Protein: P43681 - metric: balanced_accuracy

Total (train): 705

ROC curve

AUC_train = 1.000
AUC_test = 0.968
Random

Pareto Chart with Highlighted Best Attempt


Trials
Pareto Front Trials
Best Trial (# 2785)

Confusion Matrix

Confusion Matrix (nomr.)

Calibration curve

train: 0.0146
test: 0.0704
perfectly_calibrated
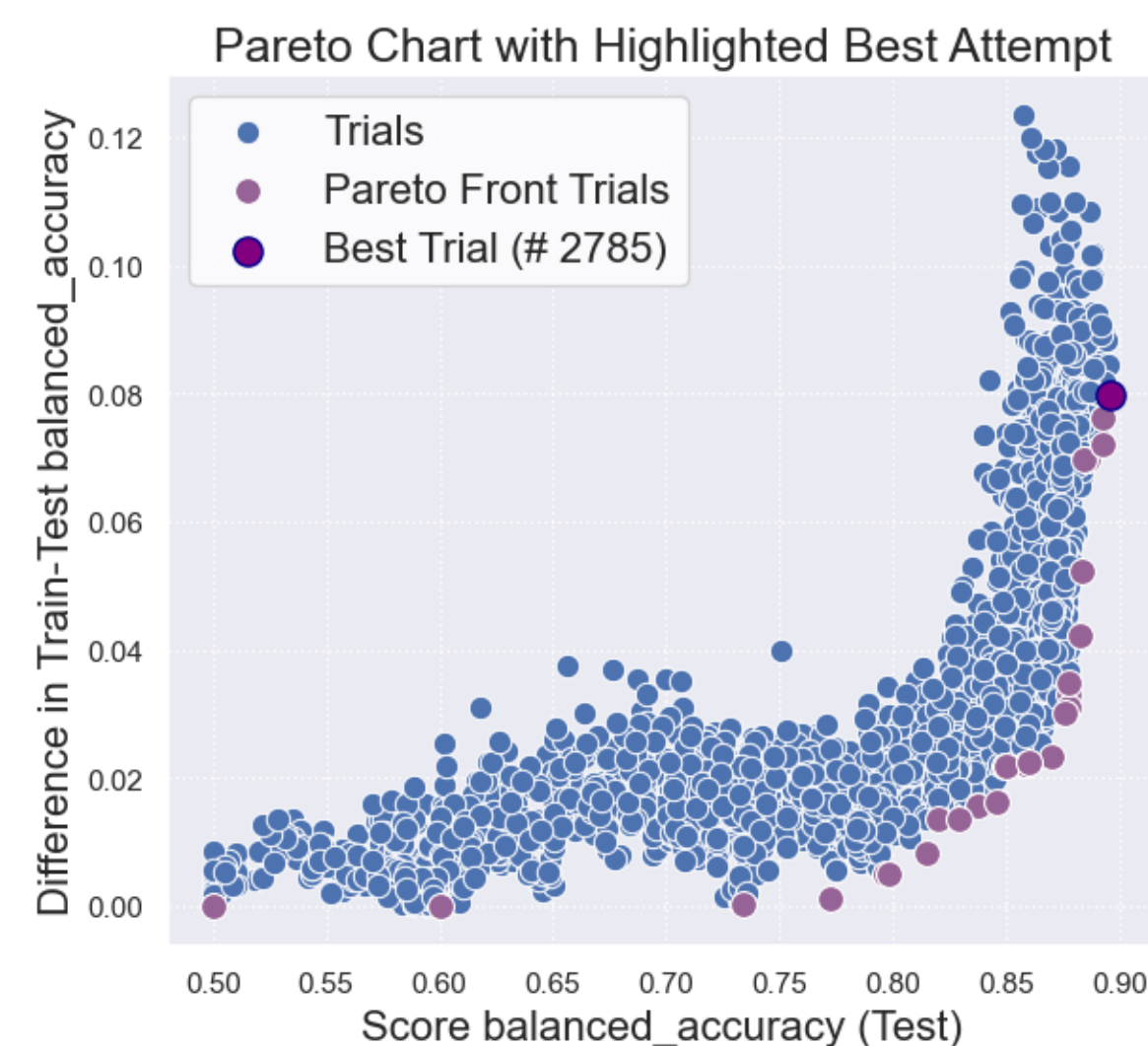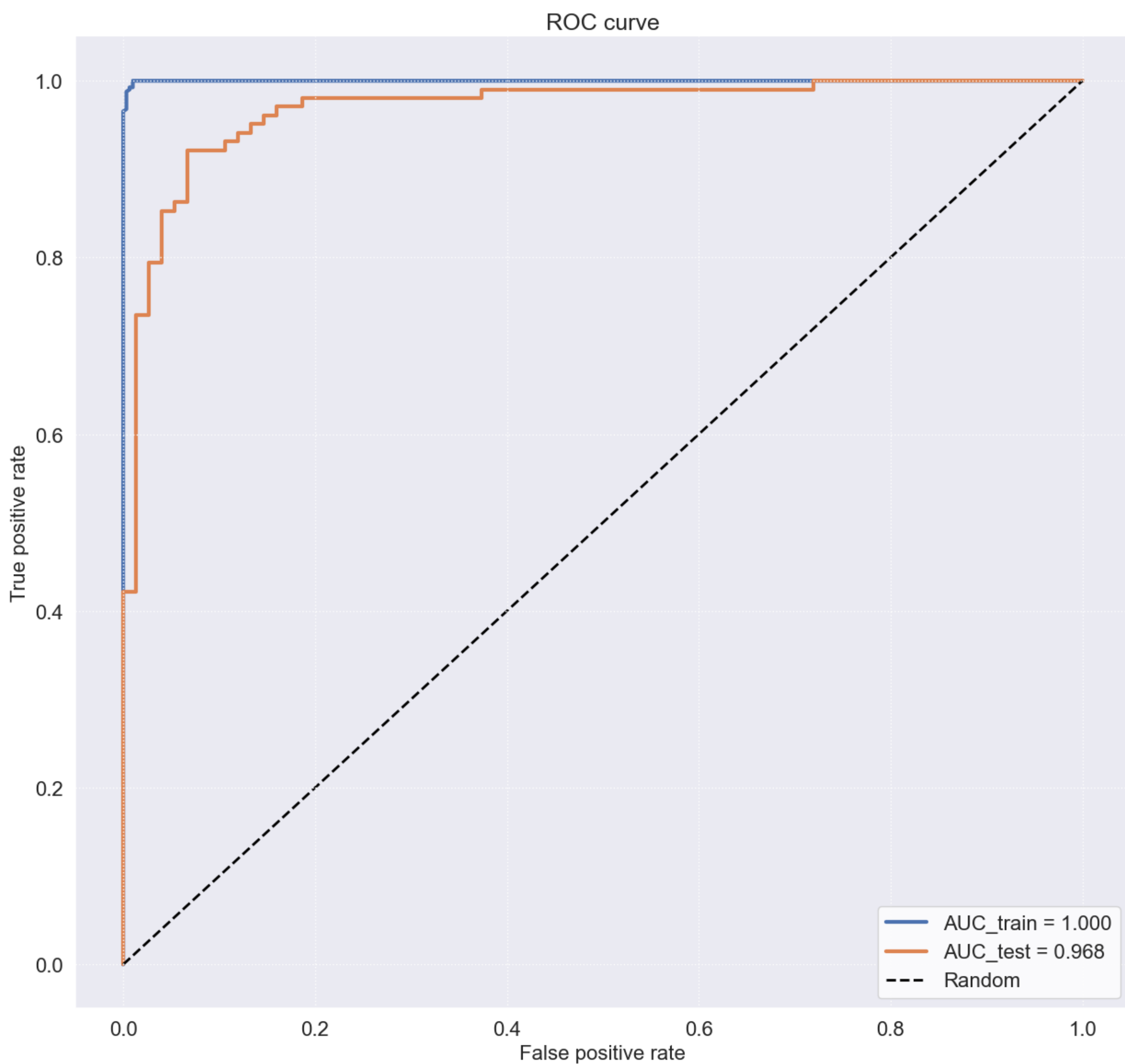
XGBoost Parameters	Value
alpha	4.3999
colsample_bytree	0.8627
gamma	0.3092
lambda	1.8821
learning_rate	0.0532
max_depth	10.0
min_child_weight	3.0
n_estimators	815.0
reg_alpha	0.0351
reg_lambda	0.0772
scale_pos_weight	6.5148
subsample	0.9051

