3DVisualization

May 13, 2024

1 Loading dependencies

[1]:
```
%pip install rdkit tensorrt py3Dmol
```

```
Requirement already satisfied: rdkit in /opt/conda/lib/python3.11/site-packages
(2023.9.6)
Requirement already satisfied: tensorrt in /opt/conda/lib/python3.11/site-
packages (10.0.1)
Requirement already satisfied: py3Dmol in /opt/conda/lib/python3.11/site-
packages (2.1.0)
Requirement already satisfied: numpy in /opt/conda/lib/python3.11/site-packages
(from rdkit) (1.26.4)
Requirement already satisfied: Pillow in /opt/conda/lib/python3.11/site-packages
(from rdkit) (10.2.0)
Requirement already satisfied: tensorrt-cu12 in /opt/conda/lib/python3.11/site-
packages (from tensorrt) (10.0.1)
Note: you may need to restart the kernel to use updated packages.
```

1.1 Get library

[2]:
```
# Normal Lib
import os
import numpy as np
from typing import cast
```

[3]:
```
# keras
from keras import Model
from keras.layers import Conv3D, Input, MaxPooling3D, BatchNormalization,␣
↪Dense, Dropout, Flatten,Activation, GlobalAveragePooling3D
import tensorflow as tf
import keras
```

```
2024-05-12 06:17:16.355246: I tensorflow/core/platform/cpu_feature_guard.cc:210]
This TensorFlow binary is optimized to use available CPU instructions in
performance-critical operations.
To enable the following instructions: AVX2 FMA, in other operations, rebuild
TensorFlow with the appropriate compiler flags.
2024-05-12 06:17:17.168338: W
```

```
tensorflow/compiler/tf2tensorrt/utils/py_utils.cc:38] TF-TRT Warning: Could not
find TensorRT
```

[4]:
```
print(tf.config.list_physical_devices('GPU'))
```

```
[PhysicalDevice(name='/physical_device:GPU:0', device_type='GPU')]
```

[5]:
```
import py3Dmol
```

[6]:
```
import csv
```

1.2 Get data and labels zip

[7]:
```
protein_folder = './protein'
protein_list = os.listdir(protein_folder)

ligand_folder = './ligand'
ligand_list = os.listdir(ligand_folder)

label_folder = './label'
label_list = os.listdir(label_folder)
```

[8]:
```
hit_Protein = './protein/3qzr.pdb'
```

[9]:
```
hitLead_Protein = './protein/5c1u.pdb'
```

[10]:
```
no_Protein = './protein/3qzr.pdb'
```

[11]:
```
# ligand_14748_path = os.path.join(ligand_folder, ligand_14748)
hitLead_Ligand = './ligand/5c1u-CR_model22.pdb'
```

[12]:
```
# ligand_14748_path = os.path.join(ligand_folder, ligand_14748)
hit_Ligand = './ligand/5c1u-GC376_model97.pdb'
```

[13]:
```
no_Ligand = './ligand/5c1u-FOPMC_model71.pdb'
```

[14]:
```
csv_path = './Final/CSV/resultSFCNN.csv'
```

[15]:
```
totalSize = len(ligand_list)
totalSize
```

[15]:
```
16786
```

[16]:
```
# Generate random array of integers from 0 to totalSize - 1
permu = np.random.RandomState(seed=69).permutation(totalSize)
```

[17]:
```
train_num, validate_num, test_num = 0,0,0
```

[18]:
```
iDataset_num = totalSize
ratio = (60,20,20)
```

[19]:
```
train_num = int(iDataset_num * (ratio[0]/ (ratio[0]+ratio[1]+ratio[2])))
# val_num = int(iDataset_num * (ratio[1]/ (ratio[0]+ratio[1]+ratio[2])))
# test_num = int(iDataset_num * (ratio[2]/ (ratio[0]+ratio[1]+ratio[2])))

val_num = 100
test_num = 500
last_num = 2000
```

[20]:
```
train_list_IDs = permu[:train_num]
val_list_IDs = permu[train_num:(train_num+val_num)]
test_list_IDs = permu[(train_num+val_num):(train_num+val_num+test_num)]
last_list_IDs = permu[(train_num+val_num+test_num):
 ↪(train_num+val_num+test_num+last_num)]
```

[21]:
```
train_list_IDs
```

[21]:
```
array([ 1592, 14669,  5474, …,  3035,  6871,  6499])
```

[22]:
```
datatset_path = './Final/CSV/dataset.csv'
```

1.3 Get features

[23]:
```
from utils.preprocessing import get_data_batch
```

1.4 Get metric

[24]:
```
from utils.evaluation import regression_metrics, classification_metric
```

