Protein: P09619 - metric: balanced_accuracy

Total (train): 859

ROC curve

	AUC_train = 1.000
	AUC_test = 0.932
	Random

Pareto Chart with Highlighted Best Attempt

- Trials
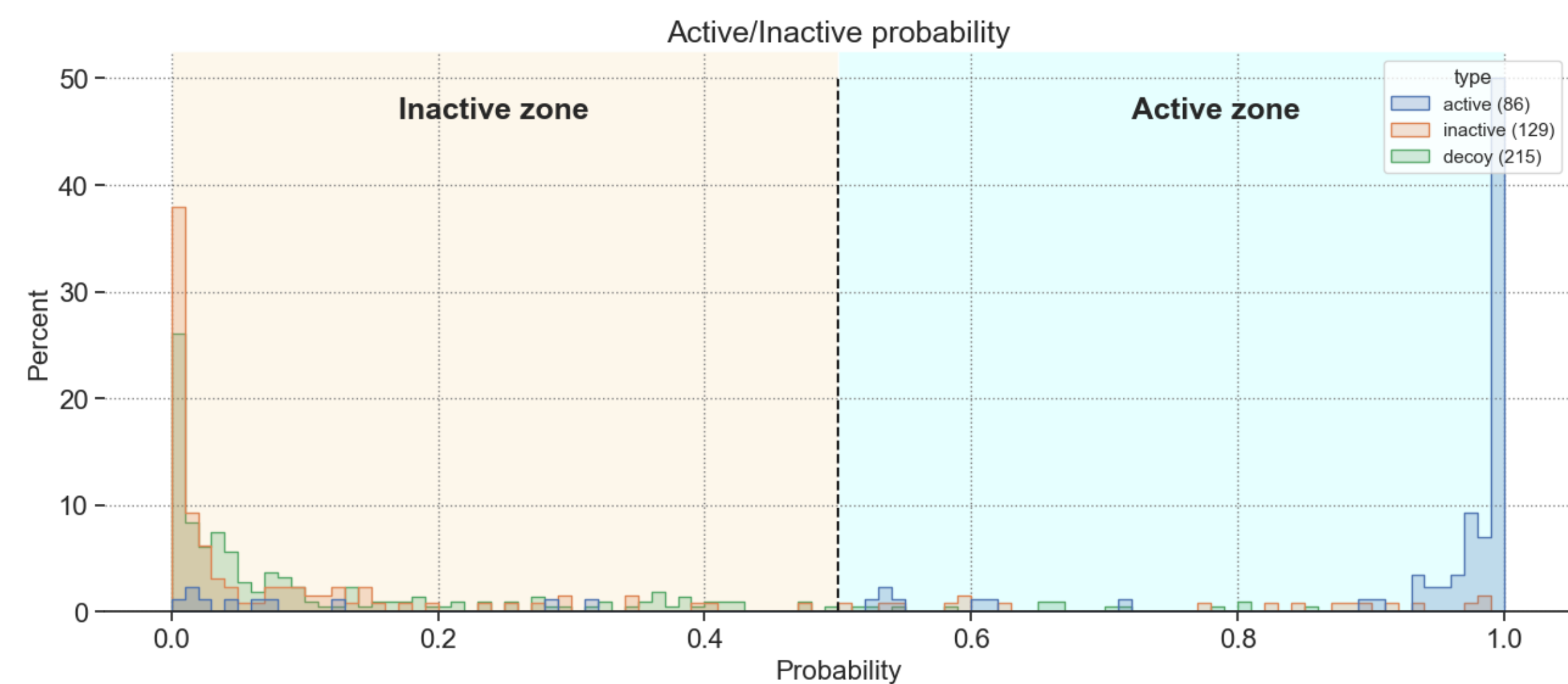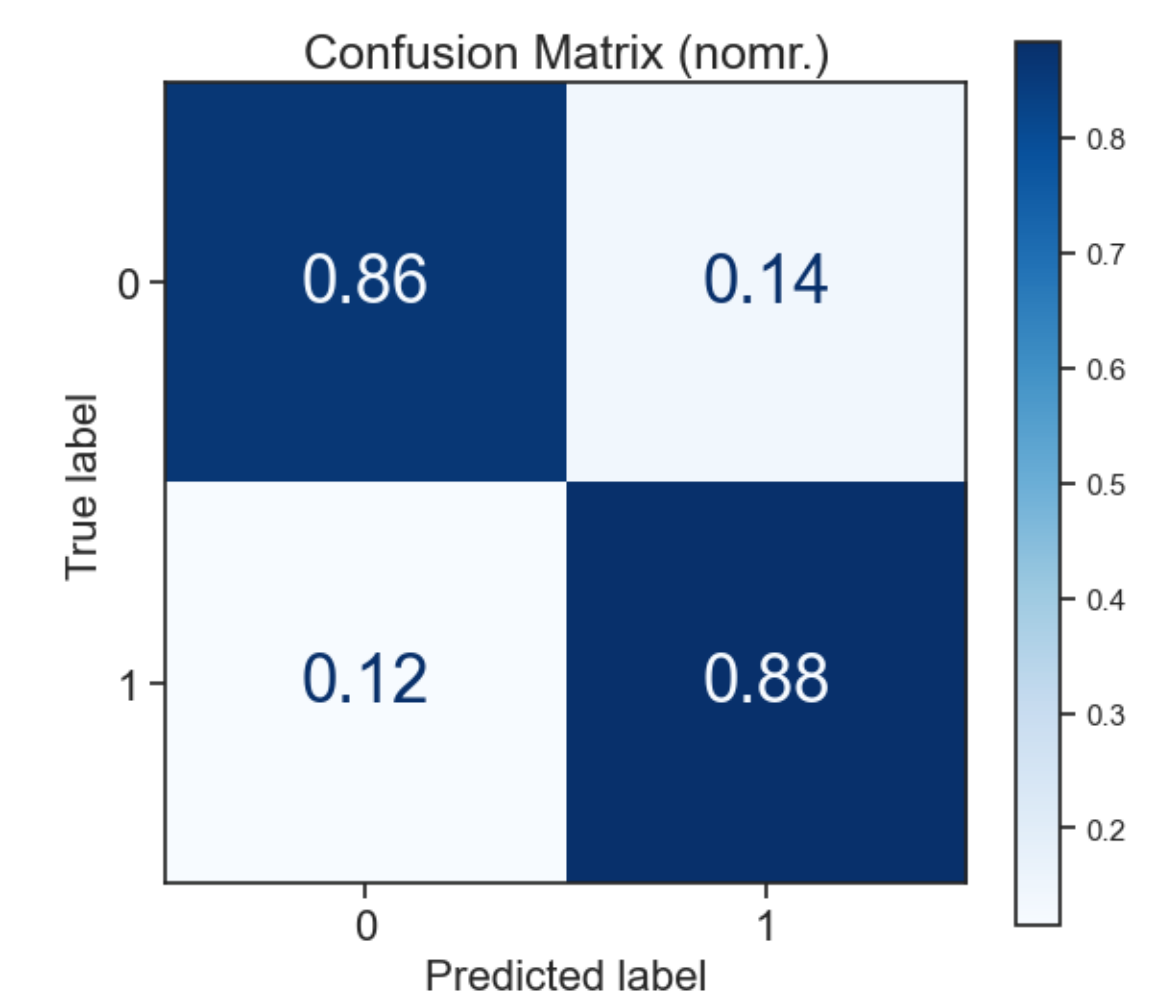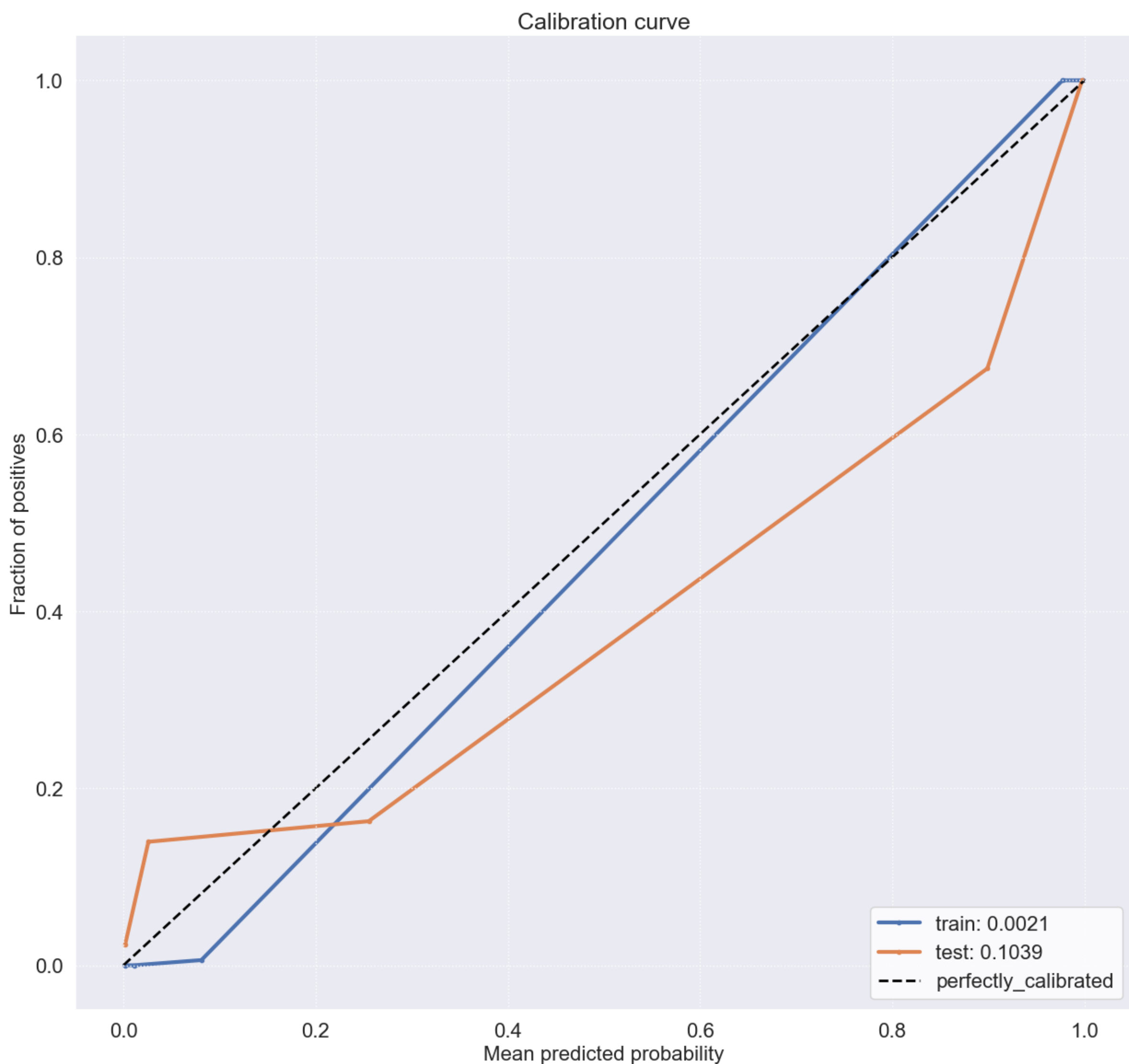- Pareto Front Trials
- Best Trial (# 162)
