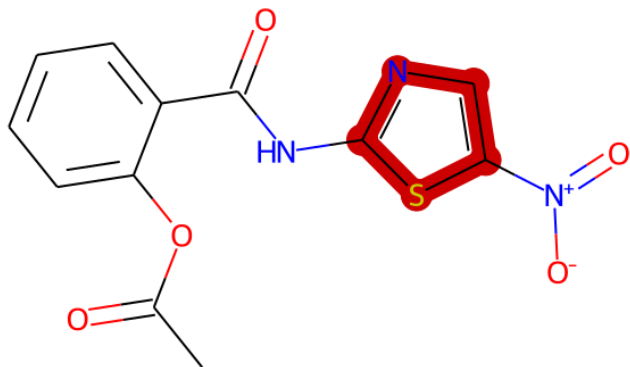zinc_id: ZINC000003956788
smiles: CC(=O)Oc1ccccc1C(=O)Nc1ncc([N+](=O)[O-])s1
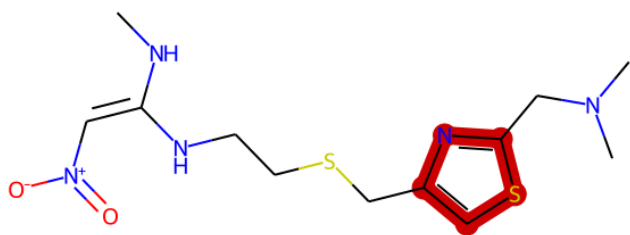QuerySmiles: s:1:c:n:c:c:1

