

DeepChemDatasets

October 27, 2020

1 DeepChem datasets

```
[2]: import tensorflow as tf
import rdkit
print(tf.__version__)
import sys
#!conda install -y -c conda-forge rdkit deepchem==2.3.0
import deepchem as dc
tf.config.experimental.list_physical_devices('GPU')
print("Num GPUs Available: ", len(tf.config.experimental.
    ↳list_physical_devices('GPU')))
import rdkit
```

1.15.0

```
C:\Users\ella_\conda\envs\tensorflow1\lib\site-
packages\sklearn\externals\joblib\__init__.py:15: FutureWarning:
sklearn.externals.joblib is deprecated in 0.21 and will be removed in 0.23.
Please import this functionality directly from joblib, which can be installed
with: pip install joblib. If this warning is raised when loading pickled models,
you may need to re-serialize those models with scikit-learn 0.21+.
  warnings.warn(msg, category=FutureWarning)
```

```
WARNING:tensorflow:
The TensorFlow contrib module will not be included in TensorFlow 2.0.
For more information, please see:
  * https://github.com/tensorflow/community/blob/master/rfcs/20180907-contrib-
sunset.md
  * https://github.com/tensorflow/addons
  * https://github.com/tensorflow/io (for I/O related ops)
If you depend on functionality not listed there, please file an issue.
```

Num GPUs Available: 1

```
[3]: tasks, datasets, transformers = dc.molnet.load_delaney(featurizer='GraphConv')
train_dataset, valid_dataset, test_dataset = datasets
```

```
Loading dataset from disk.
Loading dataset from disk.
```

Loading dataset from disk.

```
[17]: print(test_dataset.get_task_names())
      test_dataset.get_shape()
```

```
['NR-AR', 'NR-AR-LBD', 'NR-AhR', 'NR-Aromatase', 'NR-ER', 'NR-ER-LBD', 'NR-PPAR-
gamma', 'SR-ARE', 'SR-ATAD5', 'SR-HSE', 'SR-MMP', 'SR-p53']
```

```
[17]: ((784, 1024), (784, 12), (784, 12), (784,))
```

```
[18]: for X, y, w, id in test_dataset.itorsamples():
      print(y, id)
```

```
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCC(=O)C1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1.]
Cc1ccc(Nc2nccc(N(C)c3ccc4c(C)n(C)nc4c3)n2)cc1S(N)(=O)=O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
CC(C)OC(=O)OCOP(=O)(CO[C@H](C)Cn1cnc2c(N)ncnc21)OCOC(=O)OC(C)C
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
CC(=O)N[C@H]([C@H](O)CC(=O)C(=O)O)[C@H](O)[C@H](O)[C@H](O)CO
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(C=Cc1ccc(O)c(O)c1)O[C@H]1C[C@@](OC(=O)
)C=Cc2ccc(O)c(O)c2)(C(=O)O)C[C@H](O)[C@H]1O
[0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 1. 1.] CO[C@H](C(=O)[C@H](O)[C@H](C)O)[C@H]1Cc
2cc3cc(O[C@H]4C[C@@H](O[C@H]5C[C@H](O)[C@H](OC)[C@H](C)O5)[C@H](OC(=O)O)[C@
H](C)O4)c(C)c(O)c3c(O)c2C(=O)[C@H]1O[C@H]1C[C@H](O[C@H]2C[C@H](O[C@H]3C[C@
)(O)[C@H](OC(C)=O)[C@H](C)O3)[C@H](O)[C@H](C)O2)[C@H](O)[C@H](C)O1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
CCCCCCC(=O)CCCCC/C=C/C[C@H](O)[C@H](O)[C@H](N)(CO)C(=O)O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1.] CCC1OC(=O)C[C@H](O)[C@H](C)[C@H](O)[C@H]
2O[C@H](C)C[C@H](N(C)C)[C@H]2O)[C@H](CC(=O)C[C@H](C)C(=O)C=C[C@]2(C)OC2C1C
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)CCOC(=O)c1cccc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] Cc1cc(C)c(C)c(O)c1
[0. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.] CCC(=O)OCCC(C)CCC=C(C)C
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)COC(=O)c1cccc1O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0.]
CC(C)CCCCCCCOC(=O)c1ccc(C(=O)O)CCCCCCC(C)C)c(C(=O)O)CCCCCCC(C)C)c1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCCCC(=O)O.OCCN(CCO)CCO
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCC(=O)OCC(C)OC(=O)CCCCCCC
[0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCOC(C)=O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(=O)OCCC1CCCC1
[0. 0. 0. 1. 0. 0. 0. 1. 0. 0. 0. 0. 0.] COP(=O)(OC)OC(=CC1)c1cc(Cl)c(Cl)cc1Cl
[0. 1. 1. 0. 0. 0. 1. 0. 1. 1. 1. 0.] CCN(CC)C(=S)SSC(=S)N(CC)CC
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0.]
CCCCCN(CCCC)C(=O)C(CCC(=O)[O-])NC(=O)c1ccc(Cl)c(Cl)c1
[0. 0. 1. 1. 0. 0. 0. 0. 0. 0. 0. 1. 0.]
CCCCC1cc(O)c2c(c1)OC(C)(C)[C@H]1CCC(C)=C[C@H]21
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C1CCOC1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN1C(C)(C)CCCC1(C)C
```

[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC1=CCC(C(C)(C)O)CC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCN(Cc1cccc(S(=O)(=O)O)c1)c1cccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(=O)c1ccc(O)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1cc(C(C)(C)C)cc(C)c1CC1=NCCN1
 [0. 0. 0. 0. 0. 1. 1. 1. 0. 1. 1. 0.] F[Sn](c1cccc1)(c1cccc1)c1cccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COc1ccc(O)cc1
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.]
 O=S1(=O)OCC2C(CO1)C1(C1)C(C1)=C(C1)C2(C1)C1(C1)C1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCSCc1cccc1OC(=O)NC
 [0. 0. 1. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0.] BrC1nc2cccc2s1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCC(C)Br
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] N#CCc1cccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)c1ccc(O)O1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] N#Cc1cccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] N#CCBr
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)CBr
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN1CC(O)C2=C/C(=N/NC(N)=O)C(=O)C=C21
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 Cc1ccc(C2(O)CCN(CCCC(=O)c3ccc(F)cc3)CC2)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=S(=O)(O)F
 [1. 1. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.]
 C[C@]1(O)CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@@]3(F)[C@H](O)C[C@@]21C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 N=C(N)c1ccc(OCCCOc2ccc(C(=N)N)cc2Br)c(Br)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CN1[C@H]2CCC[C@@H]1C[C@H](NC(=O)c1nn(C)c3cccc13)C2
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.] O=C(C1)/C=C/C(=O)C1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 Cc1nc2n(c(=O)c1CCN1CCC(c3noc4cc(F)ccc34)CC1)CCC[C@H]2O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 COc1cc(C(C)=O)ccc1OCCCN1CCC(c2noc3cc(F)ccc23)CC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CN(C(=O)CO)c1c(I)c(C(=O)NCC(O)CO)c(I)c(C(=O)NCC(O)CO)c1I
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 O=C1OC2(c3cccc31)c1cc(I)c(O)c(I)c10c1c2cc(I)c(O)c1I
 [0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0.]
 Nc1c(CC(=O)[O-])cccc1C(=O)c1ccc(Br)cc1.Nc1c(CC(=O)[O-])cccc1C(=O)c1ccc(Br)cc1
 [1. 0. 1. 0. 0. 0. 0. 1. 0. 0. 0. 0.] COCCCOc1ccnc(CS(=O)c2nc3cccc3[n-]2)c1C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 COCC(=O)O[C@]1(CCN(C)CCCc2nc3cccc3[nH]2)CCc2cc(F)ccc2[C@@H]1C(C)C
 [0. 0. 0. 0. 0. 0. 1. 1. 0. 0. 1. 0.] CCc1ccc(CCOc2ccc(CC3SC(=O)NC3=O)cc2)nc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCOC(C)=O
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0.]
 OCCOCCN1CCN(C2=Nc3cccc3Sc3cccc32)CC1.OCCOCCN1CCN(C2=Nc3cccc3Sc3cccc32)CC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)CCSCC(=O)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1nc[nH]c1CN1CCc2c(c3cccc3n2C)C1=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)CCCC[C@@H]1SC[C@H]2NC(=O)N[C@H]12
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 1. 0.]

C[C@] (O) (CS(=O) (=O) c1ccc(F) cc1) C(=O) Nc1ccc(C#N) c(C(F) (F) F) c1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C[N+]) (C) (C) C) OC(N)=O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C) NCC(O) COc1ccc(CCOC2CC2) cc1
[1. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] CCCCC(=O) O[C@] 1(C(=O) CO) [C@@H] (C) C[C@H] 2[C@@H] 3CCC4=CC(=O) C=C[C@] 4(C) [C@@] 3(F) [C@@H] (O) C[C@@] 21C
[1. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] CCCC(=O) O[C@] 1(C(=O) COC(=O) CC) [C@@H] (C) C[C@H] 2[C@@H] 3CCC4=CC(=O) C=C[C@] 4(C) [C@@] 3(F) [C@@H] (O) C[C@@] 21C
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(CBr) OCc1ccccc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCc1ccc(Cl) cc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=P(O) (Oc1ccccc1) Oc1ccccc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COC(=O) c1ccccc1C
[0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C) (C) C(=O) c1ccccc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(Oc1ccccc1) c1ccccc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCOC(=O) c1ccc(C) cc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1cc(C) cc(N) c1
[0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C) c1c(C(=O) Nc2ccccc2) c(-c2ccccc2) c(-c2c
cc(F) cc2) n1CC[C@@H] (O) C[C@@H] (O) CC(=O) O
[0. 0. 1. 0. 1. 1. 0. 0. 0. 0. 1. 0.]
Cc1cc(C2(c3cc(C) c(O) cc3C) OS(=O) (=O) c3ccccc32) c(C) cc1O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1ccc(S(=O) (=O) [O-]) cc1C
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1cccc(C) c1N
[0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1ccc(C) c(N) c1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1cccc(N) c1C
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1ncc(CSSCc2cnc(C) c(O) c2CO) c(CO) c1O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC=Cc1ccc(O) c(OC) c1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] FC(F) (F) C(Cl) Br
[0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.] O=C(O) c1ccc(S(=O) (=O) N(Cl) Cl) cc1
[0. 0. 1. 0. 1. 0. 0. 0. 1. 0. 0. 0. 0.] CCCCOC(=O) c1ccc(N) cc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1ccc2c(C) cccc2c1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCC(C) C(C) (COC(N)=O) COC(N)=O
[0. 0. 1. 0. 1. 1. 0. 0. 0. 0. 1. 0.]
CCN(CC) C(=O) [C@@H] 1C=C2c3cccc4 [nH] cc(c34) C[C@H] 2N(C) C1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] OC[C@@H] (O) [C@@H] (O) [C@H] (O) [C@H] (O) CO
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
CN1CCN(CCCN2c3ccccc3Sc3ccc(S(=O) (=O) N(C) C) cc32) CC1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCNCC.O=S(=O) (O) c1cc(O) ccc1O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
Cc1nn(-c2cc(NS(C) (=O) =O) c(Cl) cc2Cl) c(=O) n1C(F) F
[0. 0. 0. 1. 1. 1. 0. 1. 0. 0. 1. 0.] OC(c1ccc(Cl) cc1) (c1cncnc1) c1ccccc1Cl
[0. 0. 0. 0. 1. 0. 0. 1. 0. 0. 0. 0.] CCOC(=O) C(C) Oc1ccc(Oc2nc3ccc(Cl) cc3o2) cc1
[0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.] CCOC(=O) NCCOc1ccc(Oc2ccccc2) cc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
COc1c(O) cc2c(c1O) [C@@H] 1O[C@H] (CO) [C@@H] (O) [C@H] (O) [C@H] 1OC2=O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
Cc1onc(-c2ccccc2Cl) c1C(=O) N[C@@H] 1C(=O) N2[C@@H] (C(=O) [O-]) C(C) (C) S[C@H] 12
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(=O) O[C@H] 1C[C@@] 2(C) [C@@H] (C[C@@H] (O) [C@H] 3[C@@] 4(C) CC[C@@H] (O) [C@@H] (C) [C@@H] 4CC[C@@] 32C) /C1=C(\CCC=C(C) C) C(=O) [O-]
[0. 0. 1. 1. 0. 1. 0. 0. 0. 0. 0. 1.] N#Cc1c [nH] cc1-c1cccc2c1OC(F) (F) O2

[1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CCN(CC)C(=O)N1CCN(C)CC1.O=C(O)CC(O)(CC(=O)O)C(=O)O
 [0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.]
 CCN(CC)CCc1nc(-c2ccccc2)no1.O=C(O)CC(O)(CC(=O)O)C(=O)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CN1[C@H]2CC[C@@H]1C[C@H](OC1c3ccccc3CCc3ccccc31)C2.O=C(O)CC(O)(CC(=O)O)C(=O)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C0c1ccc(C=O)cc1
 [0. 0. 1. 0. 1. 0. 0. 0. 0. 0. 1. 0.] COP(=S)(OC)Oc1c(Cl)cc(C)cc1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 O=C(NC(=O)c1c(F)cccc1F)Nc1ccc(OC(F)(F)C(F)OC(F)(F)F)c(Cl)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCOC(=O)c1ccc(C(=O)OCCC)nc1
 [0. 0. 0. 0. 1. 0. 0. 1. 0. 0. 0. 0. 0.] CC(O)CCO
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)CCS
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCC[n+](c1ccc(C)cc1).O=S(=O)([O-])C(F)(F)F
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCC[N+](C)CCCC1.F[B-](F)(F)F
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(=O)C1CCCCC1=O
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0.] CCCC[n+](c1ccc(C)c1).O=S(=O)([O-])C(F)(F)F
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCNC=CN(C)C1
 [0. 0. 0. 0. 1. 1. 0. 1. 0. 0. 1. 0.] CC1(C(=O)Nc2ccc(O)c(Cl)c2Cl)CCCCC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCC[N+](C)CCCCC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCC[N+](C)CCCCC1.F[B-](F)(F)F
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] N=C(N)N[N+](=O)[O-]
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)(C)OOC(C)(C)C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1. 0.] CCC(C)Nc1ccc(NC(C)CC)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCNCCCC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCN(CCO)CCCC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 O=C(O)c1ccc2[nH]cc(CCCCN3CC=C(c4ccccc4)CC3)c2c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1.] CN1C2CCC1CC(OC(c1ccccc1)c1ccc(Cl)cc1)C2
 [0. 0. 0. 0. 1. 1. 0. 0. 0. 0. 0. 0.] Oc1ccc(C2CNCCc3c2cc(O)c(O)c3Cl)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Oc1ccc2[nH]cc(CCCCN3CC=C(c4ccccc4)CC3)c2c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] C[C@H](/C=C/[C@H](C)[C@H]1CC[C@H]2/C(=C/C=C3C[C@H](O)C[C@H](O)C3)CCC[C@@]21C)C(C)(C)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCOC(=O)NNc1ncc2ccccc12
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)(C)NCCNC(C)(C)C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CCCCC(F)(F)[C@@]1(O)CC[C@H]2[C@@H](CC(=O)[C@@H]2CCCCC(=O)O)O1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CC(C)=CCC/C(C)=C/CC/C(C)=C/CCC(=O)OC/C=C(\C)CCC=C(C)C
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.]
 CCN(CC)Cc1nccn1-c1ccc([N+](=O)[O-])cc1C(=O)c1ccccc1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] OC1CCCCCCCCCCC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)(C)CC(=O)OCC(=O)[C@@]12OC(C)(C)O[C@@H]
]1C[C@H]1[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@@]3(F)[C@@H](O)C[C@@]12C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CCCCC(=O)(=O)N[C@@H](Cc1ccc(OCCCC2CCNCC2)cc1)C(=O)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COC(=O)c1ccc(C(=O)O)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN(C)CCOCCO

[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C) [N+] (C) (C)CC(O)COc1cccc2ccccc12
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 Cc1ccc(S(=O)(=O)NC(=O)N[C@@H](C)Cc2ccccc2)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Nc1ccc(S(=O)(=O)NCc2ccccc2)cc1
 [0. 0. 1. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0.] CC=CC=NNC(=O)c1ccncc1
 [0. 0. 1. 1. 0. 0. 0. 0. 0. 0. 0. 1.] O=C1C(=O)c2ncccc2-c2cccnc21
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CC12CCC(C[N+](C)(CCC[N+](C)(C)C)C1)C2(C)C.COS(=O)(=O)[O-].COS(=O)(=O)[O-]
 [1. 0. 1. 0. 1. 0. 1. 0. 1. 0. 1. 1.] Nc1ccc(C(=O)Nc2ccccc2N)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C[N+](C)(C)CCOC(=O)C(O)(c1ccccc1)c1ccccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)C=CC(=O)Nc1ccc(S(=O)(=O)Nc2nccs2)cc1
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0.] FC(F)(F)C(F)(F)C(F)(F)C(F)(F)CCI
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC/C=C\CCOC(=O)CC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CO[PH](=O)OC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=CC(C)(CCC=C(C)C)OC(=O)CC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN1C(=O)CC[C@H]1c1cccnc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C[C@H]1C[C@@H](O)CC(C)(C)C1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] ClP(Cl)c1ccccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C1COC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1c(O)cccc1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCOC(=O)CC([O-])C(=O)OCC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] c1ccc(CCc2ccccc2)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COC(=O)c1ccccc1
 [0. 1. 0. 0. 0. 1. 1. 0. 1. 0. 0. 0. 0.] C=CC(=O)OCC(C)OCC(C)OC(=O)C=C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1ccc(CO)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C/C=C(/C)C#N
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0.] C=CC(=O)OCC[N+](C)(C)C
 [0. 0. 0. 0. 1. 0. 0. 1. 0. 0. 0. 0. 0.] O=C(C=Cc1ccccc1)OCc1ccccc1
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] N#Cc1ccccc1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] CCCCCCCCCCCCCC[N+](C)(C)Cc1ccccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(N)C12CC3CC(CC(C3)C1)C2
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)(N)Cc1ccc(Cl)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCC(CC)COC(=O)COc1ccc(Cl)cc1C
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.] COc1cc(NCc2ccc3nc(N)nc(N)c3c2C)cc(OC)c1OC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN(C)CC[C@H](c1ccc(Br)cc1)c1ccccc1
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.]
 O[C@@H](c1cc(C(F)(F)F)nc2c(C(F)(F)F)cccc12)[C@H]1CCCCN1
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.]
 O=C(O)CCC(=O)O.c1ccc(C2(c3ccccc3)CC2C2=NCCN2)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC1NCCOC1c1ccccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCc1ncc(C(=O)O)s1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 O=C(CCOCOCOCOCOCOC(=O)Nc1c(I)cc(I)c(C(=O)O)c1I)Nc1c(I)cc(I)c(C(=O)O)c1I
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCC(CO)CCC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1cccc2[nH]nnc12
 [0. 0. 0. 1. 0. 0. 0. 1. 0. 0. 0. 0.]
 CCCCCCCCCC(=O)OC[C@H](O)[C@H]1OC[C@H](OCCO)[C@H]1OCCO
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CS(=O)(=O)OCC(O)C(O)COS(C)(=O)=O

