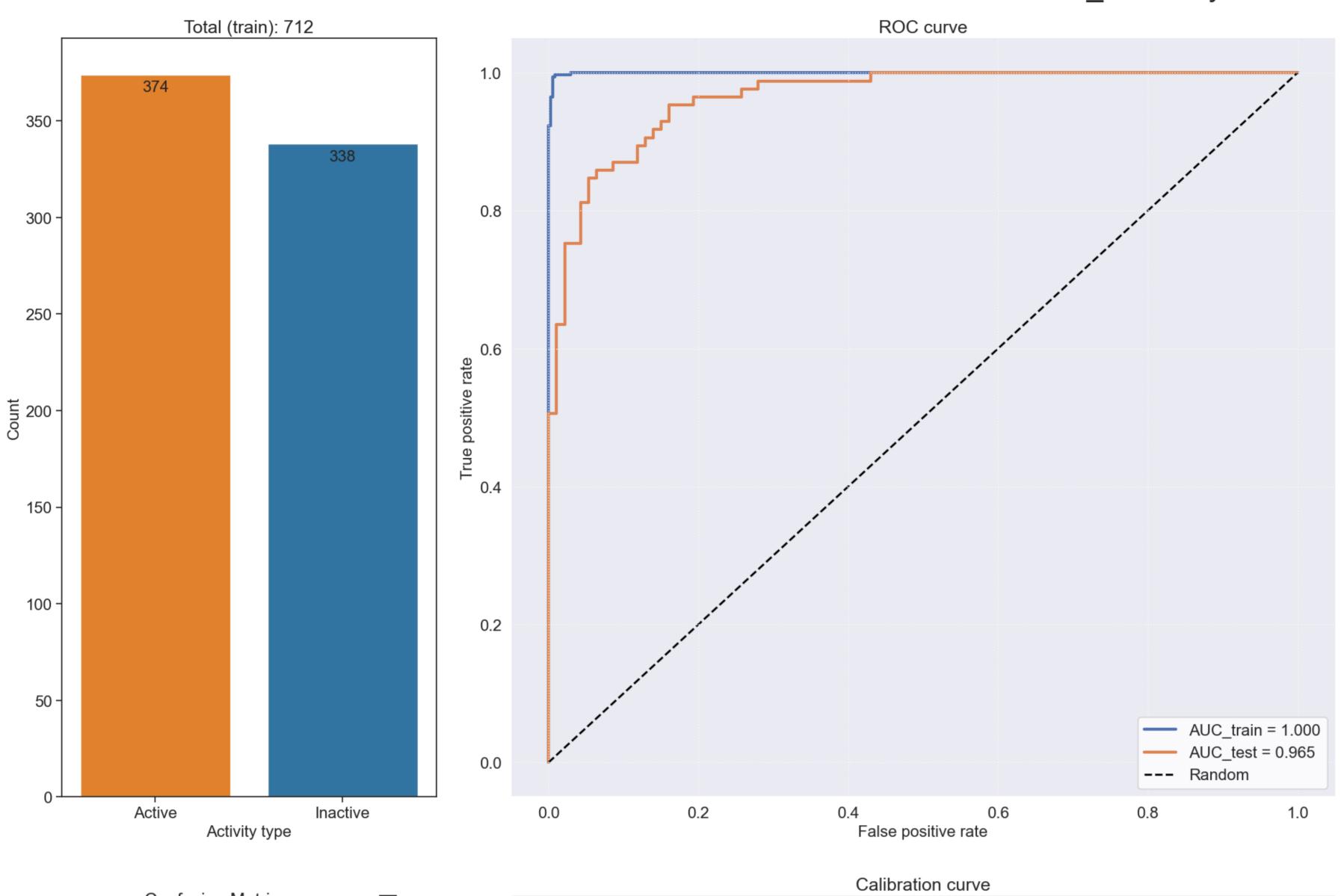
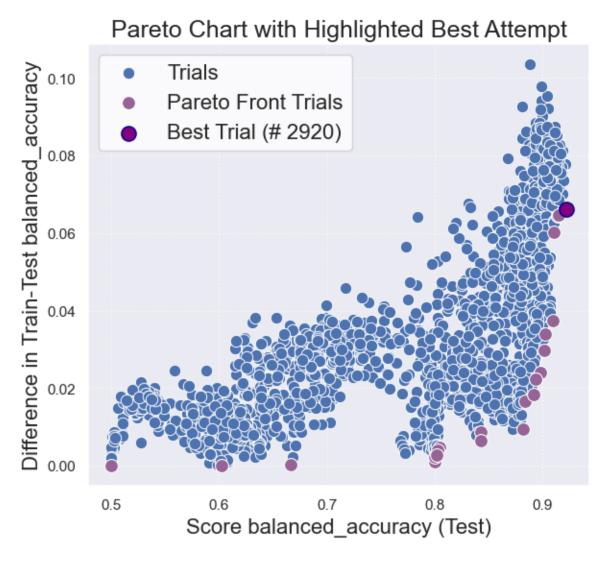
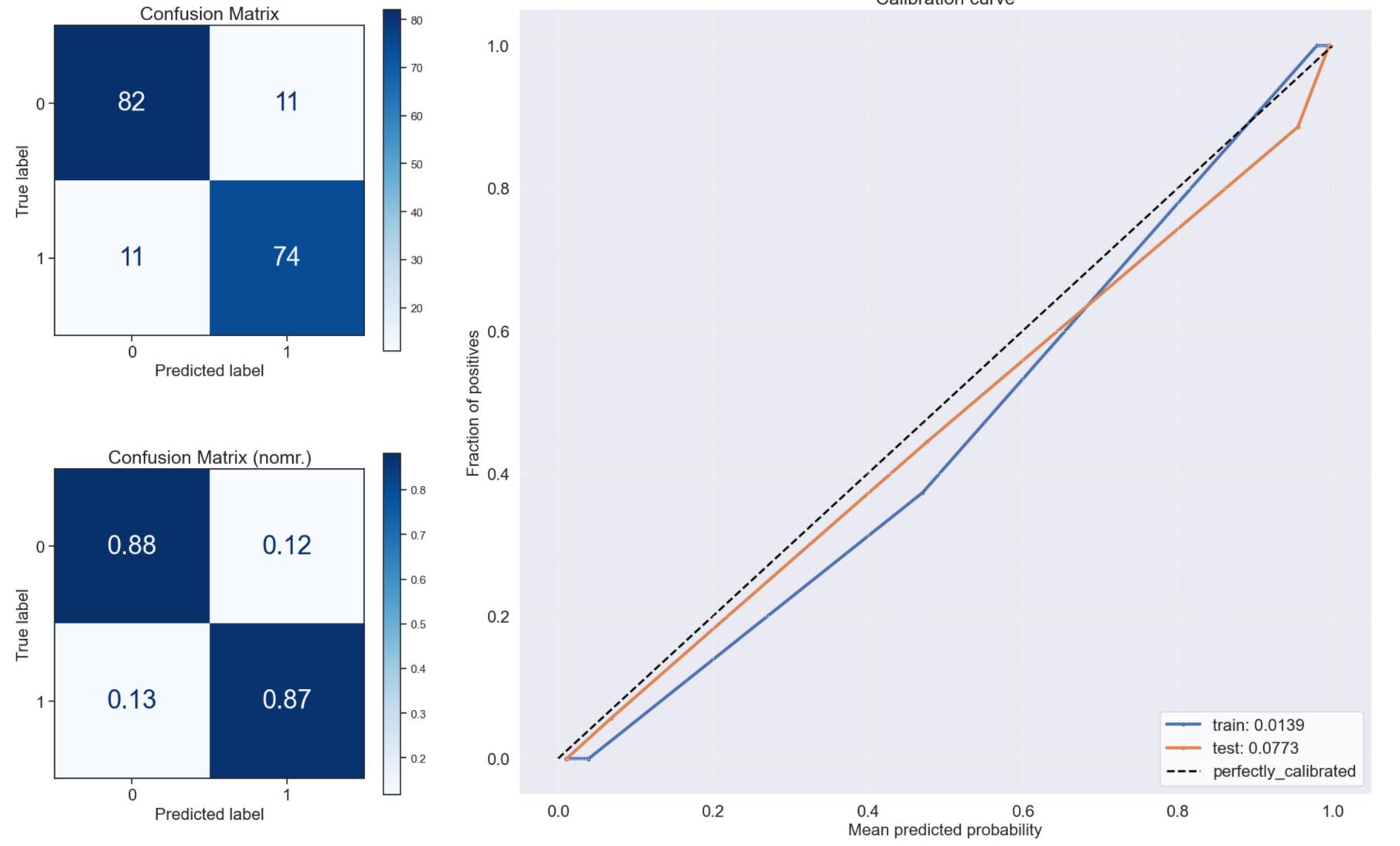
Protein: Q08499 - metric: balanced_accuracy





