

## Supplementary information

### Structure-based virtual screening of non-benzofuran inhibitors against *M. tuberculosis* Pks13-TE for anti-tuberculosis phenotypic discovery

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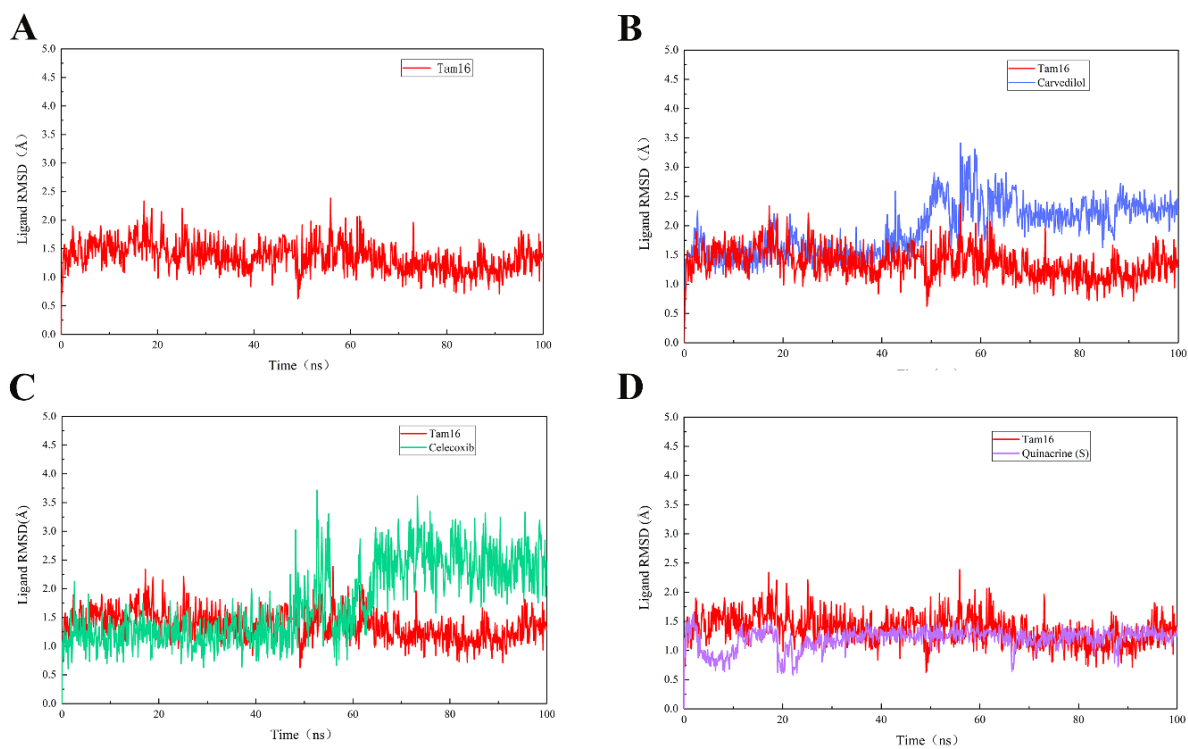


Figure S1. The RMSD values of ligands monitored by desmond. (A-D) The RMSD values of ligands calculated for the systems including Pks13-TE complexed with Tam16, carvedilol, celecoxib and quinacrine respectively.

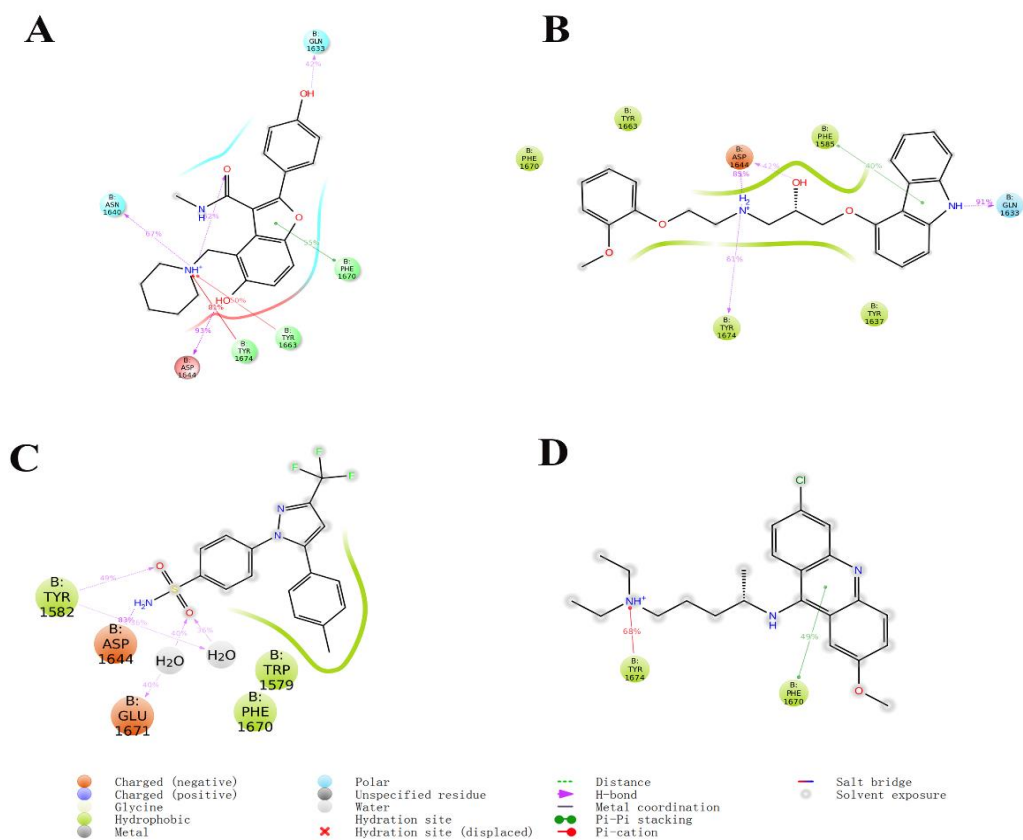


Figure S2. 2D interaction diagrams of the complexes of Pks13-TE with Tam16, carvedilol, celecoxib and quinacrine after 100 ns' MD simulations. (A) Tam16, (B) Carvedilol, (C) Celecoxib, (D) Quinacrine.

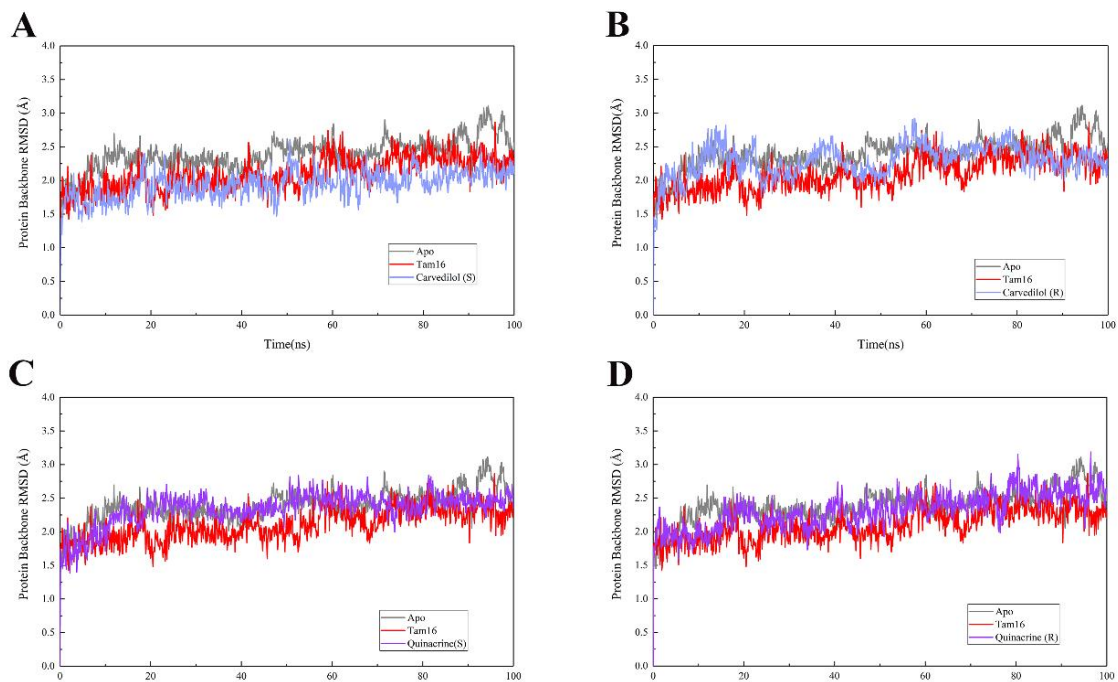


Figure S3. The RMSD values monitored by desmond. (A-D) The RMSD values of protein backbone of apo state of the Pks13-TE, and Pks13-TE complexed with native ligand Tam16, carvedilol (S), carvedilol (R), quinacrine (S), quinacrine (R).

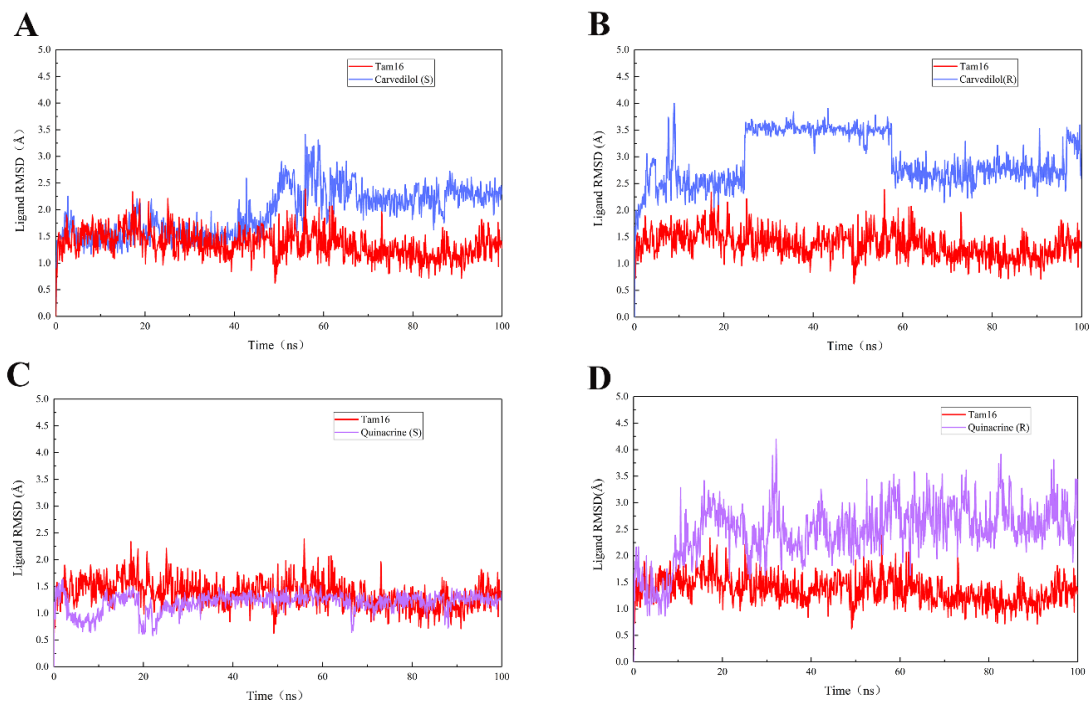


Figure S4. The RMSD values of ligands monitored by desmond. (A-D) The RMSD values of ligands calculated for the systems including Pks13-TE complexed with Tam16, carvedilol (S), carvedilol (R), quinacrine (S), quinacrine (R).

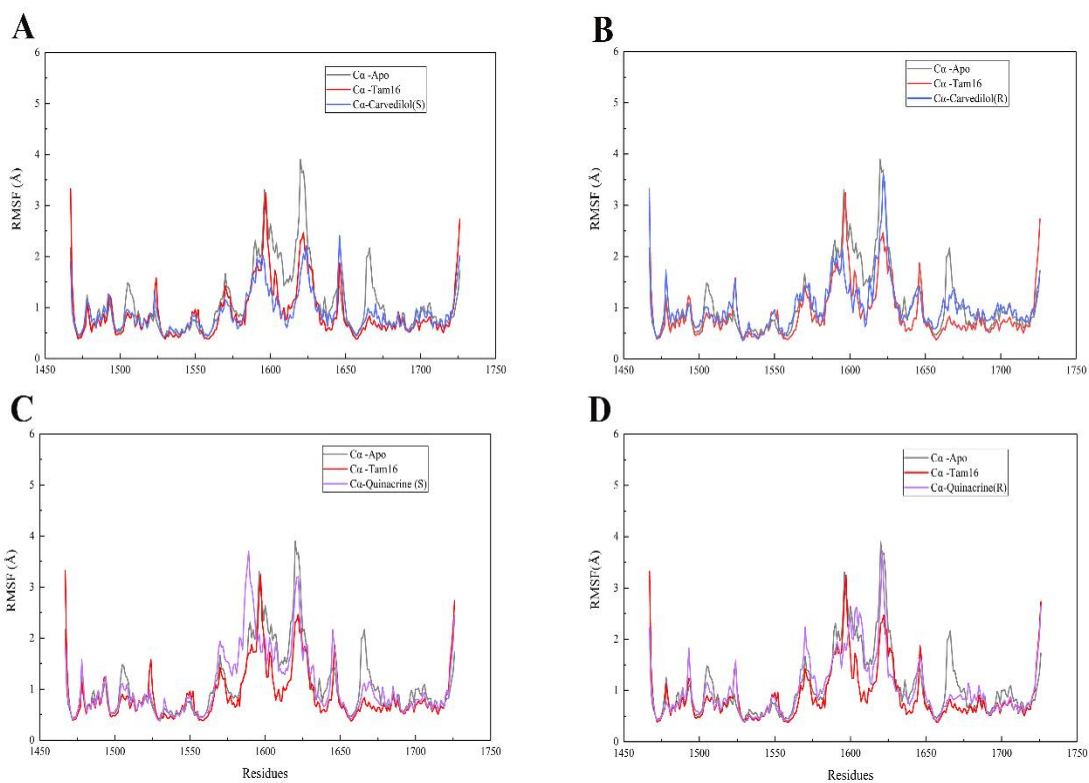


Figure S5. The RMSF monitored by desmond. (A-D) The RMSF of protein C $\alpha$  of apo state of the Pks13-TE, and Pks13-TE complexed with Tam16 overlapped with carvedilol (S), carvedilol (R), quinacrine (S), quinacrine (R). in the same frame, respectively.



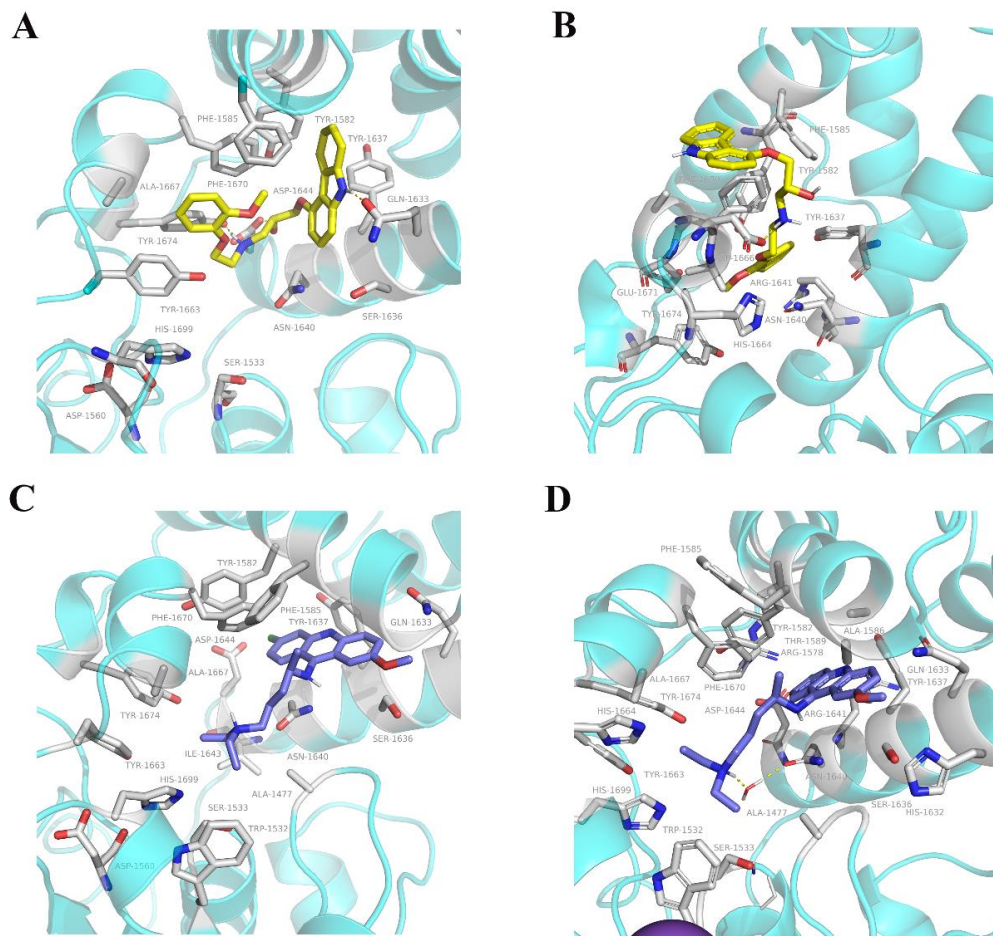


Figure S6. The binding poses of the complexes of Pks13-TE with carvedilol (S), carvedilol (R), quinacrine (S), quinacrine (R) after 100 ns' MD simulations, where the hydrogen bond interactions were displayed as yellow dashes. (A) carvedilol (S), (B) carvedilol (R), (C) quinacrine (S), (D) quinacrine (R). The pictures were produced by PyMol.

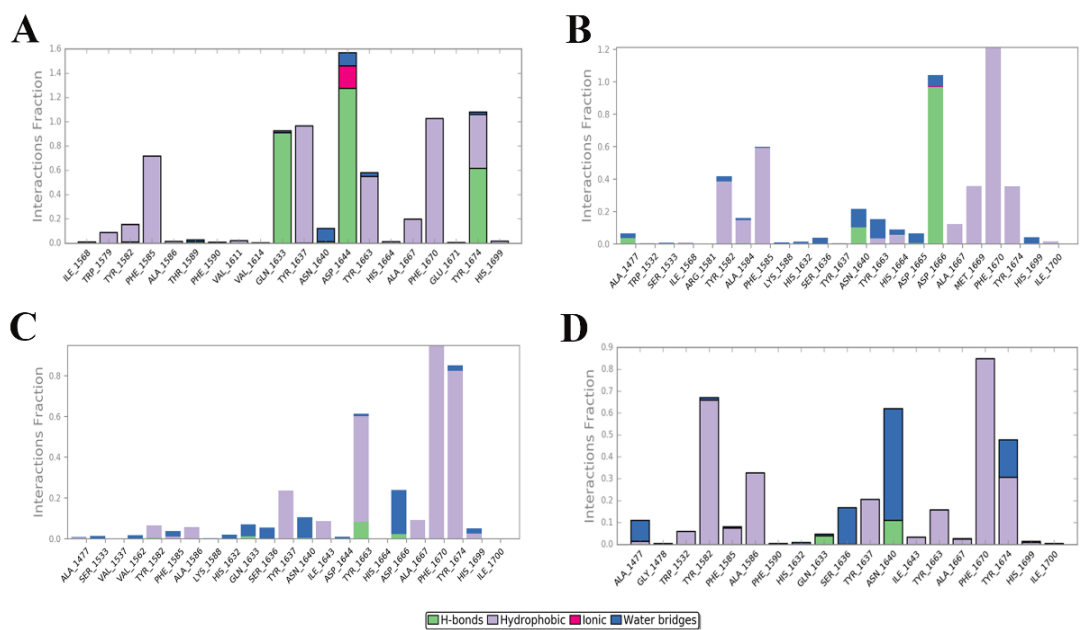


Figure S7. The interactions between protein and the ligand were monitored across the MD simulation. (A-D) The normalized stacked bar chart of carvedilol (S), carvedilol (R), quinacrine (S), quinacrine (R) complexed with Pks13-TE.

