Protein: P29317 - metric: balanced_accuracy

Total (train): 204

ROC curve

AUC_train = 0.999
AUC_test = 0.998
Random

Pareto Chart with Highlighted Best Attempt

- Trials
- Pareto Front Trials
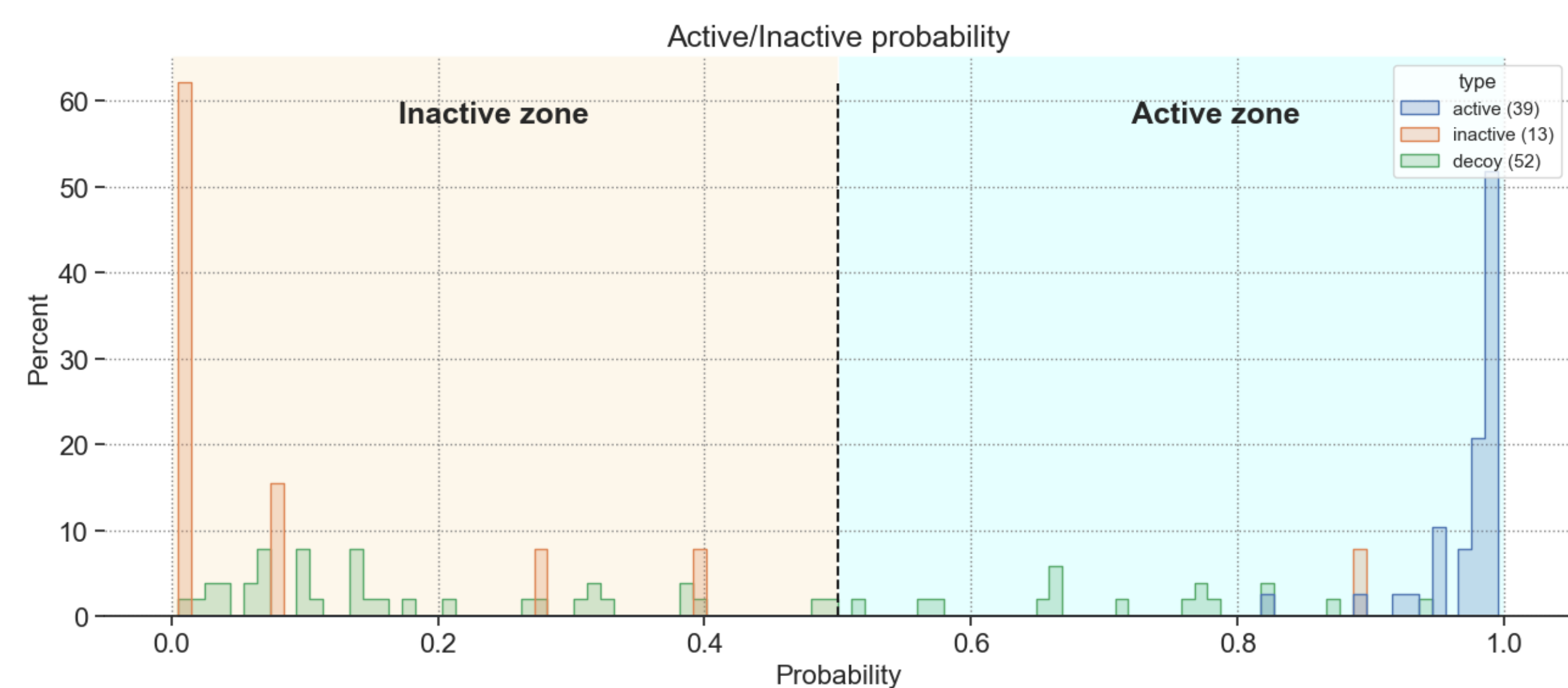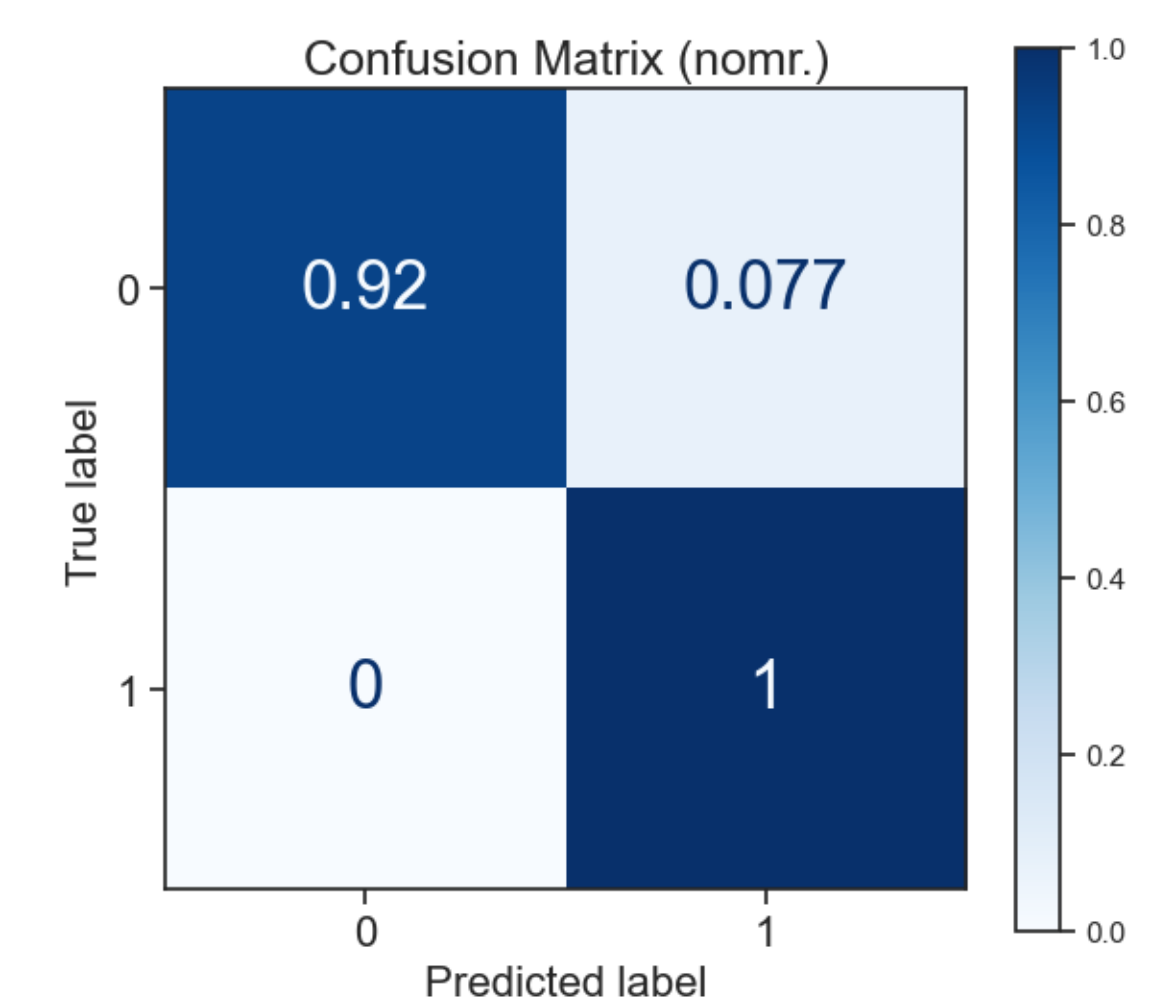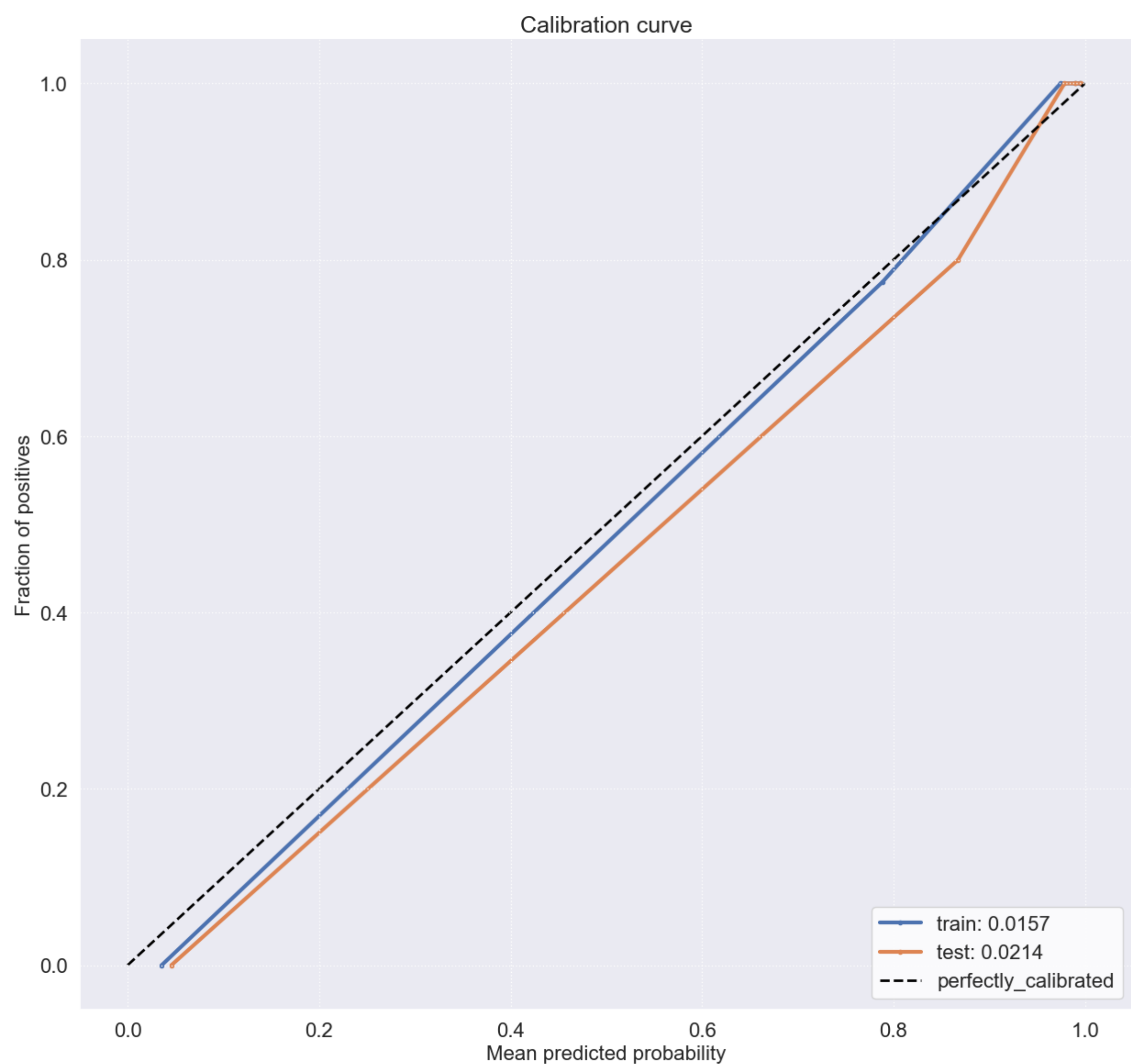- Best Trial (# 1443)