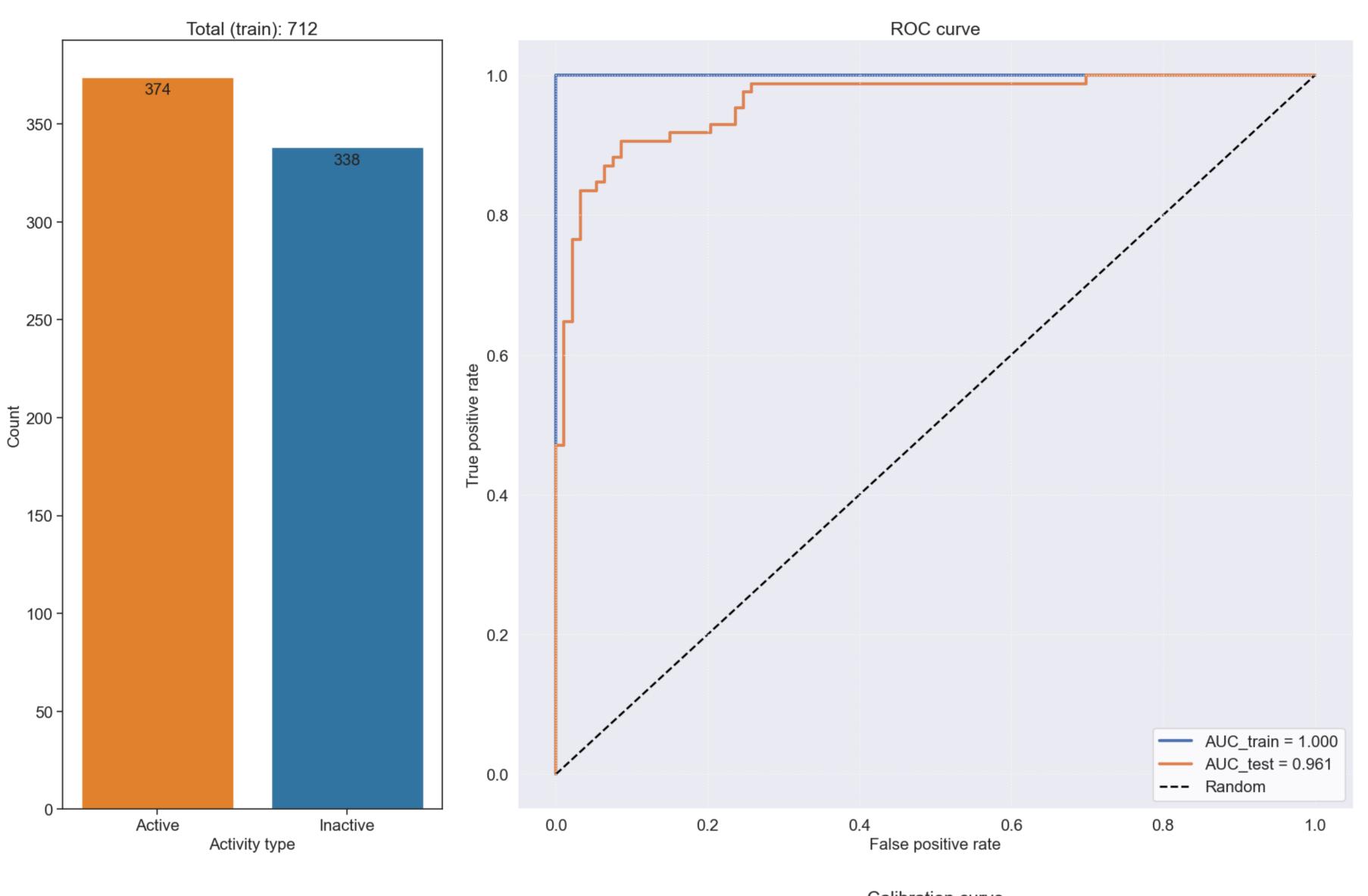
XGBoost Parameters	Value
alpha	3.317
colsample_bytree	0.8856
gamma	0.6016
lambda	1.8777
learning_rate	0.0263
max_depth	6.0
min_child_weight	2.0
n_estimators	760.0
reg_alpha	0.2266
reg_lambda	0.7455
scale_pos_weight	2.5314
subsample	0.8067

