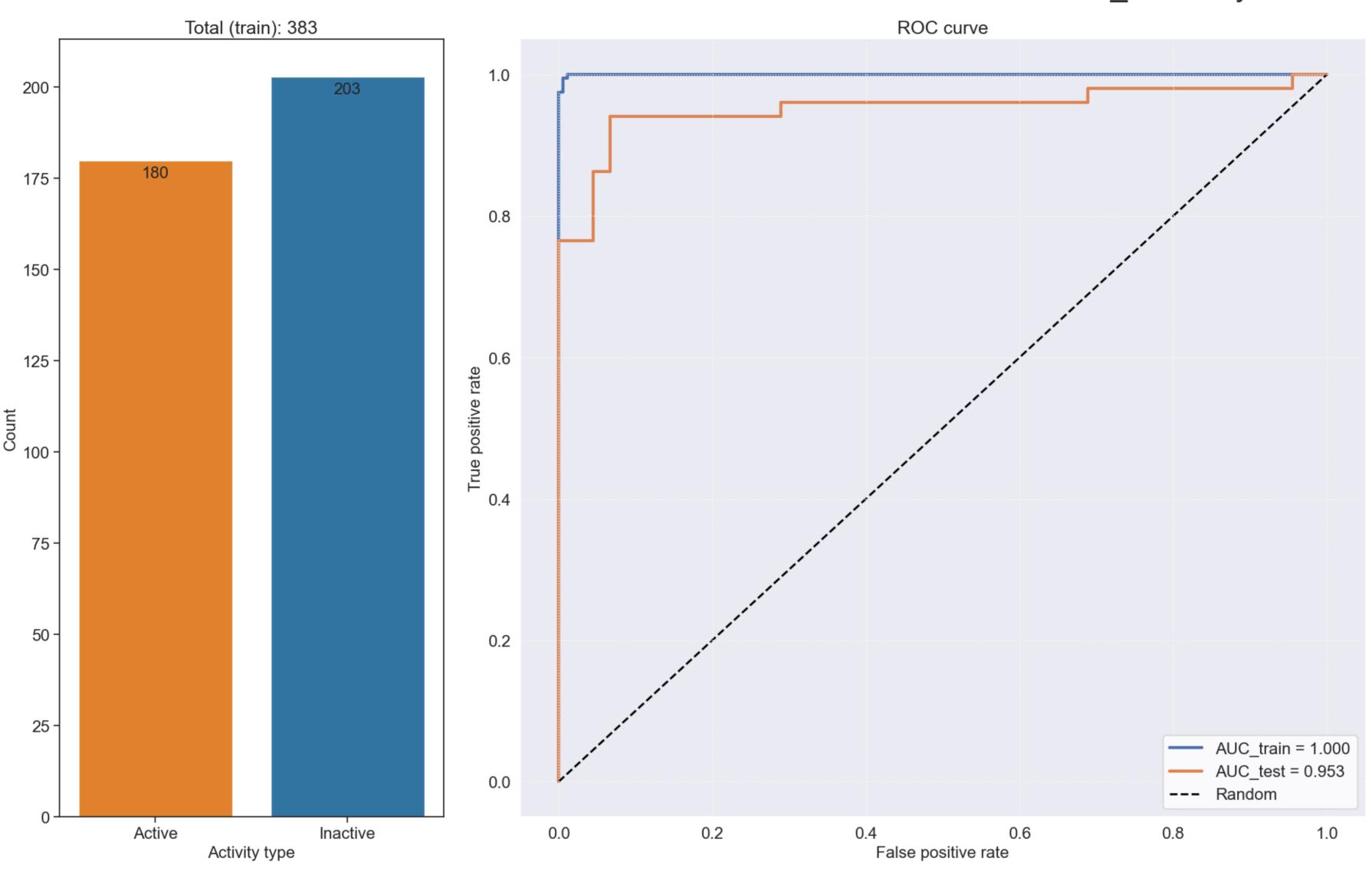
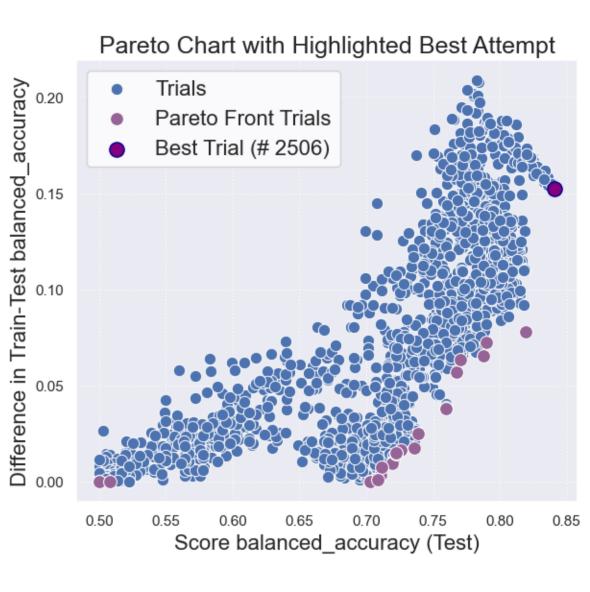
