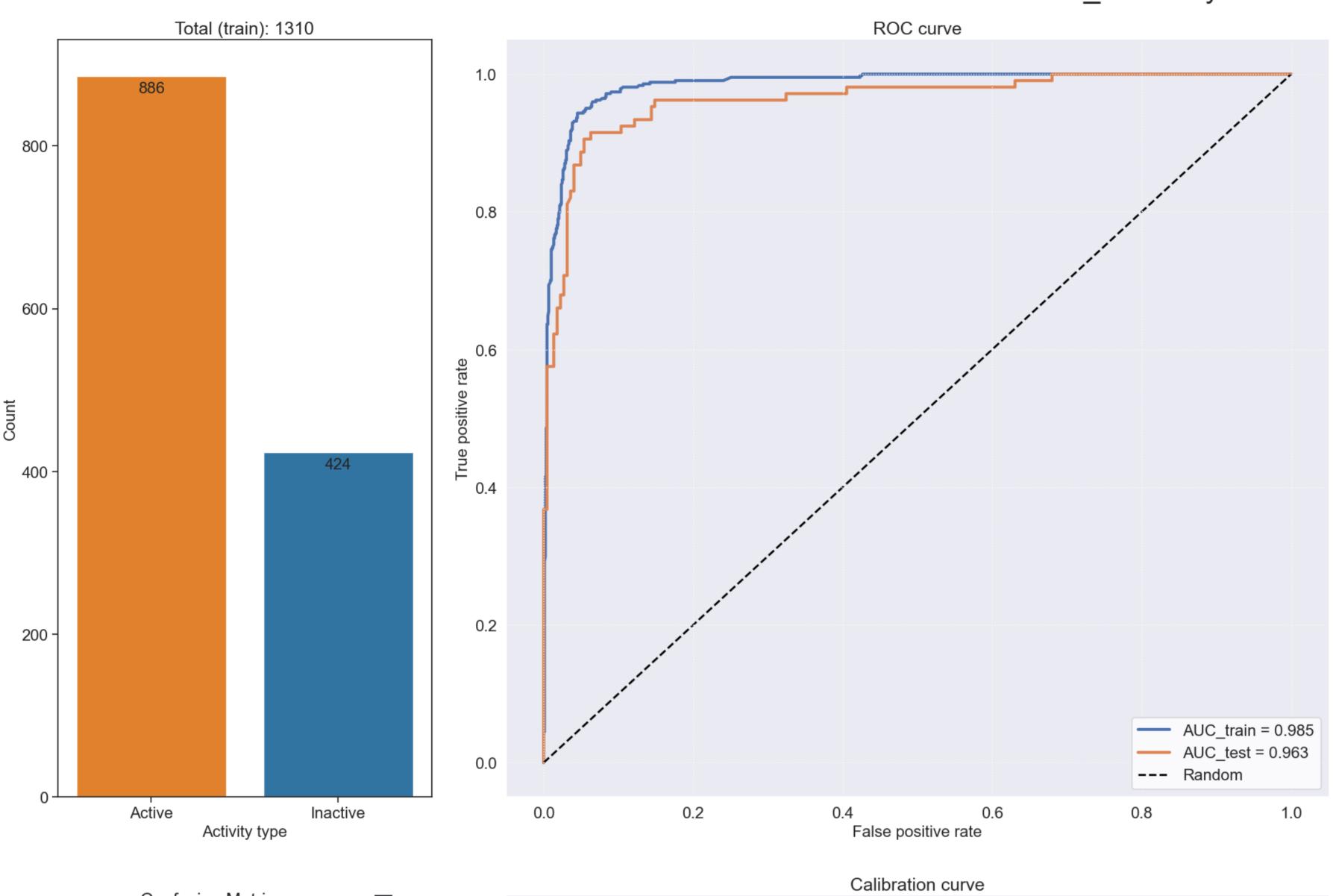
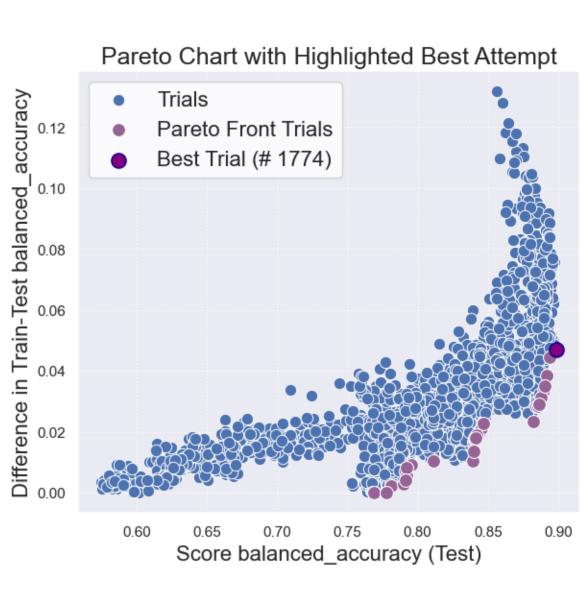
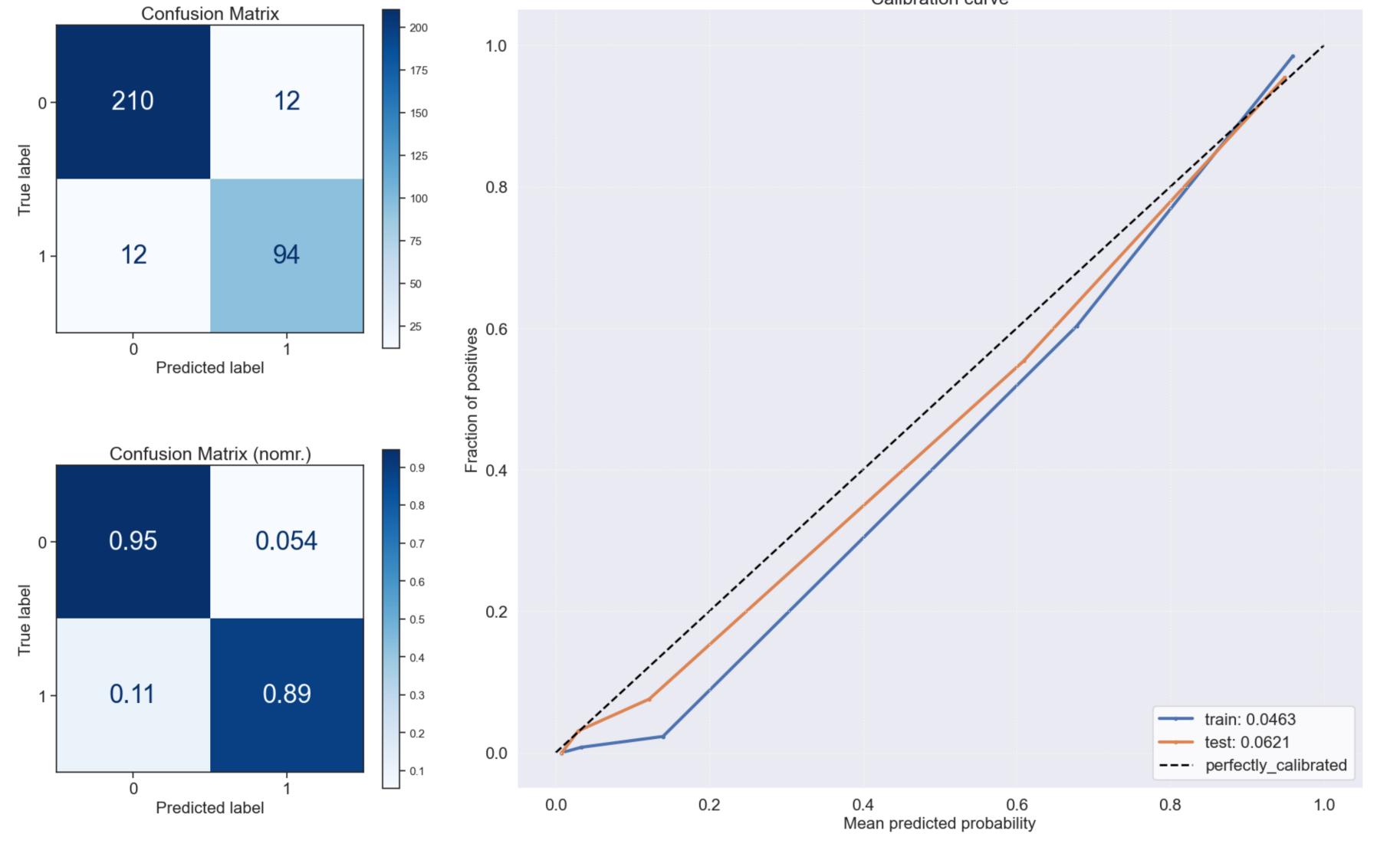
Protein: Q9NZ42 - metric: balanced_accuracy