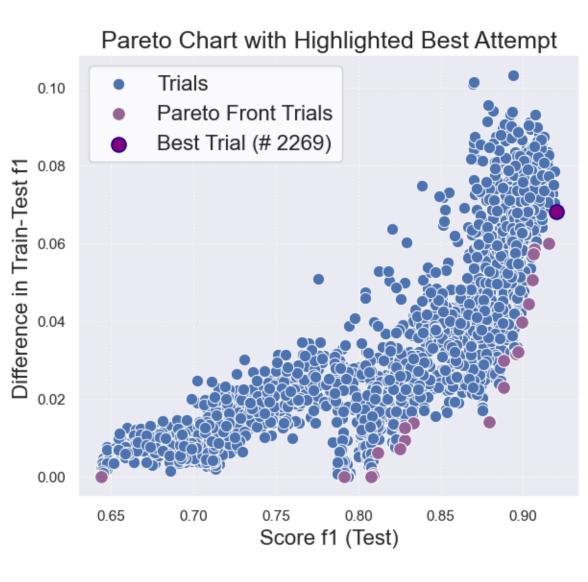


			Active/Inactive	e probability	,	
40		Inactive zone			Active zone	type active (85) inactive (93) decoy (178)
30						
Percent 00						
10						
0 —	0.0	0.2	0.4	0.6	0.8	1.0
			Proba	ability		