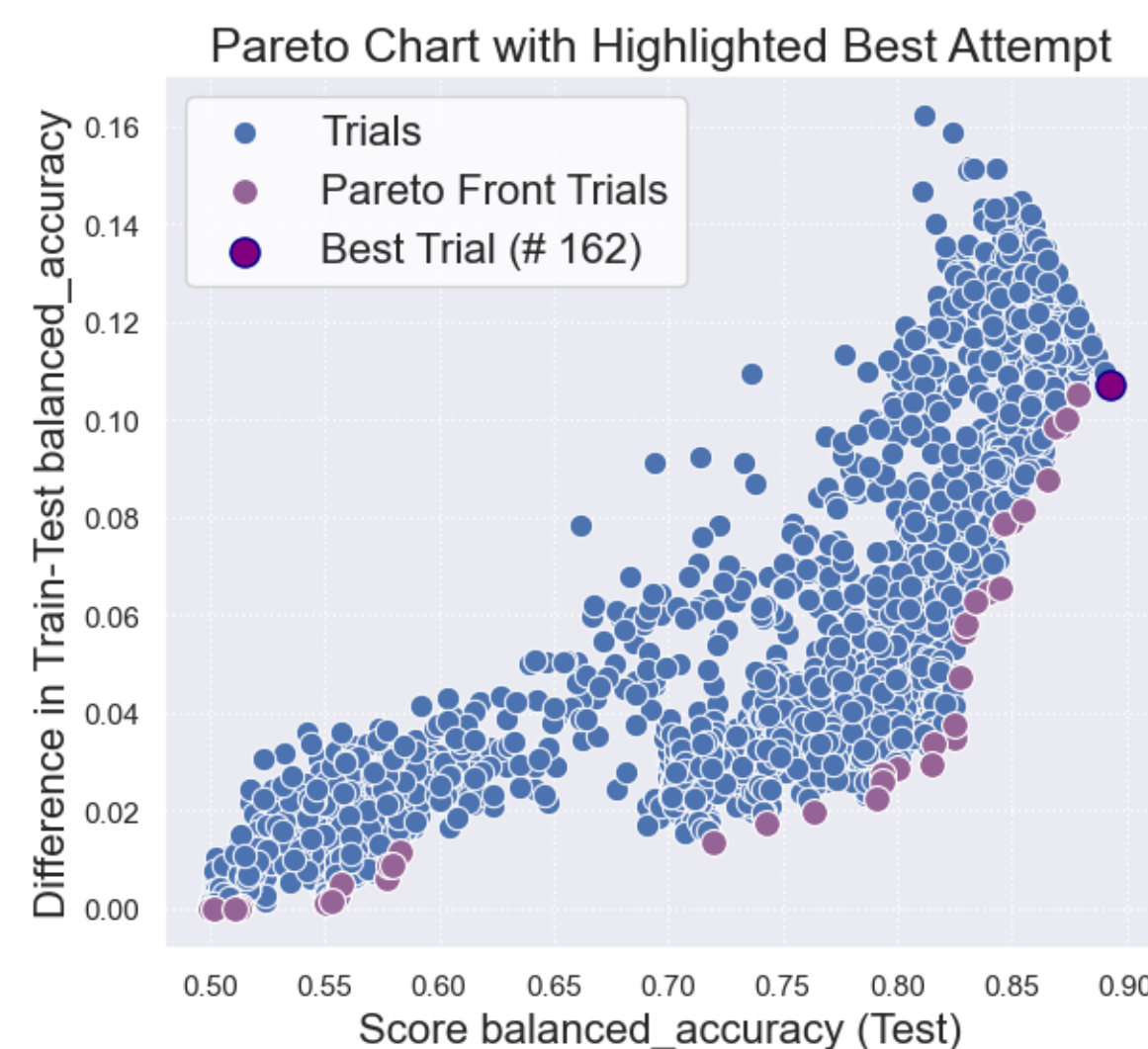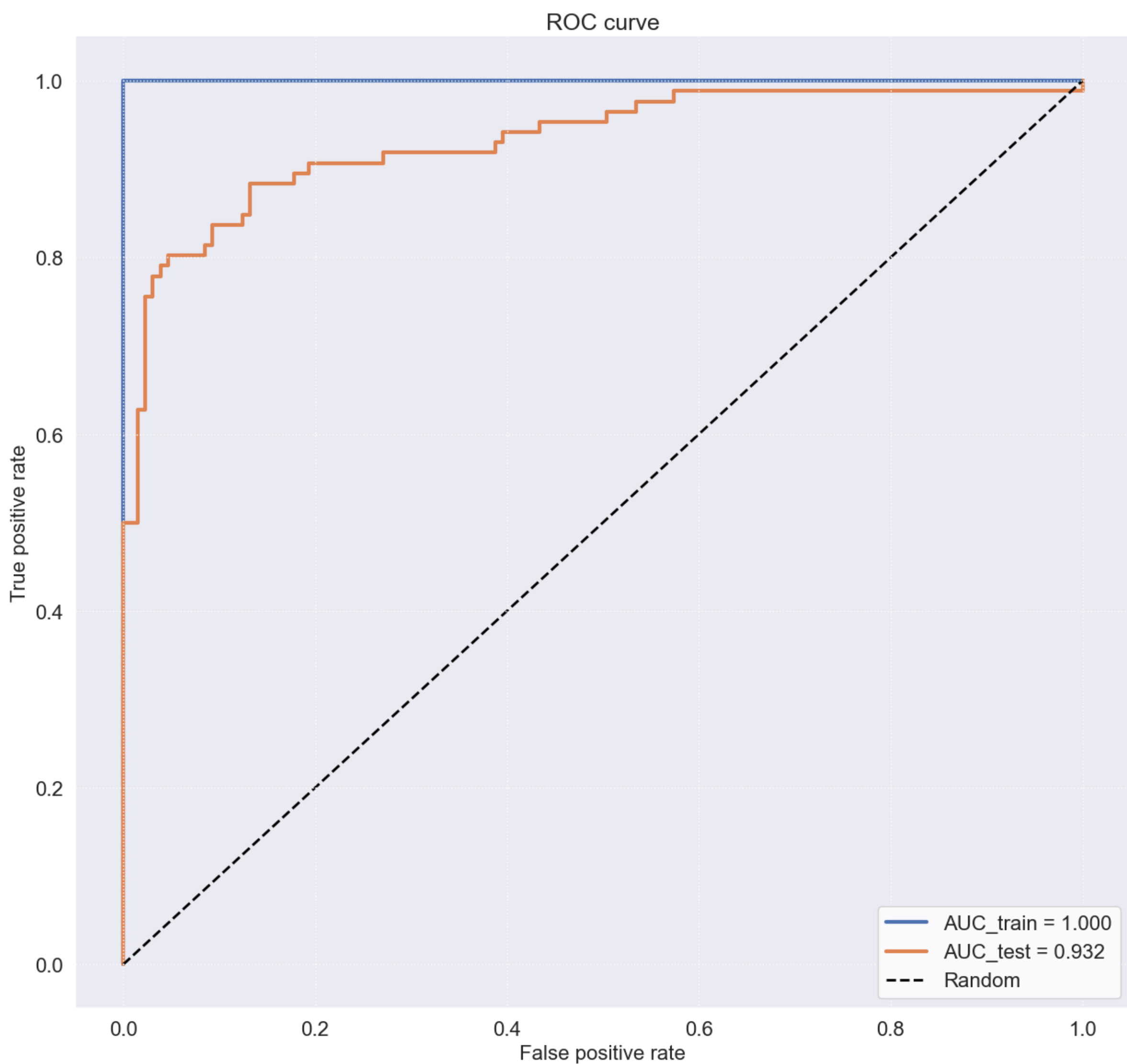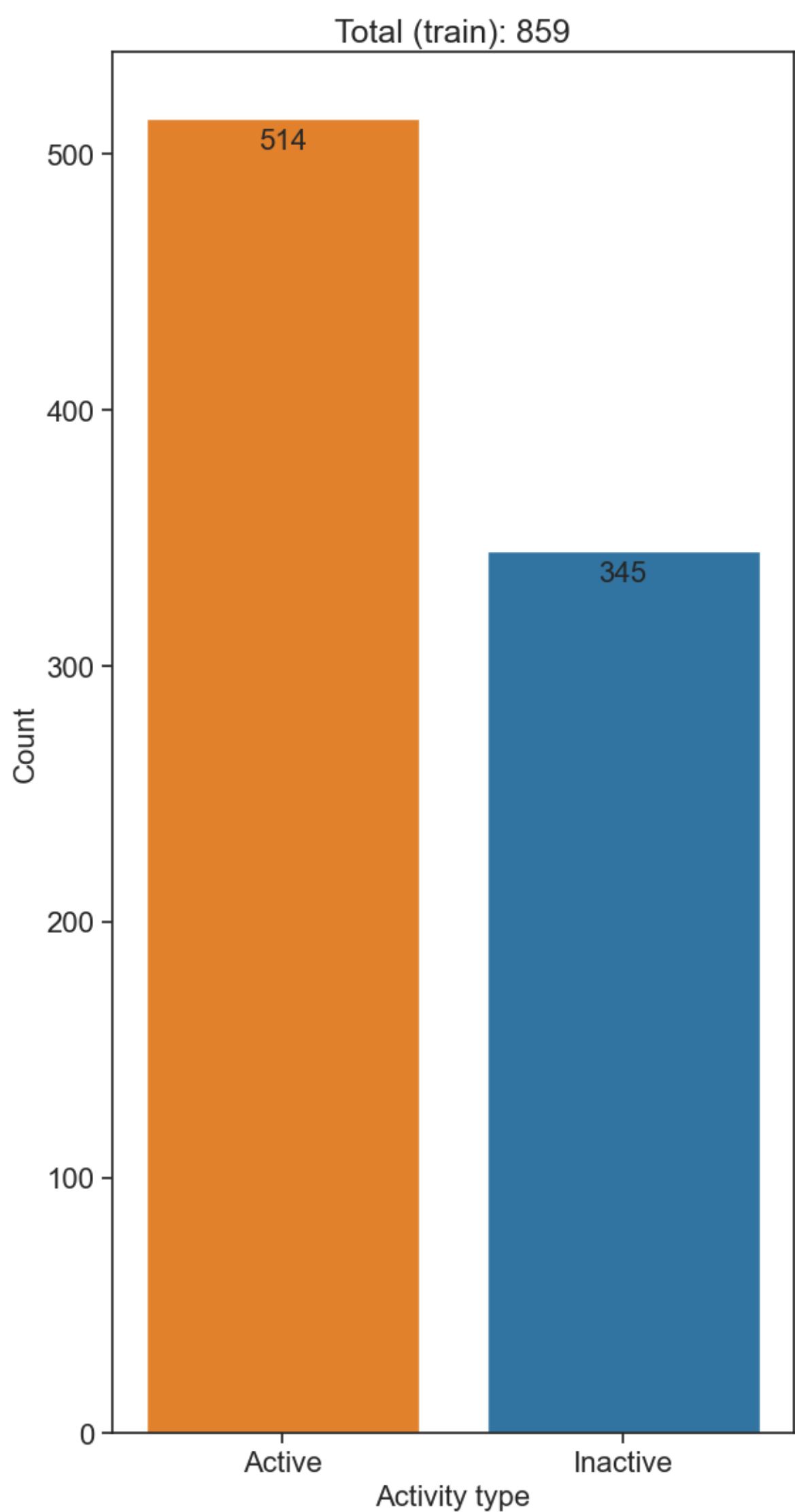
XGBoost Parameters	Value
alpha	1.5916
colsample_bytree	0.526
gamma	0.2089
lambda	4.628
learning_rate	0.2471
max_depth	6.0
min_child_weight	1.0
n_estimators	631.0
reg_alpha	0.2192
reg_lambda	0.9673
scale_pos_weight	3.4603
subsample	0.5835