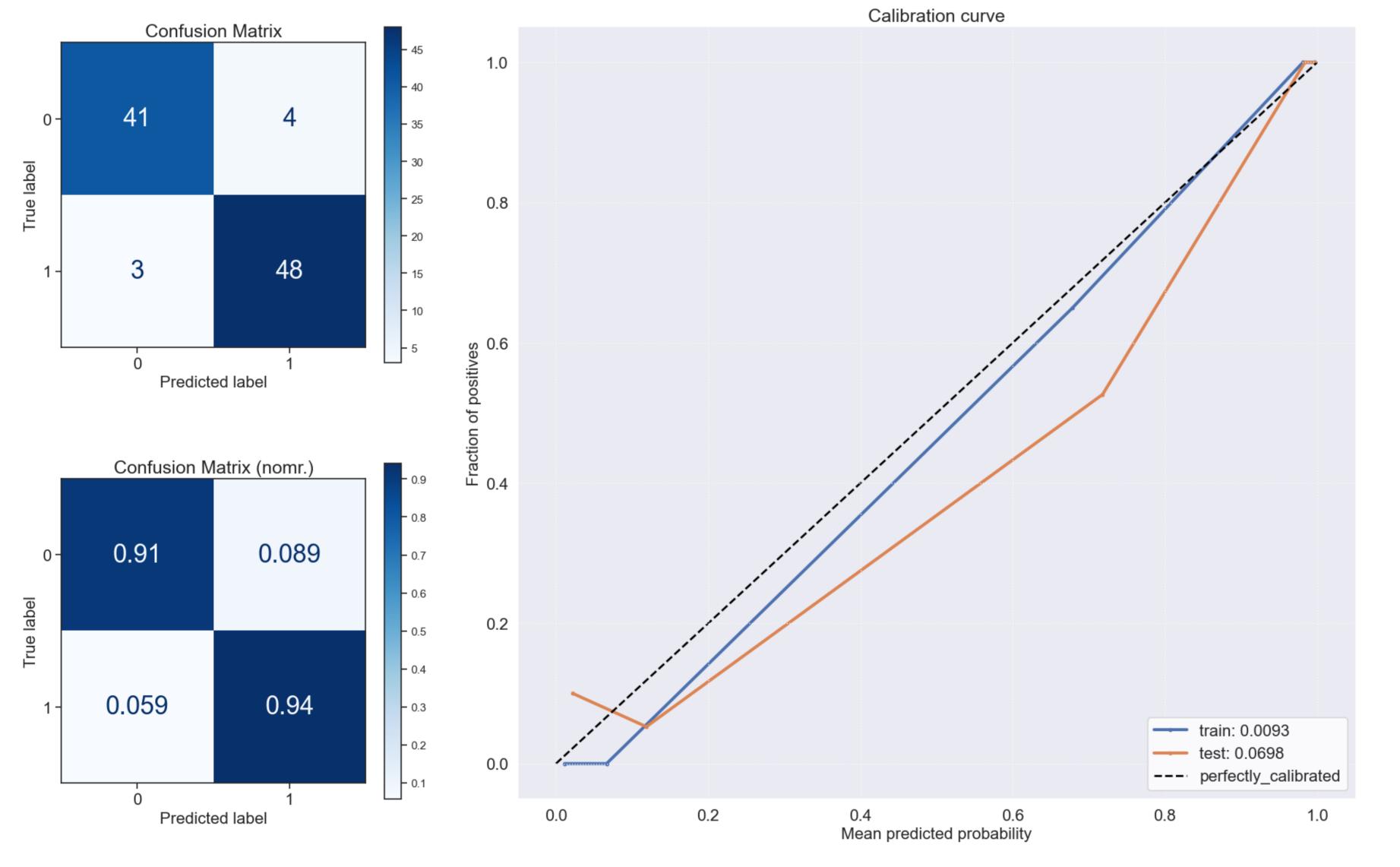
Protein: Q14524 - metric: balanced_accuracy





