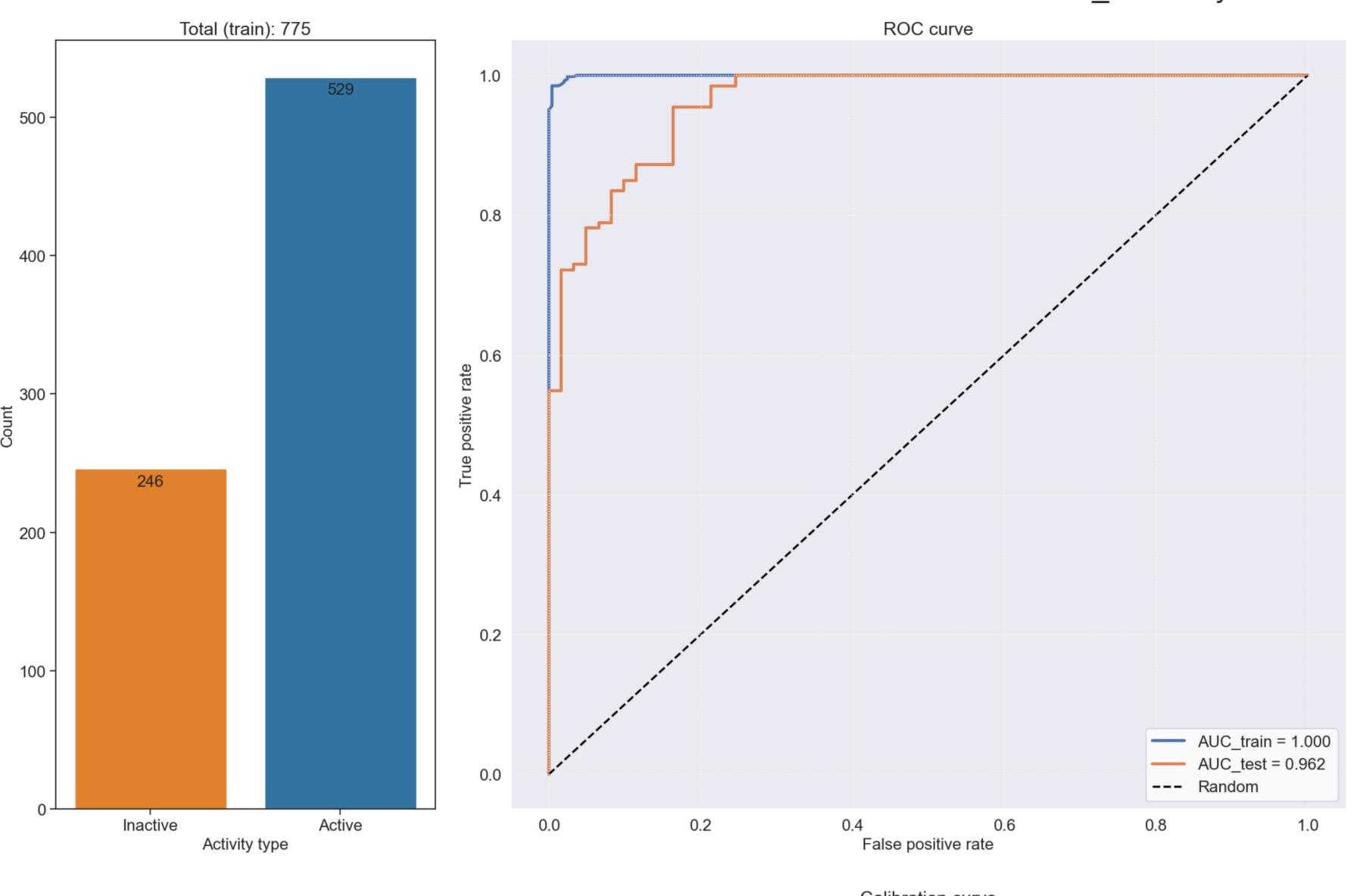
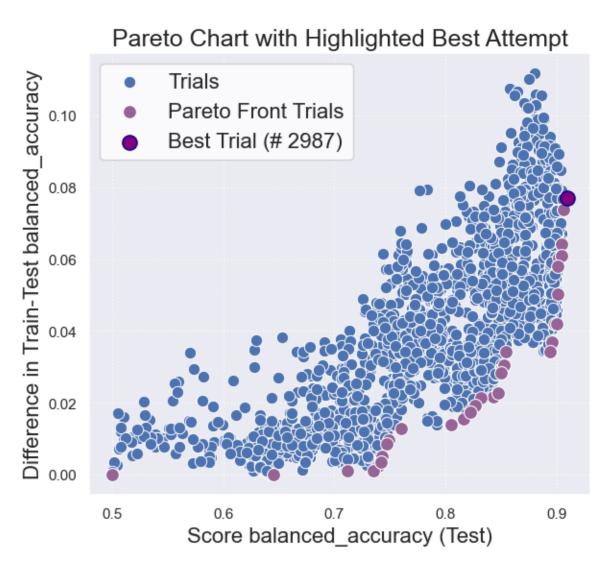
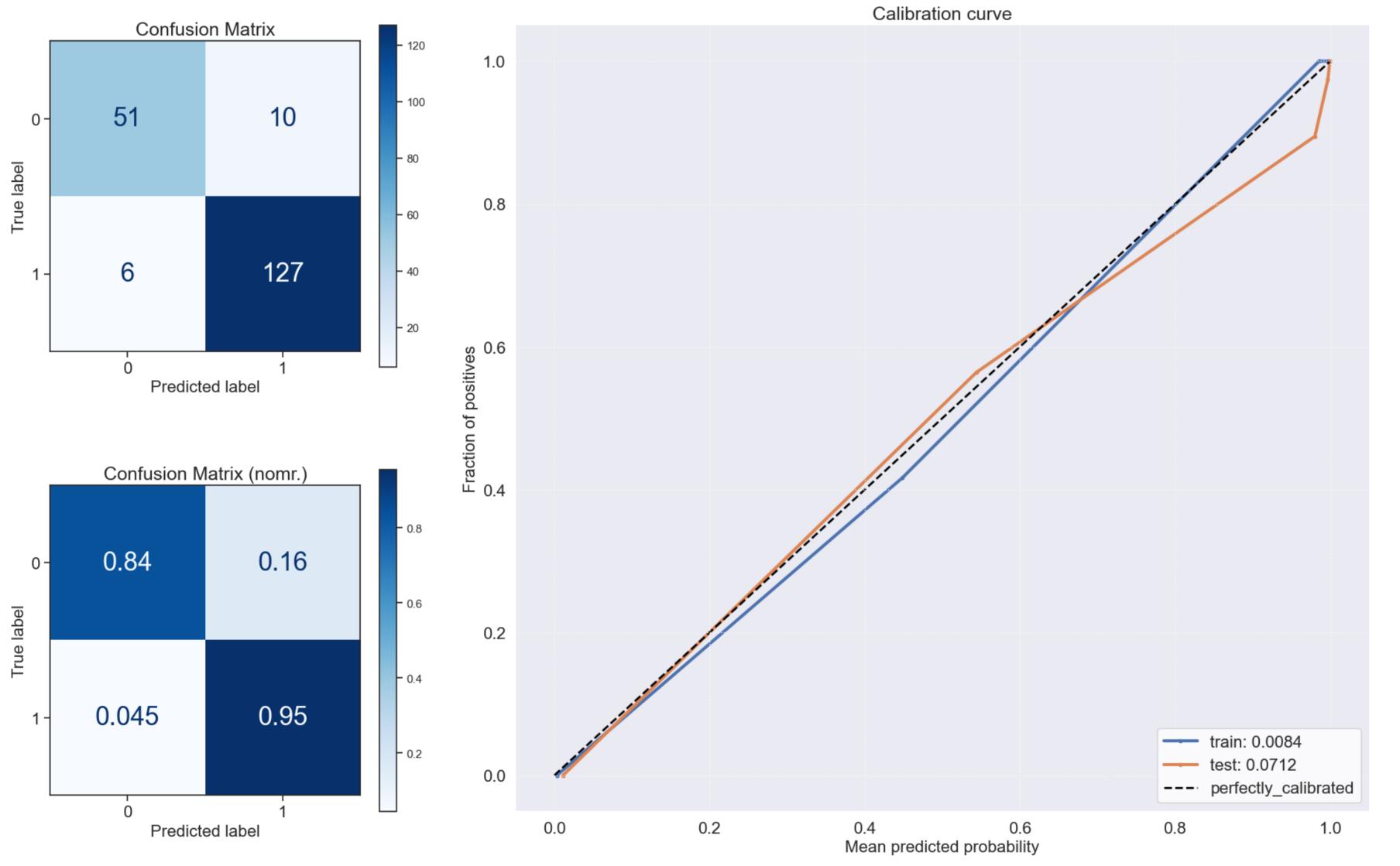
## Protein: P22894 - metric: balanced\_accuracy