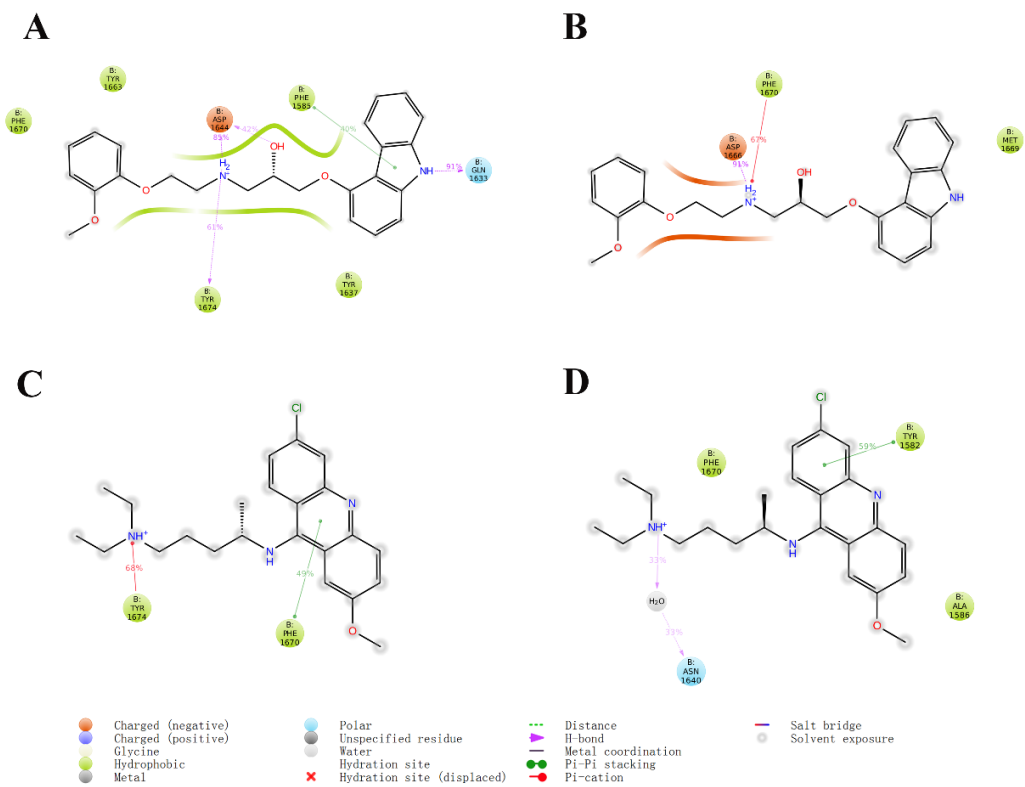


Figure S8. 2D interaction diagrams of the complexes of Pks13-TE with carvedilol (S), carvedilol (R), quinacrine (S), quinacrine (R) after 100 ns' MD simulations. (A) carvedilol (S), (B) carvedilol (R), (C) quinacrine (S), (D) quinacrine (R).

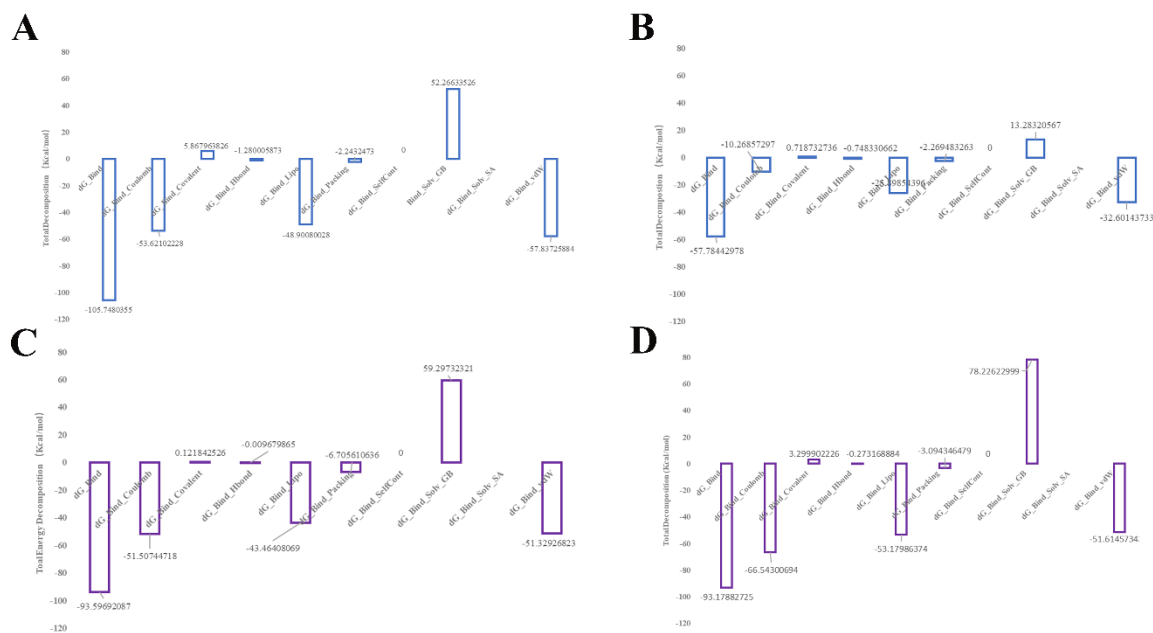


Figure S9. The binding free energy of the extracted structures of protein-ligand complex from the equilibrium stage of MD simulation was calculated by MM/GBSA method. (A-D) The binding free energy of carvedilol (S), carvedilol (R), quinacrine (S), quinacrine (R) complexed with Pks13-TE.

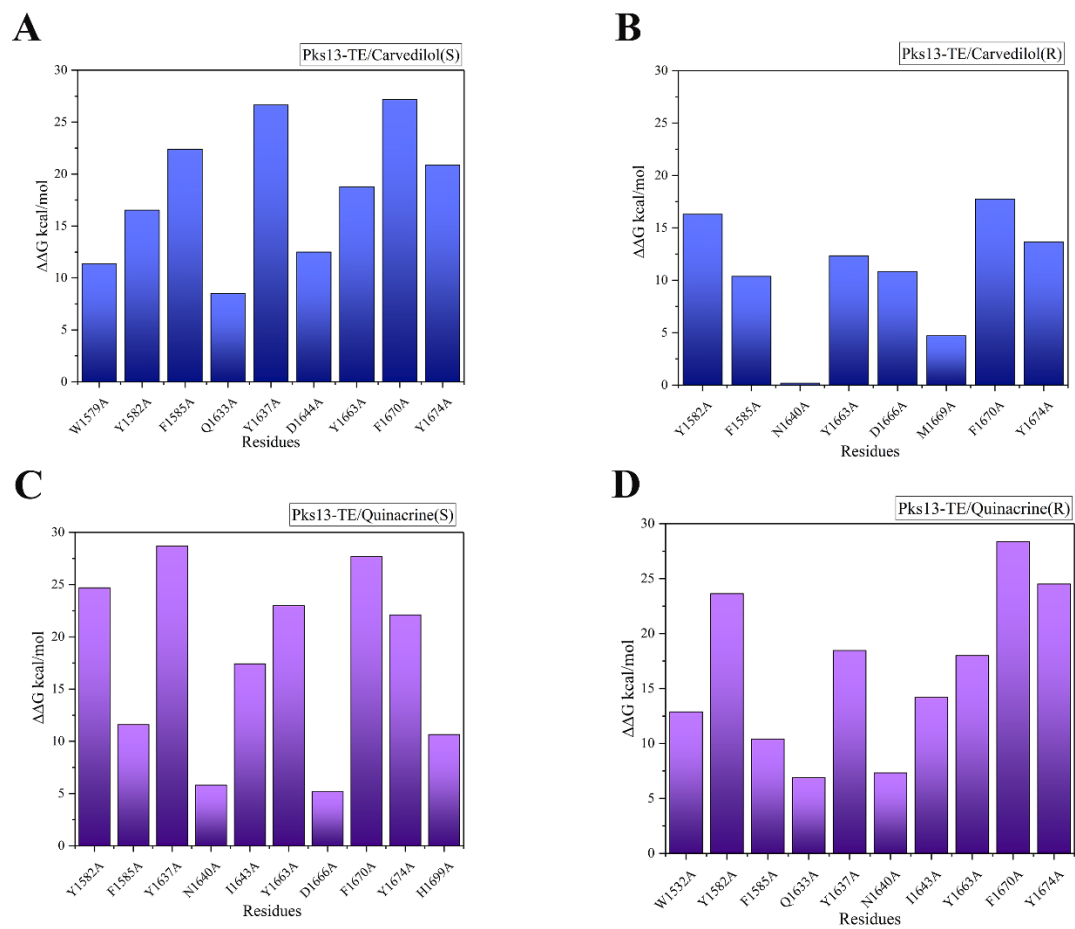


Figure S10. The results of alanine scanning mutagenesis. (A) Pks13-TE/Carvedilol (s), (B) Pks13-TE/Carvedilol (R), (C) Pks13-TE/Quinacrine (S) (D) Pks13-TE/Quinacrine (R).

Table S1. The decoy set generated by RADER (RApid DEcoy Retriever).

Smile formats of decoys	Zinc ID
<chem>O=C(OCC)c1c(c2ccccc2)oc2ccc(O)c(CN3CCC(C)CC3)c12</chem>	1
<chem>COc1cc(ccc1SC)CN1C[C@H](C)CN(c2c1cccc2)C(=O)C</chem>	ZINC81577446
<chem>O=C(N1CCc2c1cccc2)CSc1nc2c(n1c1cccc1)cccc2</chem>	ZINC06383089
<chem>Fc1ccc(cc1)Cc1noc(c1)C(=O)N1CCC(CC1)Oc1cccc1F</chem>	ZINC11880533
<chem>Clc1cccc1C(=O)N1CCN(CC1)Cc1csc(n1)c1cccc1</chem>	ZINC24257773
<chem>CC(N(C(=O)c1ccc(s1)c1ccc2c(c1)OCO2)Cc1cccc1)C</chem>	ZINC23322769
<chem>Cc1ccc(cc1)N(C(=O)c1cc2ccccc2oc1=O)Cc1cccc1</chem>	ZINC02725711
<chem>N#CCcn1cc(c(n1)c1cccc1)CN1CC[C@H](C1)c1ccc(cc1)OC</chem>	ZINC92783194
<chem>COC(=O)C1=C(C(=O)OC)[C@H]2N([C@@H]1c1c2ccc(c1)c1cccc1)c1ccc(cc1)</chem>	ZINC40148544
<chem>Fc1ccc(cc1)OCCOC(=O)c1cn(c2ccc(cc2)F)c(=O)c2c1cccc2</chem>	ZINC21360125
<chem>COC(=O)c1ccc2c(c1)CCN2S(=O)(=O)c1ccc(c(c1)C(F)(F)F)Cl</chem>	ZINC24350265
<chem>CC(CC(=O)[C@@H]1CCCN(C1)c1ncc(n1)c1cccc2c1cccc2)C</chem>	ZINC15063737
<chem>O=C(Cc1coc2c1c1cccc1cc2)OCC(=O)c1cc(n(c1C)C1CC1)C</chem>	ZINC03427885
<chem>FC(Oc1ccc(cc1)[C@@H](S(=O)(=O)c1ccc2c(c1)OCCCO2)C)F</chem>	ZINC68142044
<chem>O=C(N(c1cccc1)Cc1cccc1)c1ccc(o1)Cc1c(C)noc1C</chem>	ZINC28241946
<chem>Cc1cc(C)c2c(c1)nc(s2)N(C(=O)Cc1cccc1)C[C@H]1CCCO1</chem>	ZINC11141399
<chem>Fc1ccc(cc1)Cc1nc(c(s1)C(=O)N1CCN(CC1)c1ccc(cc1)F)C</chem>	ZINC40088795
<chem>Cc1ccc(cc1)CSc1nnc(n1c1cccc1Cl)c1ccncc1</chem>	ZINC04358244
<chem>COc1cccc(c1)c1nnc(n1c1cccc1)SCc1cc(F)cc(c1)F</chem>	ZINC04358258
<chem>Brc1ccc(cc1)c1nc(SCC(=O)N(C)C)c2c(n1)cccc2</chem>	ZINC03332868
<chem>O=C(c1ccc2c(c1)cccc2)[C@H]1CCCN(C1)C(=O)c1noc(c1)C(C)C</chem>	

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ZINC12441914  
COc1ccc2c(c1)nc(cc2C)SCC(=O)N1CCc2c1cccc2  
ZINC02634091  
Cc1ccc(c(c1)C)S(=O)(=O)N1CCN(CC1)C(=O)c1cccc1C(F)(F)F  
ZINC16600247  
Cc1ccc(c(c1)N(S(=O)(=O)C)CCCC(=O)N1[C@H](C)Cc2c1cccc2)C  
ZINC13671724  
Fc1ccc(cc1)OCCN(C(=O)c1cc(nc2c1cccc2)c1ccncc1)C  
ZINC09932648  
CCN(S(=O)(=O)c1cc(ccc1C)C(=O)N1CCc2c(C1)cccc2)CC  
ZINC15338904  
CCOC(=O)c1c(C)oc2c1cc(cc2)OC(=O)c1cc(F)c(c(c1F)F)F  
ZINC15338904  
O=C(c1cccc1C)Oc1cc(=O)n(c(n1)c1cccc1)c1cccc1  
ZINC04114529  
Cc1ccc(cc1)c1noc(n1)CN(C(=O)c1ccc(cc1)Cl)C(C)C  
ZINC06736943  
CC1CCN(CC1)C(=O)CCSc1nc(cc(n1)C(F)(F)F)c1ccc(cc1)C  
ZINC06032647  
COc1ccc(cc1)c1nc(sc1C)[C@H]1OCCN(C1)Cc1cccc1  
ZINC72087635  
C=CCn1c(SCc2c(Cl)cccc2Cl)nnc1c1cccc1OC  
ZINC05500121  
CC(Sc1nnc2c(n1)n(CCc1cccc1)c1c2cc(cc1)C)C  
ZINC05477920  
Cc1cc(C)cc(c1)n1nnc(c1C)C(=O)OCc1cccc(c1)C(F)(F)F  
ZINC46914125  
CC(Oc1cccc1CS(=O)(=O)c1ccc2c(c1)OCCCO2)C  
ZINC55344628  
COc1ccc(cc1)c1nn2c(c1)c(ncc2)SCc1ccc(cc1)C  
ZINC16842877  
Clc1cccc(c1)N(S(=O)(=O)c1cccc(c1)C(=O)N(C(C)C)C(C)C)C  
ZINC78877991  
COc1cccc1CCN(C(=O)c1se(nc1C)C1CCCC1)C  
ZINC80039940  
CCN(S(=O)(=O)c1ccc(c(c1)C(=O)Oc1ccc(cc1)Cl)Cl)CC  
ZINC01162364  
Cc1ccc(c(c1)C)C(=O)C1CCN(CC1)C(=O)CCc1ncc(o1)c1cccc1  
ZINC24455550  
FC(CSc1nnc(n1c1cccc1C(C)C)c1ccncc1)F  
ZINC78535715  
CCOc1ccc(cc1)c1nn2c(c1)c(ncc2)SCc1cccc(c1)Cl  
ZINC16842884  
COc1cccc(c1)CN(S(=O)(=O)c1cc(F)cc(c1)F)C[C@@H]1CCCO1

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ZINC64402630  
O=C(Oc1ccc(cc1Br)Cl)CCc1c(C)nc2n(c1C)nc(c2)C

