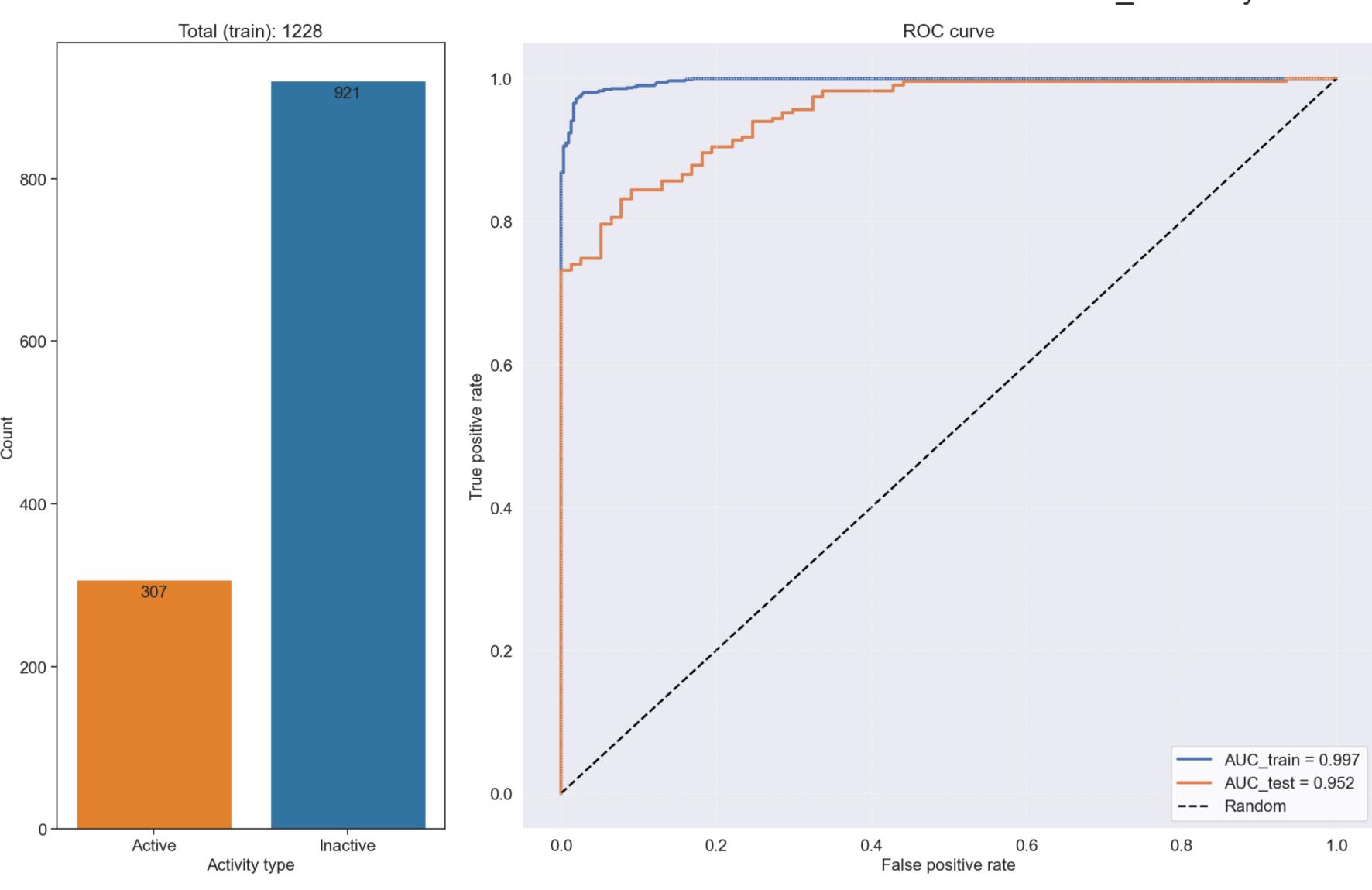
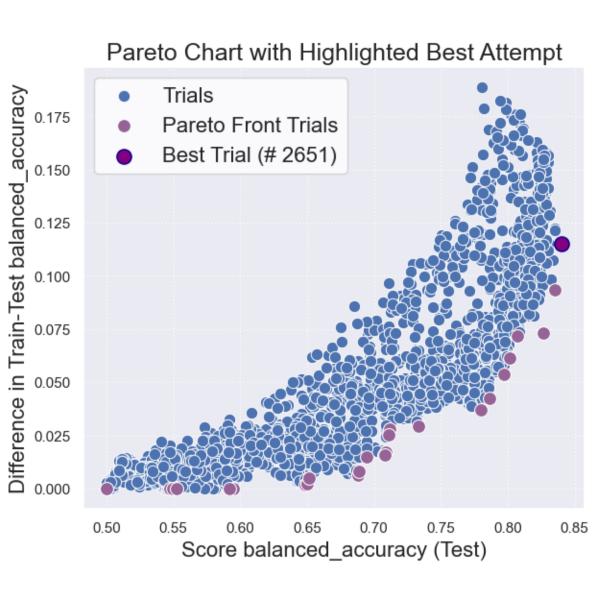