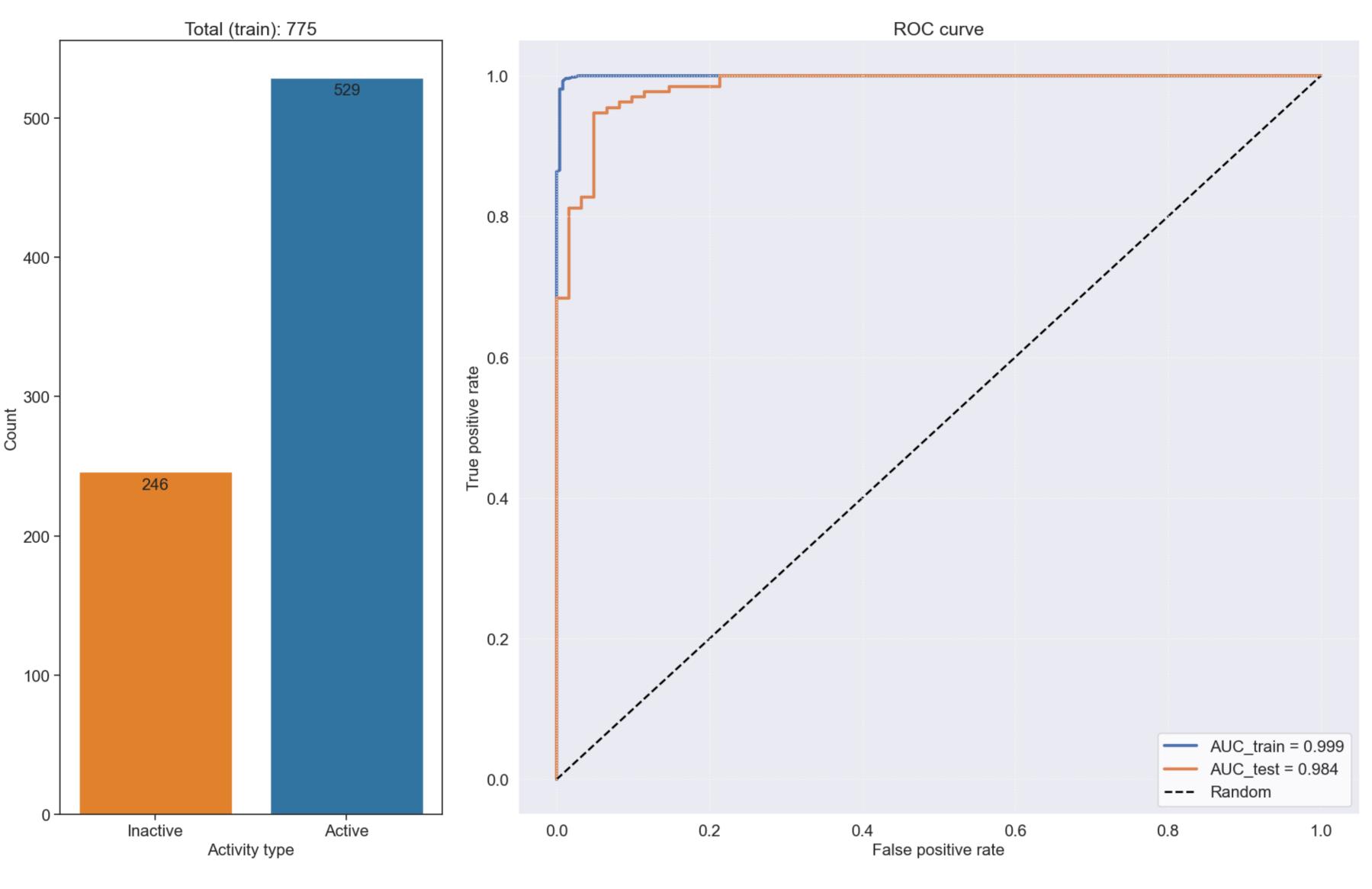
XGBoost Parameters	Value
alpha	4.985
colsample_bytree	0.8228
gamma	0.0453
lambda	4.1631
learning_rate	0.5452
max_depth	7.0
min_child_weight	3.0
n_estimators	636.0
reg_alpha	0.1904
reg_lambda	0.9167
scale_pos_weight	1.2082
subsample	0.8972