1

zinc_id: ZINC000001530737
smiles: CN/C(=C/[N+](=O)[O-])NCCSCc1csc(CN(C)C)n1
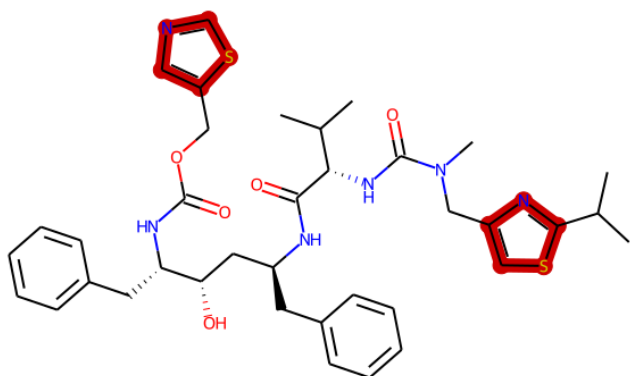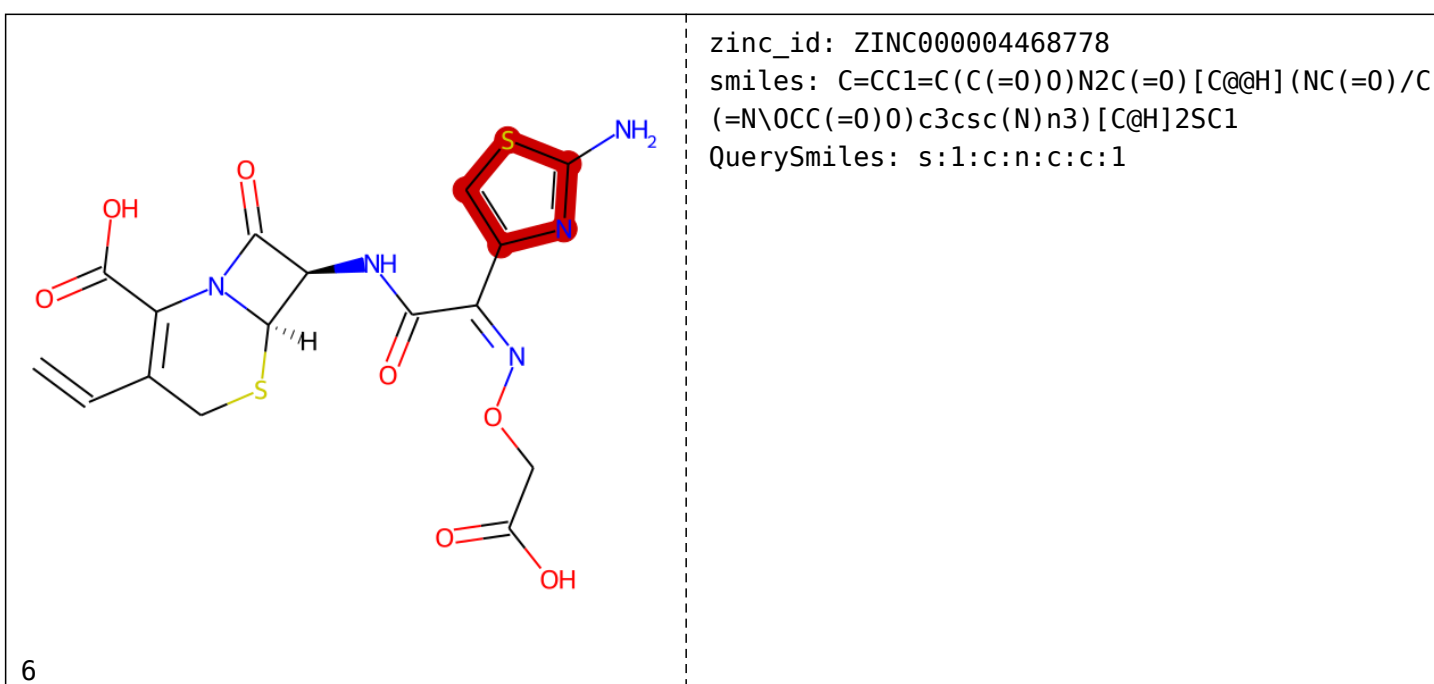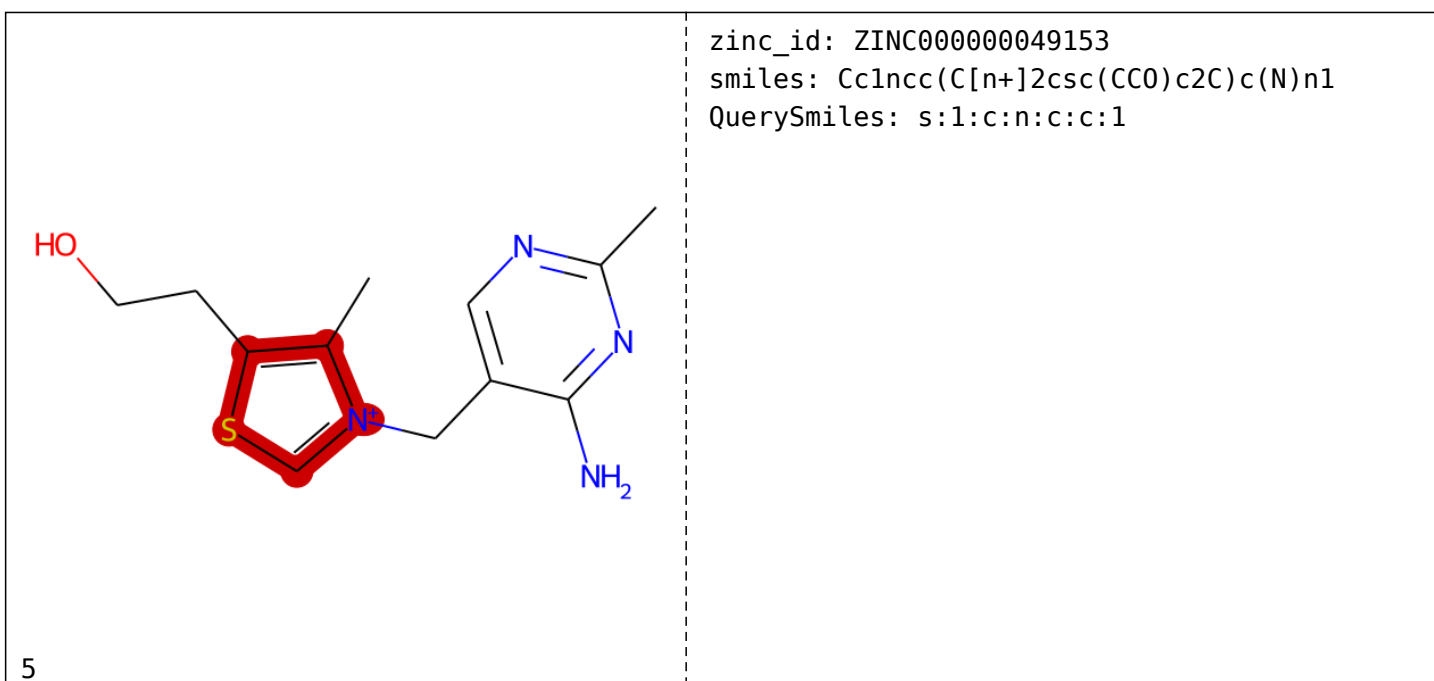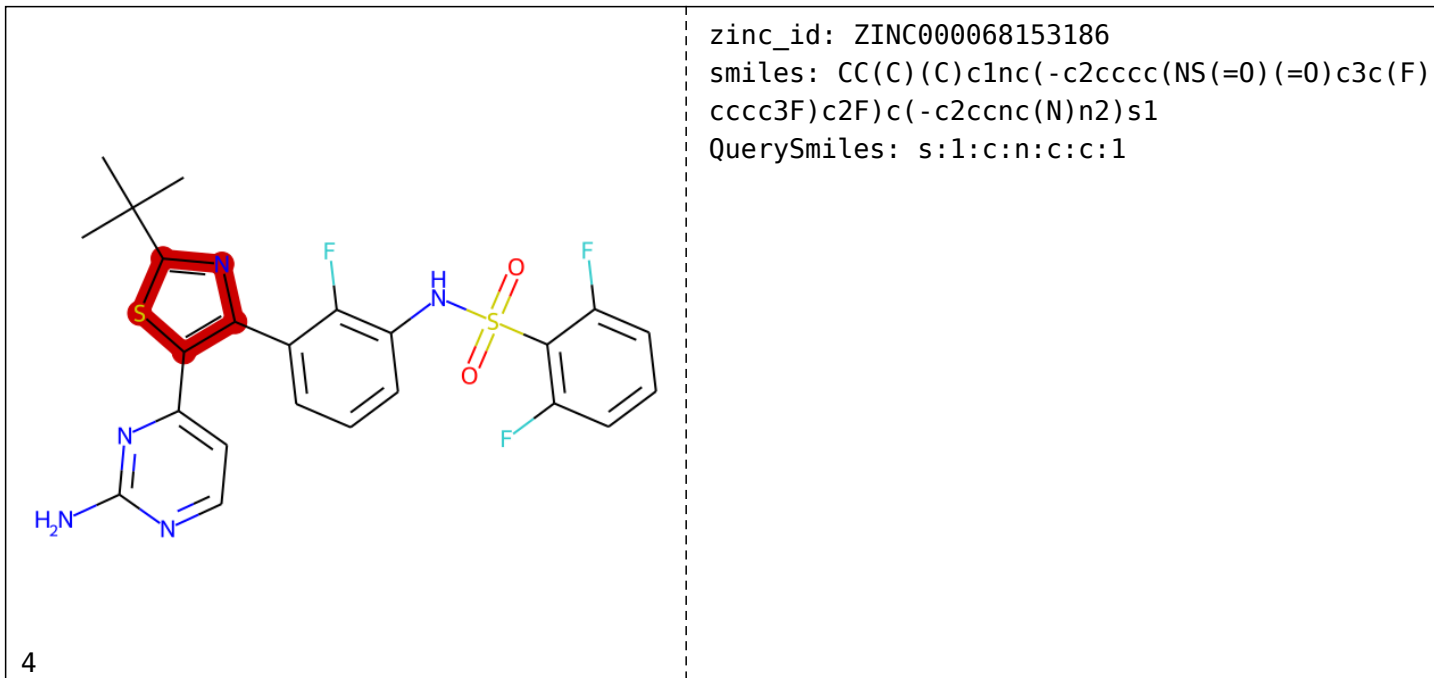QuerySmiles: s:1:c:n:c:c:1

2

zinc_id: ZINC000003944422
smiles: CC(C)c1nc(CN(C)C(=O)N[C@H](C(=O)N[C@@H](Cc2ccccc2)C[C@H](O)[C@H](Cc2ccccc2)NC(=...
QuerySmiles: s:1:c:n:c:c:1

