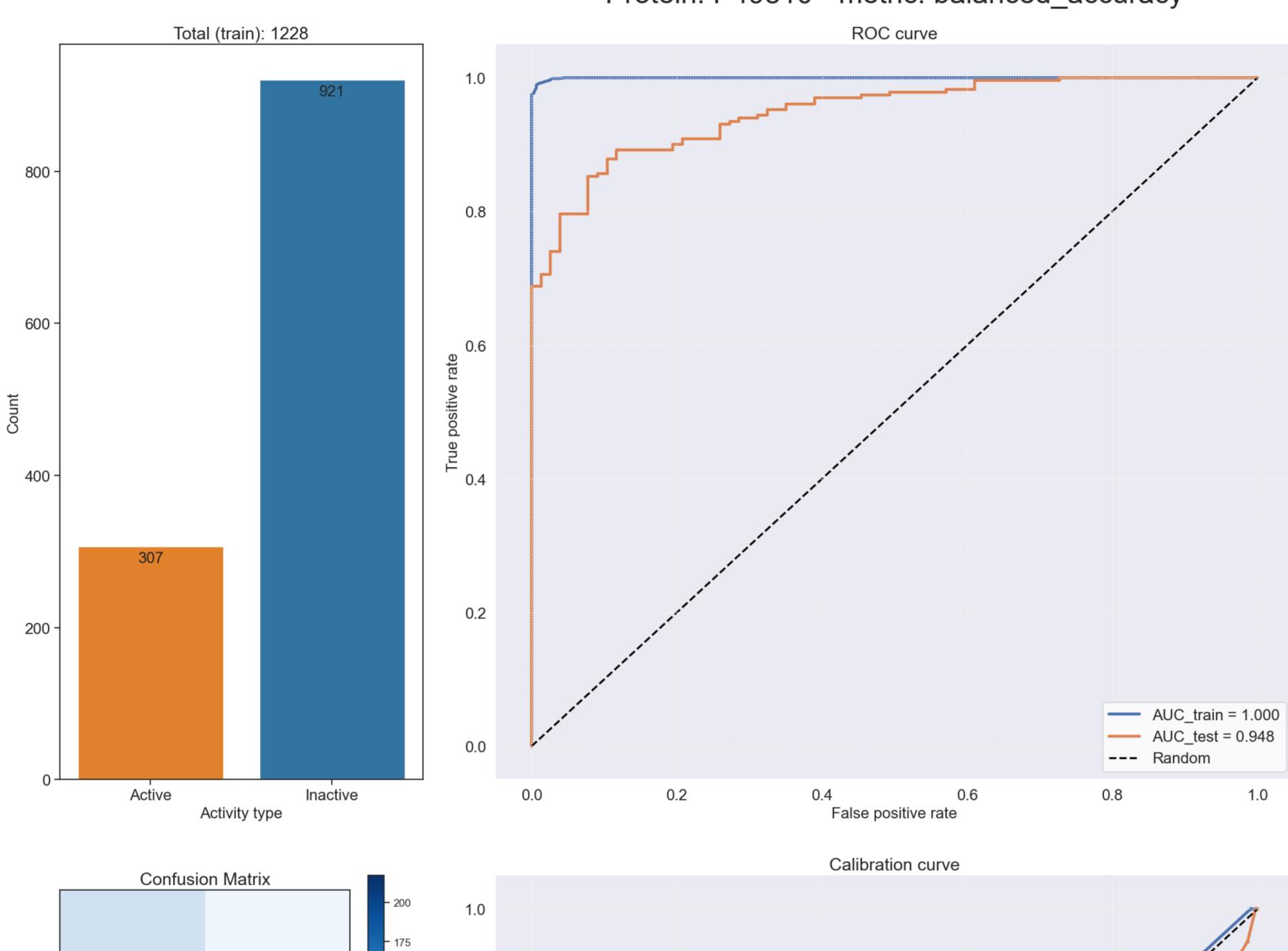
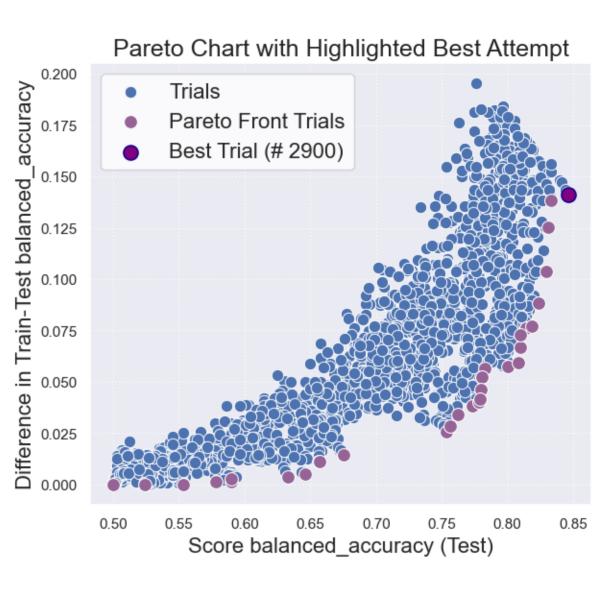
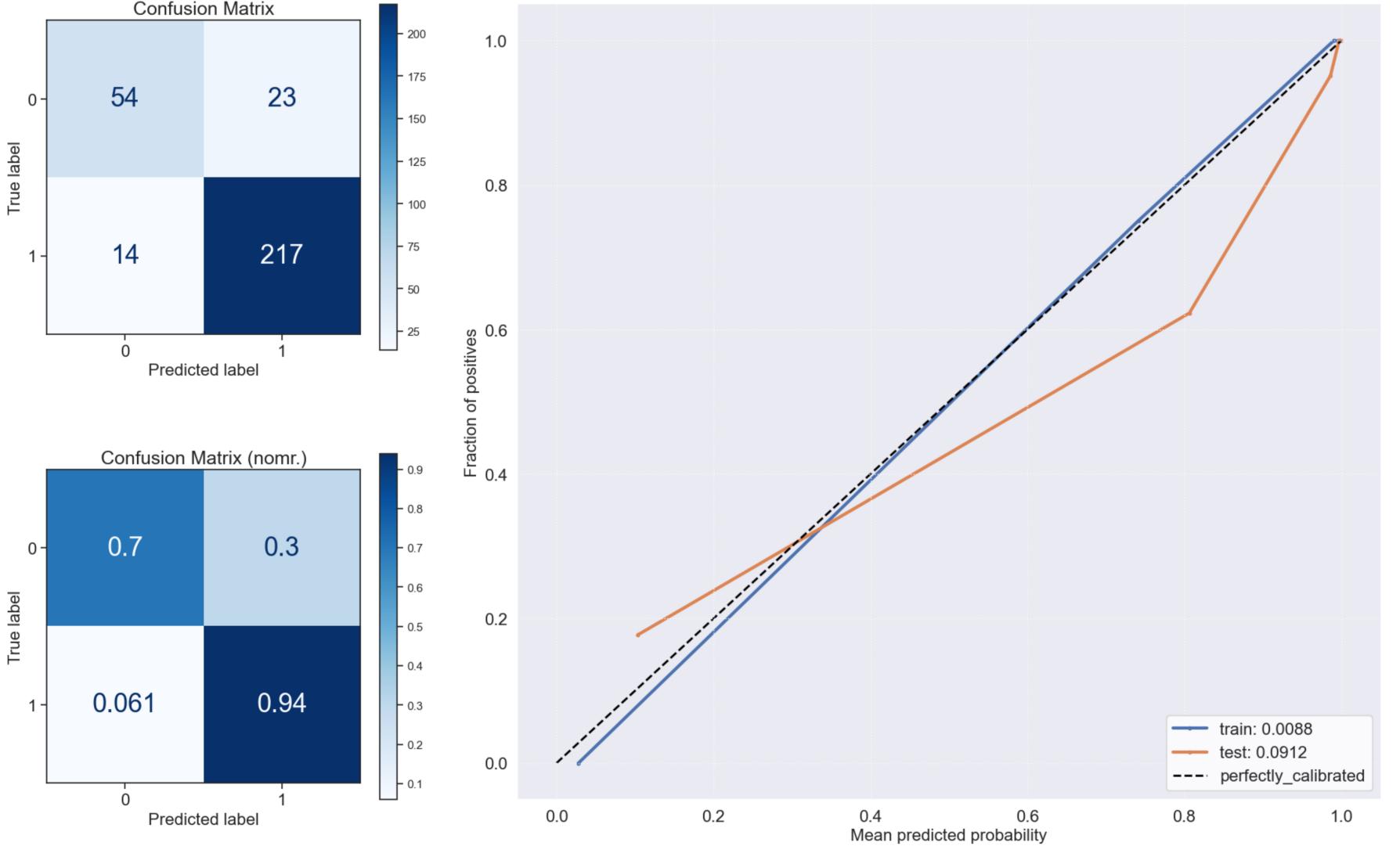
Protein: P49810 - metric: balanced_accuracy





