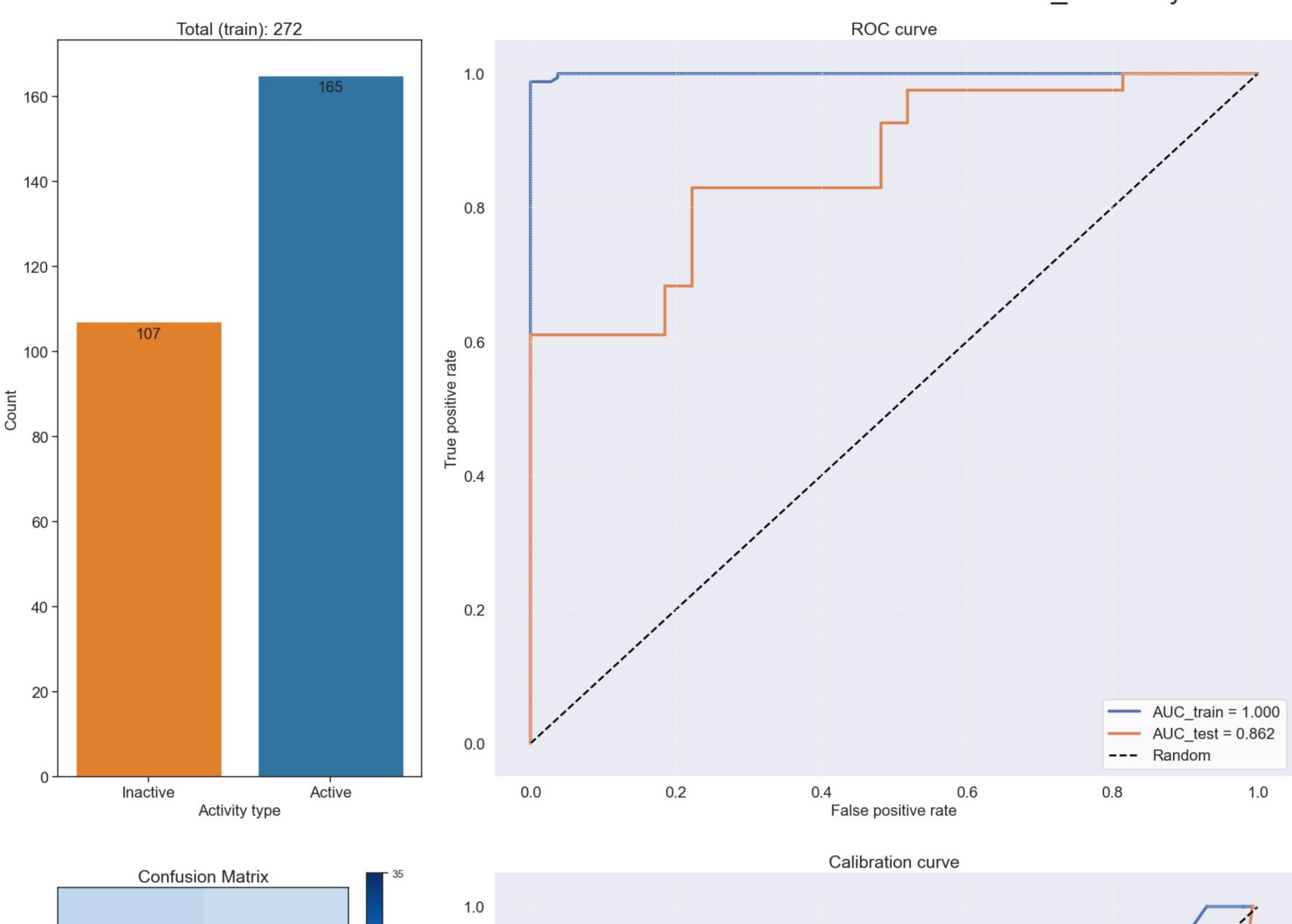
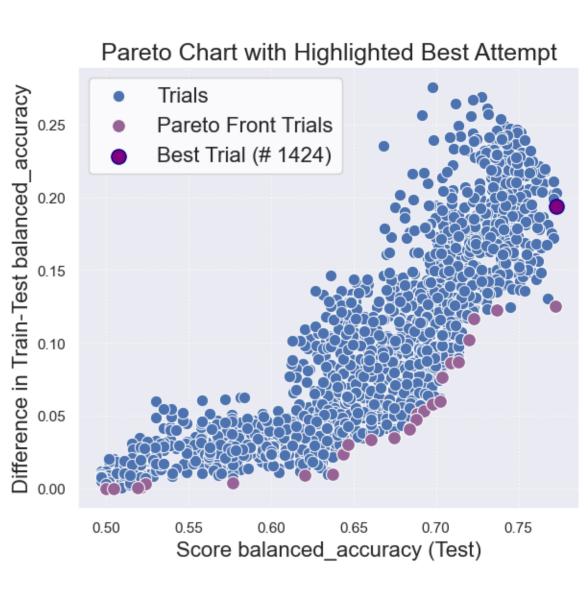
