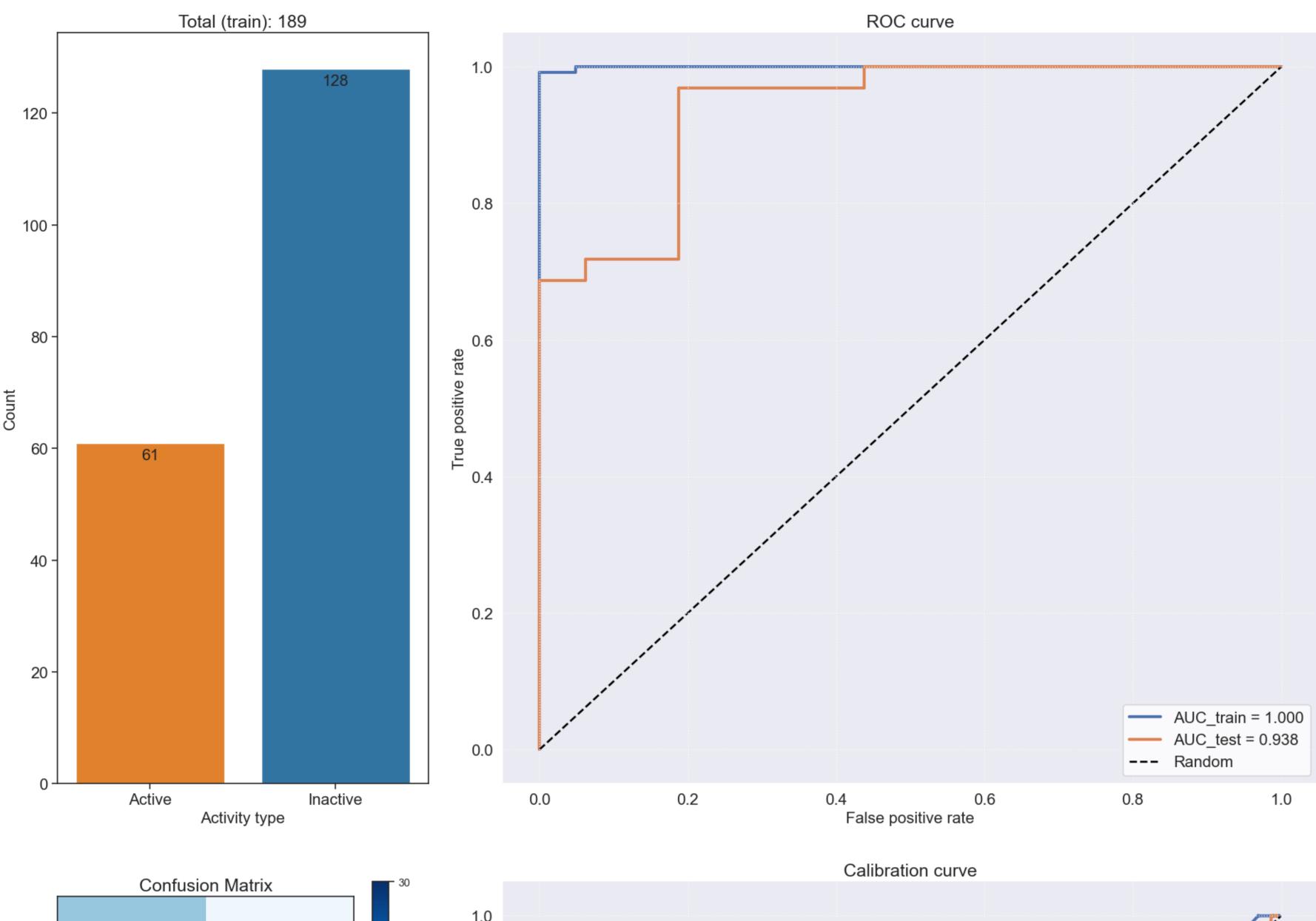
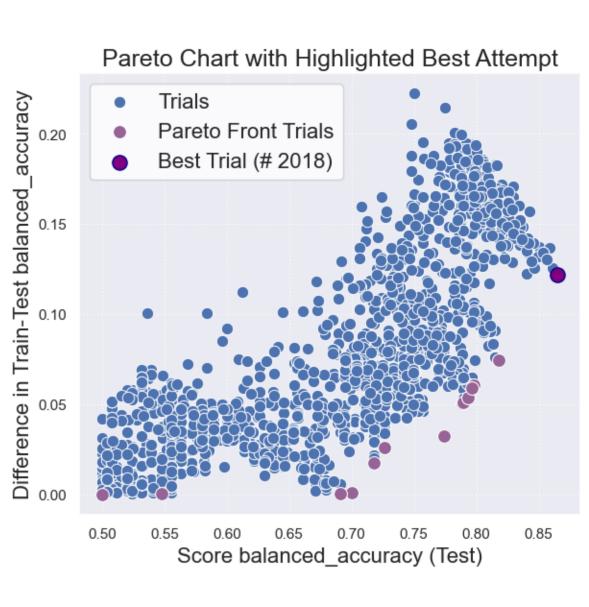
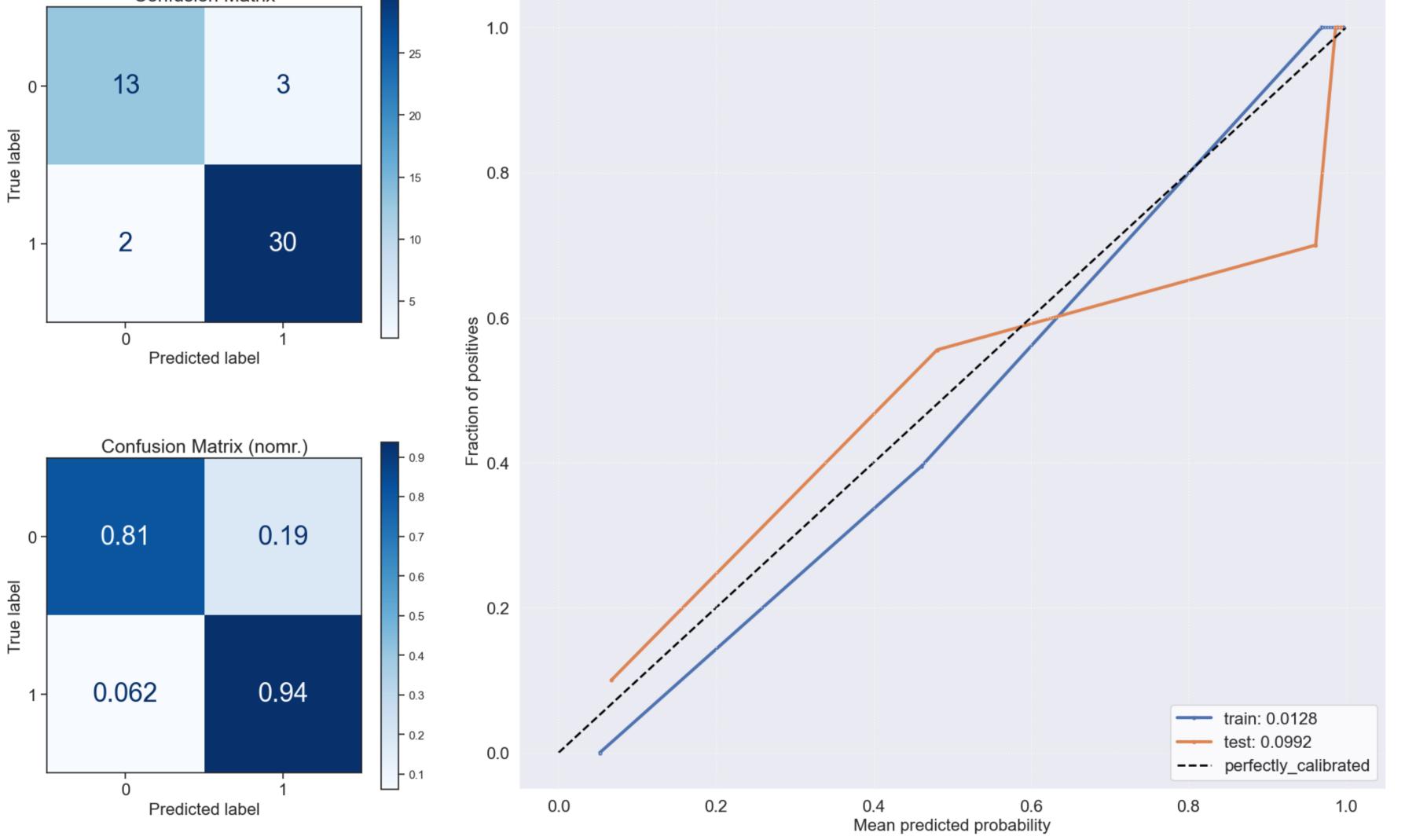
Protein: Q14432 - metric: balanced_accuracy