3

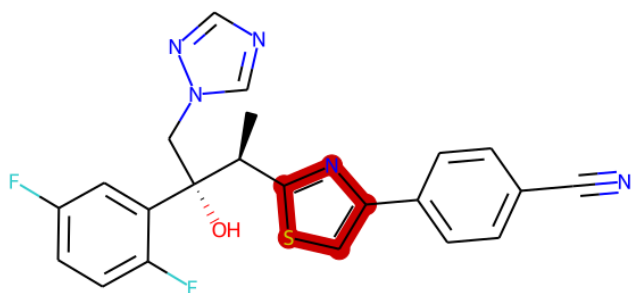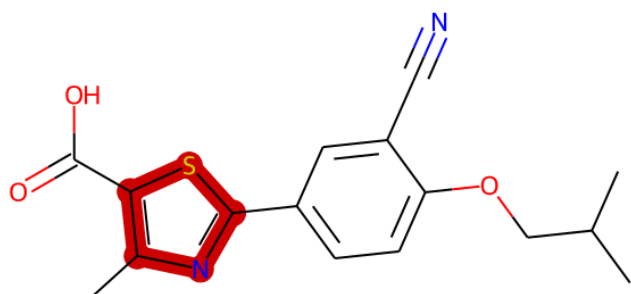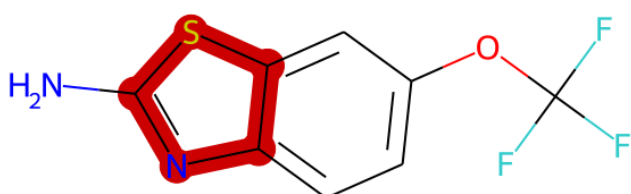|	
4	zinc_id: ZINC000068153186 smiles: CC(C)(C)c1nc(-c2cccc(NS(=O)(=O)c3c(F)cccc3F)c2F)c(-c2ccnc(N)n2)s1 QuerySmiles: s:1:c:n:c:c:1
5	zinc_id: ZINC000000049153 smiles: Cc1ncc(C[n+]2csc(CCO)c2C)c(N)n1 QuerySmiles: s:1:c:n:c:c:1
6	zinc_id: ZINC000004468778 smiles: C=CC1=C(C(=O)O)N2C(=O)[C@@H](NC(=O)/C(=N\OCC(=O)O)c3csc(N)n3)[C@H]2SC1 QuerySmiles: s:1:c:n:c:c:1

zinc_id: ZINC000001485935
smiles: C[C@@H](c1nc(-c2ccc(C#N)cc2)cs1)[C@](O)(Cn1cncn1)c1cc(F)ccc1F
QuerySmiles: s:1:c:n:c:c:1

7

zinc_id: ZINC000000005423
smiles: Cc1nc(-c2ccc(OCC(C)C)c(C#N)c2)sc1C(=O)O
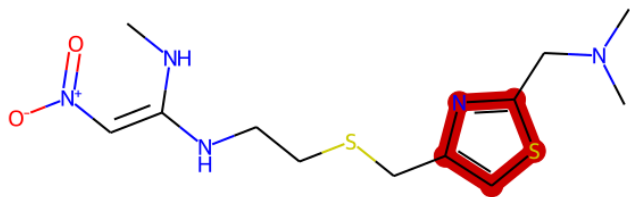QuerySmiles: s:1:c:n:c:c:1

8

zinc_id: ZINC000000006481
smiles: Nc1nc2ccc(OC(F)(F)F)cc2s1
QuerySmiles: s:1:c:n:c:c:1

9

zinc_id: ZINC000001530736
smiles: CN/C(=C\[N+](=O)[O-])NCCSCc1csc(CN(C)C)n1
QuerySmiles: s:1:c:n:c:c:1
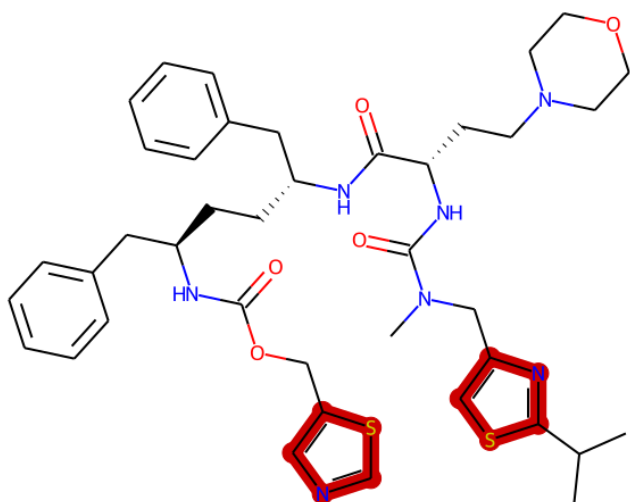
10

zinc_id: ZINC000085537014
smiles: CC(C)c1nc(CN(C)C(=O)N[C@@H](CCN2CCOCC2)C(=O)N[C@H](CC[C@H](Cc2ccccc2)NC(=O)OCc2...
QuerySmiles: s:1:c:n:c:c:1