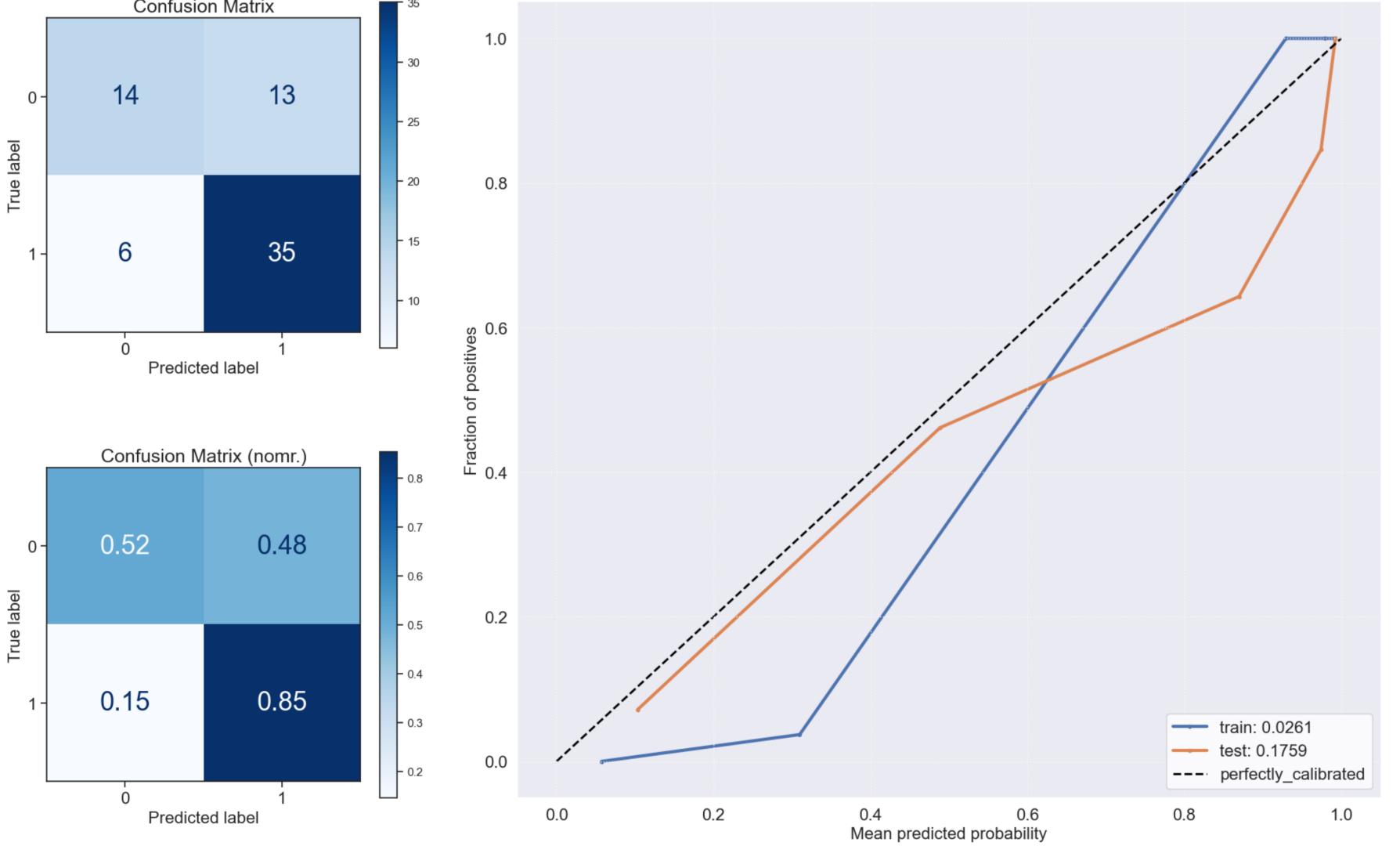
Protein: P06241 - metric: balanced_accuracy





