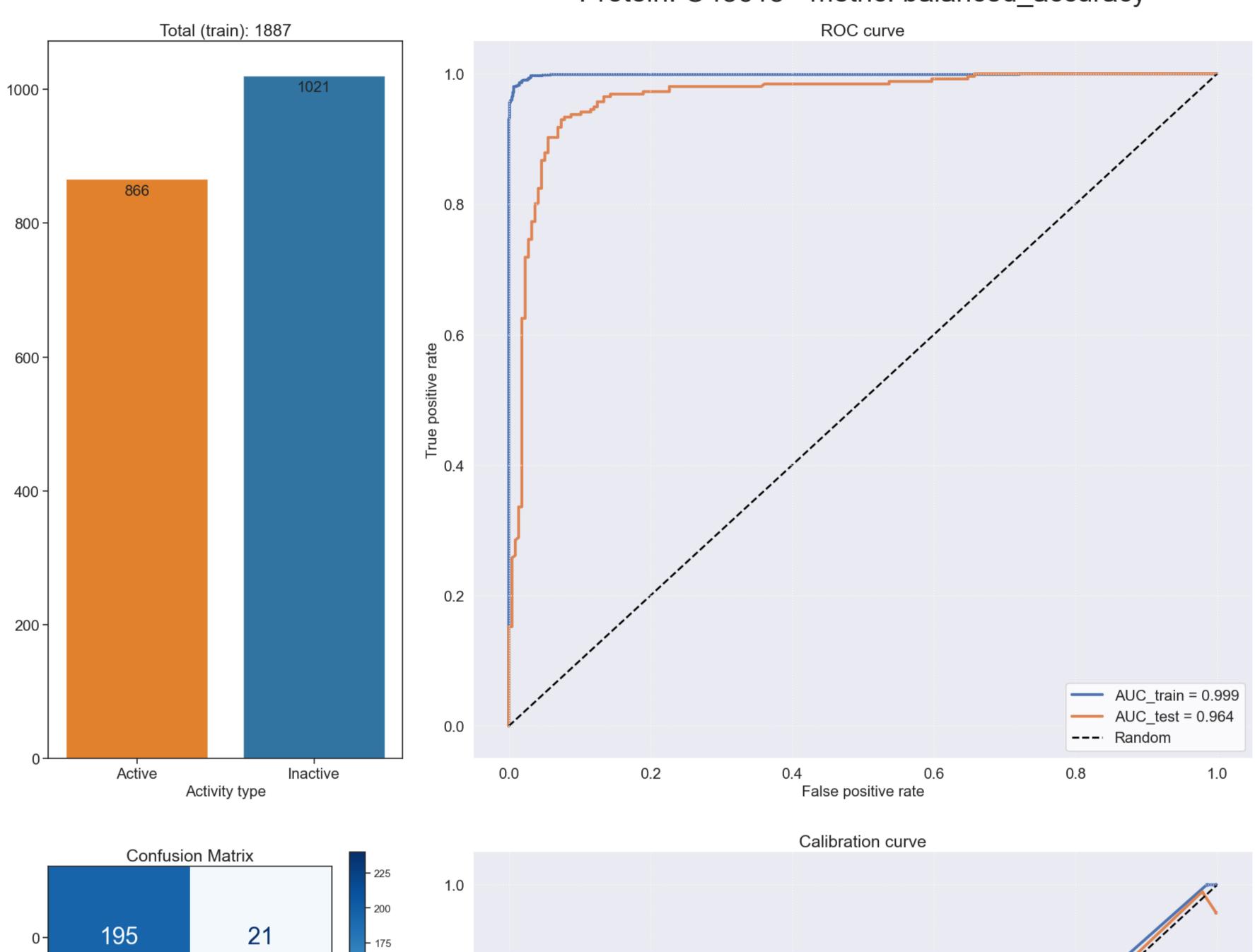
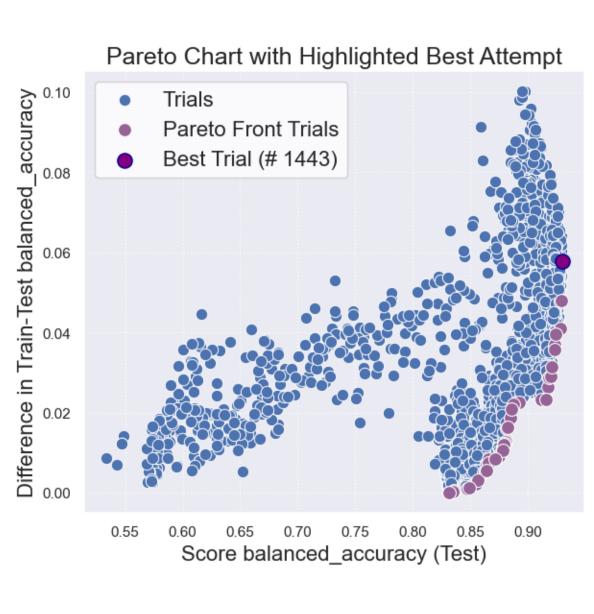
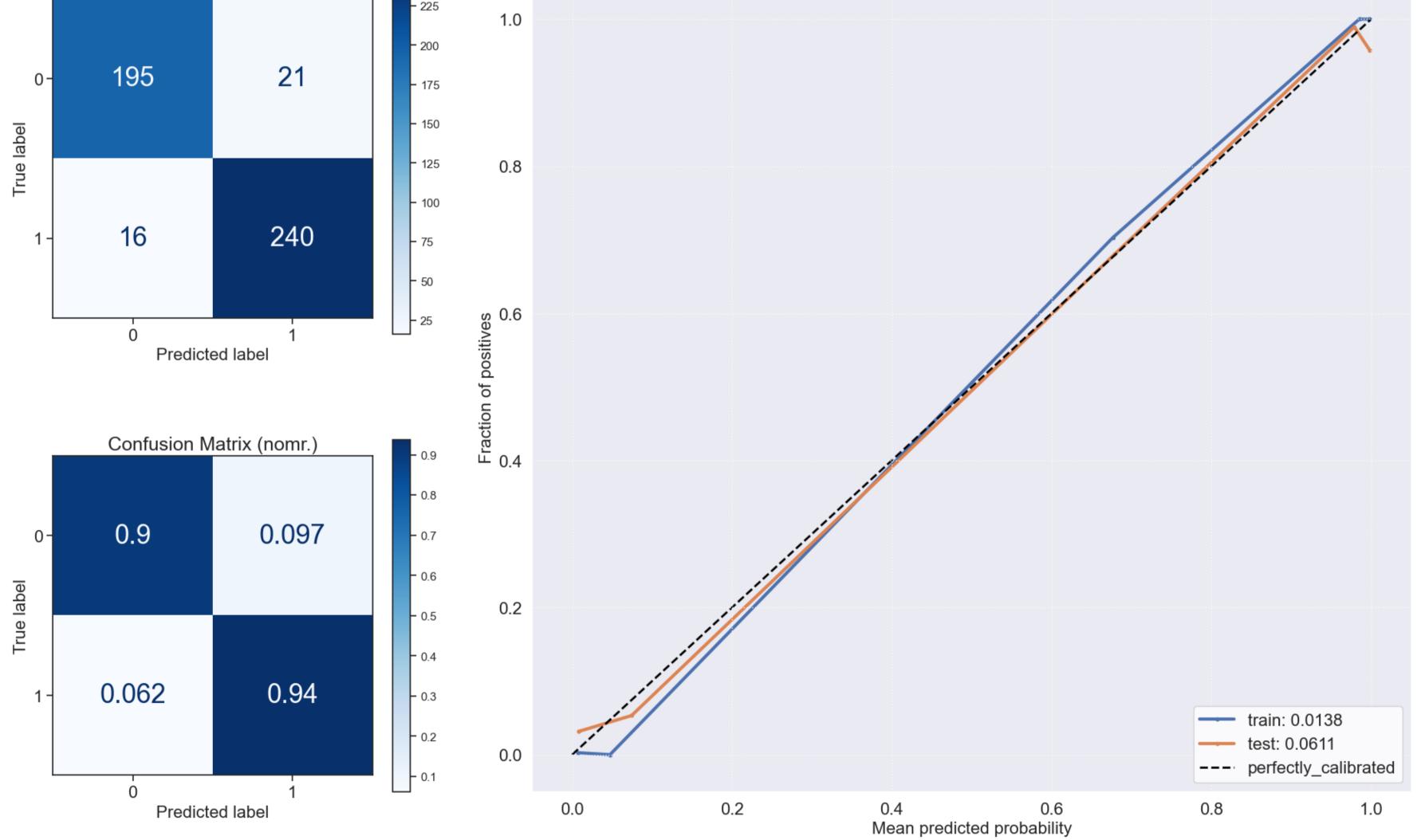
Protein: O43613 - metric: balanced_accuracy