11

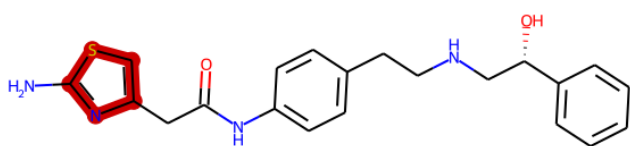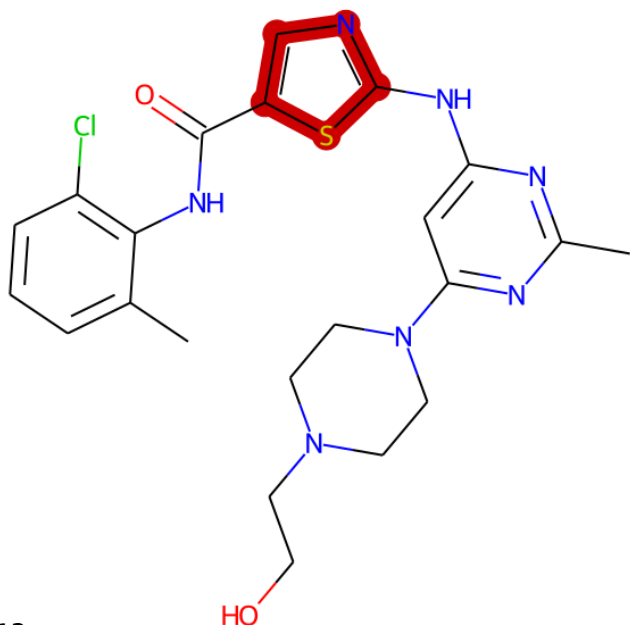zinc_id: ZINC000001996784
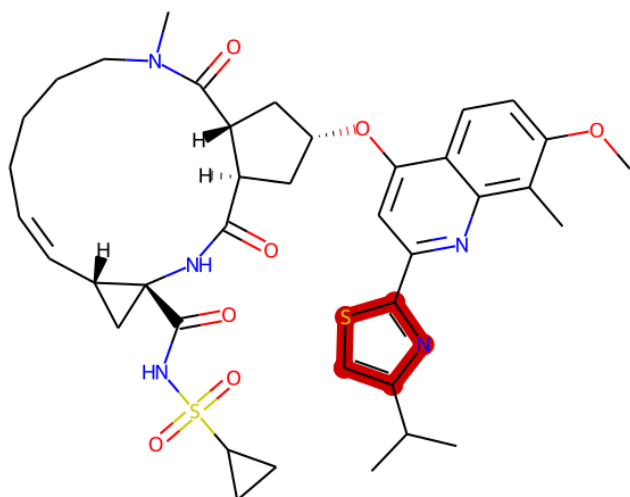smiles: Nc1nc(CC(=O)Nc2ccc(CCNC[C@H](O)c3ccccc3)cc2)cs1
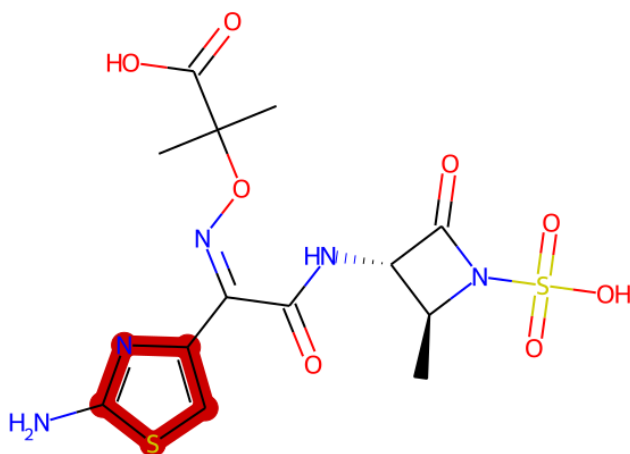QuerySmiles: s:1:c:n:c:c:1

12

zinc_id: ZINC000003986735
smiles: Cc1nc(Nc2ncc(C(=O)Nc3c(C)cccc3Cl)s2)cc(N2CCN(CCO)CC2)n1
QuerySmiles: s:1:c:n:c:c:1

13

zinc_id: ZINC000164760756
smiles: COc1ccc2c(O[C@@H]3C[C@H]4C(=O)N[C@]5(C(=O)NS(=O)(=O)C6CC6)C[C@@H]5/C=C\CCCN(C)...
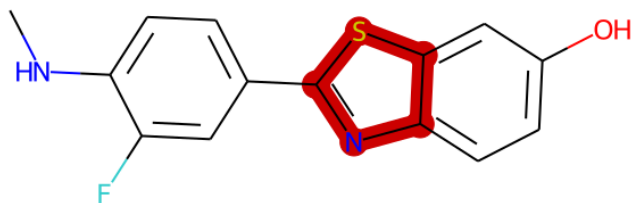QuerySmiles: s:1:c:n:c:c:1

14

zinc_id: ZINC000003830264
smiles: C[C@H]1[C@H](NC(=O)/C(=N\OC(C)(C)C(=O)O)c2csc(N)n2)C(=O)N1S(=O)(=O)O
QuerySmiles: s:1:c:n:c:c:1

15

```
zinc_id: ZINC000034220093
smiles: CNc1ccc(-c2nc3ccc(O)cc3s2)cc1F
QuerySmiles: s:1:c:n:c:c:1
```
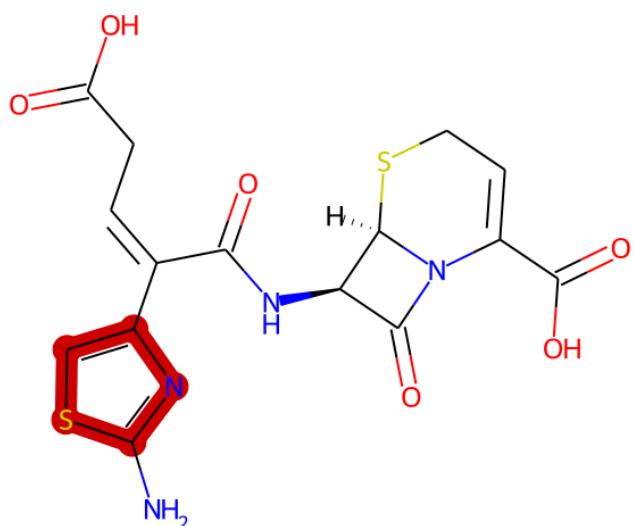
16


```
zinc_id: ZINC000003871967
smiles: Nc1nc(/C(=C/CC(=O)O)C(=O)N[C@@H]2C(=O
)N3C(C(=O)O)=CCS[C@H]23)cs1
QuerySmiles: s:1:c:n:c:c:1
```
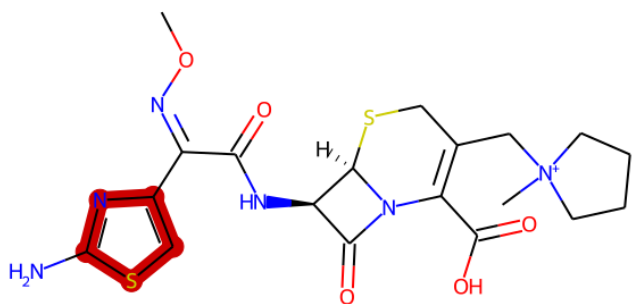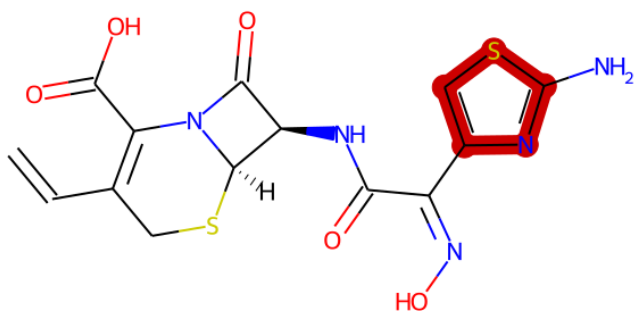
17


```
zinc_id: ZINC000003871923
smiles: CO/N=C(\C(=O)N[C@@H]1C(=O)N2C(C(=O)O)
=C(C[N+]3(C)CCCC3)CS[C@H]12)c1csc(N)n1
QuerySmiles: s:1:c:n:c:c:1
```
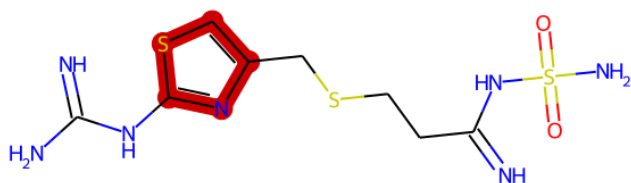
18