[0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.] C=CCN(CC=C)CC=C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=CCn1c(=O)n(CC=C)c(=O)n(CC=C)c1=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(NCO)NCO
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1cccc(O)c1C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1ccc(C)c(O)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1cc(C)cc(O)c1
 [0. 0. 1. 0. 1. 0. 0. 1. 1. 0. 1. 0.] CN(C)c1ccc(N)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1.] COc1cc2c(cc1O)CCN[C@]21CS[C@@H]2c3c(OC(C)=O)c(C)c4c(c3[C@H](COC1=O)N1[C@@H](O)[C@@H]3Cc5cc(C)c(OC)c(O)c5[C@H]([C@H]21)N3C)OC4
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Nc1cc(=O)nc(N)[nH]1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1coc2c1CCC(C)C2
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Nc1c[n+](N2CCOCC2)no1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)(Cl)Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0.] O=C(O)Cc1ccc(OCCNC[C@H](O)c2ccccc2)cc1
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.] CN1CCCN(C(c2ccccc2)c2ccc(Cl)cc2)CC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 Cn1cc(NC(=O)c2cc(NC(=O)c3cc(NC=O)cn3C)cn2C)cc1C(=O)NCCC(=N)N
 [0. 0. 0. 0. 0. 1. 1. 0. 0. 0. 0. 0. 0.]
 CC(=O)O[C@H]1CC[C@@]2(C)C(=CC[C@H]3[C@@H]4CC=C(c5ccnc5)[C@@]4(C)CC[C@@H]32)C1
 [0. 0. 1. 1. 0. 0. 0. 0. 0. 1. 0. 0.] c1ccc(-c2ccc(C(c3ccccc3)n3ccnc3)cc2)cc1
 [1. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCC(=O)O[C@]1(C(=O)CO)CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3[C@@H](O)C[C@@]21C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CC[N+](C)(CC)CCOC(=O)C(O)(c1ccccc1)C1CCCC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)c1ccc(OCCn2ccnc2)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0.] CCCCCCCCNC(C)C(O)c1ccc(SC(C)C)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 COc1cc(OC)nc(NC(=O)[N-]S(=O)(=O)c2ncccc2OCC(F)(F)F)n1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN/C(=N/[N+](=O)[O-])NCC1CCOC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CC1(C)OC[C@@H]2O[C@@]3(C(=O)[O-])OC(C)(C)O[C@H]3[C@@H]2O1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=Cc1ccccc1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Nc1cccc(Cl)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCOc1ccc(N)c([N+](=O)[O-])c1
 [1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1ccc(-c2nc3ccc(C)cn3c2CC(=O)N(C)C)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CN1CCCC(n2nc(Cc3ccc(Cl)cc3)c3ccccc3c2=O)CC1
 [0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0.] O=C1C=C2C=C[C@@H]3C[C@@]2(O1)[C@H]1CCCCN31
 [0. 0. 1. 1. 0. 0. 0. 0. 0. 1. 0. 0.]
 Clc1ccc(CO/N=C(\Cn2ccnc2)c2ccc(Cl)cc2Cl)c(Cl)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCCCCCCOP(=O)([O-])OCC[N+](C)(C)C
 [0. 0. 1. 0. 0. 0. 0. 1. 0. 0. 0. 0.] CC(=O)Nc1ccccc1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCc1cc(C(N)=S)ccn1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(=O)Nc1cccc(O)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CO/N=C1\CN(c2nc3c(cc2F)c(=O)c(C(=O)O)cn3C2CC2)CC1CN
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=CCCC#N

[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=CC/C=C/C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCOC(=O)CC
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0.] CC1=CCC(=C(C)C)CC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCOC(=O)COC(=O)c1cccc1C(=O)OCCCC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 Fc1ccc([C@@H]2CCNC[C@H]2COC2ccc3c(c2)OC(=O)3)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCSC(=O)N(CC(C)C)CC(C)C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] NC1=NC(=O)C(c2cccc2)O1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCC(=O)c1ccc(O)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] CCCCCCCC(=O)Oc1c(Br)cc(C#N)cc1Br
 [1. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(=O)OCC(=O)[C@@]1(O)[C@H](C)C[C@H]2[C@@H]
]3C[C@H](F)C4=CC(=O)C=C[C@]4(C)[C@H]3[C@@H](O)C[C@@]21C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCC
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCC=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC1=CC(=O)CC(C)(C)C1=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCCCCC(=O)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)CCCCCCCCCCCC(=O)O
 [0. 1. 0. 0. 1. 1. 1. 1. 0. 0. 0. 1.] O=C(CC1)C(C1)C1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] CCC(C)c1ccc(O)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCC(=O)N(C)C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] CCC(C)c1cccc1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN(C)CCCCCN(C)C
 [0. 0. 0. 0. 1. 1. 0. 1. 0. 0. 0. 0.] O=C(O)c1nn(Cc2ccc(C1)cc2C1)c2cccc12
 [0. 0. 0. 1. 0. 0. 0. 1. 0. 0. 1. 0.] CC[C@H](C)C(=O)O[C@H]1C[C@@H](C)C=C2C=C[C@
 H](C)[C@H](CC[C@@H]3C[C@@H](O)CC(=O)O3)[C@H]21
 [0. 0. 1. 0. 0. 0. 0. 1. 0. 0. 1. 0.]
 O=C(Nc1cccc([N+](=O)[O-])c1)c1cc2cccc2cc1O
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN(C)c1ccc(O)c2c1C[C@H]1C[C@H]3[C@H](N(C)C
)C(O)=C(C(N)=O)C(=O)[C@@]3(O)C(O)=C1C2=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCC1CCCC1=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC1=CC(C)C(C=O)C(C)C1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 O=S(=O)([O-])c1ccc2cc(O)c(S(=O)(=O)[O-])cc2c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] NC[C@H]1O[C@H](O[C@@H]2[C@@H](N)C[C@@H](N)
 [C@H](O[C@H]3O[C@H](CO)[C@@H](O)[C@H](N)[C@H]3O)[C@H]2O)[C@H](N)C[C@@H]1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.]
 Cc1ccc(C(=O)c2cc(O)c(O)c([N+](=O)[O-])c2)cc1
 [0. 0. 0. 0. 0. 1. 0. 1. 1. 1. 0. 0.] N#C[Au-]C#N
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.]
 Cc1ccc(O)c([C@H](CCN(C(C)C)C(C)C)c2cccc2)c1
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CC(C)N1CCN(c2ccc(OC[C@H]3CO[C@](Cn4cncn4)(c4ccc(C1)cc4C1)O3)cc2)CC1
 [0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0.]
 CCCCCCCCCCn1cc[n+](C)c1.O=S(=O)([N-]S(=O)(=O)C(F)(F)F)C(F)(F)F
 [0. 0. 0. 1. 0. 0. 0. 1. 0. 0. 1. 0.]
 CCCCCCCCCCn1cc[n+](C)c1.O=S(=O)([O-])C(F)(F)F
 [0. 0. 0. 1. 0. 0. 0. 0. 0. 1. 0. 0.] Clc1ccc(CSC(Cn2ccnc2)c2ccc(C1)cc2C1)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]

COc1cc2nc(N3CCN(C(=O)C4CCCO4)CC3)nc(N)c2cc1OC
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] OCCOC1CCCCC1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
CNCC(O)c1ccc(OC(=O)C(C)(C)C)c(OC(=O)C(C)(C)C)c1
[0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 1. 0. 0.] O=C(OCC(O)CO)c1cccc1Nc1ccnc2cc(Cl)ccc12
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN(C/C=C/c1cccc1)Cc1cccc2cccc12
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=NN1CCN(N=O)CC1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=C(C)[C@H]1CC=C(C)C(=O)C1
[0. 0. 1. 0. 0. 1. 0. 1. 0. 0. 0. 0. 0.] Oc1cccc1O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] ClC(Cl)(Cl)Cl
[0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 1. 0. 0.] O=[N+]([O-])c1ccc(O)c([N+](=O)[O-])c1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCC(Br)(CC)C(=O)NC(N)=O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC1=C(/C=C/C(C)=C/C=C/C(C)=C/C=C\C=C(C)\C=C\C=C(C)\C=C\C2=C(C)CCCC2(C)C(C)(C)CCC1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1c([N+](=O)[O-])ccc1[N+](=O)[O-]
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
CC1=C(C(=O)O)N2C(=O)[C@OH](NC(=O)[C@H](N)C3=CCC=CC3)[C@H]2SC1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCC(CC)COC(=O)COc1cc(Cl)c(Cl)cc1Cl
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCOCCOC(=O)COc1cc(Cl)c(Cl)cc1Cl
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)c1cccnc1C(=O)O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(O)C(C)O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCC[N+]1(C)CCCC1.F[B-](F)(F)F
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCC(=O)c1cccc(Cl)c1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCOS(=O)(=O)[O-].CCn1cc[n+](C)c1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCC[n+]1ccc(C)cc1.F[B-](F)(F)F
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCCCCCCCCBr
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=[N+]([O-])c1ccc(F)c(Cl)c1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC[n+]1cccc1.F[B-](F)(F)F
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCN1cc[n+](C)c1.Cl[Fe-](Cl)(Cl)Cl
[0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0.]
O=C(Nc1ccc(F)cc1F)c1cccnc1Oc1cccc(C(F)(F)F)c1
[0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0.] OCC=Cc1cccc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C/C=C(\C)C(C)=O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCC(CC)c1cccc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1cc(CC(=O)O)c(C)n1-c1ccc(Cl)cc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCC(CC)C(=O)OCCOCCOCCOC(=O)C(CC)CCCC
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=P([O-])(O)C(O)(Cc1cccnc1)P(=O)([O-])O
[0. 0. 0. 0. 1. 1. 0. 0. 0. 0. 0. 1. 0.] Cc1cc(C(C)(C)c2cc(C)c(O)c(C)c2)cc(C)c1O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCSC(=O)Cl
[0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0.] O=C(O)C(Cc1cc(I)c(O)c(I)c1)c1cccc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(O)COC(C)(C)C
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C1COC1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(=O)/C=C/c1cccc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)Br
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] NCc1cccc1Sc1cccc1CO
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] c1ccc(CNCCNCc2cccc2)cc1

[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCc1ccc(C(=O)O)cc1
 [0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0.] O=C(O)c1cccc1-c1ccc(C(F)(F)F)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=CCCCCCCCC(=O)OC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(=O)Oc1ccc(C)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C([O-])c1nc(O)nc(O)n1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] [O-][n+]1cccc(CO)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] OC[C@H]1O[C@@H](O)[C@H](O)[C@@H](O)[C@@H]1
 O[C@@H]1O[C@H](CO)[C@H](O)[C@H](O)[C@H]1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CNc1c2c(nn1C)CCCC2
 [1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(O)C(=O)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Nc1nnc(-c2cccc(Cl)c2Cl)c(N)n1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)c1cc(C(=O)O)cc([N+](=O)[O-])c1
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 1. 0. 0. 0.] CCOCN(C(=O)CCl)c1c(C)cccc1CC
 [0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 1. 1. 1.] CC(=O)O[C@H]1C[C@H](O[C@H]2[C@@H](O)C[C@H]
 (O[C@H]3[C@@H](O)C[C@H](OC4CC[C@@]5(C)C(CC[C@@H]6[C@@H]5CC[C@]5(C)[C@@H](C7=CC(=O)OC7)[C@@H](O)C[C@]65O)C4)O[C@@H]3C)O[C@@H]2C)O[C@H](C)[C@H]1O[C@@H]1O[C@H](CO)
 [C@@H](O)[C@H](O)[C@H]1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COc1cc2c(cc1OC)C(C(C(=O)N(CCc1ccc(OC)c(OC)
 c1OC)CCc1ccc(OC)c(OC)c1OC)c1cccc1)=NCC2
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COC(=O)C(CN)c1c[nH]c2ccc(OC)cc12
 [0. 1. 1. 0. 0. 0. 1. 1. 1. 1. 0. 1.]
 CN1CCC(Nc2ncc3ncnc(Nc4ccc(F)c(Cl)c4)c3n2)CC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1cccc(C)c1NC(=O)c1cccc1C(=O)O
 [0. 1. 0. 0. 0. 1. 0. 0. 1. 0. 0. 1. 1.] OB(O)O[Hg]c1cccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(=O)c1sc(C)nc1C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCC(=O)C(=O)CC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC1(C)S[C@@H]2[C@H](NC(=O)[C@H](N)c3cccc3
)C(=O)N2[C@H]1C(=O)OCOC(=O)[C@@H]1N2C(=O)C[C@H]2S(=O)(=O)C1(C)C
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0.] CN[C@@H]1[C@H](O[C@H]2[C@H](O[C@@H]3[C@@H]
 (NC(=N)N)[C@H](O)[C@@H](NC(=N)N)[C@H](O)[C@H]3O)O[C@@H](C)[C@]2(O)CO)O[C@@H](CO)
 [C@H](O)[C@H]1O.CN[C@@H]1[C@H](O[C@H]2[C@H](O[C@@H]3[C@@H](NC(=N)N)[C@H](O)[C@@H]
) (NC(=N)N)[C@H](O)[C@H]3O)O[C@@H](C)[C@]2(O)CO)O[C@@H](CO)[C@H](O)[C@H]1O
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0.] CN[C@@H](C)[C@H](O)c1cccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN1C(=O)C(O)N=C(c2cccc2)c2cc(Cl)ccc21
 [0. 0. 1. 0. 0. 0. 0. 1. 0. 0. 1. 0. 0.] CCC(C)(CC)c1cc(NC(=O)c2c(OC)cccc2OC)on1
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)NC(=O)N1CC(=O)N(c2cc(Cl)cc(Cl)c2)C1=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CC1(C)S[C@@H]2[C@H](NC(=O)C(C(=O)[O-])c3cccc3)C(=O)N2[C@H]1C(=O)[O-]
 [0. 0. 0. 1. 0. 1. 0. 0. 0. 0. 0. 0. 0.]
 CC/C(=C(\c1cccc1)c1ccc(OCCN(C)C)cc1)c1cccc1.O=C(O)CC(O)(CC(=O)O)C(=O)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] ClC=CCCl
 [0. 0. 1. 0. 0. 0. 0. 1. 0. 0. 1. 0. 0.] NCCS(=O)(=O)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=c1[nH]c(=O)n(C2CCC02)cc1F
 [0. 0. 0. 0. 1. 1. 0. 0. 0. 0. 0. 0. 0.] CC(C)(C)c1cc(CCC(=O)OCC(COC(=O)CCc2cc(C(C)
 (C)C)c(O)c(C(C)(C)C)c2)(COC(=O)CCc2cc(C(C)(C)C)c(O)c(C(C)(C)C)c2)COC(=O)CCc2cc(C
 (C)(C)C)c(O)c(C(C)(C)C)c2)cc(C(C)(C)C)c1O
 [0. 0. 0. 0. 1. 1. 0. 0. 0. 0. 0. 0. 0.] CC(C)C(=O)OCC(C)(C)C(OC(=O)C(C)C)C(C)C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCN

[0. 0. 1. 0. 0. 0. 0. 1. 0. 0. 0. 0.] Cc1cccc2sc(N)nc12
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 1. 0.] COc1cccc2sc(N)nc12
 [0. 0. 1. 0. 1. 0. 0. 0. 0. 0. 0. 0.] COc1ccc2nc(N)sc2c1
 [0. 0. 1. 0. 1. 0. 0. 0. 1. 0. 0. 0.] COc1ccc2nc(N)sc2c1
 [0. 0. 0. 0. 1. 1. 0. 0. 0. 0. 0. 0.] ClC1C(Cl)C(Cl)C(Cl)C(Cl)C1Cl
 [0. 0. 1. 0. 0. 0. 1. 1. 1. 0. 0. 0.] Cc1ccc(O)c(N)c1
 [0. 0. 1. 0. 0. 0. 0. 1. 0. 0. 0. 0.] Cc1ccc(N)cc1O
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.]
 Cl[C@H]1[C@H](Cl)[C@@H](Cl)[C@H](Cl)[C@@H](Cl)[C@@H]1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.]
 Cl[C@H]1[C@H](Cl)[C@@H](Cl)[C@H](Cl)[C@H](Cl)[C@H]1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCO(=O)OCC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C[Si](C)(C)O[Si](O)(O)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] OCCc1ccncc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=C(C)C(=O)OCCOP(=O)(O)O
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 1. 1.] O=C(c1cc(O)c(O)c1)c1ccc(O)c(O)c1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)(C)NC(=O)[C@H]1CN(Cc2cccnc2)CCN1C[C@H](O)C[C@@H](Cc1cccc1)C(=O)N[C@H]1c2cccc2C[C@H]1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.]
 O=C1[C@H](CC[C@H](O)c2ccc(F)cc2)[C@@H](c2ccc(O)cc2)N1c1ccc(F)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=[N+]([O-])c1c(Cl)c(Cl)cc(Cl)c1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] FC(Cl)(Cl)C(F)(Cl)Cl
 [0. 1. 0. 0. 0. 0. 0. 1. 1. 0. 0. 0.] O=[N+]([O-])c1cc(Cl)c(Cl)c(Cl)c1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 NS(=O)(=O)c1cc2c(cc1Cl)N=C(CSCc1cccc1)NS2(=O)=O
 [0. 0. 0. 0. 0. 1. 0. 0. 0. 0. 1. 0.]
 COc1c(C(C)(C)C)cc([N+](=O)[O-])c(C)c1[N+](=O)[O-]
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C1COCCN1
 [0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0.] CCCCC(CC)COC(=O)c1cccc1C(=O)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.]
 CCCCNC1ccc(C(=O)OCCOCCOCCOCCOCCOCCOCCOCCOCCO)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CCN(CC)C(=O)C1CN2CCc3cc(OC)c(OC)cc3G2CC1OC(C)=O
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.] COc1ccc(NC(C)=O)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] BrCc1ccc(Br)cc1
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 O=C(O)c1ccc2cccc2c1O.OCC1cc(C(O)CNCCCCOCCCCc2cccc2)ccc1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCC(C(=O)OCCN(CC)CC)(c1cccc1)c1cccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN1CCN(C2Cc3cccc3Sc3ccc(Cl)cc32)CC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCC1CCC[C@@H](c2cccc(O)c2)C1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCC(CC)C(C)CCOC(C)=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CC(C)NCC(O)COc1ccc(COCCOC(C)C)cc1.CC(C)NCC(O)COc1ccc(COCCOC(C)C)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C[C@@H]1C(=O)N=C2Nc3cccc(Cl)c3CN21
 [0. 0. 0. 0. 0. 0. 1. 0. 1. 0. 0. 1.] O=CCCC=O
 [0. 0. 0. 0. 0. 1. 0. 0. 0. 1. 1. 0.] CC(Cc1ccc(O)c(O)c1)C(C)Cc1ccc(O)c(O)c1
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.] N#C[Fe-2](C#N)(C#N)(C#N)(C#N)N=O
 [0. 0. 1. 0. 0. 0. 0. 1. 0. 0. 0. 0.] c1ccc2c(c1)ccc1c3cccc3ccc21