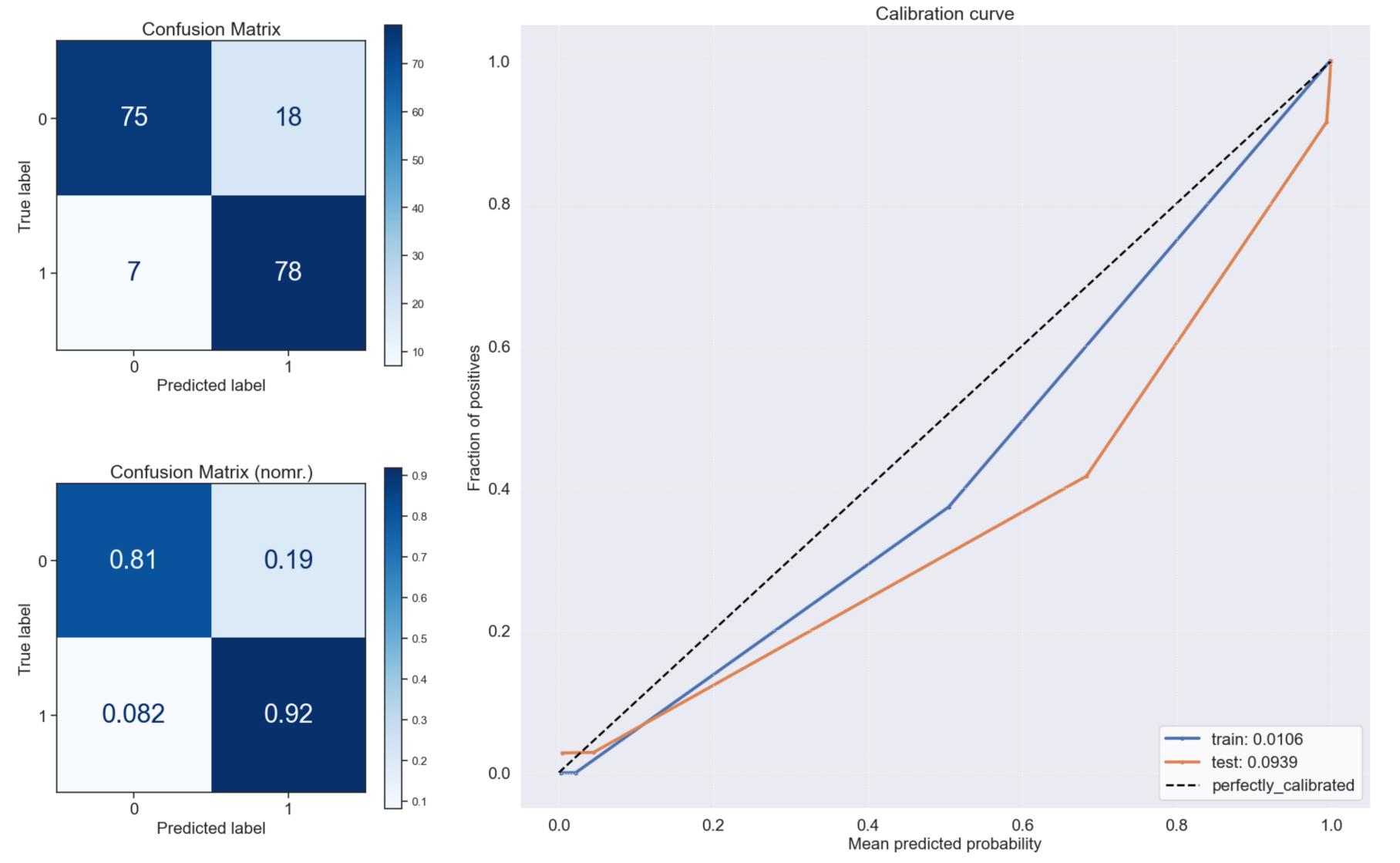
Metric	Train	Test
AUC	0.9996	0.9647
accuracy	0.9846	0.8764
balanced accuracy	0.9852	0.8762
recall_(sens)	0.997	0.8706
specificity	0.9733	0.8817
precision	0.9712	0.8706
f1_score	0.9846	0.8764