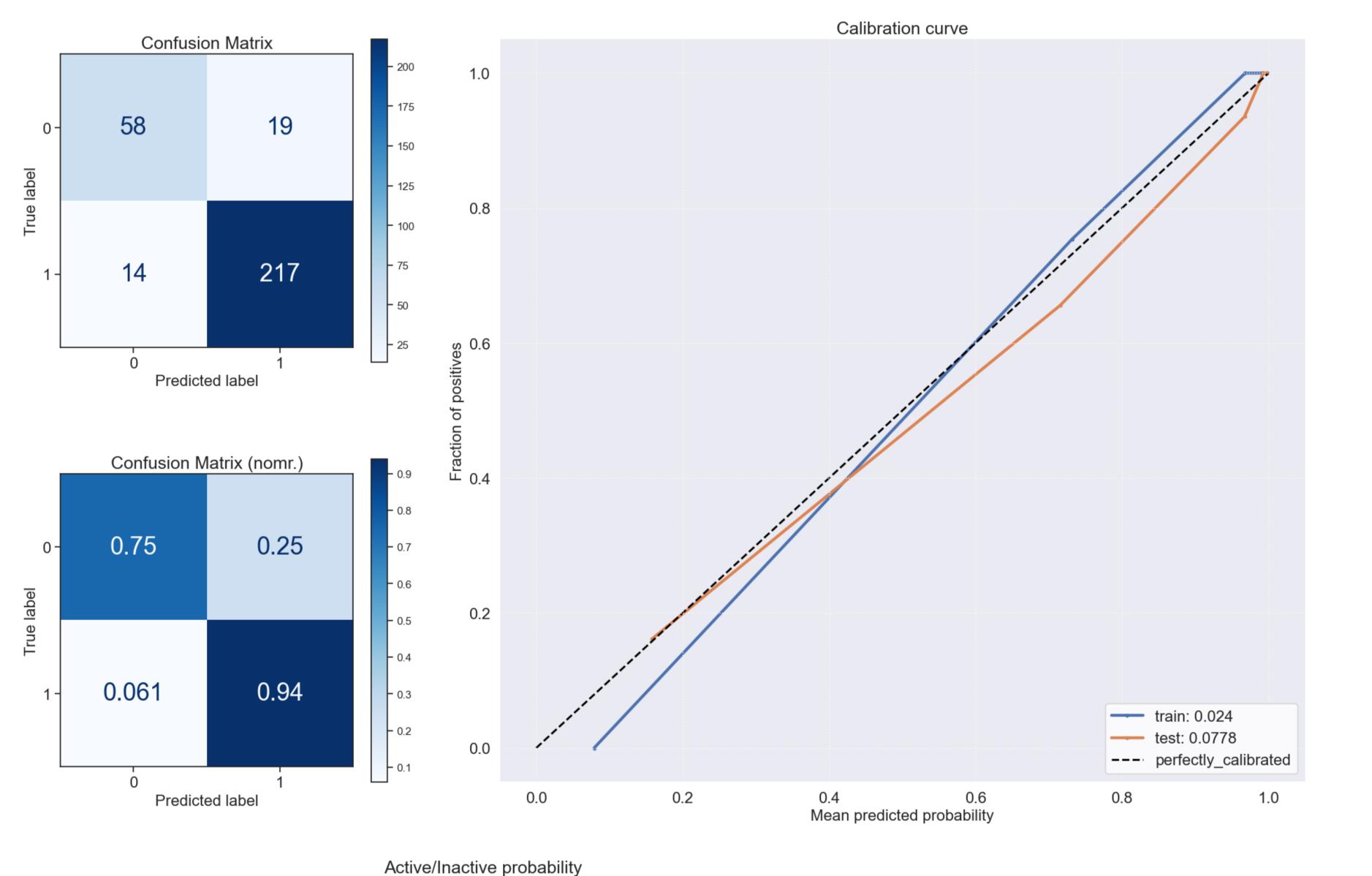
Protein: P49768 - metric: balanced_accuracy