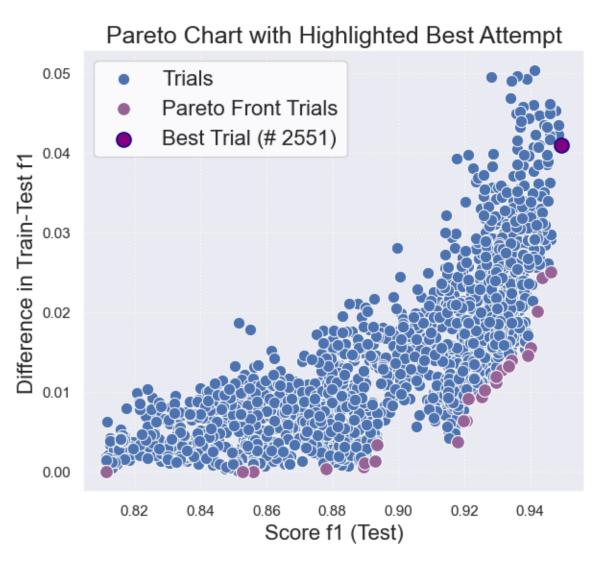


		Ac	tive/Inactiv	e probabilit	у		
60	lna	ctive zone			Active	zone	type active (133) inactive (61) decoy (194)
40							
Percent							
20							
10				_			
0 —	0.0 0.	2 0	).4 Proba	0.6 bility		0.8	1.0