1.5 Get Validate

[25]:
```
def model_val_dataset(val_dataset_idx, protein_folder, label_folder,␣
 ↪label_list, batch_size, save_path):
  dataset_len = len(val_dataset_idx)
  runs = dataset_len // batch_size
  last_batch = dataset_len - batch_size*runs
  model = keras.models.load_model(save_path+'.keras')
  # Casting model to keras model
  model = cast(keras.models.Model, model)

  ba_Actual, stat_Actual, ba_Pred, stat_Pred = [], [], [], []
  print("----------------------- Start ValDataset -----------------------")
  for i in range(int(runs+1)):
```

```
    print("Get dataset on batch "+str(i+1))
    # If it is not the last batch
    if i != runs+1:
      gridList, baList, statList = get_data_batch(val_dataset_idx,␣
↪protein_folder, ligand_folder, ligand_list, label_folder, label_list,␣
↪batch_size, i)
    else:
      gridList, baList, statList = get_data_batch(val_dataset_idx,␣
↪protein_folder, ligand_folder, ligand_list, label_folder, label_list,␣
↪last_batch, i)

    print("----------------------- Predict ValDataset -----------------------")
    result = model.predict(gridList, verbose=2)
    gridList = []
    pred_reg, pred_class = result

    baList = [value for value in baList.tolist()]
    statList = [value for value in statList.tolist()]


    pred_reg = [value[0] for value in pred_reg.tolist()]
    pred_class = [value[0] for value in pred_class.tolist()]

    if ba_Actual == []:
      ba_Actual = baList
      stat_Actual = statList
      ba_Pred = pred_reg
      stat_Pred = pred_class
    else:
      ba_Actual.extend(baList)
      stat_Actual.extend(statList)
      ba_Pred.extend(pred_reg)
      stat_Pred.extend(pred_class)

    baList, statList = [], []
  print(ba_Actual, ba_Pred)
  PearsonR, MSE = regression_metrics(ba_Actual, ba_Pred)
  print("------------------------------------------------------------")
  precision, recall, specificity, NPV, MCC = classification_metric(stat_Actual,␣
↪stat_Pred)
  return PearsonR, MSE, precision, recall, specificity, NPV, MCC, ba_Actual,␣
↪ba_Pred, stat_Actual, stat_Pred
```

1.6 Get Train

[26]:
```
def model_train_dataset(model: keras.Model, train_dataset_idx, protein_folder,␣
↪label_folder, label_list, batch_size, epochs, save_path: str, best_path):
  dataset_len = len(train_dataset_idx)
  runs = dataset_len // batch_size
  last_batch = dataset_len - batch_size*runs
  cur = 1
  # PearsonR, MSE, RMSE, precision, recall, auc, f1_score, MCC = 0,0,0,0,0,0,0,0
  # checkPearsonR, checkMCC, checkRMSE = 0,0,999
  log_txt = "log.txt"
  log_path = os.path.join(save_path, log_txt)
  readline = ''
  if os.path.exists(log_path):
    log_file = open(log_path,"r+")
    readline = log_file.readline()
    log_file.close()
  else:
    with open(log_path, 'w+') as f:
      f.write('0/'+str(runs))
      f.close()

  if readline == '' or int(readline.split('/')[0]) > runs or int(readline.
↪split('/')[0]) == 0:
    cur = 1
    model.save(save_path + '.keras')
  else:
    cur = int(readline.split('/')[0])

  check = 0

  print("---------------------- Start TrainDataset -----------------------")
  for i in range(int(cur-1),int(runs+1)):
    print("======================Batch "+␣
↪str(i+1)+"==============================")
    model = keras.models.load_model(save_path + '.keras') # type: ignore
    print("Get dataset")
    # get_data_batch(dataset_idx, protein_folder, ligand_folder, ligand_list,␣
↪label_folder, label_list, batch_size, index)
    # get_data_batch(train_list_IDs, protein_folder, ligand_folder,␣
↪ligand_list, label_folder, label_list, 32, 0)
    if i != runs+1:
      gridList, baList, statList = get_data_batch(train_dataset_idx,␣
↪protein_folder, ligand_folder, ligand_list, label_folder, label_list,␣
↪batch_size, i)
    else:
```

```
    gridList, baList, statList = get_data_batch(train_dataset_idx,␣
↪protein_folder, ligand_folder, ligand_list, label_folder, label_list,␣
↪last_batch, i)

    if len(gridList) == 0 or len(baList) == 0 or len(statList) == 0:
      raise ValueError(f'Empty List: gridList: {len(gridList)}, baList:␣
↪{len(baList)}, statList: {len(statList)}')
    print("----------------------- Train TrainDataset ------------------------")
    model.fit(gridList, [baList, statList], epochs= epochs,verbose=0)
    gridList, baList, statList = [], [], []
    # PearsonR, MSE, RMSE, precision, recall, auc, f1_score, MCC =␣
↪model_val_dataset(val_dataset_idx, protein_folder, label_folder, label_list,␣
↪batch_size, epochs, save_path, best_path)
    print("Save")
    model.save(save_path+'.keras')
    log_file = open(log_path,"r+")
    readline = log_file.write(str(i)+'/'+str(runs))
    log_file.close()
    # if PearsonR > checkPearsonR and MCC > checkMCC and RMSE < checkRMSE:
    #   model.save(best_path)
    #   checkPearsonR = PearsonR
    #   checkMCC = MCC
    #   checkRMSE = RMSE
    if check == 0 and batch_size*i >= 2000:
      check +=1
      model.save(best_path + '.keras')
  return model
```

