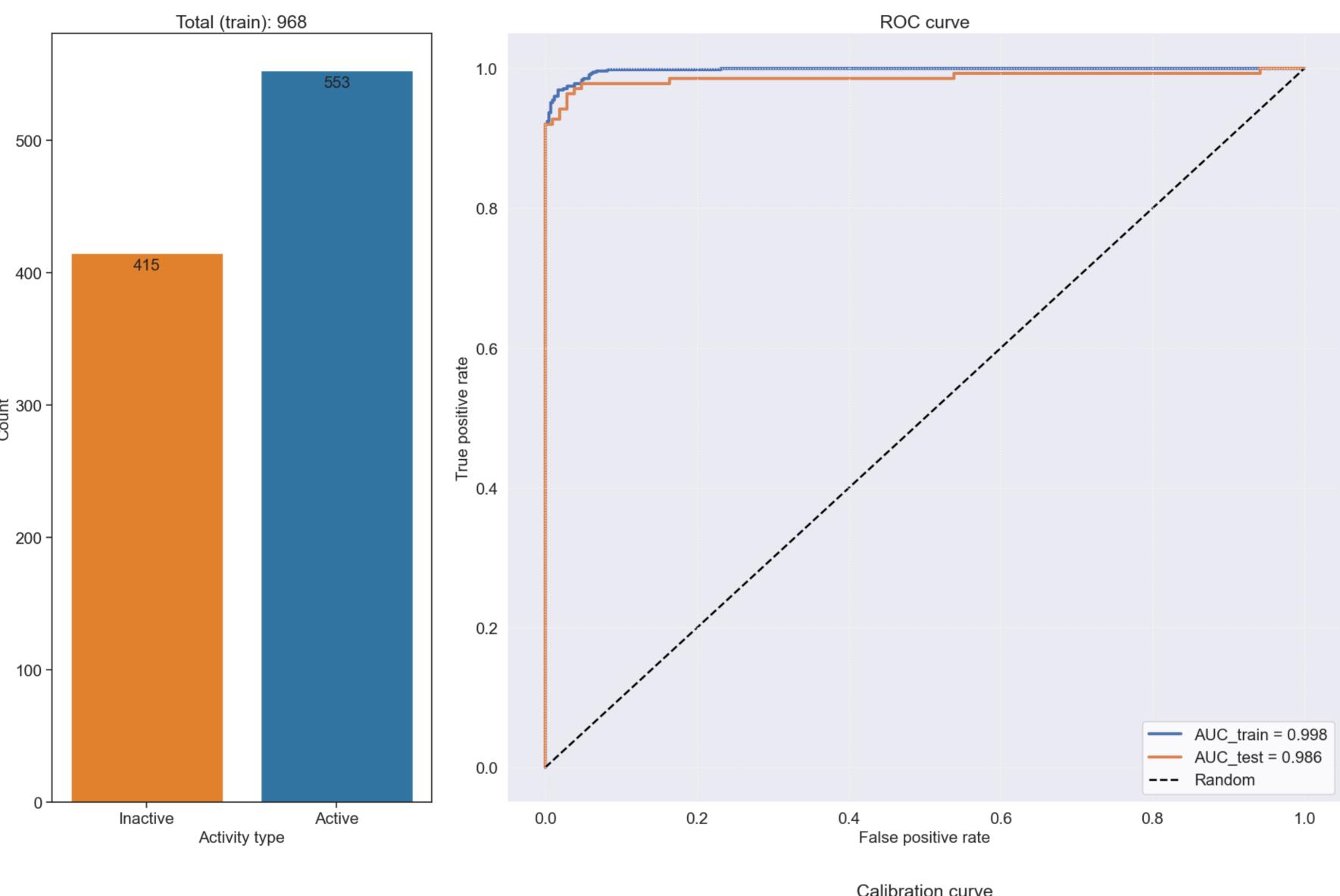
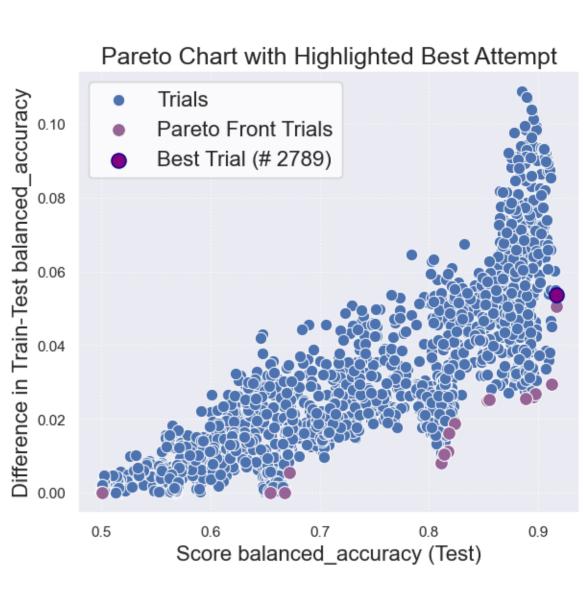
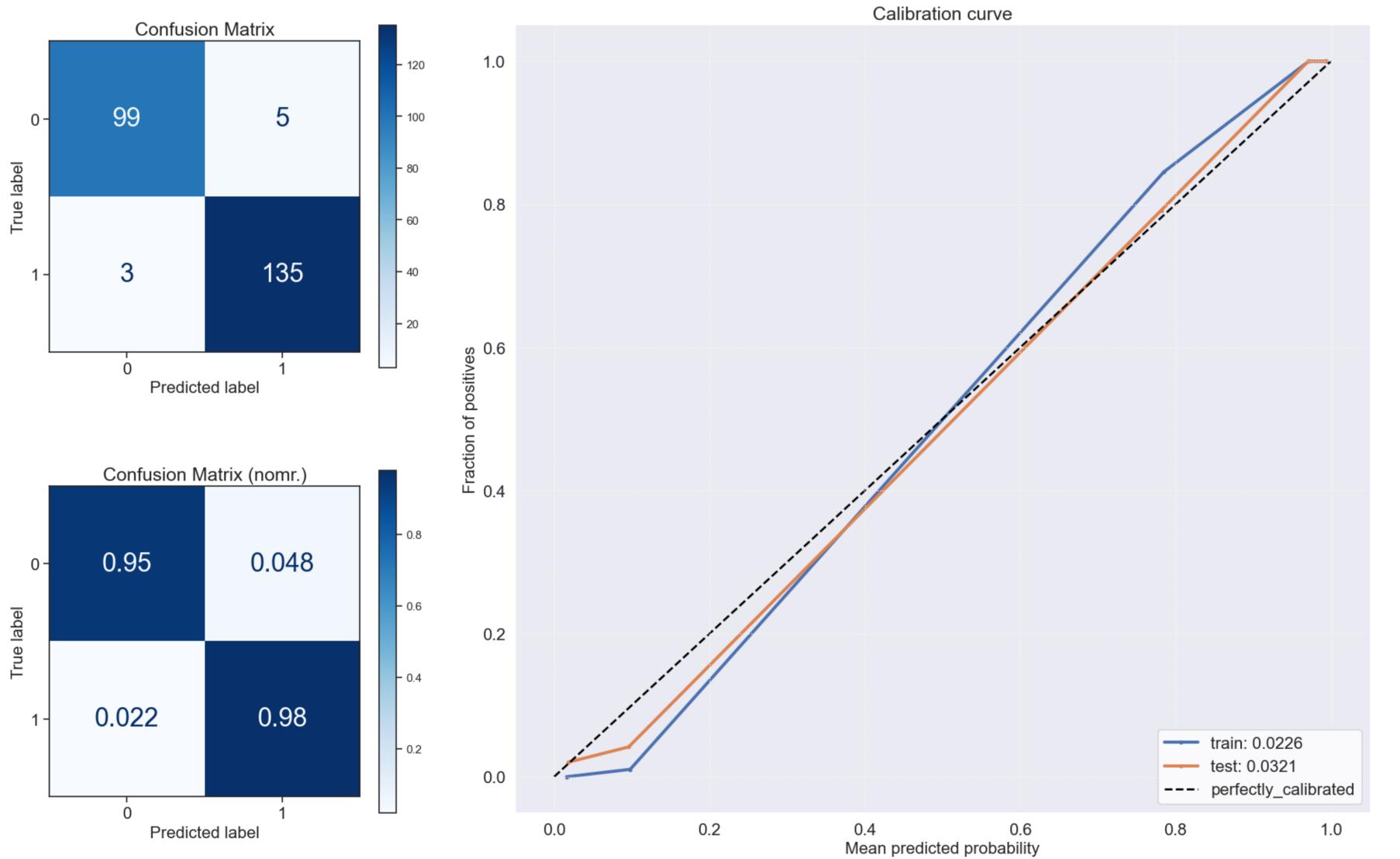
Protein: Q03181 - metric: balanced_accuracy





