Protein: P35462 - metric: balanced_accuracy

Total (train): 2957

ROC curve

- AUC_train = 0.997
- AUC_test = 0.966
- Random

Pareto Chart with Highlighted Best Attempt

- Trials
- Pareto Front Trials
- Best Trial (# 1120)
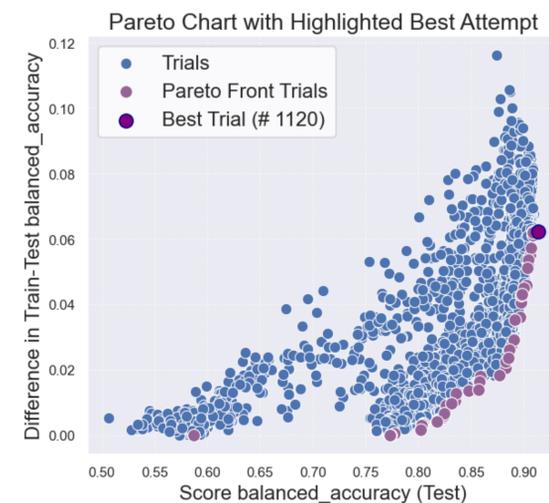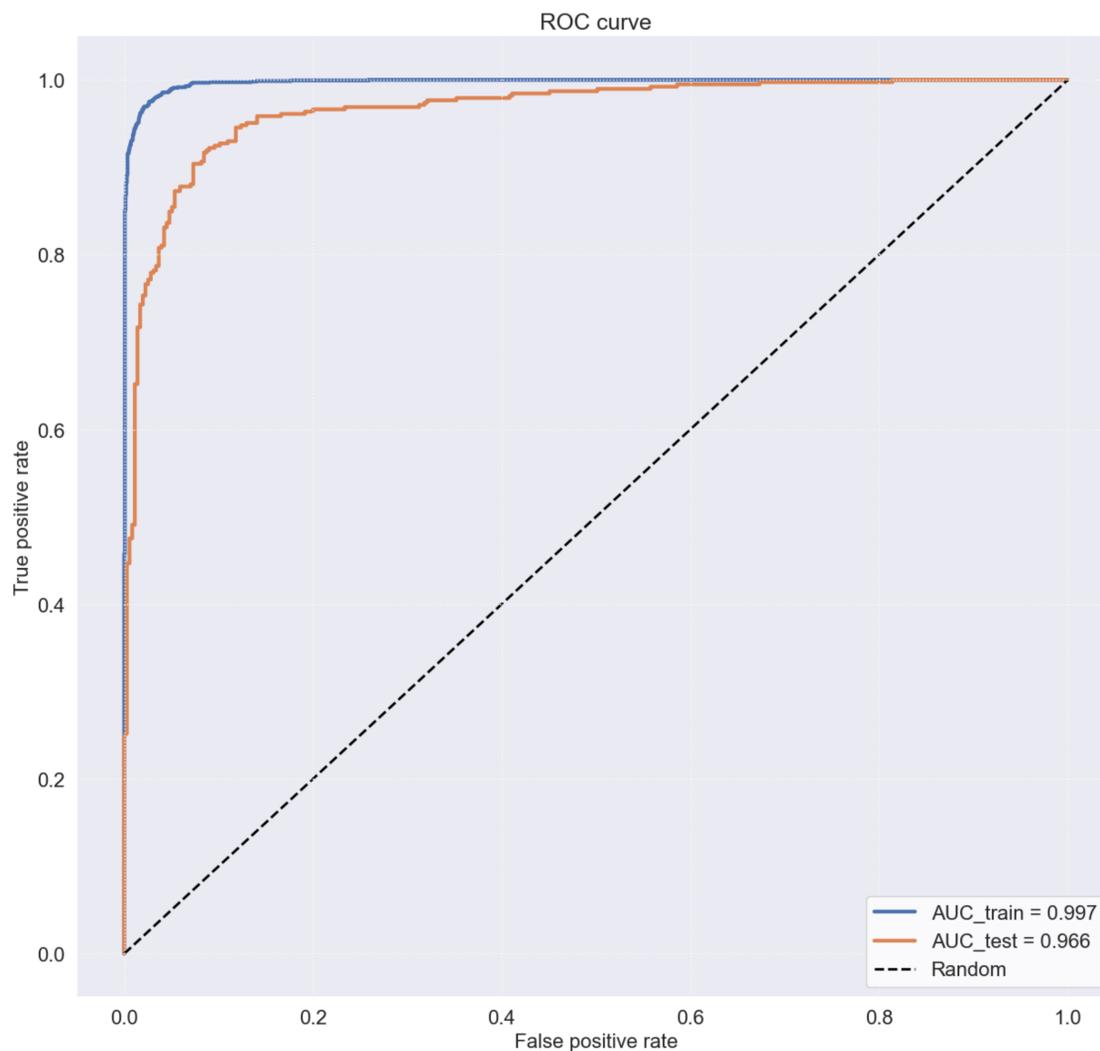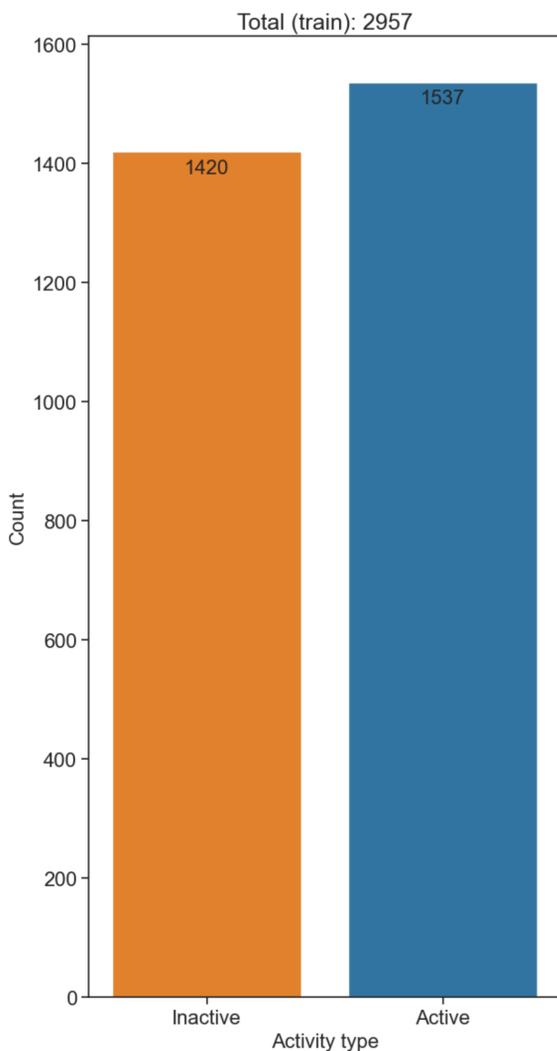
XGBoost Parameters	Value
alpha	0.1323
colsample_bytree	0.7064
gamma	0.1743
lambda	4.567
learning_rate	0.0608
max_depth	4.0
min_child_weight	1.0
n_estimators	740.0
reg_alpha	0.2751
reg_lambda	0.1234
scale_pos_weight	1.336
subsample	0.7641

Confusion Matrix

	0	1
0	313	42
1	25	360

Confusion Matrix (nomr.)