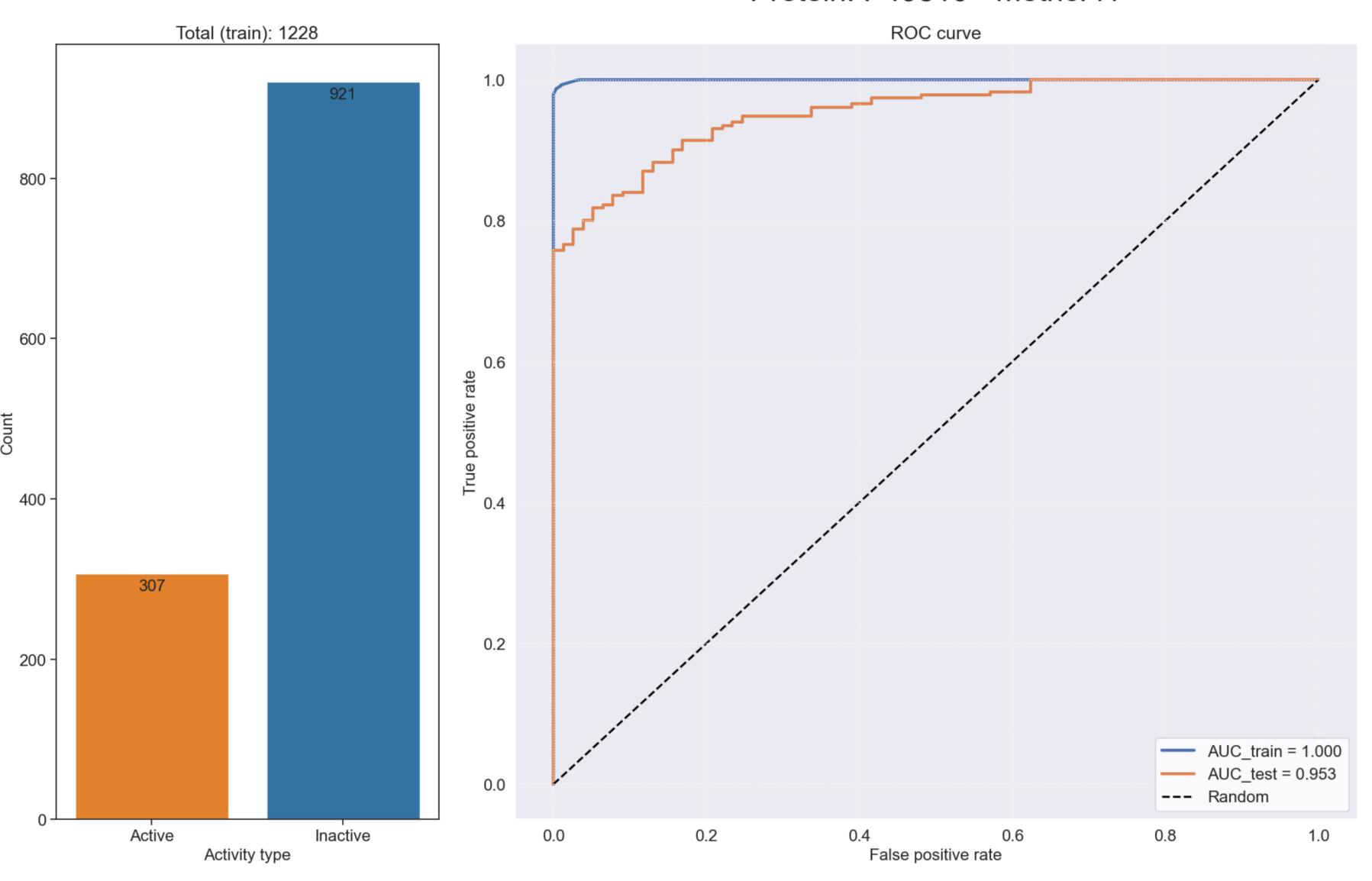
XGBoost Parameters	Value
alpha	0.6704
colsample_bytree	0.9962
gamma	0.0751
lambda	2.8912
learning_rate	0.0406
max_depth	10.0
min_child_weight	1.0
n_estimators	969.0
reg_alpha	0.3215
reg_lambda	0.4357
scale_pos_weight	1.0522
subsample	0.5344

