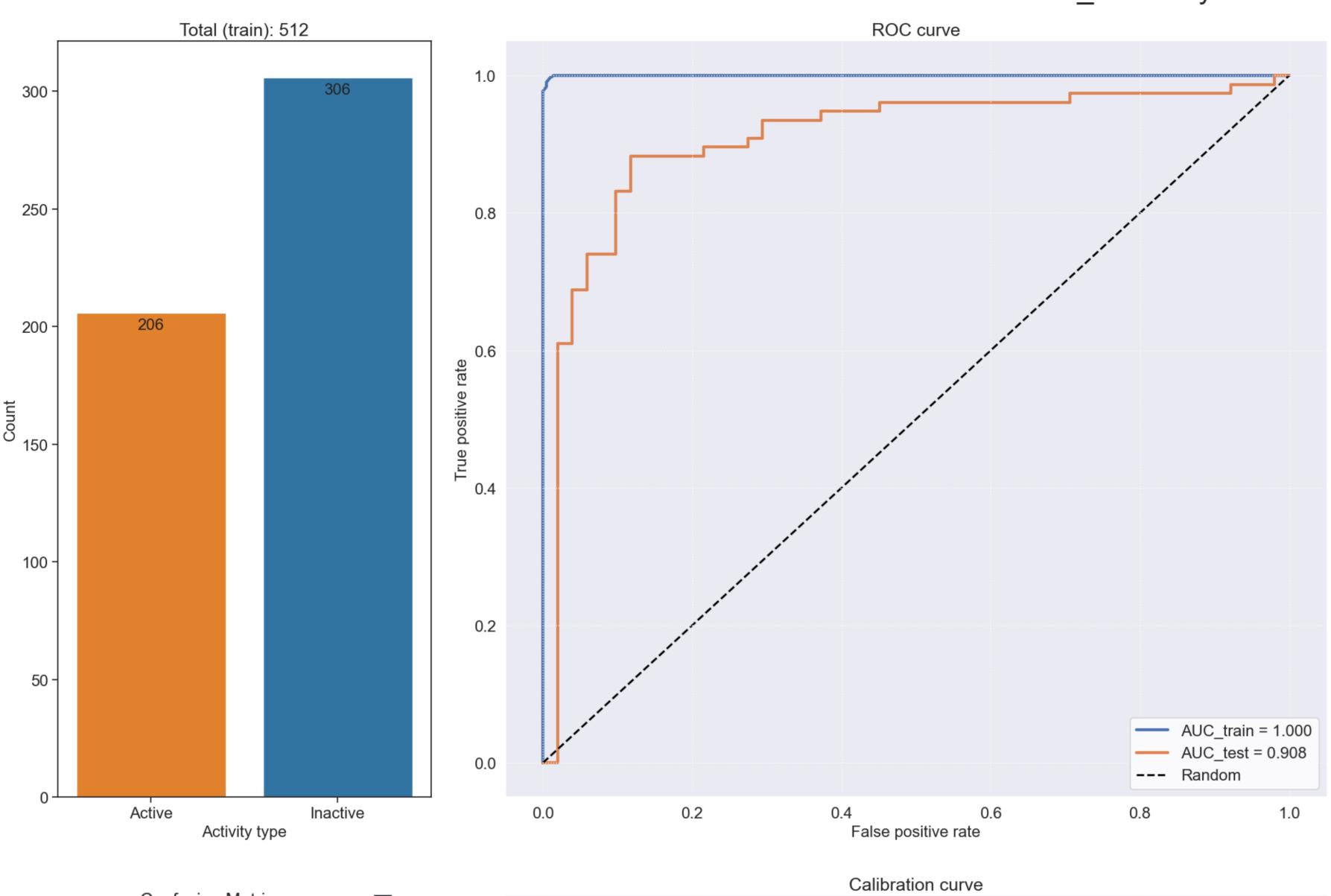
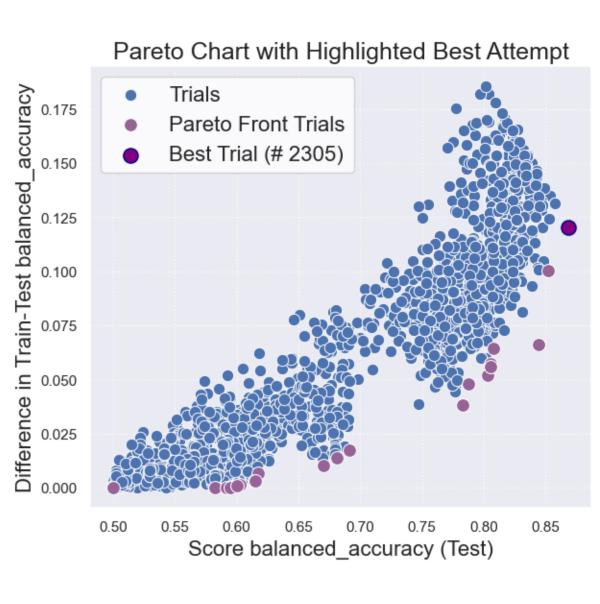
