AFP-ANN

def build\_model():

model = Sequential()

model.add(layers.Dense(200, input\_dim=512))

model.add(Dropout(0.3))

model.add(layers.Dense(100))

model.add(Dropout(0.3))

model.add(layers.Dense(50))

model.add(Dropout(0.3))

model.add(layers.Dense(1))

sgd = keras.optimizers.SGD(lr=0.0001)

model.compile(loss='mse',optimizer='sgd', metrics=['RootMeanSquaredError'])

return model

model=KerasRegressor(build\_fn=build\_model,epochs=150,batch\_size=256,verbose=0)

ECFP-ANN

def build\_model():

model = Sequential()

model.add(layers.Dense(100, input\_dim=1024))

model.add(Dropout(0.3))

model.add(layers.Dense(50))

model.add(Dropout(0.3))

model.add(layers.Dense(25))

model.add(Dropout(0.3))

model.add(layers.Dense(1))

sgd = keras.optimizers.SGD(lr=0.0001)

model.compile(loss='mse',optimizer='sgd', metrics=['RootMeanSquaredError'])

return model

model=KerasRegressor(build\_fn=build\_model,epochs=150,batch\_size=256,verbose=0)

model.fit(X\_train,y\_train,verbose=0)

MACCS-ANN

def build\_model():

model = Sequential()

model.add(layers.Dense(400, input\_dim=167))

model.add(Dropout(0.3))

model.add(layers.Dense(200))

model.add(Dropout(0.3))

model.add(layers.Dense(100))

model.add(Dropout(0.3))

model.add(layers.Dense(1))

sgd = keras.optimizers.SGD(lr=0.0001)

model.compile(loss='mse',optimizer='sgd', metrics=['RootMeanSquaredError'])

return model

model=KerasRegressor(build\_fn=build\_model,epochs=150,batch\_size=256,verbose=0)

model.fit(X\_train,y\_train,verbose=0)

Mordred-ANN

def build\_model():

model = Sequential()

model.add(layers.Dense(400, input\_dim=1104))

model.add(Dropout(0.05))

model.add(layers.Dense(200))

model.add(Dropout(0.05))

model.add(layers.Dense(100))

model.add(Dropout(0.05))

model.add(layers.Dense(1))

sgd = keras.optimizers.SGD(lr=0.01)

model.compile(loss='mse',optimizer='sgd', metrics=['RootMeanSquaredError'])

return model

model=KerasRegressor(build\_fn=build\_model,epochs=150,batch\_size=256,verbose=0)

model.fit(X\_train,y\_train,verbose=0)

RDKFP-ANN

def build\_model():

model = Sequential()

model.add(layers.Dense(200, input\_dim=1024))

model.add(Dropout(0.3))

model.add(layers.Dense(100))

model.add(Dropout(0.3))

model.add(layers.Dense(50))

model.add(Dropout(0.3))

model.add(layers.Dense(1))

sgd = keras.optimizers.SGD(lr=0.0001)

model.compile(loss='mse',optimizer='sgd', metrics=['RootMeanSquaredError'])

return model

model=KerasRegressor(build\_fn=build\_model,epochs=150,batch\_size=256,verbose=0)

model.fit(X\_train,y\_train,verbose=0)

AFP-GBR

fit1=GradientBoostingRegressor(learning\_rate=0.03,max\_depth=5, max\_features='sqrt',min\_samples\_leaf=10, min\_samples\_split=7,n\_estimators=500,random\_state=42)

ECFP-GBR

fit1=GradientBoostingRegressor(learning\_rate=0.01,max\_depth=10, max\_features='sqrt',min\_samples\_leaf= 1,min\_samples\_split=2,n\_estimators=500,random\_state=42)

MACCS-GBR

fit1=GradientBoostingRegressor(learning\_rate=0.0207,max\_depth=10, max\_features='log2',min\_samples\_leaf= 6,min\_samples\_split=2,n\_estimators=400,random\_state=42)

Mordred-GBR

fit1=GradientBoostingRegressor(learning\_rate=0.0170,max\_depth=7, max\_features='sqrt',min\_samples\_leaf= 1,min\_samples\_split=19,n\_estimators=400,random\_state=42)

RDKFP-GBR

fit1=GradientBoostingRegressor(learning\_rate=0.014,max\_depth=10, max\_features='sqrt',min\_samples\_leaf= 17,min\_samples\_split=24,n\_estimators=450,random\_state=42)

AFP-RF

fit1=RandomForestRegressor(max\_depth=10, max\_features='sqrt',min\_samples\_leaf= 1,min\_samples\_split=3,n\_estimators=500,random\_state=42)

ECFP-RF

fit1=RandomForestRegressor(max\_depth=3, max\_features='sqrt',min\_samples\_leaf= 2,min\_samples\_split=3,n\_estimators=1000,random\_state=42)

MACCS-RF

fit1=RandomForestRegressor(max\_depth=10, max\_features='sqrt',min\_samples\_leaf= 1,min\_samples\_split=4,n\_estimators=550,random\_state=42)

Mordred-RF

fit1=RandomForestRegressor(max\_depth=10, max\_features='sqrt',min\_samples\_leaf= 1,min\_samples\_split=5,n\_estimators=800,random\_state=42)

RDKFP-RF

fit1=RandomForestRegressor(max\_depth=10, max\_features='sqrt',min\_samples\_leaf= 1,min\_samples\_split=3,n\_estimators=700,random\_state=42)

AFP-SVM

fit1=SVR(C=0.0256 , kernel='poly',max\_iter= 5000,coef0=1,degree=4,gamma=0.0249)

ECFP-SVM

fit1=SVR(C=1000, kernel='poly',max\_iter= 10000,coef0=0,degree=2,gamma=0.0041)

MACCS-SVM

fit1=SVR(C=741.8451, kernel='poly',max\_iter= 10000,coef0=0,degree=2,gamma=0.0015)

Mordred-SVM

fit1=SVR(C=0.8956 , kernel='rbf',max\_iter= 5100,gamma=0.0003)

RDKFP-SVM

fit1=SVR(C=1000, kernel='poly',max\_iter= 10000,coef0=0,degree=2,gamma=0.0036)