[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)c1cccc1C(c1ccc(O)cc1)c1ccc(O)cc1
 [1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cn1sc(Cl)cc1=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCC1CCC(=O)O1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)COc1ccc(Cl)cc1
 [0. 0. 0. 1. 0. 0. 0. 1. 0. 0. 1. 0.]
 CCCCCCCCCCn1cc[n+](C)c1.O=S(=O)([O-])C(F)(F)F
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 COc1cccc(C(=O)NN(C(=O)c2cc(C)cc(C)c2)C(C)(C)C)c1C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C#CCOC(=O)/C=C(C)/C=C/CC(C)CCCC(C)C
 [0. 0. 1. 0. 0. 0. 0. 1. 0. 0. 1. 0.] COC(C)(C)CCCC(C)C/C=C/C(C)=C/C(=O)OC(C)C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1cc(=O)[nH]o1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)CCCc1c[nH]c2cccc12
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 O=C(O)[C@H]1[C@@H](O)CC[C@H]2CN3CCc4c([nH]c5cccc45)[C@@H]3C[C@@H]21
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COc1ccc2cc([C@H](C)C(=O)[O-])ccc2c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CC(=O)OCC1=C(C(=O)[O-])N2C(=O)[C@@H](NC(=O)CSc3ccncc3)[C@H]2SC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1ccsc1/C=C/C1=NCCCN1C
 [0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.] CC1(C)[C@@H](OC(=O)CCC(=O)[O-])CC[C@@]2(C)
 [C@H]1CC[C@]1(C)[C@@H]2C(=O)C=C2[C@@H]3C[C@@](C)(C(=O)[O-])CC[C@]3(C)CC[C@]21C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC[C@@]1([C@@H]2O[C@@H]([C@H]3O[C@@](O)(CO)
) [C@H](C)C[C@@H]3C)C[C@@H]2)CC[C@H]([C@]2(C)CC[C@]3(C[C@H](O)[C@@H](C)[C@@H]([C
 @H](C)[C@@H](OC)[C@H](C)C(=O)[O-])O3)O2)O1
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.]
 COc1ccc2cccc2c1C(=O)N[C@@H]1C(=O)N2[C@@H](C(=O)[O-])C(C)(C)S[C@H]12
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCC(NC(C)C)C(O)c1ccc(O)c(O)c1
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 O=S(=O)([O-])c1ccc(N=Nc2c(O)ccc3cccc23)cc1
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 1. 0.] O=C1OC2(c3ccc(O)cc3O)c3cc(O)ccc32)c2cccc21
 [0. 0. 0. 1. 0. 1. 0. 0. 0. 0. 1. 0.] CCOP(=O)(OCC)Oc1nc(Cl)c(Cl)cc1Cl
 [0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 1. 1. 0.]
 CCNc1ccc(C(=C2C=CC(=[N+](CC)CC)C=C2)c2ccc(N(CC)CC)cc2)c2cccc12
 [0. 0. 0. 0. 1. 0. 0. 0. 1. 0. 0. 0.] COc1cc(/C=C/c2cccc2)oc(=O)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCC(CO)CCCCCCC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0.] CN(C)C(=S)[S-]
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] CC(C)(C)c1cccc(C(C)(C)C)c1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 Cc1cccc(C)c1NC(=O)c1cc(S(N)(=O)=O)c(Cl)cc1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] OC1OC[C@@H](O)[C@H](O)[C@H]1O
 [0. 0. 1. 0. 0. 0. 1. 1. 0. 0. 1. 0.]
 COc1cc(C(=O)NS(=O)(=O)c2cccc2C)ccc1Cc1cn(C)c2ccc(NC(=O)OC3CCCC3)cc12
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Nc1ccn([C@H]2CC[C@@H](CO)O2)c(=O)n1
 [0. 0. 1. 0. 1. 1. 0. 0. 0. 0. 1. 0.]
 N[C@@H](Cc1cc(I)c(Oc2ccc(O)c(I)c2)c(I)c1)C(=O)O
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 N[C@@H](Cc1cc(I)c(Oc2cc(I)c(O)c(I)c2)c(I)c1)C(=O)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CN(CCO)CC(O)Cn1cnc2c1c(=O)n(C)c(=O)n2C.O=C(O)c1cccnc1

[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCN(C(C)=O)c1cccc(-c2ccnc3c(C#N)cnn23)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CC(=O)N[C@@H]1[C@@H](NC(=N)N)C=C(C(=O)O)O[C@H]1[C@H](O)[C@H](O)CO
 [1. 1. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.]
 CC[N+]1(CCOC(=O)C(O)(c2ccccc2)c2ccccc2)CCCCC1
 [0. 0. 1. 0. 1. 0. 0. 0. 0. 0. 0. 0.] c1ccc2c(c1)CCc1cccc1N2
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)c1cc(Cl)ccc1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)c1c(Cl)cccc1Cl
 [1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)c1cccc(Cl)c1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)c1ccc(Cl)cc1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0.] O=C1C=CC(=O)N1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=Cc1c(Cl)cccc1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=Cc1ccc(Cl)c(Cl)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCC(=O)O[C@H]1[C@H](O[C@@H]2[C@@H](C)[C@H]
 (O[C@H]3C[C@@](C)(OC)[C@@H](O)[C@H](C)O3)[C@@H](C)C(=O)O[C@H](CC)[C@@](C)(O)[C@H]
](O)[C@@H](C)C(=O)[C@H](C)C[C@@]2(C)O)O[C@H](C)C[C@@H]1N(C)C.CCCCCCCCCCCCCOS(=O)(
 =O)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C[C@H]1CC[C@@H]2[C@@H](C)[C@H]3[C@H](C[C@H]
]4[C@@H]5CC=C6CC(O[C@@H]7O[C@H](CO)[C@H](O)[C@H](O[C@@H]8O[C@H](CO)[C@@H](O)[C@H]
](O)[C@H]8O)[C@H]7O[C@H]7O[C@@H](C)[C@H](O)[C@@H](O)[C@H]7O)CC[C@]6(C)[C@H]5CC[C
 @@]43C)N2C1
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.] C=CC(=O)NCOC
 [1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCc1ccc(C(=O)c2ccccc2)c(O)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCC#N
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C1c2ccccc2CN2C(=O)c3ccccc3CN12
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] ClCCCCBr
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCCBr
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COc1nccnc1NS(=O)(=O)c1ccc(N)cc1
 [0. 0. 1. 0. 1. 0. 0. 0. 1. 0. 1. 1.] CCCOc1ccc2nc(NC(=O)OC)sc2c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN1CCCC(CN2c3ccccc3Sc3ccccc32)C1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 O=C(CCN1CCN(CCO)CC1)N1c2ccccc2Sc2ccc(C(F)(F)F)cc21
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCBr
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(Cl)c1ccc(F)c(Cl)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=S(=O)(Cl)c1c(Cl)cccc1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCOC(=O)CCCC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 O=C(O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCC1CCCC(=O)O1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC=C(C)C(=O)OCCC(C)CCC=C(C)C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC/C=C\CCOC(=O)c1ccccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 C=C(C)C(=O)OCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCOC(=O)CCC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] ClC1=C(Cl)C2(Cl)C(CBr)CC1(Cl)C2(Cl)Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1. 0.]
 O=[N+]([O-])c1ccc(O/N=C/c2cc(Br)c(O)c(Br)c2)c([N+](=O)[O-])c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]

O=S1(=O)OC(c2cc(Br)c(O)c(Br)c2)(c2cc(Br)c(O)c(Br)c2)c2ccccc21
[0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCOP(=S)(OCC)Oc1cc(Cl)c(Br)cc1Cl
[0. 0. 1. 0. 0. 0. 0. 0. 0. 1. 1. 0.] CN(C)c1ccc(C(=C2C=CC(=[N+](C)C)C=C2)c2cccc
c2)cc1.CN(C)c1ccc(C(=C2C=CC(=[N+](C)C)C=C2)c2ccccc2)cc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCOC(=O)c1cnc2cc(OCC(C)C)c(OCC(C)C)cc2c1O
[0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 1. 0.] C#CCOS(=O)OC1CCCC10c1ccc(C(C)(C)C)cc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=c1cc(O)c(Cl)c[nH]1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)(C)NCC(O)c1cc(Cl)c(N)c(C(F)(F)F)c1
[1. 1. 0. 1. 1. 1. 0. 0. 0. 0. 0. 0.]
C[C@]12CC[C@H]3[C@@H](CCC4=C(O)C(=O)CC[C@@]43C)[C@H]1CCC2=O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
C[C@@H](NCCCc1cccc(C(F)(F)F)c1)c1cccc2ccccc12
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] CCCCCc1ccc(C)cc1O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCOC(=O)c1cccc1O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CO/N=C(\C(=O)N[C@@H]1C(=O)N2C(C(=O)[O-])=C
(C[n+])3ccc(N)n3CCO)CS[C@H]12)c1csc(N)n1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCCCCCSC#N
[0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.]
CC1(C)[C@@H](C(=O)OCc2coc(Cc3ccccc3)c2)[C@H]1/C=C1\CCSC1=O
[0. 0. 1. 0. 1. 0. 0. 0. 0. 0. 0. 0.] CCOP(=S)(OCC)Oc1cc(-c2ccccc2)on1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCCCCN1CCCCC1=O
[0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.] CN(C)C(=O)Nc1ccc(OC(=O)NC(C)(C)C)c1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cl[Sn](Cl)(Cl)Cl
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] NCc1ccc(S(N)(=O)=O)cc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC1CC(CC2CCC(N)C(C)C2)CCC1N
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(O)(P(=O)([O-])O)P(=O)([O-])O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=[Si]=O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CO[Si](C)(OC)c1cccc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1ccc(S(=O)(=O)[N-]Cl)cc1
[0. 0. 1. 0. 0. 0. 0. 1. 0. 0. 1. 0.] [O-]c1cccc1-c1cccc1
[0. 0. 1. 0. 0. 0. 0. 1. 0. 0. 0. 0.] O=[N+]([O-])c1cccc2cccc([N+](=O)[O-])c12
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
O=[N+]([O-])c1cc([N+](=O)[O-])c2ccc(S(=O)(=O)O)cc2c1O
[0. 0. 1. 0. 0. 0. 0. 1. 0. 0. 0. 0.] O=[N+]([O-])c1cc([N+](=O)[O-])c2ccccc2c1
[0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.] O=[N+]([O-])c1cccc2c([N+](=O)[O-])cccc12
[0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 1. 0.] Nc1ccc(Cc2ccc(N)c(Cl)c2)cc1Cl
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCOC(=O)[C@H](C)O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCOC(=O)CC
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(COC(C)(C)C)OCCCO
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
CC1=C(CC(=O)O)c2cc(F)ccc2/C1=C\c1ccc(S(C)(=O)=O)cc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
OC[C@H]1O[C@H](O[C@]2(CC1)O[C@H](CC1)[C@@H](O)[C@@H]2O)[C@H](O)[C@@H](O)[C@H]1Cl
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] CC[C@H](C)[C@H]1O[C@]2(C=C[C@@H]1C)C[C@@H]
1C[C@@H](CC=C(C)[C@@H](O[C@H]3C[C@H](OC)[C@@H](O[C@H]4C[C@H](OC)[C@@H](NH2+)C[C@H](C)O4)
[C@H](C)O3)[C@@H](C)C=CC=C3CO[C@@H]4[C@H](O)C(C)=C[C@@H](C(=O)O1)[C@]3
4O)O2.O=C([O-])c1cccc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]

CN[C@H]1CC[C@@H](c2ccc(Cl)c(Cl)c2)c2ccccc21
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(Nc1ccc(/C=C/c2ccc(NC(=O)c3cc(S(=O)(=O)O)c4ccnc4c3O)cc2S(=O)(=O)O)c(S(=O)(=O)O)c1)c1cc(S(=O)(=O)O)c2ccnc2c1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCO P(=S)(OCC)SCSC(C)(C)C
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CN(CC(=O)N1CCOCC1)Cc1c(Cl)cccc1NC(=O)c1ccccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN1CCN(C2=Nc3ccccc3Cc3ccccc32)CC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(Cn1c(=O)sc2ccc(Cl)cc21)N1CCN(CCO)CC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 COc1cc(C[C@@H]2NCCc3cc(O)c(O)cc32)cc(OC)c1OC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C1CCC(N2C(=O)c3ccccc3C2=O)C(=O)N1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCOCOCOC
 [0. 0. 0. 0. 1. 1. 0. 1. 0. 0. 0. 0.] O=C(O)/C=C/C(=O)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)/C=C\C(=O)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCC(C)=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCC(=O)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCC=O
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 1. 0. 0.]
 CC(C)=CC1C(C(=O)OCc2coc(Cc3ccccc3)c2)C1(C)C
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.] CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@H]2C[C@@](C)(OC)[C@@H](O)[C@H](C)O2)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@H](N(C)C)[C@H]2O)[C@](C)(O)C[C@@H](C)C(=O)[C@H](C)[C@@H](O)[C@]1(C)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCC(=O)OC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] c1cc(-c2ccncc2)ccn1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN=C=S
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)=CCO
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COP(=O)(OC)O/C(C)=C/C(=O)N(C)C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C1CCOCOC1
 [0. 0. 0. 0. 1. 1. 0. 0. 0. 0. 0. 0.] CC(C)=CC1
 [0. 0. 1. 0. 0. 0. 0. 1. 0. 0. 1. 0.]
 O=C1c2c(O)ccc(Nc3ccc(CCO)cc3)c2C(=O)c2c([N+](=O)[O-])ccc(O)c21
 [0. 0. 0. 1. 0. 0. 0. 0. 0. 1. 0. 0. 0. 1.]
 O=C1C(O)=C([C@H]2CC[C@H](c3ccc(Cl)cc3)CC2)C(=O)c2ccccc21
 [1. 0. 0. 0. 1. 0. 0. 1. 0. 0. 1. 0.] Oc1ccc(-c2ccccc2)c(Cl)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C1CCCCCCCCC(=O)OCCO1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=[PH]1Oc2ccccc2-c2ccccc21
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=[N+]([O-])C1(Br)COCOC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(NC(C)(C)C)C(=O)c1cccc(Cl)c1
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.]
 CC#CCC(C)[C@H](O)/C=C/C1[C@H]2C/C(=C/CCCC(=O)O)C[C@H]2C[C@H]1O
 [0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)Cn1cnc2c(N)nc3ccccc3c21
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN(C)CCCN(C)CCCN(C)C
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.] NCCCCOCCOCCCN
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] N#CSc1ccc(N)c([N+](=O)[O-])c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(=O)N[C@H]1[C@@H](O[C@@H]2C(C(=O)[O-])C[C@@H](O[C@@H]3[C@@H](CO)O[C@H](OC4C(C(=O)[O-])O[C@@H](OC5[C@H]6CO[C@H](O6)[C@H](

NS(=O)(=O)[O-][C@H]5O[C@H](O)[C@H]4O[C@H](NC(C)=O)[C@H]3C[C@H](O)[C@H]2O[C@H]1C[C@H](COS(=O)(=O)O)[C@@H](O)[C@@H]2OC(C(=O)[O-])=C[C@H](O)[C@H]2O[C@@H]1O
 [1. 1. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.]
 C=C[C@H]1CN2CC[C@H]1C[C@H]2[C@H](OC(=O)OCC)c1ccnc2ccc(OC)cc12
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)=CCC[C@@](C)(O)[C@H]1CC=C(C)CC1
 [1. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.]
 O=C1c2c(O)ccc2[C@H]([C@@H]2O[C@H](CO)[C@@H](O)[C@H](O)[C@H]2O)c2cc(CO)cc(O)c21
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(N)Cc1ccc(O)cc1
 [0. 0. 1. 0. 0. 1. 0. 0. 0. 0. 1. 0.] O=C1c2cccc2C(=O)c2c1ccc(O)c2O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COc1cc(OC)cc(OC)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCC(=O)C(CC(C)N(C)C)(c1cccc1)c1cccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1c(N(C)C)c(=O)n(-c2cccc2)n1C
 [1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN(C)CCO
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN(C)c1cccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0.] C[As](C)(=O)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC1(C)C(=O)NC(=O)NC1=O
 [0. 0. 1. 0. 1. 1. 0. 0. 0. 1. 1. 1.] O=C(c1ccc(O)cc1O)c1ccc(O)cc1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=C(C)C(=O)OCCOC1CC2CC1C1C=CCC21
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] OCC(c1ccc(Cl)cc1)c1ccc(Cl)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCN(CC)CCOC(=O)c1ccc(N)cc1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCN(CC)C(=O)c1ccc(O)c(OC)c1
 [0. 0. 0. 0. 1. 1. 0. 0. 0. 0. 0. 0.]
 C1CNCCN1.C[C@]12CC[C@@H]3c4ccc(OS(=O)(=O)O)cc4CC[C@H]3[C@@H]1CCC2=O
 [1. 1. 0. 0. 1. 1. 0. 0. 0. 0. 0. 0.]
 CCCCC(=O)O[C@H]1CC[C@H]2[C@@H]3CCc4cc(O)ccc4[C@H]3CC[C@]12C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CC(=O)OC(C)OC(=O)C(C)c1ccc(-c2cccc2)c(F)c1
 [1. 1. 0. 0. 1. 1. 0. 0. 0. 0. 0. 0.]
 CCCCCC(=O)O[C@H]1CC[C@H]2[C@@H]3CCc4cc(O)ccc4[C@H]3CC[C@]12C
 [1. 1. 0. 0. 1. 1. 0. 0. 0. 0. 0. 0.]
 CCC(=O)Oc1ccc2c(c1)CC[C@@H]1[C@@H]2CC[C@]2(C)[C@@H](OC(=O)CC)CC[C@@H]12
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCN(CC)CCNC(=O)c1cc(S(C)(=O)=O)ccc1OC
 [0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0.] FC(F)(F)c1cccc1-n1ccnc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] N#CC(C#N)=Cc1cc(O)c(O)c(O)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] N#CC(C#N)=Cc1ccc(O)c(O)c1
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 1.]
 O=C(O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 O=C(O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.]
 O=C(O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 O=S(=O)(O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COC(=O)[C@@H]1CC2=CC(=O)CC[C@]2(C)[C@@]23O
 [C@@H]2C[C@@]2(C)[C@@H](CC[C@@]24CCC(=O)O4)[C@H]13
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)CC(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@@H]
 (CC(C)C)[C@@H](O)CC(=O)N[C@@H](C)C(=O)N[C@@H](CC(C)C)[C@@H](O)CC(=O)O)C(C)C)C(C)

C

[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN(C)CCc1ccc(O)cc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC1(C)S[C@@H]2[C@H](N)C(=O)N2[C@H]1C(=O)O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] c1cc2c(c(N3CCNCC3)c1)OCCO2
[0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
CC1(CN2CCC(n3c(=O)[nH]c4cccc43)CC2)OCc2cccc2-n2cccc21
[0. 0. 1. 1. 0. 0. 0. 1. 1. 0. 1. 0.]
CN1C(=O)[C@@H](NC(=O)c2cc3cccc3[nH]2)N=C(c2cccc2)c2cccc21
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
O=c1[nH]c2cc(C(F)(F)F)c(N3CCOCC3)cc2n(CP(=O)(O)O)c1=O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
COC1=CC=C2[C@H]3Cc4ccc(OC)c5c4[C@@]2(CCN3C)[C@H]1O5
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
[0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 1. 0.] Cc1ccc(N(SC(F)(Cl)Cl)S(=O)(=O)N(C)C)cc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(=O)Nc1ccc(S(=O)(=O)Cl)cc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1ccc([N+](=O)[O-])cc1Cl
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1.]
COC(=O)Nc1cc(Sc2cccc2)ccc1N=C(NC(=O)OC)NC(=O)OC
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)[C@@]1(NC(=O)[C@@H]2C[C@@H]3c4cccc5[nH]cc(c45)C[C@H]3N(C)C2)O[C@@]2(O)[C@@H]3CCCN3C(=O)[C@H](Cc3cccc3)N2C1=O
[1. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
C[C@@H](CO)NC(=O)[C@@H]1C=C2c3cccc4[nH]cc(c34)C[C@H]2N(C)C1
[0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 1. 0.]
CCN(CC)C(=O)N[C@@H]1C=C2c3cccc4[nH]cc(c34)C[C@@H]2N(C)C1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=CCN1CCc2nc(N)sc2CC1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
CN(C(=O)Cc1cccc1)[C@H]1CC[C@@]2(CCCO2)C[C@@H]1N1CCCC1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
CN1C[C@@H](NS(=O)(=O)N(C)C)C[C@@H]2c3cccc4c3c(cn4C)C[C@H]21
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
C=CCN1CC[C@]23c4c5ccc(O)c4O[C@H]2C(=O)CC[C@@]3(O)[C@H]1C5.CI
[0. 0. 1. 1. 0. 0. 0. 1. 0. 1. 1. 0.] CC(C)(C)NSc1nc2cccc2s1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0.]
C=CCC1=C(C)C(OC(=O)C2C(C=C(C)C)C2(C)C)CC1=O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC1=CC(=O)CCC1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)c1cccc1C(C)C
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C=NC1CCC(CC2CCC(N=C=O)CC2)CC1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCOC(C)O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=C(C)C(=O)OCC[N+](C)(C)C
[0. 0. 1. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0.] c1ccc2sc(SN(C3CCCC3)C3CCCC3)nc2c1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)C(=O)OCC(C)(C)C(O)C(C)C
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1cccc(Cl)c1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C1=CCCC=CCCC=CCC1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=C(C)C#N
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COP(N)(=O)SC
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCSP(=O)(SCCCC)SCCCC
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COCC(=O)N(c1c(C)cccc1C)C(C)C(=O)OC