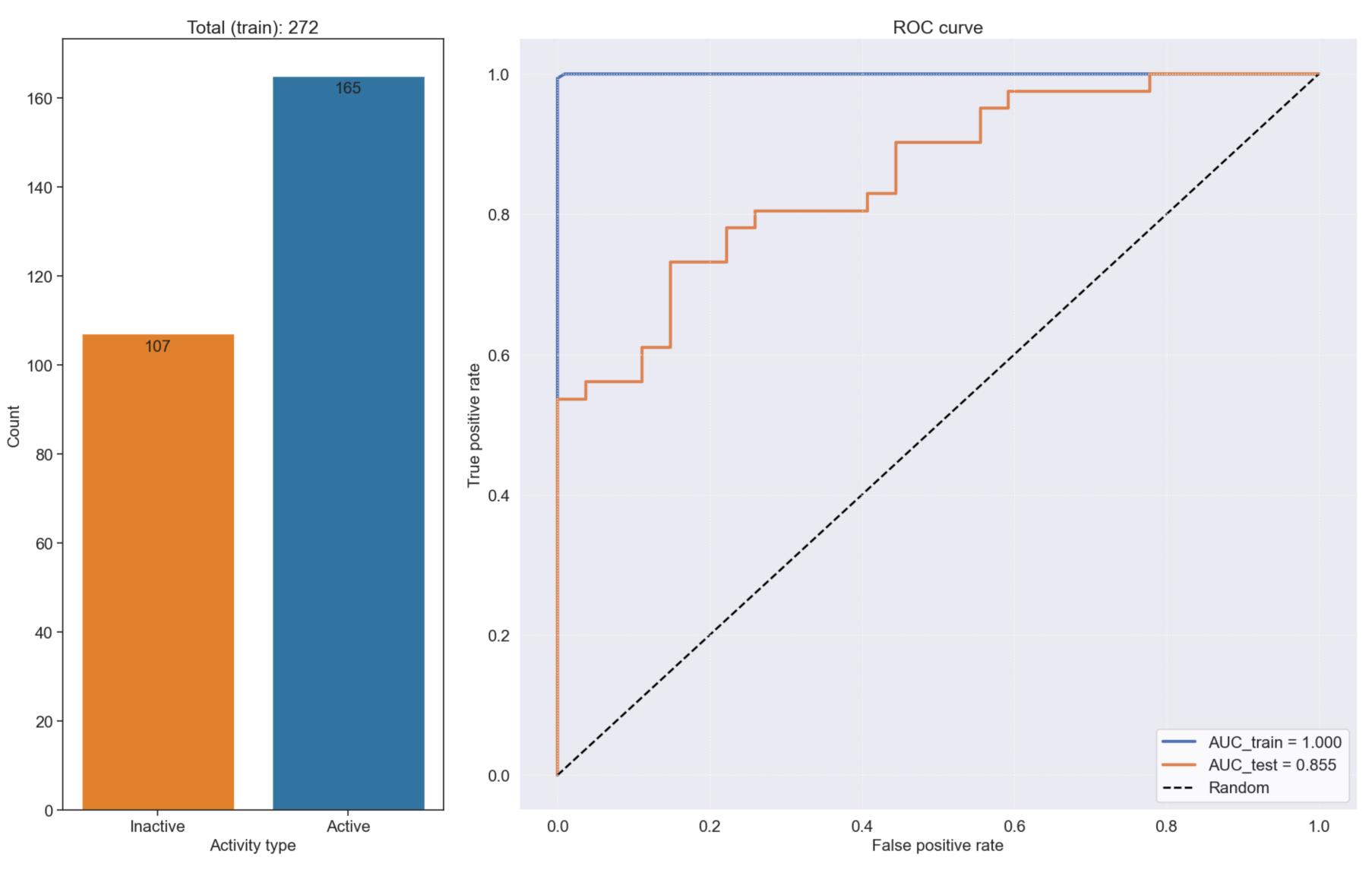
XGBoost Parameters	Value
alpha	2.3463
colsample_bytree	0.8495
gamma	0.6424
lambda	0.4644
learning_rate	0.0277
max_depth	9.0
min_child_weight	1.0
n_estimators	628.0
reg_alpha	0.5145
reg_lambda	0.9611
scale_pos_weight	3.1216
subsample	0.7249

