```
pd version:  2.2.3
sklearn version:  1.5.2
xgb version:  2.1.1
Tran and val dataset size:  (7581, 1865)
Test dataset size: (494, 1865)
Tran and val extractants number:  (280, 5)
Splits number:  3
Train size for one split:  5990
Val size for one split: 1591
Val SMILES number:  42
x_trainVal shape:  (7581, 1860)
y_trainVal shape:  (7581,)
x_test shape:  (494, 1860)
y_test shape:  (494,)
Top 10 models:
Rank 2831:
Parameters: {'alpha': 0.1, 'colsample_bytree': 1.0, 'lambda': 1.5, 'learning_rate'
: 0.3, 'max_depth': 18, 'min_child_weight': 1, 'n_estimators': 100}
Mean Train Score: 0.9621153213387629
Mean Test Score: 0.716221277051517
-------------------------------------------------
Rank 1792:
Parameters: {'alpha': 0.01, 'colsample_bytree': 1.0, 'lambda': 1, 'learning_rate':
 0.5, 'max_depth': 21, 'min_child_weight': 0.5, 'n_estimators': 50}
Mean Train Score: 0.9622729294989579
Mean Test Score: 0.7152308793709065
-------------------------------------------------
Rank 786:
Parameters: {'alpha': 0, 'colsample_bytree': 1.0, 'lambda': 1, 'learning_rate': 0.
3, 'max_depth': 21, 'min_child_weight': 0.5, 'n_estimators': 200}
Mean Train Score: 0.9622729294989579
Mean Test Score: 0.7142343434153228
-------------------------------------------------
Rank 780:
Parameters: {'alpha': 0, 'colsample_bytree': 1.0, 'lambda': 1, 'learning_rate': 0.
3, 'max_depth': 18, 'min_child_weight': 1, 'n_estimators': 200}
Mean Train Score: 0.9621153213387629
Mean Test Score: 0.7125923719208513
-------------------------------------------------
Rank 1793:
Parameters: {'alpha': 0.01, 'colsample_bytree': 1.0, 'lambda': 1, 'learning_rate':
 0.5, 'max_depth': 21, 'min_child_weight': 0.5, 'n_estimators': 100}
Mean Train Score: 0.9622729294989579
Mean Test Score: 0.7124219497874261
-------------------------------------------------
Best parameters found:  {'alpha': 0.1, 'colsample_bytree': 1.0, 'lambda': 1.5, 'le
arning_rate': 0.3, 'max_depth': 18, 'min_child_weight': 1, 'n_estimators': 100}
Model saved as xbg_model.sav
[[132  35   0]
 [ 41 188  10]
 [  5  49  34]]
              precision    recall  f1-score   support

           0       0.74      0.79      0.77       167
           1       0.69      0.79      0.74       239
           2       0.77      0.39      0.52        88

    accuracy                           0.72       494
   macro avg       0.74      0.65      0.67       494
weighted avg       0.72      0.72      0.71       494
```