1.7 Get Model

[27]:
```
def combine_embedding(drop_rate, input_shape= (52,52,52,11)):
  inp = Input(shape= input_shape, name='Input_Complexes')

  ## Check there are atoms
  x1 = Conv3D(filters= 8, kernel_size=(1,1,1), padding='same',␣
↪bias_initializer='zeros', kernel_initializer='glorot_uniform')(inp)
  x1 = BatchNormalization()(x1)
  x1 = Activation('relu')(x1)

  x1 = Conv3D(8, kernel_size=(3,3,3))(x1)
  x1 = BatchNormalization()(x1)
  x1 = Activation('relu')(x1)

  x1 = Conv3D(32,kernel_size=(3,3,3),padding='same')(x1)
  x1 = BatchNormalization()(x1)
  x1 = Activation('relu')(x1)
```

```
x1 = MaxPooling3D(pool_size=2)(x1)

x1 = Conv3D(64,kernel_size=(1,1,1),padding='same')(x1)
x1 = BatchNormalization()(x1)
x1 = Activation('relu')(x1)

x1 = Conv3D(64,kernel_size=(3,3,3),padding='same')(x1)
x1 = BatchNormalization()(x1)
x1 = Activation('relu')(x1)

x1 = MaxPooling3D(pool_size=2)(x1)

x1 = Conv3D(128,kernel_size=(1,1,1),padding='same')(x1)
x1 = BatchNormalization()(x1)
x1 = Activation('relu')(x1)

x1 = Conv3D(128,kernel_size=(3,3,3),padding='same')(x1)
x1 = BatchNormalization()(x1)
x1 = Activation('relu')(x1)
x1 = MaxPooling3D(pool_size=2)(x1)

x1 = Conv3D(256,kernel_size=(1,1,1),padding='same')(x1)
x1 = BatchNormalization()(x1)
x1 = Activation('relu')(x1)

x1 = Conv3D(256,kernel_size=(3,3,3),padding='same')(x1)
x1 = BatchNormalization()(x1)
x1 = Activation('relu')(x1)
x1 = MaxPooling3D(pool_size=2)(x1)

  # Global Pooling
x2 = GlobalAveragePooling3D()(x1)

x2 = Dense(256)(x2)
x2 = BatchNormalization()(x2)
x2 = Activation('relu')(x2)
x2 = Dropout(0.5)(x2)

# Flattening
x1 = Flatten()(x1)

x1 = Dense(256)(x1)
x1 = BatchNormalization()(x1)
x1 = Activation('relu')(x1)
x1 = Dropout(0.5)(x1)

# Regression Output
```

```
  d1 = Dense(1,kernel_regularizer=keras.regularizers.l2(0.01))(x1)
  # Classification Output
  d2 = Dense(1, activation='sigmoid')(x2)

  return Model(inputs=[inp], outputs=[d1,d2], name='Embedding')
```

1.8 Create model

[28]:
```
from utils.preprocessing import set_grid
fake_grid, x,y,z = set_grid('./protein/3qzq.pdb')
shape = np.shape(fake_grid)
shape
```

[28]: (52, 52, 52, 14)

[29]:
```
model = combine_embedding(0.5, shape)
model.summary()
```

```
2024-05-12 06:17:19.055664: I
tensorflow/core/common_runtime/gpu/gpu_device.cc:1928] Created device
/job:localhost/replica:0/task:0/device:GPU:0 with 10367 MB memory:  -> device:
0, name: NVIDIA GeForce RTX 3060, pci bus id: 0000:81:00.0, compute capability:
8.6
```

Model: "Embedding"

Layer (type)	Output Shape	Param #	Connected to
Input_Complexes (InputLayer)	(None, 52, 52, 52, 14)	0	-
conv3d (Conv3D)	(None, 52, 52, 52, 8)	120	Input_Complexes[…
batch_normalization (BatchNormalizatio…	(None, 52, 52, 52, 8)	32	conv3d[0][0]
activation (Activation)	(None, 52, 52, 52, 8)	0	batch_normalizat…
conv3d_1 (Conv3D)	(None, 50, 50, 50, 8)	1,736	activation[0][0]
batch_normalizatio… (BatchNormalizatio…	(None, 50, 50, 50, 8)	32	conv3d_1[0][0]

```
activation_1 (Activation)        (None, 50, 50, 50, 8)          0   batch_normalizat…

conv3d_2 (Conv3D)                (None, 50, 50, 50, 32)      6,944   activation_1[0][…

batch_normalizatio… (BatchNormalizatio…  (None, 50, 50, 50, 32)   128   conv3d_2[0][0]

activation_2 (Activation)        (None, 50, 50, 50, 32)         0   batch_normalizat…

max_pooling3d (MaxPooling3D)     (None, 25, 25, 25, 32)         0   activation_2[0][…

conv3d_3 (Conv3D)                (None, 25, 25, 25, 64)      2,112   max_pooling3d[0]…

batch_normalizatio… (BatchNormalizatio…  (None, 25, 25, 25, 64)   256   conv3d_3[0][0]

activation_3 (Activation)        (None, 25, 25, 25, 64)         0   batch_normalizat…

conv3d_4 (Conv3D)                (None, 25, 25, 25, 64)    110,656   activation_3[0][…

batch_normalizatio… (BatchNormalizatio…  (None, 25, 25, 25, 64)   256   conv3d_4[0][0]

activation_4 (Activation)        (None, 25, 25, 25, 64)         0   batch_normalizat…

max_pooling3d_1 (MaxPooling3D)   (None, 12, 12, 12, 64)         0   activation_4[0][…

conv3d_5 (Conv3D)                (None, 12, 12, 12, 128)     8,320   max_pooling3d_1[…

batch_normalizatio… (BatchNormalizatio…  (None, 12, 12, 12, 128)  512   conv3d_5[0][0]

activation_5 (Activation)        (None, 12, 12, 12, 128)        0   batch_normalizat…

conv3d_6 (Conv3D)                (None, 12, 12, 12, 128)   442,496   activation_5[0][…
```