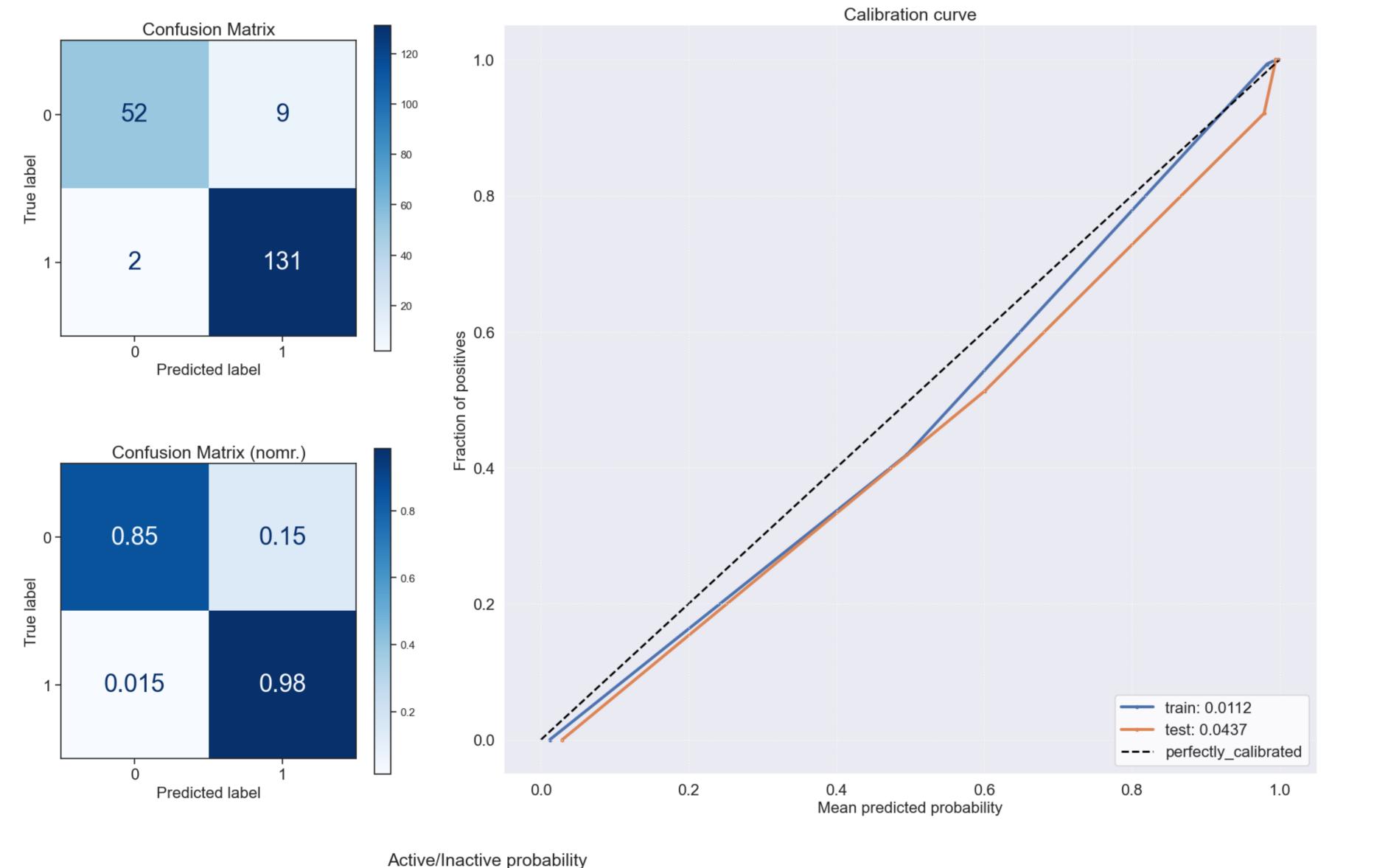
Metric	Train	Test
AUC	0.9995	0.9624
accuracy	0.991	0.9175
balanced accuracy	0.9869	0.8955
recall_(sens)	0.9981	0.9549
specificity	0.9756	0.8361
precision	0.9888	0.927
f1_score	0.9909	0.9167

