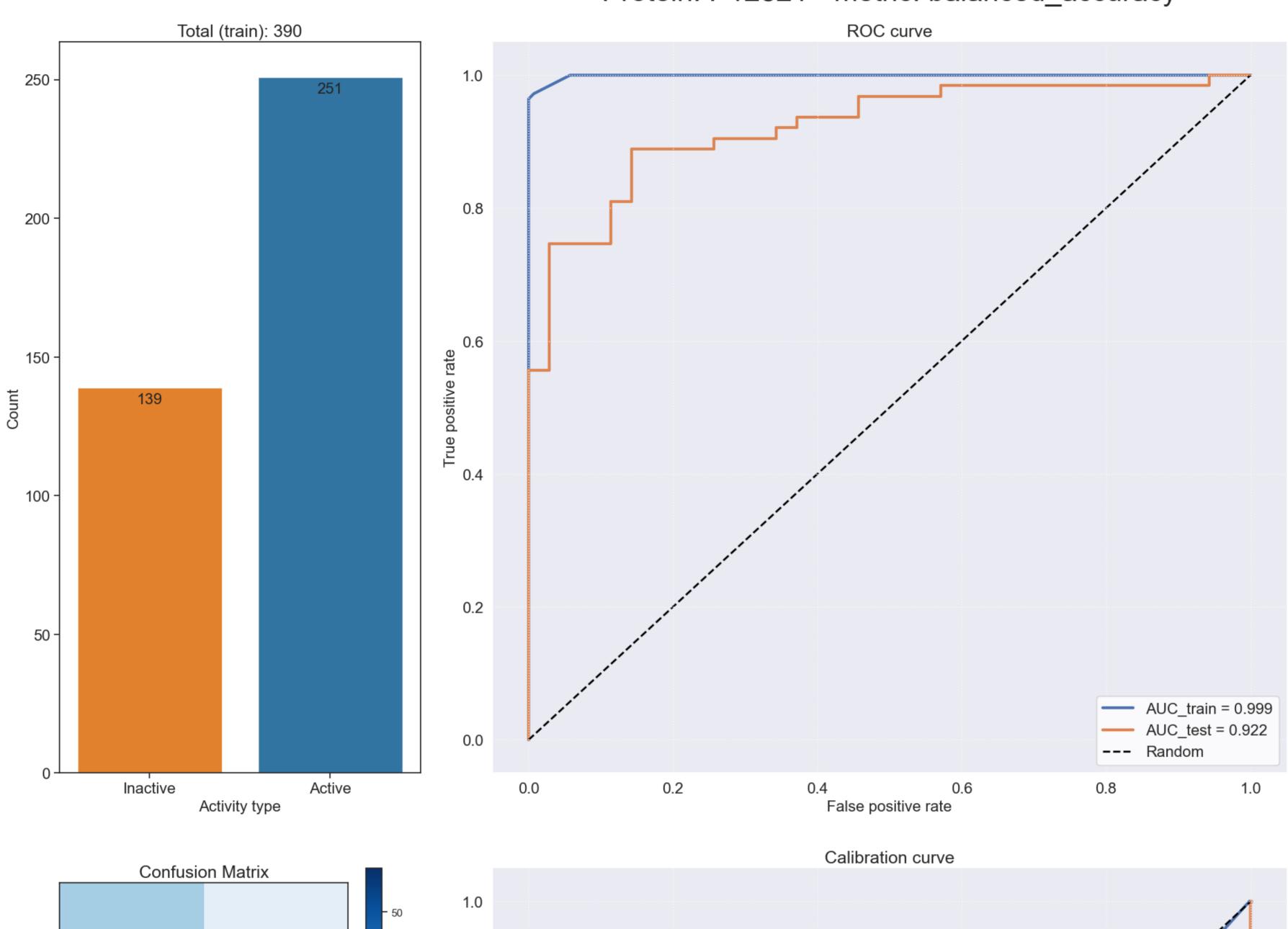
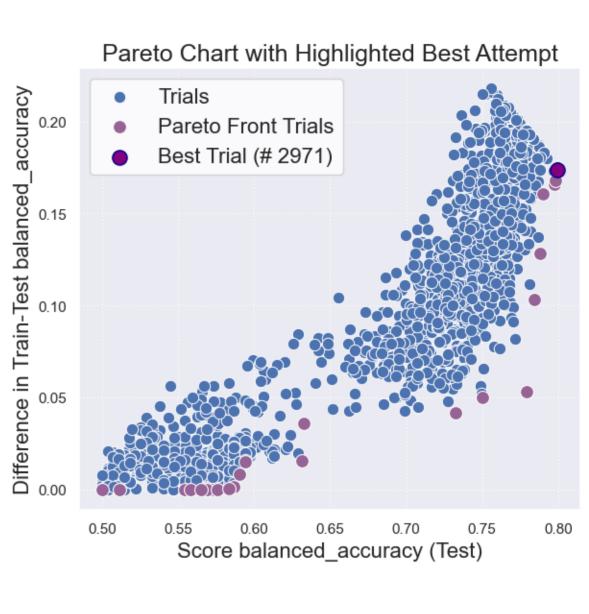