[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C[N+]1(C)CCCCC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 Cn1cc(C2=C(c3cn(C4CCN(Cc5cccn5)CC4)c4cccc34)C(=O)NC2=O)c2cccc21
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 O=C(NOC[C@H](O)CO)c1ccc(F)c(F)c1Nc1ccc(I)cc1F
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 1. 1.] O=C1CN=C(c2cccc2)c2cc(Cl)ccc2N1CC1CC1
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Nc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCOC(=O)CCC(C)=O
 [1. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 C[C@]12C[C@H](O)[C@H]3[C@@H](CCC4=CC(=O)C=C[C@@]43C)[C@H]1CC[C@]2(O)C(=O)CO
 [1. 1. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.]
 C[C@]12CC(=O)[C@H]3[C@@H](CCC4=CC(=O)C=C[C@@]43C)[C@H]1CC[C@]2(O)C(=O)CO
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CNC(=O)CSP(=O)(OC)OC
 [1. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0.] CCCN(CCC)S(=O)(=O)c1ccc(C(=O)O)cc1
 [0. 0. 0. 1. 0. 0. 0. 1. 0. 0. 0. 0.] C=C(C)[C@H]1CCC2=CCC[C@@H](C)[C@]2(C)C1
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.] C=CC(C)=CCC=C(C)C
 [0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0.]
 C=C(C)[C@@H]1CCC2=CC(=O)C[C@@H](C)[C@]2(C)C1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCOC(=O)CC(C)C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCCN(CCCCCCCCCC)CCCCCCCCC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC1=CCCC(C)(C)C12CCC(C)O2
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 1. 0. 0.]
 c1cc(C(c2ccc(OCC3C03)cc2)c2ccc(OCC3C03)cc2)ccc1OCC1CO1
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC1(CO)CN(c2cccc2)NC1=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=C(C)C(=O)OCCCCCCCCCOC(=O)C(=C)C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCC(=O)OCc1cccc1
 [0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 1. 0.] Cc1cccc(Nc2cccc2)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=S(=O)([O-])CC(O)CC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=CCOCC(CC)(CO)COCC=C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] NS(=O)(=O)c1cccc1Cl
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 1. 0. 0.]
 CCC(C)(CCC(C)C)C(=O)O[Sn](C)(C)OC(=O)C(C)(CC)CCC(C)C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)(C)C1CCCC1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0.] CC(C)CP(=S)([S-])CC(C)C
 [1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COc1ccc(CC2c3cc(OC)c(OC)cc3CC[N+]2(C)CCC(=O)OCCCCOC(=O)CC[N+]2(C)CCc3cc(OC)c(OC)cc3C2Cc2ccc(OC)c(OC)c2)cc1OC.O=S(=O)([O-])c1cccc1.O=S(=O)([O-])c1cccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COc1c(N2CCOCC2)cnn(C)c1=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN1CCC(=C2c3cccc3CCc3ccnc32)CC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CC(=O)OC[C@H]1O[C@@H](n2ncc(=O)[nH]c2=O)[C@H](OC(C)=O)[C@H]1OC(C)=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CCOC(=O)[C@H](CCc1cccc1)N[C@@H](C)C(=O)N1CCC[C@H]1C(=O)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN(C)C(=O)Nc1ccc(Cl)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1ccc(S(=O)(=O)N=C=O)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] NC(=O)c1cccc1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C1C[C@@H]2OCC=C3CN4CC[C@]56c7cccc7N1[C@H]5[C@H]2[C@H]

3C[C@H]46

[0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.] O=c1oc2ccccc2c(O)c1Cc1c(O)c2ccccc2oc1=O
[0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.] O=C1NCC2(CCN(Cc3ccccc3)CC2)O1
[0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.] CCOC(=O)Nc1ccc(NCc2ccc(F)cc2)nc1N
[0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.]
CC(C)[N+]1(C)C2CCC1CC(OC(=O)C(CO)c1ccccc1)C2
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] N=C(N)NCc1cccc(I)c1.N=C(N)NCc1cccc(I)c1
[0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.] CC(C)NC(C)Cc1ccc(I)cc1
[0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0.] Clc1cc(C(Cl)(Cl)Cl)cnc1Cl
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1cn[nH]c1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
NC(=O)c1nnc([C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O)c1O
[0. 0. 0. 0. 1. 0. 0. 1. 0. 0. 0. 0.] C#CCN(C)CCCOc1ccc(Cl)cc1Cl
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCC#N
[0. 0. 0. 0. 0. 1. 0. 0. 1. 1. 0. 1.] N#Cc1c(Cl)c(Cl)c(Cl)c(C#N)c1Cl
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1ccc(C)c(O)c1C
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=C(C)C(=O)OCCOCC
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)[C@@H]1CC[C@@H](C)C[C@H]1O
[0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 1. 0.] O=C=Nc1ccc(Cl)c(Cl)c1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] COP(=S)(OC)Oc1nc(Cl)c(Cl)cc1Cl
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
C#CCOC(=O)[C@@H](C)Oc1ccc(Oc2ncc(Cl)cc2F)cc1
[0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.] CC1(C)CON(Cc2ccccc2Cl)C1=O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCSC(=O)N(CC)C1CCCCC1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COC(=O)C(C)Oc1ccc(Oc2ccc(Cl)cc2Cl)cc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCNC(=O)NC(=O)/C(C#N)=N/OC
[0. 0. 1. 0. 1. 0. 0. 0. 0. 0. 0. 0.] Cc1cc(C2CC2)nc(Nc2ccccc2)n1
[0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0.]
COc1cc2nc(N(C)CCCNC(=O)C3CCC03)nc(N)c2cc1OC
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
CN(C)C(=O)Oc1cc(OC(=O)N(C)C)cc(C(O)CNC(C)(C)C)c1
[1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] CCC(=O)O[C@]1(C(=O)SCF)[C@H](C)C[C@H]2C3C[C@H](F)C4=CC(=O)C=C[C@]4(C)[C@@]3(F)[C@@H](O)C[C@@]21C
[1. 0. 0. 0. 1. 1. 0. 0. 0. 0. 0. 0.]
C[C@@]12CCC[C@H]1[C@@H]1CC[C@H]3C[C@@H](O)CC[C@]3(C)[C@H]1CC2
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
CC(=O)SC[C@@H](Cc1ccccc1)C(=O)NCC(=O)OCc1ccccc1
[0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCN1CCC[C@@H]2Cc3n[nH]cc3C[C@H]21
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] CCC[C@@]1(CCc2ccccc2)CC(O)=C([C@H](CC)c2ccc(NS(=O)(=O)c3ccc(C(F)(F)F)cn3)c2)C(=O)O1
[0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 1. 0.] CO[C@H]1C[C@@H]2CC[C@@H](C)[C@@](O)(O2)C(=O)C(=O)N2CCCC[C@H]2C(=O)O[C@H]([C@H](C)C[C@@H]2CC[C@@H](O)[C@H](OC)C2)CC(=O)[C@H](C)C=C(C)[C@@H](O)[C@@H](OC)C(=O)[C@H](C)C[C@H](C)C=CC=CC=C1C
[1. 0. 0. 1. 1. 0. 0. 1. 0. 0. 0. 0.] CCC(C)(C)C(=O)O[C@H]1C[C@@H](C)C=C2C=C[C@H](C)[C@H](CC[C@@H]3C[C@@H](O)CC(=O)O3)[C@H]21
[0. 0. 0. 0. 0. 0. 0. 1. 0. 1. 1. 1.]
CC(C)=CCOc1ccc(/C=C/C(=O)c2ccc(OCC=C(C)C)cc2OCC(=O)O)cc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C1NC(=O)[C@@]2(CC0c3ccc(F)cc32)N1

[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C/C=C(/CC[C@@H] (C) [C@H] 1CC [C@H] 2C3=CC [C@H]
 4 [C@H] (C) [C@@H] (O)CC [C@] 4 (C) [C@H] 3CC [C@@] 21C)C(C)C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] OC [C@H] (O) [C@@H] (O) [C@H] (O) [C@H] (O)CO
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCCOC(=O)(=O)O.OCCN(CCO)CCO
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] [O-]c1cccc1
 [0. 1. 1. 0. 0. 0. 1. 1. 0. 0. 1. 1.] c1ccc2c(c1)c1ccc3ccc4cccc2c4c31
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=CCNCC=C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1. 0.] CCCCC/C=C/C=C/C=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C1CCC2CCCCC2C1
 [0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0.] CCCCCCCCCC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=C(C)C(=O)OCCCCCCCCC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=CC(=O)NC(C)(C)CC(C)=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(=O)CC(C)(C)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CN(C)C(=O)C1(N2CCCC2)CCN(CCC2(c3ccc(C1)c(C1)c3)CN(C(=O)c3cccc3)CCO2)CC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C([O-])C(Cl)Cl
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 1.] O=C([O-])Cc1cccc1Nc1c(Cl)cccc1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Clc1cc(Cl)c(Cl)nc1Cl
 [0. 0. 1. 0. 0. 0. 0. 0. 1. 0. 0.] NNC(=S)NN
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] NC(=O)Nc1ccc(Cl)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] [O-][n+]1ccc(Cl)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCC/C=C\C/C=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN1C(=O)CC(=O)N(c2cccc2)c2cc(Cl)ccc21
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCc1occc(=O)c1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC1=C(O)C(=O)C(C)O1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COc1ccc(CCO)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCC(C)C(O)CC
 [1. 0. 0. 0. 1. 1. 0. 1. 1. 0. 1. 0.] Oc1ccc(/C=C/c2cc(O)cc(O)c2)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C1C[N+]([O-])=C(c2cccc2)c2cc(Cl)ccc2N1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(/C=C/c1cccc(F)c1)NC1CC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)Cc1csc(-c2ccc(Cl)cc2)n1
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 1. 0.] O=C(Nc1ccc(Br)cc1)c1cc(Br)c(Br)s1
 [0. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0.] O=C(O)Cc1cn(-c2cccc2)nc1-c1ccc(Cl)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1cccc(C)c1NC(=O)CN1CCCC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] NS(=O)(=O)c1ccc(Cl)c(S(N)(=O)=O)c1
 [0. 0. 0. 0. 0. 0. 1. 0. 1. 0. 0.] COc1ccc(C=CC(=O)c2ccc(OC)cc2OC)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(NCN1CCOCC1)c1cnccn1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COc1cccc2c1C(=O)c1c(O)c3c(c(O)c1C2=O)C[C@@
](O)(C(=O)CO)C[C@@H]3O[C@H]1C[C@H](N)[C@H](O[C@@H]2CCCCO2)[C@H](C)O1
 [1. 1. 0. 0. 1. 1. 0. 0. 0. 0. 0. 0.]
 CCCCCC(=O)O[C@H]1CC[C@H]2[C@@H]3CC[C@H]4CC(=O)C=C(C)[C@]4(C)[C@H]3CC[C@]12C
 [0. 0. 0. 0. 0. 0. 1. 0. 1. 0. 0.] C=C/C(C)=C/C=C(\C)CCC=C(C)C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCC(=O)OCCOc1cccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(=O)CCC1=C(C)CCCC1(C)C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COc1cc(C=O)ccc1OC(=O)C(C)C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN1N=C(C(N)=O)CCC1=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@@]43C)[C@@H]1CC[C@H]2C(=O)O

[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1sccc1Br
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(CCC1)NCCc1cccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 [O-] [n+] 1cccc(/C(C1)=N/OC[C@H](O)CN2CCCC2)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0.]
 CC[C@@]1(O)C(=O)OCc2c1cc1n(c2=O)Cc2c-1nc1cccc1c2/C=N/OC(C)(C)C
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0.]
 C=CCNc1nc(NCC=C)nc(N2CCN(C(c3ccc(F)cc3)c3ccc(F)cc3)CC2)n1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1.]
 CC[C@@]1(O)C(=O)OCc2c1cc1n(c2=O)Cc2cc3c([N+](=O)[O-])cccc3nc2-1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCCCCCOS(=O)(=O)[O-]
 [1. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] S=c1[nH]c2cccc2[nH]1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(=O)N[C@@H]1C(O[C@H]2O[C@H](C(=O)O)C(O)[C@H](O)[C@H]2O)[C@H](O)[C@H]2O[C@H](O)[C@H]1O
 [0. 0. 1. 0. 0. 0. 0. 1. 0. 0. 1. 1.] S=C1NC=NC2N=CNC12
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCOC(=O)CCCC(=O)OCCCCC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCC(=O)OC
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0.] OC/C=C/CO
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 1. 0.] Cc1c(Cl)cccc1Nc1cccc1C(=O)O
 [0. 0. 1. 1. 0. 0. 0. 1. 0. 0. 1. 0.] OCc1c[nH]c2cccc12
 [0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0.] Cc1cccc(Nc2cc(Cl)nc(SCC(=O)O)n2)c1C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CNCC(O)c1ccc(O)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=CCCl
 [0. 0. 1. 0. 1. 0. 0. 1. 1. 1. 0. 0.] O=C(CCl)c1cccc1
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COP(=S)(OC)Oc1ccc([N+](=O)[O-])cc1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COC(=O)c1cccc1C(=O)O
 [0. 1. 1. 0. 1. 0. 0. 1. 1. 1. 0. 1.] CC(=O)Nc1ccc(C(=O)CC1)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCC(=O)c1cccc1C(=O)O
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Nc1ccc(Cl)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] c1ccc(CCCc2cccn2)cc1
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCOC(=O)c1cn2nc(OP(=S)(OCC)OCC)cc2nc1C
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 1. 0. 1.]
 CCC(C)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1OC(=O)C=C(C)C
 [0. 0. 0. 0. 0. 1. 0. 1. 0. 1. 1. 1.]
 CCC(C)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1OC(=O)OC(C)C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CCN(CC)c1c([N+](=O)[O-])cc(C(F)(F)F)c(N)c1[N+](=O)[O-]
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CC1(C)[C@@H]2CC[C@@]1(C)[C@H](OC(=O)CSC#N)C2
 [0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)N(C(=O)SCC(Cl)=CC1)C(C)C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CC(=O)OCC1=C(C(=O)O)N2C(=O)[C@@H](N)[C@H]2SC1
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 1. 0.] COC(=O)Nc1nc2cccc2[nH]1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C1CCCCC1C1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC1(C)[C@@H]2CC[C@@]1(C)C(=O)C2
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] NC(N)=O.OO
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCC(=O)Cl

[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0.] CCCCCOC(C)=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCCCCCC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCCCCCC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] OCCCCCO
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=CCCCCCCCCCCCC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCCCCCC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CSc1ccc(Cl)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Clc1ccc2ccccc2c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1ccccc1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CS(=O)(=O)c1ccc(Cl)cc1
 [0. 0. 1. 1. 1. 0. 0. 0. 0. 0. 1. 0.] Oc1ccc2ccc3cccc4ccc1c2c34
 [0. 0. 0. 0. 1. 1. 0. 0. 0. 0. 1. 0.] CC(C)COC(=O)c1ccc(O)cc1
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cn1c(N)nc2c3ccnnc3ccc21
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] NC(=O)CI
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.] IC(I)I
 [0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0.]
 COc1ccc2c(c1)c(CC(=O)O)c(C)n2C(=O)c1ccc(Cl)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=CCOC(CO)(COCC=C)COCC=C
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 1. 0.] CCc1ccc(O)c(C(C)(C)C)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 Cc1c(C)c([N+](=O)[O-])c(C(C)(C)C)c([N+](=O)[O-])c1C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C#CCN(C)[C@H](C)Cc1ccccc1
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 1. 0.]
 O=C1CN(N=Cc2ccc(-c3ccc([N+](=O)[O-])cc3)o2)C(=O)[N-]1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCN(CCC#N)c1ccccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COC(=O)CCCC(=O)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] OC[C@H](Cc1ccccc(O)c1)[C@H](CO)Cc1ccccc(O)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] COc1cc(Cl)ccc1Oc1ccc(Cl)cc1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1ccc(O)c(C(=O)c2ccccc2)c1
 [0. 0. 0. 0. 1. 1. 0. 0. 0. 0. 1. 0.] O=C(c1ccccc1)c1ccc(O)c1
 [0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(c1ccccc1)c1ccccc1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN1CCc2cc3c(cc2C1O)OC3
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] CCCCCCCCCCOC(=O)c1ccc(O)cc1
 [0. 0. 0. 0. 1. 1. 0. 0. 0. 0. 0. 0.] O=C(Oc1ccccc1)c1ccc(O)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1. 0.]
 CCCC(c1cc(C(C)(C)C)c(O)cc1C)c1cc(C(C)(C)C)c(O)cc1C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=c1[nH]cnc2nc[nH]c12
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 C=C1CC[C@H]2[C@@](C)(CC[C@@H](O)[C@@]2(C)CO)[C@@H]1C/C=C1/C(=O)OC[C@H]1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN1CC(=O)NC1=N
 [1. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0.] CC1(C)O[C@H]2CC(=O)OC[C@@]23[C@H]1CC(=O)[C
 @]1(C)[C@@H]3CC[C@@]2(C)[C@H](c3ccoc3)OC(=O)[C@H]3O[C@]321
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] OC[C@H]1O[C@@H](O[C@@H]2[C@@H](CO)O[C@@H](
 O)[C@H](O)[C@H]2O)[C@H](O)[C@@H](O)[C@@H]1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CN(C)CCN(Cc1ccccc1)c1ccccc1.O=C(O)CC(O)(CC(=O)O)C(=O)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=CCC1(C(C)CCC)C(=O)N=C([S-])NC1=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Clc1ccccc1

```

[0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1.] CCOC(=O)C(O)(c1ccc(Cl)cc1)c1ccc(Cl)cc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
CCCCCCCCC[C@@H](C[C@@H]1OC(=O)[C@H]1CCCCC)OC(=O)C(CC(C)C)NC=O
[0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.] CCC1C01
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] FC(F)OC(F)(F)C(F)Cl
[1. 1. 0. 0. 1. 1. 0. 0. 0. 0. 0. 0.]
C#C[C@]1(O)CC[C@H]2[C@@H]3CCC4=C(CCC(=O)C4)[C@H]3CC[C@@]21C
[0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 1. 0.]
O=S1OCC2C(CO1)C1(Cl)C(Cl)=C(Cl)C2(Cl)C1(Cl)Cl
[0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 1. 0.]
ClC1=C(Cl)[C@]2(Cl)[C@H]3[C@H]([C@@H]4C[C@H]3[C@H]3O[C@@H]43)[C@@]1(Cl)C2(Cl)Cl
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] ClCC1C01
[1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
O=C(O[C@@H]1Cc2c(O)cc(O)cc2O[C@@H]1c1cc(O)c(O)c(O)c1)c1cc(O)c(O)c(O)c1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)NCC1CCc2cc(CO)c([N+](=O)[O-])cc2N1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCn1cnc2c1c(=O)n(CCCC(C)=O)c(=O)n2C
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] c1cnc(N2CCN(Cc3ccc4c(c3)OC(=O)C2)nc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1ccc(=O)n(-c2cccc2)c1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
Cc1nc2ccccn2c(=O)c1CCN1CCC(C(=O)c2ccc(F)cc2)CC1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
O=c1[nH]c2cccc2n1CCCN1CCN(C(c2cccc2)c2cccc2)CC1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] NC(=O)CN1CC(O)CC1=O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCC(=O)c1ccc2c(c1)N(CCCN(C)C)c1cccc1S2
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCn1c(=O)[nH]c(=O)c2[nH]cnc21
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCNCC(O)COc1cccc1C(=O)CCc1cccc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
CCOc1nc2cccc(C(=O)O)c2n1Cc1ccc(-c2cccc2-c2nnn[nH]2)cc1
[1. 1. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.]
CC(=O)[C@H]1CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3CC[C@]12C
[1. 1. 0. 0. 1. 1. 0. 1. 0. 0. 0. 0.]
C[C@]12CC[C@H]3[C@@H]([C@@H]4CCC4=CC(=O)CC[C@@]43C)[C@@H]1CC[C@@H]2O
[1. 1. 0. 0. 1. 1. 0. 0. 0. 0. 1. 1.]
C[C@]12CC[C@@H]3c4ccc(O)cc4CC[C@H]3[C@@H]1CC[C@H]2O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] COc1ccc2c(c1OC)CN1CCc3cc4c(cc3C1C2)OC(=O)C4

```

```

[19]: tasks, datasets, transformers = dc.molnet.load_tox21()
      train_dataset, valid_dataset, test_dataset = datasets

```

```

Loading dataset from disk.
Loading dataset from disk.
Loading dataset from disk.