	0	1
0	0.88	0.12
1	0.065	0.94

Calibration curve

- train: 0.024
- test: 0.0676
- perfectly_calibrated

Active/Inactive probability

- Inactive zone
- Active zone
- type
  - active (385)
  - inactive (355)
  - decoy (734)
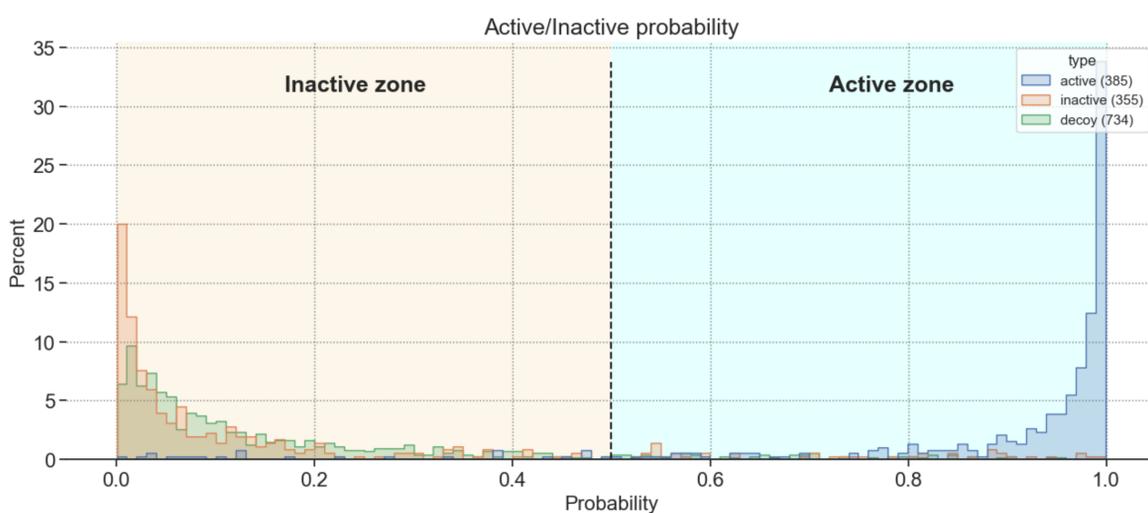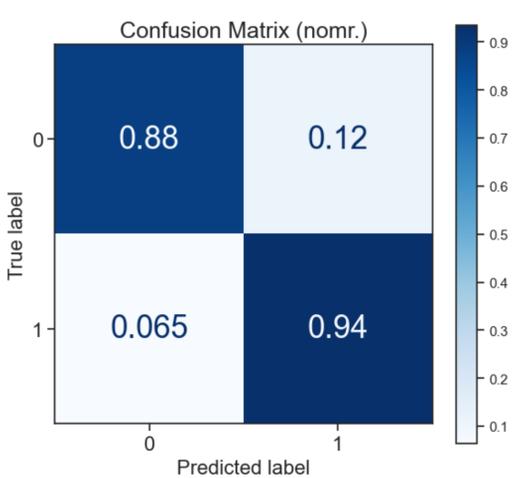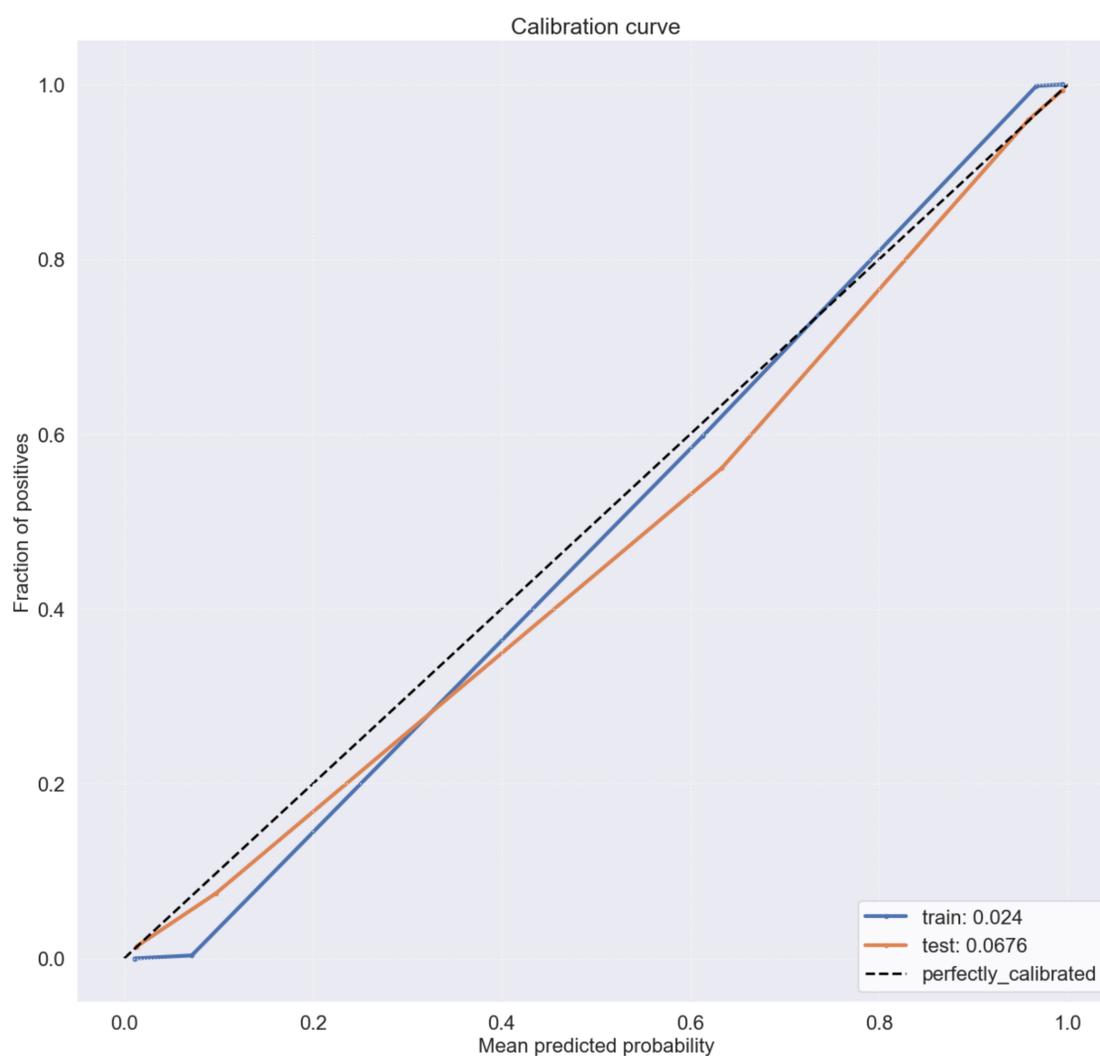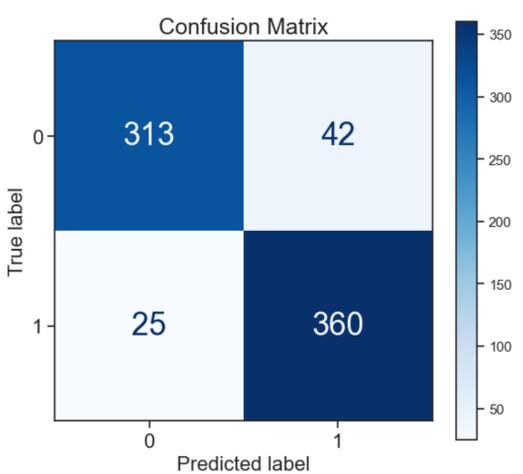
Metric	Train	Test
AUC	0.9972	0.966
accuracy	0.9726	0.9095
balanced accuracy	0.9722	0.9084
recall_(sens)	0.9831	0.9351
specificity	0.9613	0.8817
precision	0.9649	0.8955
f1_score	0.9726	0.9093