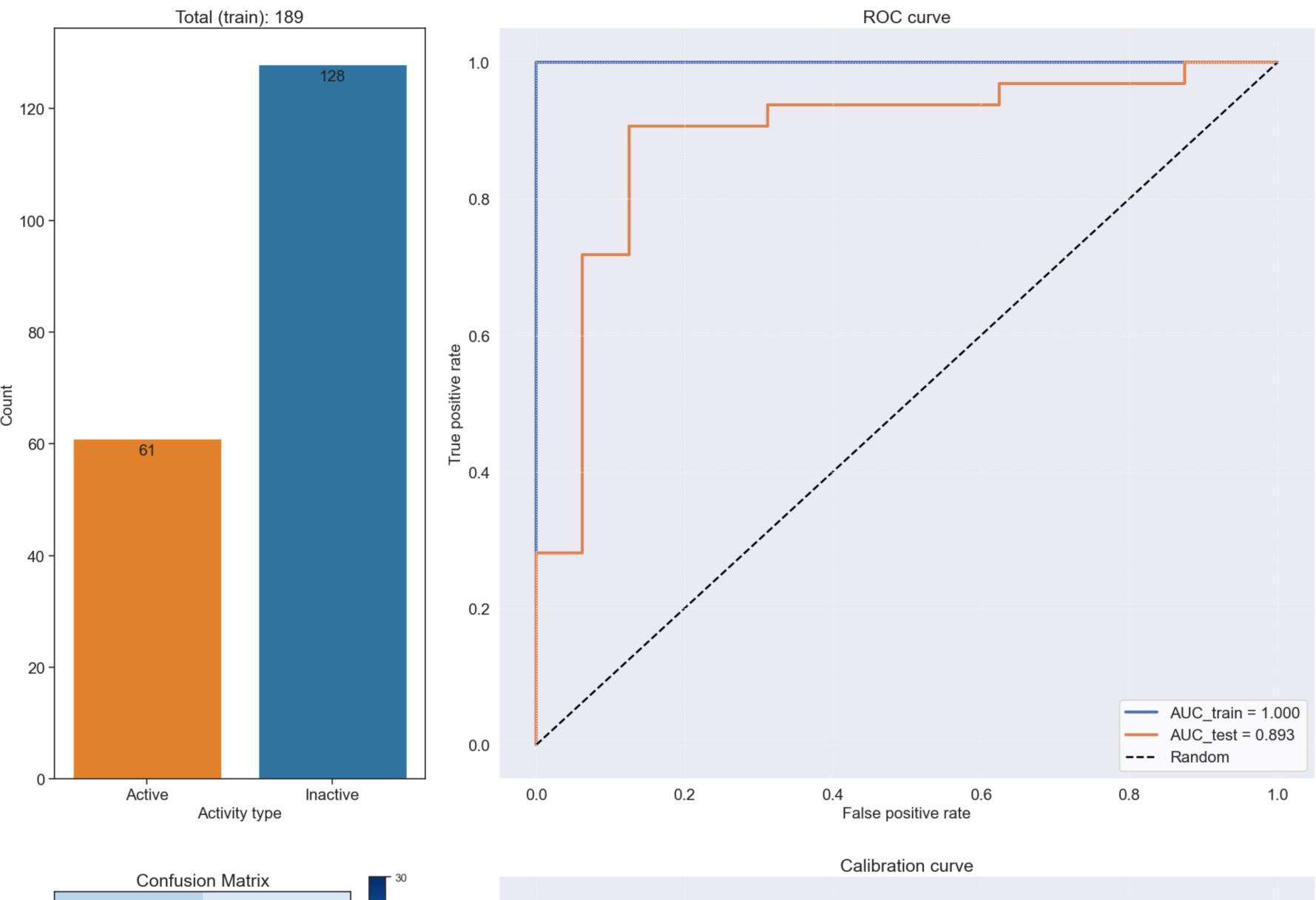
XGBoost Parameters	Value
alpha	4.7262
colsample_bytree	0.6761
gamma	0.3978
lambda	0.6
learning_rate	0.7462
max_depth	8.0
min_child_weight	1.0
n_estimators	262.0
reg_alpha	0.7788
reg_lambda	0.8967
scale_pos_weight	1.6573
subsample	0.8362