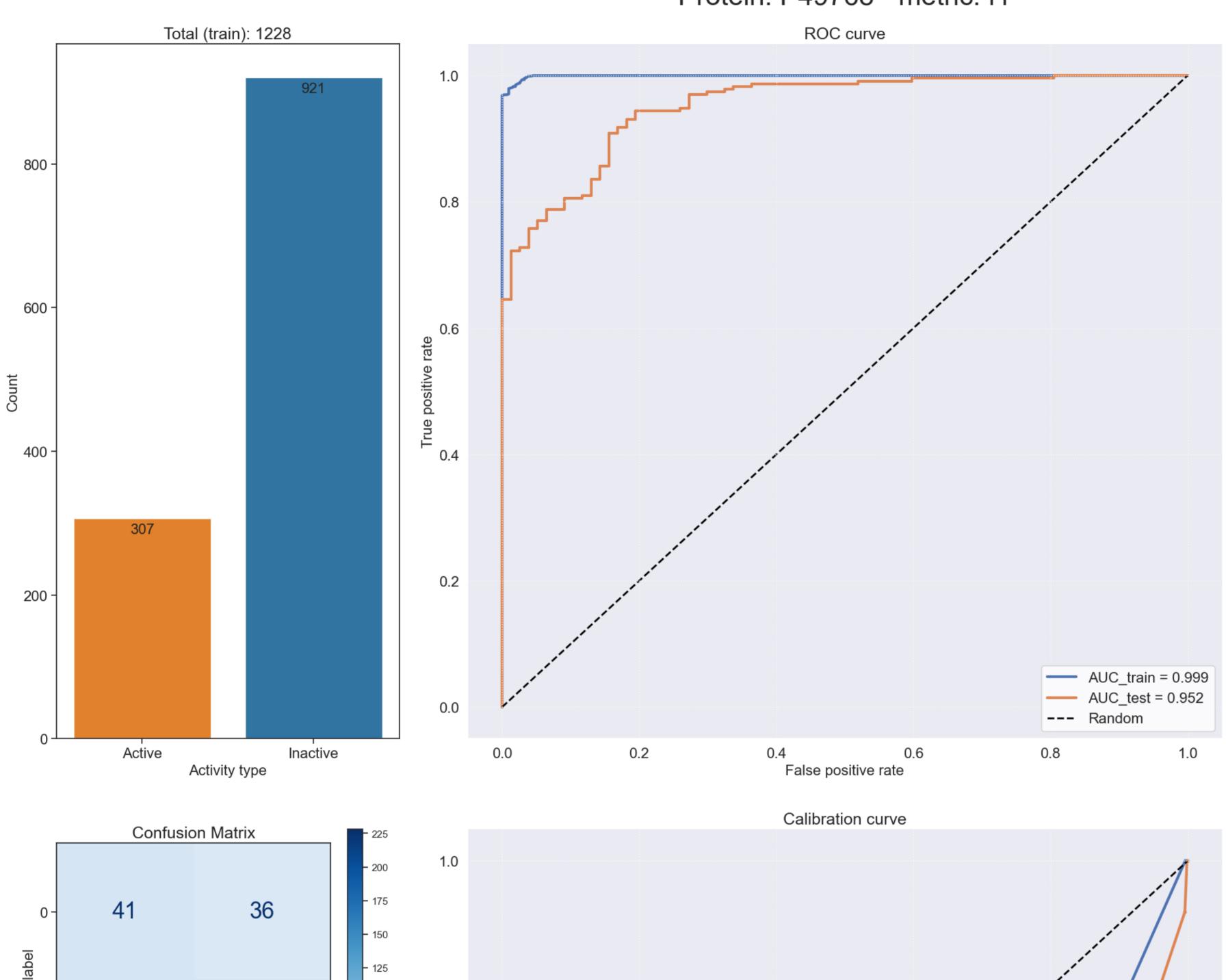
XGBoost Parameters	Value
alpha	2.1688
colsample_bytree	0.9973
gamma	0.6146
lambda	2.7472
learning_rate	0.145
max_depth	3.0
min_child_weight	3.0
n_estimators	997.0
reg_alpha	0.1424
reg_lambda	0.0299
scale_pos_weight	1.0789
subsample	0.9224

