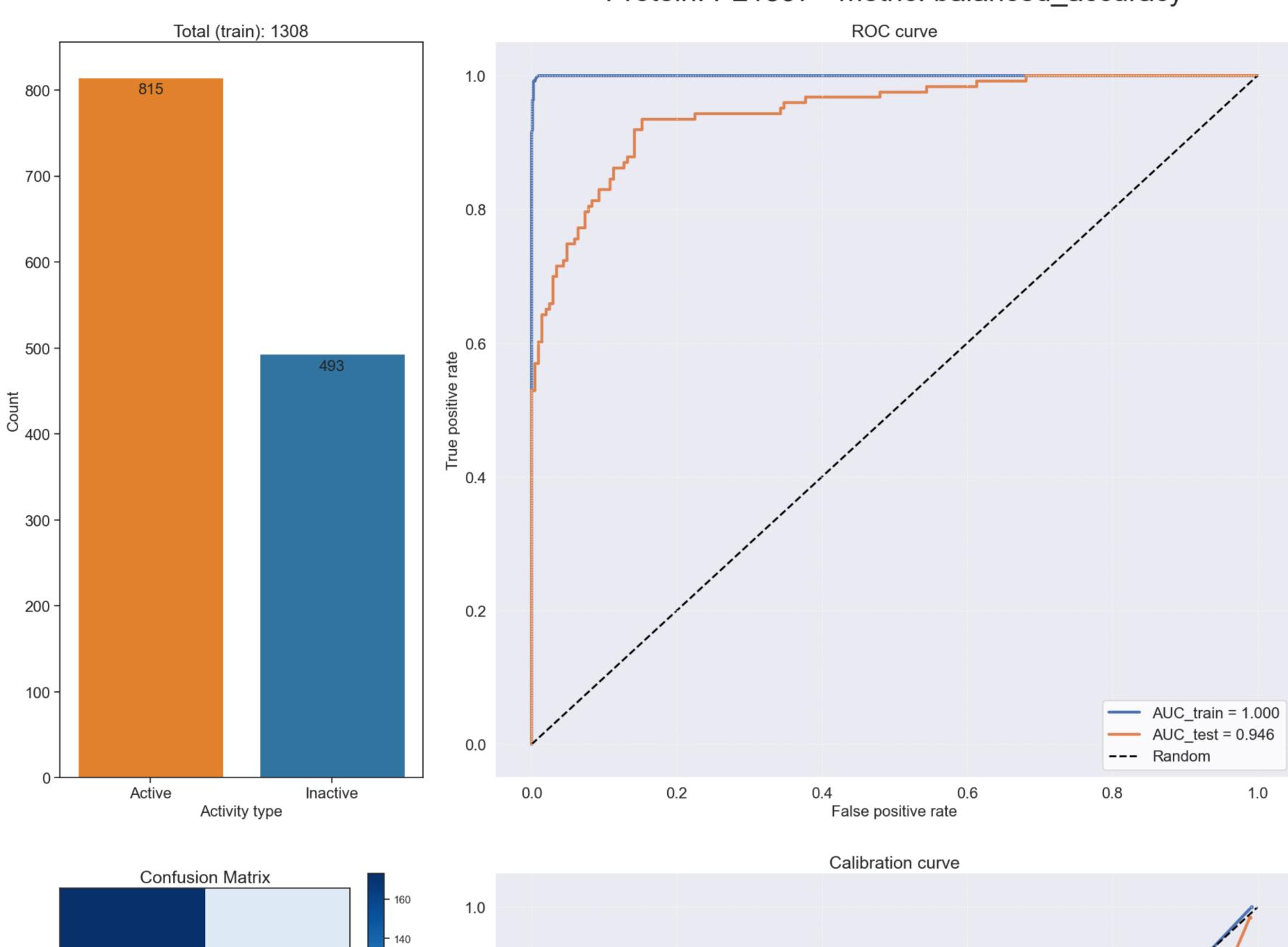
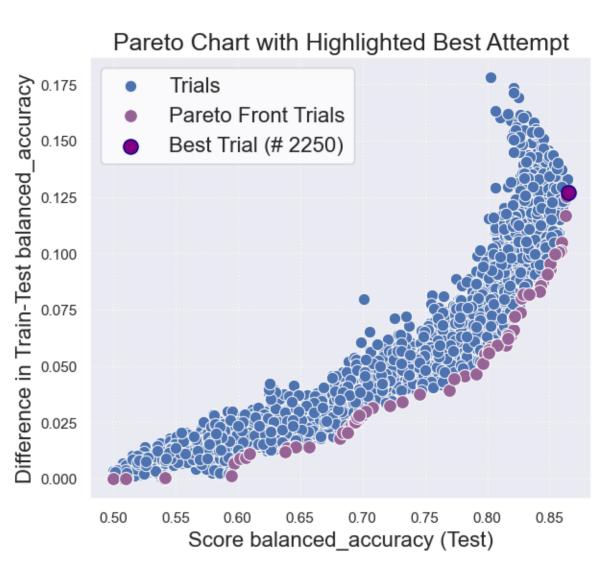
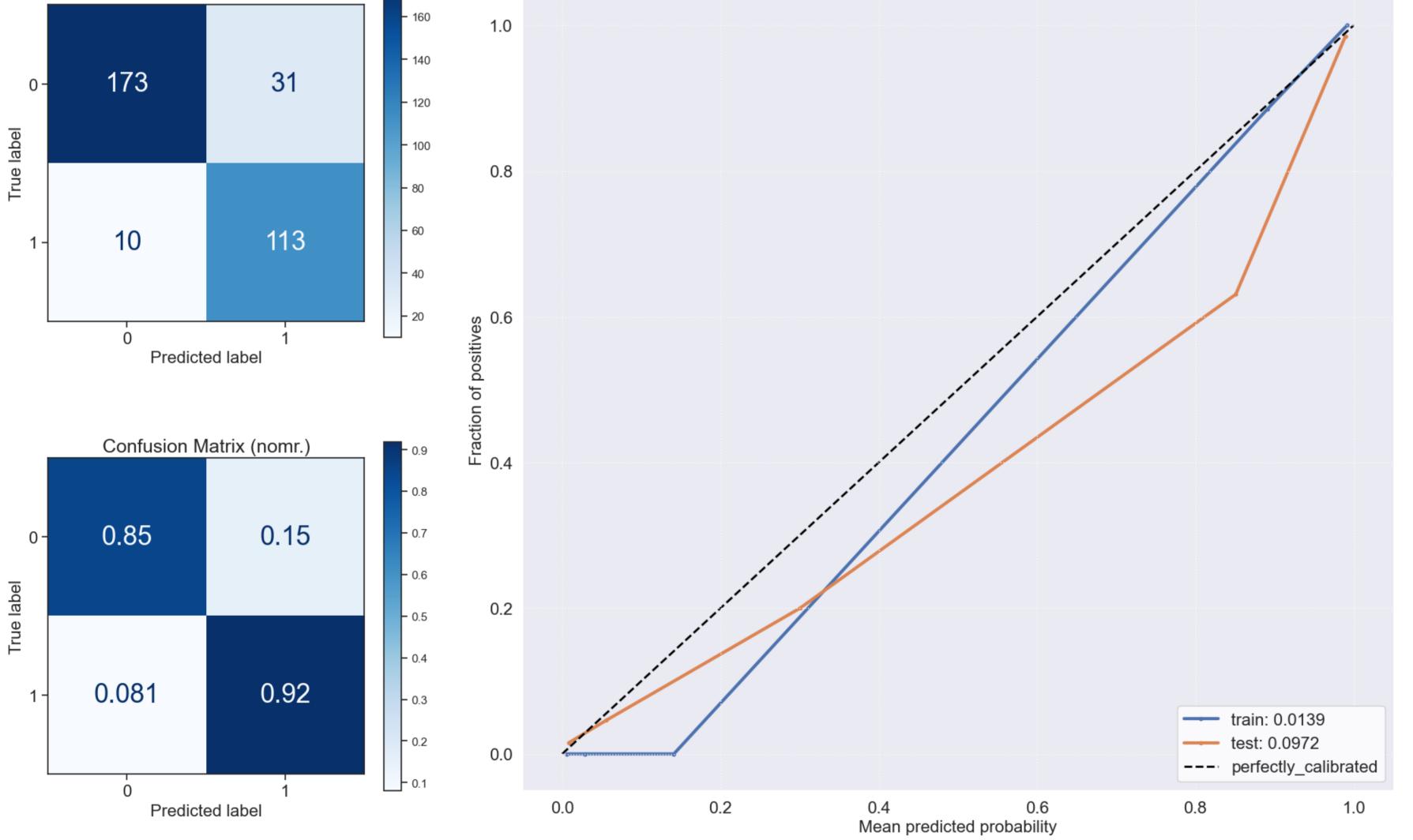
Protein: P21397 - metric: balanced_accuracy