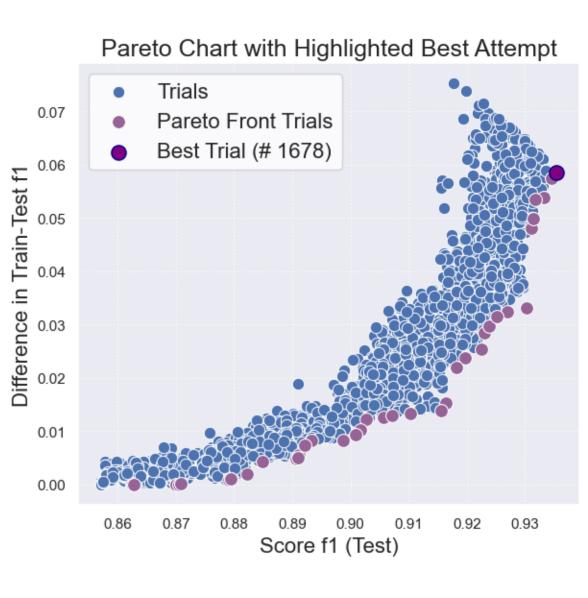


			Active/Inacti	ve probability		
60		Inactive zone			Active zone	inactive (77) decoy (307)
40						
20						
10						
0 —	0.0	0.2	0.4 Prob	0.6 ability	0.8	1.0