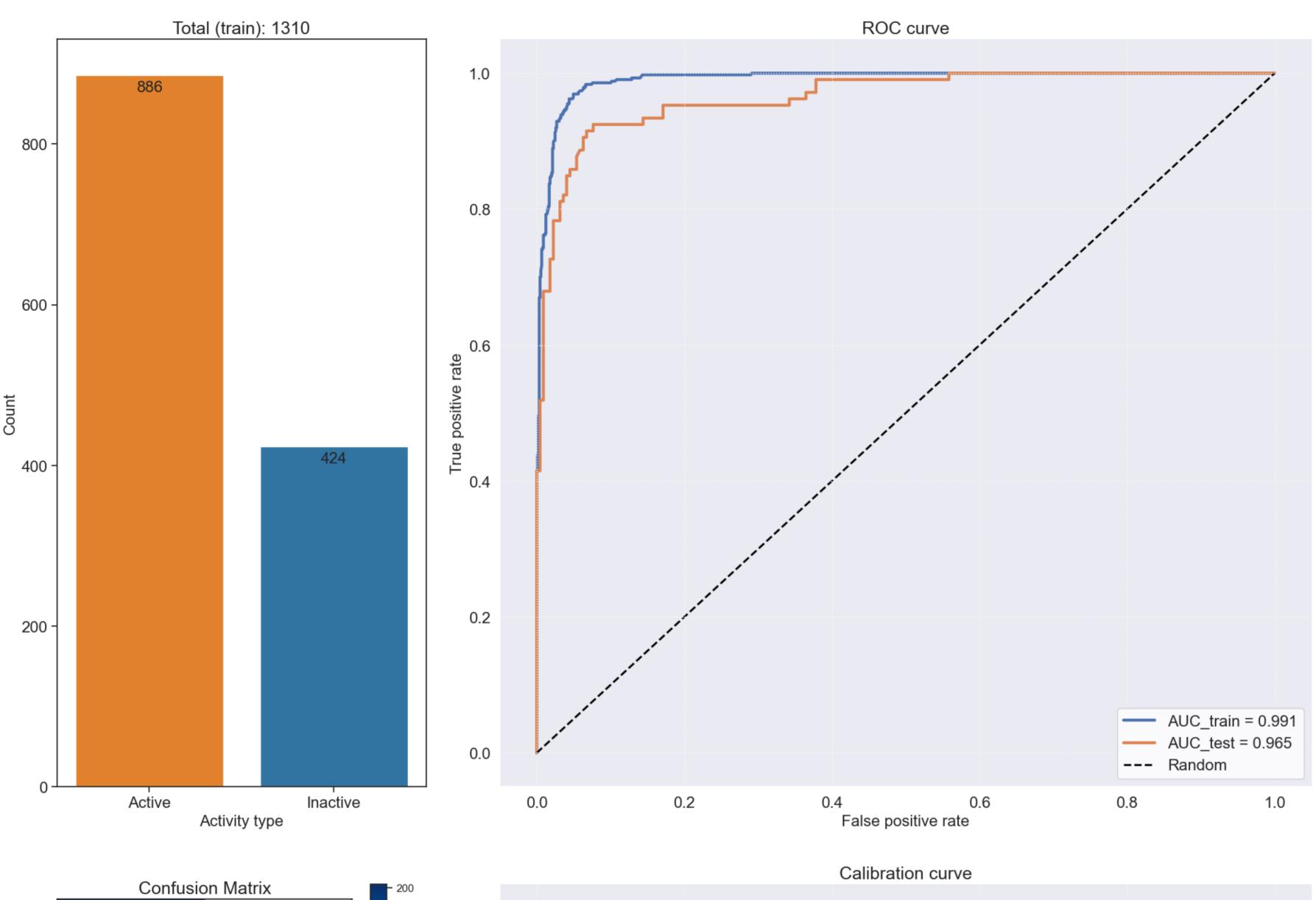
XGBoost Parameters	Value
alpha	1.0539
colsample_bytree	0.5073
gamma	0.4198
lambda	1.6492
learning_rate	0.034
max_depth	8.0
min_child_weight	10.0
n_estimators	485.0
reg_alpha	0.0316
reg_lambda	0.2162
scale_pos_weight	2.0261
subsample	0.7816