zinc_id: ZINC000003927198
smiles: C=CC1=C(C(=O)O)N2C(=O)[C@@H](NC(=O)/C
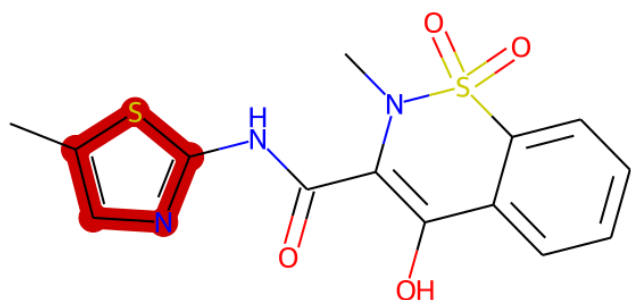(=N\O)c3csc(N)n3)[C@H]2SC1
QuerySmiles: s:1:c:n:c:c:1

19

zinc_id: ZINC000001530636
smiles: N=C(N)Nc1nc(CSCCC(=N)NS(N)(=O)=O)cs1
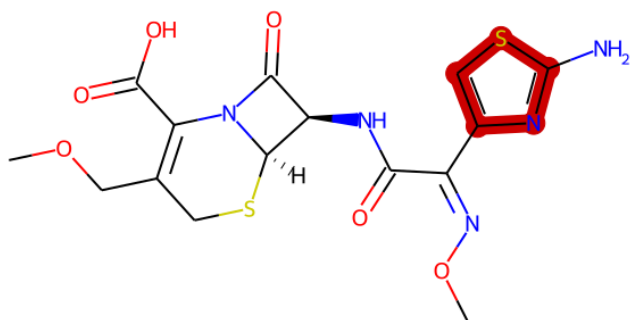QuerySmiles: s:1:c:n:c:c:1

20

zinc_id: ZINC000013129998
smiles: Cc1cnc(NC(=O)C2=C(O)c3ccccc3S(=O)(=O)
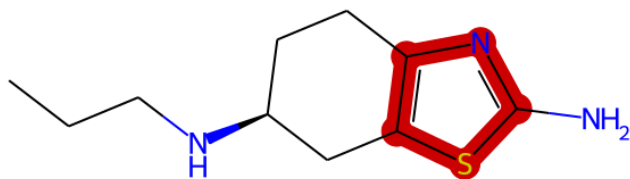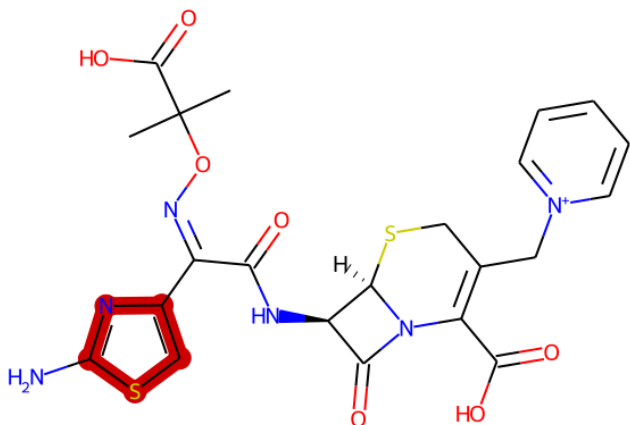N2C)s1
QuerySmiles: s:1:c:n:c:c:1

21

zinc_id: ZINC000003830453
smiles: COCC1=C(C(=O)O)N2C(=O)[C@@H](NC(=O)/C
(=N\OC)c3csc(N)n3)[C@H]2SC1
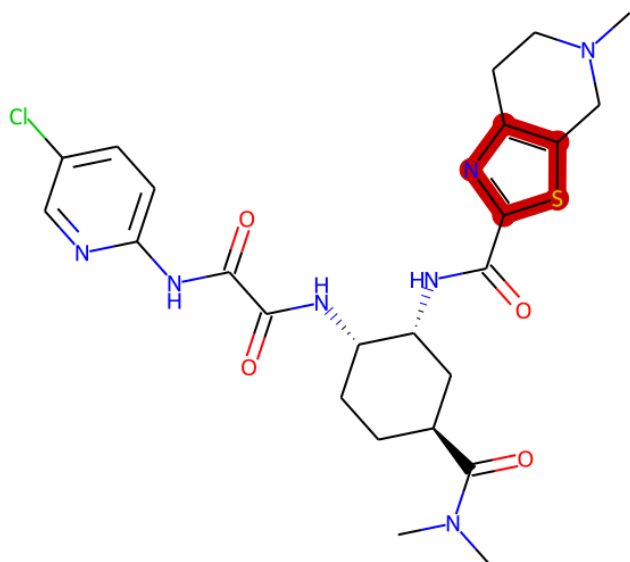QuerySmiles: s:1:c:n:c:c:1

22

zinc_id: ZINC000003781664
smiles: CCCN[C@H]1CCc2nc(N)sc2C1
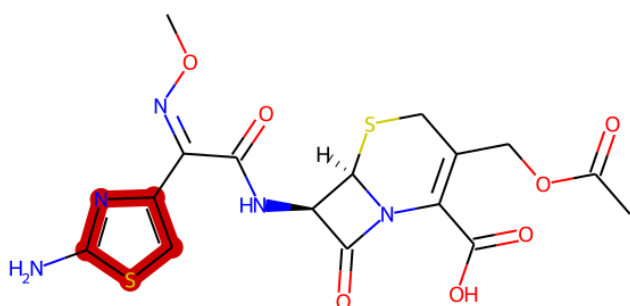QuerySmiles: s:1:c:n:c:c:1