XGBoost Parameters	Value
alpha	0.1365
colsample_bytree	0.746
gamma	0.0813
lambda	2.6206
learning_rate	0.038
max_depth	7.0
min_child_weight	2.0
n_estimators	457.0
reg_alpha	0.1509
reg_lambda	0.234
scale_pos_weight	1.994
subsample	0.9118

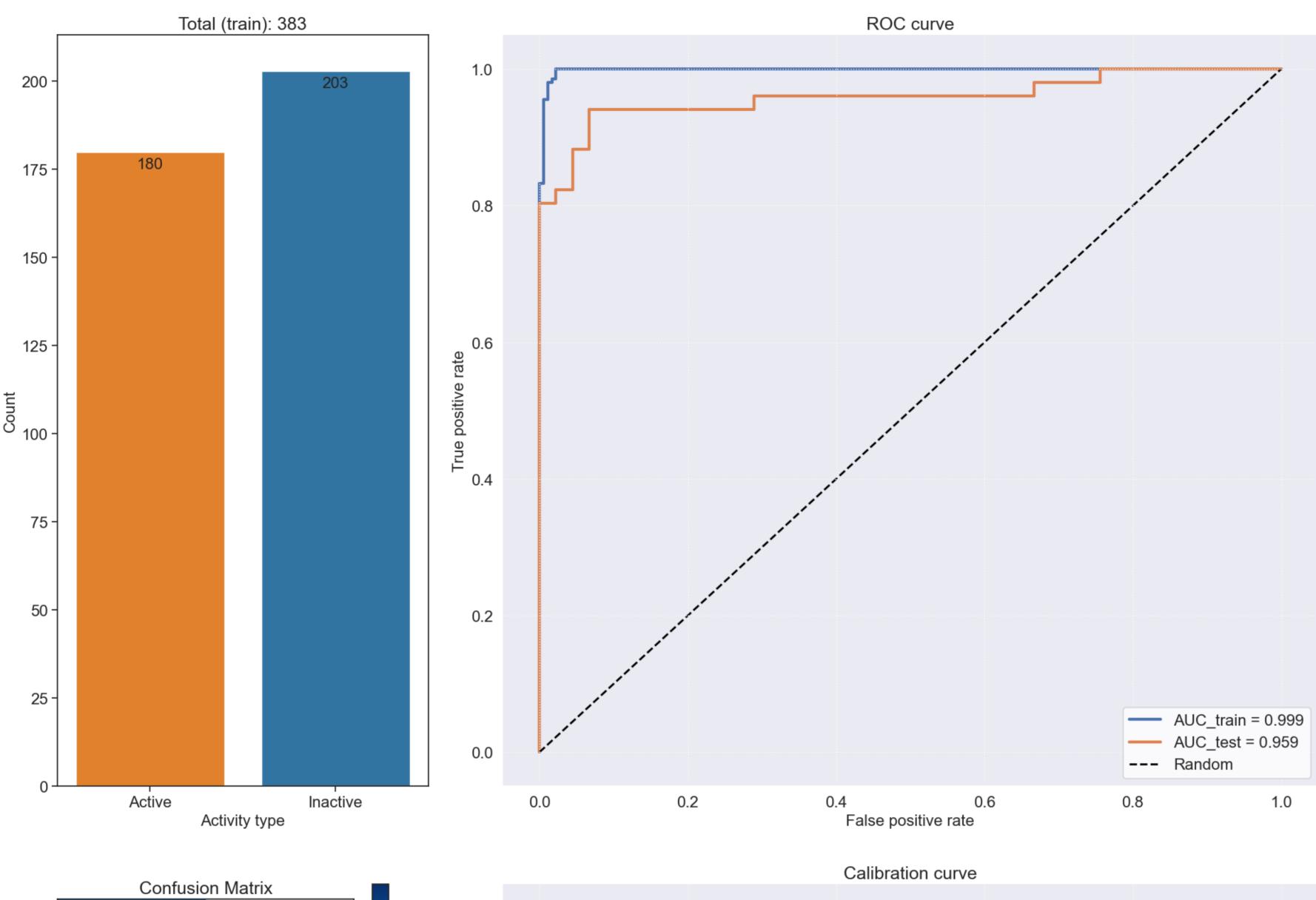


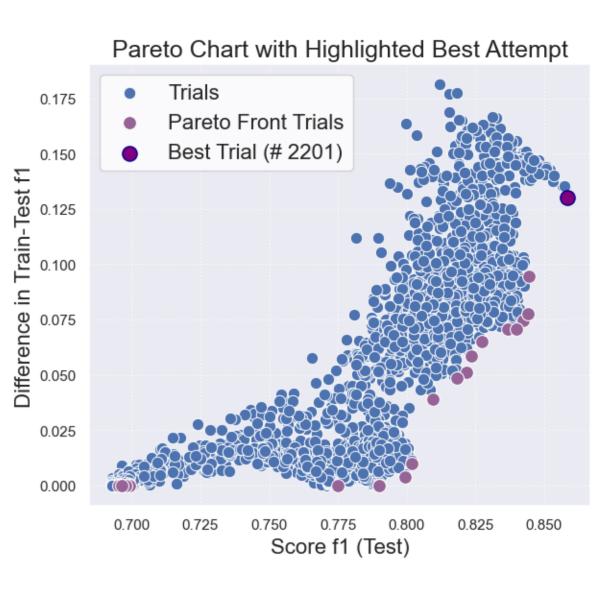
50		Inactive zone			Active		type active (51) inactive (45)
40							decoy (96)
Perc							
10							
0							
,	0.0	0.2	0.4 Pro	0. bability	6	0.8	1.0

