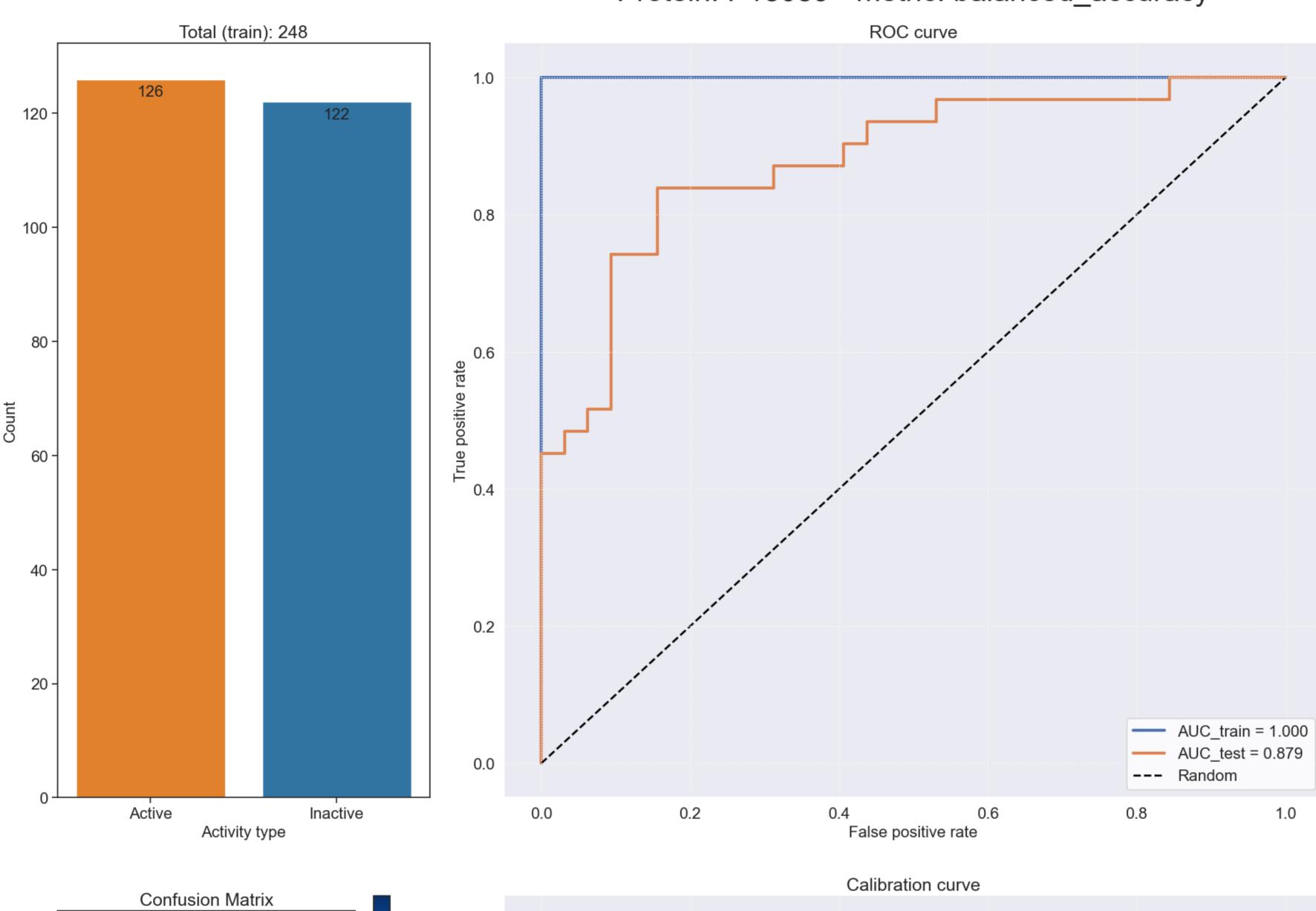
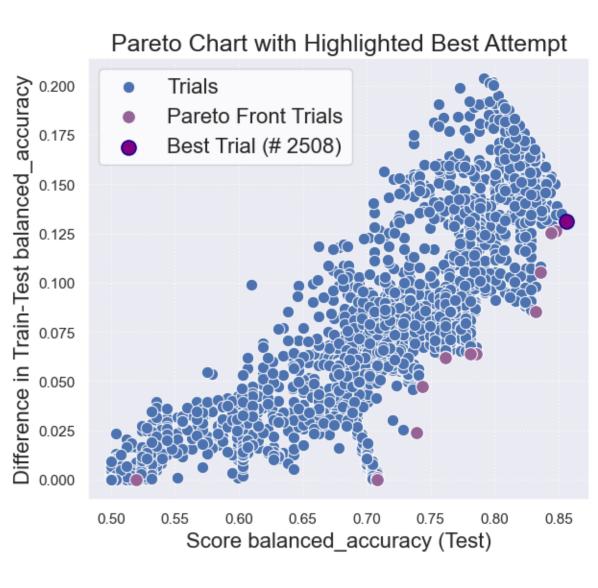
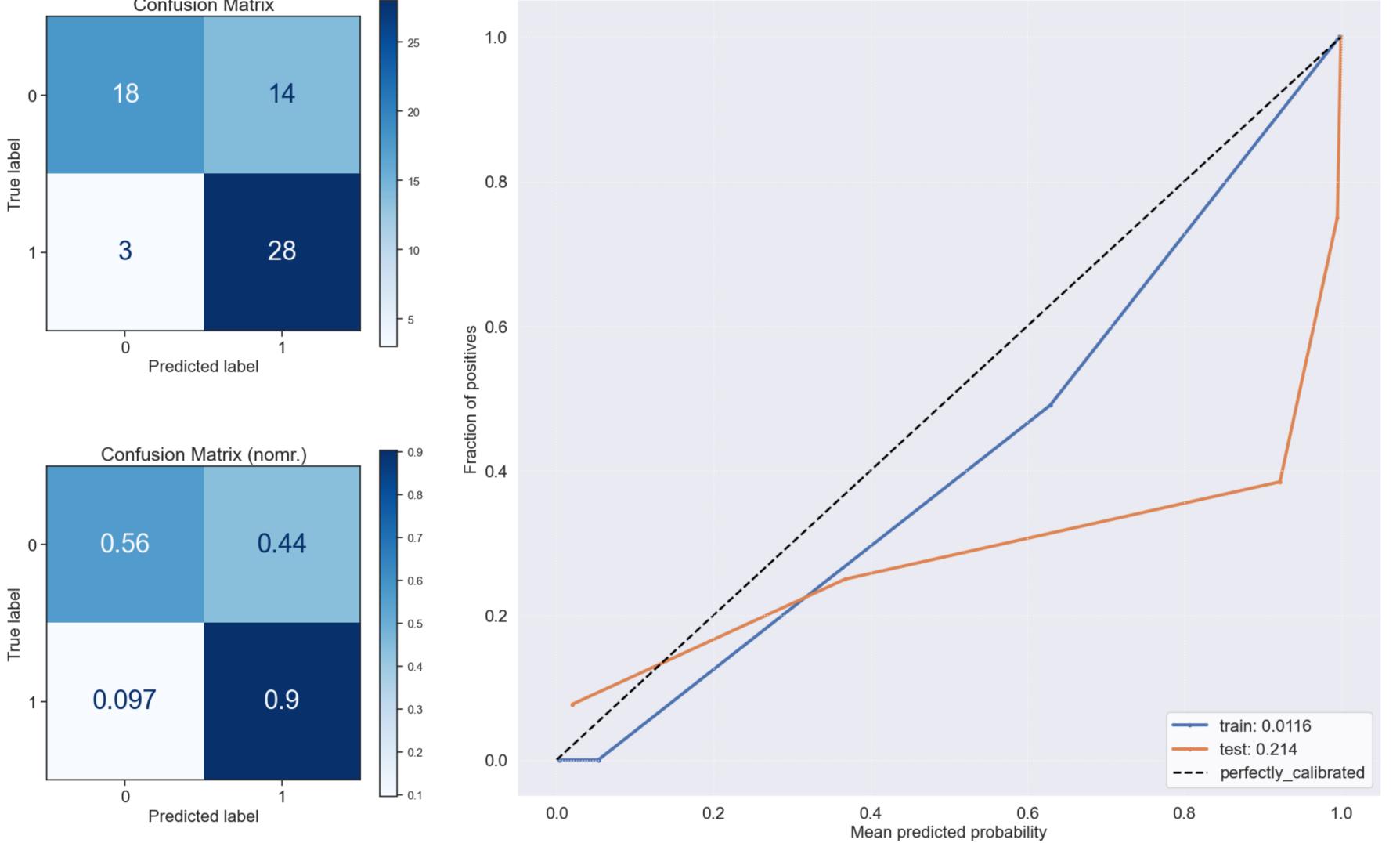
Protein: P18089 - metric: balanced_accuracy