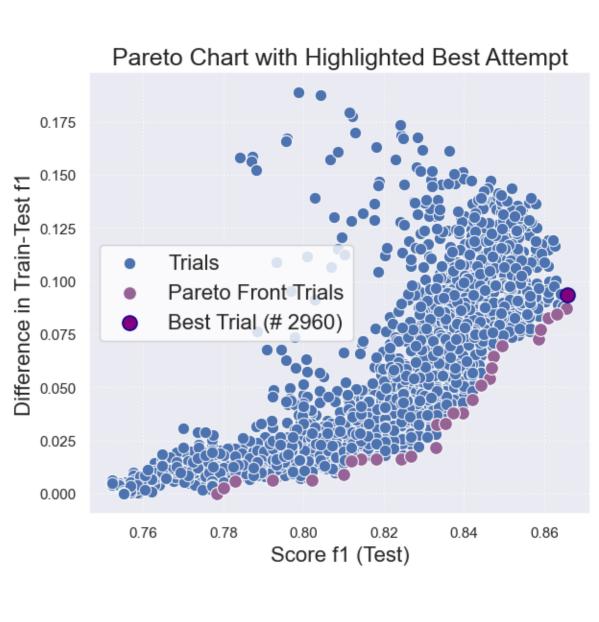


Active/Inactive probability						
30	Ina	ctive zone			Active zone	type active (41) inactive (27) decoy (68)
25						
Percent 51						
<u> </u>						
10						
5						
0						
U	0.0	2	0.4	0.6	0.8	1.0
			Probabilit	У		

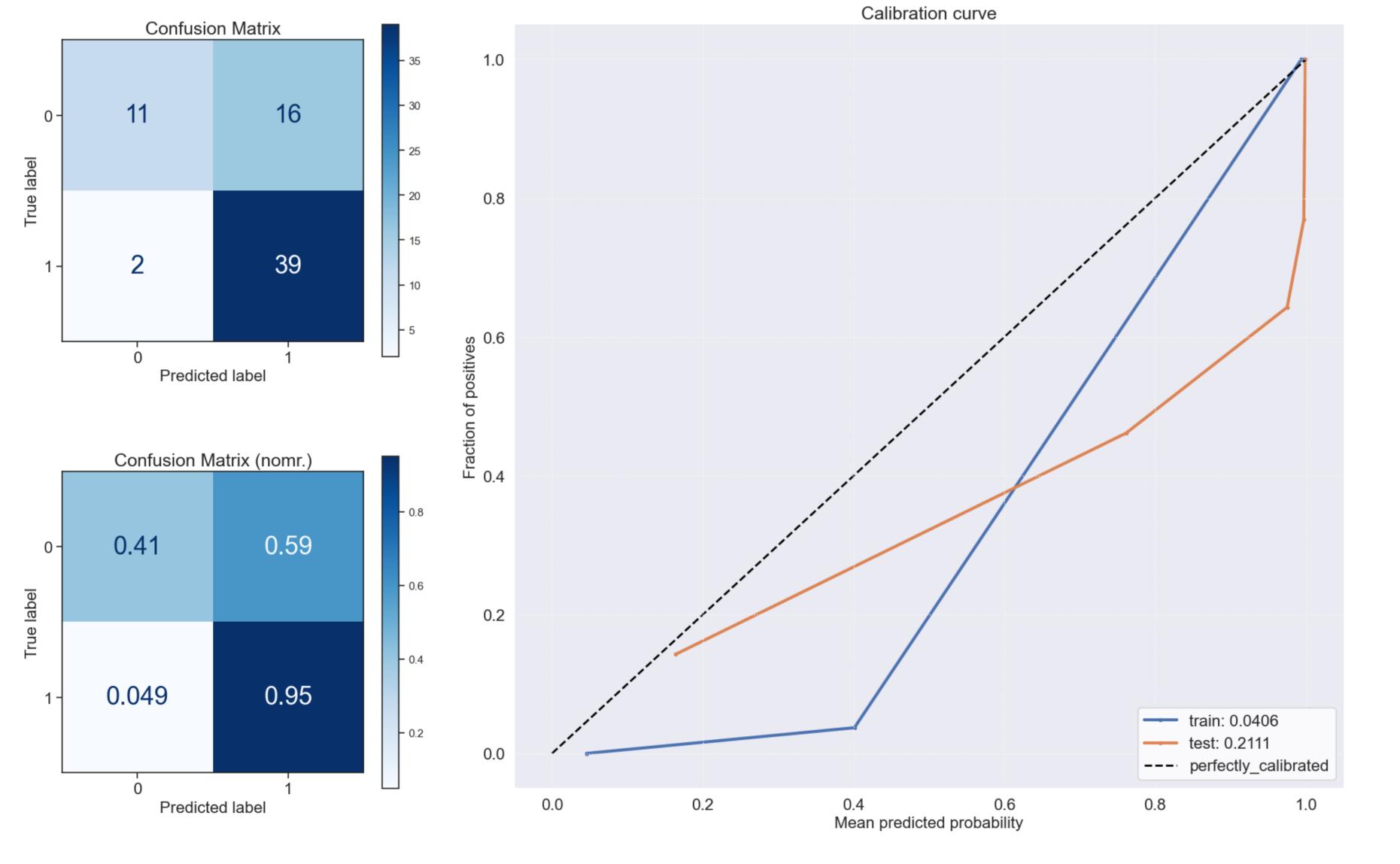
Metric	Train	Test
AUC	0.9996	0.8618
accuracy	0.9779	0.7206
balanced accuracy	0.972	0.6861
recall_(sens)	1.0	0.8537
specificity	0.9439	0.5185
precision	0.9649	0.7292
f1_score	0.9778	0.7108