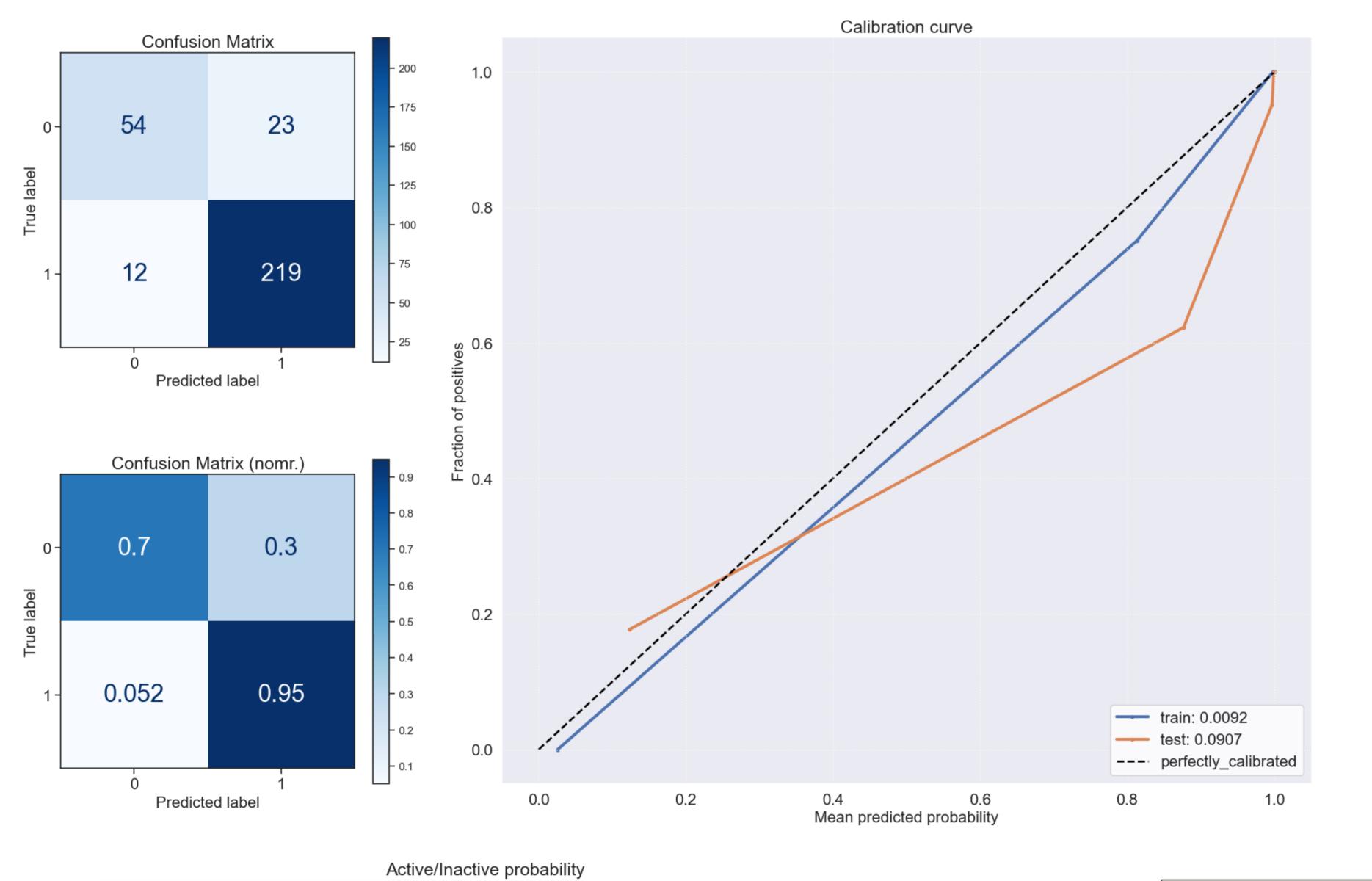
Metric	Train	Test
AUC	0.9997	0.9484
accuracy	0.9919	0.8799
balanced accuracy	0.9859	0.8203
recall_(sens)	0.9978	0.9394
specificity	0.9739	0.7013
precision	0.9914	0.9042
f1_score	0.9918	0.8773

