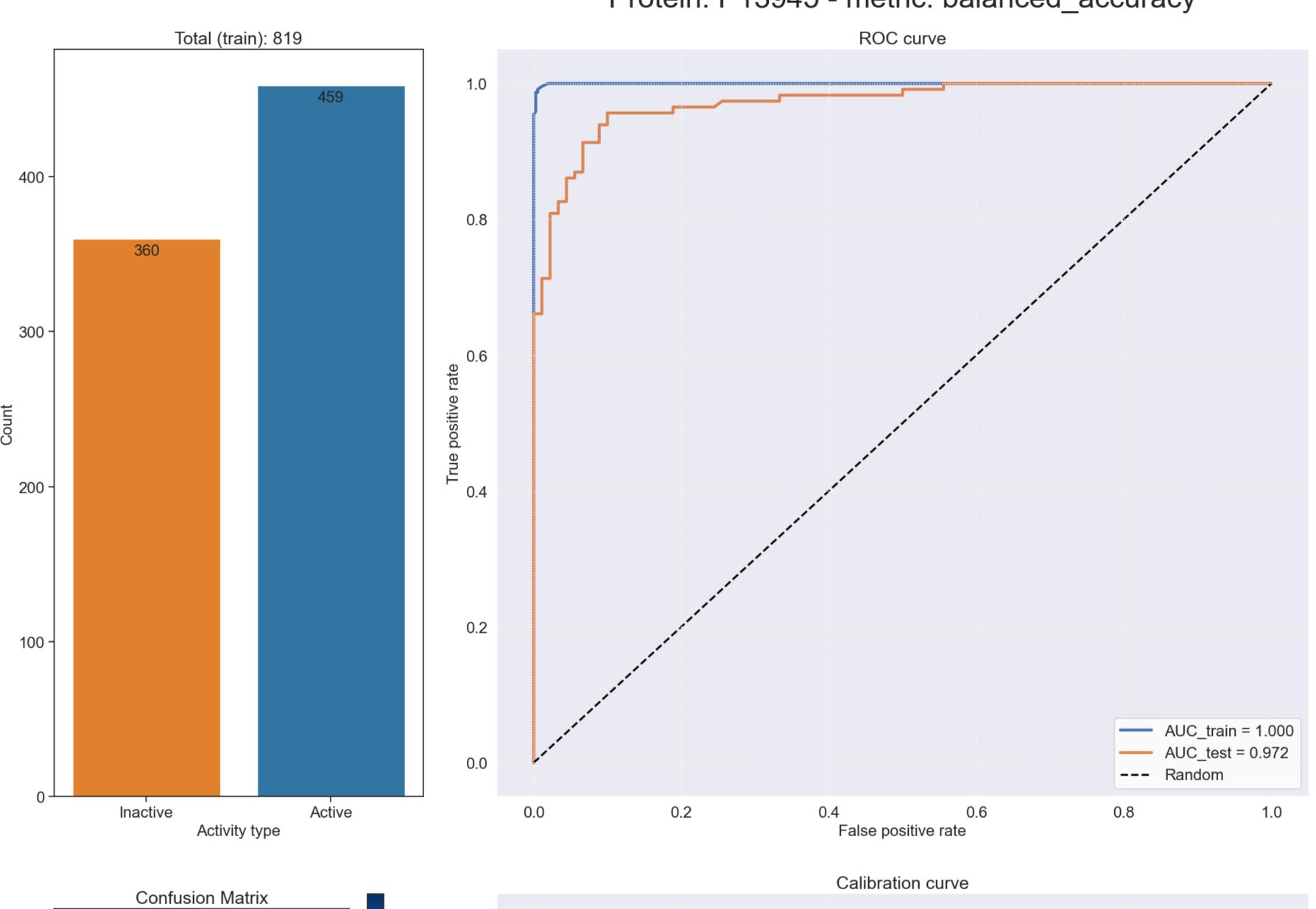
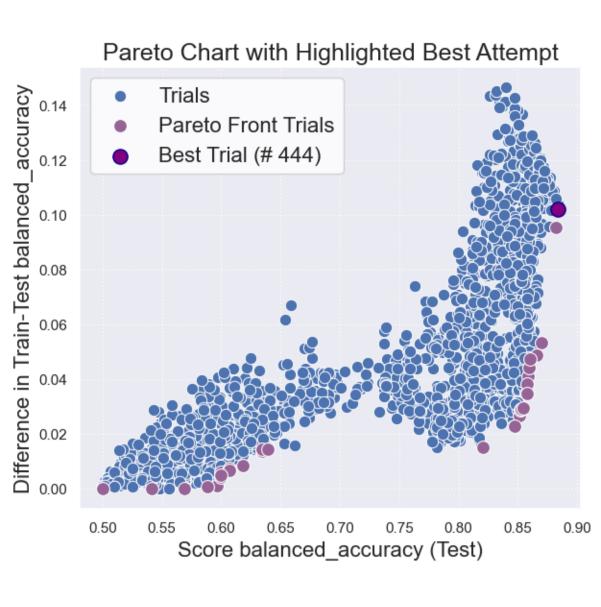
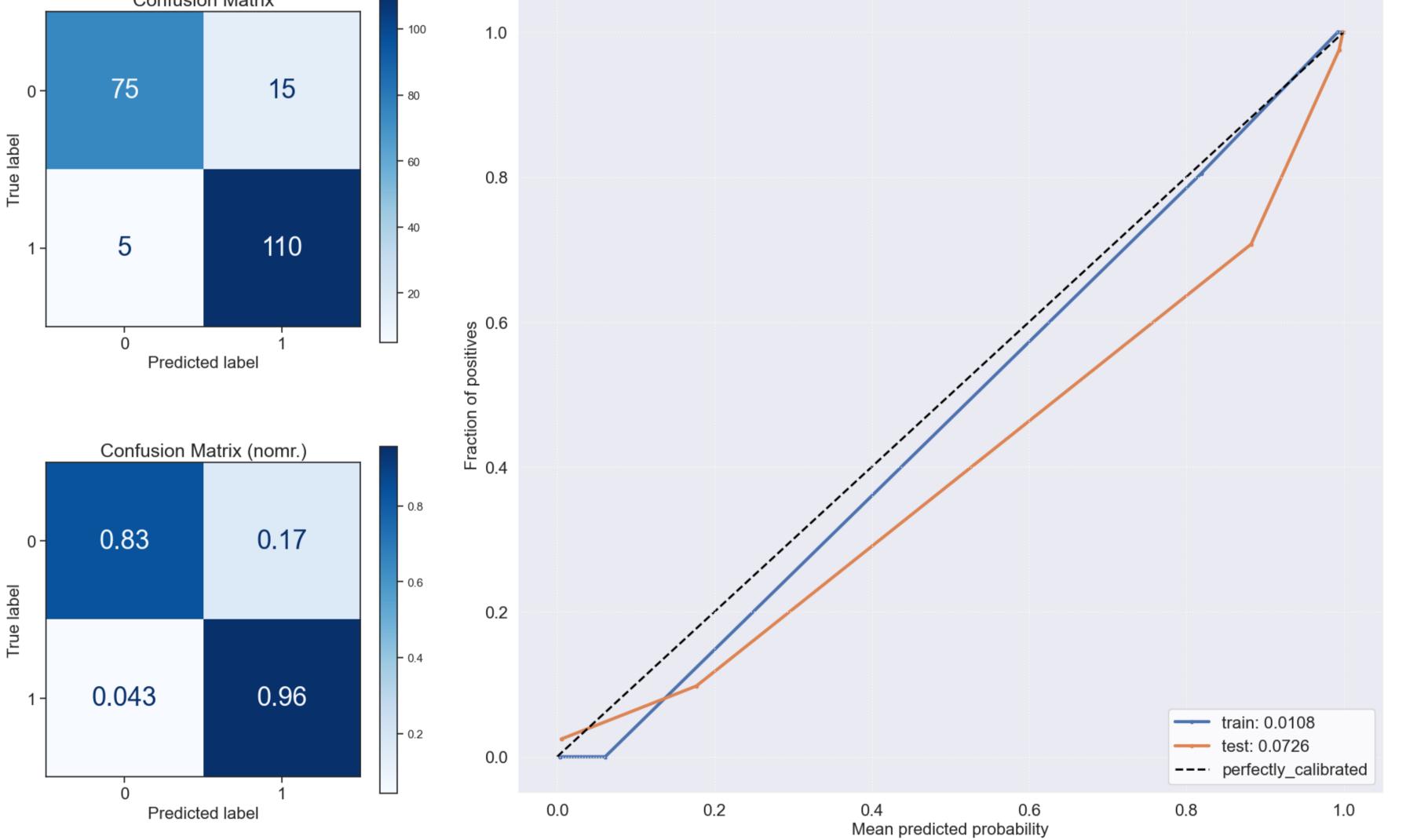
## Protein: P13945 - metric: balanced\_accuracy