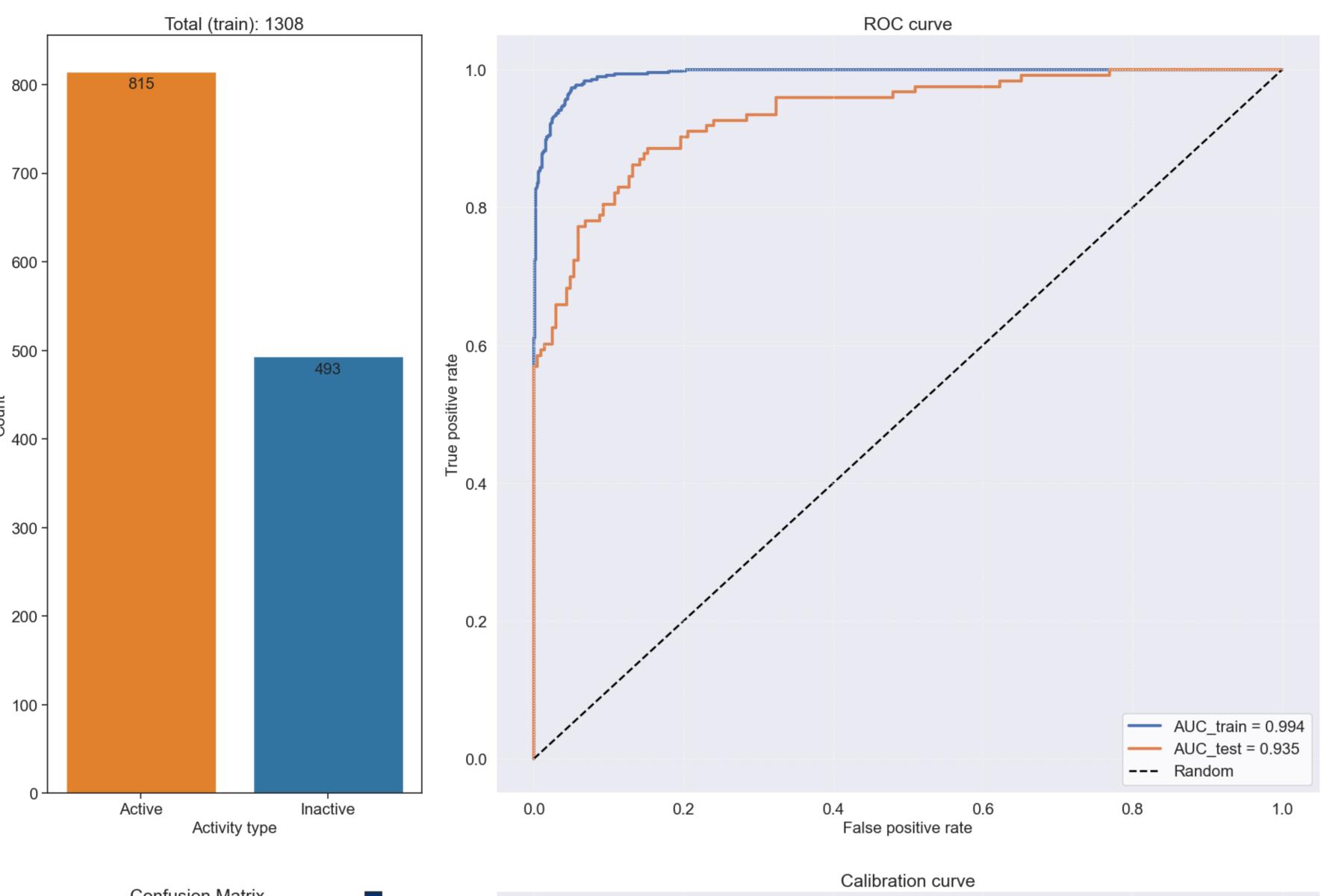
XGBoost Parameters	Value
alpha	1.474
colsample_bytree	0.7269
gamma	0.1044
lambda	1.0856
learning_rate	0.0829
max_depth	7.0
min_child_weight	1.0
n_estimators	399.0
reg_alpha	0.4235
reg_lambda	0.9679
scale_pos_weight	3.7487
subsample	0.885