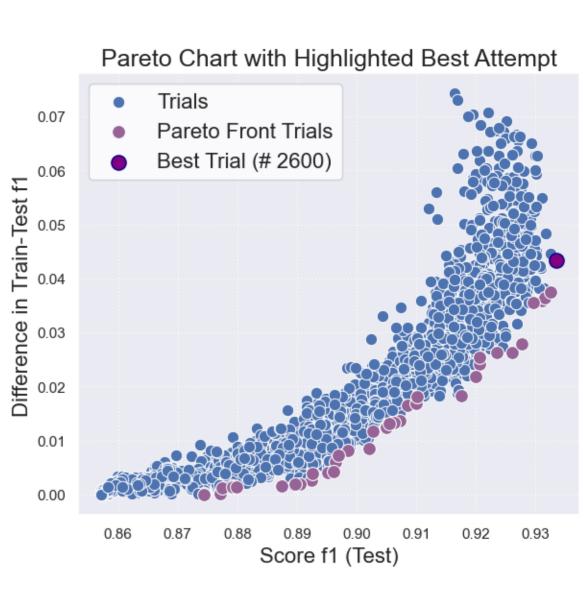


		Active/inde	tive probability		
50	Inacti	ve zone		Active zone	type active (231) inactive (77) decoy (308)
40					, , ,
Percent 20					
10					
0 —	0.0 0.2	0.4	0.6	0.8	1.0
		Pro	bability		

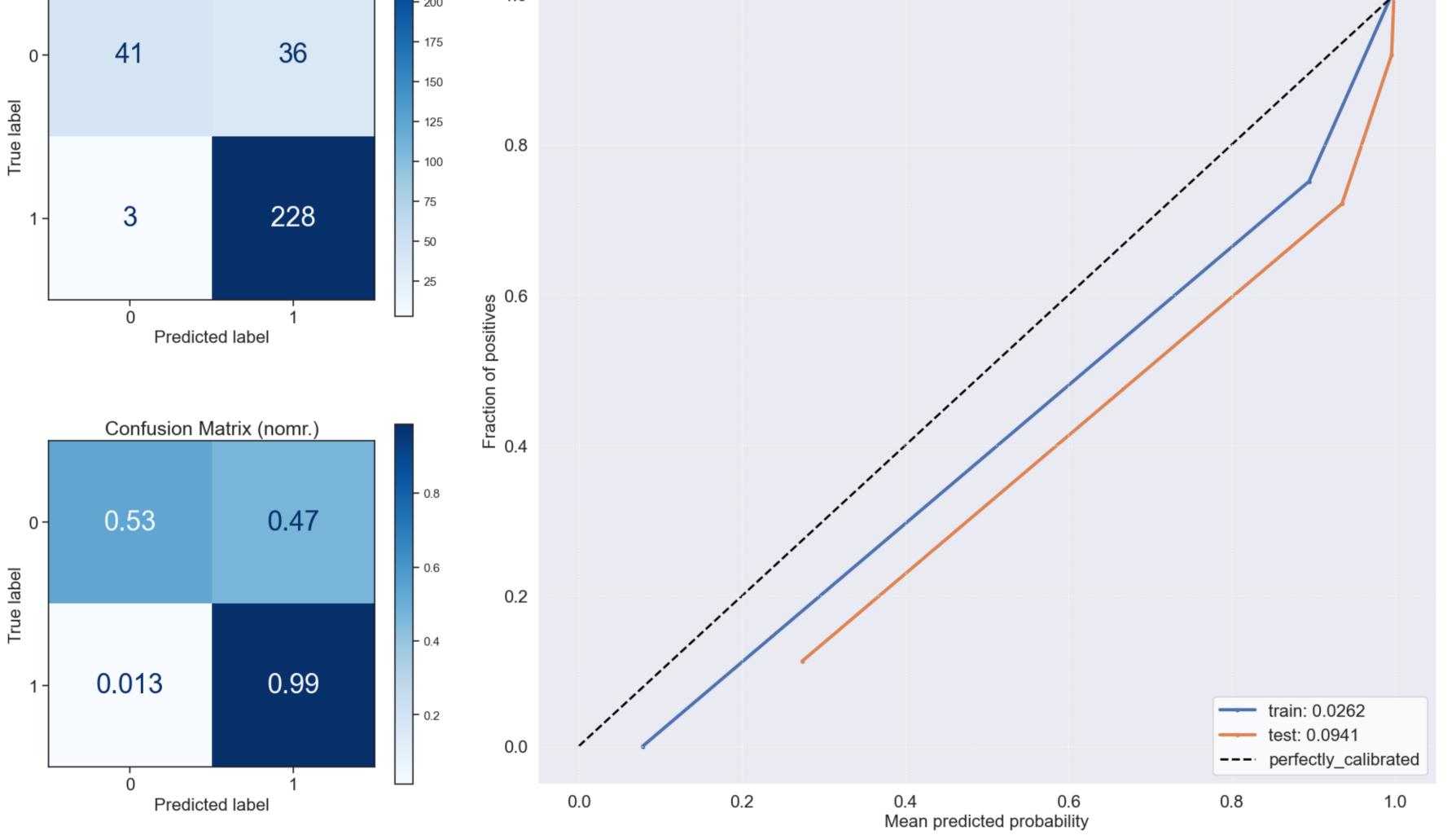
Metric	Train	Test
AUC	0.9967	0.9519
accuracy	0.9707	0.8929
balanced accuracy	0.9555	0.8463
recall_(sens)	0.9859	0.9394
specificity	0.9251	0.7532
precision	0.9753	0.9195
f1_score	0.9705	0.8916