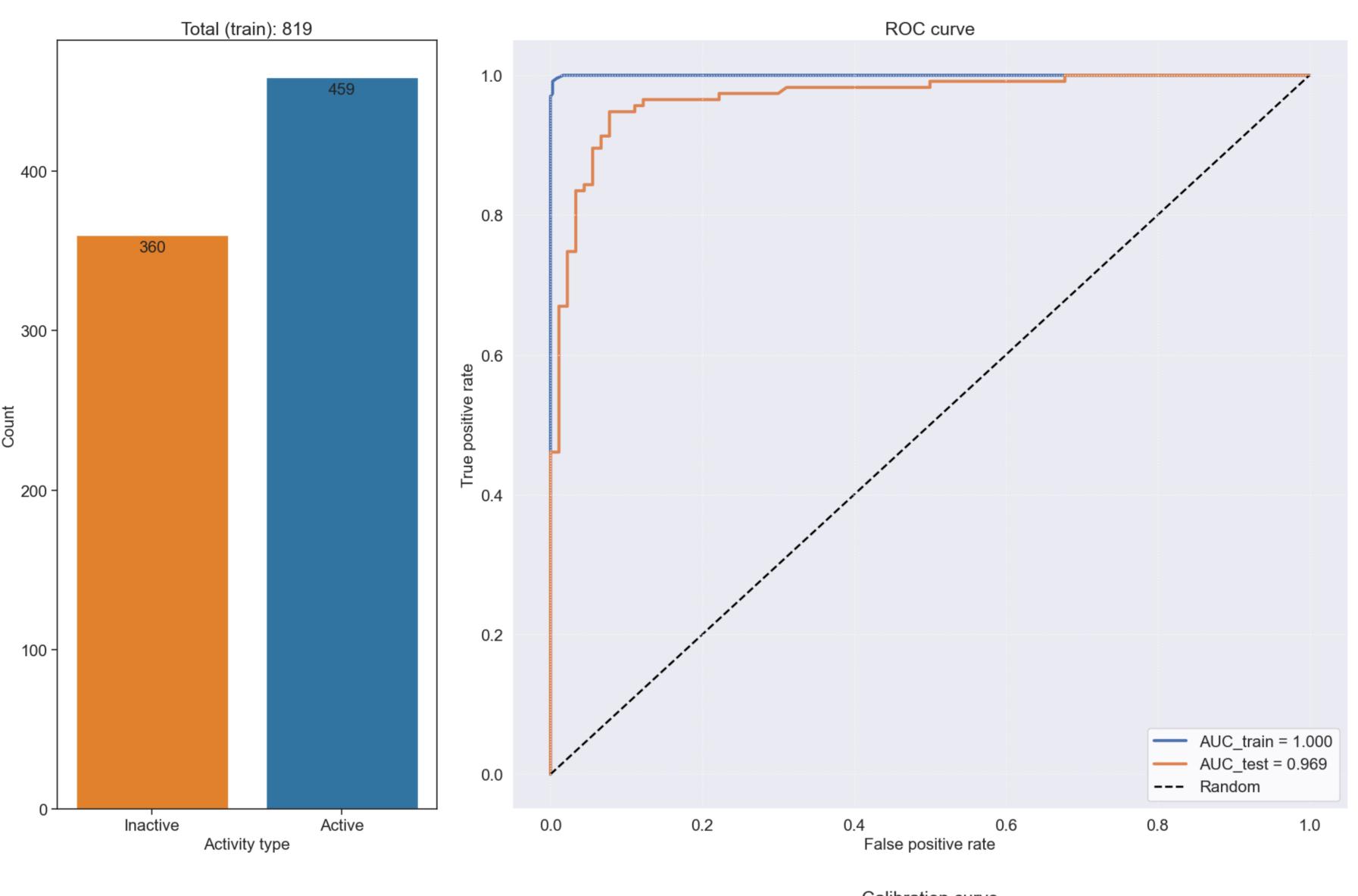
XGBoost Parameters	Value
alpha	1.1531
colsample_bytree	0.5625
gamma	0.1528
lambda	0.485
learning_rate	0.1793
max_depth	7.0
min_child_weight	2.0
n_estimators	718.0
reg_alpha	0.7789
reg_lambda	0.0849
scale_pos_weight	1.9434
subsample	0.6707