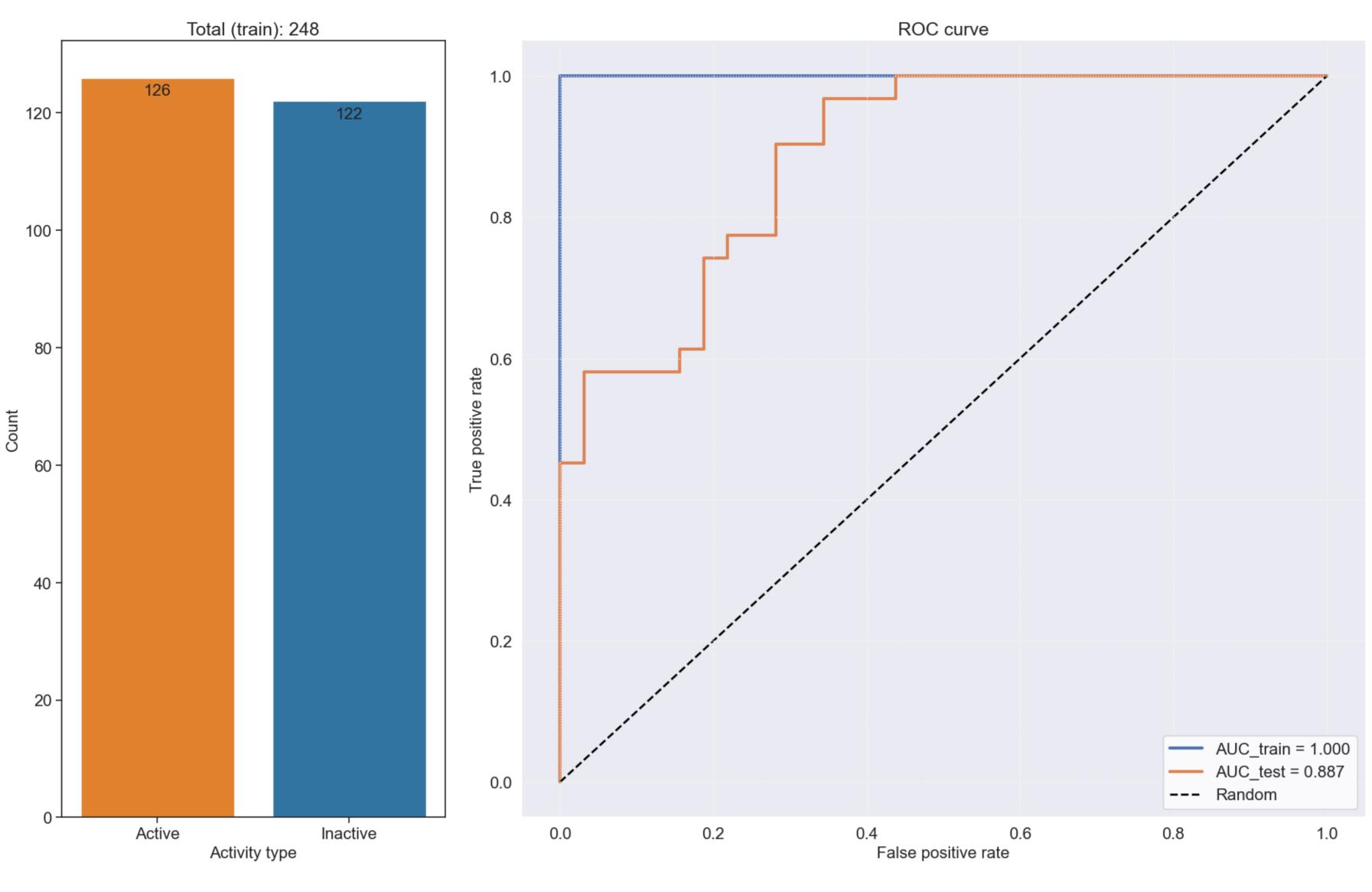
XGBoost Parameters	Value
alpha	3.0337
colsample_bytree	0.8496
gamma	0.2838
lambda	2.335
learning_rate	0.4234
max_depth	8.0
min_child_weight	1.0
n_estimators	342.0
reg_alpha	0.9749
reg_lambda	0.8468
scale_pos_weight	33.9549
subsample	0.7487

