cccc2[nH]1

ZINC42009545 Nc1ccc(S[C@]2(C(=O)O)CCSC2)nc1

ZINC09427748 Cc1ccc2[nH]c(=O)c(C3=NN(C(=O)CCC(=O)O)[C@@H](c4cccs4)C3)c(-c3cccc3)c2c1

ZINC05023605 O=C(NCCCC1N[C@@H]1CCC[C@H](C(=O)O)C1

ZINC13034931 COC[C@H](C)NC(=O)CSc1nc2nc(C)c(CC(=O)O)c(C)n2n1

ZINC44483555 O=C(O)Cc1esc(NC(=O)c2ccc(Br)cc2O)n1

ZINC54295843 O=C(O)C[C@H]1CCCN(C(=O)Cn2ccc(=O)[nH]c2=O)C1

ZINC13345871 O=C(O)c1ccc2c(=O)[nH]c(CSc3nnc4sc5c(c34)CCC5)nc2c1

ZINC51021810 O=C(O)c1cn(CCSc2nnc3[nH]cnc23)nn1

ZINC67223670 Oe1cccc(CN[C@H]2CCOc3ccc(Br)cc32)c1

ZINC42009545 Nc1ccc(S[C@]2(C(=O)O)CCSC2)nc1

ZINC63074746 CC1(C)CCCN1c1ccc(N)cc1C(=O)O

ZINC37593143 Cn1c(=O)c2[nH]c(N(CC(=O)O)C3CC3)nc2n(C)c1=O

ZINC41049309 C[C@H](CSc1ccc(N)en1)C(=O)O

ZINC48235688 O=C1CCc2cc(S(=O)(=O)Nc3cc([N+](=O)[O-])ccc3NCCO)c(F)cc2N1

ZINC41049355 C[C@H](CC(=O)O)Sc1ccc1N

ZINC09882922 C[C@H](Sc1nc2ccc(Cl)cc2[nH]1)C(N)=O

ZINC13462198 O=C(O)c1ccc(-c2ccc([C@@H]3Ne4cccc4C(=O)N3C[C@H]3CCCC3)o2)cc1

ZINC08581704 O=C(Nc1ccc(N2CCC[C@H](O)C2)cc1)c1snc2c(O)nnc12

ZINC13333434 C[C@@H](C(=O)O)n1c(SCC(=O)Nc2c(F)cccc2F)nc2cccc2c1=O

ZINC01484020 COC(=O)[C@@]1(Cc2ccc(O)cc2)OC(=O)C(O)=C1c1ccc(O)cc1

ZINC49235738 O=C(O)c1cc(S(=O)(=O)Nc2nc(C3CC3)es2)c[nH]1

ZINC06075024 CC(C)(C)NC(=O)[C@H](c1ccc2ccc2c1)N(Cc1cccs1)C(=O)c1snc(C(N)=O)c1N

ZINC37846369 O=C(NCCCCO)C1CCN(C(=O)c2cc(Br)c[nH]2)CC1

ZINC36360901 Cc1ccc(N2CCN([C@@H](C(=O)O)c3cn(C)c4ccc(C(=O)O)cc34)CC2)c(C)c1

ZINC00108671 CC(C)(CO)Nc1ccsc1C(=O)O

ZINC19915382 O=c1[nH][nH]c(=O)c2c(NCc3ccc(Br)o3)cccc12

ZINC13192345 O=C(O)CCn1c(SCC(=O)NC(=O)NC2CCCC2)nnc1-c1cccs1

ZINC48916580 CC[C@@H]1CO[C@H](C)CN1C(=O)NC(=O)COCC(=O)O

ZINC40577813 CO[C@H]1C[C@H](C(=O)O)N(C(=O)N2CCOC[C@@H]2)C1

ZINC16901242 Cc1ccc(O)c(N[C@@H]2CC(=O)N(c3ccc(CC(=O)O)cc3)C2=O)c1

ZINC56214098 O=C1CNC(N=C(O)c2cncn2-c2cccc2)=N1

ZINC29010049 O=C(O)CC1(CC(=O)Nc2ccc3c(e2)NC(=O)CO3)CCCC1

ZINC54176766 CC[C@@H](C/C(N)=N/O)NS(=O)(=O)c1ccc1Br

ZINC39690357 C[C@@H]1OC2=NC(CSc3nnc3C)=NC(=O)C2=C1C(=O)O

ZINC13334714 C[C@H](C(=O)O)n1c(SCC(=O)c2c(-c3cccc3)[nH]c3cccc23)nc2cccc2c1=O

ZINC39692709 CC1=C2C(CSc3nnc(Nc4cccc4Cl)s3)=CC(=O)N=C2S[C@H]1C(=O)O

ZINC36360901 Cc1ccc(N2CCN([C@@H](C(=O)O)c3en(C)c4ccc(C(=O)O)cc34)CC2)c(C)c1

ZINC44888489 Cc1cn2c(CC(=O)N[C@H](C)c3nn[nH]3)esc2n1

ZINC39680423 CC1=C(C)[C@@H]2C(=O)N(C)[C@H](SCC3=CC(=O)N=C4S[C@@H](C(=O)O)C(C)=C34)N[C@H]2S1

ZINC13052620 C[C@H](O)Cn1c(Sc2ccc(C#N)cc2F)nc2cc(C(=O)O)ccc2c1=O

ZINC07785061 CC1=C(C(=O)O)N=C2CC(C)(C)CC(NN3CC(=O)NC3=O)=C21

ZINC59119291 O=C(NCc1ccnc(N2CCCC2)c1)NC[C@H](O)c1ccc(F)cc1

ZINC66135692 Cc1nc(N)nc(CCCOe2ccc(Cl)cc2Cl)c1C(N)=O

ZINC13025602 CCc1ccc([C@H](C)NC(=O)CSc2nc3ccc3c(=O)n2[C@@H](C(=O)O)C(C)C)cc1

ZINC37321158 O[C@@H]1CCC[C@@H](NCc2ccc(I)o2)C1

ZINC19862340 COc1cc(-c2[nH]c(=S)[nH]c(=O)c2CCCC(=O)O)cc(OC)c1OC

ZINC09882922 C[C@H](Sc1nc2ccc(Cl)cc2[nH]1)C(N)=O

ZINC13252851 Cc1ccc(C)c(OCC(=O)NNC(=O)[C@H]2CC=CC[C@H]2C(=O)O)c1

ZINC28706707 COc1cc([C@H]2NC(=O)NC(C)=C2C(=O)O)ccc1OCCn1ccc2ccnc21

ZINC40802040 Ne1c(OC2CCCC2)nnc1N1CCC(C(=O)O)CC1

ZINC08791503 Cc1c(CC(=O)NC[C@@H](O)c2cccc2)c(=O)oc2c(O)c(O)ccc12

ZINC49132349 C[C@@H](NC(=O)C(=O)Nc1ccc(F)c(C(N)=O)c1)c1ccc2c(e1)CCCC2

ZINC39605434 CC[C@H](C(=O)N)C[C@@H](C(=O)NCCCCO)C2(CCNCC2)C1c1cccc1

ZINC62828819 CO[C@H]1CCC[C@@H]1NC(=O)Nc1sc(C)c(C)c1C(=O)O

ZINC54336003 C[C@H]1CCC[C@@H](NC(=O)NC[C@@H](C)C(=O)O)C1

ZINC36356879 O=C(O)Cn1cc([C@H](C(=O)O)N2CCN(CC(=O)N3CCCC3)CC2)c2ccc(F)cc21

ZINC31861953 Cc1sc(N)c(C(=O)O)c1-c1ccc2c(e1)N(C)C(=O)[C@@H](C)O2

ZINC12706160 Cc1ccc([C@H](C(=O)NC[C@H]2CCCO2)N(C(=O)c2snc(C(N)=O)c2N)e2cccc(C)c2C)cc1

ZINC02793054 CC1=C(C)C[C@@H](C(=O)O)[C@@H](C(=O)NNC(=O)c2cccs2)C1

ZINC44616484 CC[C@@H](C(=O)O)N(C)C(=O)CN1C(=O)NC(C)(C)C1=O

ZINC63521498 COc1ccc2c(e1)=C1CCN[C@@H](c3ccc(OCC(N)=O)c(OC)c3)[C@H]1N=2

ZINC36360901 Cc1ccc(N2CCN([C@@H](C(=O)O)c3en(C)c4ccc(C(=O)O)cc34)CC2)c(C)c1

ZINC20064387 C=C1C=C(O)N2C(=NC(NC3CCCC3)=N[C@@H]2c2ccenc2)N1

ZINC17878453 NC1=NC(=O)[C@@H]([C@]2(O)C(=O)N(CCCc3ccc3)c3ccc32)S1

ZINC67314503 Ce1ccc(NC(=O)N2CC=C(c3ccc(O)cc3)CC2)cc1C(N)=O

ZINC39465523 CC(C)S(=O)(=O)c1cc2c(cc1Cc1ccc1)[C@@H]1CO[P@](=O)(O)NN1CC2

ZINC05728860 O=C(N/N=C/c1ccc(Br)c1)c1c[nH][nH]c1=O

ZINC05728860 O=C(N/N=C/c1ccc(Br)c1)c1c[nH][nH]c1=O

ZINC13689147 NC1=C(c2nc(-c3ccc3)es2)C(=O)CN1/N=C/c1ccc(O)c1

ZINC37843341 O=S(=O)(CCCCI)/N=c1\ccc2nc(O)c(O)[nH]c-2c1

ZINC04611000 N#C/C(=C\c1ccc(Br)cc1)c1nn(CCO)c(N)c1C#N

ZINC35622399 C/C(=N\c1cc(-e2ccc(F)c2)n[nH]1)c1c(O)[nH]c(=O)sc1=O

ZINC47633170 C[C@H](CNC(=O)NC1CCC(O)CC1)N1CCN(c2ccccc2)CC1

ZINC43751419 CN1N=C(C(=O)Nc2nc(C(F)F)n[nH]2)CCC1=O

ZINC32521236 Cc1c(NC(=O)CS2nnc(=O)[nH]2)c(=O)n(-c2ccccc2)n1C

ZINC13345871 O=C(O)c1ccc2c(=O)[nH]c(CSe3nenc4se5c(e34)CCC5)nc2c1

ZINC40802040 Ne1c(OC2CCCC2)nenc1N1CCC(C(=O)O)CC1

ZINC55156947 COc1ccc(Br)cc1N[C@H](C)C(=O)Nc1ccc1C(N)=O

ZINC13223721 C[C@H](Sc1nc2ccccc2c(=O)n1CCCCC(=O)O)C(=O)NC(=O)NC1CCCCC1

ZINC37419823 Ce1ccnc2nc(C(=O)NC3(C(=O)O)CCCC3)nn12

ZINC47965760 C[C@H](NC(=O)C(=O)Nc1ccc1C(N)=O)c1ccc2c(e1)CCCC2

ZINC32614381 O=C1NC[C@@H](c2ccccc2)[C@@H]1C(=O)N/N=C\c1cc(O)ccc1[N+](=O)[O-]

ZINC22263984 O=C(CN1C(=O)N[C@]2(CCCc3ccc32)C1=O)Nc1nccc1O

ZINC13203328 O=C(O)Cn1c(SCC(=O)NC(=O)NC2CCCC2)nnc1-c1cccs1

ZINC65371303 O=C1C[C@H]([C@@H]2C=NN=C2C(=O)O)C2=C(c3ccnc3)N=N[C@@H]2N1

ZINC00072843 O=C(O)COc1ccc(Br)cc1/C=C1/NC(=O)NC1=O

ZINC15958932 O=C1[C@@H]2[C@H](Cc3ccc(O)c(O)c3)N[C@@]3(C(=O)Nc4ccc43)[C@H]2C(=O)N1Cc1ccc2c(e1)OCO2

ZINC27305831 NC(=O)c1cn(-e2ccc(O)cc2Cl)c2cc(-e3cnc(F)c3)ccc2c1=O

ZINC60407333 Cc1ccc(CN(CCN(C)C)C(=O)C2CCN(C(N)=O)CC2)o1

ZINC33175270 COCCn1c(SC/C(O)=N/c2nen[nH]2)nc2csc2c1=O

ZINC39869881 CN1C(=O)/C(=C2\SC(Nc3ccc3C(N)=O)=NC2=O)c2ccccc21

ZINC58158061 Cc1c(C(=O)O)[nH]c2c1/C(=N/N1CC(=O)NC1=O)CC(C)(C)C2

ZINC59119291 O=C(NCc1cenc(N2CCCC2)c1)NC[C@H](O)c1ccc(F)cc1

ZINC10127193 CC(=O)OCC1=C(C(=O)O)N2C(=O)[C@@H](NC(=O)[C@H](C)Cn3cc(Cl)cn3)[C@H]2S1

ZINC45692702 NC(=O)c1cc(NC(=O)N2CC=C(c3c[nH]c4nccc34)CC2)ccc1F

ZINC23140693 O=C(Nc1nc[nH]n1)[C@@H]1CCCN(C(=O)c2ccoc2)C1

ZINC31158121 COC(=O)[C@]1(Cc2ccc(O)cc2)OC(=O)C(O)=C1c1ccc(O)cc1

ZINC44658189 CC(C)CN1C(=O)N(C)C(O)=C(C(=O)CSe2nc(-c3ccc3)n[nH]2)[C@H]1N

ZINC16429960 N#Cc1c(N)[nH]c(=S)c(C#N)c1-c1cccnc1

ZINC45666617 O=C(Cc1ccc2ccccc2c1)NNC(=O)N[C@@H]1CCCCNC1=O

ZINC39593164 Oc1cccc(/C=N/N2C(S)=NN[C@H]2[C@H]2N=NC3=C2CCC3)c1

ZINC39593169 Oc1cccc(/C=N/N2C(S)=NN[C@H]2[C@@H]2N=NC3=C2CCC3)c1

ZINC62206512 CCc1cccc(C)c1NC(=O)C(=O)NC[C@H](O)c1ccc(Cl)cc1

ZINC40377405 CC[C@](C)(NS(=O)(=O)c1ccc(Br)s1)/C(N)=N/O

ZINC16102314 C/C(=N)NC(=O)c1cc(O)c(O)c(O)c1c1cccc(Br)c1

ZINC54304143 CN(C(=O)N1CCC[C@@H](CC(=O)O)C1)[C@@H]1CCS(=O)(=O)C1

ZINC54124366 NC(=O)[C@@H]1CCCN(c2ccc(CNc3nnc4sccc34)cc2)C1

ZINC17067428 O=C1C/C=C/c2nc(O)c([N+](=O)[O-])c(=O)[nH]2=CO[C@H]2C=CC=C[C@@H]12

ZINC50019827 CCN(c1cc(C(=O)O)c(N)cc1F)C1CC1

ZINC00803597 COc1cc([C@H]2C(C#N)=C(N)Oe3e2c(C)nn3-e2ccc(C)cc2)ccc1OCC(N)=O

ZINC13302017 O=C1COe2ccc(-c3csc(NS(=O)(=O)c4cc(C(=O)O)es4)n3)cc2N1

ZINC40819448 CC(C)C[C@@H](NC(=O)c1ccnc1N)c1nc2ccccc2c(=O)[nH]1

ZINC40079682 COc1ccc(C(=O)C2=C(O)C(=O)N(CCOCCO)[C@H]2c2ccc(O)c2)c(C)c1

ZINC12139893 O=C1N[C@H](c2ccc(O)cc2)[C@@H](C(=O)c2ccccc2)[C@](O)(C(F)(F)F)N1

ZINC10127189 CC(=O)OCC1=C(C(=O)O)N2C(=O)[C@H](NC(=O)[C@@H](C)Cn3cc(Cl)en3)[C@H]2SC1

ZINC33175270 COCCn1c(SC/C(O)=N/e2nc[nH]2)nc2ccsc2e1=O

ZINC15958851 Cc1cccc2c1NC(=O)[C@@]21N[C@@H](CCC(=O)O)[C@H]2C(=O)N(Cc3ccc4c(c3)OCO4)C(=O)[C@H]21

ZINC59248894 CCOc1ccc(NC(=O)/C(C#N)=C/c2cc(C)n(-c3ccc(C(=O)O)c(Cl)c3)c2C)cc1

ZINC42711086 COC(=O)[C@H](C)CN(C)C(=O)N1C[C@H](O)C[C@H]1C(=O)O

ZINC44218213 N[C@@H](CC(=O)O)c1ccc2oc(C(=O)c3ccc(Br)cc3)cc2c1

ZINC58915575 C[C@H](NC(=O)[C@H]1CC(=O)N(e2ccc3c(c2)OCCO3)C1)c1ccc(NC(N)=O)cc1

ZINC42524631 CC[C@@](C)(NS(=O)(=O)c1sccc1Br)/C(N)=N/O

ZINC13572491 COCCCN1C(=O)[C@@H]2[C@@H](Cc3ccc(O)c(O)c3)N[C@@]3(C(=O)Nc4ccccc43)[C@@H]2C1=O

ZINC39678701 CCC(=O)N1C[C@@H](C(=O)NCC(=O)OC(C)C)C2(CCNCC2)C1

ZINC15958932 O=C1[C@@H]2[C@H](Cc3ccc(O)c(O)c3)N[C@@]3(C(=O)Nc4ccccc43)[C@@H]2C(=O)N1Cc1ccc2c(c1)OCO2

ZINC65347481 O=C(O)c1enc(O)c(-e2cc(O)cc(F)c2)c1

ZINC48353955 C[C@@H](CNC(=O)N[C@H](C)c1nnc1C)N1CCc2sccc2C1

ZINC41681672 C[C@H]1CN(C(=O)NC(=O)COCC(=O)O)CC(C)(C)O1

ZINC14331468 NC(=O)Cc1csc(NC(=O)c2cc(Br)ccc2O)n1

ZINC36231435 Nc1ccc(OC[C@@H]2CCCCO2)c(C(=O)O)c1

ZINC13405935 Ce1oc2nc(CSc3nnc(NCC(C)C)s3)[nH]c(=O)e2c1C(=O)O

ZINC13299596 COc1cc(/C=N/Nc2c(Cl)c(Cl)nc(C(=O)O)c2Cl)cc(Cl)c1OCC(N)=O

ZINC13196675 C=CCNC(=O)NC(=O)CSc1nnc(-e2ccc(C)cc2)n1CCC(=O)O

ZINC05809264 COc1cc([C@@H]2C(C(=O)O)=C(CO)Oe3cc4c(cc32)OCO4)cc(OC)c1O

ZINC02389067 O=C(O)C[C@@H](NC(=O)OCC1c2ccccc2-e2ccccc21)c1ccccc1Br

ZINC40735066 CC1(C)C[C@H]2C[C@](C)(CN2c2nnc(NNC(=O)c3ccccc3)e2N)C1

ZINC13123337 Cc1ccc(-n2nc(C)c3c2NC2=C(C(=O)CC(C)(C)C2)[C@@H]3e2ccccc2OCC(=O)O)cc1

ZINC52889957 N#Cc1enc(SCe2csc(-c3ccc(C(N)=O)cc3)n2)nc1N

ZINC13252779 Cc1cc(C)cc(OCC(=O)NNC(=O)[C@H]2CC=CC[C@@H]2C(=O)O)c1

ZINC25490225 O=C1NC(=O)[C@H](Cc2cc([N+](=O)[O-])c(O)cc2[N+](=O)[O-])N1

ZINC28465560 CC(C)([C@@H](C#N)C(N)=O)[C@H](C(N)=O)c1nc(-c2ccc(Cl)cc2)cs1

ZINC58197506 C=CCN(Cc1cc(Br)ccc1F)C(=O)[C@@H](C)NC(N)=O

ZINC48353954 C[C@H](NC(=O)NC[C@@H](C)N1CCc2sccc2C1)c1nnc1C

ZINC02755022 CC(C)c1cc(C(=O)NNC(=O)[C@H]2CC=CC[C@H]2C(=O)O)cs1



ZINC13302017 O=C1COe2ccc(-c3esc(NS(=O)(=O)c4cc(C(=O)O)cs4)n3)cc2N1

ZINC38011379 Cc1n[nH]cc1CNC1CC(c2ccccc2Br)C1

ZINC37593143 Cn1c(=O)c2[nH]c(N(CC(=O)O)C3CC3)nc2n(C)c1=O

ZINC42422737 CCO[C@H]1CCCN(S(=O)(=O)c2[nH]ncc2C(=O)O)C1

ZINC20682496 COCCNC(=O)c1ccc2c(c1)[C@H]1C=CC[C@H]1[C@@H](c1ccc(O)cc1O)N2

ZINC13244937 C[C@@H](C(=O)O)n1c(SCC(=O)N(CCC(N)=O)c2ccccc2Cl)nnc1-c1cccs1

ZINC16577284 CC1(C)S[C@@H]2[C@@H](NC(=O)NC3CCCC3)C(=O)N2[C@@H]1C(=O)O

ZINC12867121 CC(C)C[C@H](NC(=O)OC(C)C)C(=O)N1CCC(C(=O)NCC2CCC(C(=O)O)CC2)CC1

ZINC65371302 O=C1C[C@@H]([C@@H]2C=NN=C2C(=O)O)C2=C(c3ccccc3)N=N[C@@H]2N1

ZINC58915581 C[C@@H](NC(=O)[C@H]1CC(=O)N(c2ccc3c(c2)OCCO3)C1)c1ccc(NC(N)=O)cc1

ZINC37931598 Cc1oc2nc[nH]c(=O)c2c1C(=O)N(C)CCC(=O)O

ZINC05830065 O=C(CCC1CCCC1)NNC(=O)[C@H]1CC=CC[C@@H]1C(=O)O

ZINC44610090 O=C(O)CC[C@@H]1CCCN(c2cncc3nnnn23)C1

ZINC12473237 Cc1ccc(N(C(=O)c2ncc(C(N)=O)c2N)[C@@H](C(=O)NC[C@H]2CCCO2)c2ccc(F)cc2)c(C)c1

ZINC65371302 O=C1C[C@H]([C@@H]2C=NN=C2C(=O)O)C2=C(c3ccccc3)N=N[C@@H]2N1

ZINC65537545 O=C(Cc1nc2ccccc2c(=O)[nH]1)N[C@H]1CCc2nccn2C1

ZINC00814141 CCOc1cc([C@@H]2C(C#N)=C(N)O)c3c2c(C)nn3-c2ccccc2)ccc1OCC(N)=O

ZINC08994119 O=C(O)c1ccc(-n2c(S)nncc2-c2cc(C3CC3)n[nH]2)cc1

ZINC39554914 NC(=O)c1cc(-c2esc(NC(=O)c3ccc(Cl)s3)n2)c[nH]1

ZINC13046872 COc1ccc(CNC(=O)[C@H](C)Sc2nc3cc(C(=O)O)ccc3c(=O)n2CCO)cc1OC

ZINC67402115 CCc1ncc(CN)[C@H](C)C(=O)N2CCC(C(N)=O)CC2)s1

ZINC16022092 COCCN1C(=O)[C@@H]2[C@@H](Cc3ccc(O)c(O)c3)N[C@@]3(C(=O)Nc4ccc(F)cc43)[C@@H]2C1=O

ZINC59403420 Cc1ccccc(-e2n[nH]c(N=C(O)CNC(=O)c3ccccc3)n2)n1

ZINC41670938 Nc1ccc(SCc2occc2C(=O)O)cn1

ZINC65407310 Nc1nc(N2CCOCC2)cc(N2C[C@H](O)[C@@H](N3CCCC3)C2)n1

ZINC39693602 N#CCNC(=O)[C@H]1CN(C(=O)c2ccccc2F)CC12CCNCC2

ZINC40548144 O=C1c2[nH]nc(-c3cc(Cl)ccc3O)c2[C@@H](c2ccc(F)cc2)N1[C@H]1CCS(=O)(=O)C1

ZINC62828474 COC(=O)C(C)C)NC(=O)Nc1sc(C)c(C)c1C(=O)O

ZINC54124366 NC(=O)[C@@H]1CCCN(c2ccc(CNc3nnc4sccc34)cc2)C1

ZINC20567045 COCCCN1C(=O)[C@@H]2[C@@H](Cc3ccc(O)c(O)c3)N[C@@]3(C(=O)Nc4ccc(F)cc43)[C@@H]2C1=O