## Protein: P22894 - metric: f1





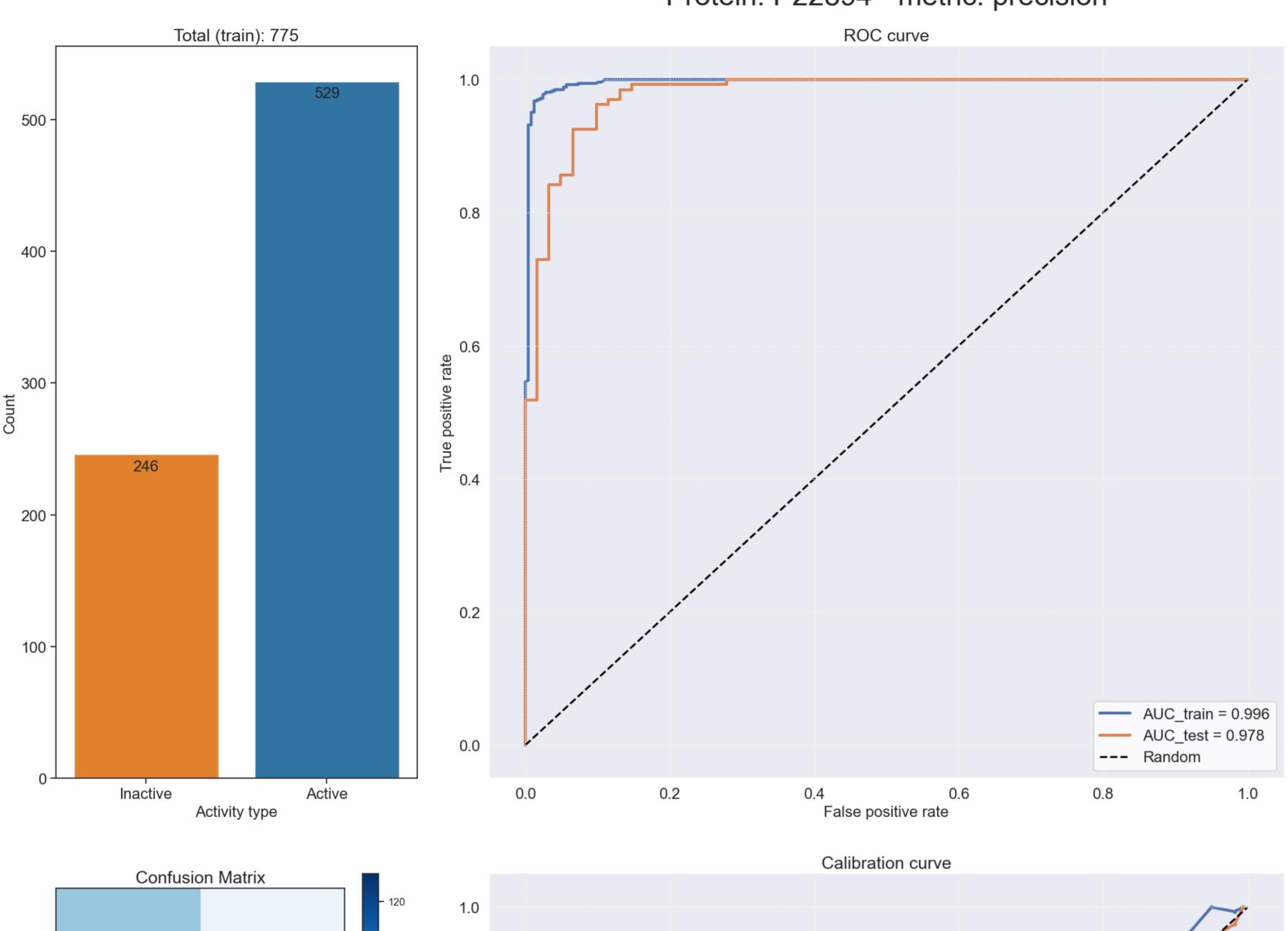
XGBoost Parameters	Value
alpha	4.3461
colsample_bytree	0.5753
gamma	0.3526
lambda	2.4726
learning_rate	0.0211
max_depth	8.0
min_child_weight	1.0
n_estimators	834.0
reg_alpha	0.141
reg_lambda	0.281
scale_pos_weight	2.2012
subsample	0.6354

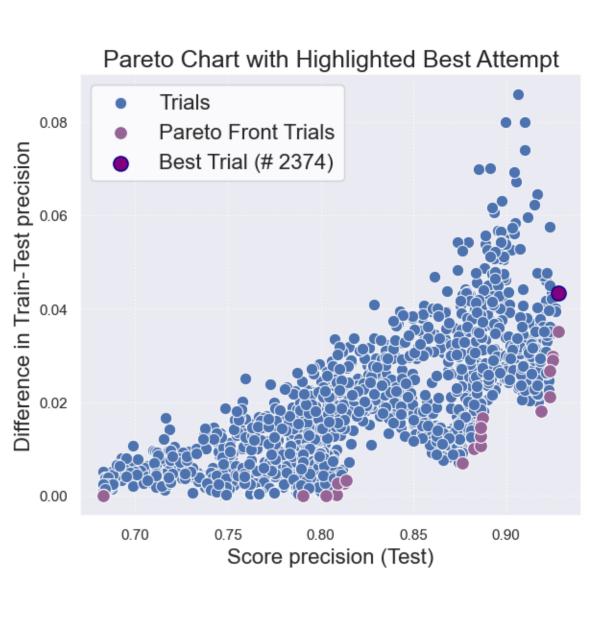


Active/mactive probability							
		Inactive zone				one ac ina	pe tive (133) active (61) coy (194)
30							
ercent							
20							
10							
0—	0.0	0.2	0.4 Proba	0.6 ability	0.	8	1.0

