Protein: P06276 - metric: balanced_accuracy

Total (train): 1592 — bar chart showing Inactive (533) and Active (1059) counts.

ROC curve — AUC_train = 1.000, AUC_test = 0.970, Random.

**Pareto Chart with Highlighted Best Attempt** — Trials, Pareto Front Trials, Best Trial (# 1209).

Confusion Matrix

	Predicted 0	Predicted 1
True 0	114	19
True 1	15	251

Confusion Matrix (nomr.)

	Predicted 0	Predicted 1
True 0	0.86	0.14
True 1	0.056	0.94

Calibration curve — train: 0.0023, test: 0.0657, perfectly_calibrated.

Active/Inactive probability — Inactive zone, Active zone; type: active (266), inactive (133), decoy (399).

XGBoost Parameters	Value
alpha	1.6131
colsample_bytree	0.9023
gamma	0.0009
lambda	2.9916
learning_rate	0.175
max_depth	10.0
min_child_weight	2.0
n_estimators	680.0
reg_alpha	0.1941
reg_lambda	0.4153
scale_pos_weight	1.7258
subsample	0.9361
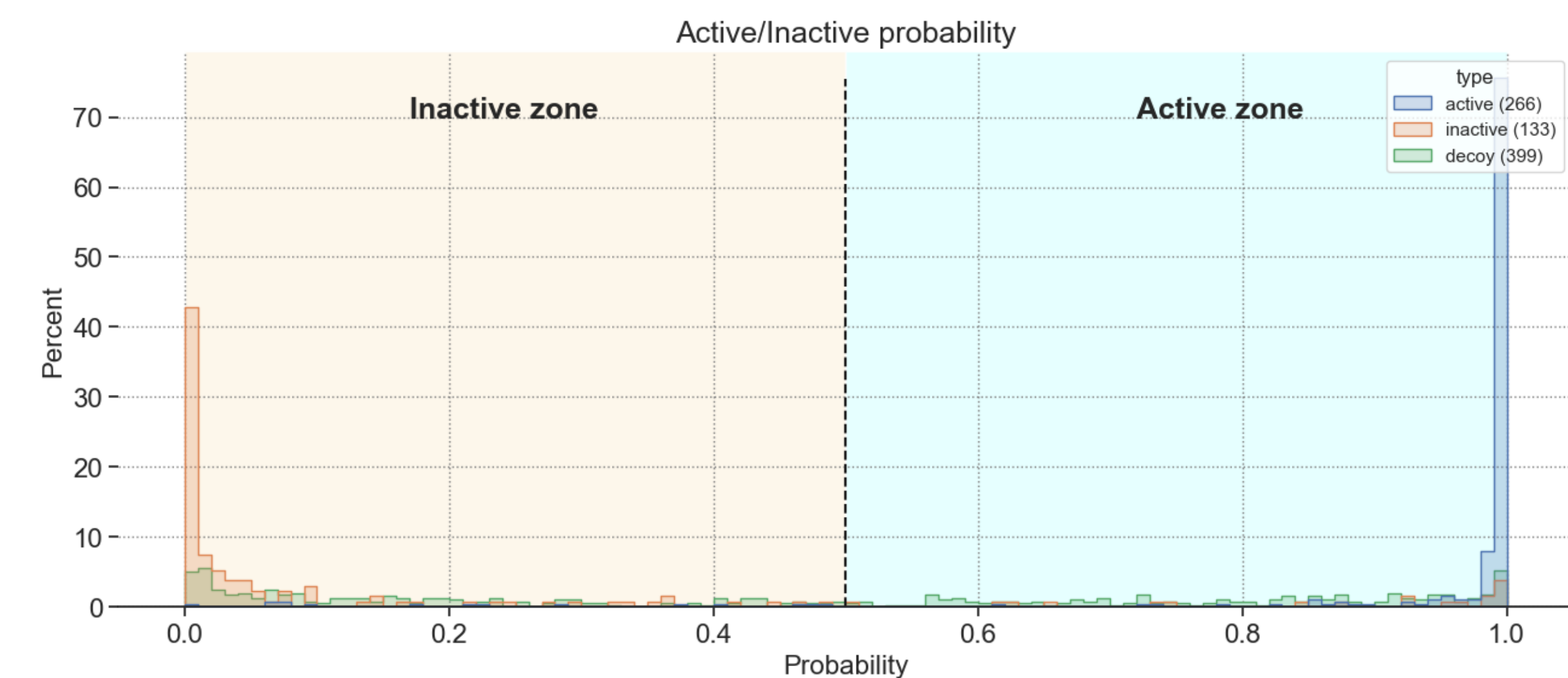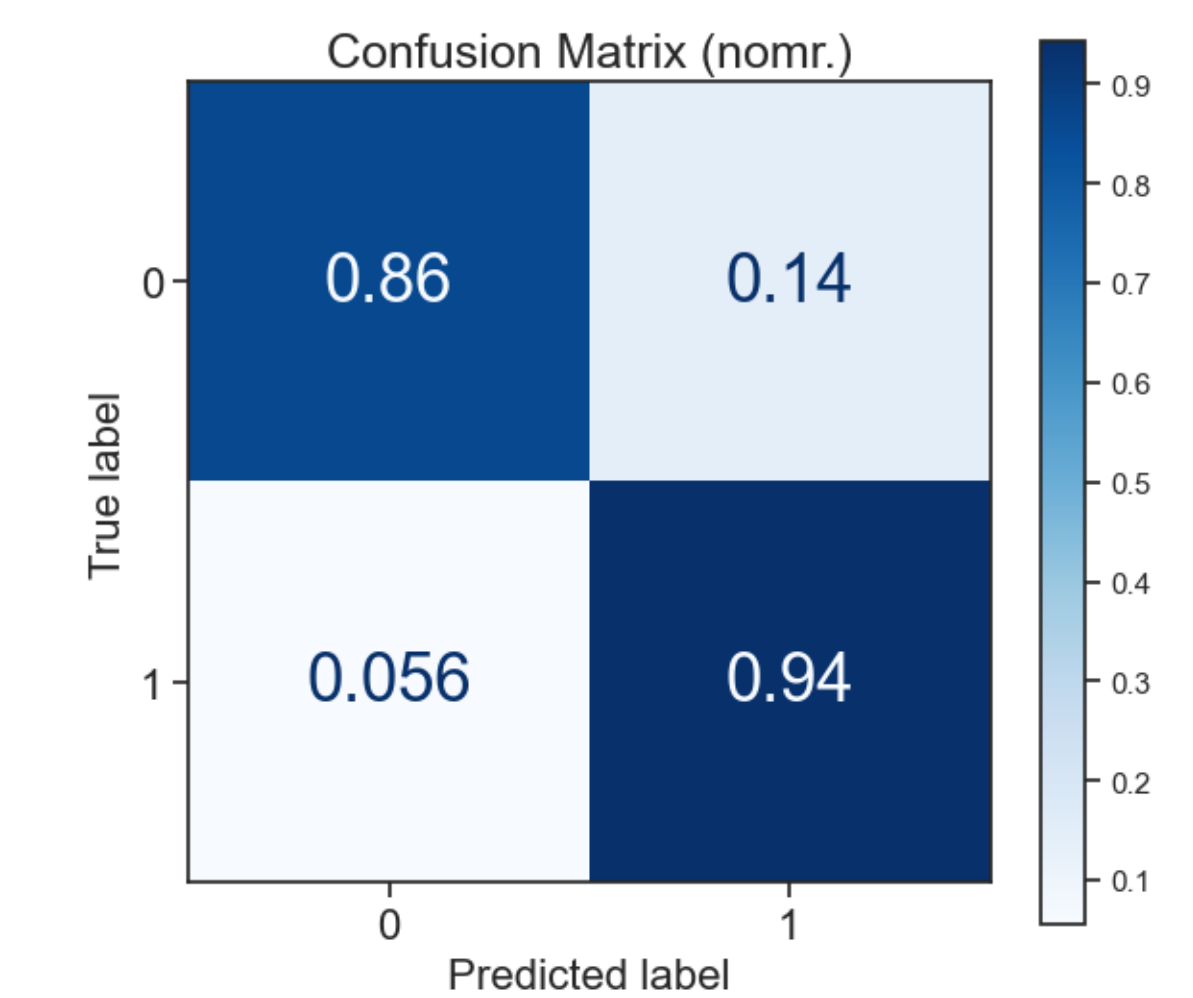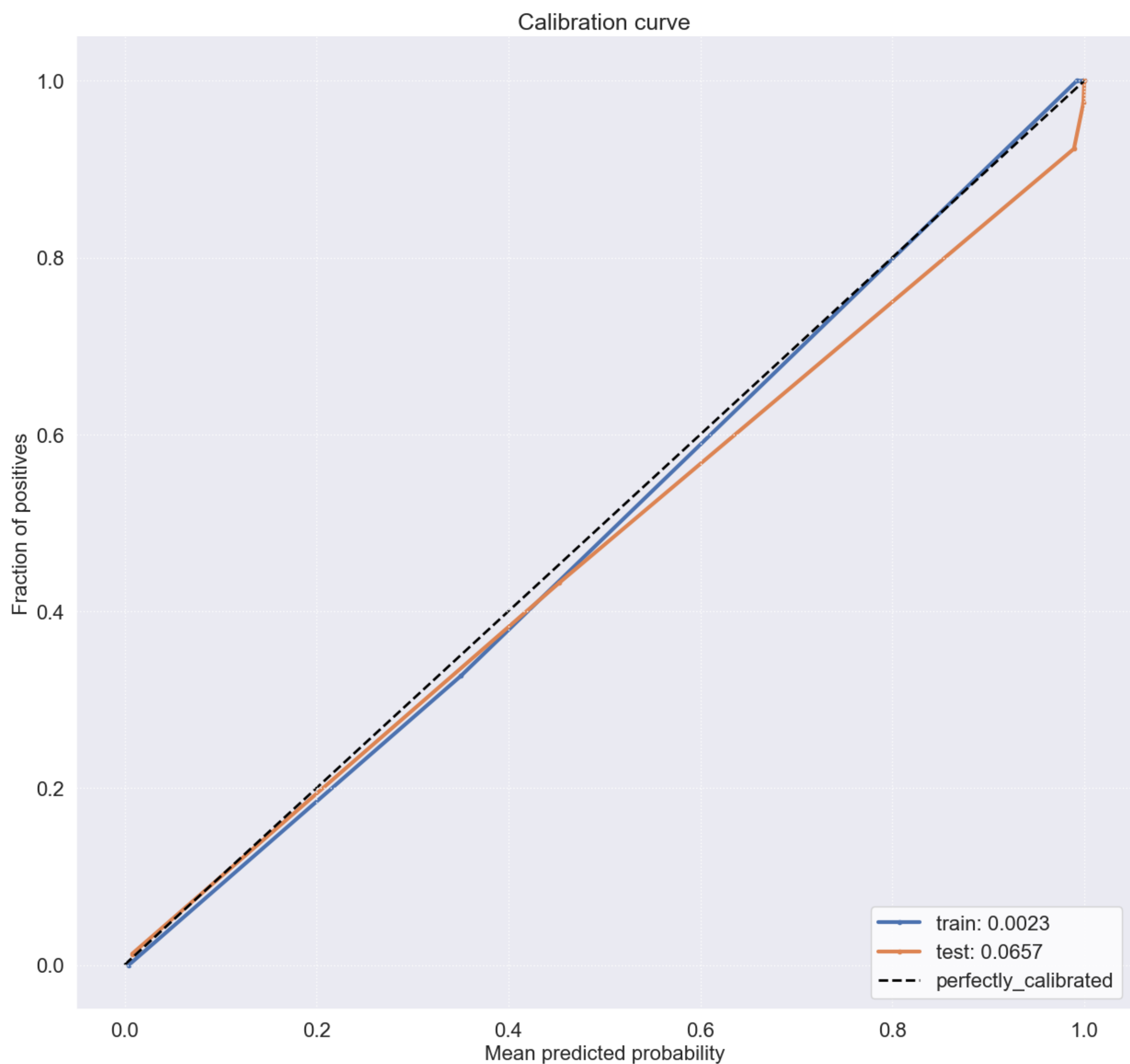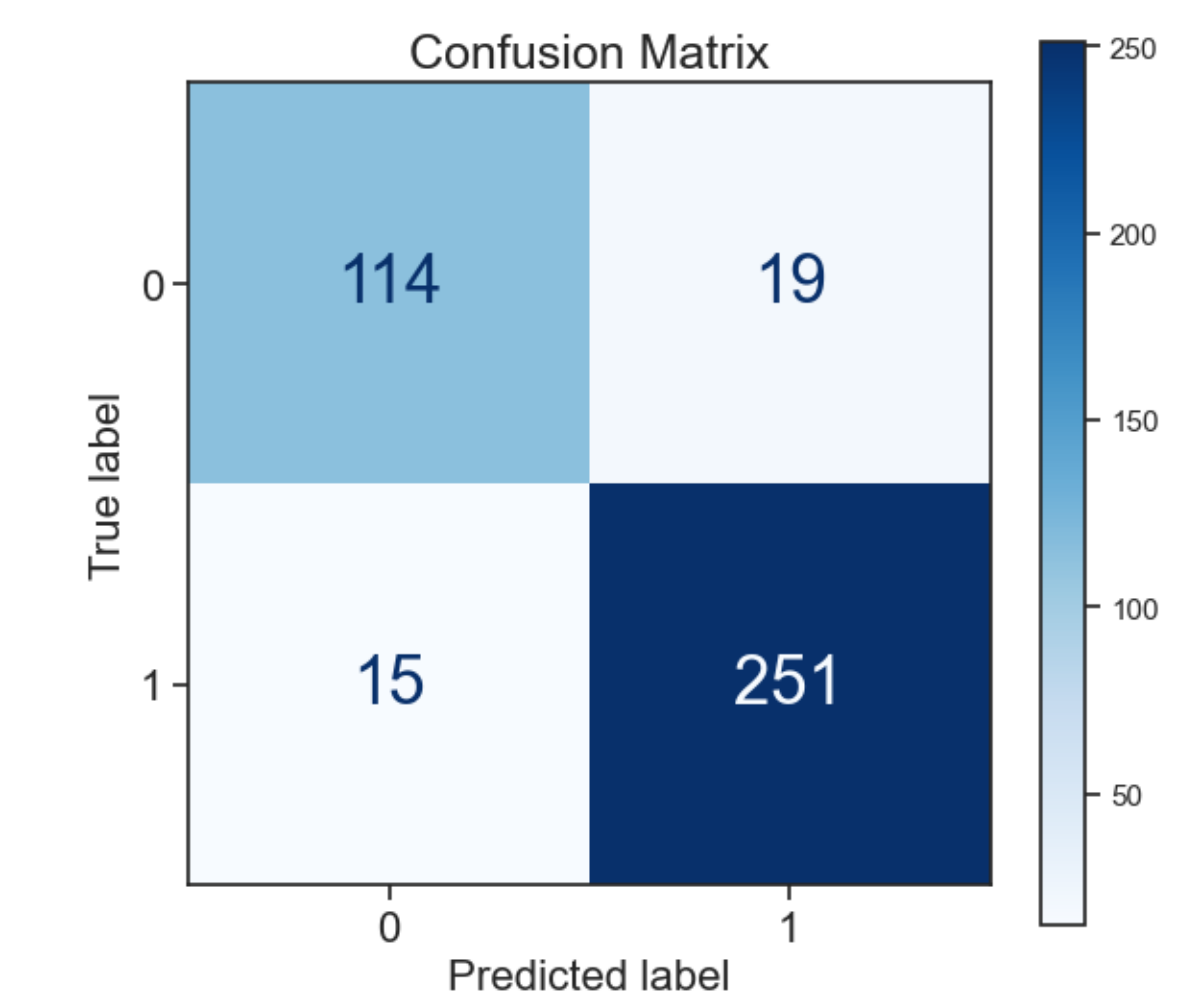
Metric	Train	Test
AUC	1.0	0.9696
accuracy	0.9975	0.9148
balanced accuracy	0.9962	0.9004
recall_(sens)	1.0	0.9436
specificity	0.9925	0.8571
precision	0.9962	0.9296
f1_score	0.9975	0.9145