Protein: Q08499 - metric: f1





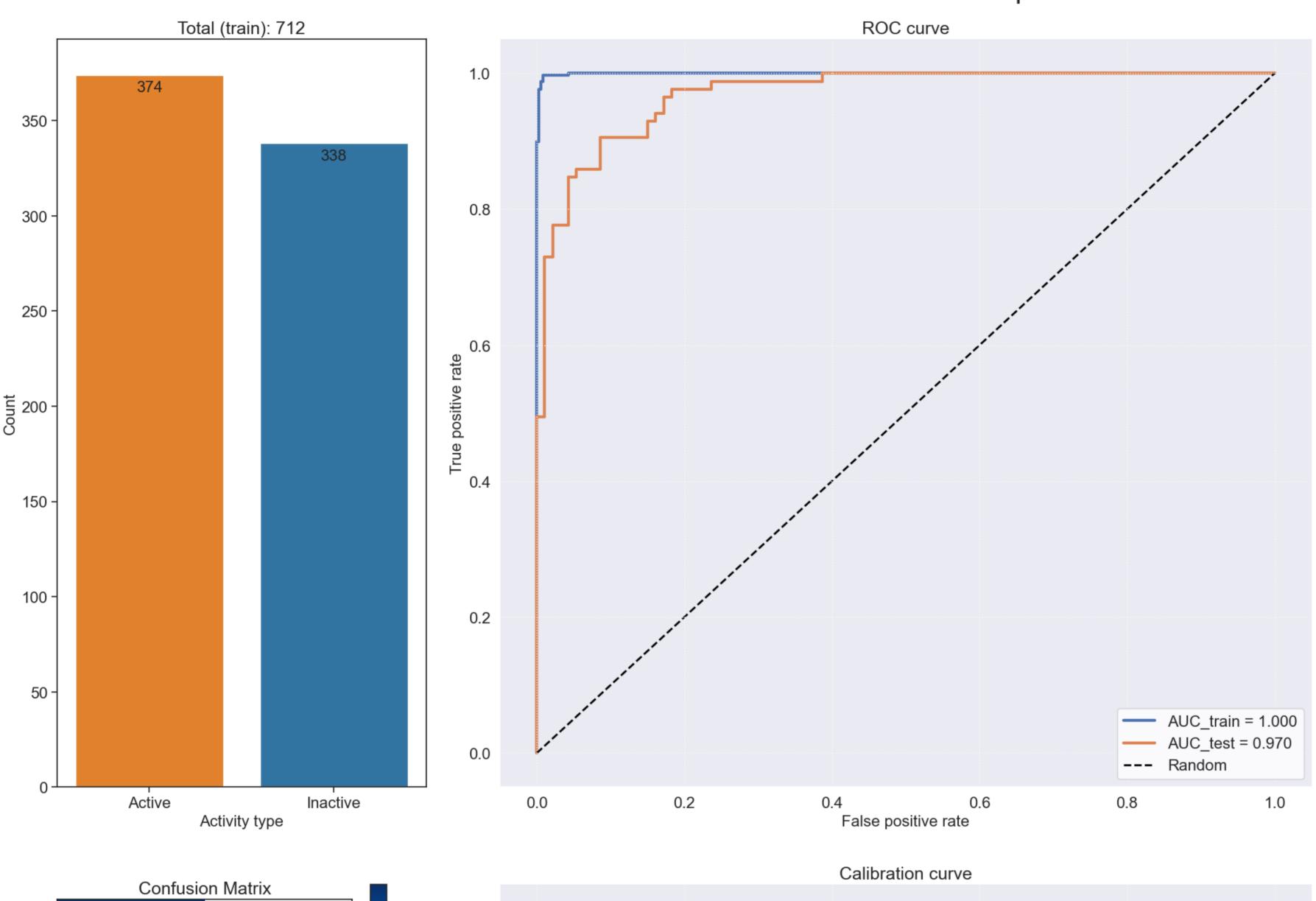
XGBoost Parameters	Value
alpha	3.3107
colsample_bytree	0.9035
gamma	0.5717
lambda	1.4305
learning_rate	0.164
max_depth	4.0
min_child_weight	1.0
n_estimators	466.0
reg_alpha	0.1676
reg_lambda	0.6924
scale_pos_weight	20.6149
subsample	0.9532

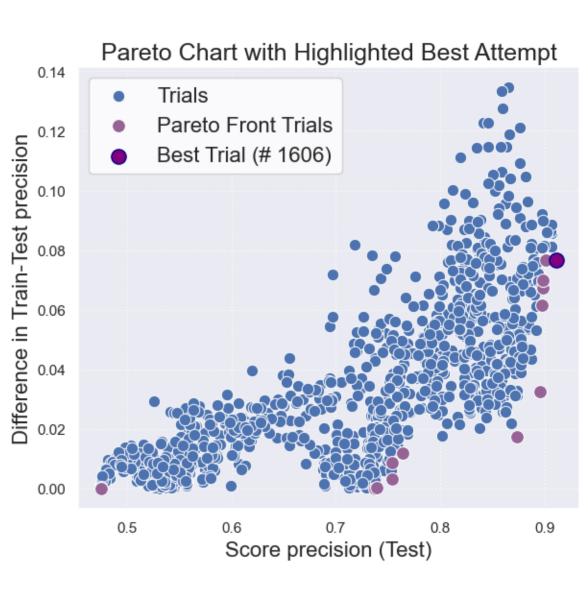


		Active	e/Inactive probabil	lity		
00	Ina			Active	zone type active inactive decoy	(85) ve (93)
50						
Percent 6						
30 -···						
20						
10						
0—	0.0 0.	2 0.4	0. Probability		.8 1	.0