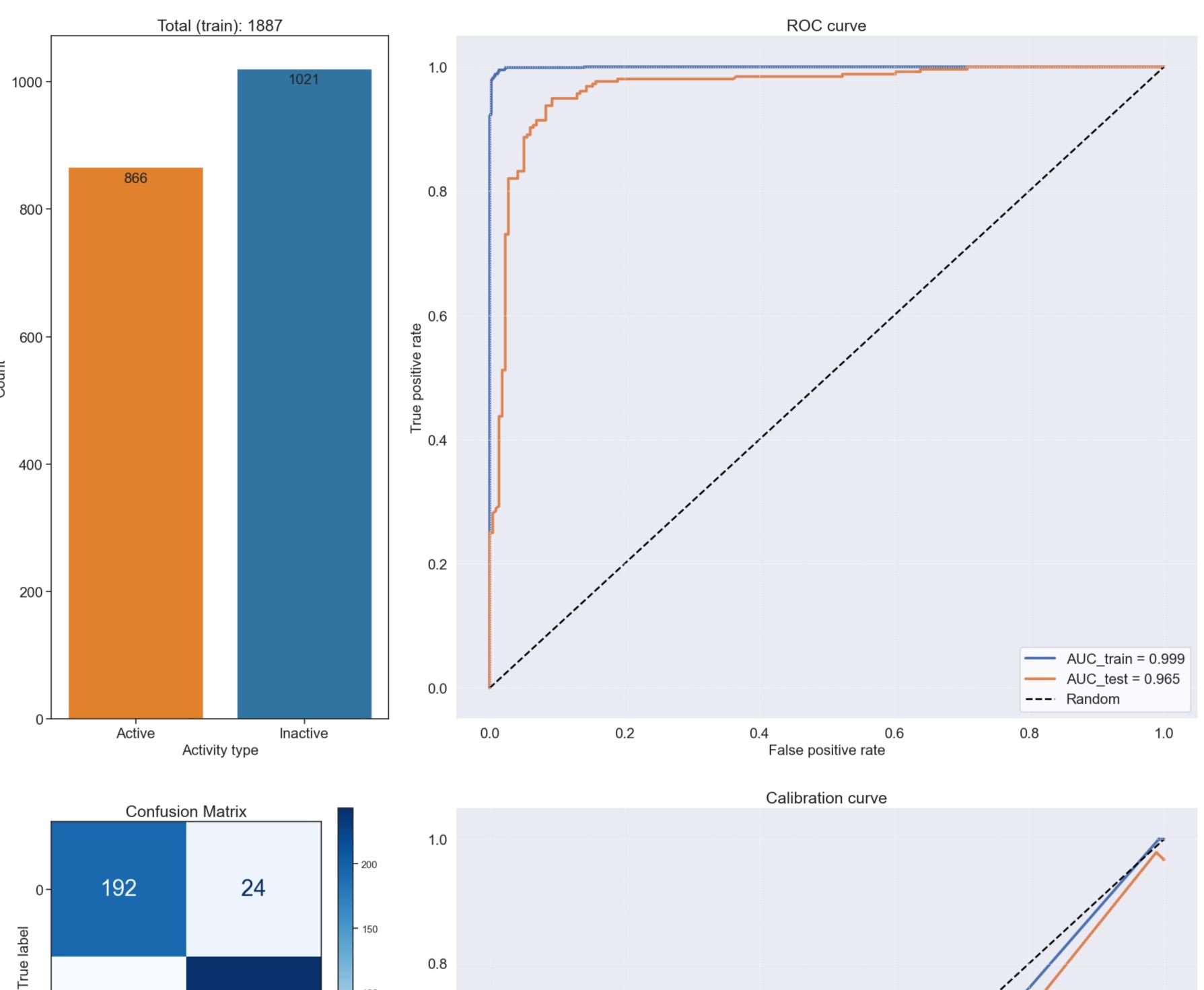
XGBoost Parameters	Value
alpha	0.6461
colsample_bytree	0.5131
gamma	0.3648
lambda	3.2673
learning_rate	0.0667
max_depth	4.0
min_child_weight	1.0
n_estimators	747.0
reg_alpha	0.1874
reg_lambda	0.6728
scale_pos_weight	1.0689
subsample	0.8822

