Graph_Neural_Network

November 6, 2020

[1]:
```
#from chembl_webresource_client.new_client import new_client
import matplotlib
import pandas as pd
#import modin.pandas as pd
import torch
from torch import nn
from torch import optim
from torch.utils.data import DataLoader

import EMNN.gnn

import EMNN.gnn.emn_implementations
from EMNN.losses import LOSS_FUNCTIONS
from EMNN.train_logging import LOG_FUNCTIONS
from EMNN.gnn.molgraph_data import MolGraphDataset, molgraph_collate_fn
from EMNN.train_logging import feed_net
from EMNN.train_logging import compute_mse
import datetime
```

[2]:
```
drug_c = pd.read_csv("drugCentral.csv")
endogenous = pd.read_csv("endogenous.csv")
in_trails = pd.read_csv("in-trials.csv")
world = pd.read_csv("world.csv")
df1 = pd.read_csv('Bioactivities2.csv',sep='\t',low_memory=False)
```

[3]:
```
# uniprot_id = "O15648"
# records = new_client.target.filter(target_components__accession=uniprot_id)
# print([(x['target_chembl_id'], x['pref_name']) for x in records])
```

[4]:
```
# chembl_id = "CHEMBL5686"
# records = new_client.activity.filter(target_chembl_id=chembl_id)
# len(records)
```

[5]:
```
# Bio = records[0:7870]
```

[6]:
```
# df= pd.DataFrame(list(Bio.all()))
```

[7]:
```
# pd.DataFrame(df).to_csv("Bioactivities.csv", index=True, sep='\t')
```

[8]:
```
data = pd.read_csv("Bioactivities.csv",sep='\t')
```

[3]:
```
df1.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 64726 entries, 0 to 64725
Data columns (total 48 columns):
 #   Column                       Non-Null Count  Dtype
---  ------                       --------------  -----
 0   Unnamed: 0                   64726 non-null  int64
 1   Molecule ChEMBL ID           64726 non-null  object
 2   Molecule Max Phase           64726 non-null  int64
 3   Molecular Weight             64726 non-null  float64
 4   #RO5 Violations              64726 non-null  object
 5   AlogP                        64726 non-null  object
 6   Compound Key                 64726 non-null  object
 7   Smiles                       64726 non-null  object
 8   Standard Type                64726 non-null  object
 9   Standard Relation            64726 non-null  object
 10  Standard Value               64726 non-null  float64
 11  Standard Units               64726 non-null  object
 12  Uo Units                     64726 non-null  object
 13  Potential Duplicate          64726 non-null  bool
 14  Assay ChEMBL ID              64726 non-null  object
 15  Assay Description            64726 non-null  object
 16  Assay Type                   64726 non-null  object
 17  BAO Format ID                64726 non-null  object
 18  BAO Label                    64726 non-null  object
 19  Assay Organism               64726 non-null  object
 20  Assay Tissue ChEMBL ID       64726 non-null  object
 21  Assay Tissue Name            64726 non-null  object
 22  Assay Cell Type              64726 non-null  object
 23  Assay Subcellular Fraction   64726 non-null  object
 24  Target ChEMBL ID             64726 non-null  object
 25  Target Name                  64726 non-null  object
 26  Target Organism              64726 non-null  object
 27  Target Type                  64726 non-null  object
 28  Document ChEMBL ID           64726 non-null  object
 29  Source ID                    64726 non-null  int64
 30  Source Description           64726 non-null  object
 31  Cell ChEMBL ID               64726 non-null  object
 32  mol                          64726 non-null  object
 33  HeavyAtomCount               64726 non-null  int64
 34  HAccept                      64726 non-null  int64
 35  HDonor                       64726 non-null  int64
```

```
 36  Heteroatoms                 64726 non-null  int64
 37  RingCount                   64726 non-null  int64
 38  SaturatedRings              64726 non-null  int64
 39  AliphaticRings              64726 non-null  int64
 40  AromaticRings               64726 non-null  int64
 41  Ipc                         64726 non-null  float64
 42  HallKierAlpha               64726 non-null  float64
 43  NumValenceElectrons         64726 non-null  int64
 44  MolLogP                     64726 non-null  float64
 45  AMW                         64726 non-null  float64
 46  NumRotatableBonds           64726 non-null  int64
 47  logValue                    64726 non-null  float64
dtypes: bool(1), float64(7), int64(13), object(27)
memory usage: 23.3+ MB
```