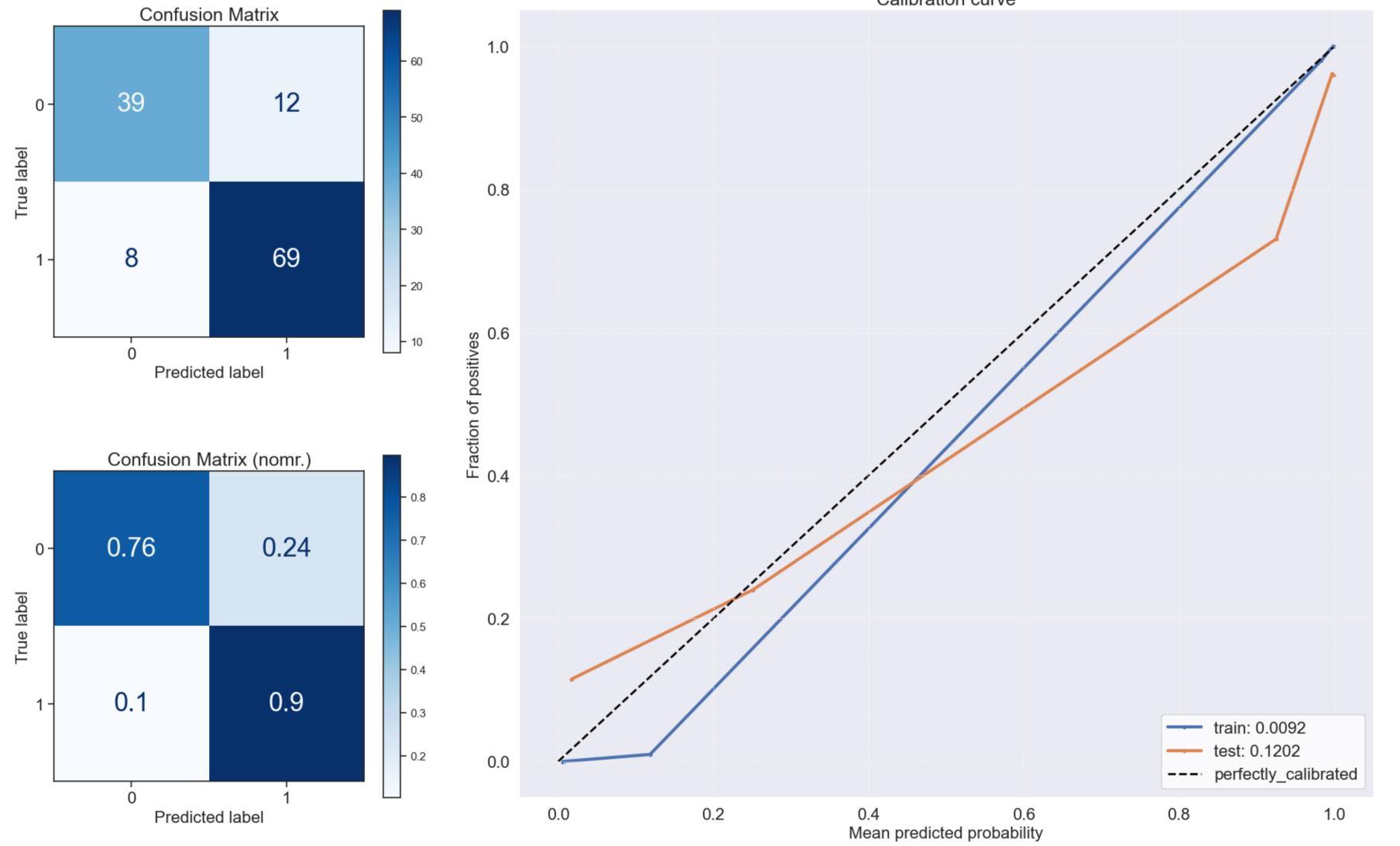
Protein: P08913 - metric: balanced_accuracy