ZINC17044889 COc1cc([C@@H]2CC(=O)Nc3nc(-c4ccccc4)[nH]c(=O)c32)ccc1OCC(N)=O

ZINC44930858 COC(=O)c1ccc(S(=O)(=O)NCc2nnn[nH]2)c(Br)s1

ZINC30981370 Cc1ccc(SCC(=O)Nc2nc(-c3e[nH]c(C(N)=O)c3)es2)cc1

ZINC67458914 Cc1cc2nc(CNC(=O)c3cc(CN4CCC[C@@H](O)C4)on3)[nH]e2cc1C

ZINC09012191 COc1cc([C@H](c2c(O)n[nH]e2C)c2c(C)n[nH]e2O)ccc1OC(=O)c1ccc(Br)c1

ZINC02263084 CC(C)C[C@@H]1CCc2c(sc3e2-c2nnc(SCC(N)=O)n2-c2nnc(SCC(N)=O)n2-3)C1

ZINC27244164 CCc1ccc(N2C[C@H](C(=O)Nc3cccc(C(N)=O)c3)CC2=O)cc1

ZINC09110631 Cn1c(=O)[nH]c(=O)c2c1nc(N1CCNCC1)n2[C@@H](O)COc1ccc2ccccc2c1

ZINC66250841 Cn1cc(S(=O)(=O)N=c2[nH]c(CN3CCCC3)es2)cc1C(N)=O

ZINC08994119 O=C(O)c1ccc(-n2c(S)nncc2-c2cc(C3CC3)n[nH]2)cc1

ZINC39709594 CCOc1ccc([C@@H](C2=C(C)N=N[C@@H]2O)c2c(C)n[nH]e2O)cc1

ZINC66482149 C[C@H](NC[C@@H](O)CN1C[C@@H](C)O[C@H](C)C1)c1nnc2ccccc12

ZINC65474512 NC(=O)c1ccc(NC(=O)[C@@]23CCC(=O)N2e2cc(Cl)ccc2S3)ccc1F

ZINC62012485 C[C@@H](c1ccccc1N)(C)[C@@H](c1ccccc1)[C@@H](C)N

ZINC12941110 O=C(O)Cc1csc(NC(=O)C2CCN(c3ccc(C(F)F)en3)CC2)n1

ZINC17092753 Cc1c(C(N)=O)sc(NC(=O)CN(C)C)c2cnn(C)c2C)c1C(=O)OC(C)C

ZINC17575813 O=C(NNC(=O)c1c[nH]c(=S)n1-c1ccc1)1ccc1O

ZINC44345938 CC(C)CN1C[C@@H](C(=O)N[C@H](C)c2nn[nH]2)CC1=O

ZINC43425967 O=C(O)c1cn(CCN2CCO[C@@H]3CCC[C@@H]32)nn1

ZINC44218023 N[C@@H](CC(=O)O)c1c(-c2ccc2Cl)nn(-c2ccc2)c1Cl

ZINC18068440 C/C(O)=C1\C(=O)c2ccc2\C1=N\N

ZINC40112620 Nc1ncnc1C(=O)N[C@H](c1ccc1)N1CCc2secc2C1

ZINC36356879 O=C(O)Cn1cc([C@H](C(=O)O)N2CCN(CC(=O)N3CCCC3)CC2)c2ccc(F)cc21

ZINC63822788 CC1=C2[C@@H](c3ccc(F)c3F)CC(=O)N[C@@H]2N(c2ccc(O)nn2)N1

ZINC45375934 O=C(NCc1ccc(N2CCOCC2)nc1)N[C@@H]1CCCCN1=O

ZINC43223297 O=C(NCc1ccc1C(F)F)[C@H]1CNC[C@@H]1C(=O)NC[C@H]1CCCO1

ZINC46814957 N#Cc1c(F)ccc1N1CCN(C(=O)c2ccc3c(O)[nH]c(=S)nc3e2)CC1

ZINC58431849 COc1ccc1NC(=O)c1ccc2c(O)[nH]c(=S)nc2c1

ZINC62832103 CC[C@H](C#N)N(C)c1ccc(N)cc1C(=O)O

ZINC13564105 Cc1nc(O)c2nsc(C(=O)Nc3ccc(N4CCC[C@@H](O)C4)cc3)e2n1

ZINC66930695 NC(=O)c1ccc(OCC(=O)NC[C@]2(O)CCCc3ccc32)c1

ZINC16688278 CCOc1cc(/C=C2/NC(=S)NC2=O)cc([N+](=O)[O-])c1O

ZINC09334391 O=C(NC1CC1)c1c(O)c2c([nH]c1=O)CCCC2

ZINC55476972 Cn1c(C(=O)NNC(=O)c2nn(-c3ccc3)cc2O)cc2ccc21

ZINC42956539 Cn1nc(O)c2c(C(=O)NNc3ccc(C1)c3)cc(C3CC3)nc21

ZINC20228158 COc1cc([N+](=O)[O-])cc(/C=N/NC(=O)Cn2cnn2)c1O

ZINC41033318 Cn1nc([N+](=O)[O-])c1NC1(C(=O)O)CCCCC1

ZINC08581704 O=C(Nc1ccc(N2CC[C@H](O)C2)cc1)c1snc2c(O)ncnc12

ZINC04861208 Cc1nc(SCC(N)=O)[nH]c(=O)c1C

ZINC63823888 CC1=C2[C@@H](c3c(F)ccc3F)CC(=O)N[C@@H]2N(c2ccc(O)nn2)N1

ZINC23143211 O=C1C[C@H](/C(O)=N/c2n[nH]2)CN1c1ccc2c(c1)OCCO2

ZINC16282732 Cc1cc(O)ccc1N[C@H]([C@@H](Nc1ccc(O)cc1C)n1nnc2ccc21)n1nnc2ccc21

ZINC03847021 C[C@H](CO)c1c(O)c(O)c2c(c1O)C(=O)C(=O)[C@H]1C(C)(C)CCC[C@]21C

ZINC39605432 CC[C@H](C(=O)N1C[C@H](C(=O)NCCCO)C2(CCNCC2)C1)c1ccc1

ZINC01425496 CN1C(=O)N[C@H](c2ccc(O)cc2)C2=C1CN(c1ccc(N3CC4=C(C3=O)[C@@H](c3ccc(O)cc3)NC(=O)N4C)cc1)C

ZINC54681330 N[C@@H](Cc1cc(Br)c2c(c1)OCO2)c1ccc1

ZINC66080059 Cc1nc2nc(=S)nc(CN3CCC[C@@H](CCC(N)=O)C3)n2c(C)c1C

ZINC15899888 O=C(NNC(=S)NC[C@H]1CCCO1)c1ccc(Br)s1

ZINC26258525 CSc1nc2nc(C)c(C/C(O)=N/c3n[nH]3)c(C)n2n1

ZINC01425499 CN1C(=O)N[C@@H](c2ccc(O)cc2)C2=C1CN(c1ccc(N3CC4=C(C3=O)[C@H](c3ccc(O)cc3)NC(=O)N4C)cc1)C

ZINC13123816 CC1(C)CC(=O)C(Sc2nnc(-c3ccc(O)cc3)n2C[C@@H]2CCCO2)=C(O)C1

ZINC19300404 CN(C)[C@@H]1c2ccc2C2(CCN(C(=O)C3=NCC(=O)CC3)CC2)[C@H]1O

ZINC08328762 C[C@]1(c2cc3ccc3o2)NC(=O)N(CC(=O)Nc2secc2C(N)=O)C1=O

ZINC58385468 CC(=O)N/C=C\c1ccc1)C(=O)N[C@H](C)c1ccc2[nH]c(=O)[nH]e2c1

ZINC47969262 CC(C)[C@@H](NC(=O)C(=O)Nc1ccc1C(N)=O)c1ccc(Cl)cc1

ZINC20682501 COCCNC(=O)c1ccc2c(c1)[C@H]1C=CC[C@@H]1[C@@H](c1ccc(O)cc1O)N2

ZINC44713564 COc1ccc2nc(CCN(C(=O)[C@@H]3CN(C(=O)c4cc(C)n(C)n4)CC34CCNCC4)[nH]e2c1

ZINC65692295 Nc1nc2nc(CSc3c(F)cc(F)cc3F)cc(O)n2n1

ZINC27643925 O[C@@H]1C[C@@H]2[C@@H](C[C@@H](O)[C@@H]2/C=C/[C@@H](O)COe2cccc(C(F)(F)F)e2)O1

ZINC02793057 CC1=C(C)C[C@@H](C(=O)NNC(=O)c2cccs2)[C@@H](C(=O)O)C1

ZINC04163015 COc1cc([C@H]2NC(=O)NC(C)=C2C(=O)OCCSC)cc([N+](=O)[O-])c1O

ZINC41069992 Ce1cccc(C)c1NS(=O)(=O)c1cc(Br)ene1NN

ZINC66952604 CN(C)C(=O)Cc1cccc1NC(=O)NC[C@@]1(O)CCc2cccc21

ZINC45375936 O=C(NCc1ccc(N2CCOCC2)nc1)N[C@H]1CCCCNC1=O

ZINC60368200 O=C(CNC(=O)c1cc2c(s1)CCCC2)Nc1ncccc1O

ZINC67044320 Ce1cccc(C(=O)NNC(=O)NCCc2en3c(n2)CCCC3)c1

ZINC47110816 C[C@@H]1CCCN(CCCNC(=O)c2ccc3c(O)[nH]c(=S)nc3c2)C1

ZINC39232679 COc1ccc2c(CCN(=O)[C@H](C)S[C@@H]3NC(C1)=NC4=NC=N[C@@H]43)c[nH]e2c1

ZINC41919221 O=C1COCC(=O)N1[C@]1(C(=O)O)CCOe2cccc21

ZINC63823011 CC1=C2[C@@H](NC(=O)C[C@@H]2e2cccc2)N(c2ccc(O)nn2)N1

ZINC36998628 CC[C@H](Ne1enn(CC(N)=O)c1)c1cc(Br)ccc1O

ZINC06058013 O=C(N/N=C/c1cccc(O)c1)c1c(O)n2c3c(cccc3c1=O)CCC2

ZINC36356879 O=C(O)Cn1cc([C@H](C(=O)O)N2CCN(CC(=O)N3CCCC3)CC2)c2ccc(F)cc21

ZINC39345493 Ce1c(NC(=O)c2n[nH]2)cccc1[C@@H]1Ne2cc(Cl)ccc2O1

ZINC63521500 COc1ccc2c(c1)=C1CCN[C@@H](c3ccc(OCC(N)=O)c(OC)c3)[C@@H]1N=2

ZINC39733845 C[C@H](S[C@@H]1NN=C(SCC(N)=O)S1)C(=O)C1=c2cccc2=N[C@@H]1C

ZINC65347480 O=C(O)c1cc(O)nc1-c1cc(O)cc(F)c1

ZINC44928654 O=C(CS[C@@H]1CCS(=O)(=O)C1)NCc1nn[nH]1

ZINC13259179 O=C(O)C[C@@H](NC(=O)C1CCN(C(=O)c2cccc3cccc23)CC1)e1cccc1C1

ZINC16033039 COc1ccc(CN2C(=O)[C@@H]3[C@H](CCC(N)=O)N[C@]4(C(=O)Nc5c(C)cccc54)[C@@H]3C2=O)cc1

ZINC66621391 Ce1c(C(=O)Nc2nn[nH]2)nnn1-c1cccc2enccc12

ZINC45216077 C[C@](N)(C#N)CCSc1nccc(=O)[nH]1

ZINC40802040 Ne1c(OC2CCCC2)nene1N1CCC(C(=O)O)CC1

ZINC40055067 O=C(C1=C(O)C(=O)N(CCCO)[C@H]1e1encc1)c1cccc(OCe2ccc(F)cc2)c1

ZINC03946853 COc1cc(/C=N/Nc2[nH]c(=O)nn2C)cc([N+](=O)[O-])c1O

ZINC63789192 CN1CNN=C1Sc1ccc(C(=O)NNC(=O)CC2=c3cccc3=NC2)cc1

ZINC19862340 COc1cc(-c2[nH]c(=S)[nH]c(=O)c2CCCC(=O)O)cc(OC)c1OC

ZINC49235738 O=C(O)c1cc(S(=O)(=O)Nc2nc(C3CC3)cs2)c[nH]1

ZINC66234044 Cn1cene1CCNC(=O)NCc1cc(F)cc2c1OCOC2

ZINC67065747 C[C@H](NC(=O)NNC(=O)CC1CCCC1)c1ccc2c(c1)CC(=O)N2

ZINC16033039 COc1ccc(CN2C(=O)[C@@H]3[C@H](CCC(N)=O)N[C@]4(C(=O)Nc5c(C)cccc54)[C@@H]3C2=O)cc1

ZINC44923455 Ce1nn(C)c(=O)c(C(=O)N[C@@H](C)c2nn[nH]2)c1C

ZINC16102314 C/C(=N)NC(=O)c1cc(O)c(O)c(O)c1c1cccc(Br)c1

ZINC20721099 COc1ccc(N2C[C@@H](C(=O)Nc3nc[nH]n3)CC2=O)c(OC)c1

ZINC06431618 C[C@H](OC(=O)C=C/c1cc(Br)ccc1F)C(=O)NC(N)=O

ZINC37843341 O=S(=O)(CCCC1)/N=c1\ccc2nc(O)c(O)[nH]c-2c1

ZINC63521504 COc1ccc2c(c1)=C1CCN[C@@H](c3ccc(OCC(N)=O)c(OC)c3)[C@@H]1N=2

ZINC40085178 COc1ccc(C(=O)C2=C(O)C(=O)N(CCOCCO)[C@H]2e2cccc3cccc23)cc1C

ZINC40358147 CC(C)CC(=O)C1=C(O)C(=O)N(CC(C)C)[C@@H]1c1ccc(O)cc1O

ZINC40053293 COc1ccc2cc(C(=O)C3=C(O)C(=O)N(CCCO)[C@H]3c3cccc(O)c3)oc12

ZINC37931598 Ce1oc2nc[nH]c(=O)c2c1C(=O)N(C)CCC(=O)O

ZINC38187042 O=C1NC(S)=N/C1=C/c1cc2cccc2[nH]1

ZINC39448679 N#Cc1enc(Cl)nc1NC(=N/O)/C(=N/O)c1cccc1

ZINC64885779 Cc1cccc(C2(C(=O)NNC(=O)NCCCN3ccnc3)CC2)c1

ZINC06403499 COc1cc([C@H]2C(C(=O)O)=C(CO)Oc3cc4c(cc32)OCO4)cc(OC)c1O

ZINC66482149 C[C@H](NC[C@@H](O)CN1C[C@H](C)O[C@H](C)C1)c1nnc2cccc12

ZINC44345274 C[C@H](NC(=O)c1nc2scn2c1=O)c1nn[nH]1

ZINC40053293 COc1cccc2cc(C(=O)C3=C(O)C(=O)N(CCCO)[C@H]3c3cccc(O)c3)oc12

ZINC13450878 COc1ccc(NC(=O)[C@H](C)Se2nc(C)c(CCC(=O)O)c(=O)[nH]2)cc1OC

ZINC04861208 Cc1nc(SCC(N)=O)[nH]c(=O)c1C

ZINC38556246 CC1=C[C@H]([C@H]2NN[C@H](SCC(=O)c3cccc3Cl)N2N)N=N1

ZINC50672095 Cc1ccc([C@@H](C)NS(=O)(=O)c2cc(Br)nc2N)o1

ZINC27244157 CCc1ccc(N2C[C@@H](C(=O)Nc3ccc(C(N)=O)c3C)CC2=O)cc1

ZINC03101251 O=C(N/N=C/c1cc([N+](=O)[O-])ccc1O)C(=O)Nc1ccc(F)cc1

ZINC12377926 O=C1N[C@H](c2ccc(O)cc2)[C@@H](C(=O)c2cccs2)[C@](O)(C(F)(F)F)N1

ZINC37994608 CC(C)N(CC(=O)O)c1cc2c(cc1[N+](=O)[O-])CC(=O)N2

ZINC05000164 O=C(Nc1cccc(F)c1F)[C@@H]1C[C@H](O)CN1C(=O)Nc1cccc1

ZINC50649174 Cc1cc(F)ccc1NS(=O)(=O)c1c(N)nc2scn12

ZINC09410142 COc1cc([C@H]2CC(=O)Nc3nc(-c4cccc4)[nH]c(=O)c32)ccc1OCC(N)=O

ZINC13123816 CC1(C)CC(=O)C(Se2nnc(-c3ccc(O)cc3)n2C[C@H]2CCCO2)=C(O)C1

ZINC40096581 O=C(C1=C(O)C(=O)N(CCO)[C@@H]1c1cccc(Cl)c1)c1ccc2c(c1)OCCO2

ZINC67402115 Cc1ncc(CN(C)[C@H](C)C(=O)N2CCC(C(N)=O)CC2)s1

ZINC67588578 O=C(O)c1[nH]ncc1CN1CCC[C@@H](c2n[nH]cc2-c2cccc2)C1

ZINC65508179 NC(=O)c1enc2n1CCN(C(=O)[C@H]1CCCC3=c4cccc4=N[C@H]31)C2

ZINC65419302 Cc1cenc(NCCNC(=O)[C@H]2CCCN(C(=O)N(C)C)C2)c1

ZINC48732625 O=C(c1n[nH]c(O)n1)N1CCN(c2nccs2)CC1

ZINC54124365 NC(=O)[C@H]1CCCN(c2ccc(CNc3nenc4sccc34)cc2)C1

ZINC05316121 O=[N+](O-)]c1ccc2nc(C(=N/O)[C@@H](O)c3cccc3)c(O)nc2c1

ZINC64185694 O=C(N[C@H](CC1=c2cccc2=NC1)C(=O)NC[C@H]1NN=C2CCCN21)c1cccs1

ZINC53819720 COc1ccc(NC(=O)c2ccc3c(O)[nH]c(=S)nc3c2)cc1F

ZINC63823004 CCC(C)(C)C1CCC(NC(=O)C(=O)Nc2cc(C(N)=O)ccc2C)CC1

ZINC05885477 O=c1c2cc(Br)ccc2nc(-c2cccc2Cl)n1NC[C@]1(O)OC[C@@H](O)[C@@H](O)[C@H]1O

ZINC13450878 COc1ccc(NC(=O)[C@H](C)Se2nc(C)c(CCC(=O)O)c(=O)[nH]2)cc1OC

ZINC38612381 CC1=C([C@H](c2cccc(Br)c2)c2c(C)n[nH]e2O)[C@@H](O)N=N1

ZINC36239754 C[C@@H](C(=O)O)N1C(=O)CSC=C1c1ccc([N+](=O)[O-])c1

ZINC63810477 O=C(Nc1cccc(-n2ccn2)c1)c1ccc2c(O)[nH]c(=S)nc2c1

ZINC44887028 C[C@H](NC(=O)c1ccc(Cn2cccn2)o1)c1nnn[nH]1

ZINC66812791 Ne1encc(NC[C@@H](O)COc2ccc(I)cc2)n1

ZINC41553135 Cc1c(NC(=O)C(=O)N[C@@H]2CCCC[C@H]2C(C)(C)C)cccc1C(N)=O

ZINC63818704 COc1ccc2c(c1)=C(CCNC(=O)C(=O)Nc1ccc(O)cc1)CN=2

ZINC40053253 COc1cccc2cc(C(=O)C3=C(O)C(=O)N(CCCO)[C@H]3c3ccc(C(C)(C)C)cc3)oc12

ZINC44931949 Cn1enc(S(=O)(=O)Nc2nnn[nH]2)c1Cl

ZINC08615652 Cc1cc(C)c2c(=S)nc(N)nc-2[nH]1

ZINC67223670 Oe1cccc(CN[C@H]2CCOe3ccc(Br)cc32)c1

ZINC04183833 O=C1N[C@H](c2ccc(O)cc2)[C@@H](C(=O)c2cccc2)[C@](O)(C(F)(F)F)N1

ZINC43732368 NC(=O)COc1ccc(C2=C(C(=O)c3ccc3)[C@@]3(ON2)C(=O)Nc2cccc23)cc1

ZINC47886765 NC(=O)C1CCN(C(=O)e2cccc2NC(=O)/C=C/e2cccs2)CC1

ZINC32610336 O=C(O)[C@H]1CC=CC[C@H]1C(=O)Nc1cc(-c2cccc2)n[nH]1

ZINC16156646 COC(=O)c1cc(Br)ccc1-c1cccc(/C=N\N=C(/N)e2nonc2N)o1

ZINC17878453 NC1=NC(=O)[C@@H]([C@]2(O)C(=O)N(CCCc3cccc3)e3cccc32)S1

ZINC23143208 O=C1C[C@@H](/C(O)=N/e2nen[nH]2)CN1c1ccc2c(c1)OCCO2

ZINC39681925 O=C(NCCF)[C@H]1CN(C(=O)C2CCOCC2)CC12CCNCC2

ZINC60626442 O=C(Nc1cccc(N2CCOC2=O)e1)c1ccc2c(O)[nH]c(=S)nc2c1

ZINC65372530 Cc1ccc(C)c2c1=N[C@H](C)C=2CC(=O)N[C@@H]1C[C@H]2C(=O)NCC(=O)N2C1

ZINC43238061 Cn1cc([C@@H](CN)Se2ccc(Br)cc2)en1

ZINC39715405 O=C(Nc1ccc2c(c1)N[C@H](c1cccc3cccc13)O2)c1nen[nH]1

ZINC41670938 Ne1ccc(SCe2occc2C(=O)O)en1

ZINC40109332 O=C(C1=C(O)C(=O)N(CCO)[C@@H]1c1ccc(Cl)cc1)c1cccc(OCc2ccc(F)cc2)c1

ZINC37448213 COc1ccc([C@H]2[C@@H](C(N)=O)C(=O)N[C@@](O)(c3cccc3)[C@@H]2C#N)cc1[N+](=O)[O-]

ZINC00943112 C[C@H](Nc1n[nH]e(=O)[nH]c1=O)C(=O)N/N=C/e1cccc1I

ZINC44278219 Cc1c(Br)c(O)c(/C=C/C(N)=O)c(C)c1[N+](=O)[O-]

ZINC44930540 C[C@H](NS(=O)(=O)N1C[C@@H](C)O[C@H](C)C1)c1nnn[nH]1

ZINC03039109 CCOc1ccc(NC(=O)Nc2cc(C(=O)O)ccc2N2C[C@@H]3C[C@H](C2)Cn2c3cccc2=O)cc1

ZINC13416288 Cc1se2nenc(SCc3nc4sc(C(=O)O)c(C)c4c(=O)[nH]3)c2c1C

ZINC60368200 O=C(CNC(=O)c1cc2c(s1)CCCC2)Nc1cccc1O

ZINC32116836 O=C1NC(=S)N=C(O)/C1=C/e1ccc(Se2ccc(Cl)cc2)c([N+](=O)[O-])c1

ZINC16688278 CCOc1cc(/C=C2/NC(=S)NC2=O)cc([N+](=O)[O-])c1O

ZINC67458914 Cc1cc2nc(CNC(=O)c3cc(CN4CCC[C@@H](O)C4)on3)[nH]c2cc1C

ZINC39551757 Cc1nc(NC2cccc(-n3enen3)e2)cc([C@H]2CCCN2)n1

ZINC62084382 C[C@H](CNS(=O)(=O)c1cc(Br)enc1N)CN1CCCC1

ZINC43259797 COC1CCN([C@H](c2ccc(Br)s2)[C@@H](C)N)CC1

ZINC39593164 Oe1cccc(/C=N/N2C(S)=NN[C@H]2[C@H]2N=NC3=C2CCC3)c1

ZINC39593169 Oe1cccc(/C=N/N2C(S)=NN[C@H]2[C@H]2N=NC3=C2CCC3)c1

ZINC20756365 COc1ccc(CN2C(=O)[C@@H]3[C@@H](CCC(N)=O)N[C@@]4(C(=O)Nc5c(C)cccc54)[C@@H]3C2=O)cc1

ZINC39396295 O=C(N[C@H]1NC(SCe2ccc(F)cc2)=NS1)c1nen[nH]1

ZINC32918666 Cn1c(=O)c(-c2noc(O)n2)nn(-c2cccc2)c1=O

ZINC16282739 Cc1cc(O)ccc1N[C@H]([C@H](Nc1ccc(O)cc1C)n1nne2cccc21)n1nne2cccc21

ZINC49556841 O=C(O)c1cc(S(=O)(=O)Nc2nc3c(s2)CCCC3)c[nH]1

ZINC60626442 O=C(Nc1cccc(N2CCOC2=O)e1)c1ccc2c(O)[nH]c(=S)nc2c1

ZINC05208363 COc1ccc2c1C(=O)c1c(O)c3c(c(O)c1C2=O)C[C@@](O)(/C(C)=N\NC(=O)c1cccc1)C[C@H]3O