[10]:
```
data = data.dropna(subset=['canonical_smiles', 'molecule_chembl_id']).
↪drop_duplicates(subset=['molecule_chembl_id'])
```

[11]:
```
data.type.value_counts()
```

[11]:
```
Potency     5798
Activity      53
INH           36
IC50          10
Ki             3
Ki/Km          1
Name: type, dtype: int64
```

[12]:
```
data.canonical_smiles
```

[12]:
```
0              OC[C@H]1O[C@H](CNC2CCCC2)[C@@H](O)[C@@H]1O
1       OC[C@H]1O[C@H](CNCc2ccc(Cl)cc2Cl)[C@@H](O)[C@@…
2            OC[C@H]1O[C@H](CNC2CCCCCC2)[C@@H](O)[C@@H]1O
3       OC[C@H]1O[C@H](CNCc2ccc(-c3ccccc3)cc2)[C@@H](O…
4        Cc1ccc(CNC[C@H]2O[C@H](CO)[C@@H](O)[C@@H]2O)cc1C
                                 …
7846    COc1ccc(CC(=O)Nc2ccc(S(=O)(=O)Nc3cc(C)on3)cc2)…
7857    Cc1cc(NC(=O)c2ccc(NC(=O)Cc3ccc(Cl)c(Cl)c3)cc2)no1
7863     Cc1cc(NC(=O)c2csc(NC(=O)Cc3ccc(Cl)c(Cl)c3)n2)no1
7868    OC[C@H]1O[C@H](CNc2ccc3ccccc3c2)[C@@H](O)[C@@H]1O
7869    OC[C@H]1O[C@H](CNc2ccc(Cl)c(Cl)c2)[C@@H](O)[C@…
Name: canonical_smiles, Length: 5901, dtype: object
```

[3]:
```
data_reduced = df1[['Smiles','logValue']]
```

[9]:
```
data_reduced.info()
```

```
<class 'pandas.core.frame.DataFrame'>
```

```
RangeIndex: 64726 entries, 0 to 64725
Data columns (total 2 columns):
 #   Column    Non-Null Count  Dtype
---  ------    --------------  -----
 0   Smiles    64726 non-null  object
 1   logValue  64726 non-null  float64
dtypes: float64(1), object(1)
memory usage: 1011.5+ KB
```

[14]:
```
drop_low_types = data_reduced[(data_reduced['type'] == 'IC50') |␣
↪(data_reduced['type']== 'Activity') | (data_reduced['type']== 'INH') |␣
↪(data_reduced['type']== 'Ki')| (data_reduced['type']== 'Ki/Km')].index
```