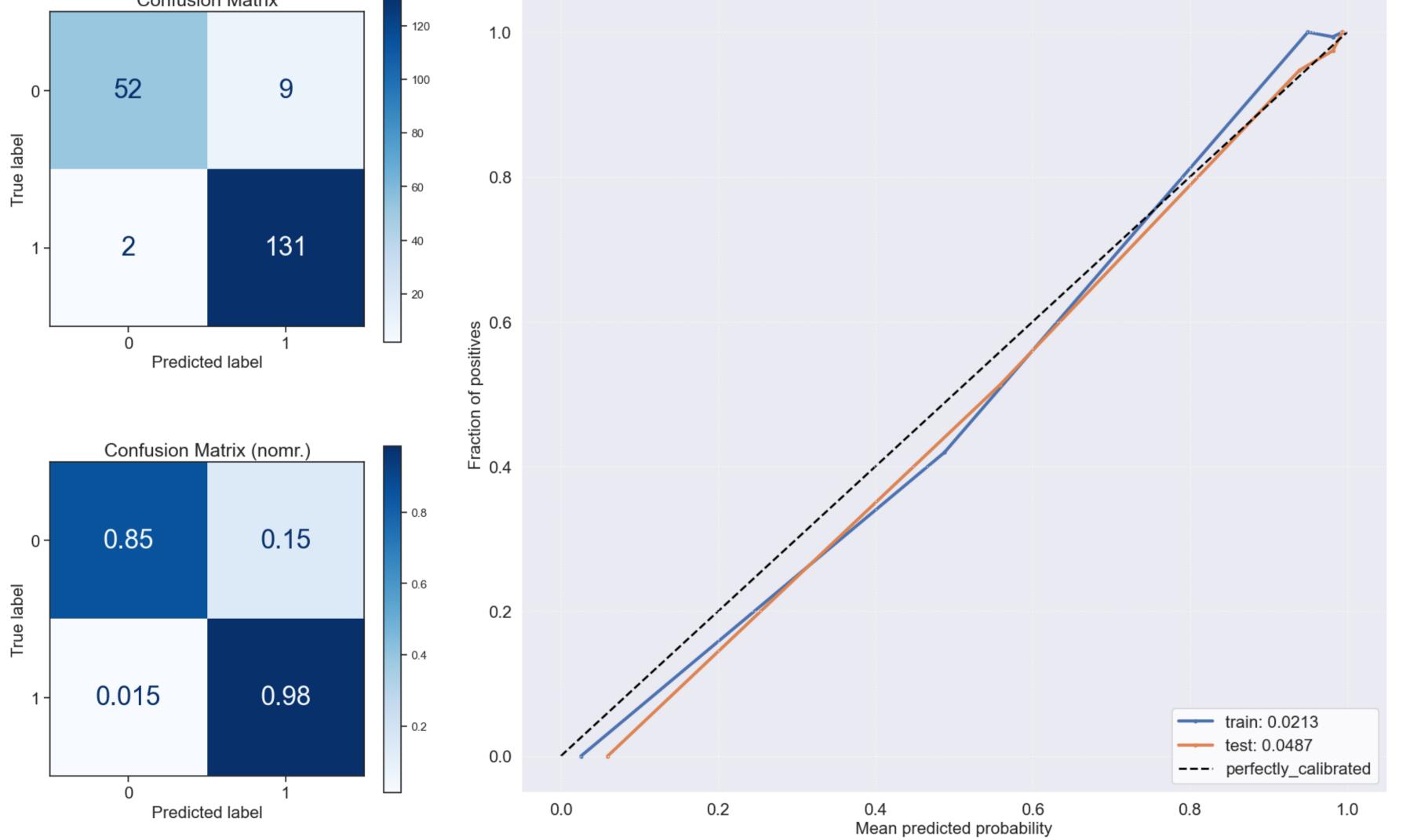
Metric	Train	Test
AUC	0.9993	0.9845
accuracy	0.9858	0.9433
balanced accuracy	0.9776	0.9187
recall_(sens)	1.0	0.985
specificity	0.9553	0.8525
precision	0.9796	0.9357
f1_score	0.9857	0.9423