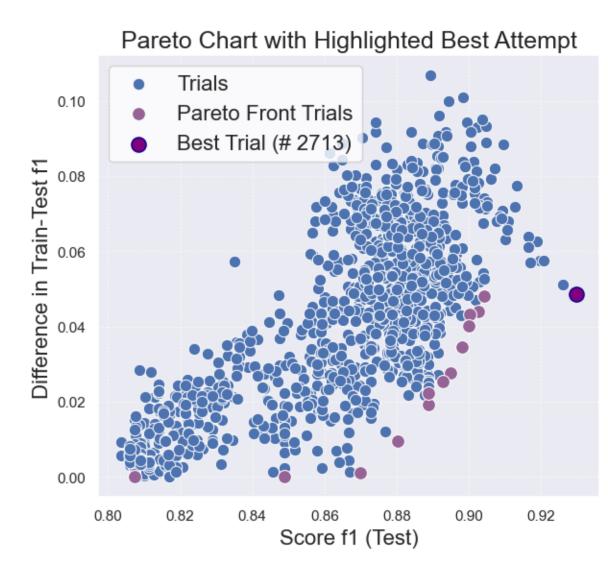


		Active/I	nactive probability		
40	_		•		type
	Ina	ctive zone		Active zone	active (32) inactive (16)
35					decoy (48)
30					
25					
Percent					
9 -					
15					
10					
5				П	
0 —					
	0.0	.2 0.4	0.6	0.8	1.0
			Probability		