```

```

[20]: tasks

```

```

[20]: ['NR-AR',
      'NR-AR-LBD',

```

```
'NR-AhR',
'NR-Aromatase',
'NR-ER',
'NR-ER-LBD',
'NR-PPAR-gamma',
'SR-ARE',
'SR-ATAD5',
'SR-HSE',
'SR-MMP',
'SR-p53']
```

```
[21]: datasets
```

```
[21]: (<deepchem.data.datasets.DiskDataset at 0x151d1e9ca88>,
<deepchem.data.datasets.DiskDataset at 0x151d1ea5188>,
<deepchem.data.datasets.DiskDataset at 0x151d1ea3408>)
```

```
[22]: for X, y, w, id in test_dataset.itersamples():
print(y, id)
```

```
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCC(=O)C1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1.]
Cc1ccc(Nc2nccc(N(C)c3ccc4c(C)n(C)nc4c3)n2)cc1S(N)(=O)=O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
CC(C)OC(=O)OCOP(=O)(CO[C@H](C)Cn1cnc2c(N)ncnc21)OCOC(=O)OC(C)C
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
CC(=O)N[C@H]([C@@H](O)CC(=O)C(=O)O)[C@@H](O)[C@H](O)[C@H](O)CO
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(C=Cc1ccc(O)c(O)c1)O[C@@H]1C[C@@](OC(=O)C=Cc2ccc(O)c(O)c2)(C(=O)O)C[C@@H](O)[C@@H]1O
[0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 1. 1.] CO[C@H](C(=O)[C@@H](O)[C@@H](C)O)[C@@H]1Cc2cc3cc(O[C@H]4C[C@@H](O[C@@H]5C[C@@H](O)[C@@H](OC)[C@@H](C)O5)[C@@H](OC(=O)O)[C@@H](C)O4)c(C)c(O)c3c(O)c2C(=O)[C@H]1O[C@H]1C[C@@H](O[C@H]2C[C@@H](O[C@H]3C[C@](C)(O)[C@@H](OC(C)=O)[C@H](C)O3)[C@H](O)[C@@H](C)O2)[C@H](O)[C@@H](C)O1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
CCCCCCC(=O)CCCCC/C=C/C[C@@H](O)[C@H](O)[C@@](N)(CO)C(=O)O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1.] CCC1OC(=O)C[C@@H](O)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@H](N(C)C)[C@H]2O)[C@@H](CC(=O)C[C@@H](C)C(=O)C=C[C@]2(C)OC2C1C
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)CCOC(=O)c1cccc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] Cc1cc(C)c(C)c(O)c1
[0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0.] CCC(=O)OCCC(C)CCC=C(C)C
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)COC(=O)c1cccc1O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0.]
CC(C)CCCCCCCOC(=O)c1ccc(C(=O)OCCCCCCC(C)C)c(C(=O)OCCCCCCC(C)C)c1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCCCC(=O)O.OCCN(CCO)CCO
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCC(=O)OCC(C)OC(=O)CCCCCCCC
[0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCCOC(C)=O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(=O)OCCC1CCCC1
```


[0. 0. 0. 1. 0. 0. 0. 1. 0. 0. 0. 0.] COP(=O) (OC)OC(=CC1)c1cc(Cl)c(Cl)cc1Cl
 [0. 1. 1. 0. 0. 0. 1. 0. 1. 1. 1. 0.] CCN(CC)C(=S)SSC(=S)N(CC)CC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0.]
 CCCCCN(CCCCC)C(=O)C(CCC(=O) [O-])NC(=O)c1ccc(Cl)c(Cl)c1
 [0. 0. 1. 1. 0. 0. 0. 0. 0. 1. 0.]
 CCCCCc1cc(O)c2c(c1)OC(C)(C)[C@@H]1CCC(C)=C[C@@H]21
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C1CCOC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN1C(C)(C)CCCC1(C)C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC1=CCC(C(C)(C)O)CC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCN(Cc1cccc(S(=O)(=O)O)c1)c1cccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(=O)c1ccc(O)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1cc(C(C)(C)C)cc(C)c1CC1=NCCN1
 [0. 0. 0. 0. 0. 1. 1. 1. 0. 1. 1. 0.] F[Sn](c1cccc1)(c1cccc1)c1cccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COc1ccc(O)cc1
 [0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.]
 O=S1(=O)OCC2C(CO1)C1(Cl)C(Cl)=C(Cl)C2(Cl)C1(Cl)Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCSCc1cccc1OC(=O)NC
 [0. 0. 1. 0. 0. 0. 0. 1. 0. 0. 0. 0.] BrC1nc2cccc2s1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCC(C)Br
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] N#CCc1cccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)c1ccc(CO)o1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] N#Cc1cccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] N#CCBr
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)CBr
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN1CC(O)C2=C/C(=N/NC(N)=O)C(=O)C=C21
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 Cc1ccc(C2(O)CCN(CCCC(=O)c3ccc(F)cc3)CC2)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=S(=O)(O)F
 [1. 1. 0. 0. 1. 0. 0. 0. 0. 0. 0.]
 C[C@]1(O)CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@@]3(F)[C@@H](O)C[C@@]21C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 N=C(N)c1ccc(OCCCOc2ccc(C(=N)N)cc2Br)c(Br)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CN1[C@H]2CCC[C@@H]1C[C@H](NC(=O)c1nn(C)c3cccc13)C2
 [0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.] O=C(Cl)/C=C/C(=O)Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 Cc1nc2n(c(=O)c1CCN1CCC(c3noc4cc(F)ccc34)CC1)CCC[C@H]2O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 COc1cc(C(C)=O)ccc1OCCCN1CCC(c2noc3cc(F)ccc23)CC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CN(C(=O)CO)c1c(I)c(C(=O)NCC(O)CO)c(I)c(C(=O)NCC(O)CO)c1I
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0.]
 O=C1OC2(c3cccc31)c1cc(I)c(O)c(I)c10c1c2cc(I)c(O)c1I
 [0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.]
 Nc1c(CC(=O) [O-])cccc1C(=O)c1ccc(Br)cc1.Nc1c(CC(=O) [O-])cccc1C(=O)c1ccc(Br)cc1
 [1. 0. 1. 0. 0. 0. 0. 1. 0. 0. 0.] COCCCOc1ccnc(CS(=O)c2nc3cccc3[n-]2)c1C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 COCC(=O)O[C@]1(CCN(C)CCCc2nc3cccc3[nH]2)CCc2cc(F)ccc2[C@@H]1C(C)C

[0. 0. 0. 0. 0. 0. 1. 1. 0. 0. 1. 0.] CCc1ccc(CCOc2ccc(CC3SC(=O)NC3=O)cc2)nc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCOC(C)=O
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.]
 OCCOCCN1CCN(C2=Nc3cccc3Sc3cccc32)CC1.OCCOCCN1CCN(C2=Nc3cccc3Sc3cccc32)CC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)CCSCC(=O)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1nc[nH]c1CN1CCc2c(c3cccc3n2C)C1=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)CCCC[C@@H]1SC[C@@H]2NC(=O)N[C@H]12
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 1. 0.]
 C[C@] (O) (CS(=O) (=O) c1ccc(F) cc1) C(=O) Nc1ccc(C#N) c(C(F) (F) F) c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C[N+](C)(C)C)OC(N)=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)NCC(O)COc1ccc(COCC2CC2)cc1
 [1. 1. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] CCCCC(=O)O[C@]1(C(=O)CO)[C@@H](C)C[C@H]2[C
 @H]3CCC4=CC(=O)C=C[C@]4(C)[C@@]3(F)[C@@H](O)C[C@@]21C
 [1. 1. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] CCCC(=O)O[C@]1(C(=O)CO)(C)C[C@H]2[C
 @H]3CCC4=CC(=O)C=C[C@]4(C)[C@@]3(F)[C@@H](O)C[C@@]21C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(CBr)OCc1cccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCc1ccc(Cl)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=P(O)(Oc1cccc1)Oc1cccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COC(=O)c1cccc1C
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.] CC(C)(C)C(=O)c1cccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(Oc1cccc1)c1cccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COC(=O)c1ccc(C)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1cc(C)cc(N)c1
 [0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)c1c(C(=O)Nc2cccc2)c(-c2cccc2)c(-c2c
 cc(F)cc2)n1CC[C@@H](O)C[C@@H](O)CC(=O)O
 [0. 0. 1. 0. 1. 1. 0. 0. 0. 0. 1. 0.]
 Cc1cc(C2(c3cc(C)c(O)cc3C)OS(=O)(=O)c3cccc32)c(C)cc1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1ccc(S(=O)(=O)[O-])cc1C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1cccc(C)c1N
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.] Cc1ccc(C)c(N)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1cccc(N)c1C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1ncc(CSSCc2cnc(C)c(O)c2CO)c(CO)c1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC=Cc1ccc(O)c(OC)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] FC(F)(F)C(Cl)Br
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.] O=C(O)c1ccc(S(=O)(=O)N(Cl)Cl)cc1
 [0. 0. 1. 0. 1. 0. 0. 0. 1. 0. 0. 0.] CCCCCO(=O)c1ccc(N)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1ccc2c(C)cccc2c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCC(C)C(C)(COC(N)=O)COC(N)=O
 [0. 0. 1. 0. 1. 1. 0. 0. 0. 0. 1. 0.]
 CCN(CC)C(=O)[C@@H]1C=C2c3cccc4[nH]cc(c34)C[C@H]2N(C)C1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] OC[C@@H](O)[C@@H](O)[C@H](O)[C@H](O)CO
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CN1CCN(CCCN2c3cccc3Sc3ccc(S(=O)(=O)N(C)C)cc32)CC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCNCC.O=S(=O)(O)c1cc(O)ccc1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 Cc1nn(-c2cc(NS(C)(=O)=O)c(Cl)cc2Cl)c(=O)n1C(F)F
 [0. 0. 0. 1. 1. 1. 0. 1. 0. 0. 1. 0.] OC(c1ccc(Cl)cc1)(c1cncnc1)c1cccc1Cl
 [0. 0. 0. 0. 1. 0. 0. 1. 0. 0. 0. 0.] COC(=O)C(C)Oc1ccc(Oc2nc3ccc(Cl)cc3o2)cc1

[0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.] CCOC(=O)NCCOc1ccc(Oc2ccccc2)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 COc1c(O)cc2c(c1O)[C@@H]1O[C@H](CO)[C@@H](O)[C@H](O)[C@H]1OC2=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 Cc1onc(-c2ccccc2Cl)c1C(=O)N[C@@H]1C(=O)N2[C@@H](C(=O)[O-])C(C)(C)S[C@H]12
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(=O)O[C@H]1C[C@@]2(C)[C@@H](C[C@@H](O)[C
 @H]3[C@@]4(C)CC[C@@H](O)[C@@H](C)[C@@H]4CC[C@@]32C)/C1=C(\CCC=C(C)C)C(=O)[O-]
 [0. 0. 1. 1. 0. 1. 0. 0. 0. 0. 0. 1.] N#Cc1c[nH]cc1-c1cccc2c1OC(F)(F)O2
 [1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CCN(CC)C(=O)N1CCN(C)CC1.O=C(O)CC(O)(CC(=O)O)C(=O)O
 [0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.]
 CCN(CC)CCc1nc(-c2ccccc2)no1.O=C(O)CC(O)(CC(=O)O)C(=O)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CN1[C@H]2CC[C@@H]1C[C@H](OC1c3ccccc3CCc3ccccc31)C2.O=C(O)CC(O)(CC(=O)O)C(=O)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COc1ccc(C=O)cc1
 [0. 0. 1. 0. 1. 0. 0. 0. 0. 0. 1. 0.] COP(=S)(OC)Oc1c(Cl)cc(C)cc1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 O=C(NC(=O)c1c(F)cccc1F)Nc1ccc(OC(F)(F)C(F)OC(F)(F)F)c(Cl)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCOC(=O)c1ccc(C(=O)OCCC)nc1
 [0. 0. 0. 0. 1. 0. 0. 1. 0. 0. 0. 0.] CC(O)CCO
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)CCS
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCC[N+]1ccc(C)cc1.O=S(=O)([O-])C(F)(F)F
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCC[N+]1(C)CCCC1.F[B-](F)(F)F
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(=O)C1CCCCC1=O
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.] CCCC[N+]1cccc(C)c1.O=S(=O)([O-])C(F)(F)F
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCC1C=CN(C)C1
 [0. 0. 0. 0. 1. 1. 0. 1. 0. 0. 1. 0.] CC1(C(=O)Nc2ccc(O)c(Cl)c2Cl)CCCCC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCC[N+]1(C)CCCCC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCC[N+]1(C)CCCCC1.F[B-](F)(F)F
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] N=C(N)N[N+](=O)[O-]
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)(C)OOC(C)(C)C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1. 0.] CCC(C)Nc1ccc(NC(C)CC)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCNCCCC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCN(CCO)CCCC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 O=C(O)c1ccc2[nH]cc(CCCCN3CC=C(c4ccccc4)CC3)c2c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1.] CN1C2CCC1CC(OC(c1ccccc1)c1ccc(Cl)cc1)C2
 [0. 0. 0. 0. 1. 1. 0. 0. 0. 0. 0. 0.] Oc1ccc(C2CNCCc3c2cc(O)c(O)c3Cl)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Oc1ccc2[nH]cc(CCCCN3CC=C(c4ccccc4)CC3)c2c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] C[C@@H](/C=C/[C@@H](C)[C@H]1CC[C@H]2/C(=C/
 C=C3C[C@@H](O)C[C@H](O)C3)CCC[C@@]21C)C(C)(C)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCOC(=O)NNc1ncc2ccccc12
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)(C)NCCNC(C)(C)C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CCCCC(F)(F)[C@@]1(O)CC[C@H]2[C@@H](CC(=O)[C@@H]2CCCCC(=O)O)O1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CC(C)=CCC/C(C)=C/CC/C(C)=C/CCC(=O)OC/C=C(\C)CCC=C(C)C
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.]

CCN(CC)Cc1nccn1-c1ccc([N+](=O)[O-])cc1C(=O)c1ccccc1C1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] OC1CCCCCCCCCCC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)(C)CC(=O)OCC(=O)[C@@]12OC(C)(C)O[C@@H
]1C[C@H]1[C@@H]3CCC4=CC(=O)C=C[C@]4(C)[C@@]3(F)[C@@H](O)C[C@@]12C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CCCC(S(=O)(=O)N[C@@H](Cc1ccc(OCCCC2CCNCC2)cc1)C(=O)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COC(=O)c1ccc(C(=O)O)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN(C)CCOCCO
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)[N+](C)(C)CC(O)COc1cccc2ccccc12
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 Cc1ccc(S(=O)(=O)NC(=O)N[C@@H](C)Cc2ccccc2)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Nc1ccc(S(=O)(=O)NCc2ccccc2)cc1
 [0. 0. 1. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0.] CC=CC=NNC(=O)c1ccncc1
 [0. 0. 1. 1. 0. 0. 0. 0. 0. 0. 0. 1. 0.] O=C1C(=O)c2ncccc2-c2cccnc21
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CC12CCC(C[N+](C)(CCC[N+](C)(C)C)C1)C2(C)C.COS(=O)(=O)[O-].COS(=O)(=O)[O-]
 [1. 0. 1. 0. 1. 0. 1. 0. 1. 0. 1. 1.] Nc1ccc(C(=O)Nc2ccccc2N)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C[N+](C)(C)CCOC(=O)C(O)(c1ccccc1)c1ccccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)C=CC(=O)Nc1ccc(S(=O)(=O)Nc2nccs2)cc1
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0.] FC(F)(F)C(F)(F)C(F)(F)C(F)(F)CCI
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC/C=C\CCOC(=O)CC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CO[PH](=O)OC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=CC(C)(CCC=C(C)C)OC(=O)CC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN1C(=O)CC[C@H]1c1cccnc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C[C@H]1C[C@@H](O)CC(C)(C)C1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] ClP(Cl)c1ccccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C1COC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1c(O)cccc10
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCOC(=O)CC([O-])C(=O)OCC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] c1ccc(CCc2ccccc2)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COC(=O)c1ccccc1
 [0. 1. 0. 0. 0. 1. 1. 0. 1. 0. 0. 0. 0.] C=CC(=O)OCC(C)OCC(C)OC(=O)C=C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1ccc(CO)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C/C=C(/C)C#N
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0.] C=CC(=O)OCC[N+](C)(C)C
 [0. 0. 0. 0. 1. 0. 0. 1. 0. 0. 0. 0. 0.] O=C(C=Cc1ccccc1)OCc1ccccc1
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] N#Cc1ccccc10
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] CCCCCCCCCCCCCC[N+](C)(C)Cc1ccccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(N)C12CC3CC(CC(C3)C1)C2
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)(N)Cc1ccc(Cl)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCC(CC)COC(=O)COc1ccc(Cl)cc1C
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.] COc1cc(NCc2ccc3nc(N)nc(N)c3c2C)cc(OC)c1OC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN(C)CC[C@@H](c1ccc(Br)cc1)c1ccccc1
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.]
 O[C@@H](c1cc(C(F)(F)F)nc2c(C(F)(F)F)cccc12)[C@H]1CCCCN1
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.]
 O=C(O)CCC(=O)O.c1ccc(C2(c3ccccc3)CC2C2=NCCN2)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC1NCCOC1c1ccccc1

[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCc1ncc(C(=O)O)s1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 O=C(CCOCOCOCOCOCOC(=O)Nc1c(I)cc(I)c(C(=O)O)c1I)Nc1c(I)cc(I)c(C(=O)O)c1I
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCC(CO)CCC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1cccc2[nH]nnc12
 [0. 0. 0. 1. 0. 0. 0. 1. 0. 0. 0. 0. 0.]
 CCCCCCCCCC(=O)OC[C@@H](O)[C@H]1OC[C@H](OCCO)[C@H]1OCCO
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CS(=O)(=O)OCC(O)C(O)COS(C)(=O)=O
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0.] C=CCN(CC=C)CC=C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=CCn1c(=O)n(CC=C)c(=O)n(CC=C)c1=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(NCO)NCO
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1cccc(O)c1C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1ccc(C)c(O)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1cc(C)cc(O)c1
 [0. 0. 1. 0. 1. 0. 0. 1. 1. 0. 1. 0. 0.] CN(C)c1ccc(N)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1.] COc1cc2c(cc1O)CCN[C@]21CS[C@@H]2c3c(OC(C)=
 O)c(C)c4c(c3[C@H](COc1=O)N1[C@@H](O)[C@@H]3Cc5cc(C)c(OC)c(O)c5[C@H]([C@H]21)N3C)
 OCO4
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Nc1cc(=O)nc(N)[nH]1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1coc2c1CCC(C)C2
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Nc1c[n+](N2CCOCC2)no1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)(Cl)Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0.] O=C(O)Cc1ccc(OCCNC[C@H](O)c2cccc2)cc1
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0.] CN1CCCN(C(c2cccc2)c2ccc(Cl)cc2)CC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 Cn1cc(NC(=O)c2cc(NC(=O)c3cc(NC=O)cn3C)cn2C)cc1C(=O)NCCC(=N)N
 [0. 0. 0. 0. 0. 1. 1. 0. 0. 0. 0. 0. 0.]
 CC(=O)O[C@H]1CC[C@@]2(C)C(=CC[C@H]3[C@H]4CC=C(c5cccn5)[C@@]4(C)CC[C@@H]32)C1
 [0. 0. 1. 1. 0. 0. 0. 0. 0. 0. 1. 0. 0.] c1ccc(-c2ccc(C(c3cccc3)n3ccnc3)cc2)cc1
 [1. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCC(=O)O[C@]1(C(=O)CO)CC[C@H]2[C@@H]3CCC
 4=CC(=O)CC[C@]4(C)[C@H]3[C@@H](O)C[C@@]21C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CC[N+](C)(CC)CCOC(=O)C(O)(c1cccc1)C1CCCC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)c1ccc(OCCn2ccnc2)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0.] CCCCCCCNC(C)C(O)c1ccc(SC(C)C)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 COc1cc(OC)nc(NC(=O)[N-]S(=O)(=O)c2ncccc2OCC(F)(F)F)n1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN/C(=N/[N+](=O)[O-])NCC1CCOC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CC1(C)OC[C@@H]2O[C@@]3(C(=O)[O-])OC(C)(C)O[C@H]3[C@@H]2O1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=Cc1cccc1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Nc1cccc(Cl)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COc1ccc(N)c([N+](=O)[O-])c1
 [1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1ccc(-c2nc3ccc(C)cn3c2CC(=O)N(C)C)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CN1CCCC(n2nc(Cc3ccc(Cl)cc3)c3cccc3c2=O)CC1
 [0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.] O=C1C=C2C=C[C@@H]3C[C@@]2(O1)[C@H]1CCCCN31
 [0. 0. 1. 1. 0. 0. 0. 0. 0. 0. 1. 0. 0.]

