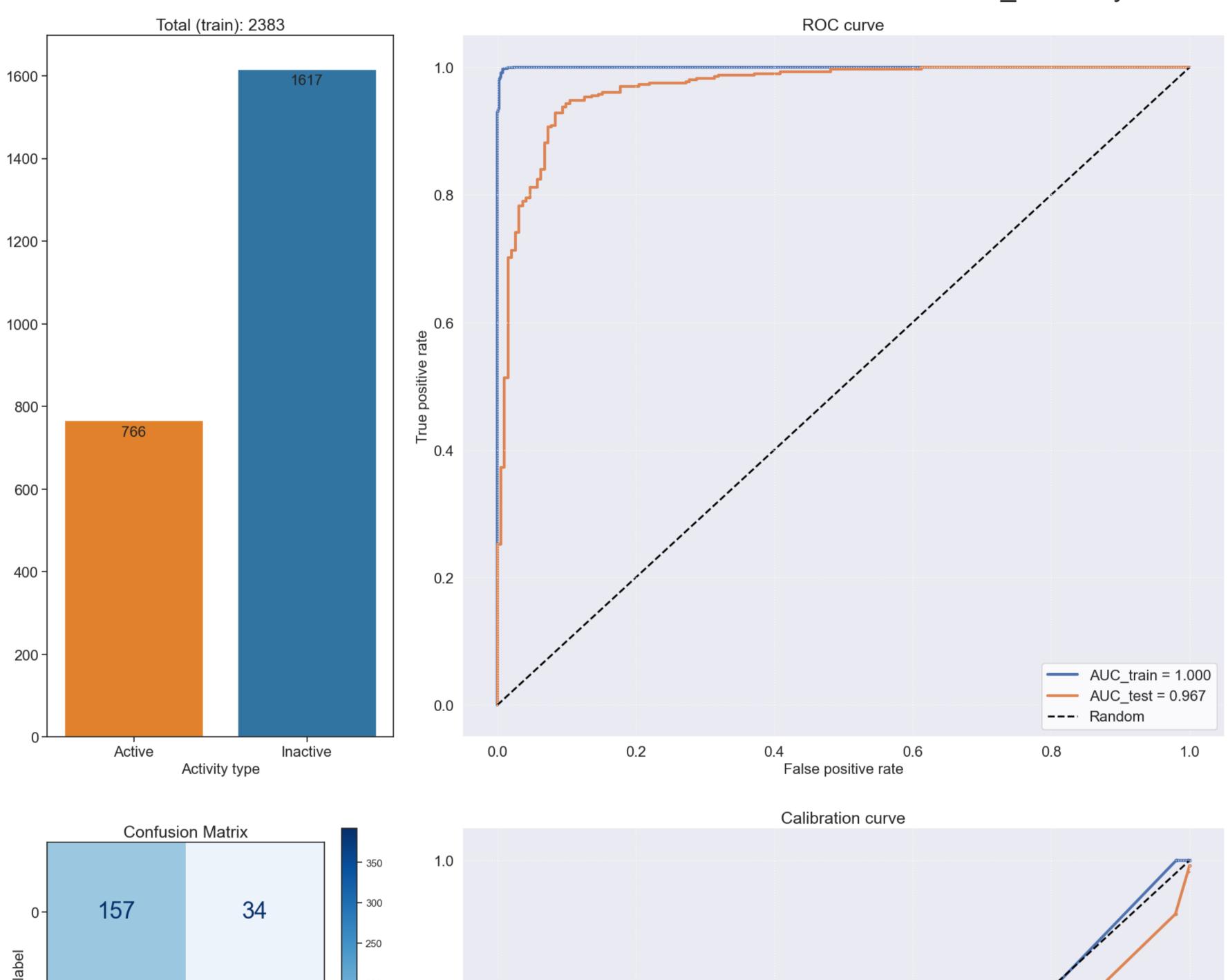
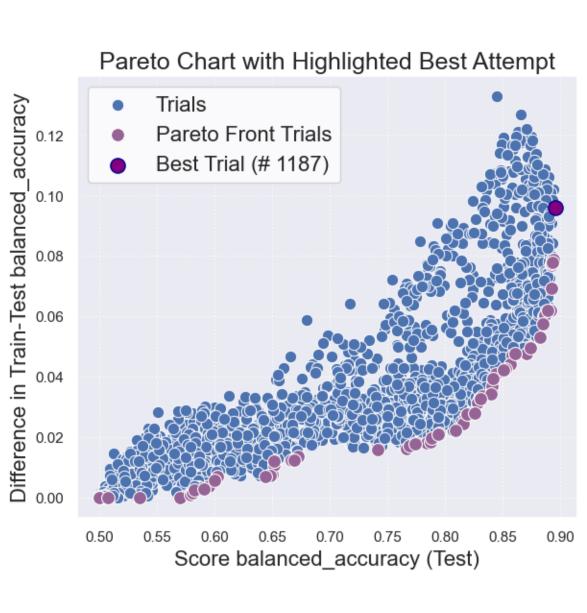