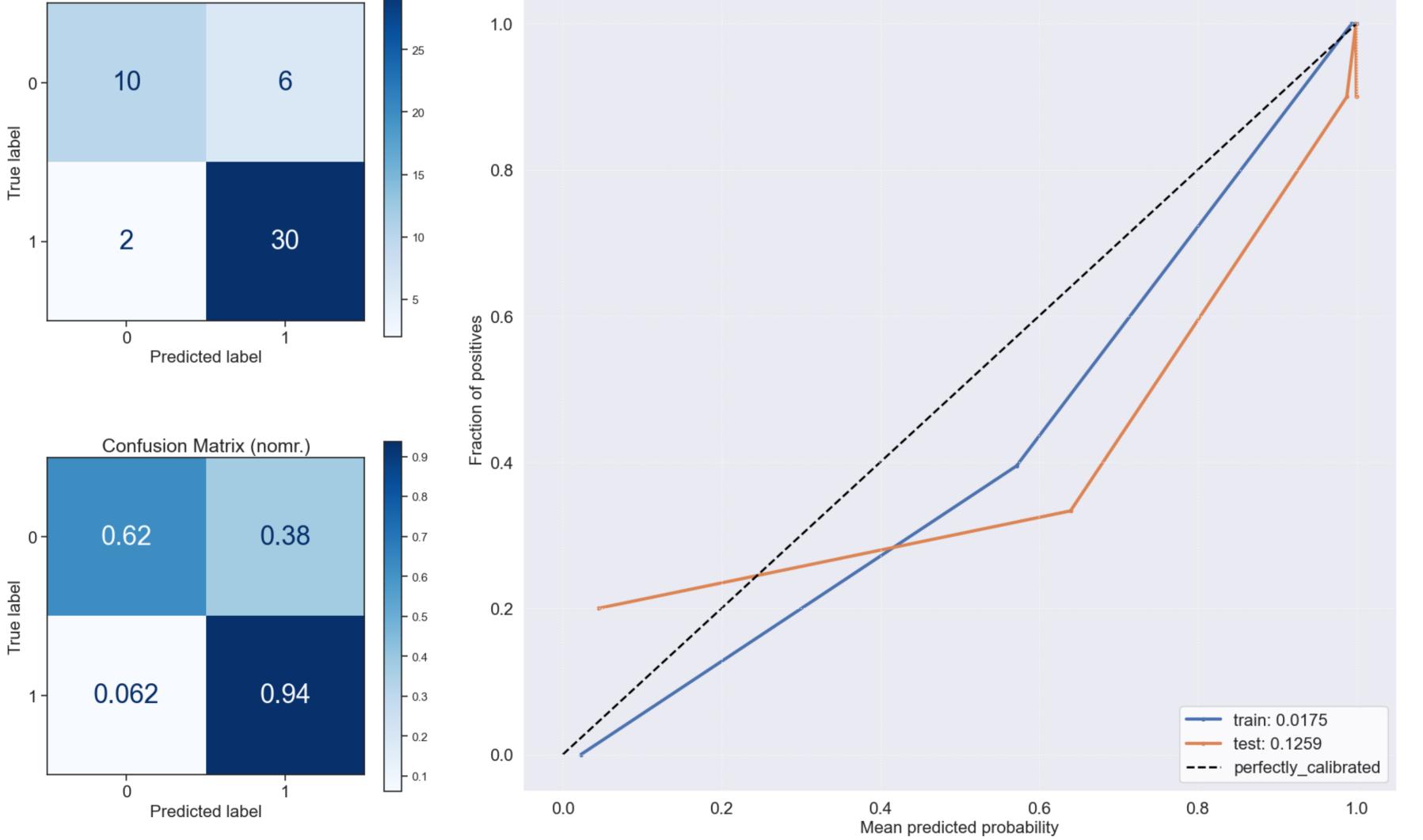
Metric	Train	Test
AUC	0.9996	0.9375
accuracy	0.9947	0.8958
balanced accuracy	0.9961	0.875
recall_(sens)	0.9922	0.9375
specificity	1.0	0.8125
precision	1.0	0.9091
f1_score	0.9947	0.895