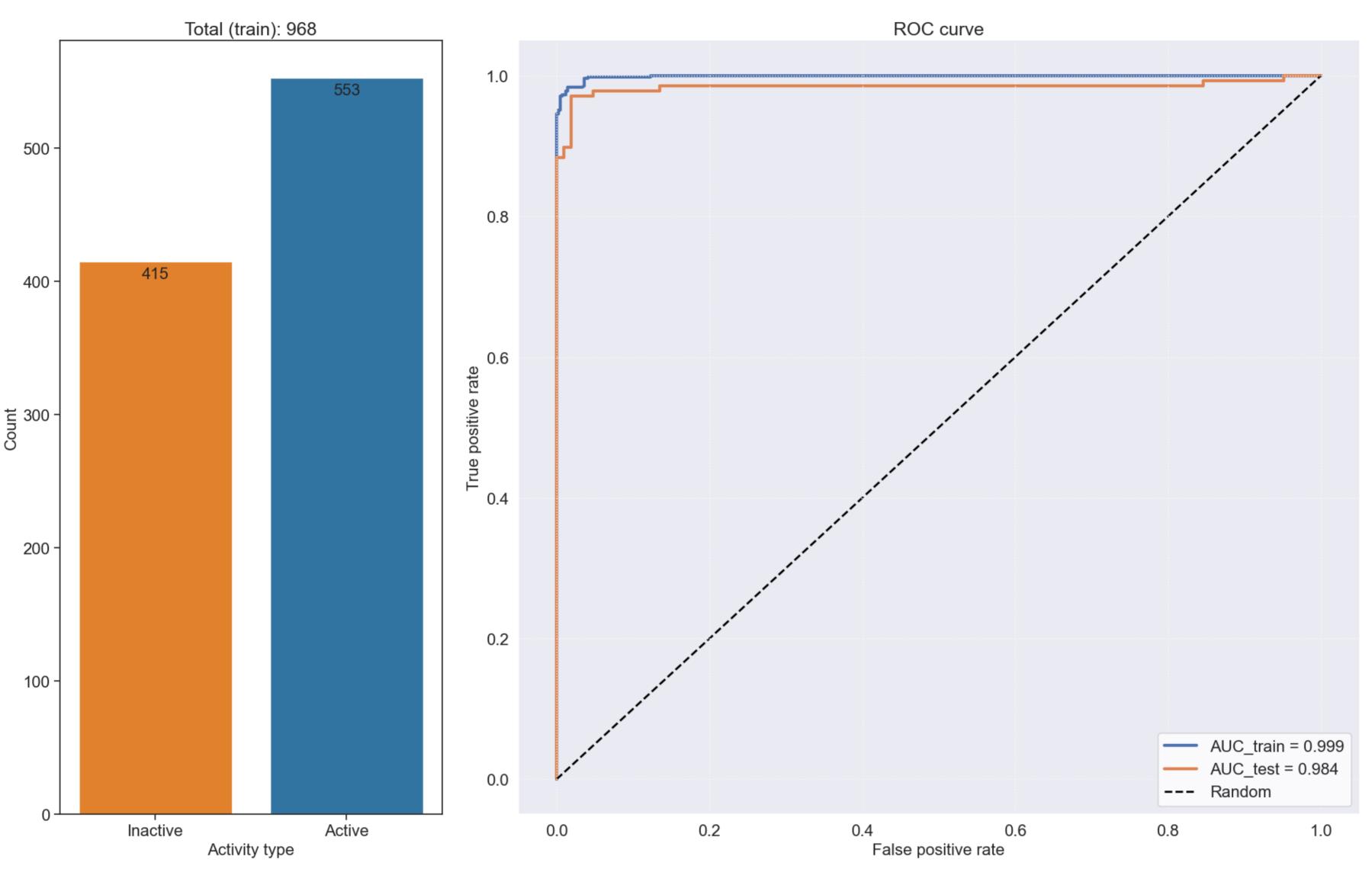
XGBoost Parameters	Value
alpha	0.0143
colsample_bytree	0.6947
gamma	0.7189
lambda	1.5612
learning_rate	0.0362
max_depth	4.0
min_child_weight	1.0
n_estimators	784.0
reg_alpha	0.5294
reg_lambda	0.2892
scale_pos_weight	1.0404
subsample	0.606