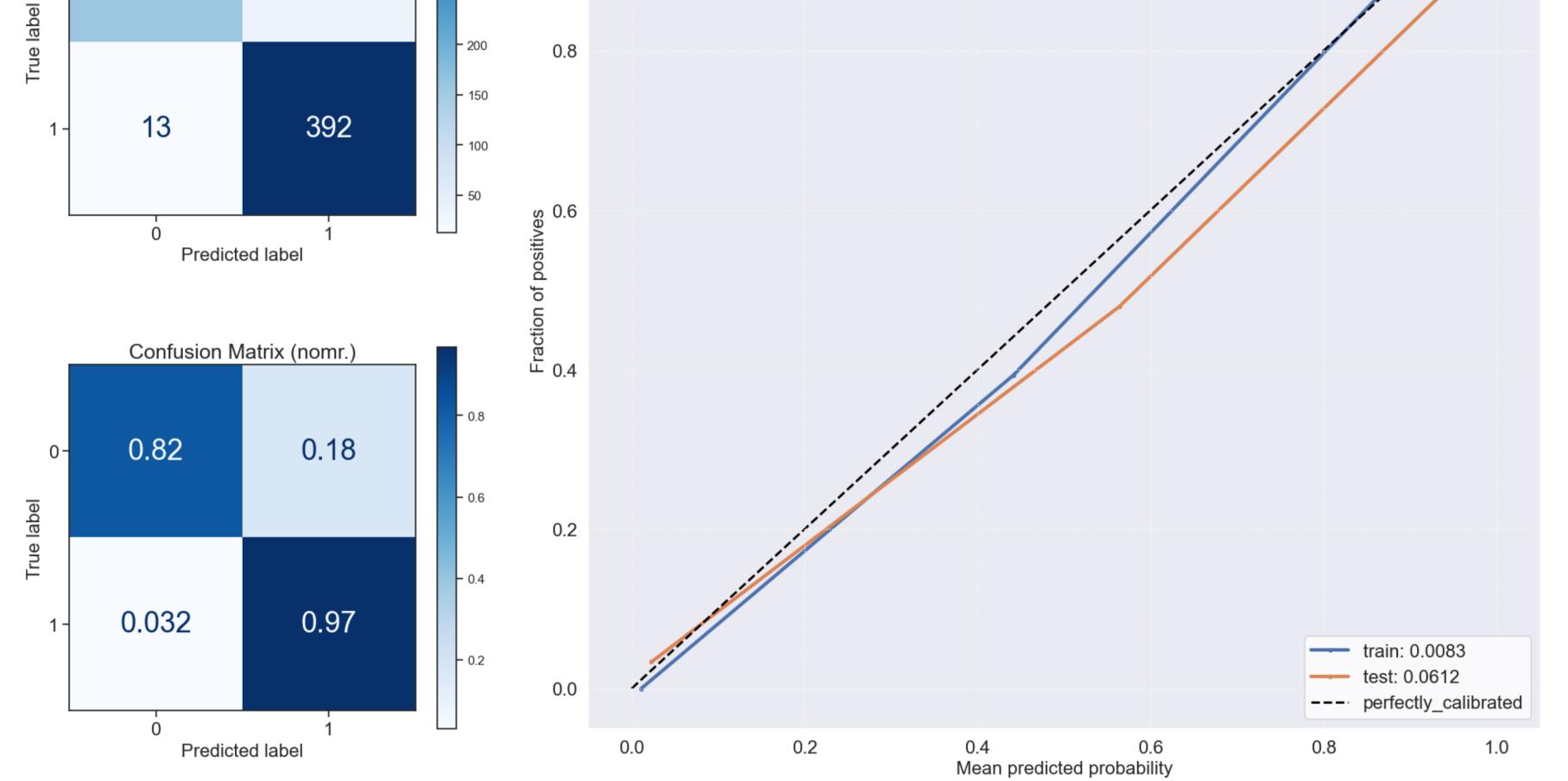
Protein: P0DMS8 - metric: balanced_accuracy