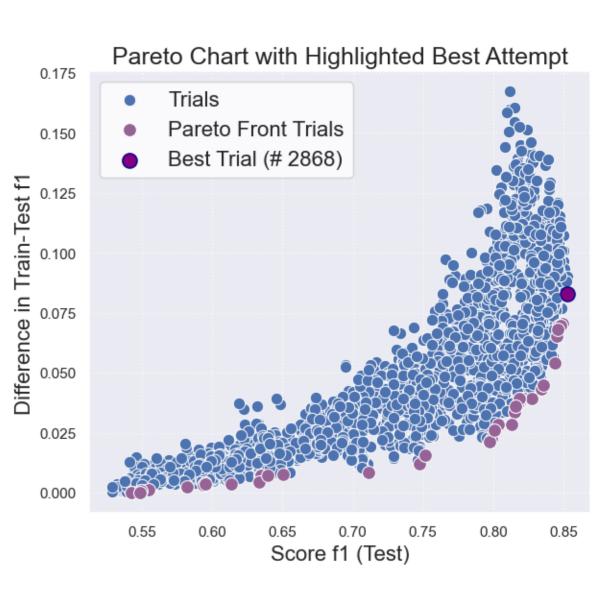


			Active/Inactive	probability		
25		Inactive zone			Active zone	type active (106) inactive (222) decoy (328)
20 25 15						
5						
U -	0.0	0.2	0.4 Probak	0.6 pility	0.8	1.0