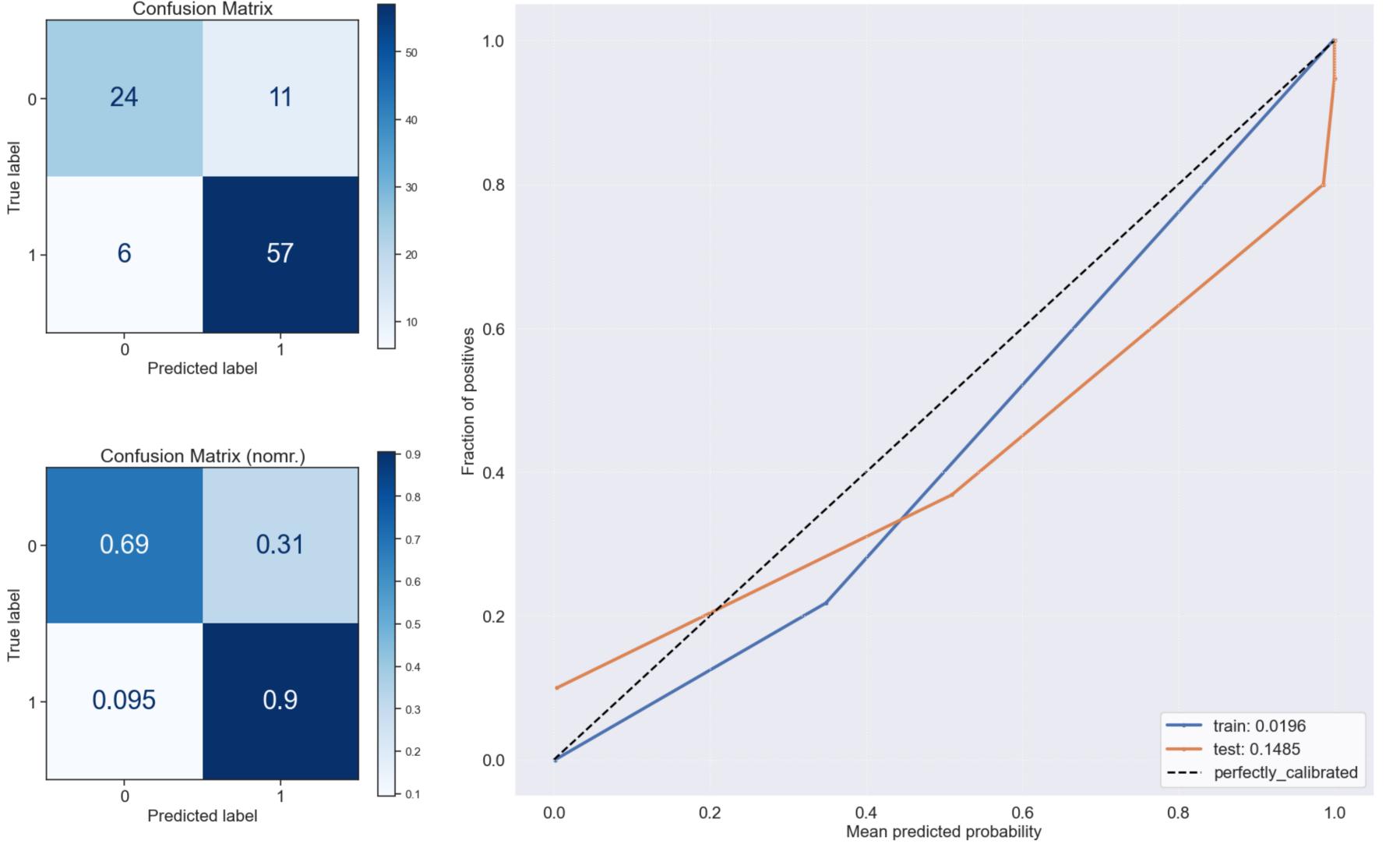
Protein: P12821 - metric: balanced_accuracy





XGBoost Parameters	Value
alpha	2.9381
colsample_bytree	0.6595
gamma	0.2636
lambda	3.3876
learning_rate	0.8742
max_depth	7.0
min_child_weight	2.0
n_estimators	931.0
reg_alpha	0.0281
reg_lambda	0.3527
scale_pos_weight	25.4566
subsample	0.9174

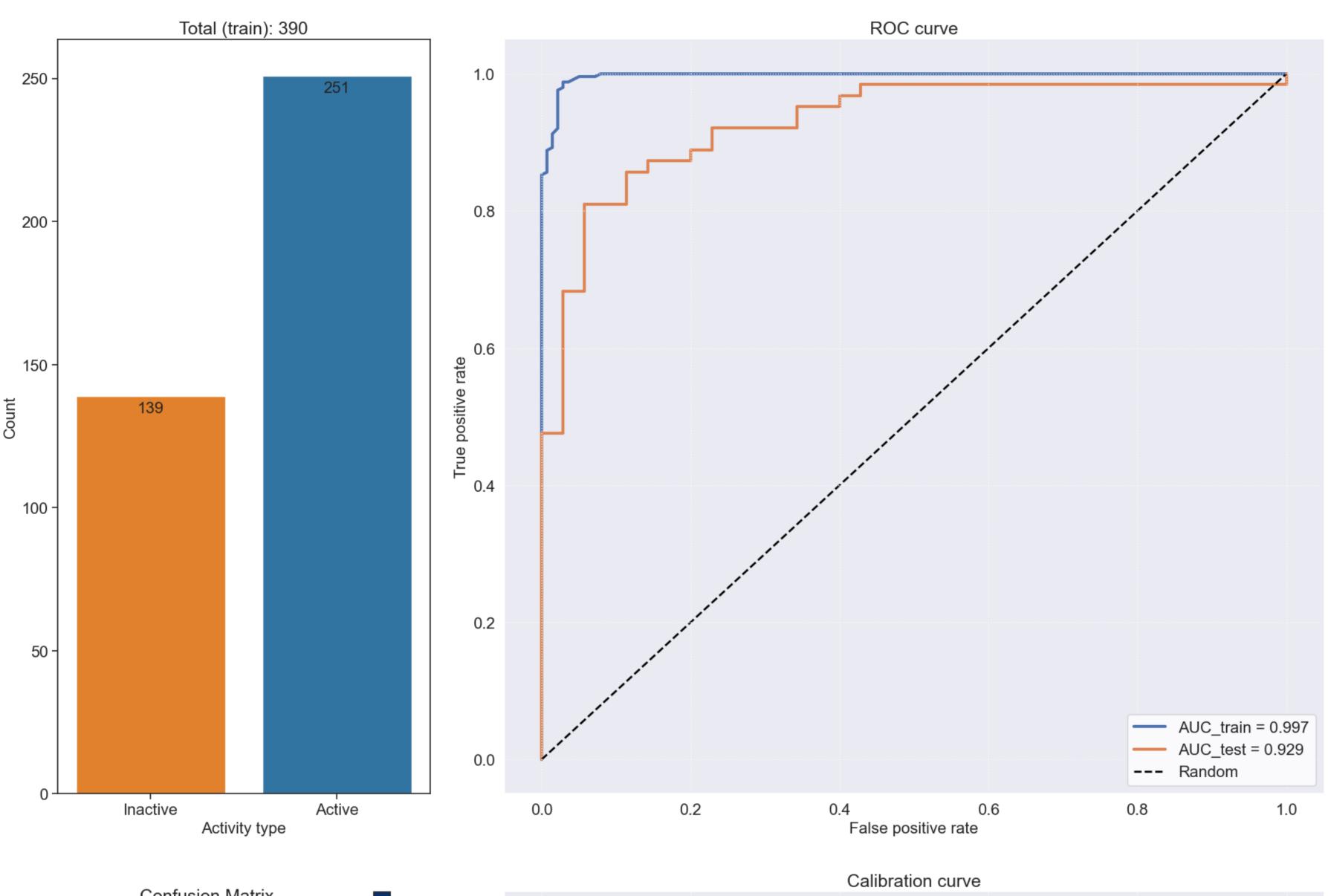


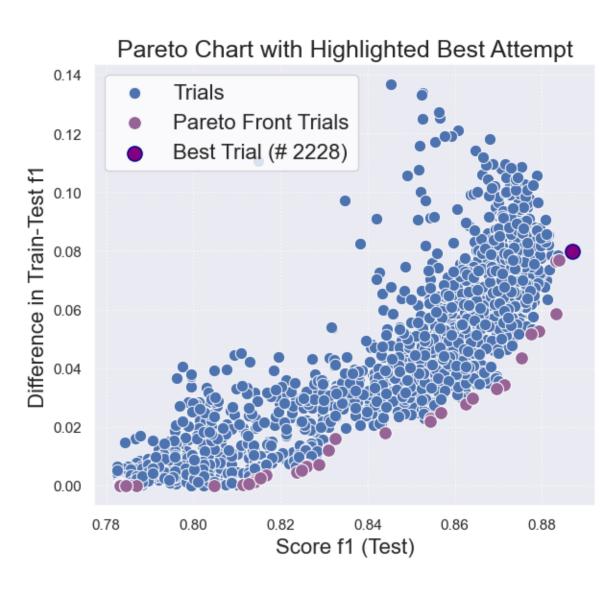
00	Ina				ctive zone	inactive (35) decoy (98)
50						
Percent 05						
30						
20						
0				П		
	0.0	.2 0	.4 Probability	0.6	0.8	1.0

Active/Inactive probability

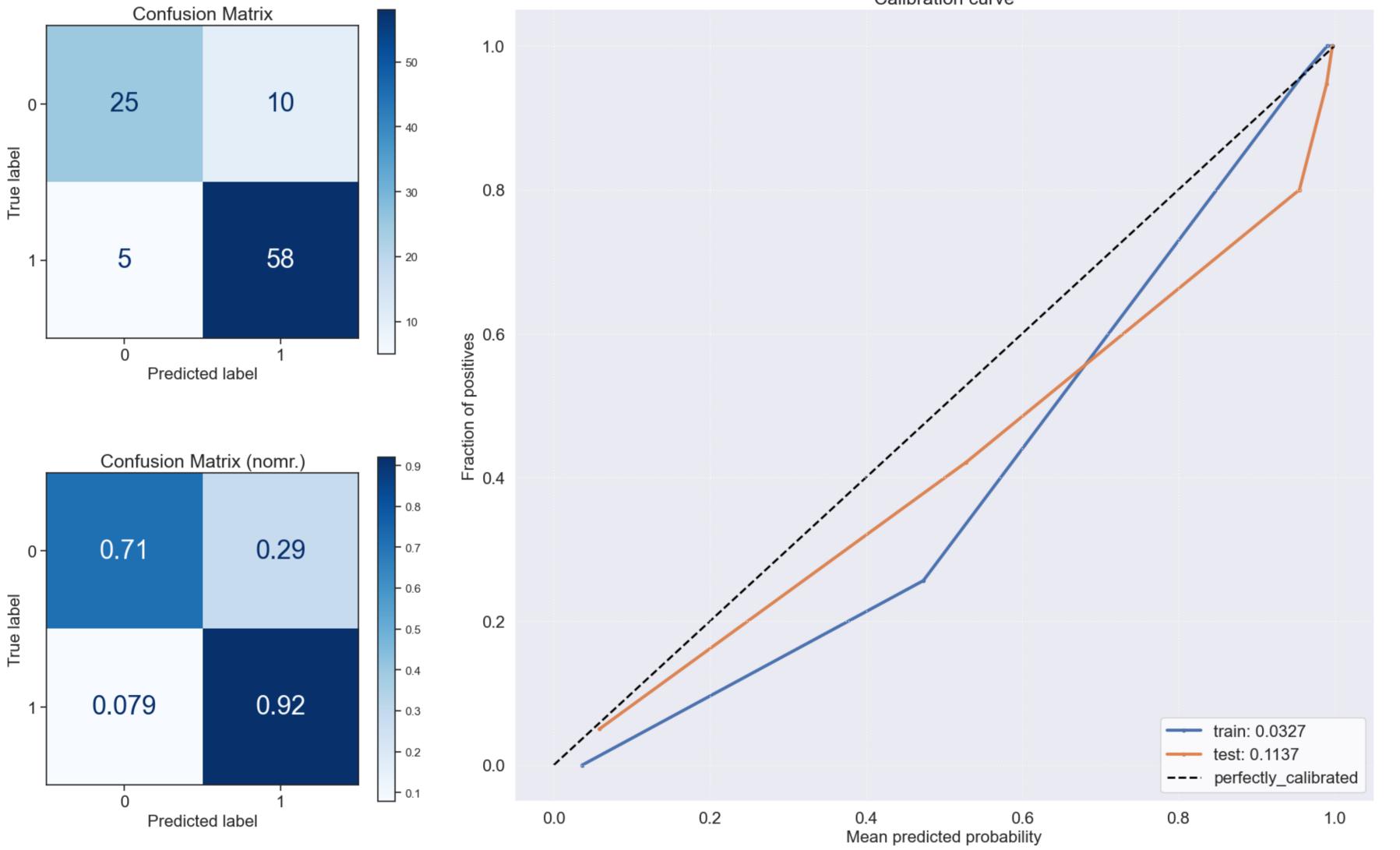
Metric	Train	Test
AUC	0.9991	0.922
accuracy	0.9795	0.8265
balanced accuracy	0.9712	0.7952
recall_(sens)	1.0	0.9048
specificity	0.9424	0.6857
precision	0.9691	0.8382
f1_score	0.9793	0.8232

Protein: P12821 - metric: f1





XGBoost Parameters	Value
alpha	3.3445
colsample_bytree	0.768
gamma	0.815
lambda	3.1744
learning_rate	0.048
max_depth	10.0
min_child_weight	1.0
n_estimators	932.0
reg_alpha	0.147
reg_lambda	0.6921
scale_pos_weight	3.9626
subsample	0.7743

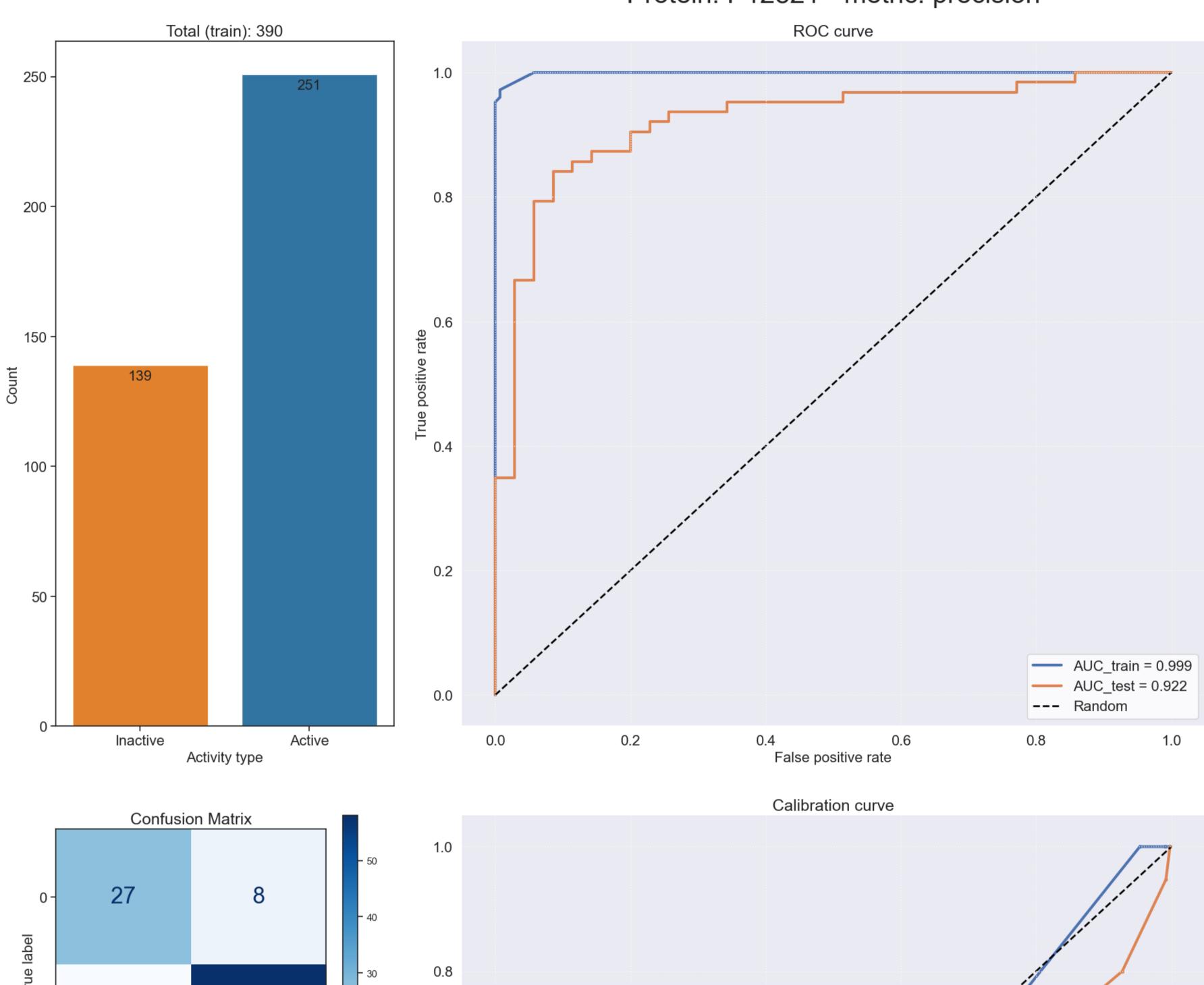


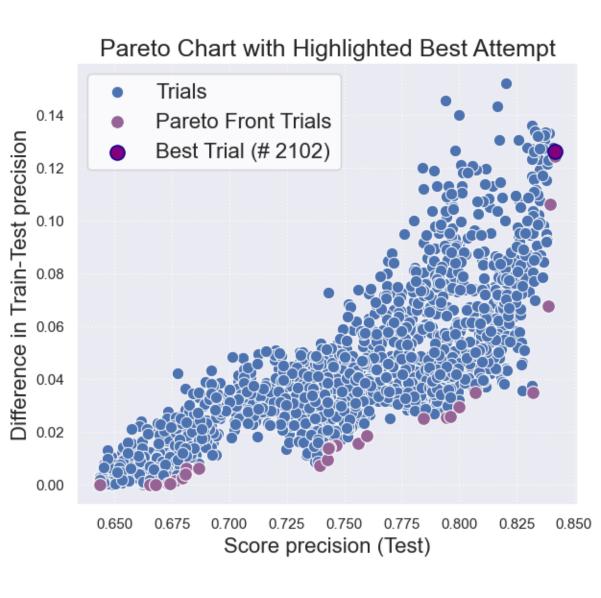
50		Inactive zone				Active zo	type active inacti	e (63) ve (35)
40							 	
Percent 30							 	
00								
10							 	
0					<u></u>			
	0.0	0.2	0.4	0. pability	.0	0.8	1	.0

Active/Inactive probability

Metric	Train	Test
AUC	0.9971	0.9288
accuracy	0.9564	0.8469
balanced accuracy	0.9388	0.8175
recall_(sens)	1.0	0.9206
specificity	0.8777	0.7143
precision	0.9366	0.8529
f1_score	0.9557	0.844

Protein: P12821 - metric: precision



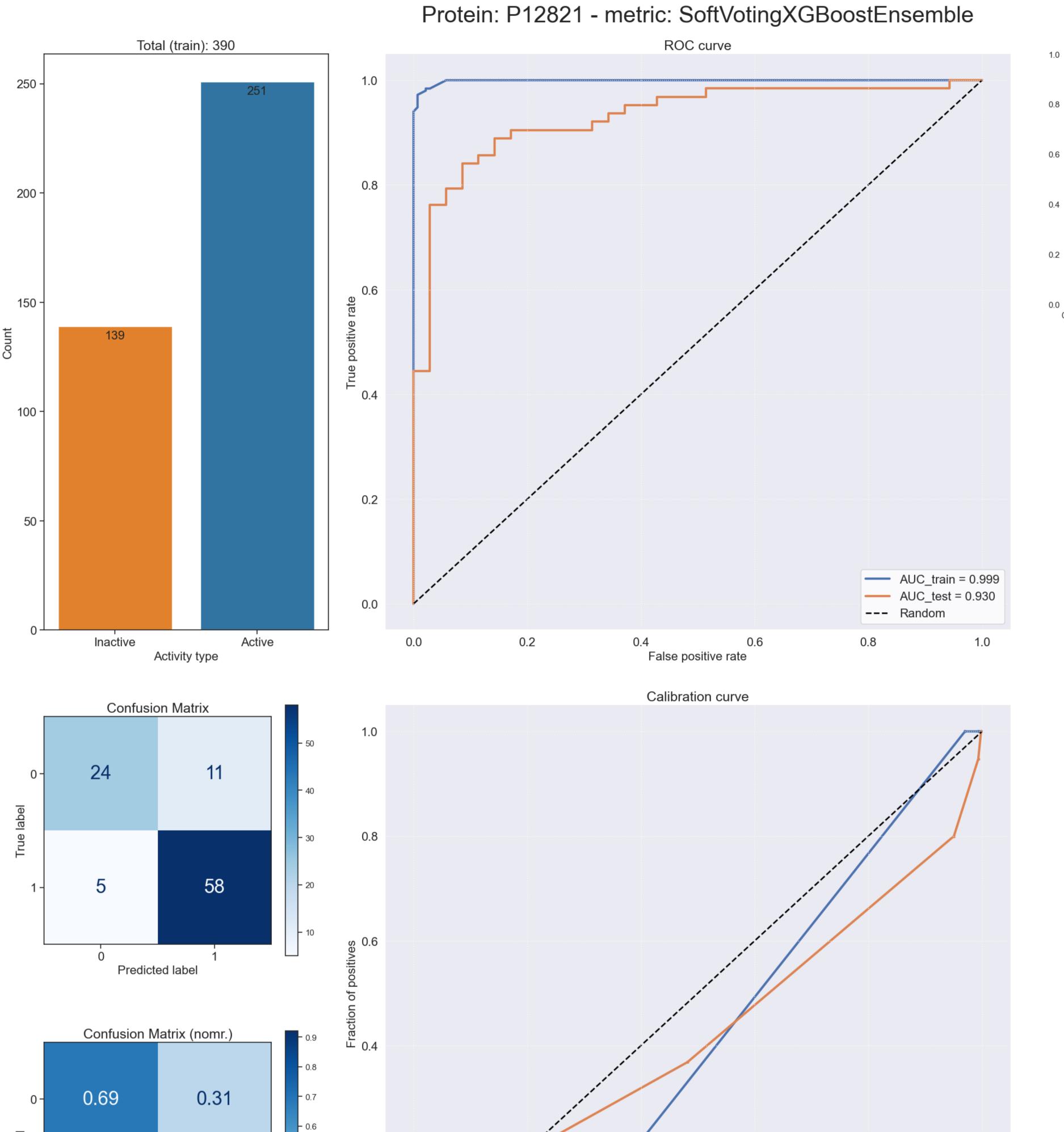


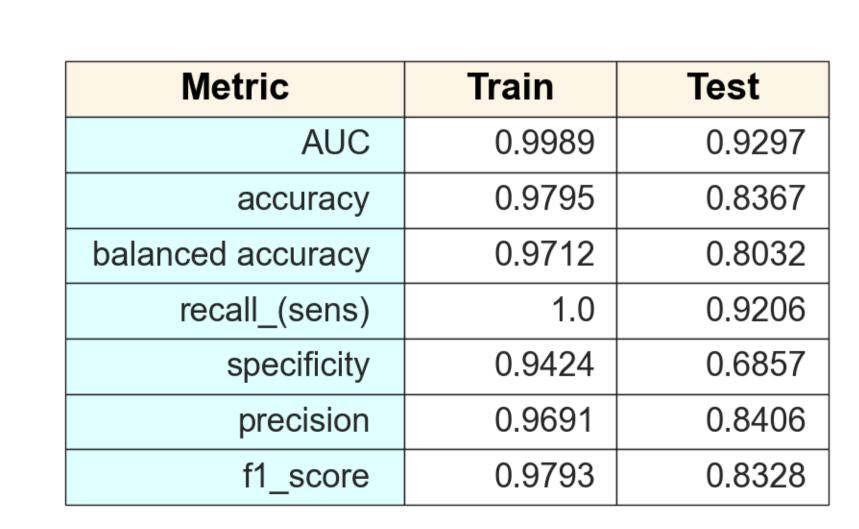
XGBoost Parameters	Value
alpha	0.7945
colsample_bytree	0.6258
gamma	0.0018
lambda	3.1348
learning_rate	0.0462
max_depth	8.0
min_child_weight	2.0
n_estimators	801.0
reg_alpha	0.2074
reg_lambda	0.3517
scale_pos_weight	2.2539
subsample	0.8254

label O	27	8	- 50 - 40	1.0						
True label			- 30	0.8						
1 -	5	58	- 20					مممر		
	0 Predicte	1 ed label	- 10	of positives 9.						
ı	Confusion M	latrix (nomr.)	0.9	Fraction 6.0			, proportion			
label O	0.77	0.23	- 0.8 - 0.7 - 0.6 - 0.5	0.2		, received				
True label	0.079	0.92	- 0.4 - 0.3 - 0.2	0.0	, e e e e e e e e e e e e e e e e e e e				train: 0.	
	0 Predicte	1 ed label	- 0.1		0.0	0.2	0.4 Mean predicte	0.6 ed probability	0.8	1.0

		Ac	ctive/Inactive p	robability		
40	Ina				Active zone	inactive (35) decoy (98)
Percent 08						
20						
10 	0.0 0	0.2	0.4 Probabilit	0.6 y	0.8	1.0

Metric	Train	Test
AUC	0.999	0.922
accuracy	0.9769	0.8673
balanced accuracy	0.9676	0.846
recall_(sens)	1.0	0.9206
specificity	0.9353	0.7714
precision	0.9654	0.8788
f1_score	0.9767	0.8659





--- train: 0.0217

--- test: 0.1174

0.8

0.4 0.6 Mean predicted probability

--- perfectly_calibrated

1.0

0.0

0.2

0.6

		Acti	ive/Inactiv	e probabi	lity			
50	Inacti	ve zone			Activ	e zone	type active inactive decoy	e (35)
40								
Percent								
20								
0 —		<u> </u>	1-7 - <mark>-</mark> -					
0.	.0 0.2	0.4	4 Proba	0. ability	6	0.8	1.	0

0.2

0.0

0.0

0.2

- 0.5

- 0.4

- 0.3

0.2

0.92

True label

0.079

Predicted label