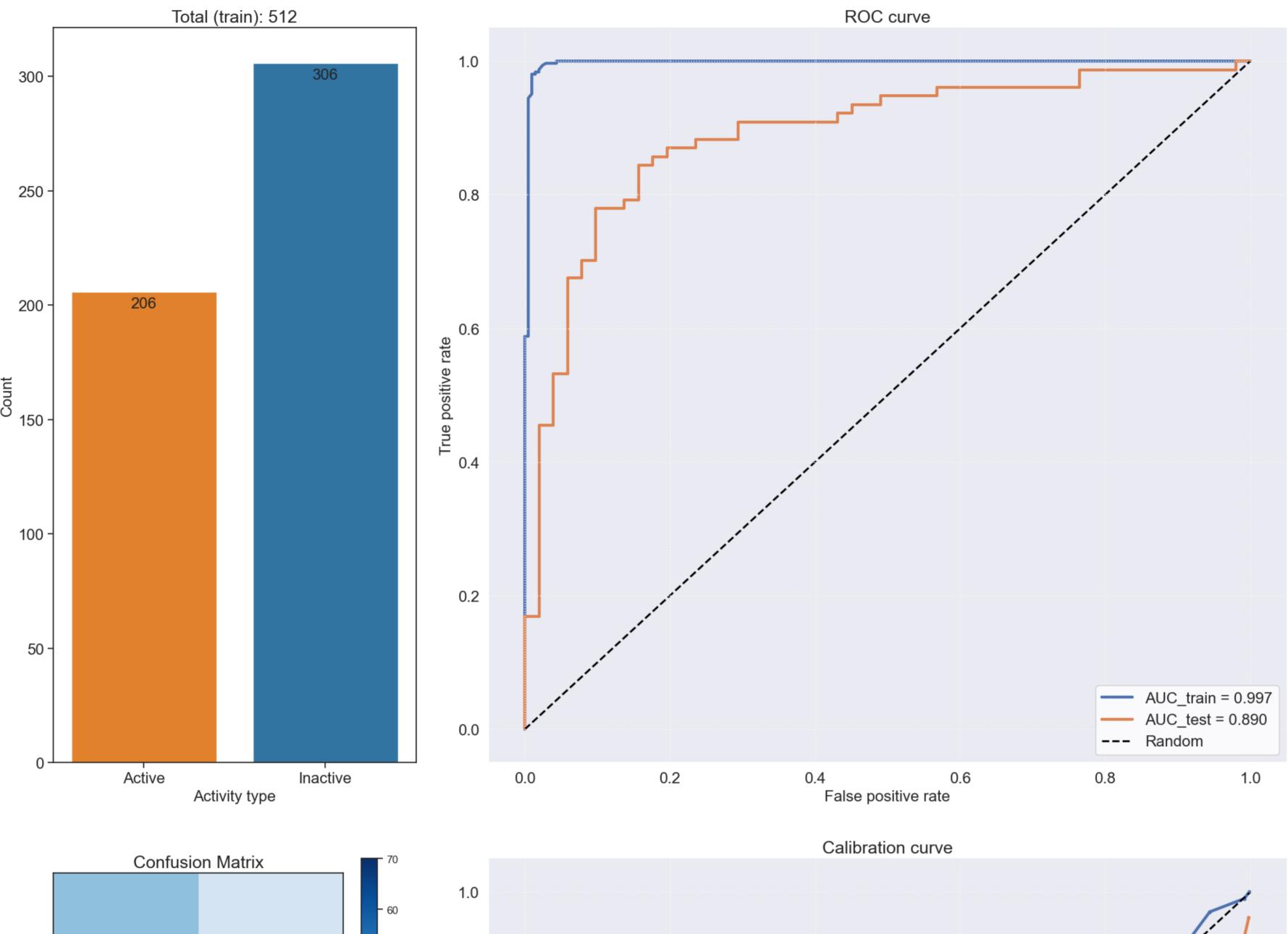
XGBoost Parameters	Value
alpha	3.1597
colsample_bytree	0.9737
gamma	0.0129
lambda	4.6342
learning_rate	0.3801
max_depth	3.0
min_child_weight	2.0
n_estimators	460.0
reg_alpha	0.5099
reg_lambda	0.6544
scale_pos_weight	7.27
subsample	0.9528