Confusion Matrix

	0	1
0	111	18
1	10	76

Confusion Matrix (nomr.)

	0	1
0	0.86	0.14
1	0.12	0.88

Calibration curve

	train: 0.0021
	test: 0.1039
	perfectly_calibrated

Active/Inactive probability

Inactive zone   Active zone

type
- active (86)
- inactive (129)
- decoy (215)
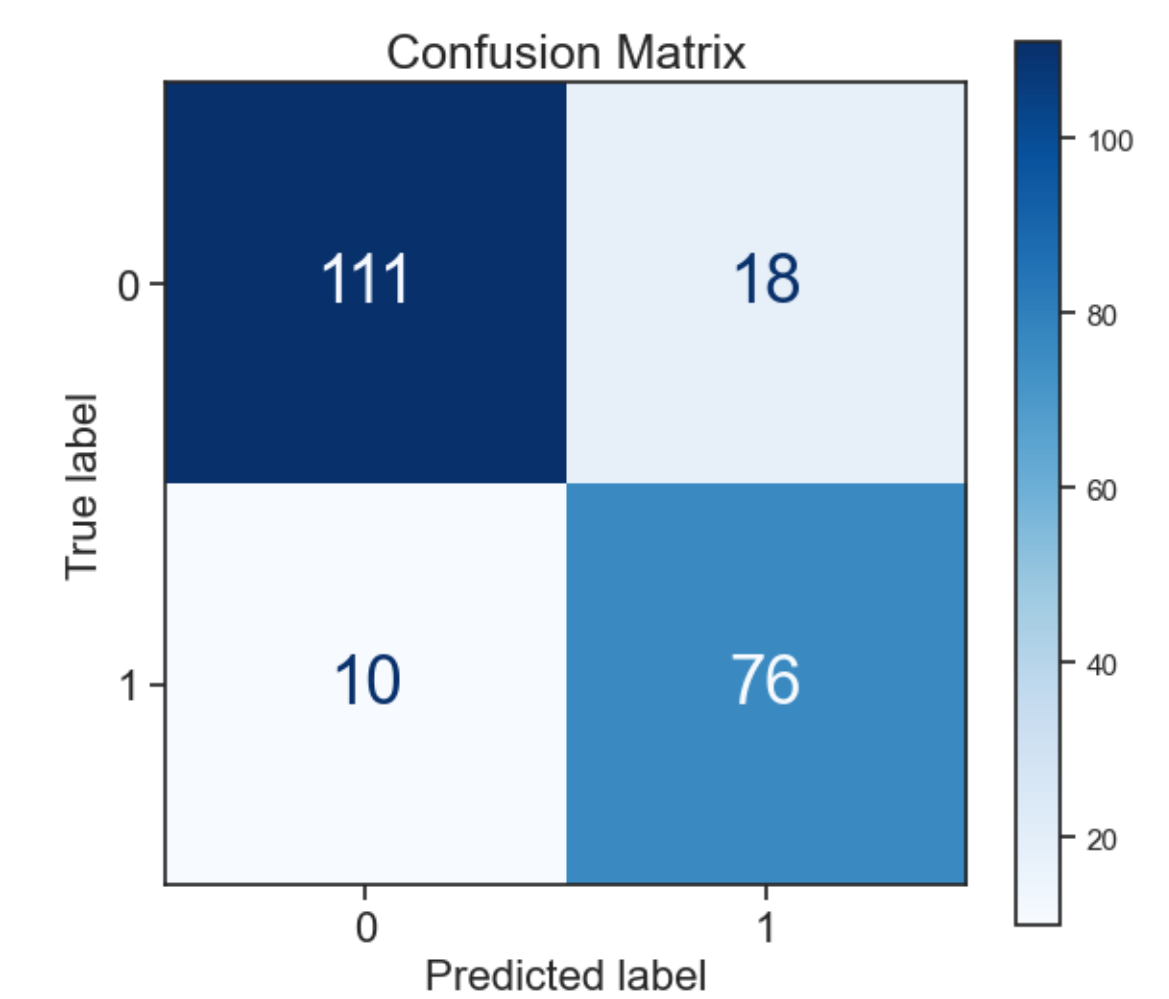
Metric	Train	Test
AUC	1.0	0.9321
accuracy	1.0	0.8698
balanced accuracy	1.0	0.8721
recall_(sens)	1.0	0.8837
specificity	1.0	0.8605
precision	1.0	0.8085
f1_score	1.0	0.8706

Protein: P09619 - metric: f1

Total (train): 859

ROC curve

AUC_train = 1.000
AUC_test = 0.930
Random

Pareto Chart with Highlighted Best Attempt

- Trials
- Pareto Front Trials
- Best Trial (# 1240)
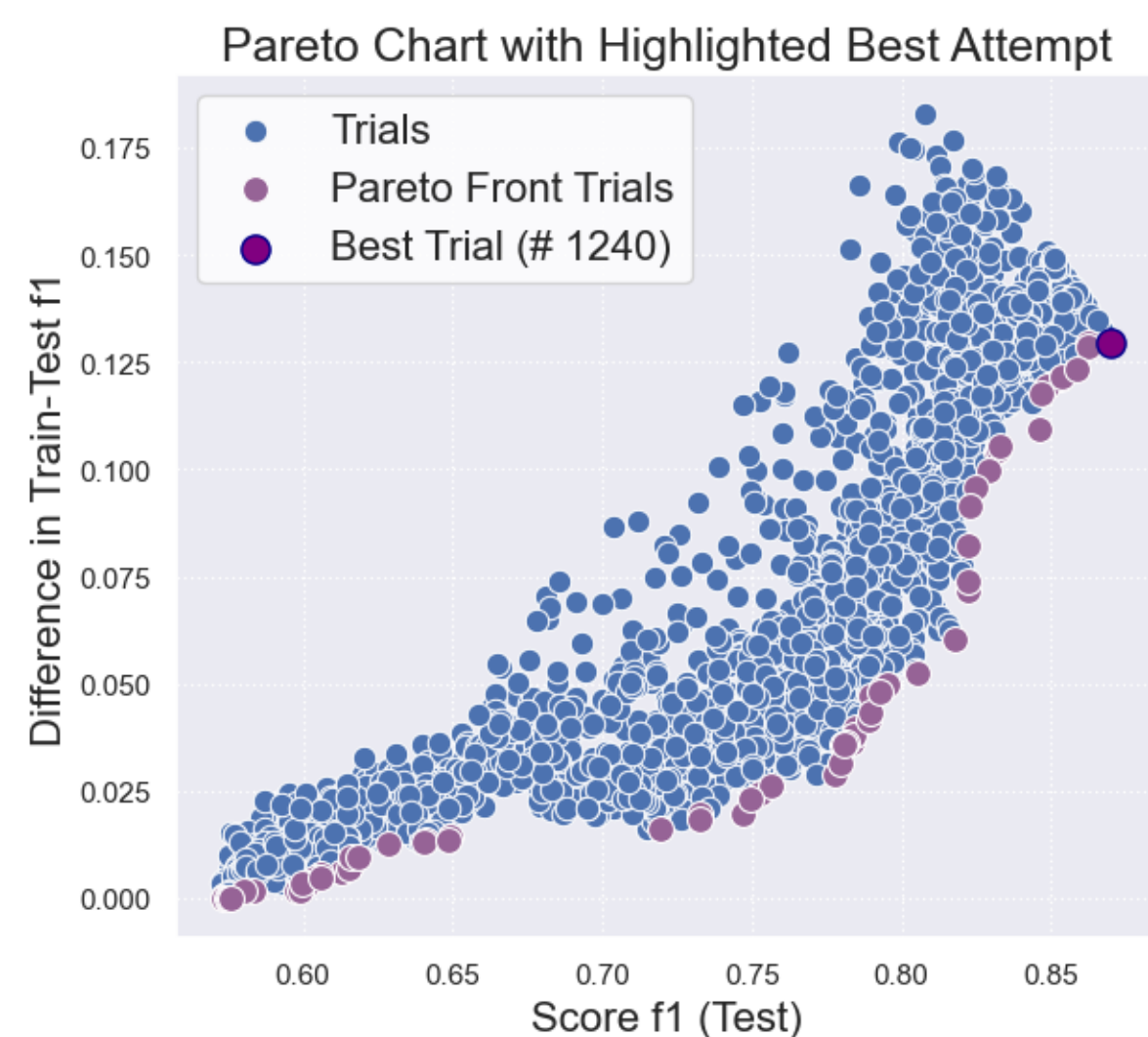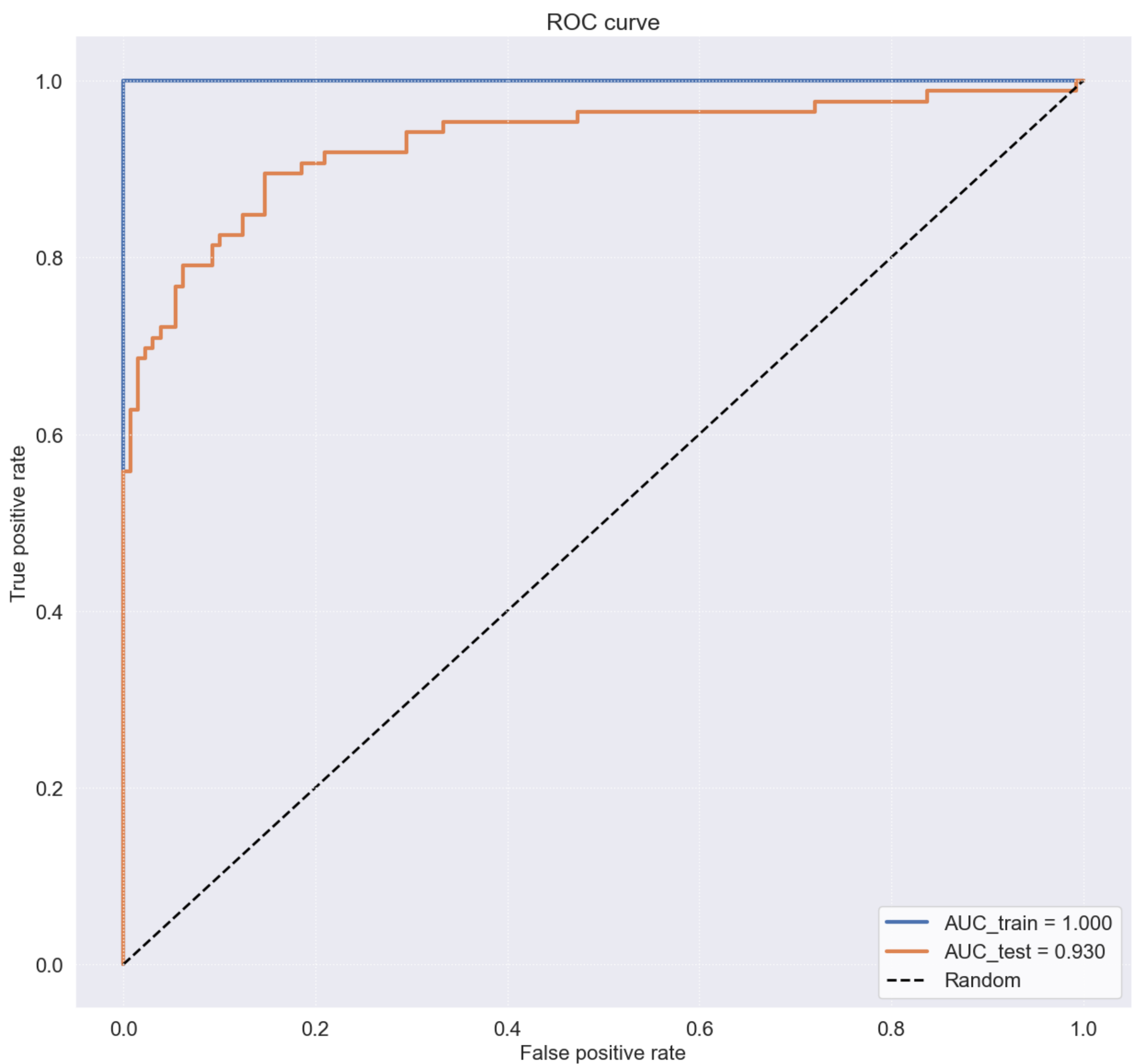
XGBoost Parameters	Value
alpha	1.9227
colsample_bytree	0.7857
gamma	0.2252
lambda	2.0426
learning_rate	0.0312
max_depth	9.0
min_child_weight	1.0
n_estimators	660.0
reg_alpha	0.395
reg_lambda	0.6874
scale_pos_weight	2.843
subsample	0.8562

Confusion Matrix

	Predicted 0	Predicted 1
True 0	110	19
True 1	11	75

Calibration curve

train: 0.0057
test: 0.1047
perfectly_calibrated

Confusion Matrix (nomr.)