ZINC40053405 Cc1nc(C)c(C(=O)C2=C(O)C(=O)N(CCCO)[C@H]2c2cccc(Oc3cccc3)c2)s1

ZINC40554938 C[C@H](C(=O)NC(C)C)N1CCC(C(=O)Nc2enen2)CC1

ZINC36356879 O=C(O)Cn1cc([C@H](C(=O)O)N2CCN(CC(=O)N3CCCC3)CC2)c2ccc(F)cc21

ZINC40109575 O=C(C1=C(O)C(=O)N(CCO)[C@H]1c1cccc1)c1ccc(OCc2cccc2Cl)cc1

ZINC40781477 COC[C@@H](C)Nc1nenc(Nc2cccc2Br)c1N

ZINC41992163 Nn1cnne1S[C@@](C(=O)O)(c1ccc(Cl)cc1)C1CC1

ZINC16911119 CC[C@H](Oe1cccc1/C=C1/SC(=O)N(e2ccc(O)cc2C)C1=O)C(=O)O

ZINC04557120 CCCC(=O)Nc1nnc2c1nen2[C@@H]1C[C@@H]2O[P@@](=O)(O)OC[C@H]2O1

ZINC33573060 O=C1CNC(c2cccc2)=C2C=C(Br)C=C[C@H]2N1

ZINC17067422 O=C1C(/C=C/e2nc(O)c([N+](=O)[O-])c(=O)[nH]2)=CO[C@@H]2C=CC=C[C@H]12

ZINC39960835 COc1cccc1[C@@H](C1=C(C)N=N[C@@H]1O)c1c(C)n[nH]e1O

ZINC13196780 CCNC(=O)NC(=O)[C@H](C)Sc1nnc(-c2ccc(C)cc2)n1CCC(=O)O

ZINC61622259 Ce1ccc(-e2n[nH]c(NC(=O)c3ccc(NC4CC4)nc3)n2)s1

ZINC41062484 Cc1n[nH]c(Se2ccc(C#N)cc2N)n1

ZINC13394483 O=C(O)[C@H]1CCCN(C(=O)CSe2nmmn2-c2ccc(O)cc2)C1

ZINC22263984 O=C(CN1C(=O)N[C@]2(CCc3ccc32)C1=O)Nc1ncccc1O

ZINC44785706 N/C(=N/O)C1(C(=O)NCe2cccc(Br)c2)CCOCC1

ZINC38011379 Cc1n[nH]cc1CNC1CC(c2ccc2Br)C1

ZINC36231435 Nc1ccc(OC[C@@H]2CCCCO2)c(C(=O)O)c1

ZINC66833439 CCN(C(=O)[C@H]1CC(=O)N(C2CCC(C)CC2)C1)[C@H]1CC(O)=NC1=O

ZINC12379556 CC(=O)Nc1c(O)nc(SCC(=O)Nc2ccc(Br)cn2)[nH]e1=O

ZINC17067424 O=C1C(/C=C/c2nc(O)c([N+](=O)[O-])c(=O)[nH]2)=CO[C@H]2C=CC=C[C@H]12

ZINC44165545 O=C(NC[C@H]1CCCO1)[C@@H]1CSC[C@H](c2ccc3c(c2)OCCO3)n1

ZINC31823605 C=CCNC(=O)NC(=O)[C@H](C)Se1nc(N)c2c(C)c(C)sc2n1

ZINC23143211 O=C1C[C@H](/C(O)=N/c2n[nH]2)CN1c1ccc2c(c1)OCCO2

ZINC65581407 NC(=O)Cc1ccc(OCC(=O)N[C@@H]2CCSc3c(F)cccc32)cc1

ZINC13564105 Cc1nc(O)c2nsc(C(=O)Nc3ccc(N4CCC[C@@H](O)C4)cc3)c2n1

ZINC48967763 O=C(O)c1ccc(Br)cc1NC(=O)N1CCC[C@H](O)C1

ZINC13270706 Cc1cccc(-c2nnc(S[C@@H](C)C(=O)NC(=O)NC3CC3)n2CCC(=O)O)c1

ZINC11869123 Cc1ccc(CNc2nc(CN(CCO)[C@H]3CS(=O)(=O)C[C@@H]3O)nc3ccc23)cc1

ZINC58296359 Cc1cc2n(n1)C[C@H](CNCCS(=O)(=O)c1cccc1)CN2

ZINC55196670 Cc1cccc2c1[C@H](NC(=O)C(C)(C)NC(=O)c1cccs1)C(=O)N2

ZINC12749044 O=C(C[C@H]1C(=O)NCCN1Cc1ccc(C(F)(F)F)e1)NCCN1CCNC1=O

ZINC09130177 O=C1N[C@@H](c2ccc(O)c2)[C@@H](C(=O)c2ccc(Cl)cc2)[C@](O)(C(F)(F)F)N1

ZINC63822928 CC1=C2[C@@H](c3cccs3)CC(=O)N[C@@H]2N(c2ccc(O)nn2)N1

ZINC17092753 Cc1c(C(N)=O)sc(NC(=O)CN(C)C)c2c1c(=O)OC(C)C

ZINC07251982 NC(=O)NC(=O)CSc1nc(-c2ccc2Br)n[nH]1

ZINC15958932 O=C1[C@@H]2[C@H](Cc3ccc(O)c(O)c3)N[C@@]3(C(=O)Nc4cccc43)[C@@H]2C(=O)N1Cc1ccc2c(c1)OCO2

ZINC08791503 Cc1c(CC(=O)NC[C@@H](O)c2ccc2)c(=O)oc2c(O)c(O)ccc12

ZINC60494468 COCCNC(=O)C1CCN([C@H](C)C(=O)NC(=O)NC2CCCC2)CC1

ZINC44713839 CCC(CC)C(=O)N1C[C@@H](C(=O)N[C@H](C)c2c(C)n[nH]e2C)C2(CNCC2)C1

ZINC40077275 COc1ccc(C(=O)C2=C(O)C(=O)N(CCOCCO)[C@H]2c2ccc(Cl)cc2Cl)cc1

ZINC13206378 Cc1cccc(-c2nnc(SCC(=O)N[C@H](C)c3ccc4c(c3)CCCC4)n2CC(=O)O)c1

ZINC01434644 O=C(NN1C(=O)c2ccc2N[C@H]1c1ccc(O)c1)c1ccc1

ZINC66833439 CCN(C(=O)[C@H]1CC(=O)N(C2CCC(C)CC2)C1)[C@H]1CC(O)=NC1=O

ZINC16282735 Cc1cc(O)ccc1N[C@@H]([C@H](Nc1ccc(O)cc1C)n1nnc2ccc21)n1nnc2ccc21

ZINC02480157 COc1ccc2ccc(OC)c([C@@H]3NC(=S)NC(C)=C3C(N)=O)c2c1

ZINC18211452 NC1=C(O)C(=O)[C@H](c2ccc2)O1

ZINC16611283 CC[C@@H](C)n1c(O)c([C@@H]2NCCc3c2[nH]e2ccc32)c(=O)[nH]c1=O

ZINC16102314 C/C(=N)NC(=O)c1cc(O)c(O)c(O)c1c1ccc(Br)c1

ZINC34138251 COc1cc([N+](=O)[O-])cc(/C=C\c(=O)NC(=O)N(C)C2=O)c1O

ZINC34863228 COCCN(Cc1nc2ccc2c(=O)[nH]1)C(=O)c1enn(-c2ccc(O)nn2)c1C

ZINC02339711 CCOc1ccc([C@@H]2C3=C(CC(C)C)CC3=O)Nc3[nH]c(N)nc(=O)c32cc1

ZINC31875846 COc1cc(/C=N)NC(=O)[C@@H]2COc3ccc3O2)c(Br)c(Br)c1O

ZINC35678695 CC(=O)OCC1=C(C(=O)O)N2C(=O)[C@H](NC(=O)[C@H](C)n3nce(Cl)e3C)[C@H]2SC1

ZINC09431503 CC(=O)OCC1=C(C(=O)O)N2C(=O)[C@H](NC(=O)[C@@H](C)n3cc(Cl)c(C)n3)[C@H]2SC1

ZINC44714238 CC[C@H](C)CC(=O)N1C[C@H](C(=O)N[C@@H](C)e2c(C)n[nH]e2C)C2(CCNCC2)C1

ZINC40096977 O=C(C1=C(O)C(=O)N(CCOCCO)[C@@H]1c1ccc(O)cc1)c1ccc2ccccc2o1

ZINC04861208 Cc1nc(SCC(N)=O)[nH]c(=O)c1C

ZINC06787870 CCCn1c(N)c(C(=O)CN(C)Ce2cccc(F)e2)c(=O)[nH]c1=O

ZINC13564105 Cc1nc(O)c2nsc(C(=O)Nc3ccc(N4CCC[C@@H](O)C4)cc3)c2n1

ZINC39869854 Cc1ccc(/C=C2/SC(Nc3cccc3C(N)=O)=NC2=O)o1

ZINC04786974 Nn1c(SCC(=O)NC2CC2)mnc1-c1cccc1Br

ZINC15082922 Cc1cc(=O)[nH]c(SCC(=O)Nc2[nH]c(C)c(C)c2C#N)n1

ZINC12901265 Ce1c(CC(=O)N[C@H](CO)c2cccc2)c(=O)oc2c(O)c(O)ccc12

ZINC41539105 Cc1nn(C)c(C)c1c(C=O)C1=C(O)C(=O)N(C)[C@@H]1c1ccccc1

ZINC18211452 NC1=C(O)C(=O)[C@H](e2cccc2)O1

ZINC62207833 CCC(CC)(CNC(=O)C(=O)Nc1ccc2c(c1)CCC(=O)N2)N(C)C

ZINC39624190 CCCCNC(=O)[C@H]1CN(C(=O)C2CCOCC2)CC12CCNCC2

ZINC50649174 Cc1cc(F)ccc1NS(=O)(=O)c1c(N)nc2scn12

ZINC44755163 Cc1nc(-c2c[nH]c(C(=O)Nc3ccc4oc(O)nc4c3)c2)es1

ZINC63822017 CC1=C2[C@@H](NC(=O)C[C@H]2e2cccc2Cl)N(c2ccc(O)nn2)N1

ZINC63823893 CC1=C2[C@@H](NC(=O)C[C@H]2c2c(F)cccc2F)N(c2ccc(O)nn2)N1

ZINC40054987 Cc1ccc([C@H]2C(C(=O)c3cccc(OCc4ccc(F)cc4)c3)=C(O)C(=O)N2CCCO)cc1

ZINC43238068 C[C@@H](N)[C@H](Sc1ccc(Br)cc1)c1enn(C)c1

ZINC20475209 C[C@H]1CN([C@H](CN)c2cc(Br)es2)C[C@@H](C)O1

ZINC20431210 CN1C(=O)Ce2ccc([C@@H](N)Cc3ccc(Br)cc3)ccc21

ZINC20567045 COCCCN1C(=O)[C@@H]2[C@H](Cc3ccc(O)c(O)c3)N[C@@]3(C(=O)Nc4ccc(F)cc43)[C@@H]2C1=O

ZINC63831541 CC1=C2[C@@H](c3ccc4c(c3)OCCO4)CC(=O)N[C@@H]2N(c2ccc(O)nn2)N1

ZINC40052968 O=C(C1=C(O)C(=O)N(CCO)[C@@H]1c1cccc1F)c1ccc2c(c1)OCCO2

ZINC38702170 Cc1cc(C)c(O)c(-c2n[nH]e3e2[C@@H](c2ccc(OCC(N)=O)cc2)N([C@@H]2CCS(=O)(=O)C2)C3=O)c1

ZINC01472215 CCCc1nn(-c2cccc2)e2c1[C@H](c1ccc(O)c(O)c1)C(C#N)=C(N)O2

ZINC39658826 O=C(NC[C@H]1CCCO1)[C@H]1CN(C(=O)[C@@H]2CC=CCC2)CC12CCNCC2

ZINC43307515 CN(C)[C@@H](CNC(=O)NN[C@@]1(C)CCS(=O)(=O)C1)c1cccc1Cl

ZINC12900585 COCCCN1C(=O)[C@@H]2[C@H](Cc3c[nH]e4cccc34)N[C@@]3(C(=O)Nc4cccc43)[C@@H]2C1=O

ZINC13572491 COCCCN1C(=O)[C@@H]2[C@H](Cc3ccc(O)c(O)c3)N[C@@]3(C(=O)Nc4cccc43)[C@@H]2C1=O

ZINC33893497 CCc1ccc(N2C(=O)[C@H]3ON(CCN(=O)[C@@H](c4ccc(O)c(O)c4)[C@H]3C2=O)cc1

ZINC05372313 CC[C@@]1(O)Cc2c(O)c3c(c(O)c2[C@@H](O)C1)C(=O)c1c(OC)cccc1C3=O

ZINC23143208 O=C1C[C@@H](C(O)=N/e2n[nH]2)CN1c1ccc2c(c1)OCCO2

ZINC44658189 CC(C)CN1C(=O)N(C)C(O)=C(C(=O)CSc2nc(-c3cccs3)n[nH]2)[C@H]1N

ZINC36339450 CCC[C@@](C)(NC(=O)c1ene2nncn2c1C)C(=O)O

ZINC37466401 NC[C@H](c1ccc(F)cc1)N1CCN(CC(F)(F)F)CC1

ZINC67267965 Cc1ccc([C@H](CNC(=O)CCc2c(C)nc3nc(N)nn3e2C)N(C)C)cc1

ZINC39345493 Cc1c(NC(=O)c2n[nH]2)ccc1[C@@H]1Ne2cc(Cl)ccc2O1

ZINC13640520 COCCNC(=O)c1ccc2c(c1)[C@@H]1C=CC[C@H]1[C@H](c1ccc(O)cc1O)N2

ZINC00086260 CcC1c(O)c2c(=O)n(C)c(=O)n(C)c2n(C)c1=O

ZINC04814153 O=C(Nc1cccc1)[C@H]1CC(O)=N/C(=N)c2ccc(F)cc2)N1

ZINC67588578 O=C(O)c1[nH]ncc1CN1CCC[C@@H](c2n[nH]cc2-c2cccc2)C1

ZINC16033039 COc1ccc(CN2C(=O)[C@@H]3[C@H](CCC(N)=O)N[C@]4(C(=O)Nc5c(C)cccc54)[C@@H]3C2=O)cc1

ZINC43240598 Cc1ccc([C@@H]([C@H](C)N)N2CCC[C@@H]2c2ccnc2)s1

ZINC44483555 O=C(O)Cc1esc(NC(=O)c2ccc(Br)cc2O)n1

ZINC51255376 CN(Cc1cccc1Br)C[C@]1(CN)CCOC1

ZINC13469380 CCOC(=O)c1c(NC(=O)[C@@H]2CC=CC[C@@H]2C(=O)O)sc2c1CCC[S@]2=O

ZINC12473989 Ce1ccc(N(C(=O)e2snc(C(N)=O)e2N)[C@H](C(=O)NC[C@H]2CCCO2)c2ccc(O)cc2)c(C)c1

ZINC37321394 O[C@H]1CCC[C@H](N[C@@H]2CCOc3c(Cl)cc(Cl)cc32)C1

ZINC35955485 COc1ccc(-c2c(N)n(C[C@H]3CCCO3)c(=O)c3cc(N)ccc23)cc1

ZINC64370103 CCn1c(SCC(=O)N2CCC(C(N)=O)CC2)mnc1-c1se2ncccc2e1N

ZINC56908817 COc1nn(C)cc1C(=O)N1CCC[C@H](C(=O)Nc2cccc(NS(C)(=O)=O)e2)C1

ZINC61461221 Ce1ccc2nc([C@@H]3CCCN3C(=O)c3cnc4nc(O)[nH]c(=O)e4c3)[nH]c2c1

ZINC15957797 COc1cccc1CN1C(=O)[C@@H]2[C@H](CC(N)=O)N[C@]3(C(=O)Nc4cccc43)[C@@H]2C1=O

ZINC11888518 Cc1noc(C)c1S(=O)(=O)OC(C)(C)C(=O)O

ZINC66952665 O=C(NC[C@]1(O)CCc2cccc21)Nc1cc(Br)c[nH]e1=O

ZINC23130755 NC[C@@H]1CN(C2CCN(c3cccc(-n4cccn4)c3)CC2)CCO1

ZINC49543509 O=C(CC[C@H]1NC(=O)c2cccc2N=C1O)Nc1ccc2cc[nH]c2c1

ZINC39978610 CCOC(=O)N1CCC2=C3C(O)=N[C@@H]([C@@H]4C=CC=N4)N[C@H]3S[C@@H]2C1

ZINC13025319 CCCNC(=O)NC(=O)CSc1ne2cccc2c(=O)n1[C@H](C(=O)O)C(C)C

ZINC13405935 Cc1oc2nc(CSc3nnc(NCC(C)C)s3)[nH]c(=O)e2c1C(=O)O

ZINC66482149 C[C@H](NC[C@@H](O)CN1C[C@H](C)O[C@H](C)C1)c1nnc2ccccc12

ZINC13405935 Cc1oc2nc(CSc3nnc(NCC(C)C)s3)[nH]c(=O)e2c1C(=O)O

ZINC63521500 COc1ccc2c(c1)=C1CCN[C@@H](c3ccc(OCC(N)=O)c(OC)c3)[C@@H]1N=2

ZINC19323678 CCCC12CN3CC(C)(CN(C1)C3c1[nH]c(=O)[nH]c(=O)c1C)C2=O

ZINC38128012 N[C@@H](Cc1c(F)cccc1Cl)c1ccc2e1OCCO2

ZINC12703087 Cc1cccc(CN2CCC[C@](O)(CNCc3enn(C)c3C)C2=O)c1

ZINC09501249 Ce1c(C#N)c(NC(=O)CN2Cc3cccc3C[C@H]2C(N)=O)n(C[C@@H]2CCCO2)c1C

ZINC39604934 O=C(NC[C@H]1CCCO1)[C@@H]1CN(C(=O)[C@H]2CC=CCC2)CC12CCNCC2

ZINC39022546 CC1=N[C@@H]2C(=N1)C([N+](=O)[O-])=C1Nc3nonc3NC1=C2[N+](=O)[O-]

ZINC22263737 C=CCn1c(=S)[nH]c2cc(C(=O)Nc3ncccc3O)ccc2c1=O

ZINC41034862 C[C@@H]1CCC[C@](NS(=O)(=O)c2cc(Br)sc2Br)(C(=O)O)C1

ZINC39668846 CC(=O)N1C[C@H](C(=O)NC[C@@H]2OCCc3cccc32)C2(CCNCC2)C1

ZINC64008962 CC1=C2C=C(C(=O)Nc3cccc(-c4nn[nH]4)c3)S[C@H]2N(C)N1

ZINC39545437 CON(C(=O)[C@@H]1CC(Cl)=C2Nc3cccc3CN21)c1cccc1O

ZINC66134887 Cc1n[nH]c([C@H](C)Oc2ccc(Cl)cc2Br)c1C(=O)NN

ZINC16739640 COc1ccc([C@@H]2c3sc(=O)[nH]c3S[C@@H]3C(=O)N(C(N)=O)C(=O)[C@@H]32)cc1

ZINC15958932 O=C1[C@@H]2[C@H](Cc3ccc(O)c(O)c3)N[C@@]3(C(=O)Nc4cccc43)[C@@H]2C(=O)N1Cc1ccc2c(e1)OCO2

ZINC38994706 Cc1cccc1N1C(=O)[C@H]([C@H]2NCCc3e2[nH]c2cccc32)C(O)=N[C@@H]1O

ZINC63351980 C[C@H](NC(=O)N[C@H]1C[C@H]1c1cccc(F)c1)c1ccc(NS(C)(=O)=O)e1

ZINC13123337 Cc1ccc(-n2nc(C)c3e2NC2=C(C(=O)CC(C)(C)C2)[C@@H]3c2cccc2OCC(=O)O)cc1

ZINC00192117 Cn1c(=O)[nH]c(=O)c2c1nc(N1CCCCC1)n2CCC(=O)O

ZINC57742680 Cc1nc(NS(C)(=O)=O)sc1C(=O)N[C@@H]1CCC(=O)N[C@H]1c1ccc1

ZINC46814957 N#Cc1c(F)cccc1N1CCN(C(=O)c2ccc3c(O)[nH]c(=S)nc3e2)CC1

ZINC12473908 Ce1ccc(N(C(=O)e2snc(C(N)=O)e2N)[C@@H](C(=O)NC[C@@H]2CCCO2)e2ccc(O)cc2)c1

ZINC00987723 CCOc1ccc(N=C2N=C(O)C[C@@H](C(=O)Nc3ccc(C)cc3)N2)cc1



ZINC58157772 CCNC(=O)NC(=O)[C@@H](C)N1CCCN(e2nc(C)es2)CC1

ZINC47633170 C[C@H](CNC(=O)NC1CCC(O)CC1)N1CCN(e2ceccc2)CC1

ZINC52806460 CC(C)[C@@H](NNC(=O)c1cc(Br)c[nH]1)C(=O)NC(C)(C)C

ZINC64008961 CC1=C2C=C(C(=O)Nc3ccc(-c4nn[nH]4)c3)S[C@@H]2N(C)N1

ZINC65249534 COe1ccc(C)cc1NC(=O)c1c(O)c2cccnc2[nH]c1=O

ZINC34138251 COe1cc([N+](=O)[O-])cc(/C=C\C(=O)NC(=O)N(C)C2=O)c1O

ZINC04163015 COe1cc([C@H]2NC(=O)NC(C)=C2C(=O)OCCSC)cc([N+](=O)[O-])c1O

ZINC20328995 COe1cc([C@@H]2CC(=O)Nc3sc4c(C)c(C#N)c(N)nc4c32)ccc1O

ZINC58162059 C[C@H]1Oe2ccc(NC(=O)NC[C@@H]([C@@H]3CCOC3)N3CCCC3)cc2NC1=O

ZINC32996184 CCCCN1e(N)e(N(CC)C(=O)Cc2n[nH]c(=O)c3cccnc23)c(=O)[nH]c1=O

ZINC66482149 C[C@H](NC[C@@H](O)CN1C[C@@H](C)O[C@H](C)C1)c1nnc2cccnc12

ZINC48353955 C[C@@H](CNC(=O)N[C@H](C)c1nnc1C)N1CCc2ccc2C1

ZINC65376303 CC(=O)N1C[C@H]2CN(C(=O)CC3CCC(=O)CC3)C[C@@]2(C(=O)O)C1

ZINC40095593 COe1ccc1[C@@H]1C(C(=O)c2ccc3c(e2)C[C@H](C)O3)=C(O)C(=O)N1CCO

ZINC43285836 C[C@H](N)[C@H](c1cc(Br)es1)N1CCC[C@@H]1c1cccnc1

ZINC58431849 COe1ccc1NC(=O)c1ccc2c(O)[nH]c(S)nc2c1

ZINC05690460 CCCOe1ccc(C(=O)cc1Cc1c(O)nc(S)nc1O

ZINC06760828 CC(C)CCNC(=O)C(=O)Nc1sc2c(c1C(=O)O)CCC2

ZINC40085702 CCOe1ccc(C(=O)C2=C(O)C(=O)N(CCO)[C@H]2e2ccc(Oc3cccnc3)c2)cc1C

ZINC44887174 C[C@H](NC(=O)c1cnc1-c1cccnc1)c1nnc1[nH]1

ZINC64185687 O=C(N[C@@H](CC1=C2cccnc2=NC1)C(=O)NC[C@@H]1NN=C2CCCN21)c1cccnc1

ZINC13204063 CCNC(=O)NC(=O)[C@H](C)Sc1nnc(-c2ccc(Cl)cc2)n1CC(=O)O

ZINC57742680 Cc1nc(NS(C)(=O)=O)sc1C(=O)N[C@@H]1CCC(=O)N[C@H]1c1cccnc1

ZINC37720741 NCCc1cc(Br)ccc1OC[C@H]1CCCCO1

ZINC33833474 CC(=O)OC[C@@]1(O)[C@H]2CC[C@@H]3[C@@]45CCCC(C)(C)[C@@H]4[C@H](OC(C)=O)[C@](O)(OC5)[C@]3(

ZINC41026300 NC(=O)c1c(Nc2nc(N3CCN(CCO)CC3)nc3e2enn3-c2cccnc2)se2e1CCC2

ZINC07251982 NC(=O)NC(=O)CSc1nc(-c2cccnc2Br)n[nH]1

ZINC26573431 CC(C)c1nnc(/N=C\O)C2=NN(C)C(=O)CC2)s1

ZINC08860312 COe1cc([C@H]2C(C(=O)Nc3cccnc3C)=C(C)Nc3nnc32)ccc1OCC(N)=O

ZINC43307515 CN(C)[C@@H](CNC(=O)NN[C@@]1(C)CCS(=O)(=O)C1)c1cccnc1C1

ZINC63822639 CC1=C2[C@@H](c3cccnc3C)CC(=O)N[C@@H]2N(e2ccc(O)nn2)N1

ZINC41237985 Cc1cc(NS(=O)(=O)CCNS(=O)(=O)c2c(C)noc2C)no1

ZINC17044889 COe1cc([C@@H]2CC(=O)Nc3nc(-c4cccnc4)[nH]c(=O)c32)ccc1OCC(N)=O

ZINC66952287 CC(=O)Nc1cc(NC(=O)NC[C@@]2(O)CCc3cccnc32)ccc1C

ZINC39746384 C[C@@H]1NNC(=O)C2=C1[C@@H](C)O[C@H]2NC(=O)COC(=O)CC1(C[C@@H]2Nc3cccnc3S2)CCCC1

ZINC67273382 O=C1NC(=O)C2(CCC(C(=O)N[C@H]3C[C@@H]3c3cccnc3C(F)F)CC2)N1

ZINC09329295 Cn1c(=O)c2c(nc(NN/C=C3\C(=O)NC(=O)N(e4cccnc4)C3=O)n2C)n(C)c1=O

ZINC09329295 Cn1c(=O)c2c(nc(NN/C=C3\C(=O)NC(=O)N(e4cccnc4)C3=O)n2C)n(C)c1=O

ZINC66229911 Cc1nnc(C)c(C)c1S(=O)(=O)N=C\O)[C@@H](C)NC(=O)C1CCC1

ZINC09410142 COe1cc([C@H]2CC(=O)Nc3nc(-c4cccnc4)[nH]c(=O)c32)ccc1OCC(N)=O

ZINC47073212 O=C(NCCc1nnc2n1CCCC2)c1ccc2c(=O)[nH]c(S)nc2c1

ZINC36320697 CN(C1CCOCC1)[C@H](CN)c1c(Cl)cccnc1C1

ZINC18211452 NC1=C(O)C(=O)[C@H](e2cccnc2)O1

ZINC06810409 CC(=O)OCC1=C(C(=O)O)N2C(=O)[C@H](NC(=O)c3cccnc3)C[C@@H]2SC1

ZINC66229912 Cc1nn(C)c(C)c1S(=O)(=O)/N=C(O)[C@H](C)NC(=O)C1CCC1

ZINC23140693 O=C(Nc1nc[nH]n1)[C@@H]1CCCN(C(=O)c2ccoc2)C1

ZINC67236017 O=C(NCCn1ccn1)NNC(=O)[C@@H]1C[C@@H]1c1cccc(F)c1

ZINC03911303 COc1ccc(NC(=O)C(=O)c2c(O)[nH]e3ccccc23)cc1OC

ZINC40100221 COc1ccc(C(=O)C2=C(O)C(=O)N(CCOCCO)[C@H]2c2ccc(Cl)c(Cl)c2)c1

ZINC40085222 COc1ccc(C(=O)C2=C(O)C(=O)N(CCO)[C@H]2c2ccc(Br)c2)c1C

ZINC44658189 CC(C)CN1C(=O)N(C)C(O)=C(C(=O)CSc2nc(-c3cccs3)n[nH]2)[C@H]1N

ZINC39899244 CCCOc1ccc([C@H]2c3c(-c4cc(Cl)ccc4O)n[nH]c3C(=O)N2Cc2ccnc2)c1

ZINC67157716 CCCC(=O)N1CSC[C@@H]1C(=O)Nc1nc(S(C)(=O)=O)n[nH]1

ZINC54176713 CC[C@H](C/C(N)=N/O)NS(=O)(=O)c1ccc(Br)s1

ZINC41605860 Ce1ccc(C)c(NC(=O)[C@@H](C)Sc2nnc(O)[nH]e2=O)c1

ZINC04087196 CCN1CCc2c(sc(NC(=O)c3ccc([N+](=O)[O-])s3)c2C(N)=O)C1

ZINC15017291 COc1ccc([C@@H]2[C@@H](C(N)=O)C(=O)N[C@](O)(c3ccccc3)[C@@H]2C#N)cc1[N+](=O)[O-]