Protein: P06276 - metric: f1

Total (train): 1592

ROC curve

AUC_train = 1.000
AUC_test = 0.969
Random

Pareto Chart with Highlighted Best Attempt

Trials
Pareto Front Trials
Best Trial (# 2410)
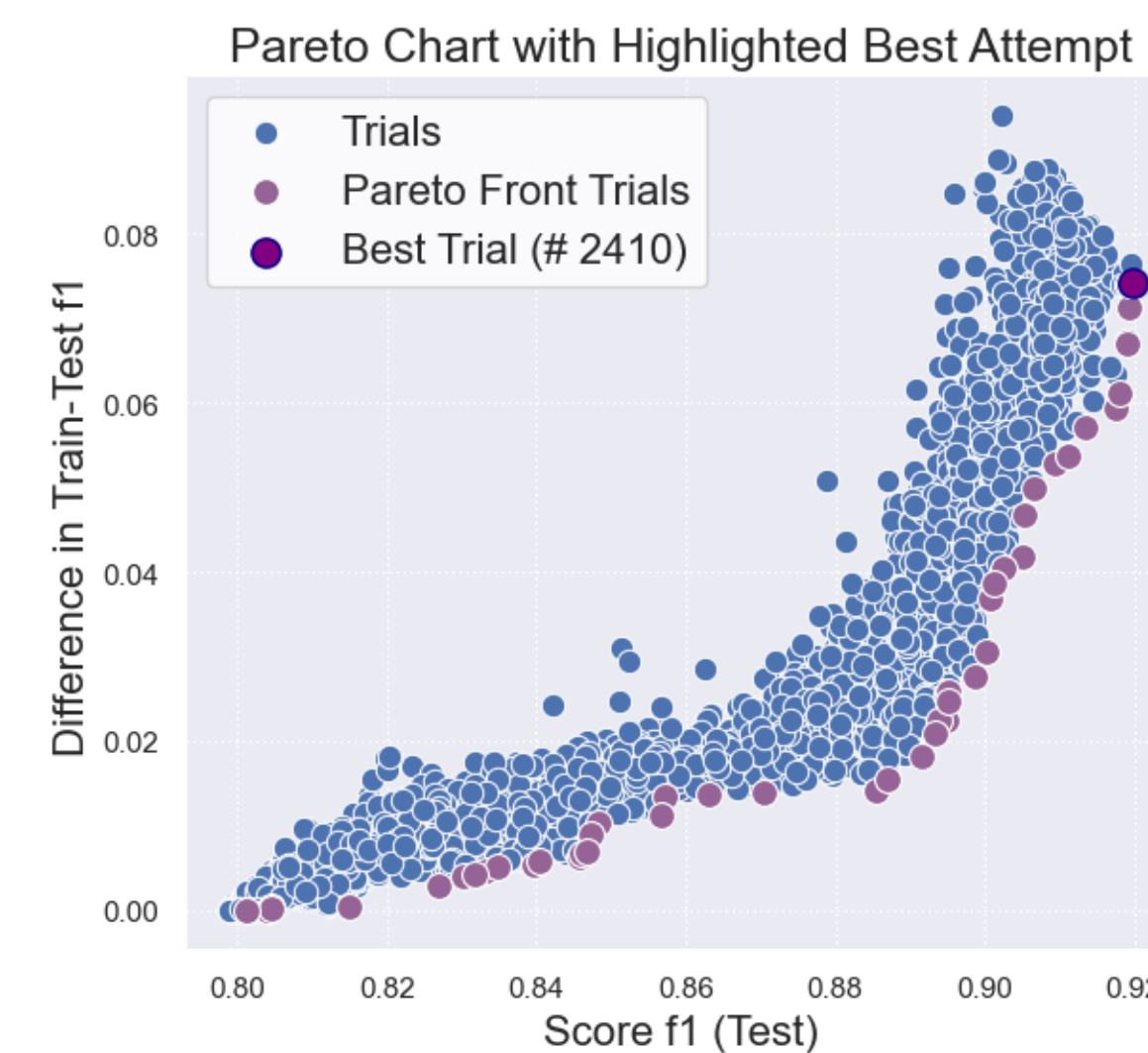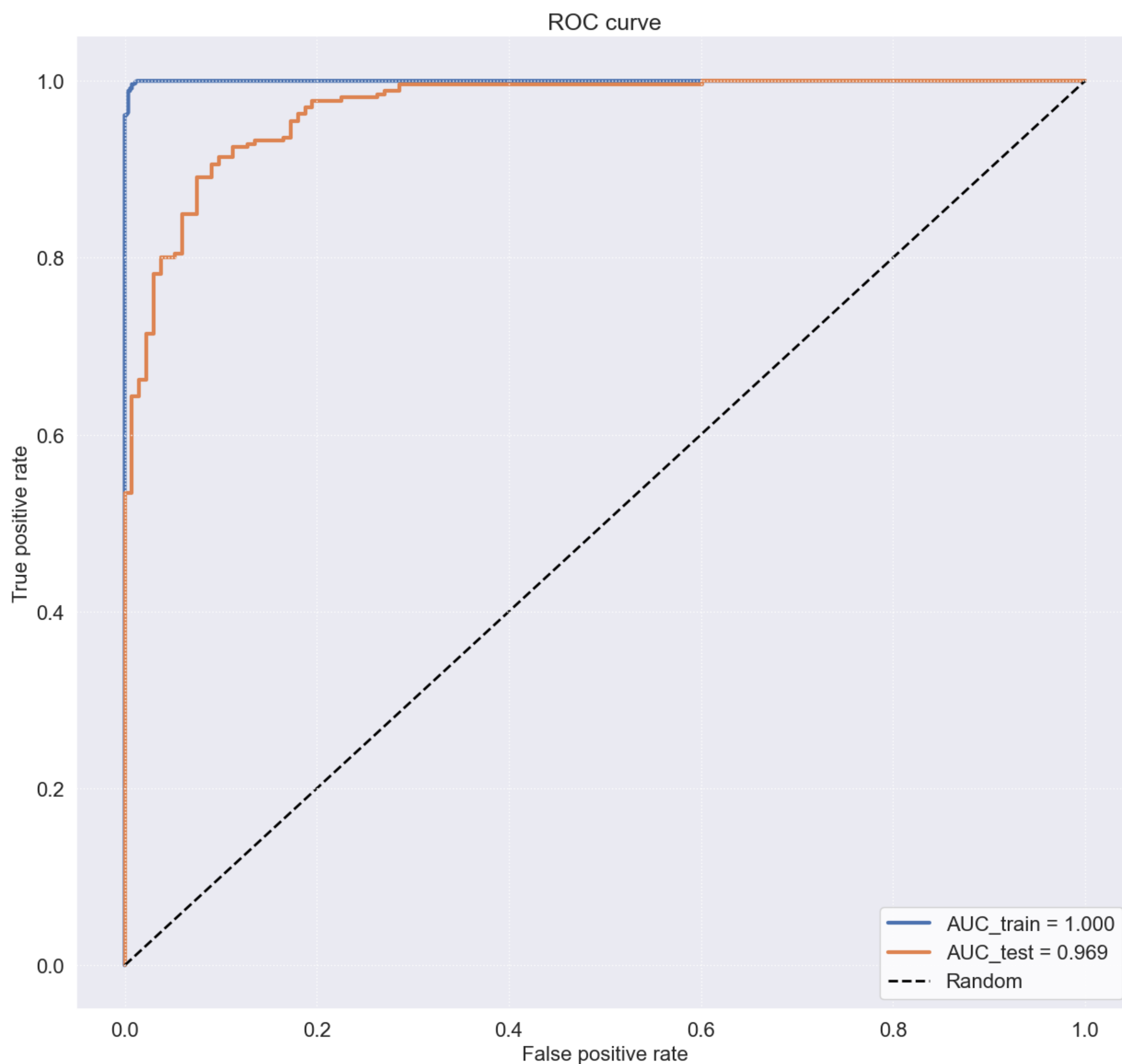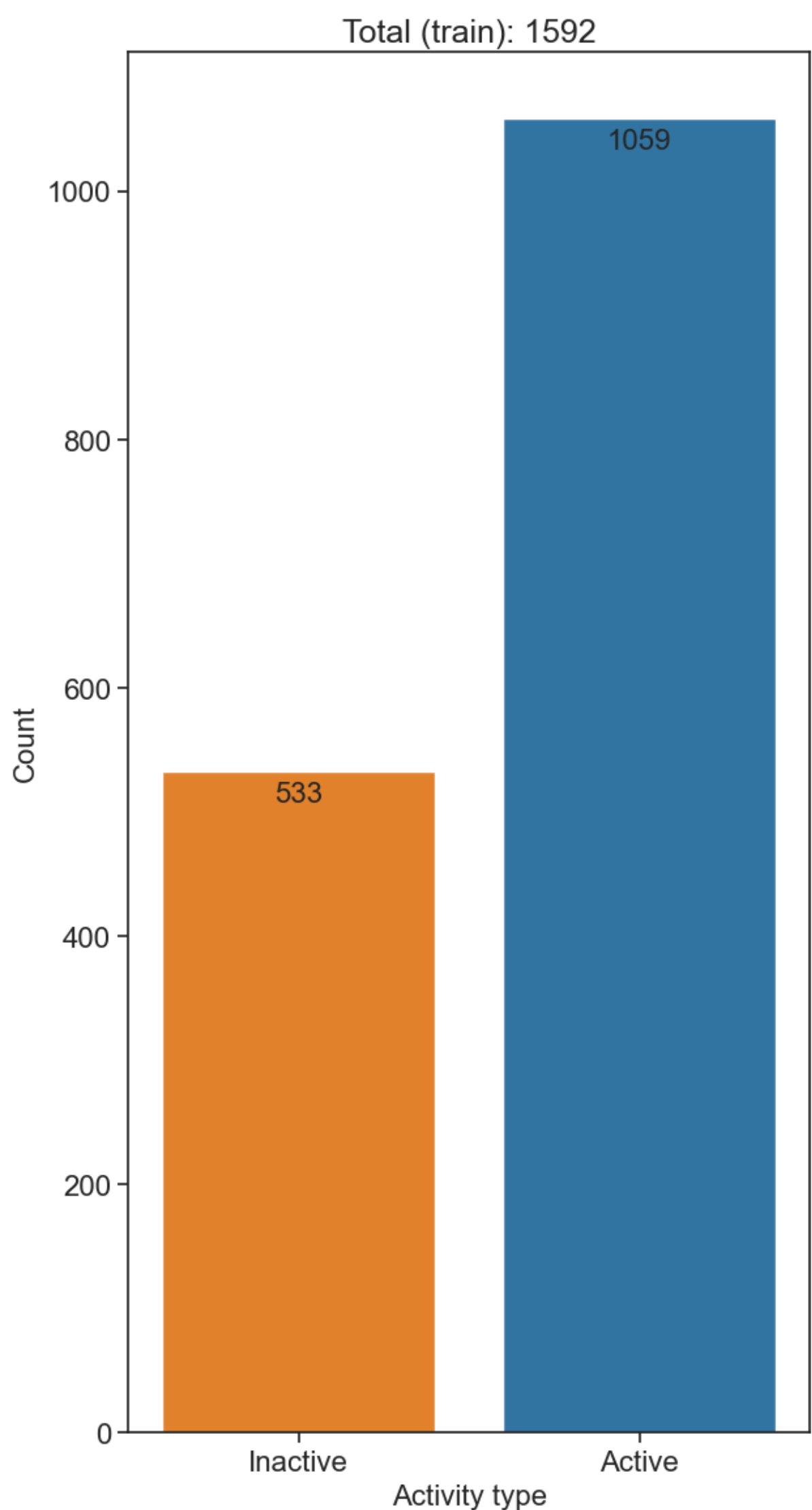
XGBoost Parameters	Value
alpha	2.2958
colsample_bytree	0.819
gamma	0.5903
lambda	2.9638
learning_rate	0.1333
max_depth	7.0
min_child_weight	1.0
n_estimators	830.0
reg_alpha	0.769
reg_lambda	0.206
scale_pos_weight	3.0693
subsample	0.5764