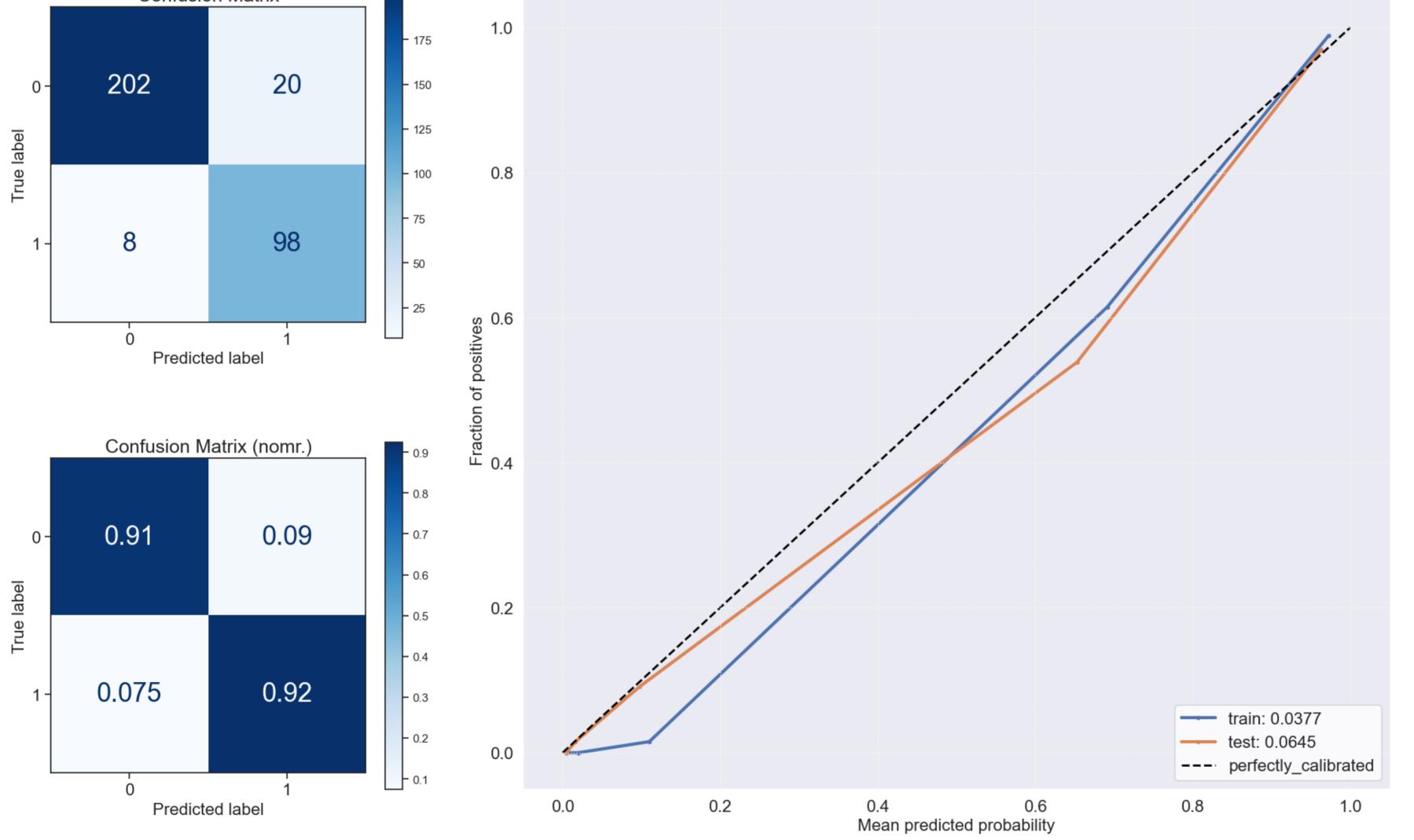
Metric	Train	Test
AUC	0.985	0.9631
accuracy	0.9427	0.9268
balanced accuracy	0.9448	0.9164
recall_(sens)	0.9505	0.8868
specificity	0.9391	0.9459
precision	0.8818	0.8868
f1_score	0.9433	0.9268