ZINC05523774 O=C1N[C@@H](c2ccc(F)cc2)[C@@H](C(=O)c2ccnc2)[C@@](O)(C(F)(F)F)N1

ZINC47343057 O/C(=Nc1nc(-e2cccn2)n[nH]1)e1ccc(-n2cn2)cc1

ZINC47007441 Ce1c([C@@H](C)NC(=O)NNe2c(F)c(F)c(F)c2F)cnn1C

ZINC47110816 C[C@@H]1CCCN(CCCNC(=O)c2ccc3c(O)[nH]c(=S)nc3c2)C1

ZINC40112620 Nc1ncnc1C(=O)NC[C@H](c1ccccc1)N1CCc2secc2C1

ZINC39676238 C[C@H](Oe1ccccc1)C(=O)N1C[C@@H](C(=O)NCc2nc3ccccc3e(=O)[nH]2)C2(CCNCC2)C1

ZINC39495613 O=CC[C@H](NC=O)c1ccc(-e2ccccc2O)c(O)c1-c1ccccc1O

ZINC34972163 Ce1ccc(C)c(-e2nnc(S)n2N)c1

ZINC07725352 N#Cc1c(CCCNC(=O)C2c3ccccc3Oe3ccccc32)n[nH]e1N

ZINC59146832 Cc1nn(-e2ccc([N+](=O)[O-])cc2[N+](=O)[O-])c(C)c1/C=N/NC(=O)[C@H](N)CC(C)C

ZINC63521498 COc1ccc2c(c1)=C1CCN[C@@H](c3ccc(OCC(N)=O)c(OC)c3)[C@H]1N=2

ZINC48733572 O=C(Nc1n[nH]c(C(F)(F)F)n1)e1ensn1

ZINC34863228 COCCN(Ce1nc2ccccc2c(=O)[nH]1)C(=O)c1enn(-e2ccc(O)nn2)c1C

ZINC31895693 Ce1cc(NC(=O)C2CCN(C(=O)c3ccc(O)nn3)CC2)no1

ZINC47965762 C[C@@H](NC(=O)C(=O)Nc1secc1C(N)=O)c1ccc2c(c1)CCCC2

ZINC31818108 Cc1nn(-e2ccc(O)nn2)c2c1[C@H](c1ccc(F)c(Br)c1)CC(O)=N2

ZINC06147391 O=C1Ne2ccccc2/C1=N/NC(=O)c1nc2ccccc2c(=O)[nH]1

ZINC12737654 C[C@@H](NC(=O)CCe1nnc(=S)[nH]e1O)c1ccc1Cl

ZINC37404646 Ce1nnc(CSc2nc(=O)[nH]c(C)c2C(=O)O)o1

ZINC40358206 C=CCN1C(=O)C(O)=C(C(=O)CC(C)C)[C@@H]1c1ccc(O)cc1O

ZINC25027857 CC[C@H](C)NC(=O)[C@H](C)N1CCN(Cc2nc(N)c3ccccc3n2)CC1

ZINC14052033 NC(=O)N[C@@H](CC(=O)N1CCN(c2ccccc2)CC1)c1cccs1

ZINC53819720 COc1ccc(NC(=O)c2ccc3c(O)[nH]c(=S)nc3c2)cc1F

ZINC40820358 O=C(c1cc(=O)[nH]c(O)n1)N1CCC[C@@H]1c1c[nH]e2cc(Cl)ccc12

ZINC38570961 CC[C@H](C)N1C(=O)N=C(O)[C@@H]([C@@H]2c3[nH]c4ccccc4e3CCN2C)[C@H]1O

ZINC40095297 C[C@H]1Cc2cc(C(=O)C3=C(O)C(=O)N(CCO)[C@@H]3c3ccccc(Br)c3)ccc2O1

ZINC11658229 O=C(C[C@@H]1NC(=O)NC1=O)NNC(=O)c1cn(-e2ccccc2)nc1-c1ccccc1

ZINC39958156 C[C@H]1CN(CC2=N[C@@H]3C(=N2)C(O)=NC(=O)N3C)C[C@H](C)O1

ZINC50176943 CNC(=O)c1cc(NC(=O)C(=O)N[C@H]2CCC(C)(C)c3ccccc32)ccc1F

ZINC64886547 O=C(NCCn1ccn1)NNC(=O)c1cc(Cl)se1Cl

ZINC12901265 Ce1c(CC(=O)N[C@H](CO)c2ccccc2)c(=O)oc2c(O)c(O)ccc12

ZINC55243565 Cc1n[nH]c(SCC(=O)N2Cc3cccc3C[C@@H]2C(N)=O)n1

ZINC41062484 Cc1n[nH]c(Se2ccc(C#N)cc2N)n1

ZINC16853037 Ce1nc(/C=C/e2enc(O)[nH]e2=O)c(CCC(C)C)c(=O)[nH]1

ZINC66402994 CN(C)[C@@H](CNC(=O)Nc1cc(C(F)F)c[nH]e1=O)c1ccco1

ZINC22116712 CC/C=C(\C(=O)O)c1esc(N)n1

ZINC66783234 Ce1ccse1C(=O)NNC(=O)c1cccc(-n2nc(O)ccc2=O)c1

ZINC50224864 NCe1cn(Ce2mnc(-c3ccc(Br)s3)o2)nn1

ZINC64024435 Ce1nnc(NNC(=O)e2ccc(N3CCe4cccc4C3)cc2)nc1O

ZINC59719269 COe1ccc([C@@H]2N(c3cccc3)N=C(C(C)=O)N2e2ccc3[nH]c(=O)[nH]e3e2)ccc1OCC(N)=O

ZINC20611483 COe1cccc1CN1C(=O)[C@@H]2[C@H](CCC(N)=O)N[C@@]3(C(=O)Nc4c(C)ccc43)[C@@H]2C1=O

ZINC65537545 O=C(CCe1nc2cccc2c(=O)[nH]1)N[C@H]1CCe2nccn2C1

ZINC16739640 COc1ccc([C@@H]2c3sc(=O)[nH]e3S[C@@H]3C(=O)N(C(N)=O)C(=O)[C@@H]3)cc1

ZINC31818108 Ce1nn(-c2ccc(O)nn2)c2c1[C@H](c1ccc(F)c(Br)c1)CC(O)=N2

ZINC37164220 O=C(O)c1c(NS(=O)(=O)e2cc[nH]e2)sc2c1CCCC2

ZINC64024435 Ce1nnc(NNC(=O)e2ccc(N3CCe4cccc4C3)cc2)nc1O

ZINC66122289 Ce1ccc(C(=O)NNC(=S)N[C@@H](C)e2ccc(Cl)cc2Cl)c(=O)[nH]1

ZINC66925388 O=C(CCNC(=O)NC[C@@]1(O)CCCe2cccc21)NC1CCCC1

ZINC24543918 COc1cc([C@H]2C3=C(CC(C)C)CC3=O)Nc3[nH]c(=O)[nH]c(=O)e32)cc1e1O

ZINC44452571 NC(=O)NC(=O)c1c(NC(=O)c2cccc(Cl)e2)sc2c1CCCC2

ZINC39468579 O=C(c1cc(=O)[nH]c(=O)[nH]1)N1CCC[C@@H](Nc2ccc(F)c(F)e2)C1

ZINC12900585 COCCCN1C(=O)[C@@H]2[C@H](Cc3c[nH]e4cccc34)N[C@@]3(C(=O)Nc4cccc43)[C@@H]2C1=O

ZINC41605860 Ce1ccc(C)c(NC(=O)[C@@H](C)Sc2nnc(O)[nH]e2=O)c1

ZINC06787870 CCCn1c(N)c(C(=O)CN(C)Ce2cccc(F)e2)c(=O)[nH]e1=O

ZINC67458914 Ce1cc2nc(CNC(=O)e3cc(CN4CCC[C@@H](O)C4)on3)[nH]e2cc1C

ZINC50094285 CC1(C)Ce2nc(Ce3ccc(Br)cc3)nc2[C@@H](N)C1

ZINC65419870 COe1ccc(C(=O)N2C[C@@H]3CN(C(=O)C4CC4)C[C@@]3(C(=O)O)C2)o1

ZINC25027857 CC[C@H](C)NC(=O)[C@H](C)N1CCN(Ce2nc(N)c3cccc3n2)CC1

ZINC08615652 Ce1cc(C)c2c(=S)nc(N)nc-2[nH]1

ZINC40348968 Cn1cc(NS(=O)(=O)e2c(N)cc(Cl)cc2Cl)ccc1=O

ZINC37164220 O=C(O)c1c(NS(=O)(=O)e2cc[nH]e2)sc2c1CCCC2

ZINC62675251 Cn1cc(S(=O)(=O)N=C(\O)e2ccc(-c3ccco3)[nH]e2=O)en1

ZINC15070035 COe1cccc1-n1cc(CNC[C@@]2(O)CCCN(C)C2=O)en1

ZINC36587167 CC(C)N(C(=O)Cc1cccc(Cl)e1Cl)[C@H](C(=O)NC1CCCCC1)c1c(O)cc(O)cc1O

ZINC66926216 Ce1ccse1C(=O)NNC(=O)NC[C@@]1(O)CCCe2cccc21

ZINC36386875 C[C@H](C(=O)e1c(N)n(C)c(=O)n(C)c1=O)N1CCC[C@H]1c1cccs1

ZINC40109332 O=C(C1=C(O)C(=O)N(CCO)[C@@H]1e1ccc(Cl)cc1)e1cccc(OCe2ccc(F)cc2)c1

ZINC48721252 C[C@@H](Cn1ccn1)NC(=O)C(O)=N/e1nncs1

ZINC44452611 Ce1ccc(C(=O)Nc2sc3c(e2C(=O)NC(N)=O)CCC3)cc1C

ZINC08253665 NC(=O)[C@@H]1C[C@@H](O)[C@H](O)[C@H]2[C@@H]1N(c1cccc1)C(=S)N2Cc1cccs1

ZINC16670586 Ce1cc(C)c(SCC(=O)e2c(N)n(C3CC3)c(=O)[nH]e2=O)c(C)c1

ZINC40819448 CC(C)C[C@@H](NC(=O)e1ccene1N)e1nc2cccc2c(=O)[nH]1

ZINC05345261 COCCCN1C(=O)[C@@H]2[C@@H](C)N[C@@]3(C(=O)Nc4c(Cl)cccc43)[C@@H]2C1=O

ZINC54029016 Ce1cc(C)c(NC(=O)CNC(=O)NCCN2ccene2)c(C)c1

ZINC39899244 CCCOe1cccc([C@H]2e3c(-c4cc(Cl)ccc4O)n[nH]e3C(=O)N2Ce2ccene2)c1

ZINC23828369 CC(C)CN(C(=O)CN(C)Cc1ccco1)c1c(N)(CC(C)C)c(=O)[nH]c1=O

ZINC13270561 Ce1cccc(-c2nnc(S[C@@H](C)C(=O)NC(=O)NC3CC3)n2CC(=O)O)c1

ZINC45216077 C[C@](N)(C#N)CCSc1nccc(=O)[nH]1

ZINC40268165 CS(=O)(=O)N1CCN([C@H](C(=O)O)e2c[nH]c3ccc(OCC#N)cc23)CC1

ZINC64617988 CN(C)S(=O)(=O)N=C(O)CCN1C(=O)NC2(CCCC2)C1=O

ZINC50396373 O=C1NCCC[C@@H]1NCc1cc(F)ccc1Br

ZINC17067428 O=C1C(C=C/e2nc(O)c([N+](=O)[O-])c(=O)[nH]2)-CO[C@H]2C=CC=C[C@@H]12

ZINC66909127 O=C(NCCC(=O)N1CCCCC1)NC[C@]1(O)CCc2ccc2c1

ZINC21324986 C/C(=N)\c1nnc(SCC(=O)N[C@H](C)e2ccccc2)n1N)e1cccn1

ZINC66790916 CCn1c(O)c2ccc(C(=O)NNC(=O)CCC(C)C)cc2nc1=S

ZINC42524631 CC[C@@](C)(NS(=O)(=O)c1sccc1Br)/C(N)=N/O

ZINC13151895 CC(=O)c1ccc2c(c1)[C@H]1[C@H](Cl)[C@H](Sc3ccccc3[N+](=O)[O-])C[C@@H]1[C@H](C(=O)O)N2

ZINC54124365 NC(=O)[C@H]1CCCN(e2ccc(CNc3nnc4sccc34)cc2)C1

ZINC65370360 COc1ccc2e(c1)[C@H](NC(=O)c1cc3n(n1)CCNC3)CC(C)(C)O2

ZINC13245490 CC(C)[C@H](C(=O)O)n1c(SCC(=O)N(CCC(N)=O)e2ccccc2)nc2ccccc2c1=O

ZINC58180947 Ce1ccc([C@@H](CNC(=O)CCe2c(C)[nH]c(=O)[nH]e2=O)N(C)C)cc1

ZINC64890804 CCCn1c(=O)c(=O)[nH]c2cc(C3=N[C@@H]([C@H](NS(=O)(=O)c4ccccc4)C(C)C)ON3)ccc21

ZINC03847021 C[C@H](CO)c1c(O)c(O)c2c(c1O)C(=O)C(=O)[C@H]1C(C)(C)CCC[C@]21C

ZINC09431466 CC(=O)OCC1=C(C(=O)O)N2C(=O)[C@H](NC(=O)Cn3nc(C)c(Cl)c3C)[C@@H]2SC1

ZINC20328995 COc1cc([C@@H]2CC(=O)Nc3c4c(C)c(C#N)c(N)nc4c32)ccc1O

ZINC65427031 Ce1nn(C)c(C)c1C(=O)N1C[C@@H]2CN(C(=O)C3CC3)C[C@]2(C(=O)O)C1

ZINC66390648 C[C@H](N[C@@H](C)c1ccc(N2CCN(C)CC2)c(F)c1)C(=O)NC(=O)NC1CC1

ZINC01425496 CN1C(=O)N[C@H](e2ccc(O)cc2)C2=C1CN(e1ccc(N3CC4=C(C3=O)[C@@H](c3ccc(O)cc3)NC(=O)N4C)cc1)C

ZINC34783375 Ce1c(C(=O)NN)sc2c1c(=O)n(CC(=O)NC1CCCCC1)c(=O)n2CC(C)C

ZINC59383264 CNC(=S)N/N=C/c1cc([N+](=O)[O-])cc(Br)c1O

ZINC40408296 O=C1Nc2ccc(O)cc2/C1=C/e1ccc(/C=C2/C(=O)Nc3ccc(O)cc32)n1

ZINC12783824 C[C@@H]1Oe2ccc(NC(=O)c3ccccc3SC[C@]3(C)NC(=O)NC3=O)cc2NC1=O

ZINC14074751 Ce1c(C#N)c(NC(=O)CN(CC(N)=O)C(C)C)n(C2CCCC2)c1C

ZINC60626442 O=C(Nc1cccc(N2CCOC2=O)c1)c1ccc2c(O)[nH]c(=S)nc2c1

ZINC39685702 CC(C)C(=O)N1C[C@@H](C(=O)N[C@H](C(=O)NC(C)(C)C)C2(CCNCC2)C1

ZINC13345871 O=C(O)c1ccc2c(=O)[nH]c(CSc3nnc4se5c(c34)CCC5)nc2c1

ZINC67000318 Ce1ccc(C#N)cc1NC(=O)C(=O)NC[C@]1(O)CCc2ccc2c1

ZINC62828819 CO[C@H]1CCC[C@@H]1NC(=O)Nc1sc(C)c(C)c1C(=O)O

ZINC13450878 COc1ccc(NC(=O)[C@H](C)Sc2nc(C)c(CCC(=O)O)c(=O)[nH]2)cc1OC

ZINC13196931 CCCNC(=O)NC(=O)CSc1nnc(-e2ccc(C)cc2)n1CCC(=O)O

ZINC23338448 Cc1n[nH]c(N=C(O)N2CCC[C@H](C(=O)N3CCOCC3)C2)n1

ZINC26258525 CSc1nc2nc(C)c(C/C(O)=N/c3nen[nH]3)c(C)n2n1

ZINC40053253 COc1ccc2cc(C(=O)C3=C(O)C(=O)N(CCCO)[C@H]3c3ccc(C(C)C)cc3)oc12

ZINC20558928 C[C@@H]1C[C@@H]1c1ccc([C@@H](CN)N2CCc3ccc3C2)o1

ZINC37538602 C=C1[C@@H](O)[C@H]2/C=C/C[C@@H](C)C=C(C)C(=O)[C@@H](O)CCC(=O)[C@]23C(=O)N[C@H](Cc2c[nH]

ZINC63521504 COc1ccc2c(c1)=C1CCN[C@H](c3ccc(OCC(N)=O)c(OC)c3)[C@@H]1N=2

ZINC04832459 COc1ccc([C@@H]2[C@@H](C(N)=O)C(=O)N[C@@](O)(c3ccccc3)[C@@H]2C#N)cc1

ZINC39676236 C[C@H](O)c1ccc1C(=O)N1C[C@H](C(=O)NCe2nc3ccccc3c(=O)[nH]2)C2(CCNCC2)C1

ZINC67157152 CC(=O)N[C@H](CC(=O)NC[C@@H](O)c1ccc(F)c1)c1c(F)ccc1F

ZINC64185691 O=C(N[C@@H](CC1=e2ccccc2=NC1)C(=O)NC[C@H]1NN=C2CCCN21)e1cccs1

ZINC63281448 COc1cc2c(cc1OC)=N[C@@H](C(=O)N[C@@H](C)C(=O)N[C@@H]1Nc3ccccc3S1)C=2

ZINC62012685 C[C@@H](N)[C@H](c1cenc1)N(C)[C@H](C)c1ccccc1)c1

ZINC39396295 O=C(N[C@H]1NC(SCc2ccc(F)cc2)=NS1)c1n[nH]1

ZINC14960513 CCN(CC)C(=O)[C@H]1CCCN(Cc2ccc(C(=O)NCC3(O)CCCC3)c(=O)[nH]2)C1

ZINC39715405 O=C(Nc1ccc2c(c1)N[C@H](c1ccccc3cccc13)O2)c1n[nH]1

ZINC44658189 CC(C)CN1C(=O)N(C)C(O)=C(C(=O)CSc2nc(-c3cccs3)n[nH]2)[C@H]1N

ZINC06359840 CCCC[C@]1(CC)C(=N)NC(=O)NC1=O

ZINC64886428 Cc1ccc(-e2enc(CCC(=O)NNC(=O)NCCCn3cenc3)o2)cc1

ZINC40707512 CCNc1nnc(N2CCN(Cc3ccc4c(c3)OCO4)CC2)c1N

ZINC49544857 COCc1nnc(NC(=O)c2enc3ccc(C)n3e2=O)s1

ZINC55196670 Cc1ccccc2c1[C@H](NC(=O)C(C)C)NC(=O)c1cccs1)C(=O)N2

ZINC03594174 COc1ccc([C@H]2c3cc4c(cc3O[C@](O)(CO)[C@@H]2C(=O)O)OCO4)c(OC)c1

ZINC29856798 CNC(=O)NC(=O)[C@H](C)N1CCN(c2ccc(F)c2C#N)CC1

ZINC02343584 CCOc1ccccc1/C=N/NC(=O)c1nnn(-e2none2N)e1CN1CCCC1

ZINC09010075 O=c1[nH]c(O)c(/C=N/e2ccccc2Sc2ccccc2)c(=O)[nH]1

ZINC40577874 C[C@@H]1COCCN1C(=O)N(CC(=O)O)[C@H]1CCS(=O)(=O)C1

ZINC63878202 Cc1ccc(C(N)=O)cc1NS(=O)(=O)c1ccccc2nsnc12

ZINC39467309 COC1=C[C@H]2CN3N[P@@](=O)(c4ccccc4O)OC[C@H]3C[C@@H]2CC1=O

ZINC45216077 C[C@](N)(C#N)CCSc1nccc(=O)[nH]1

ZINC45410416 Cc1ccccc(OCC(=O)NNC(=O)NC2CCN(C3CC3)CC2)c1

ZINC09882922 C[C@H](Sc1nc2ccc(Cl)cc2[nH]1)C(N)=O

ZINC39345493 Cc1c(NC(=O)c2n[nH]2)ccc1[C@@H]1Nc2cc(Cl)ccc2O1

ZINC48353954 C[C@H](NC(=O)NC[C@@H](C)N1Cc2sccc2C1)c1mnn1C

ZINC50224864 NCc1cn(Cc2nnc(-c3ccc(Br)s3)o2)nn1

ZINC18068440 C/C(O)=C1\C(=O)c2ccccc2\C1=N\N

ZINC67106460 C/C(=C/C(=O)NNc1nnc(C)c(O)n1)c1ccccc1C1

ZINC62982325 NCC#Cc1ccc(CN2CC[C@@H](N3CCCC3)C2)s1

ZINC36597690 Cc1ccc(CN(C(=O)c2ccc(O)c2O)[C@H](C(=O)NC2CCCC2)c2c(O)cc(O)cc2O)o1

ZINC38556246 CC1=C[C@@H]([C@H]2NN[C@H](SCC(=O)c3ccccc3Cl)N2)N=N1

ZINC23140693 O=C(Nc1nc[nH]n1)[C@@H]1CCCN(C(=O)c2ccc2)C1

ZINC02343584 CCOc1ccccc1/C=N/NC(=O)c1nnn(-e2none2N)e1CN1CCCC1

ZINC64797194 C#CCOc1cc([C@@H]2CC(=O)Nc3c2sc(C(=O)O)c3-c2ccc(OC)cc2)ccc1OC

ZINC19751015 Cc1cc2nc([C@@H](C)N)n(Cc3ccccc3Cl)c2cc1C

ZINC35851539 COc1ccc(Cl)cc1N1C(=O)[C@H]2[C@H](CCC(N)=O)N[C@@]3(C(=O)Nc4ccccc43)[C@@H]2C1=O