Confusion Matrix

Confusion Matrix (nomr.)

Calibration curve

train: 0.0098
test: 0.0673
perfectly_calibrated

Active/Inactive probability

type
active (266)
inactive (133)
decoy (399)
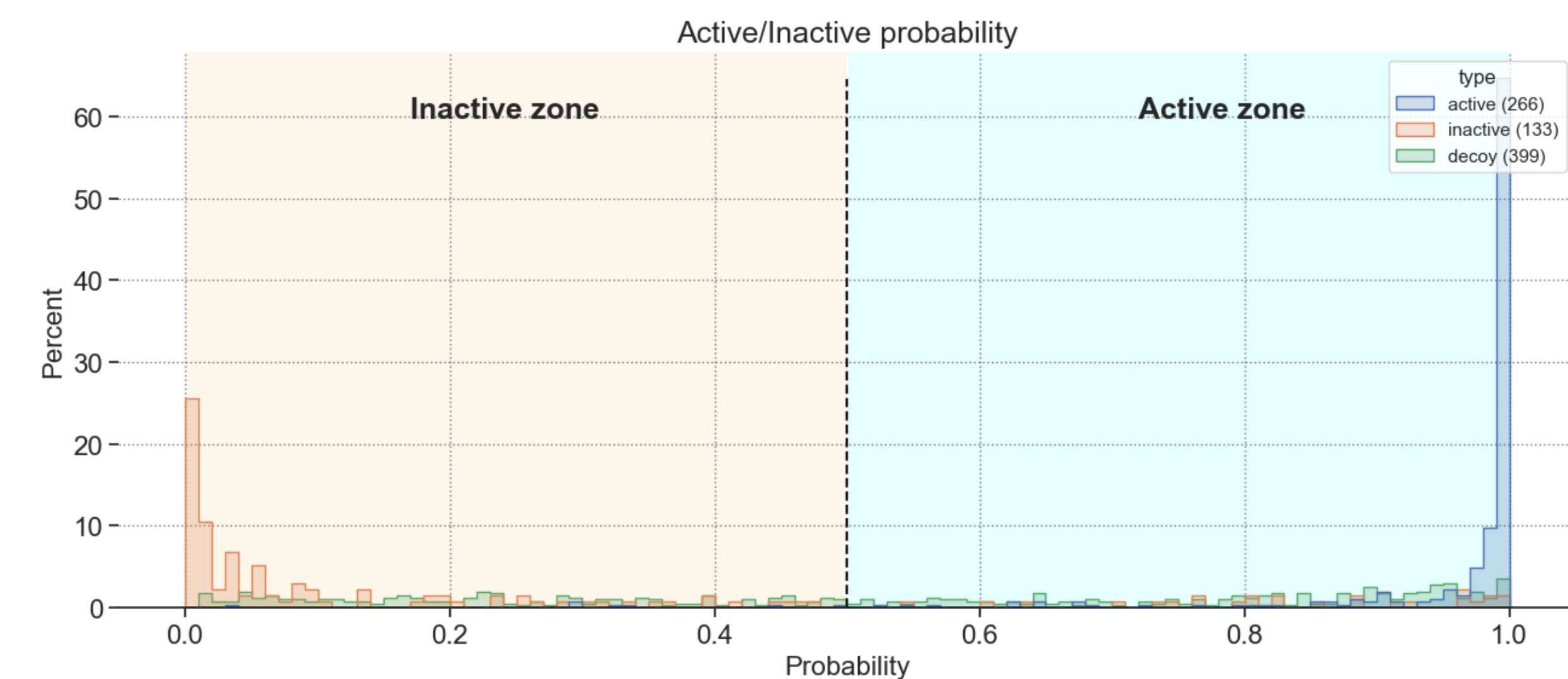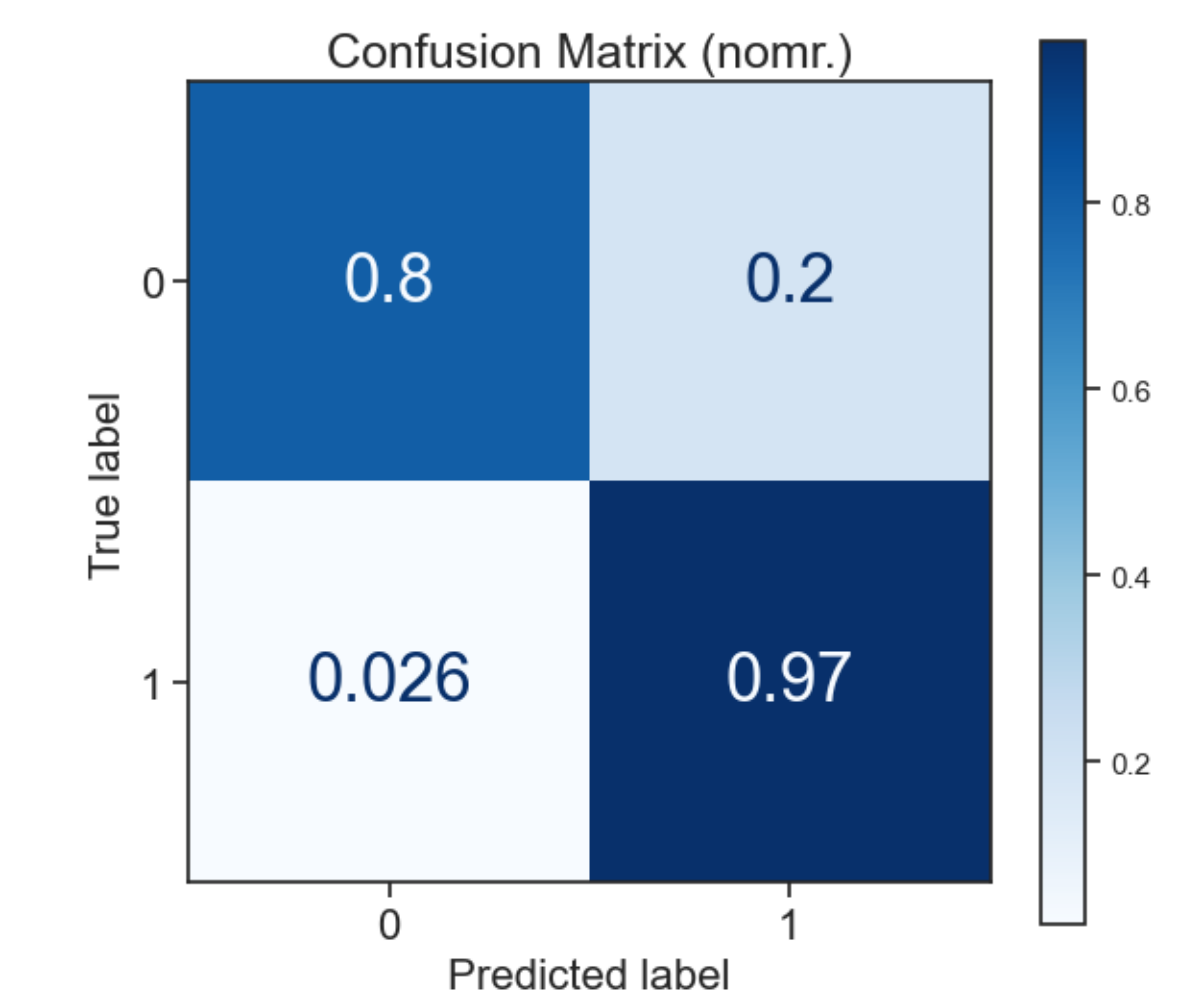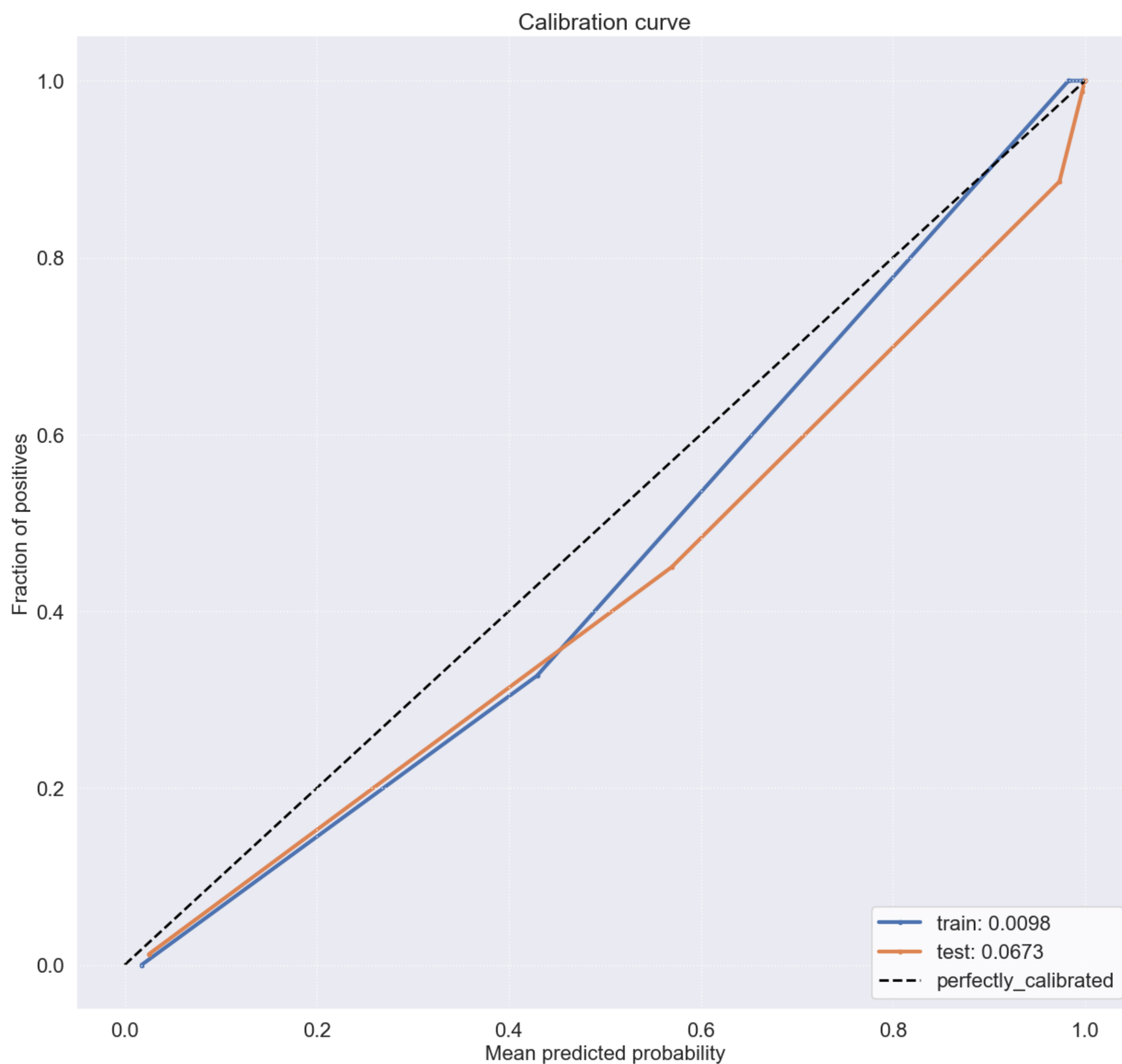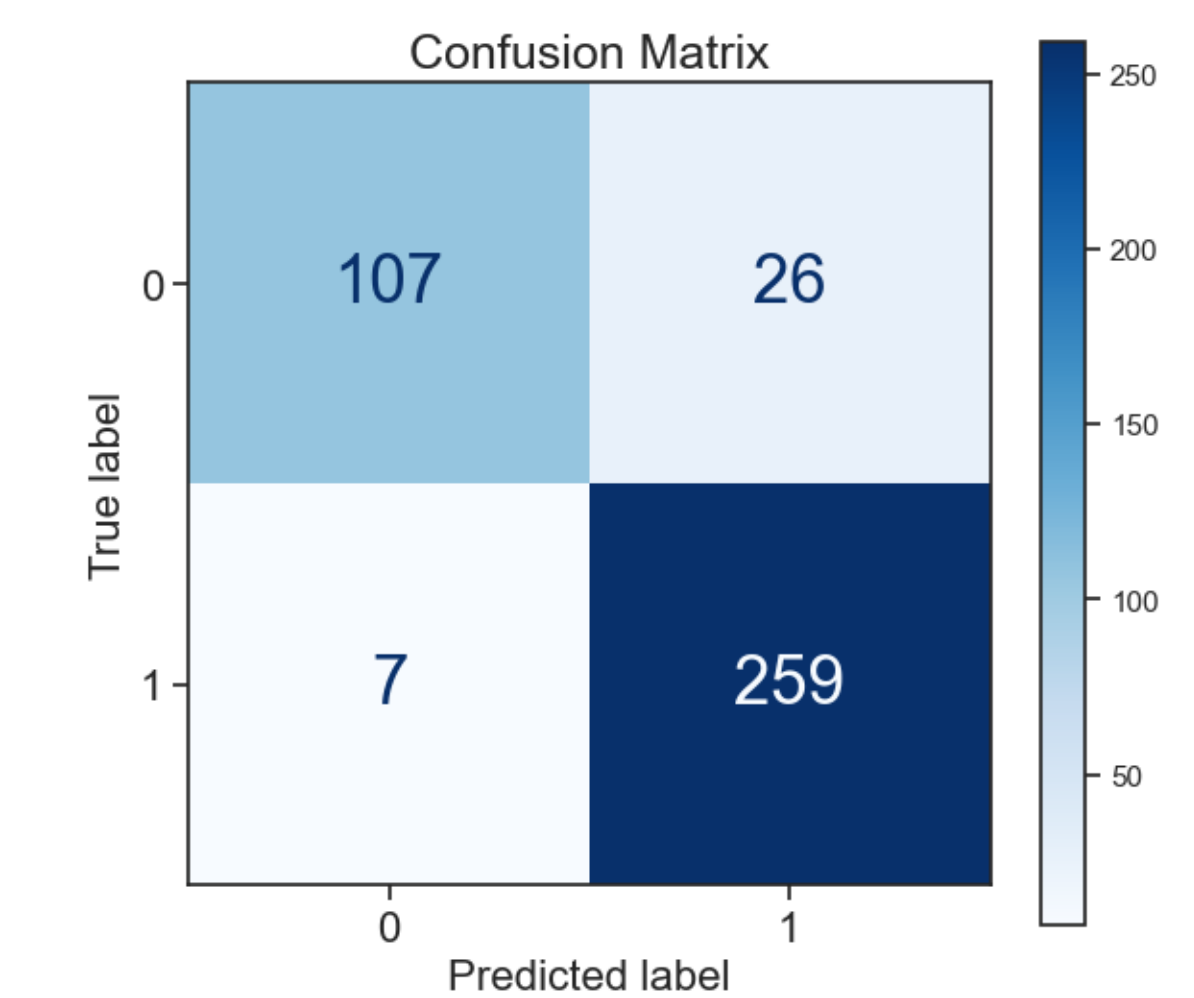
Metric	Train	Test
AUC	0.9998	0.9692
accuracy	0.9918	0.9173
balanced accuracy	0.9878	0.8891
recall_(sens)	1.0	0.9737
specificity	0.9756	0.8045
precision	0.9879	0.9088
f1_score	0.9918	0.9155

Protein: P06276 - metric: precision

Total (train): 1592

ROC curve

Pareto Chart with Highlighted Best Attempt

- Trials
- Pareto Front Trials
- Best Trial (# 2394)

ROC curve legend:
- AUC_train = 1.000
- AUC_test = 0.967
- Random

Confusion Matrix

	Predicted 0	Predicted 1
True 0	116	17
True 1	14	252

Confusion Matrix (nomr.)