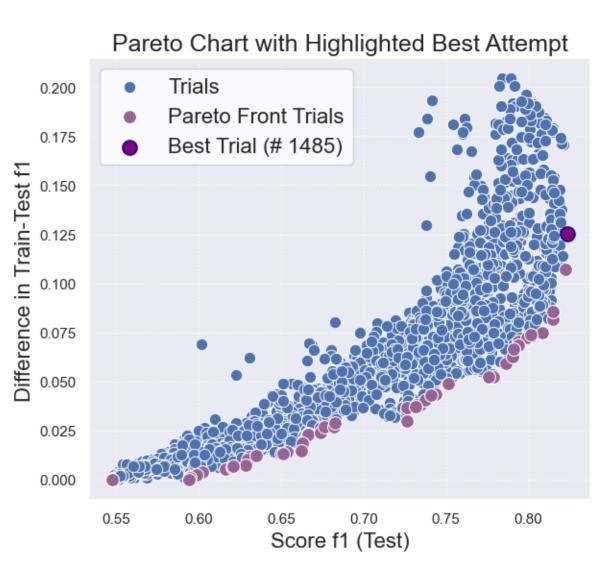


35	Active/Inactive probability					
22	Ina	ctive zone		Active	inact	e (123) tive (204) by (326)
25	П					
Percent 15						
10						
5						
,	0.0	2 0.4	(Probability	0.6).8	1.0