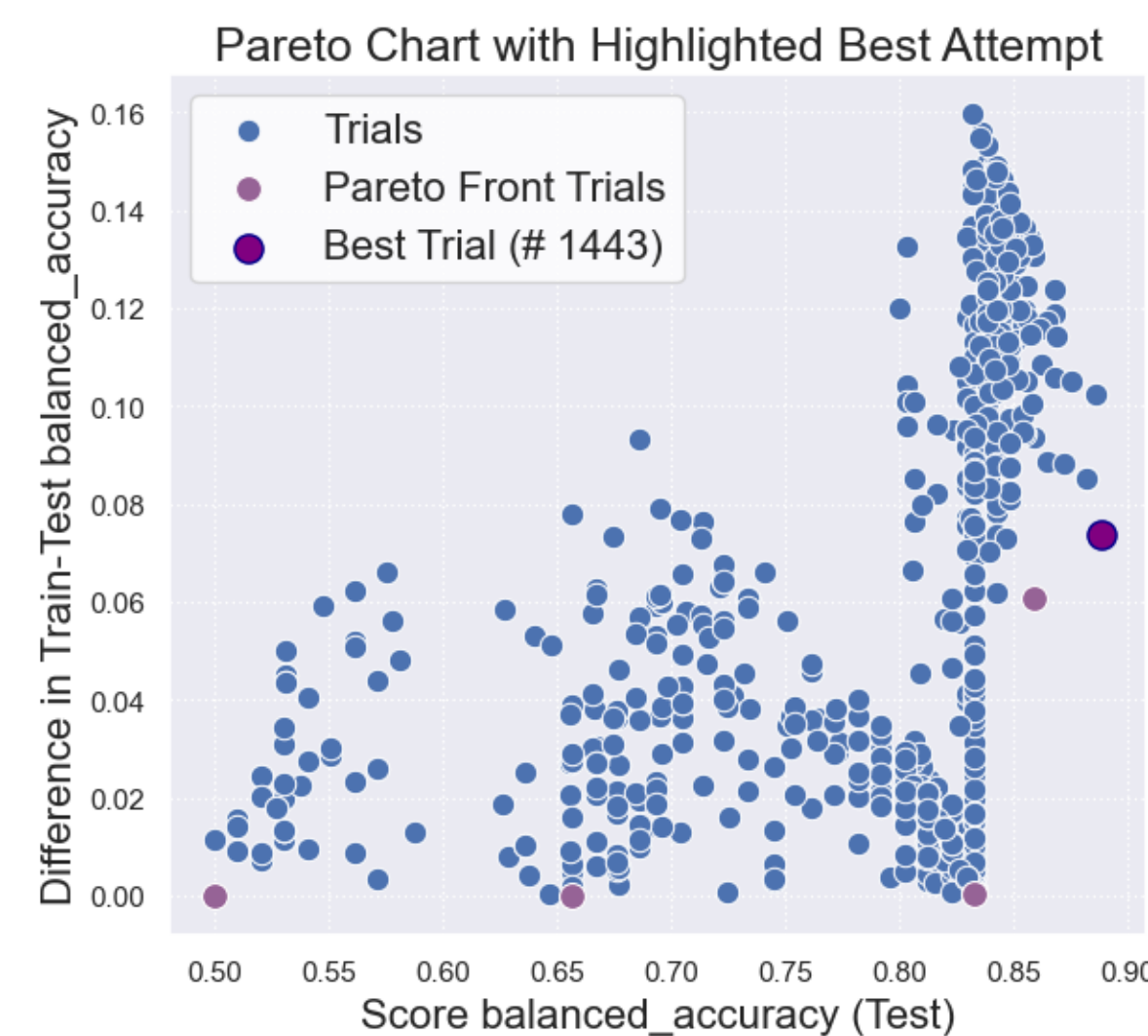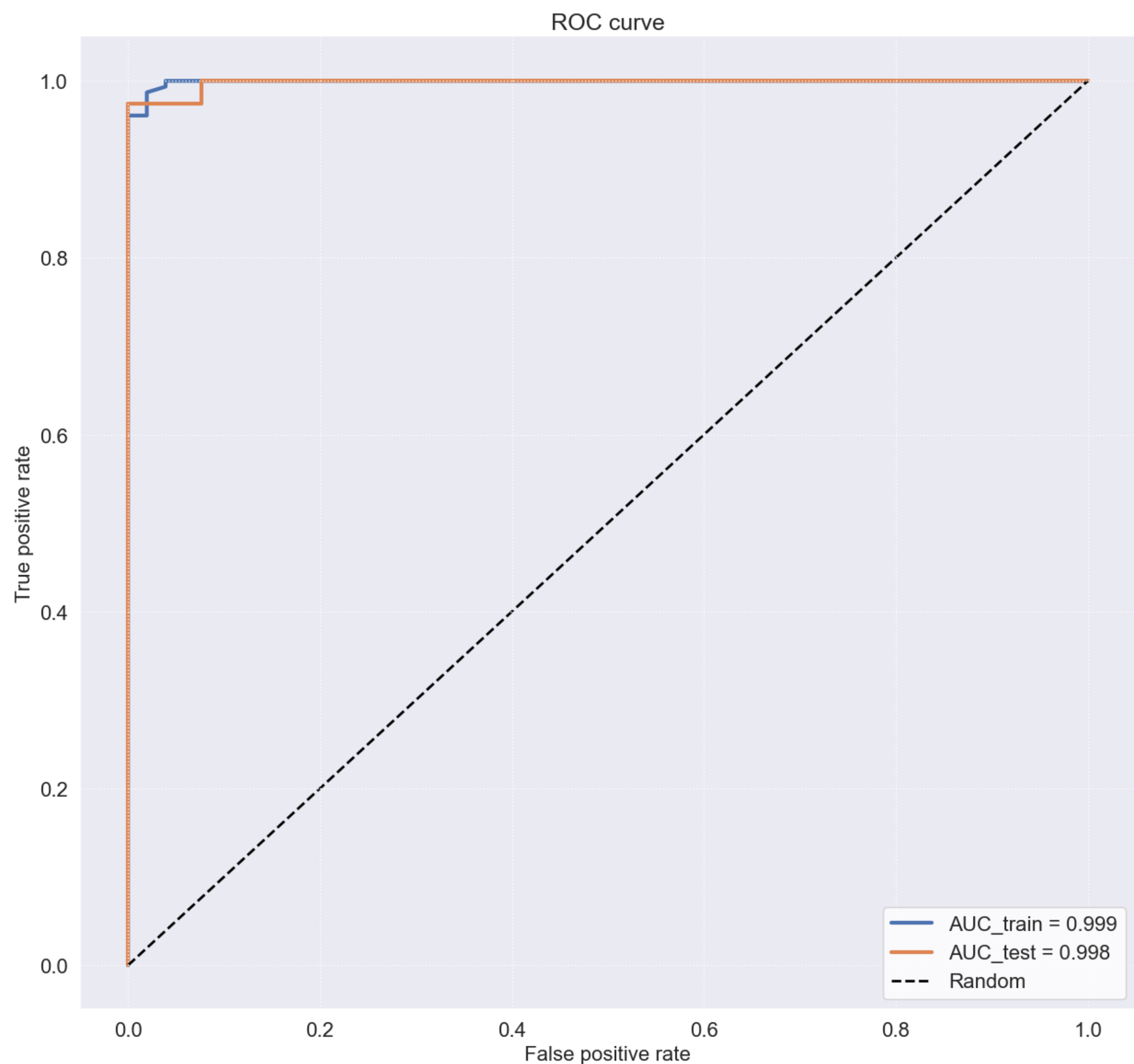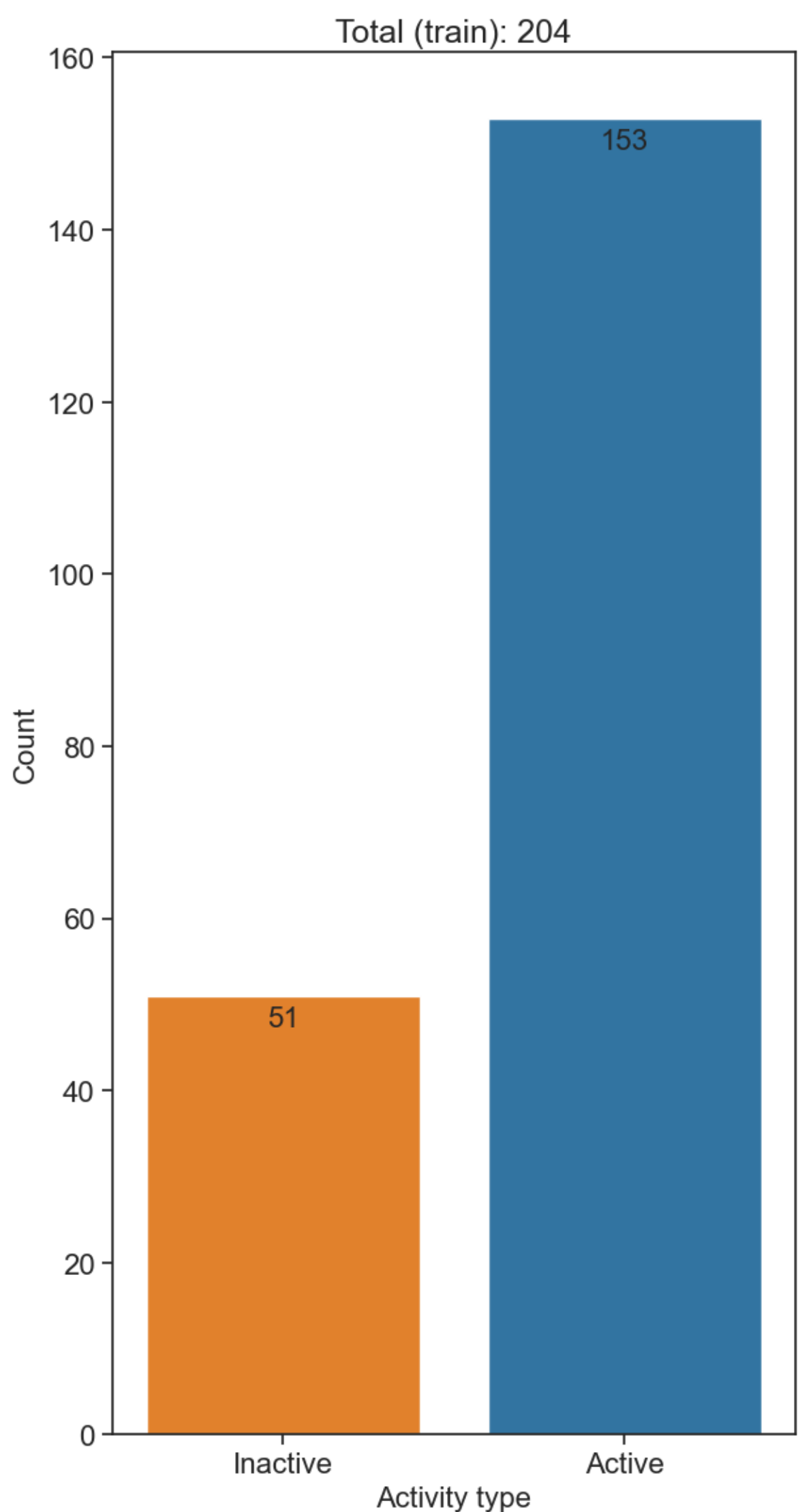
XGBoost Parameters	Value
alpha	2.8189
colsample_bytree	0.592
gamma	0.4424
lambda	1.6954
learning_rate	0.6814
max_depth	6.0
min_child_weight	1.0
n_estimators	111.0
reg_alpha	0.675
reg_lambda	0.3696
scale_pos_weight	1.0198
subsample	0.8813