batch_normalizatio… (BatchNormalizatio…	(None, 12, 12, 12, 128)	512	conv3d_6[0][0]
activation_6 (Activation)	(None, 12, 12, 12, 128)	0	batch_normalizat…
max_pooling3d_2 (MaxPooling3D)	(None, 6, 6, 6, 128)	0	activation_6[0][…
conv3d_7 (Conv3D)	(None, 6, 6, 6, 256)	33,024	max_pooling3d_2[…
batch_normalizatio… (BatchNormalizatio…	(None, 6, 6, 6, 256)	1,024	conv3d_7[0][0]
activation_7 (Activation)	(None, 6, 6, 6, 256)	0	batch_normalizat…
conv3d_8 (Conv3D)	(None, 6, 6, 6, 256)	1,769,728	activation_7[0][…
batch_normalizatio… (BatchNormalizatio…	(None, 6, 6, 6, 256)	1,024	conv3d_8[0][0]
activation_8 (Activation)	(None, 6, 6, 6, 256)	0	batch_normalizat…
max_pooling3d_3 (MaxPooling3D)	(None, 3, 3, 3, 256)	0	activation_8[0][…
flatten (Flatten)	(None, 6912)	0	max_pooling3d_3[…
global_average_poo… (GlobalAveragePool…	(None, 256)	0	max_pooling3d_3[…
dense_1 (Dense)	(None, 256)	1,769,728	flatten[0][0]
dense (Dense)	(None, 256)	65,792	global_average_p…
batch_normalizatio… (BatchNormalizatio…	(None, 256)	1,024	dense_1[0][0]
batch_normalizatio… (BatchNormalizatio…	(None, 256)	1,024	dense[0][0]
activation_10 (Activation)	(None, 256)	0	batch_normalizat…

```
activation_9          (None, 256)                 0   batch_normalizat…
(Activation)

dropout_1 (Dropout)   (None, 256)                 0   activation_10[0]…

dropout (Dropout)     (None, 256)                 0   activation_9[0][…

dense_2 (Dense)       (None, 1)                 257   dropout_1[0][0]

dense_3 (Dense)       (None, 1)                 257   dropout[0][0]


Total params: 4,216,994 (16.09 MB)

Trainable params: 4,214,082 (16.08 MB)

Non-trainable params: 2,912 (11.38 KB)
```

[30]:
```
optimizer=keras.optimizers.Adam(learning_rate=1e-4)

loss=['mean_squared_error', "binary_crossentropy"]
model.compile(optimizer= optimizer,
              loss= loss, run_eagerly=True)
```

1.9 Save paths

[31]:
```
save_path = './SFCNN/Model1'
best_path = './SFCNN/Best1'
```

1.10 Set hyperparameters

[32]:
```
batch_size = 32
epochs = 150
```

1.11 Train

[33]:
```
trained_model = model_train_dataset(model, train_list_IDs, protein_folder,␣
 ↪label_folder, label_list, batch_size, epochs, save_path, best_path)
```

```
---------------------- Start TrainDataset ----------------------
======================Batch 1==============================

/opt/conda/lib/python3.11/site-packages/keras/src/saving/saving_lib.py:396:
UserWarning: Skipping variable loading for optimizer 'adam', because it has 98
```

```
variables whereas the saved optimizer has 2 variables.
  trackable.load_own_variables(weights_store.get(inner_path))

Get dataset
---------------------- Train TrainDataset ----------------------

2024-05-12 06:17:27.244799: I
external/local_xla/xla/stream_executor/cuda/cuda_dnn.cc:465] Loaded cuDNN
version 8907

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======================Batch 2==============================
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---------------------- Train TrainDataset ----------------------
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2 New test

[34]:
```
model = cast(keras.models.Model, keras.models.load_model(save_path+'.keras'))
```

[35]:
```
model.summary()
```

```
Model: "Embedding"
```

Layer (type)	Output Shape	Param #	Connected to
Input_Complexes (InputLayer)	(None, 52, 52, 52, 14)	0	-
conv3d (Conv3D)	(None, 52, 52, 52, 8)	120	Input_Complexes[…
batch_normalization (BatchNormalizatio…	(None, 52, 52, 52, 8)	32	conv3d[0][0]
activation (Activation)	(None, 52, 52, 52, 8)	0	batch_normalizat…
conv3d_1 (Conv3D)	(None, 50, 50, 50, 8)	1,736	activation[0][0]
batch_normalizatio… (BatchNormalizatio…	(None, 50, 50, 50, 8)	32	conv3d_1[0][0]