ZINC60951539  
CCOC(=O)[C@H](Oc1ccc2c(c1)oc(c(c2=O)c1ccc(cc1)Cl)C)C

ZINC01447928  
O=C(N1CCc2c(C1)cccc2)C1CCN(CC1)S(=O)(=O)c1ccc(cc1)C(C)C

ZINC15338906  
COC(=O)c1ccc(c(c1)S(=O)(=O)N(c1cccc1)CC1CC1)F

ZINC84042181  
O=C(OC1CN(C1)c1nc2c(s1)cccc2)Cc1ccc(cc1)C(C)C

ZINC77157695  
CC(Oc1cccc(c1)C(=O)[C@@H]1CCCN(C1)Cc1nc(s1)C)C

ZINC20449419  
Fc1ccc(cc1)C(=O)N(c1ccc(n1)c1cccc1)C[C@H]1CCCO1

ZINC00882120  
COc1cc(ccc1SC)CN(Cn1c(=O)c2c3c1cccc3ccc2)C

ZINC58540728  
O=C(OCC)c1c(c2cccc2)oc2ccc(O)c(CN3CC(C)CCC3)c12  
2

O=C([C@H](Oc1cccc(c1)Cl)C)Nc1cccc1C(=O)N1CCCCC1

ZINC01024980  
Clc1ccc(c(c1)S(=O)(=O)NCc1cccc1Cn1ccn1)Cl

ZINC10959016  
O=C([C@H](Sc1ccc2c(c1)OCCO2)C)Nc1ccc(cc1)Br

ZINC05018689  
COc1cc(OC)c(cc1NC(=O)c1ccc(cc1)SC(F)F)F

ZINC87401071  
Clc1cccc1CS(=O)(=O)NCc1cm(c1)c1cccc1

ZINC76350745  
COc1ccc(cc1)c1onc(c1)C(=O)Nc1cccc1Br

ZINC27579916  
CC([C@@H](C(=O)Nc1ccc2c(c1)CCC(=O)N2C)Oc1cccc(c1)Cl)C

ZINC94074751  
COc1ccc2c(c1)o/c(=N\c1cccc1F)/c(c2)C(=O)Nc1cccc1

ZINC01512508  
CCCCN(c1ccc(cc1)C(=O)N1CC[C@@H](c2c1ccc2)C(=O)N)C

ZINC89447974  
O=C([C@H]1CCCN1C(=O)CC(C)(C)C)Nc1cc(ccc1F)c1ccc1

ZINC80719329  
CCOC(=O)C1=C(C)Nc2c([C@@H]1c1ccc(cc1)Cl)cm2c1ccc(cc1)Cl

ZINC08873386  
O=C(C[C@]12C[C@@H]3C[C@H](C1)C[C@](C2)(C3)Br)Nc1ccc(nc1)n1cccc1

ZINC25007209  
Clc1ccc(cc1)Cc1nc2n(n1)c(N[C@@H](c1cccc1)C)c1c(n2)CCC1

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ZINC46022886

O=C(N[C@H](c1ccc2c(c1)OCO2)C)COc1cc(C)ccc1C(C)C

ZINC25243639

C[C@H]1[C@H](C)CCC[C@H]1NC(=O)COC(=O)c1cc(n(c1C)c1ccc(cc1)F)C

ZINC05659057

Clc1ccc(cc1)[C@@H](n1ccn1)CNCc1sc2c(n1)CCC2

ZINC93080367

Cc1cccc(c1)c1cccc(c1)C(=O)NC[C@@H]1Cc2c(O1)c(ccc2)c1cncn1

ZINC11880534

O=C(Nc1cccc1Cl)CCc1c(C)nc2n(c1C)nc(c2)c1cccc(c1)F

ZINC09609623

O=C([C@H](Sc1cccc1F)C)Nc1c(C)nn(c1C)c1cccc1

ZINC42096168

C[C@@H]1[C@H](C)CCC[C@H]1NC(=O)CCc1nnc(o1)c1ccc(cc1)Cl

ZINC73397821

Cc1cccc(c1)CN1CCc2c(C1=O)cccc2OCC(=O)Nc1cccc(c1C)C

ZINC02716548

O=C(c1ccc(cc1C)n1cncn1)N[C@H](c1ccc(c(c1)Cl)Cl)C

ZINC78877988

CCCc1nc2ccc(cc2c(=O)n1Cc1ccc(cc1)c1cccc1OC)N

ZINC01331495

Fc1ccc(nc1)Nc1cccc(n1)[C@H]1CCCN1C(=O)c1nccc2c1cccc2

ZINC72375307

Cc1cc(C(=O)NCC2(CC2)c2cccc2)c2c(n1)n(nc2C)C(C)(C)C

ZINC48302135

O=C([C@H](Sc1ncc2n1cccc2)C)Nc1c(Cl)cc(cc1Cl)Cl

ZINC26371943

Cc1cccc(c1)NC(=O)[C@@H]1CCCN(C1)c1ccnc(n1)c1cccc(c1)F

ZINC64662855

Clc1ccc(s1)[C@@H](NC(=O)N1CCN(CC1)c1cccc1Cl)C

ZINC28410322

O=C([C@@H](n1nc(ccc1=O)c1ccc(cc1)F)C)Nc1cccc(c1Cl)Cl

ZINC49059628

COc1ccc(cc1)C(=O)Nc1ccc2c(c1)CN(CC2)C(=O)c1cccc1

ZINC09038226

O=C(Nc1ccc2c(c1)c(=O)n(c2)C)Cc1cccc1)CCc1cccc1

ZINC01331520

Cc1ccc(o1)[C@H](NC(=O)c1c(C)nn(c1Cl)Cc1cccc1)C

ZINC78918756

CC(Oc1ncccc1CNC(=O)c1cc2cc(Cl)ccc2nc1)C

ZINC48303389

O=C(OC(C)(C)C)NC1CCN(CC1)C(=O)c1cccc2c1cccc2

ZINC40119483

C[C@@H]1CCCN(C1)c1ncnc(c1N)N(Cc1cccc1)Cc1cccc1

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ZINC40709444

O=C(Nc1ccc2c(c1)OC1(O2)CCCC1)COc1ccc(c(c1)Cl)F

ZINC25039380

COc1ccc(cc1c1cc2C[C@@H](Oc2c(c1)Cl)CNC(=O)C(C)C)OC

ZINC14961175

CS(=O)(=O)Nc1ccc(cc1)CCc1nc2c(n1c1cccc1)cccc2

ZINC15870797

CNS(=O)(=O)c1cccc1N1CCN(CC1)Cc1c(F)cccc1Cl

ZINC69080511

O=C(Nc1ccc(cc1)c1nnc(o1)c1ccc(c1)C)CCc1cccc1

ZINC04826338

O=C(c1ccc(cc1)n1nc2c(c1=O)cccc2)NCc1cccc1Cl

ZINC21703395

Clc1cccc(c1)[C@@H](N(C(=O)NCc1ncc(o1)c1cccc1)C)C

ZINC80017871

Brc1ccc(cc1)NC(=O)c1enn2c1nc(cc2C(F)F)C1CC1

ZINC01009241

Cc1cccc(c1)Cn1nc(c(c1C)NS(=O)(=O)c1ccc(c1)F)C

ZINC39974968

COc1ccc(cc1NC(=O)C1CCN(CC1)C(=O)c1cccc1C)Cl

ZINC00780514

O=C(c1cccc1OCc1cccc1C)N[C@H](c1c(C)onc1C)C

ZINC70950870

O=C(c1c(Cl)cccc1Cl)Nc1cccc(c1)Oc1ccenn1

ZINC85292404

O=C(N[C@@H]1CC(C)(C)C2c1enn2c1ccc(cc1)F)Cc1cccn1

ZINC12441920

C=CCNC(=O)c1ccc(o1)c1c(nen1C1CCCCC1)c1ccc(cc1)F

ZINC64669548

O=C(C1CC1)Nc1ccc2c(c1)c(=O)n(c(n2)C)Cc1ccc(cc1)c1cccc1

ZINC01331500

O=C(OCC)c1c(c2cccc2)oc2ccc(O)c(CN3CCCC3)c12

3

COc1cccc2c1CC[C@H]2NC(=O)C[C@@H](c1ccc(cc1)Cl)O

ZINC89321299

O=C(Nc1ccc(cc1C)N1CCOCC1)Nc1enn(c1)C(C)(C)C

ZINC62388975

C[C@@H]1O[C@H](C)CN(C1)c1ccc(cc1F)NC(=O)Nc1c(C)nn(c1C)C(C)C

ZINC58201511

O[C@@H](c1ccncc1)CN[C@H]1CCCOc2c1cccc2C(C)C

ZINC90711032

C[C@@H](C(=O)NC(C)(C)C)NC(=O)c1ccc(c1C)Br

ZINC79738311

CCCN1ncc(c1)NC(=O)Nc1cc(Cl)ccc1N1CCOCC1

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ZINC72500877

O=C(Nc1ccc(c(c1)C)N(C)C)NCc1ccc(nc1)N1C[C@H](C)O[C@@H](C1)C

ZINC58548072

O=C(Nc1cc(Cl)ccc1N(C)C)Nc1enn(c1)C[C@@H]1CCCO1

ZINC77497376

O=C(Nc1cccc1O[C@H]1COCC1)Nc1ccc(c(c1)F)N1CCOCC1

ZINC84506050

COc1cccc(c1)N1CCC[C@H](C1)NC(=O)Nc1enn(c1)C(C)(C)C

ZINC93277784

CCn1nc(c(c1C)NC(=O)N[C@H](c1ccc(cc1)N1CCOCC1)C)C

ZINC89478505

C[C@@H](C(=O)Nc1cccc1)NC(=O)c1ccc(c(c1)Cl)Cl

ZINC78649092

CCn1nc(c(c1C)CNC(=O)Nc1cccc1N1C[C@H](C)O[C@@H](C1)C)C

ZINC67264867

CCOe1cc(ccc1NC(=O)Nc1ccc2c(c1)COC2)N1CCN(CC1)C

ZINC92168523

O=C(Nc1ccc(cc1C)N1CCOCC1)Nc1ccc(nc1)N1CCCC1

ZINC65789270

CCn1ncc(c1)NC(=O)Nc1ccc(cc1)N1C[C@H](C)O[C@@H](C1)C

ZINC72941147

COc1cc(CNC(=O)c2c[nH]nc2c2c(F)cccc2F)cc(c1)F

ZINC91789343

COe1cccc1NC1CCN(CC1)C(=O)Nc1ccnn1C(C)C

ZINC85358020

O=C(N1CCCC[C@H]1c1cccn1C)Nc1cccc(c1)N1CCNC1=O

ZINC83055102

COc1n(C)nc(c1NC(=O)Nc1cccc(c1)N1CCC(CC1)C)C

ZINC88390161

CCn1c(=O)n(c2c1cc(NC(=O)NC1CCCC1)c(c2)N1CCCCC1)CC

ZINC64591078

Cc1ccc(c(c1)N(C)C)CNC(=O)c1ccc([nH]c1=O)c1cccc1

ZINC84794884

O=C(Nc1cc(Cl)ccc1N1CCOCC1)NCc1cn2c(n1)cccc2C

ZINC69254417

C[C@H](C(=O)NCc1cccc1)NC(=O)c1cccc(c1Cl)F

ZINC79716970

COe1ccc2c(c1)NC1(c3n2ccc3)CCN(CC1)C(=O)NCc1ccc1

ZINC35446990

CCCNC(=O)Nc1nn(c2c1c(ccc2)N1CCOCC1)c1ccc(cc1)F

ZINC77340268

O=C(Nc1cc2c(cc1N(C)C)n(c(=O)n2C)C)Nc1ccc(c(c1)Cl)F

ZINC64591113

COe1cccc(c1)NC(=O)NCc1nn2c(c1)CN(CC2)C1CCCCC1

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ZINC82148360  
O=C(N(Cc1ccccc1Cl)C)N[C@H](c1nc2c([nH]1)cccc2)C(C)C  
ZINC43105956  
Cc1cc(C)cc(c1)n1ccnc(c1=O)NCCc1c[nH]c2c1cccc2  
ZINC06914980  
Clc1cccc(c1)N1CCN(CC1)C(=O)Nc1cccc(c1)N1CCNC1=O  
ZINC40120461  
COc1ccccc1N1CCC[C@H](C1)NC(=O)Nc1c(C)nn(c1C)CC  
ZINC89478931  
CCNc1ccnc(n1)NCc1ccnc1N1CCN(CC1)c1ccccc1C  
ZINC67773168  
O=C(Nc1cc2c(cc1N1CCCC1)n(c(=O)n2C)C)Nc1ccc(cc1)F  
ZINC20428092  
C[C@@H]1O[C@H](C)CN(C1)c1ccc(cc1)NC(=O)NCCc1nc2n(c1)cccc2  
ZINC50081720  
O=C(Nc1cccc(c1C)C)Cc1[nH]nc(n1)Cc1ccc(cc1)C  
ZINC65232641  
O=C(Nc1ccc2c(c1)CCCN2C)NC[C@@H](c1ccc(o1)C)N1CCOCC1  
ZINC64562043  
O=C(N[C@@H](c1ccccc1Cl)C)CNC(=O)c1ccc(cc1Cl)Cl  
ZINC17908249  
O=C(Nc1ccc(cc1C)N1CCOCC1)NCc1nc2c(n1C)cccc2  
ZINC58129226  
COc1ccc(en1)CNC(=O)c1cc2c([nH]1)cc(cc2)Br  
ZINC44366103  
O=C(Nc1ccc(cc1)N1C[C@H](C)O[C@H](C1)C)NCc1nc2c(n1C)cccc2  
ZINC64716690  
O=C(Nc1cc(Cl)ccc1N1CCOCC1)NCc1ccc2c(c1)OCCO2  
ZINC43398239  
O=C(C1CC1)Nc1ccc(cc1)C(=O)Nc1ccc(c(c1)Cl)Cl  
ZINC15411526  
O=C(Nc1ccc2c(c1)CCCN2C)NCc1ccc(nc1)N1CCO[C@@H](C1)C  
ZINC64561736  
COc1c2c(CCN([C@H]2NC(=O)Nc2ccccc2Cl)C)cc2c1OCO2  
ZINC20112649  
O=C(NCc1cccs1)CNc1ccc(c(c1)Br)C  
ZINC32754379  
COc1ccc2c(c1)c(CCNC(=O)C)cc(c2)c1ccccc1)N  
ZINC00023738  
O=C(c1cc2ccccc2c(=O)[nH]1)Nc1ccc(cc1)OCc1ccccc1  
ZINC60739617  
O=C(Nc1cc2c(cc1N1CCCC1)n(c(=O)n2C)C)Nc1ccc(c(c1)C)C  
ZINC20853274  
C[C@@H]1CCN([C@H]2[C@@H]1CCCC2)C(=O)CNC(=O)c1cc2c([nH]1)cccc

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ZINC79532916

O=C(OCC)c1c(c2ccccc2)oc2ccc(O)c(CN3CCCCC3)c12

4

COc1ccc(cc1S(=O)(=O)N(C1CC1)Cc1ccc(cc1)F)Br

ZINC12783192

CCcn1c(SCc2ccc3c(c2)cccc3)nnc1Cc1ccccc1

ZINC02838334

Fe1ccccc1N(c1ccc(n1)COc1ccccc1C(F)(F)F)C(=O)C

ZINC31789553

Clc1ccc(c1C)n1c(SCCC(F)(F)F)nc2c(c1=O)cccc2

ZINC06852311

COc1ccccc1C(=O)N(c1ccc(c1)Cl)Cc1cccs1

ZINC27662778

Cc1cc(C)c(c(c1)C)CSc1ncn(n1)Cc1cc2ccccc2cc1C

ZINC16267198

Cc1ccccc(c1)CN(C(=O)[C@@H]1C[C@@H]1c1ccc(s1)C)Cc1ccccc1

ZINC79000768

FC(c1ccccc1)c1ccc(n1)[C@H]1OCCN(C1)Cc1ccccc1(F)F

ZINC72087697

CCOC(=O)c1c(Br)c2c(n1Cc1ccc(cc1)F)cc(s2)C

ZINC01350647

CCOCC(=O)N(c1ccccc1C(C)C)c1nc2c(s1)cccc2

ZINC74361984

N#Cc1ccc(cc1Cl)S(=O)(=O)N(c1ccccc1)Cc1ccccc1

ZINC71990203

Cc1ccccc(c1)C(=O)Oc1c(Cc2ccccc2)c(=O)oc2c1cccc2

ZINC02435033

C=CCN(C(=O)c1ccc(s1)c1ccccc1Cl)CC(F)(F)F

ZINC64934631

CCS(=O)(=O)c1ccc(c(c1)C(=O)N(Cc1ccccc1)C)Cl

ZINC67166017

O=C(c1ccccc1)C1CCN(CC1)Cc1ccc(s1)c1ccccc1

ZINC78432890

COc1cc(F)ccc1S(=O)(=O)N1CCC(CC1)Cc1ccccc1

ZINC00836068

COc1ccc(cc1)N(S(=O)(=O)c1ccccc1)Cc1ccccc1F

ZINC23657901

C=CCSc1nnc(n1C1CCCC1)c1ccc(cc1)Br

ZINC09143345

Cc1nc(SCc2ccccc2)F)nc(c1)Oc1cc(C)cc(c1)C

ZINC37510458

COc1ccc(cc1)OCc1ccc(n1)c1ccc(c(c1)Cl)Cl

ZINC01046828

O=C(O[C@H](c1ccc2c(c1)cccc2)C)CCC(=O)c1ccc(cc1)F

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ZINC72079229  
COc1cccc1CN(S(=O)(=O)c1cccc1C(F)(F)F)C  
ZINC03458014  
Cc1ccc(cc1)S(=O)(=O)CC(=O)N(C1CCCCC1)C1CCCCC1  
ZINC01115027  
CC(c1ccc(cc1)S(=O)(=O)N(Cc1ccc(o1)Br)C)C  
ZINC30420292  
C[C@@H]1CC[C@@H](CC1)N(C(=O)CSc1ccc(en1)C(F)(F)F)C1CC1  
ZINC71865631  
N#C[C@H](C(=O)[C@@H](Oc1ccc(cc1)c1cccc1)C)c1ccc(en1)F  
ZINC80442473  
C=CCn1c(SCCC(C)C)nnc1c1ccc(cc1)Br  
ZINC59265873  
CCOc1ccc(cc1)N(c1nc2c(s1)cccc2)C(=O)CC1CCC1  
ZINC73851190  
CCc1ccc(cc1)[C@H](C(=O)N1CCCc2c1ccc(c2)S(=O)(=O)C)C  
ZINC67972031  
FC(c1cc(Sc2cccc(c2)C(F)(F)F)nc(n1)c1cccn1)(F)F  
ZINC03041160  
O=C(C1(CC1)c1cccc(c1)C(F)(F)F)Oc1cccc(c1)S(=O)(=O)C  
ZINC66313378  
N#Cc1c(Cl)nc(c1Cl)Cl)N(Cc1cccc1)Cc1cccc1  
ZINC22402112  
CCn1c(SCc2ccc(c(c2)Cl)Cl)nnc1c1cccc1  
ZINC05500126  
CCn1c(nnc1c1ccc(cc1)C(C)(C)C)SCc1ccc(cc1)C  
ZINC05500140  
Fc1ccc(cc1)COC1CCN(CC1)S(=O)(=O)c1ccc(cc1)Cl  
ZINC92556781  
Br1ccc(s1)CN(C(=O)c1cccc1C(=O)c1cccc1)C  
ZINC14302980  
Clc1ccc(cc1)c1nc(en1c1cccc1)SCC(=O)C(C)(C)C  
ZINC04089461  
Cc1ccc(cc1)c1nc2ccc(cc2c(c1)C)C(=O)OCC(=O)c1ccc(cc1)F)C  
ZINC02079736  
N#Cc1ccc(cc1)c1ccc(cc1)OC(=O)C(Oc1ccc(cc1)Cl)(C)C  
ZINC06515322  
Cc1cc(ccc1SCc1ccc(cc1)C(=O)N1CCOCC1)C(C)(C)C  
ZINC01083928  
CCOc1ccc(cc1)[C@@H]1CCCN1S(=O)(=O)c1cc(F)cc(c1)F  
ZINC10516665  
O=C(c1cccc(c1)C(F)(F)F)COc1ccc(cc1)S(=O)(=O)C  
ZINC72573550  
COc1ccc(cc1)OCc1ccc(cc1)c1ccc(cc1)C(F)(F)F

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ZINC01046831  
CCN(c1cccc(c1)C)C(=O)CSc1cc(C)c2c(n1)c(C)cc(c2)C  
ZINC40167201  
COc1ccc(cc1)CN1CCC[C@@H](C1)c1scc(n1)C(F)(F)F  
ZINC93772347  
COc1ccc(cc1)[C@@H](N(S(=O)(=O)Cc1cccc1Cl)C)C  
ZINC76350786  
Cc1ccc(cc1)Oc1cc(C)nc(n1)SCc1cccc1Cl  
ZINC37510467  
CC(COc1nc(C)cc(c1S(=O)(=O)c1cccc(c1)C(F)(F)F)C)C  
ZINC01388739  
N#CCCN1cc(c(n1)c1ccc(c(c1)F)F)/C=C/c1ccc2c(n1)cccc2  
ZINC09368158  
Cc1ccc(cc1)N(S(=O)(=O)c1ccc(cc1)Cl)C(=O)c1cccc(c1)C  
ZINC01467588  
O=C(OCC)c1c(c2cccc2)oc2ccc(O)c(CN3CCOCC3)c12  
5  
O=C(C1CCN(CC1)C(=O)c1cc(C)cc(c1)C)Nc1ccc2c(c1)OCO2  
ZINC15175508  
Cc1cnn(c1)Cc1ccc(cc1)NC(=O)c1cnc2n1cc(C)cc2  
ZINC90562891  
Clc1ccc2c(c1)cc(c(n2)C)C(=O)NCc1ccnc1n1ccn1  
ZINC24590467  
O=C1c2nc3c(n2C[C@])(N1Cc1cccc1)(C)C(=O)NC1CCCCC1)cccc3  
ZINC21860391  
Clc1cccc(c1)[C@H](N1CCOCC1)CNc1onc(n1)C1CC1  
ZINC76685942  
COc1ccc(cc1)CNc1nc2c(nnn2c2c1cccc2)c1cccc1  
ZINC05035185  
O=C(NC1CCCCC1)CCn1cnc2c(c1=O)c(C)c(n2c1cccc1)C  
ZINC21885781  
Clc1cccc(c1)C(=O)N1CCN(CC1)CCNC(=O)c1cscc1  
ZINC44451988  
COc1ccc(cc1)CCNC(=O)Cn1c(=O)oc2c1ccc(c2)Cl  
ZINC07866377  
O=C(N1CCN(CC1)C(=O)c1cccc1F)Nc1ccc(cc1)C(=O)C  
ZINC25237422  
O=C(CCc1ncc(o1)c1ccc(c(c1)C)C)NCc1ccc2c(c1)OCO2  
ZINC12617310  
CC(=O)O[C@H](c1ccc(cc1)F)C(=O)NCc1ccc2c(c1)OCO2  
ZINC01345004  
O=C(CCc1c(C)noc1C)NCC#CCOc1cccc2c1nccc2  
ZINC90742851  
COc1cc(ccc1OC)C(=O)Nc1cenn1Cc1cccc(c1)C