	Predicted 0	Predicted 1
True 0	0.87	0.13
True 1	0.053	0.95

Calibration curve

- train: 0.0072
- test: 0.062
- perfectly_calibrated
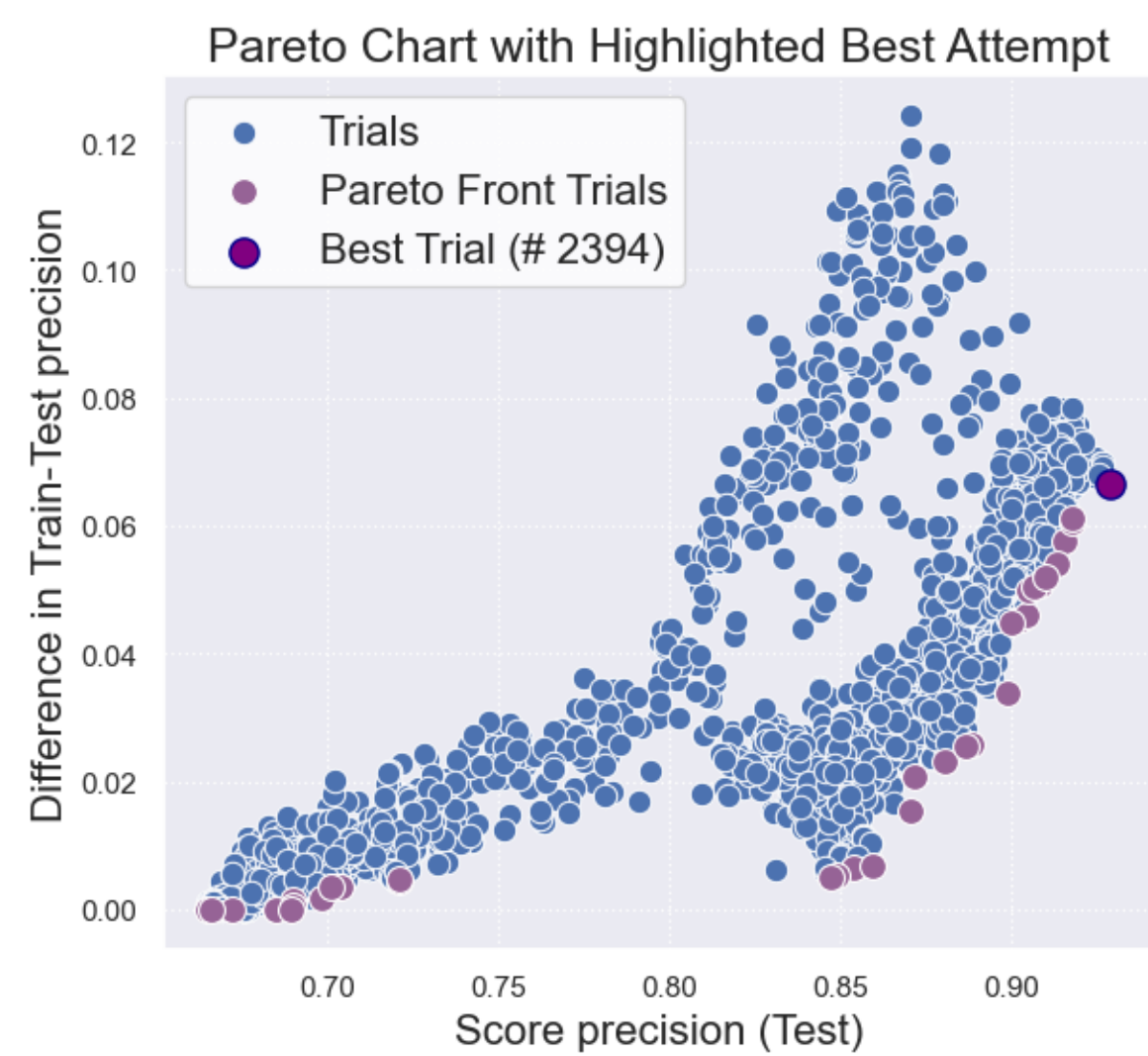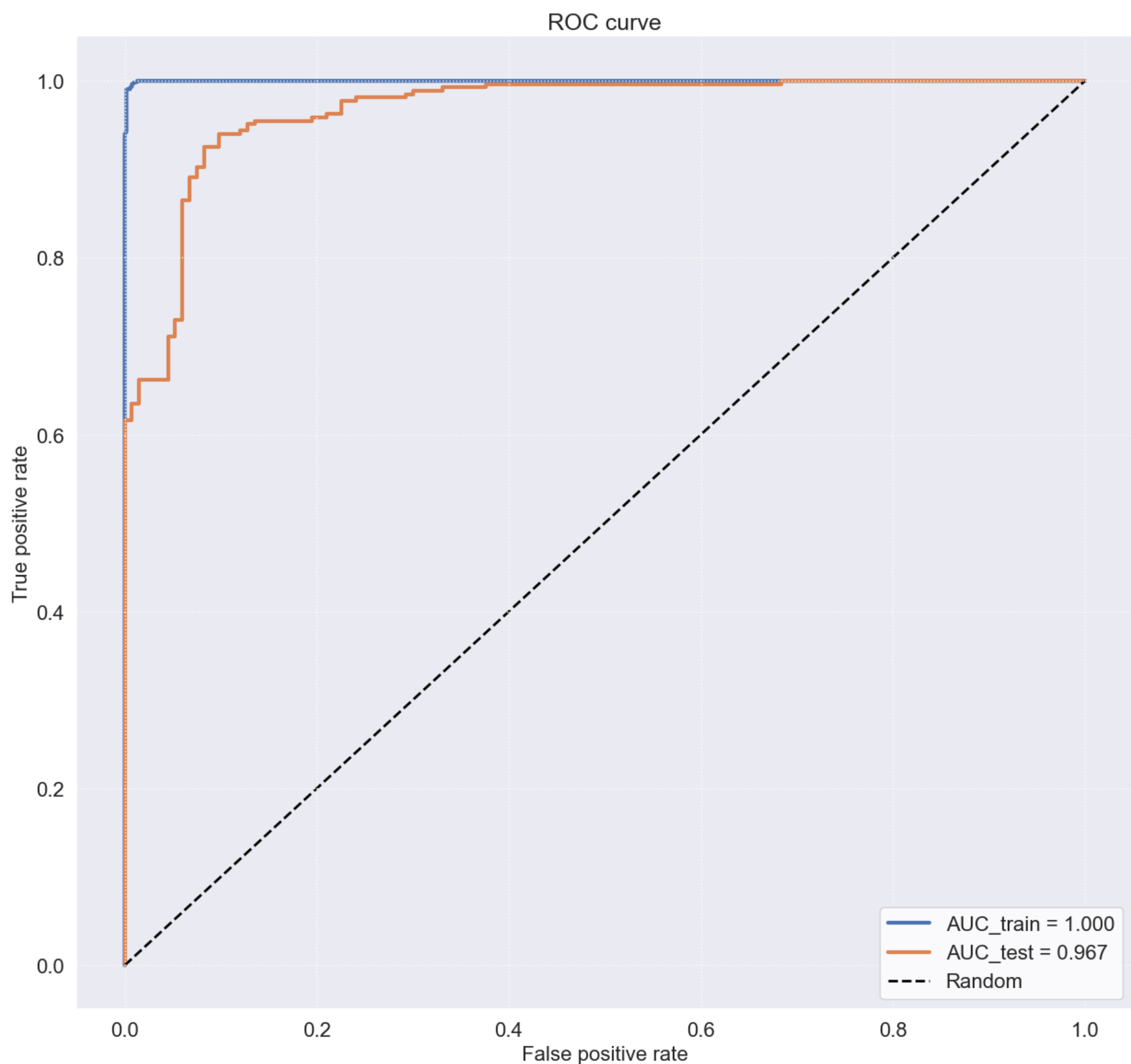
XGBoost Parameters	Value
alpha	2.8757
colsample_bytree	0.9562
gamma	0.021
lambda	0.4009
learning_rate	0.2531
max_depth	4.0
min_child_weight	3.0
n_estimators	928.0
reg_alpha	0.4133
reg_lambda	0.5917
scale_pos_weight	1.0184
subsample	0.9614

Active/Inactive probability

type:
- active (266)
- inactive (133)
- decoy (399)

