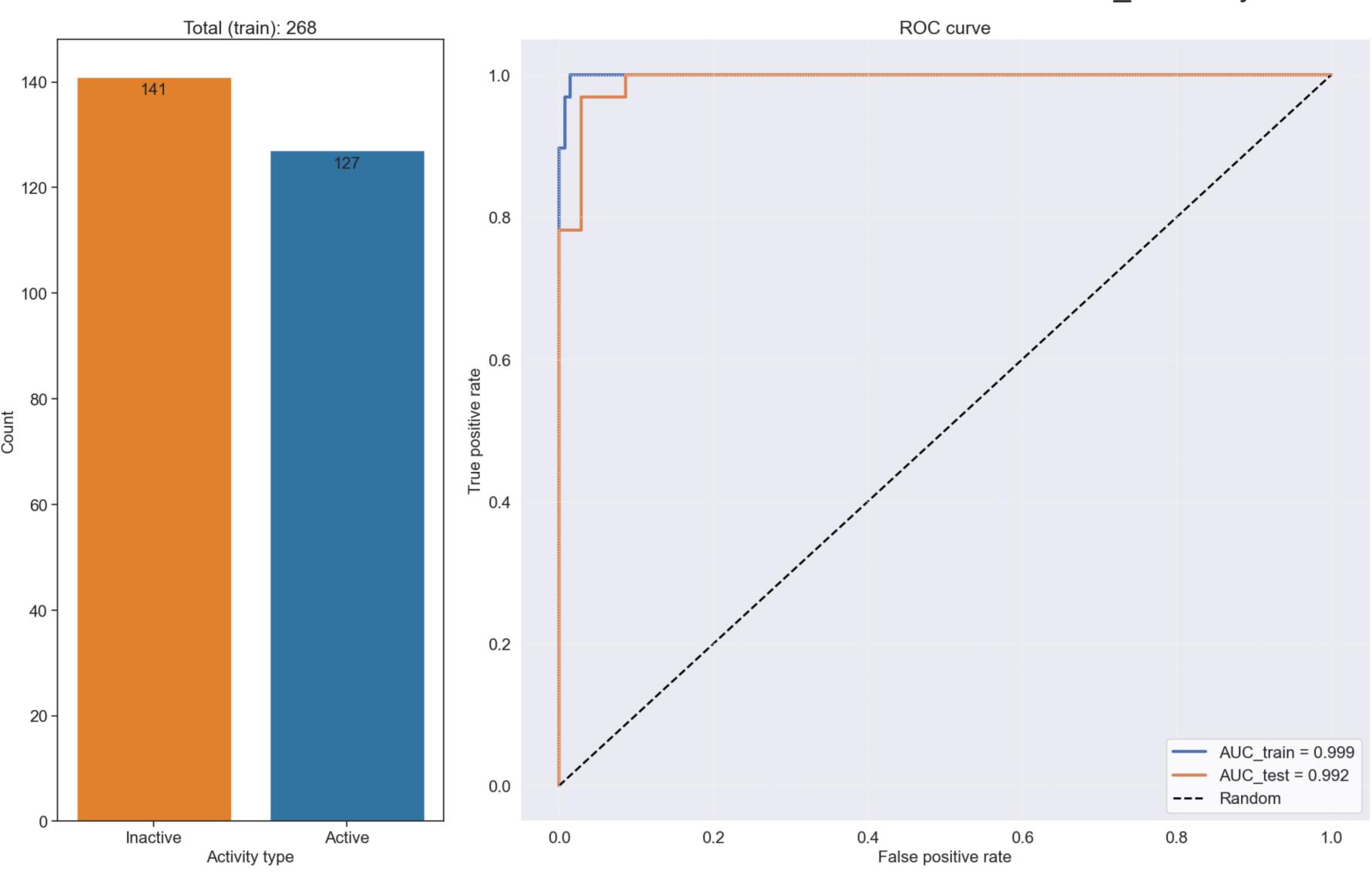
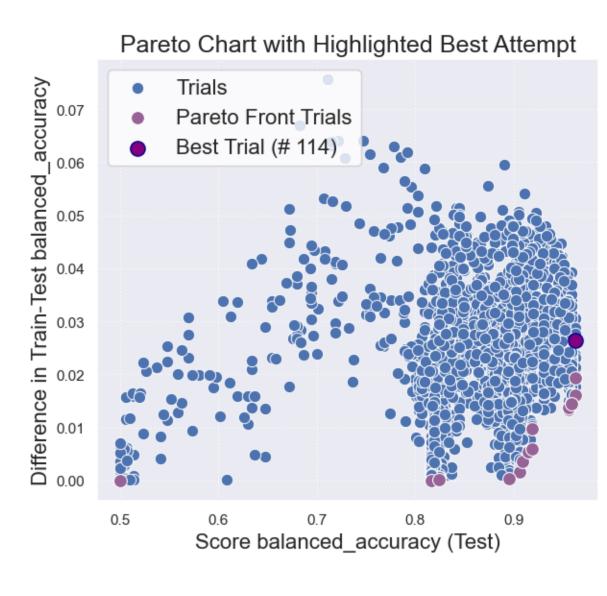