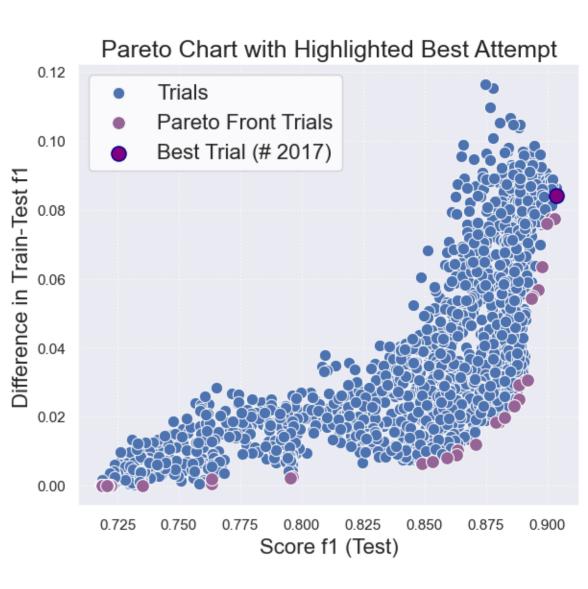


Active/Inactive probability						
70		active zone			e zone	type active (115) inactive (90) decoy (205)
50						
Percent 0 04						
20						
10						
0-	0.0	0.2	).4	0.6	0.8	1.0
Probability						