C1c1ccc(CO/N=C(\Cn2ccnc2)c2ccc(C1)cc2C1)c(C1)c1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCCCCCCOP(=O)([O-])OCC[N+](C)(C)C
[0. 0. 1. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0.] CC(=O)Nc1ccccc1O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCc1cc(C(N)=S)ccn1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(=O)Nc1ccc(O)c1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
CO/N=C1\CN(c2nc3c(cc2F)c(=O)c(C(=O)O)cn3C2CC2)CC1CN
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=CCCC#N
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=CC/C=C/C
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCOC(=O)CC
[0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0.] CC1=CCC(=C(C)C)CC1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCOC(=O)COC(=O)c1ccccc1C(=O)OCCCC
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
Fc1ccc([C@@H]2CCNC[C@H]2COc2ccc3c(c2)OC(=O)O)cc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCSC(=O)N(CC(C)C)CC(C)C
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] NC1=NC(=O)C(c2ccccc2)O1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCC(=O)c1ccc(O)cc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] CCCCCC(=O)Oc1c(Br)cc(C#N)cc1Br
[1. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(=O)OCC(=O)[C@@]1(O)[C@H](C)C[C@H]2[C@@H]
]3C[C@H](F)C4=CC(=O)C=C[C@]4(C)[C@H]3[C@@H](O)C[C@@]21C
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCC
[0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCC=O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC1=CC(=O)CC(C)(C)C1=O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCCCC(=O)O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)CCCCCCCCCCC(=O)O
[0. 1. 0. 0. 1. 1. 1. 1. 0. 0. 0. 1.] O=C(CC1)C(C1)C1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] CCC(C)c1ccc(O)cc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCC(=O)N(C)C
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] CCC(C)c1ccccc1O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN(C)CCCCCN(C)C
[0. 0. 0. 0. 1. 1. 0. 1. 0. 0. 0. 0.] O=C(O)c1nn(Cc2ccc(C1)cc2C1)c2ccccc12
[0. 0. 0. 1. 0. 0. 0. 1. 0. 0. 1. 0.] CC[C@H](C)C(=O)O[C@H]1C[C@@H](C)C=C2C=C[C@
H](C)[C@H](CC[C@@H]3C[C@@H](O)CC(=O)O3)[C@H]21
[0. 0. 1. 0. 0. 0. 0. 1. 0. 0. 1. 0.]
O=C(Nc1ccc([N+](=O)[O-])c1)c1cc2ccccc2cc1O
[0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN(C)c1ccc(O)c2c1C[C@H]1C[C@H]3[C@H](N(C)C
)C(O)=C(C(N)=O)C(=O)[C@@]3(O)C(O)=C1C2=O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCC1CCCC1=O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC1=CC(C)C(C=O)C(C)C1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
O=S(=O)([O-])c1ccc2cc(O)c(S(=O)(=O)[O-])cc2c1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] NC[C@H]1O[C@H](O[C@@H]2[C@@H](N)C[C@@H](N)
[C@H](O[C@H]3O[C@H](CO)[C@@H](O)[C@H](N)[C@H]3O)[C@H]2O)[C@H](N)C[C@@H]1O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.]
Cc1ccc(C(=O)c2cc(O)c(O)c([N+](=O)[O-])c2)cc1
[0. 0. 0. 0. 0. 1. 0. 1. 1. 1. 0. 0.] N#C[Au-]C#N
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.]
Cc1ccc(O)c([C@H](CCN(C(C)C)C(C)C)c2ccccc2)c1

[0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CC(C)N1CCN(c2ccc(OC[C@H]3CO[C@](Cn4cncn4)(c4ccc(Cl)cc4Cl)O3)cc2)CC1
 [0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0.]
 CCCCCCCCCCn1cc[n+](C)c1.O=S(=O)([N-])S(=O)(=O)C(F)(F)F)C(F)(F)F
 [0. 0. 0. 1. 0. 0. 0. 1. 0. 0. 1. 0.]
 CCCCCCCCCCn1cc[n+](C)c1.O=S(=O)([O-])C(F)(F)F
 [0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 1. 0. 0.] Clc1ccc(CSC(Cn2ccnc2)c2ccc(Cl)cc2Cl)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 COc1cc2nc(N3CCN(C(=O)C4CCCO4)CC3)nc(N)c2cc1OC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] OCCOc1cccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CNCC(O)c1ccc(OC(=O)C(C)(C)C)c(OC(=O)C(C)(C)C)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 1. 0. 0.] O=C(OCC(O)CO)c1cccc1Nc1ccnc2cc(Cl)ccc12
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN(C/C=C/c1cccc1)Cc1cccc2cccc12
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=NN1CCN(N=O)CC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=C(C)[C@H]1CC=C(C)C(=O)C1
 [0. 0. 1. 0. 0. 1. 0. 1. 0. 0. 0. 0.] Oc1cccc1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] ClC(Cl)(Cl)Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 1. 0.] O=[N+]([O-])c1ccc(O)c([N+](=O) [O-])c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCC(Br)(CC)C(=O)NC(N)=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC1=C(/C=C/C(C)=C/C=C/C(C)=C/C=C\C=C(C)\C=C
 \C=C(C)\C=C\C2=C(C)CCCC2(C)C)C(C)(C)CCC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1c([N+](=O) [O-])cccc1 [N+](=O) [O-]
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1ccc([N+](=O) [O-])cc1 [N+](=O) [O-]
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CC1=C(C(=O)O)N2C(=O)[C@H](NC(=O)[C@H](N)C3=CCC=CC3)[C@H]2SC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCC(CC)COC(=O)COc1cc(Cl)c(Cl)cc1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCOC(=O)COc1cc(Cl)c(Cl)cc1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)c1cccnc1C(=O)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(O)C(C)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCC [N+](C)CCCC1.F [B-](F)(F)F
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCC(=O)c1cccc(Cl)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCOS(=O)(=O) [O-] .CCn1cc[n+](C)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCC [n+](C)ccc(C)cc1.F [B-](F)(F)F
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCCCCCCCCCBr
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=[N+]([O-])c1ccc(F)c(Cl)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC [n+](C)cccc1.F [B-](F)(F)F
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCn1cc[n+](C)c1.Cl [Fe-](Cl)(Cl)Cl
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 1. 0.]
 O=C(Nc1ccc(F)cc1F)c1cccnc1Oc1ccc(C(F)(F)F)c1
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.] OCC=Cc1cccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C/C=C(\C)C(C)=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCC(CC)c1cccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1cc(CC(=O)O)c(C)n1-c1ccc(Cl)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCC(CC)C(=O)OCCOCCOCCOCC(=O)C(CC)CCCC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=P([O-])(O)C(O)(Cc1cccnc1)P(=O)([O-])O
 [0. 0. 0. 0. 1. 1. 0. 0. 0. 0. 0. 1.] Cc1cc(C(C)(C)c2cc(C)c(O)c(C)c2)cc(C)c1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCSC(=O)Cl

[0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0.] O=C(O)C(Cc1cc(I)c(O)c(I)c1)c1cccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(O)COC(C)(C)C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C1COC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(=O)/C=C/c1cccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)Br
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] NCc1cccc1Sc1cccc1CO
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] c1ccc(CNCCNCc2cccc2)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCc1ccc(C(=O)O)cc1
 [0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0.] O=C(O)c1cccc1-c1ccc(C(F)(F)F)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=CCCCCCCCC(=O)OC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(=O)Oc1ccc(C)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C([O-])c1nc(O)nc(O)n1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] [O-][n+]1cccc(CO)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] OC[C@H]1O[C@@H](O)[C@H](O)[C@@H](O)[C@@H]1
 O[C@@H]1O[C@H](CO)[C@H](O)[C@H](O)[C@H]1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CNc1c2c(nn1C)CCCC2
 [1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(O)C(=O)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Nc1nnc(-c2cccc(C1)c2C1)c(N)n1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)c1cc(C(=O)O)cc([N+](=O)[O-])c1
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 1. 0. 0.] CCOCN(C(=O)CC1)c1c(C)cccc1CC
 [0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 1. 1.] CC(=O)O[C@H]1C[C@H](O[C@H]2[C@@H](O)C[C@H]
 (O[C@H]3[C@@H](O)C[C@H](OC4CC[C@@]5(C)C(CC[C@@H]6[C@@H]5CC[C@]5(C)[C@@H](C7=CC(=O)OC7)[C@@H](O)C[C@]65O)C4)O[C@@H]3C)O[C@@H]2C)O[C@H](C)[C@H]1O[C@@H]1O[C@H](CO)
 [C@@H](O)[C@H](O)[C@H]1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COc1cc2c(cc1OC)C(C(C(=O)N(CCc1ccc(OC)c(OC)
 c1OC)CCc1ccc(OC)c(OC)c1OC)c1cccc1)=NCC2
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COC(=O)C(CN)c1c[nH]c2ccc(OC)cc12
 [0. 1. 1. 0. 0. 0. 1. 1. 1. 1. 0. 1.]
 CN1CCC(Nc2ncc3ncnc(Nc4ccc(F)c(Cl)c4)c3n2)CC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1cccc(C)c1NC(=O)c1cccc1C(=O)O
 [0. 1. 0. 0. 0. 1. 0. 0. 1. 0. 0. 1.] OB(O)O[Hg]c1cccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(=O)c1sc(C)nc1C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCC(=O)C(=O)CC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC1(C)S[C@@H]2[C@H](NC(=O)[C@H](N)c3cccc3
)C(=O)N2[C@H]1C(=O)OCOC(=O)[C@@H]1N2C(=O)C[C@H]2S(=O)(=O)C1(C)C
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.] CN[C@@H]1[C@H](O[C@H]2[C@H](O[C@@H]3[C@@H]
 (NC(=N)N)[C@H](O)[C@@H](NC(=N)N)[C@H](O)[C@H]3O)O[C@@H](C)[C@]2(O)CO)O[C@@H](CO)
 [C@H](O)[C@H]1O.CN[C@@H]1[C@H](O[C@H]2[C@H](O[C@@H]3[C@@H](NC(=N)N)[C@H](O)[C@@H]
) (NC(=N)N)[C@H](O)[C@H]3O)O[C@@H](C)[C@]2(O)CO)O[C@@H](CO)[C@H](O)[C@H]1O
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.] CN[C@@H](C)[C@H](O)c1cccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN1C(=O)C(O)N=C(c2cccc2)c2cc(Cl)ccc21
 [0. 0. 1. 0. 0. 0. 0. 1. 0. 0. 1. 0.] CCC(C)(CC)c1cc(NC(=O)c2c(OC)cccc2OC)on1
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)NC(=O)N1CC(=O)N(c2cc(Cl)cc(Cl)c2)C1=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CC1(C)S[C@@H]2[C@H](NC(=O)C(C(=O)[O-])c3cccc3)C(=O)N2[C@H]1C(=O)[O-]
 [0. 0. 0. 1. 0. 1. 0. 0. 0. 0. 0. 0.]
 CC/C=C(\c1cccc1)c1ccc(OCCN(C)C)cc1)c1cccc1.O=C(O)CC(O)(CC(=O)O)C(=O)O

[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] ClC=CCCl
 [0. 0. 1. 0. 0. 0. 0. 1. 0. 0. 1. 0.] NCCS(=O)(=O)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=c1[nH]c(=O)n(C2CCCO2)cc1F
 [0. 0. 0. 0. 1. 1. 0. 0. 0. 0. 0. 0.] CC(C)(C)c1cc(CCC(=O)OCC(COC(=O)CCc2cc(C(C)(C)C)c(O)c(C(C)(C)C)c2)(COC(=O)CCc2cc(C(C)(C)C)c(O)c(C(C)(C)C)c2)cc(C(C)(C)C)c1O
 [0. 0. 0. 0. 1. 1. 0. 0. 0. 0. 0. 0.] CC(C)C(=O)OCC(C)(C)C(OCC(=O)C(C)C)C(C)C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCN
 [0. 0. 1. 0. 0. 0. 0. 1. 0. 0. 0. 0.] Cc1cccc2sc(N)nc12
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 1. 0.] COc1cccc2sc(N)nc12
 [0. 0. 1. 0. 1. 0. 0. 0. 0. 0. 0. 0.] COc1ccc2nc(N)sc2c1
 [0. 0. 1. 0. 1. 0. 0. 0. 1. 0. 0. 0.] COc1ccc2nc(N)sc2c1
 [0. 0. 0. 0. 1. 1. 0. 0. 0. 0. 0. 0.] ClC1C(Cl)C(Cl)C(Cl)C(Cl)C1Cl
 [0. 0. 1. 0. 0. 0. 1. 1. 1. 0. 0. 0.] Cc1ccc(O)c(N)c1
 [0. 0. 1. 0. 0. 0. 0. 1. 0. 0. 0. 0.] Cc1ccc(N)cc1O
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.]
 Cl[C@H]1[C@H](Cl)[C@@H](Cl)[C@H](Cl)[C@@H](Cl)[C@@H]1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.]
 Cl[C@H]1[C@H](Cl)[C@@H](Cl)[C@H](Cl)[C@H](Cl)[C@H]1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCO(=O)OCC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C[Si](C)(C)O[Si](O)(O)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] OCCc1ccncc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=C(C)C(=O)OCCOP(=O)(O)O
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 1. 1.] O=C(c1cc(O)c(O)c(O)c1)c1ccc(O)c(O)c1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)(C)NC(=O)[C@H]1CN(Cc2cccnc2)CCN1C[C@H](O)C[C@@H](Cc1cccc1)C(=O)N[C@H]1c2cccc2C[C@H]1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.]
 O=C1[C@H](CC[C@H](O)c2ccc(F)cc2)[C@@H](c2ccc(O)cc2)N1c1ccc(F)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=[N+]([O-])c1c(Cl)c(Cl)cc(Cl)c1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] FC(Cl)(Cl)C(F)(Cl)Cl
 [0. 1. 0. 0. 0. 0. 0. 1. 1. 0. 0. 0.] O=[N+]([O-])c1cc(Cl)c(Cl)c(Cl)c1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 NS(=O)(=O)c1cc2c(cc1Cl)N=C(CSCc1cccc1)NS2(=O)=O
 [0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0. 1. 0.]
 COc1c(C(C)(C)C)cc([N+](=O)[O-])c(C)c1[N+](=O)[O-]
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C1COCCN1
 [0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0.] CCCCC(C)COC(=O)c1cccc1C(=O)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.]
 CCCCNC1ccc(C(=O)OCCOCCOCCOCCOCCOCCOCCOCCOCCO)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CCN(CC)C(=O)C1CN2CCc3cc(OC)c(OC)cc3C2CC1OC(C)=O
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.] COc1ccc(NC(C)=O)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] BrCc1ccc(Br)cc1
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 O=C(O)c1ccc2cccc2c1O.OCCc1cc(C)CNCCCCOCCCCc2cccc2)ccc1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCC(C(=O)OCCN(CC)CC)(c1cccc1)c1cccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN1CCN(C2Cc3cccc3Sc3ccc(Cl)cc32)CC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCC1CCC[C@H](c2cccc(O)c2)C1

[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCC(CC)C(C)CCOC(C)=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CC(C)NCC(O)COc1ccc(COCCOC(C)C)cc1.CC(C)NCC(O)COc1ccc(COCCOC(C)C)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C[C@@H]1C(=O)N=C2Nc3cccc(Cl)c3CN21
 [0. 0. 0. 0. 0. 0. 1. 0. 1. 0. 0. 1. 0.] O=CCCC=O
 [0. 0. 0. 0. 0. 1. 0. 0. 0. 1. 1. 0. 0.] CC(Cc1ccc(O)c(O)c1)C(C)Cc1ccc(O)c(O)c1
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0.] N#C[Fe-2](C#N)(C#N)(C#N)(C#N)N=O
 [0. 0. 1. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0.] c1ccc2c(c1)ccc1c3cccc3ccc21
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)c1cccc1C(c1ccc(O)cc1)c1ccc(O)cc1
 [1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cn1sc(Cl)cc1=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCC1CCC(=O)O1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)COc1ccc(Cl)cc1
 [0. 0. 0. 1. 0. 0. 0. 1. 0. 0. 1. 0. 0.]
 CCCCCCCCCCn1cc[n+](C)c1.O=S(=O)([O-])C(F)(F)F
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 COc1cccc(C(=O)NN(C(=O)c2cc(C)cc(C)c2)C(C)(C)C)c1C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C#CCOC(=O)/C=C(C)/C=C/CC(C)CCCC(C)C
 [0. 0. 1. 0. 0. 0. 0. 1. 0. 0. 1. 0. 0.] COC(C)(C)CCCC(C)C/C=C/C(C)=C/C(=O)OC(C)C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1cc(=O)[nH]o1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)CCCc1c[nH]c2cccc12
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 O=C(O)[C@H]1[C@@H](O)CC[C@H]2CN3CCc4c([nH]c5cccc45)[C@H]3C[C@@H]21
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COc1ccc2cc([C@H](C)C(=O)[O-])ccc2c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CC(=O)OCC1=C(C(=O)[O-])N2C(=O)[C@H](NC(=O)CSc3ccncc3)[C@H]2SC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1ccsc1/C=C/C1=NCCCN1C
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0.] CC1(C)[C@@H](OC(=O)CCC(=O)[O-])CC[C@@]2(C)
 [C@H]1CC[C@]1(C)[C@@H]2C(=O)C=C2[C@@H]3C[C@@](C)(C(=O)[O-])CC[C@]3(C)CC[C@]21C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC[C@@]1([C@@H]2O[C@@H]([C@H]3O[C@@](O)(CO)
) [C@H](C)C[C@@H]3C)C[C@@H]2C)CC[C@H]([C@]2(C)CC[C@]3(C[C@H](O)[C@@H](C)[C@@H]([C
 @H](C)[C@@H](OC)[C@H](C)C(=O)[O-])O3)O2)O1
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0.]
 COc1ccc2cccc2c1C(=O)N[C@@H]1C(=O)N2[C@@H](C(=O)[O-])C(C)(C)S[C@H]12
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCC(NC(C)C)C(O)c1ccc(O)c(O)c1
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 O=S(=O)([O-])c1ccc(N=Nc2c(O)ccc3cccc23)cc1
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 1. 0. 0.] O=C1OC2(c3ccc(O)cc3O)c3cc(O)ccc32)c2cccc21
 [0. 0. 0. 1. 0. 1. 0. 0. 0. 0. 1. 0. 0.] CCOP(=O)(OCC)Oc1nc(Cl)c(Cl)cc1Cl
 [0. 0. 0. 1. 0. 0. 0. 0. 0. 1. 1. 0. 0.]
 CCNc1ccc(C(=C2C=CC(=[N+](CC)CC)C=C2)c2ccc(N(CC)CC)cc2)c2cccc12
 [0. 0. 0. 0. 1. 0. 0. 0. 1. 0. 0. 0. 0.] COc1cc(/C=C/c2cccc2)oc(=O)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCC(CO)CCCCCCC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0.] CN(C)C(=S)[S-]
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0.] CC(C)(C)c1cccc(C(C)(C)C)c1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 Cc1cccc(C)c1NC(=O)c1cc(S(N)(=O)=O)c(Cl)cc1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] OC1OC[C@@H](O)[C@H](O)[C@H]1O
 [0. 0. 1. 0. 0. 0. 1. 1. 0. 0. 1. 0. 0.]