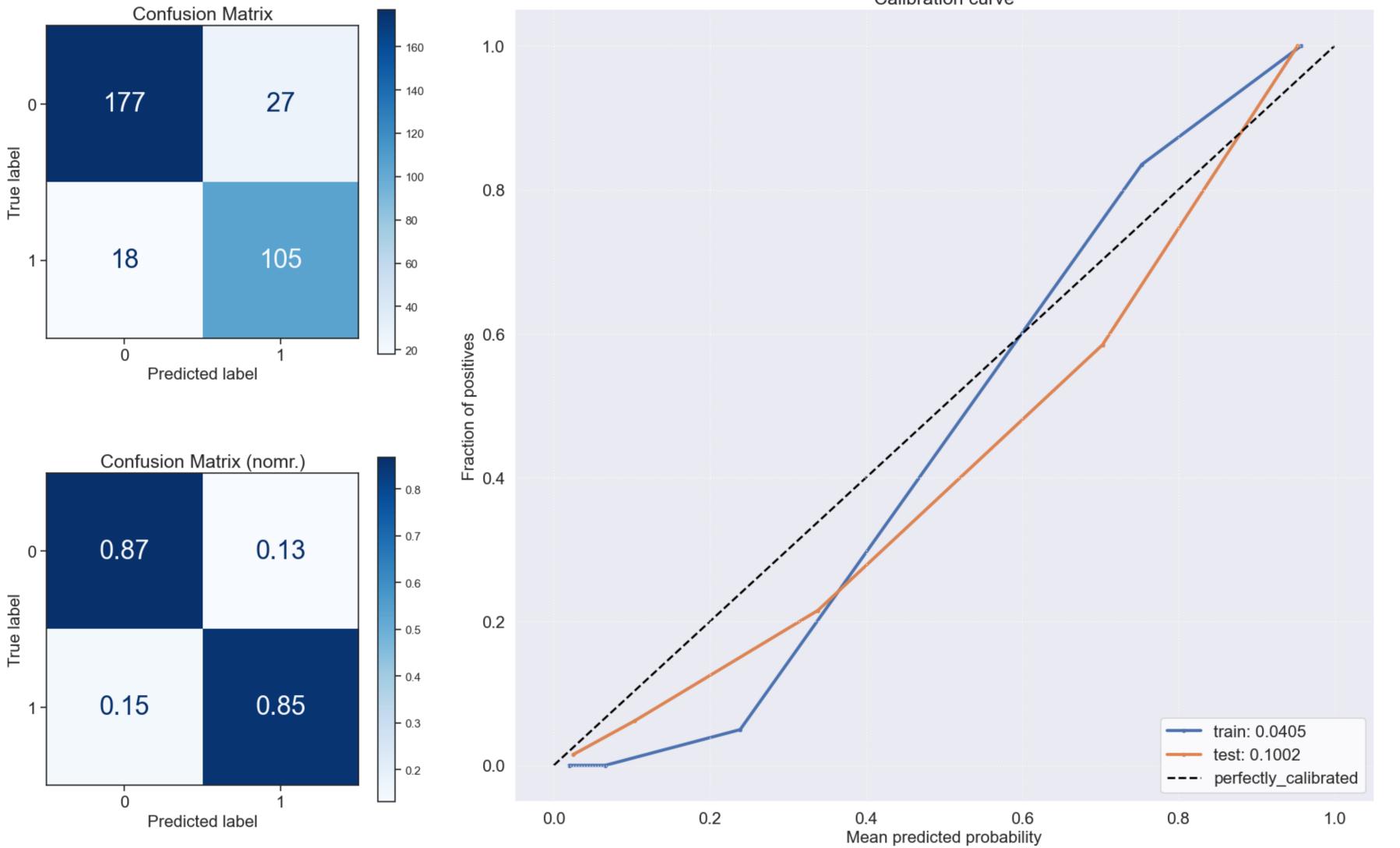
Metric	Train	Test
AUC	0.9998	0.9458
accuracy	0.9885	0.8746
balanced accuracy	0.9908	0.8834
recall_(sens)	1.0	0.9187
specificity	0.9816	0.848
precision	0.9705	0.7847
f1_score	0.9886	0.8761