```
activation_1          (None, 50, 50,              0   batch_normalizat…
(Activation)          50, 8)

conv3d_2 (Conv3D)     (None, 50, 50,          6,944   activation_1[0][…
                      50, 32)

batch_normalizatio…   (None, 50, 50,            128   conv3d_2[0][0]
(BatchNormalizatio…   50, 32)

activation_2          (None, 50, 50,              0   batch_normalizat…
(Activation)          50, 32)

max_pooling3d         (None, 25, 25,              0   activation_2[0][…
(MaxPooling3D)        25, 32)

conv3d_3 (Conv3D)     (None, 25, 25,          2,112   max_pooling3d[0]…
                      25, 64)

batch_normalizatio…   (None, 25, 25,            256   conv3d_3[0][0]
(BatchNormalizatio…   25, 64)

activation_3          (None, 25, 25,              0   batch_normalizat…
(Activation)          25, 64)

conv3d_4 (Conv3D)     (None, 25, 25,        110,656   activation_3[0][…
                      25, 64)

batch_normalizatio…   (None, 25, 25,            256   conv3d_4[0][0]
(BatchNormalizatio…   25, 64)

activation_4          (None, 25, 25,              0   batch_normalizat…
(Activation)          25, 64)

max_pooling3d_1       (None, 12, 12,              0   activation_4[0][…
(MaxPooling3D)        12, 64)

conv3d_5 (Conv3D)     (None, 12, 12,          8,320   max_pooling3d_1[…
                      12, 128)

batch_normalizatio…   (None, 12, 12,            512   conv3d_5[0][0]
(BatchNormalizatio…   12, 128)

activation_5          (None, 12, 12,              0   batch_normalizat…
(Activation)          12, 128)

conv3d_6 (Conv3D)     (None, 12, 12,        442,496   activation_5[0][…
                      12, 128)
```

batch_normalizatio… (BatchNormalizatio…	(None, 12, 12, 12, 128)	512	conv3d_6[0][0]
activation_6 (Activation)	(None, 12, 12, 12, 128)	0	batch_normalizat…
max_pooling3d_2 (MaxPooling3D)	(None, 6, 6, 6, 128)	0	activation_6[0][…
conv3d_7 (Conv3D)	(None, 6, 6, 6, 256)	33,024	max_pooling3d_2[…
batch_normalizatio… (BatchNormalizatio…	(None, 6, 6, 6, 256)	1,024	conv3d_7[0][0]
activation_7 (Activation)	(None, 6, 6, 6, 256)	0	batch_normalizat…
conv3d_8 (Conv3D)	(None, 6, 6, 6, 256)	1,769,728	activation_7[0][…
batch_normalizatio… (BatchNormalizatio…	(None, 6, 6, 6, 256)	1,024	conv3d_8[0][0]
activation_8 (Activation)	(None, 6, 6, 6, 256)	0	batch_normalizat…
max_pooling3d_3 (MaxPooling3D)	(None, 3, 3, 3, 256)	0	activation_8[0][…
flatten (Flatten)	(None, 6912)	0	max_pooling3d_3[…
global_average_poo… (GlobalAveragePool…	(None, 256)	0	max_pooling3d_3[…
dense_1 (Dense)	(None, 256)	1,769,728	flatten[0][0]
dense (Dense)	(None, 256)	65,792	global_average_p…
batch_normalizatio… (BatchNormalizatio…	(None, 256)	1,024	dense_1[0][0]
batch_normalizatio… (BatchNormalizatio…	(None, 256)	1,024	dense[0][0]
activation_10 (Activation)	(None, 256)	0	batch_normalizat…

```
activation_9 (Activation)        (None, 256)                0   batch_normalizat…

dropout_1 (Dropout)              (None, 256)                0   activation_10[0]…

dropout (Dropout)                (None, 256)                0   activation_9[0][…

dense_2 (Dense)                  (None, 1)                257   dropout_1[0][0]

dense_3 (Dense)                  (None, 1)                257   dropout[0][0]


Total params: 12,645,160 (48.24 MB)

Trainable params: 4,214,082 (16.08 MB)

Non-trainable params: 2,912 (11.38 KB)

Optimizer params: 8,428,166 (32.15 MB)
```

[36]:
```
test1_list_IDs = permu[12000:12100]
```

[37]:
```
PearsonR, MSE, precision, recall, specificity, NPV, MCC, ba_Actual, ba_Pred,␣
↪stat_Actual, stat_Pred = model_val_dataset(val_list_IDs, protein_folder,␣
↪label_folder, label_list, batch_size, save_path)
```