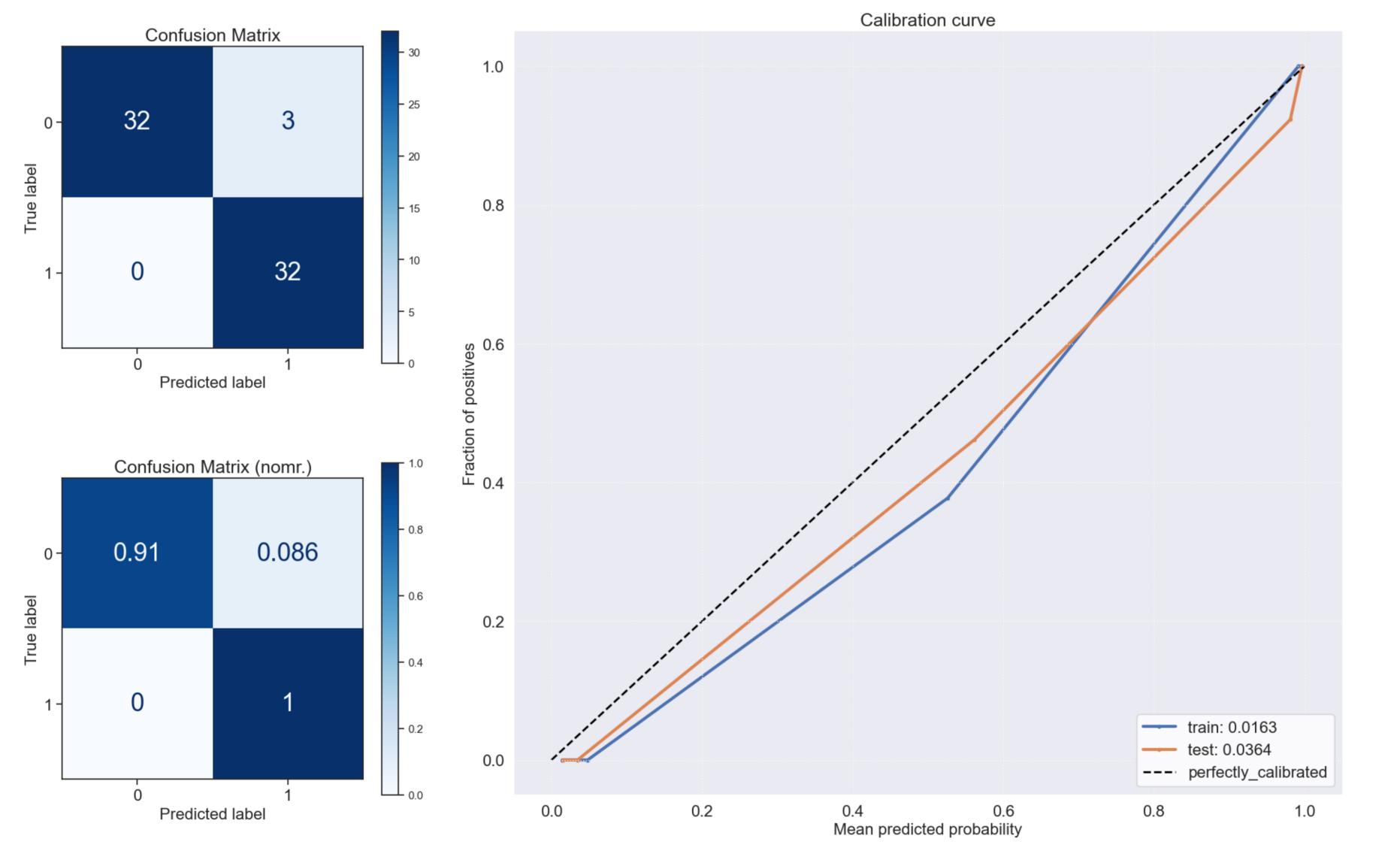
Protein: Q13093 - metric: balanced_accuracy