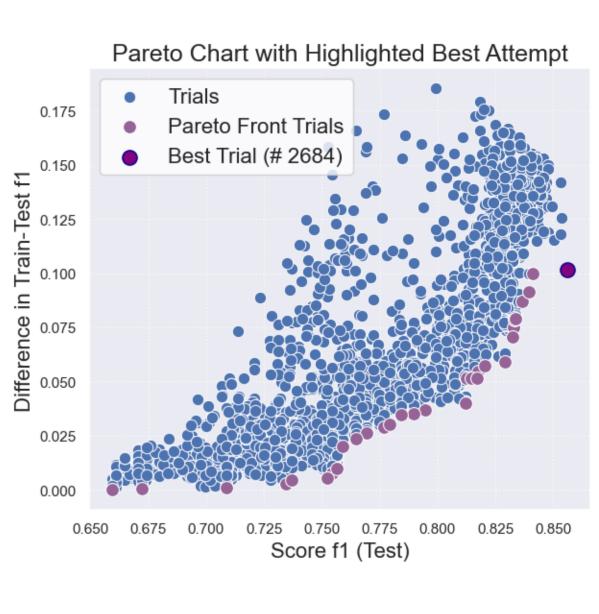


			Active/Inacti	ve probability		
70 		Inactive zone			Active zone	active (31) inactive (32)
50						
Percent 30						
20						
10 	0.0	0.2	0.4	0.6	0.8	10
	0.0	0.2		ability	0.0	1.0