Active/Inactive probability

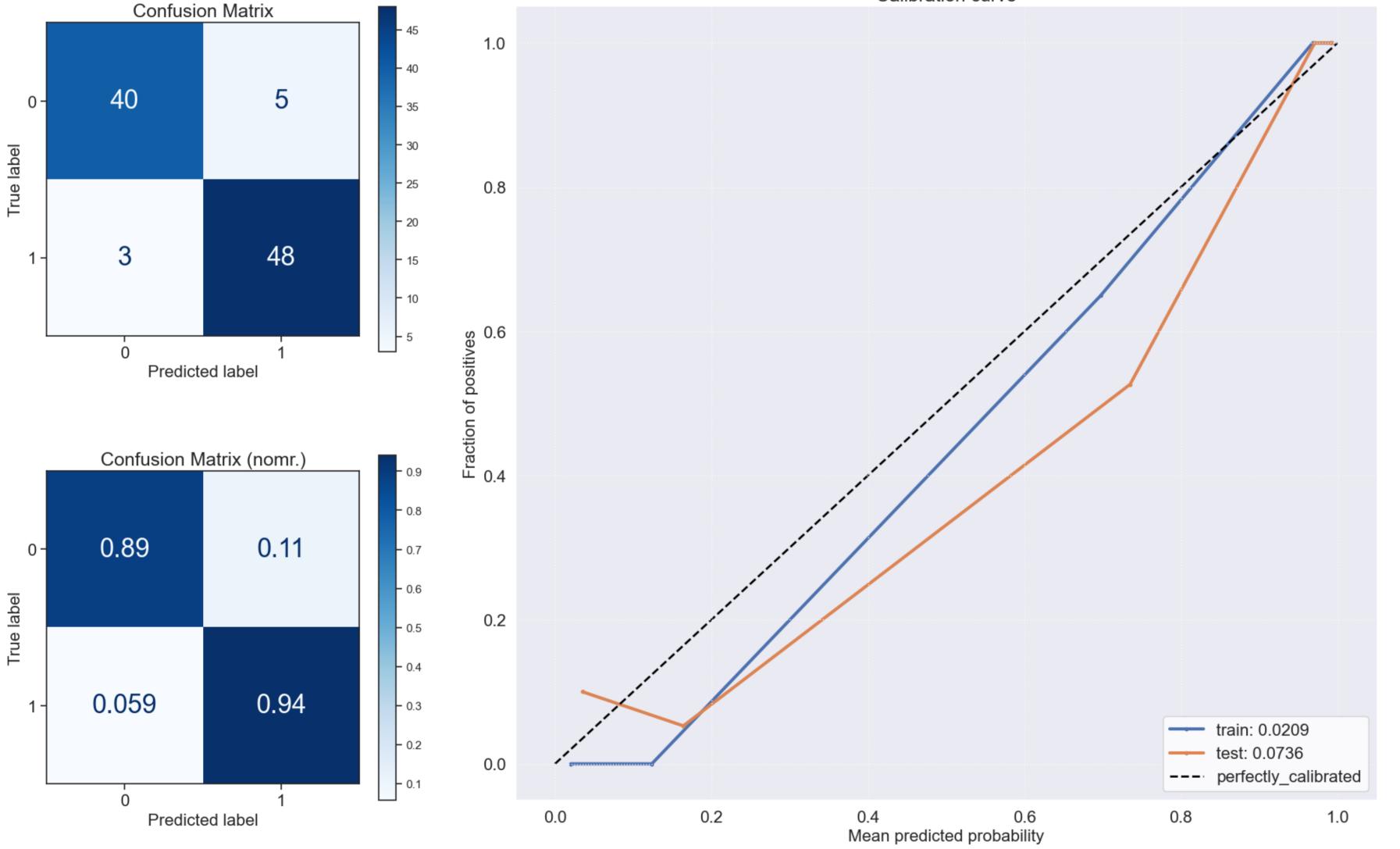
Metric	Train	Test
AUC	0.9998	0.9525
accuracy	0.9922	0.9271
balanced accuracy	0.9917	0.9261
recall_(sens)	1.0	0.9412
specificity	0.9833	0.9111
precision	0.9854	0.9231
f1_score	0.9922	0.927