Confusion Matrix

Calibration curve

train: 0.0157
test: 0.0214
perfectly_calibrated

Confusion Matrix (nomr.)

Active/Inactive probability

type
active (39)
inactive (13)
decoy (52)
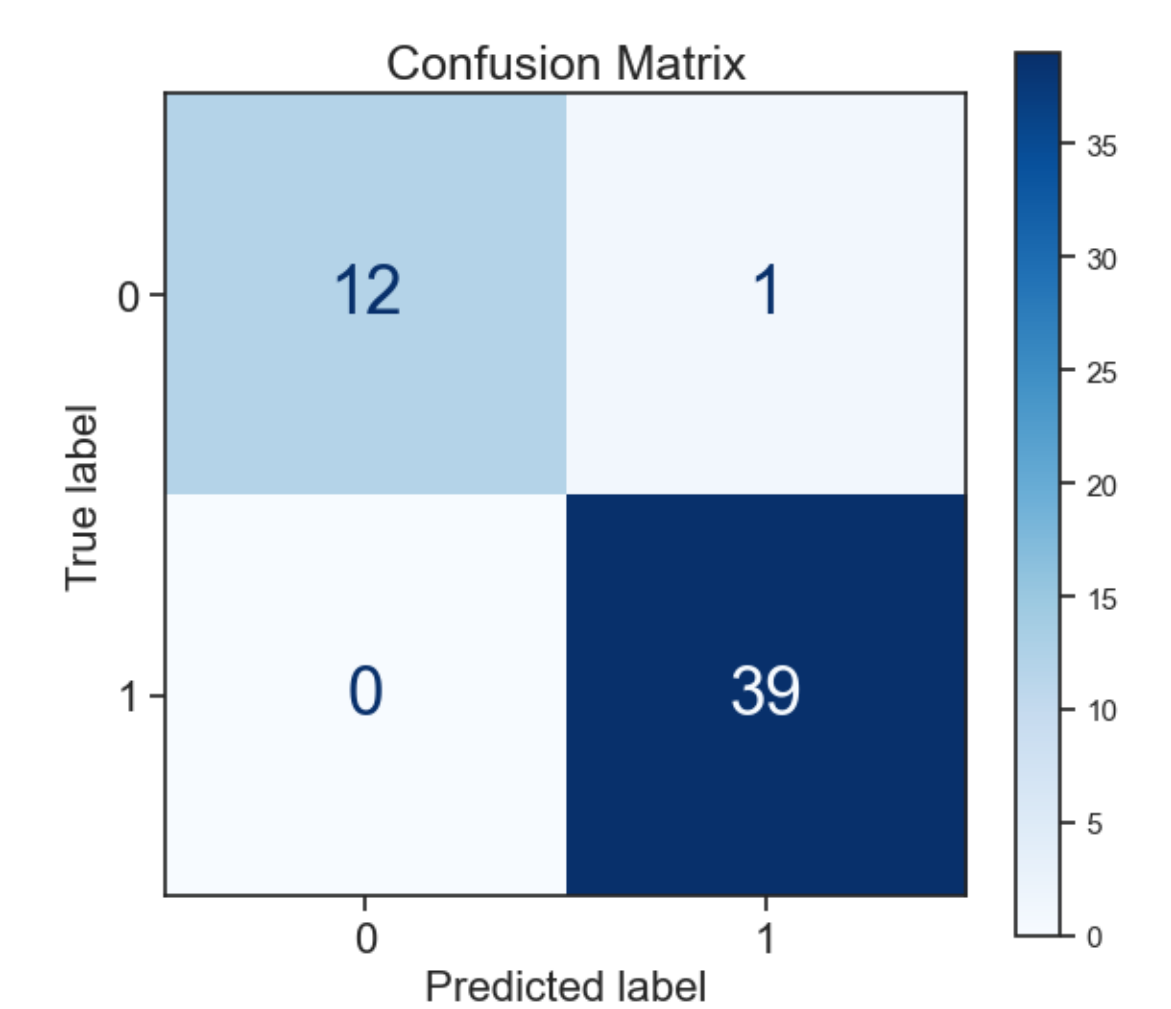
Metric	Train	Test
AUC	0.999	0.998
accuracy	0.9804	0.9808
balanced accuracy	0.9608	0.9615
recall_(sens)	1.0	1.0
specificity	0.9216	0.9231
precision	0.9745	0.975
f1_score	0.9801	0.9805

Protein: P29317 - metric: f1

Total (train): 204

Inactive: 51
Active: 153

ROC curve

AUC_train = 0.999
AUC_test = 0.955
Random

Pareto Chart with Highlighted Best Attempt

- Trials
- Pareto Front Trials
- Best Trial (# 4)

Confusion Matrix

	Predicted 0	Predicted 1
True 0	9	4
True 1	0	39

Confusion Matrix (nomr.)

	Predicted 0	Predicted 1
True 0	0.69	0.31