CCOC1CC(C(=O)NS(=O)(=O)C2CCCCC2C)CCC1CC1CN(C)C2CCC(NC(=O)OC3CCCC3)CC12
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Nc1ccn([C@H]2CC[C@@H](CO)O2)c(=O)n1
 [0. 0. 1. 0. 1. 1. 0. 0. 0. 0. 1. 0.]
N[C@@H](Cc1cc(I)c(Oc2ccc(O)c(I)c2)c(I)c1)C(=O)O
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
N[C@@H](Cc1cc(I)c(Oc2cc(I)c(O)c(I)c2)c(I)c1)C(=O)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
CN(CCO)CC(O)Cn1cnc2c1c(=O)n(C)c(=O)n2C.O=C(O)c1cccnc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCN(C(C)=O)c1cccc(-c2ccnc3c(C#N)cnn23)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
CC(=O)N[C@@H]1[C@@H](NC(=N)N)C=C(C(=O)O)O[C@H]1[C@H](O)[C@H](O)CO
 [1. 1. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.]
CC[N+]1(CCOC(=O)C(O)(c2ccccc2)c2ccccc2)CCCCC1
 [0. 0. 1. 0. 1. 0. 0. 0. 0. 0. 0. 0.] c1ccc2c(c1)CCc1ccccc1N2
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)c1cc(Cl)ccc1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)c1c(Cl)ccc1Cl
 [1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)c1cccc(Cl)c1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)c1ccc(Cl)cc1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0.] O=C1C=CC(=O)N1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=Cc1c(Cl)ccc1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=Cc1ccc(Cl)c(Cl)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCC(=O)O[C@H]1[C@H](O[C@@H]2[C@@H](C)[C@H](O[C@H]3C[C@@](C)(OC)[C@@H](O)[C@H](C)O3)[C@@H](C)C(=O)O[C@H](CC)[C@@](C)(O)[C@H](O)[C@@H](C)C(=O)[C@H](C)C[C@@]2(C)O)O[C@H](C)C[C@@H]1N(C)C.CCCCCCCCCCOC(=O)(=O)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C[C@H]1CC[C@@H]2[C@@H](C)[C@H]3[C@H](C[C@H]4[C@@H]5CC=C6CC(O[C@@H]7O[C@H](CO)[C@H](O)[C@H](O[C@@H]8O[C@H](CO)[C@@H](O)[C@H](O)[C@H]8O)[C@H]7O)[C@H]7O[C@H]7O[C@@H](C)[C@H](O)[C@@H](O)[C@H]7O)CC[C@]6(C)[C@H]5CC[C@@]43C)N2C1
 [0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.] C=CC(=O)NCOC
 [1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCOCc1ccc(C(=O)c2ccccc2)c(O)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCC#N
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C1c2ccccc2CN2C(=O)c3ccccc3CN12
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] ClCCCCBr
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCBr
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COc1nccnc1NS(=O)(=O)c1ccc(N)cc1
 [0. 0. 1. 0. 1. 0. 0. 0. 1. 0. 1. 1.] CCCOc1ccc2nc(NC(=O)OC)sc2c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN1CCC(CN2c3ccccc3Sc3ccccc32)C1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
O=C(CCN1CCN(CCO)CC1)N1c2ccccc2Sc2ccc(C(F)(F)F)cc21
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCBr
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(Cl)c1ccc(F)c(Cl)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=S(=O)(Cl)c1c(Cl)ccc1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCOC(=O)CCCC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
O=C(O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCC1CCCCC(=O)O1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC=C(C)C(=O)OCCC(C)CCC=C(C)C

[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC/C=C\CCOC(=O)c1cccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 C=C(C)C(=O)OCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCOC(=O)CCC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] ClC1=C(Cl)C2(Cl)C(CBr)CC1(Cl)C2(Cl)Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1. 0.]
 O=[N+]([O-])c1ccc(O/N=C/c2cc(Br)c(O)c(Br)c2)c([N+](=O)[O-])c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 O=S1(=O)OC(c2cc(Br)c(O)c(Br)c2)(c2cc(Br)c(O)c(Br)c2)c2cccc21
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCOP(=S)(OCC)Oc1cc(Cl)c(Br)cc1Cl
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 1. 1. 0.] CN(C)c1ccc(C(=C2C=CC(=[N+](C)C)C=C2)c2cccc
 c2)cc1.CN(C)c1ccc(C(=C2C=CC(=[N+](C)C)C=C2)c2cccc2)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCOC(=O)c1cnc2cc(OCC(C)C)c(OCC(C)C)cc2c1O
 [0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 1. 0.] C#CCOS(=O)OC1CCCC1Oc1ccc(C(C)(C)C)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=c1cc(O)c(Cl)c[nH]1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)(C)NCC(O)c1cc(Cl)c(N)c(C(F)(F)F)c1
 [1. 1. 0. 1. 1. 1. 0. 0. 0. 0. 0. 0. 0.]
 C[C@]12CC[C@H]3[C@@H](CCC4=C(O)C(=O)CC[C@@]43C)[C@@H]1CCC2=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 C[C@@H](NCCCc1ccc(C(F)(F)F)c1)c1ccc2cccc12
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] CCCCCc1ccc(C)cc1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCOC(=O)c1cccc1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CO/N=C(\C(=O)N[C@@H]1C(=O)N2C(C(=O)[O-])=C
 (C[n+]3ccc(N)n3CCO)CS[C@H]12)c1csc(N)n1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCCCCSC#N
 [0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.]
 CC1(C)[C@@H](C(=O)OCc2coc(Cc3cccc3)c2)[C@H]1/C=C1\CCSC1=O
 [0. 0. 1. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0.] CCOP(=S)(OCC)Oc1cc(-c2cccc2)on1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCCCCN1CCCCC1=O
 [0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.] CN(C)C(=O)Nc1ccc(OC(=O)NC(C)(C)C)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cl[Sn](Cl)(Cl)Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] NCc1ccc(S(N)(=O)=O)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC1CC(CC2CCC(N)C(C)C2)CCC1N
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(O)(P(=O)([O-])O)P(=O)([O-])O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=[Si]=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CO[Si](C)(OC)c1cccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1ccc(S(=O)(=O)[N-]Cl)cc1
 [0. 0. 1. 0. 0. 0. 0. 1. 0. 0. 1. 0.] [O-]c1cccc1-c1cccc1
 [0. 0. 1. 0. 0. 0. 0. 1. 0. 0. 0. 0.] O=[N+]([O-])c1cccc2cccc([N+](=O)[O-])c12
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 O=[N+]([O-])c1cc([N+](=O)[O-])c2ccc(S(=O)(=O)O)cc2c1O
 [0. 0. 1. 0. 0. 0. 0. 1. 0. 0. 0. 0.] O=[N+]([O-])c1cc([N+](=O)[O-])c2cccc2c1
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.] O=[N+]([O-])c1cccc2c([N+](=O)[O-])cccc12
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 1. 0.] Nc1ccc(Cc2ccc(N)c(Cl)c2)cc1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCOC(=O)[C@H](C)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCOC(=O)CC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(COC(C)(C)C)OCCCO
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]

CC1=C(CC(=O)O)c2cc(F)ccc2/C1=C\c1ccc(S(C)(=O)=O)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
OC[C@H]1O[C@H](O[C@]2(CC1)O[C@H](CC1)[C@@H](O)[C@@H]2O)[C@H](O)[C@@H](O)[C@H]1C1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] CC[C@H](C)[C@H]1O[C@]2(C=C[C@@H]1C)C[C@@H]
1C[C@@H](CC=C(C)[C@@H](O[C@H]3C[C@H](OC)[C@@H](O[C@H]4C[C@H](OC)[C@@H]([NH2+]C)[
C@H](C)O4)[C@H](C)O3)[C@@H](C)C=CC=C3CO[C@@H]4[C@H](O)C(C)=C[C@@H](C(=O)O1)[C@]3
4O)O2.O=C([O-])c1ccccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
CN[C@H]1CC[C@@H](c2ccc(Cl)c(Cl)c2)c2ccccc21
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(Nc1ccc(/C=C/c2ccc(NC(=O)c3cc(S(=O)(=O)
O)c4ccnc4c3O)cc2S(=O)(=O)O)c(S(=O)(=O)O)c1)c1cc(S(=O)(=O)O)c2ccnc2c1O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCO P(=S)(OCC)SCSC(C)(C)C
[0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
CN(CC(=O)N1CCOCC1)Cc1c(Cl)cccc1NC(=O)c1ccccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN1CCN(C2=Nc3ccccc3Cc3ccccc32)CC1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(Cn1c(=O)sc2ccc(Cl)cc21)N1CCN(CCO)CC1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
COc1cc(C[C@@H]2NCCc3cc(O)c(O)cc32)cc(OC)c1OC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C1CCC(N2C(=O)c3ccccc3C2=O)C(=O)N1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCOCOCOC
[0. 0. 0. 0. 1. 1. 0. 1. 0. 0. 0. 0. 0.] O=C(O)/C=C/C(=O)O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)/C=C\C(=O)O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCC(C)=O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCC(=O)O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCC=O
[0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 1. 0. 0.]
CC(C)=CC1C(C(=O)OCc2coc(Cc3ccccc3)c2)C1(C)C
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0.] CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@H]2C[C@@]
(C)(OC)[C@@H](O)[C@H](C)O2)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@H](N(C)C)[C@H]2O)
[C@](C)(O)C[C@@H](C)C(=O)[C@H](C)[C@@H](O)[C@]1(C)O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCC(=O)OC
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] c1cc(-c2ccncc2)ccn1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN=C=S
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)=CCO
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COP(=O)(OC)O/C(C)=C/C(=O)N(C)C
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C1CCOCOC1
[0. 0. 0. 0. 1. 1. 0. 0. 0. 0. 0. 0. 0.] CC(C)=CC1
[0. 0. 1. 0. 0. 0. 0. 1. 0. 0. 1. 0.]
O=C1c2c(O)ccc(Nc3ccc(CCO)cc3)c2C(=O)c2c([N+](=O)[O-])ccc(O)c21
 [0. 0. 0. 1. 0. 0. 0. 0. 0. 1. 0. 0. 0. 1.]
O=C1C(O)=C([C@H]2CC[C@H](c3ccc(Cl)cc3)CC2)C(=O)c2ccccc21
 [1. 0. 0. 0. 1. 0. 0. 1. 0. 0. 1. 0.] Oc1ccc(-c2ccccc2)c(Cl)c1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C1CCCCCCCCC(=O)OCCO1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=[PH]1Oc2ccccc2-c2ccccc21
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=[N+]([O-])C1(Br)COCOC1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(NC(C)(C)C)C(=O)c1cccc(Cl)c1

[0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.]
CC#CCC(C) [C@H] (O)/C=C/C1 [C@H] 2C/C(=C/CCCC(=O)O)C [C@H] 2C [C@H] 1O
[0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)Cn1cnc2c(N)nc3cccc3c21
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN(C)CCCN(C)CCCN(C)C
[0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0.] NCCOCCOCCOCCCN
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] N#CSc1ccc(N)c([N+](=O)[O-])c1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(=O)N [C@H] 1 [C@@H] (O [C@@H] 2C(C(=O) [O-])C [C@@H] (O [C@@H] 3 [C@@H] (CO)O [C@H] (OC4C(C(=O) [O-])O [C@@H] (OC5 [C@H] 6CO [C@H] (O6) [C@H] (NS(=O) (=O) [O-]) [C@H] 5O) [C@H] (O) [C@H] 4O) [C@H] (NC(C)=O) [C@H] 3C) [C@H] (O) [C@H] 2O)O [C@H] (COS(=O) (=O)O) [C@@H] (O [C@@H] 2OC(C(=O) [O-])=C [C@H] (O) [C@H] 2O) [C@@H] 1O
[1. 1. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0.]
C=C [C@H] 1CN2CC [C@H] 1C [C@H] 2 [C@H] (OC(=O)OCC) c1ccnc2ccc(OC) cc12
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)=CCC [C@@] (C) (O) [C@H] 1CC=C(C) CC1
[1. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.]
O=C1c2c(O)cccc2 [C@H] ([C@@H] 2O [C@H] (CO) [C@@H] (O) [C@H] (O) [C@H] 2O) c2cc(CO) cc(O) c21
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(N)C c1ccc(O) cc1
[0. 0. 1. 0. 0. 1. 0. 0. 0. 0. 1. 0.] O=C1c2cccc2C(=O) c2c1ccc(O) c2O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COc1cc(OC) cc(OC) c1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCC(=O)C(CC(C)N(C)C) (c1cccc1) c1cccc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1c(N(C)C) c(=O) n(-c2cccc2) n1C
[1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN(C)CCO
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN(C) c1cccc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0.] C[As] (C) (=O)O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC1(C)C(=O)NC(=O)NC1=O
[0. 0. 1. 0. 1. 1. 0. 0. 0. 1. 1. 1.] O=C(c1ccc(O) cc1O) c1ccc(O) cc1O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=C(C)C(=O)OCCOC1CC2CC1C1C=CCC21
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] OCC(c1ccc(Cl) cc1) c1ccc(Cl) cc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCN(CC)CCOC(=O) c1ccc(N) cc1Cl
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCN(CC)C(=O) c1ccc(O) c(OC) c1
[0. 0. 0. 0. 1. 1. 0. 0. 0. 0. 0. 0.]
C1CNCCN1.C [C@] 12CC [C@@H] 3c4ccc(OS(=O) (=O)O) cc4CC [C@H] 3 [C@@H] 1CCC2=O
[1. 1. 0. 0. 1. 1. 0. 0. 0. 0. 0. 0.]
CCCCC(=O)O [C@H] 1CC [C@H] 2 [C@@H] 3CCc4cc(O) ccc4 [C@H] 3CC [C@] 12C
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
CC(=O)OC(C)OC(=O)C(C) c1ccc(-c2cccc2) c(F) c1
[1. 1. 0. 0. 1. 1. 0. 0. 0. 0. 0. 0.]
CCCCCCC(=O)O [C@H] 1CC [C@H] 2 [C@@H] 3CCc4cc(O) ccc4 [C@H] 3CC [C@] 12C
[1. 1. 0. 0. 1. 1. 0. 0. 0. 0. 0. 0.]
CCC(=O)O c1ccc2c(c1)CC [C@@H] 1 [C@@H] 2CC [C@] 2(C) [C@@H] (OC(=O)CC)CC [C@@H] 12
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCN(CC)CCNC(=O) c1cc(S(C) (=O)=O) ccc1OC
[0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0.] FC(F) (F) c1cccc1-n1ccnc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] N#CC(C#N)=Cc1cc(O) c(O) c(O) c1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] N#CC(C#N)=Cc1ccc(O) c(O) c1
[0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 1.]
O=C(O)C(F) (F)C(F) (F)C(F) (F)C(F) (F)C(F) (F)C(F) (F)C(F) (F)C(F) (F)C(F) (F)C(F) (F)F
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)C(F) (F)C(F) (F)C(F) (F)C(F) (F)C(F) (F)C(F) (F)C(F) (F)F
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
O=C(O)C(F) (F)C(F) (F)C(F) (F)C(F) (F)C(F) (F)C(F) (F)C(F) (F)C(F) (F)C(F) (F)C(F) (F)F

[0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.]
 O=C(O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 O=S(=O)(O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CDC(=O)[C@@H]1CC2=CC(=O)CC[C@]2(C)[C@@]23O
 [C@@H]2C[C@@]2(C)[C@@H](CC[C@@]24CCC(=O)O4)[C@H]13
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)CC(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@@H]
 (CC(C)C)[C@@H](O)CC(=O)N[C@@H](C)C(=O)N[C@@H](CC(C)C)[C@@H](O)CC(=O)O)C(C)C)C(C)
 C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN(C)CCc1ccc(O)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC1(C)S[C@@H]2[C@H](N)C(=O)N2[C@H]1C(=O)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] c1cc2c(c(N3CCNCC3)c1)OCCO2
 [0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0.]
 CC1(CN2CCC(n3c(=O)[nH]c4cccc43)CC2)OCc2cccc2-n2cccc21
 [0. 0. 1. 1. 0. 0. 0. 1. 1. 0. 1. 0.]
 CN1C(=O)[C@@H](NC(=O)c2cc3cccc3[nH]2)N=C(c2cccc2)c2cccc21
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 O=c1[nH]c2cc(C(F)(F)F)c(N3CCOCC3)cc2n(CP(=O)(O)O)c1=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CDC1=CC=C2[C@H]3Cc4ccc(OC)c5c4[C@@]2(CCN3C)[C@H]1O5
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
 [0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 1. 0.] Cc1ccc(N(SC(F)(Cl)Cl)S(=O)(=O)N(C)C)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(=O)Nc1ccc(S(=O)(=O)Cl)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1ccc([N+](=O)[O-])cc1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1.]
 COCC(=O)Nc1cc(Sc2cccc2)ccc1N=C(NC(=O)OC)NC(=O)OC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)[C@@]1(NC(=O)[C@@H]2C[C@@H]3c4cccc5[n
 H]cc(c45)C[C@H]3N(C)C2)O[C@@]2(O)[C@@H]3CCCN3C(=O)[C@H](Cc3cccc3)N2C1=O
 [1. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 C[C@@H](CO)NC(=O)[C@@H]1C=C2c3cccc4[nH]cc(c34)C[C@H]2N(C)C1
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 1. 0.]
 CCN(CC)C(=O)N[C@@H]1C=C2c3cccc4[nH]cc(c34)C[C@@H]2N(C)C1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=CCN1CCc2nc(N)sc2CC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CN(C(=O)Cc1cccc1)[C@H]1CC[C@@]2(CCCO2)C[C@@H]1N1CCCC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CN1C[C@@H](NS(=O)(=O)N(C)C)C[C@@H]2c3cccc4c3c(cn4C)C[C@H]21
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 C=CCN1CC[C@]23c4c5ccc(O)c4O[C@H]2C(=O)CC[C@@]3(O)[C@H]1C5.CI
 [0. 0. 1. 1. 0. 0. 0. 1. 0. 1. 1. 0.] CC(C)(C)NSc1nc2cccc2s1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0.]
 C=CCC1=C(C)C(OC(=O)C2C(C=C(C)C)C2(C)C)CC1=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC1=CC(=O)CCC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)c1cccc1C(C)C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C=NC1CCC(CC2CCC(N=C(=O)CC2)CC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCOC(C)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=C(C)C(=O)OCC[N+](C)(C)C