Protein: P21397 - metric: f1





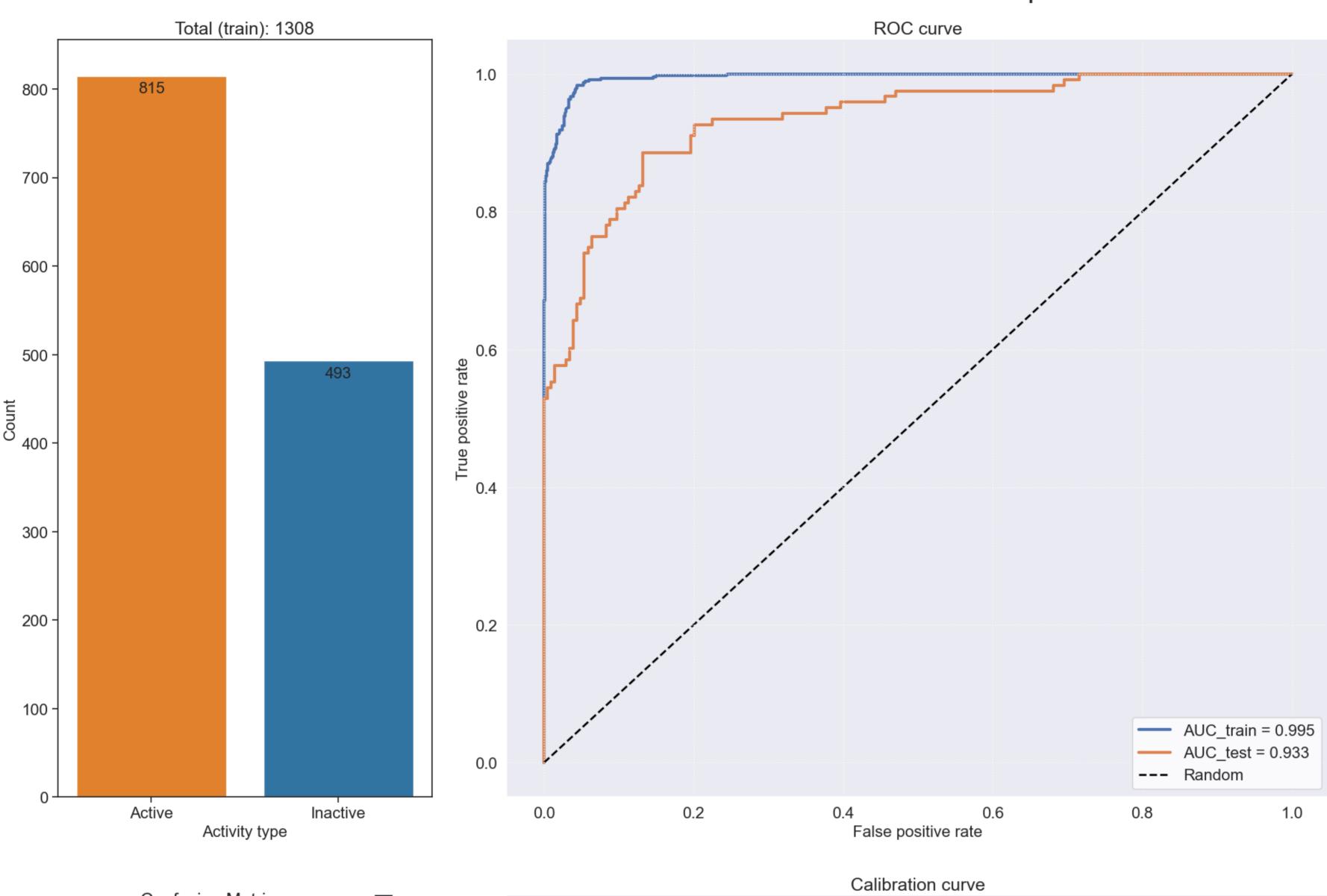
XGBoost Parameters	Value
alpha	1.1019
colsample_bytree	0.7126
gamma	0.1514
lambda	1.2376
learning_rate	0.0245
max_depth	6.0
min_child_weight	2.0
n_estimators	985.0
reg_alpha	0.9706
reg_lambda	0.8484
scale_pos_weight	1.6239
subsample	0.5174

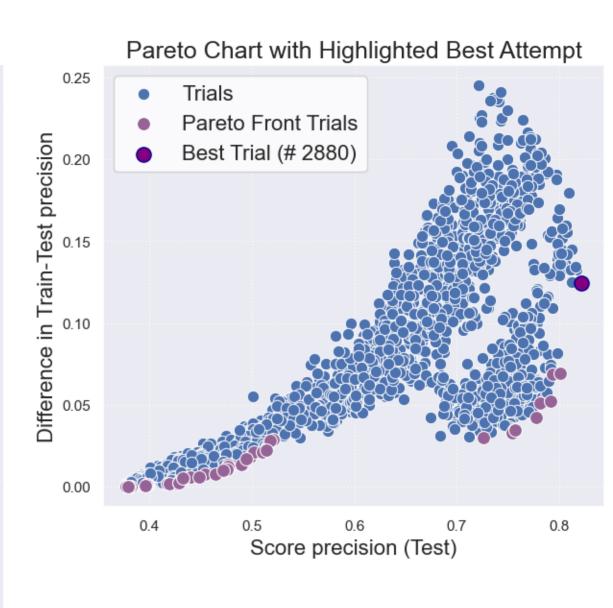


		Active/Inactive	ve probability		
8 -	Inactive zone			Active zone	type active (123) inactive (204) decoy (326)
6-					
Percent - 4					
2					
0					
0.0	0.2	0.4 Proba	0.6 ability	0.8	1.0