True 1	0	1

Calibration curve

train: 0.0312
test: 0.0691
perfectly_calibrated

Active/Inactive probability

Inactive zone / Active zone

type:
- active (39)
- inactive (13)
- decoy (52)

XGBoost Parameters	Value
alpha	4.1279
colsample_bytree	0.8298
gamma	0.0697
lambda	0.0903
learning_rate	0.2515
max_depth	3.0
min_child_weight	1.0
n_estimators	758.0
reg_alpha	0.5369
reg_lambda	0.498
scale_pos_weight	99.3476
subsample	0.9358
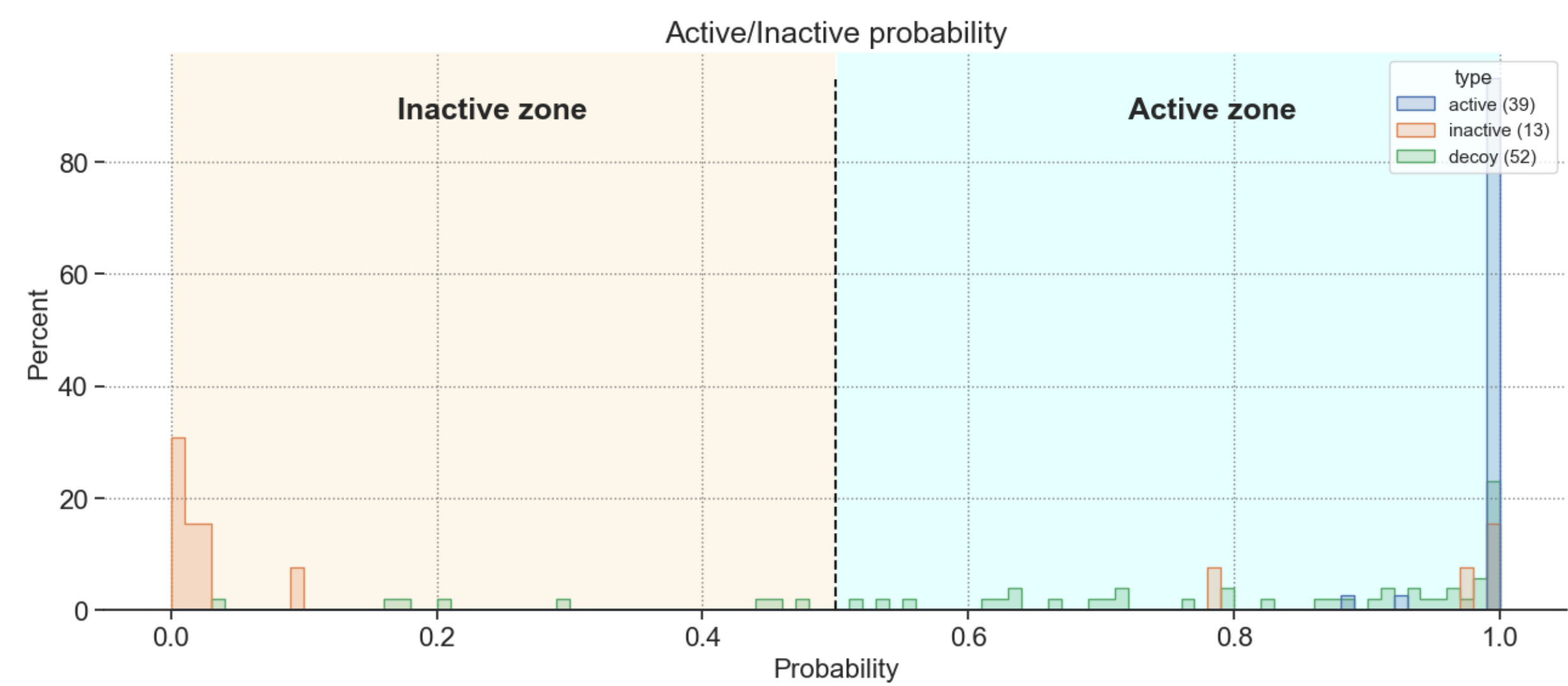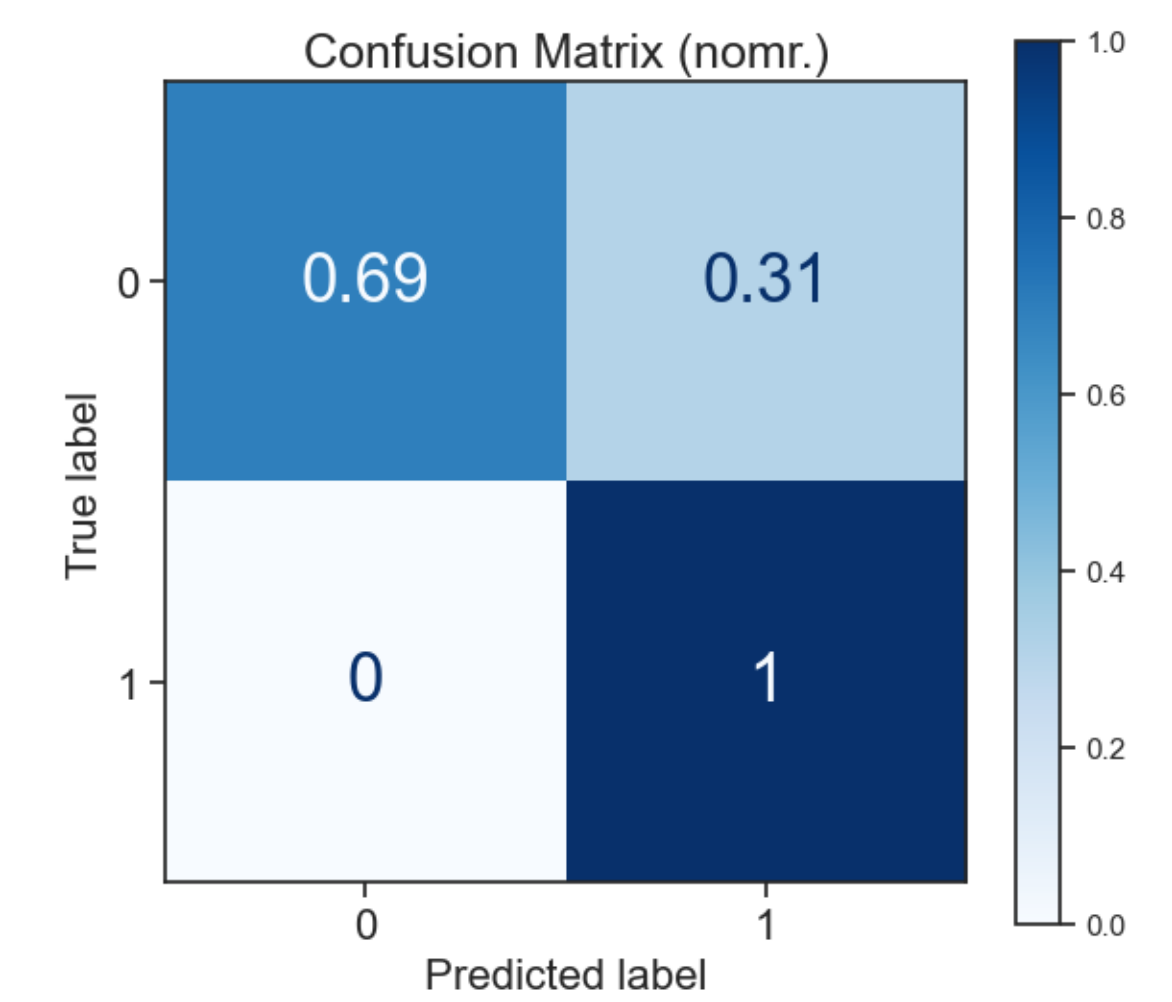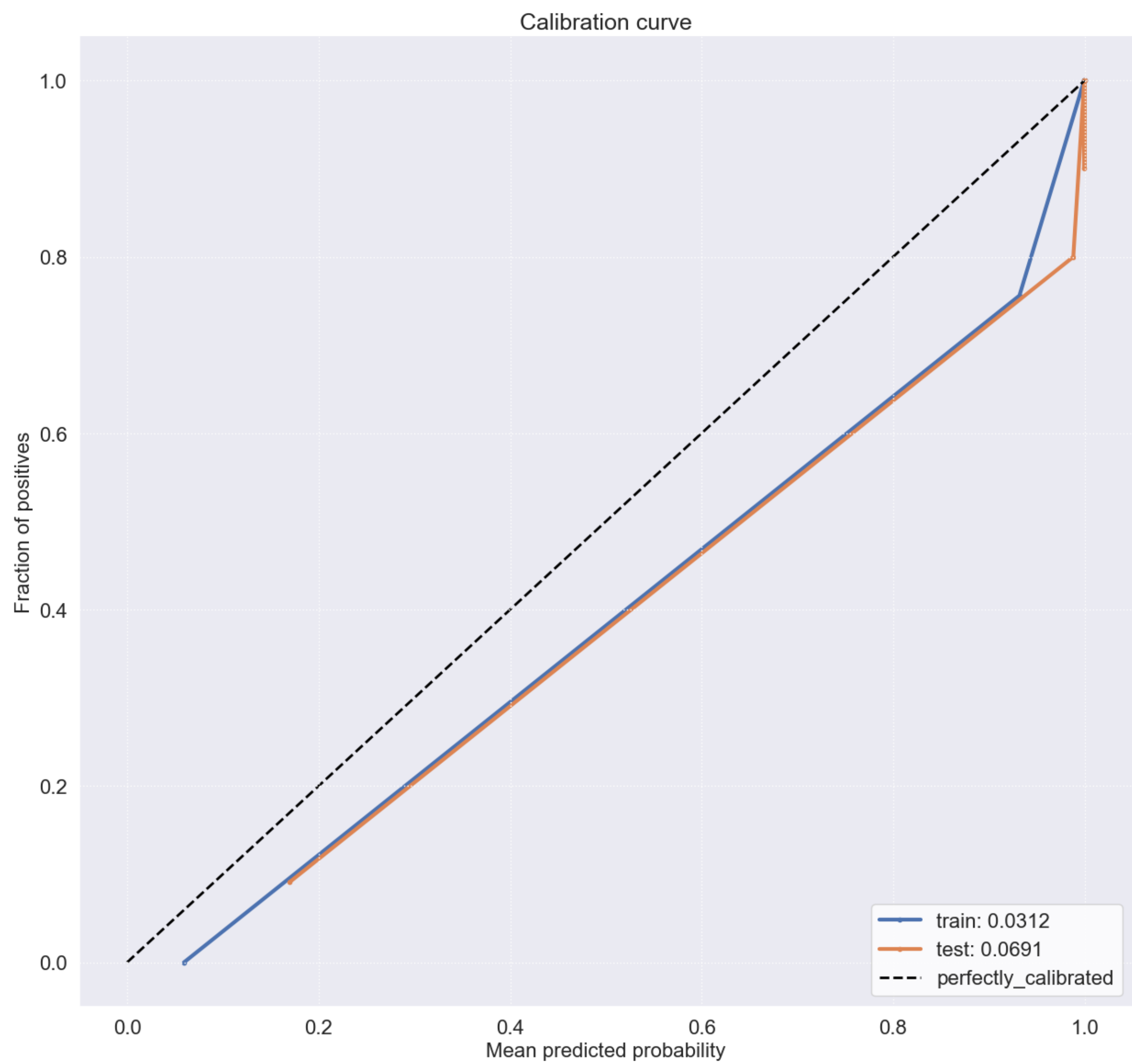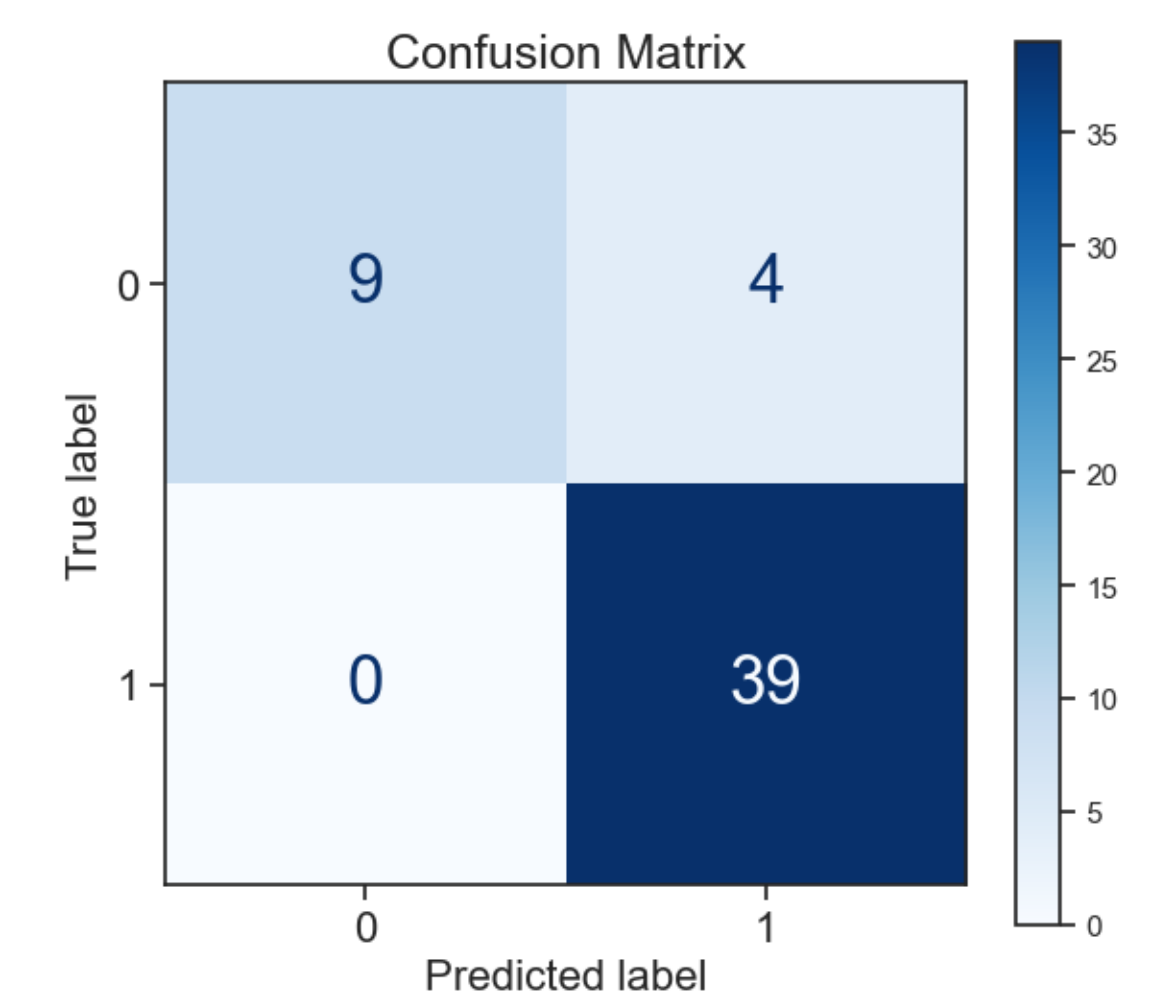
Metric	Train	Test
AUC	0.9987	0.9546
accuracy	0.9559	0.9231
balanced accuracy	0.9118	0.8462
recall_(sens)	1.0	1.0
specificity	0.8235	0.6923
precision	0.9444	0.907
f1_score	0.9544	0.918