Protein: P49810 - metric: f1





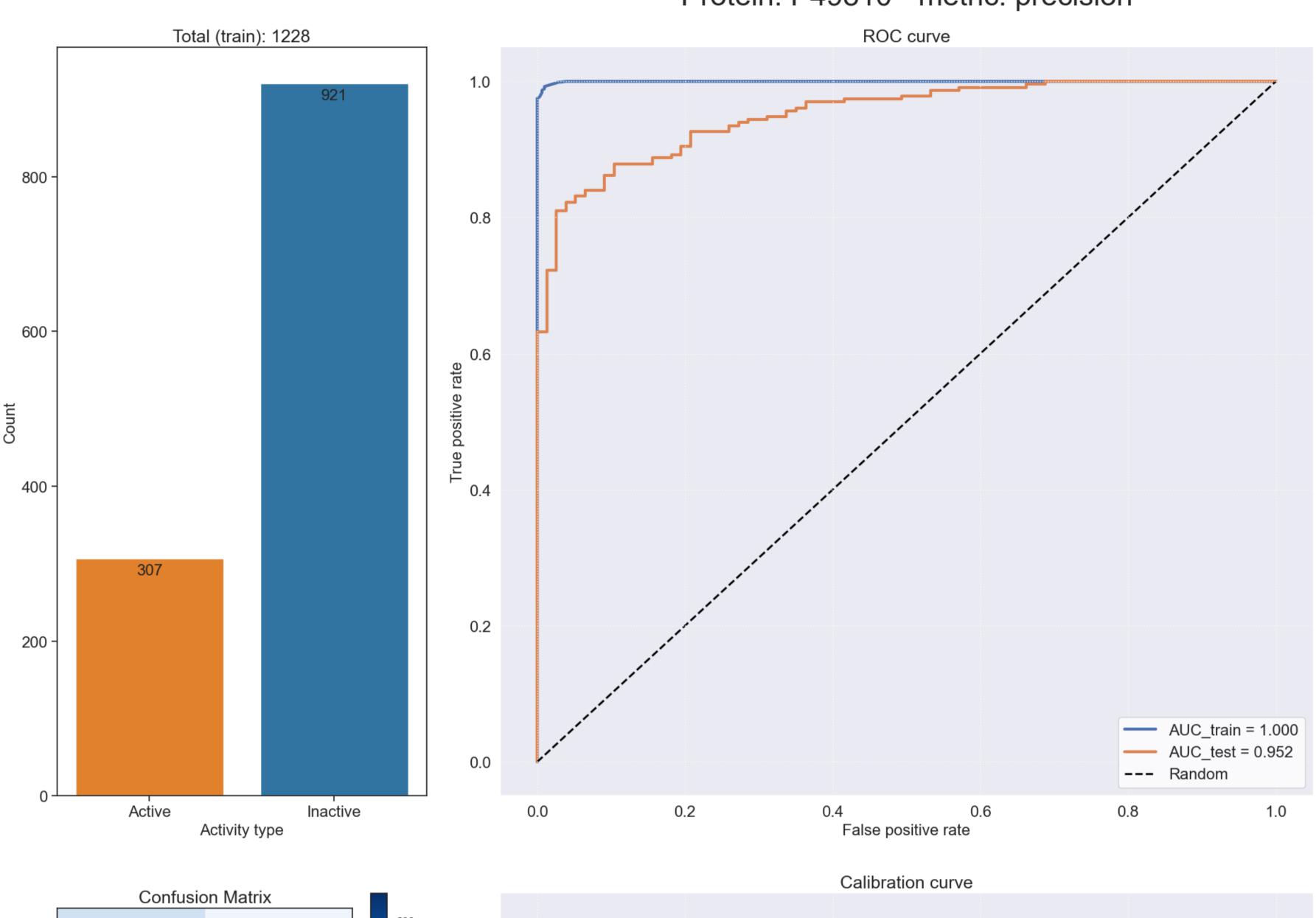
XGBoost Parameters	Value
alpha	0.0915
colsample_bytree	0.8102
gamma	0.1289
lambda	0.6002
learning_rate	0.1249
max_depth	9.0
min_child_weight	2.0
n_estimators	624.0
reg_alpha	0.0164
reg_lambda	0.7705
scale_pos_weight	4.9177
subsample	0.9343

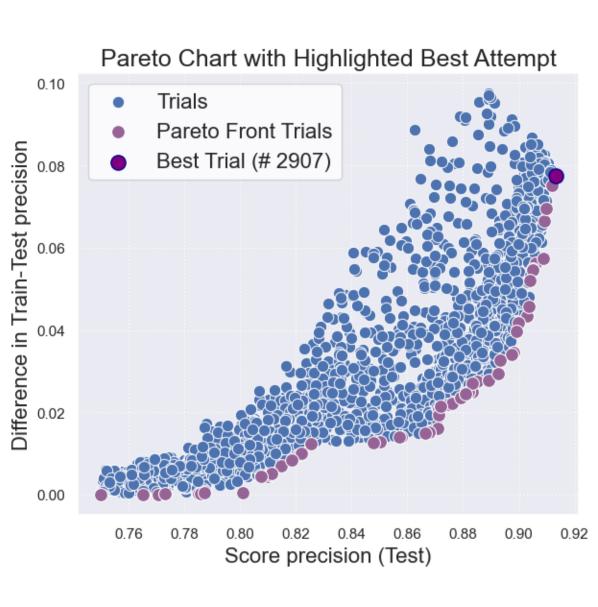


80					
00	Inactive :	zone	A	Active zone	active (231) inactive (77)
70					
60					
50					
# 50		ļ.			
Percent 04		-			
Pe					
30					
20					
10 -					
10	L	-			
0					
	0.0 0.2	0.4	0.6	0.8	1.0
		Probab	ility		