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ZINC30528291  
COC1CCN(CC1)C(=O)Nc1ccc(nc1)Oc1cccc(c1)CC  
ZINC48388916  
COc1ccnc(c1)NC(=O)c1cc(ccc1Cl)N1CCCC1=O  
ZINC89982308  
Cc1ccnc(c1)[C@@H](C1CC1)NC(=O)c1cnc(nc1)c1ccnc1  
ZINC95389202  
Cc1cccc(c1)CNC(=O)N1CCC(CC1)c1nnc2n1cccc2  
ZINC79157880  
CC(=O)Nc1cccc(c1)COC(=O)c1cn(nc1c1cccc1)C  
ZINC93157335  
O=C(Cn1ncc(c(c1=O)Cl)Cl)Nc1ccc(cc1)OC(F)(F)F  
ZINC06251408  
Cc1cccc1Oc1ncccc1CNCc1cccn1c1nccn1  
ZINC67787525  
COc1ccc(cc1)Nc1nc(nc2c1enn2c1cccc1)N(C)C  
ZINC16915074  
Fc1cccc(c1)CN(C(=O)NCc1nnc2n1CCCCC2)C1CC1  
ZINC79884500  
O=c1ccc2c(o1)ccc(c2)NC(=O)c1cc(mn1C(C)(C)C)C1CC1  
ZINC54254269  
Clc1ccc(nc1)C(=O)NC[C@@H](c1onc(n1)c1cccc1)C  
ZINC89955798  
CNC(=O)[C@H]1Oe2cccc2N(C1)C(=O)c1ccc(cc1)OC(F)F  
ZINC15617091  
CC(Cc1c(C)nc(nc1C)NC[C@@H]1CCCN(C1)c1nccn1)C  
ZINC91687446  
COc1cccc(c1)[C@H]1N(C2CC2)C(=O)c2c([C@@H]1C(=O)NCc1cccc1)cccc2  
ZINC35972389  
COc1ccc(cc1NC(=O)c1ccc(nc1)n1cnc2c1cccc2)Cl  
ZINC92148251  
O=C(C[C@@H]1OC(=O)c2c1cccc2)NCc1ccnc1Oc1cccc(c1)F  
ZINC40106614  
COC(CNC(=O)c1ccc2c(c1)ncn2c1ccc(cc1F)F)OC  
ZINC37866809  
O=C(Nc1ccc(cc1F)Cl)CCn1nnc(n1)c1cccc(c1)C(F)(F)F  
ZINC12749585  
COc1cccc2c1oc(c2)C(=O)NCc1nc2n(c1)cc(cc2)Cl  
ZINC73900861  
CCCN1C[C@@H](CC1=O)Nc1cc(nc2n1ncc2)c1cccc1F  
ZINC72122403  
CC([C@@H](C(=O)Nc1ccc(cc1)N1CCOC1=O)Oc1cccc(c1)Cl)C  
ZINC94035221  
Clc1ccc(cc1)Cn1ncc(c1)NC(=O)c1ccnc1N(C)C

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ZINC81311247

O=C(Cc1cccc1)N[C@H]1CCN(C1)C(=O)c1nc2n(c1C)cc(cc2)Cl

ZINC77892667

O=C(COc1ccc2c(c1)oc(=O)c1c2CCC1)NCCc1cccc1

ZINC09470904

COC(=O)CNC(=O)c1cc(nc2c1cccc2)c1ccc2c(c1)ccc(c2)OC

ZINC17440545

COc1c(Cl)cc(cc1OC)C(=O)N1CCC(CC1)NC(=O)C(C)C

ZINC60424957

CO[C@]1(C)C[C@@H](C1(C)C)NC(=O)c1nmn(c1C)c1ccc(cc1)F

ZINC73268901

CNC(=O)c1ccc(cc1)OCc1onc(n1)c1ccc(cc1)C(C)C

ZINC32783542

O=C(Nc1ccc(c(c1)Cl)F)COc1ccc2c(c1)c(=O)n1c(n2)CCC1

ZINC08991553

COC(=O)COc1ccc(c2c1cccc2)NC(=O)N1CC[C@H](C[C@@H]1C)C

ZINC92076457

COc1nc2cccc2nc1N1CCC[C@H](C1)C(=O)Nc1ccc(cc1C)F

ZINC86077281

CC[C@H]1CN(CC[C@H]1NC(=O)OC(C)(C)C)C(=O)c1oc(cc1C)C

ZINC95441484

O=C(c1ccnc1N1CCCC1)NCc1ccnc(c1)OC1CCC1

ZINC90013783

COc1cc(cc(c1)OC)Nc1c(nnn1c1ccc(cc1)Cl)C(=O)C

ZINC20443918

Cc1cc(C)n2c(n1)c(Cl)c(n2)C(=O)NCCN1CCc2c1cccc2

ZINC12148426

Cc1ccc(cc1)N1CCC[C@@H](C1)NC(=O)c1ccc(cc1)n1mcc1

ZINC89772455

O=C(OCC)c1c(c2cccc2)oc2ccc(O)c(CN(C)C)c12

6

O=C(N(Cc1cccc1N1CCCC1)C)N[C@H]1CCCN2c1nnc2C

ZINC80183845

O=C(N1CC[C@H](CC1)OC(C)(C)C)NC[C@@H]1CCCN(C1)c1nccn1

ZINC94061592

CC[C@H](n1ncc(c1C1CC1)C(=O)N[C@H]1CCCN(C1)c1cmn(c1)C)C

ZINC89815650

Cc1ccc(cc1)OCCN(C(=O)Nc1cnc2c(c1)c(C)nn2)C

ZINC48104536

COc1cccc(c1)c1nm2c(c1)CN(CCC2)C(=O)NCc1ccc1

ZINC65270311

O=C(Cn1nc(c(c1)c1cccc1)N(C)C)Nc1ccc2c(c1)OCCO2

ZINC62006973

CCOc1ccc(cc1Cl)NC(=O)N(Cc1mnc2n1cccc2)C

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ZINC78801160  
CC(Cn1ccc2c1ccc(c2)NC(=O)N(Cc1ncnn1C)C)C  
ZINC81066554  
O=C1OCCN1c1cc(NCc2cnn(n2)c2ccccc2)ccc1C  
ZINC72743107  
COc1cccc(c1)[C@@H]1CCCN1C(=O)Nc1enn(c1)C[C@@H]1CCCO1  
ZINC81081342  
O=C(N(Cc1ncn1C)C)Nc1ccc2c(c1)OC1(O2)CCCC1  
ZINC92729917  
CN(c1cccc1)CCCNc1nc(nc2c1cnn2C)c1ccncc1  
ZINC72447101  
COc1cccc1CN1CCN(CC1)C(=O)N[C@@H](c1c(C)noc1C)C  
ZINC73234798  
COc1ccc(cc1)[C@@H]1CCN(C1)C(=O)NCc1ccc(nc1)n1ccn1  
ZINC58227478  
CCc1ccc(o1)[C@@H]1COCCN1C(=O)Nc1ccc(nc1)N1CCCC1  
ZINC76780306  
CC(C[C@@H]1COCCN1C(=O)Nc1cccc(c1)c1nnc2n1CCC2)C  
ZINC73029754  
O=C(N1CCN(CC1)c1ccccn1)NCc1ccnc(c1)OC(C)(C)C  
ZINC92430436  
O=C(N1CCC(CC1)OC(C)(C)C)Nc1cccc1n1nc(nc1C)C  
ZINC89271752  
O=C1CCCCN1c1cccc(c1)NC(=O)c1cnn(c1n1cccc1)C  
ZINC25238071  
CCn1ccc(c1)CN1CCC(CC1)n1ccc1NC(=O)C1CCCC1  
ZINC12439659  
O=C(N(Cc1ncn1C(F)F)C)Nc1ccc2c(c1)OCCCO2  
ZINC76035731  
COc1cc(CN[C@H](c2cccc(c2)n2ncnc2)C)cc2c1OCCO2  
ZINC80241608  
O=C(N(Cc1ncn1C(F)F)C)N[C@H](c1ccc2c(c1)OCO2)C  
ZINC79061988  
C[C@@H]1CCN(C[C@@H]1n1cnc1)C(=O)NCc1ccnc(c1)OC(C)(C)C  
ZINC92431420  
COc1ccc(cc1)NC(=O)N1CCN(CC1)Cc1nc2c(o1)cccc2  
ZINC35534218  
COc1ccc(cc1OC(F)F)NC(=O)N1CCN(CC1)c1cccc1  
ZINC43995542  
O=C(N(Cc1nnc(n1C)C1CC1)C)Nc1cc(ccc1F)n1cccc1  
ZINC81067125  
O=C(N1CCN(CC1)c1ccccn1)Nc1cccc1n1nc(cc1C)C  
ZINC44209255  
COc1cccc(c1)CN(C(=O)Nc1cccc1n1nc(nc1C)C)C

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ZINC89271768  
COc1cc(CNc2ccc(cc2)OCc2nccn2C)cc2c1OCO2  
ZINC75917385  
O=C(N1CCN(CC1)c1cccc1)Nc1ccc(cc1)N1CCOC1=O  
ZINC56767297  
COc1ccc(cc1O)CN(Cc1c(C)nn(c1Oc1cccn1)C)C  
ZINC92405348  
CC(Oc1cccc(c1)[C@H](NC(=O)N1CCN(CC1)c1nccn1)C)C  
ZINC46663293  
COc1cc(CN[C@H](c2cccc(c2)n2ncnc2)C)cc2c1OCO2  
ZINC80241859  
COc1ccc(c(c1)OC)NC(=O)N1CCN(CC1)c1cccc1OC  
ZINC05393867  
O=C(N(Cc1cn(nc1C(C)C)C)C)Nc1cmn(c1)C(C)(C)C  
ZINC93275001  
C[C@@H]1CN(C[C@@H](O1)C)Cc1cccc1NC(=O)N(Cc1noc(c1)C)C  
ZINC47569847  
O=C(c1ccc(nc1)N1CCOCC1)N[C@@H](c1ccc(cc1)n1cncc1)C  
ZINC12549539  
CCOc1cccc1N1CCN(CC1)C(=O)Nc1c(C)noc1CC  
ZINC89415085  
COc1ccc(cc1)NC(=O)N1CCN(C[C@H]1C)C(=O)OC(C)(C)C  
ZINC72274848  
COc1cc(NC2CCN(CC2)C(=O)c2ccn(n2)C(C)C)cc(c1)OC  
ZINC80597553  
COc1ccc(cc1)N1CCCN(CC1)C(=O)Nc1cmn(c1)C(C)(C)C  
ZINC93274225  
C[C@@H](c1ccc(cc1)n1ccn1)Nc1nc(nc(n1)N(C)C)C(C)C  
ZINC91425089  
O=C(N1CCC[C@H]1c1cccn1C)Nc1cccc(c1)N1CCOC1=O  
ZINC58105640  
C[C@@H]1CN(CCC2CCN(CC2)C(=O)Nc2noc(c2)C(C)C)C[C@@H](O1)C  
ZINC78628254  
CO[C@]1(C)C[C@H](C1(C)C)NC(=O)N1CC[C@H](CC1)c1nnc2n1cccc2  
ZINC74941271  
CC(=O)N(c1ccc(cc1)NCc1c(C)nn(c1Oc1cccn1)C)C  
ZINC83472902  
CCNc1ccnc(n1)N1CCC[C@@H](C1)c1nccn1Cc1cccn1  
ZINC92001638  
CCc1mn(c(c1)CNC(=O)N1CC[C@@H](C[C@@H]1c1ccco1)C)OC)C  
ZINC91168872  
Fc1ccc(c(c1)OCC1CC1)NC(=O)N1CCC(CC1)n1cn1  
ZINC77724106  
O=C(OCC)c1c(c2ccccc2)oc2ccc(O)c(CN3CCCC3)c12

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Cc1ccc(cc1)n1nc(c(c1n1cccc1)C(=O)Nc1ccc2c(c1)OCCO2)C  
ZINC15681406

COc1ccc(c(c1)[C@H]1CCCN1C(=O)Nc1c(C)nn(c1C)CC)OC  
ZINC89228452

Clc1cccc(c1)NC(=O)N1CCN(CC1)c1cc(C)nc(n1)N1CCCCC1  
ZINC65363941

O=C(N1CCC[C@H](C1)N(c1nc2cccc2nc1NC1CC1)C)OC(C)(C)C  
ZINC95074088

COc1cccc(c1)NC(=O)N1CCn2c([C@@H]1c1ccc(c(c1)OC)OC)ccc2  
ZINC05256272

COc1cccc(c1)NC(=O)N(c1ccc(cc1)F)Cc1nnc2n1CCCCC2  
ZINC04518177

COc1cc(OC)ccc1NC(=O)c1cnn(c1n1cccc1)c1cccc(c1)F  
ZINC20980279

CCn1nc(c2c1nc(C)cc2C(=O)Nc1ccc(c(c1)Cl)N1CCOCC1)C  
ZINC36616754

Cc1ccc(cc1)n1nc(c(c1n1cccc1)C(=O)NCc1ccc2c(c1)OCO2)C  
ZINC15681394

COc1cccc1NC(=O)N1CCC(CC1)n1c2ncccc2nc1C(F)(F)F  
ZINC32949911

O=C(c1cnn(c1n1cccc1)C)NCc1cccc(c1)Cn1cnc2c1cccc2  
ZINC72047288

O=C(N1CCN(CC1)c1cenc(n1)N1CCCCC1)Nc1ccc2c(c1)cccc2  
ZINC72437298

O=C(OC(C)(C)C)N[C@@H]1CC[C@@H](CC1)N(Cc1cnc2n1c(C)cc(n2)C)C  
ZINC93888535

COc1cc(ccc1OC)c1nc2n(c1NCc1ccc3c(c1)OCO3)ccc(c2)C  
ZINC04848441

CC(Oc1cccc1NC(=O)N1CCC[C@@H](C1)c1nnc2n1CCCCC2)C  
ZINC92733208

O=C(OC(C)(C)C)N[C@@H]1CCN(C1)c1nccn2c1cc(n2)c1cccc1  
ZINC71328516

CC(=O)Nc1ccc(cc1)N(Cc1nc2n(c1)cccc2)Cc1nc2n(c1)cccc2  
ZINC12618924

O=C(C[C@@H](n1nc(cc1C)C)C)Nc1ccc2c(c1)nc(n2C)CN1CCCCC1  
ZINC19573130

C1CCCN(CC1)c1ccc(en1)CNc1cc(nc2n1ncn2)c1cccc1  
ZINC71955247

C[C@@H]1O[C@H](C)CN(C1)C(CNC(=O)c1cc(nc2c1cnn2C(C)C)C(C)C)(C)C  
ZINC25407693

CCN(C(=O)Nc1cc(Cl)ccc1N1CCOCC1)Cc1ccc2c(c1)OCO2  
ZINC40103423

Cc1cc(n(n1)c1cccc1NC(=O)N(Cc1ccc2c(c1)OCO2)C)C

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ZINC44209076  
O=C(N1CCN(CC1)c1nc(C)nc(c1)n1cccc1)Nc1ccc(c(c1)Cl)C  
ZINC90607872  
CCOc1cccc1NC(=O)C1CCN(CC1)c1nc2ncccc2n2c1ccc2  
ZINC33012044  
COc1ccc(cc1)[C@H](c1nccn1C)Nc1nc2cc(nn2c2c1cccc2)C  
ZINC26698091  
CCOc1ccc(cc1)C1=CCN(CC1)C(=O)N[C@H](c1nnc2n1cccc2)C  
ZINC93287278  
Cc1ccc(cc1)Oc1cc(nc(n1)C)N1CCN(CC1)C(=O)Nc1cccc1  
ZINC12224300  
COc1cccc1NC(=O)N(c1cccc1)Cc1nnc2n1CCCCC2  
ZINC05223367  
CN(C(=O)Nc1ccnm1C(C)C)Cc1c(C)nn(c1C)c1cccc1  
ZINC43451645  
CCc1ccc(cc1)[C@H]1Nc2nccn2[C@@H](C1)c1cc(OC)c(c(c1)OC)OC  
ZINC02915479  
O=C(N1CCC[C@@H]1c1ccc2c(c1)OCCO2)NCCCn1enc2c1cccc2  
ZINC43858227  
CN(C(=O)Nc1nn(c2c1c(ccc2)Oc1ccnc1)Cc1cccc1)C  
ZINC77380114  
COc1cccc(c1)[C@@H]1CCCN1C(=O)Nc1enc2c(c1)cnn2C(C)C  
ZINC48064198  
CC[C@@H]1CCCN1c1nnc(c1N)N1CCN(CC1)c1ccc(cc1)OC  
ZINC40727647  
Cc1ccc2n(c1)cc(n2)COc1ccc(cc1)C(=O)Nc1ccc(nc1)N(C)C  
ZINC12673894  
COc1ccc(c(c1)OC)N[C@H]1N(Cc2ccc3c(c2)OCO3)C(=O)c2c1cccc2  
ZINC04915523  
COc1cccc(c1)n1nnc(c1C)C(=O)Nc1ccc(cc1)N1CCCCC1  
ZINC58406886  
COc1ccc(cc1)NC(=O)N1CCC(CC1)n1c(C)nc2c1nccc2)C  
ZINC32949886  
COc1cccc(c1)CNC(=O)N1CCN(CC1)c1nc2cccc2n2c1ccc2  
ZINC64450072  
Fc1ccc(cc1)n1ncc2c1nc(N[C@H](c1cccc1)C)nc2N1CCOCC1  
ZINC36656933  
O=C(N1CCN(CC1)C(=O)c1ccc1)Nc1ccc(c(c1)Cl)N1CCCCC1  
ZINC72055301  
COc1cc(ccc1OC)NC(=O)c1c(C)nn(c1n1cccc1)c1ccc(cc1)C  
ZINC15681379  
O=C(N1CCC(CC1)c1enn(c1)C)Nc1nn(cc1C)c1cccc1Cl  
ZINC92190338  
CCOc1ccc(cc1)[C@H]1N(CCn2c1ccc2)C(=O)Nc1ccc2c(c1)OCO2

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ZINC05256221  
O=C(N1CCN(CC1)C(=O)OC(C)(C)C)Nc1cccc1N1CCCCC1