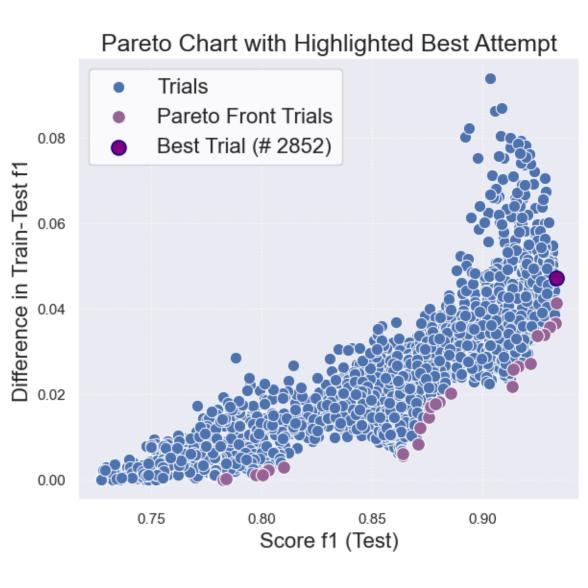


35			ive probability		
20	Inactive			Active zone	type active (138) inactive (104) decoy (242)
20					
Percent					
10					
5 					
	0.0 0.2	0.4 Prob	0.6 pability	0.8	1.0