XGBoost Parameters	Value
alpha	4.844
colsample_bytree	0.6838
gamma	0.3624
lambda	1.3544
learning_rate	0.0081
max_depth	5.0
min_child_weight	2.0
n_estimators	721.0
reg_alpha	0.2351
reg_lambda	0.3182
scale_pos_weight	12.0612
subsample	0.7184

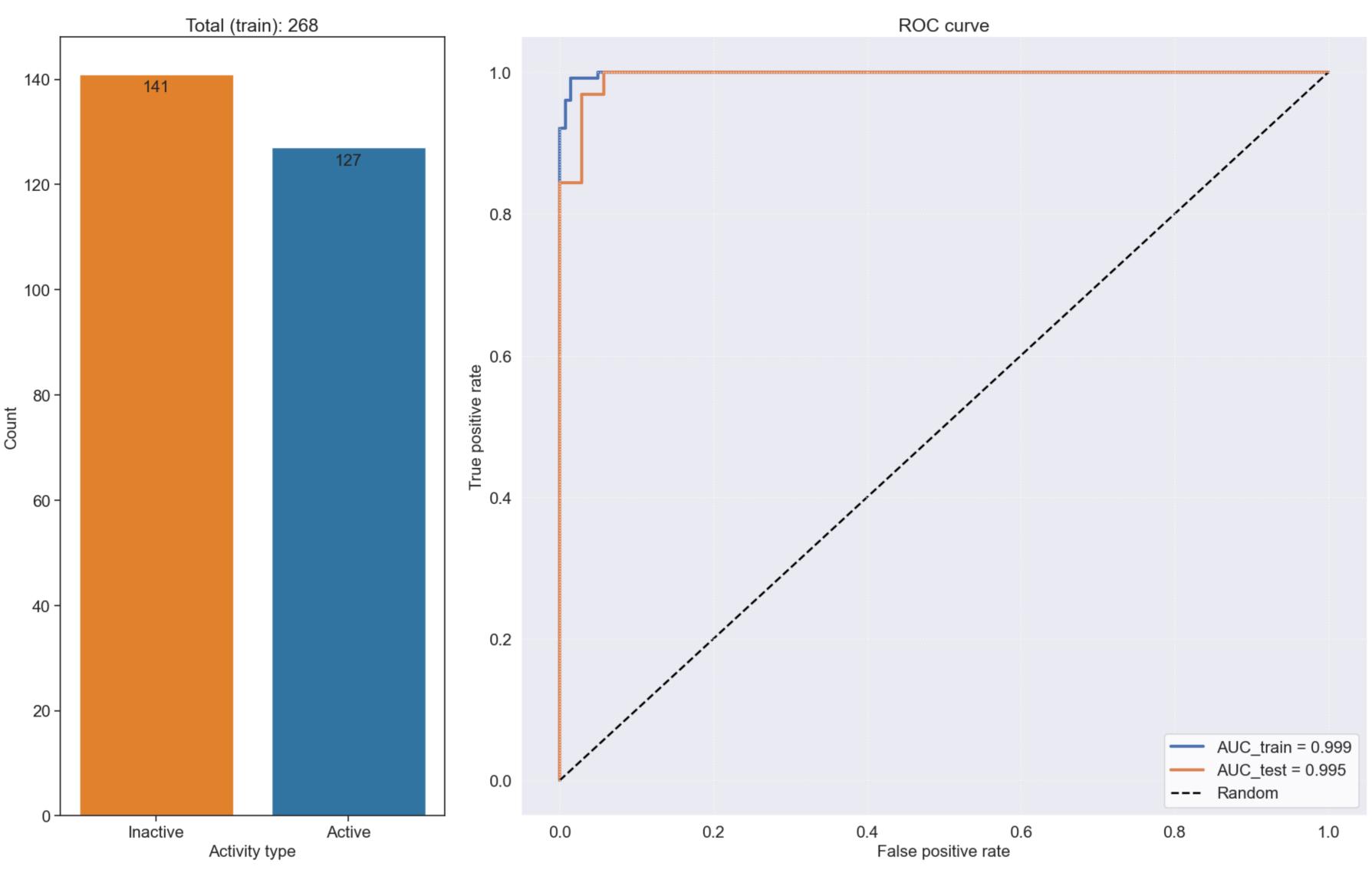


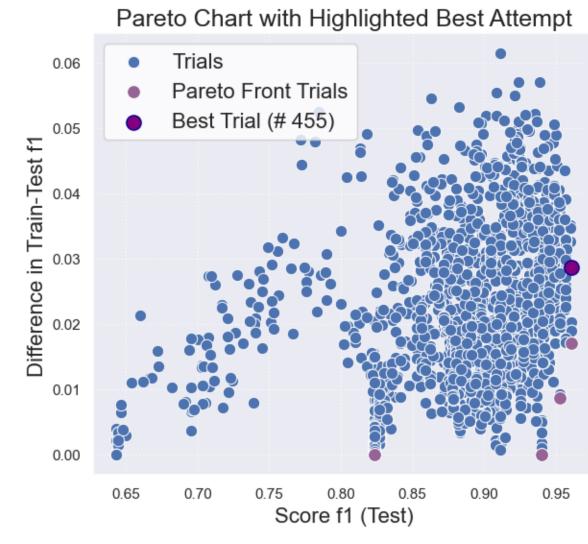
50					Active		type active (32) nactive (35) decoy (67)
30							
Percent 0.00							
90							
20							
10						П	
0					B B		
	0.0	0.2	0.4 Proba	0.9 ability	6 0).8	1.0

