BAF

AFP-ANN

def build\_model():

model = Sequential()

model.add(layers.Dense(400, input\_dim=512))

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)

ECFP-ANN

def build\_model():

model = Sequential()

model.add(layers.Dense(300, input\_dim=1024))

model.add(Dropout(0.3))

model.add(layers.Dense(150))

model.add(Dropout(0.3))

model.add(layers.Dense(75))

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(100, input\_dim=167))

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)

Mordred-ANN

def build\_model():

model = Sequential()

model.add(layers.Dense(400, input\_dim=1027))

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=0.001)

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=0.0810,max\_depth=10, max\_features='sqrt',min\_samples\_leaf=8, min\_samples\_split=9,n\_estimators=300,random\_state=42)

ECFP-GBR

fit1=GradientBoostingRegressor(learning\_rate=0.07445,max\_depth=10, max\_features='log2',min\_samples\_leaf= 8,min\_samples\_split=14,n\_estimators=1000,random\_state=42)

MACCS-GBR

fit1=GradientBoostingRegressor(learning\_rate=0.0245,max\_depth=6, max\_features='sqrt',min\_samples\_leaf= 2,min\_samples\_split=2,n\_estimators=850,random\_state=42)

Mordred-GBR

fit1=GradientBoostingRegressor(learning\_rate=0.0502,max\_depth=5, max\_features='sqrt',min\_samples\_leaf= 2,min\_samples\_split=2,n\_estimators=650,random\_state=42)

RDKFP-GBR

fit1=GradientBoostingRegressor(learning\_rate=0.0403,max\_depth=10, max\_features='sqrt',min\_samples\_leaf= 19,min\_samples\_split=12,n\_estimators=600,random\_state=42)

AFP-RF

fit1=RandomForestRegressor(max\_depth=10, max\_features='sqrt',min\_samples\_leaf= 1,min\_samples\_split=2,n\_estimators=600,random\_state=42)

ECFP-RF

fit1=RandomForestRegressor(max\_depth=2, max\_features='sqrt',min\_samples\_leaf= 1,min\_samples\_split=3,n\_estimators=600,random\_state=42)

MACCS-RF

fit1=RandomForestRegressor(max\_depth=10, max\_features='sqrt',min\_samples\_leaf= 1,min\_samples\_split=2,n\_estimators=650,random\_state=42)

Mordred-RF

fit1=RandomForestRegressor(max\_depth=10, max\_features='sqrt',min\_samples\_leaf= 1,min\_samples\_split=2,n\_estimators=800,random\_state=42)

RDKFP-RF

fit1=RandomForestRegressor(max\_depth=10, max\_features='sqrt',min\_samples\_leaf= 1,min\_samples\_split=2,n\_estimators=950,random\_state=42)

AFP-SVM

fit1=SVR(C=1.5539 , kernel='poly',max\_iter=10000,coef0=1,degree=2,gamma=0.0267)

ECFP- SVM

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

MACCS- SVM

fit1=SVR(C=1000, kernel='poly',max\_iter= 10000,coef0=0,degree=2,gamma=0.0033)

Mordred- SVM

fit1=SVR(C=1000, kernel='poly',max\_iter= 10000,coef0=0,degree=2,gamma=0.0001)

RDKFP- SVM

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