ZINC71902105  
CN(C(=O)Nc1cccc2c1OCCO2)Cc1c(C)nn(c1C)c1cccc1

ZINC56722146  
COc1cc(CNc2cc(C)nc3n2nc(c3)c2ccc(cc2)C)cc(c1OC)OC

ZINC01340699  
COc1cc(cc(c1OC)OC)c1nc2n(c1N[C@@H]1CC[C@@H](CC1)C)ccn2

ZINC09726993  
COc1ccc(cc1)CNc1c(nc2n1ccnc2)c1cc2OCOc2cc1Cl

ZINC72342053  
COc1cccc(c1)N1CCn2c(C1)nc1c2ccc(c1)NC(=O)c1cccc1

ZINC13729324  
OC(=O)c1c(c2ccccc2)oc2ccc(O)c(CN3CCCCC3)c12

8  
O=C(Nc1ccc2c(c1)CCC(=O)N2)NCC1(C)Cc2c(C1)cccc2

ZINC92226553  
O=C(Nc1c(C)cccc1C(C)C)Nc1ccc2c(c1)CC(=O)N2

ZINC73175120  
O=C1NC(=NC1=C(Nc1cccc1)Nc1cccc1)c1cccc1

ZINC06161349  
O=C(Nc1c(C)n[nH]c1C)N[C@@H]1CCO[C@@H]1c1ccc(c(c1)F)Cl

ZINC91046428  
O=C(N[C@H]1CCCOc2c1ccc1c2cccc1)NC[C@@H]1CCC[C@@H]1O

ZINC84459479  
Nc1c(ncnc1NC1CCCC1)NCc1cccc1Cl

ZINC40800451  
O=C(Nc1ccc2c(c1)CCC(=O)N2)NCc1ccc(c(c1)F)C

ZINC31731350  
O=C(Nc1c(C)n[nH]c1C)Nc1cccc(c1)C#Cc1cccn1

ZINC89869535  
CCOc1cc(cc(c1O)Br)[C@H]1N=C(O)c2c(N1)cccc2

ZINC04108247  
O=C(Nc1cccc2c1ccnc2)NC[C@@]1(O)CCc2c1cccc2

ZINC66906739  
O[C@@H]1CC[C@H](CC1)NC(=O)Nc1ccc(cc1)N1CC[C@H](C1)C

ZINC71880073  
O=C1Nc2c(C1)cc(cc2)N[C@@H](C(=O)Nc1cc(C)ccc1C)C

ZINC72997192  
O=C1NCCN1c1cccc(c1)C(=O)NCc1ccc2c(c1)c1CCCCc1[nH]2

ZINC71388768  
O=C(Nc1ccc2c(c1)NC(=O)CC2)NC[C@H]1C[C@]21CCc1c2cccc1

ZINC88390801  
O=C1C[C@@H](CNC(=O)N[C@@H]2[C@H](C)Cc3c2ccccc3)c2c(N1)cccc2

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ZINC89941424  
O=C(Nc1cnc1C)NCc1ccc(c1)Br)O  
ZINC89280621  
O=C(N[C@@H](c1ccc2c(c1)CCC(=O)N2)C)Nc1ccc(cc1)F  
ZINC47719370  
CC(=O)Nc1ccc(cc1)[C@H]1NC(=O)c2c(N1)cc(c2)F)C  
ZINC76864564  
CC(=O)Nc1ccc(c1)C(=O)Nc1cc(Cl)cc(c1O)C)F  
ZINC71909937  
O=C(Nc1cccc(c1F)Cl)Nc1ccc2c(c1)CC(=O)N2  
ZINC73176429  
O=C(Nc1ccc(cc1n1cccc1)Cl)Nc1c(C)n[nH]c1C  
ZINC89869989  
CC(=O)Nc1cccc(c1)NC(=O)c1ccc2c(c1O)cccc2  
ZINC78787771  
O=C1CCc2c(N1)ccc(c2)N[C@H](C(=O)Nc1ccc(cc1)Cl)C  
ZINC27017441  
O=C(Nc1cccc(c1C)Cl)C[C@@H]1Nc2cccc2NC1=O  
ZINC00092690  
COc1ccc(c1)NC(=O)N[C@H]1[C@@H](O)Cc2c1cccc2)Cl  
ZINC69038330  
O=C(Nc1ccc(cc1)Cl)Nc1ccc2c(c1)C(=O)NCC2  
ZINC70953725  
O=C1NC(=C([C@@H](N1)c1ccc(cc1)Cl)C(=O)Nc1cc(Cl)ccc1C)C  
ZINC04953313  
O=C(N[C@H]1[C@@H](O)Cc2c1cccc2)Nc1cc(Cl)ccc1N(C)C  
ZINC77496998  
CC([C@H]1Nc2ccc(cc2NC1=O)C(=O)NC1CCCC1)C  
ZINC06785265  
O=C1Nc2c(C1)cc(cc2)N[C@H](C(=O)Nc1cccc(c1Cl)Cl)C  
ZINC72997462  
CCC(=O)Nc1ccc2c(c1)[C@@H]1C=CC[C@@H]1[C@@H](N2)c1ccc(c1)O)O  
ZINC14457516  
CC(=O)Nc1ccc(cc1NC(=O)c1cc(C)cc(c1O)C)C  
ZINC94101486  
COc1cccc1[C@@H](c1c(O)ccc2c1cc(O)cc2)NC(=O)C  
ZINC00319173  
O=C1N[C@@H](c2cccc2F)[C@H]([C@@](N1)(O)C(F)(F)F)C(=O)c1cccc1  
ZINC04387407  
O=C1CCc2c(N1)ccc(c2)N[C@@H](C(=O)Nc1cccc(c1C)C)C  
ZINC27020380  
COc1cccc(c1O)[C@@H]1Nc2c([C@H]3[C@H]1CC=C3)cccc2C(=O)NC(C)C  
ZINC20694362  
CCn1ccc2c1cc(cc2)NC(=O)N[C@H]1[C@@H](O)Cc2c1cccc2

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ZINC76327279

O=C(NC1(CCOCC1)c1ccc(cc1F)F)Nc1c(C)n[nH]c1C

ZINC89683622

O=C(Nc1ccc2c(c1)CCC(=O)N2)NC1CCCCCCC1

ZINC78262636

O=C(Nc1c(C)cc(nc1Cl)C)N[C@@H]1[C@H](O)Cc2c1cccc2

ZINC80156532

Oc1ccc(cc1)[C@H]1Nc2ccc(cc2[C@@H]2[C@H]1CC=C2)C(=O)NC[C@@H]1C

ZINC13638220

Nc1c(ncnc1NC1CCCC1)N[C@H](c1cccc1)C

ZINC40708532

O=C(c1c(O)ccc2c1cccc2)NCc1c(C)ncc2c1CCNC2

ZINC72411886

CC(=O)Nc1ccc(cc1NC(=O)c1c(O)c(Cl)cc(c1Cl)Cl)C

ZINC94101484

O=C(Nc1ccc(nc1C)Br)NC[C@]1(C)CCCC[C@@H]1O

ZINC91190239

O=C(Nc1ccc2c(c1)CCC(=O)N2)NCc1ccc2c(c1)CCC2

ZINC58544382

Oc1ccc(cc1)[C@@H]([C@H](NCc1cc(Cl)c2c(c1)OCCCO2)C)O

ZINC21866255

O=C(Nc1cccc2c1ccnc2)N[C@H]1[C@@H](O)Cc2c1cccc2

ZINC67474594

Clc1ccc(c(c1)NC(=O)Nc1c(C)n[nH]c1C)N1CCCCC1

ZINC89854362

O[C@@H]1CC[C@H](CC1)NC(=O)Nc1ccc(c(c1)Cl)N1CCCCC1

ZINC72055304

O=C(NC)c1c(c2cccc2)oc2ccc(O)c(CN3CCCCC3)c12

9

O=C(Nc1cccc2c1cccc2)Nc1ccc(cc1)N1CCNC1=O

ZINC55084064

O=C1NCCN(C1)c1cccc1NC(=O)NCc1cccc2c1cccc2

ZINC49027179

OC[C@H](Cc1c[nH]c2c1cccc2)Nc1ccc2c(n1)cc(cc2)F

ZINC78667064

O=C(C[C@@H]1Nc2cc(C)c(cc2NC1=O)C)Nc1ccc(cc1)N(C)C

ZINC00938434

O=C(c1[nH]nc(c1Cl)C1CC1)NCCc1c[nH]c2c1cccc2

ZINC88564842

O=C(Nc1cccc(c1)N1CCCNC1=O)NCC1CCC(CC1)(C)C

ZINC89223472

O=C(Nc1cc(F)ccc1N1CCCCC1)Nc1ccc2c(c1)CC(=O)N2

ZINC73189185

CC(c1ccc(cc1)NC(=O)N1CCC2(CC1)NC(=O)c1c(N2)c(C)ccc1)C

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ZINC34812079  
O=C(Nc1cc(C)cc2c1nccc2)Nc1ccc(cc1)NC1CCOCC1  
ZINC92144245  
O=C(Nc1ccc(c(c1)Cl)N1CCNC(=O)C1)N[C@H]1CCCC[C@H]1C  
ZINC48560942  
OC[C@H](c1ccc(cc1)CC)NC(=O)c1c[nH]c2c1cc(F)cc2  
ZINC91082959  
O=C1NC(=C([C@H](N1)c1ccc(cc1)N(C)C)C(=O)Nc1cc(Cl)ccc1C)C  
ZINC04953319  
CC[C@@H]1CC[C@H](CC1)NC(=O)Nc1cccc(c1)N1CCNC1=O  
ZINC79676184  
CCCCNC(=O)N1CCC2(CC1)NC(=O)c1c(N2)cccc1Cl  
ZINC34812101  
O=C(Nc1cccc(c1)N1CCNC1=O)NCc1ccc(cc1)Cl  
ZINC47893972  
O[C@@H]1CC[C@H](CC1)NC(=O)Nc1cc(ccc1N1CCOCC1)C(F)(F)F  
ZINC71901090  
O=C(Nc1ccc(cc1)C(F)(F)F)Nc1ccc(cc1)N1CCNC1=O  
ZINC58208834  
O=C(Nc1ccc2c(c1)COC2)Nc1ccc(cc1)NC1CCOCC1  
ZINC92150102  
O=C(N[C@@H](c1ccc(c(c1)F)C)C)Nc1cccc(c1)N1CCNC1=O  
ZINC88360086  
Brc1cc(NCCc2c[nH]c3e2cccc3)c(c(c1)F)C(=O)N  
ZINC92826587  
O=C(Nc1cccc1N(C)C)N[C@H](c1ccc2c(c1)CCC(=O)N2)C  
ZINC79493827  
O=C1NCCN(C1)c1cccc1NC(=O)Nc1ccc(cc1)C(C)(C)C  
ZINC49412624  
O=C(Nc1ccc2c(c1)CC(=O)N2)Nc1ccc(c(c1)F)N(C(C)C)C  
ZINC73182544  
COc1cc(CNC(=O)Nc2ccc3c(c2)CCCN3C)ccc1O  
ZINC64561787  
O=C(Nc1ccc2c(c1)CCCN2C)Nc1cc(C)c(c(c1)C)NC(=O)C  
ZINC79799342  
O=C(Nc1ccc2c(c1)CCC(=O)N2)NCc1ccc(cc1N(C)C)C  
ZINC84869510  
Fc1ccc(c(c1)NC1CC1)NC(=O)c1c[nH]c2c1cc(F)cc2  
ZINC91071980  
CCN1CC(=O)Nc2c1ccc(c2)C(=O)Nc1ccc(cc1NC1CC1)F  
ZINC90063836  
O=C(NC1(CCCC1)c1cccc1)Nc1cccc(c1)N1CCNC1=O  
ZINC73027580  
O=C(NC1(C)Cc2c(C1)cccc2)Nc1ccc(c(c1)Cl)N1CCNC(=O)C1

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	ZINC91974585
O=C(Nc1ccc2c(c1)CCC(=O)N2)NCc1ccc(c(c1)F)N(C)C	
	ZINC58617260
O=C(NC1(C)CCCCC1)Nc1cccc(c1)N1CCNC1=O	
	ZINC69631109
O=C(C[C@H]1Nc2ccccc2NC1=O)Nc1ccc(cc1)N1CCCCC1	
	ZINC04115925
O=C(NC1(C)Cc2c(C1)cccc2)Nc1ccc(c1)N1CCCNC1=O	
	ZINC92056745
Cc1ccc2c(c1)C(=O)NC1(N2)CCN(CC1)C(=O)NCc1cccc1	
	ZINC40427056
O=C(Nc1ccc2c(c1)CCCN2C)Nc1ccc2c(c1)CC(=O)N2	
	ZINC73186625
CC(Nc1ccc(cc1)NC(=O)c1cccc(c1)N1CCCNC1=O)F)C	
	ZINC81424996
O=C1NCCN(C1)c1cccc1NC(=O)Nc1ccc(cc1)C(F)(F)F	
	ZINC49413065
CCn1ccc2c1cc(cc2)NC(=O)NC[C@@H]1CC(=O)Nc2c1cccc2	
	ZINC78611261
O=C(NC(c1ccc(cc1)Cl)(C)C)Nc1cccc(c1)N1CCNC1=O	
	ZINC67033918
O=C(N[C@@H]1CCc2c1cccc2O)CCc1c[nH]c2c1cc(C)cc2	
	ZINC81400264
CCN1CC(=O)Nc2c1ccc(e2)C(=O)Nc1cc(F)ccc1NC(C)C	
	ZINC89573861
O=C(Nc1ccc2c(c1)CC(=O)N2)Nc1cccc(c1)N1CCCCC1	
	ZINC73185844
O=C(Nc1cccc(c1)N1CCNC1=O)NC[C@H]1CCC(c2c1cccc2)(C)C	
	ZINC93923481
O=C(Nc1ccc2c(c1)n(C)cc2)Nc1cc(C)c(c(c1)C)NC(=O)C	
	ZINC79807187
O=C(Cc1n[nH]c2c1cccc2)Nc1ccc(cc1)Nc1cccc1	
	ZINC72035548
O=C(N[C@H]1CCc2c1cccc2O)NCc1ccc(cc1)N1CCOCC1	
	ZINC73821750
C[C@H](c1ccc(cc1)N1[C@H](C)CNC1=O)NC(=O)NC1(C)Cc2c(C1)cccc2	
	ZINC92222389
O=C(Nc1ccc(cc1)C)N1CCOCC1)NC[C@]1(O)CCCc2c1cccc2	
	ZINC66952128
CC(Nc1nc(N[C@@]23C[C@H]4C[C@@H](C2)C[C@@H](C3)C4)nc(n1)NC(C)	
	ZINC05255802
O=C(OCC)c1c(c2ccc(O)cc2)oc2ccc(O)c(CN3CCCCC3)c12	
	10
O=C(Nc1ccc2c(c1)NC(=O)[C@H](O2)C)NC[C@H](N(c1cccc1)C)C	

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ZINC76188803  
OCCNc1nc(N[C@H](c2ccccc2)C)nc2c1enn2c1ccc(cc1)F  
ZINC38486261  
O=C(Nc1cccc(c1)NC(=O)c1ccc2c(c1)OCCCO2)NC1CC1  
ZINC42662959  
O=C(C[C@@H]1C(=O)NCCN1C(=O)Nc1ccccc1)Nc1cc(Cl)cc(c1)Cl  
ZINC02241676  
CCOC(=O)C1=C(CNc2cccc3c2nccc3)NC(=O)N[C@@H]1c1cc(C)ccc1C  
ZINC01422885  
O=C(N[C@H](c1cccc(c1)NC(=O)C)C)Nc1ccc2c(c1)OC(O2)(F)F  
ZINC43851235  
O=C(Nc1c(C)nn(c1C)C(C)C)Nc1ccc(c(c1)Cl)NC(=O)C  
ZINC47398505  
CC(NC(=O)N[C@H]1CCN2[C@@H](C1)C(=O)Nc1c(C2=O)cc(cc1)c1ccccc1F)C  
ZINC08300073  
Oc1cccc(c1)NC(=O)c1enn2c1N[C@H](C[C@H]2C(F)(F)F)c1ccc1  
ZINC00866687  
O=C(Nc1ccccc1)NC1CCN(CC1)C(=O)Nc1cnc2c(c1)cccc2  
ZINC67540740  
Cc1nc(Nc2ccc(cc2)NC(=O)Nc2cccc(c2)C)nc(c1)N1CCOCC1  
ZINC17135392  
COc1ccccc1NC(=O)Nc1ccc2c(c1)C(=O)Nc1c(O2)cccc1  
ZINC38901344  
CC1=C(C(=O)Nc2ccccc2)[C@H](N=C(N1)Nc1nc2c(o1)cccc2)c1ccccc1  
ZINC17093570  
COc1cccc(c1)N1C(=O)Nc2c([C@@]1(O)C(=O)N[C@@H]1CC[C@@H](CC1)C  
ZINC04672646  
CCOc1ccc(cc1)NC(=O)Nc1ccc2c(c1)C(=O)Nc1c(O2)cccc1  
ZINC38715307  
CC(NC(=O)N[C@H]1CCN2[C@@H]1C(=O)Nc1c(C2=O)cc(cc1)c1ccc(cc1)Cl)C  
ZINC08296671  
C=CCNC(=O)N[C@H]1CCN2[C@@H](C1)C(=O)Nc1c(C2=O)cc(cc1)c1ccccc1F  
ZINC08300084  
O=C(Nc1cc(C)c(c(c1)C)NC(=O)C)Nc1ccc(nc1)N1CCCC1  
ZINC79783926  
O=C(Nc1nn(cc1C)c1ccccc1Cl)Nc1ccc(c(c1)NC(=O)C)C  
ZINC92190362  
COc1ccc(cc1)NC(=O)N[C@@H](c1ccc(cc1)N1[C@H](C)CNC1=O)C)F  
ZINC92118092  
O=C(Nc1ccc(cc1)N1CCCC1)CNc1cc2OCC(=O)Nc2cc1Cl  
ZINC71887053  
COc1ccc(cc1)NC(=O)C1=C(C)NC(=O)N[C@H]1c1ccccc1OC  
ZINC05851027  
COc1ccc(c(c1)[C@@H](NC(=O)Nc1ccccc1)c1nccn1C)C)O

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ZINC77445679  
Oc1cccc(c1)NC(=O)c1ccc(cc1)NC(=O)N1CCN(CC1)c1cccc1  
ZINC71279776  
O=C(Nc1ccc2c(c1)OCO2)N[C@@H]1CC[C@@H](C1)C(=O)Nc1ccc(cc1)F  
ZINC72427323  
COc1ccc(cc1)CNC(=O)Nc1ccc2c(c1)C(=O)Nc1c(O2)cccc1  
ZINC38715310  
O=C(NC1(CCCCC1)C(=O)Nc1ccc2c(c1)OCCO2)Nc1c(C)cccc1C  
ZINC04982202  
COc1cccc(c1)NC(=O)C1=C(C)NC(=O)N[C@H]1c1ccc(cc1)N(C)C  
ZINC05129385  
COc1ccc(cc1)NC(=O)C1=C(C)Nc2n([C@H]1c1cccc(c1)O)c1cccc1n2  
ZINC09289257  
O=C(N[C@H](c1ccc2c(c1)NC(=O)CO2)C)Nc1ccc(c(c1)C)N(C)C  
ZINC76138628  
COc1ccc(cc1)NC(=O)[C@@H]1C[C@@H](N[C@@]21C(=O)Nc1c2cc(C)cc1Cl)C  
ZINC35828190  
O=C(Nc1nn(cc1C)c1cccc1Cl)NC[C@@](c1ccc(O)C  
ZINC92187808  
CCOc1cccc1NC(=O)C1=C(C)NC(=O)N[C@@H]1c1cccc(c1)OC  
ZINC00641189  
O=C(Nc1ccc2c(c1)OC1(O2)CCCC1)NC[C@H](c1ccc(O)O  
ZINC76096203  
CC(NC(=O)c1ccc(cc1C)NC(=O)N1CCN(CC1)c1ccc(cc1)O)C  
ZINC66683658  
CCN1CCN(CC1)c1ccc(c(c1)C)NC(=O)c1ccc(cc1)NC(=O)N  
ZINC22238034  
CCOc1ccc(cc1)NC(=O)N1CCC2(CC1)NC(=O)c1c(N2)c(C)ccc1  
ZINC40427060  
O=C(Nc1ccnn1C1CCCC1)Nc1cc(C)c(c(c1)C)NC(=O)C  
ZINC79800348  
CCNC(=O)N1CCc2c1cc(cc2)NC(=O)c1ccc2c(c1)CCCC(=O)N2  
ZINC84791062  
O=C(Nc1cccc1)Nc1ccc(cc1)C(=O)NC1CCC2(CC1)OCCO2  
ZINC40151653  
O=C(Nc1cccc1C(=O)Nc1c(C)nn(c1C)C)Nc1cccc1  
ZINC01024008  
CCOc1cccc1NC(=O)C1=C(C)NC(=O)N[C@@H]1c1ccc(cc1)N(C)C  
ZINC00641225  
O=C(C1=C(C)Nc2n([C@@H]1C(C)C)ncc2C(=O)Nc1cccc1)Nc1cccc1  
ZINC20134931  
COc1cc(CNC(=O)Nc2nn(cc2C)c2cccc2Cl)ccc1O  
ZINC92189662  
CC(=O)Nc1ccc(cc1)NC(=O)c1ccc(cc1)N1CCNC1=O)Cl