Protein: Q14524 - metric: f1





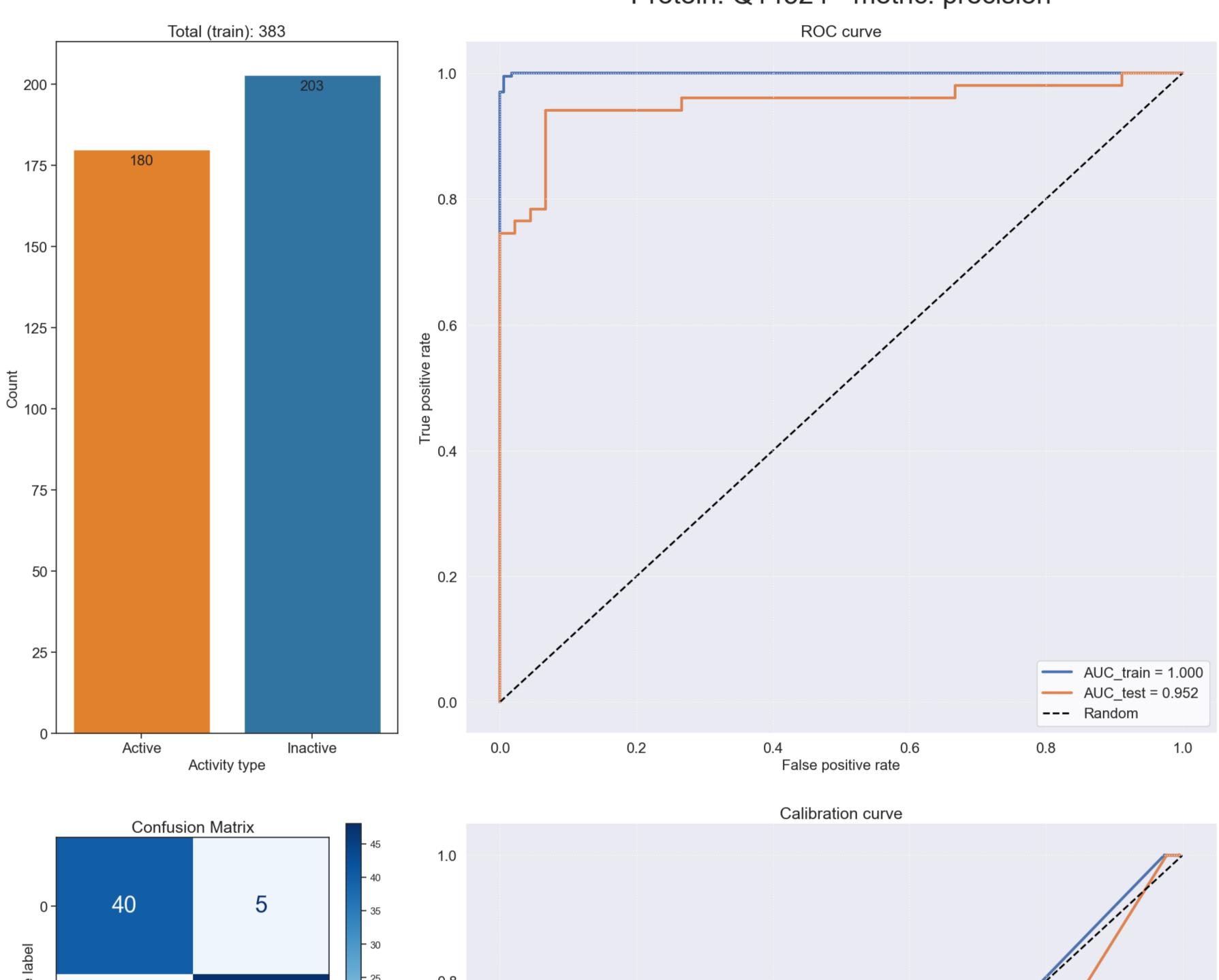
XGBoost Parameters	Value
alpha	2.0824
colsample_bytree	0.7352
gamma	0.8581
lambda	0.8554
learning_rate	0.1441
max_depth	10.0
min_child_weight	2.0
n_estimators	506.0
reg_alpha	0.2308
reg_lambda	0.5568
scale_pos_weight	2.0814
subsample	0.801

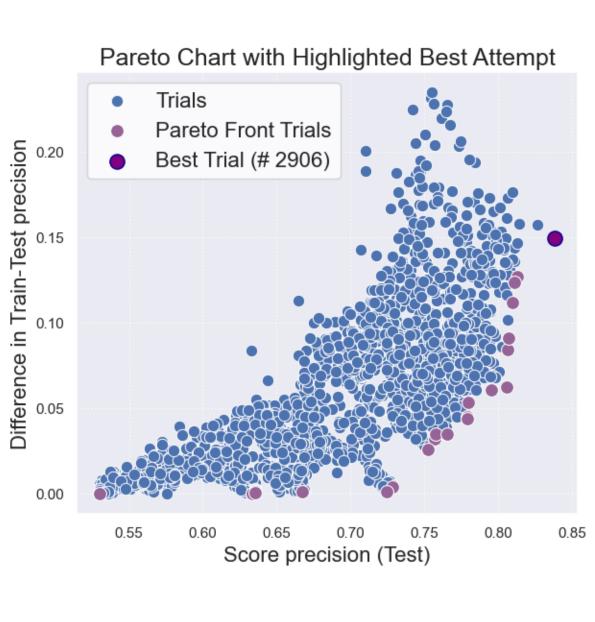


			Active/Inactiv	e probability		
00		Inactive zone			Active zone	type active (51) inactive (45) decoy (96)
25						
Percent 02						
15						
5						
0						
	0.0	0.2	0.4 Proba	0.6 ability	0.8	1.0