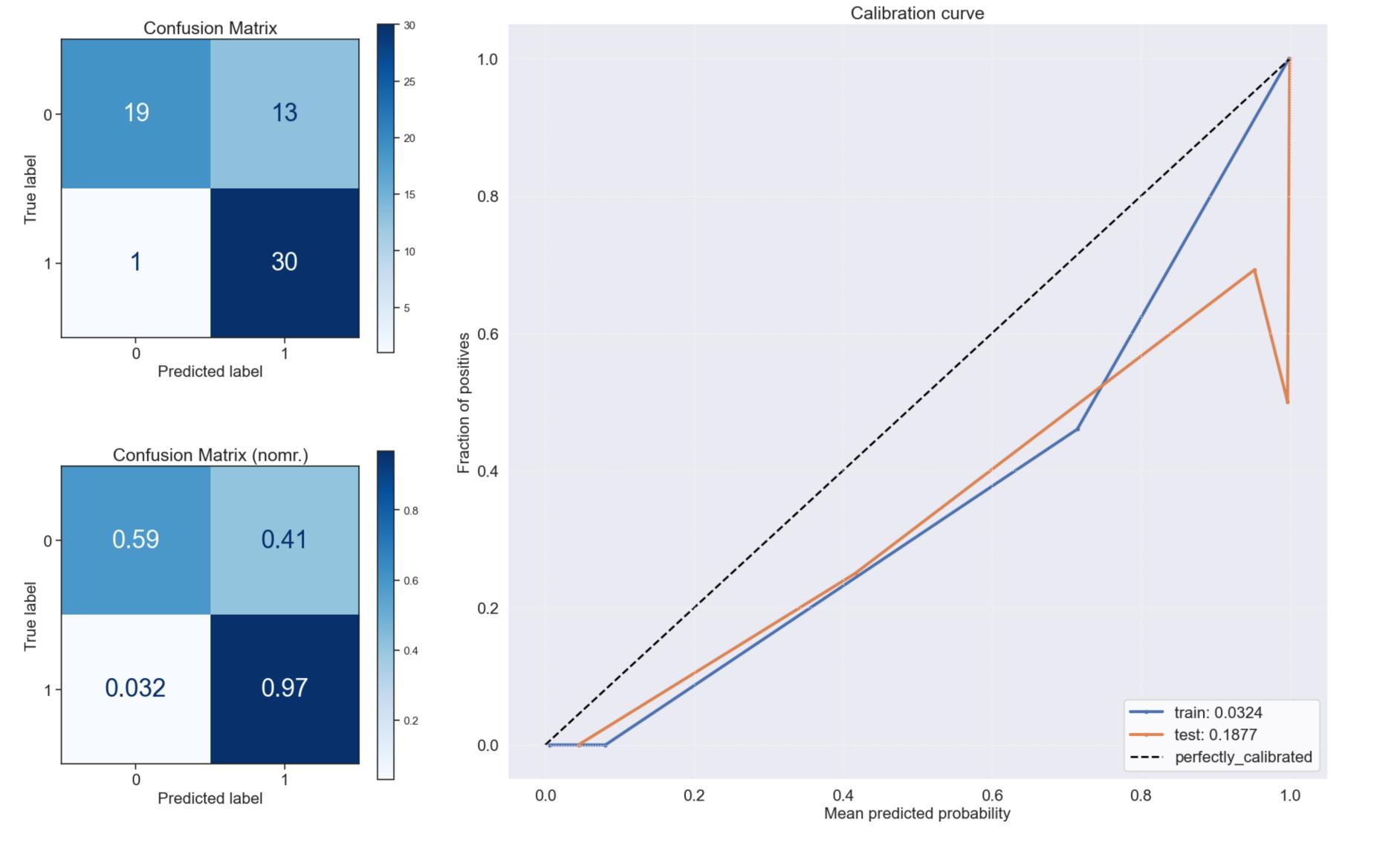
Metric	Train	Test
AUC	1.0	0.879
accuracy	0.9879	0.7302
balanced accuracy	0.9881	0.7329
recall_(sens)	1.0	0.9032
specificity	0.9762	0.5625
precision	0.976	0.6667
f1_score	0.9879	0.7225