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ZINC72048257

CCCN(C(=O)[C@@]1(O)N(c2cccc(c2)OC)C(=O)Nc2c1cc(Br)cc2

ZINC09836180

COc1ccc(cc1NC(=O)[C@H](Nc1ccc2c(c1)NC(=O)[C@@H](O2)C)C)Cl

ZINC08729126

O=C(N[C@@H]1CCCc2c1cnn2C)Nc1ccc(cc1)C(=O)NC1CCCC1

ZINC47757736

Oc1cccc(c1)[C@H]1C(=C(C)Nc2n1nc(n2)c1cccc1)C(=O)Nc1cccc1

ZINC00950576

O=C(Nc1cccc1)Nc1ccc(cc1)NC(=O)c1ccc2c(c1)OCCCO2

ZINC22976116

O=C(OCC)c1c(c2ccccc2)oc2cccc(CN3CCCC3)c12

11

Clc1ccc(c(c1)Cl)[C@@H](NC(=O)c1ccc(cc1)CN1CCCC1=O)C

ZINC25450702

Cc1nn(c(c1CNC(=O)[C@@]12C[C@H]3C[C@@H](C1)C[C@@H](C2)C3)C)Cc

ZINC10903257

O=C(C(C)C)NC[C@@H]1CCCN(C1)C(=O)c1ccc(cc1F)c1ccc(cc1)C

ZINC78610108

Clc1ccc(cn1)CNc1cnn(c1)c1ccc(cc1)C(F)(F)F

ZINC92846212

CCOc1cccc1c1cccc(c1)C(=O)NCC#Cc1cccn1

ZINC89330914

CC[C@@H](c1ccc(cc1)Cl)NC(=O)c1ccc(cc1OC)OC

ZINC21592619

Cc1ccc2n(c1)c(NCc1ccc3c(c1)OCO3)c(n2)c1ccc(cc1)N(C)C

ZINC04848454

COc1ccc(cc1Br)[C@@H](NC(=O)N1CCCC[C@H]1C)C

ZINC45182519

COc1ccc(cc1Br)C(=O)Nc1ccc(cc1)OC(C)C

ZINC08569129

C[C@@H](c1onc(n1)C(C)(C)C)Nc1cccc1CCC(F)(F)F

ZINC89099375

CC[C@@H](c1ccc(cc1)Br)NC(=O)N(Cc1cenn1)C

ZINC43233147

C[C@@H](c1nnc(o1)c1cccc1)Nc1cccc1CCC(F)(F)F

ZINC89099379

O=C(Nc1cccc(c1N(C)C)Cl)CCC(=O)c1ccc2c(c1)CCC2

ZINC72071626

O=C(c1cccc(c1)OC[C@@H]1CCCO1)N[C@H]1CCC[C@@H](C1)C(F)(F)F

ZINC73803812

Cc1cccc(c1)Cn1cccc1NC(=O)c1cccc(c1Cl)Cl

ZINC30528339

O=C(N([C@H](c1ccc2c(c1)cccc2)C)C1CC1)N[C@H](c1cenn1)C

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ZINC86340154  
CCc1ccc(cc1)C(=O)N1CCC[C@H](C1)c1cccc(c1)C(=O)NC(C)C  
ZINC33034836  
COc1cc(C)c2c(c1C)C[C@@H](CC2)[C@@H](C(=O)NCc1ccc1)C  
ZINC04222628  
O=C(Nc1cccc1CN1CCc2c1cccc2)CCc1ccnc1  
ZINC55588491  
O=C(c1cccn(c1=O)Cc1cccc1)Nc1ccc(c1)C(F)(F)F  
ZINC01391155  
Clc1ccc(en1)NC(=O)[C@@H](Oc1cccc(c1)C(C)(C)C)C  
ZINC78494956  
Fc1ccc(cc1)NC(=O)c1cc(n1c1cccc1)c1ccc(c1)C)C  
ZINC04376704  
CN(C(=O)c1cccc1C(=O)Nc1c(C)cccc1C)Cc1cccc1  
ZINC32968964  
CCN1CCN(CC1)c1ccc(cc1NC(=O)N([C@H](c1ccc1)C)C)Cl  
ZINC69570090  
CC(Oc1cccc1NC(=O)[C@@H](Oc1cccc1Cl)C)C  
ZINC10683994  
Clc1ccc(cc1)C1=CCN(CC1)C(=O)N[C@H](c1ccnc1)C  
ZINC83642733  
Cc1ccc(cc1)c1occ(n1)CNc1cccc1C(F)(F)F  
ZINC80700011  
COc1cccc(c1)Nc1ncc2c(n1)CCN(C2)Cc1cccc1Cl  
ZINC15778817  
O=C(C1CCCC1)NCCc1nc2c(n1[C@H](c1cccc1)C)cccc2  
ZINC04906606  
Fc1ccc2c(c1)CCN(C2)C(=O)Nc1cccc(c1)OC(F)(F)F  
ZINC91948729  
FC(COc1ncccc1CN[C@H]1CCOc2c1cc(C)cc2C)F  
ZINC90942028  
Cc1ccc(o1)CN(C(=O)Nc1cccc(c1)C)Cc1cccc1  
ZINC04422125  
COc1cc(ccc1OC)[C@H](NC(=O)c1cccc(c1)C(F)(F)F)C  
ZINC20029669  
O=C(Nc1cccc(c1)C)CN(c1ncc(cc1Cl)C(F)(F)F)C  
ZINC33012140  
Cc1ccc(cc1)C(=O)C1CCN(CC1)C(=O)Nc1cccc1C(C)(C)C  
ZINC56543450  
Fc1cccc(c1)Cn1cccc(c1=O)C(=O)Nc1ccc(c1)Cl)C  
ZINC05268837  
O=C(Nc1ccnc1Cl)COc1ccc(c2c1cccc2)Cl  
ZINC03458292  
COc1cccc1[C@@H](N(C(=O)Nc1ccc(cc1Br)F)C)C

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ZINC48451715  
Clc1ccc(c(c1)Cl)C(=O)NCc1c(C)nn(c1C)Cc1cccc1  
ZINC10903254  
CC[C@H](NC(=O)[C@@H]1CC[C@@H](N(C1)C(=O)C1CCCC1)c1ccc(c(c1)  
ZINC37614011  
COc1cccc(c1)c1nc2cccc2c(c1)C(=O)Nc1cccc1  
ZINC00669098  
O=C(C[C@@H](n1cccn1)C)Nc1ccc(c(c1)C(F)(F)F)Cl  
ZINC20990656  
O=C([C@@H]1CC(=O)N(C1)c1ccc(cc1)C(C)C)Nc1ccc(cc1Cl)Cl  
ZINC01158789  
Fc1ccc(cc1)N1CC[C@H](C1)CNC(=O)N(Cc1ccc(c(c1)F)F)C  
ZINC66345415  
CCOc1ccc(cc1)NC(=O)COc1c(C)cc(cc1Cl)Cl  
ZINC01184967  
CC[C@@H]1CCCN(C1)C(=O)Nc1cccc(c1)OCC(F)(F)F  
ZINC44309426  
O=C(c1ccc(c(c1)F)F)Nc1ccc(cc1C(F)(F)F)n1cccn1  
ZINC31967400  
COc1ccc(cc1C(=O)Nc1ccc(cc1)Oc1cccc1)Cl  
ZINC02736562  
CCCCOc1ccc2c(c1)c(C(=O)Nc1cccc(c1)C)c(o2)C  
ZINC46086082  
Cc1ccc(c(c1)C)C(=O)NCCCC1(CCCCC1)C1OCCO1  
ZINC75148678  
O=C(NC)c1c(c2ccc(O)cc2)oc2ccc(O)c(CN3CCCC3)c12  
12  
O=C(Nc1cc(Cl)ccc1O)CNC(=O)c1c[nH]c2c1cccc2  
ZINC49027811  
O=C(Nc1cc(ccc1O)C(F)(F)F)Nc1cc(ccc1O)C(F)(F)F  
ZINC13829413  
CC[C@H](NC(=O)c1cccc2c1N[C@@H]([C@@H]1[C@@H]2C=CC1)c1ccc(cc1  
O)O)C  
ZINC13640364  
O=C(N[C@@H]1CCc2c1cccc2O)N[C@H](c1nc2c([nH]1)cccc2)C(C)C  
ZINC73441816  
O=C([C@@H](Oc1ccc(c(c1)Cl)Cl)C)NC1(CCCC1)C(=O)N  
ZINC70885462  
O=C(N[C@@H]1CCc2c1cccc2O)Nc1cc(=O)[nH]c2c1cccc2  
ZINC85408454  
COc1ccc(c(c1)N)NC(=O)c1cc(c(s1)Br)C  
ZINC94533163  
COc1ccnc(c1)NC(=O)c1nc([nH]c1C)c1cccc(c1)Cl  
ZINC89982313

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O=C(N[C@@H]1CCc2c1cccc2O)NC[C@@]1(O)CCc2c1cccc2  
ZINC74712388

Cc1nc2cccc2c(c1)C(=O)N1CCC(CC1)NC(=O)c1ccc[nH]1  
ZINC65489732

O=C(C1CCN(CC1)C(=O)c1cccc1)Nc1ccc2c(c1)[nH]nc2C  
ZINC91836553

O=C(Nc1cccc(c1)C(=O)N)COc1ccc(cc1)Br  
ZINC09498427

O=C(N[C@H](c1nc2c([nH]1)cccc2)C)NCc1c(O)ccc2c1CCCC2  
ZINC73528787

O=C(Nc1ccc(cc1)C(F)(F)F)N[C@H]1[C@H](O)[C@@H](C[C@@H]1c1cccc1)  
ZINC72321898

OCCCNc1nc(Nc2cc(Cl)ccc2O)nc2c1cccc2  
ZINC41150246

CCc1ccc(cc1)C(NC(=O)Cc1c(C)nc2n(c1C)[nH]c(=O)c2)(C)C  
ZINC81702335

OC[C@H]([C@H](c1ccc(cc1)N)O)NC(=O)c1ccc(cc1Cl)Cl  
ZINC66142159

CC(CC(=O)Nc1ccc2c(c1)[C@H]1C=CC[C@H]1[C@H](N2)c1ccc(cc1O)O)C  
ZINC20682361

O=C(N[C@H]1CCc2c1cccc2O)Nc1ccc2c(c1)nc([nH]2)C(F)F  
ZINC93351610

CCCc1cc(c(cc1OC)O)c1n[nH]cc1c1ccc2c(c1)OCCCO2  
ZINC18097097

O=C(N[C@@H]1CCc2c1cccc2O)NC[C@H](c1c(F)cccc1F)O  
ZINC74712425

O=C(Nc1ccc2c(c1)nc([nH]2)C(F)F)NCC1(O)CCCCC1  
ZINC93351635

OC[C@@H](c1ccc(cc1)Cl)NC(=O)N[C@H]1CCc2c1cccc2O  
ZINC89226240

CC(NC(=O)c1cccc2c1N[C@@H]([C@@H]1[C@H]2C=CC1)c1ccc(cc1O)O)C  
ZINC20682022

COc1ccc(cc1Nc1ccc(n1)C(=O)Nc1ccc(c(c1)F)C)C  
ZINC38512058

CCCNC(=O)c1cccc2c1N[C@@H]([C@@H]1[C@H]2C=CC1)c1ccc(cc1O)O  
ZINC20682029

O=C(Nc1ccc(cc1)c1cc[nH]n1)NC[C@@]1(O)CCc2c1cccc2  
ZINC77711243

N#Cc1ccc(cc1Cl)NC(=O)N1C[C@@H](C[C@@H]1C1CCCC1)O  
ZINC78462355

O=C(Cc1c(C)nc2c(c1C)c(=O)[nH]n2C)NCC(c1cccc(c1)C)(C)C  
ZINC78494952

Fe1ccc(c(c1)F)Oc1cccc1CNC(=O)c1[nH]nc(c1)C  
ZINC67654433

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O=C(N[C@@H]1CCc2c1cccc2O)N[C@H]([C@@H](c1ccc(cc1)Cl)O)C  
 ZINC80460238  
N=C(Nc1nc(=O)c(c([nH]1)C)Cc1cccc1)Nc1ccc(cc1)Cl  
 ZINC17075526  
CCNC(=O)c1cccc2c1N[C@@H]([C@@H]1[C@H]2C=CC1)c1ccc(cc1O)O  
 ZINC20682037  
O=C(C1CC1)Nc1ccc(cc1)NC(=O)c1cc2c(s1)CCCC2  
 ZINC11311613  
O=S(=O)(N1CCOCC1)NCc1ccc2c(c1)c1CCCCCc1[nH]2  
 ZINC71746561  
Cc1ccc(cc1NC(=O)c1cccc2c1ncn2)c1nc2c([nH]1)cccc2  
 ZINC35311250  
OC[C@]1(C)[C@H](O)CC[C@]2([C@H]1CC[C@H]([C@H]2CC(=O)N[C@@H](c1cccc1)C)O)C  
 ZINC43554154  
O=C(Nc1ccc2c(c1)nc([nH]2)C(F)F)NC[C@@]1(C)CCCC[C@@H]1O  
 ZINC93352933  
CCCC(=O)Nc1ccc2c(c1)[C@@H]1C=CC[C@@H]1[C@@H](N2)c1ccc(cc1O)O  
 ZINC13640493  
COc1ccc(cc1NC(=O)c1sc(c1)C)Br)N  
 ZINC94533162  
O=C(Nc1cccc1)Nc1ccc(cc1)c1cccc2c1c(N)n[nH]2  
 ZINC36176941  
Clc1ccc(cc1)[C@@H](C(=O)N1CC[C@H](CC1)c1nc2cccc2cc1N)O  
 ZINC19376222  
O=C([C@@H](Nc1ccc(cc1)N1CCCC1)C)Nc1ccc2c(c1)[nH]c(=O)[nH]2  
 ZINC12559183  
O=C(Cn1nc2c1cccc2)Nc1ccc2c(c1)[nH]c(=O)cc2C(C)(C)C  
 ZINC49472475  
COc1ccc2c(c1)[nH]c(n2)SCC(=O)Nc1cccc1Cl  
 ZINC04705491  
O=C(NCc1cc(=O)[nH]c2c1cccc2)NCC1(O)CCCCC1  
 ZINC85428531  
N=C(Nc1cccc2c1cccc2)Nc1[nH]c(C)c(c(=O)n1)Cc1cccc1  
 ZINC20477893  
OC[C@H]1[C@H]2CC[C@@H]([C@H]1NC(=O)Nc1ccc3c(c1)nc([nH]3)C(F)F)C2  
 ZINC93352642  
O=C(Nc1ccc2c(c1)CCC(=O)N2)NCCc1c[nH]c2c1cccc2  
 ZINC76103210  
C=CCN1c2ccc(cc2[C@](C1=O)(O)CC(=O)c1cccc1O)Br  
 ZINC04673158  
O=C(OCC)c1c(c2ccc(O)nc2)oc2ccc(O)c(CN3CCCCC3)c12

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CCC[C@@H](C(=O)N1CCc2c(C1)ccs2)NC(=O)c1ccc(c(c1)Cl)O  
ZINC66144135

O=C(C1CC1)N[C@@H]1CN(C[C@H]1c1ccc(cc1)C)c1ncccc1C(=O)N  
ZINC77457932

COC(=O)c1sc2c(c1CNC(=O)CC1(O)CCCC1)c(F)ccc2  
ZINC73470612

CCOc1ccc2c(c1)[nH]c(n2)SCC(=O)N[C@@H]1CCOc2c1cccc2  
ZINC26859942

COc1cc(Cl)c(cc1NC(=O)C[C@H]1Sc2cccc2NC1=O)C  
ZINC01122926

COc1ccc(cc1NS(=O)(=O)C)NC(=O)c1cc(F)ccc1Br  
ZINC29817787

O=C([C@H]1CCCN(C1)c1ncccc1C(F)(F)F)Nc1ccc2c(c1)[nH]c(=O)o2  
ZINC47079401

Cc1m(c(n1)C)c1ccc(cc1)C(=O)Nc1ccc(cc1)c1n[nH]cc1  
ZINC79478692

O=C([C@@H](c1cccc1)NC(=O)c1cc2c(s1)occ2)NC1CCCC1  
ZINC77874471

O=C(Nc1mnc(s1)C(c1cccc1)(C)C)Cc1ccc(c(c1)O)C  
ZINC89440474

COc1ccc(cc1Nc1scc(n1)C(=O)Nc1cc(C)ccc1OC)C  
ZINC38512061

CNC(=O)c1cc(Br)ccc1NC(=O)COc1ccc(cc1)C#N  
ZINC89391735

O=C(c1ccc(cc1)S(=O)(=O)Nc1cccc1F)Nc1cccc1  
ZINC21894016

O=C(c1cc(F)c(cc1Cl)F)Nc1cccc(c1)NS(=O)(=O)N(C)C  
ZINC01060717

CC(=O)Nc1cccc2c1CCN(C2)S(=O)(=O)c1c[nH]c(n1)C(C)C  
ZINC80728441

O=C(c1noc(c1)c1cccc1)Nc1ccc2c(c1)[nH]c(=O)cc2C(C)(C)C  
ZINC49472477

O=C(Nc1cccc(c1)S(=O)(=O)N(C)C)NCc1ccc(cc1)Cl  
ZINC40097270

COc1cccc(c1)CNC(=O)C1CCN(CC1)C(=O)c1cc2c([nH]1)sc2  
ZINC13358801

Oc1ccc2c(c1)CN(CC2)C(=O)NCCCc1nc2c(s1)cccc2  
ZINC79020447

Fc1ccc(cc1)NC(=O)c1cccc(c1)S(=O)(=O)NCc1cccc1  
ZINC00991163

O[C@H]1CCCN(C1)C(=O)c1cc(ccc1Cl)S(=O)(=O)NC(C)C  
ZINC67510492

N#Cc1ccc(nc1)O[C@@H]1CC[C@H](CC1)NC(=O)NCc1cccc(c1)Cl  
ZINC92148258

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C[C@@H]1O[C@H](C)CN(C1)c1ccc(cc1)NC(=O)c1[nH]cc(c1)c1csc(n1)C  
ZINC95392643

COc1cc(ccc1OC)[C@H](CN[C@H](c1cnc2c(c1)sc2)C)O  
ZINC90058480

O=C(C[C@@H]1N(C=Cc2c1cccc2)C(=O)C)Nc1ccc(c(c1)C(=O)N)F  
ZINC33064501

O=C1CCCN1Cc1ccc(cc1)CNc1ncc(cc1Cl)C(=O)N  
ZINC80156007

O=C(c1enn(c1C)C(C)C)Nc1n[nH]c(n1)c1cccc2c1cccc2  
ZINC92717341

COc1ccc(cc1Cl)NC(=O)Cc1csc(n1)Nc1cccc1  
ZINC49451250

O=C(Nc1ccc(cc1F)F)CCCC1=Nc2cccc2S(=O)(=O)N1  
ZINC15729551

O=C([C@@H](NC1=NS(=O)(=O)c2c1cccc2)C)NCc1ccc2c(c1)CCC2  
ZINC72004271

O=C(Cc1cc2OCCOc2cc1Br)Nc1ccc(cc1)C(=O)N  
ZINC79289647

CC[C@H](NC(=O)N1CC[C@H](CC1)NS(=O)(=O)c1ccc(cc1)F)C  
ZINC42844124

N#Cc1ccc(cc1)Oc1ccc(cc1)NC(=O)[C@H]1CC(=O)Nc2c1cccc2  
ZINC66037450

CCn1c(cc2c1cccc2)C(=O)N[C@H](c1cccc(c1)S(=O)(=O)NC)C  
ZINC66748953

C[C@@H](c1ccc(cc1)NC(=O)C1CC1)NC(=O)c1sc(nc1C)Cl  
ZINC81937701

Nc1ncc(en1)c1nc2cc(C)cc(c2c(c1)C(=O)N[C@H](C(F)(F)F)C)C  
ZINC23429060

O=C(Nc1ccc2c(c1)NC(=O)CS2)CCOc1cc(C)ccc1C  
ZINC24295412

CCOc1ccc(cc1)NC(=O)CSc1nc2c([nH]1)ncc(c2)Br  
ZINC05249076

O=C(N1CCCN(CC1)C(=O)c1cc2c([nH]1)ccs2)Nc1cccc1  
ZINC77867456

CCn1c(=O)[nH]c(=O)c(c1N)N(Cc1ccc(o1)c1ccc(cc1C)F)C  
ZINC92811589

CC([C@@H](c1onc(n1)c1ccnc1)NC(=O)c1cccc2c1[nH]cc2)C  
ZINC79907987

CCc1nc2onc(c2c(c1)C(=O)Nc1ccc(cc1c1[nH]nc(c1)C)C)C  
ZINC19714498

Cc1ccc(cc1C)Nc1nc(Nc2ccc3c(c2)ccn3)nc(n1)N1CCOCC1  
ZINC12235182

CCc1n[nH]c(c1)NC(=O)c1en(nc1c1ccnc1)c1cccc1  
ZINC76428184

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O=C(CN(S(=O)(=O)c1ccc2c(c1)c1CCCCc1[nH]2)C)NC[C@@H]1CCCO1  
ZINC06931437