Active/Inactive probability

type
active (102)
inactive (75)
decoy (177)
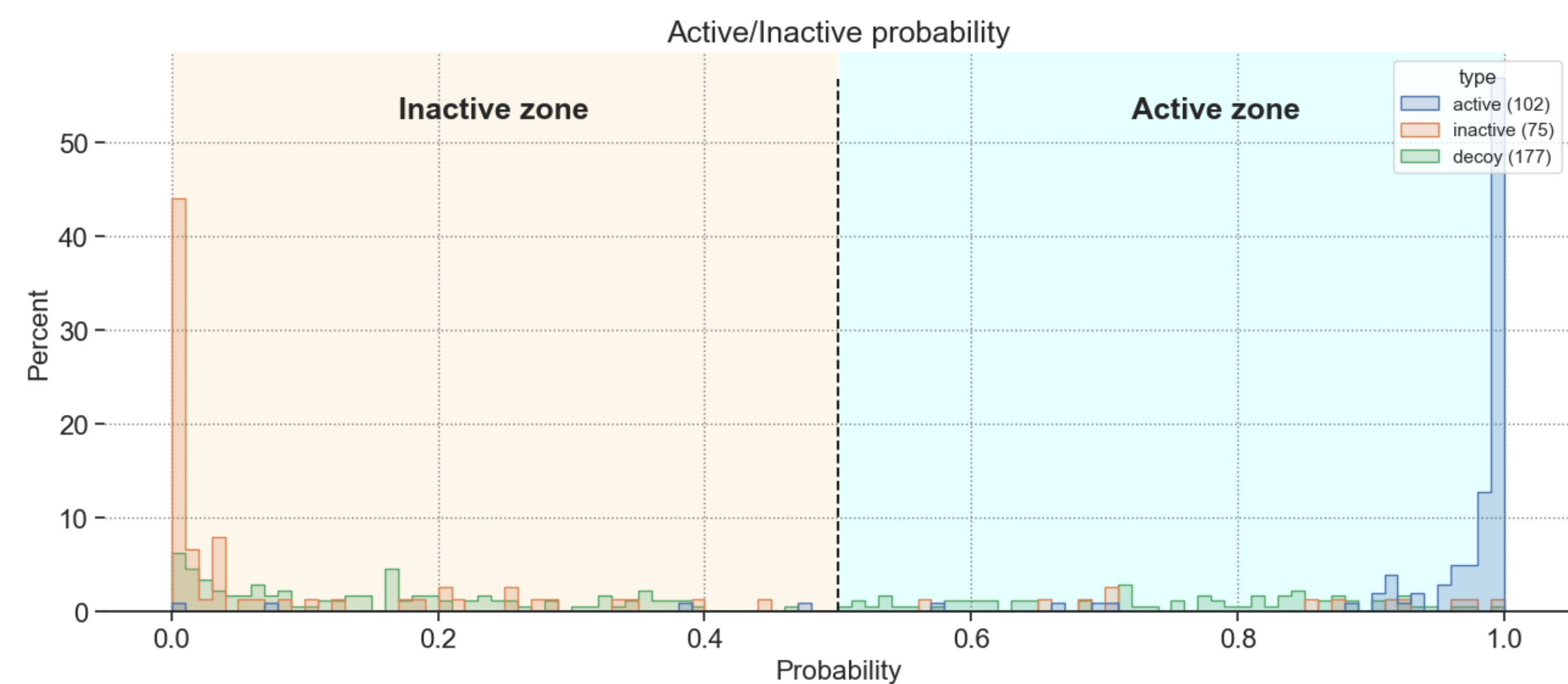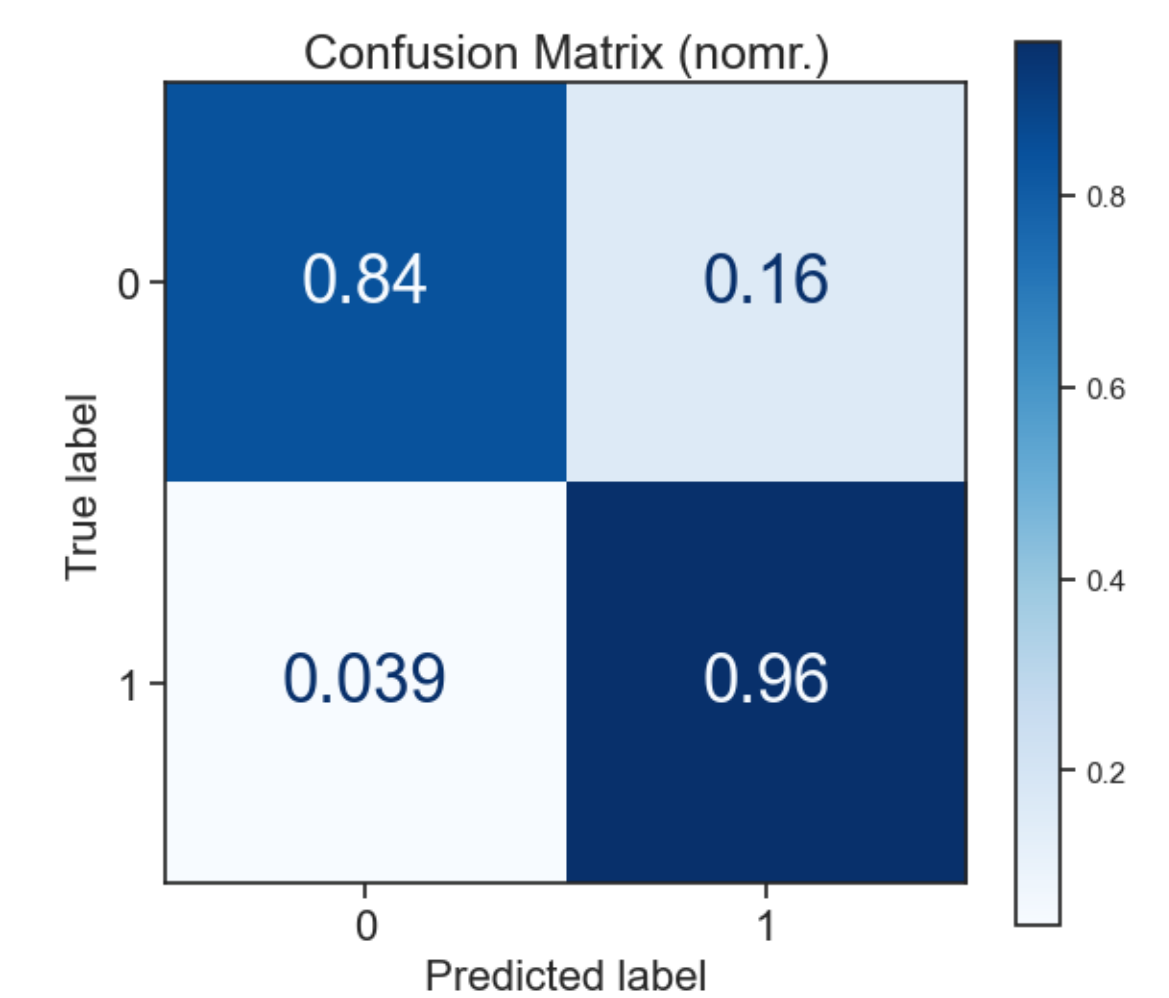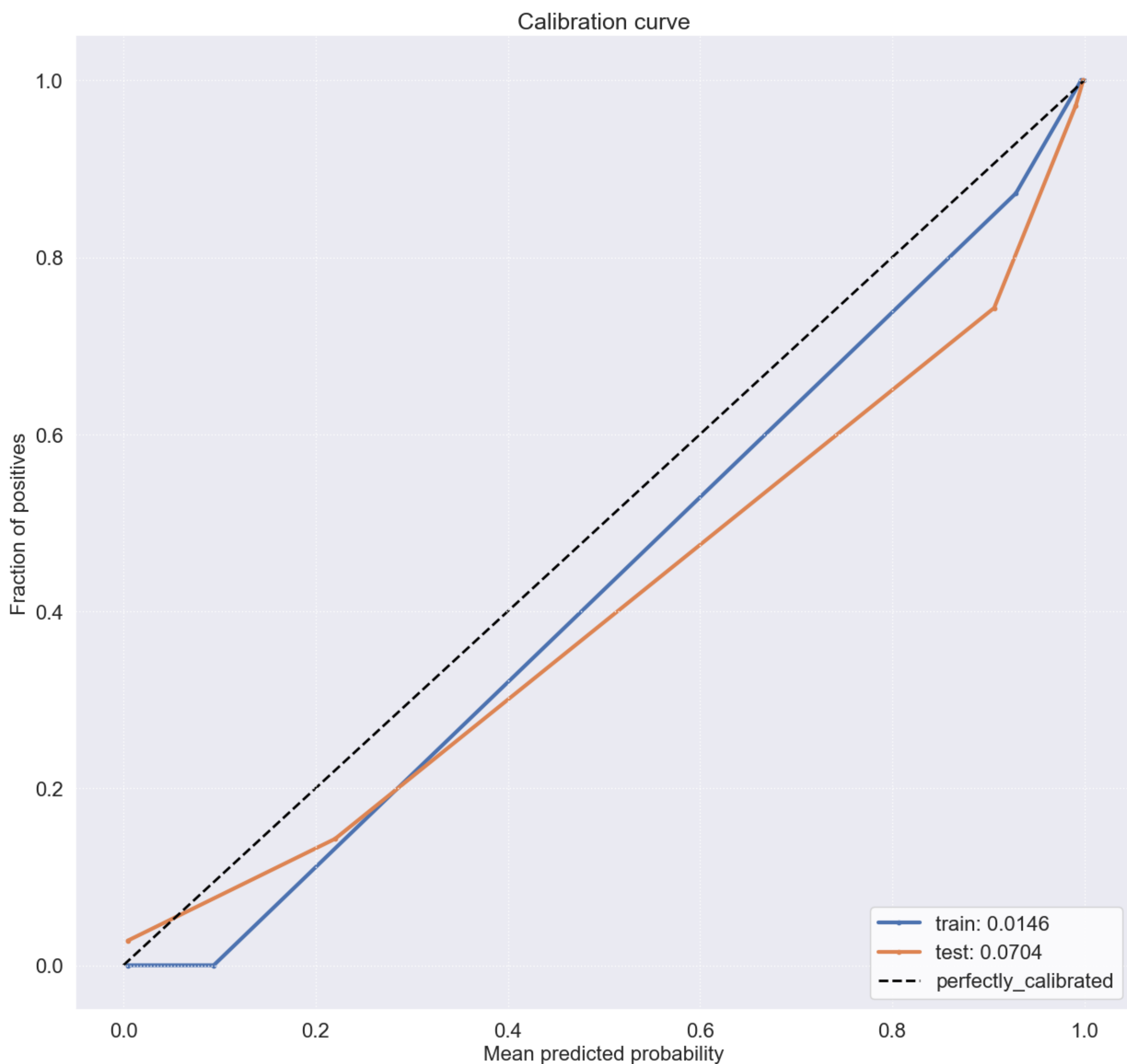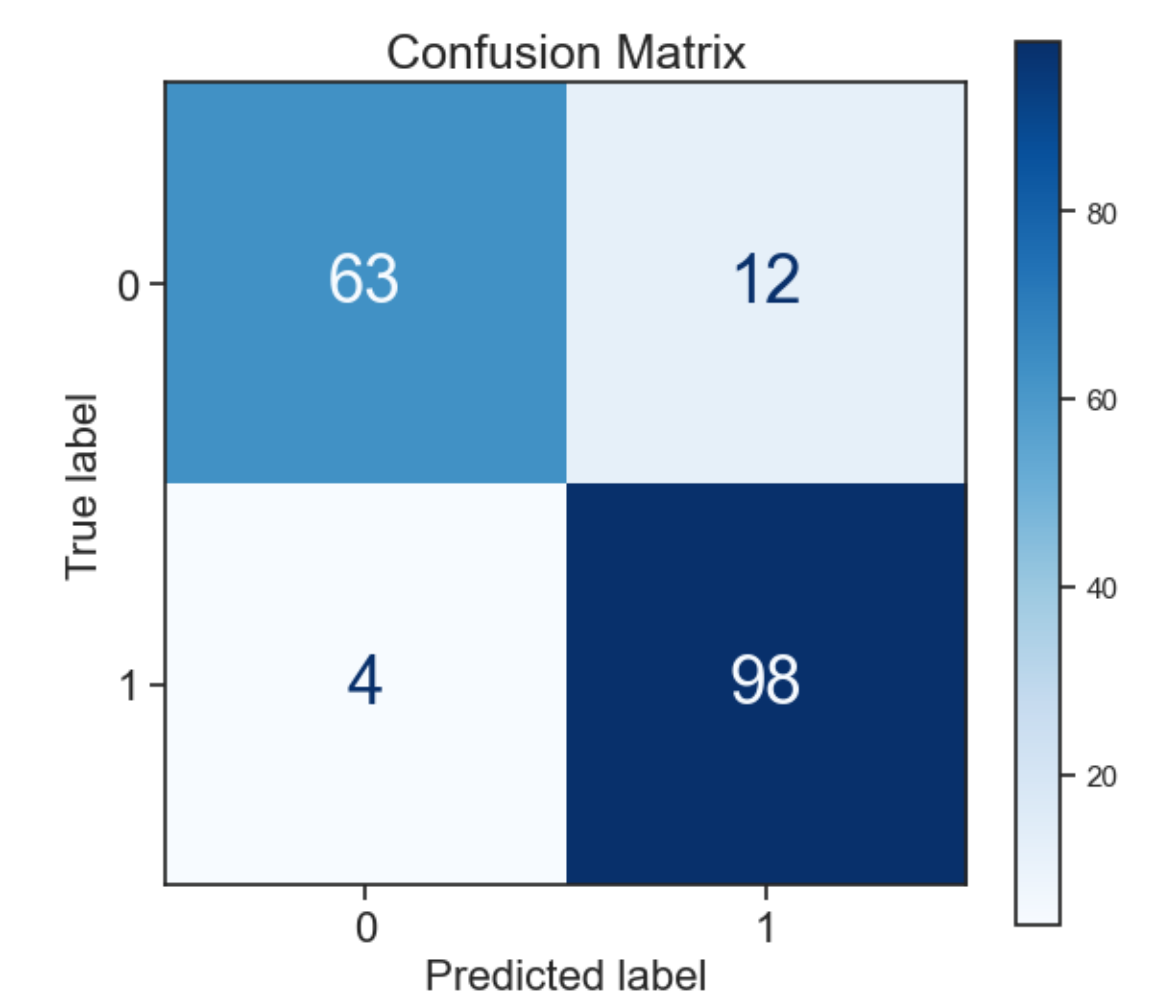
Metric	Train	Test
AUC	0.9998	0.9684
accuracy	0.9787	0.9096
balanced accuracy	0.975	0.9004
recall_(sens)	1.0	0.9608
specificity	0.95	0.84
precision	0.9643	0.8909
f1_score	0.9786	0.9088