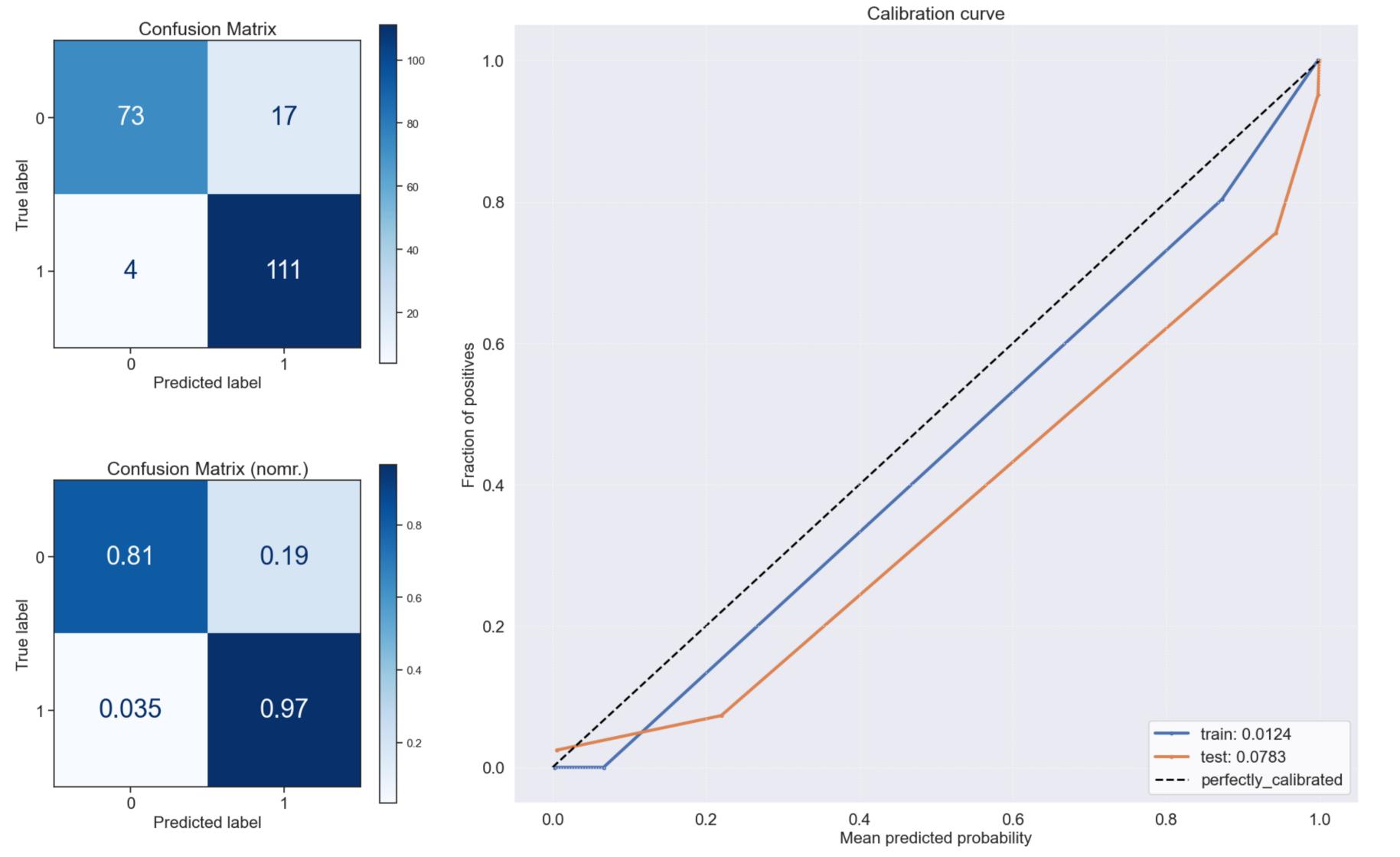
Metric	Train	Test
AUC	0.9998	0.9718
accuracy	0.9902	0.9024
balanced accuracy	0.9889	0.8949
recall_(sens)	1.0	0.9565
specificity	0.9778	0.8333
precision	0.9829	0.88
f1_score	0.9902	0.9016