```
---------------------- Start ValDataset ----------------------
Get dataset on batch 1
---------------------- Predict ValDataset ----------------------
1/1 - 0s - 279ms/step
Get dataset on batch 2
---------------------- Predict ValDataset ----------------------
1/1 - 0s - 276ms/step
Get dataset on batch 3
---------------------- Predict ValDataset ----------------------
1/1 - 0s - 275ms/step
Get dataset on batch 4
---------------------- Predict ValDataset ----------------------
1/1 - 1s - 781ms/step
[-6.2, -6.5, -5.9, -6.7, -7.2, -6.4, -5.9, -6.3, -6.7, -6.0, -6.4, -7.1, -6.2,
-7.5, -6.9, -7.3, -6.9, -7.3, -6.3, -6.8, -7.1, -6.2, -7.0, -6.8, -6.7, -7.6,
-7.5, -6.3, -6.7, -6.3, -7.9, -7.4, -6.4, -5.8, -7.1, -6.5, -6.9, -6.7, -7.1,
-6.3, -6.7, -6.6, -5.9, -7.1, -6.3, -6.7, -6.5, -7.2, -5.8, -8.1, -7.7, -6.4,
-7.4, -7.0, -6.5, -6.1, -7.0, -6.4, -7.1, -6.4, -7.0, -7.0, -6.2, -6.6, -6.3,
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-6.1, -6.6, -6.7, -6.1, -7.0, -7.2, -6.6, -7.6, -6.6, -6.2, -7.7, -6.4, -7.2,
-6.8, -6.9, -7.5, -7.2, -6.0, -6.6, -6.2, -6.2, -6.9, -6.8, -7.3, -7.0, -7.7,
-7.2, -7.5, -7.2, -7.6, -6.4, -7.2, -6.3, -6.2, -7.0] [-7.5687665939331055,
-6.028539657592773, -7.235199928283691, -7.5687665939331055, -6.280409812927246,
-6.854605674743652, -5.382704734802246, -5.382704734802246, -6.901060104370117,
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-7.027408599853516, -7.011621475219727, -6.293680191040039, -6.854605674743652,
-6.177022933959961, -7.235199928283691, -7.5687665939331055, -7.027408599853516,
-6.2170000076293945, -7.011621475219727, -7.235199928283691, -7.011621475219727,
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++++++++++++++++++++++++++Regression++++++++++++++++++++++++++
Pearson Correlation Coefficient: 0.0705369693363294
Mean Absolute Error: 0.62199855
------------------------------------------------------------
+++++++++++++++++++++Classification++++++++++++++++++++++
TP Result: 29.0
FP Result: 7.0
Precision: 0.8055556
Recall: 0.50877196
Specificity: 0.8372093
NPV: 0.5625
Phi coefficient:0.3568477471006598
```

[38]:
```
PearsonR, MSE, precision, recall, specificity, NPV, MCC, ba_Actual, ba_Pred,␣
↪stat_Actual, stat_Pred = model_val_dataset(test_list_IDs, protein_folder,␣
↪label_folder, label_list, batch_size, save_path)
```

```
---------------------- Start ValDataset -----------------------
Get dataset on batch 1
```

```
---------------------- Predict ValDataset ----------------------
1/1 - 0s - 279ms/step
Get dataset on batch 2
---------------------- Predict ValDataset ----------------------
1/1 - 0s - 276ms/step
Get dataset on batch 3
---------------------- Predict ValDataset ----------------------
1/1 - 0s - 275ms/step
Get dataset on batch 4
---------------------- Predict ValDataset ----------------------
1/1 - 0s - 275ms/step
Get dataset on batch 5
---------------------- Predict ValDataset ----------------------
1/1 - 0s - 281ms/step
Get dataset on batch 6
---------------------- Predict ValDataset ----------------------
1/1 - 0s - 277ms/step
Get dataset on batch 7
---------------------- Predict ValDataset ----------------------
1/1 - 0s - 275ms/step
Get dataset on batch 8
---------------------- Predict ValDataset ----------------------
1/1 - 0s - 278ms/step
Get dataset on batch 9
---------------------- Predict ValDataset ----------------------
1/1 - 0s - 274ms/step
Get dataset on batch 10
---------------------- Predict ValDataset ----------------------
1/1 - 0s - 280ms/step
Get dataset on batch 11
---------------------- Predict ValDataset ----------------------
1/1 - 0s - 279ms/step
Get dataset on batch 12
---------------------- Predict ValDataset ----------------------
1/1 - 0s - 280ms/step
Get dataset on batch 13
---------------------- Predict ValDataset ----------------------
1/1 - 0s - 278ms/step
Get dataset on batch 14
---------------------- Predict ValDataset ----------------------
1/1 - 0s - 276ms/step
Get dataset on batch 15
---------------------- Predict ValDataset ----------------------
1/1 - 0s - 277ms/step
Get dataset on batch 16
---------------------- Predict ValDataset ----------------------
1/1 - 3s - 3s/step
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-7.5687761306762695, -7.235220909118652, -7.027400970458984, -7.011674880981445]
++++++++++++++++++++++++++Regression++++++++++++++++++++++++++
Pearson Correlation Coefficient: 0.24535654491605263
Mean Absolute Error: 0.6146272
------------------------------------------------------------
++++++++++++++++++++++Classification++++++++++++++++++++++
TP Result: 121.0
FP Result: 26.0
Precision: 0.82312924
Recall: 0.44485295
Specificity: 0.88596493
NPV: 0.57223797
Phi coefficient:0.3616552637712131
```

Save the result into csv files

[39]:
```python
def to_csv(rows, fields, path):
    with open(path, 'w') as csvfile:
        # creating a csv writer object
        csvwriter = csv.writer(csvfile)