## Protein: P22894 - metric: precision





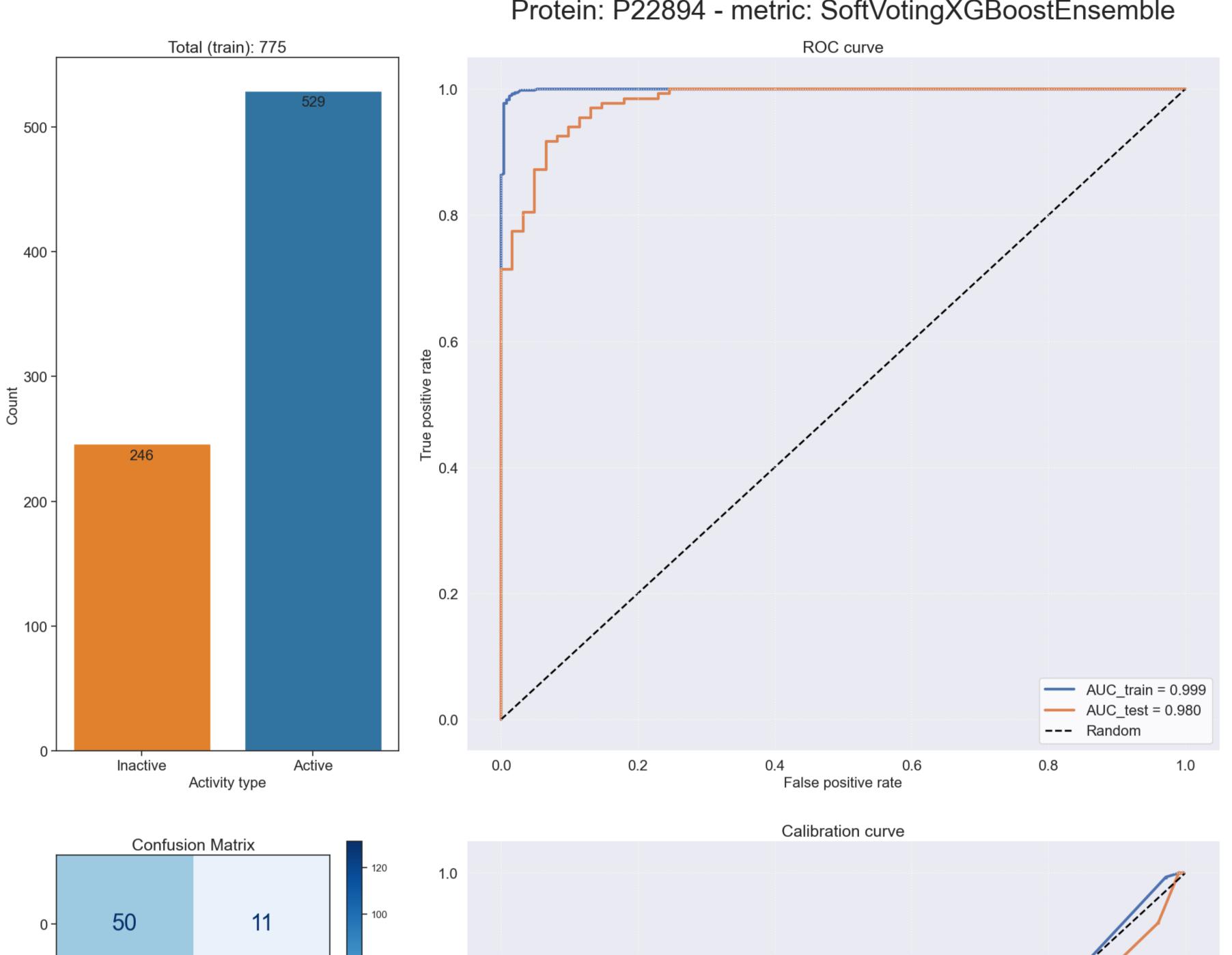
XGBoost Parameters	Value
alpha	3.7299
colsample_bytree	0.8327
gamma	0.6504
lambda	2.8885
learning_rate	0.0695
max_depth	9.0
min_child_weight	3.0
n_estimators	344.0
reg_alpha	0.008
reg_lambda	0.3005
scale_pos_weight	1.151
subsample	0.8689