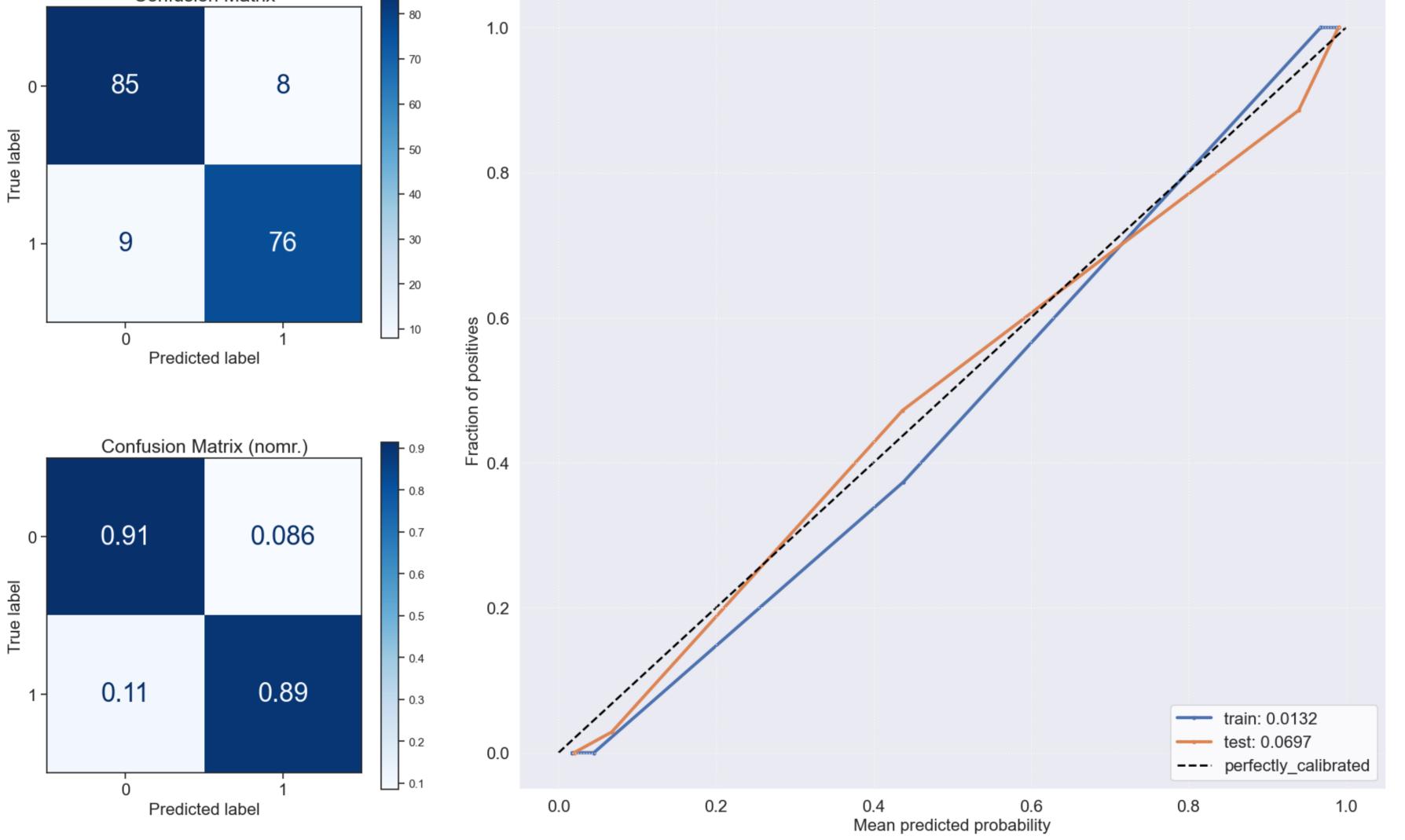
Metric	Train	Test
AUC	1.0	0.9614
accuracy	0.9874	0.8596
balanced accuracy	0.988	0.862
recall_(sens)	1.0	0.9176
specificity	0.9759	0.8065
precision	0.9741	0.8125
f1_score	0.9874	0.8594