Protein: P43681 - metric: f1

Total (train): 705

ROC curve

AUC_train = 0.999
AUC_test = 0.968
Random

Pareto Chart with Highlighted Best Attempt

Trials
Pareto Front Trials
Best Trial (# 1478)
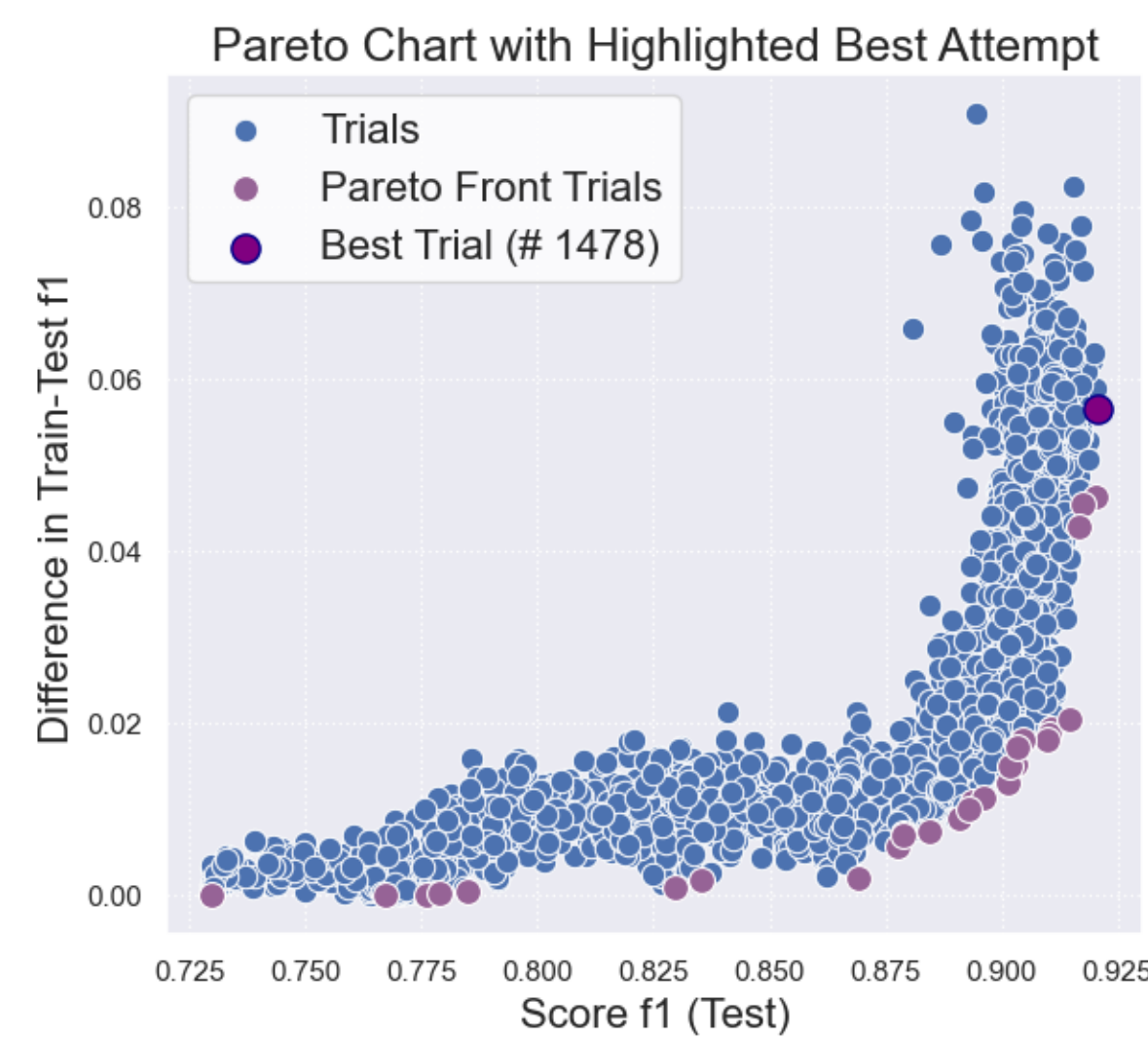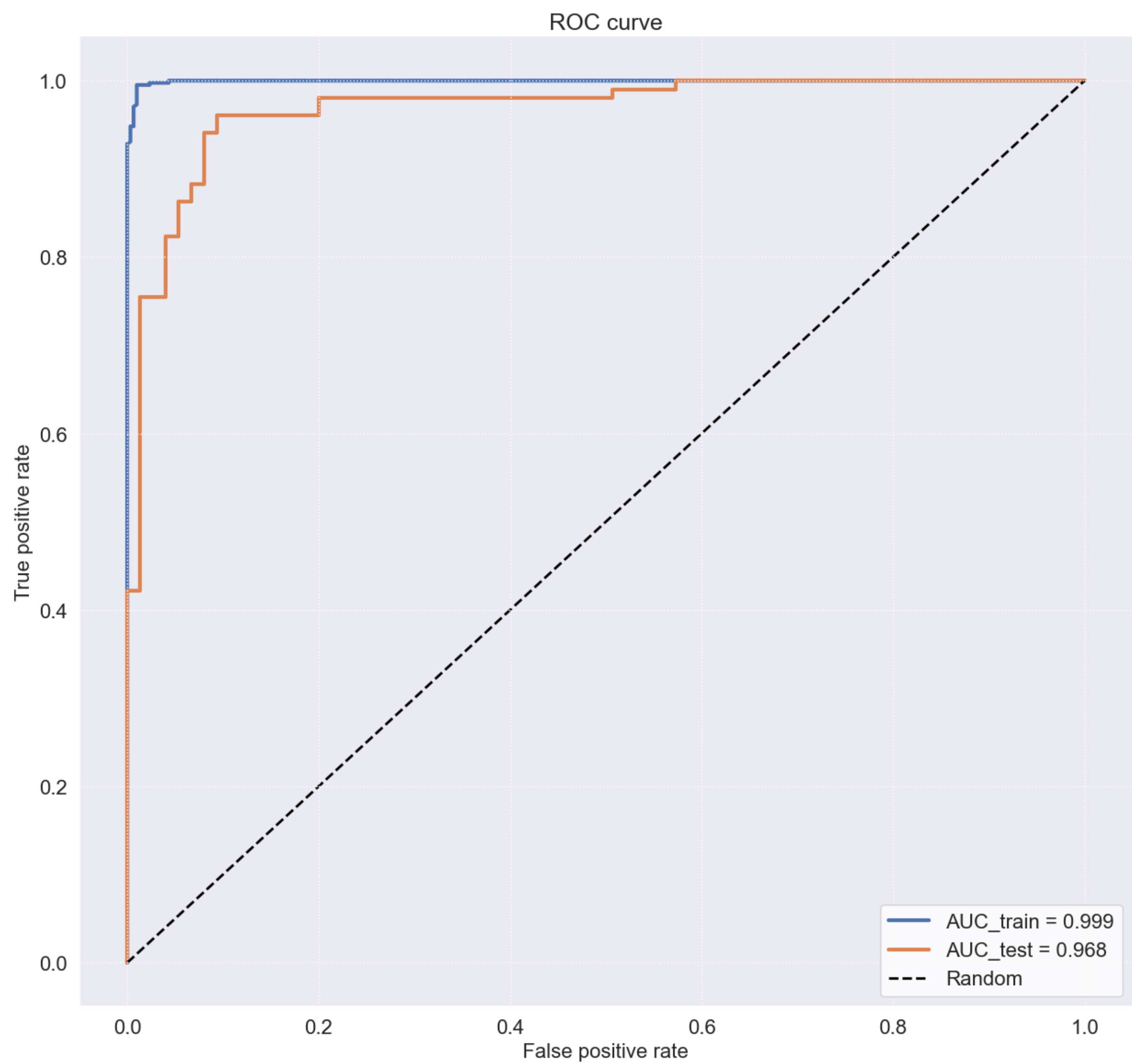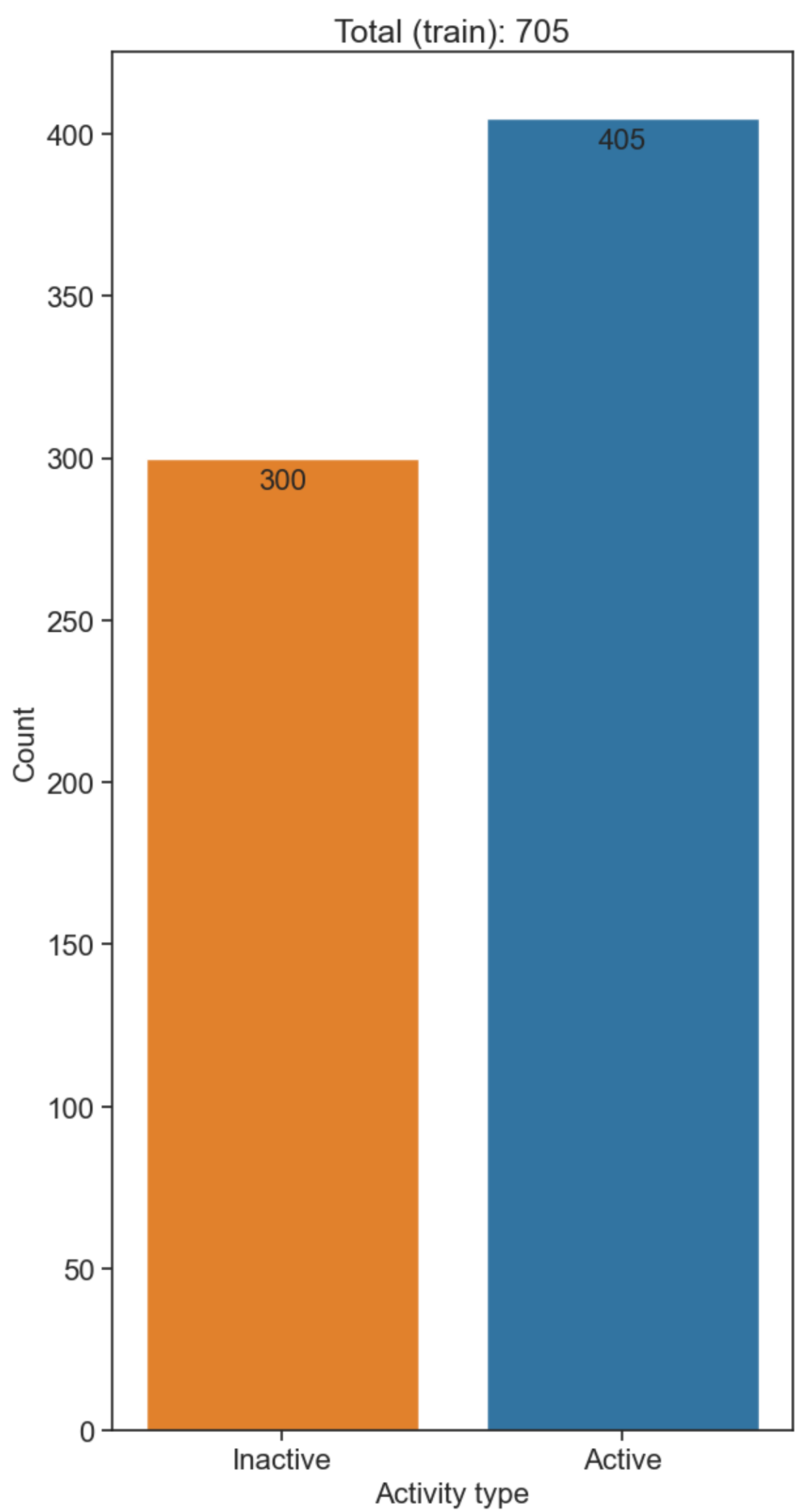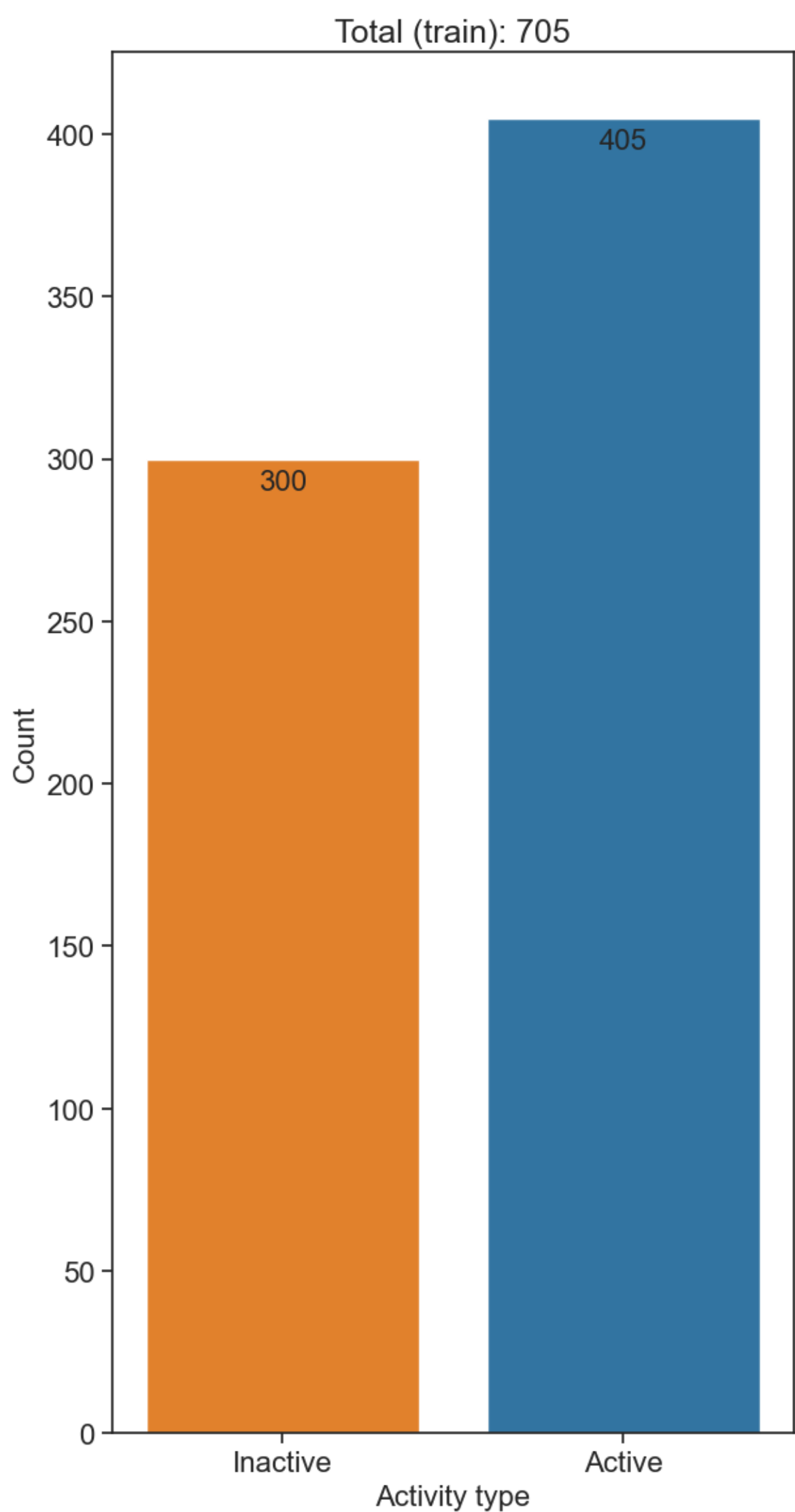
XGBoost Parameters	Value
alpha	2.5844
colsample_bytree	0.8194
gamma	0.329
lambda	4.2764
learning_rate	0.1369
max_depth	7.0
min_child_weight	3.0
n_estimators	759.0
reg_alpha	0.8019
reg_lambda	0.0172
scale_pos_weight	4.3846
subsample	0.8016

Confusion Matrix

Calibration curve

train: 0.0192
test: 0.0659
perfectly_calibrated

Confusion Matrix (nomr.)