[15]:
```
data_reduced_PotOnly = data_reduced.drop(drop_low_types)
```

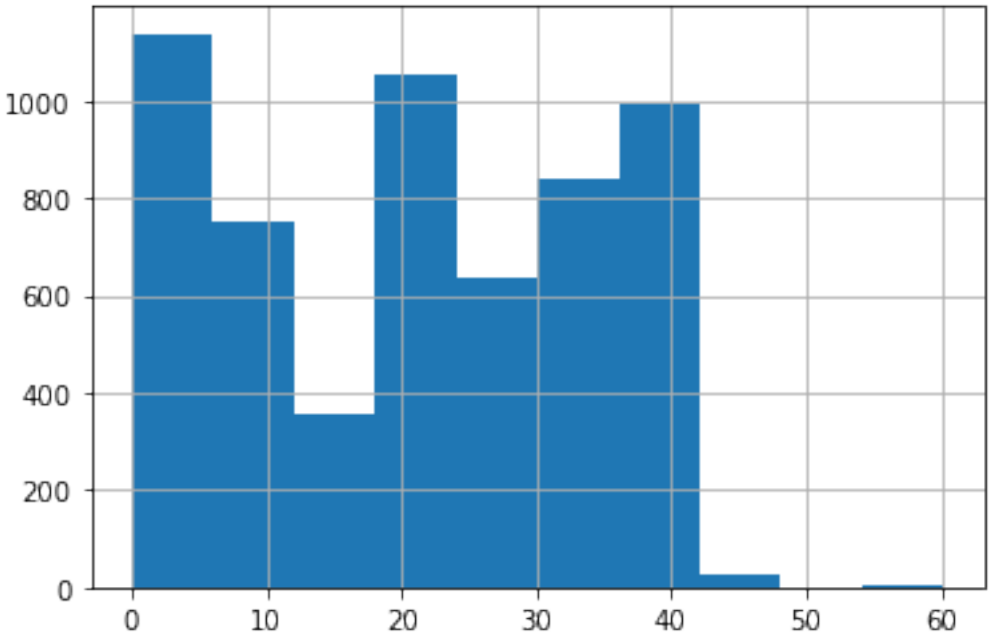
[16]:
```
data_reduced_PotOnly = data_reduced_PotOnly.dropna()
```

[17]:
```
data_reduced_PotOnly.info()
```

```
<class 'pandas.core.frame.DataFrame'>
Int64Index: 5798 entries, 66 to 6835
Data columns (total 3 columns):
 #   Column            Non-Null Count  Dtype
---  ------            --------------  -----
 0   canonical_smiles  5798 non-null   object
 1   type              5798 non-null   object
 2   value             5798 non-null   float64
dtypes: float64(1), object(2)
memory usage: 181.2+ KB
```

[18]:
```
data_reduced_PotOnly['value'].hist()
```

[18]: <AxesSubplot:>



[19]:
```
import numpy as np
data_reduced_PotOnly['logValue'] = -1 * np.log(data_reduced_PotOnly['value'])
```

[20]:
```
# data_prepared = data_reduced_PotOnly.drop(columns = "type")
data_prepared = data_reduced.drop(columns = "value")
```

[21]:
```
data_prepared
```

[21]:

	canonical_smiles	logValue
66	Cc1cc(C(=O)NNC(=O)Cc2ccc(Cl)c(Cl)c2)c(C)o1	-3.405564
67	O=C(NC(=S)Nc1ccccc1C(=O)O)c1ccc2ccccc2c1	-2.484532
68	O=C(NCCCN1CCCCCC1)c1ccc(CS(=O)(=O)Cc2ccccc2F)o1	-1.908890
69	NS(=O)(=O)c1ccc(NC(=O)Nc2ccc(C(F)(F)F)cc2)cc1	-2.599655
70	CCNC(=O)C1CCCc2c1[nH]c1ccc(Cl)cc21	-3.060175
…	…	…
6831	C[N+](C)(C)CCO	1.775492
6832	Cc1cc([C@@H]2CCCN2C)on1	-3.981209
6833	Cc1cccc(C2CN(C)CCc3c2cc(O)c(O)c3Cl)c1	0.163461
6834	CC(=O)O[C@H]1CC2(C)[C@@H](C[C@@H](O)[C@H]3[C@@…	-2.024008
6835	CC[C@@H](CO)Nc1nc(NCc2ccccc2)c2ncn(C(C)C)c2n1	0.278524

[5798 rows x 2 columns]

[22]:
```
from sklearn.preprocessing import StandardScaler
scaler = StandardScaler()
```

```
data_prepared['logValue_scaled'] = scaler.
 ↪fit_transform(data_prepared[['logValue']].values[:,0].reshape(-1, 1))
# df.insert(2, 'value_scaled', scaler.transform(data_prepared[['value']].
 ↪values[:,0].reshape(-1, 1)), True)
```

[4]:
```
# data_prepared_sacled = data_prepared.drop(columns = "logValue")
# data_prepared_sacled_np = data_prepared_sacled.to_numpy()
data_reduced_np = data_reduced.to_numpy()
```