Inactive zone / Active zone
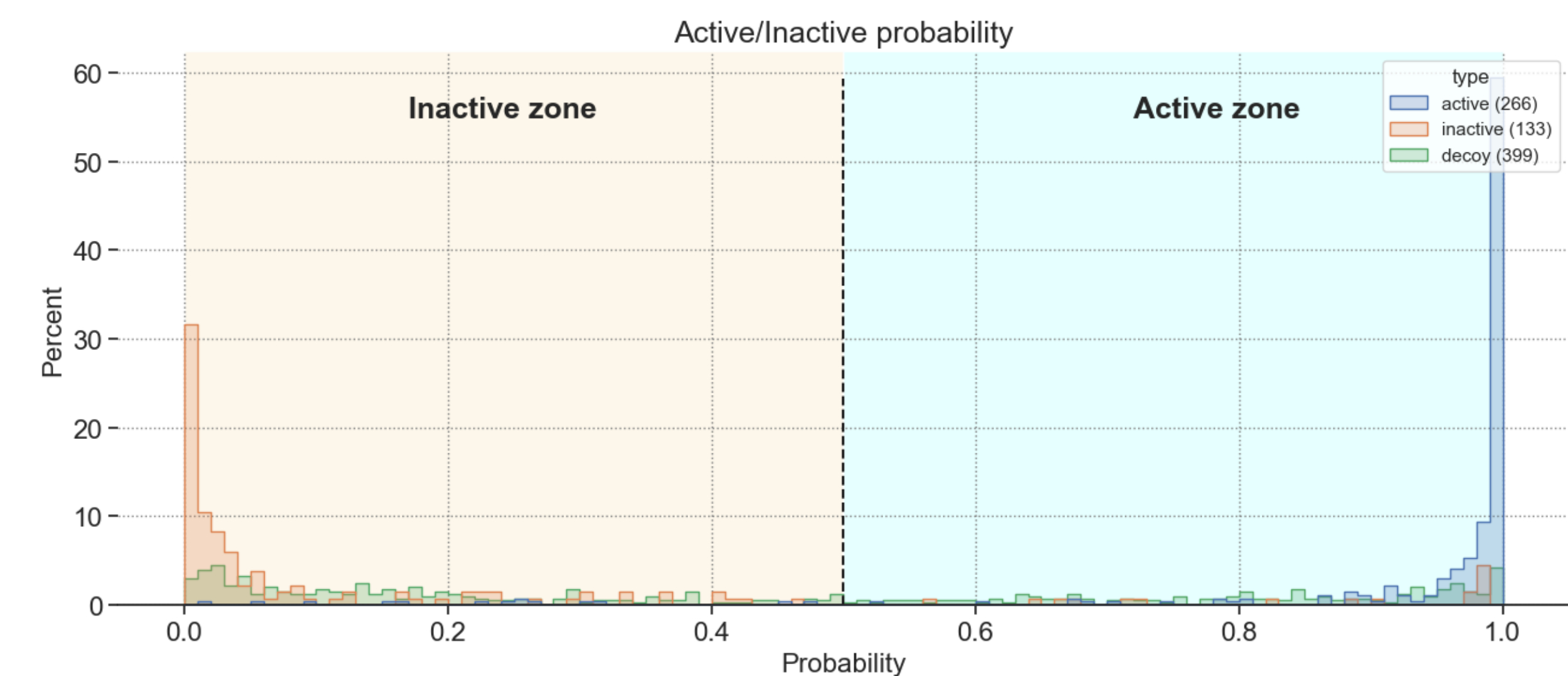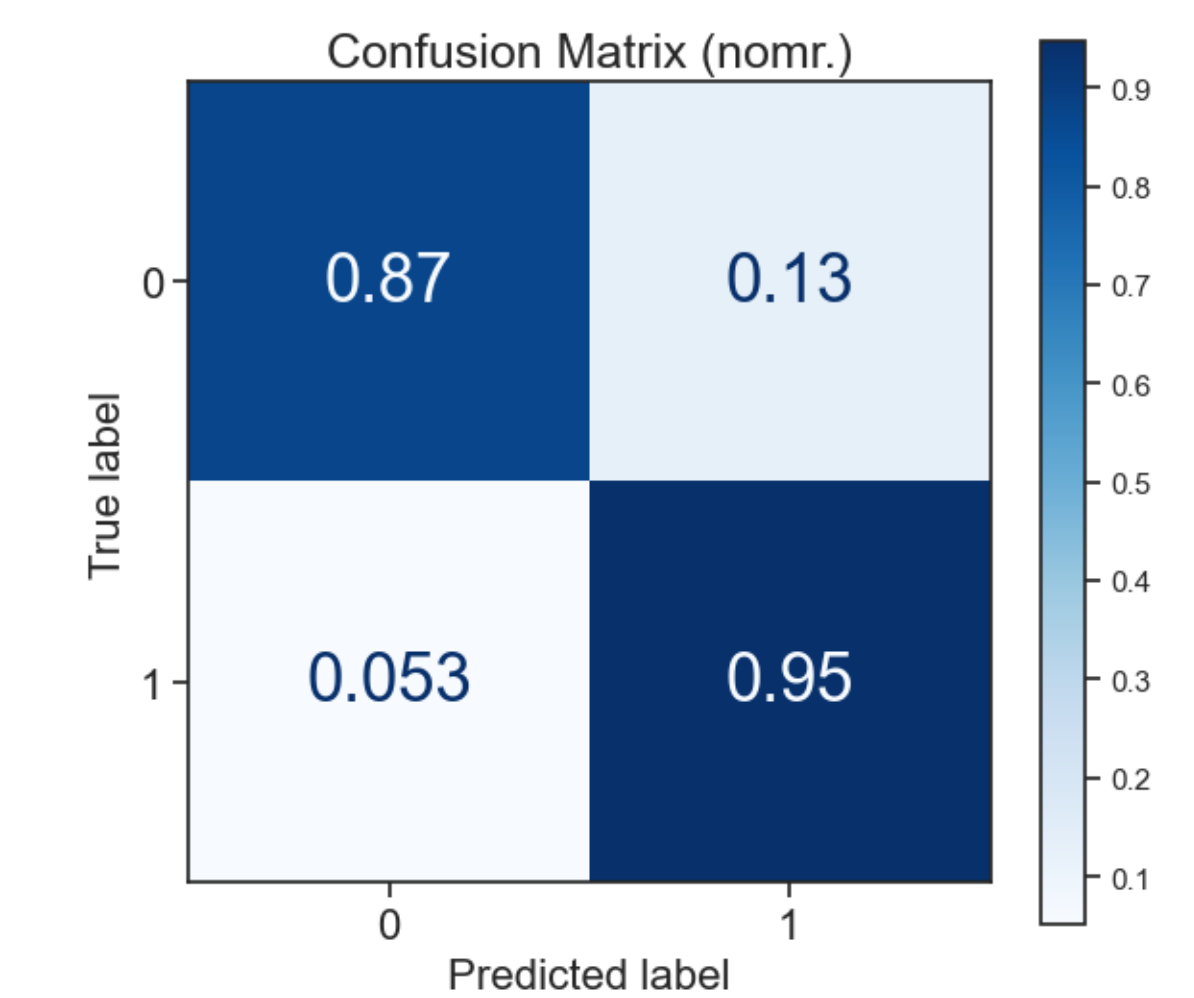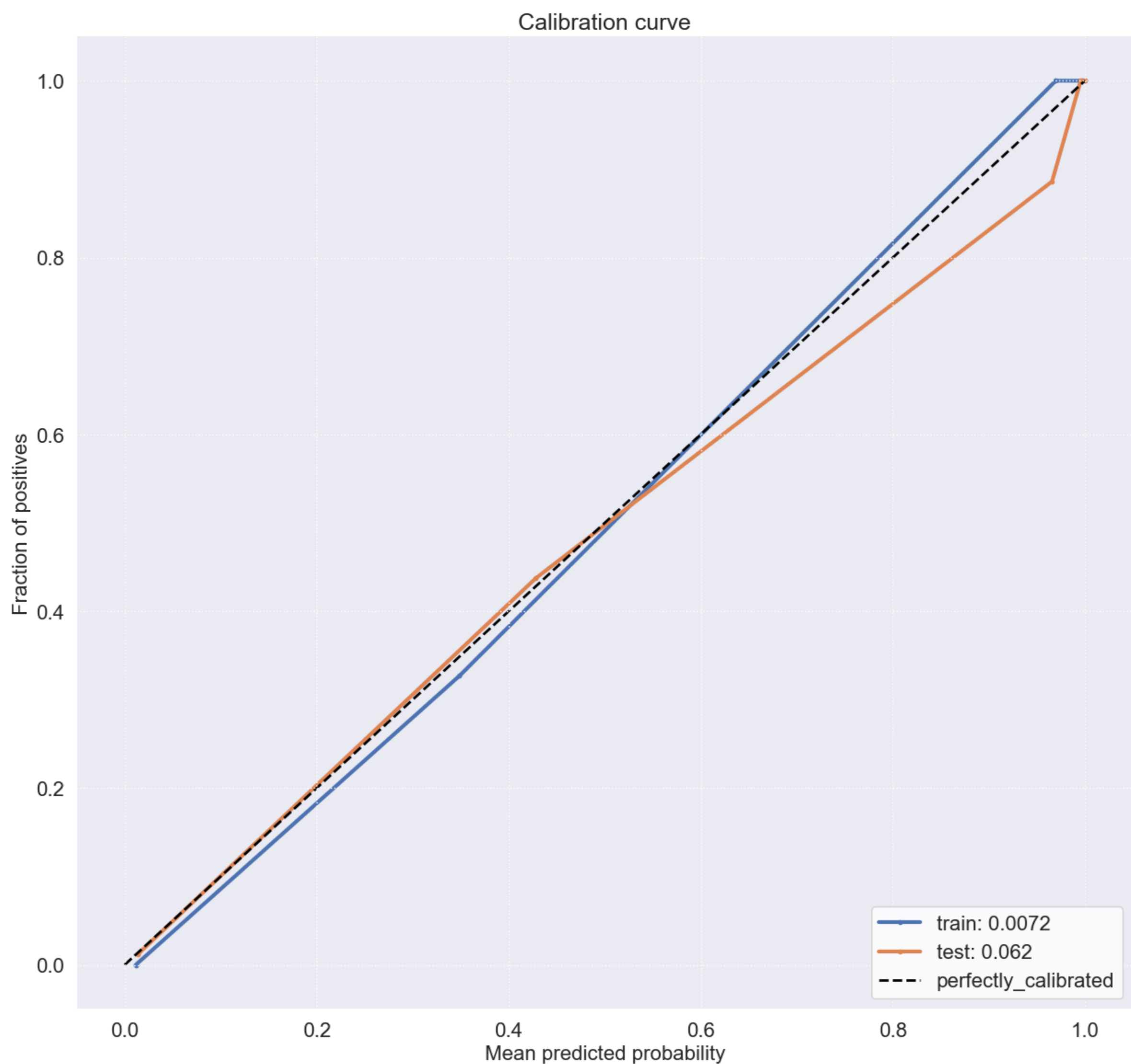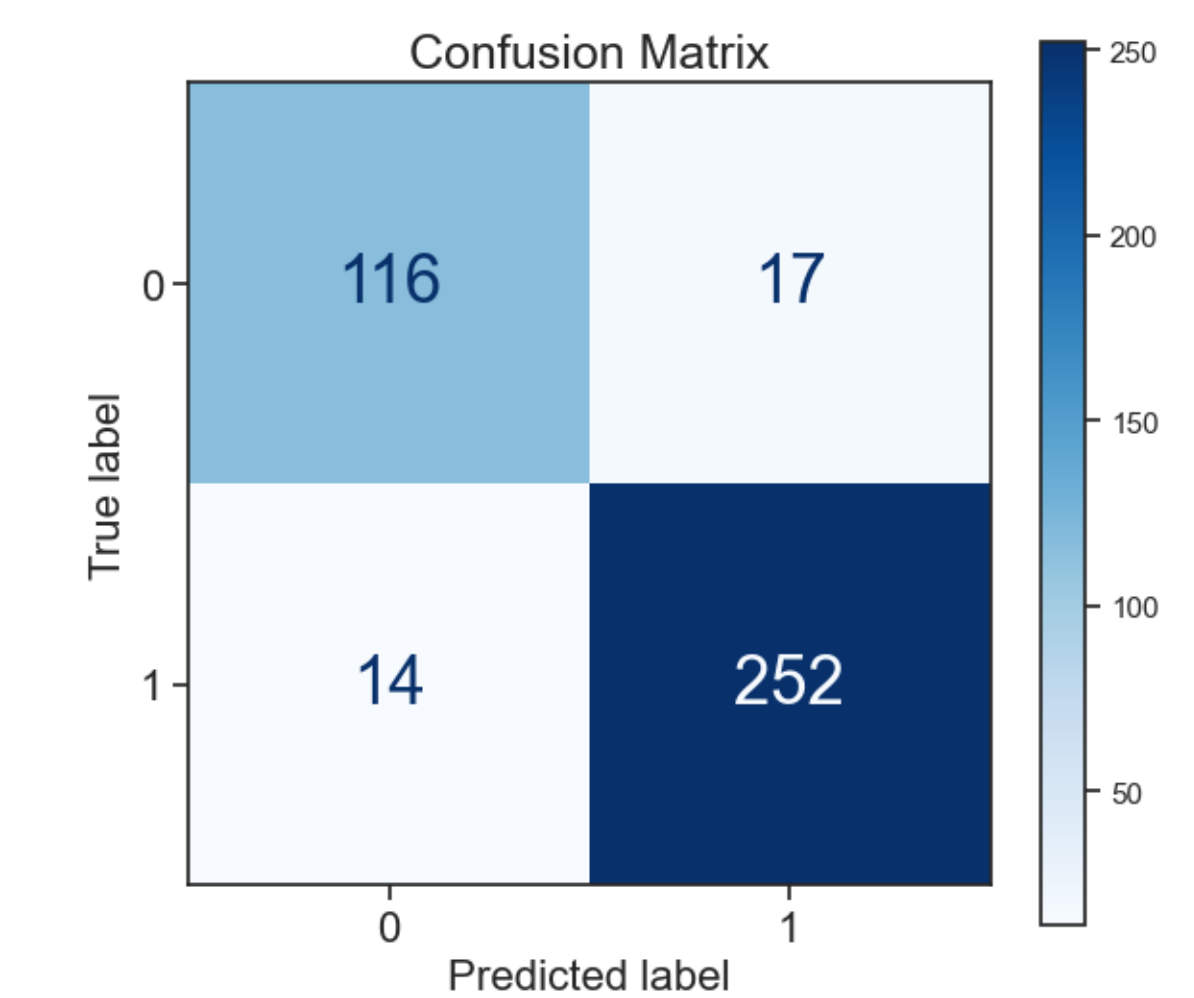
Metric	Train	Test
AUC	0.9998	0.967
accuracy	0.995	0.9223
balanced accuracy	0.9934	0.9098
recall_(sens)	0.9981	0.9474
specificity	0.9887	0.8722
precision	0.9944	0.9368
f1_score	0.995	0.9221