Active/Inactive probability

type
active (102)
inactive (75)
decoy (177)
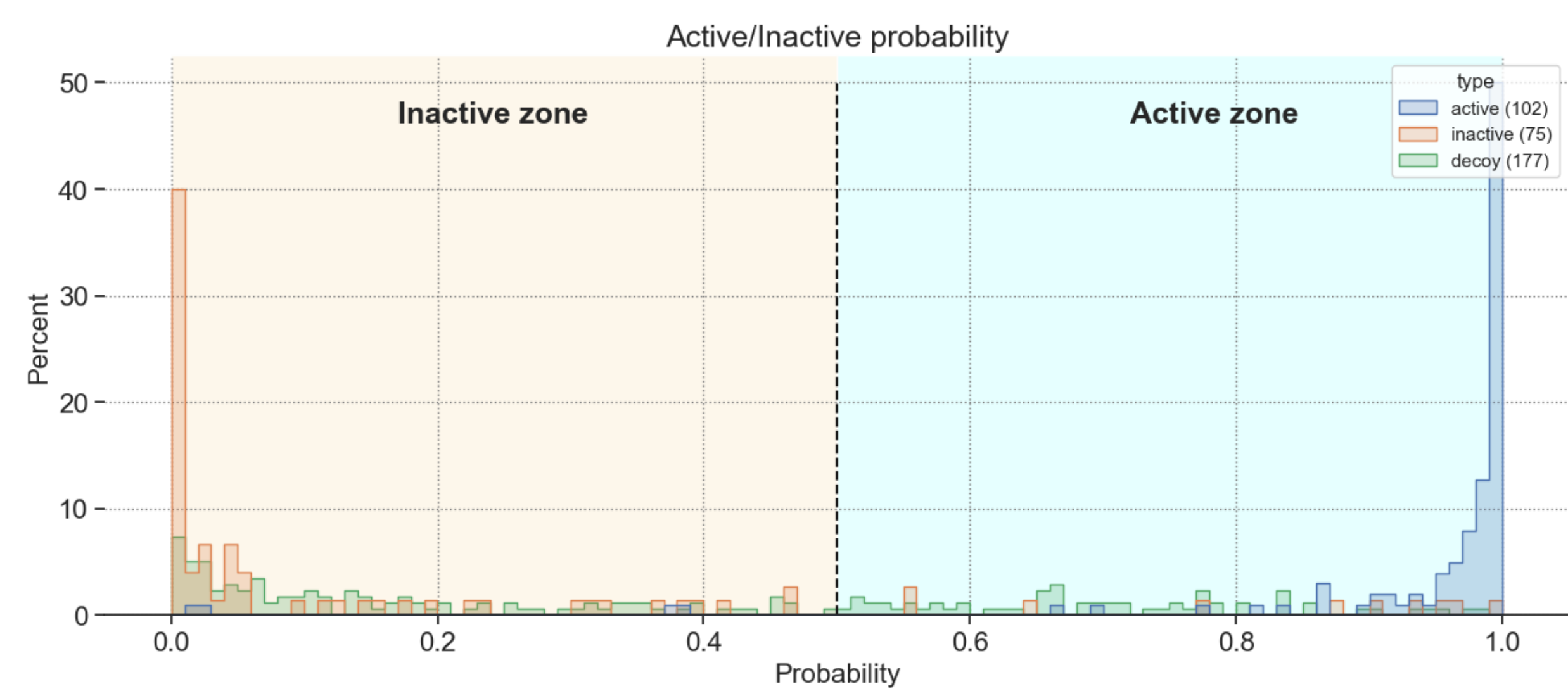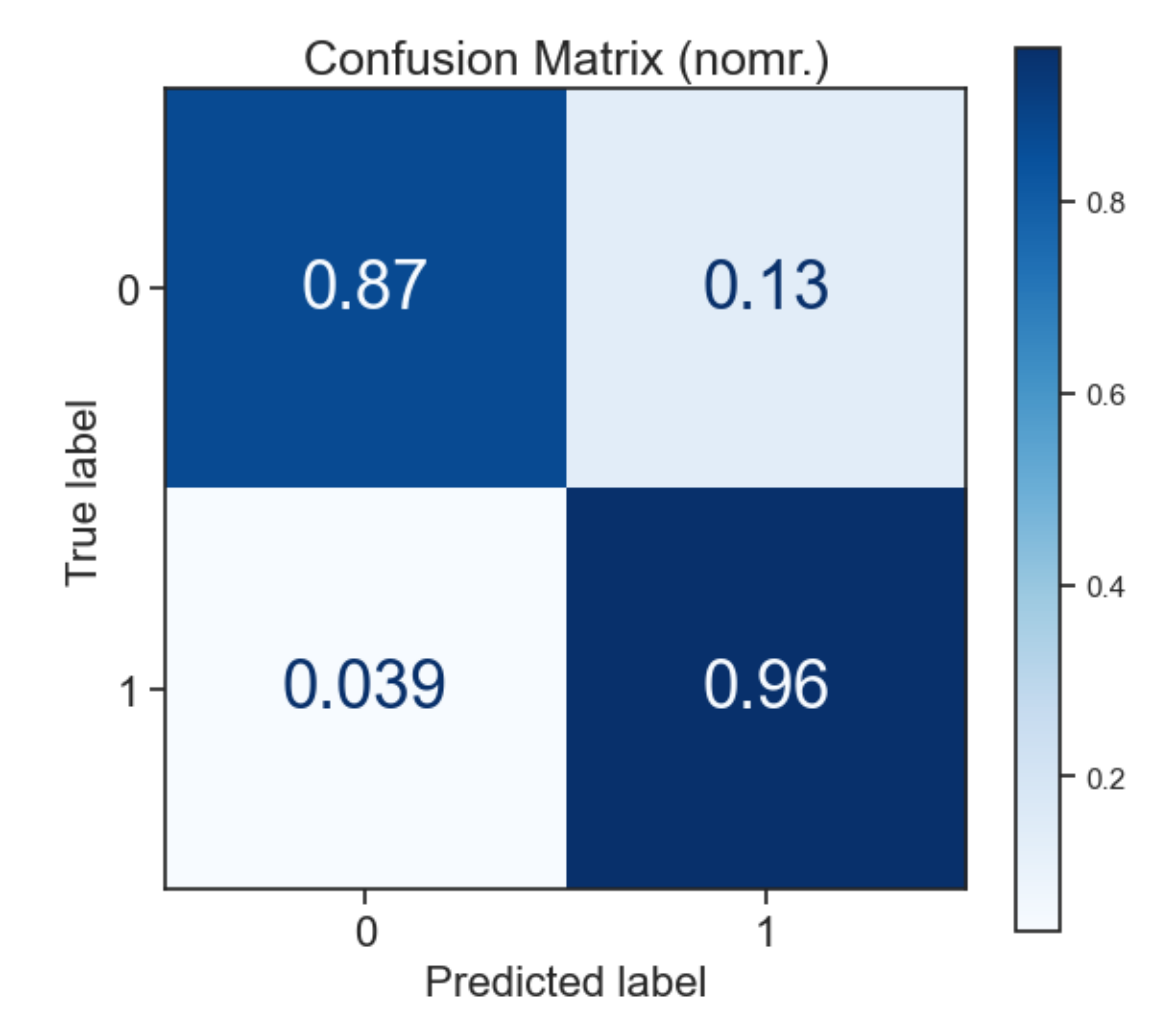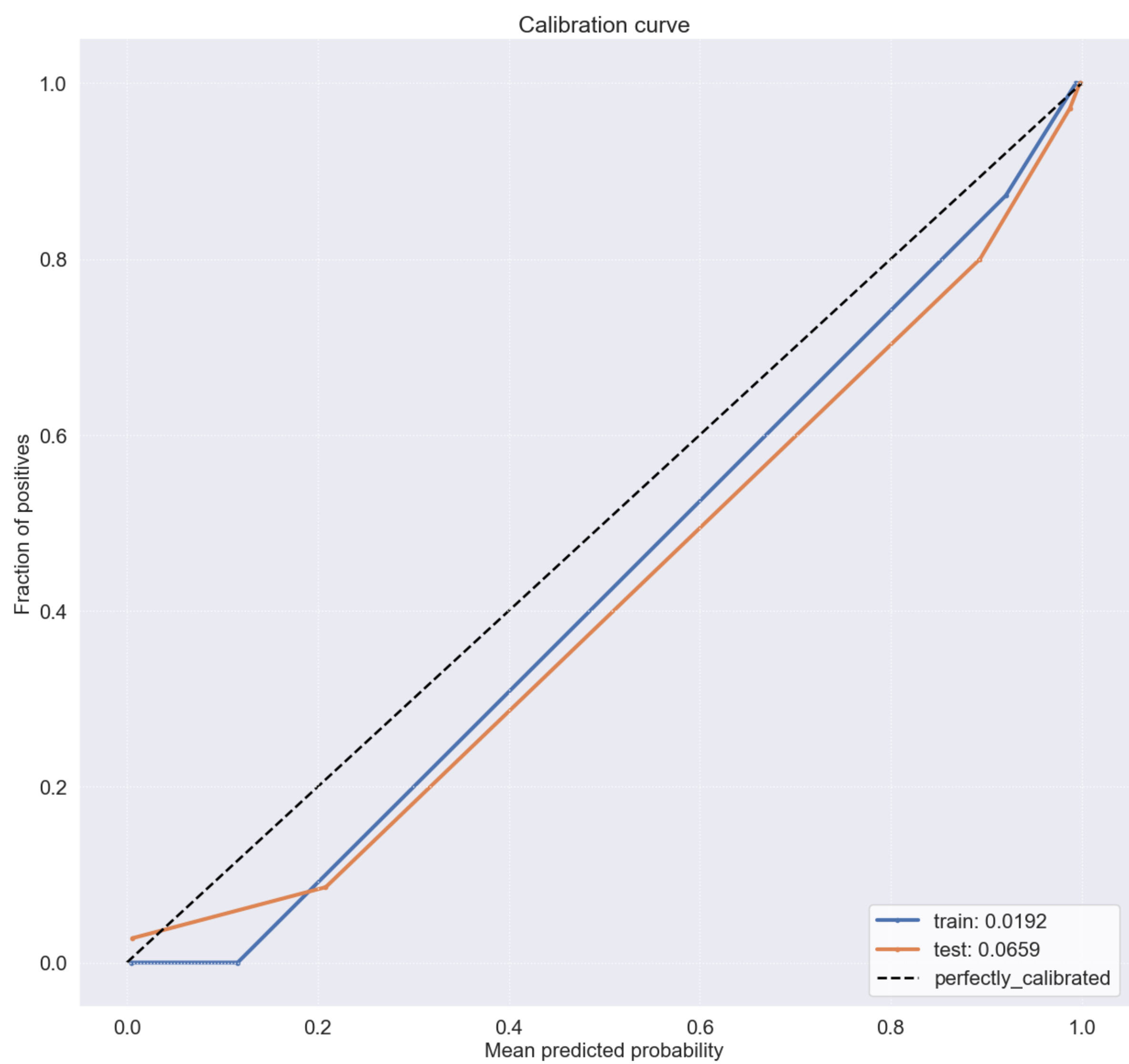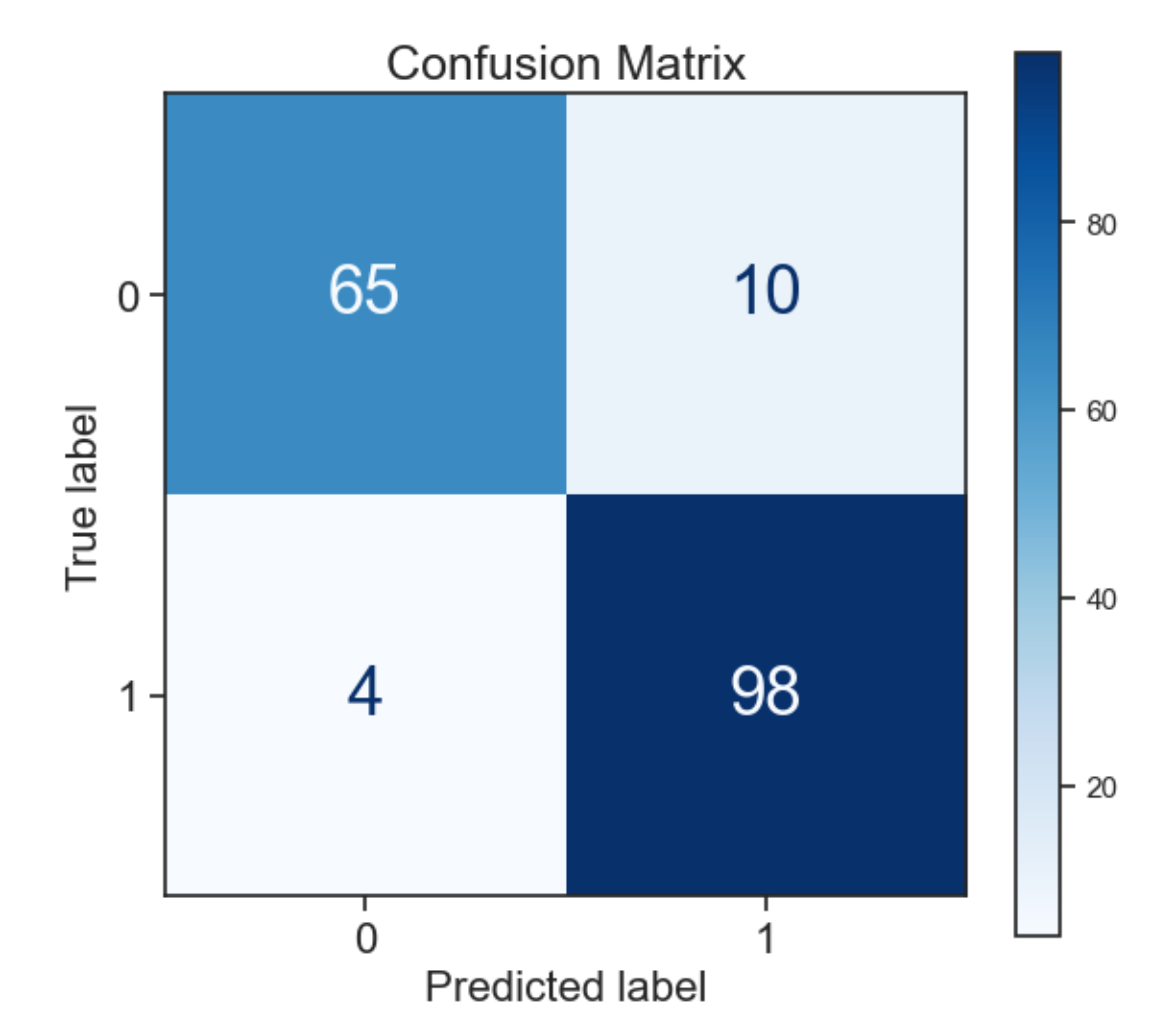
Metric	Train	Test
AUC	0.9994	0.9684
accuracy	0.9745	0.9209
balanced accuracy	0.97	0.9137
recall_(sens)	1.0	0.9608
specificity	0.94	0.8667
precision	0.9574	0.9074
f1_score	0.9744	0.9204