[63]:
```
import numpy as np
np.random.shuffle(data_reduced_np)
train, valid, test = np.split(data_reduced_np, [int(.76*data_reduced_np.
 ↪shape[0]), int(.9*data_reduced_np.shape[0])])
train = np.insert(train, 0, [None]*train.shape[0], 1)
valid = np.insert(valid, 0, [None]*valid.shape[0], 1)
test = np.insert(test, 0, [None]*test.shape[0], 1)
```

[11]:
```
import numpy as np
```

[64]:
```
len(train)
```

[64]: 49191

[65]:
```
len(valid)
```

[65]: 9062

[66]:
```
len(test)
```

[66]: 6473

[5]:
```
pd.DataFrame(train).to_csv("Data/leishmaniasis_train.csv.gz", index=False,␣
 ↪compression='gzip', sep='\t')
pd.DataFrame(valid).to_csv("Data/leishmaniasis_valid.csv.gz", index=False,␣
 ↪compression='gzip', sep='\t')
pd.DataFrame(test).to_csv("Data/leishmaniasis_test.csv.gz", index=False,␣
 ↪compression='gzip', sep='\t')
```

```
---------------------------------------------------------------------------
NameError                                 Traceback (most recent call last)
<ipython-input-5-e7e3f6327344> in <module>
----> 1 pd.DataFrame(train).to_csv("Data/leishmaniasis_train.csv.gz",␣
 ↪index=False, compression='gzip', sep='\t')
      2 pd.DataFrame(valid).to_csv("Data/leishmaniasis_valid.csv.gz",␣
 ↪index=False, compression='gzip', sep='\t')
      3 pd.DataFrame(test).to_csv("Data/leishmaniasis_test.csv.gz", index=False␣
 ↪compression='gzip', sep='\t')
```

```
NameError: name 'train' is not defined
```

[12]:
```
train_dataset = MolGraphDataset('Data/leishmaniasis_train.csv.gz')
train_dataloader = DataLoader(train_dataset, batch_size=64, shuffle=True,␣
↪collate_fn=molgraph_collate_fn)
validation_dataset = MolGraphDataset('Data/leishmaniasis_valid.csv.gz')
validation_dataloader = DataLoader(validation_dataset, batch_size=64,␣
↪collate_fn=molgraph_collate_fn)
test_dataset = MolGraphDataset('Data/leishmaniasis_test.csv.gz')
test_dataloader = DataLoader(test_dataset, batch_size=64,␣
↪collate_fn=molgraph_collate_fn)
```

[13]:
```
# ((sample_adjacency, sample_nodes, sample_edges), sample_target) =␣
↪train_dataset[0]

# net = EMNN.gnn.emn_implementations.
↪EMNImplementation(node_features=len(sample_nodes[0]),
#                                                  ␣
↪edge_features=len(sample_edges[0, 0]),
#                                                  ␣
↪out_features=len(sample_target),
#                                                   message_passes=5,␣
↪edge_embedding_size=30,
#                                                   edge_emb_depth=2,␣
↪edge_emb_hidden_dim=60,
#                                                   edge_emb_dropout_p=0.0,␣
↪att_depth=2, att_hidden_dim=50,
#                                                   att_dropout_p=0.0,␣
↪msg_depth=2, msg_hidden_dim=50,
#                                                   msg_dropout_p=0.0,␣
↪gather_width=30, gather_att_depth=2,
#                                                   gather_att_hidden_dim=15,␣
↪gather_att_dropout_p=0.0,
#                                                   gather_emb_depth=2,␣
↪gather_emb_hidden_dim=15,
#                                                   gather_emb_dropout_p=0.0,␣
↪out_depth=2, out_hidden_dim=360,
#                                                   out_dropout_p=0.1,␣
↪out_layer_shrinkage=0.6)

# if True:
#     net = net.cuda()

# optimizer = optim.Adam(net.parameters(), lr=1e-4)
# criterion = nn.MSELoss()
```