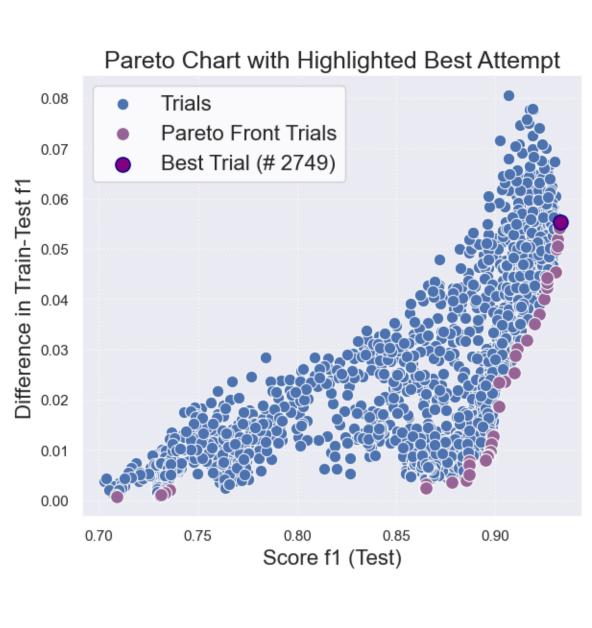


		Ac	tive/Inactive	probability		
00		active zone			Active zone	active (256) inactive (216) decoy (468)
20						
Percent						
10						
0	0.0	0.2 0	0.4 Probabi	0.6 lity	0.8	1.0