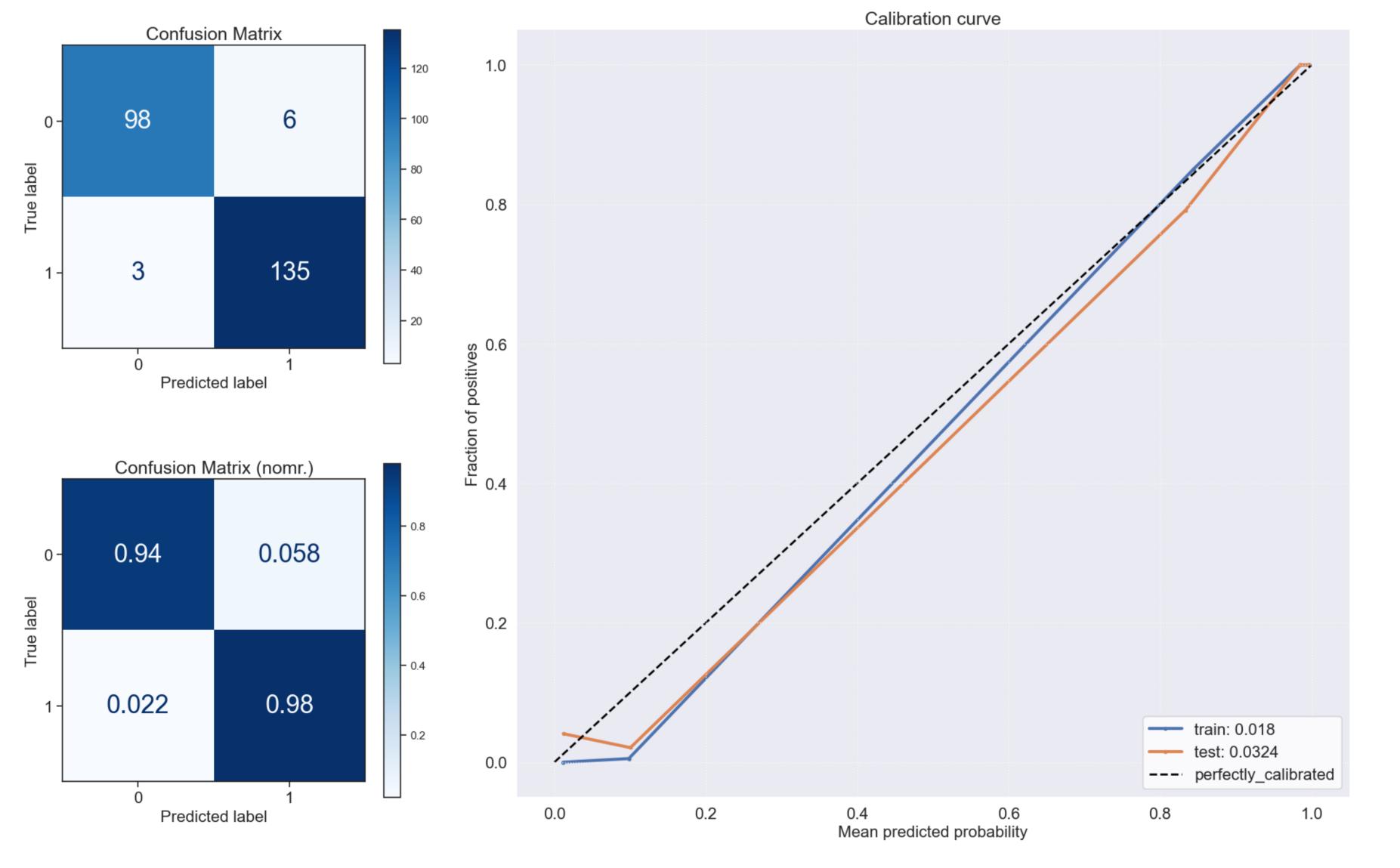
Metric	Train	Test
AUC	0.9977	0.9865
accuracy	0.968	0.9669
balanced accuracy	0.9663	0.9651
recall_(sens)	0.9783	0.9783
specificity	0.9542	0.9519
precision	0.9661	0.9643
f1_score	0.9679	0.9669