        # writing the fields
        csvwriter.writerow(fields)

        # writing the data rows
        csvwriter.writerows(rows)
```

[40]:
```
def prediction_preprocessing(_val_list_IDs):
    rows = []
    for idx, value in enumerate(_val_list_IDs):
        row = []
        row.append(ligand_list[value])
        row.append(stat_Actual[idx])
        row.append(stat_Pred[idx])
        row.append(ba_Actual[idx])
        row.append(ba_Pred[idx])
        # row = (ligand_list[value], stat_Actual[idx], stat_Pred[idx],␣
 ↪ba_Actual[idx], ba_Pred[idx])
        # print(type(row))
        rows.append(row)
    print("Rows:", len(rows))
    return rows

def protein_ligand_preprocessing(input_list):
    rows = []
    for idx, value in enumerate(input_list):
        row = []
        row.append(idx+1)
        ligand = ligand_list[value]
        pro = ligand.split('-')[0]
        protein = [value for value in protein_list if pro in value][0]
        protein_name = protein.split('.')[0]
        ligand_name = ligand.split('.')[0]
        row.append(protein_name)
        row.append(ligand_name)

        rows.append(row)
    print("Rows:", len(rows))
    return rows
```

[41]:
```
# Write Model', 'Hit_Label', 'Hit_Prediction', 'BindingAffinity_Label',␣
 ↪'BindingAffinity_Prediction -> resultSFCNN.csv
to_csv(
    prediction_preprocessing(val_list_IDs),
    fields = ['Model', 'Hit_Label', 'Hit_Prediction', 'BindingAffinity_Label',␣
 ↪'BindingAffinity_Prediction'],
    path = csv_path
)
```

```
Rows: 100
```

[42]:
```
to_csv(
    protein_ligand_preprocessing(test1_list_IDs),
    fields = ['Model', 'Protein', 'Ligand'],
```

```
    path = datatset_path
)
```

```
Rows: 100
```

3 Draw

[43]:
```
view = py3Dmol.view()
view.removeAllModels()
view.setViewStyle({'style':'outline','color':'black','width':0.1})

view.addModel(open(hitLead_Protein,'r').read(),format='pdb')
Prot=view.getModel()
Prot.setStyle({'cartoon':{'arrows':True, 'tubes':True, 'style':'oval', 'color':
 ↪'white'}})
view.addSurface(py3Dmol.VDW,{'opacity':0.8,'color':'white'})


view.addModel(open(hitLead_Ligand,'r').read(),format='mol2')
ref_m1 = view.getModel()
ref_m1.setStyle({},{'stick':{'colorscheme':'redCarbon','radius':0.2}})

view.addModel(open(hit_Ligand,'r').read(),format='mol2')
ref_m2 = view.getModel()
ref_m2.setStyle({},{'stick':{'colorscheme':'blueCarbon','radius':0.2}})

view.addModel(open(no_Ligand,'r').read(),format='mol2')
ref_m3 = view.getModel()
ref_m3.setStyle({},{'stick':{'colorscheme':'yellowCarbon','radius':0.2}})

# ref_m.setStyle({},{'cartoon':{'arrows':True, 'tubes':True, 'style':'oval',␣
 ↪'color':'red'}})
# ref_m.setStyle({'cartoon':{'arrows':True, 'tubes':True, 'style':'oval',␣
 ↪'color':'red'}})


# results=Chem.SDMolSupplier('1AZ8_lig_vina_out.sdf')

# p=Chem.MolToMolBlock(results[0],False)

# print('Reference: Magenta | Vina Pose: Cyan')
# print ('Pose: {} | Score: {}'.format(results[0].GetProp('Pose'),results[0].
 ↪GetProp('Score')))

# view.addModel(p,'mol')
# x = view.getModel()
```

```
# x.setStyle({},{'stick':{'colorscheme':'cyanCarbon','radius':0.2}})

view.zoomTo()
view.show()
```

[44]:
```
view = py3Dmol.view()
view.removeAllModels()
view.setViewStyle({'style':'outline','color':'black','width':0.1})

# view.addModel(open(hitLead_Protein,'r').read(),format='pdb')
# Prot=view.getModel()
# Prot.setStyle({'cartoon':{'arrows':True, 'tubes':True, 'style':'oval',␣
 ↪'color':'white'}})
# view.addSurface(py3Dmol.VDW,{'opacity':0.8,'color':'white'})


view.addModel(open(hitLead_Ligand,'r').read(),format='mol2')
ref_m = view.getModel()
ref_m.setStyle({},{'stick':{'colorscheme':'magentaCarbon','radius':0.2}})
# ref_m.setStyle({},{'cartoon':{'arrows':True, 'tubes':True, 'style':'oval',␣
 ↪'color':'red'}})
# ref_m.setStyle({'cartoon':{'arrows':True, 'tubes':True, 'style':'oval',␣
 ↪'color':'red'}})