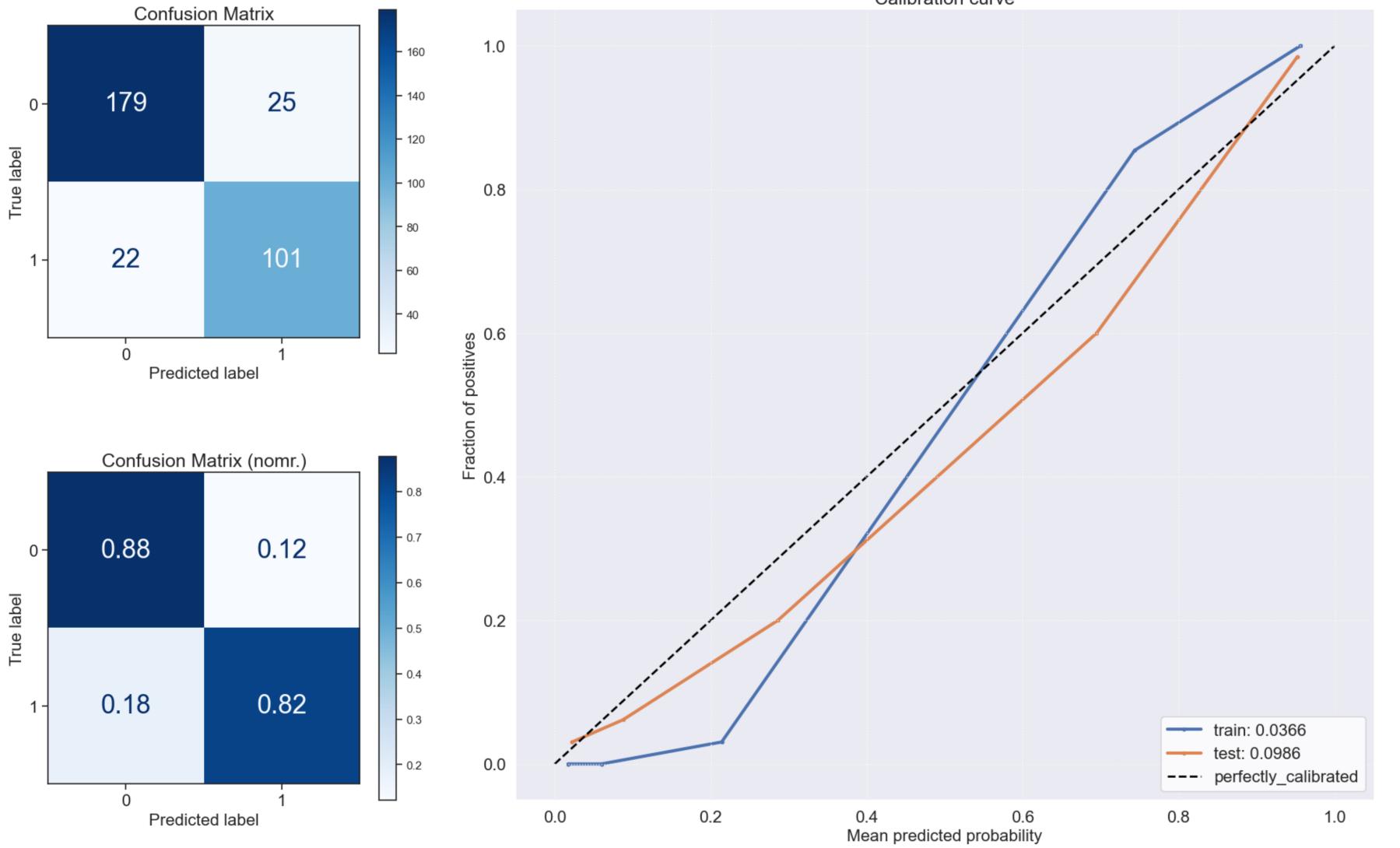
Metric	Train	Test
AUC	0.9938	0.9353
accuracy	0.9549	0.8624
balanced accuracy	0.9538	0.8607
recall_(sens)	0.9493	0.8537
specificity	0.9583	0.8676
precision	0.9323	0.7955
f1_score	0.955	0.8633

Protein: P21397 - metric: precision





XGBoost Parameters	Value
alpha	3.863
colsample_bytree	0.8004
gamma	0.5893
lambda	3.795
learning_rate	0.0936
max_depth	7.0
min_child_weight	2.0
n_estimators	208.0
reg_alpha	0.6198
reg_lambda	0.6386
scale_pos_weight	1.4275
subsample	0.8099