Protein: P43681 - metric: precision
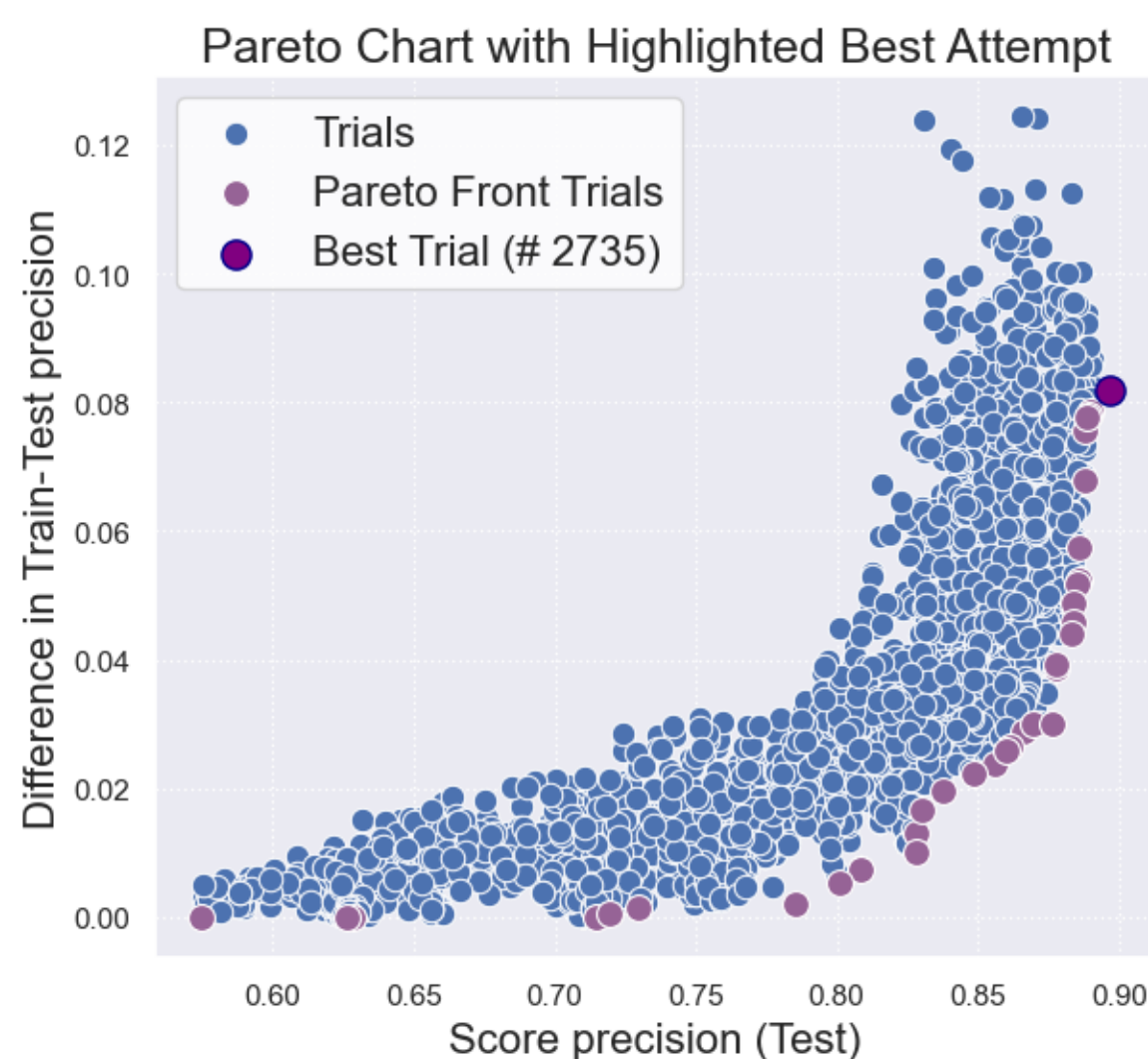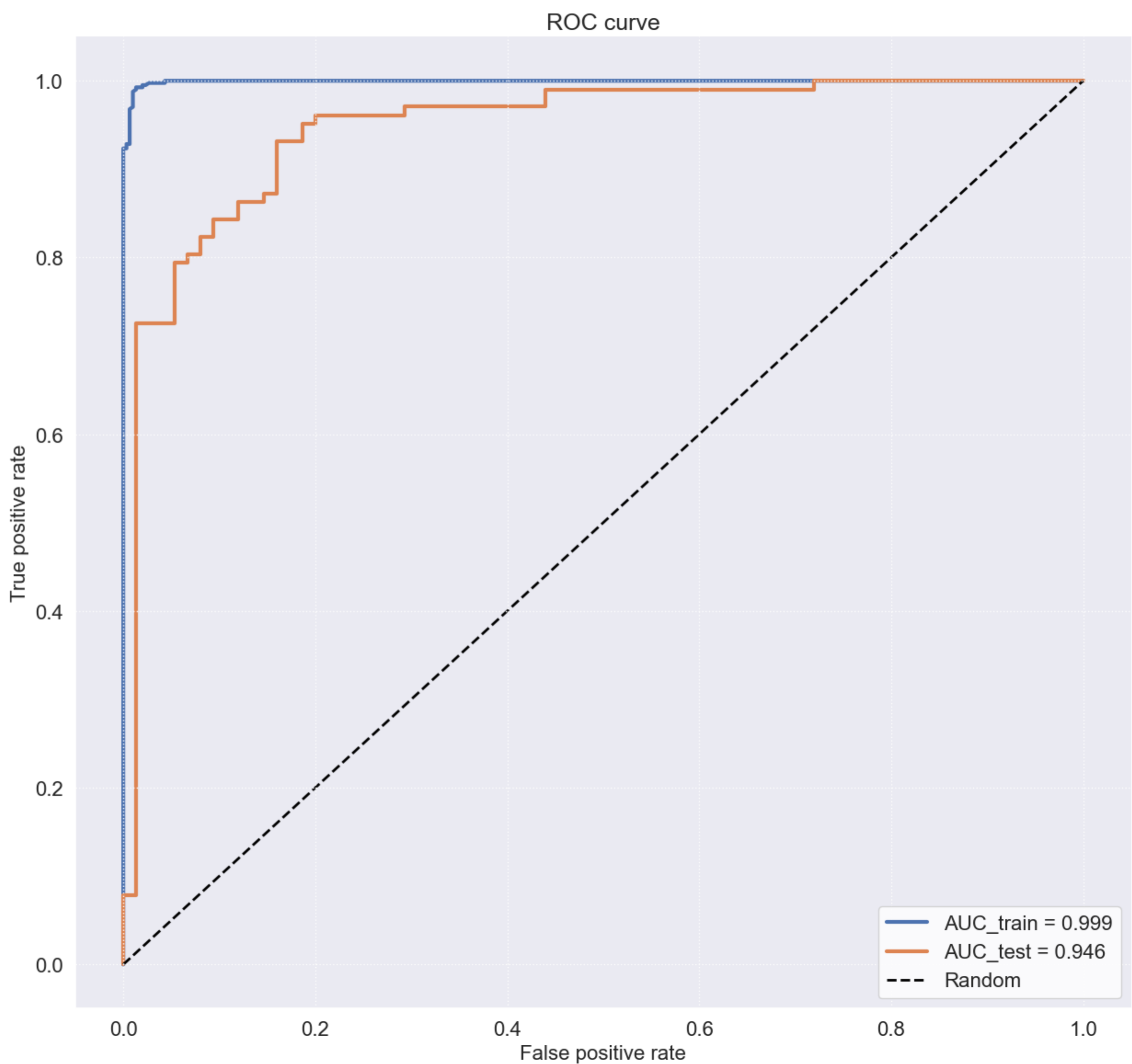
XGBoost Parameters	Value
alpha	3.8293
colsample_bytree	0.7898
gamma	0.7943
lambda	2.4134
learning_rate	0.5824
max_depth	10.0
min_child_weight	2.0
n_estimators	462.0
reg_alpha	0.1484
reg_lambda	0.0491
scale_pos_weight	1.7222
subsample	0.5384