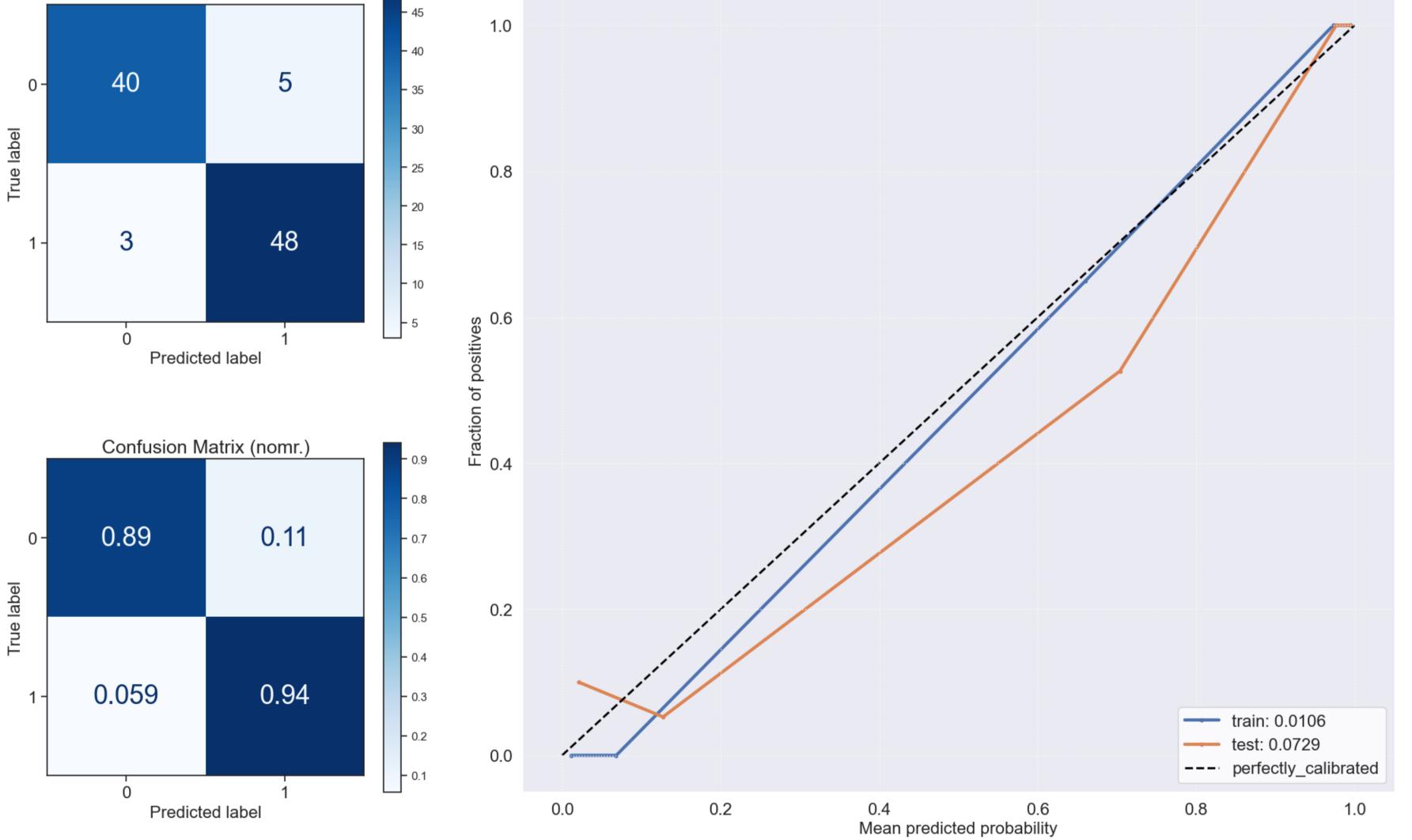
Metric	Train	Test
AUC	0.9986	0.9595
accuracy	0.9896	0.9167
balanced accuracy	0.9889	0.915
recall_(sens)	1.0	0.9412
specificity	0.9778	0.8889
precision	0.9807	0.9057
f1_score	0.9895	0.9165