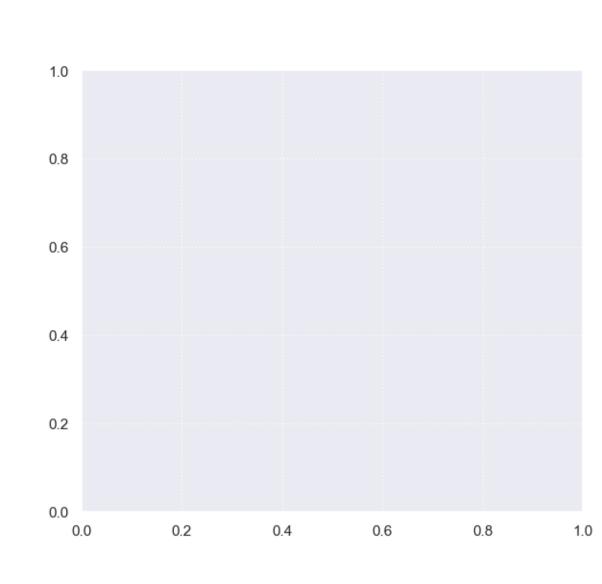


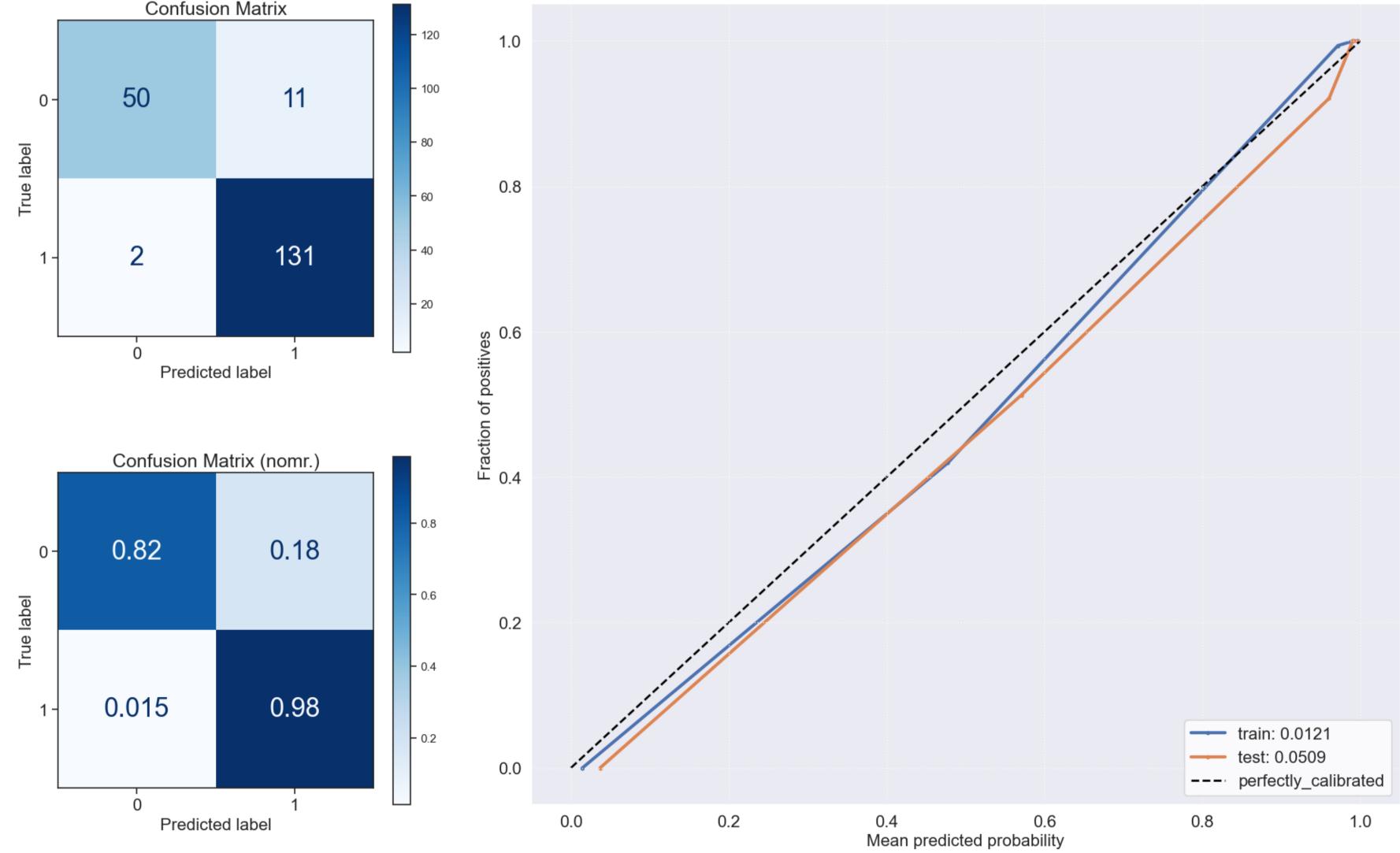
		Activ	e/Inactive probab	ility		
50	Ina			Active	zone	type active (133) inactive (61) decoy (194)
20						
10 5						
	0.0	0.2	(Probability	).6	0.8	1.0

Metric	Train	Test
AUC	0.9965	0.9779
accuracy	0.9768	0.9433
balanced accuracy	0.9678	0.9187
recall_(sens)	0.9924	0.985
specificity	0.9431	0.8525
precision	0.974	0.9357
f1_score	0.9766	0.9423

## Protein: P22894 - metric: SoftVotingXGBoostEnsemble







	Active/Inactive probability					
50 -·····	Inacti	ive zone	Active	zone type active inactive deco	e (133) ive (61) y (194)	
30						
Percent 00						
10						
0 —	0.0 0.2	0.4 Proba	5.5	).8 1	1.0	

Metric	Train	Test
AUC	0.9991	0.9799
accuracy	0.9871	0.933
balanced accuracy	0.9808	0.9023
recall_(sens)	0.9981	0.985
specificity	0.9634	0.8197
precision	0.9832	0.9225
f1_score	0.987	0.9314