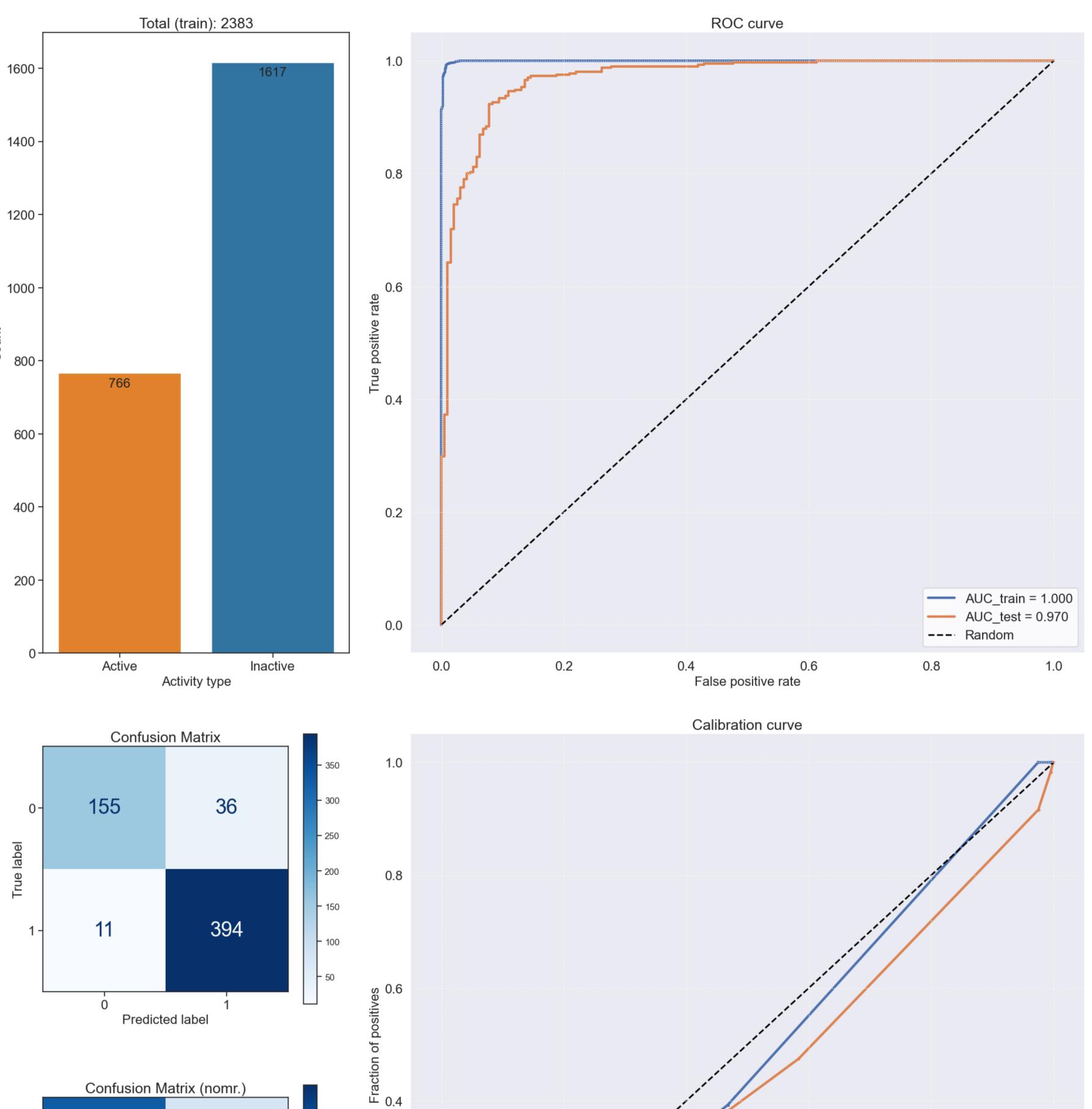
XGBoost Parameters	Value
alpha	4.4229
colsample_bytree	0.5403
gamma	0.2269
lambda	3.0044
learning_rate	0.2146
max_depth	8.0
min_child_weight	4.0
n_estimators	590.0
reg_alpha	0.2304
reg_lambda	0.1212
scale_pos_weight	1.5177
subsample	0.8084