Protein: P06276 - metric: SoftVotingXGBoostEnsemble
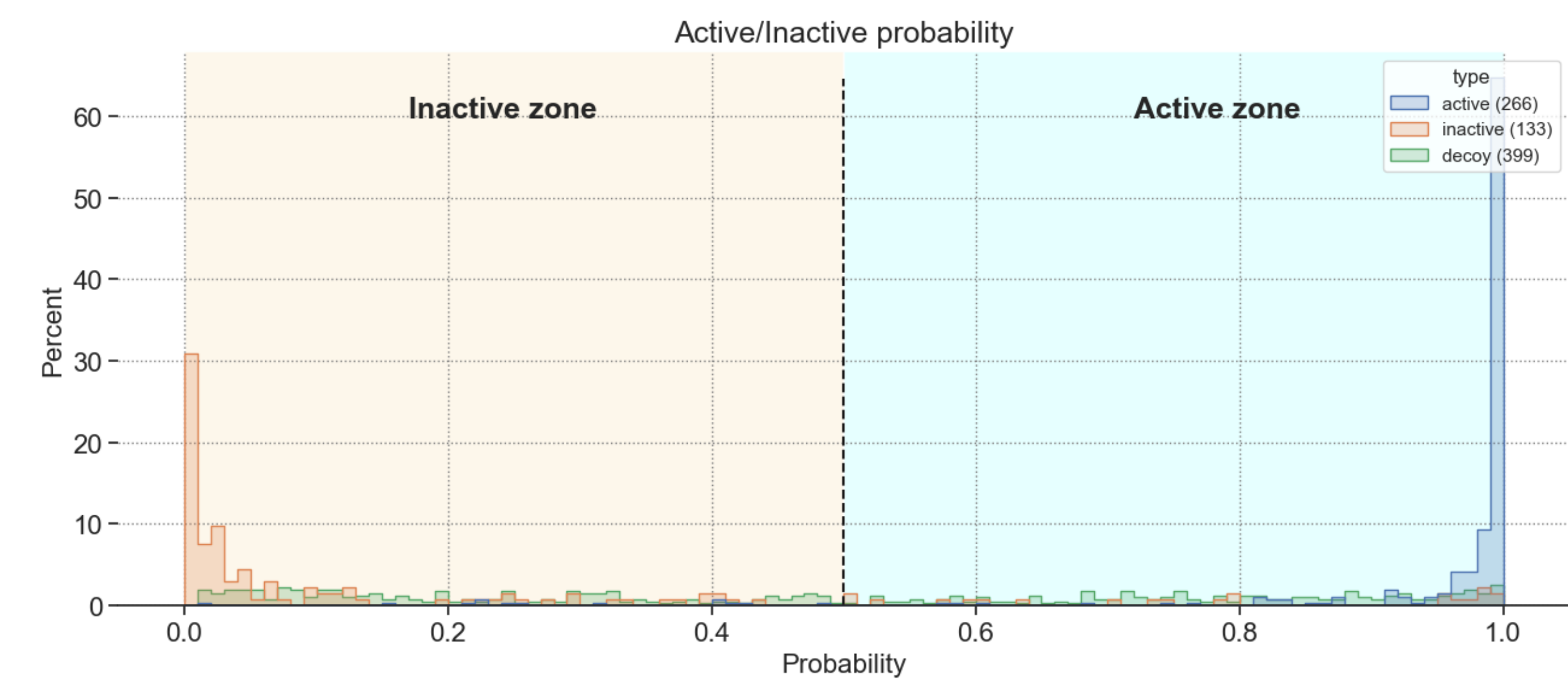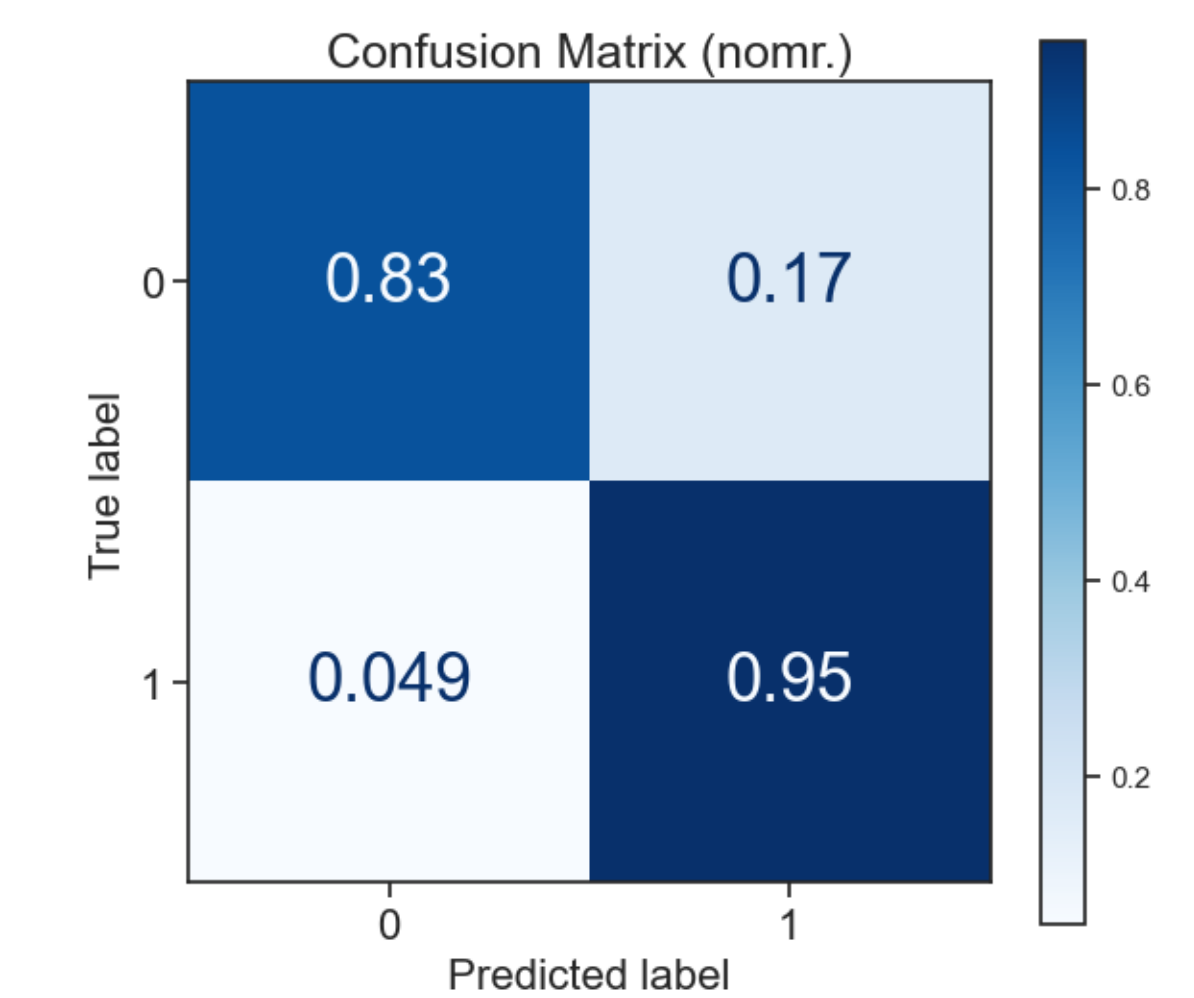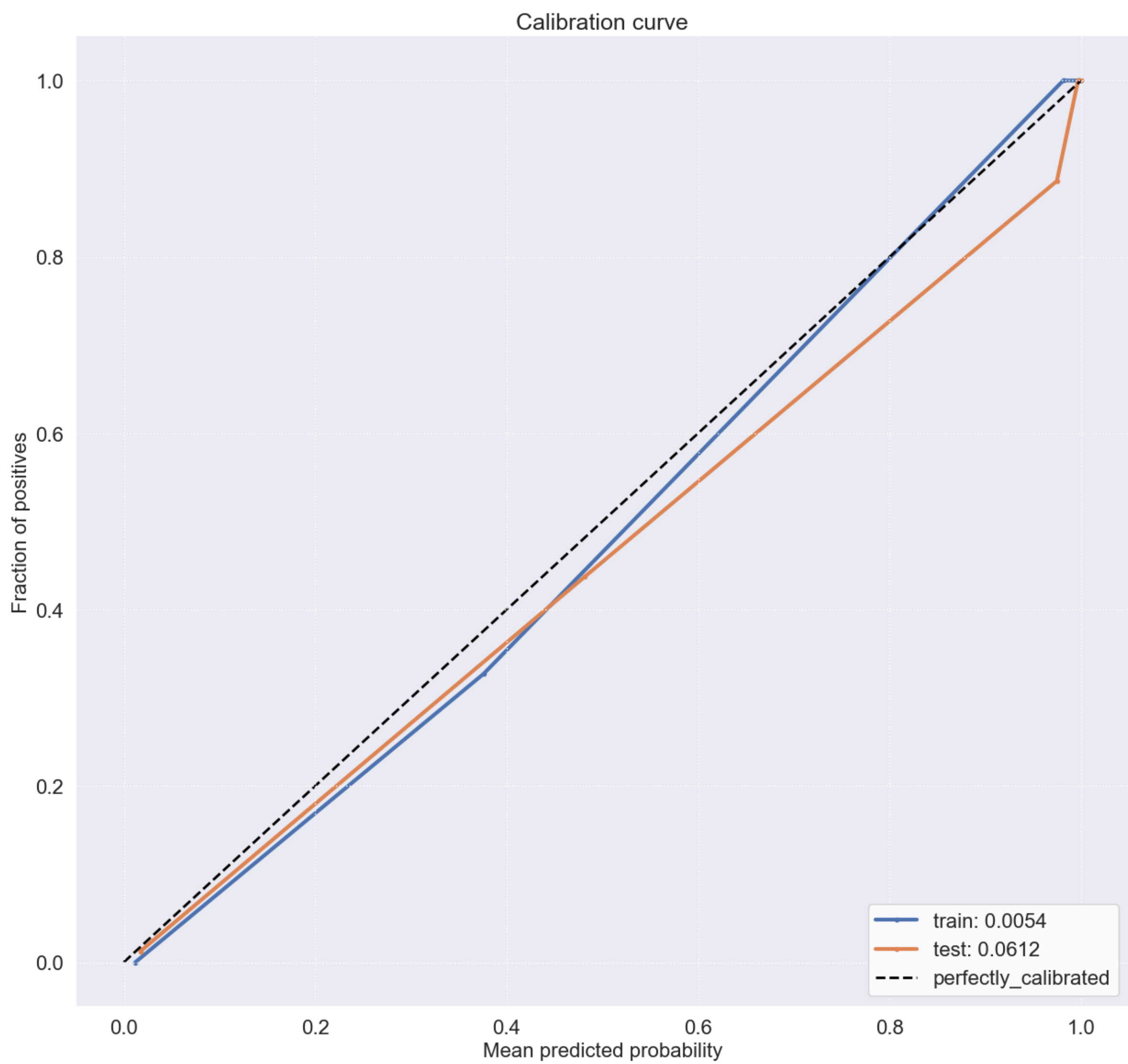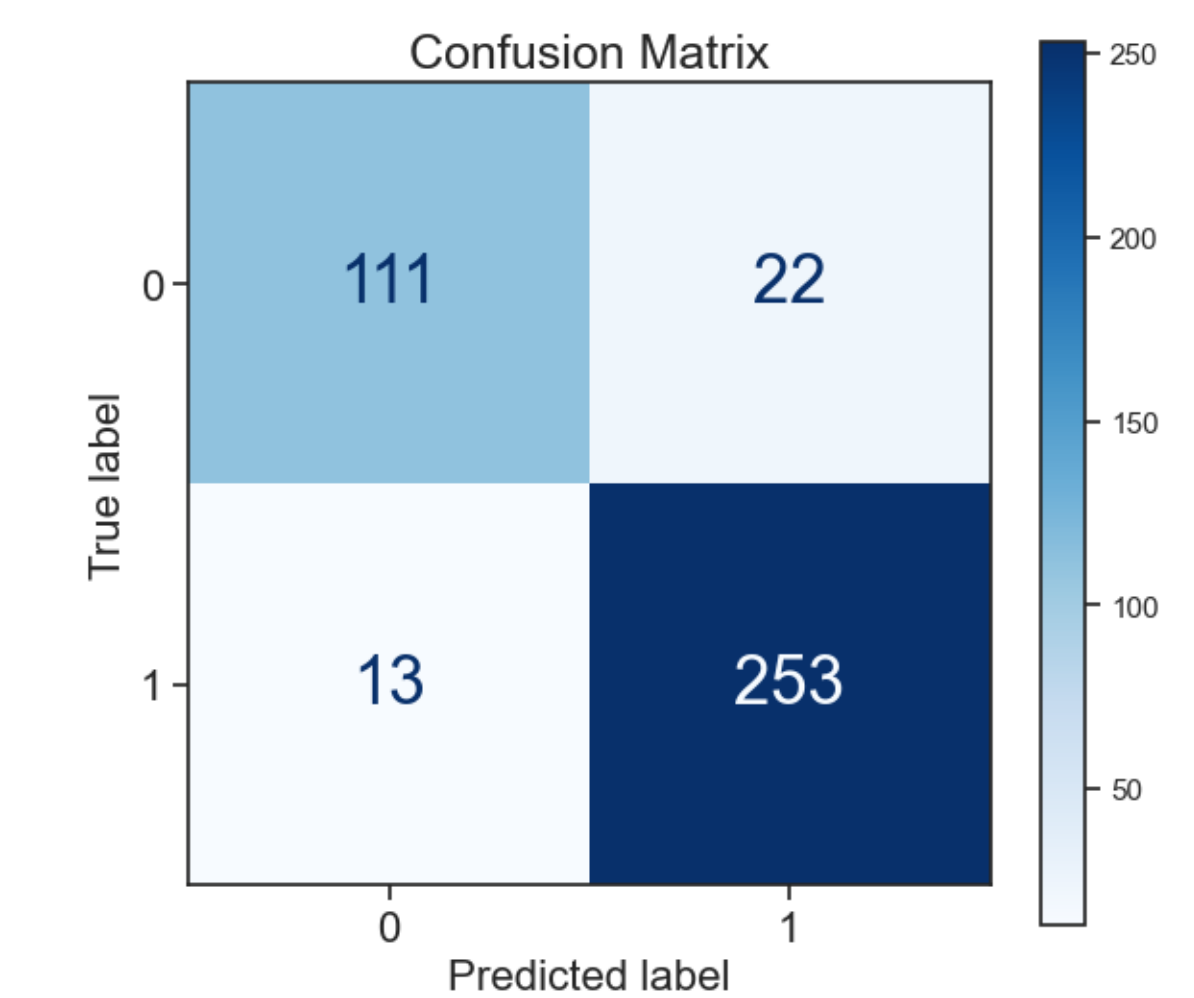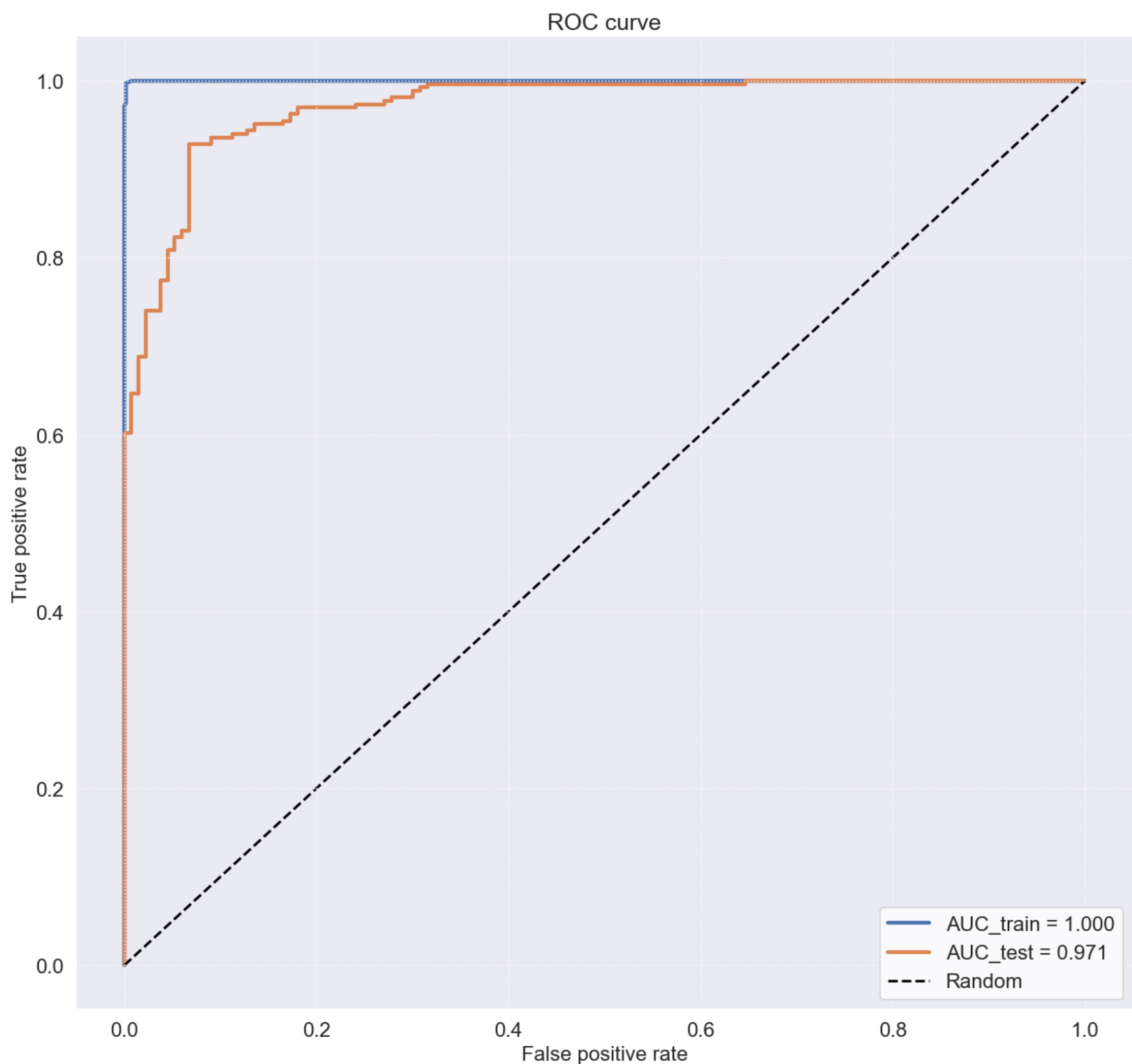