O=C(Cc1ccc(cc1)Cl)NCc1[nH]c(=O)c2c(n1)n(nc2)c1cccc1  
ZINC12408933

O=C([C@@H](NC1=NS(=O)(=O)c2c1cccc2)C)NCc1ccc(cc1C(F)(F)F)F  
ZINC72004268

O=C(Cc1c(C)[nH]c2c1cc(C)cc2C)N[C@H](c1nc2n(c1)ncs2)C  
ZINC91713399

O=C(c1ccc(=O)n(c1)Cc1cccc(c1)C(F)(F)F)Nc1cccc1C(=O)N  
ZINC07594237

COc1cc(CNc2[nH]ncn2)cc(c1OCc1ccs1)Br  
ZINC13895990

O=C(NC)c1c(c2cc(F)c(O)cc2)oc2ccc(O)c(CN3CCCCC3)c12  
14

COc1cc(ccc1OC)NC(=O)Nc1ccc2c(c1)C(=O)N1CCCC[C@@H]1CCO2  
ZINC49464580

O=C(Nc1cccc1C)Nc1ccnn1C1CCN(CC1)c1nccn1  
ZINC67714171

COc1ccc(cc1NC(=O)NC1CCN(CC1)c1nc2cccc2n(c1=O)C)C  
ZINC33169721

O=C(Nc1ccc2c(c1)OC1(O2)CCCC1)NCc1nc2n1CCC2  
ZINC43907468

COc1cc(cc(c1OC)OC)C(=O)Nc1ccc2c(c1)C(=O)Nc1c(O2)ccc(c1)C  
ZINC09134886

O=C(C[C@H]1C(=O)Nc2n1ncc2c1ccc(cc1)Cl)Nc1ccc2c(c1)OCO2  
ZINC72455862

Nc1c(ncnc1N1CCN(CC1)c1cccc1F)NCc1ccc2c(c1)OCO2  
ZINC40686290

O=C(N[C@H](c1ccc(cc1)N1CCOCC1)C)Nc1nc2c(c1)c(C)nn2C  
ZINC65455803

CCn1nc(c(c1C)NC(=O)Nc1ccn(n1)c1ncccc1Cl)C  
ZINC89877301

O=C(Nc1nn(cc1C)c1cccc1Cl)NCc1nc2n1CCCCC2  
ZINC92189837

Clc1ccc(cc1)NC(=O)C1=C(C)Nc2n([C@H]1c1ccc3c(c1)OCCCO3)ncn2  
ZINC72460428

C[C@@H]1Oc2ccc(cc2NC1=O)NC(=O)c1cccc(c1)OCc1nc2n(c1)cccc2  
ZINC15480149

c1ccc(cc1)CNc1nc(NCc2ccc3c(c2)OCO3)nc2c1ncn2  
ZINC31820365

CCcn1ncc(c1C)C(=O)Nc1ccc(cc1)[C@@H]1NC(=O)c2c(N1C)nccc2  
ZINC19525906

CCc1nn2c(n1)[C@H](CCC2)NC(=O)Nc1nn(cc1C)c1cccc1Cl  
ZINC92190105

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O=C(Nc1ccc(c(c1)Cl)n1cccn1)NCc1nnc2n1cccc2  
ZINC67287424

COc1ccc(cc1NC(=O)Nc1cc2c(cc1N1CCCC1)n(c(=O)n2C)C)Cl  
ZINC20853305

O=C(Nc1cnn(c1)C(C)(C)C)NC1CCN(CC1)c1cc(C)nc(n1)C  
ZINC93281593

O=C(c1nn(c(c1)NC(=O)c1cccc1Cl)C)Nc1ccc2c(c1)OCO2  
ZINC40755146

O=C(Nc1cnn(c1)c1ncc(en1)N1CCCCC1)NC1CCCCC1  
ZINC65231897

O=C([C@@H]1COc2c(O1)cccc2)Nc1cccc1C(=O)Nc1ccc2c(c1)OCO2  
ZINC09284110

O=C(c1ccc2c(c1)OCCO2)Nc1cccc(c1)NC(=O)c1ccc2c(c1)OCCO2  
ZINC09289106

O=C(c1nn(c(c1)NC(=O)c1cccc1Cl)C)Nc1ccc2c(c1)OCCO2  
ZINC40755148

O=C(c1ccc2c(c1)OCO2)N[C@@H]1CC[C@@H](CC1)NC(=O)c1ccc2c(c1)OCO  
ZINC01115132

COc1n(C)nc(c1NC(=O)Nc1ccc(c(c1)Cl)n1cccn1)C  
ZINC83935428

O=C(N[C@@H](c1ccc2c(c1)OCCO2)C)Nc1cnc2c(c1)c(C)nn2C  
ZINC48103147

Cc1cc(ccc1C)Nc1nc(NCc2ccc3c(c2)OCO3)nc(n1)N1CCOCC1  
ZINC12235198

COc1cccc1NC(=O)C1=C(C)Nc2n([C@H]1c1cccc(c1Cl)Cl)mm2  
ZINC01119438

COc1cc(Cl)c(cc1NC(=O)N[C@H]1CCc2c1nnc2C)OC  
ZINC80180487

O=C(C[C@@H]1C(=O)Nc2n1nc(c2c1cccc1)C)Nc1ccc2c(c1)OCCO2  
ZINC72453130

COc1cc(OC)ccc1NC(=O)C1=C(C)Nc2n([C@H]1c1cccc(c1)F)ncn2  
ZINC04383859

O=C(Nc1c(=O)n(n(c1C)C)c1cccc1)N[C@H](c1c(C)noc1C)C  
ZINC73167894

O=C(Nc1ccc2c(c1)OCO2)Nc1ccc2c(c1)CN(CC2)C(=O)c1cccc1  
ZINC38944676

Cc1ccc(cc1)NC(=O)C1=C(C)Nc2n([C@@H]1c1ccc3c(c1)OCCCO3)nc(n2)C  
ZINC72460456

COc1ccc(cc1)c1nn(cc1[C@@H]1NC(=O)NC(=C1C(=O)OC)C)c1cccc1  
ZINC00908977

O=C(Nc1ccnn1C1CCN(CC1)c1encn1)Nc1cccc(c1)F  
ZINC71315245

O=C(Nc1ccc(cc1)F)N[C@H]1CCN(C1)c1nn2c(c(c1C)C)nn2C(F)(F)F  
ZINC84019768

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O=C(Nc1n(CC(C)C)c(=O)nc2c1cccc2)Nc1ccc2c(c1)OCO2  
 ZINC10214701  
O=C(C1CCCCC1)NC1CCN(CC1)C(=O)Nc1cnc2c(c1)c(C)nn2C  
 ZINC62390818  
C=CCN1c2cc(ccc2OCC(C1=O)(C)C)NC(=O)Nc1ccc2c(c1)OCO2  
 ZINC22509750  
O=C(c1ccc(cc1)NC(=O)c1cccc2n1ncc2)Nc1ccc2c(c1)OCO2  
 ZINC77930353  
CCOC(=O)C1=C(NC(=O)N[C@@H]1c1ccc2c(c1)OCO2)c1ccc(cc1)OC  
 ZINC00831854  
COc1cc(ccc1N1CCCC1=O)NC(=O)Nc1ccc2c(c1)OCO2  
 ZINC10259392  
COc1cccc(c1OC)[C@@H]1[C@H](C(=O)Nc2ccc(cc2C)C)[C@@H](C)Nc2n1nc  
 ZINC11027450  
c1ccc2c(c1)N[C@H]([C@@H](N2)Cn1nnc2c1cccc2)Cn1nnc2c1cccc2  
 ZINC05332327  
CCOc1ccc(cc1)[C@@H]1C(=C(C)Nc2n1nnn2)C(=O)Nc1ccc(cc1)C  
 ZINC40962191  
COc1c(cccc1OC)NC(=O)Nc1ccc2c(c1)C(=O)N(C)c1c(O2)cccc1  
 ZINC49377083  
COc1cccc1NC(=O)C1=C(C)Nc2n([C@H]1c1ccc(cc1)N(C)C)nen2  
 ZINC04705342  
O=C(N[C@@]12C[C@H]3C[C@@H](C1)C[C@@H](C2)C3)NC1CCN(CC1)c1c  
c(C)nc2n1nen2  
 ZINC21175663  
CNC(=O)[C@@H]1CN(CC(=O)Nc2ccc3c(c2)OC2(O3)CCCCC2)c2c(O1)cccc2  
 ZINC09414371  
O=C(NC)c1c(c2ccc(O)cc2)oc2cc(O)cc(CN3CCCCC3)c12  
 15  
O=C1Nc2c(C1(C)C)cc(cc2)[C@@H](NCCc1[nH]nc(n1)c1ccc1)C  
 ZINC89672933  
O=C(Nc1cccc1)NC1CCN(CC1)C(=O)c1ccc(cc1O)C  
 ZINC55420200  
O=C(c1c[nH]c2c1c(Cl)ccn2)Nc1ccc(cc1)N1CCNC1=O  
 ZINC90020480  
O=C(C[C@@H]1Nc2cc(C)c(cc2NC1=O)C)Nc1ccc(cc1)OC(F)F  
 ZINC00938438  
Fc1ccc(c(c1)C(=O)Nc1cccc(c1)C(=O)Nc1ccccn1)O  
 ZINC94082922  
CCOC(=O)C1=C(CNc2cccc(c2Cl)Cl)NC(=O)NC1  
 ZINC70944053  
O=C(Nc1ccc2c(c1)cc[nH]2)NCc1ccnc(c1)N1CCOCC1  
 ZINC58330739  
O=C(Nc1c[nH]nc1)NCc1ccc(nc1)N1CCc2c(C1)cccc2

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ZINC46205021  
Clc1ccc(cc1)c1nn2c(c1)nc(cc2NC[C@@H](c1cccc(c1)O)O)C  
ZINC57710126  
O=C(Nc1ccc2c(c1)NC(=O)[C@H](O2)C)NCC(c1cccc1)(C)C  
ZINC43871120  
O=C(Nc1cccc(c1C)F)Nc1ccc(c(c1)NS(=O)(=O)C)C  
ZINC81071908  
O=C(Nc1cc(C)cc2c1nccc2)NCc1cccc(c1)c1ncn[nH]1  
ZINC92145309  
O=C(Nc1ccnn1Cc1ccc(cc1)Br)Nc1c[nH]nc1  
ZINC80539223  
CCOC(=O)[C@@H]1[C@H](NC(=O)N[C@]1(O)C(F)(F)F)c1cccc(c1Cl)Cl  
ZINC00715264  
O=C(Nc1cnc(cc1C)Cl)NCc1cccc(c1)c1n[nH]c(n1)C  
ZINC89272193  
Nc1c(ncnc1Nc1ccc2c(c1)OCCO2)NC1CCCCC1  
ZINC40708546  
CNS(=O)(=O)c1ccc(c(c1)NC(=O)N[C@]1(C)CC[C@@H](CC1)C)C  
ZINC77479310  
CCN1CC(=O)Nc2c1ccc(c2)C(=O)Nc1cccc1c1ncc[nH]1  
ZINC90057568  
O[C@@H]1CC[C@H](CC1)NC(=O)Nc1cc(ccc1n1ccn1)C(F)(F)F  
ZINC76089509  
O=C(Nc1ccc2c(c1)n[nH]n2)N[C@@H]1CCCC[C@@H]1OC1CCCC1  
ZINC89875442  
CCOc1cccc1NC(=O)C[C@H]1Nc2cc(C)c(cc2NC1=O)C  
ZINC00799411  
CSc1ccc(cc1)NC(=O)[C@@H](Nc1ccc2c(c1)CC(=O)N2)C  
ZINC72997211  
O=C(Nc1cc(c[nH]c1=O)C(F)(F)F)Nc1ccc(nc1)N1CCCC1  
ZINC65818148  
COc1cc(ccc1O)[C@@H]1O[C@@H]([C@@]([C@H]1C)(C)O)c1ccc(c(c1)OC)  
ZINC36378859  
CCNc1ccnc(n1)c1cc(NC2cccn2)nc2c1cc[nH]2  
ZINC72462774  
CC(=O)Nc1ccc(c(c1)NC(=O)N1CCCC[C@@H]1c1ncc[nH]1)Cl  
ZINC88363833  
O=C(c1cnc(nc1)Nc1cccc1)NCc1c(C)ncc2c1CCNC2  
ZINC72409786  
O=C(Nc1ccc(cc1C)F)N[C@H](c1ccc2c(c1)NC(=O)CO2)C  
ZINC43420721  
O=C1COc2c(N1)ccc(c2)C(=O)Nc1cccc1NCC(F)(F)F  
ZINC66452285  
CNC(=O)Nc1ccc(cc1)NS(=O)(=O)c1cc(Cl)ccc1Cl

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ZINC45800189  
O[C@@H](c1ccccc1Cl)CNc1nc(nc2c1CNC2)c1ccccc1  
ZINC72170384  
O=C(N[C@H]1CC(C)(C)Cc2c1cc(o2)C)NC[C@@H](C1CCOCC1)O  
ZINC76951964  
O=C1NCCN1c1ccc(c(c1)C(=O)Nc1ccc2c(c1)[nH]nc2C)F  
ZINC91837106  
C1CCC(CC1)Nc1nc(Nc2ccc(cc2)N2CCOCC2)c2c(n1)[nH]cn2  
ZINC27645129  
O=C(N[C@H]1[C@@H](O)Cc2c1cccc2)Nc1cccc(c1)c1ncc(o1)C  
ZINC66975165  
O=C(Nc1cc2OCCOc2cc1Cl)NCCc1cccc(c1)O  
ZINC77563584  
O[C@H]1CCCN(C1)C(=O)Nc1cc(ccc1C)NC(=O)c1ccccc1  
ZINC48373228  
CCOc1ccccc1NC(=O)C1=C(C)NC(=O)N[C@@H]1c1ccc(cc1)Cl  
ZINC01016443  
CCNc1c(N/C(=N/c2ccc(cc2F)F)/O)c(=O)oc2c1cccc2  
ZINC28048722  
O=C(NCc1ccc(cc1Cl)Cl)CC[C@H]1NC(=O)c2c(N=C1O)cccc2  
ZINC36596686  
O=C(N[C@@]12C[C@H]3C[C@@H](C1)C[C@@H](C2)C3)Nc1ccc2c(c1)NC(=O)[C@H](O2)C  
ZINC43871086  
O=C(N[C@H]1CCN(C1=O)c1cccc(c1)Cl)NCC1(O)CCCCC1  
ZINC79130578  
O[C@@H]1C[C@@H](N(C1)C(=O)Nc1cccc(c1)NC(=O)C)C1CCCCC1  
ZINC78469862  
C[C@@H]1CCN(CC1)C(=O)c1ccc(cc1)NC(=O)N[C@@H]1CC[C@H](CC1)O  
ZINC71998049  
COc1c(F)cc(cc1F)NC(=O)Nc1ccc(c(c1)Cl)C(=O)N  
ZINC56845481  
CCOC(=O)C1=C(C)NC(=O)N[C@@H]1c1cc(Cl)cc(c1O)Cl  
ZINC00070007  
COc1ccc(c(c1)C(=O)Nc1cccc(c1)NC(=O)N)Br  
ZINC29148616  
O=C(Nc1ccc(c(c1)C(=O)N)C)NCc1ccc2c(c1)CCCN2C  
ZINC67310296  
COc1cc(CNC(=O)Nc2ccc3c(c2)CCC(=O)N3)cc(c1)F  
ZINC92226564  
O=C(Nc1cc(ccc1C)c1ncco1)Nc1ccc(cc1)c1ccn[nH]1  
ZINC90480967  
O=C(OCC)c1c(c2ccc(O)nc2)oc2cc(O)cc(CN3CCCCC3)c12

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N#Cc1cccc(c1)COc1ccc(cc1)NC(=O)c1n[nH]c(c1)C(C)C  
ZINC76228389

COCCN1C(=O)c2cccc2[C@@H](C21CCCC2)C(=O)N=c1[nH]c2c([nH]1)cccc2  
ZINC32072240

O=C(N[C@@]12C[C@H]3C[C@@H](C1)C[C@@H](C2)C3)Cc1csc(n1)Nc1cccc  
n1  
ZINC49451284

O=C(Cc1noc2c1cccc2)Nc1ccc2c(c1)[nH]c(=O)cc2C(C)(C)C  
ZINC49472491

CC(=O)NCc1ccc(s1)C(=O)Nc1cc(F)c(c(c1)F)I  
ZINC72056212

O=C(C1CCN(CC1)C(=O)c1cc2c([nH]1)sc2)NCCC1=CCCC1  
ZINC13358811

O=C(c1ccc(cc1)CSc1ncn[nH]1)N[C@@H]1CCC[C@@H](C1)C(F)(F)F  
ZINC42851943

O=C(c1occc1CSc1cccc1)N[C@@H]1[C@H](O)Cc2c1cccc2  
ZINC89509474

CC(=O)c1sc(nc1c1cccc1)NC(=O)c1cccc2c1cc[nH]2  
ZINC81118255

C[C@@H]1CCc2c(C1)sc1c2c(=O)[nH]c(n1)CCC(=O)Nc1cc(C)ccc1C  
ZINC08280836

N#CCSc1cccc1NC(=O)CNc1ccc(c(c1)Cl)Cl  
ZINC15289087

O=C(C1CCN(CC1)C(=O)c1cc2c([nH]1)sc2)NCc1cccc1C  
ZINC13358844

N#Cc1c(=O)[nH]c(c(c1C)CCC(=O)Nc1cc(c1)N1CCCC1)C(F)(F)F)C  
ZINC08826266

OCCN(S(=O)(=O)c1cccc1)Cc1cc2cc(CC)ccc2[nH]c1=O  
ZINC00914179

OCCN([C@@H]1CCc2c1cccc2)C(=O)Nc1cccc(c1)[S@](=O)C  
ZINC85589138

OC[C@H](c1ccc(cc1)CC)NC(=O)c1cc(c1)S(=O)(=O)C  
ZINC92674145

COC(=O)[C@](C(F)(F)F)(c1c(C)[nH]c2c1cccc2)NS(=O)(=O)C  
ZINC02503968

Clc1ccc(cc1)C1(CNC(=O)c2ccc(cc2)S(=O)(=O)N)CC1  
ZINC67194500

Clc1ccc(cc1)C(=O)Nc1nnc(s1)Cc1c[nH]c2c1cccc2  
ZINC01024301

CCOc1c(ccc1Cl)NC(=O)c1cc2C(=O)CCCc2[nH]c1=O  
ZINC56191513

O=C(Nc1ccc(c(c1)Cl)F)CCc1nc2sc3c(c2c(=O)[nH]1)CCCC3  
ZINC06154139

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N#Cc1c(NCCNS(=O)(=O)c2ccc(cc2)Br)cccc1F