Protein: Q9NZ42 - metric: f1





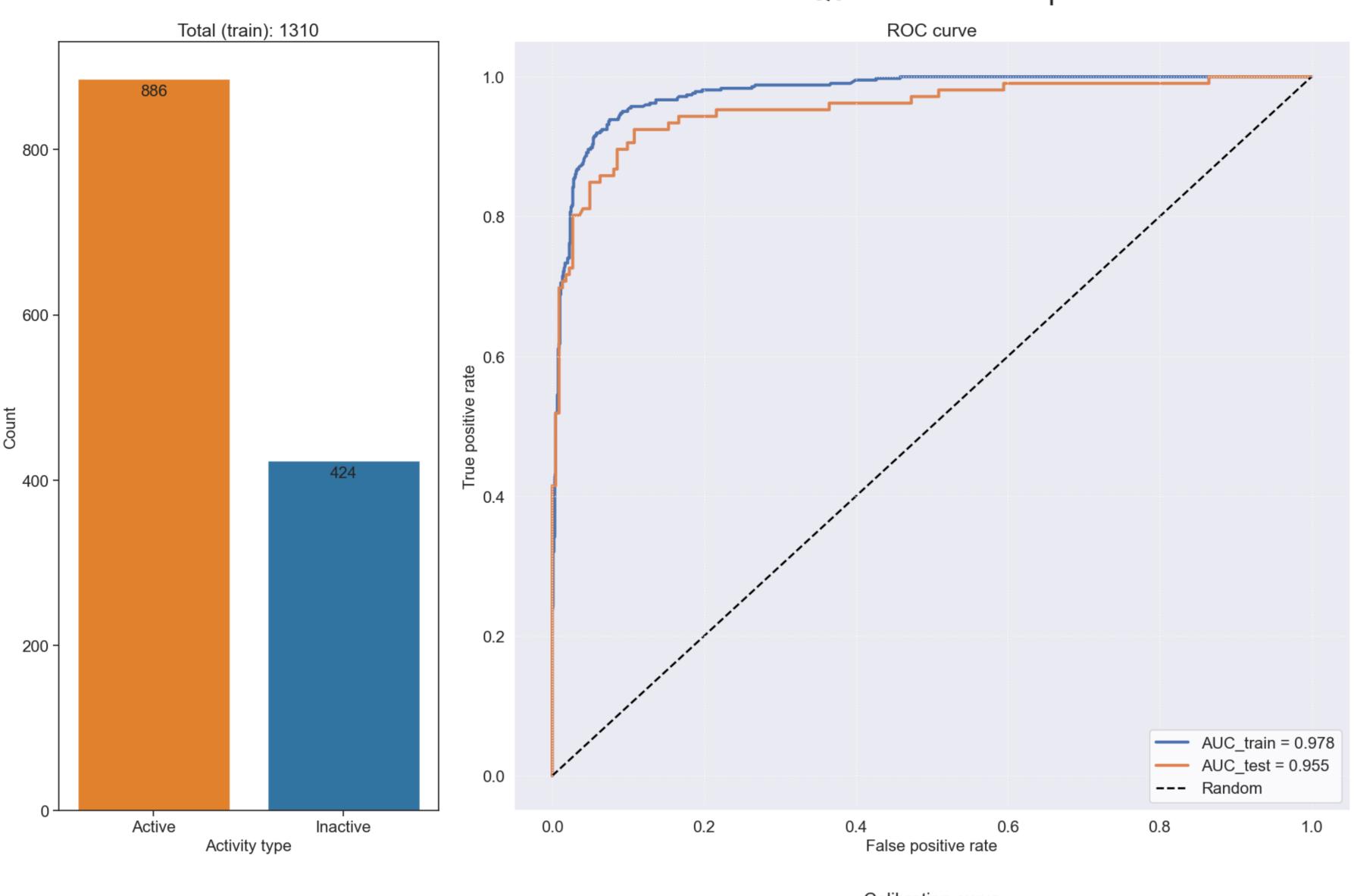
XGBoost Parameters	Value
alpha	4.7761
colsample_bytree	0.6971
gamma	0.3057
lambda	2.348
learning_rate	0.1614
max_depth	4.0
min_child_weight	3.0
n_estimators	145.0
reg_alpha	0.5422
reg_lambda	0.2279
scale_pos_weight	2.2344
subsample	0.6523

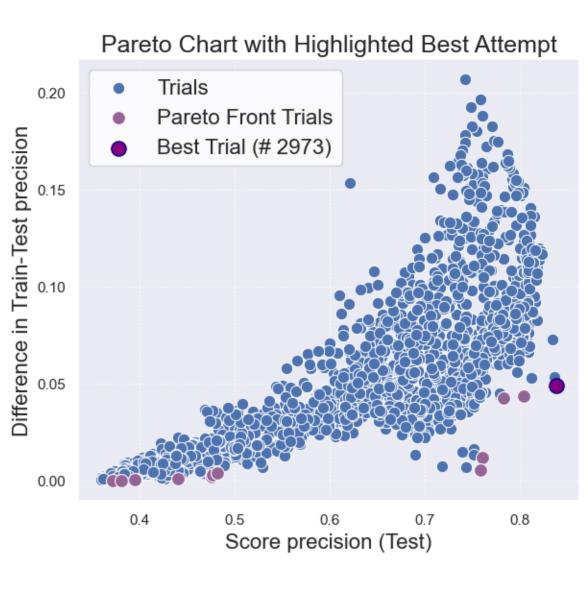


			Active/Inactiv	e probability		
35		nactive zone			Active zone	type active (106) inactive (222) decoy (328)
25						
Percent 15						п_
10 -						
0	0.0	0.2	0.4 Drobo	0.6	0.8	1.0
			Proba	Dility		