Protein: P29317 - metric: precision

Total (train): 204

ROC curve

AUC_train = 0.973
AUC_test = 0.980
Random

Pareto Chart with Highlighted Best Attempt

- Trials
- Pareto Front Trials
- Best Trial (# 2213)

Confusion Matrix

	0	1
0	11	2
1	0	39

Confusion Matrix (nomr.)

	0	1
0	0.85	0.15
1	0	1

Calibration curve

train: 0.0227
test: 0.0324
perfectly_calibrated
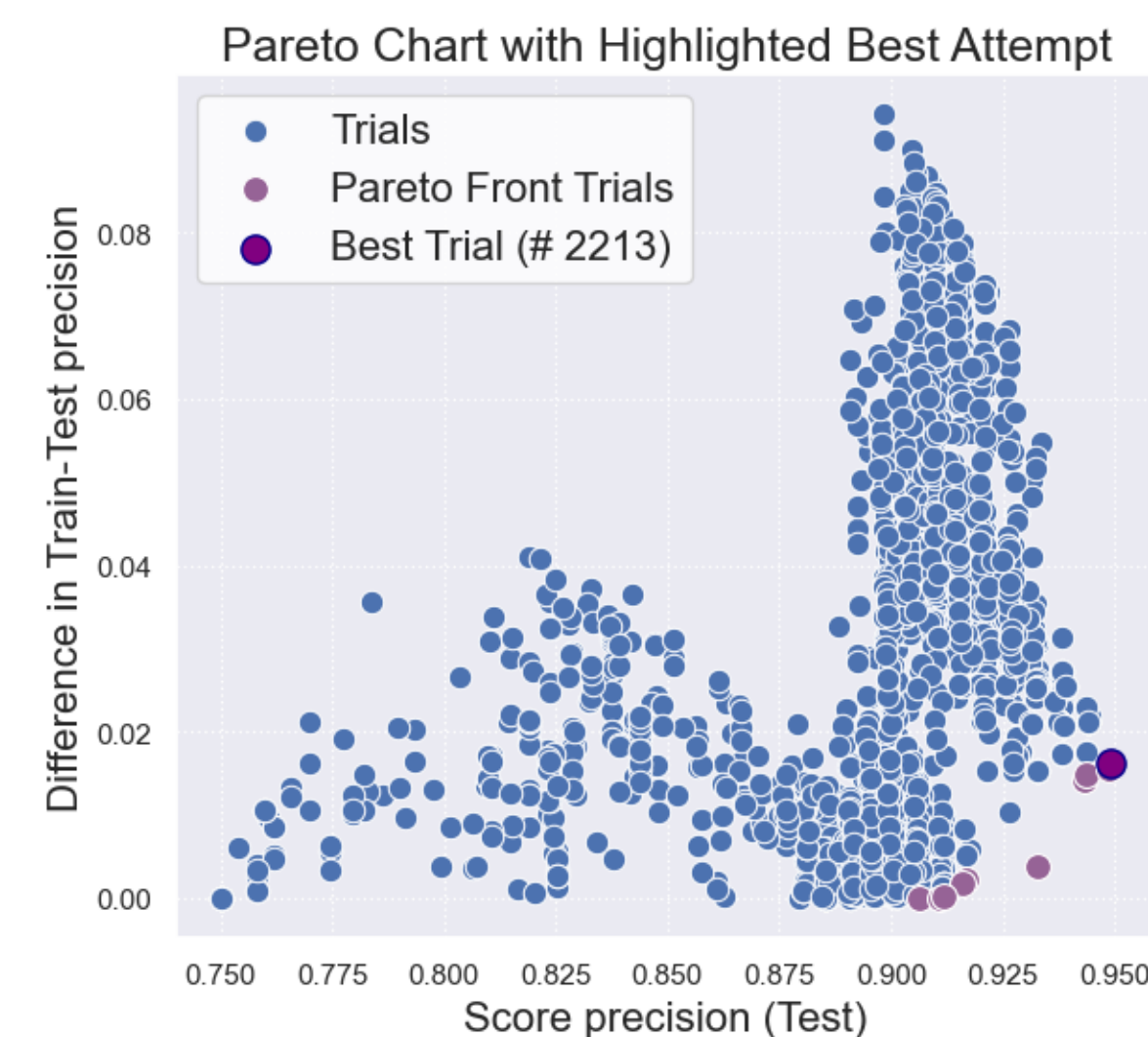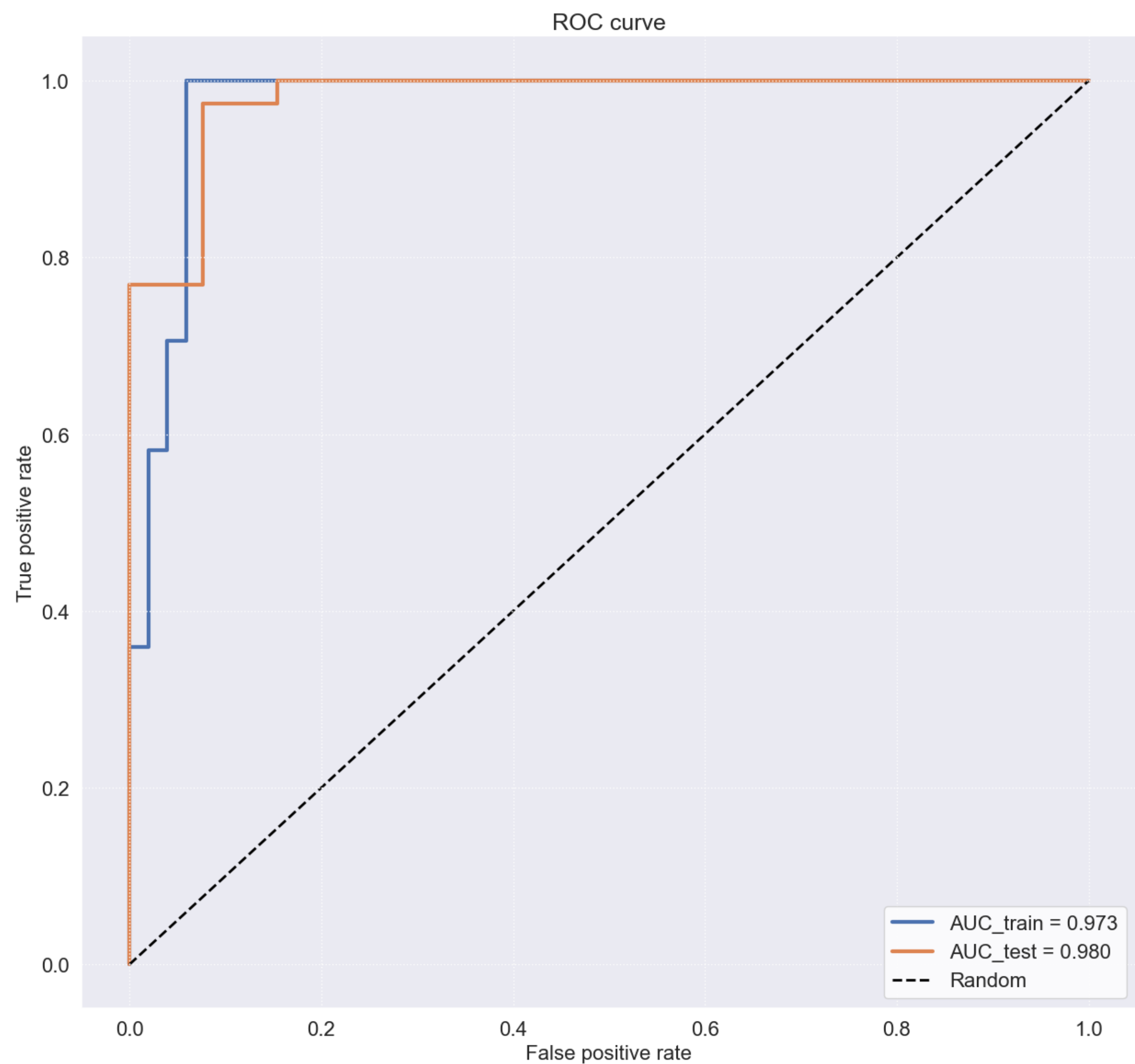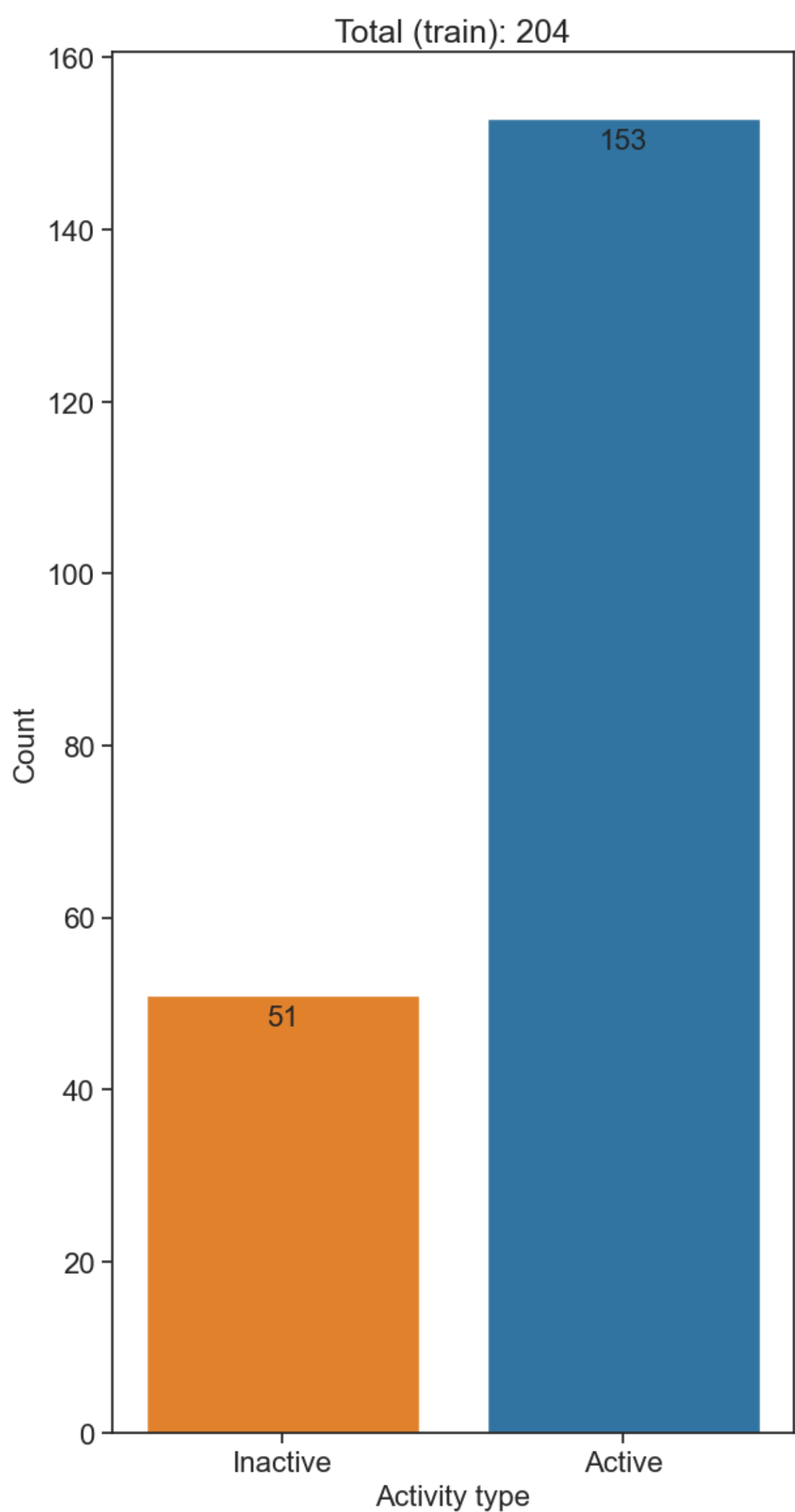
XGBoost Parameters	Value
alpha	1.9388
colsample_bytree	0.6089
gamma	0.9659
lambda	2.2733
learning_rate	0.9659
max_depth	5.0
min_child_weight	3.0
n_estimators	864.0
reg_alpha	0.1189
reg_lambda	0.2629
scale_pos_weight	18.2506
subsample	0.5862

Active/Inactive probability

type
- active (39)
- inactive (13)
- decoy (52)