23

zinc_id: ZINC000003871960
smiles: CC(C)(O/N=C(\C(=O)N[C@@H]1C(=O)N2C(C(
=O)O)=C(C[n+]3ccccc3)CS[C@H]12)c1csc(N)n1)...
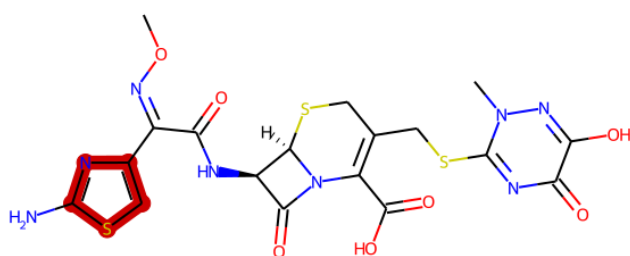QuerySmiles: s:1:c:n:c:c:1

24

zinc_id: ZINC000043200832
smiles: CN1CCc2nc(C(=O)N[C@@H]3C[C@@H](C(=O)N
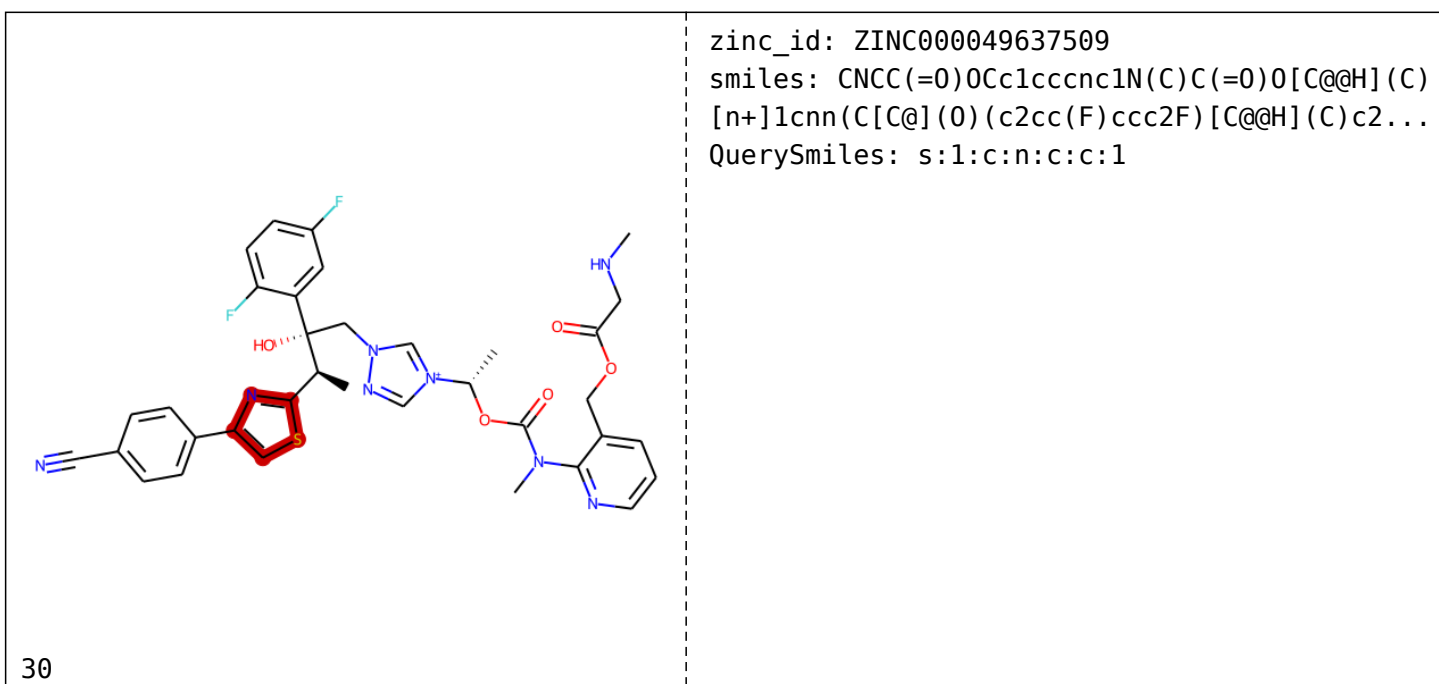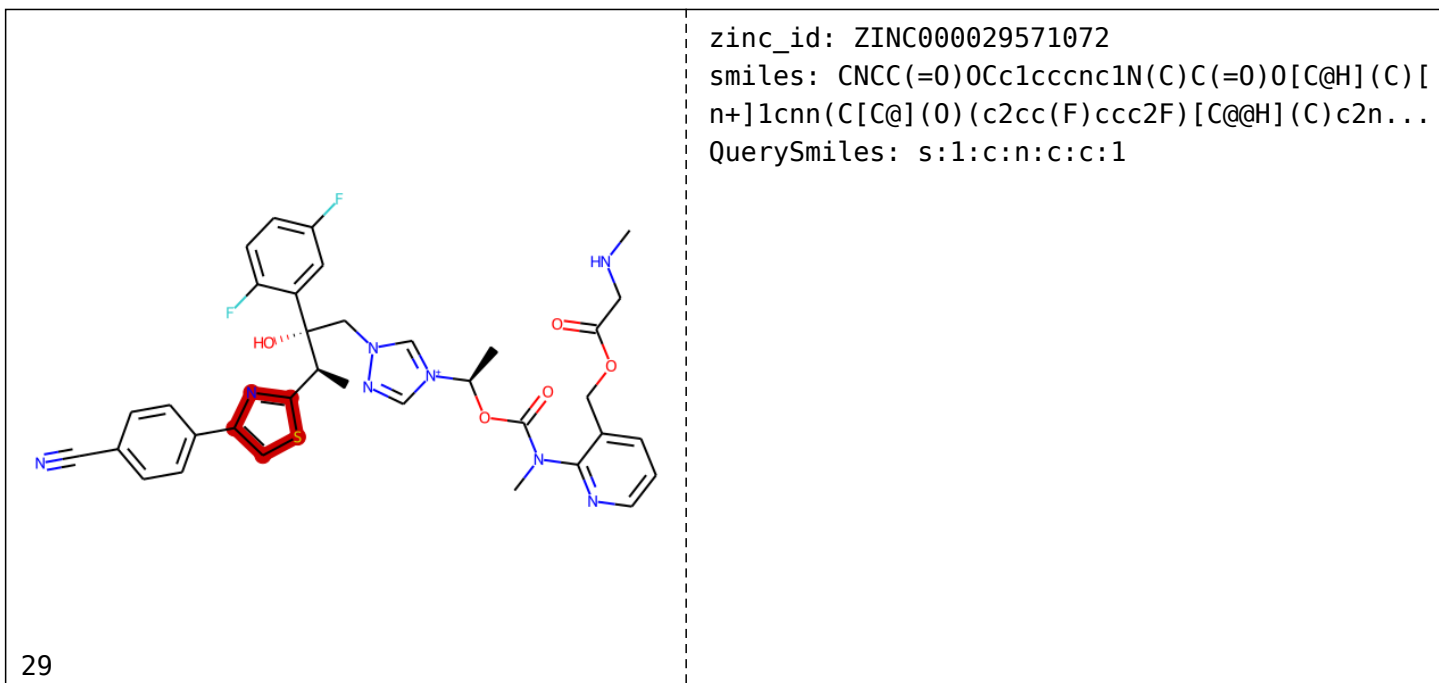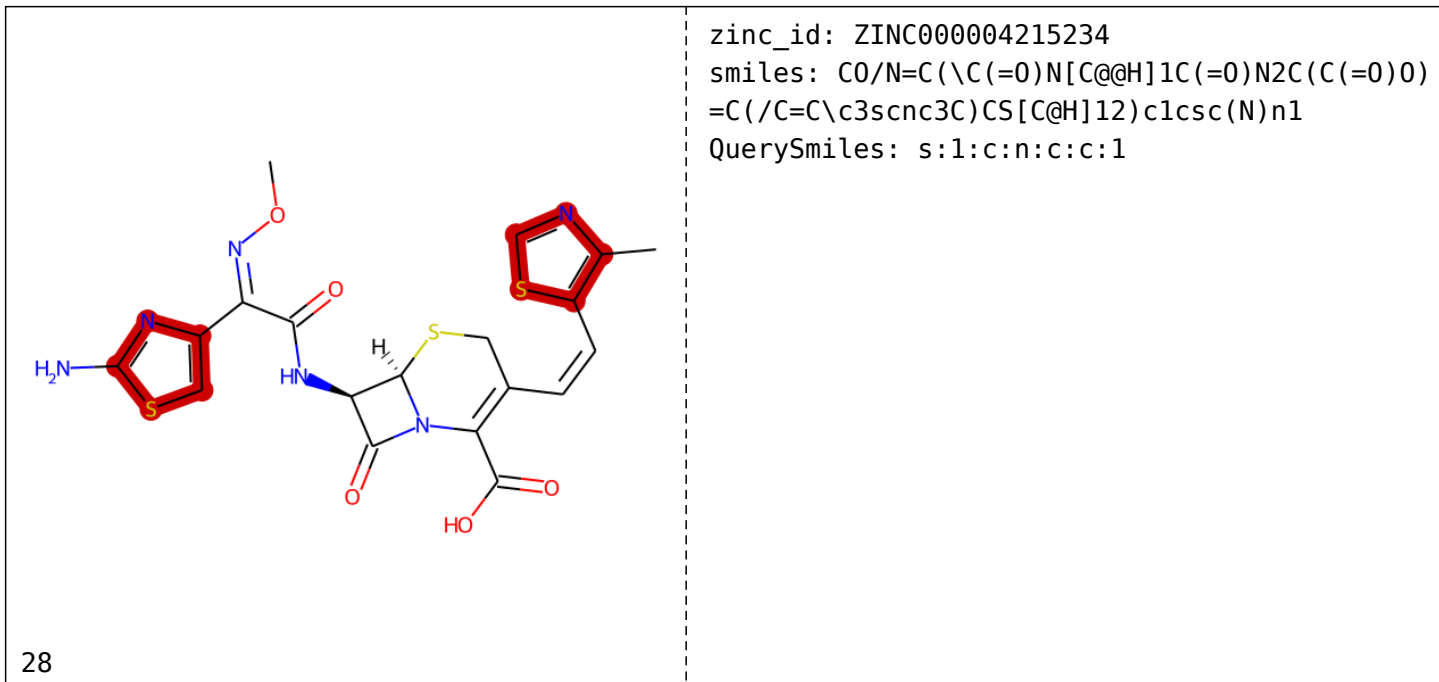(C)C)CC[C@@H]3NC(=O)C(=O)Nc3ccc(Cl)cn3)sc2C1
QuerySmiles: s:1:c:n:c:c:1