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ZINC32934556  
Fc1ccc(cc1F)OCCNS(=O)(=O)c1c[nH]c2c1c(Cl)ccn2  
ZINC93912303  
N#Cc1cccc(c1)COc1ccc(cc1)NC(=O)c1n[nH]c(c1)C1CC1  
ZINC76228394  
CCCc1cc(=O)[nH]c(n1)S[C@H](C(=O)Nc1cc(Cl)ccc1C)C  
ZINC15805399  
O=C(c1[nH]cc(c1)S(=O)(=O)NCC1(C)Cc2c(C1)cccc2)N1CCCC1  
ZINC93938673  
O=C(c1ccc(cc1)CSc1nc2c([nH]1)cccc2)NCc1cccn1  
ZINC17167591  
FC(Sc1ccc(cc1)NC(=O)c1c(C)nc([nH]c1=O)C(C)(C)C)F  
ZINC78784113  
O=C(C1CCN(CC1)C(=O)c1ccc2c(c1)[nH]cc2)NCCc1cccs1  
ZINC63252087  
O=C(Cc1csc(n1)Nc1cccn1)NCc1c(F)cccc1F  
ZINC49451235  
O=C(c1cccc1Nc1ccc(c1C)C)NCCN1CCCS1(=O)=O  
ZINC61598332  
O=C(c1cc2c(s1)c1cc[nH]c1nc2)NCc1cccc(c1)OC(F)(F)F  
ZINC77955188  
N#Cc1c(NC(=O)CNCc2cccc(c2)Cl)sc2c1CCCC2  
ZINC58120203  
O=C(Nc1ccccc1Br)CSc1nc2c([nH]1)ccn2  
ZINC05453307  
COc1cc(ccc1OC(F)F)C[C@@](c1nc2c([nH]1)cccc2)(C#N)CO  
ZINC01457661  
CCCCc1[nH]c2c(n1)cc(cc2)NS(=O)(=O)c1ccc(cc1)OC  
ZINC75106935  
Cc1ccc(cc1)c1csc2c1c(NC[C@@H](c1ccccc1)O)ncn2  
ZINC12578506  
O=C(C1CCN(CC1)C(=O)c1cc2c([nH]1)sc2)NCc1ccc(cc1)F  
ZINC13358804  
CN([C@H](c1ccc(cc1)S(=O)(=O)N)C)C[C@@H](c1ccccc1Cl)O  
ZINC58575063  
CC[C@@H](c1sc(n1)C)NC(=O)c1c[nH]nc1c1ccccc1Cl  
ZINC87312360  
CCNC(=O)c1ccc(cc1)NC(=O)C1(CCCCC1)c1cccs1  
ZINC78078134  
O=C(Nc1ncc(c(c1Cl)C)Cl)CSc1nc2c([nH]1)cc(cc2)C  
ZINC06537155  
CCS(=O)(=O)c1ccc(c(c1)NC(=O)Cc1ccc2c(c1)cccc2)O  
ZINC24152921  
C[C@@H]1CCc2c(C1)cc(s2)C(=O)NCC(=O)Nc1cccc(c1C)C

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ZINC12875937

O=C(c1ccc(c(c1)S(=O)(=O)N)Cl)N[C@@H]1C[C@@H]1C1CCCCC1

ZINC75569584

Cc1ccc(c(c1)C)c1scc(n1)C(=O)NC[C@H](c1ccc(c(c1)F)F)O

ZINC70014994

O=C(c1ccc(cc1)CSc1ncn[nH]1)Nc1cccc(c1C)Cl

ZINC69200608

N#Cc1cccc(c1)COc1ccc(cc1)NC(=O)c1[nH]cc(c1)C(=O)C

ZINC76228399

O=C(N1CCC[C@H]1c1cccc(n1)Nc1scc(n1)C)Cc1c[nH]c2c1cccc2

ZINC72375297

Cc1cc(Br)c(c(c1)C(=O)NCc1esc(n1)C1CC1)O

ZINC69973375

O=C(OCC)c1c(c2ccccc2)oc2ccc(O)c(CN3CCCC(CO)C3)c12

17

O=C([C@H](n1nc(C)c2c(c1=O)nn(c2C)c1ccc(cc1)C)C)NCCC1=CCCCC1

ZINC15942978

COc1cccc1Cn1ncc2c1CCC[C@@H]2NC(=O)c1ccc2c(c1)OCO2

ZINC19570963

CCOc1ccc2c(c1)sc(n2)N1CCC[C@H](C1)C(=O)NCc1cccc1OC

ZINC05105946

O=C(c1cccc2c1oc(c1cccc1)c(c2=O)C)NCc1ccnc1n1ncnc1

ZINC32778076

O=C(Nc1ccc(cc1)N1CCCCC1)CSc1m(c(n1)C1CC1)c1cccc1

ZINC13109765

CCOc1ccc(cc1)c1onc(n1)NC(=O)[C@H](Oc1ccc(c(c1)C)C)C

ZINC32624238

COC(=O)c1ccc(cc1)NC(=O)[C@@H](n1nc(ccc1=O)c1ccc(cc1)C)C

ZINC44390938

COc1cccc1OCC(=O)Nc1cccc(c1)c1nnc(o1)c1cccc1

ZINC02836752

O=C(c1cc(Cl)c2c(c1)OCO2)Nc1ccn(n1)CCc1cccn1

ZINC51418267

O=C(c1ccc(c(c1)S(=O)(=O)N1CCCCC1)F)Nc1ccc(en1)N1CCCCC1

ZINC72023046

COc1ccc(c(c1)CNC(=O)Cn1ncc2c1c1cccc1OC2)OC

ZINC06805325

O=C(Cn1c(=O)cc(c2c1cccc2)c1onc(n1)C1CC1)Nc1cccc(c1)Cl

ZINC67317911

COc1ccc(cc1)[C@@H](c1ccc(cc1)F)NC(=O)CCc1c(C)nc2n(c1C)ncn2

ZINC72028719

Fc1ccc(cc1)n1nc(ccc1=O)C(=O)Nc1ccnn1Cc1ccc(c(c1)F)Cl

ZINC78720530

COc1cc(Cl)c(cc1NC(=O)CSc1nc2c(n1CC)cccc2)OC

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ZINC15475083  
CCOc1cccc1NC(=O)N1CCC(CC1)n1nc2c(c1=O)cc(cc2)C  
ZINC33278465  
COc1cc(ccc1OC)NC(=O)c1nc2c(c1)c(nn2c1cccc1)C1CC1  
ZINC40088800  
O=C1NCCCC[C@H]1Oe1ccc(cc1)OC(=O)c1ccc(cc1)c1ncol  
ZINC67635551  
CCCCOc1cccc1NC(=O)c1nn2c(n1)ncc(c2)Br  
ZINC65662318  
O=C([C@H]1CCCN(C1)c1mnc(s1)n1cccc1)N[C@@H]([C@@]12C[C@H]3C[C@@H](C1)C[C@@H](C2)C3)C  
ZINC20414911  
CCc1nc2onc(c2c(c1)C(=O)N[C@H](c1ccc(cc1)N1CCOCC1)C)C  
ZINC19714499  
O=C(NC1CCCC1)CCc1nc2c(n1C)ccc(c2)S(=O)(=O)N(C)C  
ZINC26537680  
COCCn1c(cc2c1nc1c(C)ccn1c2=O)C(=O)NC1CCCCC1  
ZINC06814234  
COC(=O)c1ccc(cc1)COc1ccc(cc1)[C@H]1C[C@@H](Nc2n1ncn2)c1cccc1  
ZINC13097410  
O=C([C@H](Oc1cccc(c1)C)C)Nc1ccc(cc1)c1mnc(o1)c1cccc1  
ZINC21141774  
O=C([C@H](Oc1ccc2c(c1C)oc(=O)c1c2CCCC1)C)NCCCN1ncnc1  
ZINC06659751  
COc1cc(ccc1OC(F)F)C(=O)NCc1cccnc1n1ncnc1  
ZINC32778075  
O=C1CCCN1c1cc(ccc1Cl)C(=O)N[C@H](c1ccc(cc1)n1ncn1)C  
ZINC09949002  
O=C(C1CCN(CC1)C(=O)c1cccc1C)N[C@@H](c1ccc(cc1)n1ncn1)C  
ZINC18158178  
COc1cccc(c1)N1CCN(CC1)C(=O)CCNS(=O)(=O)c1ccc(c(c1)C)C  
ZINC12536650  
CNC(=O)c1ccc(cc1)CN(C(=O)CCc1c(C)nc2n(c1C)nc1c2cccc1)C  
ZINC12911150  
COc1c(OC)cccc1C(=O)Nc1ccc(c(c1)N1CCCC1=O)OC  
ZINC05440874  
COc1cc(ccc1OC)C(=O)N[C@H](c1onc(n1)c1ccc(cc1)F)C  
ZINC58217587  
O=C(COc1ccc(cc1Cl)Cl)OCC(=O)Nc1ccc2c(c1)OCO2  
ZINC05043717  
COc1ccc(cc1OC)CCNS(=O)(=O)c1ccc2c(c1)OCCO2  
ZINC00894123  
O=C(COc1cc(C)ccc1C)OCC(=O)N1[C@@H](C)CC(=O)Nc2c1cccc2  
ZINC07160022

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COc1ccc(cc1OC)NC(=O)COC(=O)c1c2CCCCC2nc2c1cccc2  
ZINC09664622

O=C([C@H](n1nnc1C)Cc1ccc(c1)F)Nc1cc(C)cc2c1nccc2  
ZINC92874136

C1OC[C@H](C1)Oc1nccc(c1)CNe1nenc2c1cc(o2)c1cccc1  
ZINC92900334

O=C1COc2c(N1)ccc(c2)C(=O)N(Cc1cn(nc1c1cccc1)c1cccc1)C  
ZINC25250182

CCOC(=O)[C@@H]1CCCN(C1)C(=O)Nc1ccc(cc1C(F)(F)F)n1cccn1  
ZINC58175711

O=C([C@@H]1CCCN(C1)S(=O)(=O)C)Nc1ccn(n1)Cc1cccc2c1cccc2  
ZINC02808123

COc1cccc1CNC(=O)CSc1nc2cccc2nc1N1CCCC1  
ZINC13361904

COc1cc2c(en(c(=O)c2cc1OC)CC(C)C)C(=O)NCc1cccn1  
ZINC04763154

COc1cccc(c1)N1CCN(CC1)S(=O)(=O)c1ccc(c(c1)Cl)NC(=O)C  
ZINC08693255

O=C(c1ccc2c(c1)nc(n2c1cccc1)C)Nc1ccc(cc1)S(=O)(=O)N(C)C  
ZINC12531348

CCC(NC(=O)c1ccc2c(c1)N(CC(=O)N1[C@H](C)CCC[C@H]1C)C(=O)C(O2)(C)  
C)(C)C  
ZINC12875932

CC([C@@H](c1ccc2c(c1)OCCO2)NC(=O)c1ccc(cc1)Cn1nnc2c1cccc2)C  
ZINC09257422

O=C(c1ccc2c(c1)nc(n2c1cccc1)C)NCc1cccn1n1ncc1  
ZINC32778078

COc1ccc(c(c1)OC)NC(=O)CCc1c(C)nc2n(c1C)nc(c2)c1cccc(c1)F  
ZINC09609626

O=C(NC)c1c(c2ccc(O)cc2)oc2ccc(O)c(CN3CCCC(CO)C3)c12  
18

Cc1ccc(c(c1)NC(=O)Cn1nnc(c1N)C(=O)Nc1cccc(c1)F)C  
ZINC06999123

COCCOC(=O)C1=C(C)NC(=O)N[C@H]1c1cc(Br)c(c(c1)OC)O  
ZINC04142341

COc1cc2cc(CNc3cc4OCCOc4cc3NC(=O)C)c(=O)[nH]c2cc1OC  
ZINC19022221

CCc1onc(c1NC(=O)N[C@H](c1ccc(cc1)N1[C@H](C)CNC1=O)C)C  
ZINC89441331

COc1cc(NC(=O)CC[C@H]2NC(=O)c3c(N=C2O)cccc3)cc(c1)OC  
ZINC36597285

O=C(N[C@@H]1CCc2c1cnn2C)Nc1ccc(cc1)NC(=O)c1cccc1  
ZINC43974976

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COc1cccc1NC(=O)CN1CC[C@@]2(CCC1=O)NC(=O)c1c(N2)cccc1

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ZINC19571238  
OCCc1nn2c(n1)NC(=C([C@@H]2c1ccccn1)C(=O)Nc1cccc1)C  
ZINC13132001  
O=C(Nc1ccc(cc1)NC(=O)C)COc1cc(O)c2c(c1)OC(CC2=O)(C)C  
ZINC06624187  
COc1cc(ccc1O)[C@H]1[C@@H](C(=O)Nc2ccc(cc2)Cl)[C@H](C)Nc2n1ncn2  
ZINC36701647  
OCC(NC(=O)n1ccc(n1)c1c(C)onc1c1ccc(cc1)Cl)CO  
ZINC71624613  
COc1cccc1Nc1ncccc1C(=O)Nc1ccc(nc1)N1CCNC(=O)C1  
ZINC40089078  
CCOc1cc(ccc1O)[C@@H]1NC(=O)NC(=C1C(=O)OC)CN1CCCCC1  
ZINC67285608  
Nc1c(ncnc1Nc1ccc2c(c1)OCO2)NCc1ccc2c(c1)OCO2  
ZINC40684566  
O=C([C@@H](N1CC[C@]2(CCC1=O)NC(=O)c1c(N2)nccl)C)NCCc1cccc(c1)  
ZINC72326356  
O=C([C@H](N1CC[C@]2(CCC1=O)NC(=O)c1c(N2)cccc1)C)NCCc1cccc1  
ZINC72326816  
COc1ccc(cc1)C(=O)Nc1cccc(c1)[C@H]1NC(=Nc2n1c1cccc1n2)N  
ZINC12520458  
O=C(Nc1ccc2c(c1)NC(=O)[C@@H](O2)C)CCNc1ncnc2c1cc(C)cc2  
ZINC19220695  
CNc1ccc(n1)CNC(=O)Nc1nn(cc1C)c1cccc1Cl  
ZINC92193000  
COc1cc(cc(c1O)Cl)[C@H]1NC(=O)NC(=C1C(=O)OC)[C@@H]1CCCO1)C  
ZINC00706398  
CC(=O)Nc1ccc(cc1)NC(=O)[C@H]1CC(=Nc2n1nc(c2C)c1ccc(cc1)Cl)O  
ZINC35684581  
O=C1NC(=C([C@H](N1)c1cccnc1)C(=O)NCc1ncn2n1cccc2C)C  
ZINC67981968  
O=C1NCCN(C1)c1ccc(cn1)NC(=O)c1ccc2c(c1)[nH]c(=O)n2C1CCCC1  
ZINC72071535  
N#Cc1cc2cc3OCOc3cc2nc1NCCNC(=O)Nc1cccc1C  
ZINC35292113  
O=C(Nc1cccc1)N[C@H]1CCN(C1)C(=O)c1ccc2c(n1)NC(=O)CC2  
ZINC77949126  
OC[C@H]1N(C2CCOCC2)C(=O)CO[C@@H]1c1ccc(cc1)NC(=O)Nc1cccc1  
ZINC72321536  
O=C(Nc1nn(cc1C)c1cccc1Cl)NCc1ccc(o1)C(=O)N  
ZINC92192993  
O=C(Nc1nn(cc1C)c1cccc1Cl)NCc1n[nH]c(n1)c1cccc1  
ZINC92193324  
NC(=O)Nc1ccc(cc1)NC(=O)c1cnn2c1ncc(c2)Br

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ZINC93910983  
CCNc1c(N/C(=N/c2cc(OC)cc(c2)OC)/O)c(=O)oc2c1cccc2  
ZINC45896284  
O=C1Nc2nc(nc(c2[C@H](C1)C(=O)NCCc1cccc1)N)N1CCCC1  
ZINC19820005  
N#Cc1cnn2c1NC(=C([C@H]2c1ccc(c(c1)OC)O)C(=O)Nc1ccc(cc1C)C)C  
ZINC72332732  
OCCNc1nc(NCc2ccco2)nc2c1cnn2c1ccc(cc1)Cl  
ZINC38486264  
CCOc1cc(ccc1O)[C@@H]1C(=C(C)Nc2n1cnc2)C(=O)Nc1ccc(cc1)Cl  
ZINC20175762  
O=C(Nc1ccc2c(c1)OCCO2)CC[C@H]1NC(=O)c2c(N=C1O)cccc2  
ZINC35598219  
O=C(Nc1n[nH]c(n1)c1cccc1F)NCc1cccc1n1ncnc1  
ZINC23505046  
COc1cc2cc([nH]c2c(c1OC)OC)C(=O)Nc1ccc2c(c1)NC(=O)CO2  
ZINC40082810  
O=C(Nc1cccc2c1cccc2)N[C@H]1CO[C@H]2[C@@H]1OC[C@@H]2Nc1nccc(n1)C(C)C  
ZINC08297262  
COc1ccc(cc1)NC(=O)c1ccc(cc1)CNc1nc2n(n1)c(=O)cc([nH]2)C  
ZINC21806729  
C[C@H](NC(=O)[C@H](N1CC[C@]2(CCC1=O)NC(=O)c1c(N2)nccc1)C)CCc1c  
cccc1  
ZINC72326360  
O=C(C[C@H]1NC(=O)c2c(NC1=O)cccc2)Nc1ccc2c(c1)nc(n2C)C(C)C  
ZINC85877439  
O=C(N[C@H](c1ccc2c(c1)NC(=O)CO2)C)Nc1ccc(cc1)Cn1ccn1  
ZINC69201048  
O=C(OC(C)(C)C)NC[C@@H]1CCCC[C@@H]1Nc1ncnc2c1ccc(n2)N  
ZINC90096001  
O=C1NC(=C([C@@H](N1)c1ccnc1)C(=O)NCCc1coc(n1)c1cccc1)C  
ZINC67880065  
O=C1Nc2cc(ccc2O[C@H]1C)NC(=O)c1nc(ncc1Cl)NCc1cccc1  
ZINC32932251  
O=C1NC(=C([C@H](N1)c1ccnc1)C(=O)NCCc1c(C)cccc1=O)C  
ZINC67856338  
CCNc1ccnc(n1)N[C@@H]1CC(C)(C)Cc2c1enc(n2)N1CC[C@H](CC1)O  
ZINC91636411  
O=C(C[C@@H]1C(=O)Nc2n1nc(c2c1cccc(c1)Cl)C)Nc1ccc(cc1)NC(=O)C  
ZINC72458262  
COc1cccc1NC(=O)[C@@H]1[C@@H](Nc2n([C@@]1(C)O)ncc2C#N)c1cccc  
ZINC72332754  
COc1ccc(cc1)/C=C/c1ccc2c(c1)C(=O)N1CC[C@@H]([C@H]1C(=O)N2)NC(=O)

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1-Tam1, 2-Tam2, 3-Tam3, 4-Tam4, 5-Tam5, 6-Tam6, 7-Tam9, 8-Tam10, 9-Tam12,  
10-Tam13, 11-Tam15, 12-Tam16, 13-Tam17, 14-Tam18, 15-Tam19, 16-Tam20, 17-  
Tam21, 18-Tam24.



Table S2. The results of virtual screening based on Glide SP mode and in vitro anti-tuberculosis phenotypic activity test.

ZINC ID	Glide GScore (kcal/mol)	ClogP	MIC( $\mu$ g/ml)
ZINC01530579	-12.114	4.041	32
ZINC00156831	-12.019	2.452	>100
ZINC00403010	-11.455	2.500	>100
ZINC02001884	-11.253	1.856	>100
ZINC01530731	-11.139	0.379	>100
ZINC03830247	-10.902	6.723	64
ZINC00001624	-10.663	4.255	>100
ZINC00897240	-10.620	4.428	ND
ZINC00538465	-10.602	3.797	ND
ZINC00538505	-10.538	4.520	ND
ZINC03831405	-10.389	2.785	>100
ZINC00000856	-10.382	1.741	ND
ZINC00537877	-10.294	3.003	>100
ZINC02570895	-10.062	4.372	64
ZINC00057261	-9.626	2.393	>100
ZINC00020240	-9.586	2.753	>100
ZINC01734034	-9.162	3.764	>100
ZINC00002176	-9.122	1.531	>100
RIF			<0.02

Anti-tuberculosis phenotypic activity assays against the selectable marker-free autoluminescent *Mycobacterium tuberculosis* H37Ra (UAI<sub>Ra</sub>). DMSO and rifampicin (RIF) were used as negative and positive control respectively. The activity data in the table are reported in  $\mu$ g/ml.

Table S3. G-score values of carvedilol (S), carvedilol (R), quinacrine (S), quinacrine (R).

	carvedilol (S)	carvedilol (R)	quinacrine (S)	quinacrine (R)
G-score (kcal/mol)	-12.160	-10.759	-10.902	-10.883