Protein: Q14432 - metric: f1





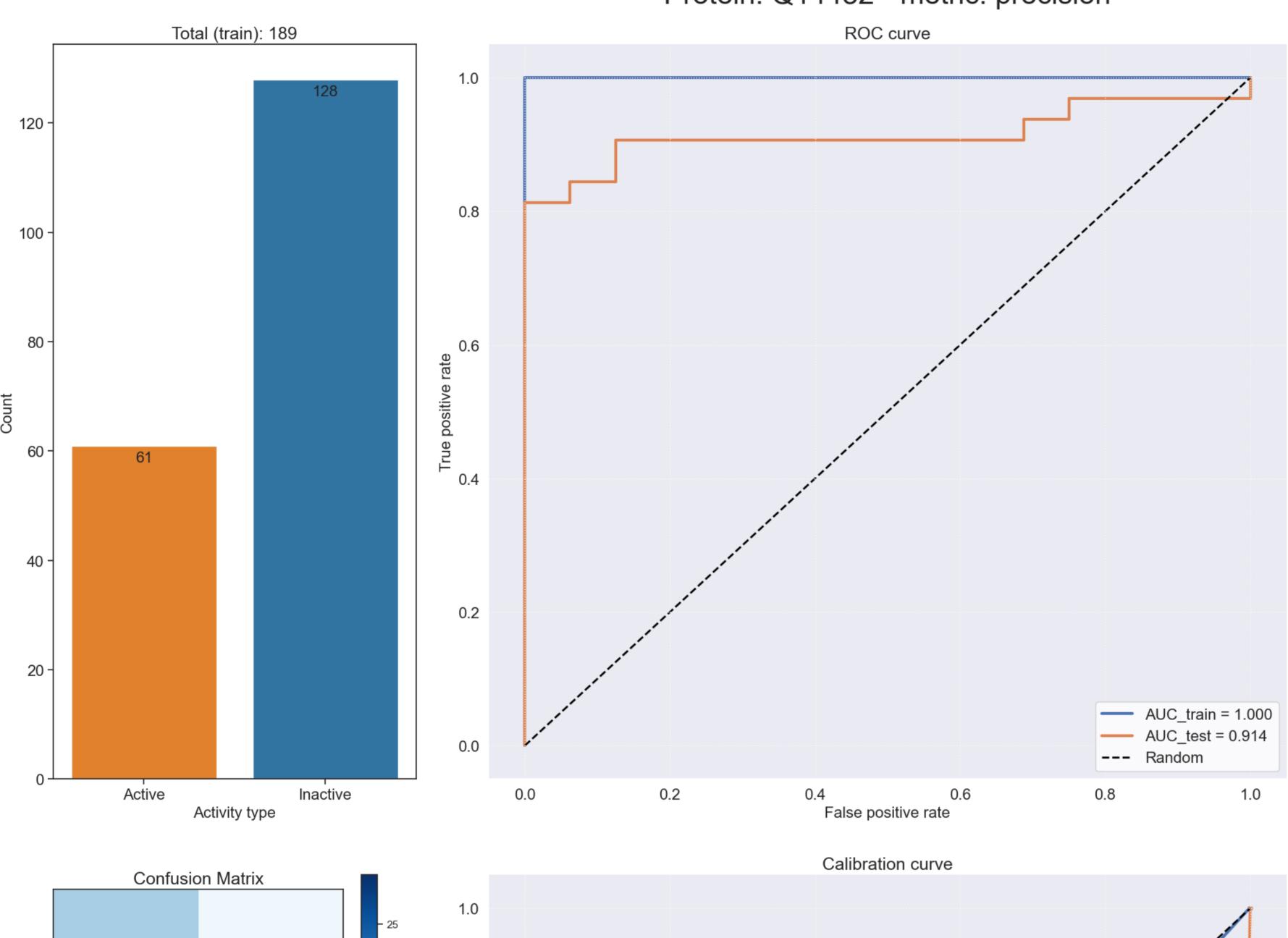
XGBoost Parameters	Value
alpha	0.969
colsample_bytree	0.7964
gamma	0.58
lambda	1.7474
learning_rate	0.9625
max_depth	10.0
min_child_weight	3.0
n_estimators	907.0
reg_alpha	0.9842
reg_lambda	0.5534
scale_pos_weight	12.227
subsample	0.6514