Protein: Q08499 - metric: precision





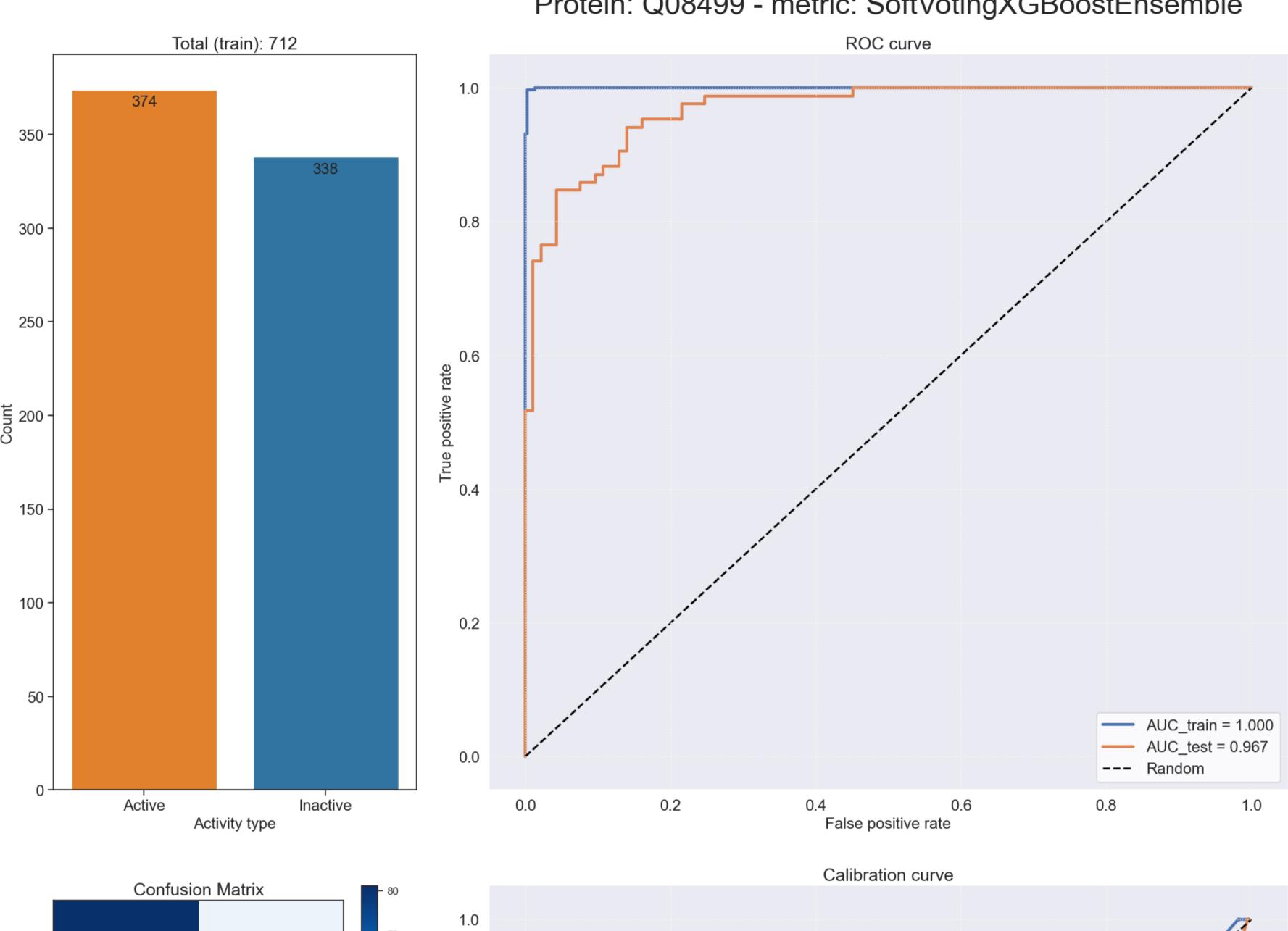
XGBoost Parameters	Value
alpha	3.6595
colsample_bytree	0.9011
gamma	0.3565
lambda	3.3463
learning_rate	0.0153
max_depth	10.0
min_child_weight	1.0
n_estimators	890.0
reg_alpha	0.6522
reg_lambda	0.7773
scale_pos_weight	1.7821
subsample	0.9736