Protein: Q14524 - metric: precision



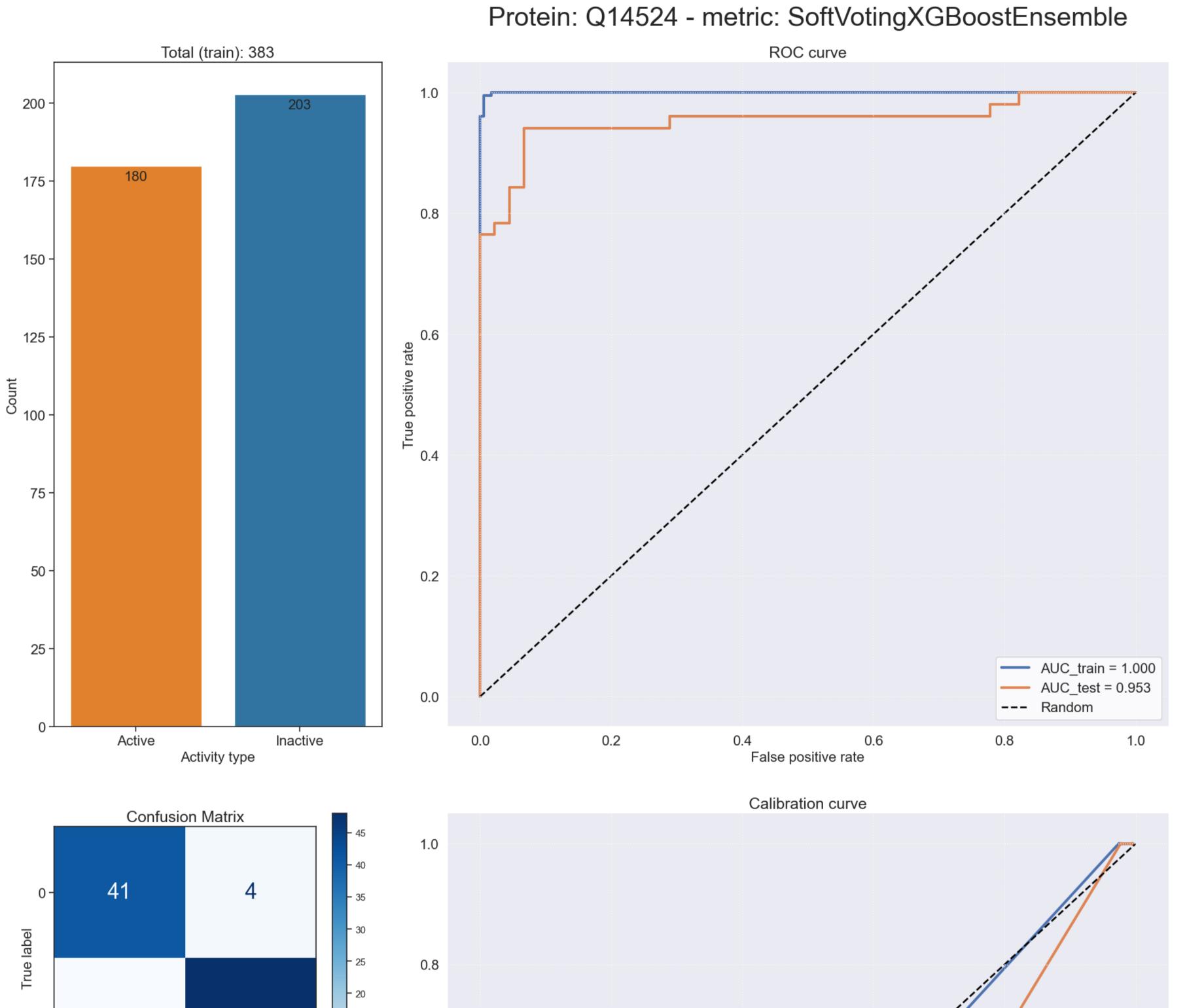


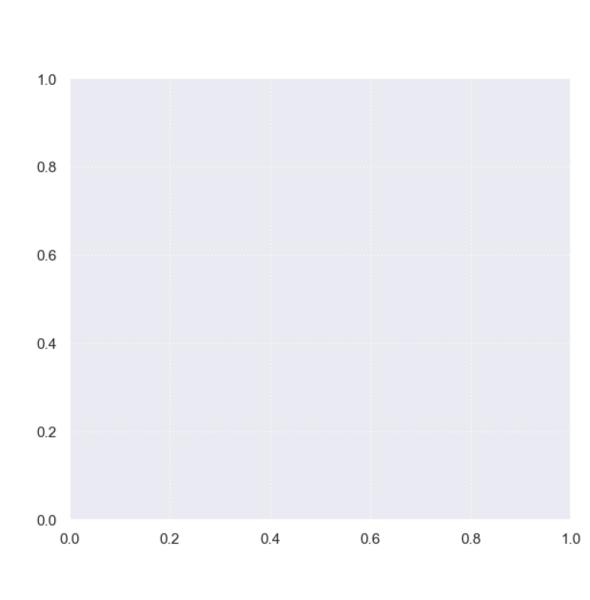
XGBoost Parameters	Value
alpha	0.4901
colsample_bytree	0.9064
gamma	0.5659
lambda	2.8064
learning_rate	0.0621
max_depth	7.0
min_child_weight	1.0
n_estimators	844.0
reg_alpha	0.0671
reg_lambda	0.7017
scale_pos_weight	1.5631
subsample	0.7889