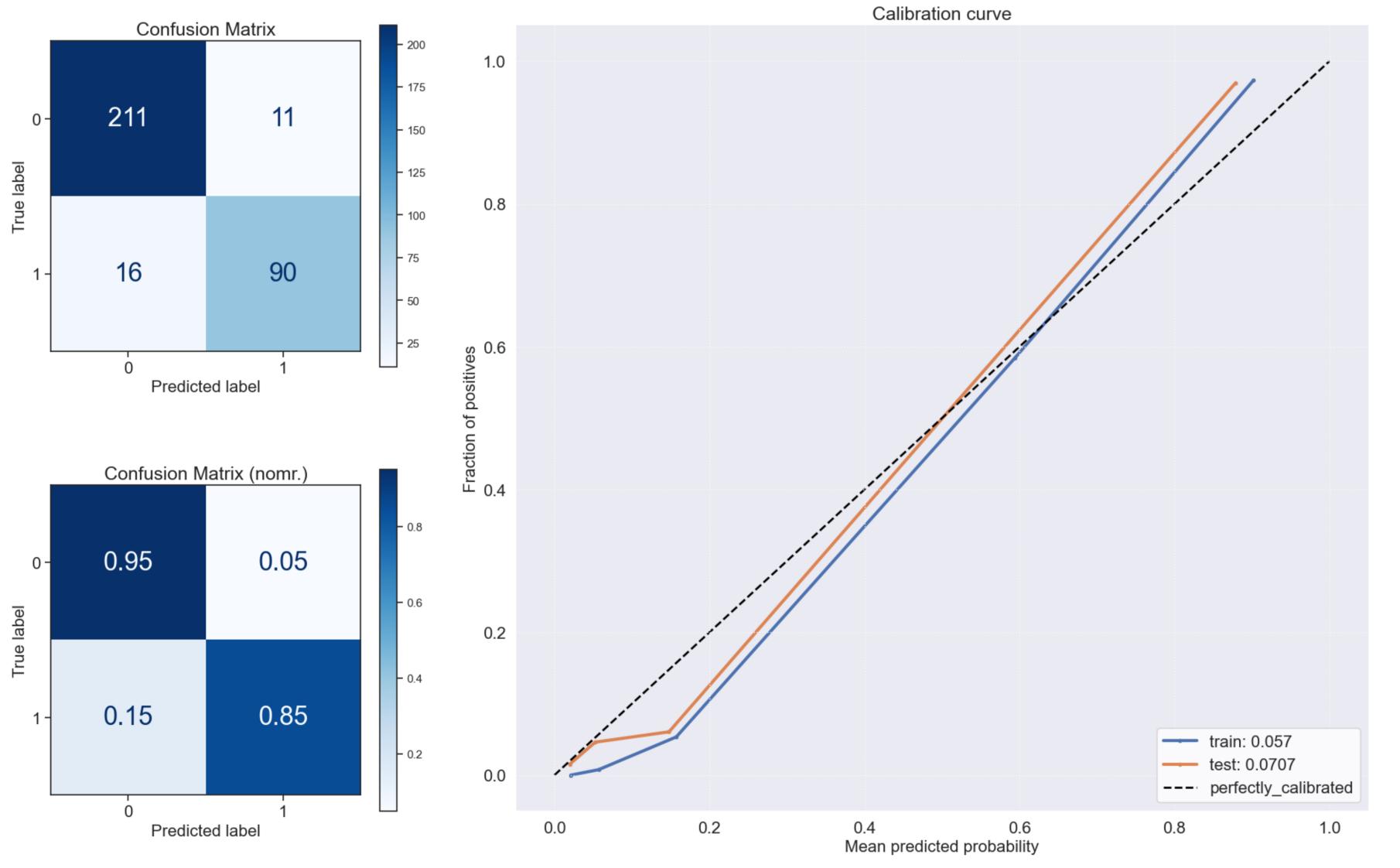
Metric	Train	Test
AUC	0.9907	0.9654
accuracy	0.9557	0.9146
balanced accuracy	0.9593	0.9172
recall_(sens)	0.9693	0.9245
specificity	0.9492	0.9099
precision	0.9013	0.8305
f1_score	0.9561	0.9157