Protein: Q03181 - metric: f1





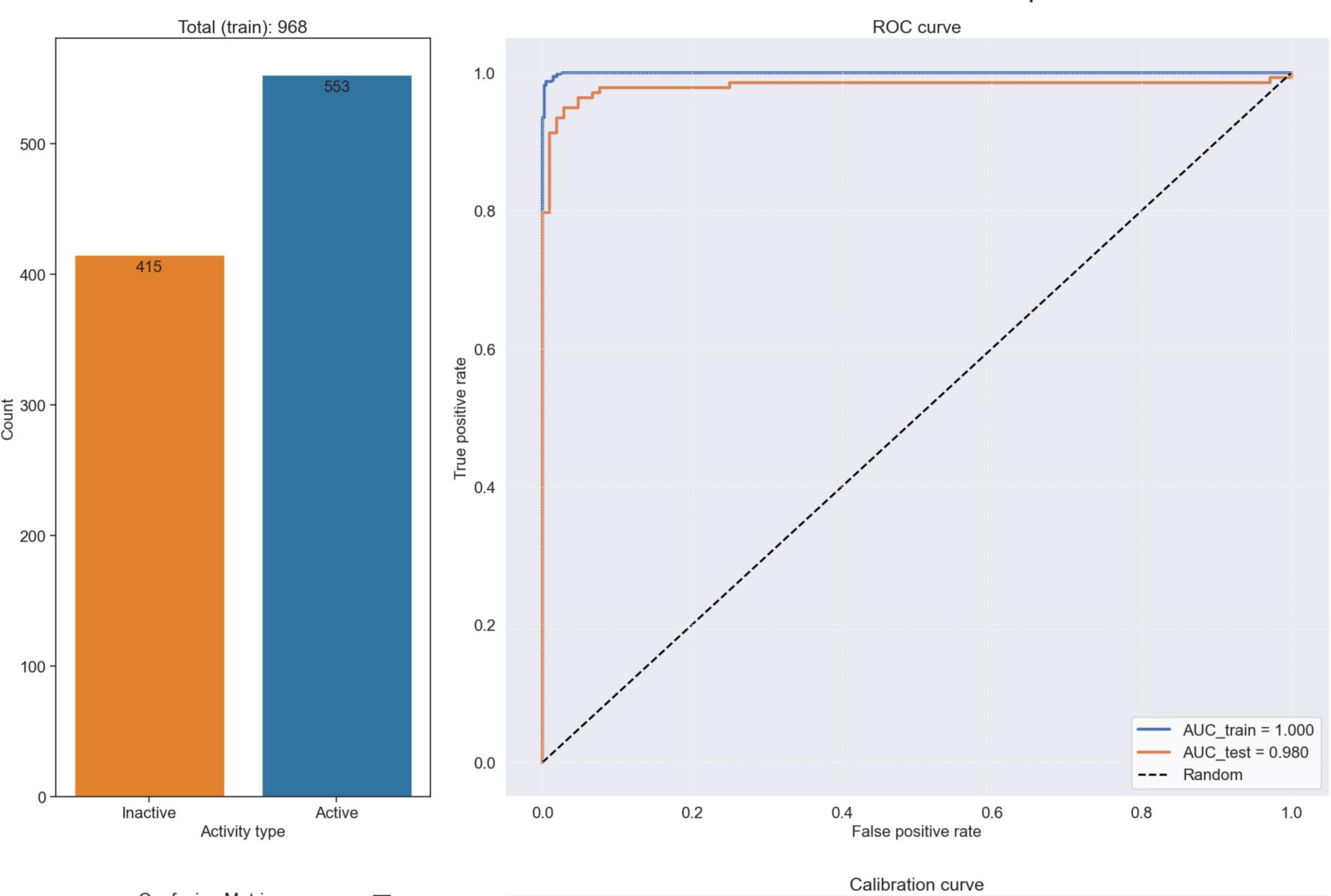
XGBoost Parameters	Value
alpha	0.4205
colsample_bytree	0.5399
gamma	0.9913
lambda	4.6324
learning_rate	0.0668
max_depth	5.0
min_child_weight	1.0
n_estimators	597.0
reg_alpha	0.1841
reg_lambda	0.8738
scale_pos_weight	1.6952
subsample	0.5308

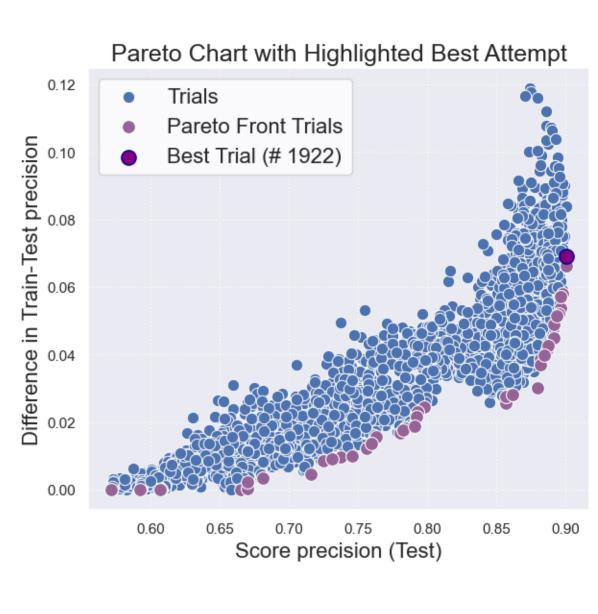


	Ac	tive/Inactive probability		
40	Inactive zone		Active zone	type active (138) inactive (104) decoy (242)
00				
Percent 05				
10				
0				
	0.0 0.2 0	.4 0.6 Probability	0.8	1.0