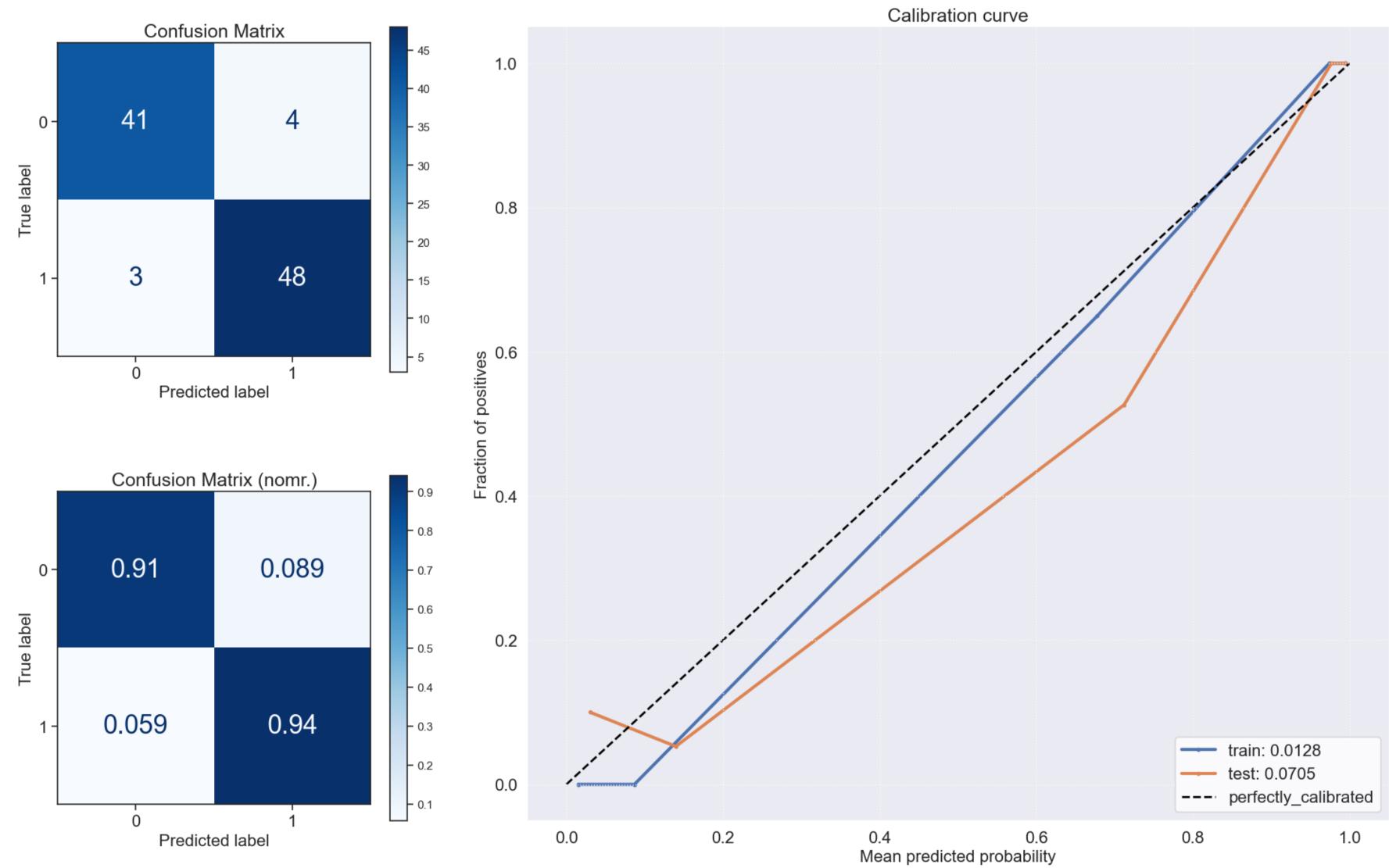


		Active/Inactive probab	oility		
50	Inactive zone		Active	zone	type active (51) inactive (45) decoy (96)
40					
Percent 08					
20					П
0					
	0.0 0.2	0.4 (Probability	0.6	0.8	1.0

Metric	Train	Test
AUC	0.9998	0.9521
accuracy	0.9922	0.9167
balanced accuracy	0.9917	0.915
recall_(sens)	1.0	0.9412
specificity	0.9833	0.8889
precision	0.9854	0.9057
f1_score	0.9922	0.9165







		Ac	tive/Inactive	probability		
40		active zone			Active zone	type active (51) inactive (45) decoy (96)
30						
Percent 0						
10						
0 —	0.0 0	.2 0	.4 Probabil	0.6 ity	0.8	1.0

Metric	Train	Test
AUC	0.9997	0.9534
accuracy	0.9922	0.9271
balanced accuracy	0.9917	0.9261
recall_(sens)	1.0	0.9412
specificity	0.9833	0.9111
precision	0.9854	0.9231
f1_score	0.9922	0.927