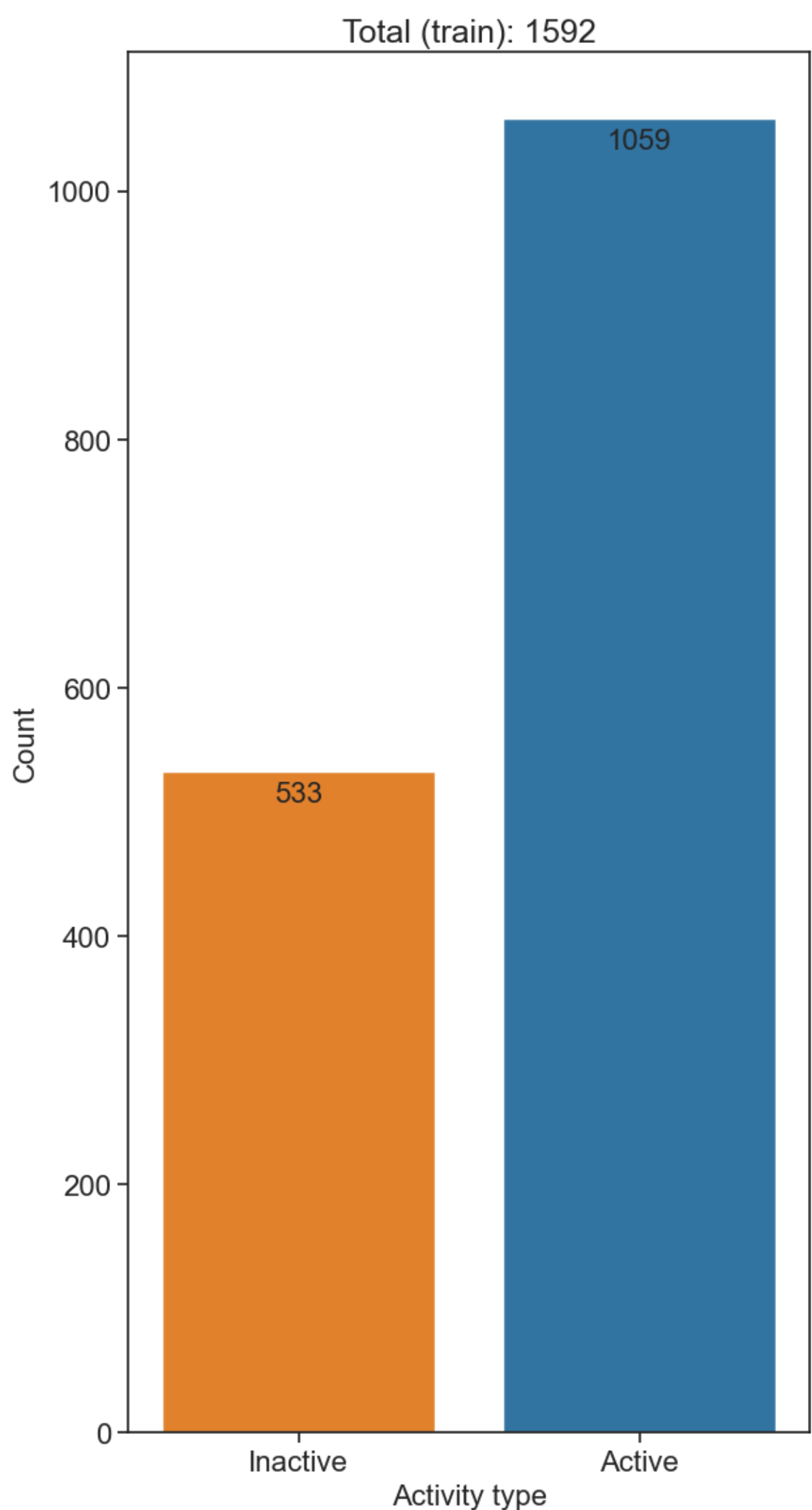
Metric	Train	Test
AUC	0.9999	0.9713
accuracy	0.9956	0.9123
balanced accuracy	0.9934	0.8929
recall_(sens)	1.0	0.9511
specificity	0.9869	0.8346
precision	0.9934	0.92
f1_score	0.9956	0.9115