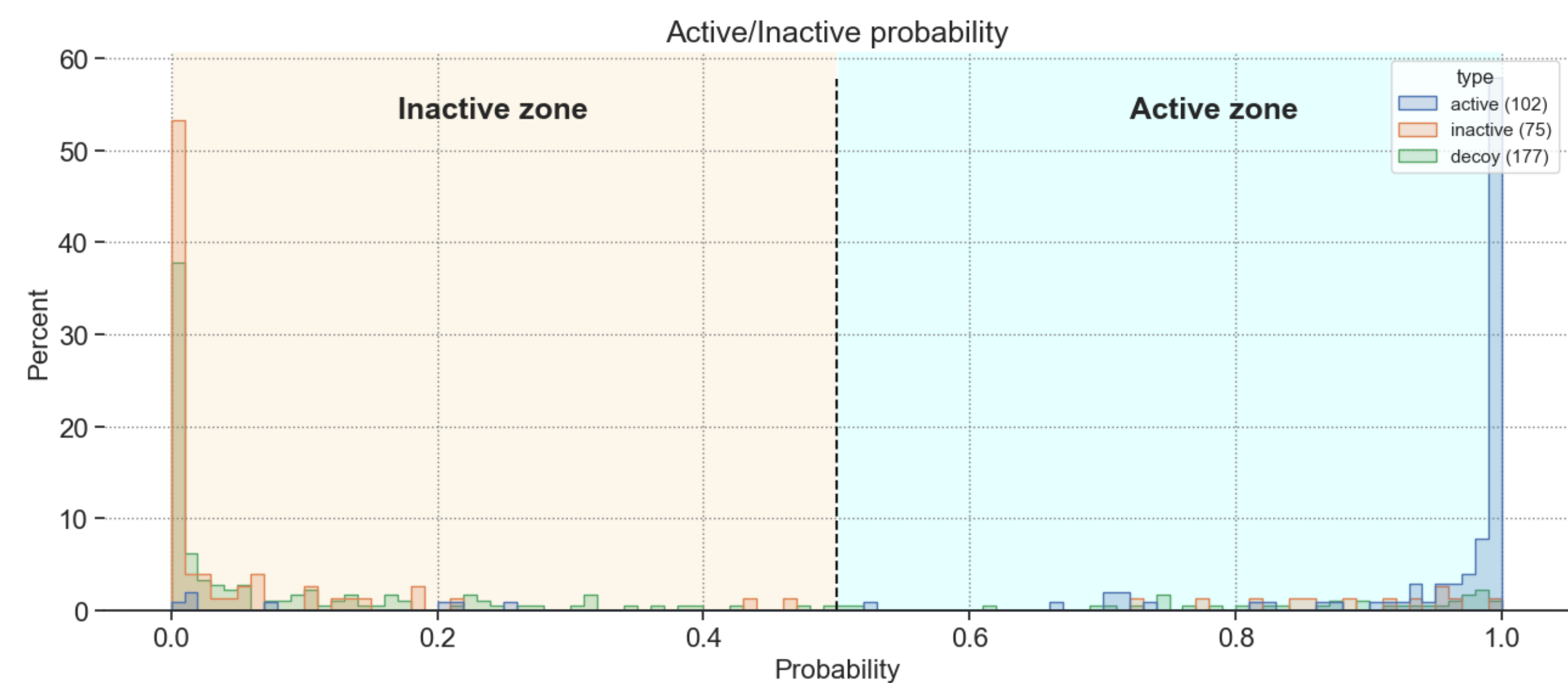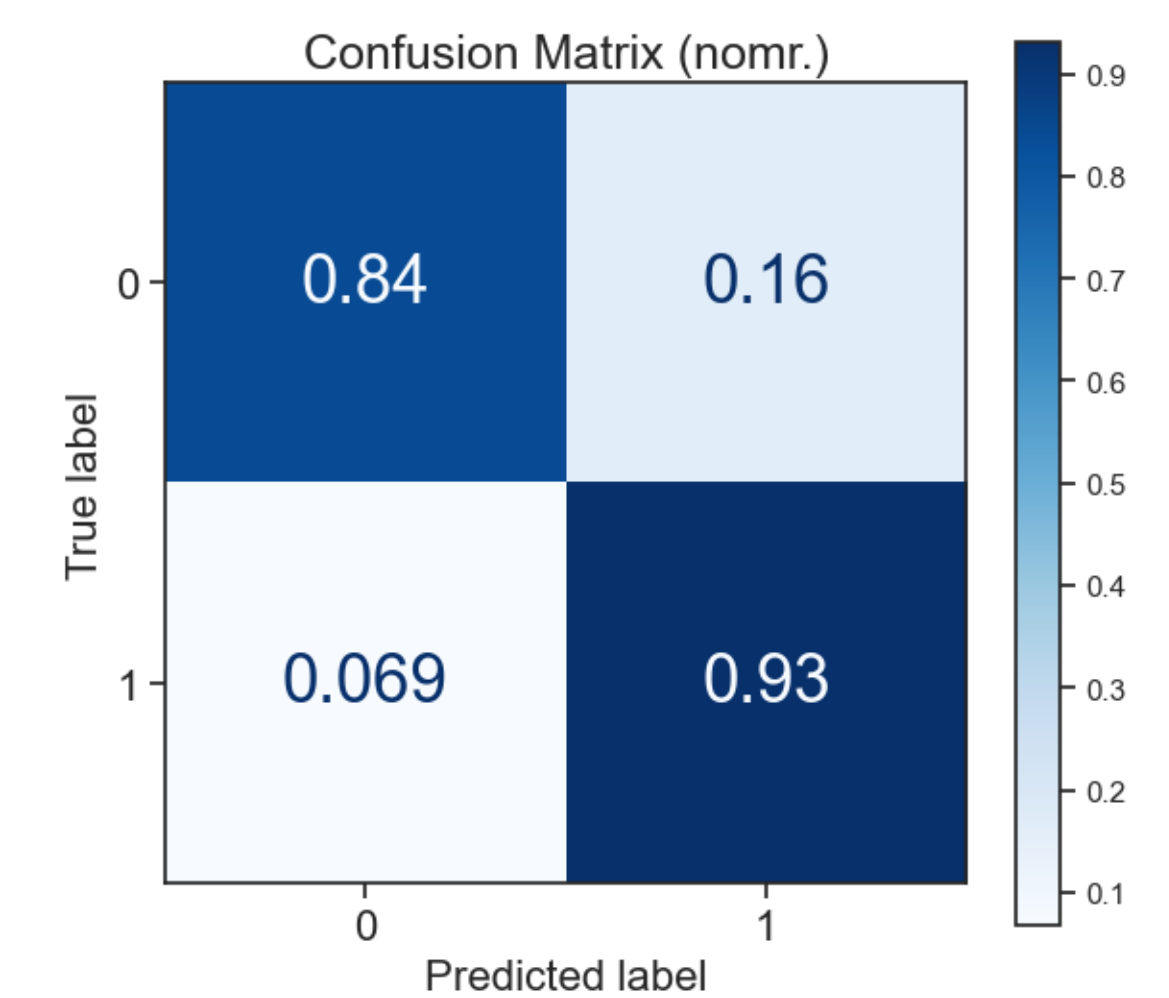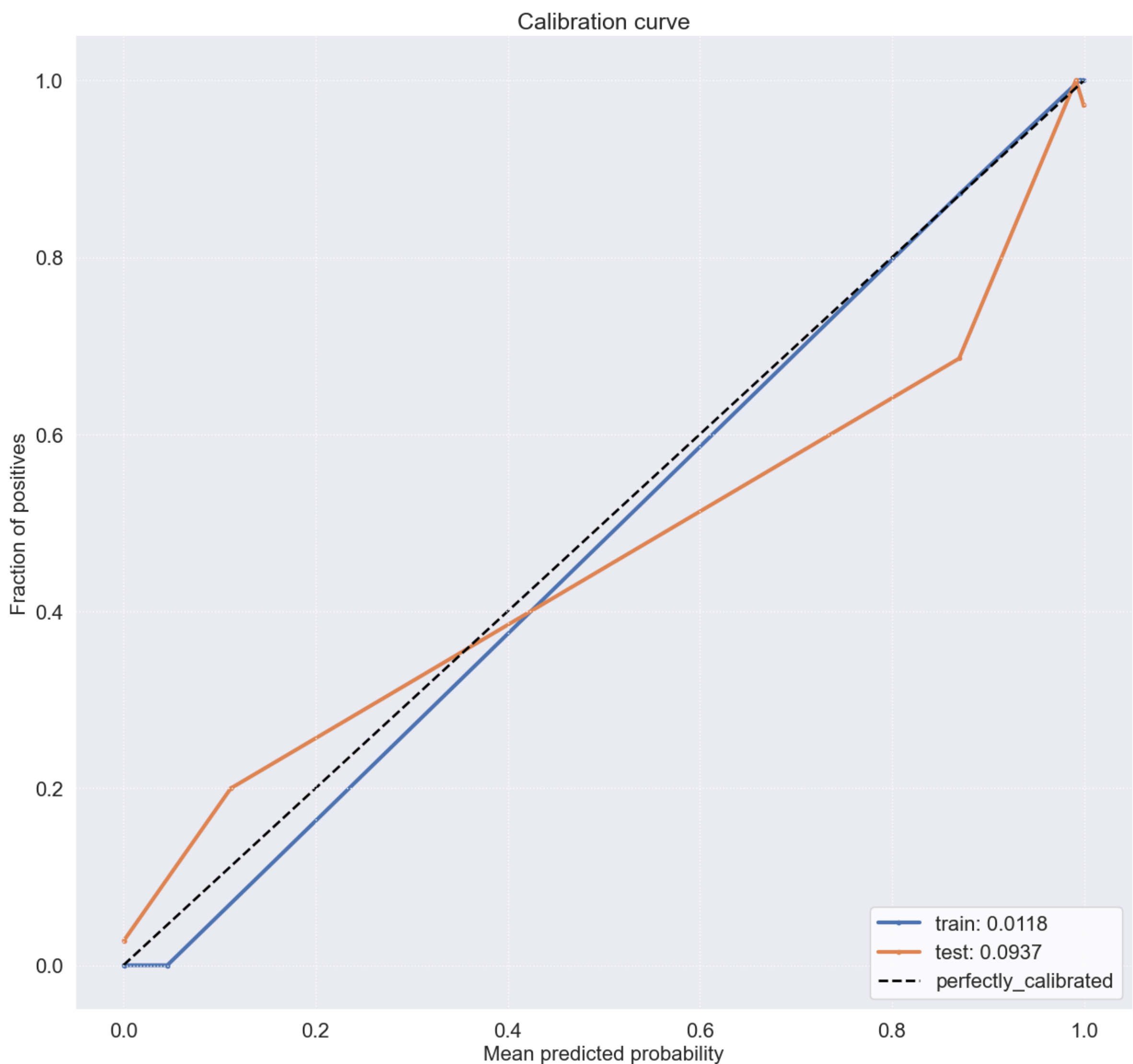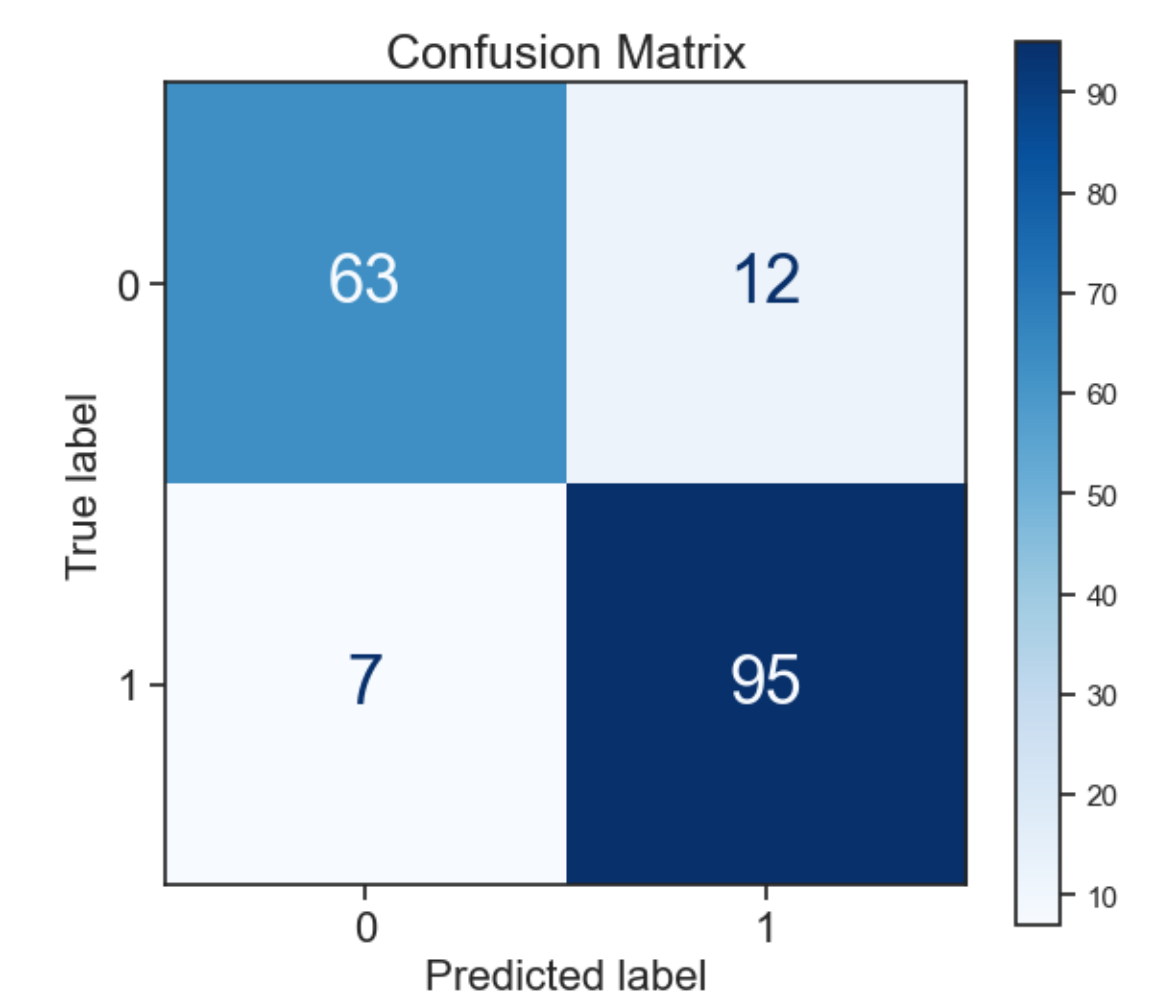
Metric	Train	Test
AUC	0.9992	0.9463
accuracy	0.9887	0.8927
balanced accuracy	0.9875	0.8857
recall_(sens)	0.9951	0.9314
specificity	0.98	0.84
precision	0.9853	0.8879
f1_score	0.9886	0.8921