Active/Inactive probability

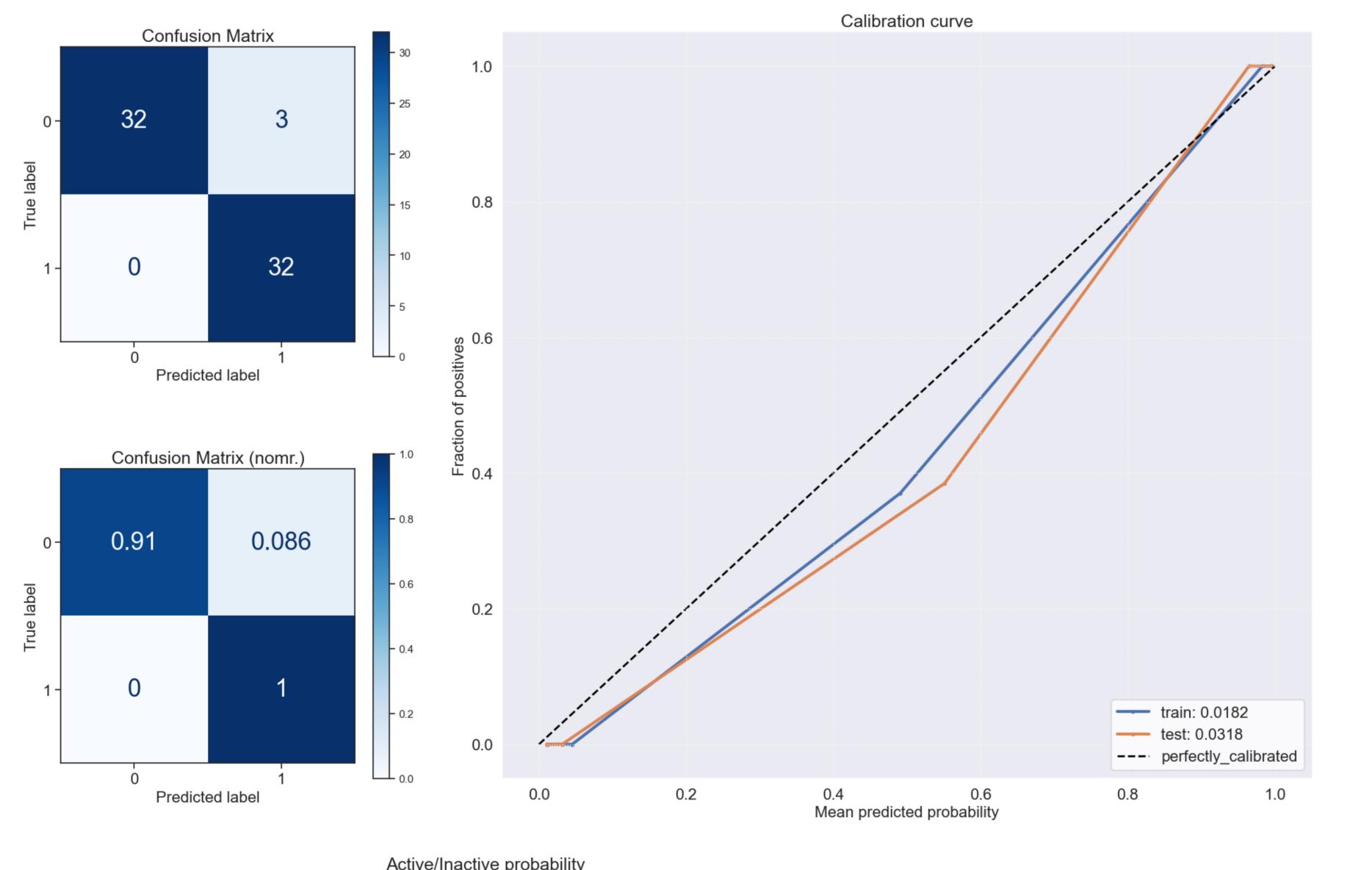
Metric	Train	Test
AUC	0.9991	0.992
accuracy	0.9813	0.9552
balanced accuracy	0.9823	0.9571
recall_(sens)	1.0	1.0
specificity	0.9645	0.9143
precision	0.9621	0.9143
f1_score	0.9814	0.9552