Protein: P06241 - metric: f1





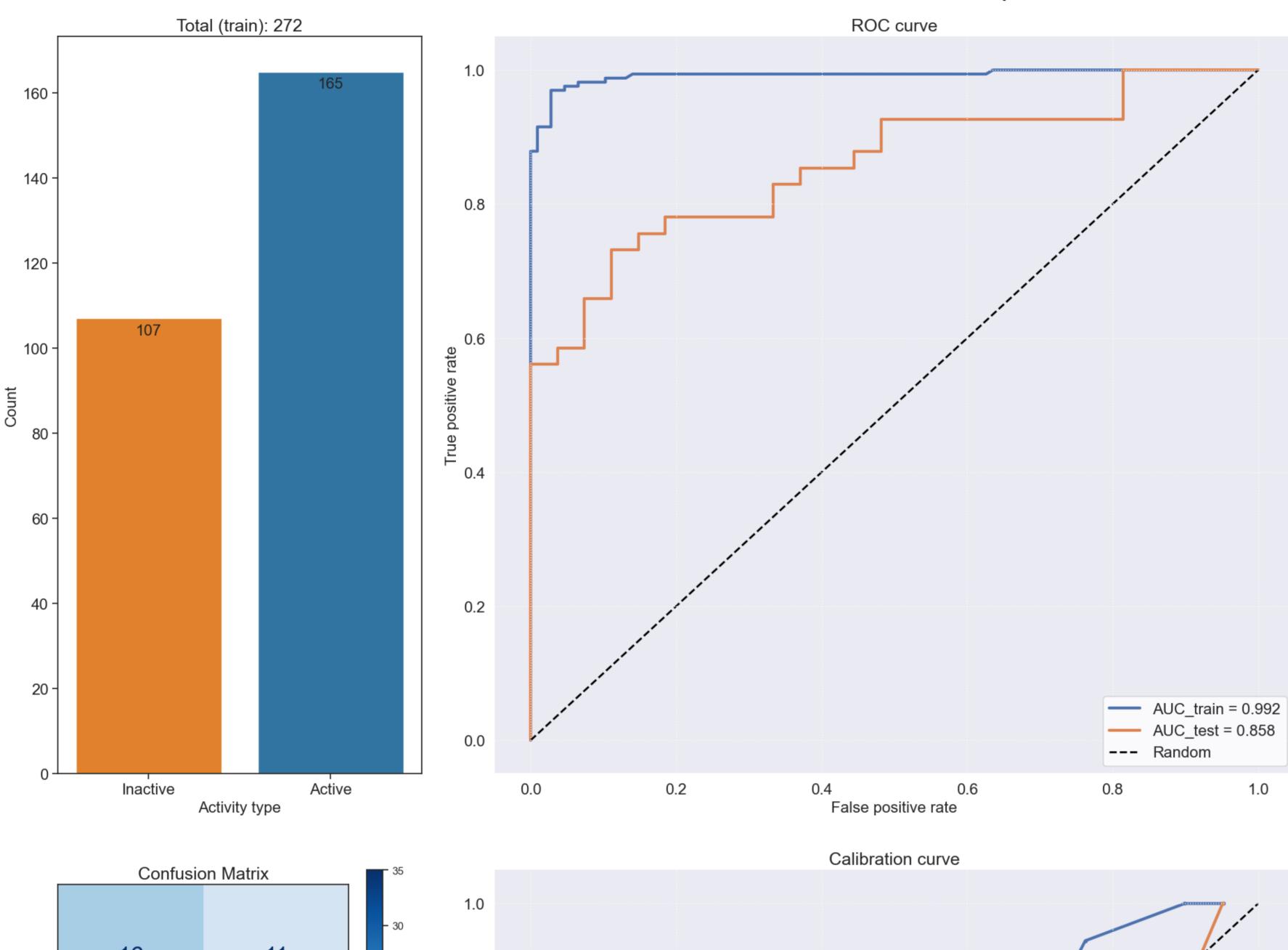
XGBoost Parameters	Value
alpha	3.8311
colsample_bytree	0.5306
gamma	0.1097
lambda	4.8321
learning_rate	0.0327
max_depth	9.0
min_child_weight	1.0
n_estimators	291.0
reg_alpha	0.5021
reg_lambda	0.6337
scale_pos_weight	48.923
subsample	0.7515

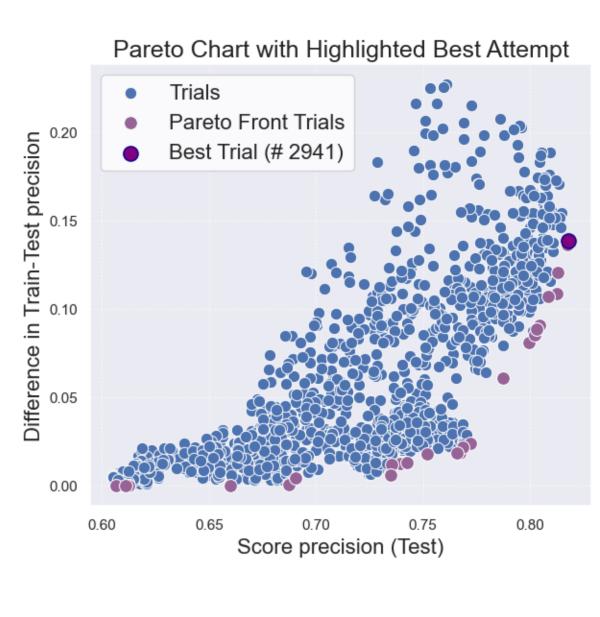


			Active/Inactiv	e probability			
60	I	nactive zone			Active z	zone	type active (41) inactive (27)
50							decoy (68)
Percent 08 08							
90							
20							
10	In Land		-7				
J	0.0	0.2	0.4 Proba	0.6 ability	0.	8	1.0