ZINC35851539 COc1ccc(Cl)cc1N1C(=O)[C@H]2[C@H](CCC(N)=O)N[C@@]3(C(=O)Nc4ccccc43)[C@@H]2C1=O

ZINC20611483 COc1ccccc1CN1C(=O)[C@@H]2[C@H](CCC(N)=O)N[C@@]3(C(=O)Nc4c(C)ccccc43)[C@@H]2C1=O

ZINC64886547 O=C(NCCCn1cenc1)NNC(=O)c1cc(Cl)sc1Cl

ZINC06557145 COC1=CC([N+](=O)[O-])=C/C(=C\c2c(O)n(C)c(=O)[nH]c2=O)C1=O

ZINC05231353 CC1(C)CC(=O)C(c2oc(N)c(C#N)c2-e2ccc2)=C(O)C1

ZINC21324569 C/C(=N\Nc1nnc(SCC(=O)Nc2c(F)ccc2F)n1N)c1cenc1

ZINC52768384 CN(C)S(=O)(=O)N=C(\O)[C@H]1CC(=O)N(c2ccccc2)C1

ZINC59198423 COc1cc(Cl)cc(/C=C2\C(=O)N(c3ccccc(Br)c3)C(=O)N=C2O)c1O

ZINC61461221 Cc1ccc2nc([C@@H]3CCCN3C(=O)c3cnc4nc(O)[nH]c(=O)c4c3)[nH]c2c1

ZINC36601330 O=C(CC[C@H]1NC(=O)c2ccccc2NC1=O)Nc1cc(F)c(F)c(F)c1

ZINC40096818 CCCCN1C(=O)C(O)=C(C(=O)c2ccc3c(c2)OCCO3)[C@H]1c1cccc(O)c1

ZINC06516291 CC(C)c1cccc(C(C)C)c1NC(=O)CSc1nc(N)cc(=O)[nH]1

ZINC45789511 CC(C)N(C)Cc1cccc1CNC(=O)NNe1ccc(-n2cccn2)nn1

ZINC40097223 CCOc1cc([C@H]2C(C(=O)c3cc4ccccc4o3)=C(O)C(=O)N2CCO)ccc1O

ZINC58431849 COc1cccc1NC(=O)c1ccc2c(O)[nH]c(S)nc2c1

ZINC06359840 CCCC[C@]1(CC)C(=N)NC(=O)NC1=O

ZINC66510661 CCn1c(=O)[nH]c2cc(C(O)=C(\C#N)C(=O)NC3CCCC3)ccc2c1=O

ZINC59146832 Cc1nn(-e2ccc([N+](=O)[O-])cc2[N+](=O)[O-])c(C)c1/C=N/NC(=O)[C@H](N)CC(C)C

ZINC40052968 O=C(C1=C(O)C(=O)N(CCCO)[C@H]1c1cccc1F)c1ccc2c(c1)OCCO2

ZINC39355973 CCOc1cccc1[C@H](C1=C(C)N=N[C@@H]1O)c1c(C)n[nH]e1O

ZINC13450878 COc1ccc(NC(=O)[C@H](C)Sc2nc(C)c(CCC(=O)O)c(=O)[nH]2)cc1OC

ZINC51068454 Cn1c(N)c(C(O)=C(\C#N)C(=O)CCc2cccc(Cl)e2)c(O)n(C)c1=O

ZINC39715405 O=C(Nc1ccc2c(c1)N[C@H](c1cccc3cccc13)O2)c1nen[nH]1

ZINC09331256 COc1cccc1N1C(=O)N=C(O)/C(=C\NN2CCOCC2)C1=O

ZINC40085178 COc1ccc(C(=O)C2=C(O)C(=O)N(CCOCCO)[C@H]2e2cccc3cccc23)cc1C

ZINC22802236 C[C@H]1CCc2c(sc3nenc(NCCCC4n[nH]c(N)c4#N)e23)C1

ZINC39232679 COc1ccc2c(CCN(C=O)[C@H](C)S[C@H]3NC(Cl)=NC4=N[C@@H]43)c[nH]e2c1

ZINC13564105 Cc1nc(O)c2nsc(C(=O)Nc3ccc(N4CCCC[C@@H](O)C4)cc3)e2n1

ZINC40053405 Cc1nc(C)c(C(=O)C2=C(O)C(=O)N(CCCO)[C@H]2c2cccc(Oc3cccc3)c2)s1

ZINC40126476 COc1cccc([C@H]2NC(=O)C(O)=C2C(=O)c2cccc(OCc3cccc3Cl)e2)e1OC

ZINC19751015 Cc1cc2nc([C@@H](C)N)n(Cc3cccc3Cl)e2cc1C

ZINC39958156 C[C@H]1CN(CC2=N[C@@H]3C(=N2)C(O)=NC(=O)N3C)[C@H](C)O1

ZINC22130310 COc1cccc(NC(=O)[C@H]2C(S)=NC(N)=C(C#N)[C@H]2e2ccc(F)cc2)c1

ZINC58366989 Cc1n[nH]c(C)c1NC(=O)CCNC(=O)NC12CC3CC(CC(C3)C1)C2

ZINC64617988 CN(C)S(=O)(=O)N=C(\O)CCN1C(=O)NC2(CCCC2)C1=O

ZINC62018619 CC(C)C[C@@H](CNC(=O)C(=O)Nc1ccc2c(c1)CCC(=O)N2)N(C)C

ZINC13271687 C=CCNC(=O)NC(=O)CSc1nnc(-e2cccs2)n1[C@@H](C(=O)O)C(C)C

ZINC45540964 Nc1c(C(=O)CSc2nc(-c3ccc(Cl)cc3)n[nH]2)c(=O)[nH]c(=O)n1C1CC1

ZINC66134886 Cc1n[nH]c([C@@H](C)O)c2ccc(Cl)cc2Br)c1C(=O)NN

ZINC51255376 CN(Cc1cccc1Br)C[C@]1(CN)CCOC1

ZINC40358147 CC(C)CC(=O)C1=C(O)C(=O)N(CC(C)C)[C@H]1c1ccc(O)cc1O

ZINC45799929 O=C(NNC(=O)c1nn(-e2ccccc2)cc1O)c1cccc(OC[C@@H]2CCCO2)c1

ZINC41181804 CC(C)(C)[C@H](N)c1nc(-e2ccc(OC(F)F)cc2)es1

ZINC06534140 Nc1cccc1-c1nnc(S)o1

ZINC66241129 N#Cc1cnn(-e2ccc(C(=O)N[C@@H]3C[C@H]3e3cccc(F)c3)cc2)c1N

ZINC07286538 COc1cc2nc(CS/C(N)=N/C(C)C)[nH]c(=O)e2cc1OC

ZINC40077275 COc1ccc(C(=O)C2=C(O)C(=O)N(CCOCCO)[C@H]2c2cccc(Cl)cc2Cl)cc1

ZINC15957797 COc1cccc1CN1C(=O)[C@@H]2[C@H](CC(N)=O)N[C@]3(C(=O)Nc4cccc43)[C@@H]2C1=O

ZINC09089994 Cc1cc(C=C2\C(=O)NC(=S)N=C2O)c(C)n1-c1cccc(I)c1

ZINC09089994 Cc1cc(C=C2\C(=O)NC(=S)N=C2O)c(C)n1-c1cccc(I)c1

ZINC48235688 O=C1CCc2cc(S(=O)(=O)Nc3cc([N+](=O)[O-])ccc3NCCO)c(F)cc2N1

ZINC25490225 O=C1NC(=O)[C@H](Cc2cc([N+](=O)[O-])c(O)cc2[N+](=O)[O-])N1

ZINC64885779 Cc1cccc(C2(C(=O)NNC(=O)NCCCn3ccnc3)CC2)c1

ZINC16853037 Ce1nc(/C=C/e2enc(O)[nH]e2=O)c(CCC(C)C)c(=O)[nH]1

ZINC23143208 O=C1C[C@@H](/C(O)=N/e2nen[nH]2)CN1c1ccc2c(c1)OCCO2

ZINC40049070 CCCOc1ccc(C(=O)C2=C(O)C(=O)N(CCCO)[C@H]2c2c(Cl)cccc2Cl)cc1C

ZINC61461221 Ce1ccc2nc([C@@H]3CCCN3C(=O)c3cnc4nc(O)[nH]c(=O)c4c3)[nH]c2c1

ZINC44218023 N[C@@H](CC(=O)O)c1c(-c2ccccc2Cl)nn(-c2ccccc2)c1Cl

ZINC06320618 Cc1cc(C(=O)N/N=C/e2cc([N+](=O)[O-])cc(Br)c2O)[nH]n1

ZINC23130755 NC[C@@H]1CN(C2CCN(c3cccc(-n4cccn4)c3)CC2)CCO1

ZINC31875846 COc1cc(/C=N\NC(=O)[C@@H]2COc3cccc3O2)c(Br)c(Br)c1O

ZINC54896816 CN(Cc1ccc(Cl)s1)c1nc2c(s1)[C@@H](N)CCC2

ZINC32116836 O=C1NC(=S)N=C(O)/C1=C/c1ccc(Se2ccc(Cl)cc2)c([N+](=O)[O-])c1

ZINC45540964 Ne1c(C(=O)CSe2nc(-c3ccc(Cl)cc3)n[nH]2)c(=O)[nH]c(=O)n1C1CC1

ZINC40141092 Ce1nc2c(C#N)enn2c(O)c1CC(=O)Nc1cccc1C(=O)NC1CCCC1

ZINC12379556 CC(=O)Nc1c(O)nc(SCC(=O)Nc2ccc(Br)cn2)[nH]c1=O

ZINC38570961 CC[C@H](C)N1C(=O)N=C(O)[C@@H]([C@@H]2c3[nH]c4cccc4c3CCN2C)[C@H]1O

ZINC17067422 O=C1C(/C=C/c2nc(O)c([N+](=O)[O-])c(=O)[nH]2)=CO[C@@H]2C=CC=C[C@H]12

ZINC04663941 Cc1cc(C(=O)N/N=C/e2cc(Br)cc([N+](=O)[O-])c2O)n[nH]1

ZINC39763575 CCNCN(=O)NC(=O)CS[C@H]1NN=C(C2=c3cccc3=NC2)N1C1CC1

ZINC67605382 Cc1cen2cc(CNC(=O)NC[C@H](O)COc3ccc4c(c3)OCO4)nc2c1

ZINC39345493 Ce1c(NC(=O)c2nen[nH]2)cccc1[C@@H]1Nc2cc(Cl)ccc2O1

ZINC06077434 CCC(C)NC(=O)[C@@H](c1ccc2ncccc2c1)N(C(=O)c1snc(C(N)=O)c1N)C1CCCC1

ZINC40100221 COc1cccc(C(=O)C2=C(O)C(=O)N(CCOCCO)[C@H]2c2ccc(Cl)c(Cl)c2)c1

ZINC40028276 C=CCN1C(=O)C(O)=C(C(=O)c2cc3cccc3o2)[C@H]1c1cc(Br)c(O)c(OC)c1

ZINC40085222 COc1ccc(C(=O)C2=C(O)C(=O)N(CCO)[C@H]2c2cccc(Br)c2)cc1C

ZINC58903681 COc1cccc([C@H]2C(C(N)=O)=C(N)Oc3c2c(C)nn3-c2ccccc2)c1

ZINC22263737 C=CCn1c(=S)[nH]c2cc(C(=O)Nc3ncccc3O)ccc2c1=O

ZINC12467760 NC(=O)c1nsc(C(=O)N(c2ccccc2)[C@@H](C(=O)NC[C@H]2CCCO2)c2c[nH]c3ccccc23)c1N

ZINC39958156 C[C@H]1CN(CC2=N[C@@H]3C(=N2)C(O)=NC(=O)N3C)C[C@H](C)O1

ZINC62828877 O=C(Nc1ccc1C(=O)O)NC1CCCC1

ZINC51262551 N#C/C(C(=O)C1CC1)=C(/O)Nc1cc2c(cc1[N+](=O)[O-])OCCO2

ZINC37731878 CCN([C@@H]1CCS(=O)(=O)C1)S(=O)(=O)c1[nH]ncc1C(=O)O

ZINC22645914 C[C@H](Se1n[nH]c(N)n1)C(=O)N(C)Cc1ccc(Br)cc1

ZINC20721099 COc1ccc(N2C[C@@H](C(=O)Nc3nc[nH]n3)CC2=O)c(OC)c1

ZINC43423750 NC[C@@H](c1ccc(Br)s1)N1CCO[C@H]2CCC[C@@H]21

ZINC60368200 O=C(CNC(=O)c1cc2c(s1)CCCC2)Nc1ncccc1O

ZINC67236017 O=C(NCCCn1cnc1)NNC(=O)[C@@H]1C[C@@H]1c1cccc(F)c1

ZINC25027857 CC[C@H](C)NC(=O)[C@H](C)N1CCN(Ce2nc(N)c3ccccc3n2)CC1

ZINC36644578 CCCCN(C(=O)[C@@H]1CC(=O)Nc2ccccc21)c1c(N)n(CCC)c(=O)[nH]c1=O

ZINC36386875 C[C@H](C(=O)c1c(N)n(C)c(=O)n(C)c1=O)N1CCC[C@H]1c1cccs1

ZINC66134887 Cc1n[nH]c([C@H](C)Oc2ccc(Cl)cc2Br)c1C(=O)NN

ZINC39899236 COc1ccc([C@H]2c3c(-c4cc(Cl)ccc4O)n[nH]e3C(=O)N2Ce2ccene2)cc1

ZINC39899236 COc1ccc([C@H]2c3c(-c4cc(Cl)ccc4O)n[nH]e3C(=O)N2Ce2ccene2)cc1

ZINC51262551 N#C/C(C(=O)C1CC1)=C(/O)Nc1cc2c(cc1[N+](=O)[O-])OCCO2

ZINC23143211 O=C1C[C@@H](/C(O)=N/e2nen[nH]2)CN1c1ccc2c(c1)OCCO2

ZINC44930540 C[C@H](NS(=O)(=O)N1C[C@@H](C)O[C@H](C)C1)c1nmm[nH]1

ZINC50396373 O=C1NCCC[C@@H]1NCc1cc(F)ccc1Br

ZINC67349739 O=S1(=O)CC[C@@H](NCCNe2ncc(Br)en2)C1

ZINC13023393 CC(C)(C)NC(=O)[C@H](c1cccs1)N(C(=O)c1snc(C(N)=O)e1N)e1ccc2c(e1)OCO2

ZINC21324569 C/C(=N)\Ne1nnc(SCC(=O)Ne2c(F)ccccc2F)n1N)c1ccccc1

ZINC12711348 NC(=O)c1nsc(C(=O)N(c2ccc(F)cc2)[C@@H](C(=O)NC[C@@H]2CCCO2)e2cccs2)e1N

ZINC19915382 O=c1[nH][nH]c(=O)c2c(NC3ccc(Br)o3)cccc12

ZINC40096581 O=C(C1=C(O)C(=O)N(CCO)[C@@H]1c1ccc(Cl)c1)c1ccc2c(c1)OCCO2

ZINC40802040 Ne1c(OC2CCCC2)nenc1N1CCC(C(=O)O)CC1

ZINC40079682 COc1ccc(C(=O)C2=C(O)C(=O)N(CCOCCO)[C@H]2c2cccc(O)c2)c(C)c1

ZINC37448211 COc1ccc([C@@H]2[C@@H](C(N)=O)C(=O)N[C@@](O)(c3ccccc3)[C@H]2C#N)cc1[N+](=O)[O-]

ZINC39996660 C=CCNC(=O)NC(=O)CS[C@H]1NN=C(C2=c3ccccc3=NC2)N1C1CC1

ZINC39763575 CCCNC(=O)NC(=O)CS[C@H]1NN=C(C2=c3ccccc3=NC2)N1C1CC1

ZINC21324992 C/C(=N)\Ne1nnc(SCC(=O)N[C@@H](C)c2ccccc2)n1N)c1ccccc1

ZINC32614381 O=C1NC[C@@H](c2ccccc2)[C@@H]1C(=O)N/N=C\c1cc(O)ccc1[N+](=O)[O-]

ZINC44713564 COc1ccc2nc(CCN(C(=O)[C@@H]3CN(C(=O)c4cc(C)n(C)n4)CC34CCNCC4)[nH]e2c1

ZINC16212879 COCCN1C(=O)C(O)=C(C(=O)c2ccc(Cl)cc2)[C@@H]1c1ccc(OCC(N)=O)cc1

ZINC65537545 O=C(CCc1nc2ccccc2c(=O)[nH]1)N[C@H]1CCc2nccn2C1

ZINC43341776 C[C@H](N)[C@H](O)c1ccc(F)cc1Br)c1ccccc1

ZINC08993831 CN(CC(=O)NN1C(=O)N[C@@](C)(CCc2ccccc2)C1=O)Cc1nc2ccccc2c(=O)[nH]1

ZINC41605860 Ce1ccc(C)c(NC(=O)[C@@H](C)Sc2nnc(O)[nH]e2=O)c1

ZINC64185694 O=C(N[C@H](CC1=c2ccccc2=NC1)C(=O)NC[C@H]1NN=C2CCCN21)c1cccs1

ZINC53819720 COc1ccc(NC(=O)c2ccc3c(O)[nH]c(S)nc3c2)cc1F

ZINC39037576 CCOc1cc([C@H](C2=C(C)N=N[C@@H]2O)c2c(C)n[nH]e2O)ccc1OC(=O)c1ccc(Cl)c1

ZINC52557329 N#Cc1nc(NC(=O)c2ccccc2NC(=O)[C@H]3C4c4ccccc4O3)e2)[nH]e1C#N

ZINC63279882 CC[C@]1(c2ccc(NC(=O)C(=O)NCCC3=c4ccccc4=NC3)cc2)CCC(=O)NC1=O

ZINC39899236 COc1ccc([C@H]2c3c(-c4cc(Cl)ccc4O)n[nH]e3C(=O)N2Cc2ccccc2)cc1

ZINC39899236 COc1ccc([C@H]2c3c(-c4cc(Cl)ccc4O)n[nH]e3C(=O)N2Cc2ccccc2)cc1

ZINC40531567 C[C@@H]1CN(C(=O)N(CC(=O)O)[C@H]2CCS(=O)(=O)C2)CCO1

ZINC05816089 Oc1c(Br)cc(C=NNc2nn[nH]2)cc1Br

ZINC41026300 NC(=O)c1c(Ne2nc(N3CCN(CCO)CC3)nc3e2nn3-c2ccccc2)se2c1CCC2

ZINC38999554 NN1[C@@H](SCC(=O)N2CCOCC2)NN[C@H]1[C@H]1C=C(c2ccc(Cl)cc2)N=N1

ZINC66134886 Cc1n[nH]c([C@@H](C)O)c2ccc(Cl)cc2Br)c1C(=O)NN

ZINC20228158 COc1cc([N+](=O)[O-])cc(/C=N/NC(=O)Cn2cnnn2)c1O

ZINC08581704 O=C(Nc1ccc(N2CCC[C@H](O)C2)cc1)c1snc2c(O)ncnc12

ZINC20611110 COc1ccccc1CN1C(=O)[C@@H]2[C@H](CC(N)=O)N[C@@]3(C(=O)Ne4ccccc43)[C@@H]2C1=O

ZINC03946853 COc1cc(/C=N/Ne2[nH]c(=O)nnc2C)cc([N+](=O)[O-])e1O

ZINC06454377 O=C1NC(=O)C(=NNc2ccc(-c3ccccc3)cc2)C(=O)N1

ZINC25027857 CC[C@H](C)NC(=O)[C@H](C)N1CCN(Ce2nc(N)c3ccccc3n2)CC1

ZINC20611110 COc1ccccc1CN1C(=O)[C@@H]2[C@H](CC(N)=O)N[C@@]3(C(=O)Ne4ccccc43)[C@@H]2C1=O

ZINC41033318 Cn1cnc([N+](=O)[O-])e1NC1(C(=O)O)CCCCC1

ZINC67349739 O=S1(=O)CC[C@@H](NCCNe2ncc(Br)en2)C1

ZINC60494468 COCCCN(C(=O)C1CCN([C@H](C)C(=O)NC(=O)NC2CCCC2)CC1

ZINC40095297 C[C@H]1Cc2cc(C(=O)C3=C(O)C(=O)N(CCO)[C@@H]3c3ccccc(Br)e3)ccc2O1

ZINC42956539 Cn1nc(O)c2c(C(=O)NNc3ccccc3Cl)c3cc(C3CC3)nc21



ZINC61381104 O=C1CCe2cc(NC(=O)c3cccc(-n4nc(O)ccc4=O)c3)ccc2N1

ZINC40096977 O=C(C1=C(O)C(=O)N(CCOCCO)[C@@H]1c1ccc(O)cc1)c1cc2ccc(O)c1

ZINC47110816 C[C@@H]1CCCN(CCCNC(=O)c2ccc3c(O)[nH]c(=S)nc3c2)C1

ZINC44713564 COe1ccc2nc(CCNC(=O)[C@@H]3CN(C(=O)c4cc(C)n(C)n4)CC34CCNCC4)[nH]c2c1

ZINC40707512 CCNc1nenc(N2CCN(Cc3ccc4c(c3)OCO4)CC2)c1N

ZINC12703087 Ce1cccc(CN2CCC[C@](O)(CNCc3enn(C)c3C)C2=O)c1

ZINC47475599 CC(C)N1C[C@H](C(=O)Nc2nc(C#N)c(C#N)[nH]2)CC1=O

ZINC41069896 C[C@H]1CCC[C@H](C)N1S(=O)(=O)c1cc(Br)enc1NN

ZINC63810477 O=C(Nc1cccc(-n2cccn2)c1)c1ccc2c(O)[nH]c(=S)nc2c1

ZINC32610336 O=C(O)[C@H]1CC=CC[C@H]1C(=O)Nc1cc(-e2ccc(O)c1)[nH]1

ZINC08860312 COe1cc([C@H]2C(C(=O)Nc3cccc3C)=C(C)Nc3nenn32)ccc1OCC(N)=O

ZINC40026252 C=CCN1C(=O)C(O)=C(C(=O)c2ccc(OC)cc2)[C@H]1c1ccc(OCC(N)=O)cc1

ZINC04087196 CCN1CCc2c(sc(NC(=O)c3ccc([N+](=O)[O-])s3)c2C(N)=O)C1

ZINC47073212 O=C(NCCc1nnc2n1CCCCC2)c1ccc2c(=O)[nH]c(S)nc2c1

ZINC38556246 CC1=C[C@@H]([C@H]2NN[C@H](SCC(=O)c3cccc3C1)N2)N=N1

ZINC40781477 COC[C@@H](C)Nc1nenc(Nc2ccc(O)c2)Br)c1N

ZINC04083625 COc1ccc(N2C(=O)[C@@H]3[C@H]([C@@H](C)O)N[C@@]4(C(=O)Nc5cccc54)[C@@H]3C2=O)cc1

ZINC40026252 C=CCN1C(=O)C(O)=C(C(=O)c2ccc(OC)cc2)[C@H]1c1ccc(OCC(N)=O)cc1

ZINC11869123 Ce1ccc(CNc2nc(CN(CCO)[C@H]3CS(=O)(=O)C[C@@H]3O)nc3cccc23)cc1

ZINC17575813 O=C(NNC(=O)c1c[nH]c(=S)n1-c1ccc(O)c1)ccc1O

ZINC12854530 COe1en(-e2ccc(C(F)(F)F)c2)nc1C(=O)OCe1nc(N)nc(N)n1

ZINC63810477 O=C(Nc1cccc(-n2cccn2)c1)c1ccc2c(O)[nH]c(=S)nc2c1

ZINC17878453 NC1=NC(=O)[C@@H]([C@]2(O)C(=O)N(CCCc3cccc3)c3cccc32)S1

ZINC15082922 Ce1cc(=O)[nH]c(SCC(=O)Nc2[nH]c(C)c(C)c2C#N)n1

ZINC40554938 C[C@H](C(=O)NC(C)C)N1CCC(C(=O)Nc2nccn2)CC1

ZINC43286070 C[C@H](N)[C@@H](c1cc(Br)es1)N1CCOC(C)C1

ZINC19323678 CCCC12CN3CC(C)(CN(C1)C3c1[nH]c(=O)[nH]c(=O)c1C)C2=O

ZINC35363867 CC(=O)Oe1ccc(N2C(=O)[C@@H]3[C@H](Cc4ccc(O)c(O)c4)N[C@@]4(C(=O)Nc5cccc54)[C@@H]3C2=O)cc1