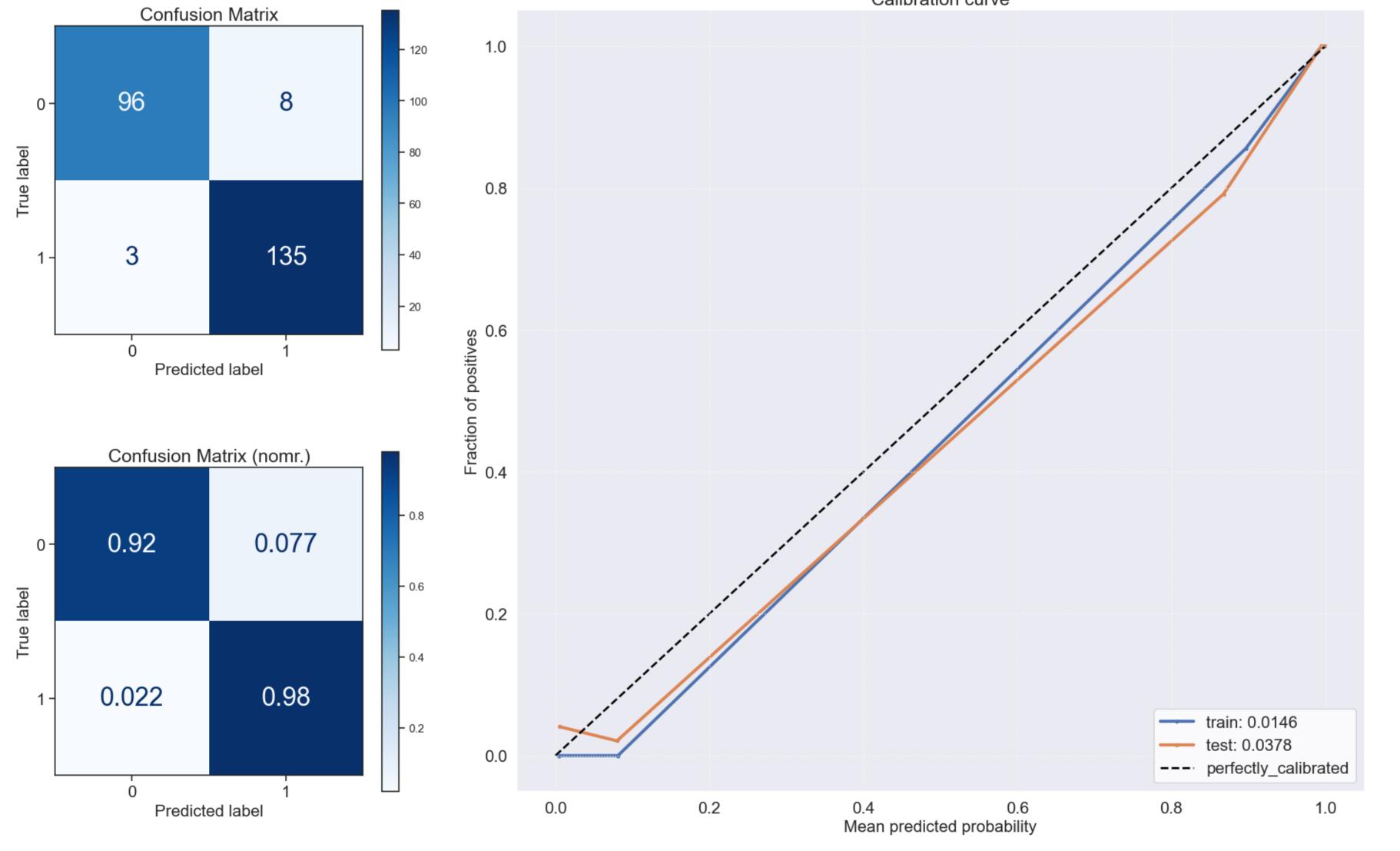
Metric	Train	Test
AUC	0.999	0.9841
accuracy	0.9783	0.9628
balanced accuracy	0.975	0.9603
recall_(sens)	0.9982	0.9783
specificity	0.9518	0.9423
precision	0.965	0.9574
f1_score	0.9782	0.9627