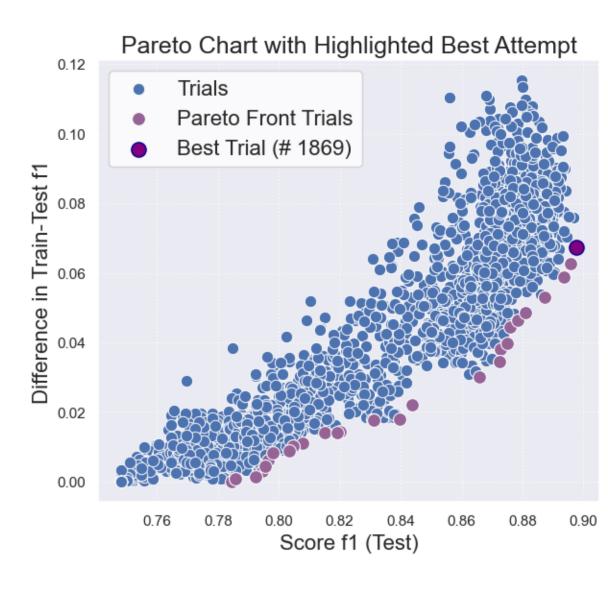


		Active/Inactive p	robability		
70 	Inactive zone			Active zone	type active (77) inactive (51) decoy (128)
50					
90					
₾ 30					
20					
0 —					
,	0.0 0.2	0.4 Probabilit	0.6 ty	0.8	1.0

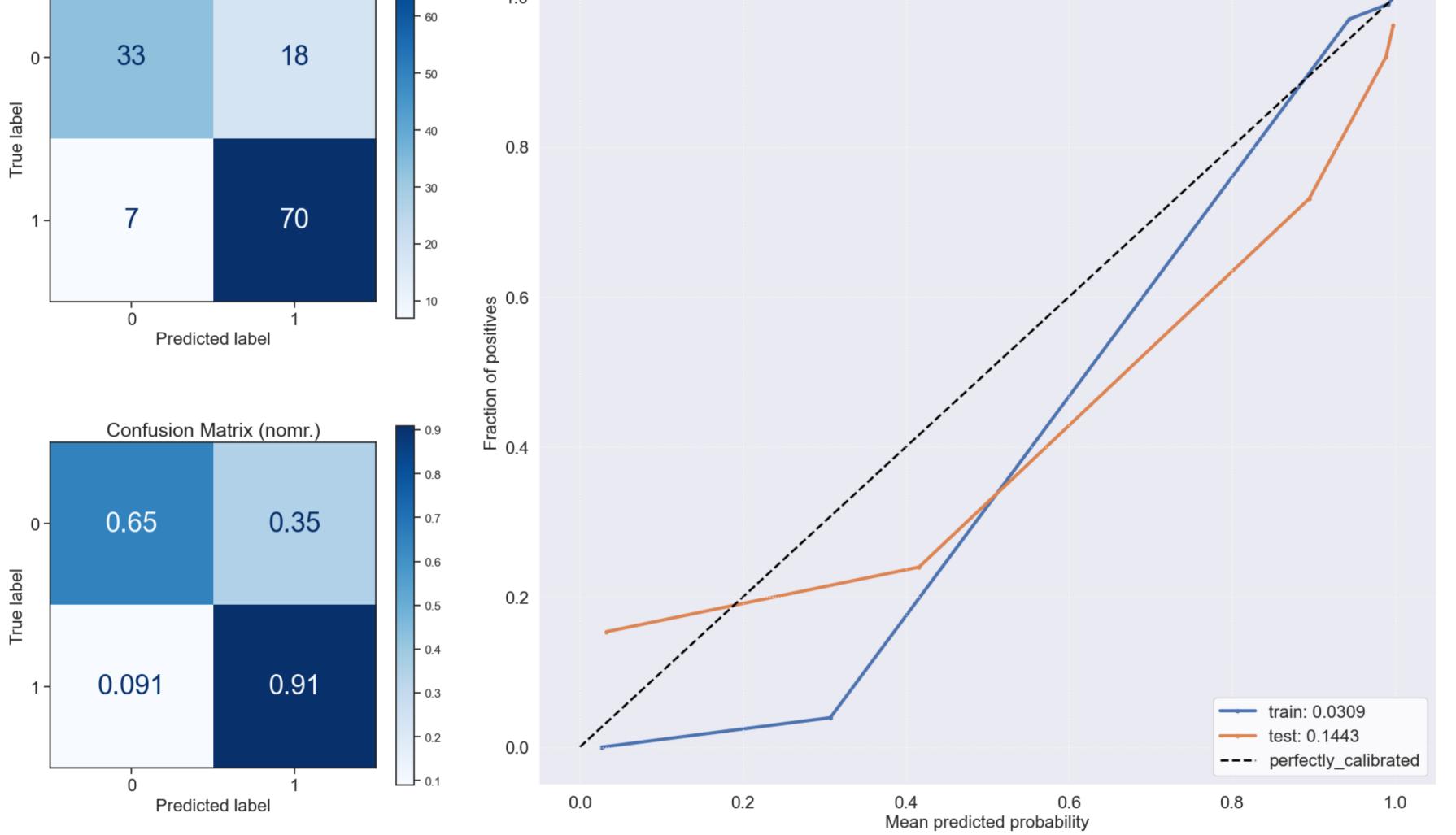
Metric	Train	Test
AUC	0.9999	0.9083
accuracy	0.9922	0.8438
balanced accuracy	0.9903	0.8304
recall_(sens)	1.0	0.8961
specificity	0.9806	0.7647
precision	0.9871	0.8519
f1_score	0.9922	0.8425