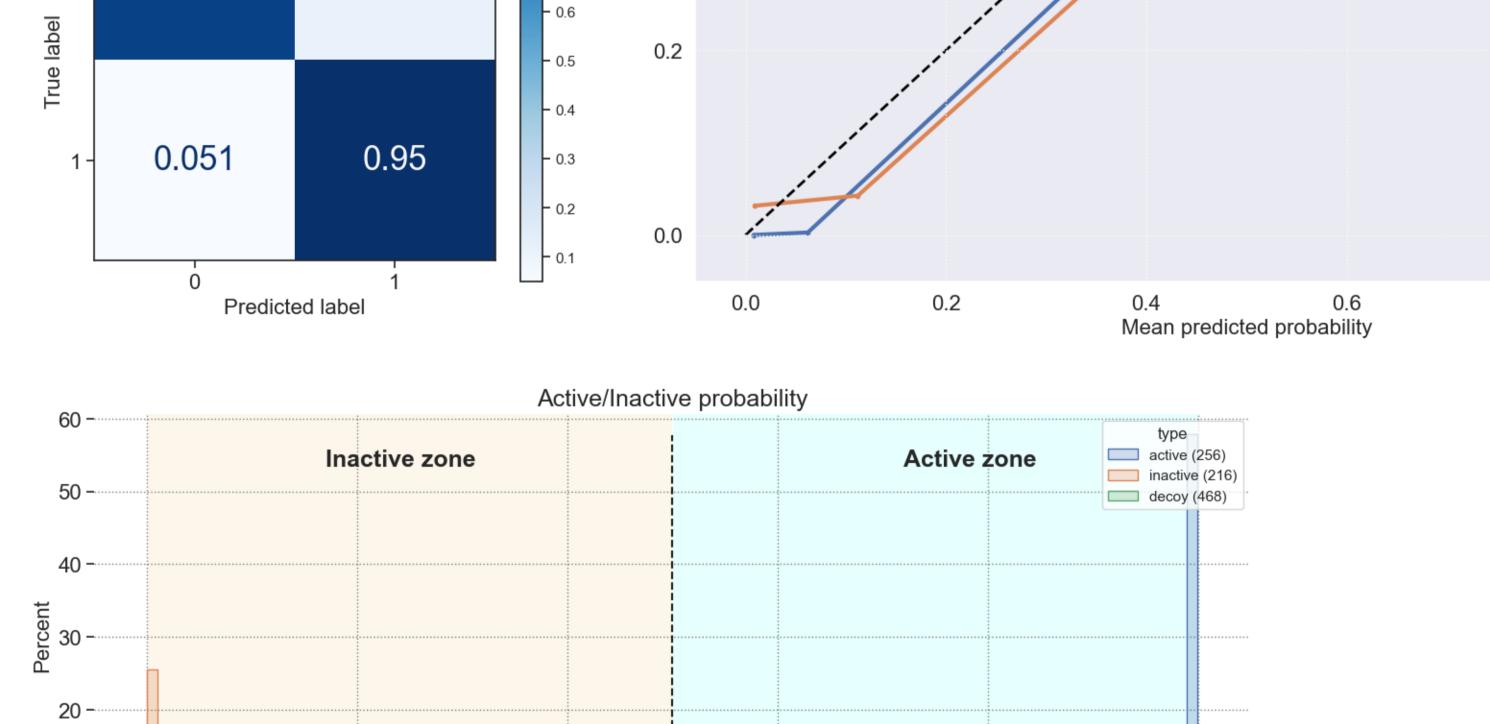
Metric	Train	Test
AUC	0.9987	0.9636
accuracy	0.9857	0.9216
balanced accuracy	0.9856	0.9201
recall_(sens)	0.9863	0.9375
specificity	0.985	0.9028
precision	0.9873	0.9195
f1_score	0.9857	0.9215

Protein: O43613 - metric: f1





XGBoost Parameters	Value
alpha	1.3429
colsample_bytree	0.5663
gamma	0.7724
lambda	4.4457
learning_rate	0.0641
max_depth	5.0
min_child_weight	1.0
n_estimators	536.0
reg_alpha	0.0177
reg_lambda	0.8236
scale_pos_weight	2.6471
subsample	0.6574



0.6

Probability

0.8

1.0

100

- 50

- 0.8

0.7

0.4

Fraction of positives

243

0.11

Predicted label

Confusion Matrix (nomr.)