	Predicted 0	Predicted 1
True 0	0.85	0.15
True 1	0.13	0.87

Active/Inactive probability

Inactive zone   Active zone

type
- active (86)
- inactive (129)
- decoy (215)
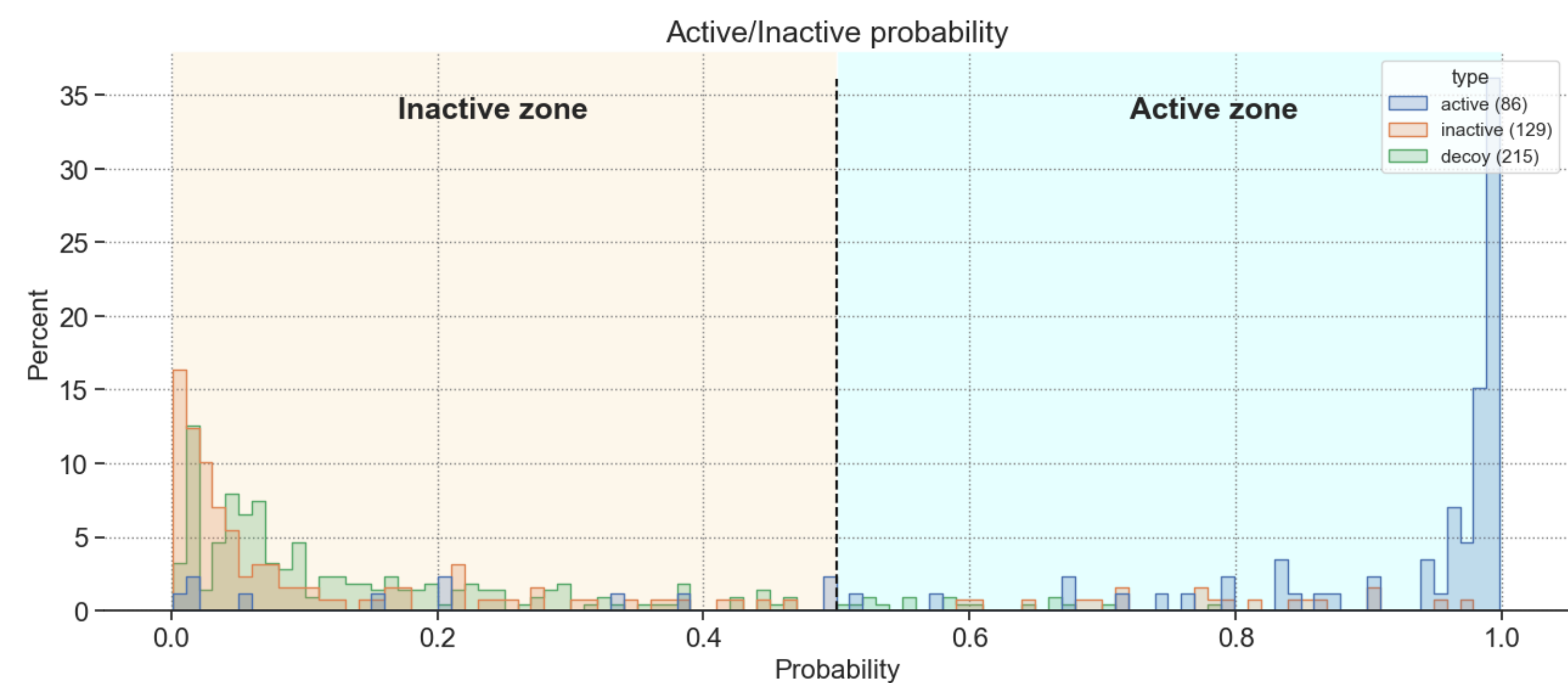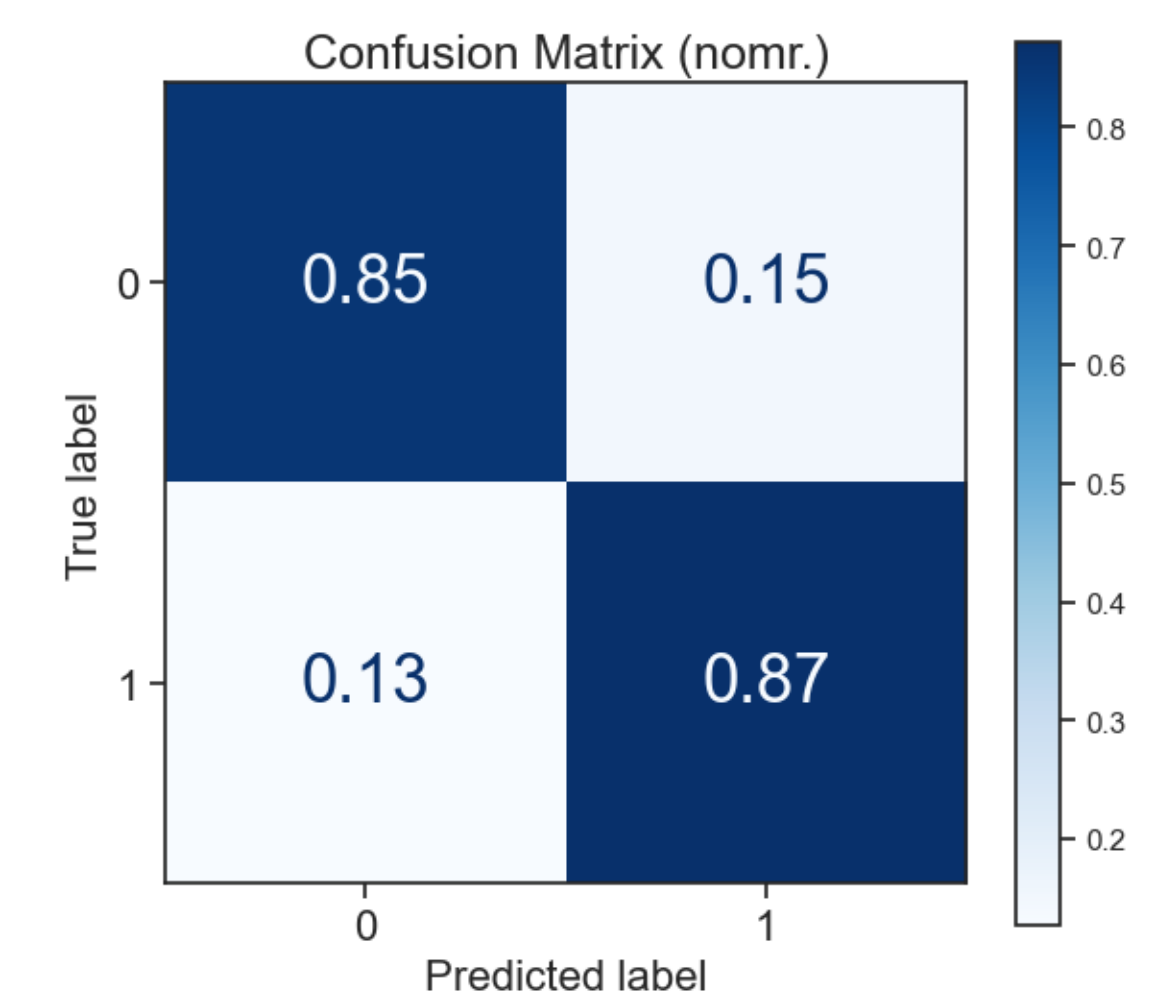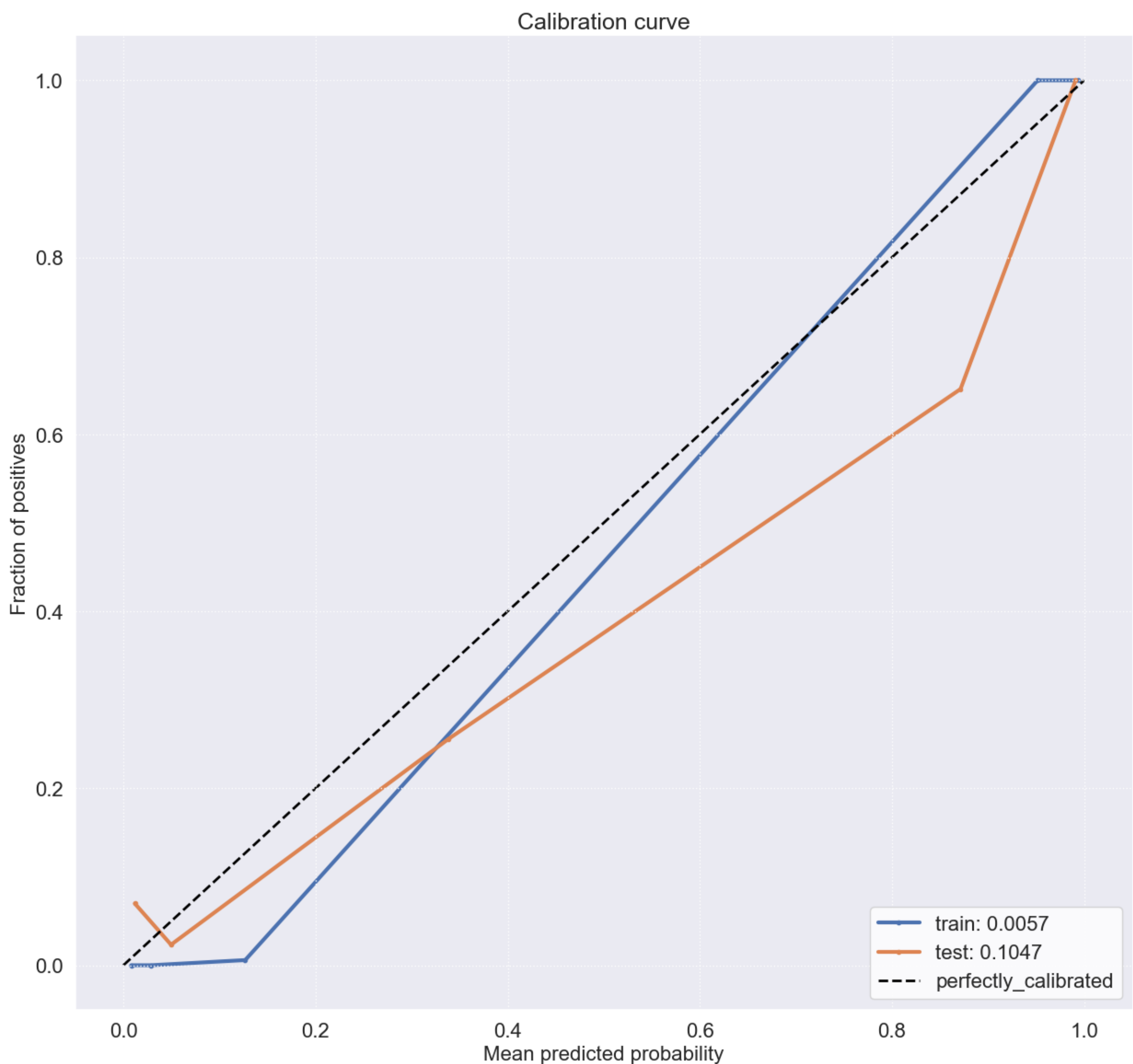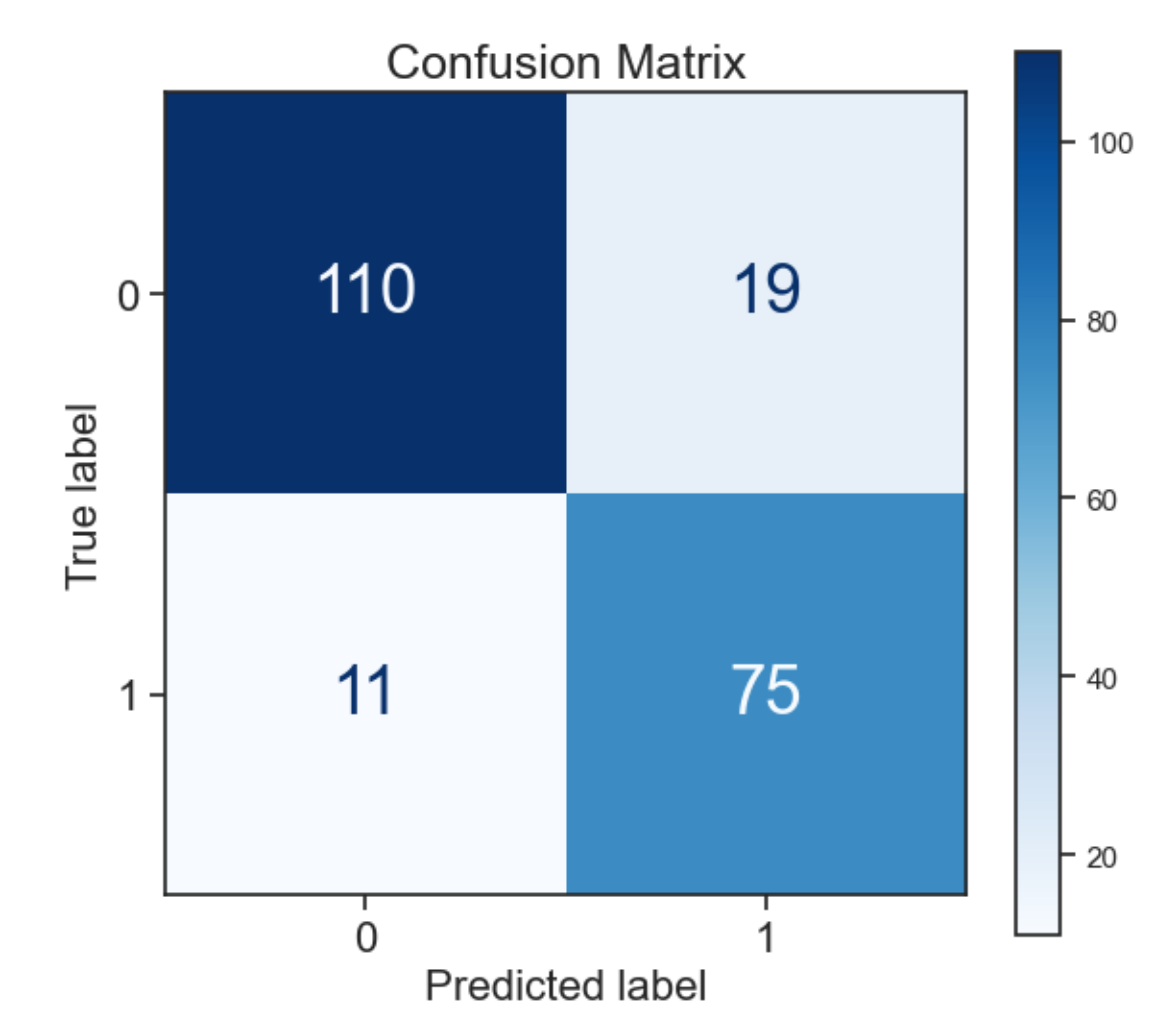
Metric	Train	Test
AUC	1.0	0.93
accuracy	1.0	0.8605
balanced accuracy	1.0	0.8624
recall_(sens)	1.0	0.8721
specificity	1.0	0.8527
precision	1.0	0.7979
f1_score	1.0	0.8613