Protein: P08913 - metric: f1





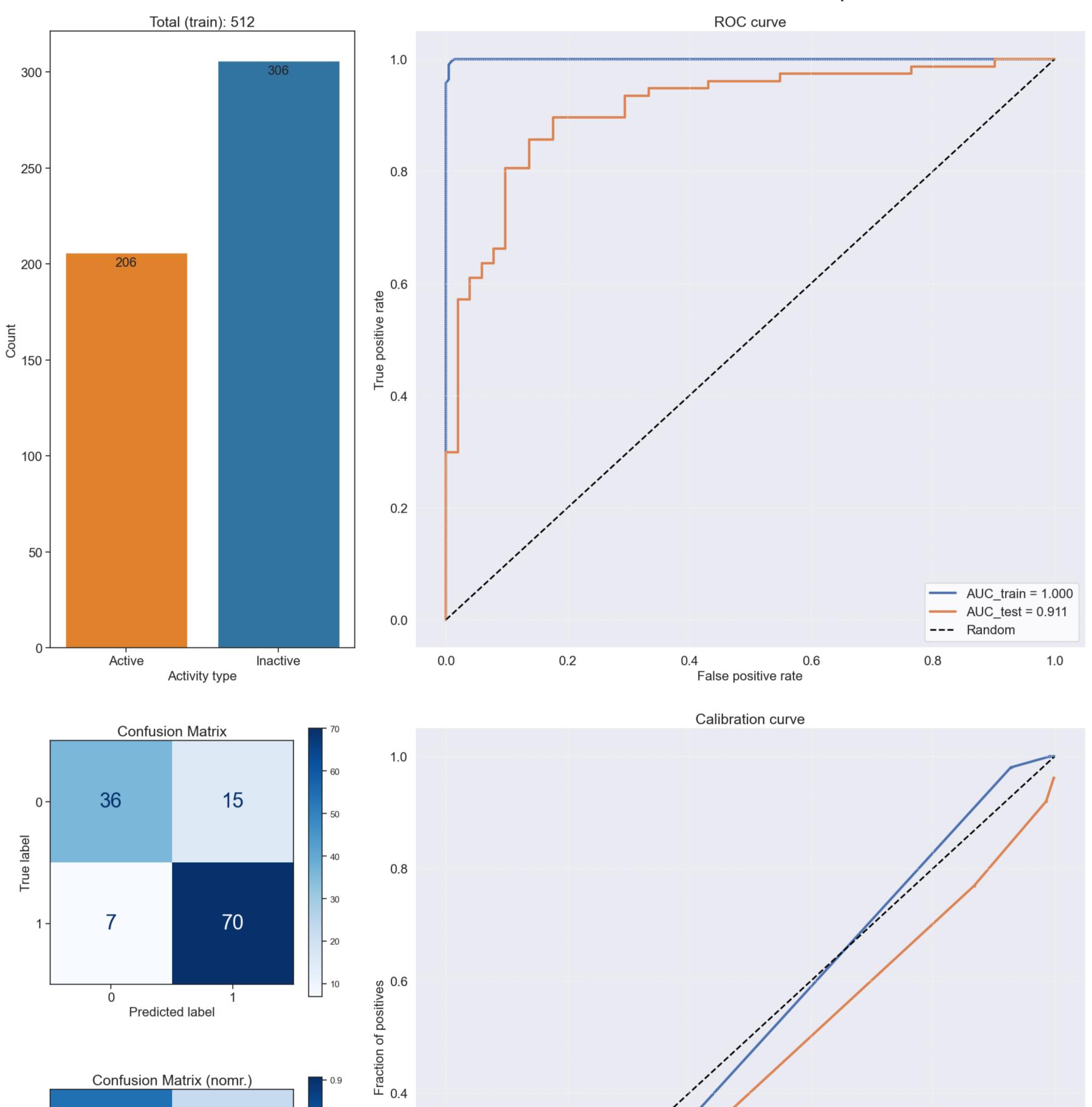
XGBoost Parameters	Value
alpha	4.5133
colsample_bytree	0.7269
gamma	0.9273
lambda	0.4191
learning_rate	0.2856
max_depth	5.0
min_child_weight	4.0
n_estimators	204.0
reg_alpha	0.1812
reg_lambda	0.2855
scale_pos_weight	5.0599
subsample	0.6654