Protein: Q9NZ42 - metric: precision





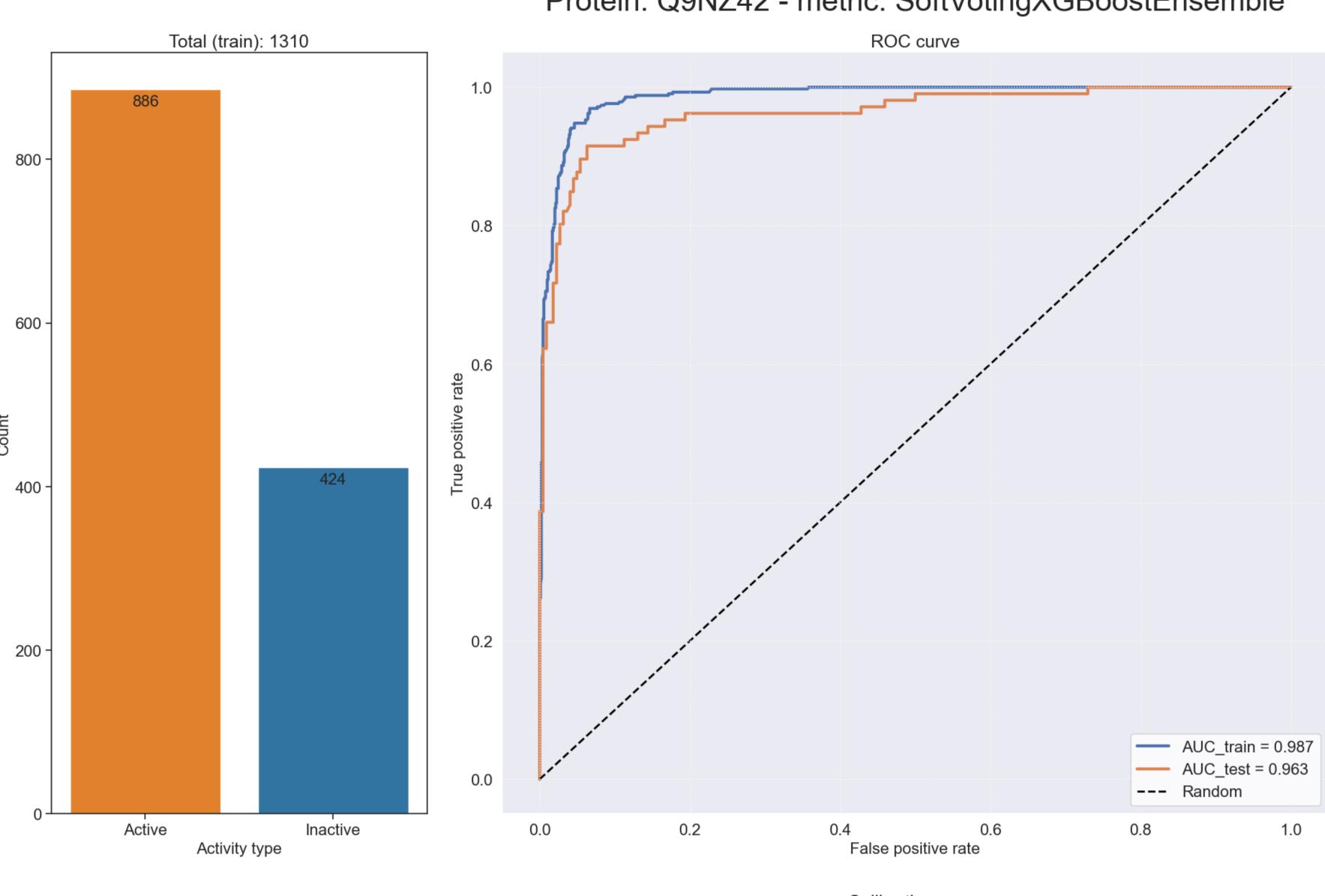
XGBoost Parameters	Value
alpha	0.141
colsample_bytree	0.948
gamma	0.7462
lambda	3.1099
learning_rate	0.0134
max_depth	3.0
min_child_weight	2.0
n_estimators	913.0
reg_alpha	0.9922
reg_lambda	0.6916
scale_pos_weight	1.3473
subsample	0.8667