Inactive zone   Active zone
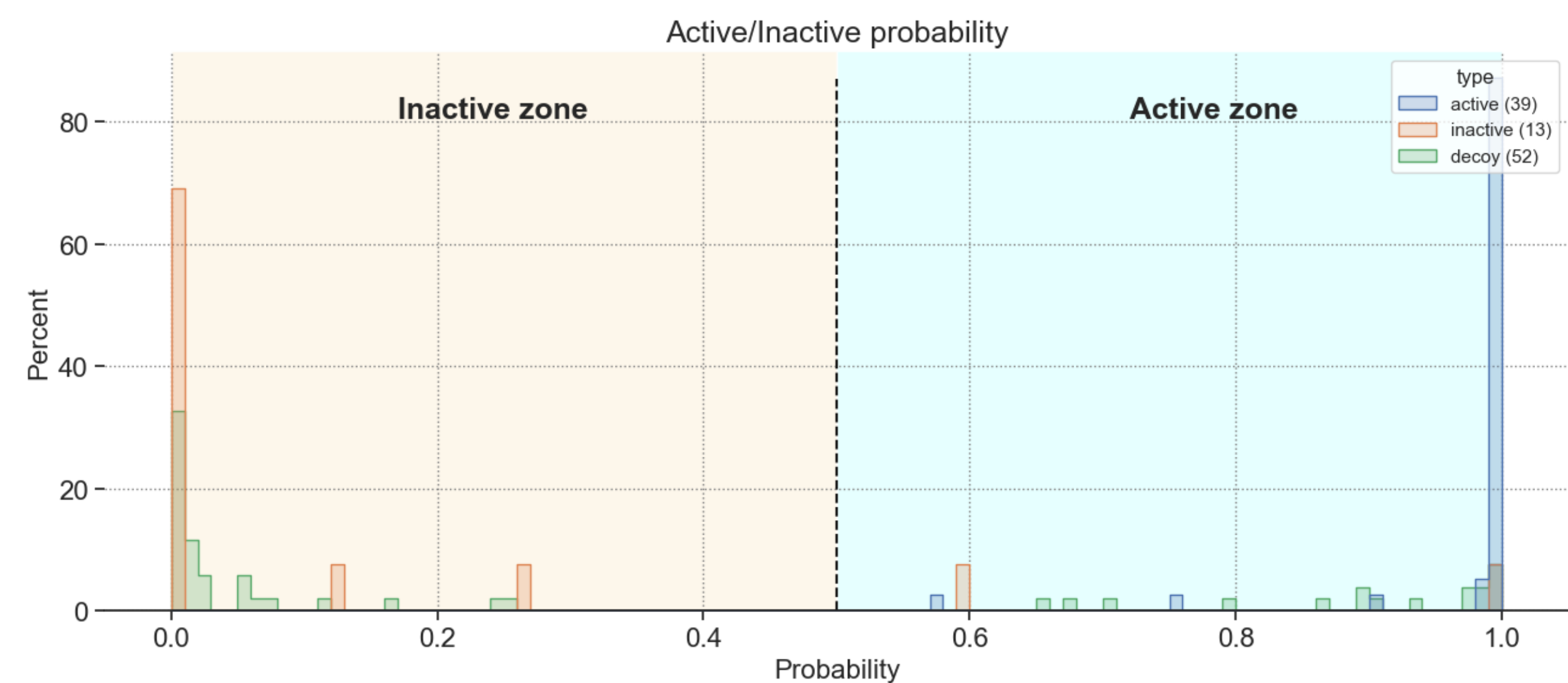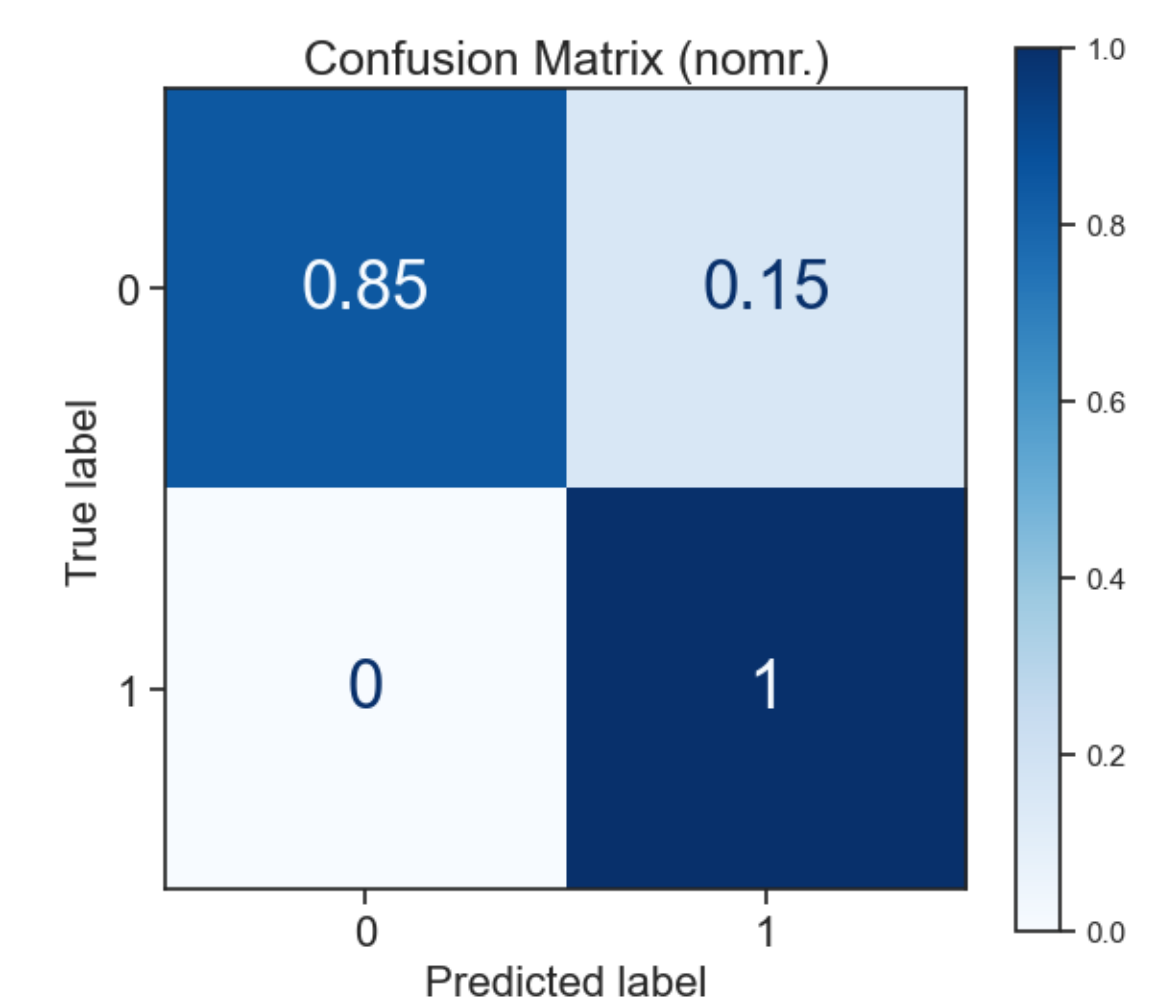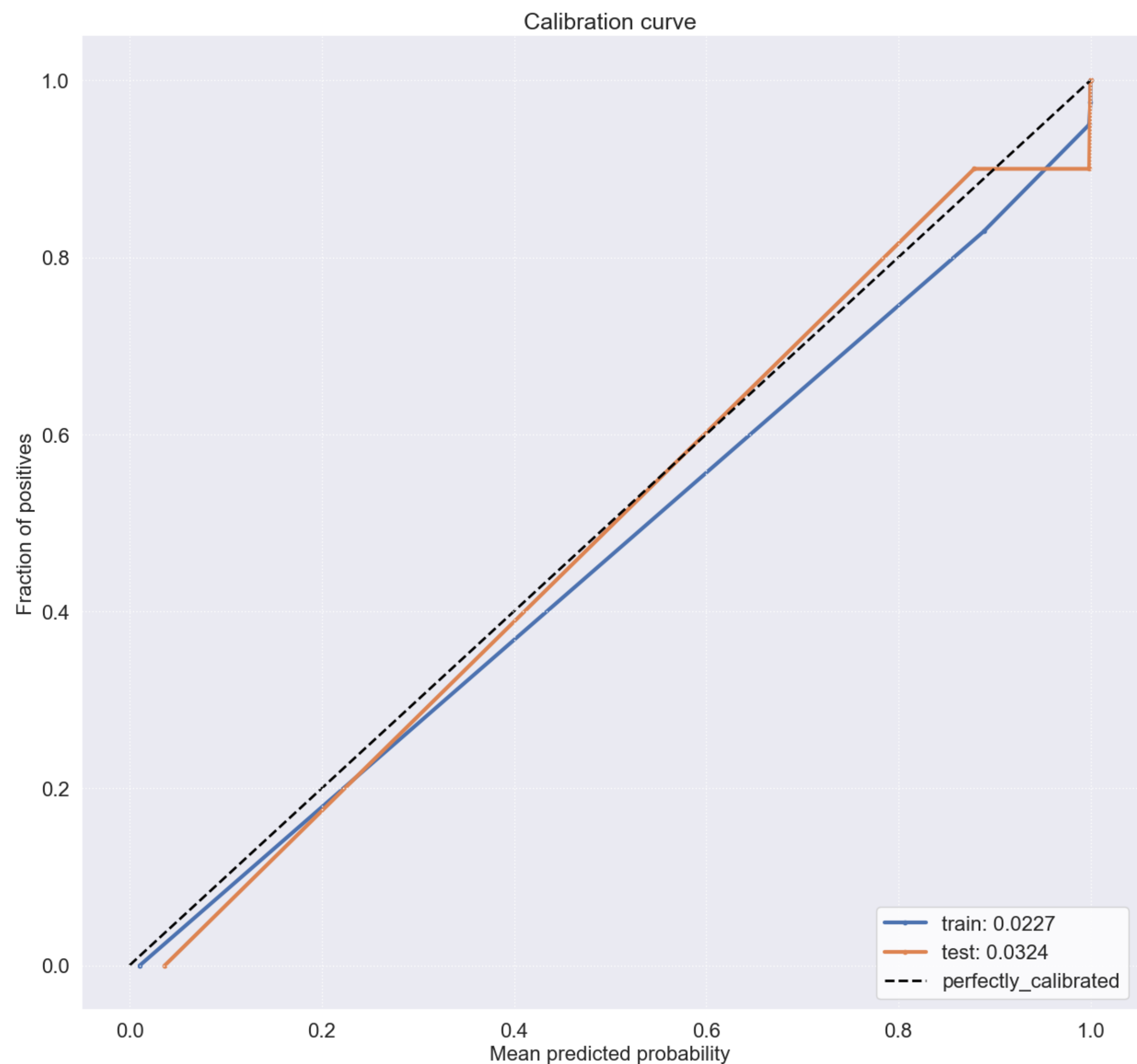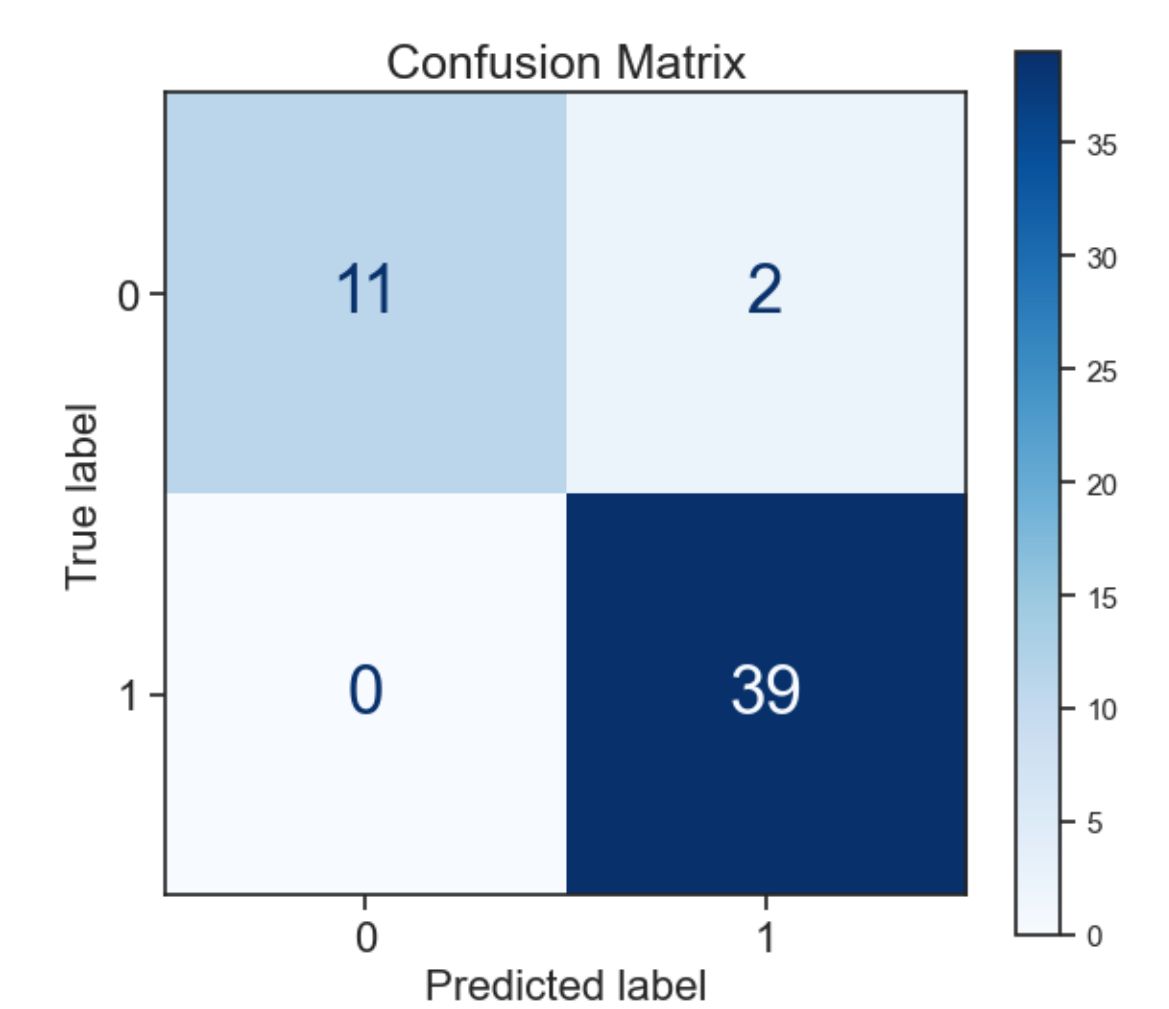
Metric	Train	Test
AUC	0.9735	0.9803
accuracy	0.9755	0.9615
balanced accuracy	0.951	0.9231
recall_(sens)	1.0	1.0
specificity	0.902	0.8462
precision	0.9684	0.9512
f1_score	0.9751	0.9604