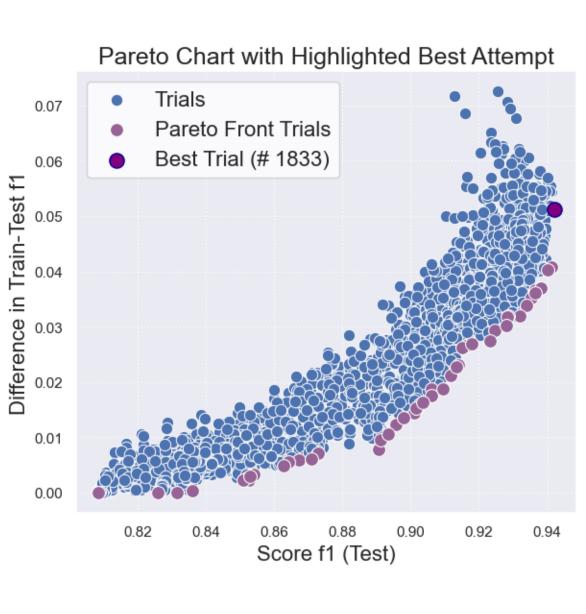


70		Active/Inactive			
60 -	Inactive zone	·		Active zone	type active (405) inactive (191)
					decoy (590)
50 -					
. 10 -					
30 -					
30					
00					
20					
10 -					
l band	<u></u>			_	
0.0	0.2	0.4	0.6	0.8	1.0
		Proba	bility		

Metric	Train	Test
AUC	0.9997	0.9673
accuracy	0.9929	0.9211
balanced accuracy	0.9892	0.8949
recall_(sens)	0.9994	0.9679
specificity	0.9791	0.822
precision	0.9902	0.9202
f1_score	0.9928	0.9198

Protein: P0DMS8 - metric: f1





XGBoost Parameters	Value
alpha	1.1022
colsample_bytree	0.867
gamma	0.7208
lambda	0.7644
learning_rate	0.0645
max_depth	6.0
min_child_weight	1.0
n_estimators	754.0
reg_alpha	0.2685
reg_lambda	0.4458
scale_pos_weight	1.7358
subsample	0.5831

		Active/Ina	ctive probability		
60 -	Inactive	zone		Active zone	active (405) inactive (191)
40					
Percent 00.					
20	7				
10 -					
0.0	0.2	0.4 Pr	0.6 obability	0.8	1.0

0.2

0.0

0.0

0.4

0.2

Predicted label

Confusion Matrix (nomr.)

Predicted label

0.19

0.97

0.81

0.027

0-

True label

Metric	Train	Test
AUC	0.9996	0.97
accuracy	0.9899	0.9211
balanced accuracy	0.9843	0.8922
recall_(sens)	1.0	0.9728
specificity	0.9687	0.8115
precision	0.9854	0.9163
f1_score	0.9899	0.9196