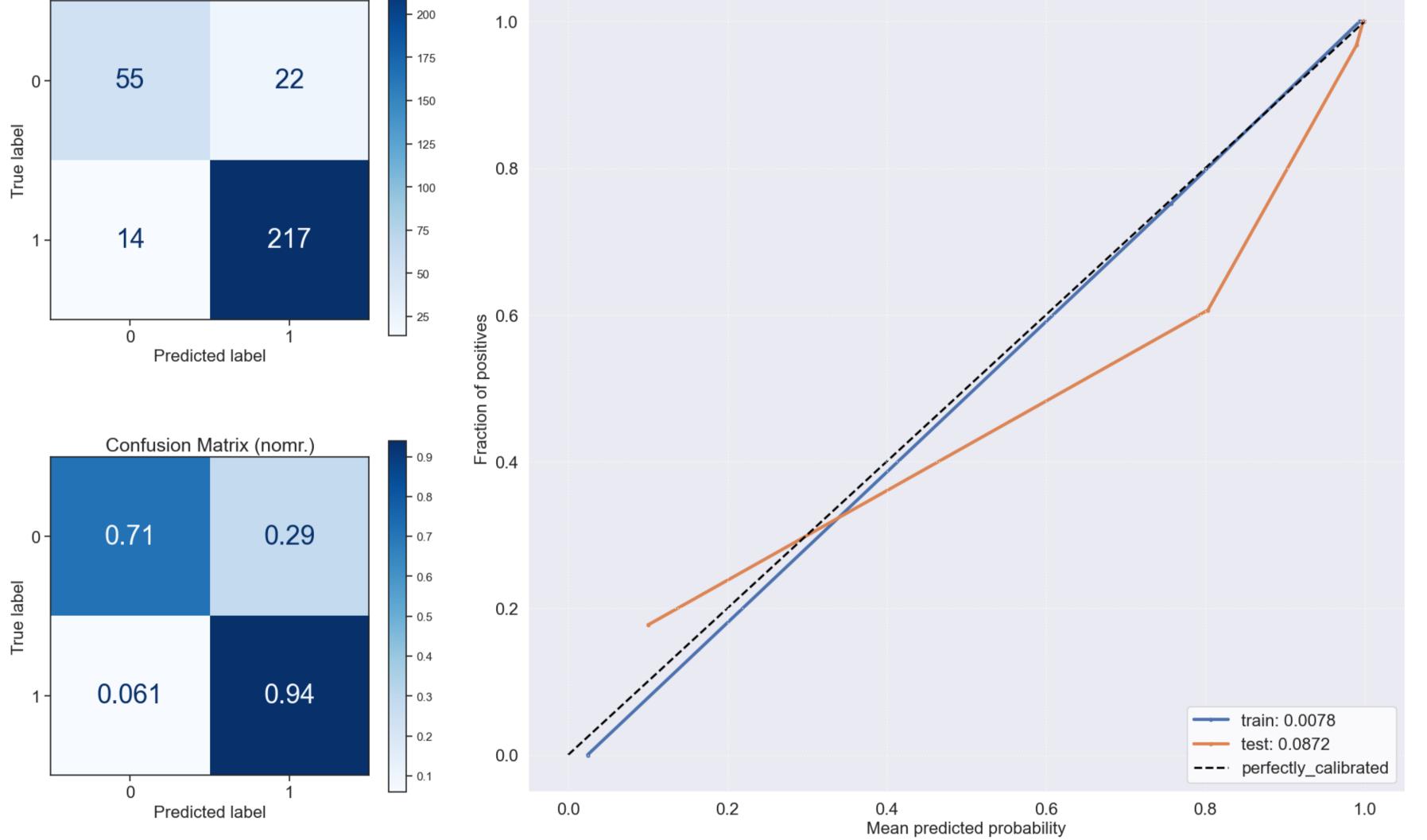
Metric	Train	Test
AUC	0.9998	0.9534
accuracy	0.991	0.8864
balanced accuracy	0.9821	0.8247
recall_(sens)	1.0	0.9481
specificity	0.9642	0.7013
precision	0.9882	0.905
f1_score	0.991	0.8833