Protein: Q13093 - metric: f1





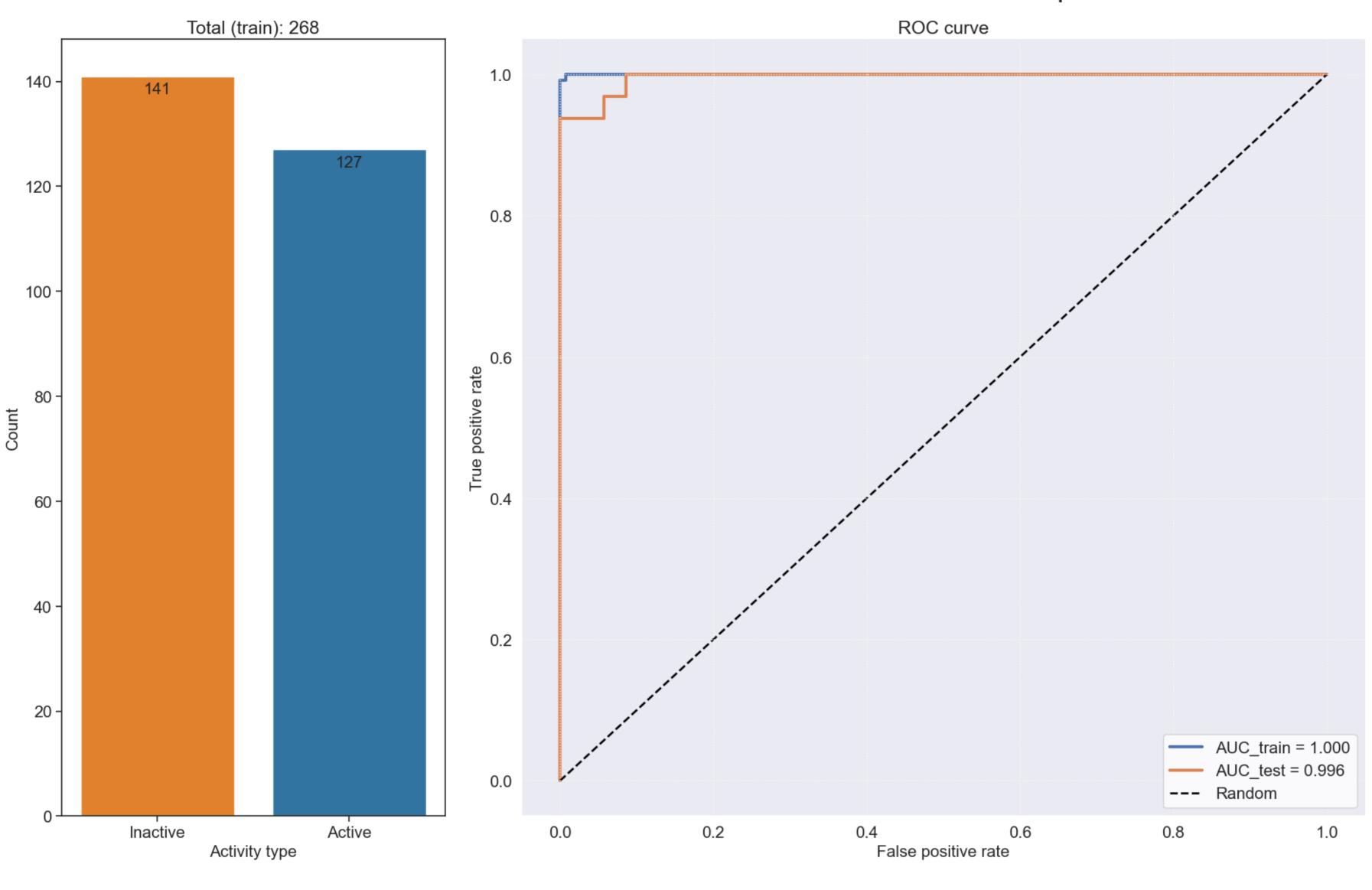
XGBoost Parameters	Value
alpha	2.3101
colsample_bytree	0.7809
gamma	0.5377
lambda	0.0244
learning_rate	0.0095
max_depth	10.0
min_child_weight	2.0
n_estimators	1000.0
reg_alpha	0.0003
reg_lambda	0.2481
scale_pos_weight	3.3494
subsample	0.8336

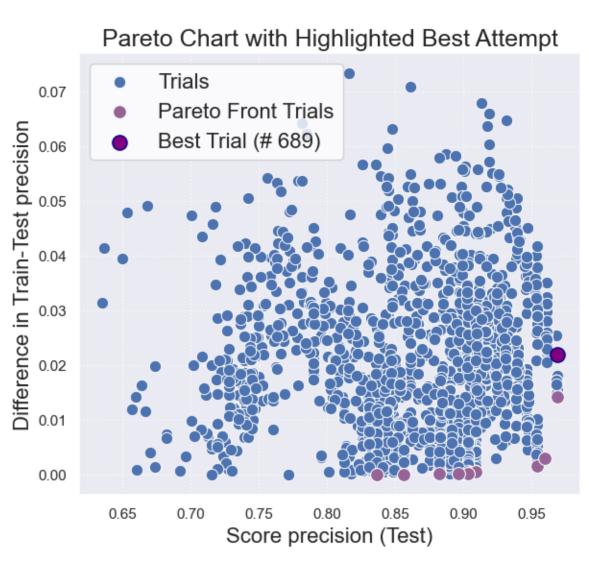


	Active/mactive probability					
50		Inactive zone			Active zone	inactive (35) decoy (67)
50						
40						
Percent 00	Π					
00						
10	7					
0 —						
	0.0	0.2	0.4	0.6	0.8	1.0
	Probability					