Protein: P18089 - metric: f1





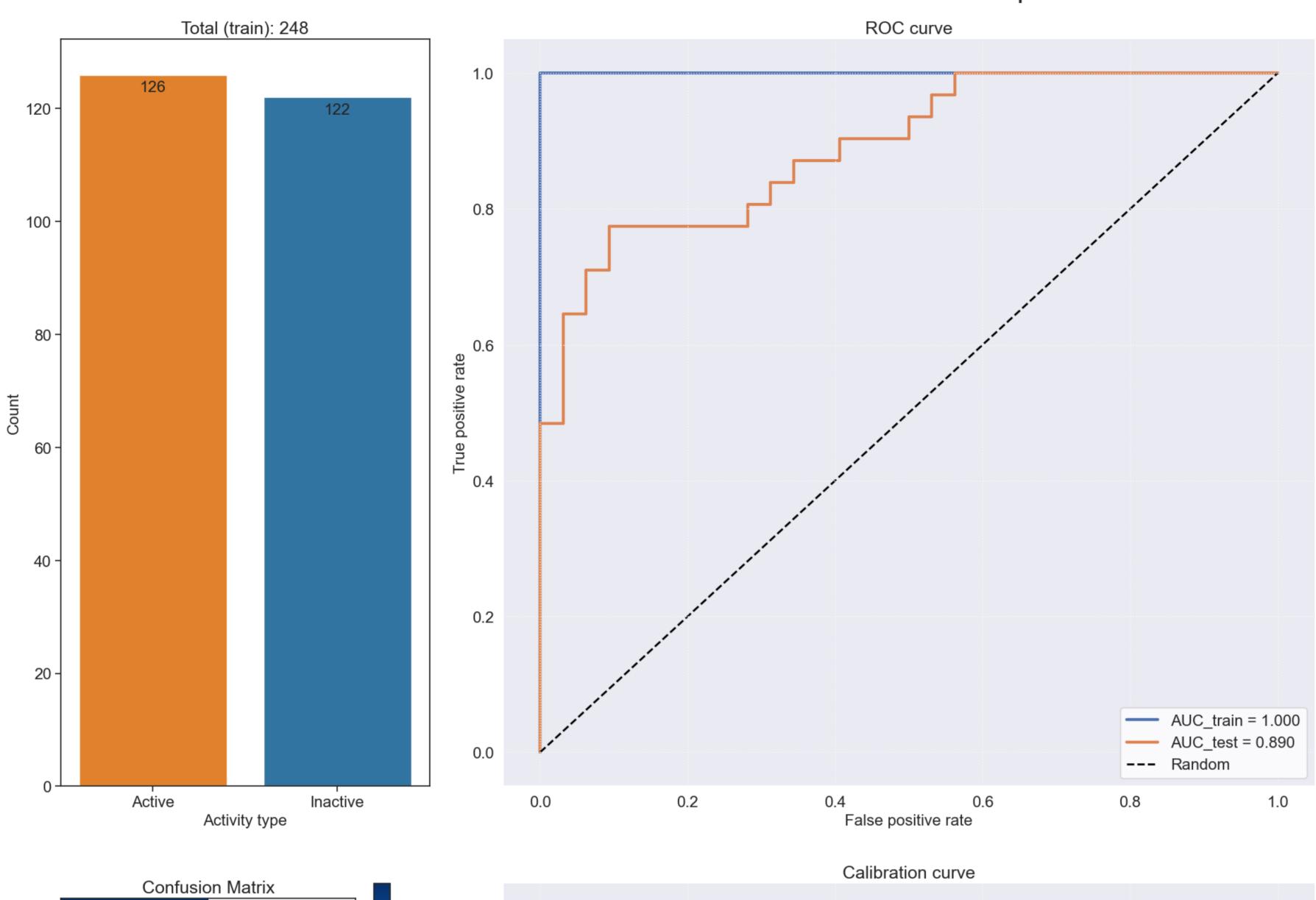
XGBoost Parameters	Value
alpha	1.0074
colsample_bytree	0.764
gamma	0.8195
lambda	2.0729
learning_rate	0.2699
max_depth	5.0
min_child_weight	1.0
n_estimators	749.0
reg_alpha	0.4758
reg_lambda	0.535
scale_pos_weight	83.9567
subsample	0.9539

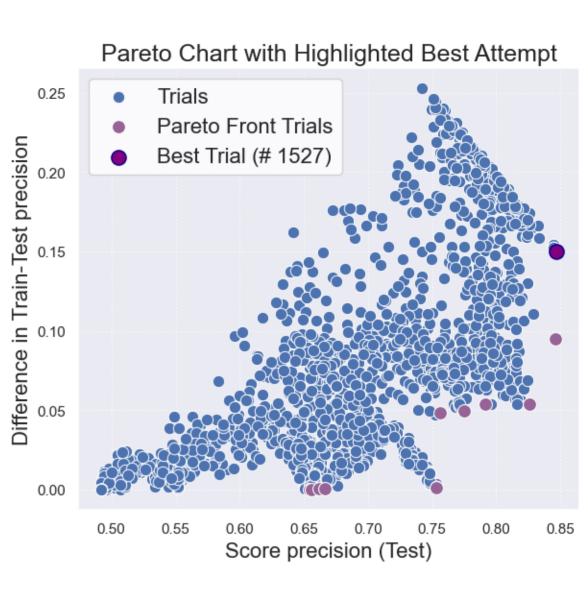


70	Active/Inactive probability					
00	Inactive zone			Active 2		type active (31) inactive (32)
50						decoy (63)
40						
Percent						
20						
10			П			
0—	0.0 0.2	0.4 Proba	0.6 ability	0.	.8	1.0