Protein: P09619 - metric: precision

Total (train): 859

ROC curve

AUC_train = 1.000
AUC_test = 0.939
Random

Pareto Chart with Highlighted Best Attempt

- Trials
- Pareto Front Trials
- Best Trial (# 2628)
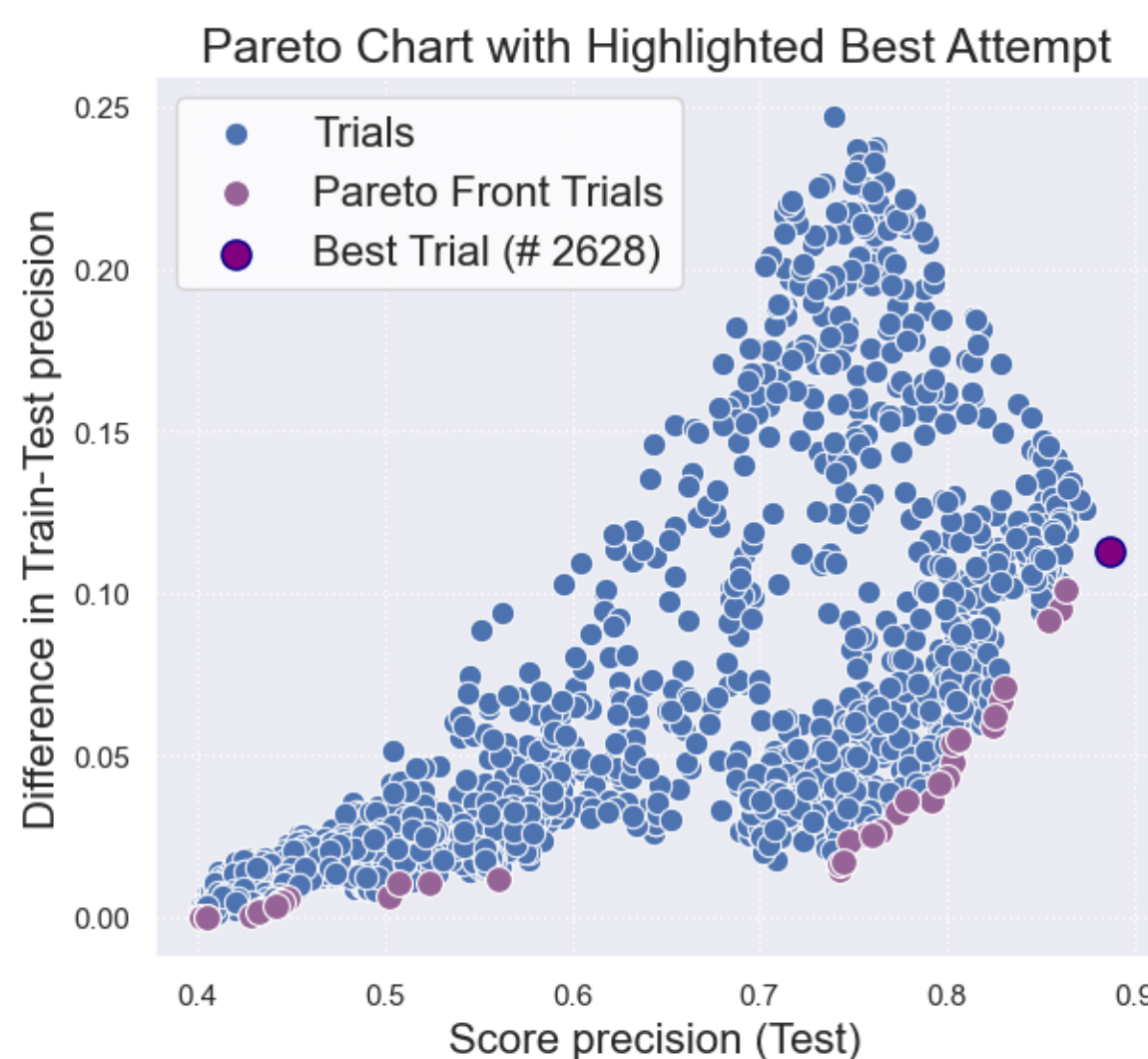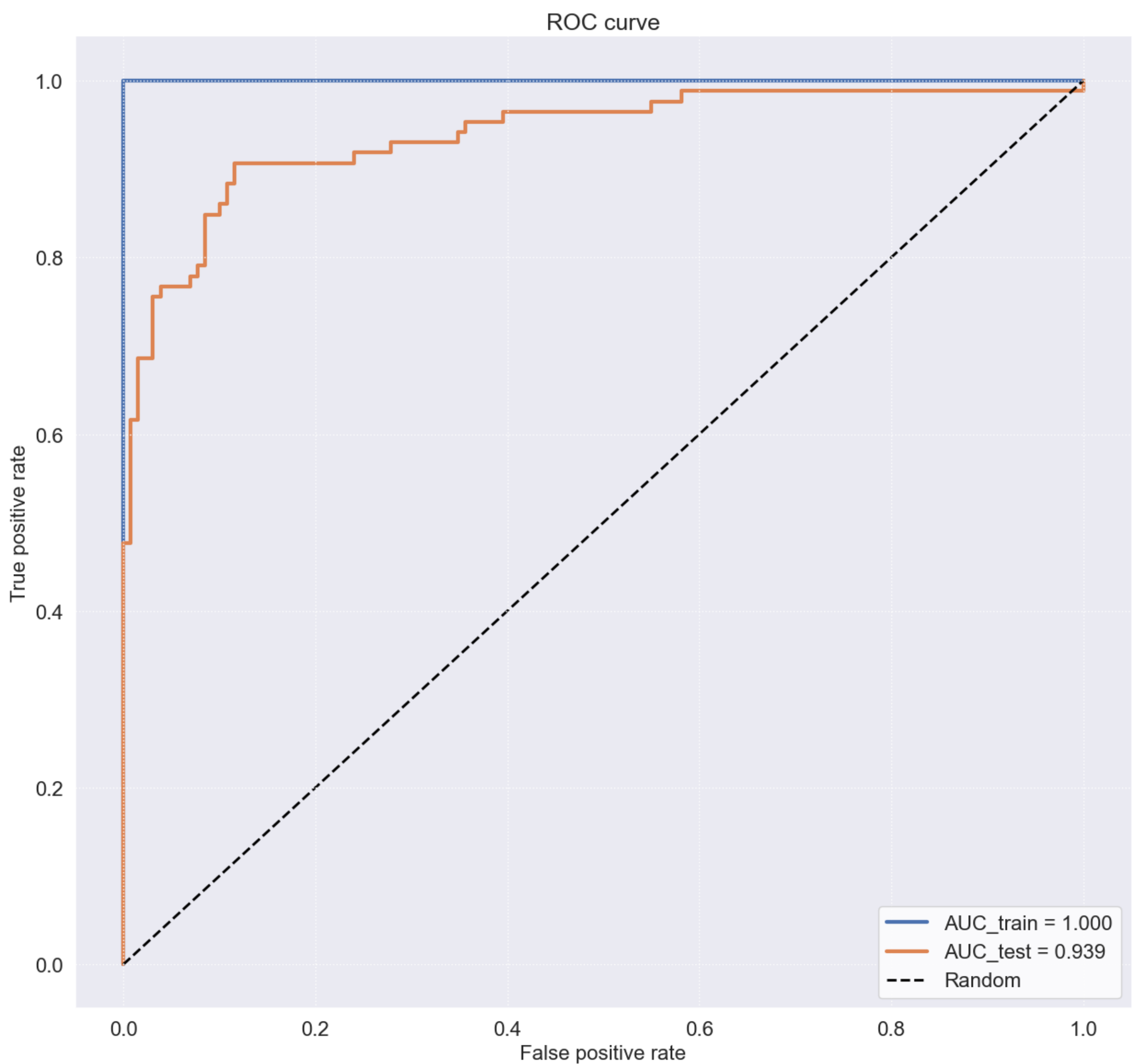
XGBoost Parameters	Value
alpha	1.3845
colsample_bytree	0.9985
gamma	0.1315
lambda	1.9582
learning_rate	0.1188
max_depth	6.0
min_child_weight	1.0
n_estimators	503.0
reg_alpha	0.3219
reg_lambda	0.7959
scale_pos_weight	1.3947
subsample	0.691

Confusion Matrix

Calibration curve

train: 0.0032
test: 0.0903
perfectly_calibrated

Confusion Matrix (nomr.)

Active/Inactive probability

type
- active (86)
- inactive (129)
- decoy (215)