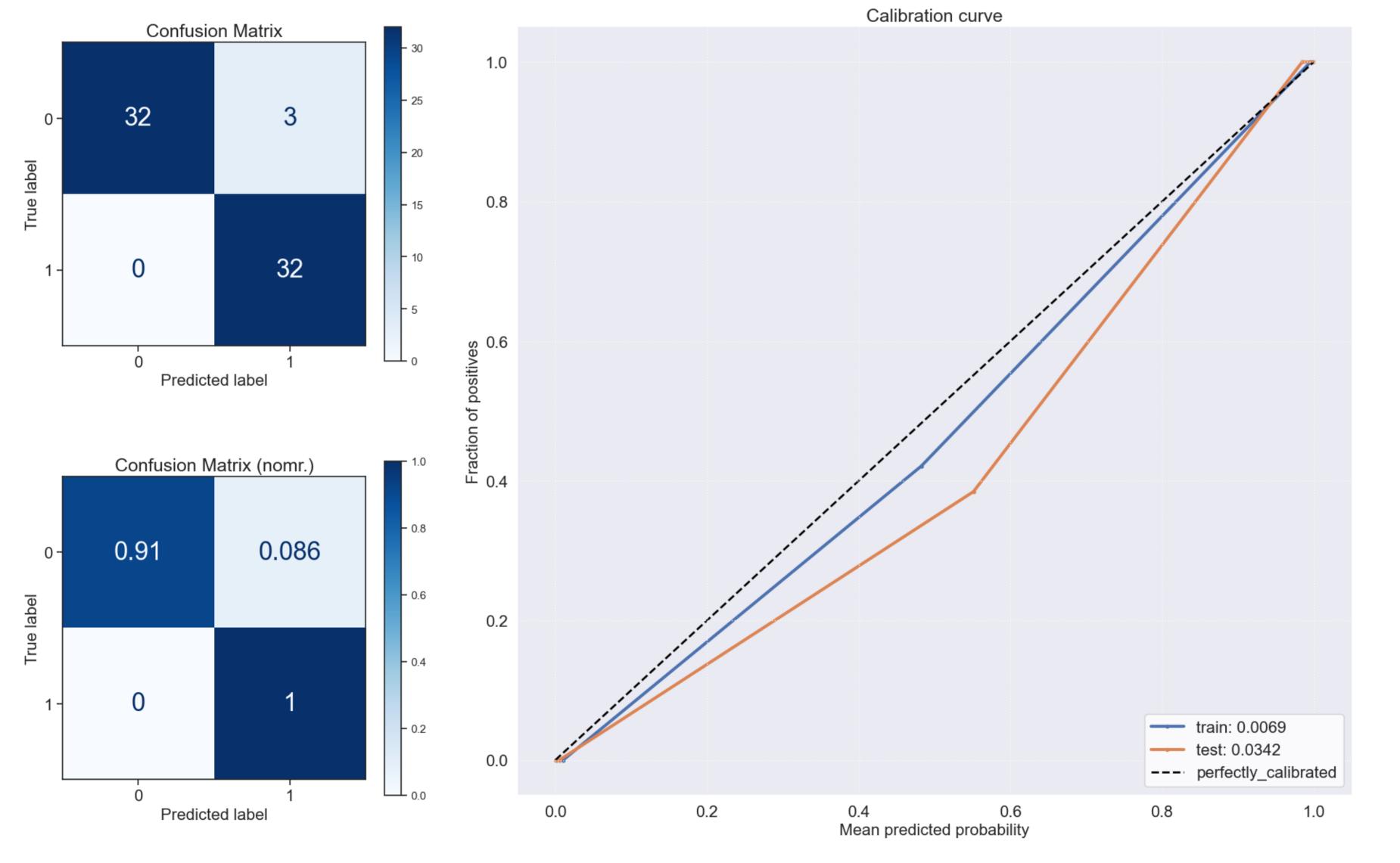
Metric	Train	Test
AUC	0.9989	0.9946
accuracy	0.9739	0.9552
balanced accuracy	0.9748	0.9571
recall_(sens)	0.9921	1.0
specificity	0.9574	0.9143
precision	0.9545	0.9143
f1_score	0.9739	0.9552

Protein: Q13093 - metric: precision





XGBoost Parameters	Value
alpha	0.6877
colsample_bytree	0.6373
gamma	0.5313
lambda	3.7865
learning_rate	0.1316
max_depth	3.0
min_child_weight	1.0
n_estimators	966.0
reg_alpha	0.0252
reg_lambda	0.1372
scale_pos_weight	3.7995
subsample	0.8651