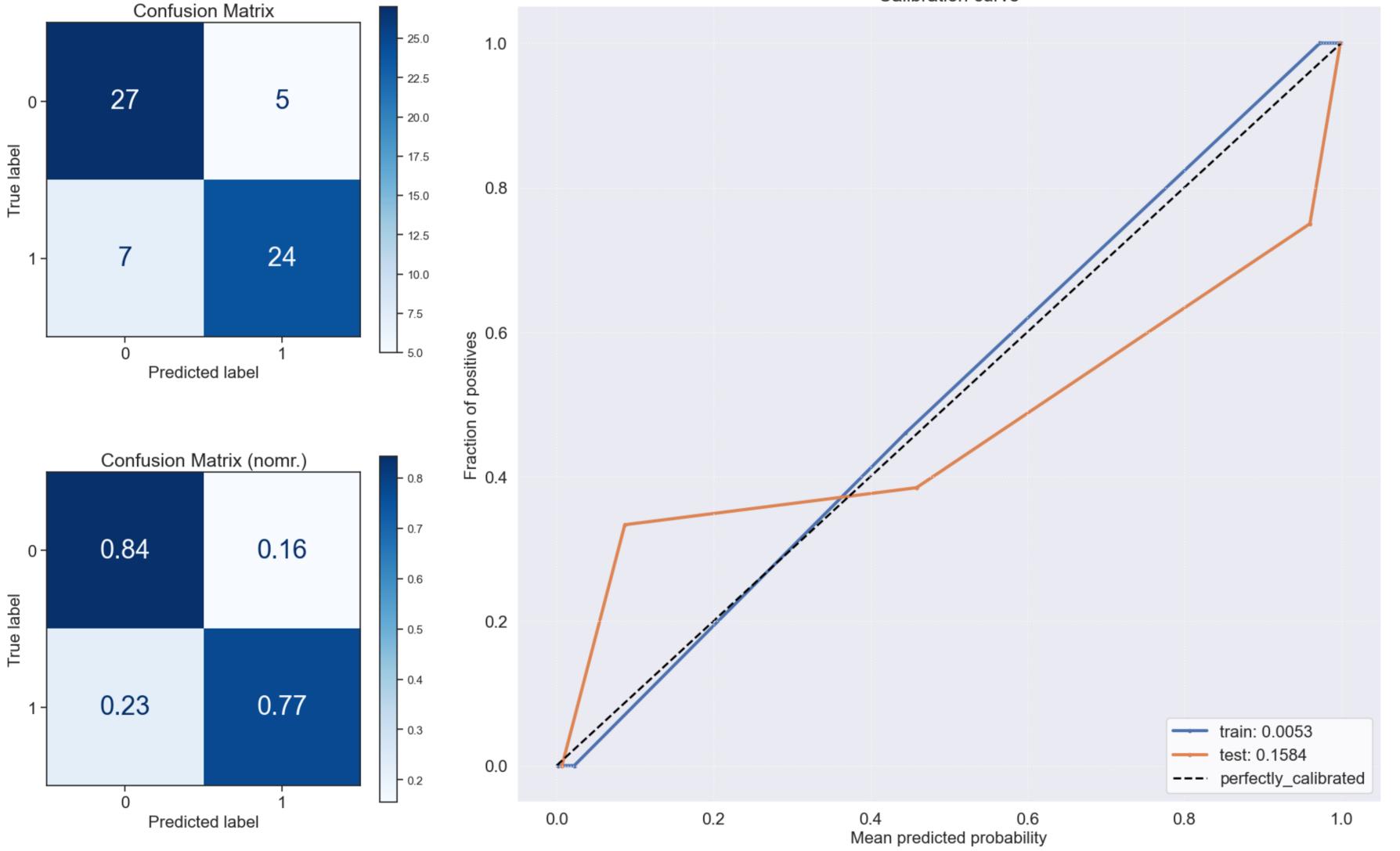
Metric	Train	Test
AUC	1.0	0.8871
accuracy	0.9516	0.7778
balanced accuracy	0.9524	0.7807
recall_(sens)	1.0	0.9677
specificity	0.9048	0.5938
precision	0.9104	0.6977
f1_score	0.9515	0.7702