## Protein: P13945 - metric: f1





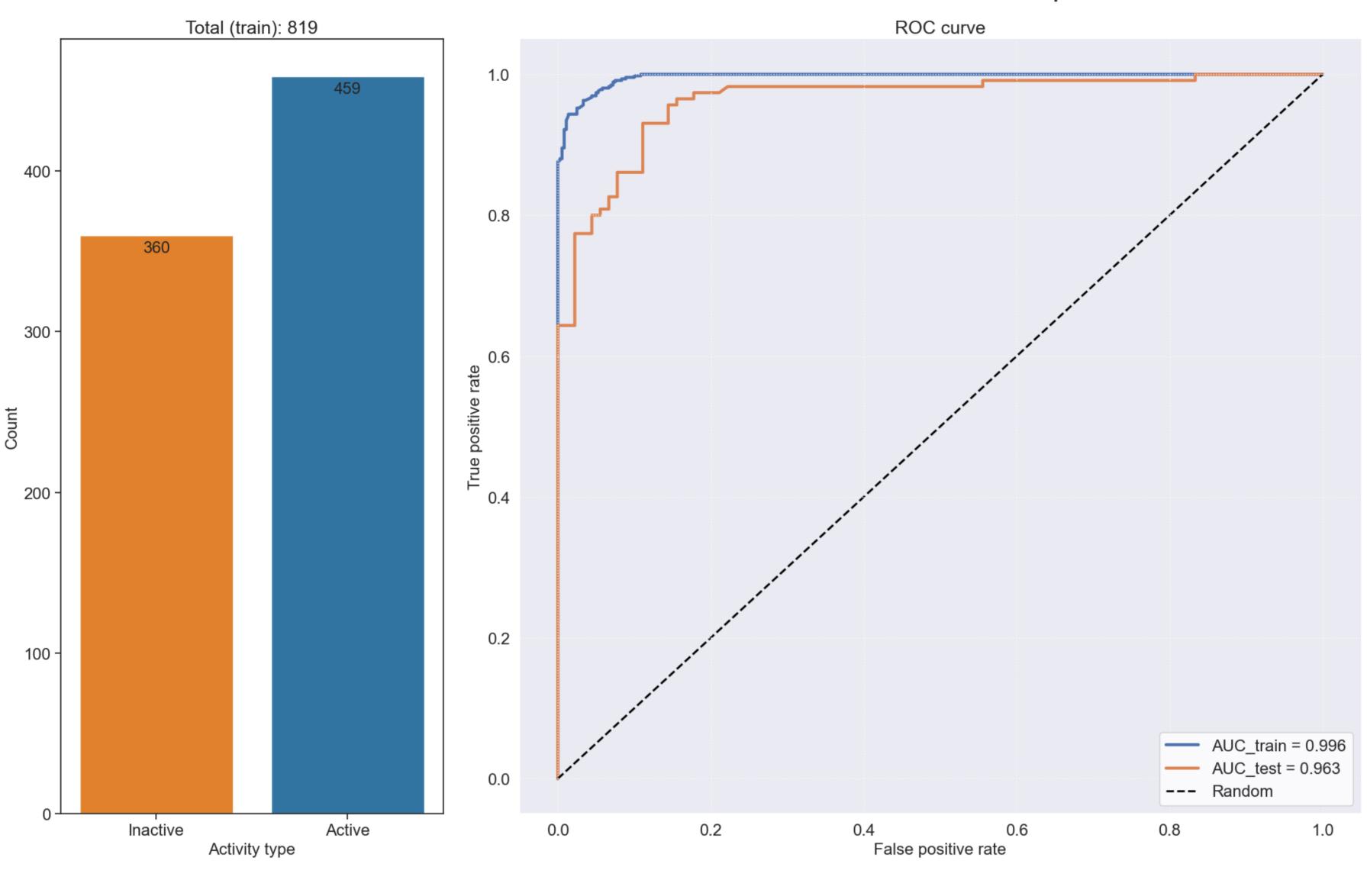
XGBoost Parameters	Value
alpha	1.5991
colsample_bytree	0.6745
gamma	0.0164
lambda	2.9563
learning_rate	0.0848
max_depth	7.0
min_child_weight	2.0
n_estimators	940.0
reg_alpha	0.6682
reg_lambda	0.2062
scale_pos_weight	6.2779
subsample	0.5343

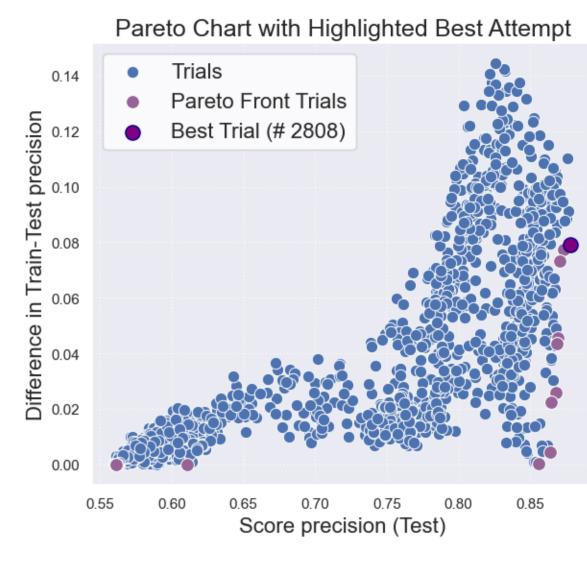


	Active/Inactive probability						
80 <del></del>		Inactive zone			Active zone	active (115)	
00							
Percent 05 05							
30							
20 <del></del> 10 <del></del>							
0 —	0.0	0.2	0.4	0.6	0.8	1.0	
	Probability						