Protein: P49810 - metric: precision





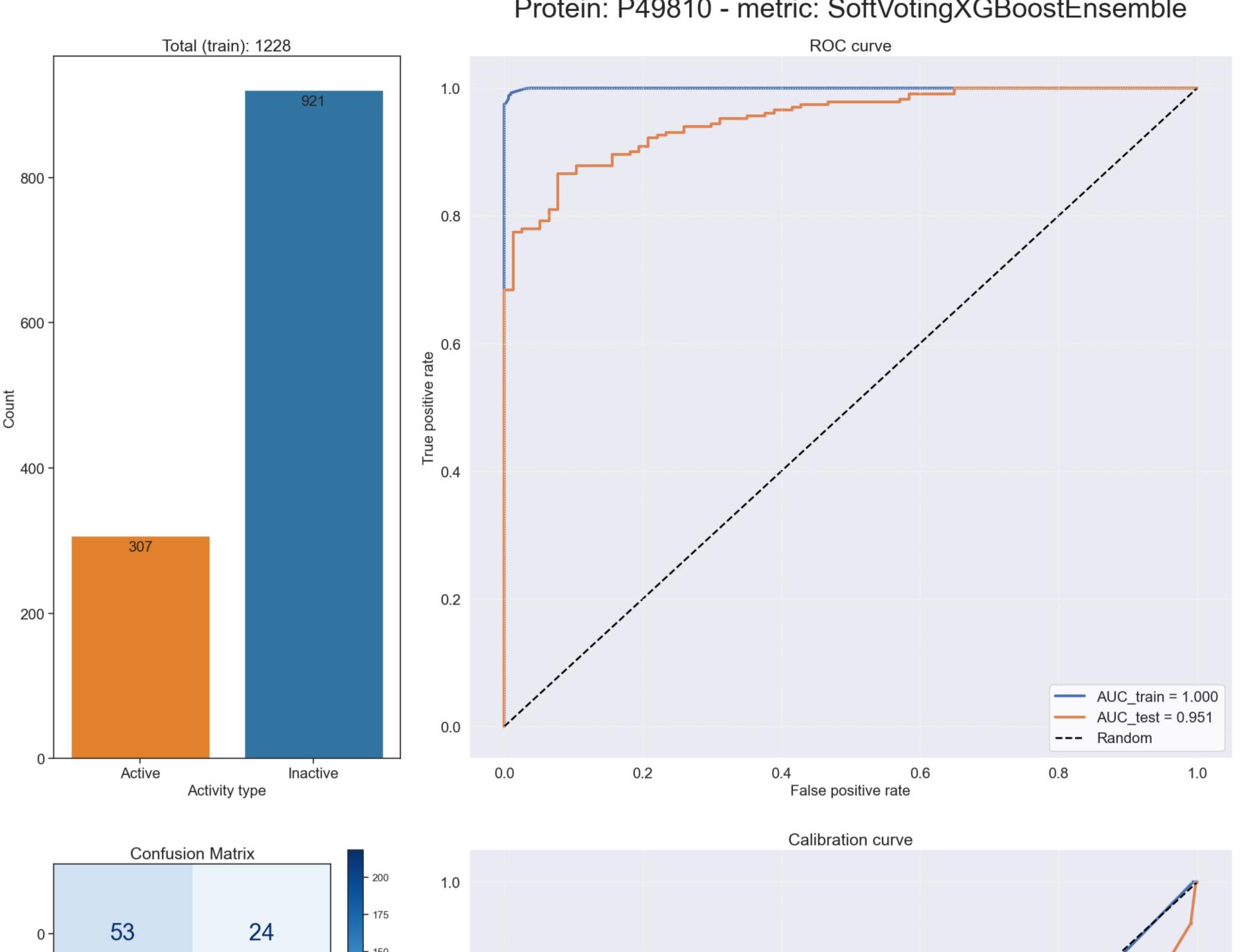
XGBoost Parameters	Value
alpha	3.0947
colsample_bytree	0.8258
gamma	0.2176
lambda	1.2772
learning_rate	0.1161
max_depth	9.0
min_child_weight	1.0
n_estimators	976.0
reg_alpha	0.3139
reg_lambda	0.5603
scale_pos_weight	1.3206
subsample	0.7715