Protein: P18089 - metric: precision





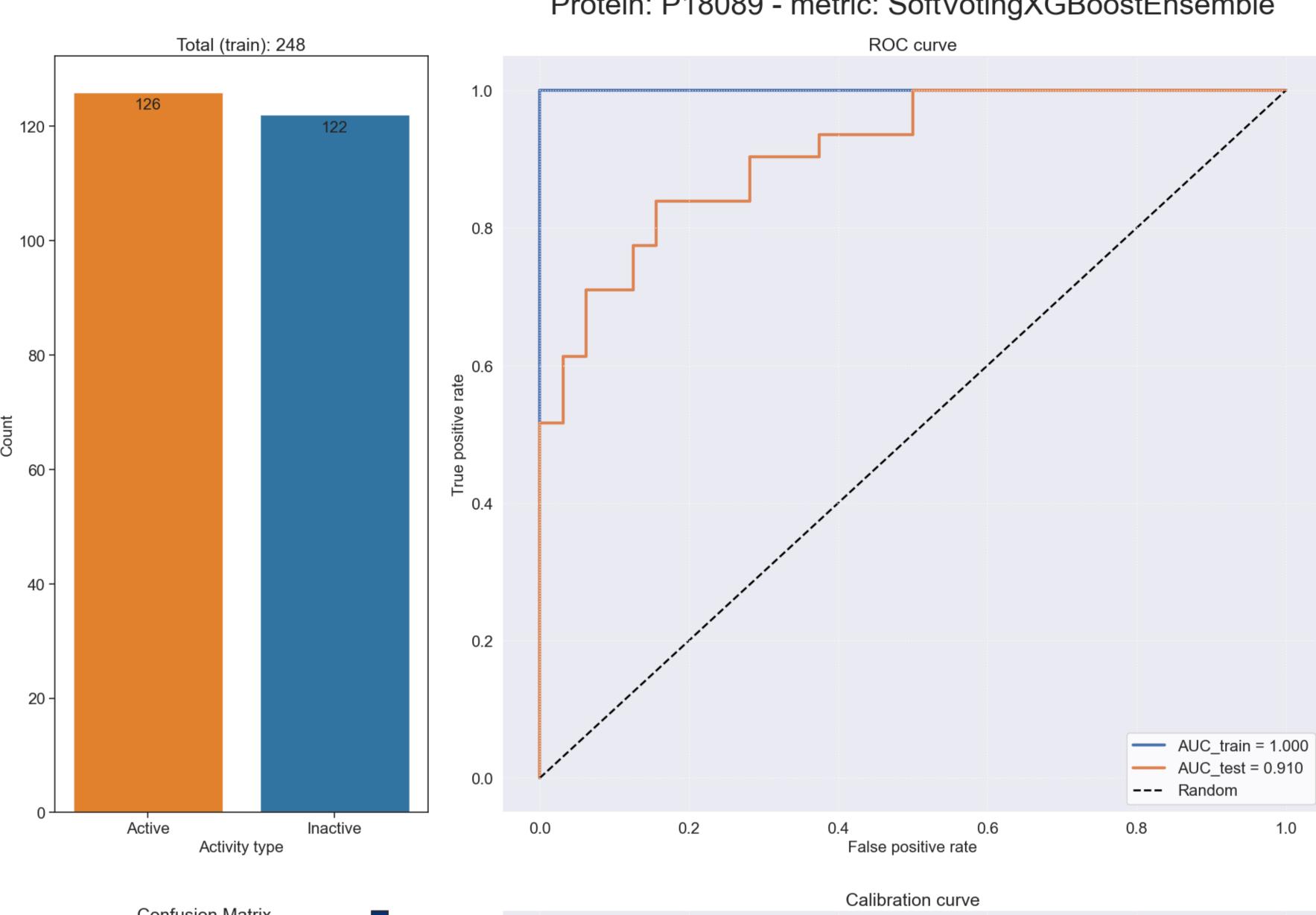
XGBoost Parameters	Value
alpha	1.9281
colsample_bytree	0.9754
gamma	0.2974
lambda	3.3889
learning_rate	0.961
max_depth	8.0
min_child_weight	1.0
n_estimators	452.0
reg_alpha	0.1586
reg_lambda	0.9857
scale_pos_weight	1.2279
subsample	0.5049