Inactive zone
Active zone
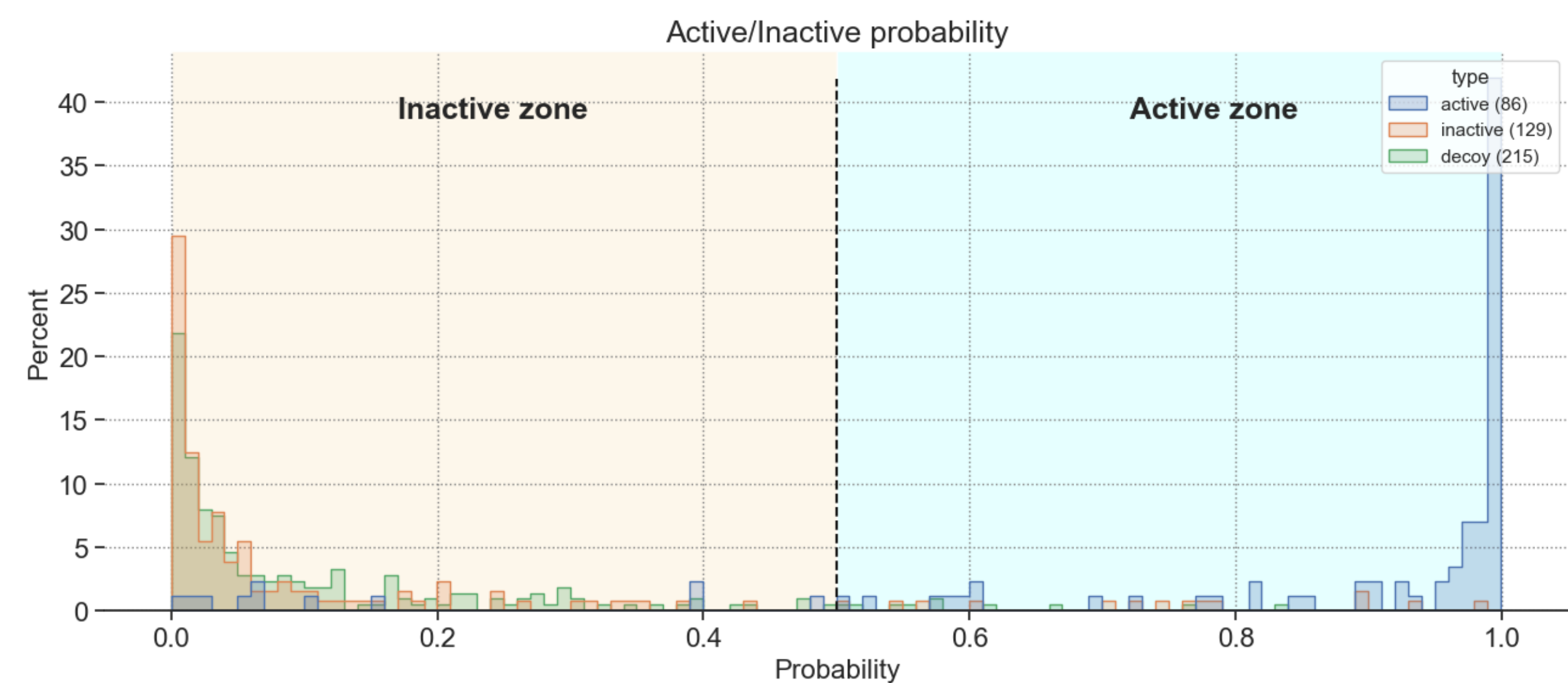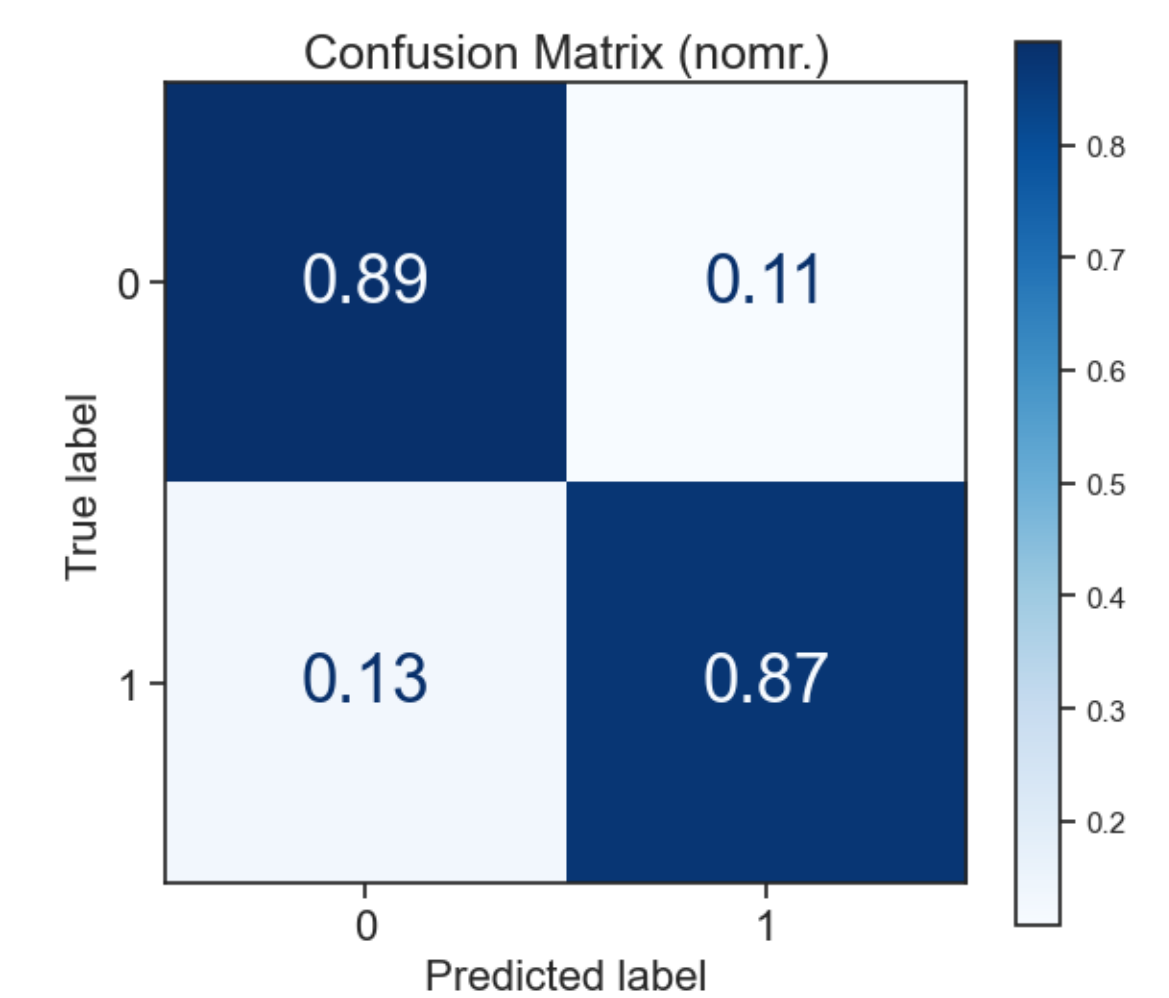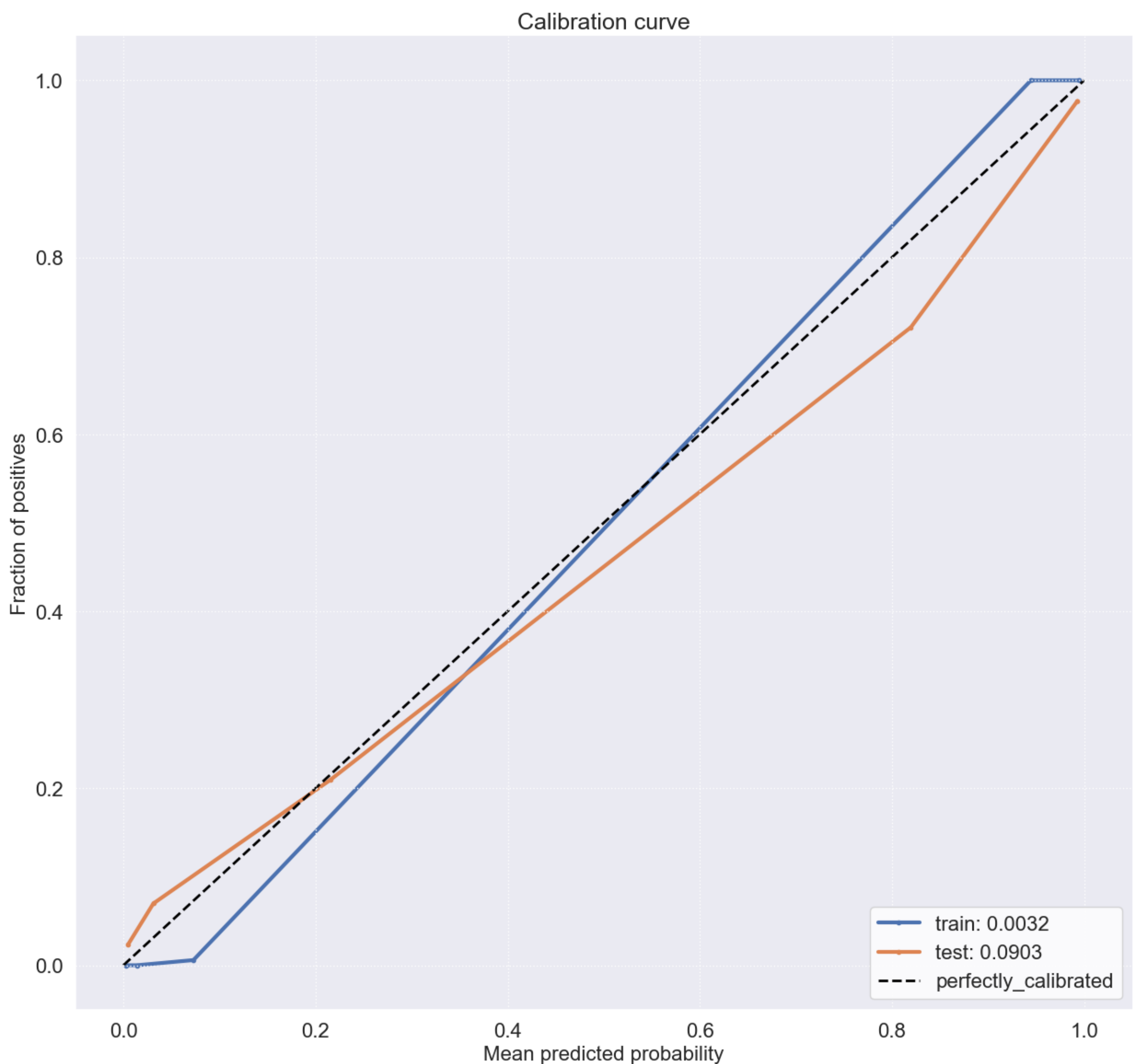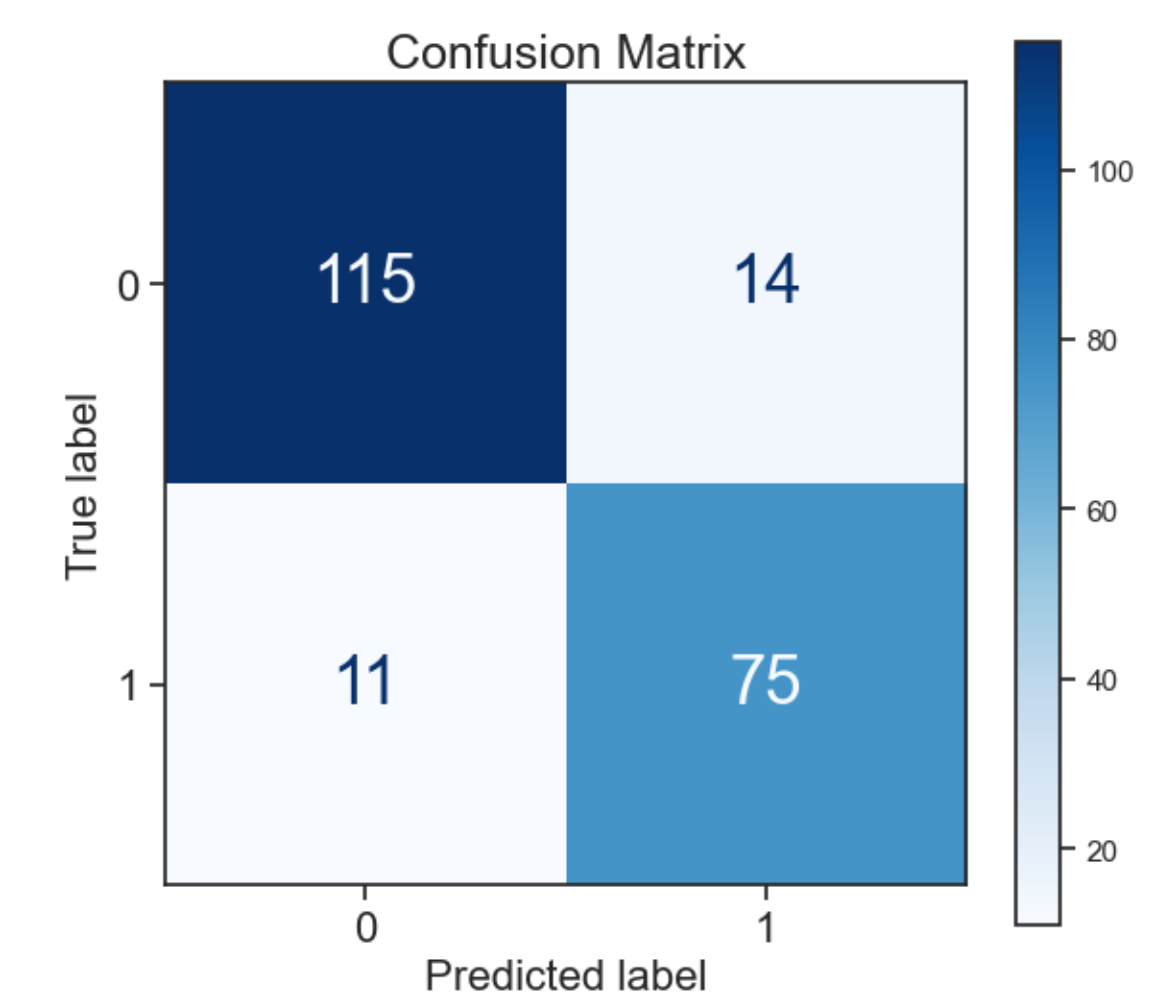
Metric	Train	Test
AUC	1.0	0.9385
accuracy	1.0	0.8837
balanced accuracy	1.0	0.8818
recall_(sens)	1.0	0.8721
specificity	1.0	0.8915
precision	1.0	0.8427
f1_score	1.0	0.884