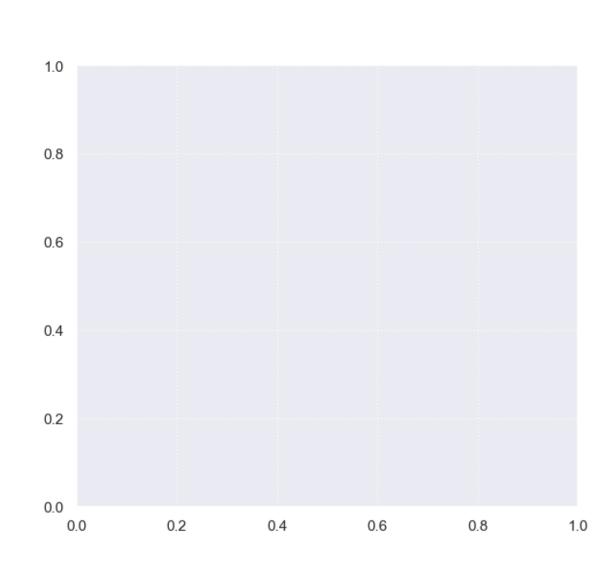


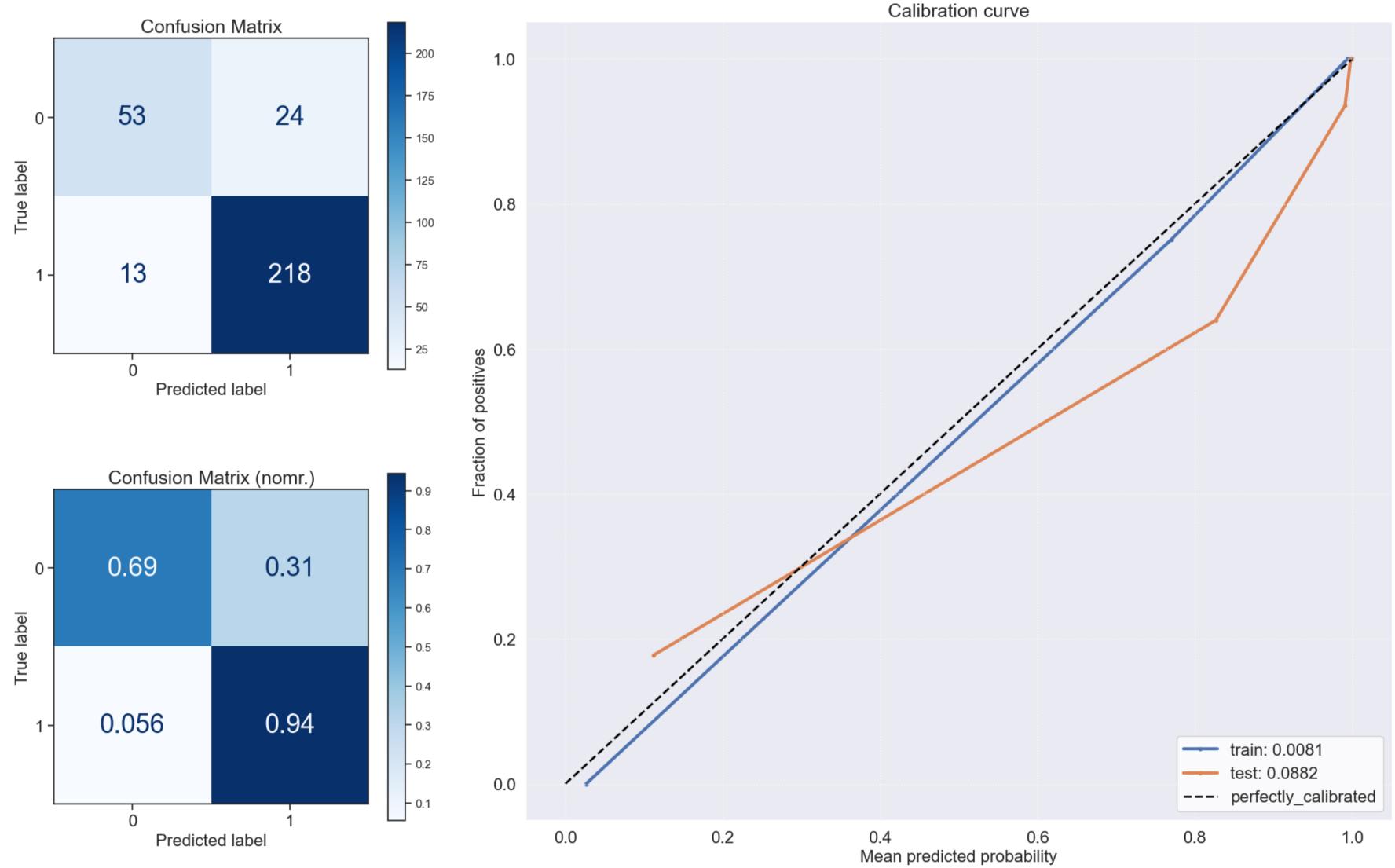
70	:	Active/Inactiv			
70	Inactive zone			Active zone	type active (231) inactive (77)
50					decoy (307)
tu 40					
Percent 30					
20					
10					
0 —	0.0 0.2	0.4 Proba	0.6 bility	0.8	1.0

Metric	Train	Test
AUC	0.9997	0.9517
accuracy	0.9919	0.8831
balanced accuracy	0.9848	0.8268
recall_(sens)	0.9989	0.9394
specificity	0.9707	0.7143
precision	0.9903	0.9079
f1_score	0.9918	0.8809

Protein: P49810 - metric: SoftVotingXGBoostEnsemble







		Active	Inactive probabil	ity		
70	Inact	tive zone		Active zo	one active	e (231) ve (77)
60					decoy	y (307)
50						
Percent 30 -						
20						
10						
· ·	0.0 0.2	0.4	0.0 Probability	6 0.8	1	.0

Metric	Train	Test
AUC	0.9997	0.9514
accuracy	0.9919	0.8799
balanced accuracy	0.9848	0.816
recall_(sens)	0.9989	0.9437
specificity	0.9707	0.6883
precision	0.9903	0.9008
f1_score	0.9918	0.8766