Protein: Q03181 - metric: precision



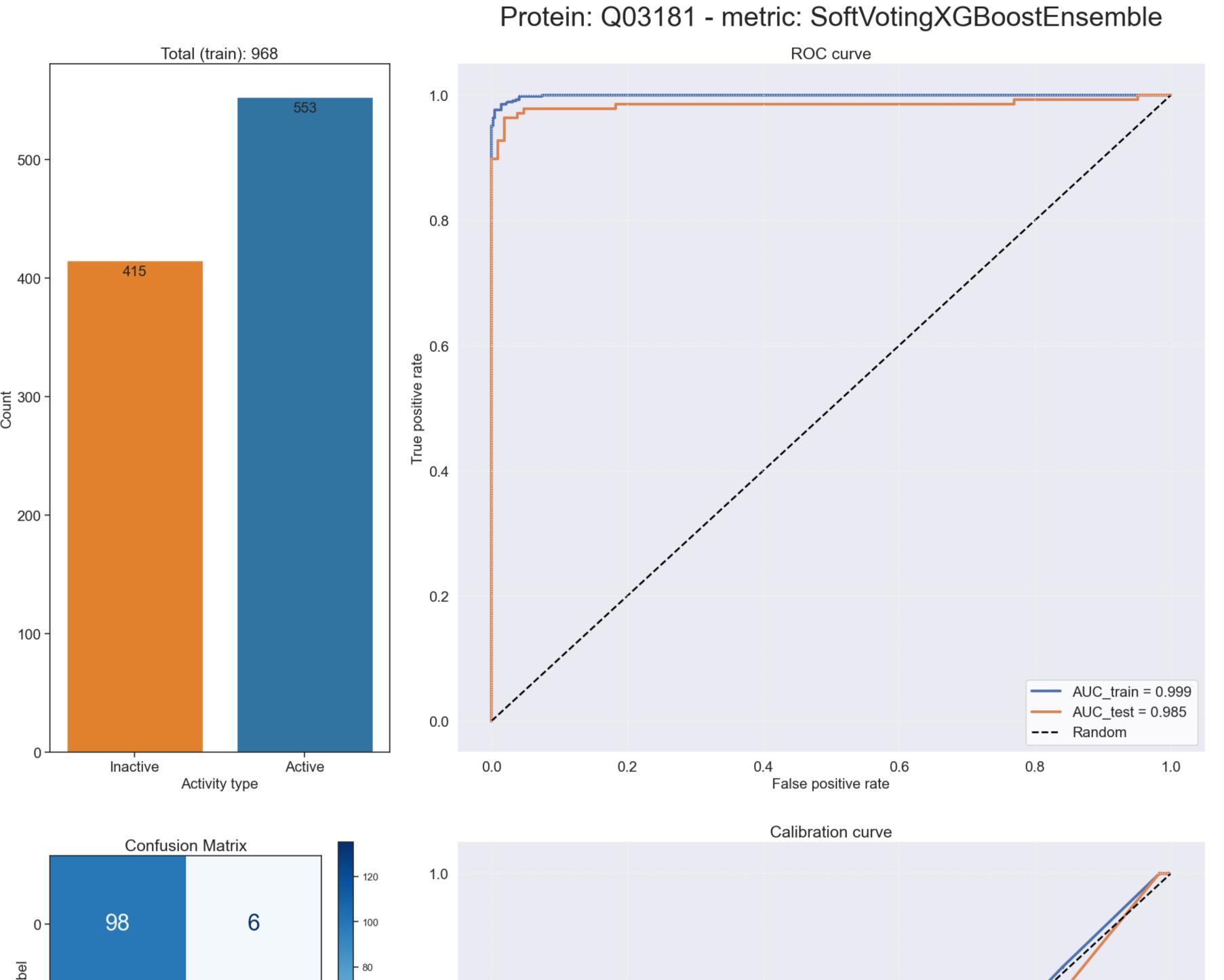


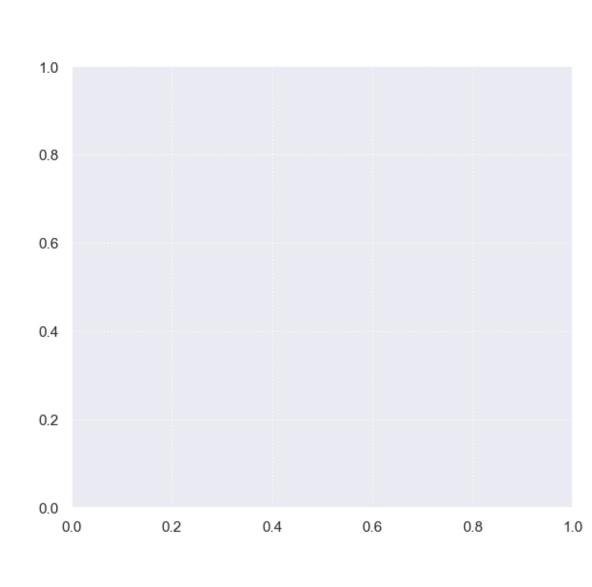
XGBoost Parameters	Value
alpha	3.8158
colsample_bytree	0.6065
gamma	0.0643
lambda	0.9116
learning_rate	0.118
max_depth	9.0
min_child_weight	3.0
n_estimators	466.0
reg_alpha	0.5088
reg_lambda	0.8562
scale_pos_weight	3.5243
subsample	0.5512