Protein: P49768 - metric: f1





XGBoost Parameters	Value
alpha	2.1987
colsample_bytree	0.5691
gamma	0.6675
lambda	4.2892
learning_rate	0.0901
max_depth	7.0
min_child_weight	2.0
n_estimators	753.0
reg_alpha	0.3291
reg_lambda	0.631
scale_pos_weight	10.4314
subsample	0.8796

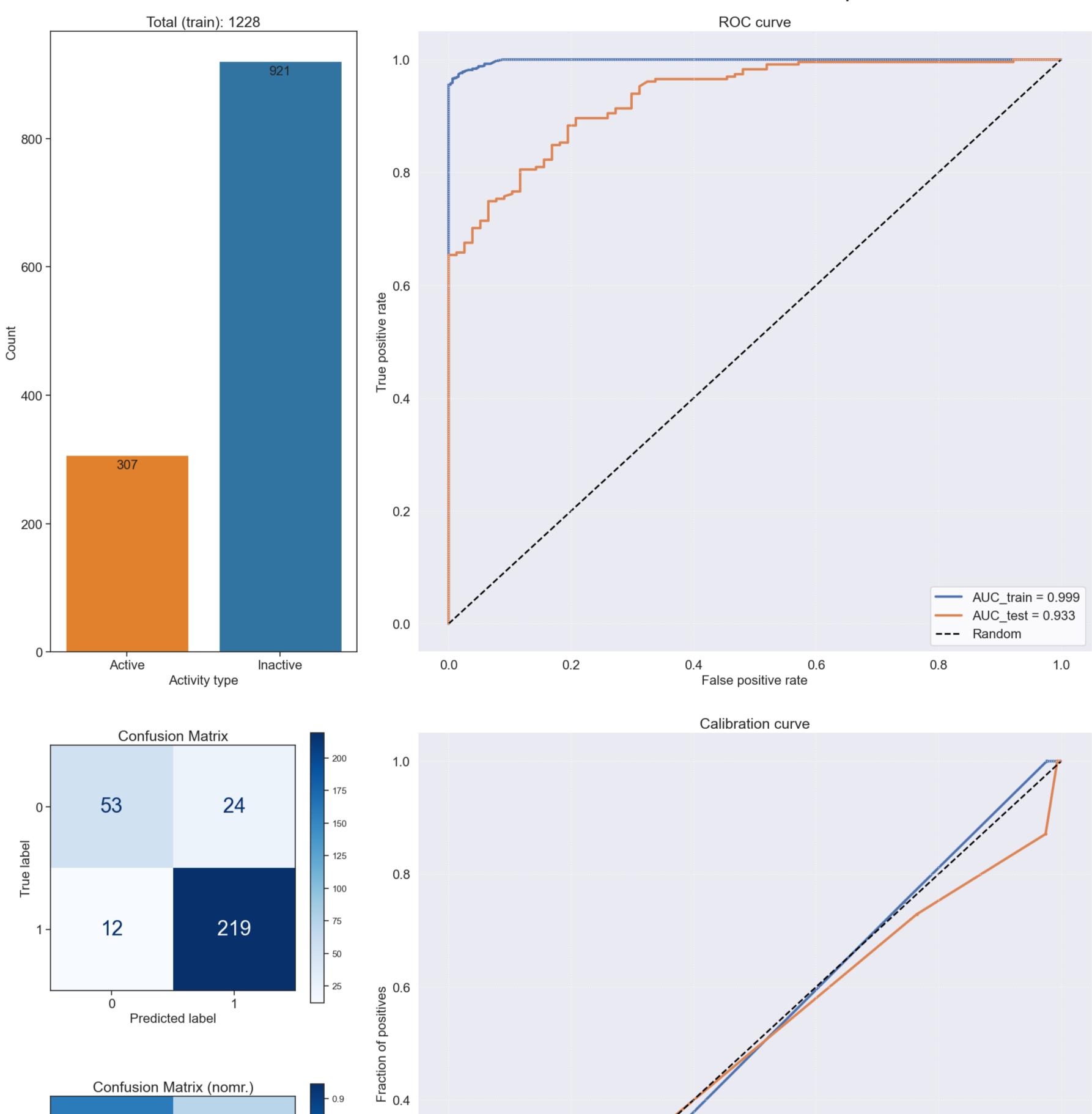


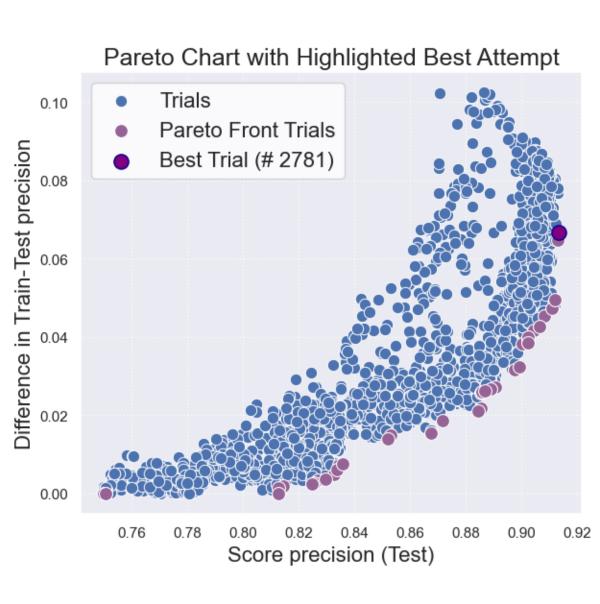
70		nactive zone		Active 2	zone act	oe ive (231) ctive (77)
70						coy (308)
00						
sent						
00						
10 -						
0						
0-	0.0	0.2	.4 0 Probability	.6 0	.8	1.0

Active/Inactive probability

Metric	Train	Test
AUC	0.9994	0.9518
accuracy	0.9658	0.8734
balanced accuracy	0.9316	0.7597
recall_(sens)	1.0	0.987
specificity	0.8632	0.5325
precision	0.9564	0.8636
f1_score	0.9649	0.8603

Protein: P49768 - metric: precision





XGBoost Parameters	Value
alpha	1.9864
colsample_bytree	0.9906
gamma	0.9844
lambda	3.6266
learning_rate	0.7496
max_depth	9.0
min_child_weight	1.0
n_estimators	546.0
reg_alpha	0.2701
reg_lambda	0.6551
scale_pos_weight	1.0747
subsample	0.9228

		Active/Inac	tive probability		
50	Inact	tive zone		Active zone	inactive (77) decoy (308)
Percent 08					
10 -					
	0.0 0.2	0.4 Pro	0.6 obability	0.8	1.0

- 0.8

- 0.7

0.6

- 0.5

- 0.4

- 0.3

0.2

0.1

0.2

0.0

0.0

0.2

Predicted label

Confusion Matrix (nomr.)