Protein: P35462 - metric: f1

Total (train): 2957

ROC curve

- AUC_train = 0.999
- AUC_test = 0.968
- Random

Pareto Chart with Highlighted Best Attempt

- Trials
- Pareto Front Trials
- Best Trial (# 1956)
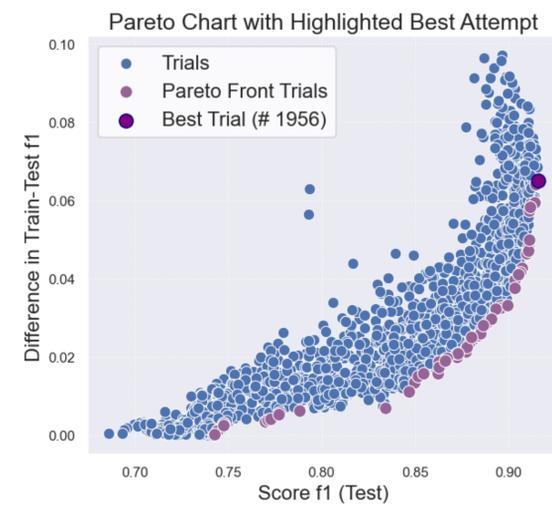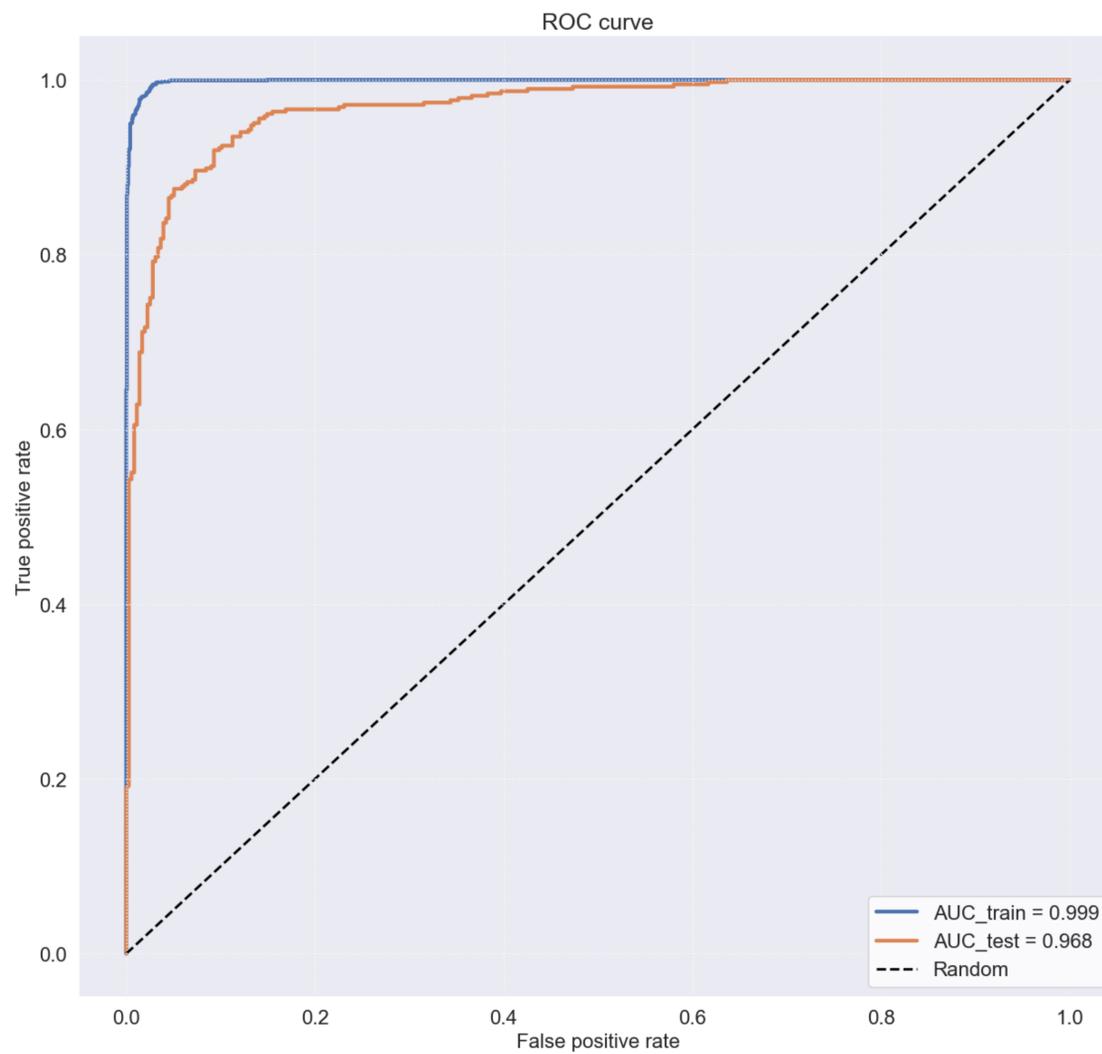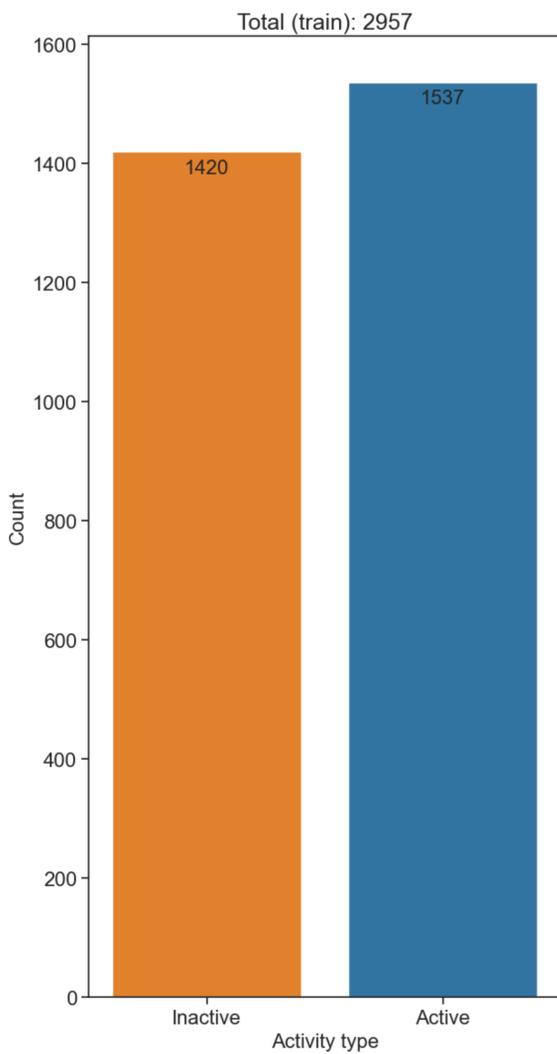
XGBoost Parameters	Value
alpha	3.1017
colsample_bytree	0.5506
gamma	0.5151
lambda	2.3617
learning_rate	0.0516
max_depth	10.0
min_child_weight	2.0
n_estimators	740.0
reg_alpha	0.2716
reg_lambda	0.8429
scale_pos_weight	2.4869
subsample	0.9822

Confusion Matrix

Confusion Matrix (nomr.)