13

0.89

0-

10 -

0.0

0.2

Metric	Train	Test
AUC	0.9995	0.9651
accuracy	0.9868	0.9216
balanced accuracy	0.9857	0.9191
recall_(sens)	0.999	0.9492
specificity	0.9723	0.8889
precision	0.977	0.9101
f1_score	0.9867	0.9214

MIGHTIC	IIaiii	1631
AUC	0.9995	0.9651
accuracy	0.9868	0.9216
balanced accuracy	0.9857	0.9191
recall_(sens)	0.999	0.9492
specificity	0.9723	0.8889
precision	0.977	0.9101
f1_score	0.9867	0.9214

- train: 0.0136

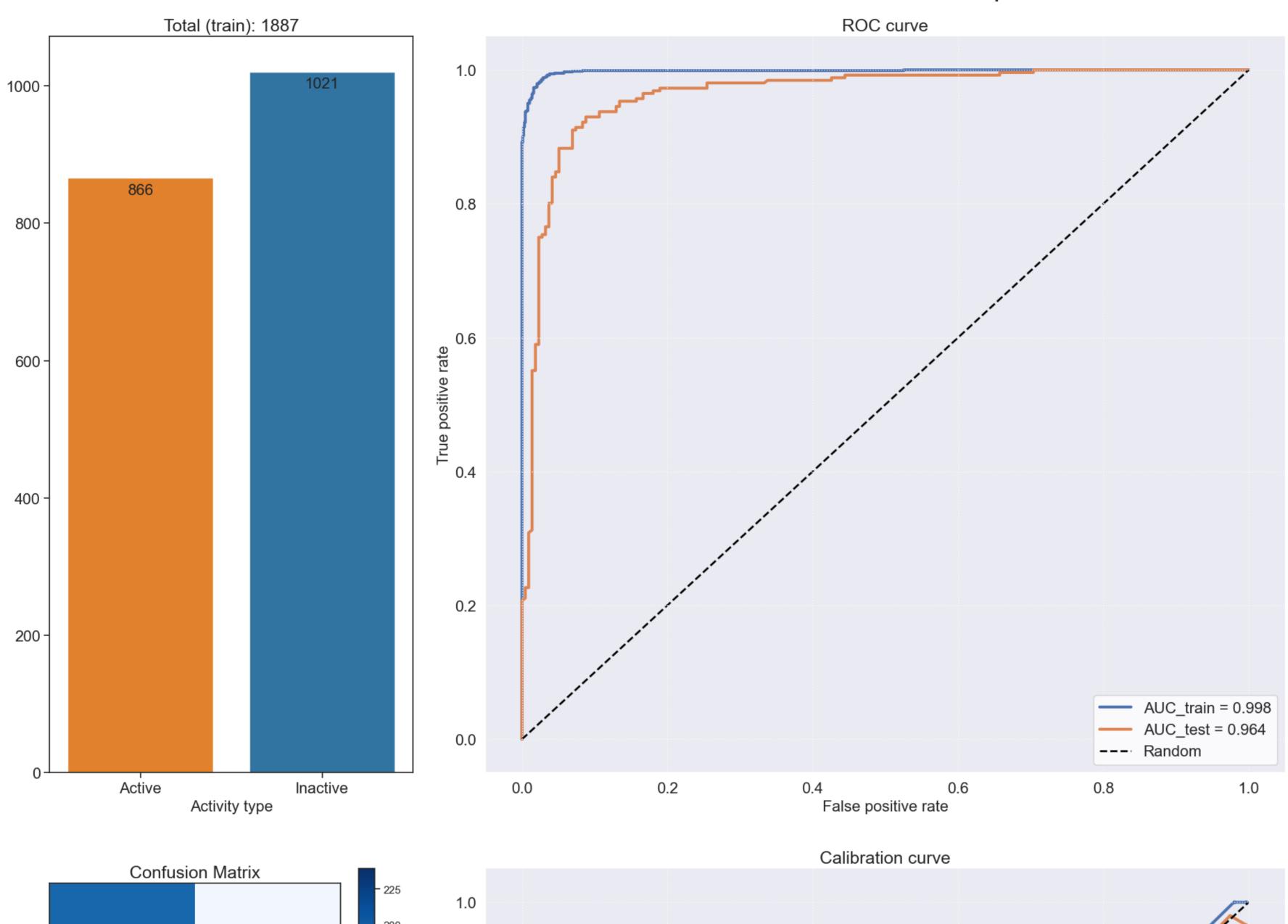
0.8

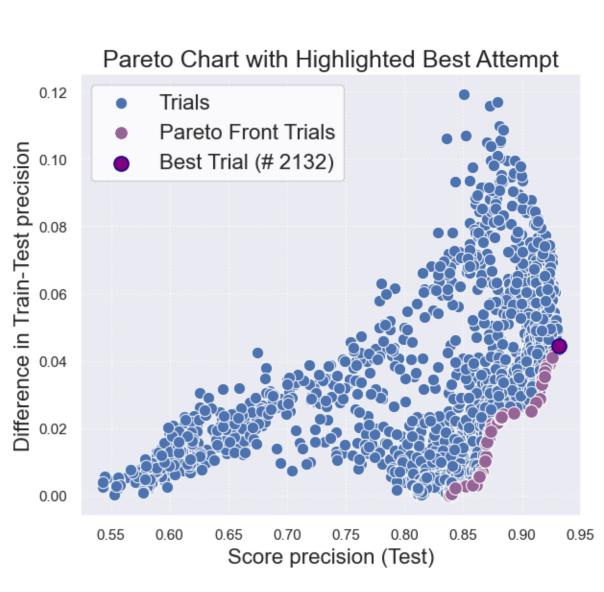
test: 0.0622

--- perfectly_calibrated

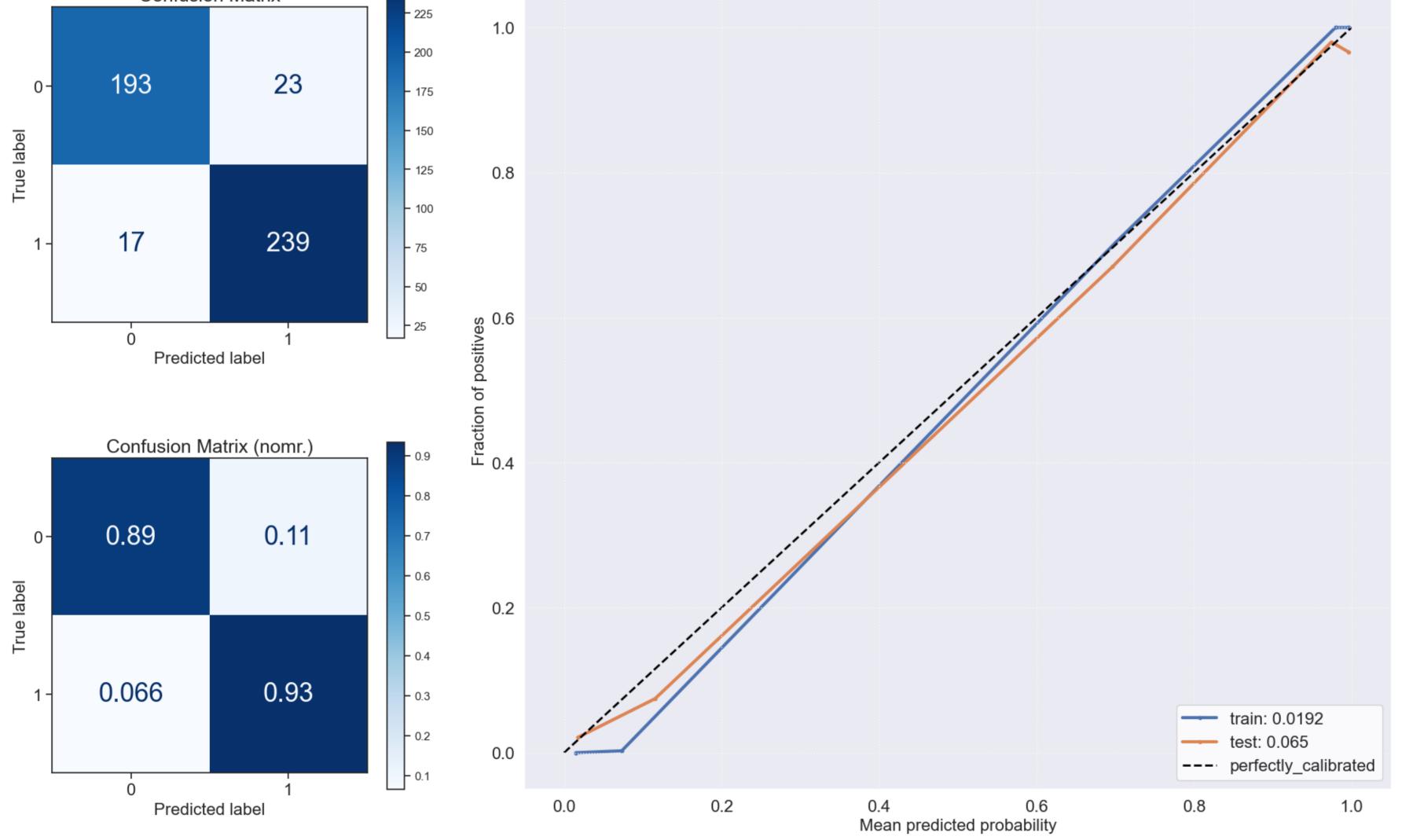
1.0

Protein: O43613 - metric: precision