--- train: 0.0119

0.8

test: 0.0594

--- perfectly_calibrated

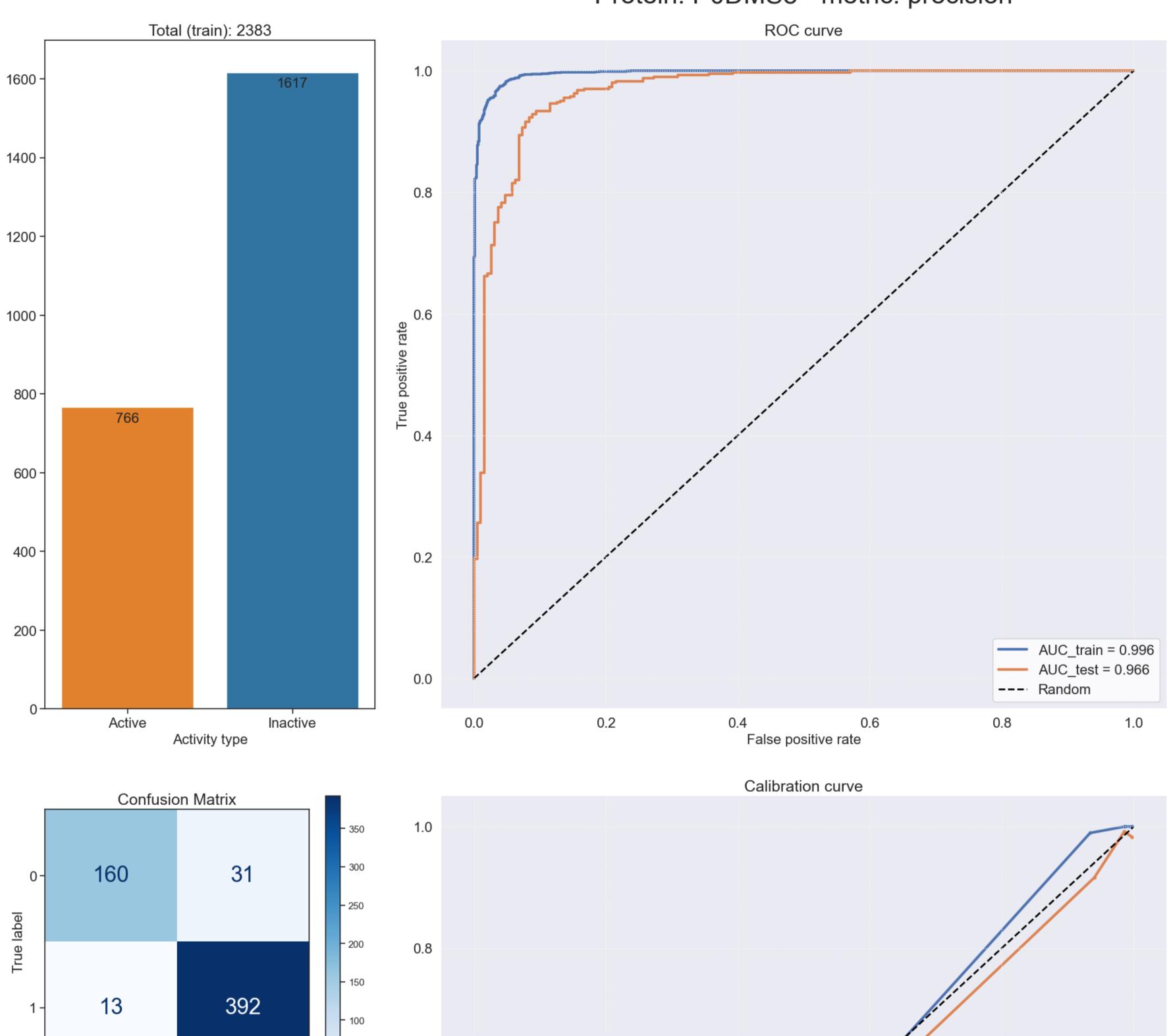
1.0

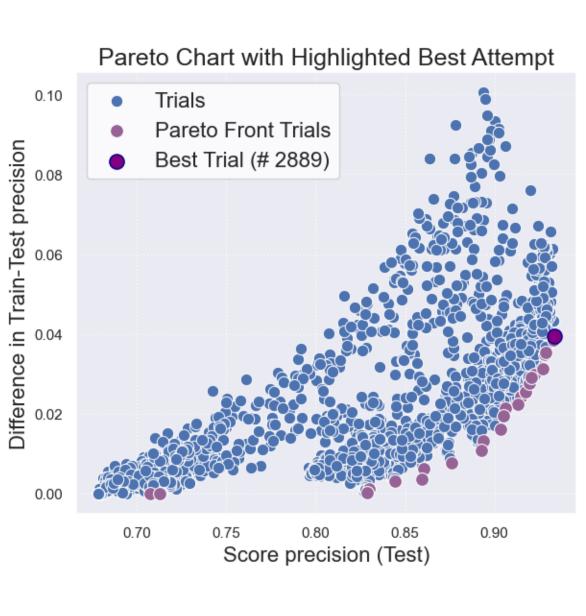
		Active/Inactive prob	pability		
60	Inactive zone		Active zone	type active (405)	Metric
50				inactive (191) decoy (590)	AUC
40					accuracy
					balanced accuracy
Percent					recall_(sens)
20					specificity
10	<u> </u>				precision
0					f1_score
0	0.0 0.2	0.4 Probability	0.6 0.8	1.0	