[14]:
```
((sample_adjacency, sample_nodes, sample_edges), sample_target) =␣
↪train_dataset[0]

net = EMNN.gnn.emn_implementations.
↪EMNImplementation(node_features=len(sample_nodes[0]),
                                                    ␣
↪edge_features=len(sample_edges[0, 0]),
                                                     out_features=len(sample_target),
                                                     message_passes=8,␣
↪edge_embedding_size=50,
                                                     edge_emb_depth=2,␣
↪edge_emb_hidden_dim=150,
                                                     edge_emb_dropout_p=0.0,␣
↪att_depth=2, att_hidden_dim=85,
                                                     att_dropout_p=0.0, msg_depth=2,␣
↪msg_hidden_dim=150,
                                                     msg_dropout_p=0.0,␣
↪gather_width=45, gather_att_depth=2,
                                                     gather_att_hidden_dim=45,␣
↪gather_att_dropout_p=0.0,
                                                     gather_emb_depth=2,␣
↪gather_emb_hidden_dim=45,
                                                     gather_emb_dropout_p=0.0,␣
↪out_depth=2, out_hidden_dim=450,
                                                     out_dropout_p=0.1,␣
↪out_layer_shrinkage=0.6)

if True:
    net = net.cuda()

optimizer = optim.Adam(net.parameters(), lr=1e-4)
criterion = nn.MSELoss()
```

[15]:
```
SAVEDMODELS_DIR = "EMNN/savedmodels/"
def evaluate_net(net, train_dataloader, validation_dataloader, test_dataloader,␣
↪criterion):
    global evaluate_called
    global DATETIME_STR
    global best_mean_train_score
    global best_mean_validation_score
    global best_mean_test_score
    global train_subset_loader

    if not evaluate_called:
        evaluate_called = True
```

```
        best_mean_train_score, best_mean_validation_score, best_mean_test_score␣
↪= 10, 10, 10
        train_subset_loader = train_dataloader

    train_output, train_loss, train_target = feed_net(net, train_subset_loader,␣
↪criterion, True)
    validation_output, validation_loss, validation_target = feed_net(net,␣
↪validation_dataloader, criterion, True)
    test_output, test_loss, test_target = feed_net(net, test_dataloader,␣
↪criterion, True)

    train_scores = compute_mse(train_output, train_target)
    train_mean_score = np.nanmean(train_scores)
    validation_scores = compute_mse(validation_output, validation_target)
    validation_mean_score = np.nanmean(validation_scores)
    test_scores = compute_mse(test_output, test_target)
    test_mean_score = np.nanmean(test_scores)

    new_best_model_found = validation_mean_score < best_mean_validation_score

    if new_best_model_found:
        best_mean_train_score = train_mean_score
        best_mean_validation_score = validation_mean_score
        best_mean_test_score = test_mean_score

        path = SAVEDMODELS_DIR + type(net).__name__ + DATETIME_STR
        torch.save(net, path)

    target_names = train_dataloader.dataset.target_names
    return {  # if made deeper, tensorboardx writing breaks I think
        'loss': {'train': train_loss, 'test': test_loss},
        'mean {}'.format("MSE"):
            {'train': train_mean_score, 'validation': validation_mean_score,␣
↪'test': test_mean_score},
        'train {}s'.format("MSE"): {target_names[i]: train_scores[i] for i in␣
↪range(len(target_names))},
        'test {}s'.format("MSE"): {target_names[i]: test_scores[i] for i in␣
↪range(len(target_names))},
        'best mean {}'.format("MSE"):
            {'train': best_mean_train_score, 'validation':␣
↪best_mean_validation_score, 'test': best_mean_test_score}
    }
```

[16]:
```
def less_log(net, train_dataloader, validation_dataloader, test_dataloader,␣
↪criterion, epoch):
```

```
    scalars = evaluate_net(net, train_dataloader, validation_dataloader,␣
 ↪test_dataloader, criterion)
    mean_score_key = 'mean {}'.format("MSE")
    print('epoch {}, training mean {}: {}, validation mean {}: {}, testing mean␣
 ↪{}: {}'.format(
          epoch + 1,
          "MSE", scalars[mean_score_key]['train'],
          "MSE", scalars[mean_score_key]['validation'],
          "MSE", scalars[mean_score_key]['test'])
    )
```