Calibration curve

- train: 0.0198
- test: 0.0699
- perfectly_calibrated

Active/Inactive probability

- type
- active (385)
- inactive (355)
- decoy (734)
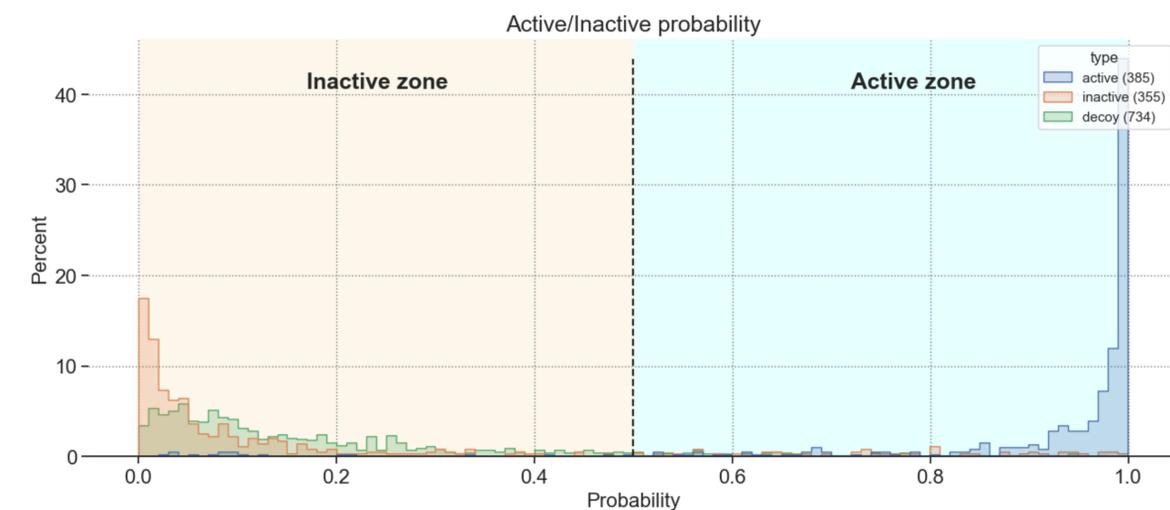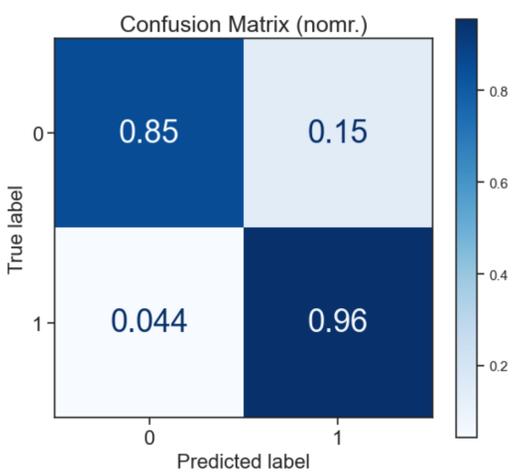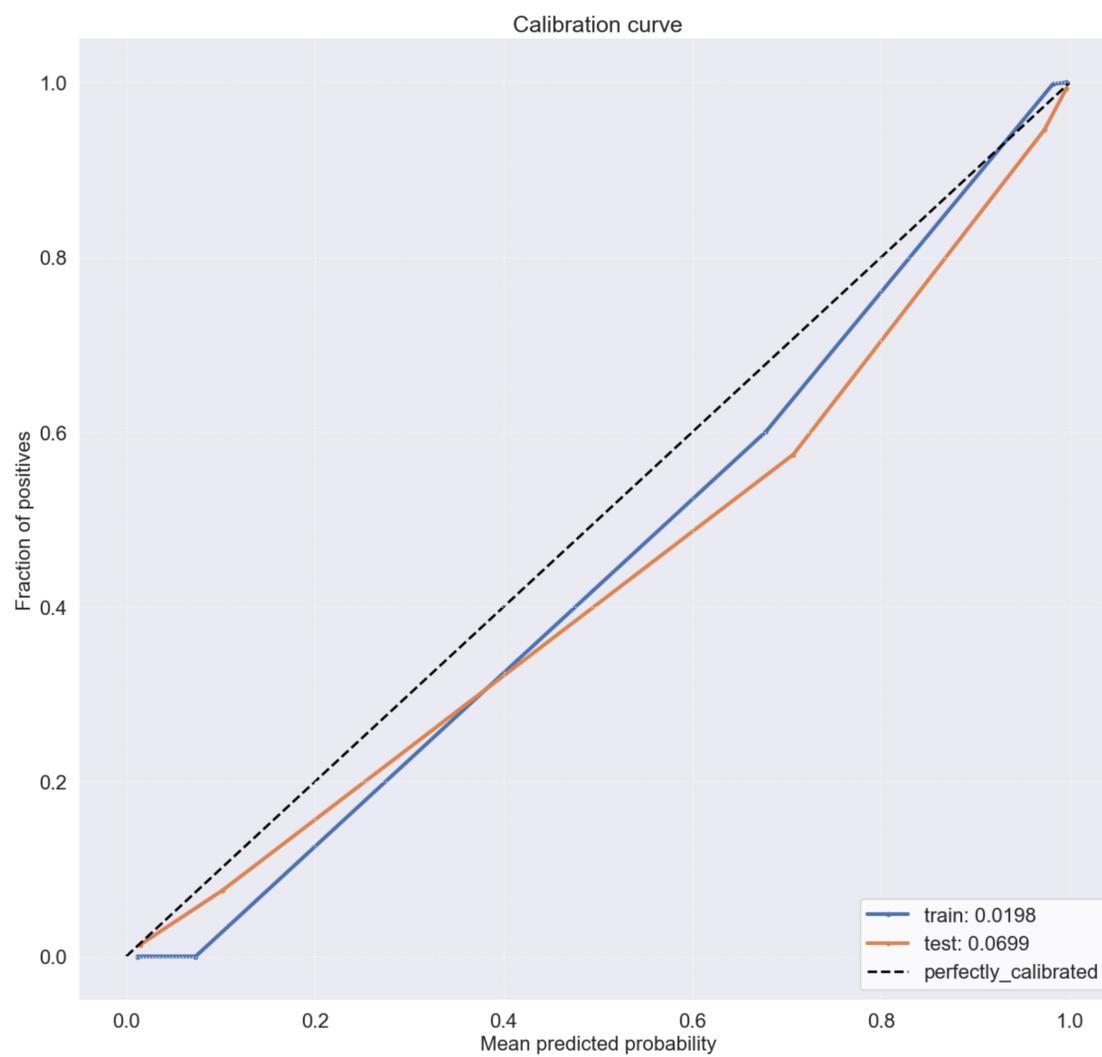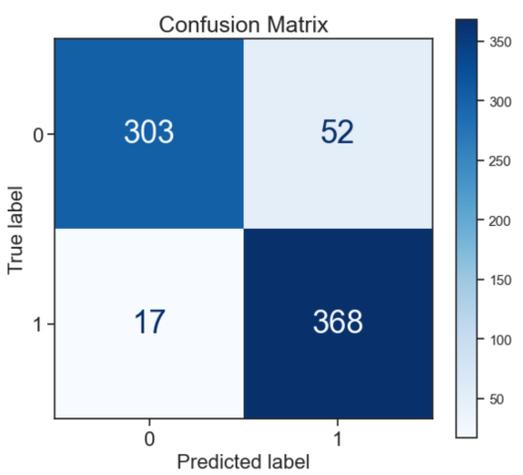
Metric	Train	Test
AUC	0.9987	0.9681
accuracy	0.9797	0.9068
balanced accuracy	0.979	0.9047
recall_(sens)	0.998	0.9558
specificity	0.9599	0.8535
precision	0.9642	0.8762
f1_score	0.9797	0.9064

Protein: P35462 - metric: precision

Total (train): 2957

ROC curve

- AUC_train = 1.000
- AUC_test = 0.966
- Random

Pareto Chart with Highlighted Best Attempt

- Trials
- Pareto Front Trials
- Best Trial (# 2995)

Confusion Matrix

Confusion Matrix (nomr.)