0.2

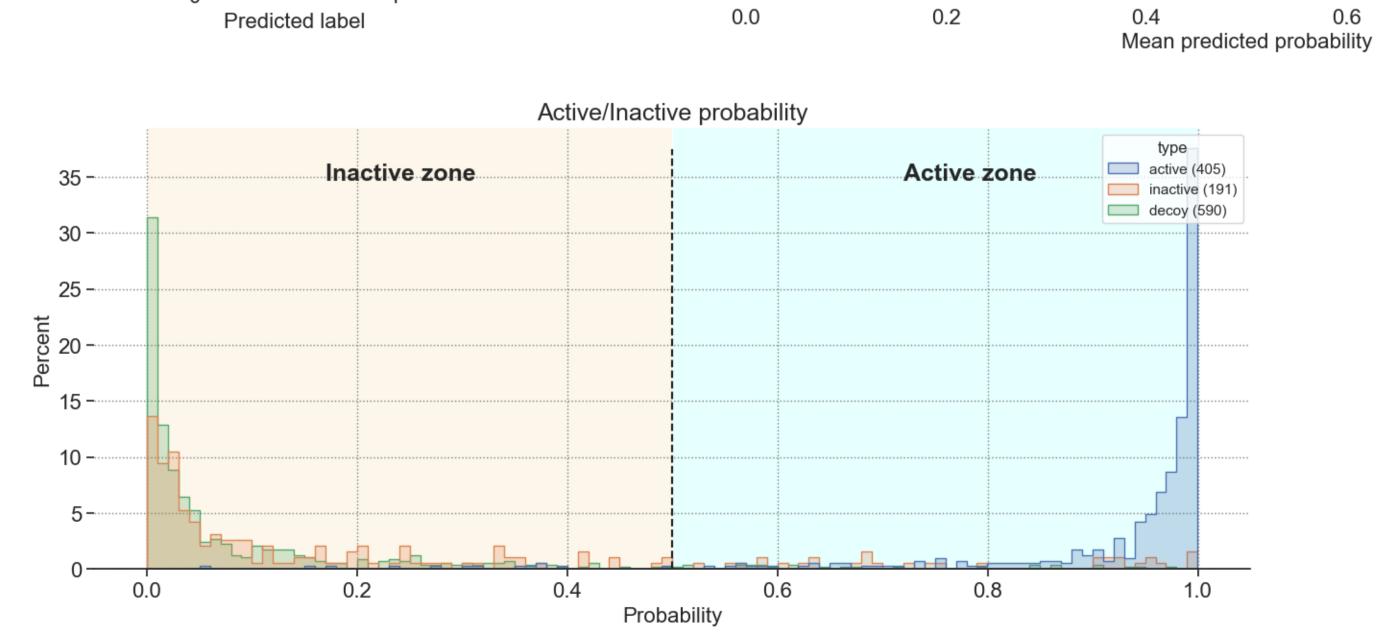
0.4 0.6 Mean predicted probability

Protein: P0DMS8 - metric: precision





XGBoost Parameters	Value
alpha	0.0502
colsample_bytree	0.9592
gamma	0.8755
lambda	0.0397
learning_rate	0.1315
max_depth	3.0
min_child_weight	1.0
n_estimators	555.0
reg_alpha	0.6885
reg_lambda	0.4809
scale_pos_weight	1.0143
subsample	0.6221



Fraction of positives

0.2

0.0

0.0

0.2

0.4

0.2

Predicted label

Confusion Matrix (nomr.)

Predicted label

0.16

0.97

0.84

0.032

0-

True label

Metric	Train	Test
AUC	0.9959	0.9662
accuracy	0.9723	0.9262
balanced accuracy	0.9645	0.9028
recall_(sens)	0.9864	0.9679
specificity	0.9426	0.8377
precision	0.9732	0.9267
f1_score	0.9722	0.9252

- train: 0.0261

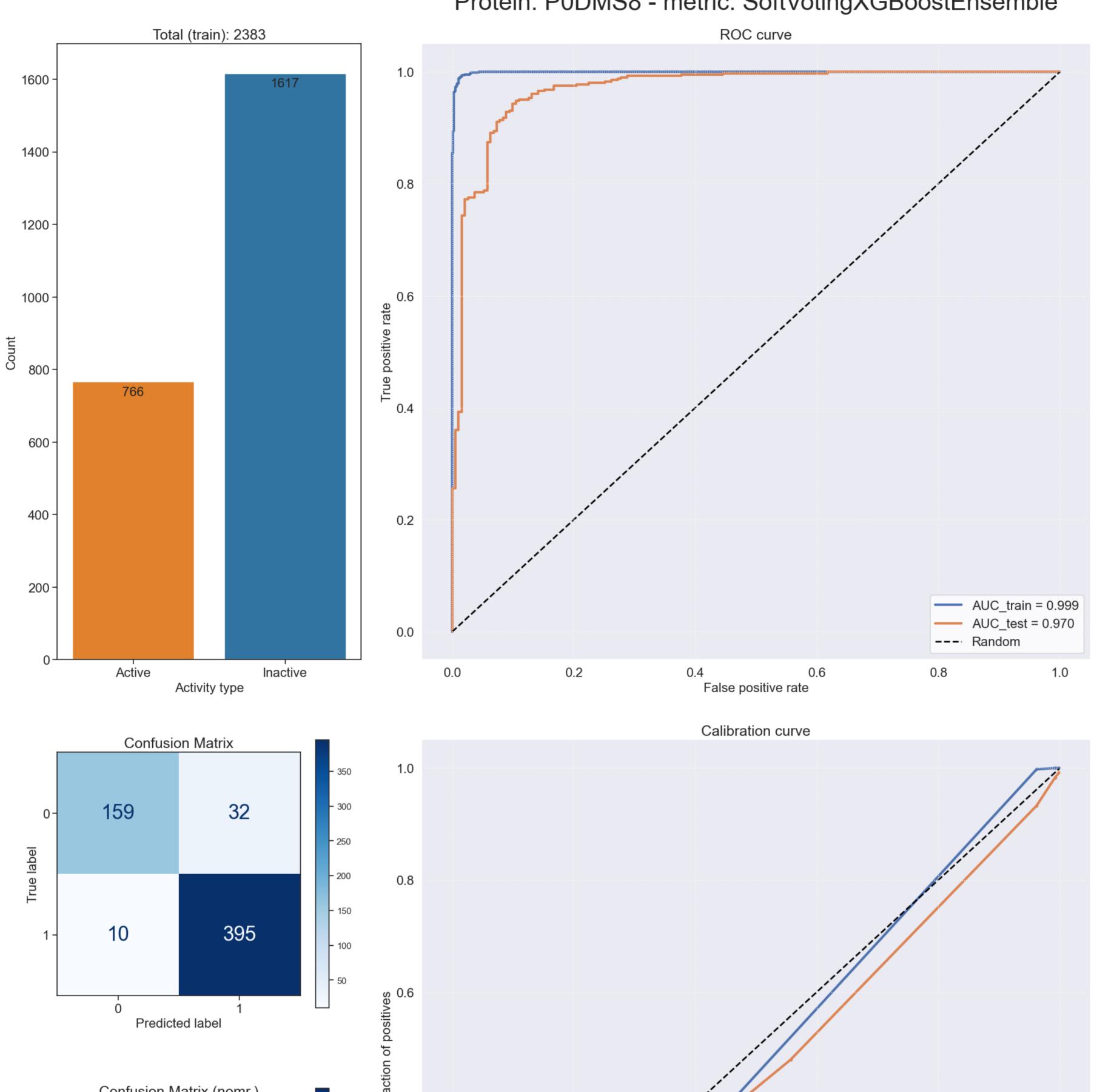
0.8

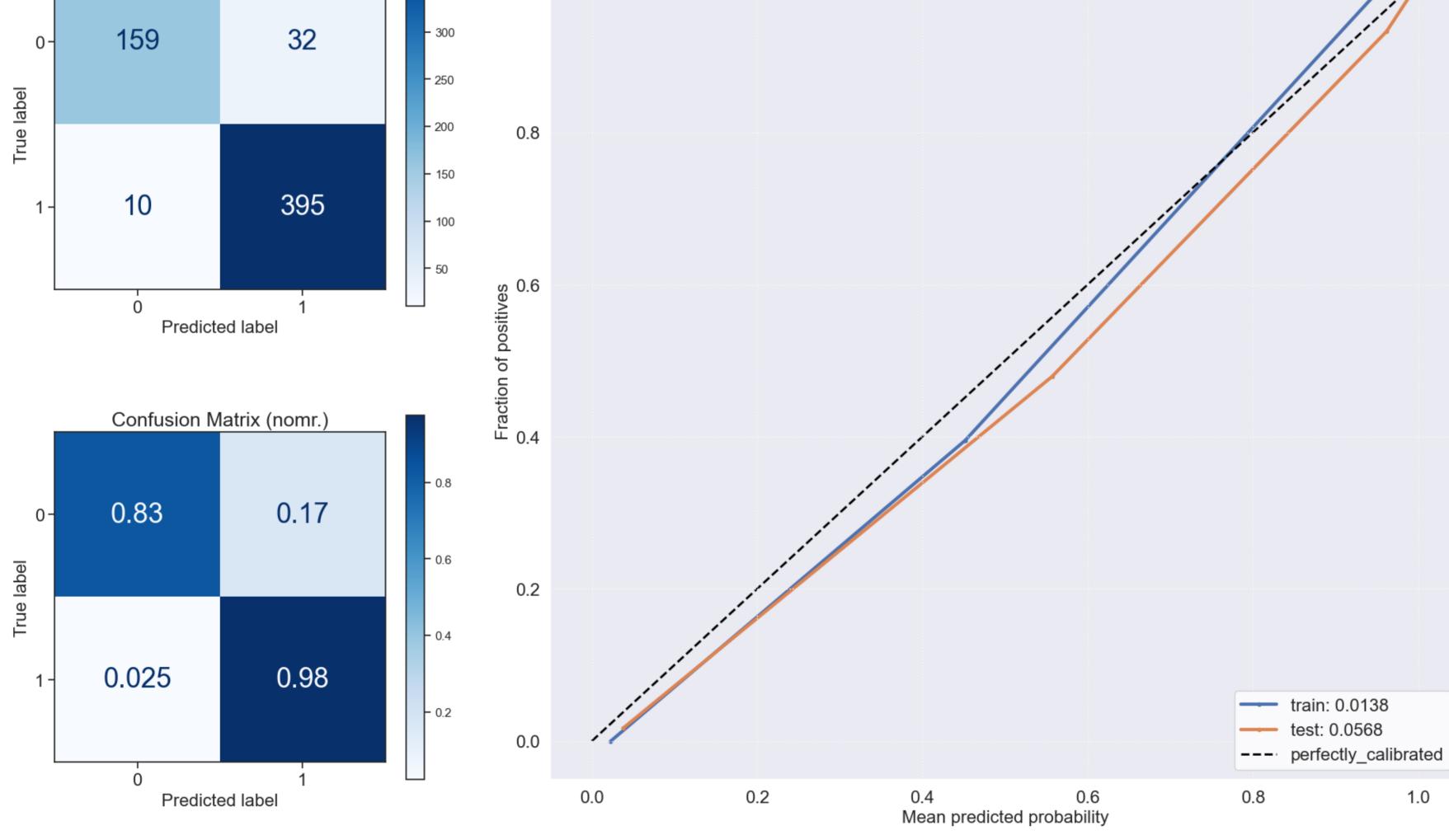
test: 0.058

--- perfectly_calibrated

1.0

Protein: P0DMS8 - metric: SoftVotingXGBoostEnsemble





		A	ctive/Inactive	e probability		
50		nactive zone			Active zone	type active (405) inactive (191) decoy (590)
40						
Percent						
20						
0-	0.0	0.2	0.4	0.6	0.8	10
	0.0	0.2	Proba		0.0	1.0

Metric	Train	Test
AUC	0.9993	0.9697
accuracy	0.9891	0.9295
balanced accuracy	0.9841	0.9039
recall_(sens)	0.9981	0.9753
specificity	0.97	0.8325
precision	0.9859	0.9251
f1_score	0.9891	0.9283

0.8

0.6

0.4

0.2

0.0

0.0

0.2

0.6