Protein: P29317 - metric: SoftVotingXGBoostEnsemble
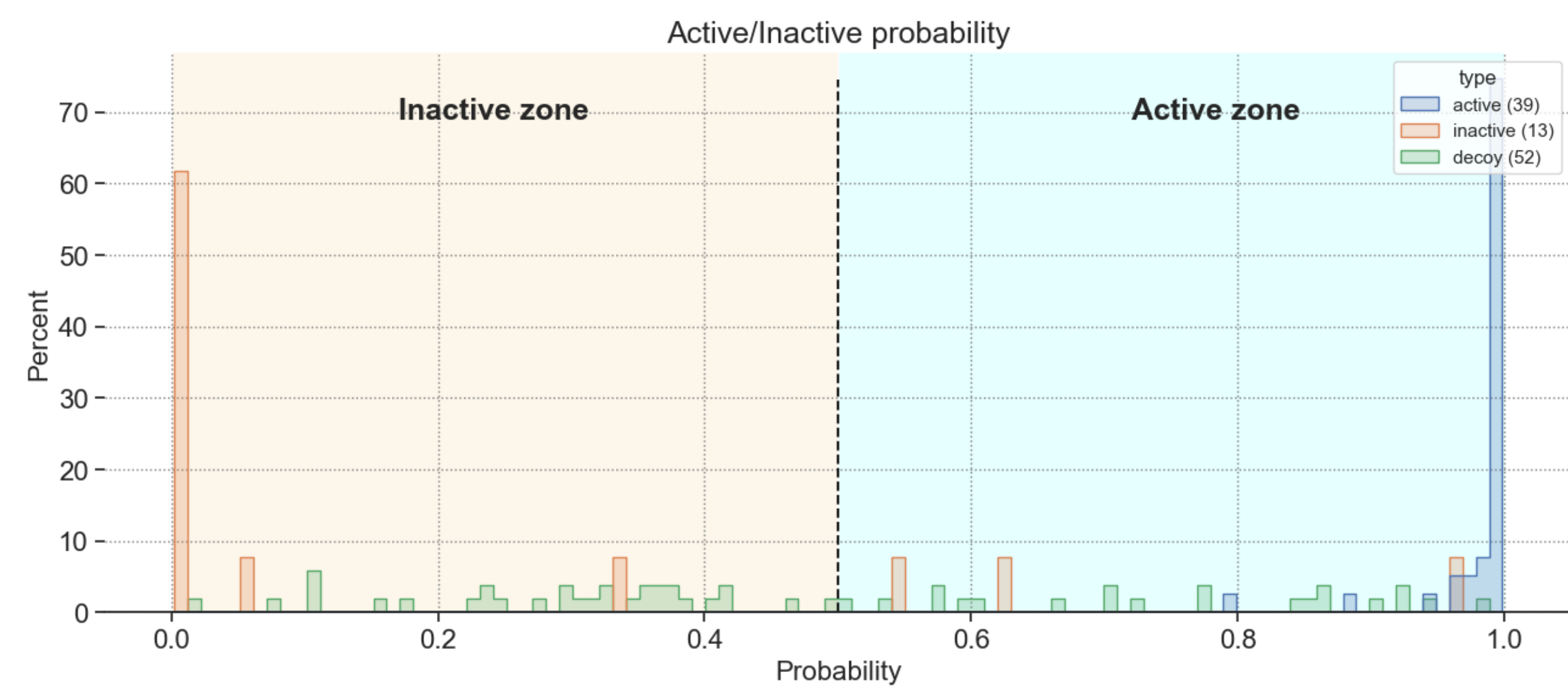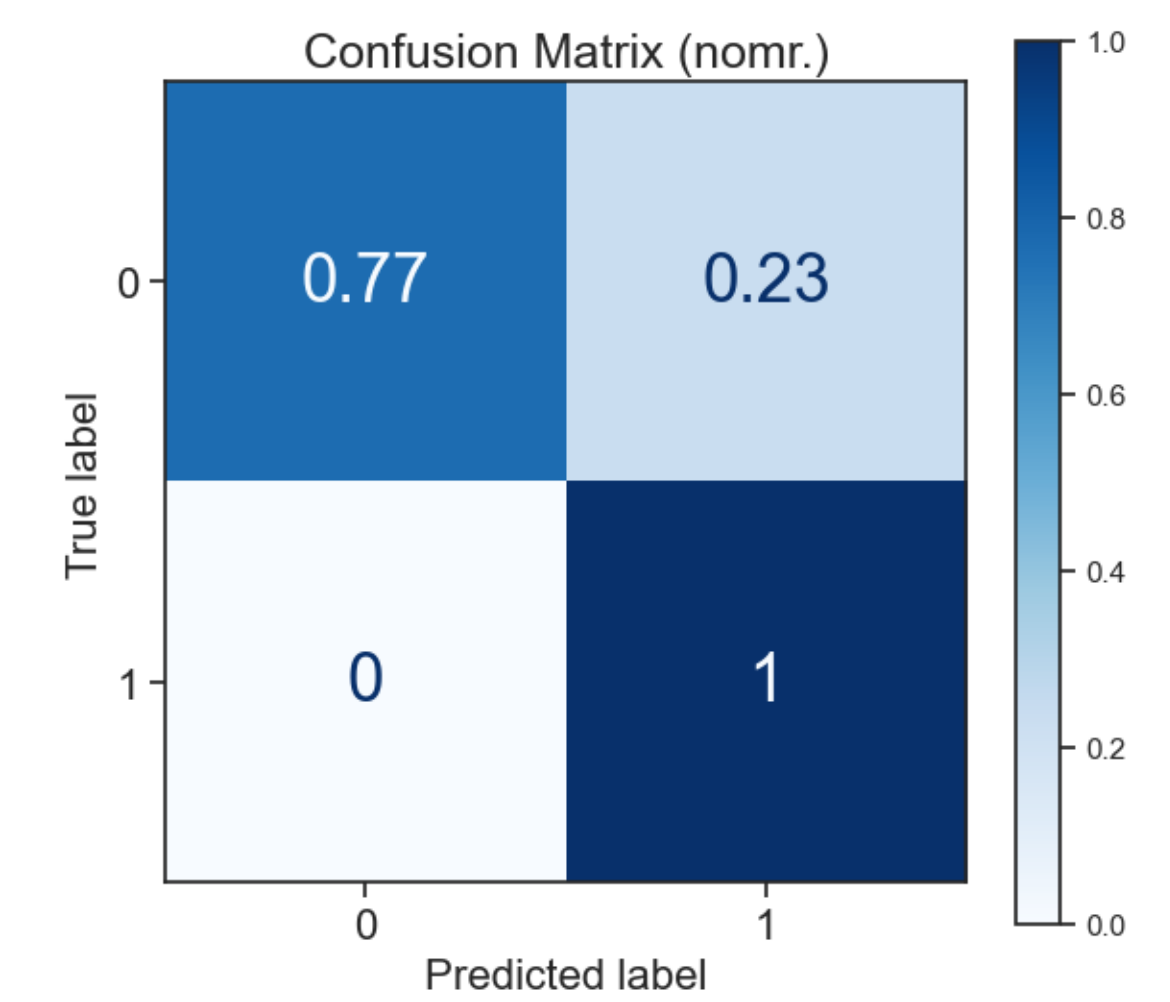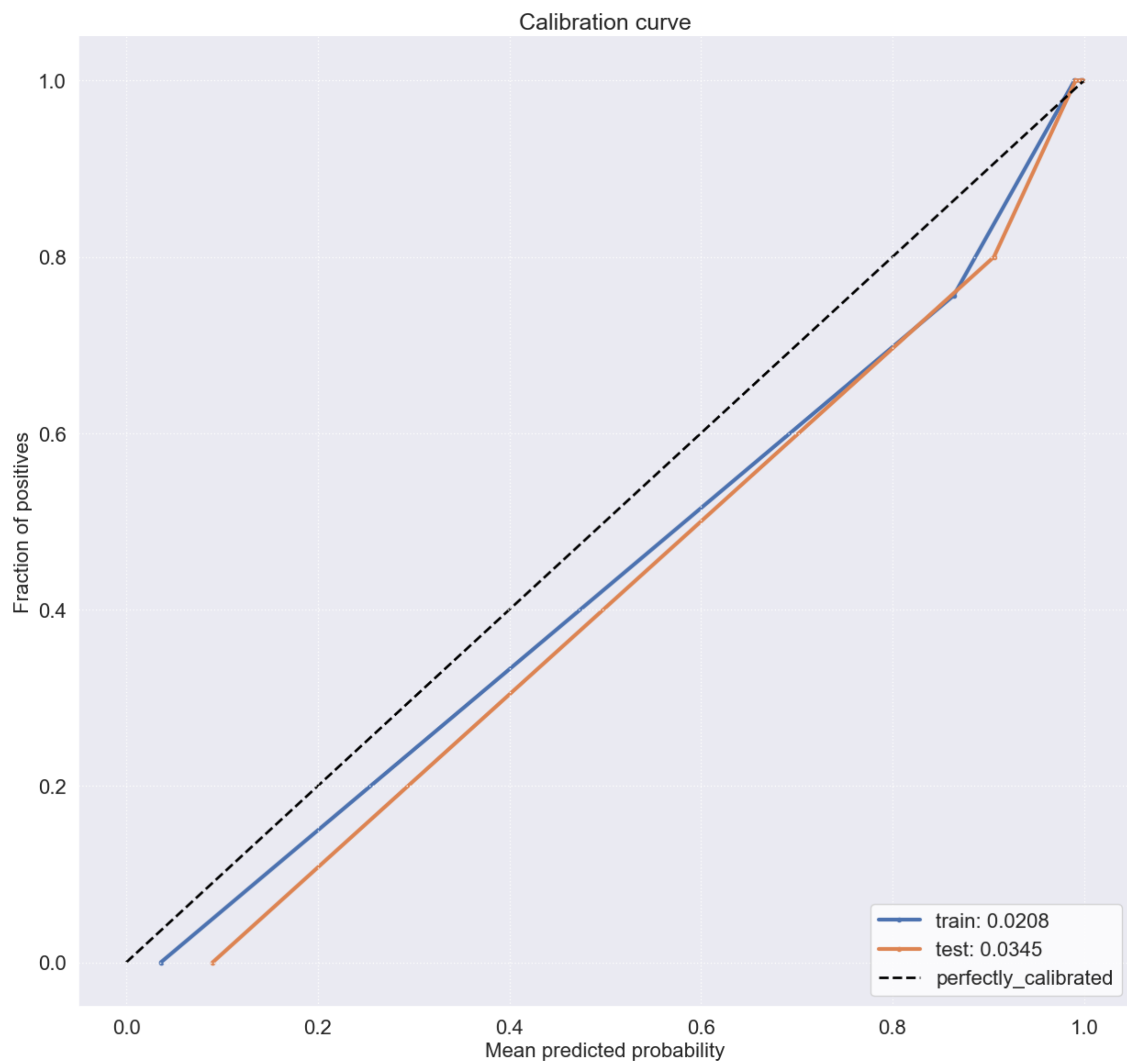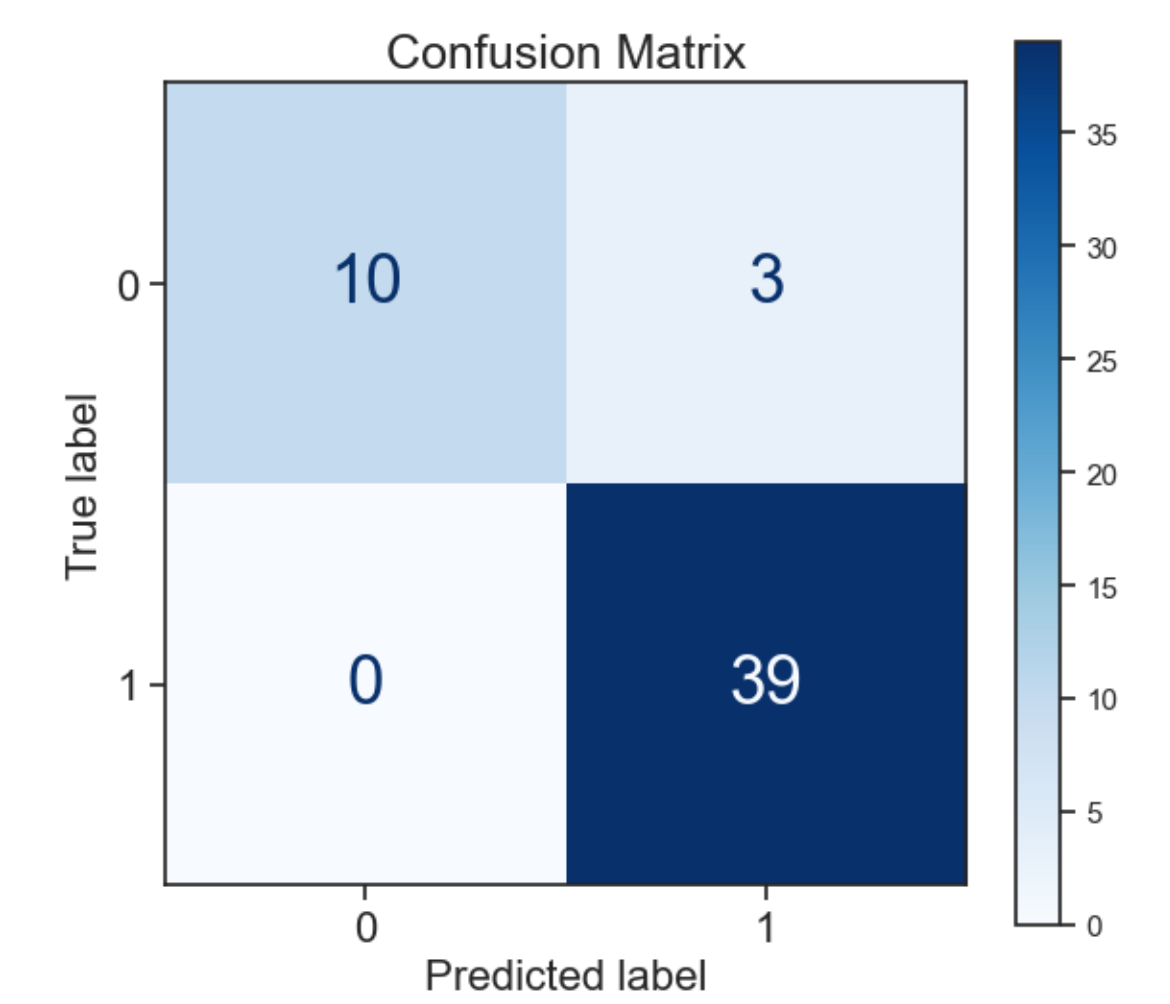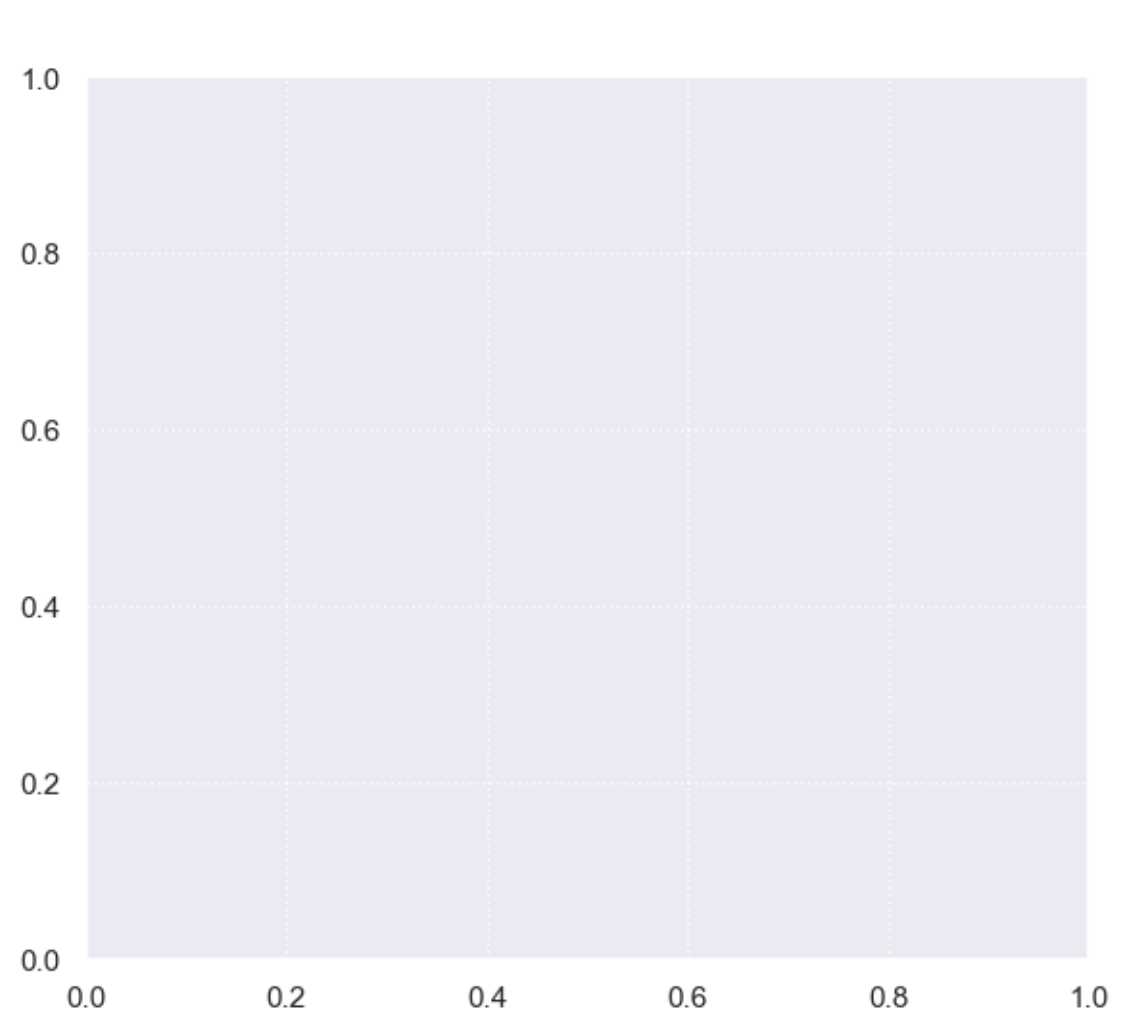