[ ]:
```
evaluate_called = False
best_mean_train_score, best_mean_validation_score, best_mean_test_score = 10,␣
 ↪10, 10
train_subset_loader = None
DATETIME_STR = datetime.datetime.now().strftime('%Y-%m-%d %H:%M:%S.%f')

for epoch in range(15):
    net.train()
    for i_batch, batch in enumerate(train_dataloader):

        if True:
            batch = [tensor.cuda() for tensor in batch]
        adjacency, nodes, edges, target = batch

        optimizer.zero_grad()
        output = net(adjacency, nodes, edges)
        loss = criterion(output, target)
        loss.backward()
        torch.nn.utils.clip_grad_value_(net.parameters(), 5.0)
        optimizer.step()

    with torch.no_grad():
        net.eval()
        less_log(net, train_dataloader, validation_dataloader, test_dataloader,␣
 ↪criterion, epoch)
```

```
epoch 1, training mean MSE: 0.5146155953407288, validation mean MSE:
0.5127953290939331, testing mean MSE: 0.5301437973976135
epoch 2, training mean MSE: 0.6003549098968506, validation mean MSE:
0.6008053421974182, testing mean MSE: 0.617516279220581
epoch 3, training mean MSE: 0.610195517539978, validation mean MSE:
0.6104124188423157, testing mean MSE: 0.6281699538230896
```

[ ]:
```
def predict(test_set):
    with torch.no_grad():
        #Change this path to predict using different trained models
```

```
        net = torch.load("EMNN/savedmodels/EMNImplementation2020-10-20 16:54:38.
↪320439")
        if True:
            net = net.cuda()
        else:
            net = net.cpu()
        net.eval()

        dataset = MolGraphDataset(test_set, prediction=True)
        dataloader = DataLoader(dataset, batch_size=50,␣
↪collate_fn=molgraph_collate_fn)

        batch_outputs = []
        for i_batch, batch in enumerate(dataloader):
            if True:
                batch = [tensor.cuda() for tensor in batch]
            adjacency, nodes, edges, target = batch
            batch_output = net(adjacency, nodes, edges)
            batch_outputs.append(batch_output)

        output = torch.cat(batch_outputs).cpu().numpy()

        df = pd.read_csv(test_set)

        df.insert(1, 'value_scaled', output, True)

        return df
```

[166]:
```
drug_c.info()
```

```
<class 'modin.pandas.dataframe.DataFrame'>
RangeIndex: 4052 entries, 0 to 4051
Data columns (total 7 columns):
 #   Column      Non-Null Count  Dtype
---  ----------  --------------  -----
 0   Unnamed: 0  4052 non-null   int64
 1   SMILES      4052 non-null   object
 2   InChI       4052 non-null   object
 3   InChIKey    4052 non-null   object
 4   ID          4052 non-null   int64
 5   INN         4052 non-null   object
 6   CAS_RN      4050 non-null   object
dtypes: object(5), int64(2)
memory usage: 221.7 KB
```

[26]:
```
in_trails_smiles= in_trails.copy()
drug_c_smiles = drug_c.copy()
```

```
endogenous_smiles = endogenous.copy()
world_smiles = world.copy()
```

[27]:
```
in_trails_smiles = in_trails_smiles.drop(columns = "zinc_id")
drug_c_smiles = drug_c_smiles.drop(['InChI', 'INN','Unnamed:␣
↪0','ID','CAS_RN','InChIKey'], axis = 1)
endogenous_smiles = endogenous_smiles.drop(columns = "zinc_id")
world_smiles = world_smiles.drop(columns = "zinc_id")
```

[28]:
```
in_trails_smiles.insert(0, 'empty', [None]*len(in_trails_smiles), True)
drug_c_smiles.insert(0, 'empty', [None]*len(drug_c_smiles), True)
endogenous_smiles.insert(0, 'empty', [None]*len(endogenous_smiles), True)
world_smiles.insert(0, 'empty', [None]*len(world_smiles), True)
```