ZINC65370360 COe1ccc2c(c1)[C@H](NC(=O)c1cc3n(n1)CCNC3)CC(C)C)O2

ZINC16212879 COCCN1C(=O)C(O)=C(C(=O)c2ccc(Cl)cc2)[C@@H]1c1ccc(OCC(N)=O)cc1

ZINC13198272 CCNC(=O)NC(=O)[C@@H](C)Se1nnc(-e2ccc(C)c2)n1CCC(=O)O

ZINC35851539 COe1ccc(Cl)cc1N1C(=O)[C@H]2[C@H](CCC(N)=O)N[C@@]3(C(=O)Nc4cccc43)[C@@H]2C1=O

ZINC35851539 COe1ccc(Cl)cc1N1C(=O)[C@H]2[C@H](CCC(N)=O)N[C@@]3(C(=O)Nc4cccc43)[C@@H]2C1=O

ZINC48260499 NC(=O)NC(=O)[C@@H](c1cccc1)N1CCO[C@H](c2ccc(F)cc2)C1

ZINC39693432 CC[C@@H](C)C(=O)N1C[C@H](C(=O)NCCNC(=O)OC(C)C)C2(CCNCC2)C1

ZINC15958851 Ce1cccc2e1NC(=O)[C@@]21N[C@@H](CCC(=O)O)[C@H]2C(=O)N(Cc3ccc4c(c3)OCO4)C(=O)[C@H]21

ZINC41163213 N[C@H](c1nc(-c2cc3cc(Br)ccc3o2)es1)C1CC1

ZINC05310018 CCCNC(=O)NC(=O)CSe1nnc(Cl)cc2[nH]1

ZINC02264694 COe1ccc(-n2c3c(c(=O)[nH]e2=O)[C@](N(C(=O)c2ccc(Cl)c2)(C(F)(F)F)C(=O)N3)cc1

ZINC64981111 Ce1cc(=O)[nH]c(SCC(=O)Nc2c(C#N)sc(=S)n2-c2ccc(O)c2)n1

ZINC66790916 CCn1c(O)c2ccc(C(=O)NCC(=O)CCC(C)C)cc2nc1=S

ZINC39958156 C[C@H]1CN(CC2=N[C@@H]3C(=N2)C(O)=NC(=O)N3C)C[C@H](C)O1

ZINC65370642 Nc1nc(NC[C@H]2C=c3ccc(F)cc3=NC2=O)cc(N2CCOCC2)n1

ZINC66390648 C[C@H](N[C@@H](C)c1ccc(N2CCN(C)CC2)c(F)c1)C(=O)NC(=O)NC1CC1

ZINC41630098 CC(C)c1cccc(C(C)C)c1NC(=O)[C@@H](C)Sc1nc(N)ccc(=O)[nH]1

ZINC40095593 COc1cccc1[C@@H]1C(C(=O)c2ccc3c(e2)C[C@H](C)O3)=C(O)C(=O)N1CCO

ZINC67574707 CN(C)C(=O)Cn1cc(C(O)=N/e2nc(-c3cccc3Cl)n[nH]2)nn1

ZINC53366727 CCCNC(=O)CN(CCC)CC(=O)NN1C(=O)NC2(CCC(C)CC2)C1=O

ZINC60368200 O=C(CNC(=O)c1cc2c(s1)CCCC2)Nc1ncccc1O

ZINC15082922 Cc1cc(=O)[nH]c(SCC(=O)Nc2[nH]c(C)c(C)c2C#N)n1

ZINC01142253 Cc1ccc(C)c(C(=O)C2=C(O)C(=O)N(c3nnc(C)s3)[C@@H]2c2ccc(O)cc2)c1

ZINC53366727 CCCNC(=O)CN(CCC)CC(=O)NN1C(=O)NC2(CCC(C)CC2)C1=O

ZINC65508179 NC(=O)c1ene2n1CCN(C(=O)[C@H]1CCCC3=c4cccc4=N[C@H]3)C2

ZINC32972785 CCCn1cc(CN/C(=N/C(=O)c2cccc(N(C)C)c2)Nc2cc(Cl)ccc2C)c(C)n1

ZINC15959687 COc1ccc(CCN2C(=O)[C@@H]3[C@H](CC(N)=O)N[C@]4(C(=O)Nc5c(C)cc(C)cc54)[C@@H]3C2=O)cc1OC

ZINC35667078 CCOc1cc(C=C(NC(C)=O)C(=O)O)cc1)c1OCc1cccc1C

ZINC12749044 O=C(C[C@H]1C(=O)NCCN1Cc1cccc(C(F)F)e1)NCCN1CCNC1=O

ZINC63941209 COC[C@H]1NN[C@@H](NC(=O)[C@@H]2CC(=O)N(CCC3=c4cc(C)ccc4=NC3)C2)S1

ZINC38117525 C[C@@](CO)(c1cc(F)c(Cl)cc1Cl)N1CCCNCC1

ZINC11617280 O=C(O)CCC(=O)N1N=C(e2c(-c3cccc3)c3cc(Cl)ccc3[nH]e2=O)C[C@H]1c1cccc1

ZINC25782523 C/C(=N)NC(=O)c1c(CN2CCCC2)nnn1-c1nonc1N)c1cc(C)sc1C

ZINC43621008 O=C(NC[C@@H](O)CN1CCCC1)Nc1cnn(-c2cccc2)n1

ZINC38701992 O=C1c2n[nH]c(-c3cc(Cl)ccc3O)c2[C@H](c2cccc2)N1[C@@H]1CCS(=O)(=O)C1

ZINC13126479 Cc1ccc2oc(-c3cc(NC(=O)e4nc[nH]n4)ccc3O)nc2c1

ZINC46814957 N#Cc1c(F)ccc1N1CCN(C(=O)c2ccc3c(O)[nH]c(=S)nc3e2)CC1

ZINC04861208 CCc1nc(SCC(N)=O)[nH]c(=O)c1C

ZINC46089269 CC1(C)Oe2cc(NC(=O)[C@@H]3CCCC[C@@H]3C(=O)O)ccc2NC1=O

ZINC66230822 C[C@H](NC(=O)C1CCC1)C(=O)/C(C#N)=C(\O)Nc1cccc(Cl)c1Cl

ZINC63775414 COc1cc2c(cc1OC)C(=O)N[C@@H](c1cc(Cl)cc([N+](=O)[O-])c1O)N2

ZINC44930540 C[C@H](NS(=O)(=O)N1C[C@@H](C)O[C@H](C)C1)c1nnn[nH]1

ZINC22263737 C=CCn1c(=S)[nH]e2cc(C(=O)Nc3ncccc3O)ccc2c1=O

ZINC13126479 Cc1ccc2oc(-c3cc(NC(=O)e4nc[nH]n4)ccc3O)nc2c1

ZINC09428205 CCOc1cc(C=C(NC(C)=O)C(=O)O)cc(Br)c1OCc1ccc(Cl)cc1

ZINC48733572 O=C(Nc1n[nH]c(C(F)F)n1)e1ens1

ZINC54176766 CC[C@@H](C/C(N)=N/O)NS(=O)(=O)c1secc1Br

ZINC20827519 Cc1cccc1NC(=O)CSc1nnc(N/N=C/e2cnn(C(C)C)c2)n1N

ZINC51068454 Cn1c(N)c(C(O)=C(\C#N)C(=O)CCc2cccc(Cl)e2)c(=O)n(C)c1=O

ZINC23828369 CC(C)CN(C(=O)CN(C)Cc1cccc1)c1c(N)n(CC(C)C)c(=O)[nH]c1=O

ZINC66234044 Cn1cnc1CCNC(=O)NCc1cc(F)cc2c1OCOC2

ZINC12783824 C[C@@H]1Oe2ccc(NC(=O)c3cccc3SC[C@]3(C)NC(=O)NC3=O)cc2NC1=O

ZINC40097223 CCOc1cc([C@H]2C(C(=O)c3cc4cccc4o3)=C(O)C(=O)N2CCO)ccc1O

ZINC64185687 O=C(N[C@@H](CC1=c2cccc2=NC1)C(=O)NC[C@@H]1NN=C2CCCN2)1c1ccs1

ZINC09058784 COCCCN1C(=O)N=C(O)/C=C2\C[C@H](c3ccc(Cl)cc3Cl)NN2)C1=O

ZINC09058784 COCCCN1C(=O)N=C(O)/C=C2\C[C@H](c3ccc(Cl)cc3Cl)NN2)C1=O

ZINC09058784 COCCCN1C(=O)N=C(O)/C=C2\C[C@H](c3ccc(Cl)cc3Cl)NN2)C1=O

ZINC09058784 COCCCN1C(=O)N=C(O)/C=C2\C[C@H](c3ccc(Cl)cc3Cl)NN2)C1=O

ZINC52768384 CN(C)S(=O)(=O)/N=C(\O)[C@H]1CC(=O)N(c2cccc2)C1

ZINC40358206 C=CCN1C(=O)C(O)=C(C(=O)CC(C)C)[C@@H]1c1ccc(O)cc1O

ZINC13393255 Cn1c(C(=O)NC/C=C/e2enc(N)[nH]2)cc(Br)c1Br

ZINC39715405 O=C(Nc1ccc2c(c1)N[C@H](c1cccc3cccc13)O2)c1nen[nH]1

ZINC38789740 C=CCOC(=O)C1=C(C)S[C@H](NC(=O)CSc2nc(CC)c(C#N)c(=O)[nH]2)N1

ZINC63557273 CCOCC[C@H]1INN[C@H](NC(=O)[C@H]2CC(=O)N(CCC3=C4cc(F)ccc4=NC3)C2)S1

ZINC16618315 Ne1c(C(=O)CSe2nnc(NC3CCCC3)s2)c(=O)[nH]c(=O)n1C1CC1

ZINC36007000 COc1cccc2c1OC(=O)[C@H]1[C@H]3C[C@H]([C@H]4Sc5[nH]c(=O)sc5[C@H]2[C@H]43)[C@H]1C(=O)O

ZINC47073212 O=C(NCCc1nnc2n1CCCC2)c1ccc2c(=O)[nH]c(S)nc2c1

ZINC61717936 COCCn1c2c(c(=O)[nH]e1=O)[C@H](C(=O)Nc1cc(F)c(F)c(F)e1)CC(O)=N2

ZINC61717936 COCCn1c2c(c(=O)[nH]e1=O)[C@H](C(=O)Nc1cc(F)c(F)c(F)e1)CC(O)=N2

ZINC07286538 COc1cc2nc(CS/C(N)=N/C(C)(C)[nH]c(=O)e2cc1OC

ZINC67001521 C[C@H]1CN(C(O)=C(C#N)C(=O)[C@H](C)NC(=O)C2CCOCC2)C[C@H](C)O1

ZINC08492620 COc1ccc([C@H]2C3=C(O)CCCC3=Nc3nc(S)nc(N)c32)cc1

ZINC39887556 COc1cccc1N1C(S)=C(C#N)C(=O)N[C@H]1c1cccc(Br)c1

ZINC20721099 COc1ccc(N2C[C@H](C(=O)Nc3nc[nH]n3)CC2=O)c(OC)c1

ZINC06074543 CC(C)(C)NC(=O)[C@H](c1ccc(F)cc1)N(C(=O)c1snc(C(N)=O)c1N)c1ccc2c(c1)OCO2

ZINC22263984 O=C(CN1C(=O)N[C@]2(CCc3cccc32)C1=O)Nc1ncccc1O

ZINC11658229 O=C(C[C@H]1NC(=O)NC1=O)NNC(=O)c1en(-c2cccc2)nc1-c1cccc1

ZINC43286072 C[C@H](N)[C@H](c1cc(Br)es1)N1CCOC(C)(C)C1

ZINC39693453 C[C@H](Oe1cccc1)C(=O)N1C[C@H](C(=O)NCCNC(=O)OC(C)(C)C2(CCNCC2)C1

ZINC24378639 C=CCNC(=O)NC(=O)[C@H](C)N(C)CC(=O)Nc1c(C)cc(C)cc1C

ZINC08581704 O=C(Nc1ccc(N2CCC[C@H](O)C2)cc1)c1snc2(O)ncnc12

ZINC53714157 N[C@H](c1cc2c(cc1Cl)OCCCO2)C1CCCCC1

ZINC12714948 Cc1cc(C)cc(N(C(=O)e2snc(C(N)=O)e2N)[C@H](C(=O)NC[C@H]2CCCO2)c2ccc(C)o2)c1

ZINC12317592 Cc1cn2cc(CNC[C@]3(O)CCCN(CC4CC4)C3=O)nc2s1

ZINC66632360 C/C(=C/C(=O)NNC(=O)NCCc1cnc1)c1cccc1Cl

ZINC49147416 CC[C@H](NS(=O)(=O)c1cc(Br)enc1NN)C(C)C

ZINC45740144 CC(C)CN(C(=O)[C@H]1CC(=O)Nc2cccc21)c1c(N)n(CC(C)C)c(=O)[nH]c1=O

ZINC66931390 O=C(Nc1cccc(C(=O)NC[C@]2(O)CCc3cccc32)e1)NC1CC1

ZINC32973114 CCCn1cc(CN/C(=N/C(=O)e2cccc(N(C)C)e2)Nc2ccc(Cl)cc2C)c(C)n1

ZINC23140693 O=C(Nc1nc[nH]n1)[C@H]1CCCN(C(=O)e2ccoc2)C1

ZINC44930540 C[C@H](NS(=O)(=O)N1C[C@H](C)O[C@H](C)C1)c1nn[nH]1

ZINC15958851 Cc1cccc2c1NC(=O)[C@]21N[C@H](CCC(=O)O)[C@H]2C(=O)N(Cc3ccc4c(c3)OCO4)C(=O)[C@H]21

ZINC43341776 C[C@H](N)[C@H](Oe1cccc(F)cc1Br)c1cccc1

ZINC15938516 COc1cc([N+](=O)[O-])cc(/C=N/NC(=O)/C=C'e2ccc3c(e2)OCO3)NC(=O)e2cccc2)c1O

ZINC40115133 Cc1nc2c(C#N)enn2c(O)c1CC(=O)N[C@H](c1ccc(F)cc1)c1cccs1

ZINC67588199 CC1=NC(=O)C2(CCN(C[C@]3(O)CCCN(CC4cccc4)C3=O)CC2)N1

ZINC16212879 COCCN1C(=O)C(O)=C(C(=O)e2ccc(Cl)cc2)[C@H]1c1ccc(OCC(N)=O)cc1

ZINC33533935 COc1cc([C@H]2C(C(=O)c3ccc(C)o3)=C(O)C(=O)N2CCc2cccc2)cc(Br)c1O

ZINC08615652 Cc1cc(C)e2c(=S)nc(N)nc-2[nH]1

ZINC19300404 CN(C)[C@H]1c2cccc2C2(CCN(C(=O)C3=NNC(=O)CC3)CC2)[C@H]1O

ZINC09058784 COCCCN1C(=O)N=C(O)/C=C2[C@H](c3ccc(Cl)cc3Cl)NN2)C1=O

ZINC09058784 COCCCN1C(=O)N=C(O)/C=C2[C@H](c3ccc(Cl)cc3Cl)NN2)C1=O

ZINC09058784 COCCCN1C(=O)N=C(O)/C=C2[C@H](c3ccc(Cl)cc3Cl)NN2)C1=O

ZINC09058784 COCCCN1C(=O)N=C(O)/C=C2[C@H](c3ccc(Cl)cc3Cl)NN2)C1=O

ZINC15961237 COc1ccc2[nH]c3c(O)n(Cc4ccc(C(=O)N5CCCC5)cc4)c(=S)nc3e2c1  
 ZINC40085702 CCOc1ccc(C(=O)C2=C(O)C(=O)N(CCO)[C@H]2e2cccc(Oc3cccc3)c2)cc1C  
 ZINC40348968 Cn1cc(NS(=O)(=O)e2c(N)cc(Cl)cc2Cl)ccc1=O  
 ZINC40377405 CC[C@](C)(NS(=O)(=O)c1ccc(Br)s1)/C(N)=N/O  
 ZINC13126479 Cc1ccc2oc(-e3cc(NC(=O)e4nc[nH]n4)ccc3O)nc2c1  
 ZINC29856798 CNC(=O)NC(=O)[C@H](C)N1CCN(c2cccc(F)c2C#N)CC1  
 ZINC50589065 Cc1nn([C@H](c2cccs2)[C@@H](C)N)c(C)c1Br  
 ZINC38995126 CC1=C[C@H]([C@H]2NN[C@H](SCc3ccc(Br)cc3)N2N)N=N1  
 ZINC03039109 CCOc1ccc(NC(=O)Nc2cc(C(=O)O)ccc2N2C[C@@H]3C[C@H](C2)Cn2c3cccc2=O)cc1  
 ZINC11869123 Cc1ccc(CNc2nc(CN(CCO)[C@H]3CS(=O)(=O)C[C@@H]3O)nc3cccc23)cc1  
 ZINC38995126 CC1=C[C@H]([C@H]2NN[C@H](SCc3ccc(Br)cc3)N2N)N=N1  
 ZINC44165545 O=C(NC[C@H]1CCCO1)[C@@H]1CSC[C@H](e2ccc3c(e2)OCCO3)N1  
 ZINC63625887 COc1ccc2c(c1)=C[C@H](C(=O)NNC(=O)COCC(=O)NC13CC4CC(CC(C4)C1)C3)N=2  
 ZINC15959687 COc1ccc(CCN2C(=O)[C@H]3[C@H](CC(N)=O)N[C@]4(C(=O)Nc5c(C)cc(C)cc54)[C@@H]3C2=O)cc1OC  
 ZINC63878202 Cc1ccc(C(N)=O)cc1NS(=O)(=O)e1cccc2nsnc12  
 ZINC39995978 CC1=C(C(=O)NNC(=O)Cn2c(S)nnc2-e2ccc(C)cc2)CCO1  
 ZINC43751419 CN1N=C(C(=O)Nc2nc(C(F)(F)F)n[nH]2)CCC1=O  
 ZINC61381104 O=C1CCc2cc(NC(=O)e3cccc(-n4nc(O)ccc4=O)c3)ccc2N1  
 ZINC20611200 COc1ccc(CCN2C(=O)[C@H]3[C@H](CC(N)=O)N[C@]4(C(=O)Nc5c4ccc(C)c5C)[C@@H]3C2=O)cc1OC  
 ZINC65419302 Cc1ccnc(NCCNC(=O)[C@H]2CCCN(C(=O)N(C)C)C2)c1  
 ZINC21324986 C/C(=N)\c1nnc(SCC(=O)N[C@H](C)e2cccc2)n1N)e1cccn1  
 ZINC00086260 CCc1c(O)e2c(=O)n(C)c(=O)n(C)c2n(C)c1=O  
 ZINC04083625 COc1ccc(N2C(=O)[C@H]3[C@H]([C@@H](C)O)N[C@]4(C(=O)Nc5cccc54)[C@@H]3C2=O)cc1  
 ZINC44713527 CC(C)(C)OC(=O)N1CC[C@H](Oe2c(N)cc(C(F)(F)F)cc2N)C1  
 ZINC04663941 Cc1cc(C(=O)N/N=C/c2cc(Br)cc([N+](=O)[O-])e2O)n[nH]1  
 ZINC66230822 [C@H](NC(=O)C1CCC1)C(=O)/C(C#N)=C(\O)Nc1cccc(Cl)c1Cl  
 ZINC29730105 Cc1occc1C(=O)NNC(=O)NCc1cnc(N2CCCC2)c1  
 ZINC49544857 COc1nnc(NC(=O)e2cnc3ccc(C)n3e2=O)s1  
 ZINC67106460 C/C(=C/C(=O)NNc1nnc(C)c(O)n1)c1cccc1Cl  
 ZINC17044889 COc1ccc([C@H]2CC(=O)Nc3nc(-e4cccc4)[nH]c(=O)c32)ccc1OCC(N)=O  
 ZINC41237985 Cc1cc(NS(=O)(=O)CCNS(=O)(=O)e2c(C)noe2C)no1  
 ZINC24543914 COc1cc([C@H]2C3=C(CC(C)C)CC3=O)Nc3[nH]c(=O)[nH]c(=O)c32)cc1C1c1O  
 ZINC05816089 Oc1c(Br)cc(C=NNe2nnn[nH]2)cc1Br  
 ZINC54681330 N[C@@H](Cc1cc(Br)c2c(c1)OCO2)c1cccc1  
 ZINC16682580 CCOC(=O)C1=C(N)n2c(s/c(=C\c3ccco3)c2=O)=C(C(N)=O)[C@@H]1c1ccc1  
 ZINC17878453 NC1=NC(=O)[C@@H]([C@]2(O)C(=O)N(CCCc3cccc3)e3cccc32)S1  
 ZINC21903832 Cc1ccc(-e2nnc(S)n2CC(=O)NNC(=O)C(C)C)cc1  
 ZINC66812793 Nc1cnc(NC[C@H](O)COc2ccc(l)cc2)n1  
 ZINC06147391 O=C1Nc2cccc2/C1=N\NC(=O)c1nc2cccc2c(=O)[nH]1  
 ZINC38117525 [C[C@@](CO)(c1cc(F)c(Cl)cc1Cl)N1CCCNCC1  
 ZINC43238068 C[C@@H](N)[C@H](Sc1ccc(Br)cc1)c1enn(C)c1  
 ZINC16033039 COc1ccc(CN2C(=O)[C@H]3[C@H](CCC(N)=O)N[C@]4(C(=O)Nc5c(C)cccc54)[C@@H]3C2=O)cc1  
 ZINC58180947 Cc1ccc([C@@H](CNC(=O)CCe2c(C)[nH]c(=O)[nH]e2=O)N(C)C)cc1  
 ZINC67167734 Cc1cccc1[C@@H](CC(=O)Nc1c(F)cccc1N1CCCC1)NC(N)=O

ZINC17092278 O=C(O)[C@H]1CCCC[C@H]1C(=O)Nc1se2c(c1C(=O)N1CCOCC1)CCCC2

ZINC39551757 Cc1nc(NC2cccc(-n3enen3)e2)cc([C@H]2CCCN2)n1

ZINC08581704 O=C(Nc1ccc(N2CCC[C@H](O)C2)cc1)c1snc2c(O)ncnc12

ZINC66250841 Cn1cc(S(=O)(=O)/N=c2/[nH]c(CN3CCCCC3)es2)cc1C(N)=O

ZINC40054987 Cc1ccc([C@H]2C(C(=O)c3cccc(OCc4ccc(F)cc4)c3)=C(O)C(=O)N2CCCO)cc1

ZINC23143208 O=C1C[C@@H](/C(O)=N/e2nen[nH]2)CN1c1ccc2c(c1)OCCO2

ZINC09089994 Cc1cc(/C=C2.C(=O)NC(=S)N=C2O)c(C)n1-c1ccc(I)c1

ZINC09089994 Cc1cc(/C=C2.C(=O)NC(=S)N=C2O)c(C)n1-c1ccc(I)c1

ZINC15082922 Cc1cc(=O)[nH]c(SCC(=O)Nc2[nH]c(C)c(C)c2C#N)n1

ZINC09041487 COCCCN1C(=O)N=C(O)C=C2.C[C@H](c3c(Cl)cccc3Cl)NN2)C1=O

ZINC09041487 COCCCN1C(=O)N=C(O)C=C2.C[C@H](c3c(Cl)cccc3Cl)NN2)C1=O

ZINC20323969 Cc1ccc(N2C(=O)NC(=O)/C(=C/NCCCN(C)C)C2=O)cc1C

ZINC08691664 O=C(N/N=C/c1ccc(F)c1)c1c(O)[nH]e2cccc2c1=O

ZINC22645914 C[C@H](Se1n[nH]c(N)n1)C(=O)N(C)Cc1ccc(Br)cc1

ZINC64890715 CC(C)[C@H](NS(=O)(=O)c1ccc1)[C@H]1N=C(c2ccc3c(e2)[nH]c(=O)c(=O)n3C(C)C)NO1

ZINC13126479 Cc1ccc2oc(-e3cc(NC(=O)e4nc[nH]n4)ccc3O)nc2c1

ZINC26258525 CSc1nc2nc(C)c(C/O)=N/e3nen[nH]3)c(C)n2n1

ZINC38702041 O=C1c2[nH]nc(-c3cc(Cl)ccc3O)e2[C@@H](c2cccc2F)N1[C@@H]1CCS(=O)(=O)C1

ZINC38702041 O=C1c2[nH]nc(-c3cc(Cl)ccc3O)e2[C@@H](c2cccc2F)N1[C@@H]1CCS(=O)(=O)C1