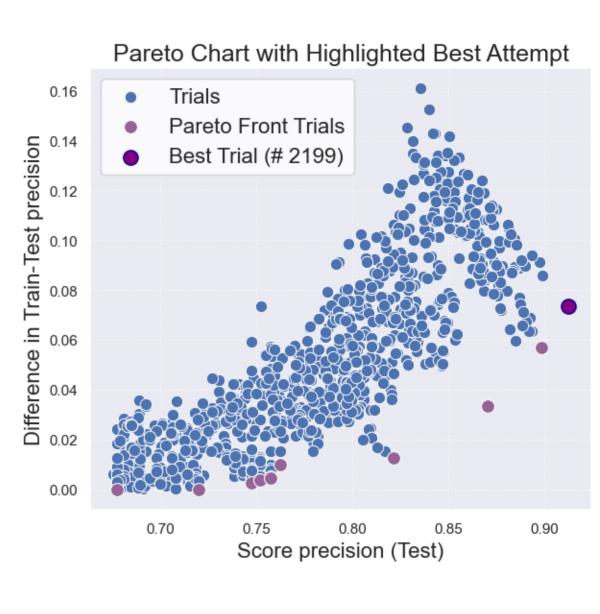


			Active/In	active probability		
		Inactive zon			Active zone	inactive (16) decoy (48)
50						
ent						
20						
0 —						
	0.0	0.2	0.4 F	0.6 Probability	0.8	1.0

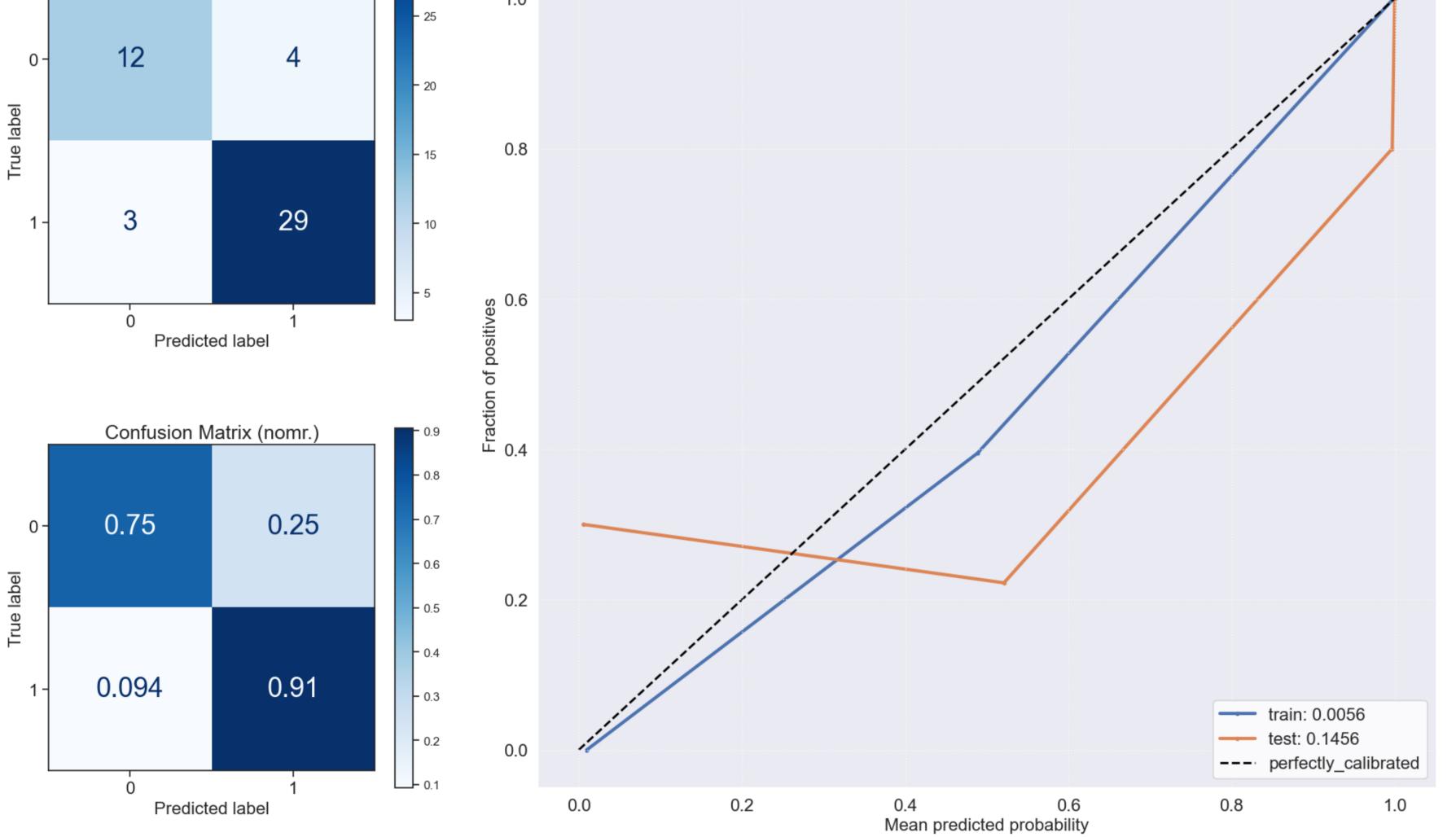
Metric	Train	Test
AUC	1.0	0.8926
accuracy	0.9683	0.8333
balanced accuracy	0.9508	0.7812
recall_(sens)	1.0	0.9375
specificity	0.9016	0.625
precision	0.9552	0.8333
f1_score	0.9678	0.8263