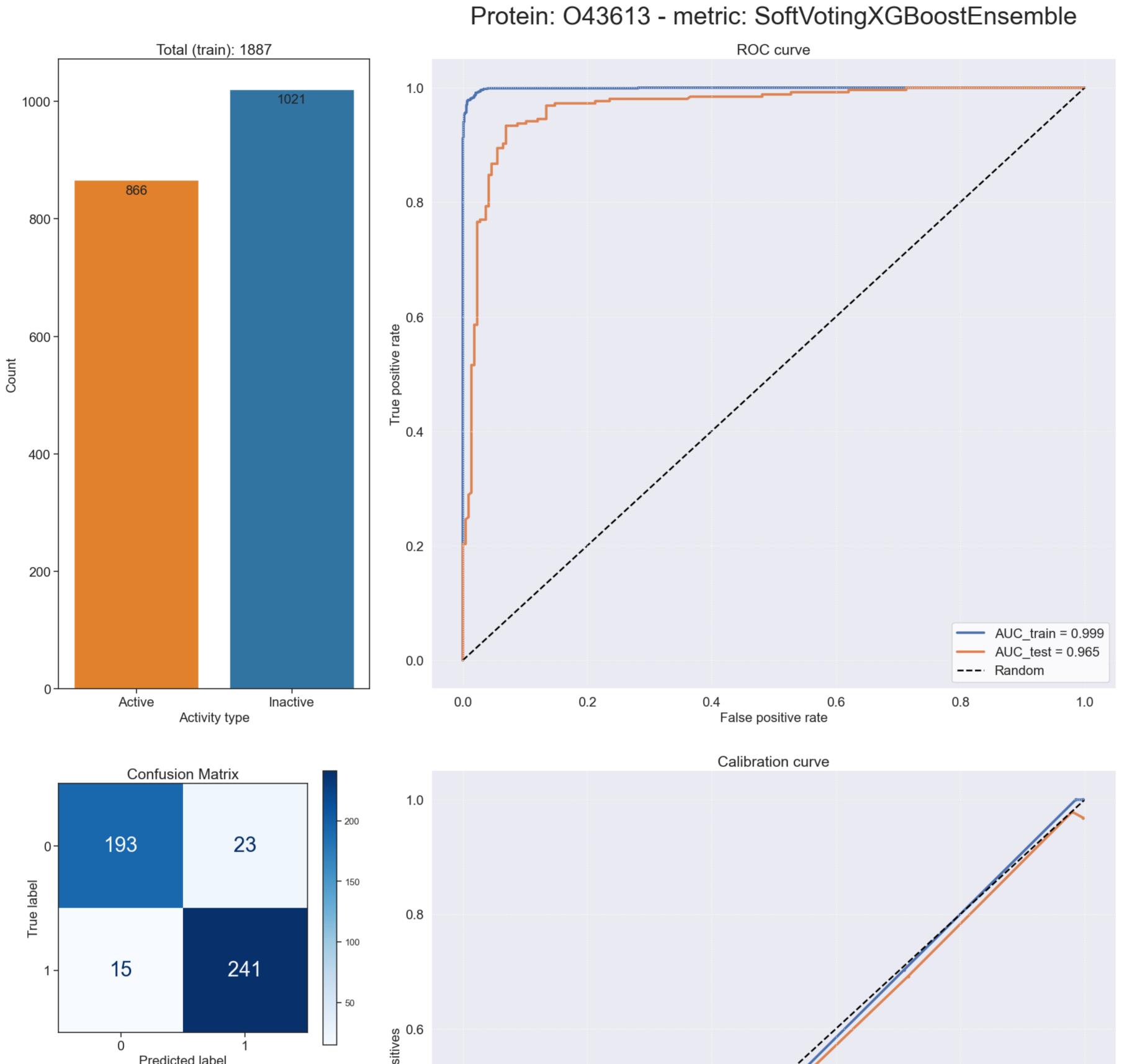


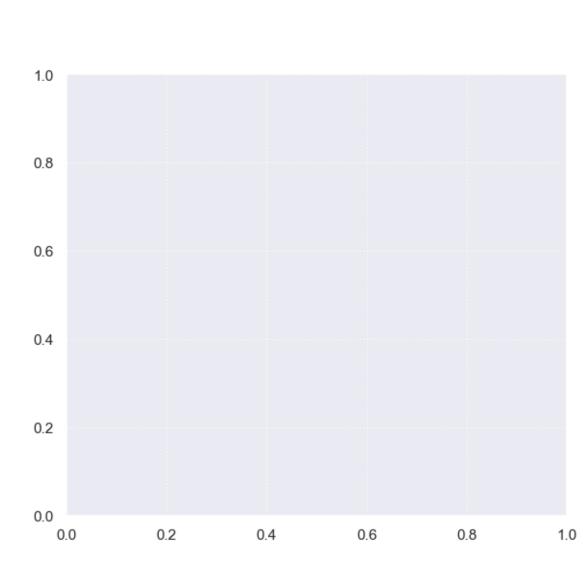
XGBoost Parameters	Value
alpha	4.45
colsample_bytree	0.545
gamma	0.4668
lambda	3.5277
learning_rate	0.0192
max_depth	10.0
min_child_weight	2.0
n_estimators	540.0
reg_alpha	0.3173
reg_lambda	0.3951
scale_pos_weight	1.4332
subsample	0.9044