25

zinc_id: ZINC000004468780
smiles: CO/N=C(\C(=O)N[C@@H]1C(=O)N2C(C(=O)O)
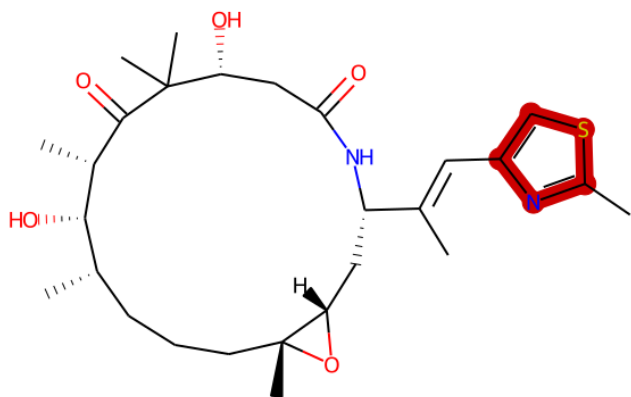=C(COC(C)=O)CS[C@H]12)c1csc(N)n1
QuerySmiles: s:1:c:n:c:c:1

26

zinc_id: ZINC000028467879
smiles: CO/N=C(\C(=O)N[C@@H]1C(=O)N2C(C(=O)O)
=C(CSc3nc(=O)c(O)nn3C)CS[C@H]12)c1csc(N)n1
QuerySmiles: s:1:c:n:c:c:1