Calibration curve

- train: 0.0105
- test: 0.0716
- perfectly_calibrated
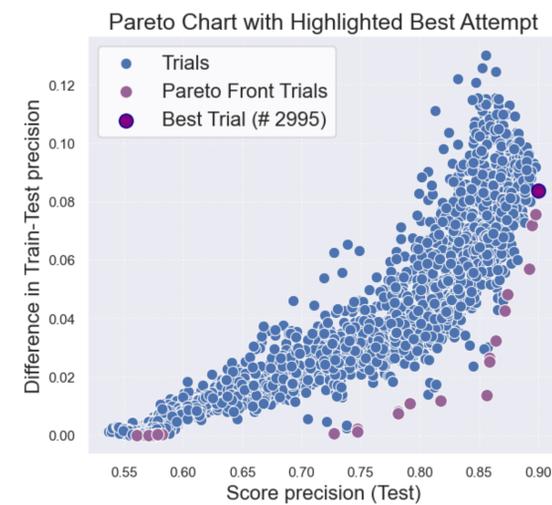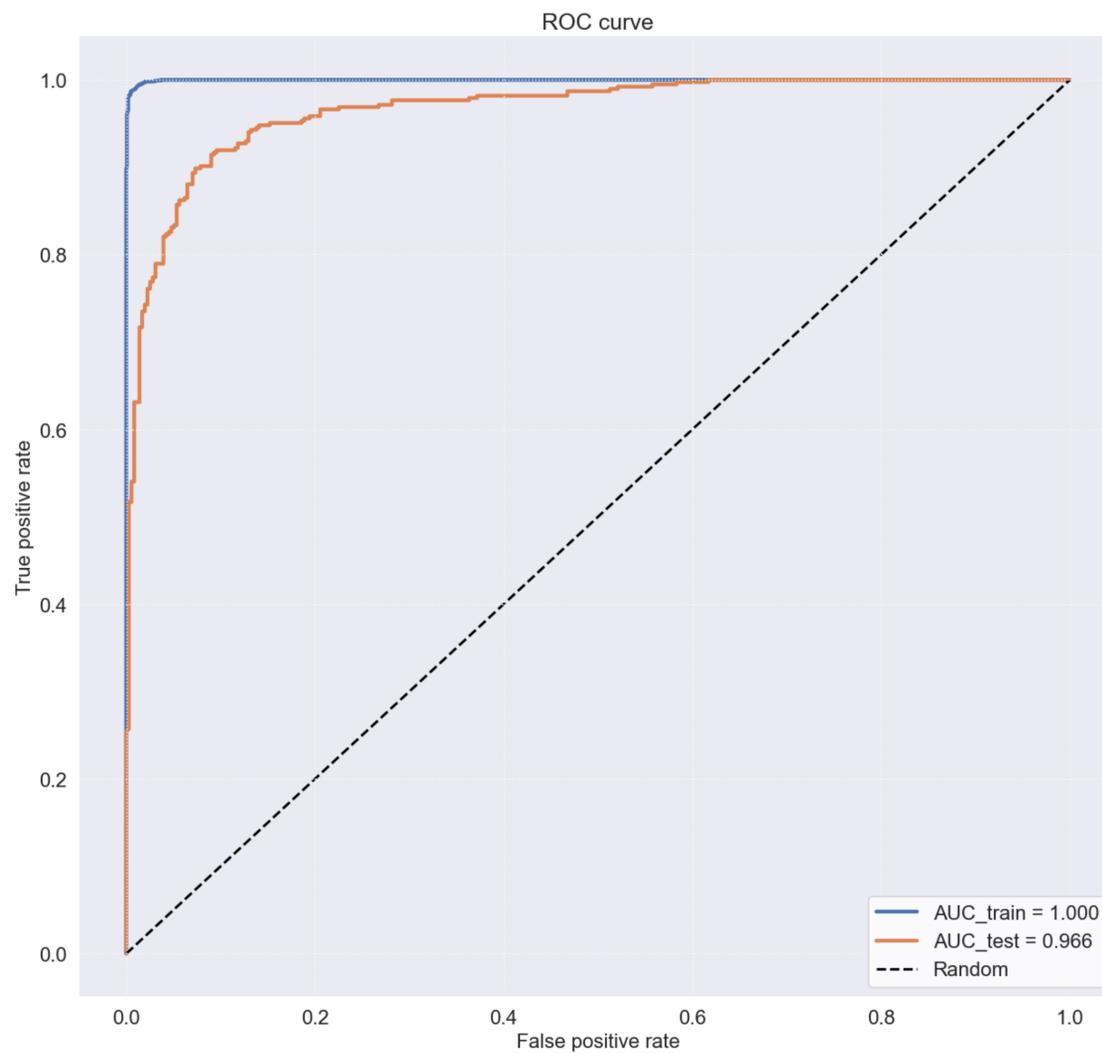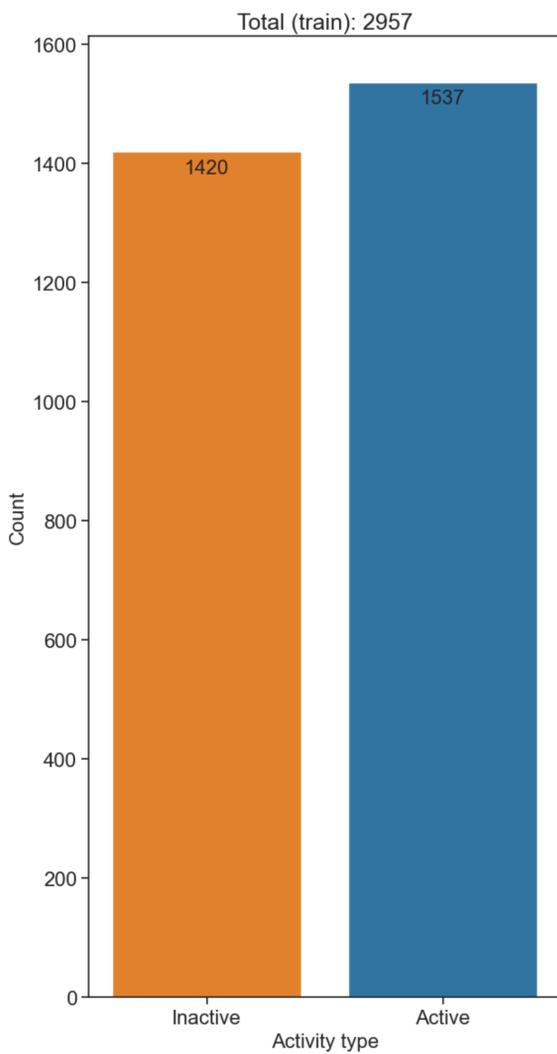
XGBoost Parameters	Value
alpha	4.2194
colsample_bytree	0.5644
gamma	0.5613
lambda	4.6635
learning_rate	0.2713
max_depth	9.0
min_child_weight	2.0
n_estimators	404.0
reg_alpha	0.0532
reg_lambda	0.4071
scale_pos_weight	1.6079
subsample	0.8494