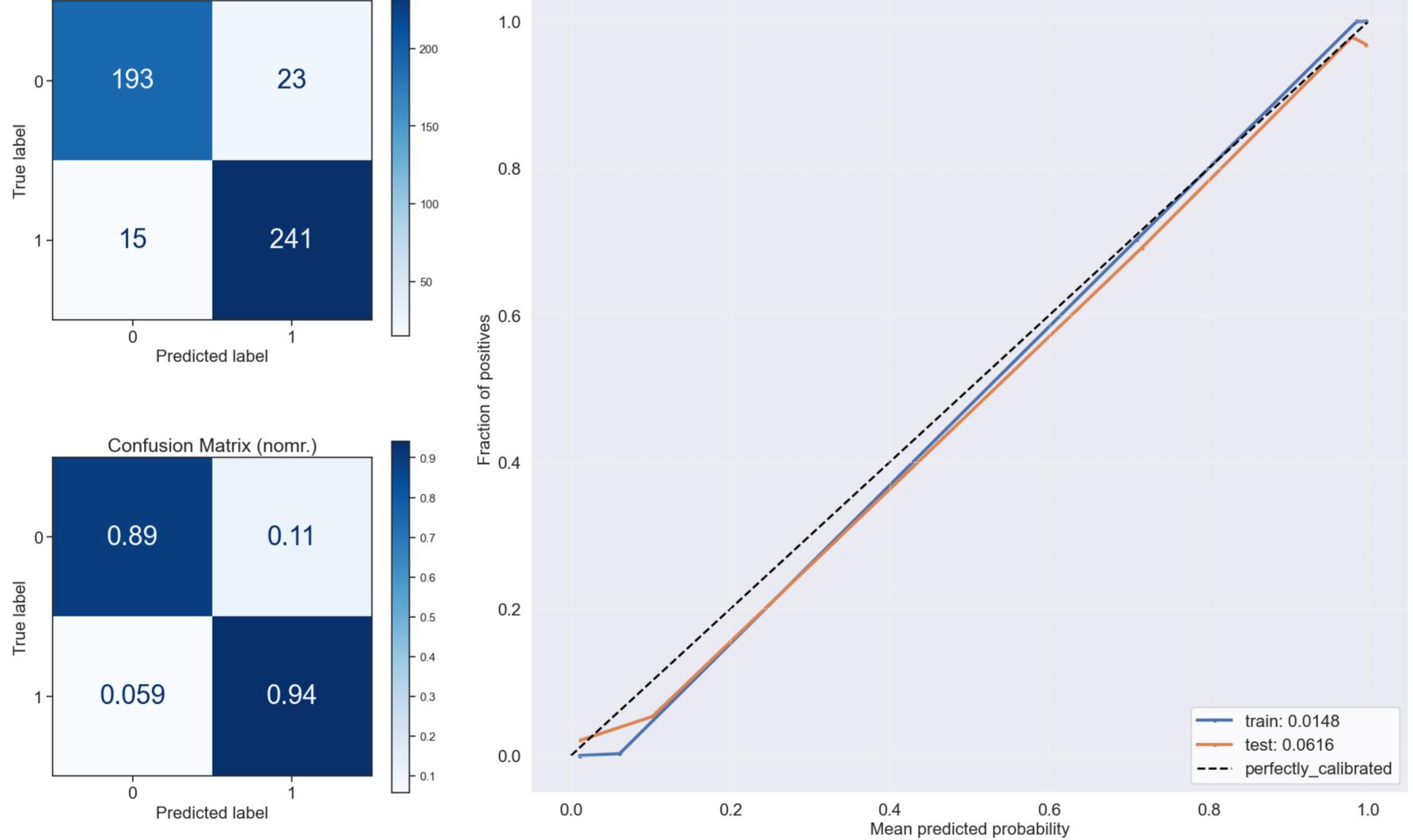


	Active/Inactive probability						
40	Ina	ictive zone			Active z	cone act	pe ive (256) ctive (216) coy (468)
30							
Percent							
10					_		
0 —	0.0 0.	.2 ().4 Proba	0.6 ability	0.	8	1.0

Metric	Train	Test
AUC	0.9981	0.964
accuracy	0.9799	0.9153
balanced accuracy	0.9791	0.9136
recall_(sens)	0.9882	0.9336
specificity	0.97	0.8935
precision	0.9749	0.9122
f1_score	0.9798	0.9151







50	Active/Inactive probability					
50 		active zone			Active zone	type active (256) inactive (216) decoy (468)
. 11 /						
Percent						
10						
0 —	0.0	0.2	0.4 Proba	0.6 ability	0.8	1.0

Metric	Train	Test
AUC	0.9991	0.9652
accuracy	0.9841	0.9195
balanced accuracy	0.9833	0.9175
recall_(sens)	0.9931	0.9414
specificity	0.9734	0.8935
precision	0.9778	0.9129
f1_score	0.9841	0.9194