Protein: Q14432 - metric: precision



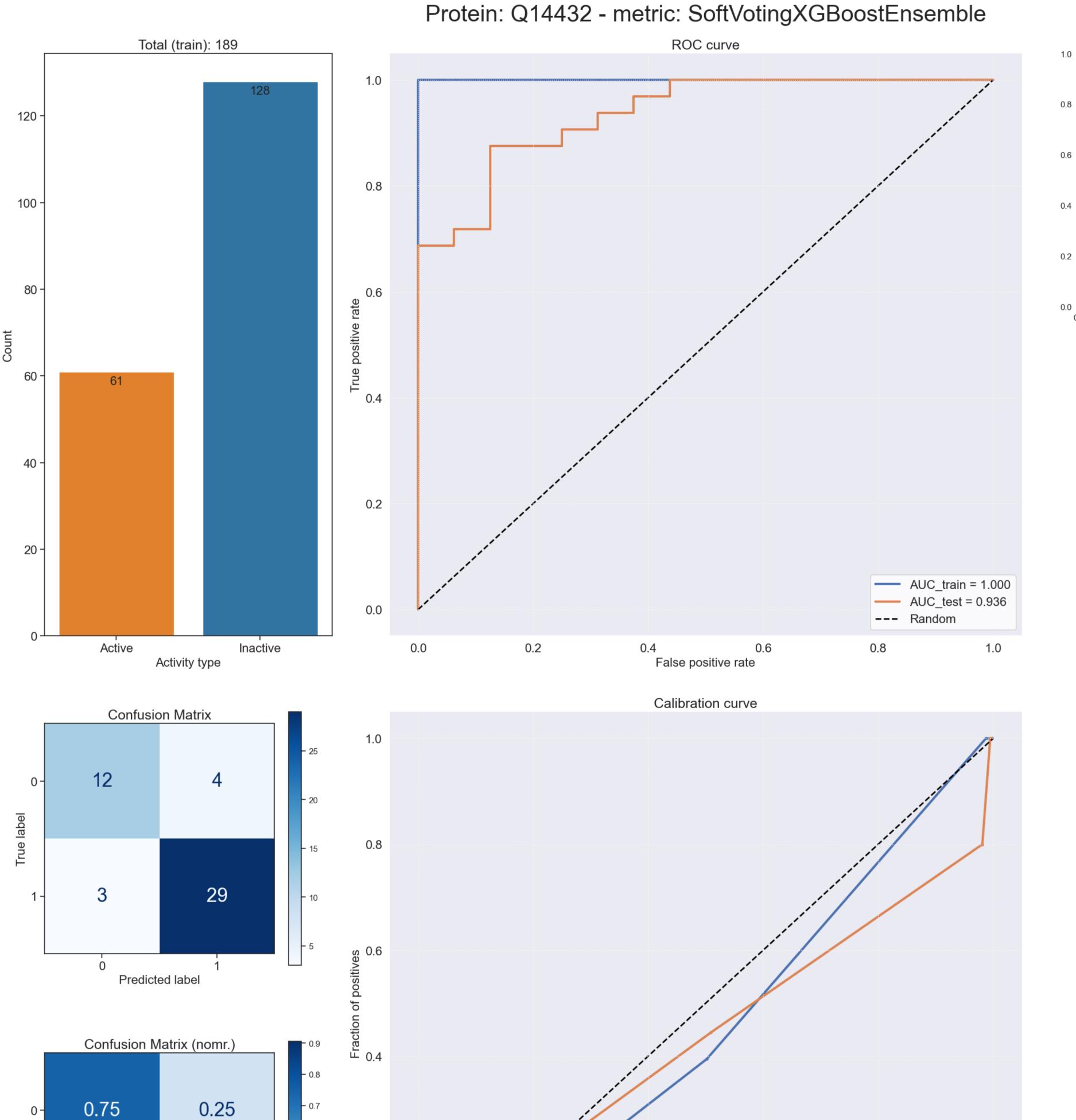


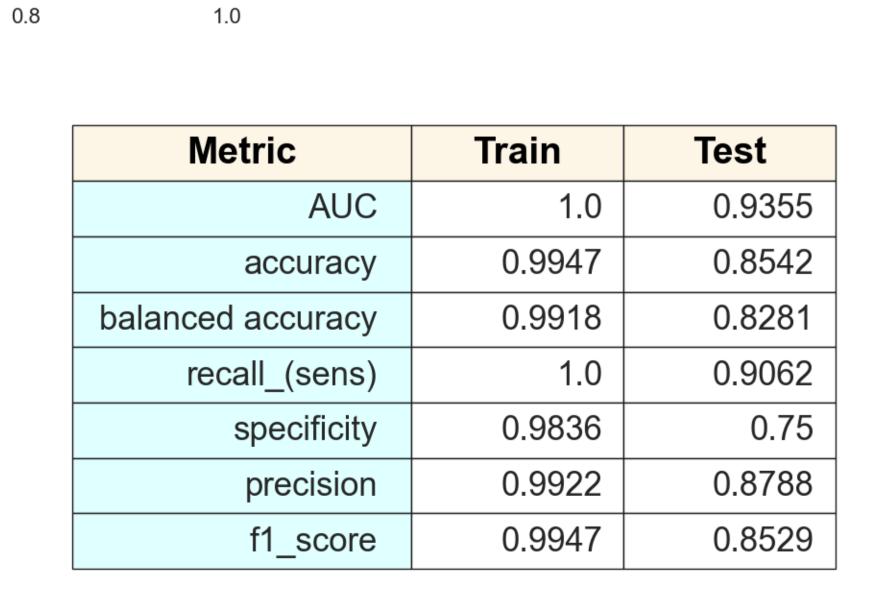
XGBoost Parameters	Value
alpha	3.6621
colsample_bytree	0.7257
gamma	0.53
lambda	0.2999
learning_rate	0.9327
max_depth	4.0
min_child_weight	2.0
n_estimators	672.0
reg_alpha	0.2862
reg_lambda	0.4829
scale_pos_weight	38.2187
subsample	0.5572



			Active/Inact	ive probability		
80		Inactive zone			Active zone	type active (32) inactive (16)
						decoy (48)
60						