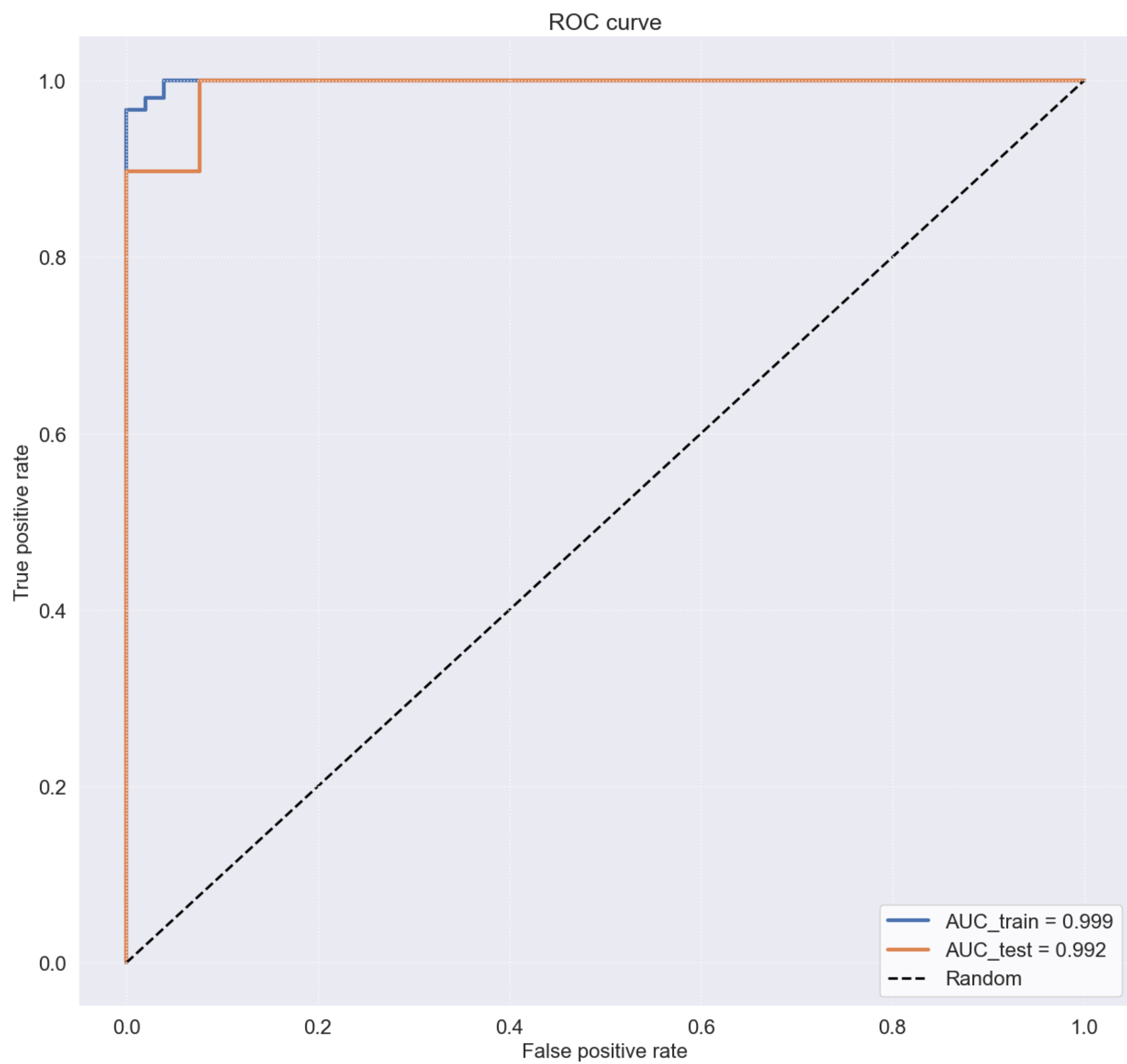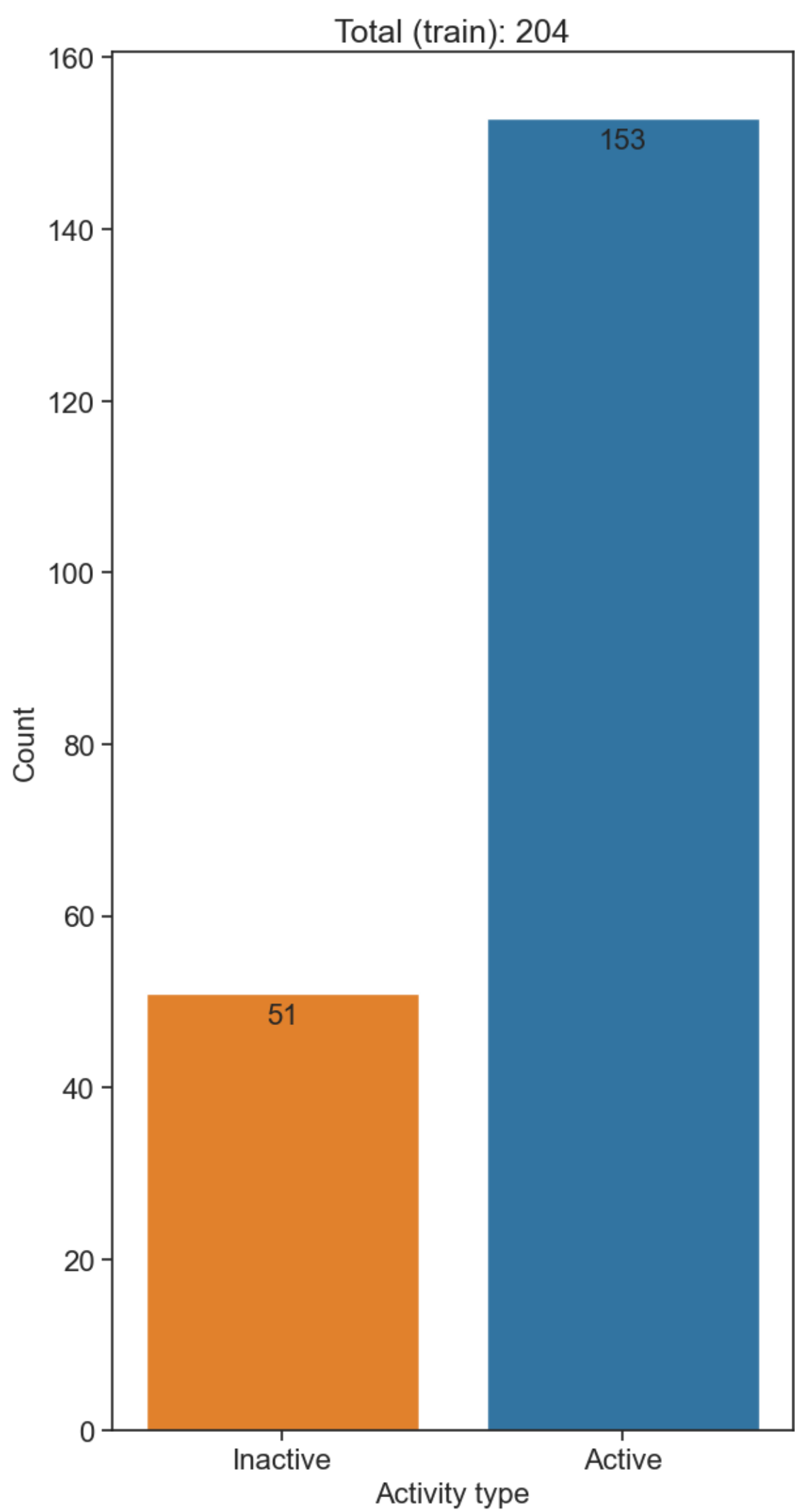
Metric	Train	Test
AUC	0.999	0.9921
accuracy	0.9706	0.9423
balanced accuracy	0.9412	0.8846
recall_(sens)	1.0	1.0
specificity	0.8824	0.7692
precision	0.9623	0.9286
f1_score	0.97	0.9396