Protein: P09619 - metric: SoftVotingXGBoostEnsemble
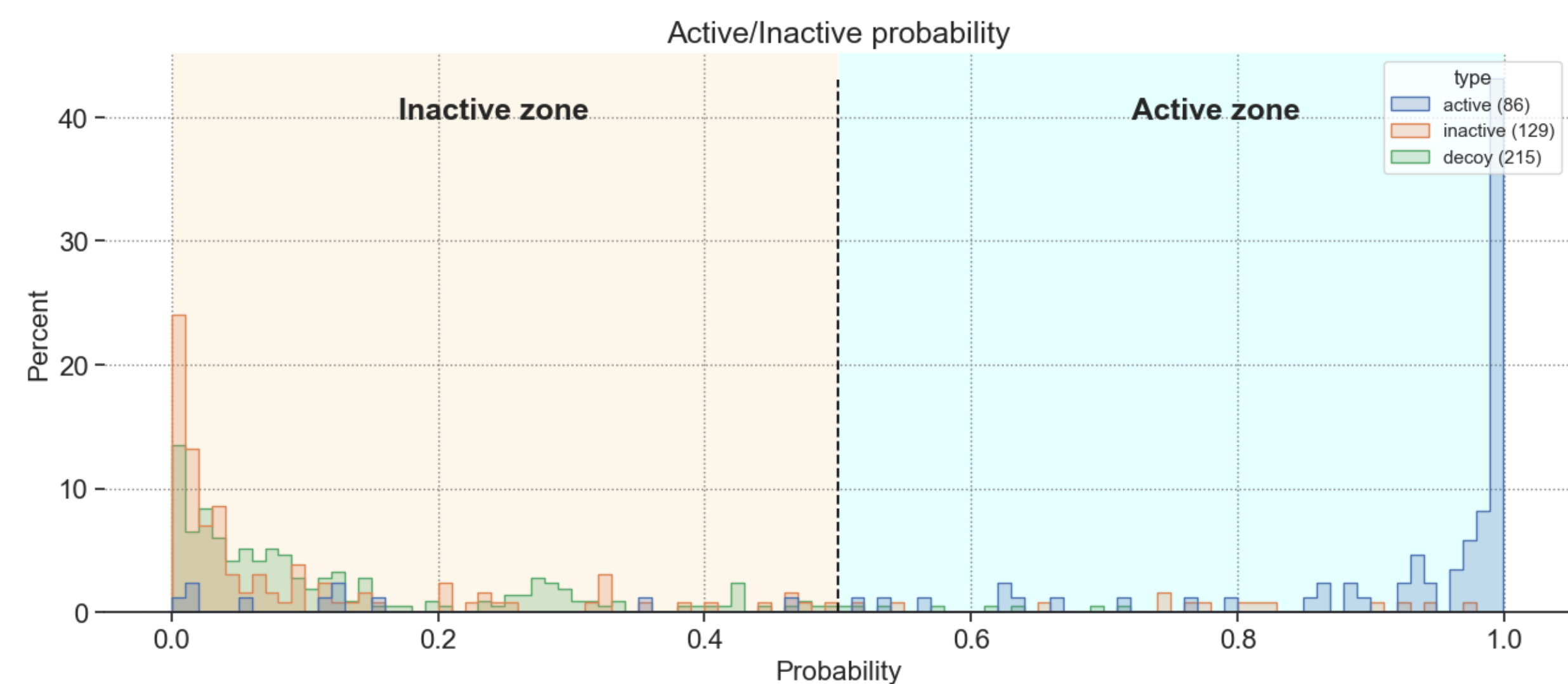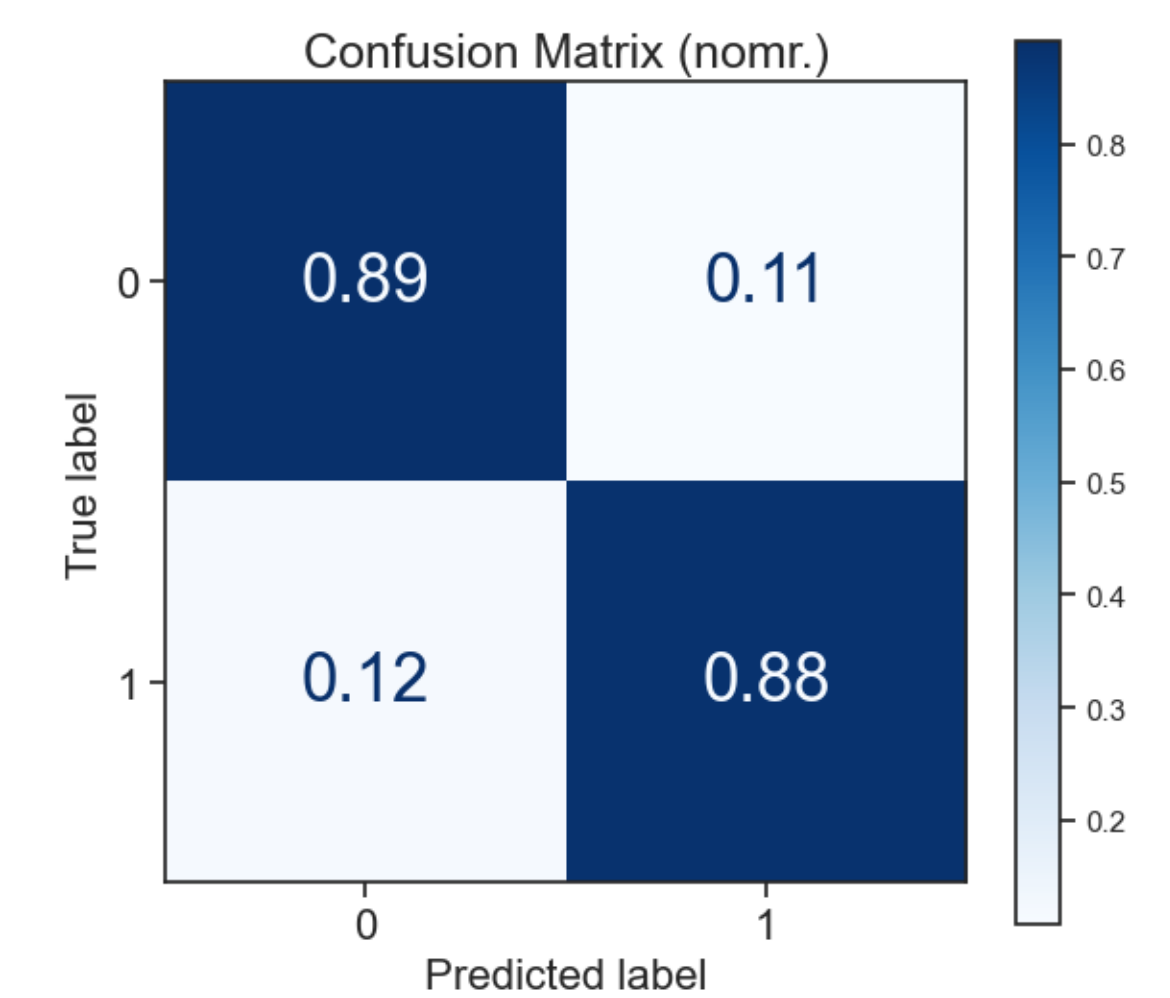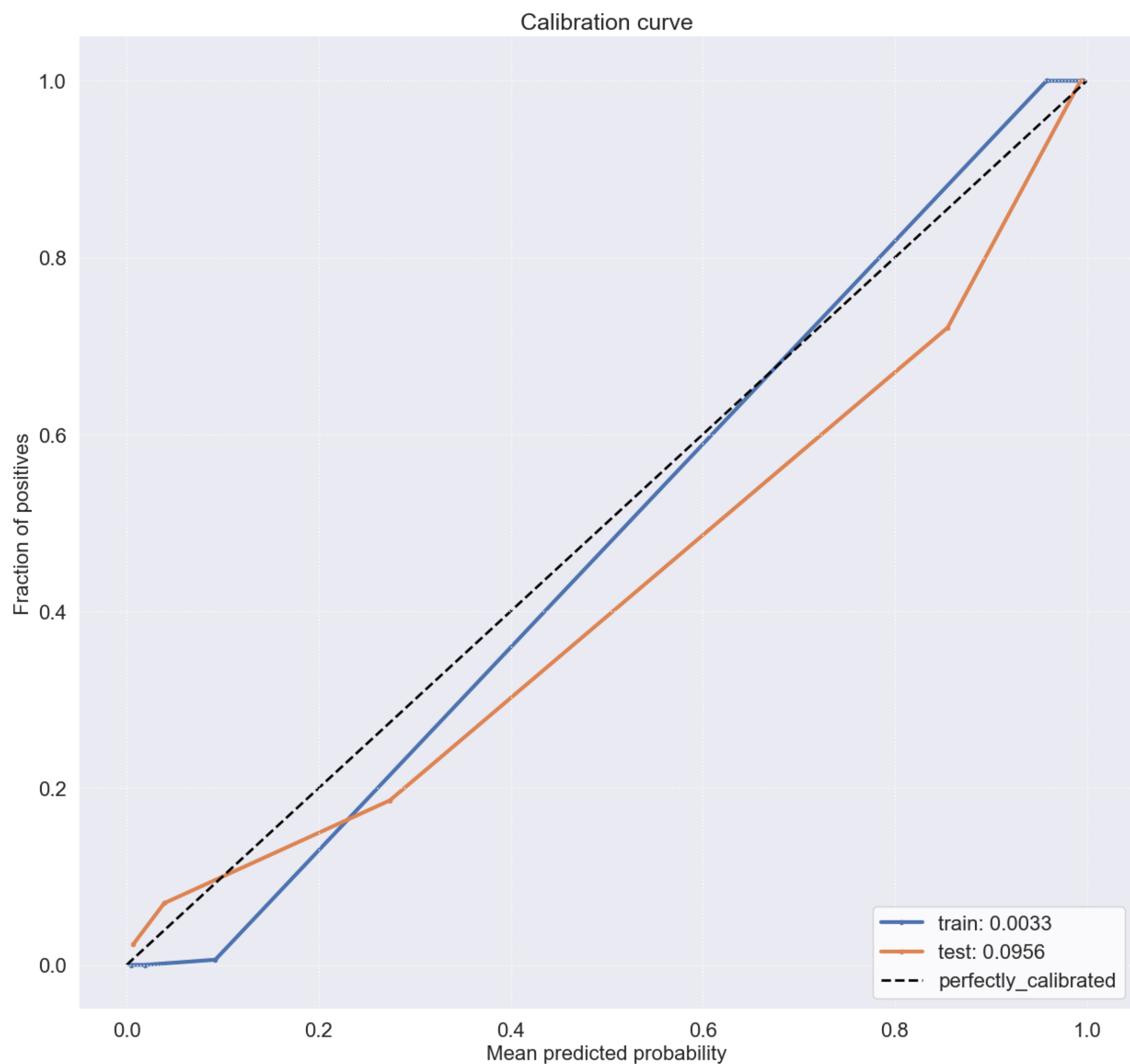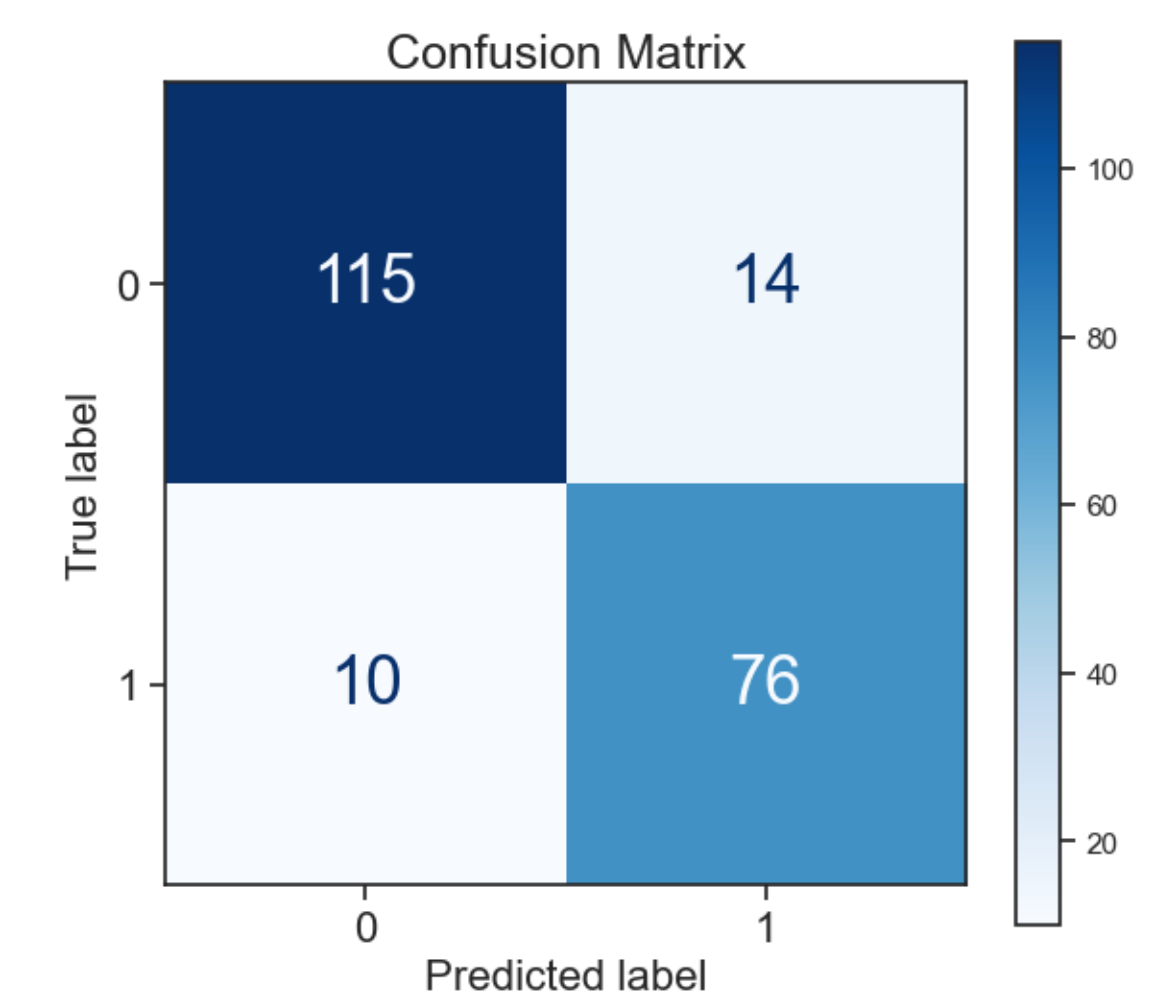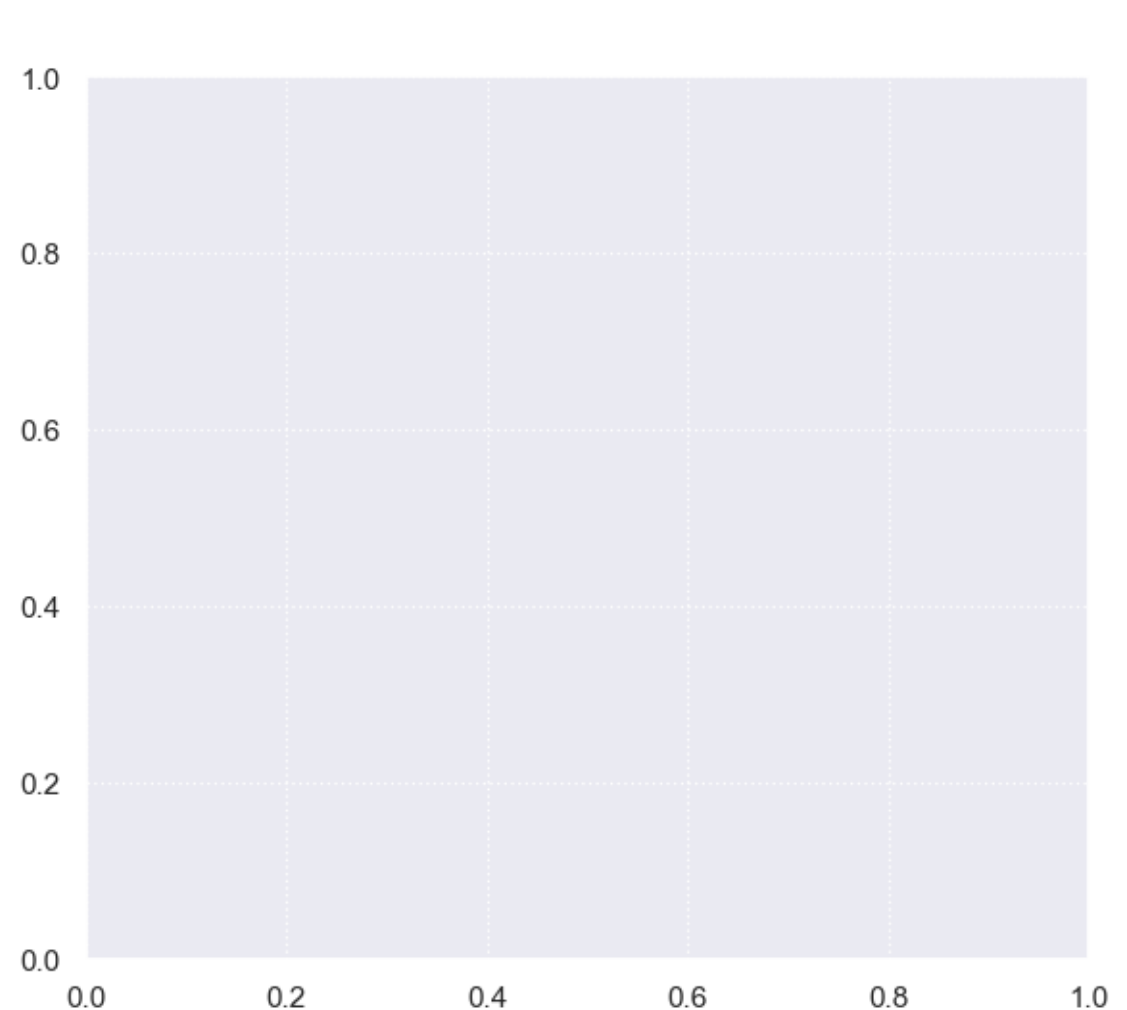