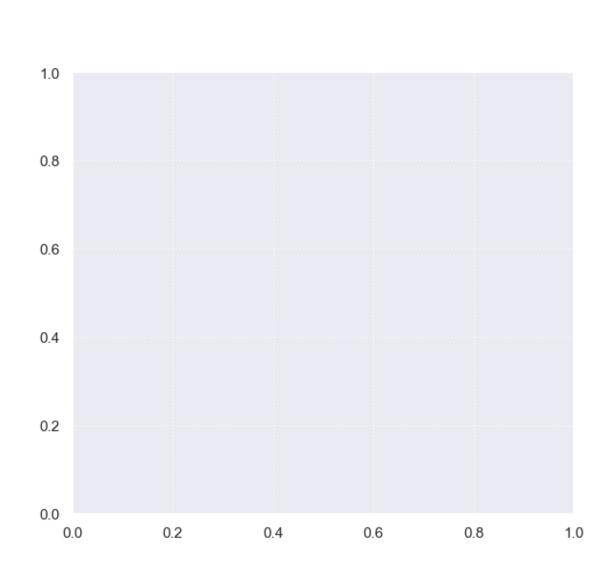


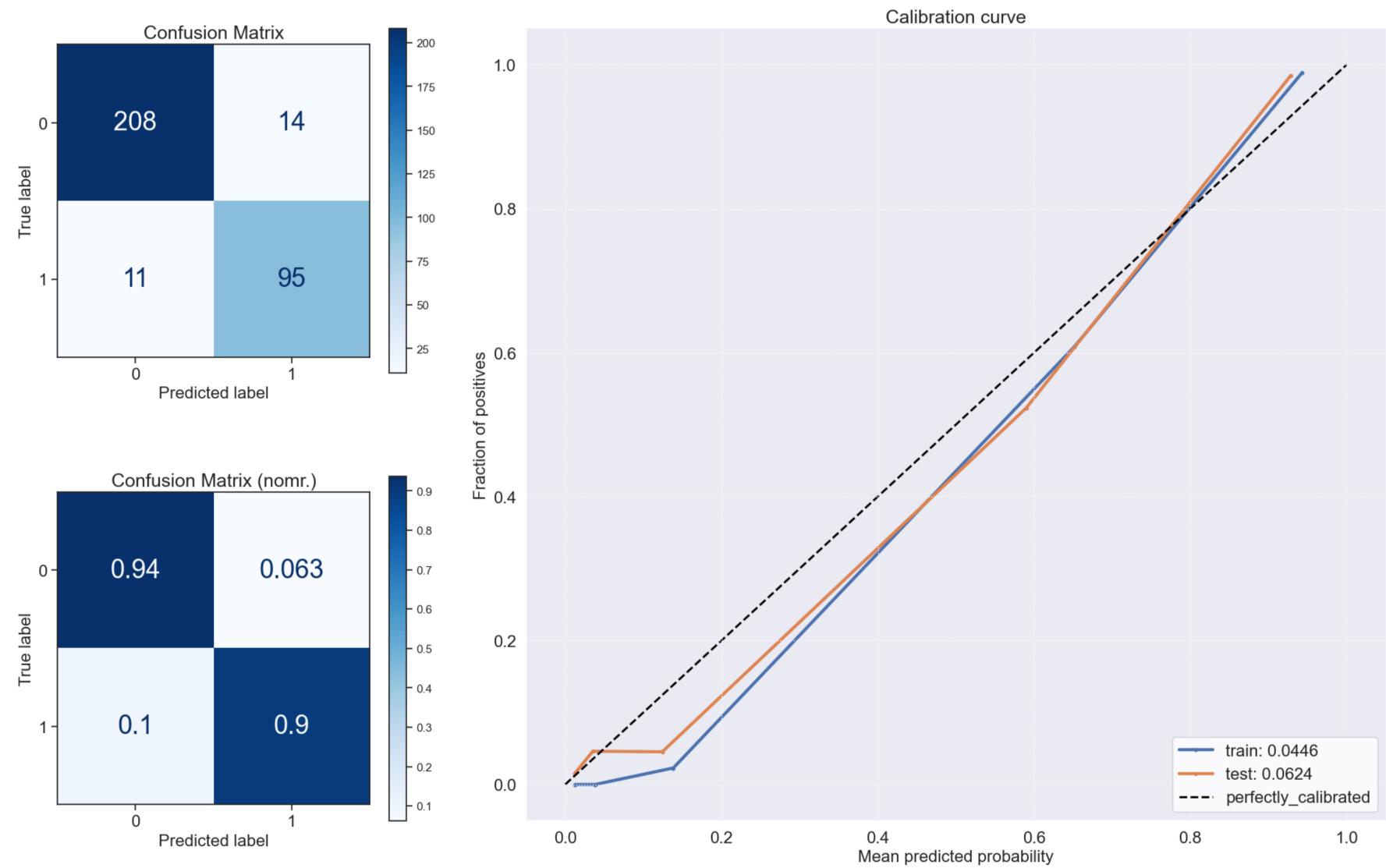
	:	Active	e/Inactive probability	:
16 14		Inactive zone		ive zone type active (106) inactive (222)
12				decoy (328)
Percent				
4				
0-				
Ŭ	0.0	0.2 0.4	0.6 Probability	0.8 1.0

Metric	Train	Test
AUC	0.9777	0.9548
accuracy	0.9321	0.9177
balanced accuracy	0.9289	0.8998
recall_(sens)	0.9198	0.8491
specificity	0.9379	0.9505
precision	0.8764	0.8911
f1_score	0.9325	0.9171

Protein: Q9NZ42 - metric: SoftVotingXGBoostEnsemble







			Active/Inac	tive probability		
20		Inactive zone			Active zone	type active (106) inactive (222) decoy (328)
Dercent						
₫ 10 5						
0 —	0.0	0.2	0.4 Pro	0.6 bability	0.8	1.0

Metric	Train	Test
AUC	0.9868	0.9633
accuracy	0.9443	0.9238
balanced accuracy	0.9453	0.9166
recall_(sens)	0.9481	0.8962
specificity	0.9424	0.9369
precision	0.8874	0.8716
f1_score	0.9447	0.9241