Active/Inactive probability

- type
- active (385)
- inactive (355)
- decoy (734)
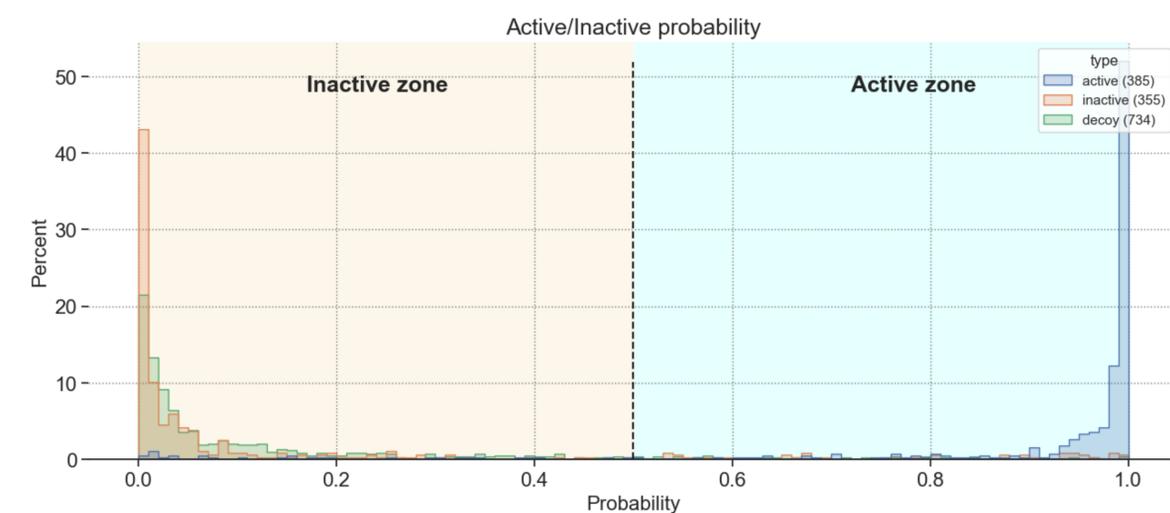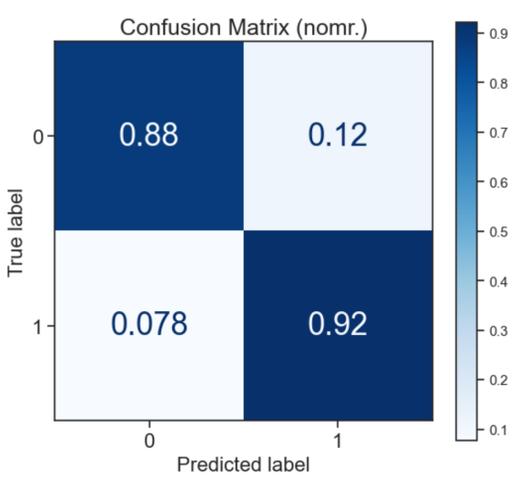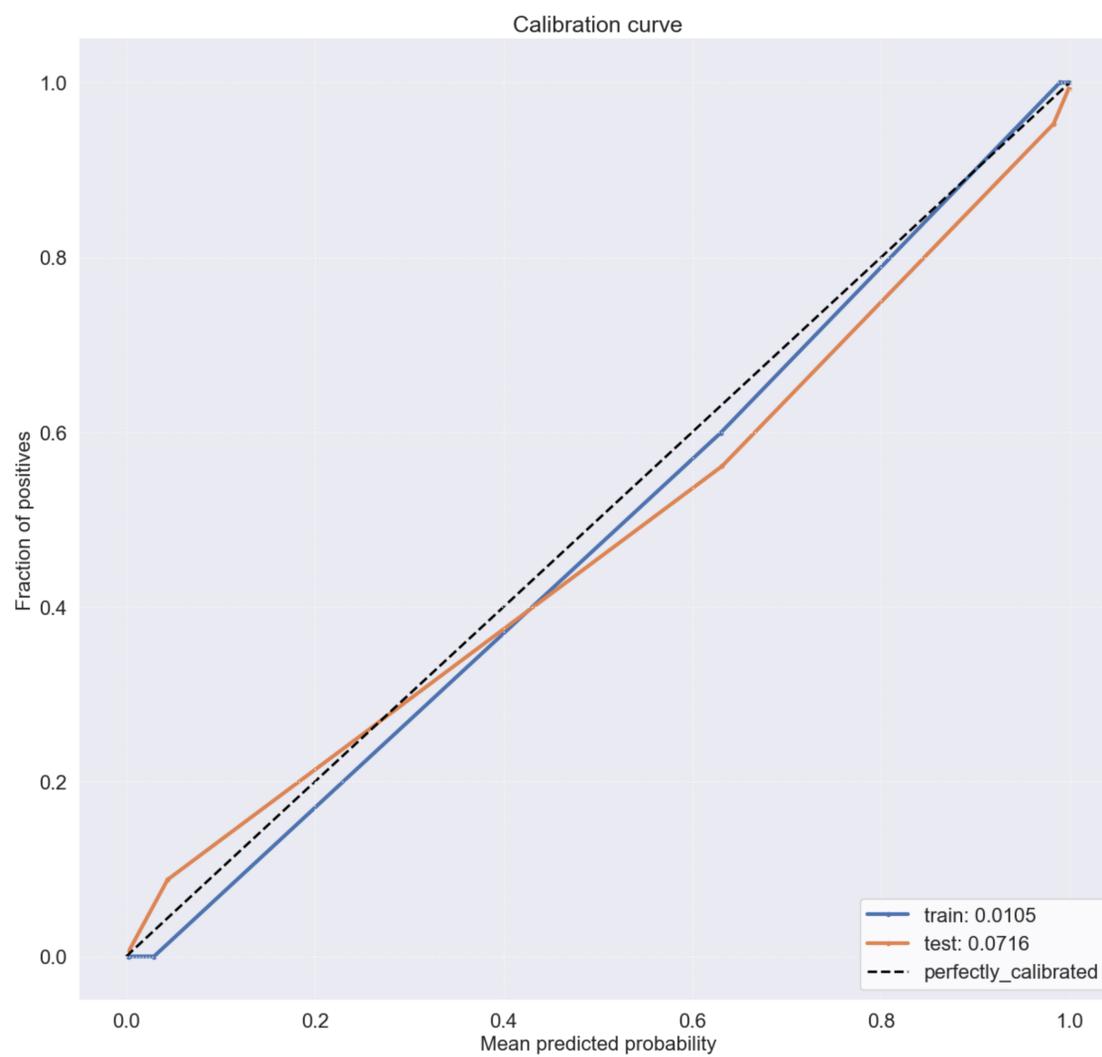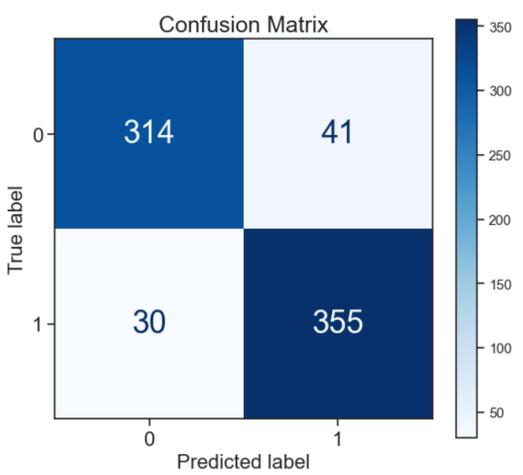
Metric	Train	Test
AUC	0.9997	0.9663
accuracy	0.9885	0.9041
balanced accuracy	0.9881	0.9033
recall_(sens)	0.998	0.9221
specificity	0.9782	0.8845
precision	0.9802	0.8965
f1_score	0.9885	0.904