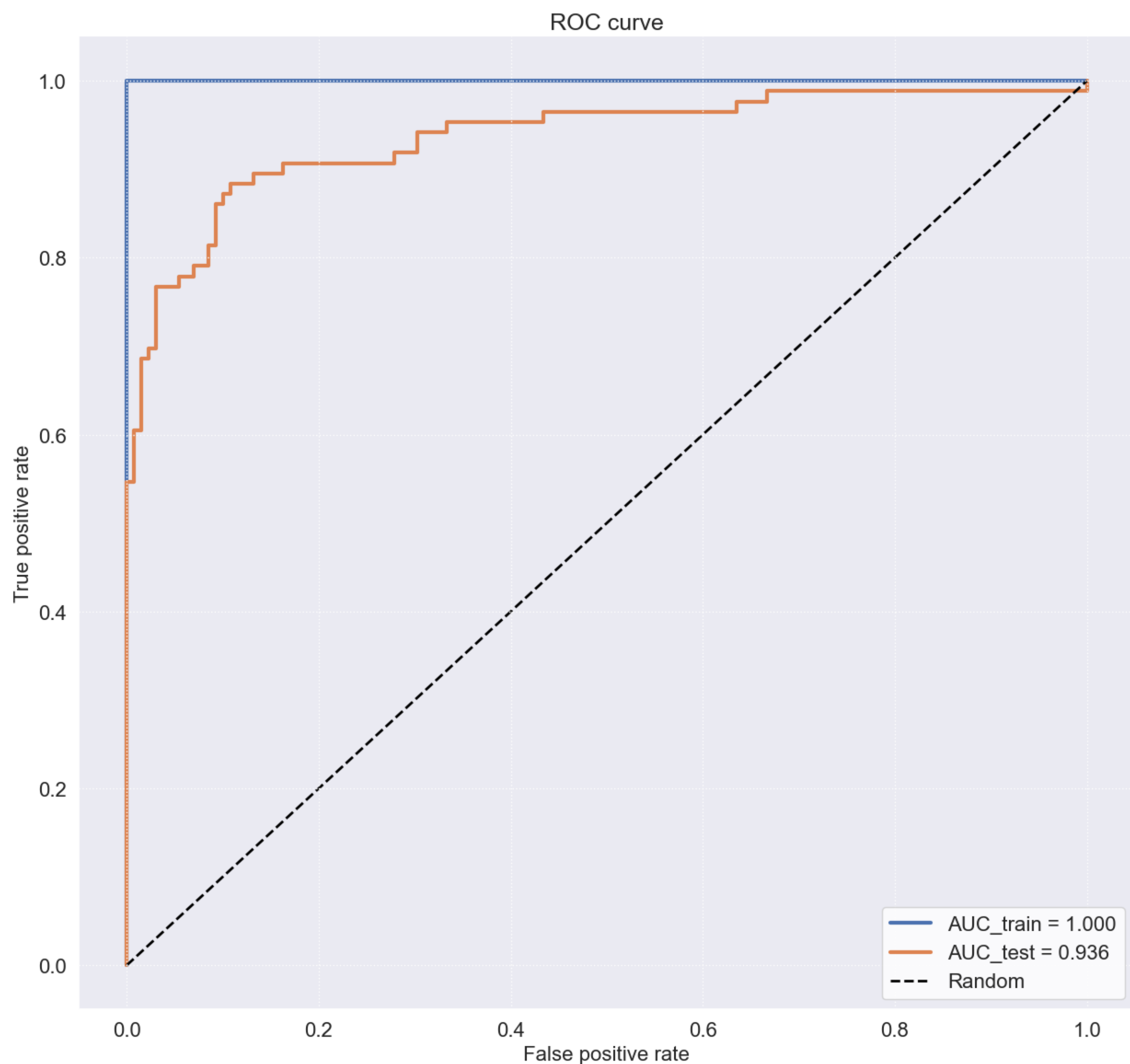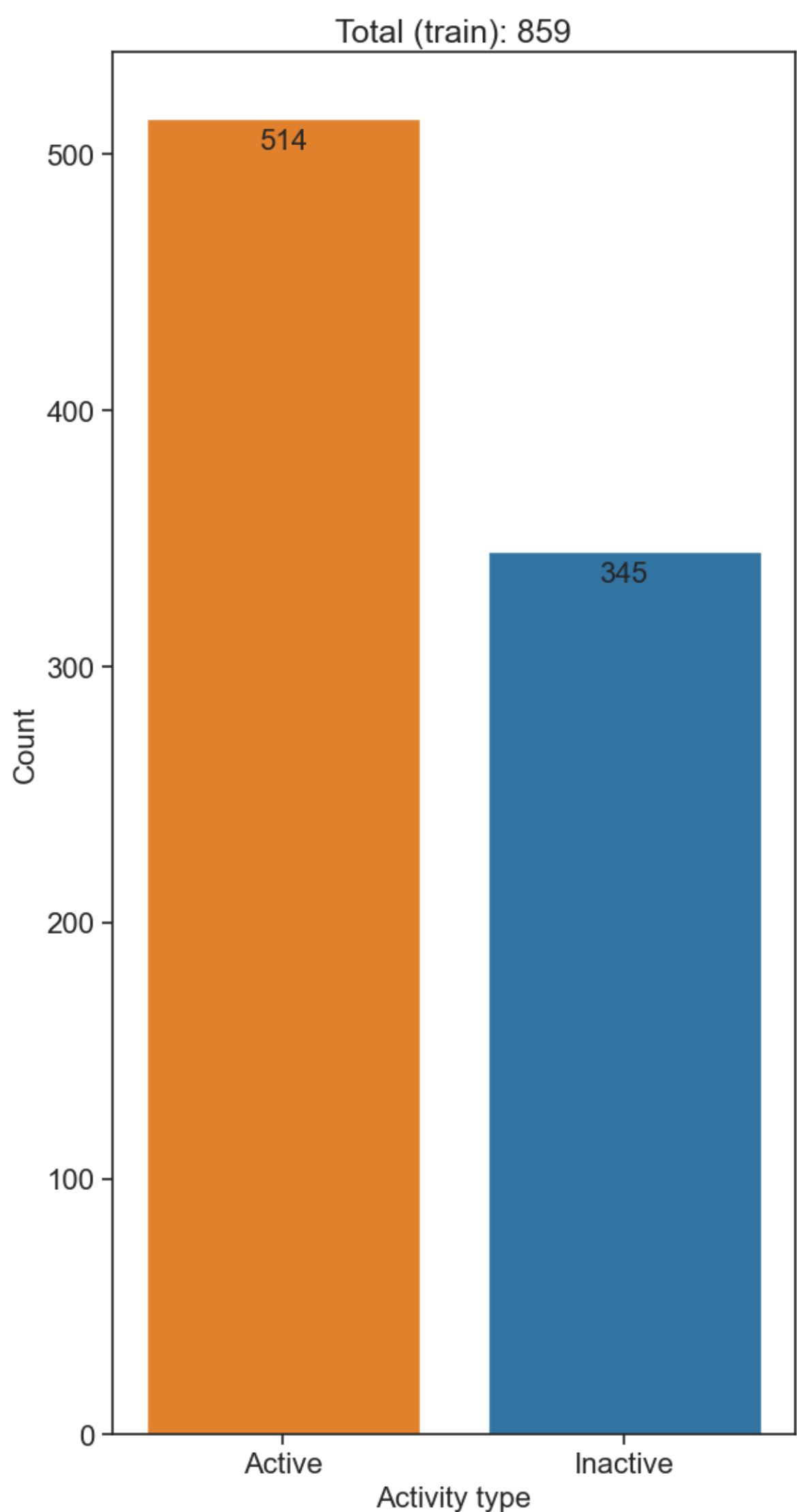
Metric	Train	Test
AUC	1.0	0.9363
accuracy	1.0	0.8884
balanced accuracy	1.0	0.8876
recall_(sens)	1.0	0.8837
specificity	1.0	0.8915
precision	1.0	0.8444
f1_score	1.0	0.8888