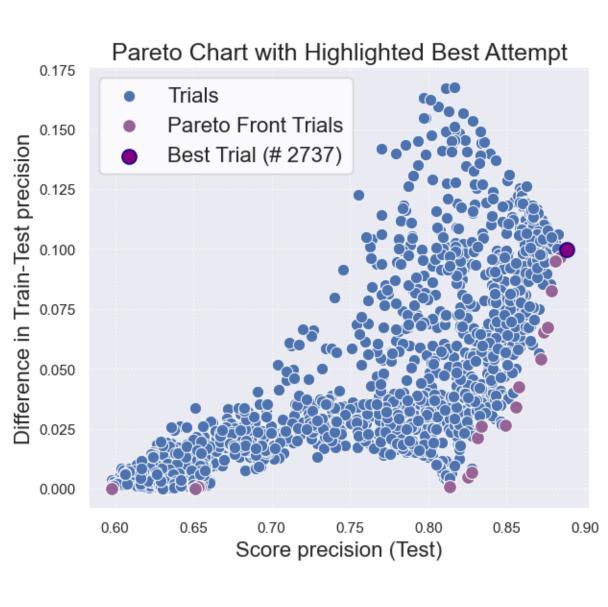


	Active/Ina	ctive probability	
50	Inactive zone	Active zone	type active (77) inactive (51) decoy (128)
40			
Percent 00			
10			
0 —	0.0 0.2 0.4	0.6 0.8	10
		obability	

Metric	Train	Test
AUC	0.9975	0.89
accuracy	0.9629	0.8047
balanced accuracy	0.9539	0.7781
recall_(sens)	1.0	0.9091
specificity	0.9078	0.6471
precision	0.9415	0.7955
f1_score	0.9626	0.7994

Protein: P08913 - metric: precision





XGBoost Parameters	Value
alpha	0.5444
colsample_bytree	0.8923
gamma	0.6661
lambda	0.4797
learning_rate	0.3955
max_depth	6.0
min_child_weight	1.0
n_estimators	277.0
reg_alpha	0.0992
reg_lambda	0.2534
scale_pos_weight	1.4119
subsample	0.607

			Active/Inactiv	e probability		
						type active (77) inactive (51) decoy (128)
40						
10 -	0.0	0.2	0.4 Proba	0.6	 	1.0
			11006	to inty		

- 0.8

- 0.7

- 0.6

- 0.5

- 0.4

- 0.3

0.2

0.2

0.0

0.0

0.2

Predicted label

Confusion Matrix (nomr.)