# results=Chem.SDMolSupplier('1AZ8_lig_vina_out.sdf')

# p=Chem.MolToMolBlock(results[0],False)

# print('Reference: Magenta | Vina Pose: Cyan')
# print ('Pose: {} | Score: {}'.format(results[0].GetProp('Pose'),results[0].
 ↪GetProp('Score')))

# view.addModel(p,'mol')
# x = view.getModel()
# x.setStyle({},{'stick':{'colorscheme':'cyanCarbon','radius':0.2}})

view.zoomTo()
view.show()
```

[45]:
```
view = py3Dmol.view()
view.removeAllModels()
view.setViewStyle({'style':'outline','color':'black','width':0.1})

view.addModel(open(hitLead_Protein,'r').read(),format='pdb')
Prot=view.getModel()
```

```
Prot.setStyle({'cartoon':{'arrows':True, 'tubes':True, 'style':'oval', 'color':
 ↪'white'}})
view.addSurface(py3Dmol.VDW,{'opacity':0.8,'color':'white'})


view.addModel(open(hitLead_Ligand,'r').read(),format='mol2')
ref_m = view.getModel()
ref_m.setStyle({},{'stick':{'colorscheme':'magentaCarbon','radius':0.2}})
# ref_m.setStyle({},{'cartoon':{'arrows':True, 'tubes':True, 'style':'oval',␣
 ↪'color':'red'}})
# ref_m.setStyle({'cartoon':{'arrows':True, 'tubes':True, 'style':'oval',␣
 ↪'color':'red'}})


# results=Chem.SDMolSupplier('1AZ8_lig_vina_out.sdf')

# p=Chem.MolToMolBlock(results[0],False)

# print('Reference: Magenta | Vina Pose: Cyan')
# print ('Pose: {} | Score: {}'.format(results[0].GetProp('Pose'),results[0].
 ↪GetProp('Score')))

# view.addModel(p,'mol')
# x = view.getModel()
# x.setStyle({},{'stick':{'colorscheme':'cyanCarbon','radius':0.2}})

view.zoomTo()
view.show()
```

[46]:
```
view = py3Dmol.view()
view.removeAllModels()
view.setViewStyle({'style':'outline','color':'black','width':0.1})

view.addModel(open(hit_Protein,'r').read(),format='pdb')
Prot=view.getModel()
Prot.setStyle({'cartoon':{'arrows':True, 'tubes':True, 'style':'oval', 'color':
 ↪'white'}})
view.addSurface(py3Dmol.VDW,{'opacity':0.8,'color':'white'})


view.addModel(open(hit_Ligand,'r').read(),format='mol2')
ref_m = view.getModel()
ref_m.setStyle({},{'stick':{'colorscheme':'magentaCarbon','radius':0.2}})
# ref_m.setStyle({},{'cartoon':{'arrows':True, 'tubes':True, 'style':'oval',␣
 ↪'color':'red'}})
```

```
# ref_m.setStyle({'cartoon':{'arrows':True, 'tubes':True, 'style':'oval',␣
 ↪'color':'red'}})


# results=Chem.SDMolSupplier('1AZ8_lig_vina_out.sdf')

# p=Chem.MolToMolBlock(results[0],False)

# print('Reference: Magenta | Vina Pose: Cyan')
# print ('Pose: {} | Score: {}'.format(results[0].GetProp('Pose'),results[0].
 ↪GetProp('Score')))

# view.addModel(p,'mol')
# x = view.getModel()
# x.setStyle({},{'stick':{'colorscheme':'cyanCarbon','radius':0.2}})

view.zoomTo()
view.show()
```

[47]:
```
view = py3Dmol.view()
view.removeAllModels()
view.setViewStyle({'style':'outline','color':'black','width':0.1})

view.addModel(open(no_Protein,'r').read(),format='pdb')
Prot=view.getModel()
Prot.setStyle({'cartoon':{'arrows':True, 'tubes':True, 'style':'oval', 'color':
 ↪'white'}})
view.addSurface(py3Dmol.VDW,{'opacity':0.8,'color':'white'})


view.addModel(open(no_Ligand,'r').read(),format='mol2')
ref_m = view.getModel()
ref_m.setStyle({},{'stick':{'colorscheme':'magentaCarbon','radius':0.2}})
# ref_m.setStyle({},{'cartoon':{'arrows':True, 'tubes':True, 'style':'oval',␣
 ↪'color':'red'}})
# ref_m.setStyle({'cartoon':{'arrows':True, 'tubes':True, 'style':'oval',␣
 ↪'color':'red'}})


# results=Chem.SDMolSupplier('1AZ8_lig_vina_out.sdf')

# p=Chem.MolToMolBlock(results[0],False)

# print('Reference: Magenta | Vina Pose: Cyan')
# print ('Pose: {} | Score: {}'.format(results[0].GetProp('Pose'),results[0].
 ↪GetProp('Score')))
```

```
# view.addModel(p,'mol')
# x = view.getModel()
# x.setStyle({},{'stick':{'colorscheme':'cyanCarbon','radius':0.2}})

view.zoomTo()
view.show()
```