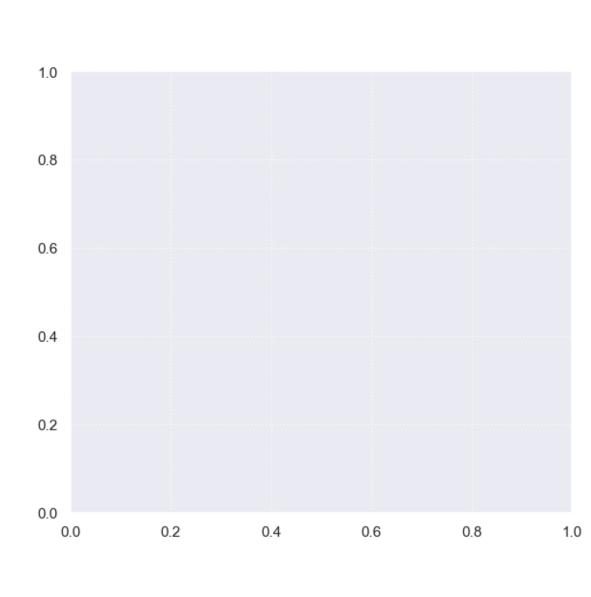


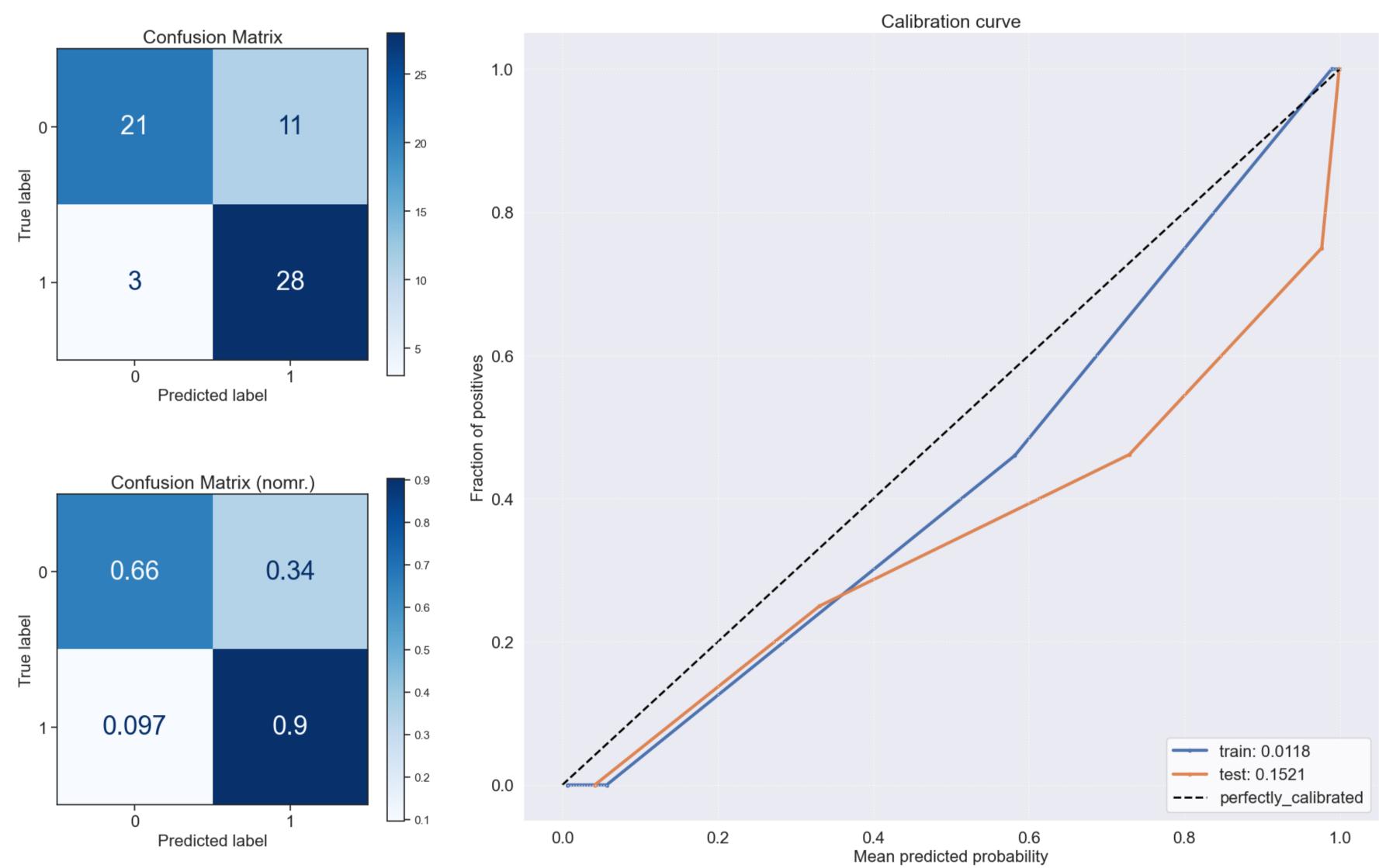
				Active/In	active p	orobability			
50 -							Active :		inactive (32) decoy (63)
30									
10			-A-A-				ΠΠ		
	0.0	0.2		0.4	Probabili	0.6 ty	0	.8	1.0

Metric	Train	Test
AUC	1.0	0.8901
accuracy	1.0	0.8095
balanced accuracy	1.0	0.809
recall_(sens)	1.0	0.7742
specificity	1.0	0.8438
precision	1.0	0.8276
f1_score	1.0	0.8092

Protein: P18089 - metric: SoftVotingXGBoostEnsemble







50	1	nactive zone			Active zone	inactive (32)
40						decoy (63)
Percent 05						
20						
10						
0	0.0	0.2	0.4 Probab	0.6 pility	0.8	1.0

Active/Inactive probability

Metric	Train	Test
AUC	1.0	0.9103
accuracy	0.9919	0.7778
balanced accuracy	0.9921	0.7797
recall_(sens)	1.0	0.9032
specificity	0.9841	0.6562
precision	0.9839	0.7179
f1_score	0.9919	0.7746