Protein: P43681 - metric: SoftVotingXGBoostEnsemble
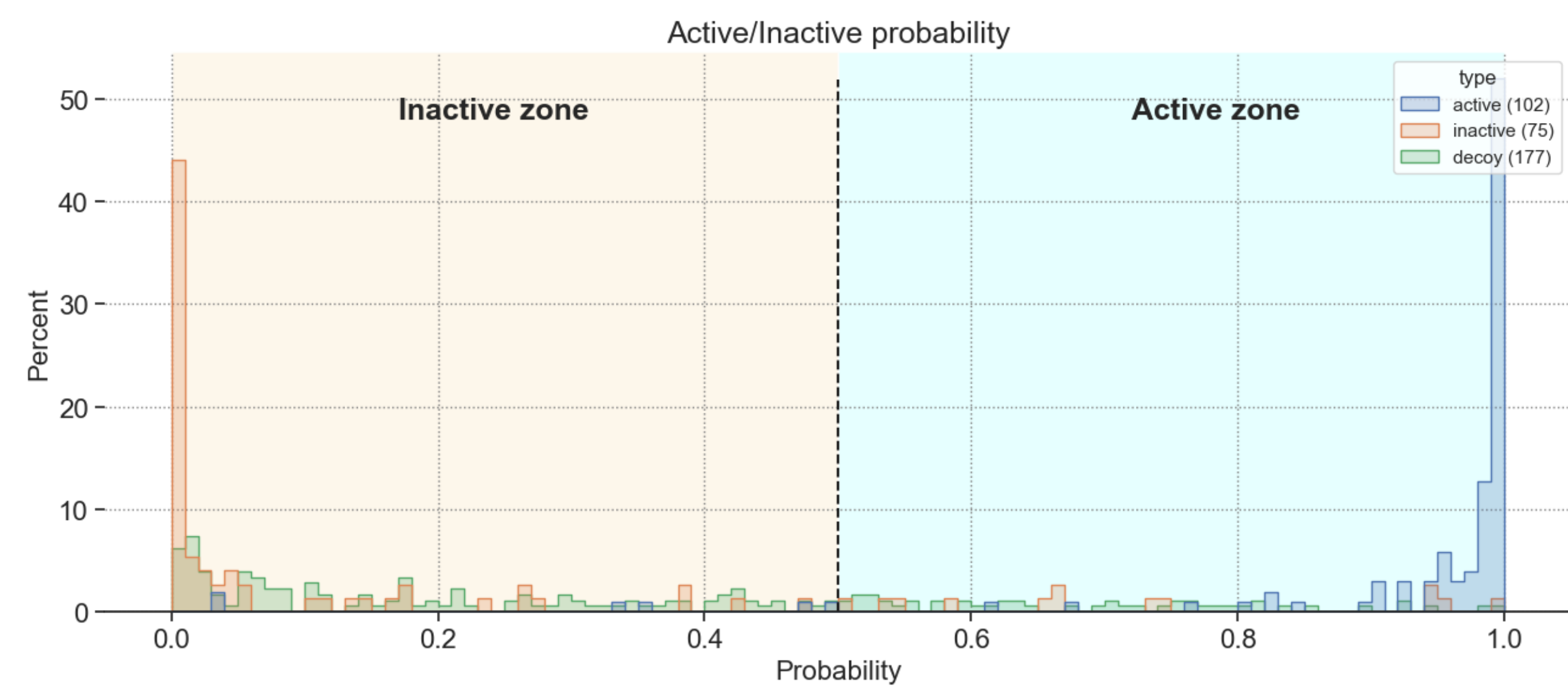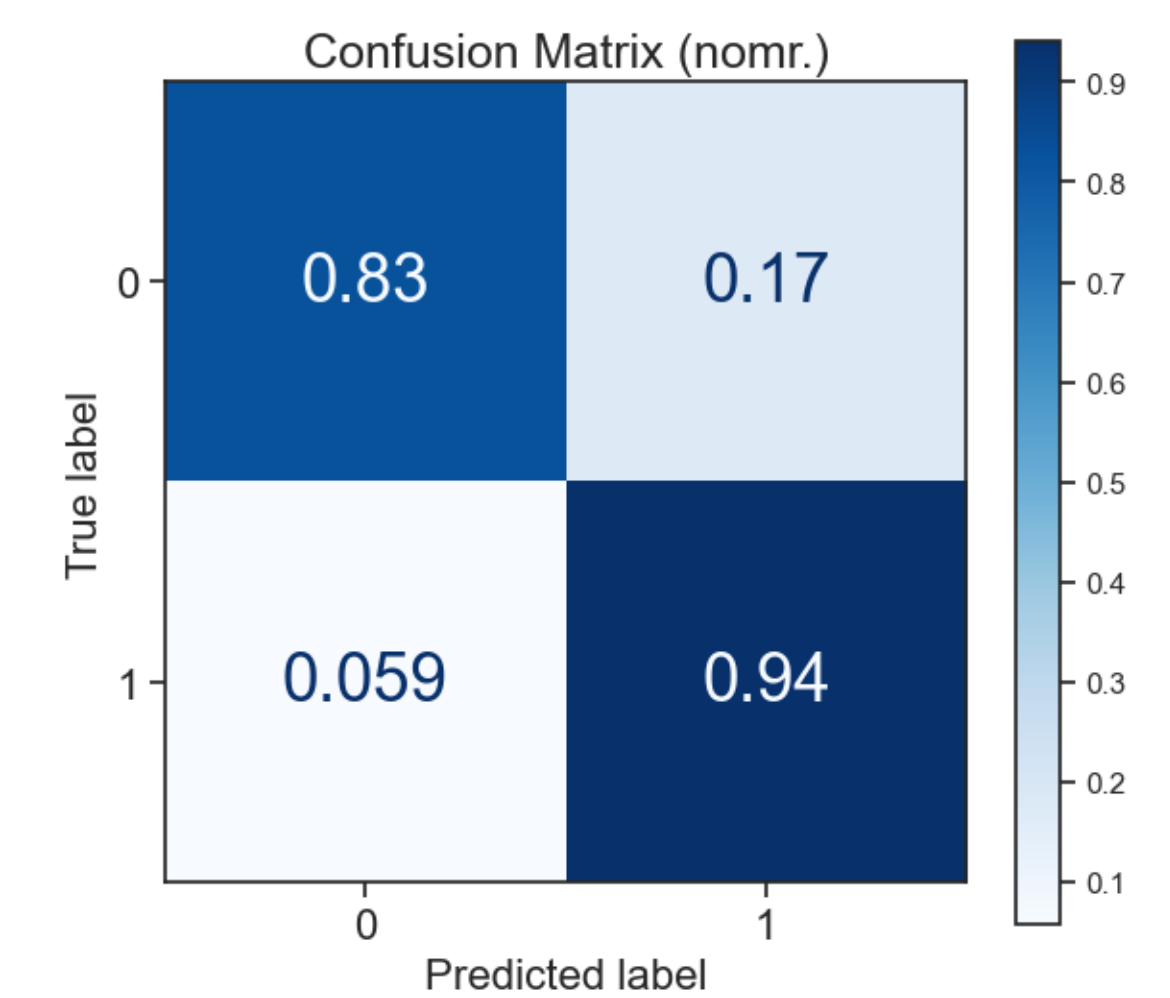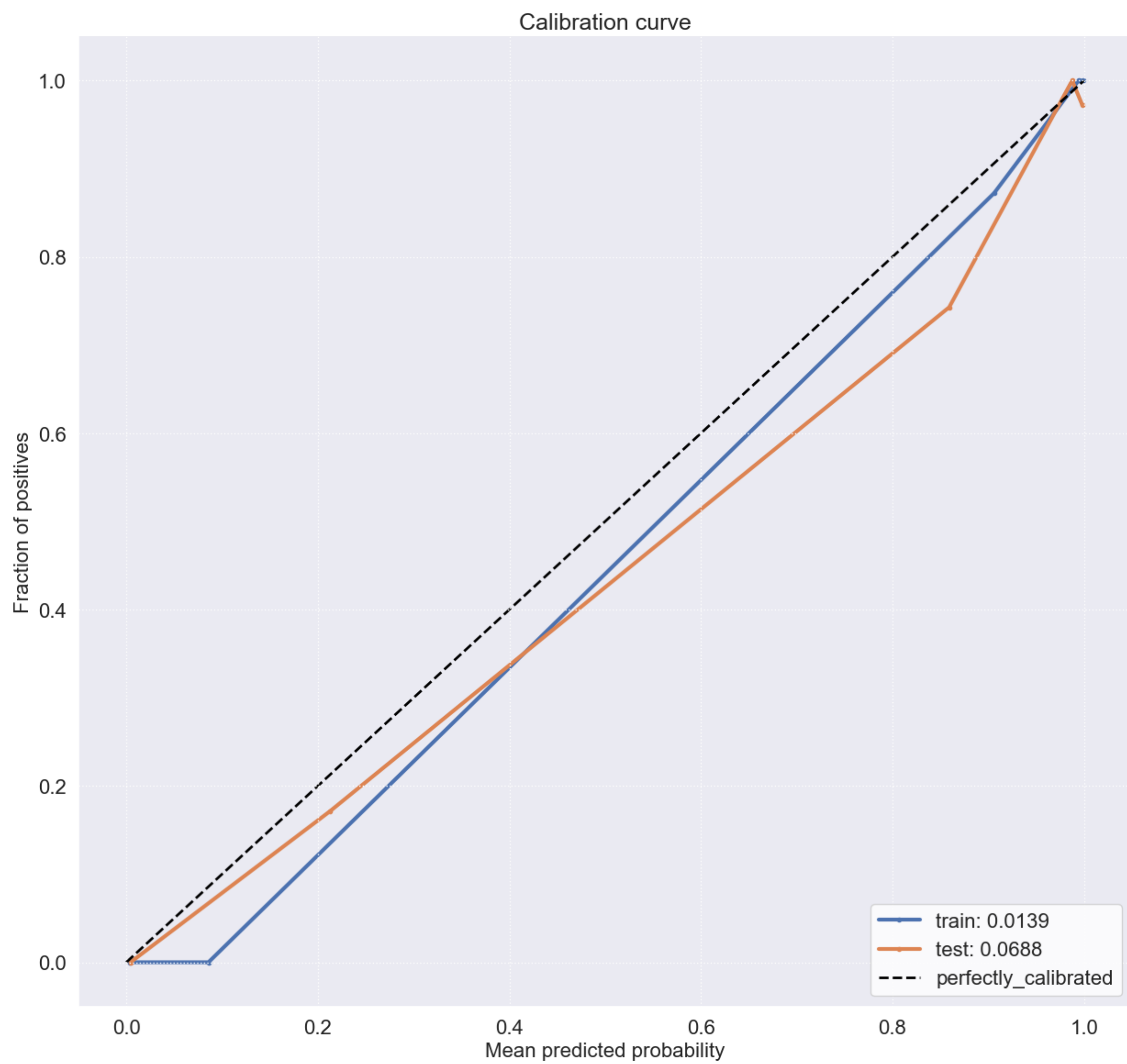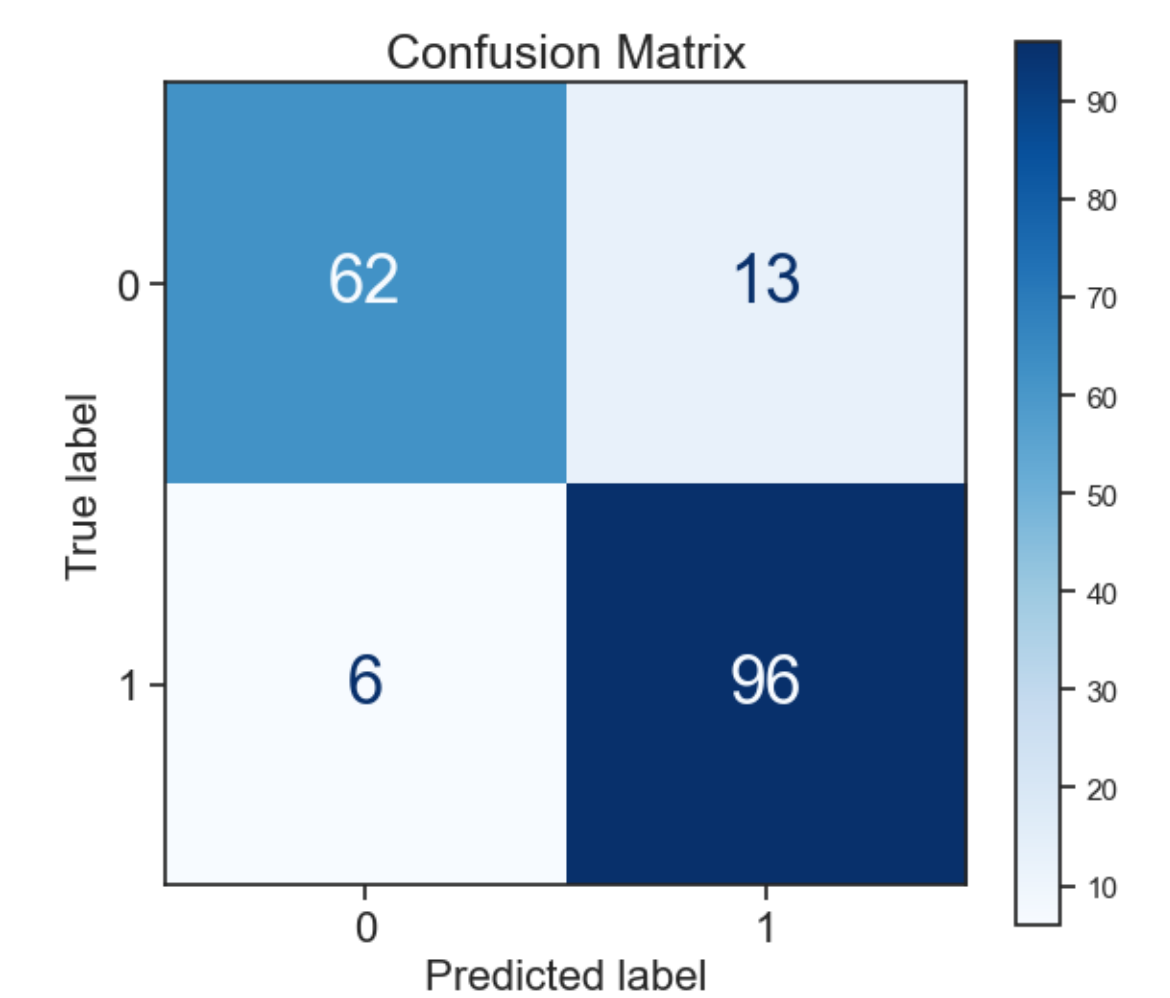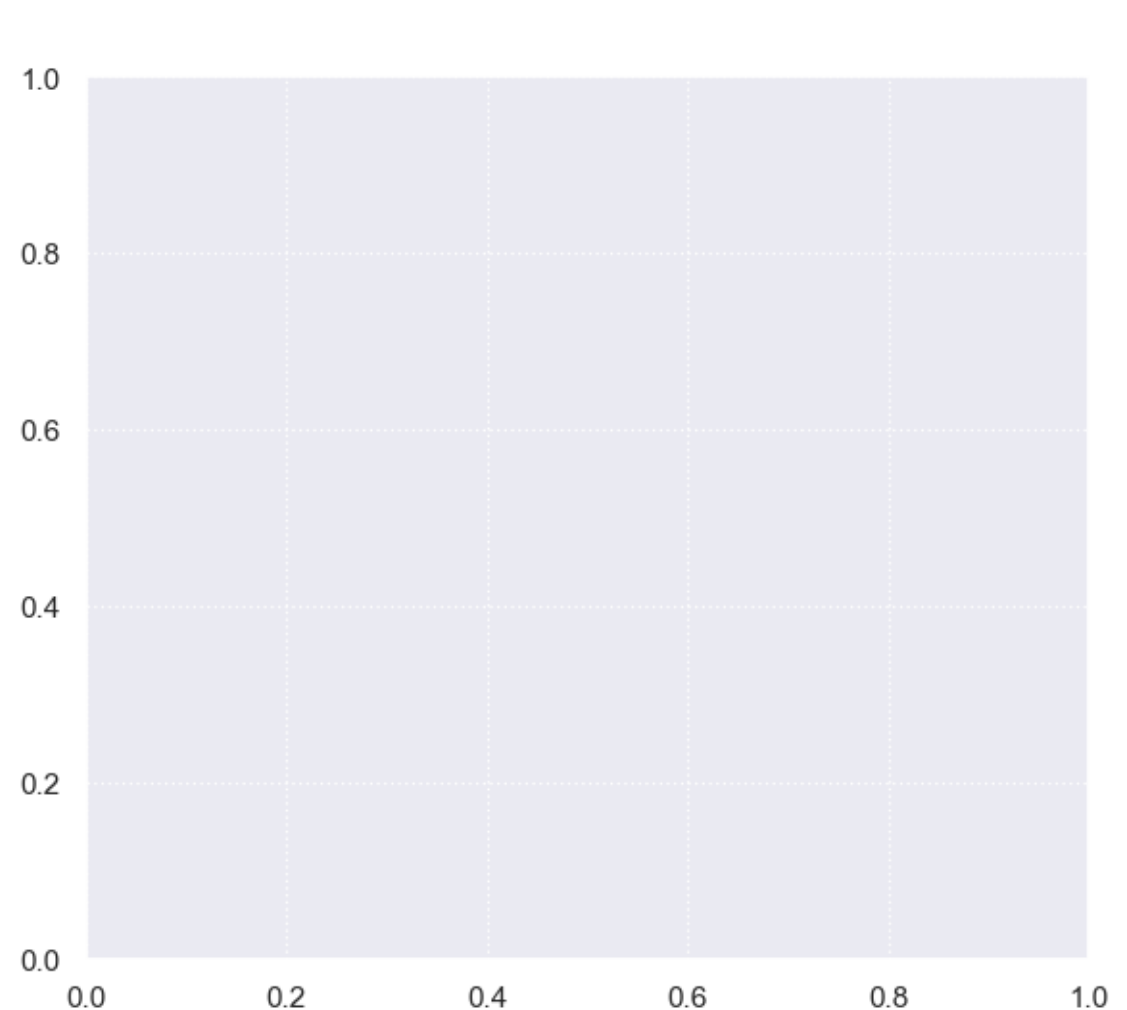