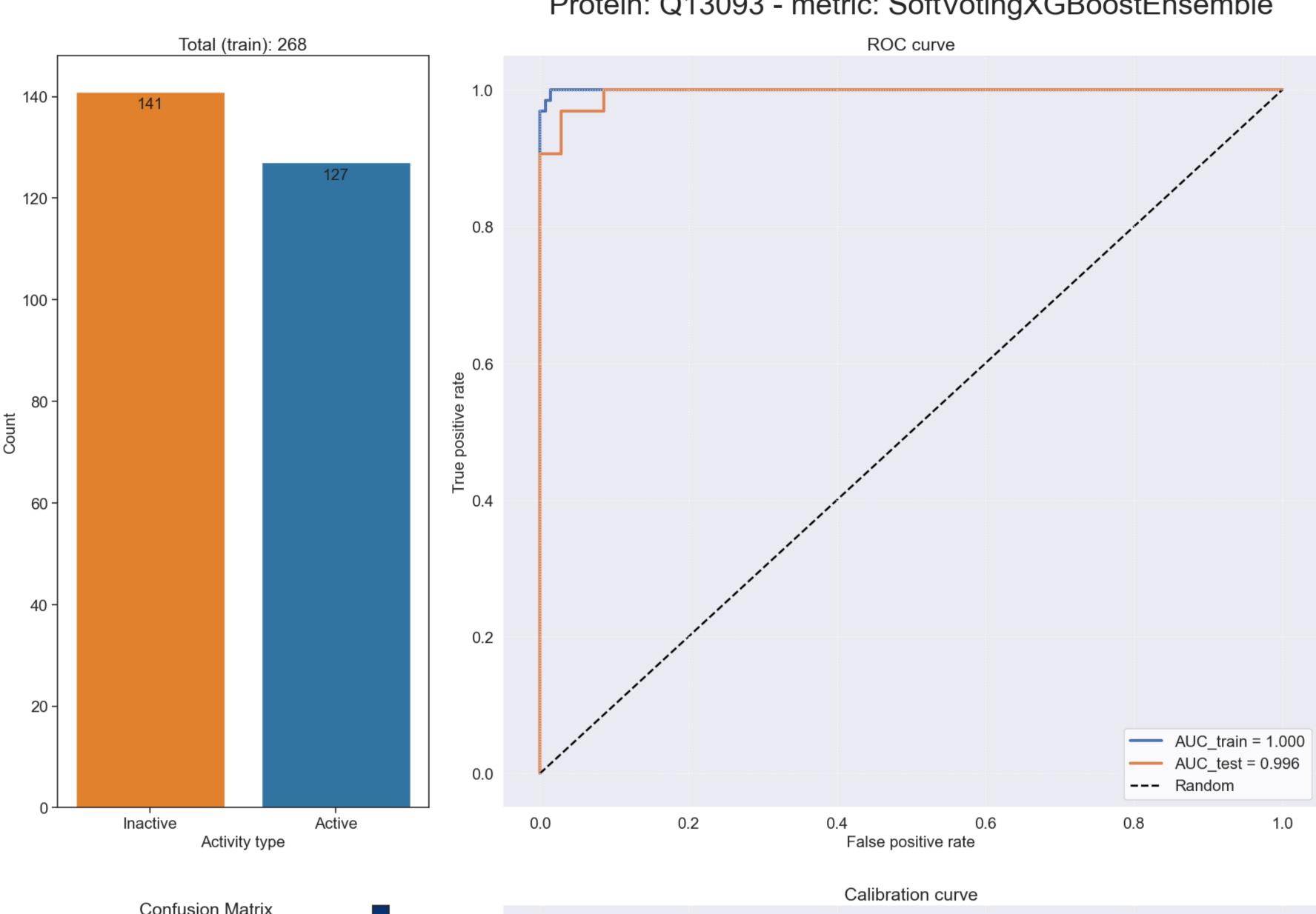


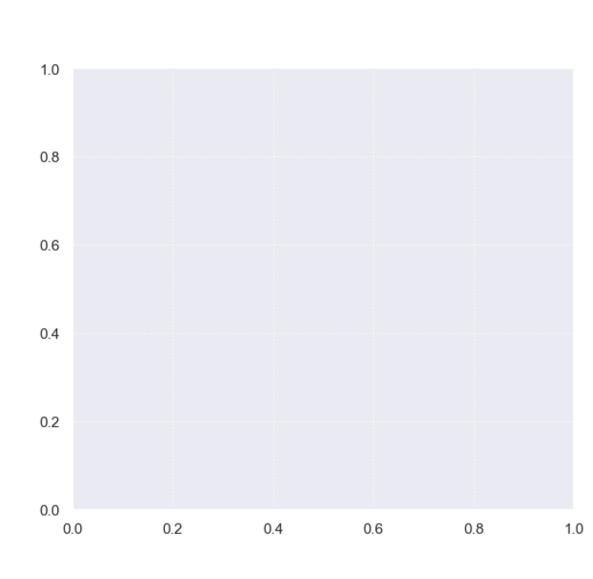
70 -		nactive zone					inactive (35) decoy (67)
00							
50							
40							
30							
20							
10						_ П_	
0 —		0.2	0.4	0.6		.8	1.0
	Probability 0.0 0.0 1.0						