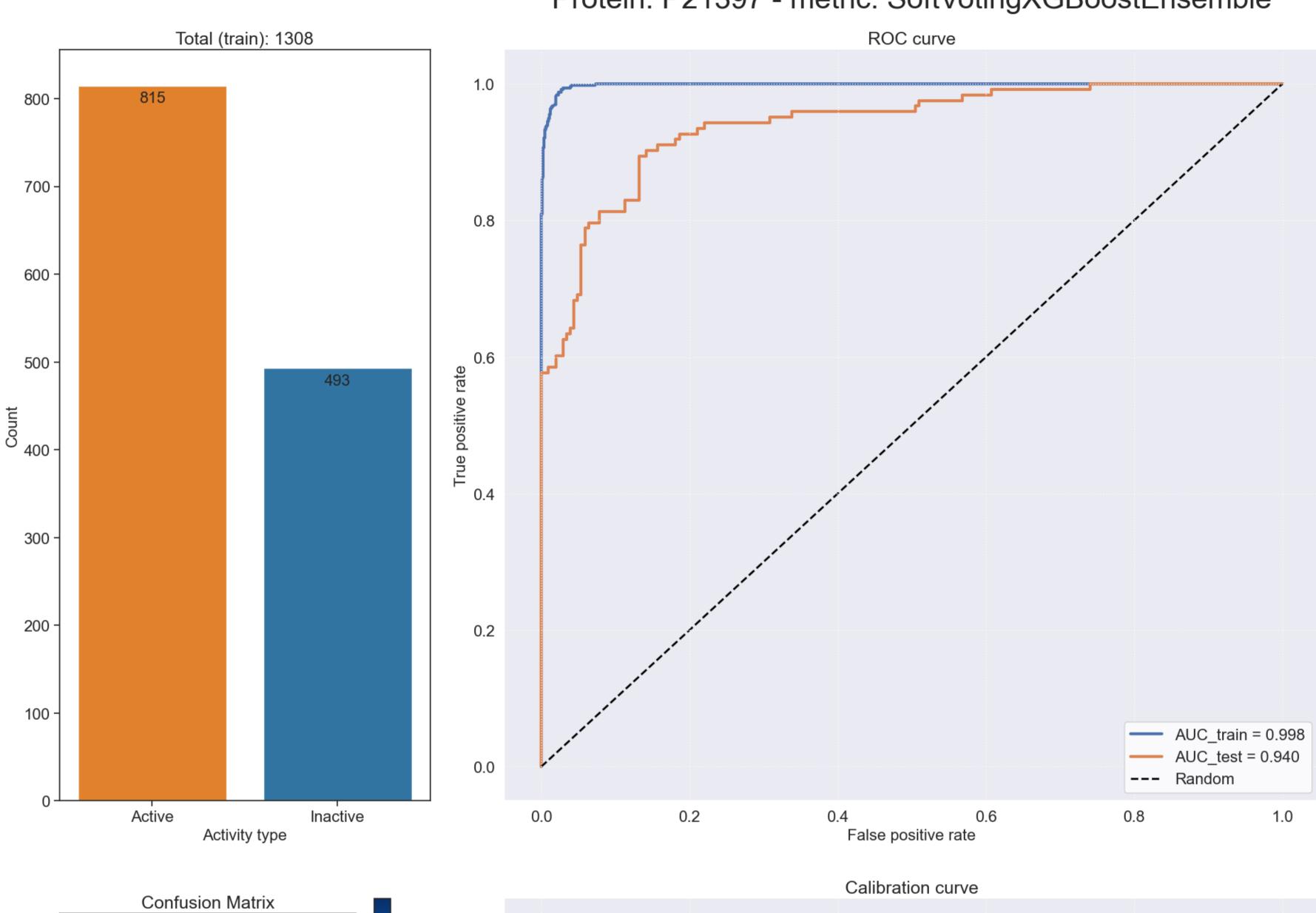


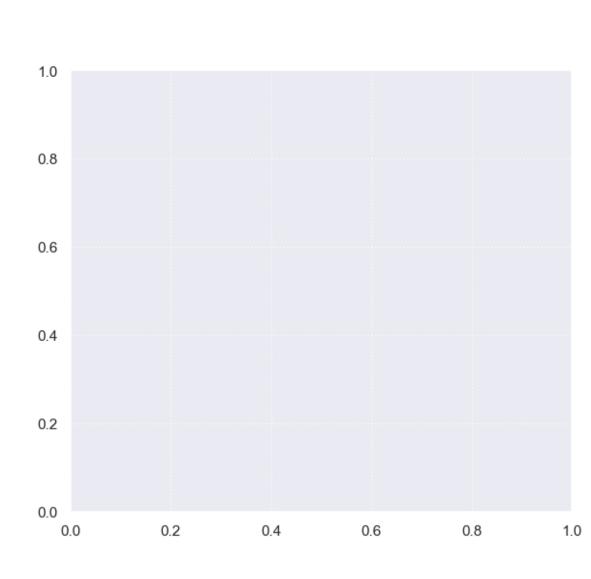
10 -		Inactive zon	е				Active zo		type active (123) inactive (204) decoy (326)
0	_								
Percent 4									
2-				_ П	П				
0 -	0.0	0.2	0.4		0.	.6	0.8		1.0
2-		0.2	0.4	Proba				h E	