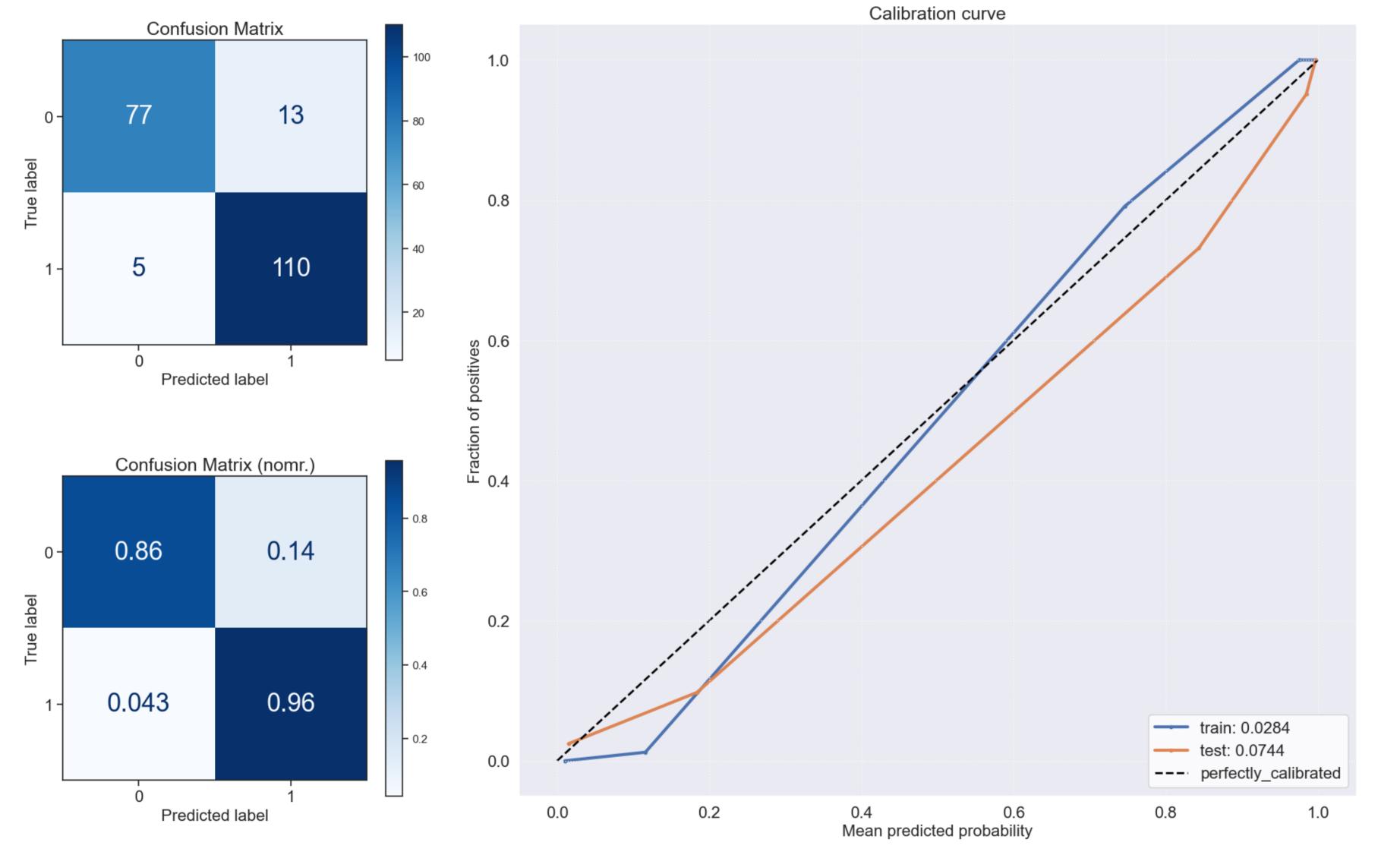
Metric	Train	Test
AUC	0.9999	0.969
accuracy	0.9866	0.8976
balanced accuracy	0.9847	0.8882
recall_(sens)	1.0	0.9652
specificity	0.9694	0.8111
precision	0.9766	0.8672
f1_score	0.9865	0.8963