ZINC66783234 Cc1ccse1C(=O)NNC(=O)c1cccc(-n2nc(O)ccc2=O)c1

ZINC40348244 Cc1csc(CNS(=O)(=O)e2ccc(Br)cc2N)n1

ZINC43238061 Cn1cc([C@@H](CN)Se2ccc(Br)cc2)cn1

ZINC63432845 CNC(=O)C1CCC(NC(=O)C(=O)Nc2cc(Cl)cc(Cl)e2)CC1

ZINC13564105 Cc1nc(O)e2nsc(C(=O)Nc3ccc(N4CCC[C@@H](O)C4)cc3)e2n1

ZINC38999559 NN1[C@@H](SCC(=O)N2CCOCC2)NN[C@@H]1[C@H]1C=C(c2ccc(Cl)cc2)N=N1

ZINC15133482 CCOC(=O)[C@@]1(C#N)[C@@H]2C=CC(C(N)=O)=CN2[C@@H](C(N)=O)[C@@H]1c1ccc(I)c1

ZINC67605382 Cc1ccn2cc(CNC(=O)NC[C@H](O)COc3ccc4c(c3)OCO4)nc2c1

ZINC67491199 COC(=O)Nc1cc(NC(=O)C(=O)NCC2(N(C)C)CCCC2)ccc1F

ZINC64981111 Cc1cc(=O)[nH]c(SCC(=O)Nc2c(C#N)sc(=S)n2-c2cccc2)n1

ZINC63941319 COc1ccc2c(c1)=C(CCN1C[C@H](C(=O)N[C@H]3NN[C@@H](C(C)C)S3)CC1=O)CN=2

ZINC00075265 O=[N+](=[O-])C[C@@H](c1ccc1)c1c(O)n[nH]c1-e1ccc1O

ZINC66620481 N#CCCN(C(=O)CCC(=O)Nc1nc(C#N)c(C#N)[nH]1)c1ccc1

ZINC63775414 COc1cc2c(cc1OC)C(=O)N[C@@H](c1cc(Cl)cc([N+](=O)[O-])c1O)N2

ZINC08295942 CC(C)C/N=C1\S[C@H]2[C@H]([C@@H](O)[C@H](O)C[C@@H]2C(N)=O)N1CC1CCCCC1

ZINC29730105 Cc1occc1C(=O)NNC(=O)NCc1cnc(N2CCCC2)c1

ZINC44163248 CSe1cccc(Ne2nnc(-c3coc([C@@H](N)C(C)C)n3)o2)c1

ZINC22263737 C=CCn1c(=S)[nH]e2cc(C(=O)Nc3ncccc3O)ccc2c1=O

ZINC47343057 O/C(=N/c1nc(-e2cccn2)n[nH]1)c1ccc(-n2enen2)cc1

ZINC06830290 CCn1c(O)c(C(=O)Nc2ccc([N+](=O)[O-])cc2O)c(=O)e2cccc21

ZINC11869123 Cc1ccc(CNc2nc(CN(CCO)[C@H]3CS(=O)(=O)C[C@@H]3O)nc3ccc23)cc1

ZINC58157772 CCNC(=O)NC(=O)[C@@H](C)N1CCCN(c2nc(C)es2)CC1

ZINC02264694 COc1ccc(-n2c3c(c(=O)[nH]e2=O)[C@](NC(=O)e2cccc(Cl)e2)(C(F)(F)F)C(=O)N3)cc1

ZINC06320618 Cc1cc(C(=O)N/N=C/e2cc([N+](=O)[O-])cc(Br)e2O)[nH]n1

ZINC16853037 Cc1nc(/C=C/c2enc(O)[nH]e2=O)c(CCC(C)C)c(=O)[nH]1

ZINC67458914 Cc1ce2nc(CNC(=O)c3cc(CN4CCC[C@@H](O)C4)on3)[nH]e2cc1C

ZINC54896816 CN(Cc1ccc(Cl)s1)c1nc2e(s1)[C@@H](N)CCC2

ZINC17965002 CCn1c(O)c2ccc(C(=O)N[C@H](C)c3ccccc3Br)cc2nc1=S

ZINC40049070 CCCOc1ccc(C(=O)C2=C(O)C(=O)N(CCCO)[C@H]2c2c(Cl)cccc2C1)cc1C

ZINC17444921 CCCc1mnc(S)n1CC(=O)NNC(=O)c1cc(C)n(-e2ccc(F)cc2)c1C

ZINC12473322 NC(=O)c1nc(C(=O)N(c2ccc(F)cc2)[C@@H](C(=O)NC[C@@H]2CCCO2)c2ccc(F)cc2)c1N

ZINC40053253 COc1cccc2cc(C(=O)C3=C(O)C(=O)N(CCCO)[C@H]3c3ccc(C(C)(C)C)cc3)oc12

ZINC00086260 CCc1c(O)c2c(=O)n(C)c(=O)n(C)c2n(C)c1=O

ZINC54453778 COc1cccc1N/C(O)=C(\C#N)C(=O)Cn1ccc([N+](=O)[O-])n1

ZINC13564105 Cc1nc(O)e2nsc(C(=O)Nc3ccc(N4CCC[C@@H](O)C4)cc3)e2n1

ZINC59595249 COc1ccc(N2C(=O)/C=C/c3c(C)[nH]c4ccccc34)C(O)=NC2=S)c(OC)c1

ZINC09410142 COc1cc([C@H]2CC(=O)Nc3nc(-c4ccccc4)[nH]c(=O)c32)ccc1OCC(N)=O

ZINC08846175 C=CCOc1ccc([C@H]2C(C#N)=C(N)Oc3ccc(N)ccc32)cc1OCC

ZINC17044889 COc1cc([C@H]2CC(=O)Nc3nc(-c4ccccc4)[nH]c(=O)c32)ccc1OCC(N)=O

ZINC38999554 NN1[C@@H](SCC(=O)N2CCOCC2)NN[C@H]1[C@H]1C=C(c2ccc(Cl)cc2)N=N1

ZINC40548144 O=C1c2[nH]nc(-c3cc(Cl)ccc3O)c2[C@@H](c2ccc(F)cc2)N1[C@H]1CCS(=O)(=O)C1

ZINC17575813 O=C(NNC(=O)c1c[nH]c(=S)n1-c1ccccc1)c1ccccc1O

ZINC09041487 COCCCN1C(=O)N=C(O)/C=C2/C[C@H](c3c(Cl)cccc3Cl)NN2)C1=O

ZINC09041487 COCCCN1C(=O)N=C(O)/C=C2/C[C@H](c3c(Cl)cccc3Cl)NN2)C1=O

ZINC17067424 O=C1C(/C=C/c2nc(O)c([N+](=O)[O-])c(=O)[nH]2)=CO[C@H]2C=CC=C[C@H]12

ZINC67574707 CN(C)C(=O)Cn1cc(C/O)=N/e2nc(-c3ccccc3Cl)n[nH]2)nn1

ZINC62828474 COC(=O)C(C)(C)NC(=O)Nc1sc(C)c(C)c1C(=O)O

ZINC62828748 Cc1cc([C@@H](C)NC(=O)Nc2sc2c(=O)O)c(C)o1

ZINC47164109 CCOC(=O)C[C@H]1C(=O)NCCN1S(=O)(=O)c1ccc2nc(O)oc2c1

ZINC40707512 CCNc1nnc(N2CCN(Cc3ccc4c(c3)OCO4)CC2)c1N

ZINC40820358 O=C(c1cc(=O)[nH]c(O)n1)N1CCC[C@@H]1c1c[nH]e2cc(Cl)ccc12

ZINC13467983 CC1=N[C@@]2(O)c3ccccc3C(=O)[C@@]2(O)C1C(=O)O[C@H]1CCCN(C)C1

ZINC39458027 Cc1c(S(=O)(=O)C(C)C)c2c(n1O)-c1nccc(-c3ccccc3O)c1C(=O)CC2

ZINC32283221 CCn1c(O)c2ccc(C(=O)N[C@@H](C)c3ccc4c(c3)OCCCO4)cc2nc1=S

ZINC39940171 [C@H]1NNC(=O)C2=C1[C@@H](C)O[C@@H]2NC(=O)CS[C@H]1NN=C(C2CC2)N1c1ccccc1

ZINC41069947 [C@H]1CCC[C@H](NS(=O)(=O)c2cc(Br)ene2NN)[C@@H]1C

ZINC07286538 COc1cc2nc(CS/C(N)=N/C(C)(C)C)[nH]c(=O)c2cc1OC

ZINC40085222 COc1ccc(C(=O)C2=C(O)C(=O)N(CCO)[C@H]2c2cccc(Br)c2)cc1C

ZINC36320697 CN(C1CCOCC1)[C@H](CN)c1c(Cl)cccc1C1

ZINC40141092 Cc1nc2c(C#N)enn2c(O)c1CC(=O)Nc1ccccc1C(=O)NC1CCCC1

ZINC61461221 Cc1ccc2nc([C@@H]3CCCN3C(=O)c3cnc4nc(O)[nH]c(=O)c4c3)[nH]c2c1

ZINC55243565 CCc1n[nH]c(SCC(=O)N2Cc3ccccc3[C@@H]2C(N)=O)n1

ZINC19902346 N#CC1=C(N)C(C#N)(C#N)[C@H](c2ccc([C@@H]3[C@H]4CCCC=C4C(C#N)=C(N)C3(C#N)C#N)cc2)[C@@H]2CC

ZINC40085178 COc1ccc(C(=O)C2=C(O)C(=O)N(CCOCCO)[C@H]2c2cccc3ccccc23)cc1C

ZINC00971479 O=c1[nH]c(O)nc2c1sc1nc(-c3ccc4c(c3)OCCCO4)cc(C(F)(F)F)c12

ZINC06058013 O=C(N/N=C/c1ccccc(O)c1)c1c(O)n2c3c(cccc3c1=O)CCC2

ZINC67588199 CC1=NC(=O)C2(CCN(C[C@]3(O)CCCN(CC4ccccc4)C3=O)CC2)N1

ZINC67267965 Cc1ccc([C@H](CNC(=O)CCc2c(C)nc3nc(N)nn3c2C)N(C)C)cc1

ZINC35363867 CC(=O)Oc1ccc(N2C(=O)[C@@H]3[C@H](Cc4ccc(O)c(O)c4)N[C@@]4(C(=O)Nc5ccccc54)[C@@H]3C2=O)cc1

ZINC00075265 O=[N+](O)C[C@@H](c1cccc1)c1c(O)n[nH]c1-c1cccc1O

ZINC64886428 Ce1ccc(-e2enc(CCC(=O)NNC(=O)NCCCn3cenc3)o2)cc1

ZINC22130310 COc1cccc(NC(=O)[C@@H]2C(S)=NC(N)=C(C#N)[C@H]2e2ccc(F)cc2)c1

ZINC36597690 Ce1ccc(CN(C(=O)c2cccc(O)c2O)[C@H](C(=O)NC2CCCC2)e2c(O)cc(O)c2O)o1

ZINC12473329 NC(=O)c1nsc(C(=O)N(c2ccc(F)cc2)[C@H](C(=O)NC[C@@H]2CCCO2)c2ccc(F)cc2)c1N

ZINC39978610 CCOC(=O)N1CCC2=C3C(O)=N[C@@H]([C@@H]4C=CC=N4)N[C@H]3S[C@@H]2C1

ZINC24378639 C=CCNC(=O)NC(=O)[C@H](C)N(C)CC(=O)Nc1c(C)cc(C)cc1C

ZINC12711216 Ce1cccc(N(C(=O)c2snc(C(N)=O)c2N)[C@H](C(=O)NC[C@@H]2CCCO2)e2cccs2)c1

ZINC22130310 COc1cccc(NC(=O)[C@@H]2C(S)=NC(N)=C(C#N)[C@H]2e2ccc(F)cc2)c1

ZINC38701992 O=C1e2n[nH]c(-e3cc(Cl)ccc3O)c2[C@H](c2cccc2)N1[C@@H]1CCS(=O)(=O)C1

ZINC15957797 COc1cccc1CN1C(=O)[C@@H]2[C@H](CC(N)=O)N[C@@]3(C(=O)Nc4cccc43)[C@@H]2C1=O

ZINC00971479 O=c1[nH]c(O)nc2c1sc1nc(-e3ccc4c(c3)OCCO4)cc(C(F)(F)F)c12

ZINC39468579 O=C(c1cc(=O)[nH]c(=O)[nH]1)N1CCC[C@@H](Nc2ccc(F)c(F)c2)C1

ZINC39693576 Ce1ccc(CC(=O)N2C[C@H](C(=O)NCCNC(=O)OC(C)C)C3(CCNCC3)C2)cc1

ZINC14960513 CCN(CC)C(=O)[C@H]1CCCN(Ce2ccc(C(=O)NCC3(O)CCCC3)c(=O)[nH]2)C1

ZINC61461221 Ce1ccc2nc([C@@H]3CCCN3C(=O)c3cnc4nc(O)[nH]c(=O)e4c3)[nH]c2c1

ZINC02264694 COc1ccc(-n2c3c(c(=O)[nH]e2=O)[C@](N(C(=O)c2cccc(Cl)c2)(C(F)(F)F)C(=O)N3)cc1

ZINC25027857 CC[C@H](C)NC(=O)[C@H](C)N1CCN(Ce2nc(N)c3cccc3n2)CC1

ZINC12474048 Ce1cc(C)cc(N(C(=O)c2snc(C(N)=O)c2N)[C@H](C(=O)NC[C@@H]2CCCO2)e2ccc(O)cc2)c1

ZINC23143211 O=C1C[C@H](/C(O)=N/c2nen[nH]2)CN1c1ccc2c(c1)OCCO2

ZINC05310018 CCCNC(=O)NC(=O)CSc1nc2ncc(Cl)cc2[nH]1

ZINC05310018 CCCNC(=O)NC(=O)CSc1nc2ncc(Cl)cc2[nH]1

ZINC41634251 Ce1nc2se([C@H](c3cccc3)N(CCO)CCO)c(O)n2n1

ZINC63557818 CCOC[C@H]1NN[C@@H](NC(=O)[C@@H]2CC(=O)N(CCC3=C4cc(C)ccc4=NC3)C2)S1

ZINC40096818 CCCCNC(=O)C(O)=C(C(=O)c2ccc3c(c2)OCCO3)[C@H]1c1cccc(O)c1

ZINC54728911 Ce1c(/C(O)=C(C#N)C(=O)Nc2cccn2)[nH]e2c1C(=O)CCC2

ZINC65373061 CN(C)c1nc2c(c(=O)[nH]1)CCN(C(=O)[C@H]1CC13CCNCC3)CC2

ZINC47343057 O/C(=N)c1nc(-e2cccn2)n[nH]1)c1ccc(-n2enen2)cc1

ZINC35653334 C[C@H](Oc1cccc1)c1n[nH]c(=S)n1N

ZINC40026252 C=CCNC(=O)C(O)=C(C(=O)c2ccc(OC)cc2)[C@H]1c1ccc(OCC(N)=O)cc1

ZINC09110631 Cn1c(=O)[nH]c(=O)c2c1nc(N1CCNCC1)n2C[C@@H](O)COc1ccc2cccce2c1

ZINC24543918 COc1cc([C@H]2C3=C(CC(C)C)CC3=O)Nc3[nH]c(=O)[nH]c(=O)c32)cc(1)c1O

ZINC09410142 COc1cc([C@H]2CC(=O)Nc3nc(-e4cccc4)[nH]c(=O)c32)ccc1OCC(N)=O

ZINC22263984 O=C(CN1C(=O)N[C@@]2(CCCc3cccc32)C1=O)Nc1cccc1O

ZINC18211452 NC1=C(O)C(=O)[C@H](c2cccc2)O1

ZINC66510661 CCn1c(=O)[nH]e2cc(/C(O)=C(C#N)C(=O)NC3CCCC3)ccc2c1=O

ZINC40109332 O=C(C1=C(O)C(=O)N(CCO)[C@@H]1c1ccc(Cl)cc1)c1cccc(OCc2ccc(F)cc2)c1

ZINC08993831 CN(CC(=O)NN1C(=O)N[C@@]([C@@H](C)CCc2cccc2)C1=O)Cc1nc2cccce2c(=O)[nH]1

ZINC59595249 COc1ccc(N2C(=O)C(=C/c3c(C)[nH]c4cccc34)C(O)=NC2=S)c(OC)c1

ZINC65063467 O=C(NC1CC1)c1ccc(Oc2ccc(NS(=O)(=O)c3ccc(Brs3)cc2)nc1

ZINC09334391 O=C(NC1CC1)c1c(O)c2c([nH]c1=O)CCCC2

ZINC00971479 O=c1[nH]c(O)nc2c1sc1nc(-e3ccc4c(c3)OCCO4)cc(C(F)(F)F)c12

ZINC20431210 CN1C(=O)Cc2cc([C@@H](N)Cc3ccc(Br)cc3)ccc21

ZINC43259797 COC1CCN([C@H](c2ccc(Brs2)[C@@H](C)N)CC1

ZINC40707512 CCNc1ncnc(N2CCN(Cc3ccc4c(c3)OCO4)CC2)c1N

ZINC14331468 NC(=O)Cc1csc(NC(=O)c2cc(Br)ccc2O)n1

ZINC40268165 CS(=O)(=O)N1CCN([C@H](C(=O)O)c2c[nH]c3ccc(OCC#N)cc23)CC1

ZINC13126479 Ce1ccc2oc(-c3cc(NC(=O)c4nc[nH]n4)ccc3O)nc2c1

ZINC54029016 Ce1cc(C)c(NC(=O)CNC(=O)NCCc2cnc2)c(C)c1

ZINC06147391 O=C1Nc2ccccc2/C1=N\NC(=O)c1nc2ccccc2c(=O)[nH]1

ZINC40115133 Ce1nc2c(C#N)cn2c(O)c1CC(=O)N[C@@H](c1ccc(F)cc1)c1ccs1

ZINC65063467 O=C(NC1CC1)c1ccc(Oc2ccc(NS(=O)(=O)c3ccc(Br)s3)cc2)nc1

ZINC39396295 O=C(N[C@H]1NC(SCc2ccc(F)cc2)=NS1)c1n[nH]1

ZINC66229911 Ce1nn(C)c(C)c1S(=O)(=O)N=C(O)[C@@H](C)NC(=O)C1CCC1

ZINC36597690 Ce1ccc(CN(C(=O)c2ccccc2O)c2O)[C@H](C(=O)NC2CCCC2)c2(O)cc(O)cc2O)o1

ZINC12711234 Ce1ccc(N(C(=O)c2snc(C(N)=O)c2N)[C@@H](C(=O)NC[C@H]2CCCO2)c2cccs2)cc1

ZINC67574707 CN(C)C(=O)Cn1cc(C(O)=N/e2nc(-c3ccccc3Cl)n[nH]2)nn1

ZINC41181804 CC(C)C[C@@H](N)c1nc(-c2ccc(OC(F)F)cc2)cs1

ZINC49417820 CC(C)S(=O)(=O)N=C(O)c1nc2n(c1=O)CCS2

ZINC61589981 NC[C@@]1(N2CCN(c3ccccc3Cl)CC2)CCCSC1

ZINC38128012 N[C@@H](Cc1c(F)ccc1Cl)c1ccccc1OCCO2

ZINC35575997 COCCOC(=O)C1=C(c2ccccc2)Nc2[nH]c(=O)[nH]c(=O)c2[C@H]1c1ccc(O)cc1

ZINC01425499 CN1C(=O)N[C@@H](c2ccc(O)cc2)C2=C1CN(c1ccc(N3CC4=C(C3=O)[C@H](c3ccc(O)cc3)NC(=O)N4C)cc1)C

ZINC39453061 COc1ccc2nc3c4c(n(-c5ccccc5O)c(=O)c3cc12)C(=O)C[C@@H](SC)N4

ZINC65489377 CCn1c(O)c2ccc(C(=O)NCc3cc(Br)cs3)cc2nc1=S

ZINC67044320 Ce1ccc(C(=O)NNC(=O)NCCc2cn3c(n2)CCCC3)c1

ZINC33533935 COc1cc([C@@H]2C(C(=O)c3ccc(C)o3)=C(O)C(=O)N2CCc2ccccc2)cc(Br)c1O

ZINC62982325 NCC#Cc1ccc(CN2CC[C@@H](N3CCCC3)C2)s1

ZINC03101251 O=C(N/N=C/c1cc([N+](=O)[O-])ccc1O)C(=O)Nc1ccc(F)cc1

ZINC65373061 CN(C)c1nc2c(c(=O)[nH]1)CCN(C(=O)[C@H]1CC13CCNCC3)CC2

ZINC22263737 C=CCn1c(=S)[nH]c2cc(C(=O)Nc3nccc3O)ccc2c1=O

ZINC05728860 O=C(N/N=C/c1ccccc(Br)c1)c1c[nH][nH]c1=O

ZINC05728860 O=C(N/N=C/c1ccccc(Br)c1)c1c[nH][nH]c1=O

ZINC07220106 Ce1ccc(NCC(=O)NNC(=O)CCCN2C(=O)NC3(CCCC3)C2=O)c(C)c1

ZINC20721099 COc1ccc(N2C[C@@H](C(=O)Nc3nc[nH]n3)CC2=O)c(OC)c1

ZINC44930858 COC(=O)c1cc(S(=O)(=O)NCc2nn[nH]2)c(Br)s1

ZINC61589982 NC[C@@]1(N2CCN(c3ccccc3Cl)CC2)CCCSC1

ZINC40085702 CCOc1ccc(C(=O)C2=C(O)C(=O)N(CCO)[C@H]2c2ccccc(Oc3ccccc3)c2)cc1C

ZINC40095297 [C@H]1Cc2cc(C(=O)C3=C(O)C(=O)N(CCO)[C@H]3c3ccccc(Br)c3)ccc2O1

ZINC37448211 COc1ccc([C@@H]2[C@@H](C(N)=O)C(=O)N[C@@](O)(c3ccccc3)[C@H]2C#N)cc1[N+](=O)[O-]

ZINC22263737 C=CCn1c(=S)[nH]c2cc(C(=O)Nc3nccc3O)ccc2c1=O

ZINC32283221 CCn1c(O)c2ccc(C(=O)N[C@@H](C)c3ccc4c(c3)OCCCO4)cc2nc1=S

ZINC39448679 N#Cc1nc(Cl)nc1NC(=N/O)/C(=N/O)c1ccccc1

ZINC16611283 CC[C@@H](C)n1c(O)c([C@@H]2NCc3e2[nH]e2ccccc32)c(=O)[nH]c1=O

ZINC39396295 O=C(N[C@H]1NC(SCc2ccc(F)cc2)=NS1)c1n[nH]1

ZINC06359840 CCCC[C@@]1(CC)C(=N)NC(=O)NC1=O

ZINC61622259 Ce1ccc(-e2n[nH]c(NC(=O)c3ccc(NC4CC4)nc3)n2)s1

ZINC67157716 CCCC(=O)N1CSC[C@@H]1C(=O)Nc1nc(S(C)(=O)=O)n[nH]1



ZINC09424629 Cc1cccc1COe1ccc(C(=O)C2=C(O)C(=O)N(Cc3ccco3)[C@H]2e2cccc(O)e2)cc1

ZINC45875575 C[C@@]1(NNC(=O)NCe2ccc(N3CCCCC3)nc2)CCS(=O)(=O)C1

ZINC17307672 CCN(C(=O)CN(C)Cc1ccse1)c1c(N)n(Ce2ccc2)c(=O)[nH]e1=O

ZINC20611110 COe1cccc1CN1C(=O)[C@@H]2[C@H](CC(N)=O)N[C@@]3(C(=O)Nc4ccccc43)[C@@H]2C1=O