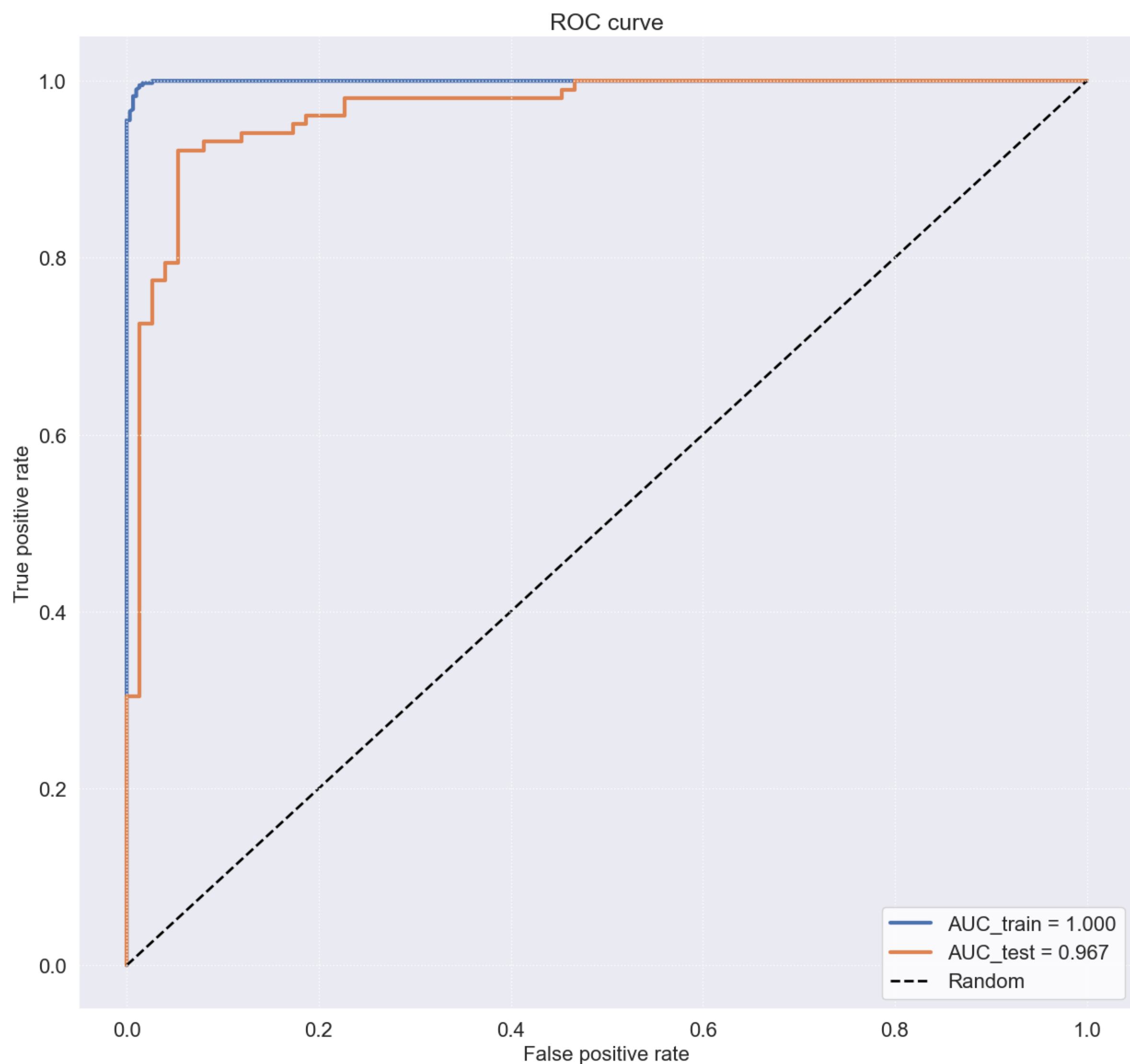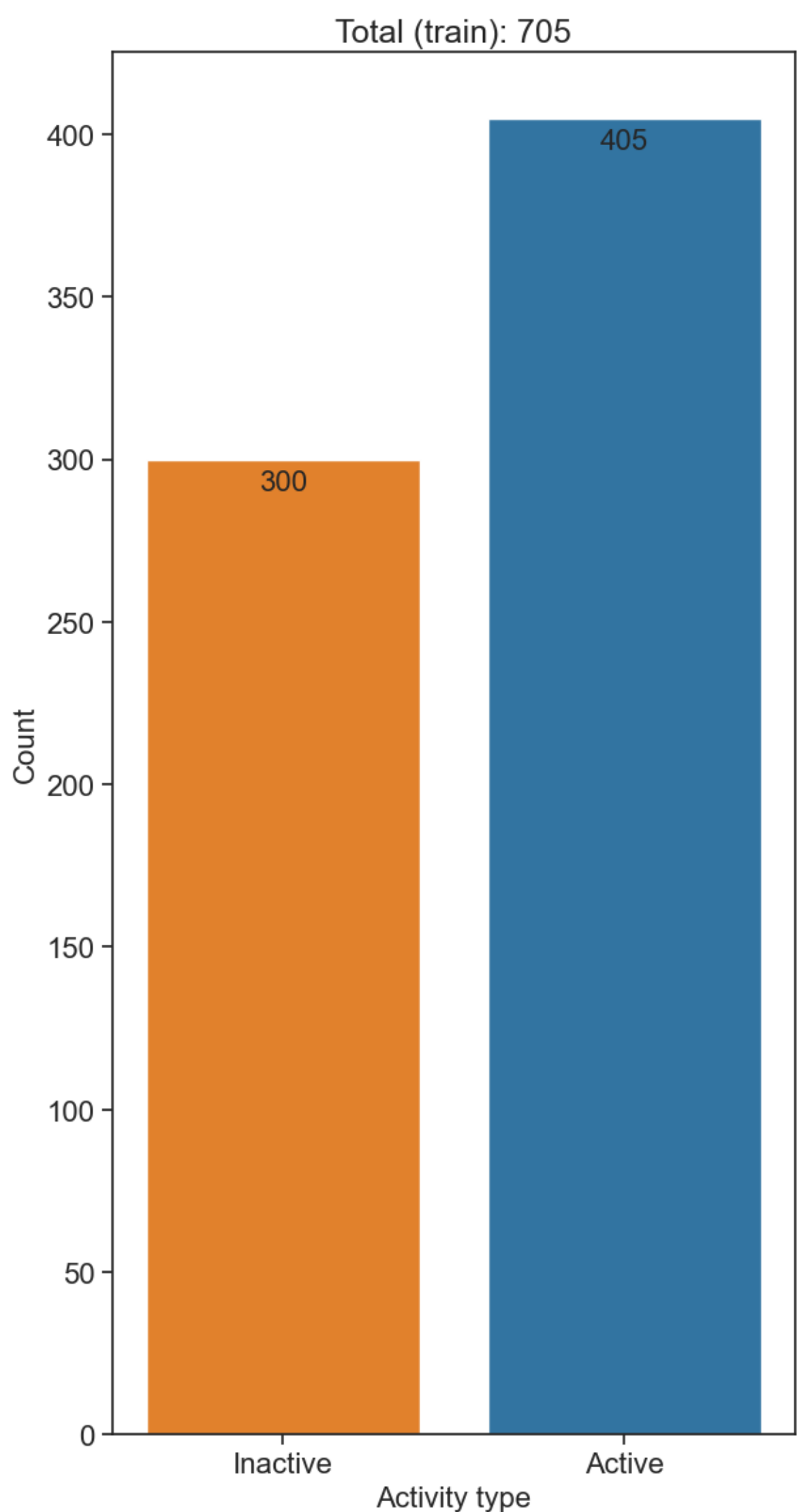
Metric	Train	Test
AUC	0.9996	0.9665
accuracy	0.983	0.8927
balanced accuracy	0.98	0.8839
recall_(sens)	1.0	0.9412
specificity	0.96	0.8267
precision	0.9712	0.8807
f1_score	0.9829	0.8918