[29]:
```
in_trails_smiles[["empty","smiles"]].to_csv("Data/in_trails_smiles.csv.gz"
                                            , index=False, compression='gzip',␣
↪sep='\t')

drug_c_smiles[["empty","SMILES"]].to_csv("Data/drug_c_smiles.csv.gz"
                                            , index=False, compression='gzip',␣
↪sep='\t')

endogenous_smiles[["empty","smiles"]].to_csv("Data/endogenous_smiles.csv.gz"
                                            , index=False, compression='gzip',␣
↪sep='\t')

world_smiles[["empty","smiles"]].to_csv("Data/world_smiles.csv.gz"
                                            , index=False, compression='gzip',␣
↪sep='\t')
```

[119]:
```
predictions_in_trails = predict("Data/in_trails_smiles.csv.gz")
predictions_drug_c = predict("Data/drug_c_smiles.csv.gz")
predictions_endogenous = predict("Data/endogenous_smiles.csv.gz")
predictions_world = predict("Data/world_smiles.csv.gz")
```

[120]:
```
predictions
```

[120]:

	empty\tsmiles	value_scaled
0	\tO=P(=O)O	[-0.06922221]
1	\tCOc1cccc2c1[C@@H]1CN(CCCCn3c(O)nc4c(sc5ncc(-…	[-0.0641703]
2	\tCN(C)c1cc(CNCC(C)(C)C)c(O)c2c1C[C@H]1C[C@H]3…	[-0.0037107468]
3	\tCN(C)c1cc(CNCC(C)(C)C)c(O)c2c1C[C@H]1C[C@H]3…	[-0.0037107468]
4	\tCN(C)c1cc(CNCC(C)(C)C)c(O)c2c1C[C@H]1C[C@H]3…	[-0.0037107468]
…	…	…
9795	\tO=C1CC2(CCCC2)CC(=O)N1CCNC[C@H]1COc2ccccc2O1	[0.14398]
9796	\tCCCCCCCCCCOc1ccc2[nH]cc(CCN)c2c1	[0.0023374557]
9797	\tCOc1cc2c(cc1OC)[C@@]13CCN4CC5=CCO[C@H]6CC(=O…	[0.09909004]

```
9798              \tCOc1ccc([C@H]2CNC(=O)C2)cc1OC1CCCC1    [-0.017078549]
9799            \tCCOC(=O)c1ccc(OC(=O)CCCCCNC(=N)N)cc1      [0.24858287]

[9800 rows x 2 columns]
```

[121]:
```
predictions.sort_values("value_scaled", ascending=False)
```

[121]:
```
                                                 empty\tsmiles   value_scaled
3612         \tCCCCCCCCCCCCCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCO     [1.0734531]
6675  \tO=S(=O)(O)OC[C@H]1O[C@@H](O[C@@]2(COS(=O)(=O…    [0.95221484]
7543  \tO=S(=O)(O)OC[C@H]1O[C@@H](O[C@]2(COS(=O)(=O)…    [0.95221484]
1570  \tCCCCCCCCC/C=C\CCCCCCCC(=O)OCC(COC(=O)CCCCCCC/…    [0.93222225]
6738  \tCCCCCCCCC/C=C\CCCCCCCC(=O)OC[C@@H](OC(=O)CCCC…     [0.8744521]
…                                                   …            …
4365             \tOC[C@H](O)[C@H](O)[C@@H](O)[C@H](O)CO   [-0.47302383]
6975           \tOC[C@H](O)[C@H](O)[C@@H](O)[C@@H](O)CO   [-0.47302383]
7277           \tOC[C@@H](O)[C@@H](O)[C@H](O)[C@H](O)CO   [-0.47302392]
3673             \tOC[C@H](O)[C@@H](O)[C@H](O)[C@H](O)CO   [-0.47302392]
4471  \tOCC(CO)N[C@H]1C[C@](O)(CO)[C@@H](O)[C@H](O)[…   [-0.51762724]

[9800 rows x 2 columns]
```