ZINC61847453 CC1(C)Ce2nc(-c3ccc(F)cc3Cl)nc2[C@@H](N)C1

ZINC19597268 CCCCOC1ccc(C2C(C#N)=C(N)SC(N)=C2C#N)cc1OC

ZINC66220146 CSc1ccc(NC(=O)C(=O)NCe2cn3c(n2)CCCC3)cn1

ZINC66229912 Cc1nn(C)c(C)c1S(=O)(=O)N=C(\O)[C@H](C)NC(=O)C1CCC1

ZINC39996660 C=CCNC(=O)NC(=O)CS[C@H]1NN=C(C2=c3ccccc3=NC2)N1C1CC1

ZINC39958156 [C@H]1CN(CC2=N[C@@H]3C(=N2)C(O)=NC(=O)N3C)C[C@H](C)O1

ZINC08581704 O=C(Nc1ccc(N2CCC[C@H](O)C2)cc1)c1snc2(O)nenc12

ZINC65506259 Cc1nn2cc(CCNc3nc(CCN)nc4sc(C)c(C)c34)nc2s1

ZINC39448113 CCCc1nnc(S)n1CC(=O)N(C)CC1=CN(c2ccc2)N[C@@H]1c1ccc(Cl)cc1

ZINC15070035 COe1cccc1-n1cc(CNC[C@]2(O)CCCN(C)C2=O)cn1

ZINC65692295 Nc1nc2nc(CSe3c(F)cc(F)cc3F)cc(O)n2n1

ZINC44930858 COC(=O)c1cc(S(=O)(=O)NCe2nnn[nH]2)c(Br)s1

ZINC64981111 Cc1cc(=O)[nH]c(SCC(=O)Nc2c(C#N)sc(=S)n2-c2ccc2)n1

ZINC66080059 Cc1nc2nc(=S)n(CN3CCC[C@H](C)C(C)C3)nc2(C)c1C

ZINC40095593 COe1cccc1[C@@H]1C(C(=O)c2ccc3c(e2)C[C@H](C)O3)=C(O)C(=O)N1CCO

ZINC24543918 COc1cc([C@H]2C3=C(CC(C)C)CC3=O)Nc3[nH]c(=O)[nH]c(=O)e32)cc(1)c1O

ZINC55758114 Cc1nc2nc(N)nn2c(C)c1CC(=O)N[C@H](C)CN1C[C@@H](C)C[C@H](C)C1

ZINC21324992 C/C(=N)Nc1nnc(SCC(=O)N[C@@H](C)c2ccc2)n1N)c1cccn1

ZINC56908817 COe1nn(C)cc1C(=O)N1CCC[C@H](C(=O)Nc2ccc(NS(C)(=O)=O)e2)C1

ZINC45621003 [C@]1(C2CC2)NC(=O)N(CC(=O)Nc2cc(Cl)c(N)c(Cl)e2)C1=O

ZINC54160628 C[C@H](N)c1enc(-e2cc(Br)c(Br)o2)s1

ZINC64152362 CC[C@@H](C)C(=O)NC[C@@H]1NN[C@H]2CCN(C(=O)CCC3=e4ccccc4=NC3)CCN21

ZINC44755163 Cc1nc(-e2c[nH]c(C(=O)Nc3ccc4oc(O)nc4c3)c2)es1

ZINC15957797 COe1cccc1CN1C(=O)[C@@H]2[C@H](CC(N)=O)N[C@@]3(C(=O)Nc4ccccc43)[C@@H]2C1=O

ZINC46618854 C=CCn1c(S)nc2cc(C(=O)N[C@@H](C)c3ccc(OCC(C)C)c(OC)c3)ccc2c1=O

ZINC09331256 COe1cccc1N1C(=O)N=C(O)/C(=C\NN2CCOCC2)C1=O

ZINC44931949 Cn1enc(S(=O)(=O)NCe2nnn[nH]2)c1Cl

ZINC24543914 COe1cc([C@@H]2C3=C(CC(C)C)CC3=O)Nc3[nH]c(=O)[nH]c(=O)e32)cc(1)c1O

ZINC39545437 CON(C(=O)[C@@H]1CC(Cl)=C2Nc3ccccc3CN21)c1ccccc1O

ZINC19323678 CCCC12CN3CC(C)(CN(C1)C3c1[nH]c(=O)[nH]c(=O)c1C)C2=O

ZINC48733572 O=C(Nc1n[nH]c(C(F)F)n1)c1ensn1

ZINC17878453 NC1=NC(=O)[C@@H]([C@]2(O)C(=O)N(CCCc3ccccc3)e3ccccc32)S1

ZINC41062484 Cc1n[nH]c(Se2ccc(C#N)cc2N)n1

ZINC08492620 COe1ccc([C@H]2C3=C(O)CCCC3=Nc3nc(S)nc(N)c32)cc1

ZINC39676238 C[C@H](Oe1cccc1)C(=O)N1C[C@@H](C(=O)NCe2nc3ccccc3e(=O)[nH]2)C2(CCNCC2)C1

ZINC26258525 CSe1nc2nc(C)c(C/C(O)=N/c3nc[nH]3)c(C)n2n1

ZINC58296359 Cc1cc2n(n1)C[C@H](CNCCS(=O)(=O)c1ccccc1)CN2

ZINC47164109 CCOC(=O)C[C@H]1C(=O)NCCN1S(=O)(=O)c1ccc2nc(O)oc2c1

ZINC00987723 CCOe1ccc(/N=C2N=C(O)C[C@@H](C(=O)Nc3ccc(C)cc3)N2)cc1

ZINC39869881 CN1C(=O)/C(=C2\SC(Nc3ccccc3C(N)=O)=NC2=O)c2ccccc21

ZINC20427795 N[C@H](Cc1nc2ccccc2o1)c1cccc(Cl)c1Cl

ZINC24543914 COc1cc([C@@H]2C3=C(CC(C)(C)CC3=O)Nc3[nH]c(=O)[nH]c(=O)c32)cc(1)c1O

ZINC09501249 Cc1c(C#N)c(NC(=O)CN2Cc3ccccc3[C@H]2C(N)=O)n(C[C@@H]2CCCCO2)c1C

ZINC40028276 C=CCN1C(=O)C(O)=C(C(=O)c2cc3ccccc3o2)[C@H]1c1cc(Br)c(O)c(OC)c1

ZINC05816089 Oe1c(Br)cc(C=NNc2nm[nH]2)cc1Br

ZINC36320697 CN(C1CCOCC1)[C@H](CN)c1c(Cl)cccc1Cl

ZINC23338448 Cc1n[nH]c(/N=C(\O)N2CCC[C@H](C(=O)N3CCOCC3)C2)n1

ZINC25784140 Nc1none1-n1nnc(C=O)N/N=C\c2c(O)ccc3ccccc23)c1CN1CCc2ccccc21

ZINC36597690 Cc1ccc(CN(C(=O)c2cccc(O)c2O)[C@H](C(=O)NC2CCCC2)c2c(O)cc(O)cc2O)o1

ZINC46618854 C=CCn1c(S)nc2cc(C(=O)N[C@@H](C)c3ccc(OCC(C)C)c(OC)c3)ccc2c1=O

ZINC08492620 COc1ccc([C@H]2C3=C(O)CCCC3=Ne3nc(S)nc(N)c32)cc1

ZINC07286538 COc1cc2nc(CS/C(N)=N/C(C)(C)[nH]c(=O)c2cc1OC

ZINC06860590 CCc1ccccc1N(C(=O)c1snc(C(N)=O)c1N)[C@H](C(=O)NC1CCCCC1)c1ccc(F)cc1

ZINC25782523 C/C(=N)NC(=O)c1c(CN2CCCC2)nmn1-c1none1N)c1cc(C)sc1C

ZINC39676236 C[C@H](Oc1ccccc1)C(=O)N1C[C@H](C(=O)NCc2nc3ccccc3c(=O)[nH]2)C2(CCNCC2)C1

ZINC38702041 O=C1e2[nH]nc(-c3cc(Cl)ccc3O)c2[C@@H](c2ccccc2F)N1[C@@H]1CCS(=O)(=O)C1

ZINC38702041 O=C1e2[nH]nc(-c3cc(Cl)ccc3O)c2[C@@H](c2ccccc2F)N1[C@@H]1CCS(=O)(=O)C1

ZINC63351980 C[C@H](NC(=O)N[C@H]1C[C@H]1c1ccccc(F)c1)c1ccc(NS(C)(=O)=O)c1

ZINC40049070 CCCOc1ccc(C(=O)C2=C(O)C(=O)N(CCCO)[C@H]2c2c(Cl)cccc2Cl)cc1C

ZINC24543918 COc1cc([C@H]2C3=C(CC(C)(C)CC3=O)Nc3[nH]c(=O)[nH]c(=O)c32)cc(1)c1O

ZINC09424629 Cc1ccccc1COc1ccc(C(=O)C2=C(O)C(=O)N(Cc3ccccc3)[C@H]2c2cccc(O)c2)cc1

ZINC48733572 O=C(Nc1n[nH]c(C(F)(F)F)n1)c1cnsn1

ZINC40028276 C=CCN1C(=O)C(O)=C(C(=O)c2cc3ccccc3o2)[C@H]1c1cc(Br)c(O)c(OC)c1

ZINC38999554 NN1[C@@H](SCC(=O)N2CCOCC2)NN[C@H]1[C@H]1C=C(c2ccc(Cl)cc2)N=N1

ZINC40126476 COc1ccc([C@H]2NC(=O)C(O)=C2C(=O)c2cccc(OCc3ccccc3Cl)c2)c1OC

ZINC40077275 COc1ccc(C(=O)C2=C(O)C(=O)N(CCOCCO)[C@H]2c2ccc(Cl)cc2Cl)cc1

ZINC38789740 C=CCOC(=O)C1=C(C)S[C@H](NC(=O)CSc2nc(C)C(C#N)c(=O)[nH]2)N1

ZINC67574707 CN(C)C(=O)Cn1cc(/C(O)=N/e2nc(-c3ccccc3Cl)n[nH]2)nn1

ZINC61622259 Cc1ccc(-e2n[nH]c(NC(=O)c3ccc(NC4CC4)nc3)n2)s1

ZINC14141828 CC(=O)N[C@H](CC(=O)Nc1sc2c(c1C(N)=O)CC[C@H](C)C2)c1ccccc1

ZINC28866467 COc1cc(OC)cc(C(=O)N[C@H](N/C(=N/C#N)Nc2ccc(Cl)nc2)C(C)(Cl)Cl)c1

ZINC58157772 CCNC(=O)NC(=O)[C@@H](C)N1CCCN(c2nc(C)es2)CC1

ZINC14074751 Cc1c(C#N)c(NC(=O)CN(CC(N)=O)C(C)C)n(C2CCCC2)c1C

ZINC12711232 Cc1ccc(N(C(=O)c2snc(C(N)=O)c2N)[C@H](C(=O)NC[C@@H]2CCCCO2)c2cccs2)cc1

ZINC67574707 CN(C)C(=O)Cn1cc(/C(O)=N/e2nc(-c3ccccc3Cl)n[nH]2)nn1

ZINC64981111 Cc1ccc(=O)[nH]c(SCC(=O)Nc2c(C#N)sc(=S)n2-c2ccccc2)n1

ZINC13126479 Cc1ccc2oc(-c3cc(NC(=O)c4nc[nH]n4)ccc3O)nc2c1

ZINC64890804 CCCn1c(=O)c(=O)[nH]c2cc(C3=N[C@@H]([C@H](NS(=O)(=O)c4ccccc4)C(C)C)ON3)ccc21

ZINC09329295 Cn1c(=O)c2c(nc(NN/C=C3/C(=O)NC(=O)N(c4ccccc45)C3=O)n2C)n(C)c1=O

ZINC09329295 Cn1c(=O)c2c(nc(NN/C=C3/C(=O)NC(=O)N(c4ccccc45)C3=O)n2C)n(C)c1=O

ZINC29493709 CCCC/N=C(N)SCC(=O)N1C[C@H](C(=O)NC)Oe2ccccc21

ZINC59403420 Cc1ccc(-e2n[nH]c(/N=C(\O)CNC(=O)c3ccccc3I)n2)n1

ZINC66390648 C[C@H](N[C@@H](C)c1ccc(N2CCN(C)CC2)c(F)c1)C(=O)NC(=O)NC1CC1

ZINC25490225 O=C1NC(=O)[C@H](Cc2cc([N+](=O)[O-])c(O)cc2[N+](=O)[O-])N1

ZINC39495613 O=CC[C@H](NC=O)c1cccc(-c2cccc2O)c(O)c1-c1cccc1O

ZINC35964152 CCN1C(=O)N[C@H](c2cccc2C(F)(F)F)C2=C1CN([C@H](Cc1cccc1)C(=O)O)C2=O

ZINC38789740 C=CCOC(=O)C1=C(C)S[C@H](NC(=O)CSc2nc(CC)c(C#N)c(=O)[nH]2)N1

ZINC49095442 CC[C@H](C)[C@H](C)NS(=O)(=O)c1cc(Br)enc1NN

ZINC22263737 C=CCn1c(=S)[nH]e2cc(C(=O)Nc3ncccc3O)ccc2c1=O

ZINC59198423 COc1cc(Cl)cc(/C=C2/C(=O)N(c3cccc(Br)c3)C(=O)N=C2O)c1O

ZINC40707512 CCNc1nenc(N2CCN(Cc3ccc4c(c3)OCO4)CC2)c1N

ZINC14960513 CCN(CC)C(=O)[C@H]1CCCN(Cc2ccc(C(=O)NCC3(O)CCCC3)c(=O)[nH]2)C1

ZINC34863228 COCCN(Cc1nc2cccc2c(=O)[nH]1)C(=O)c1enn(-e2ccc(O)nn2)c1C

ZINC23140693 O=C(Nc1nc[nH]n1)[C@@H]1CCCN(C(=O)c2ccc(O)c2)C1

ZINC66632360 C/C(=C/C(=O)NNC(=O)NCCc1ccnc1)c1cccc1Cl

ZINC62676186 N#C/C(C(=O)Nc1ccc2c(c1)OCCO2)=C(\O)CNC1cccc1[N+](=O)[O-]

ZINC38117525 [C@C@](CO)(c1cc(F)c(Cl)cc1Cl)N1CCCNCC1

ZINC04832459 COc1ccc([C@H]2[C@H](C(N)=O)C(=O)N[C@@](O)(c3cccc3)[C@H]2C#N)cc1

ZINC61622259 Cc1ccc(-e2n[nH]c(NC(=O)c3ccc(NC4CC4)nc3)n2)s1

ZINC09334391 O=C(NC1CC1)c1c(O)c2c([nH]e1=O)CCCC2

ZINC66220146 CSc1ccc(NC(=O)C(=O)NCc2cn3c(n2)CCCC3)cn1

ZINC22263737 C=CCn1c(=S)[nH]e2cc(C(=O)Nc3ncccc3O)ccc2c1=O

ZINC21903832 Cc1ccc(-e2nnc(S)n2CC(=O)NNC(=O)C(C)C)cc1

ZINC40408296 O=C1Nc2ccc(O)cc2/C1=Cc1ccc(/C=C2/C(=O)Nc3ccc(O)cc32)n1

ZINC02792642 CCOCc1c(S)nn1-c1cc2n(n1)[C@@H](C(F)(F)F)C[C@H](c1ccc(Cl)cc1)N2

ZINC61622259 Cc1ccc(-e2n[nH]c(NC(=O)c3ccc(NC4CC4)nc3)n2)s1

ZINC08647710 O=C(NNC1=NCCCN1)c1cc(OCC(F)(F)F)nc(OCC(F)(F)F)c1

ZINC16682580 CCOC(=O)C1=C(N)N2c(s/c(=C\c3ccc3)c2=O)=C(C(N)=O)[C@H]1c1ccc1

ZINC61622259 Cc1ccc(-e2n[nH]c(NC(=O)c3ccc(NC4CC4)nc3)n2)s1

ZINC13393255 Cn1c(C(=O)NC/C=C/e2enc(N)[nH]2)cc(Br)c1Br

ZINC29493709 CCCC=N(C\N)SCC(=O)N1C[C@H](C(=O)NC)Oe2cccc21

ZINC25782523 C/C(=N\NC(=O)c1c(CN2CCCC2)nnn1-e1nonc1N)c1cc(C)sc1C

ZINC42956539 Cn1nc(O)c2c(C(=O)NNc3cccc(Cl)c3)cc(C3CC3)nc21

ZINC67106460 C/C(=C/C(=O)NNc1nnc(C)c(O)n1)c1cccc1Cl

ZINC02339711 COc1ccc([C@H]2C3=C(CC(C)(C)CC3=O)Nc3[nH]c(N)nc(=O)c32)cc1

ZINC67588199 CC1=NC(=O)C2(CCN(C[C@]3(O)CCCN(CC4cccc4)C3=O)CC2)N1

ZINC53714157 N[C@H](c1ccc2c(cc1Cl)OCCCO2)C1CCCCC1

ZINC20427795 N[C@H](Cc1nc2cccc2o1)c1ccc(Cl)c1Cl

ZINC15017291 COc1ccc([C@H]2[C@H](C(N)=O)C(=O)N[C@@](O)(c3cccc3)[C@H]2C#N)cc1[N+](=O)[O-]

ZINC24543918 COc1cc([C@H]2C3=C(CC(C)(C)CC3=O)Nc3[nH]c(=O)[nH]c(=O)c32)cc(I)c1O

ZINC05231353 CC1(C)CC(=O)C(e2oc(N)c(C#N)e2-e2ccc2)=C(O)C1

ZINC09089293 CCOC(=O)[C@H]1C(O)=NC(SCC(=O)Nc2ccc(F)cc2)=C(C#N)[C@H]1c1cccc1F

ZINC66390648 C[C@H](N[C@H](C)c1ccc(N2CCN(C)CC2)c(F)c1)C(=O)NC(=O)NC1CC1

ZINC24543914 COc1cc([C@H]2C3=C(CC(C)(C)CC3=O)Nc3[nH]c(=O)[nH]c(=O)c32)cc(I)c1O

ZINC64152362 CC[C@H](C)C(=O)NC[C@H]1NN[C@H]2CCN(C(=O)CCC3=C4cccc4=NC3)CCN21

ZINC36596633 Cc1ccc(CN(C(=O)c2cc([N+](=O)[O-])ccc2O)[C@@H](C(=O)NC2CCCC2)e2cccc2O)o1

ZINC65489377 CCn1c(O)c2ccc(C(=O)Nc3cc(Br)cs3)cc2nc1=S

ZINC54728911 Cc1c(/C(O)=C(C#N)C(=O)Nc2cccc2)[nH]e2c1C(=O)CCC2

ZINC31818108	Ce1nn(-c2ccc(O)nn2)c2c1[C@H](c1ccc(F)c(Br)c1)CC(O)=N2
ZINC41069992	Ce1cccc(C)c1NS(=O)(=O)c1cc(Br)enc1NN
ZINC38999559	NN1[C@@H](SCC(=O)N2CCOCC2)NN[C@@H]1[C@H]1C=C(c2ccc(Cl)cc2)N=N1
ZINC20827519	Ce1cccc1NC(=O)CSs1nnc(N/N=C/c2enn(C(C)C)c2)n1N
ZINC31818108	Ce1nn(-c2ccc(O)nn2)c2c1[C@H](c1ccc(F)c(Br)c1)CC(O)=N2
ZINC17965002	CCn1c(O)c2ccc(C(=O)N[C@H](C)c3ccccc3Br)cc2nc1=S
ZINC06490163	CCn1cc(NC(=O)[C@@H]2C3CCC(CC3)[C@@H]2C(=O)O)c(C(=O)NC2CCCC2)n1
ZINC37448213	COe1ccc([C@H]2[C@@H](C(N)=O)C(=O)N[C@@](O)(c3ccccc3)[C@H]2C#N)cc1[N+](=O)[O-]
ZINC39940171	C[C@H]1NNC(=O)C2=C1[C@@H](C)O[C@@H]2NC(=O)CS[C@H]1NN=C(C2CC2)N1c1ccccc1
ZINC08492620	COe1ccc([C@H]2C3=C(O)CCCC3=Ne3nc(S)nc(N)c32)cc1
ZINC64890715	CC(C)[C@@H](NS(=O)(=O)c1ccccc1)[C@H]1N=C(c2ccc3c(e2)[nH]c(=O)c(=O)n3C(C)C)NO1
ZINC62676186	N#C/C(C(=O)Nc1ccc2c(c1)OCCO2)=C(\O)CNc1ccccc1[N+](=O)[O-]
ZINC12737654	C[C@@H](NC(=O)CCc1nnc(=S)[nH]e1O)c1cccce1Cl
ZINC65373061	CN(C)c1nc2c(c(=O)[nH]1)CCN(C(=O)[C@H]1CC13CCNCC3)CC2
ZINC24543914	COe1cc([C@@H]2C3=C(CC(C)C)CC3=O)Nc3[nH]c(=O)[nH]c(=O)c32)cc(1)c1O
ZINC59403420	Ce1cccc(-e2n[nH]c(N=C(\O)CNC(=O)c3ccccc3)n2)n1
ZINC66510661	CCn1c(=O)[nH]e2cc(C(O)=C(\C#N)C(=O)NC3CCCC3)ccc2c1=O
ZINC45789511	CC(C)N(C)Cc1ccccc1CNC(=O)NNc1ccc(-n2cccn2)nn1
ZINC29493709	CCCC/N=C(\N)SCC(=O)N1C[C@H](C(=O)NC)Oe2ccccc21
ZINC21903832	Ce1ccc(-e2nnc(S)n2CC(=O)NNC(=O)C(C)C)cc1

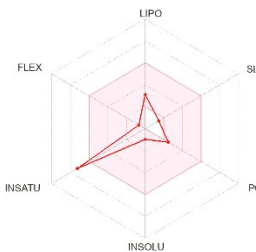
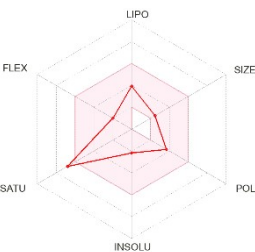
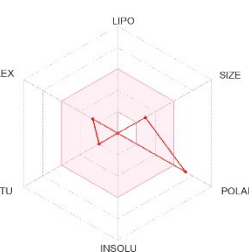
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**Table S3.** The results of virtual screening based on Glide XP mode and CA IX inhibitory activity.

Zinc ID	Glide Gscore (kcal/mol)	MIC( $\mu$ g/mL)
ZINC1799	-9.823	0.42
ZINC1532514	-9.082	>100
ZINC1531009	-8.802	>100
ZINC1543475	-8.823	>100
ZINC51581	-8.762	8.35
ZINC164392	-8.759	67.92
ZINC49135178	-8.640	>100
ZINC3812862	-8.628	8.51
ZINC3830813	-8.595	>100
ZINC1554	-8.562	1.34
ZINC3977897	-8.301	49.57
ZINC163369	-8.244	>100
ZINC61	-8.145	>100
ZINC13129998	-8.145	89.37
ZINC8577218	-8.144	58.55
ZINC51133897	-7.662	>100
ZINC7997568	-7.359	>100
ZINC1910616	-7.103	>100
AAZ	□	0.03

Inhibitory activity against CA IX. DMSO and acetazolamide (AAZ) were used as negative and positive control respectively. The activity data in the table are reported in  $\mu$ g/ml

**Table S4.** Physiochemical parameters and toxicity of proposed CA IX inhibitors.

Parameters	3-pyridinemethanol	Procodazole	Pamidronic acid
Formula	C <sub>6</sub> H <sub>7</sub> NO	C <sub>10</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub>	C <sub>4</sub> H <sub>13</sub> NO <sub>6</sub> P <sub>2</sub>
<sup>a</sup> MW (g mol <sup>-1</sup> )	109.13	190.2	233.1
<sup>b</sup> NHA	8	14	13
<sup>c</sup> NAHA	6	9	0
<sup>d</sup> NRB	1	3	4
<sup>e</sup> MR	30.36	52.45	48.85
<sup>f</sup> TPSA (Å <sup>2</sup> )	33.12	65.98	163.86
<sup>g</sup> LogS	-0.99	-2.16	2.6
<sup>h</sup> SC	Very soluble	Soluble	Highly soluble
<sup>i</sup> GI	High	High	Low
<sup>j</sup> BBB	No	Yes	No
<sup>k</sup> vROF	0	0	1
<sup>l</sup> vGhose	3	0	1
<sup>m</sup> vVeber	0	0	1
<sup>n</sup> BS	0.55	0.55	0.55
<sup>o</sup> SA	1.00	1.60	4.62
iLOGp	1.02	0.93	0
<sup>p</sup> “B-E”Ms			
<sup>q</sup> PLD <sub>50</sub> (mg kg <sup>-1</sup> )	3720	125	625
<sup>r</sup> PTC	5	3	4

<sup>a</sup> Molecular weight. <sup>b</sup> No. of heavy atoms. <sup>c</sup> No. of aromatic heavy atoms. <sup>d</sup> No. of rotatable bonds. <sup>e</sup> Molar refractivity. <sup>f</sup> Topological polar surface area. <sup>g</sup> Solubility. <sup>h</sup> Solubility class. <sup>i</sup> Gastrointestinal absorption. <sup>j</sup> Blood brain barrier penetration. <sup>k</sup> Violation of Lipinski's rule of five. <sup>l</sup> Violation of Ghose rule. <sup>m</sup> Violation of Veber rule. <sup>n</sup> Bioavailability Score. <sup>o</sup> Synthetic accessibility. <sup>p</sup> “Boiled-Egg” Method summary. <sup>q</sup> Predicted LD<sub>50</sub>. <sup>r</sup> Predicted toxicity class.

**Table S5.** The RMSD of co-ligand calculated by Glide-SP and Glide-XP.

Docking program	RMSD
Glide-SP	1.73
Glide-XP	1.72