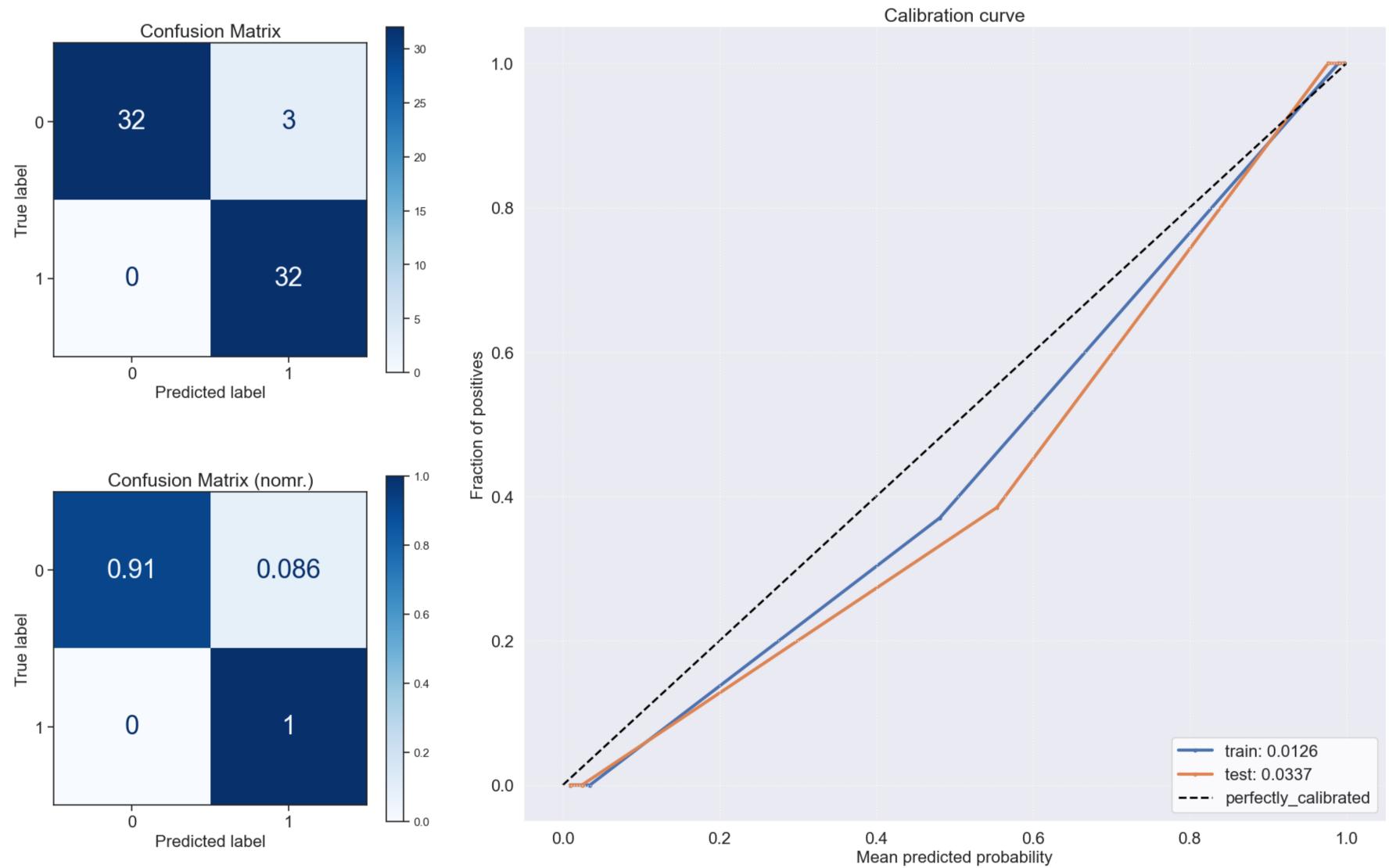
Active/Inactive probability

Metric	Train	Test
AUC	0.9999	0.9955
accuracy	0.9925	0.9552
balanced accuracy	0.9929	0.9571
recall_(sens)	1.0	1.0
specificity	0.9858	0.9143
precision	0.9845	0.9143
f1_score	0.9925	0.9552

Protein: Q13093 - metric: SoftVotingXGBoostEnsemble







	Active/Inactive probability					
50		ctive zone			tive zone	decoy (67)
- 08 Accent						
10 		2		0.6	0.8	1.0
0	0.0 0.2 0.4 0.6 0.8 1.0 Probability					

Metric	Train	Test
AUC	0.9997	0.9955
accuracy	0.9925	0.9552
balanced accuracy	0.9929	0.9571
recall_(sens)	1.0	1.0
specificity	0.9858	0.9143
precision	0.9845	0.9143
f1_score	0.9925	0.9552