[0. 0. 1. 0. 0. 0. 0. 1. 0. 0. 0. 0.] c1ccc2sc(SN(C3CCCCC3)C3CCCCC3)nc2c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)C(=O)OCC(C)(C)C(O)C(C)C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1cccc(Cl)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C1=CCCC=CCCC=CCC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=C(C)C#N
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COP(N)(=O)SC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCSP(=O)(SCCCC)SCCCC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COCC(=O)N(c1c(C)cccc1C)C(C)C(=O)OC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C[N+](C)CCCCC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 Cn1cc(C2=C(c3cn(C4CCN(Cc5cccn5)CC4)c4cccc34)C(=O)NC2=O)c2cccc21
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 O=C(NOC[C@H](O)CO)c1ccc(F)c(F)c1Nc1ccc(I)cc1F
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 1. 1.] O=C1CN=C(c2cccc2)c2cc(Cl)ccc2N1CC1CC1
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Nc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCOC(=O)CCC(C)=O
 [1. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 C[C@]12C[C@H](O)[C@H]3[C@@H](CCC4=CC(=O)C=C[C@@]43C)[C@@H]1CC[C@]2(O)C(=O)CO
 [1. 1. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.]
 C[C@]12CC(=O)[C@H]3[C@@H](CCC4=CC(=O)C=C[C@@]43C)[C@@H]1CC[C@]2(O)C(=O)CO
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CNC(=O)CSP(=O)(OC)OC
 [1. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0.] CCCN(CCC)S(=O)(=O)c1ccc(C(=O)O)cc1
 [0. 0. 0. 1. 0. 0. 0. 1. 0. 0. 0. 0.] C=C(C)[C@@H]1CCC2=CCC[C@@H](C)[C@]2(C)C1
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.] C=CC(C)=CCC=C(C)C
 [0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0.]
 C=C(C)[C@@H]1CCC2=CC(=O)C[C@@H](C)[C@]2(C)C1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCOC(=O)CC(C)C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCCN(CCCCCCCCCC)CCCCCCCCC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC1=CCCC(C)(C)C12CCC(C)O2
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 1. 0. 0.]
 c1cc(C(c2ccc(OCC3CO3)cc2)c2ccc(OCC3CO3)cc2)ccc1OCC1CO1
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC1(CO)CN(c2cccc2)NC1=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=C(C)C(=O)OCCCCCCCCOC(=O)C(=C)C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCC(=O)OCc1cccc1
 [0. 0. 0. 1. 0. 0. 0. 0. 0. 1. 0.] Cc1cccc(Nc2cccc2)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=S(=O)([O-])CC(O)CC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=CCOCC(CC)(CO)COCC=C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] NS(=O)(=O)c1cccc1Cl
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 1. 0. 0.]
 CCC(C)(CCC(C)C)C(=O)O[Sn](C)(C)OC(=O)C(C)(CC)CCC(C)C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)(C)C1CCCC1O
 [0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0.] CC(C)CP(=S)([S-])CC(C)C
 [1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COc1ccc(CC2c3cc(OC)c(OC)cc3CC[N+](C)CCC(=O)OCCCCOC(=O)CC[N+](C)CCc3cc(OC)c(OC)cc3C2Cc2ccc(OC)c(OC)c2)cc1OC.O=S(=O)([O-])c1cccc1.O=S(=O)([O-])c1cccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COc1c(N2CCOCC2)cnn(C)c1=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN1CCC(=C2c3cccc3CCc3ccnc32)CC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]

CC(=O)OC[C@H]1O[C@@H](n2ncc(=O)[nH]c2=O)[C@H](OC(C)=O)[C@@H]1OC(C)=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CCOC(=O)[C@H](CCc1cccc1)N[C@@H](C)C(=O)N1CCC[C@H]1C(=O)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN(C)C(=O)Nc1ccc(Cl)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1ccc(S(=O)(=O)N=C=O)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] NC(=O)c1cccc1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C1C[C@@H]2OCC=C3CN4CC[C@]56c7cccc7N1[C@H]5[C@H]2[C@H]3C[C@H]46
 [0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0.] O=c1oc2cccc2c(O)c1Cc1c(O)c2cccc2oc1=O
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C1NCC2(CCN(Cc3cccc3)CC2)O1
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCOC(=O)Nc1ccc(NCc2ccc(F)cc2)nc1N
 [0. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0.]
 CC(C)[N+]1(C)C2CCC1CC(OC(=O)C(CO)c1cccc1)C2
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] N=C(N)NCc1cccc(I)c1.N=C(N)NCc1cccc(I)c1
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)NC(C)Cc1ccc(I)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.] Clc1cc(C(Cl)(Cl)Cl)cnc1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1cn[nH]c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 NC(=O)c1nnc([C@@H]2O[C@H](CO)[C@@H](O)[C@H]2O)c1O
 [0. 0. 0. 0. 1. 0. 0. 1. 0. 0. 0. 0. 0. 0.] C#CCN(C)CCC0c1ccc(Cl)cc1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCC#N
 [0. 0. 0. 0. 0. 1. 0. 0. 1. 1. 0. 1.] N#Cc1c(Cl)c(Cl)c(Cl)c(C#N)c1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1ccc(C)c(O)c1C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=C(C)C(=O)OCCOCC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)[C@@H]1CC[C@@H](C)C[C@H]1O
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 1. 0.] O=C=Nc1ccc(Cl)c(Cl)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] COP(=S)(OC)Oc1nc(Cl)c(Cl)cc1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 C#CCOC(=O)[C@@H](C)Oc1ccc(Oc2ncc(Cl)cc2F)cc1
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0.] CC1(C)CON(Cc2cccc2Cl)C1=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCSC(=O)N(CC)C1CCCC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COC(=O)C(C)Oc1ccc(Oc2ccc(Cl)cc2Cl)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCNC(=O)NC(=O)/C(C#N)=N/OC
 [0. 0. 1. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1cc(C2CC2)nc(Nc2cccc2)n1
 [0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0.]
 COc1cc2nc(N(C)CCCNC(=O)C3CCC03)nc(N)c2cc1OC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CN(C)C(=O)Oc1cc(OC(=O)N(C)C)cc(C(O)CNC(C)(C)C)c1
 [1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] CCC(=O)O[C@]1(C(=O)SCF)[C@H](C)C[C@H]2C3C[C@H](F)C4=CC(=O)C=C[C@]4(C)[C@@]3(F)[C@@H](O)C[C@@]21C
 [1. 0. 0. 0. 1. 1. 0. 0. 0. 0. 0. 0. 0. 0.]
 C[C@@]12CCC[C@H]1[C@@H]1CC[C@H]3C[C@@H](O)CC[C@]3(C)[C@H]1CC2
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CC(=O)SC[C@@H](Cc1cccc1)C(=O)NCC(=O)OCc1cccc1
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCN1CCC[C@@H]2Cc3n[nH]cc3C[C@H]21
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] CCC[C@@]1(CCc2cccc2)CC(O)=C([C@H](CC)c2cc
 cc(NS(=O)(=O)c3ccc(C(F)(F)F)cn3)c2)C(=O)O1

[0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 1. 0.] CD[C@H]1C[C@@H]2CC[C@H](C)[C@@](O)(O2)C(=O)C(=O)N2CCCC[C@H]2C(=O)O[C@H]([C@H](C)C[C@@H]2CC[C@H](O)[C@H](OC)C2)CC(=O)[C@H](C)C=C(C)[C@@H](O)[C@@H](OC)C(=O)[C@H](C)C[C@H](C)C=CC=CC=C1C
 [1. 0. 0. 1. 1. 0. 0. 1. 0. 0. 0. 0.] CCC(C)(C)C(=O)O[C@H]1C[C@@H](C)C=C2C=C[C@H](C)[C@H](CC[C@H]3C[C@@H](O)CC(=O)O3)[C@H]21
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 1. 1. 1.]
 CC(C)=CCOc1ccc(/C=C/C(=O)c2ccc(OC=C(C)C)cc2OCC(=O)O)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C1NC(=O)[C@@]2(CC0c3ccc(F)cc32)N1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C/C=C(/CC[C@@H](C)[C@H]1CC[C@H]2C3=CC[C@H]4[C@H](C)[C@@H](O)CC[C@]4(C)[C@H]3CC[C@@]21C)C(C)C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] OC[C@H](O)[C@@H](O)[C@H](O)[C@H](O)CO
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCCOC(=O)(=O)O.OCCN(CCO)CCO
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] [O-]c1ccccc1
 [0. 1. 1. 0. 0. 0. 1. 1. 0. 0. 1. 1.] c1ccc2c(c1)c1ccc3ccc4cccc2c4c31
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=CCNCC=C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1. 0.] CCCCC/C=C/C=C/C=C/O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C1CCC2CCCCC2C1
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.] CCCCCCCCCC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=C(C)C(=O)OCCCCCCCCC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=CC(=O)NC(C)(C)CC(C)=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(=O)CC(C)(C)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CN(C)C(=O)C1(N2CCCC2)CCN(CCC2(c3ccc(C1)c(C1)c3)CN(C(=O)c3ccccc3)CCO2)CC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C([O-])C(Cl)Cl
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 1.] O=C([O-])Cc1ccccc1Nc1c(Cl)cccc1Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Clc1cc(Cl)c(Cl)nc1Cl
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 1. 0. 0.] NNC(=S)NN
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] NC(=O)Nc1ccc(Cl)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] [O-][n+]1ccc(Cl)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCC/C=C\CCC=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN1C(=O)CC(=O)N(c2ccccc2)c2cc(Cl)ccc21
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCc1occc(=O)c1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC1=C(O)C(=O)C(C)O1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COc1ccc(CCO)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCC(C)C(O)CC
 [1. 0. 0. 0. 1. 1. 0. 1. 1. 0. 1. 0.] Oc1ccc(/C=C/c2cc(O)cc(O)c2)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C1C[N+]([O-])=C(c2ccccc2)c2cc(Cl)ccc2N1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(/C=C/c1ccc(F)c1)NC1CC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(O)Cc1csc(-c2ccc(Cl)cc2)n1
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 1. 0.] O=C(Nc1ccc(Br)cc1)c1cc(Br)c(Br)s1
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.] O=C(O)Cc1cn(-c2ccccc2)nc1-c1ccc(Cl)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1cccc(C)c1NC(=O)CN1CCCC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] NS(=O)(=O)c1ccc(Cl)c(S(N)(=O)=O)c1
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 1. 0. 0.] COc1ccc(C=CC(=O)c2ccc(OC)cc2OC)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(NCN1CCOCC1)c1cnccn1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COc1cccc2c1C(=O)c1c(O)c3c(c(O)c1C2=O)C[C@@](O)(C(=O)CO)C[C@@H]3O[C@H]1C[C@H](N)[C@H](O[C@@H]2CCCCO2)[C@H](C)O1
 [1. 1. 0. 0. 1. 1. 0. 0. 0. 0. 0. 0.]

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CCCCC(=O)O[C@H]1CC[C@H]2[C@@H]3CC[C@H]4CC(=O)C=C(C)[C@]4(C)[C@H]3CC[C@]12C
[0. 0. 0. 0. 0. 0. 0. 1. 0. 1. 0. 0.] C=C/C(C)=C/C=C(\C)CCC=C(C)C
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCC(=O)OCCOc1cccc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(=O)CCC1=C(C)CCC1(C)C
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COc1cc(C=O)ccc1OC(=O)C(C)C
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN1N=C(C(N)=O)CCC1=O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@@]43C)[C@@H]1CC[C@@H]2C(=O)O
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1sccc1Br
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(CCC1)NCCc1cccc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
[O-][n+]1cccc(/C(Cl)=N/OC[C@H](O)CN2CCCC2)c1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0.]
CC[C@@]1(O)C(=O)OCc2c1cc1n(c2=O)Cc2c-1nc1cccc1c2/C=N/OC(C)(C)C
[0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.]
C=CCNc1nc(NCC=C)nc(N2CCN(C(c3ccc(F)cc3)c3ccc(F)cc3)CC2)n1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1.]
CC[C@@]1(O)C(=O)OCc2c1cc1n(c2=O)Cc2cc3c([N+](=O)[O-])cccc3nc2-1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCCCCCOS(=O)(=O)[O-]
[1. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0.] S=c1[nH]c2cccc2[nH]1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(=O)N[C@@H]1C(O[C@H]2O[C@H](C(=O)O)C(O)[
C@H](O)[C@H]2O)[C@H](O)[C@@H](CO)O[C@H]1O[C@@H]1C(C(=O)O)O[C@@H](O[C@H]2[C@H](O)
[C@@H](CO)OC(O)[C@@H]2NC(C)=O)[C@H](O)[C@H]1O
[0. 0. 1. 0. 0. 0. 0. 1. 0. 0. 1. 1.] S=C1NC=NC2N=CNC12
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCOC(=O)CCCC(=O)OCCCCC
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCC(=O)OC
[0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0.] OC/C=C/CO
[0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 1. 0.] Cc1c(Cl)cccc1Nc1cccc1C(=O)O
[0. 0. 1. 1. 0. 0. 0. 1. 0. 0. 1. 0.] OCc1c[nH]c2cccc12
[0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0.] Cc1cccc(Nc2cc(Cl)nc(SCC(=O)O)n2)c1C
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CNCC(O)c1ccc(O)cc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=CCCl
[0. 0. 1. 0. 1. 0. 0. 1. 1. 1. 0. 0.] O=C(CCl)c1cccc1
[0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COP(=S)(OC)Oc1ccc([N+](=O)[O-])cc1Cl
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COC(=O)c1cccc1C(=O)O
[0. 1. 1. 0. 1. 0. 0. 1. 1. 1. 0. 1.] CC(=O)Nc1ccc(C(=O)CC1)cc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCOC(=O)c1cccc1C(=O)O
[0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Nc1ccc(Cl)cc1
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] c1ccc(CCCc2cccn2)cc1
[0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCOC(=O)c1cn2nc(OP(=S)(OCC)OCC)cc2nc1C
[0. 0. 0. 0. 0. 0. 0. 1. 0. 1. 0. 1.]
CCC(C)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1OC(=O)C=C(C)C
[0. 0. 0. 0. 0. 1. 0. 1. 0. 1. 1. 1.]
CCC(C)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1OC(=O)OC(C)C
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
CCN(CC)c1c([N+](=O)[O-])cc(C(F)(F)F)c(N)c1[N+](=O)[O-]
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
CC1(C)[C@@H]2CC[C@@]1(C)[C@H](OC(=O)CSC#N)C2

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[0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)N(C(=O)SCC(C1)=CC1)C(C)C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CC(=O)OCC1=C(C(=O)O)N2C(=O)[C@@H](N)[C@H]2SC1
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 1.] COC(=O)Nc1nc2ccccc2[nH]1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=C1CCCCC1C1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC1(C)[C@@H]2CC[C@@]1(C)C(=O)C2
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] NC(N)=O.OO
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCC(=O)C1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0. 0.] CCCCCOC(C)=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCCCCCC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCCCCCC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] OCCCCCO
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=CCCCCCCCCCCCC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCCCCCCCCCCCC
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CSc1ccc(C1)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Clc1ccc2ccccc2c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1ccccc1C1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CS(=O)(=O)c1ccc(C1)cc1
 [0. 0. 1. 1. 1. 0. 0. 0. 0. 0. 1. 0.] Oc1ccc2ccc3cccc4ccc1c2c34
 [0. 0. 0. 0. 1. 1. 0. 0. 0. 0. 1. 0.] CC(C)COC(=O)c1ccc(O)cc1
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cn1c(N)nc2c3ccnc3ccc21
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] NC(=O)CI
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.] IC(I)I
 [0. 0. 0. 0. 0. 0. 1. 0. 0. 0. 0. 0.]
 COc1ccc2c(c1)c(CC(=O)O)c(C)n2C(=O)c1ccc(C1)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=CCOCC(O)(COCC=C)COCC=C
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 1. 0.] CCc1ccc(O)c(C(C)(C)C)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 Cc1c(C)c([N+](=O)[O-])c(C(C)(C)C)c([N+](=O)[O-])c1C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C#CCN(C)[C@H](C)Cc1ccccc1
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 1. 0.]
 O=C1CN(N=Cc2ccc(-c3ccc([N+](=O)[O-])cc3)o2)C(=O)[N-]1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCN(CCC#N)c1ccccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] COC(=O)CCCC(=O)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] OC[C@H](Cc1ccc(O)c1)[C@H](CO)Cc1ccc(O)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] COc1cc(C1)ccc1Oc1ccc(C1)cc1C1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1ccc(O)c(C(=O)c2ccccc2)c1
 [0. 0. 0. 0. 1. 1. 0. 0. 0. 0. 1. 0.] O=C(c1ccccc1)c1ccc(O)c1
 [0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0.] O=C(c1ccccc1)c1ccccc1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN1CCc2cc3c(cc2C1O)OC3
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] CCCCCCCCCCOC(=O)c1ccc(O)cc1
 [0. 0. 0. 0. 1. 1. 0. 0. 0. 0. 0. 0.] O=C(Oc1ccccc1)c1ccc(O)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1. 0.]
 CCCC(c1cc(C(C)(C)C)c(O)cc1C)c1cc(C(C)(C)C)c(O)cc1C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] O=c1[nH]cnc2nc[nH]c12
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 C=C1CC[C@H]2[C@@](C)(CC[C@@H](O)[C@@]2(C)CO)[C@@H]1C/C=C1/C(=O)OC[C@H]1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CN1CC(=O)NC1=N

[1. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 0.] CC1(C)O[C@H]2CC(=O)OC[C@@]23[C@H]1CC(=O)[C@]1(C)[C@@H]3CC[C@@]2(C)[C@H](c3ccoc3)OC(=O)[C@H]3O[C@]321
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] OC[C@H]1O[C@@H](O[C@@H]2[C@@H](CO)O[C@@H](O)[C@H](O)[C@H]2O)[C@H](O)[C@@H](O)[C@@H]1O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CN(C)CCN(Cc1ccccc1)c1ccccc1.O=C(O)CC(O)(CC(=O)O)C(=O)O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] C=CCC1(C(C)CCC)C(=O)N=C([S-])NC1=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Clc1ccccc1
 [0. 0. 1. 0. 0. 0. 0. 0. 0. 0. 1. 1.] CCOC(=O)C(O)(c1ccc(Cl)cc1)c1ccc(Cl)cc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CCCCCCCCC[C@@H](C[C@@H]1OC(=O)[C@H]1CCCCC)OC(=O)C(CC(C)C)NC=O
 [0. 0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.] CCC1C01
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] FC(F)OC(F)(F)C(F)Cl
 [1. 1. 0. 0. 1. 1. 0. 0. 0. 0. 0. 0.]
 C#C[C@]1(O)CC[C@H]2[C@@H]3CCC4=C(CCC(=O)C4)[C@H]3CC[C@@]21C
 [0. 0. 0. 0. 0. 0. 0. 1. 0. 0. 1. 0.]
 O=S1OCC2C(CO1)C1(Cl)C(Cl)=C(Cl)C2(Cl)C1(Cl)Cl
 [0. 0. 0. 1. 0. 0. 0. 0. 0. 0. 1. 0.]
 ClC1=C(Cl)[C@]2(Cl)[C@H]3[C@H]([C@@H]4C[C@H]3[C@H]3O[C@@H]43)[C@@]1(Cl)C2(Cl)Cl
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] ClCC1C01
 [1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 O=C(O[C@@H]1Cc2c(O)cc(O)cc2O[C@@H]1c1cc(O)c(O)c(O)c1)c1cc(O)c(O)c(O)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CC(C)NCC1CCc2cc(CO)c([N+](=O)[O-])cc2N1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCn1cnc2c1c(=O)n(CCCCC(C)=O)c(=O)n2C
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] c1cnc(N2CCN(Cc3ccc4c(c3)OC(=O)C2)nc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] Cc1ccc(=O)n(-c2cccc2)c1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 Cc1nc2cccn2c(=O)c1CCN1CCC(C(=O)c2ccc(F)cc2)CC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 O=c1[nH]c2ccccc2n1CCN1CCN(C(c2ccccc2)c2ccccc2)CC1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] NC(=O)CN1CC(O)CC1=O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCC(=O)c1ccc2c(c1)N(CCCN(C)C)c1ccccc1S2
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCn1c(=O)[nH]c(=O)c2[nH]cnc21
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.] CCCNCC(O)COc1ccccc1C(=O)CCc1ccccc1
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
 CCOc1nc2cccc(C(=O)O)c2n1Cc1ccc(-c2ccccc2-c2nnn[nH]2)cc1
 [1. 1. 0. 0. 1. 0. 0. 0. 0. 0. 0. 0.]
 CC(=O)[C@H]1CC[C@H]2[C@@H]3CCC4=CC(=O)CC[C@]4(C)[C@H]3CC[C@]12C
 [1. 1. 0. 0. 1. 1. 0. 1. 0. 0. 0. 0.]
 C[C@]12CC[C@H]3[C@@H](CCC4=CC(=O)CC[C@@]43C)[C@@H]1CC[C@@H]2O
 [1. 1. 0. 0. 1. 1. 0. 0. 0. 0. 1. 1.]
 C[C@]12CC[C@@H]3c4ccc(O)cc4CC[C@H]3[C@@H]1CC[C@H]2O
 [0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 0.] COc1ccc2c(c1OC)CN1CCc3cc4c(cc3C1C2)OC(=O)C4

[]: