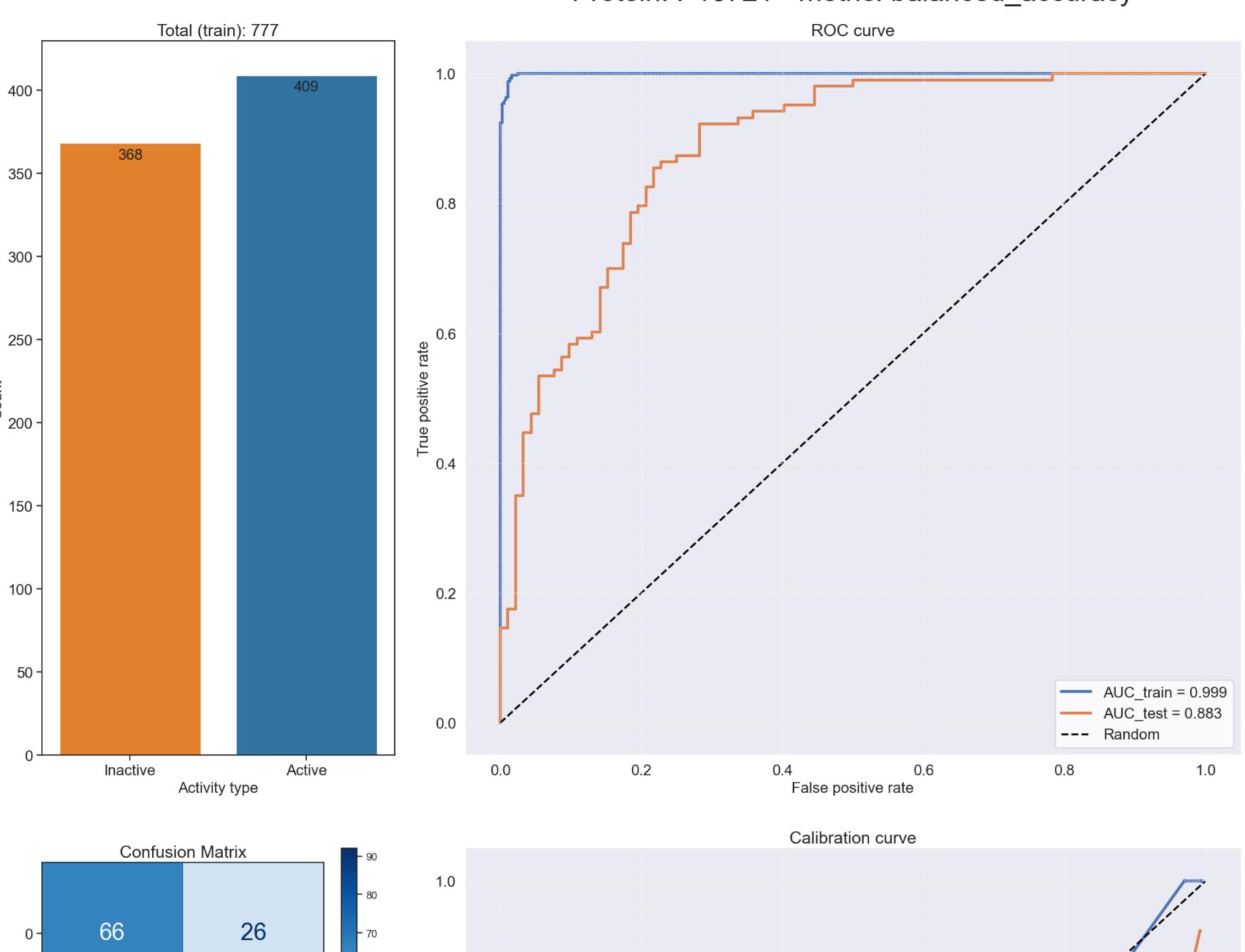
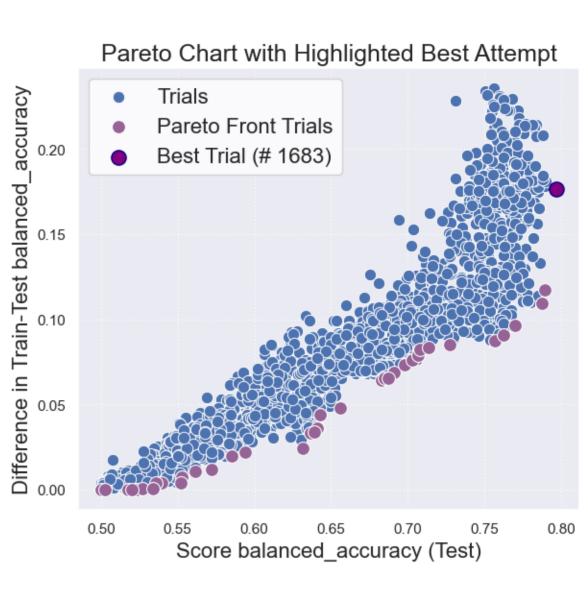
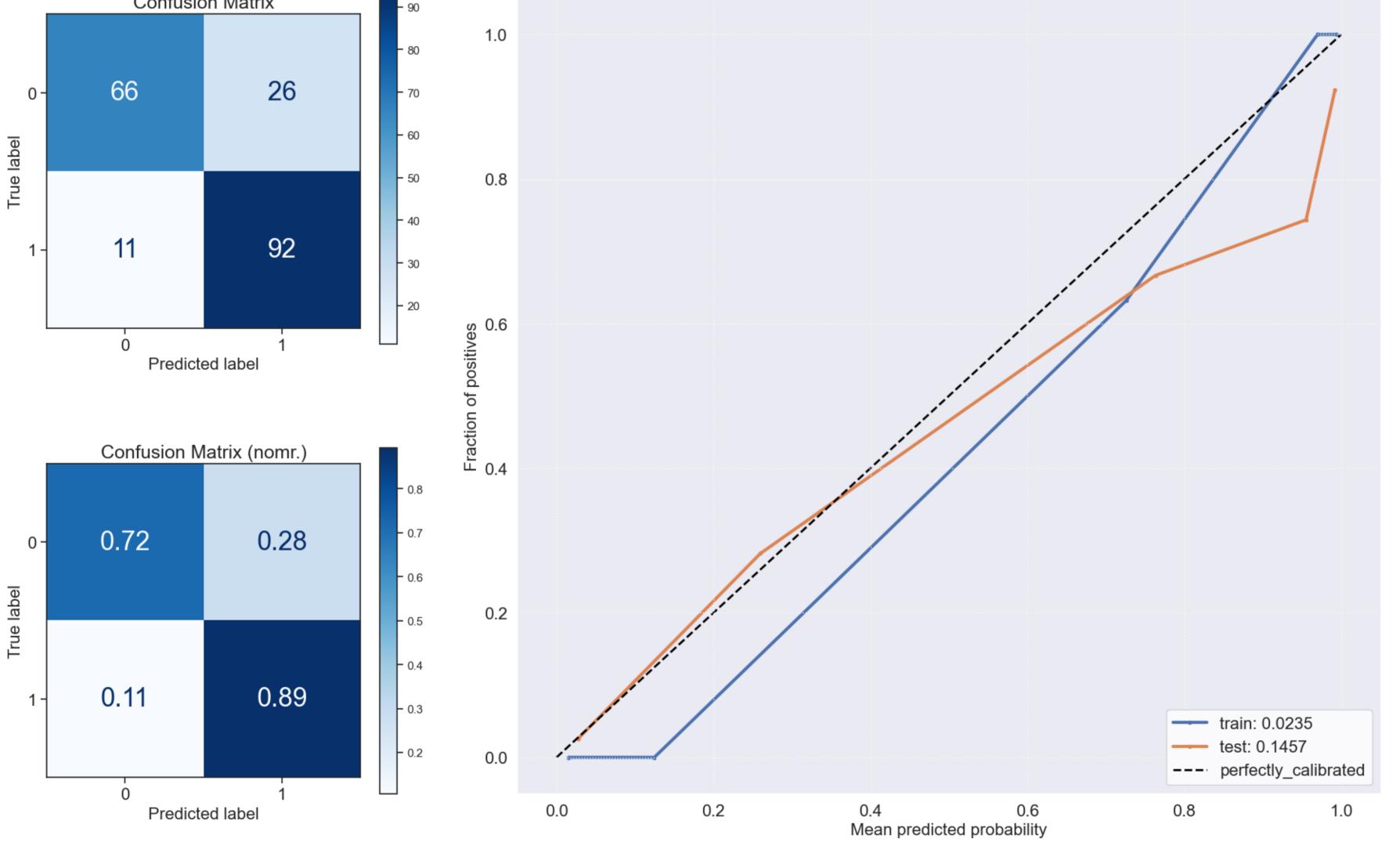
Protein: P10721 - metric: balanced_accuracy





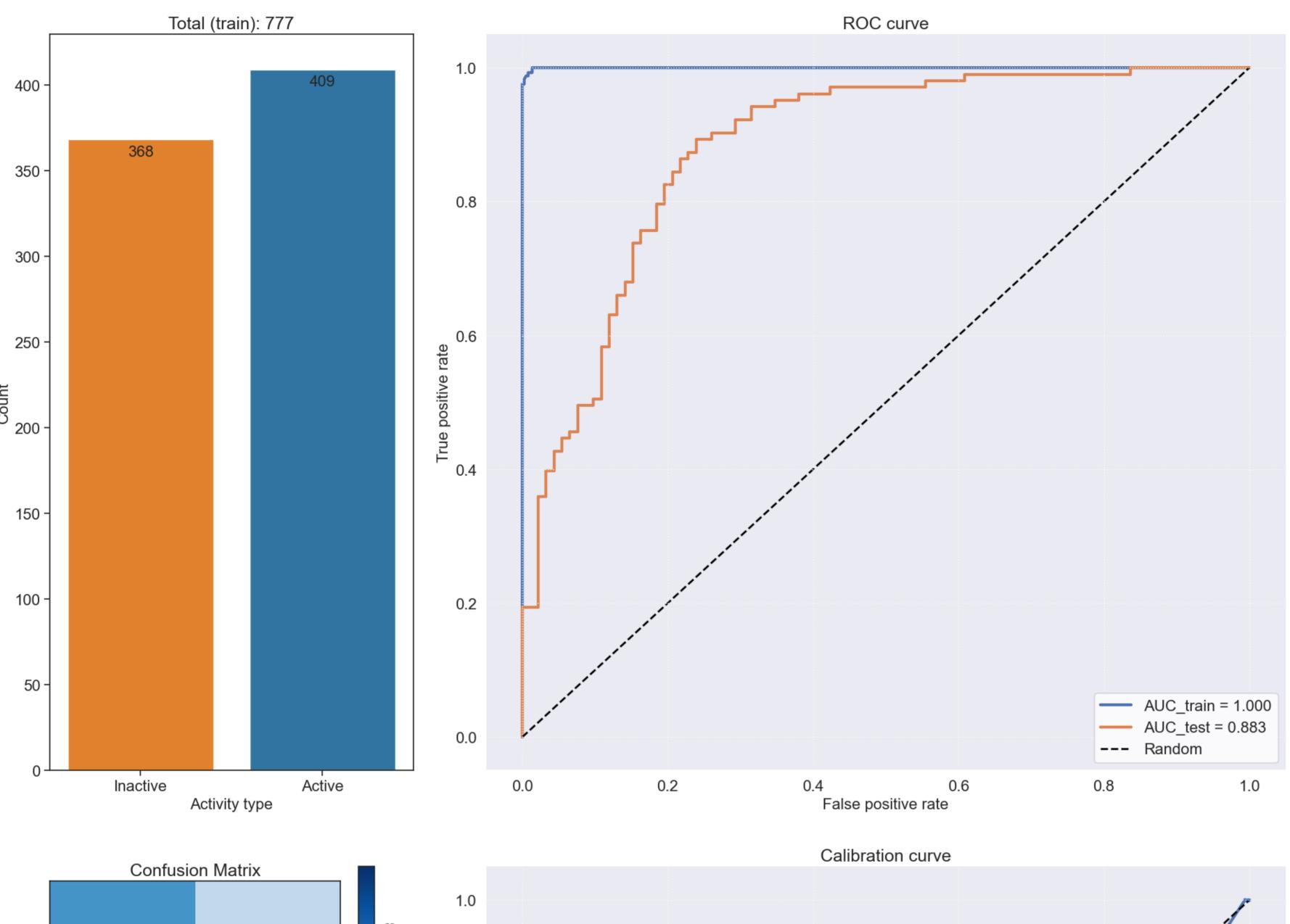
XGBoost Parameters	Value
alpha	3.2276
colsample_bytree	0.7826
gamma	0.5539
lambda	0.7981
learning_rate	0.0915
max_depth	6.0
min_child_weight	4.0
n_estimators	945.0
reg_alpha	0.4127
reg_lambda	0.2339
scale_pos_weight	2.8437
subsample	0.6777

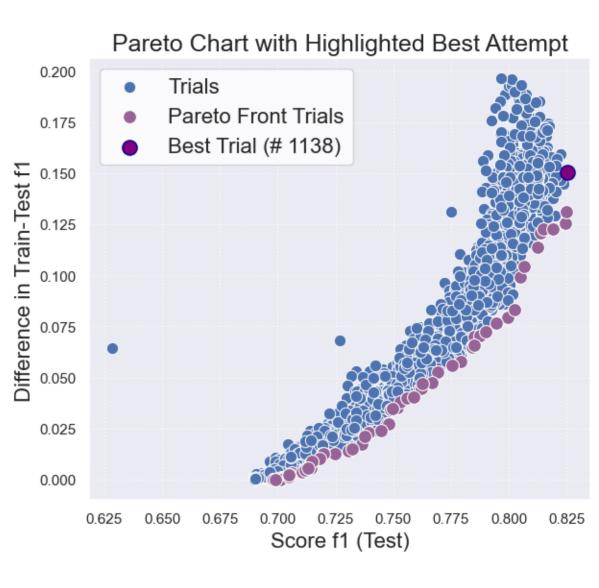


	Active/Inactive probability								
20	lna	ctive zone		A	ctive zone	type active (103) inactive (92) decoy (195)			
15									
Percent 0									
5									
5									
0	0.0 0	.2 0	.4 Probability	0.6	0.8	1.0			

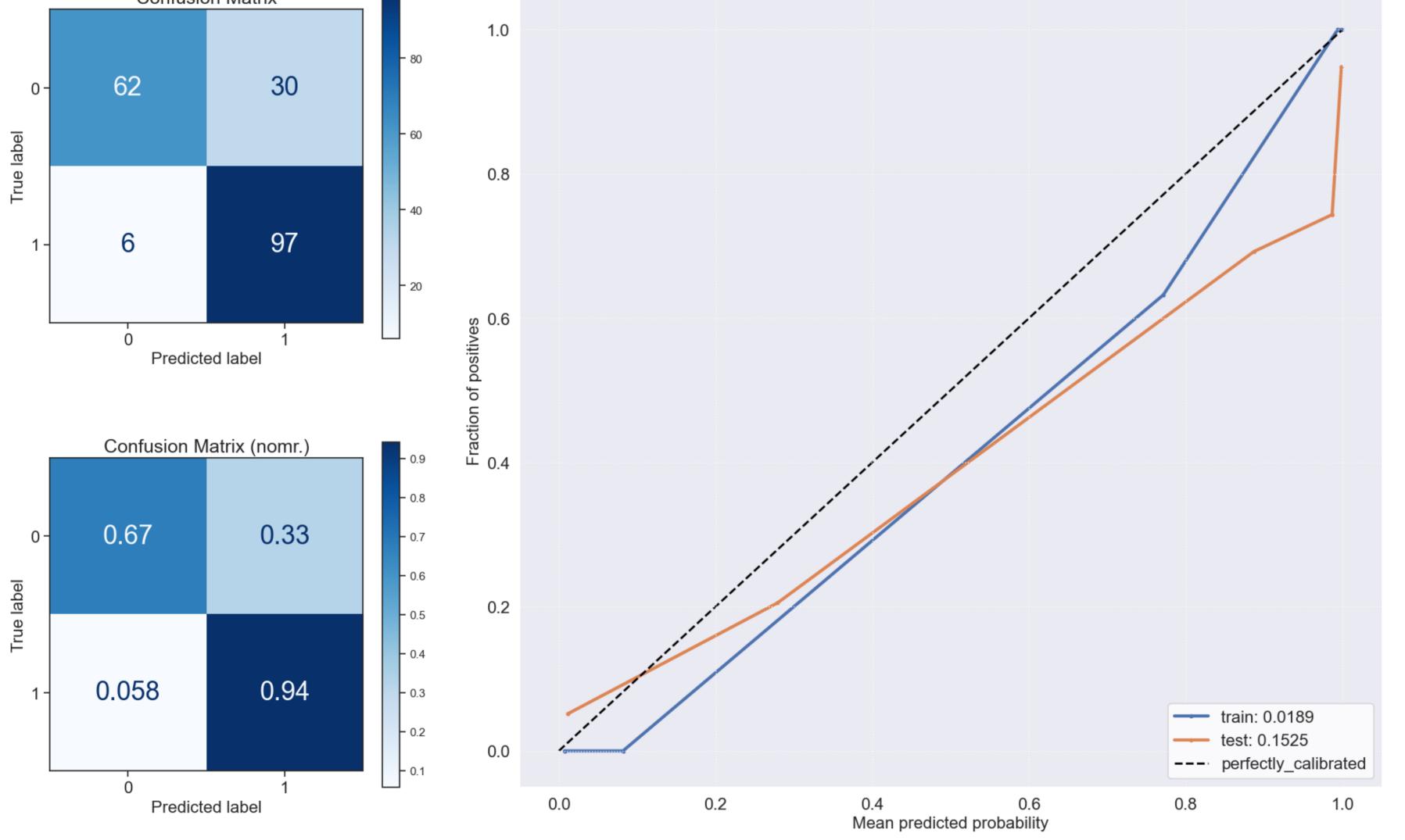
Metric	Train	Test
AUC	0.9994	0.8832
accuracy	0.9781	0.8103
balanced accuracy	0.9769	0.8053
recall_(sens)	1.0	0.8932
specificity	0.9538	0.7174
precision	0.9601	0.7797
f1_score	0.9781	0.8083

Protein: P10721 - metric: f1





XGBoost Parameters	Value
alpha	3.1706
colsample_bytree	0.8823
gamma	0.0216
lambda	0.0412
learning_rate	0.1596
max_depth	10.0
min_child_weight	6.0
n_estimators	879.0
reg_alpha	0.9436
reg_lambda	0.416
scale_pos_weight	10.4086
subsample	0.8272

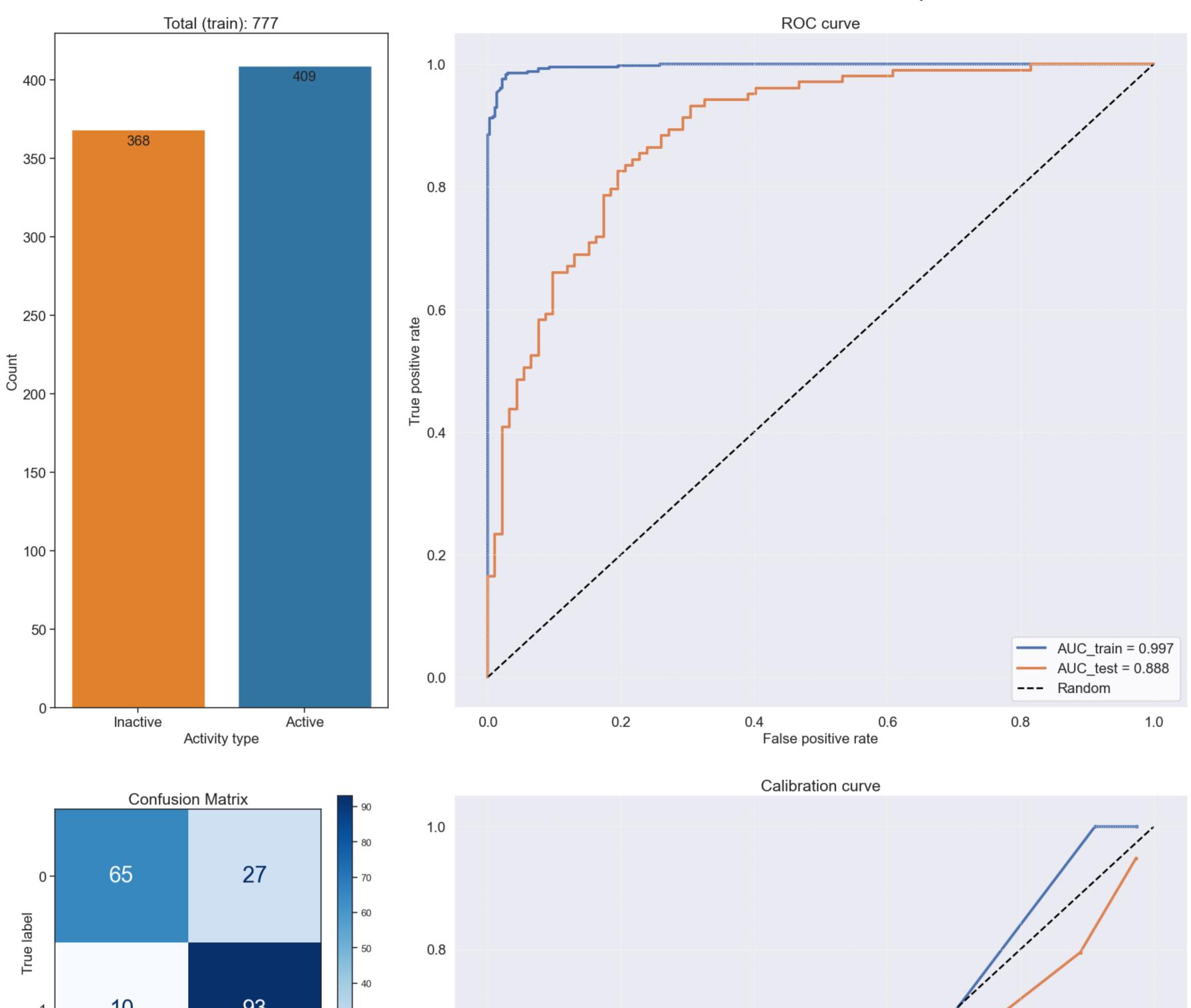


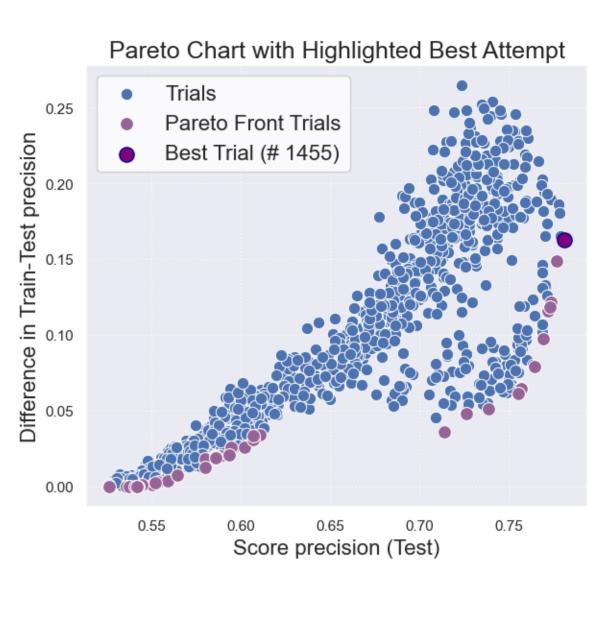
50		Inactive zone			Active zone	type active (103) inactive (92) decoy (195)
30						
Percent 00						
10						
0 —	0.0	0.2	0.4	0.6	0.8	10
	0.0	V.2	Proba		0.0	1.0

Active/Inactive probability

Metric	Train	Test
AUC	0.9998	0.8825
accuracy	0.9768	0.8154
balanced accuracy	0.9755	0.8078
recall_(sens)	1.0	0.9417
specificity	0.9511	0.6739
precision	0.9578	0.7638
f1_score	0.9768	0.8112

Protein: P10721 - metric: precision



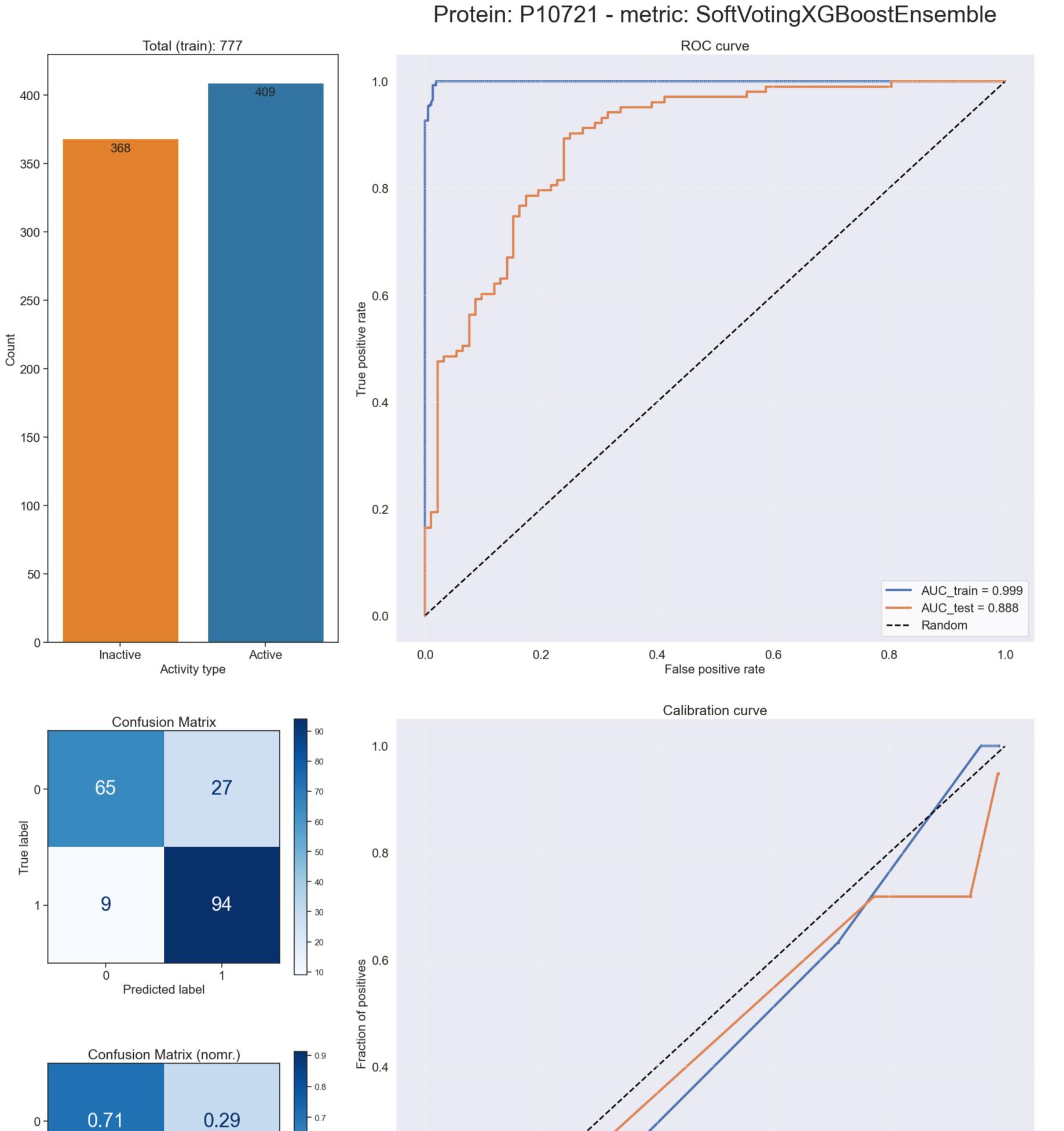


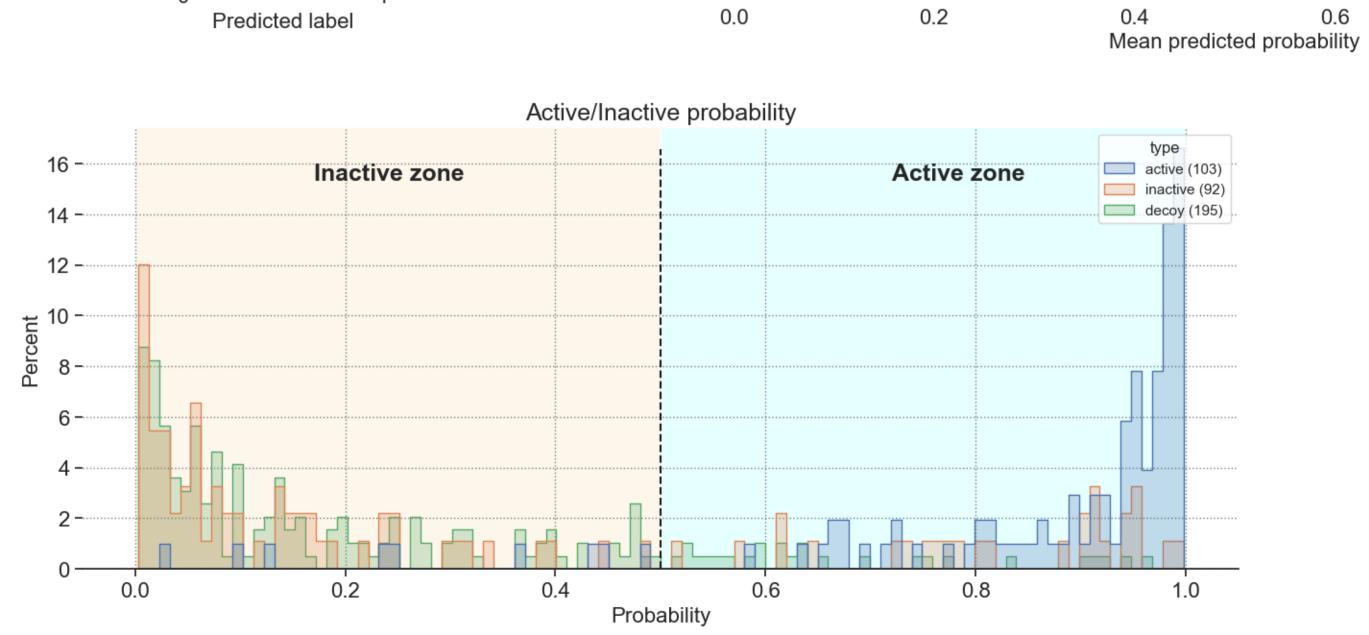
XGBoost Parameters	Value
alpha	0.8283
colsample_bytree	0.9511
gamma	0.0528
lambda	4.3388
learning_rate	0.0322
max_depth	10.0
min_child_weight	6.0
n_estimators	597.0
reg_alpha	0.5218
reg_lambda	0.7901
scale_pos_weight	1.4114
subsample	0.9988

label			- 60						
True	10	93	- 50 - 40 - 30 - 20	0.8					
	0 Predicte	1 ed label	10	tion of positives			pooro		
	Confusion M	atrix (nomr.)	0.9	Fraction 9.0					
label O	0.71	0.29	- 0.8 - 0.7 - 0.6	0.2		, or			
True label	0.097	0.9	- 0.5 - 0.4 - 0.3 - 0.2	0.0	por a distribution				train: 0.0378 test: 0.1361 perfectly_calibrated
	0 Predicte	1 ed label	0.1		0.0	0.2	0.4 Mean predicted	0.6 probability	0.8 1.0

			Active/Inact	ive probability		
16 - 14 -		Inactive zon	е		Active zone	active (103)
12 - 10 -						
Percent						
4 - 2 -			h			
0 —	0.0	0.2	0.4 Prol	0.6 pability	0.8	1.0

Metric	Train	Test
AUC	0.9968	0.8882
accuracy	0.9691	0.8103
balanced accuracy	0.9682	0.8047
recall_(sens)	0.9853	0.9029
specificity	0.9511	0.7065
precision	0.9572	0.775
f1_score	0.9691	0.8078





- 0.7

- 0.6

- 0.5

- 0.4

- 0.3

0.2

0.91

0.2

0.0

True label

0.087

Metric	Train	Test
AUC	0.9992	0.888
accuracy	0.9743	0.8154
balanced accuracy	0.9728	0.8096
recall_(sens)	1.0	0.9126
specificity	0.9457	0.7065
precision	0.9534	0.7769
f1_score	0.9742	0.8128

Metric	Train	Test
AUC	0.9992	0.888
accuracy	0.9743	0.8154
balanced accuracy	0.9728	0.8096
recall_(sens)	1.0	0.9126
specificity	0.9457	0.7065
precision	0.9534	0.7769
f1 score	0.9742	0.8128

--- train: 0.0239

--- test: 0.1398

0.8

--- perfectly_calibrated

1.0

0.8

0.6

0.4

0.2

0.0

0.0

0.2

0.6