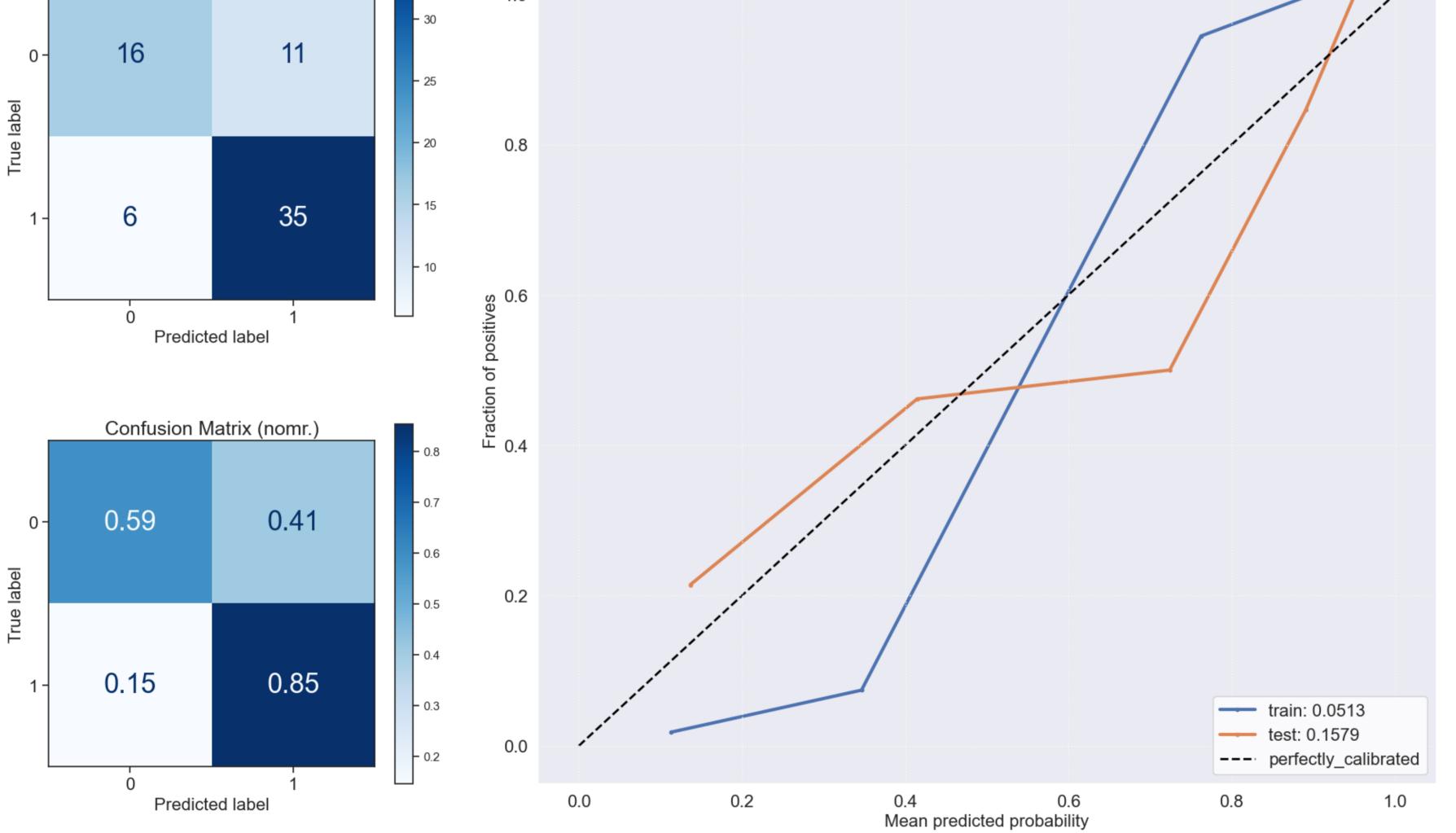
Metric	Train	Test	
AUC	1.0	0.8555	
accuracy	0.9485	0.7353	
balanced accuracy	0.9346	0.6793	
recall_(sens)	1.0	0.9512	
specificity	0.8692	0.4074	
precision	0.9218	0.7091	
f1_score	0.9478	0.7083	