27

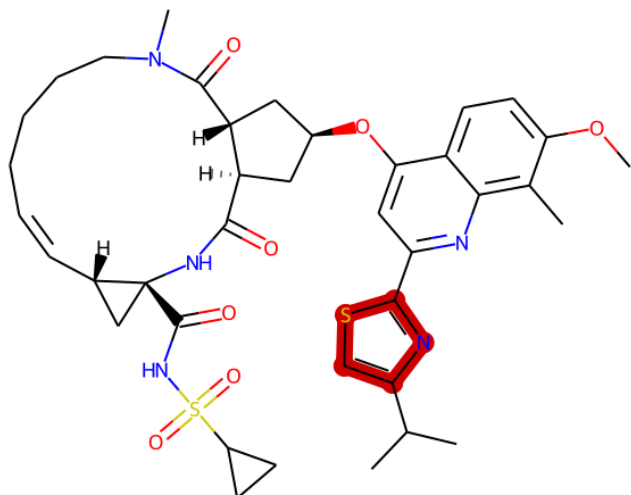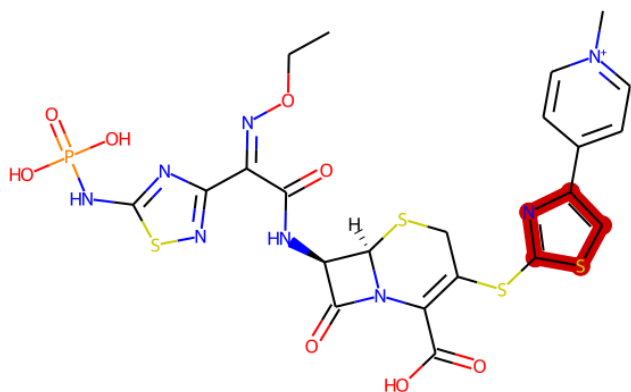|	
  28	zinc_id: ZINC000004215234 smiles: CO/N=C(\C(=O)N[C@@H]1C(=O)N2C(C(=O)O) =C(/C=C\c3scnc3C)CS[C@H]12)c1csc(N)n1 QuerySmiles: s:1:c:n:c:c:1
  29	zinc_id: ZINC000029571072 smiles: CNCC(=O)OCc1cccnc1N(C)C(=O)O[C@H](C)[n+]1cnn(C[C@](O)(c2cc(F)ccc2F)[C@@H](C)c2n... QuerySmiles: s:1:c:n:c:c:1
  30	zinc_id: ZINC000049637509 smiles: CNCC(=O)OCc1cccnc1N(C)C(=O)O[C@@H](C) [n+]1cnn(C[C@](O)(c2cc(F)ccc2F)[C@@H](C)c2... QuerySmiles: s:1:c:n:c:c:1

zinc_id: ZINC000052245489
smiles: C/C(=C\c1csc(C)n1)[C@@H]1C[C@@H]2O[C@]2(C)CCC[C@H](C)[C@H](O)[C@H](C)C(=O)C(C)(...
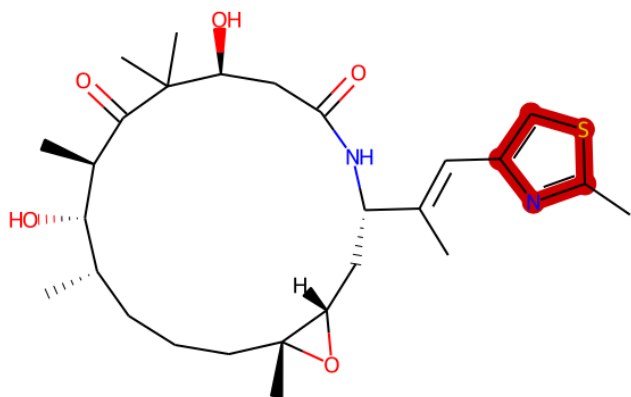QuerySmiles: s:1:c:n:c:c:1

zinc_id: ZINC000164760874
smiles: COc1ccc2c(O[C@H]3C[C@H]4C(=O)N[C@]5(C(=O)NS(=O)(=O)C6CC6)C[C@@H]5/C=C\CCCCN(C)C...
QuerySmiles: s:1:c:n:c:c:1
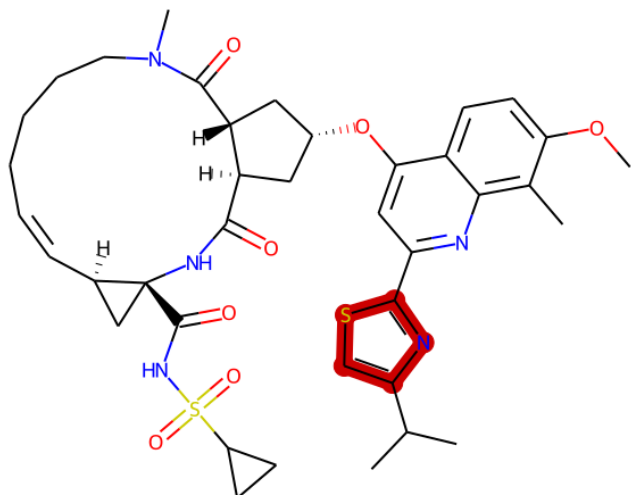

zinc_id: ZINC000003989268
smiles: CCO/N=C(\C(=O)N[C@@H]1C(=O)N2C(C(=O)O)=C(Sc3nc(-c4cc[n+](C)cc4)cs3)CS[C@H]12)c1...
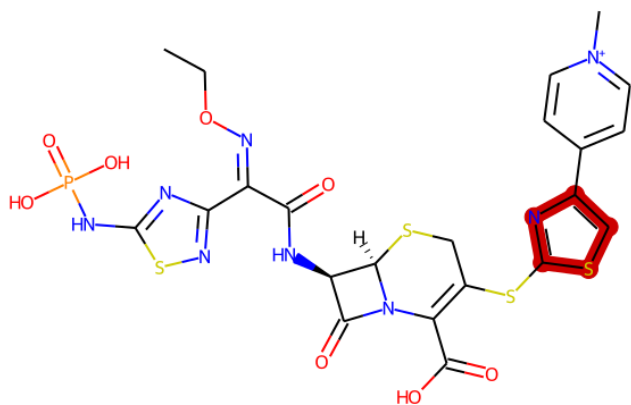QuerySmiles: s:1:c:n:c:c:1

zinc_id: ZINC000003993846
smiles: C/C(=C\c1csc(C)n1)[C@@H]1C[C@@H]2O[C@]2(C)CCC[C@H](C)[C@H](O)[C@@H](C)C(=O)C(C)...
QuerySmiles: s:1:c:n:c:c:1

34

zinc_id: ZINC000253632968
smiles: COc1ccc2c(O[C@@H]3C[C@H]4C(=O)N[C@]5(C(=O)NS(=O)(=O)C6CC6)C[C@H]5C=CCCCN(C)C(=...
QuerySmiles: s:1:c:n:c:c:1

35

zinc_id: ZINC000096006023
smiles: CCO/N=C(/C(=O)N[C@@H]1C(=O)N2C(C(=O)O)=C(Sc3nc(-c4cc[n+](C)cc4)cs3)CS[C@H]12)c1...
QuerySmiles: s:1:c:n:c:c:1

36