Predicted label

0.29

0.91

0.71

0.091

True label

Metric	Train	Test
AUC	0.9998	0.9114
accuracy	0.9922	0.8281
balanced accuracy	0.9903	0.8075
recall_(sens)	1.0	0.9091
specificity	0.9806	0.7059
precision	0.9871	0.8235
f1_score	0.9922	0.8251

Metric	Train	Test
AUC	0.9998	0.9114
accuracy	0.9922	0.8281
balanced accuracy	0.9903	0.8075
recall_(sens)	1.0	0.9091
specificity	0.9806	0.7059
precision	0.9871	0.8235
f1 score	0 9922	0.8251

- train: 0.0088

test: 0.1212

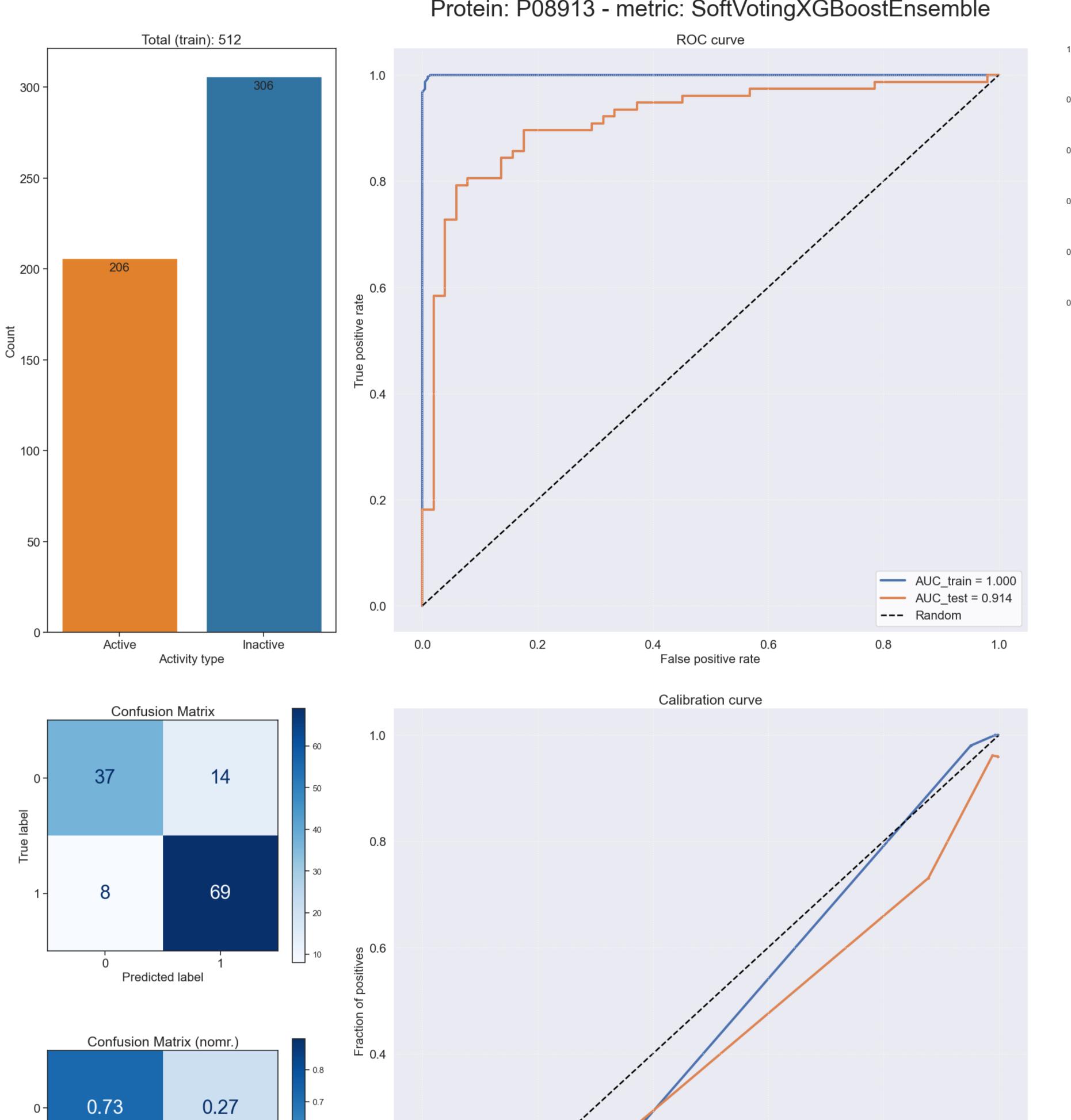
8.0

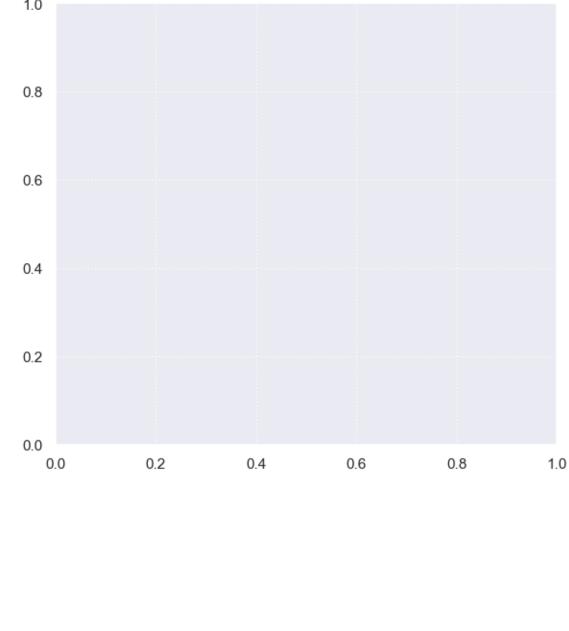