Protein: P35462 - metric: SoftVotingXGBoostEnsemble
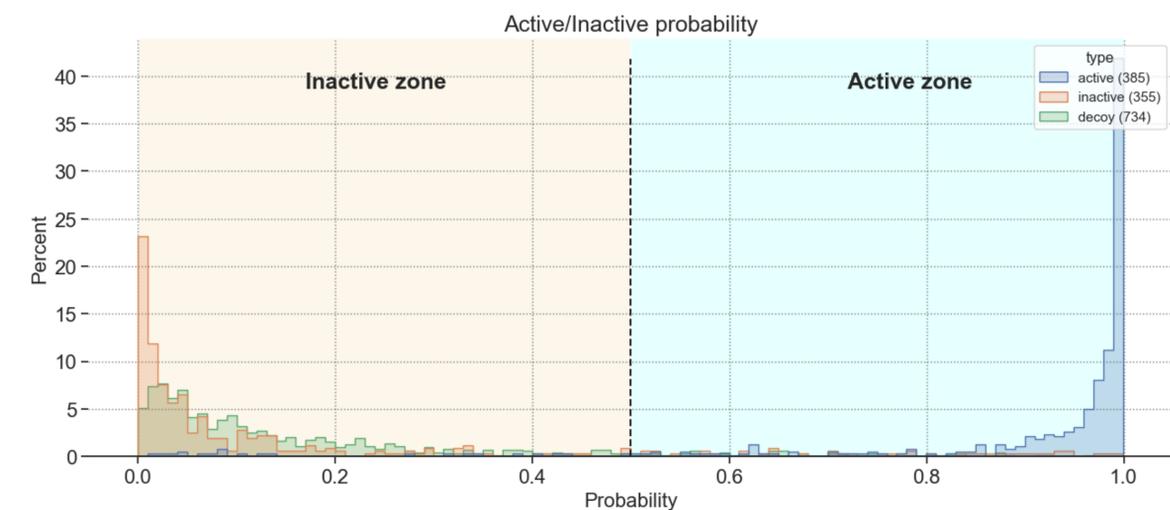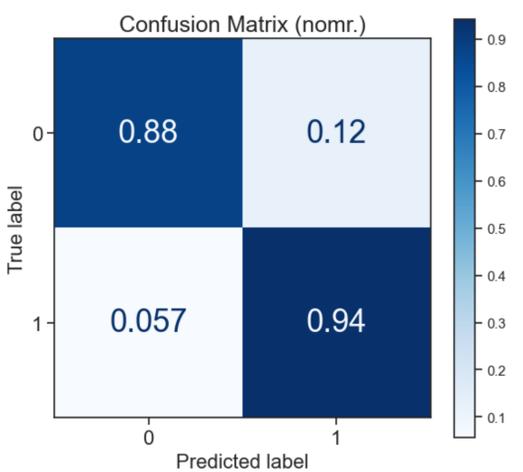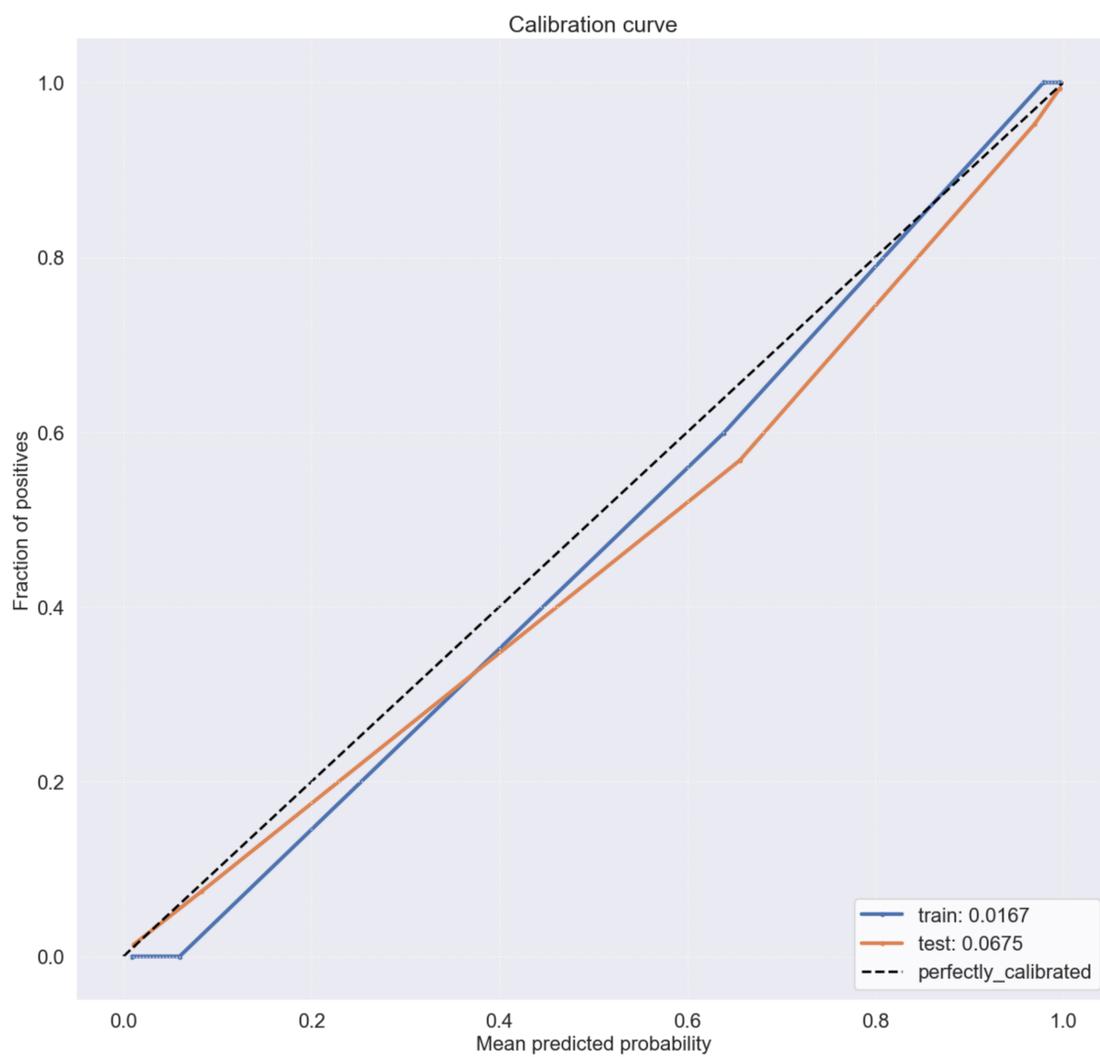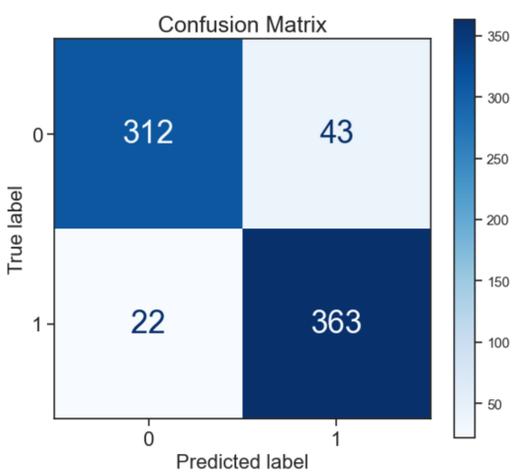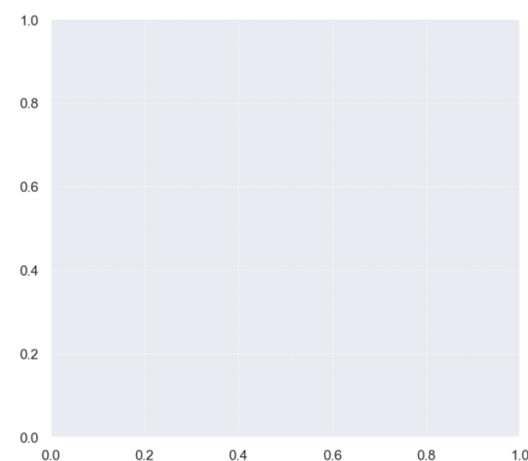