Percent 6						
20						
0						
	0.0	0.2	0.4 Prob	0.6 pability	0.8	1.0

Metric	Train	Test
AUC	1.0	0.9141
accuracy	1.0	0.8542
balanced accuracy	1.0	0.8281
recall_(sens)	1.0	0.9062
specificity	1.0	0.75
precision	1.0	0.8788
f1_score	1.0	0.8529





train: 0.009

--- perfectly_calibrated

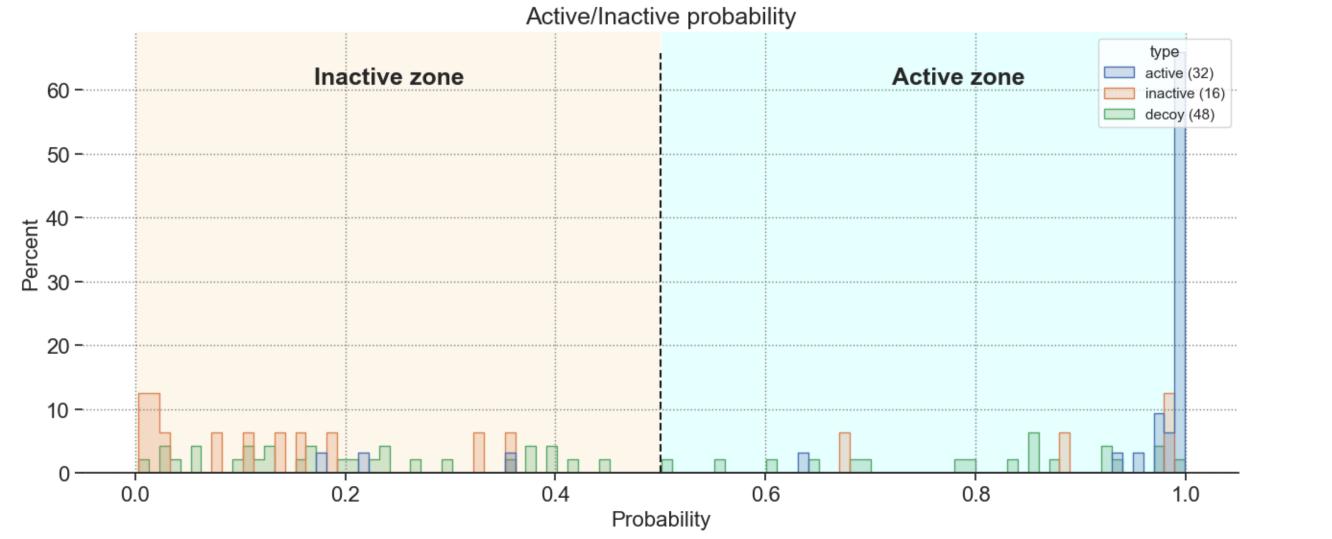
--- test: 0.1117

0.4 0.6 Mean predicted probability

0.0

0.2

0.6



- 0.6

- 0.5

0.4

- 0.3

0.2

0.91

0.2

0.0

0.0

0.2

True label

0.094

Predicted label