0.4 0.6 Mean predicted probability

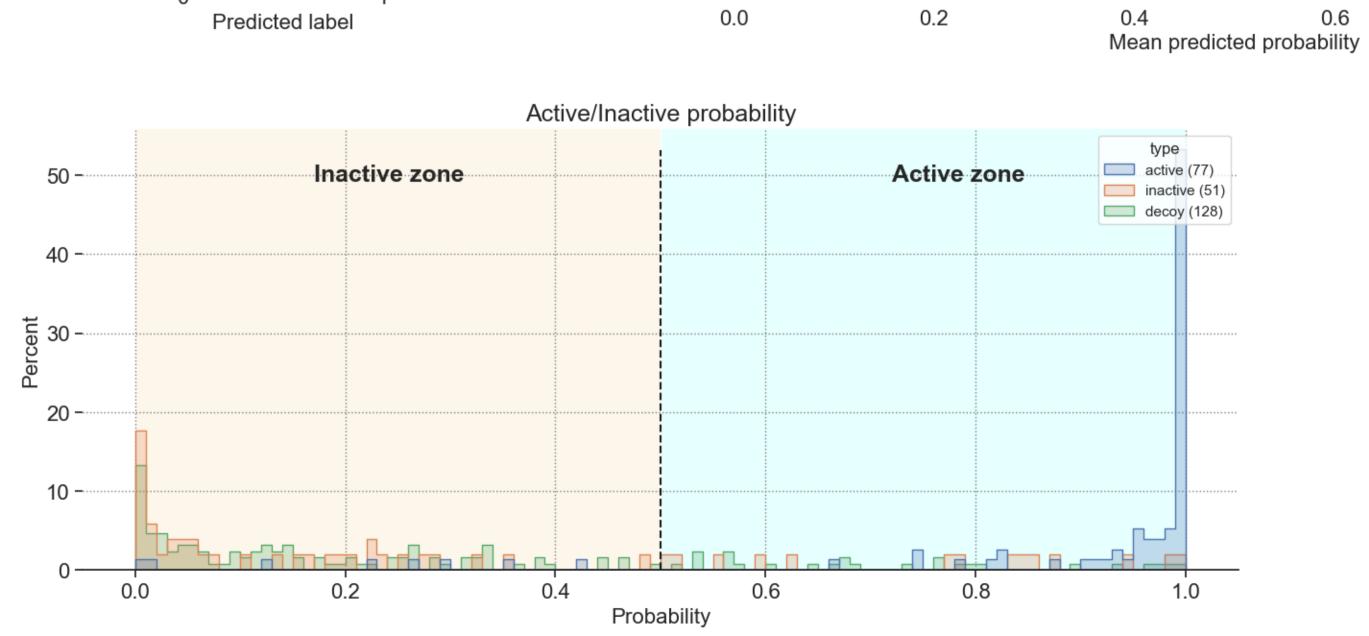
--- perfectly_calibrated

1.0

Protein: P08913 - metric: SoftVotingXGBoostEnsemble







0.2

0.0

0.0

0.2

- 0.6

- 0.5

- 0.4

- 0.3

0.2

0.9

True label

0.1

Predicted label

Metric	Train	Test
AUC	0.9998	0.9142
accuracy	0.9902	0.8281
balanced accuracy	0.9879	0.8108
recall_(sens)	1.0	0.8961
specificity	0.9757	0.7255
precision	0.9839	0.8313
f1_score	0.9902	0.826

--- train: 0.0133

--- test: 0.1185

0.8

--- perfectly_calibrated

1.0