Predicted label

0.31

0.95

0.69

0.052

True label

Metric	Train	Test
AUC	0.9985	0.9332
accuracy	0.978	0.8831
balanced accuracy	0.9636	0.8182
recall_(sens)	0.9924	0.9481
specificity	0.9349	0.6883
precision	0.9786	0.9012
f1_score	0.9779	0.8797

train: 0.018

8.0

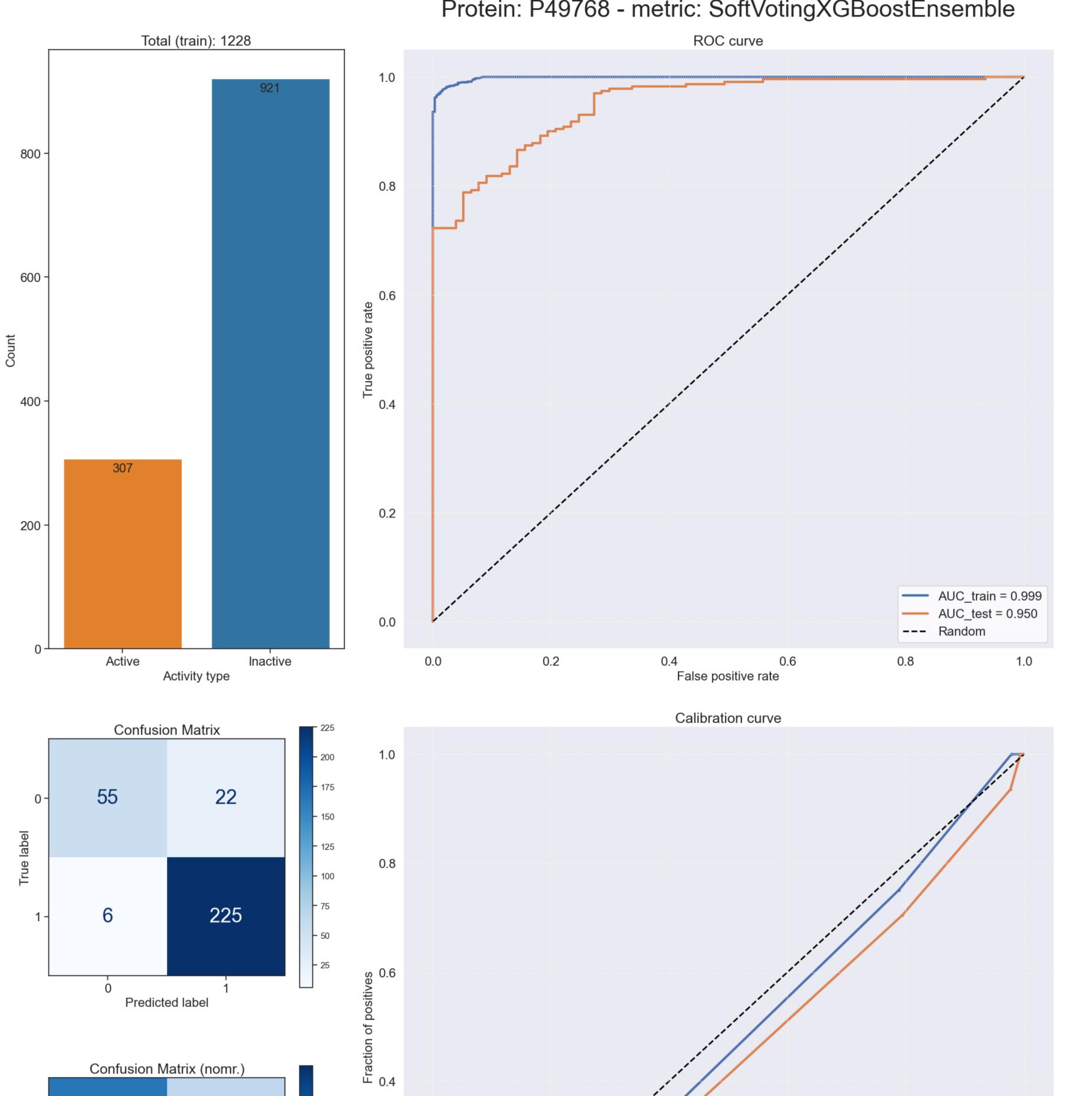
0.4 0.6 Mean predicted probability

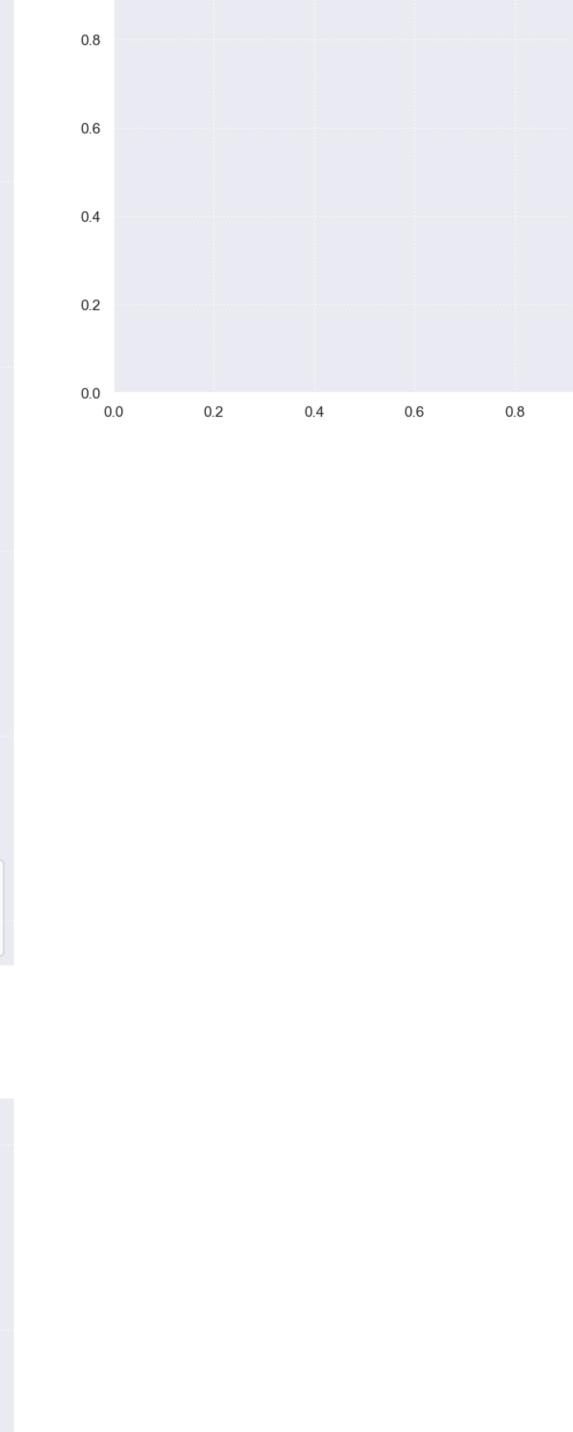
test: 0.0918

--- perfectly_calibrated

1.0

Protein: P49768 - metric: SoftVotingXGBoostEnsemble





		Ac	tive/Inactive p	robability		
40	Ina					decoy (308)
Percent 08						
20						
	0.0	.2 0).4 Probabilit	0.6 y	0.8	1.0

0.71

0.026

Predicted label

True label

0.29

0.97

- 0.6

- 0.4

0.2

0.2

0.0

0.0

0.2

Metric	Train	Test
AUC	0.9986	0.9495
accuracy	0.9756	0.9091
balanced accuracy	0.9511	0.8442
recall_(sens)	1.0	0.974
specificity	0.9023	0.7143
precision	0.9685	0.9109
f1_score	0.9751	0.9053

--- train: 0.0202

--- test: 0.0811

0.8

0.4 0.6 Mean predicted probability

--- perfectly_calibrated

1.0