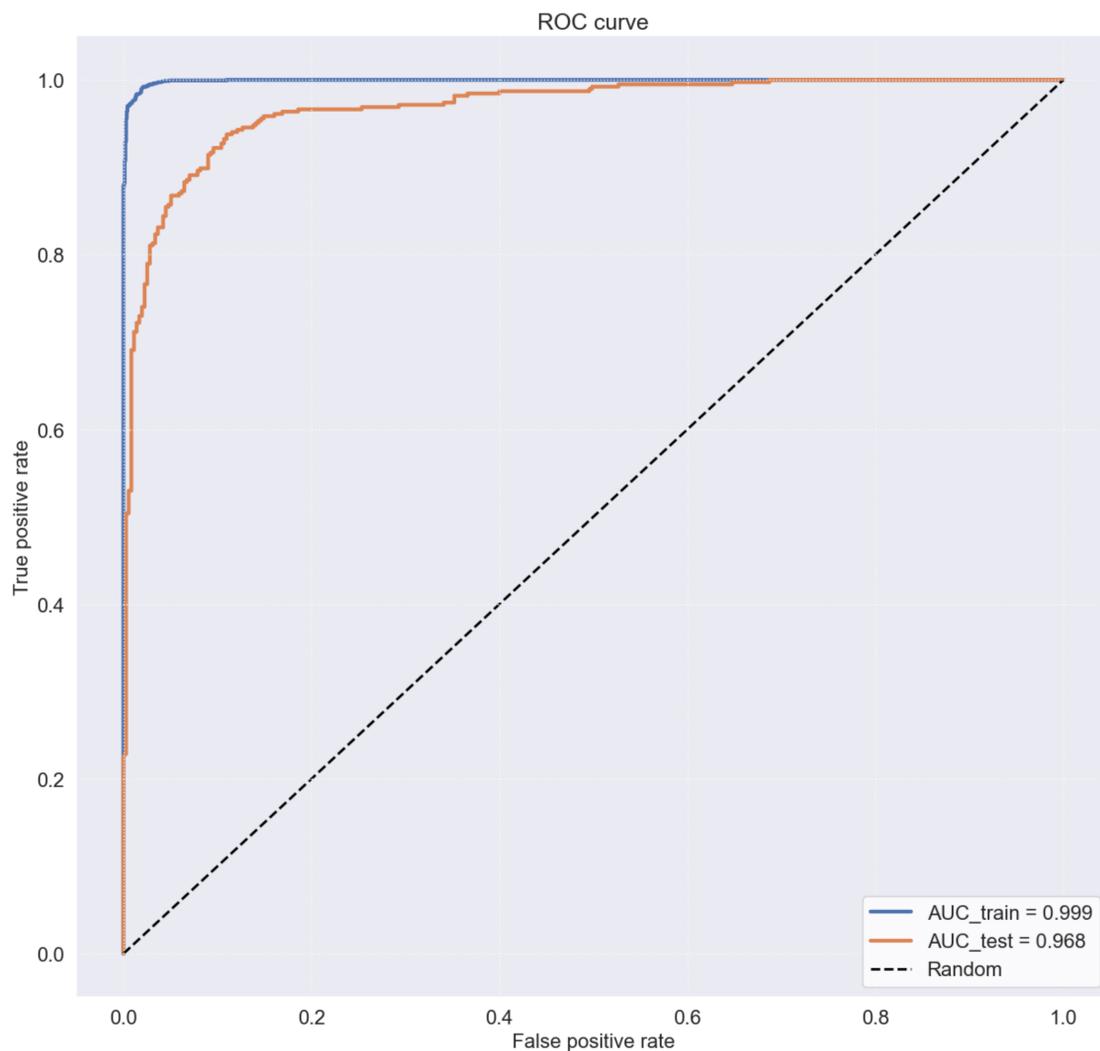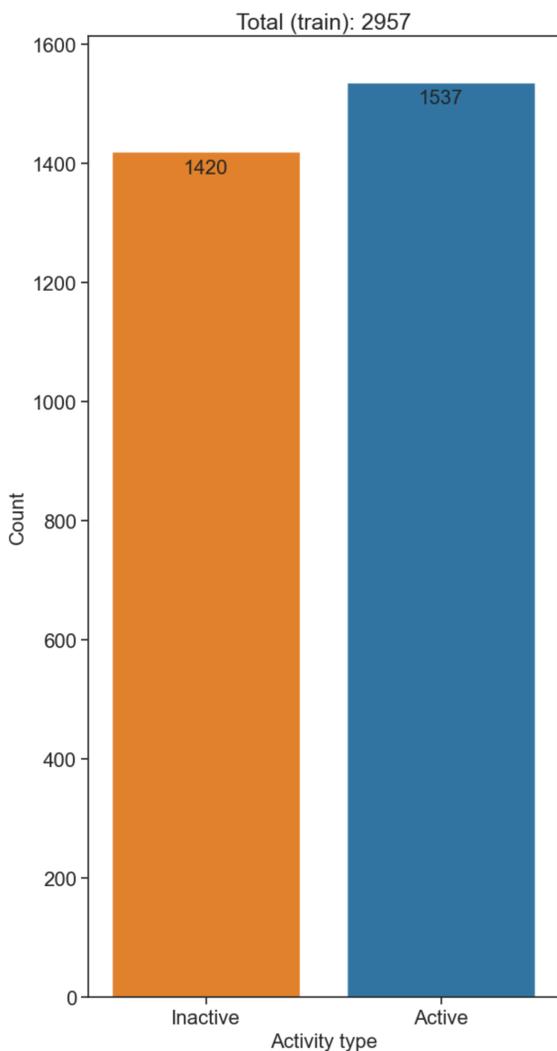
Metric	Train	Test
AUC	0.9992	0.9683
accuracy	0.9821	0.9122
balanced accuracy	0.9815	0.9109
recall_(sens)	0.9954	0.9429
specificity	0.9676	0.8789
precision	0.9708	0.8941
f1_score	0.9821	0.912