Protein: P06241 - metric: precision





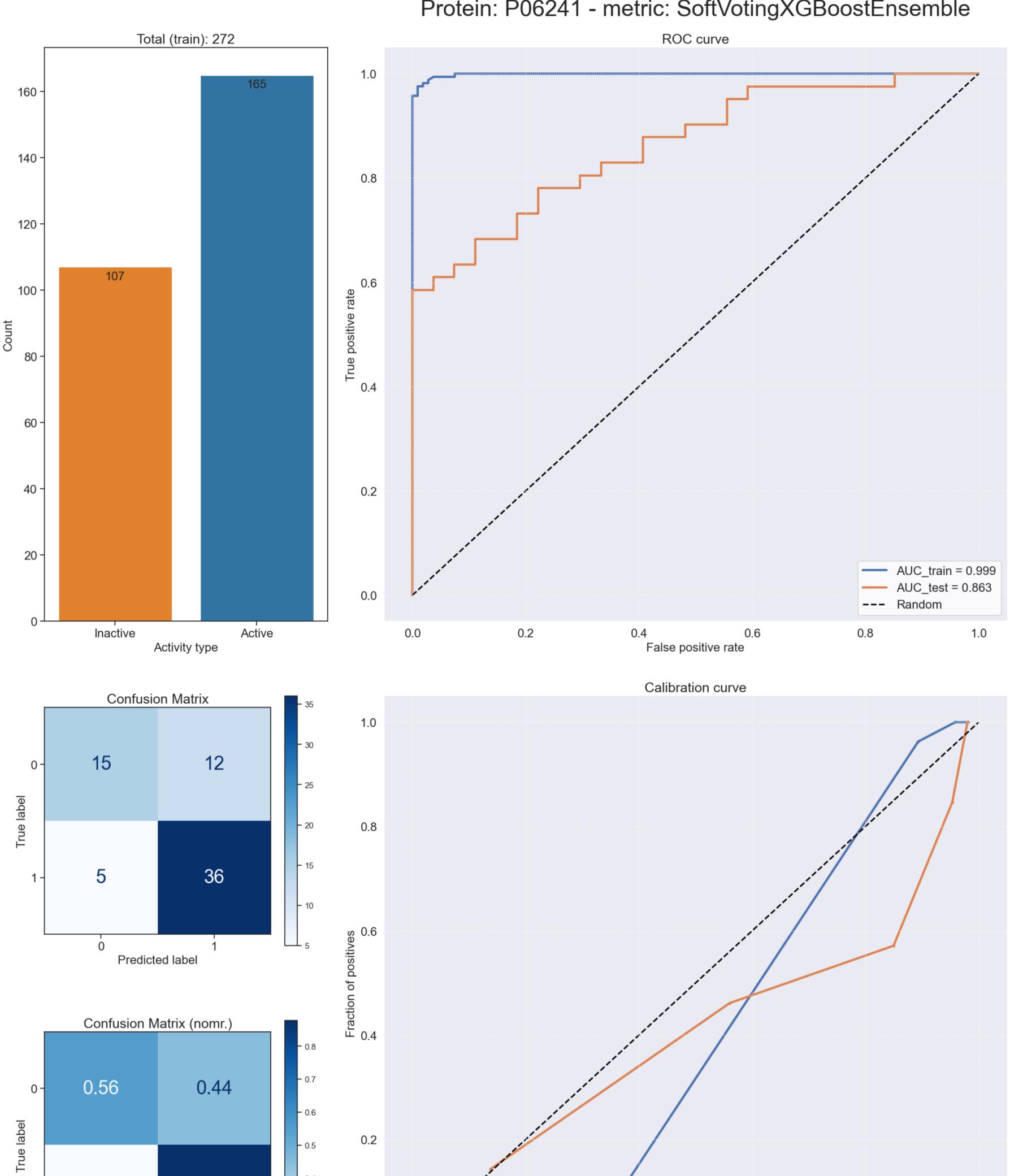
XGBoost Parameters	Value
alpha	0.8228
colsample_bytree	0.613
gamma	0.069
lambda	2.1164
learning_rate	0.0095
max_depth	6.0
min_child_weight	1.0
n_estimators	449.0
reg_alpha	0.0566
reg_lambda	0.9046
scale_pos_weight	1.1071
subsample	0.6712



	:	:	Active/Inac	tive probability	:	
12		Inactive zo	ne		active (41) inactive (27) decoy (68)	
Bercent 2 8						
Ü	0.0	0.2	0.4 Pro	0.6 bability	0.8	1.0

Metric	Train	Test
AUC	0.9922	0.8582
accuracy	0.9559	0.75
balanced accuracy	0.9489	0.7231
recall_(sens)	0.9818	0.8537
specificity	0.9159	0.5926
precision	0.9474	0.7609
f1_score	0.9556	0.7444

Protein: P06241 - metric: SoftVotingXGBoostEnsemble



Metric	Train	Test
AUC	0.9989	0.8627
accuracy	0.9559	0.75
balanced accuracy	0.9439	0.7168
recall_(sens)	1.0	0.878
specificity	0.8879	0.5556
precision	0.9322	0.75
f1_score	0.9553	0.7412

--- train: 0.0346

--- test: 0.1718

0.8

0.4 0.6 Mean predicted probability

--- perfectly_calibrated

1.0

0.8

0.6

0.4

0.2

0.0

0.0

0.2

0.6

		Acti	ve/Inactive p	orobability			
25		active zone			Active z		type active (41) inactive (27) decoy (68)
Percent 15 -							
10 5							
0 —	0.0	0.2 0.4	l Probabili	0.6	0.	8	1.0

0.2

0.0

0.0

0.2

- 0.5

- 0.4

- 0.3

0.2

0.88

0.12

Predicted label