## Protein: P13945 - metric: precision





XGBoost Parameters	Value
alpha	2.6791
colsample_bytree	0.8286
gamma	0.2938
lambda	2.7745
learning_rate	0.243
max_depth	4.0
min_child_weight	6.0
n_estimators	390.0
reg_alpha	0.3539
reg_lambda	0.003
scale_pos_weight	1.2514
subsample	0.7348

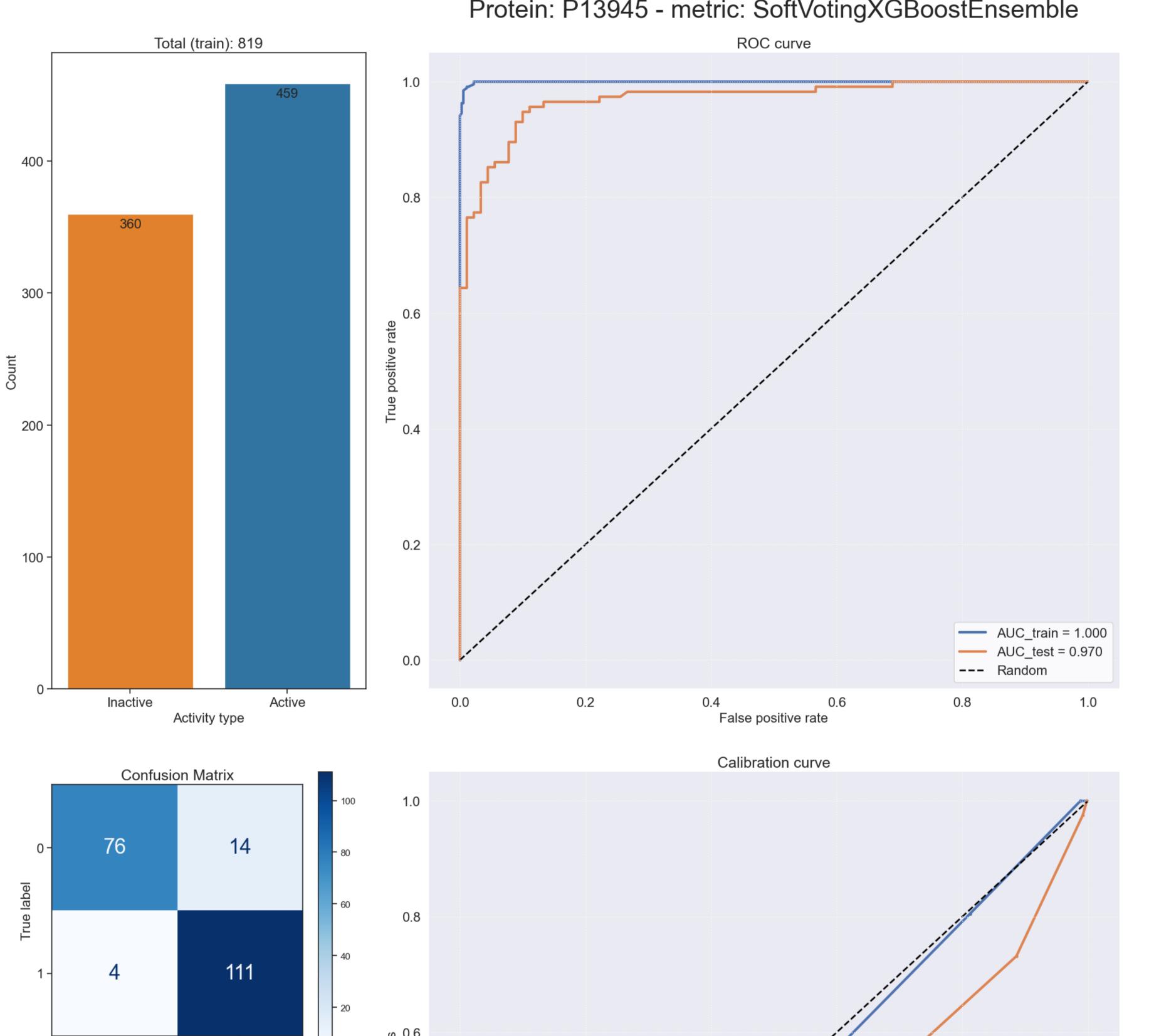


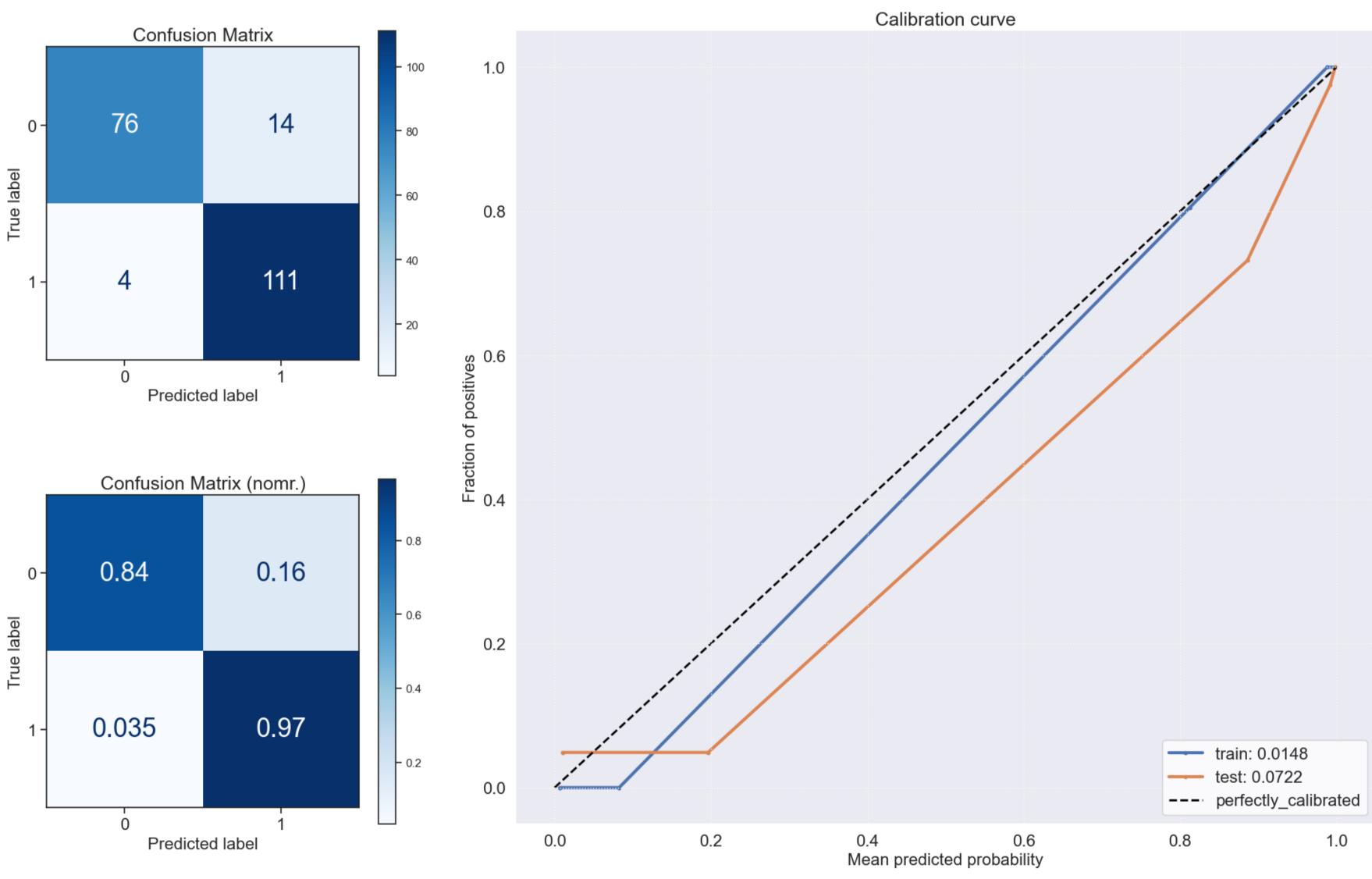
40		Inactive zone			Active zone	type active (115) inactive (90)
10				decoy (205)		
30						
Percent						
<sup>∞</sup> 20 - ·····						
10						
0-						
0	0.0	0.2	0.4 Proba	0.6	0.8	1.0
0 —	0.0	0.2	0.4 Proba		0.8	1.

Active/Inactive probability

Metric	Train	Test
AUC	0.9964	0.9632
accuracy	0.9621	0.9122
balanced accuracy	0.9608	0.906
recall_(sens)	0.9717	0.9565
specificity	0.95	0.8556
precision	0.9612	0.8943
f1_score	0.9621	0.9116

## Protein: P13945 - metric: SoftVotingXGBoostEnsemble





			Active/Inact	ive probabi	lity		
60		Inactive zone			Active	zone ac	pe tive (115) active (90)
50						de	coy (205)
Percent 0.00							
Pe 30							
20							
10							
0—	0.0	0.2	0.4 Prob	0. pability	6 0	0.8	1.0

Metric	Train	Test
AUC	0.9996	0.9703
accuracy	0.9878	0.9122
balanced accuracy	0.9861	0.9048
recall_(sens)	1.0	0.9652
specificity	0.9722	0.8444
precision	0.9787	0.888
f1_score	0.9878	0.9114

0.8

0.6

0.4

0.2

0.0

0.0

0.2

0.6