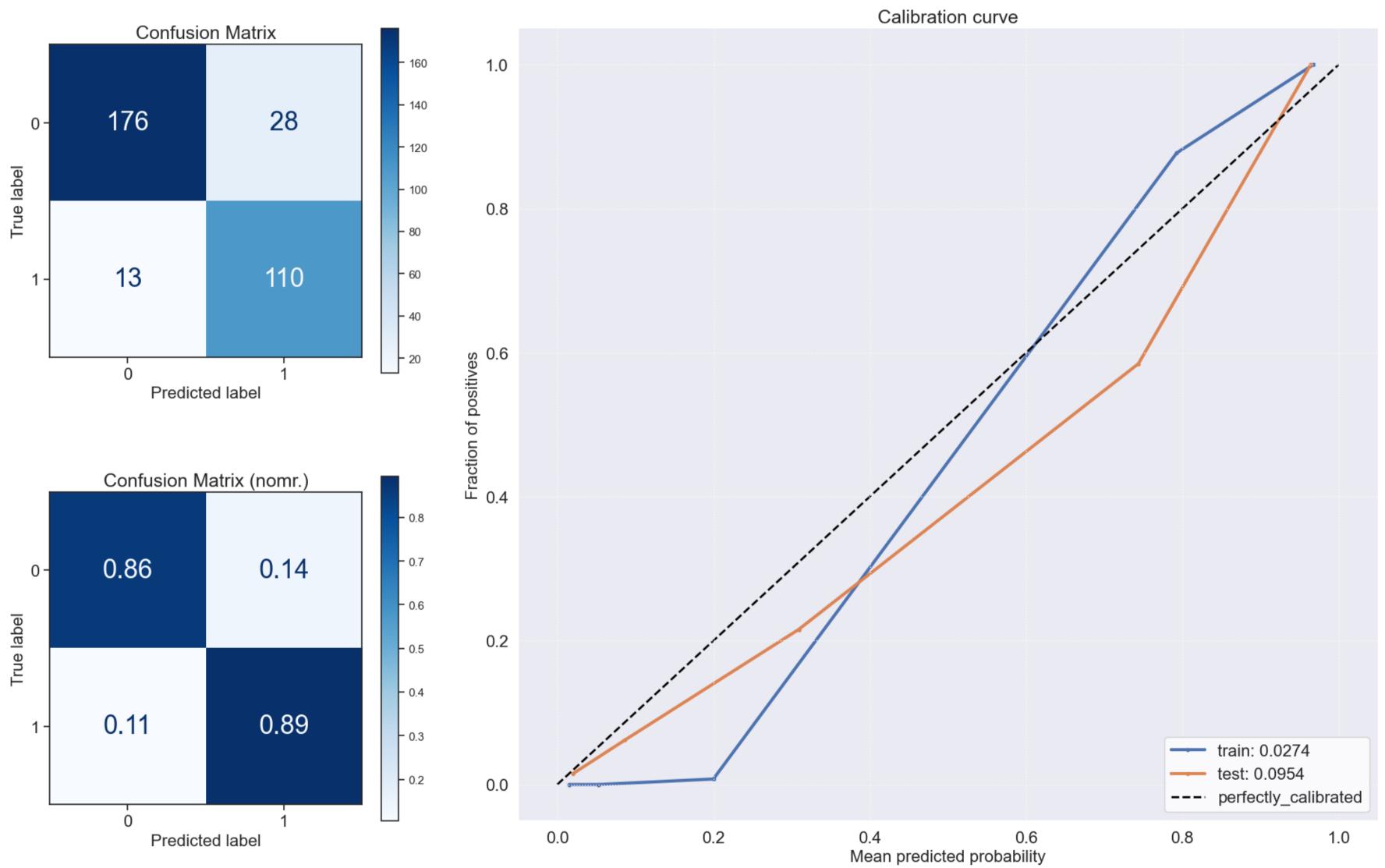
Active/Inactive probability

Metric	Train	Test
AUC	0.9952	0.9333
accuracy	0.9648	0.8563
balanced accuracy	0.9646	0.8493
recall_(sens)	0.9635	0.8211
specificity	0.9656	0.8775
precision	0.9443	0.8016
f1_score	0.9649	0.8566

Protein: P21397 - metric: SoftVotingXGBoostEnsemble







			Active	e/Inactive probab	ility		
10		Inact	ive zone		Active	zone	type active (123) inactive (204) decoy (326)
Percent	8 - 6 - 0.0 2 - 0.0	0.2).8	1.0
				Probability			

Metric	Train	Test
AUC	0.9985	0.9405
accuracy	0.9778	0.8746
balanced accuracy	0.981	0.8785
recall_(sens)	0.9939	0.8943
specificity	0.9681	0.8627
precision	0.9496	0.7971
f1_score	0.9779	0.8758