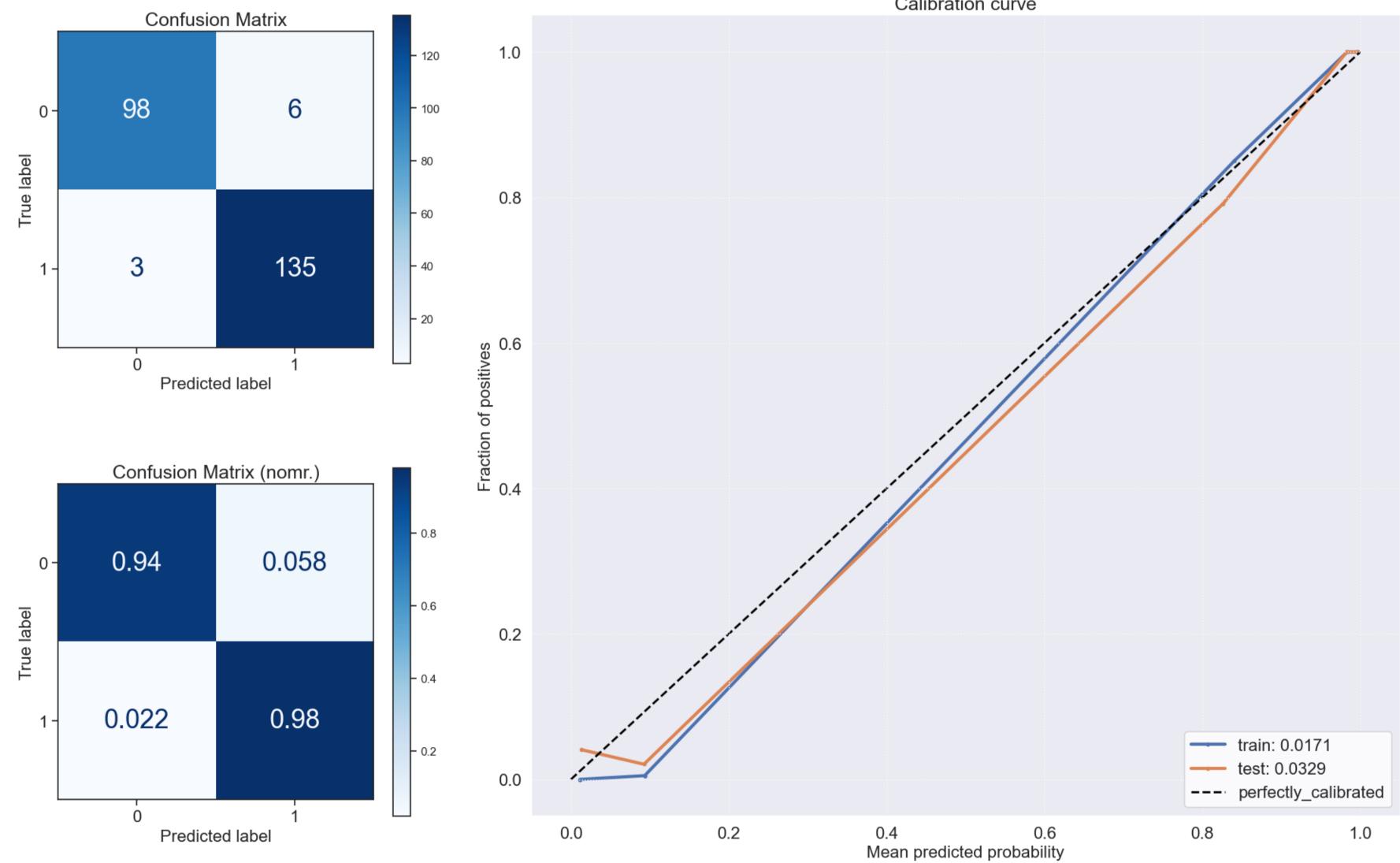


70 -			ve probability		
70	Inactive zone			Active zone	type active (138) inactive (104) decoy (242)
50					
ti 40 -					
Percent					
20					
10					_ [
0.0	0.2	0.4 Prob	0.6 ability	0.8	1.0

Metric	Train	Test
AUC	0.9996	0.9802
accuracy	0.9793	0.9545
balanced accuracy	0.9759	0.9507
recall_(sens)	1.0	0.9783
specificity	0.9518	0.9231
precision	0.9651	0.9441
f1_score	0.9793	0.9544







			Active/Inacti	ve probability		
40		Inactive zone			Active zone	type active (138) inactive (104)
30						decoy (242)
Percent 00 00 00 00 00 00 00 00 00 00 00 00 00						
E 20						
10						
0—	0.0	0.2	0.4 Prob	0.6 ability	0.8	1.0

Metric	Train	Test
AUC	0.9992	0.9846
accuracy	0.9793	0.9628
balanced accuracy	0.9762	0.9603
recall_(sens)	0.9982	0.9783
specificity	0.9542	0.9423
precision	0.9667	0.9574
f1_score	0.9793	0.9627