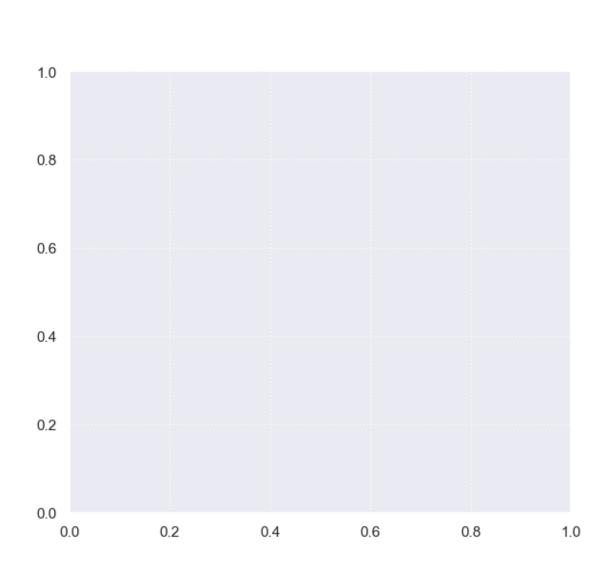


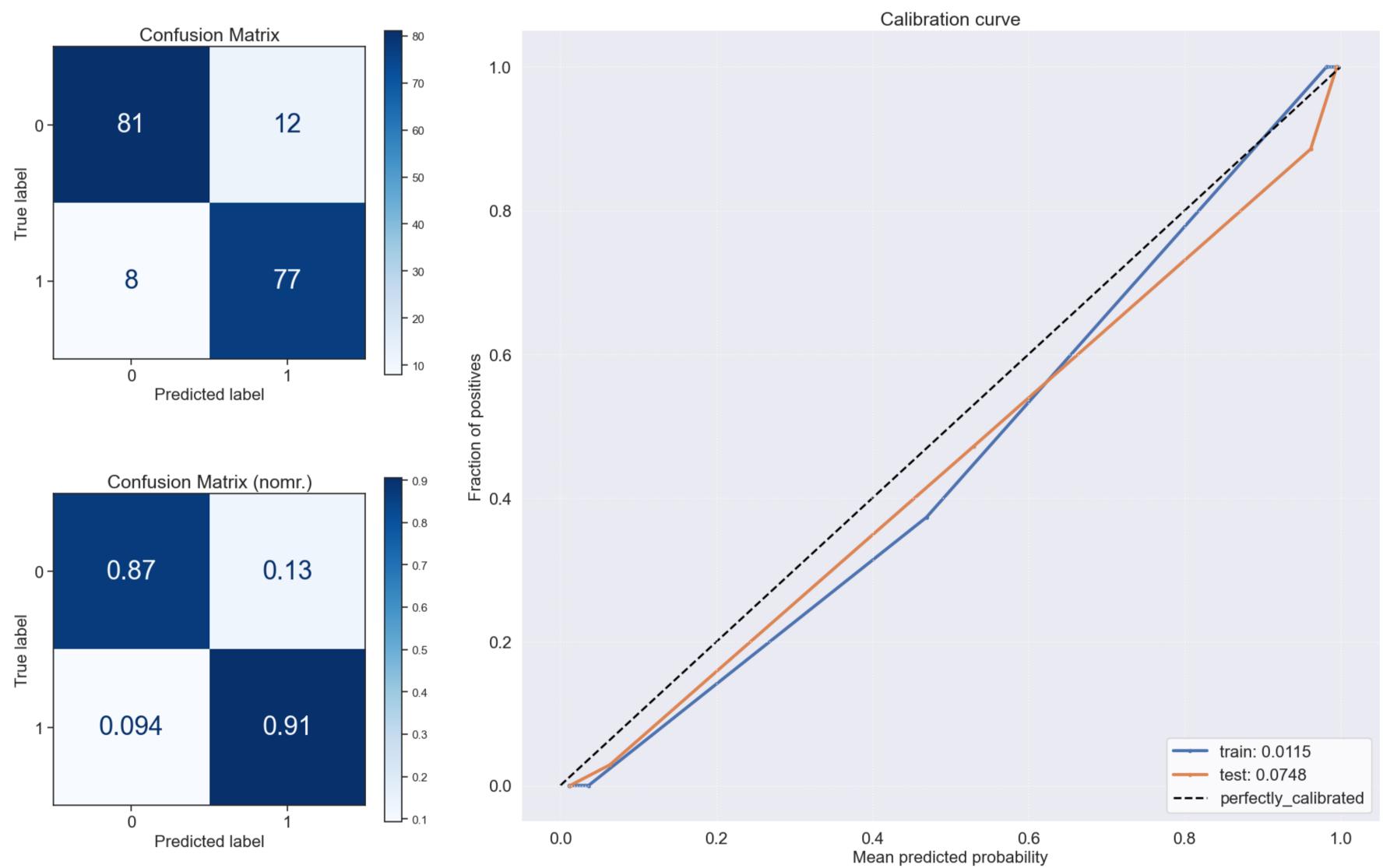
			Active/Inactiv	e probability			
40	Ir	nactive zone			Active zo	one	type active (85) inactive (93)
30							decoy (178)
Percent 05							
10							
0	0.0	0.2	0.4 Proba	0.6 ability	0.8		1.0

Metric	Train	Test
AUC	0.9995	0.9698
accuracy	0.993	0.9045
balanced accuracy	0.9932	0.904
recall_(sens)	0.997	0.8941
specificity	0.9893	0.914
precision	0.9883	0.9048
f1_score	0.993	0.9045

Protein: Q08499 - metric: SoftVotingXGBoostEnsemble







		Ac	tive/Inactive pro	bability		
50	Ina				Active zone	inactive (93) decoy (178)
Percent 30						
0 —	0.0 0.		.4 Probability	0.6	0.8	1.0

Metric	Train	Test
AUC	0.9998	0.9671
accuracy	0.9916	0.8876
balanced accuracy	0.992	0.8884
recall_(sens)	1.0	0.9059
specificity	0.984	0.871
precision	0.9826	0.8652
f1_score	0.9916	0.8877