[123]:
```
best_predicted = predictions[["empty\tsmiles"]].values[:10,0]
```

[124]:
```
best_predicted = [best_predicted[i][1:] for i in range(len(best_predicted))]
```

[125]:
```
best_predicted
```

[125]:
```
['O=P(=O)O',
 'COc1cccc2c1[C@@H]1CN(CCCCn3c(O)nc4c(sc5ncc(-c6ccccc6)nc54)c3=O)C[C@@H]1CO2',
 'CN(C)c1cc(CNCC(C)(C)C)c(O)c2c1C[C@H]1C[C@H]3[C@H](N(C)C)C(=O)[C@H](C(N)=O)C(=O
)[C@@]3(O)C(=O)[C@H]1C2=O',
 'CN(C)c1cc(CNCC(C)(C)C)c(O)c2c1C[C@H]1C[C@H]3[C@H](N(C)C)C(=O)[C@@H](C(N)=O)C(=
O)[C@@]3(O)C(=O)[C@@H]1C2=O',
 'CN(C)c1cc(CNCC(C)(C)C)c(O)c2c1C[C@H]1C[C@H]3[C@H](N(C)C)C(=O)[C@@H](C(N)=O)C(=
O)[C@@]3(O)C(=O)[C@H]1C2=O',
 'Cc1ccc2c(n1)Oc1ccc([C@@H](C)C(=O)OCC(=O)N(C)C)cc1C2',
 'CN(C)c1cc(CNCC(C)(C)C)c(O)c2c1C[C@H]1C[C@H]3[C@H](N(C)C)C(=O)[C@H](C(N)=O)C(=O
)[C@@]3(O)C(=O)[C@@H]1C2=O',
 'CCOc1cc(N)c(Cl)cc1C(=O)NC[C@@H]1CN(Cc2ccc(F)cc2)CCO1',
 'CCOc1cc(N)c(Cl)cc1C(=O)NC[C@H]1CN(Cc2ccc(F)cc2)CCO1',
 'CC(=O)C(=Cc1cc(O)c(O)c([N+](=O)[O-])c1)C(C)=O']
```

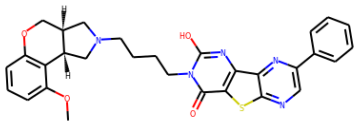
[126]:
```
import pickle
pickle.dump(best_predicted, open("Data/best_predicted_smiles.pkl", "wb"))
```

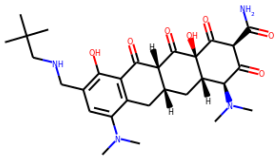
[127]:
```
best_predicted = pickle.load(open("Data/best_predicted_smiles.pkl", "rb"))
```

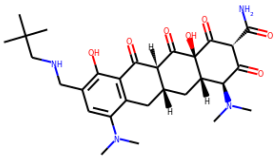
[128]:
```
import rdkit
from rdkit.Chem import AllChem as Chem
from rdkit.DataStructs import cDataStructs
best_predicted_mols = [Chem.MolFromSmiles(x) for x in best_predicted]
```

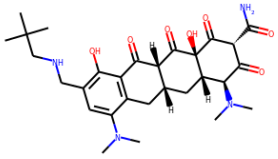
[129]:
```
rdkit.Chem.Draw.MolsToGridImage(best_predicted_mols, molsPerRow=2, maxMols=100,␣
↪subImgSize=(400, 400))
```

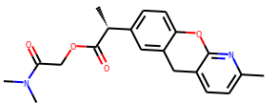
[129]:

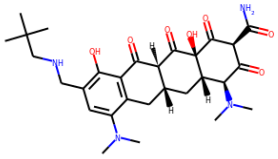


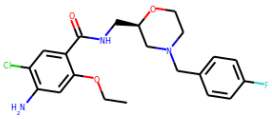


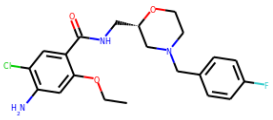


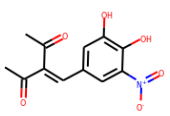












[ ]: