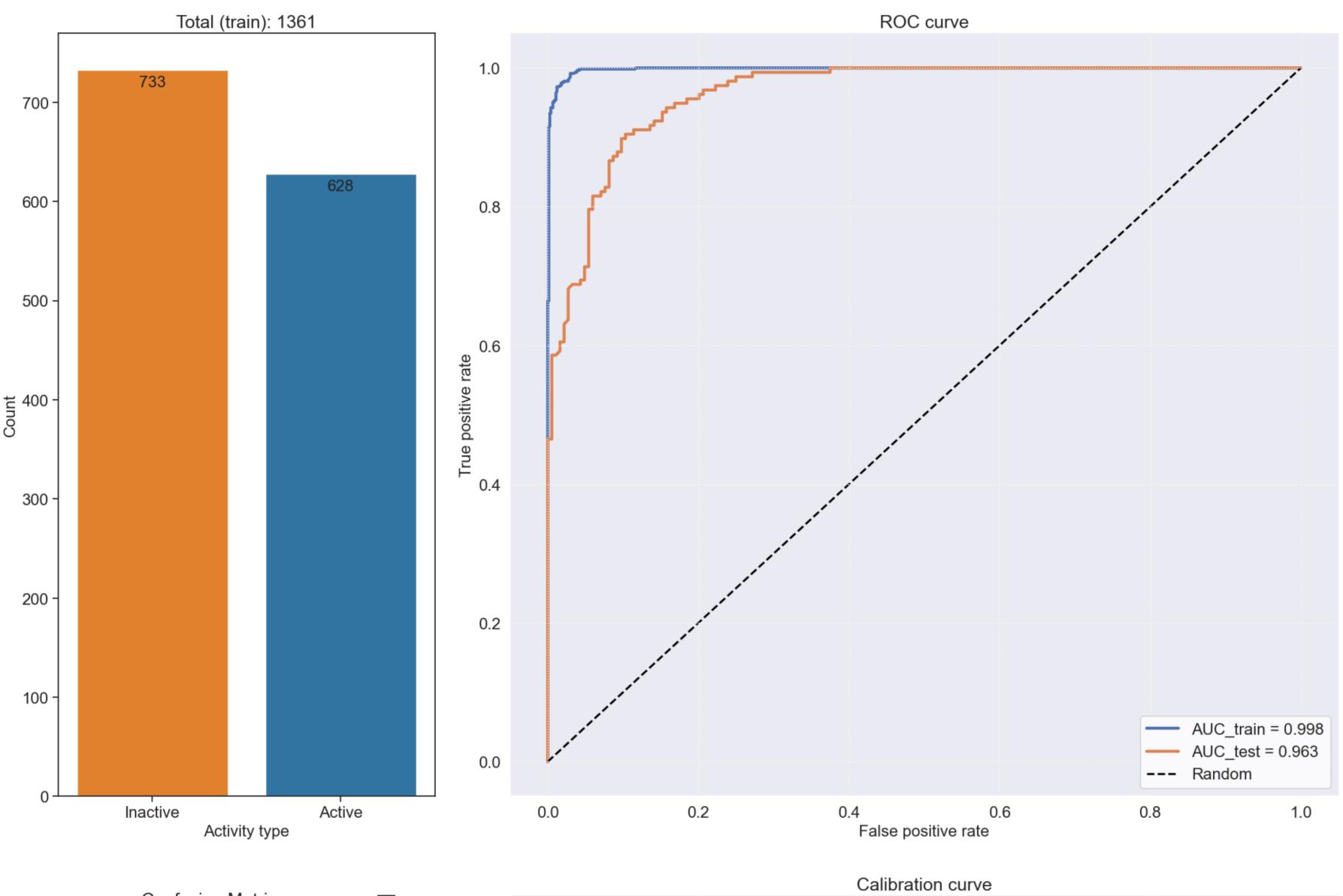
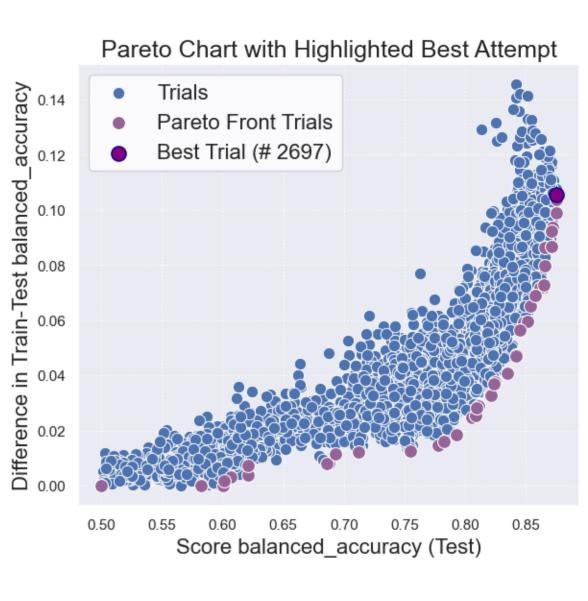
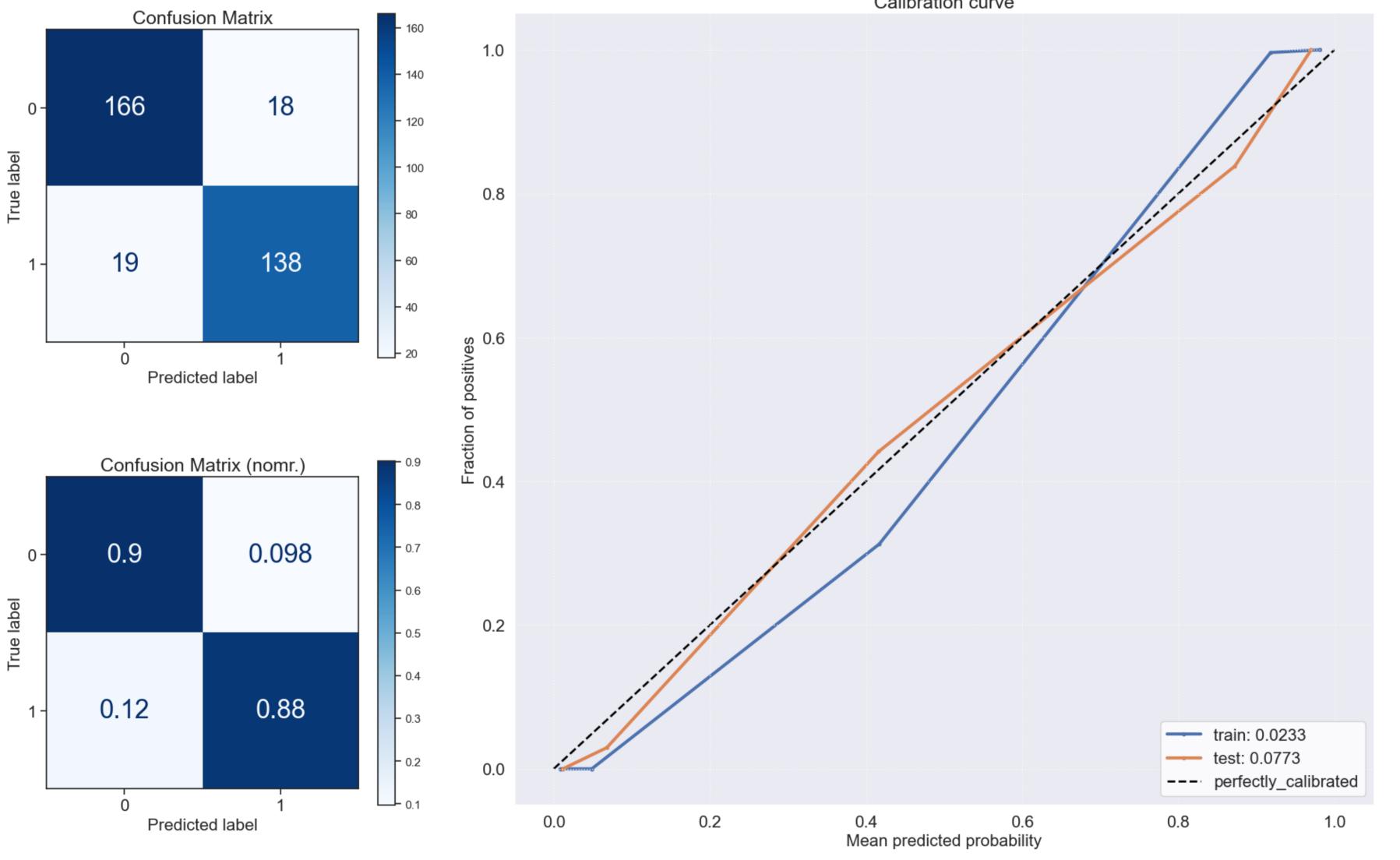
Protein: Q99720 - metric: balanced_accuracy





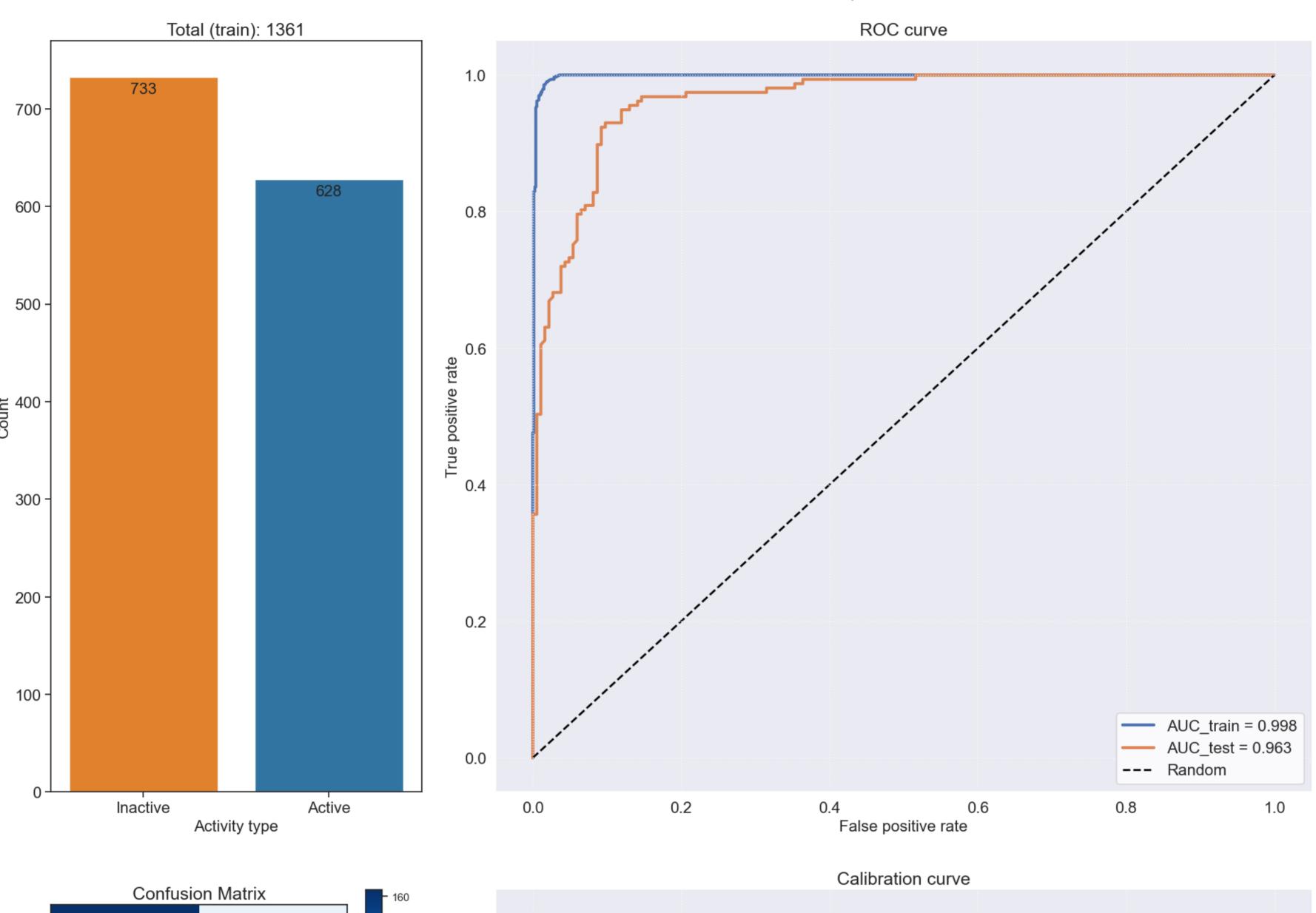
XGBoost Parameters	Value
alpha	1.4641
colsample_bytree	0.5109
gamma	0.0351
lambda	3.2515
learning_rate	0.0427
max_depth	9.0
min_child_weight	1.0
n_estimators	391.0
reg_alpha	0.1709
reg_lambda	0.5251
scale_pos_weight	1.3337
subsample	0.5724

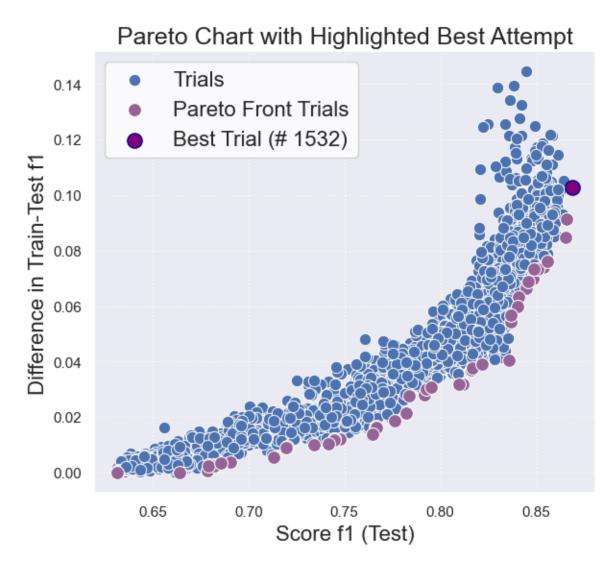


		Active/Inactive	probability		
25	Inactive zone			Active zone	inactive (184) decoy (341)
Dercent 15					
5					
0	.0 0.2	0.4 Probabi	0.6 lity	0.8	1.0

Metric	Train	Test
AUC	0.9984	0.9634
accuracy	0.9794	0.8915
balanced accuracy	0.9803	0.8906
recall_(sens)	0.992	0.879
specificity	0.9686	0.9022
precision	0.9644	0.8846
f1_score	0.9794	0.8915

Protein: Q99720 - metric: f1





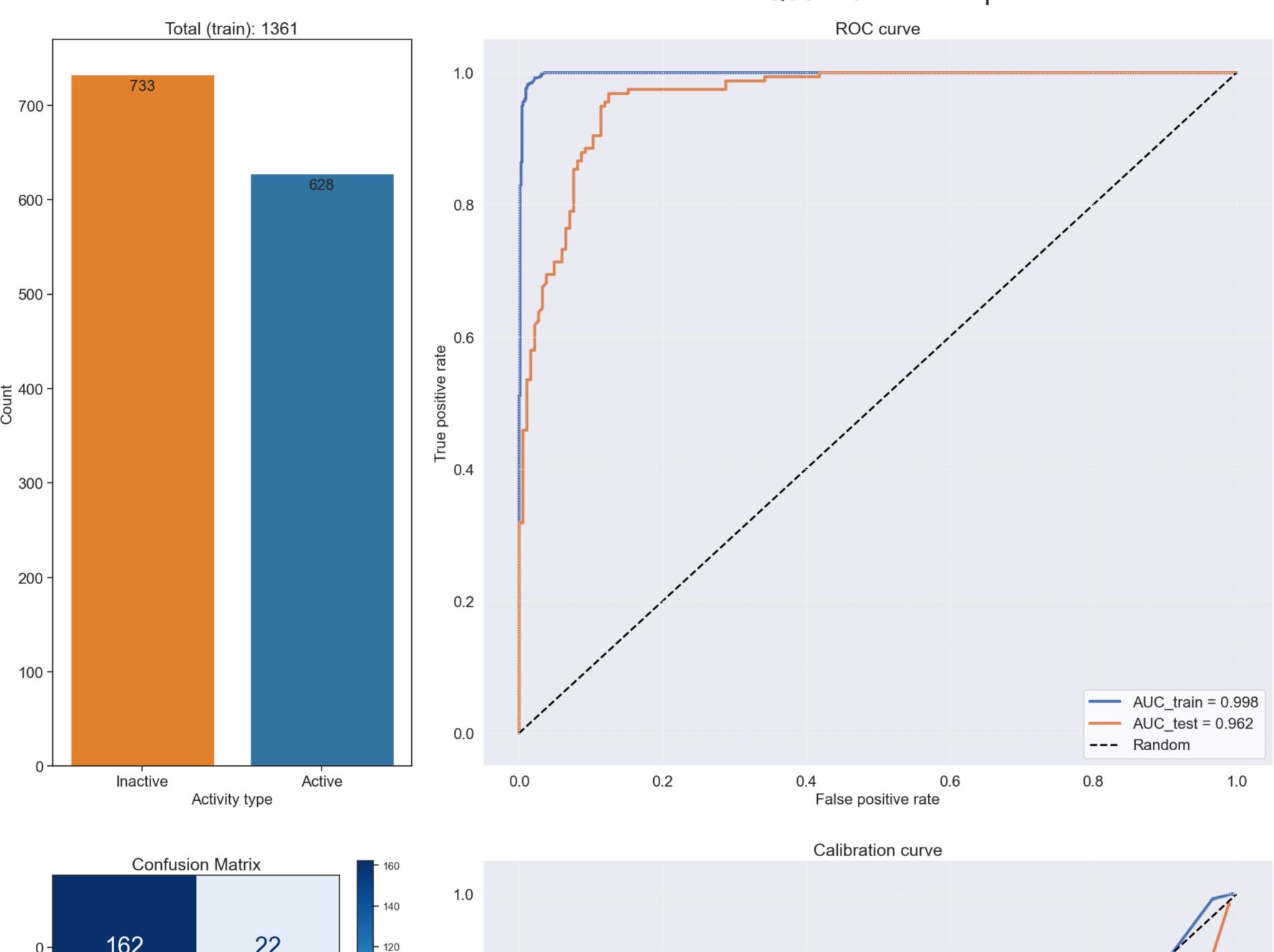
Value
4.9389
0.5707
0.261
4.9227
0.0742
8.0
3.0
954.0
0.103
0.9776
2.9636
0.9576

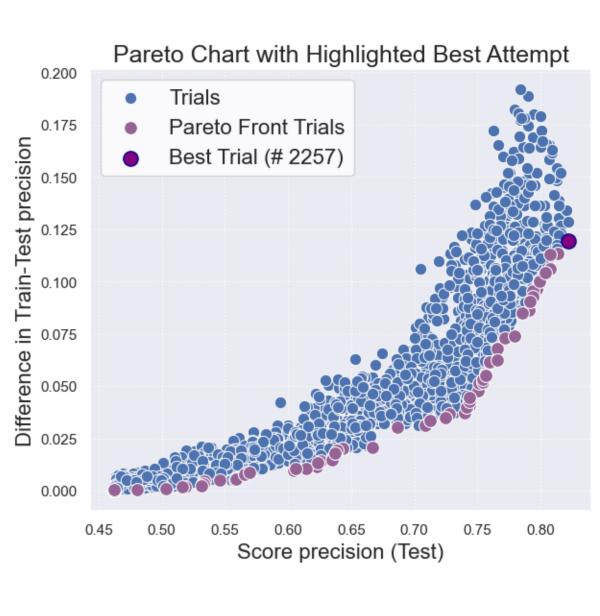
_	Confusio	n warix	- 160							
label O	163	21	- 140 - 120 - 100	1.0						
True label	11	146	- 80 - 60 - 40	0.8				pararara		
ı	0 Predicte	1 ed label	20	Fraction of positives 0 70 90			, o o o o o o o o o o o o o o o o o o o			
	Confusion M	latrix (nomr.)		ract						
True label		0.11	- 0.9 - 0.8 - 0.7 - 0.6 - 0.5	0.4		, or				
True	0.07	0.93	- 0.4 - 0.3 - 0.2 - 0.1	0.0					test: 0	0.0231 0.0753 ctly_calibrated
	0 Predicte	1 ed label			0.0	0.2	0.4 Mean predicted	0.6 d probability	0.8	1.0

		, A	Active/Inactive	e probability		
35	I	nactive zone			Active zone	type active (157) inactive (184) decoy (341)
25						
Dercent						
10						
5						
0 —	0.0	0.2	0.4	0.6	0.8	1.0
			Proba	bility		

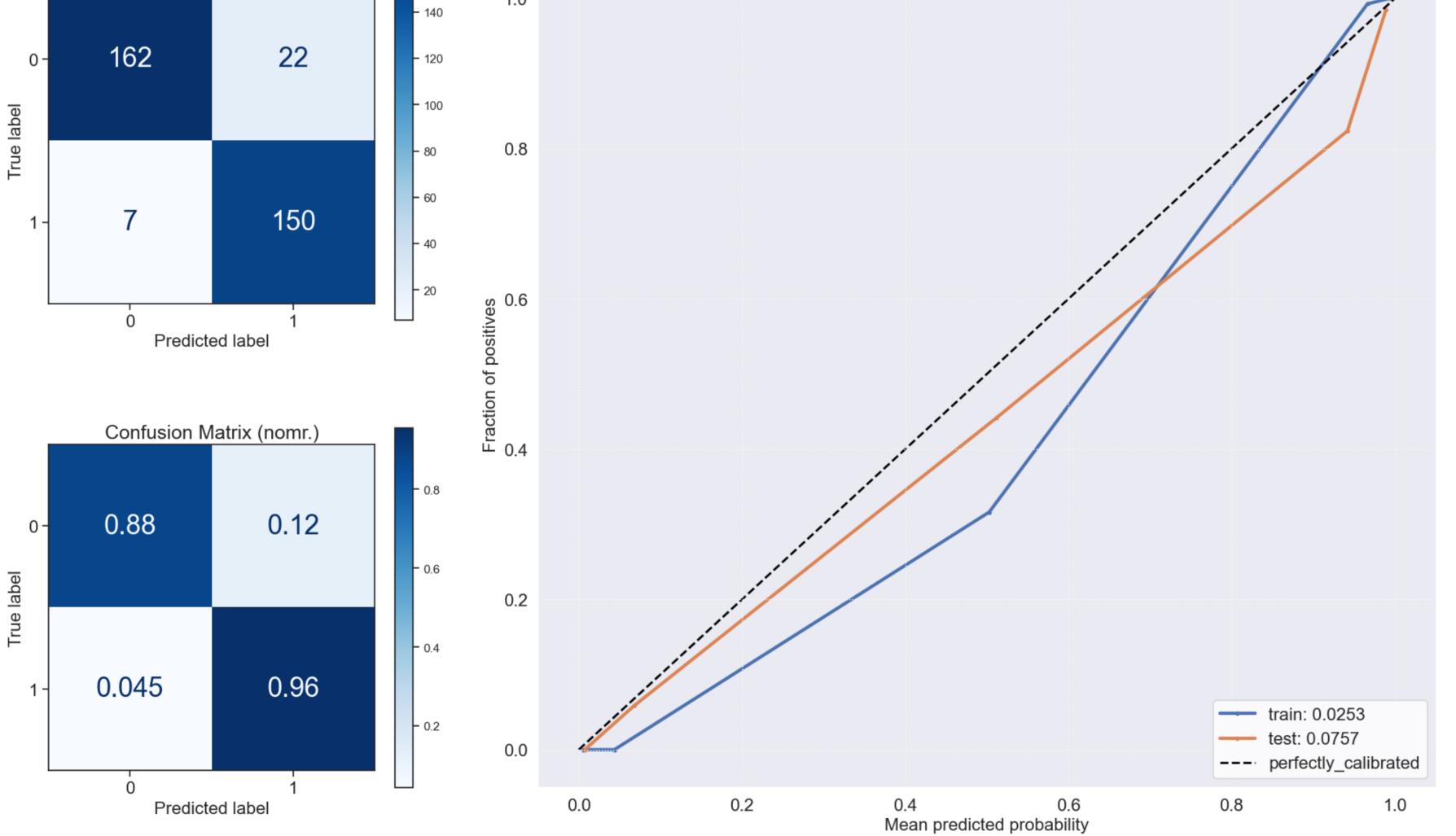
Metric	Train	Test
AUC	0.9984	0.9632
accuracy	0.9728	0.9062
balanced accuracy	0.9748	0.9079
recall_(sens)	1.0	0.9299
specificity	0.9495	0.8859
precision	0.9444	0.8743
f1_score	0.9729	0.9063

Protein: Q99720 - metric: precision





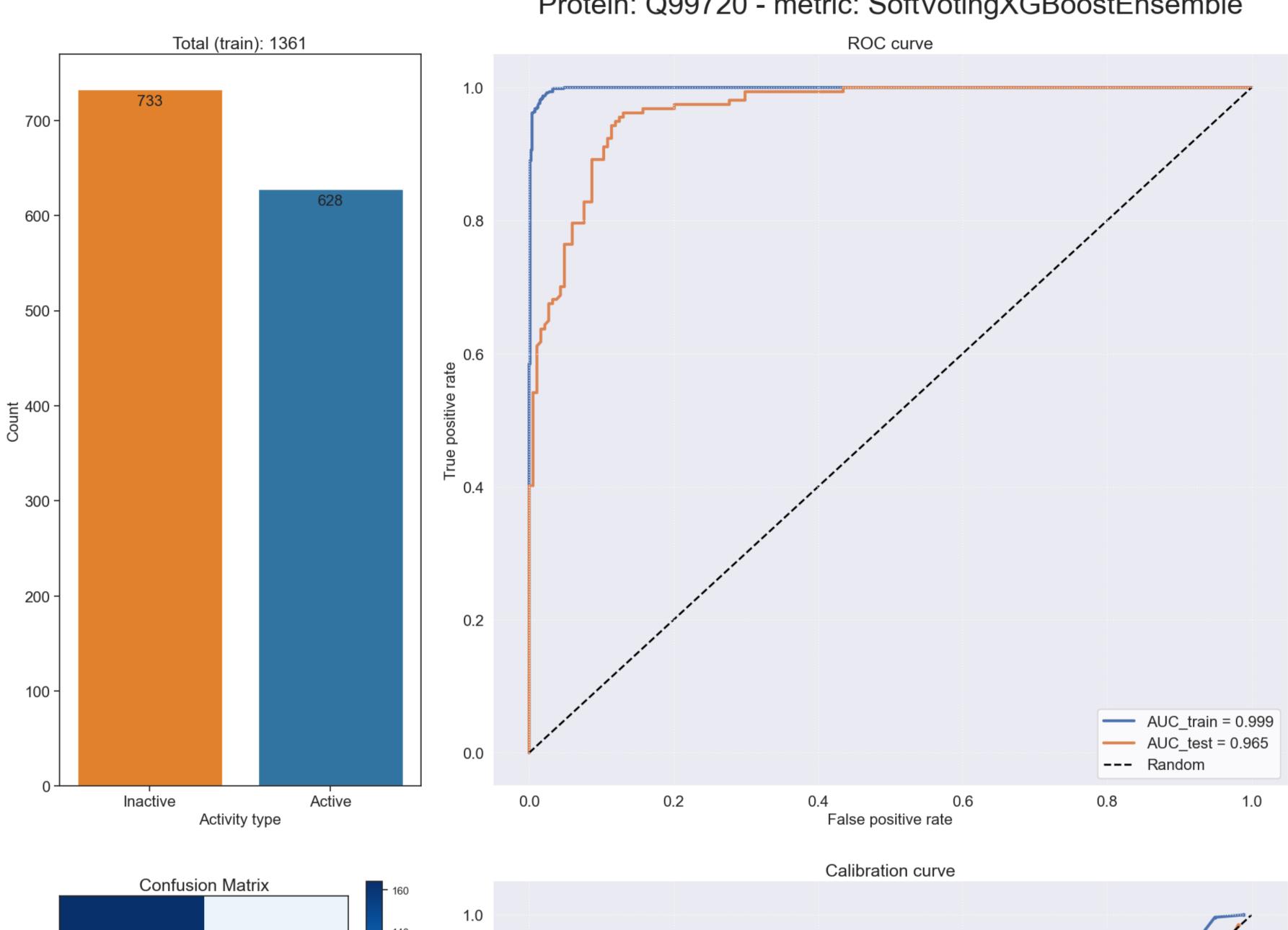
XGBoost Parameters	Value
alpha	0.3801
colsample_bytree	0.7793
gamma	0.0167
lambda	3.6012
learning_rate	0.0424
max_depth	9.0
min_child_weight	3.0
n_estimators	596.0
reg_alpha	0.2189
reg_lambda	0.3415
scale_pos_weight	3.5498
subsample	0.7963

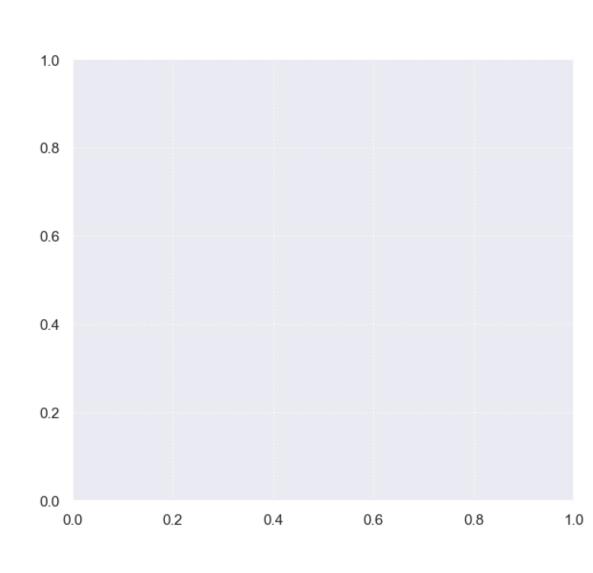


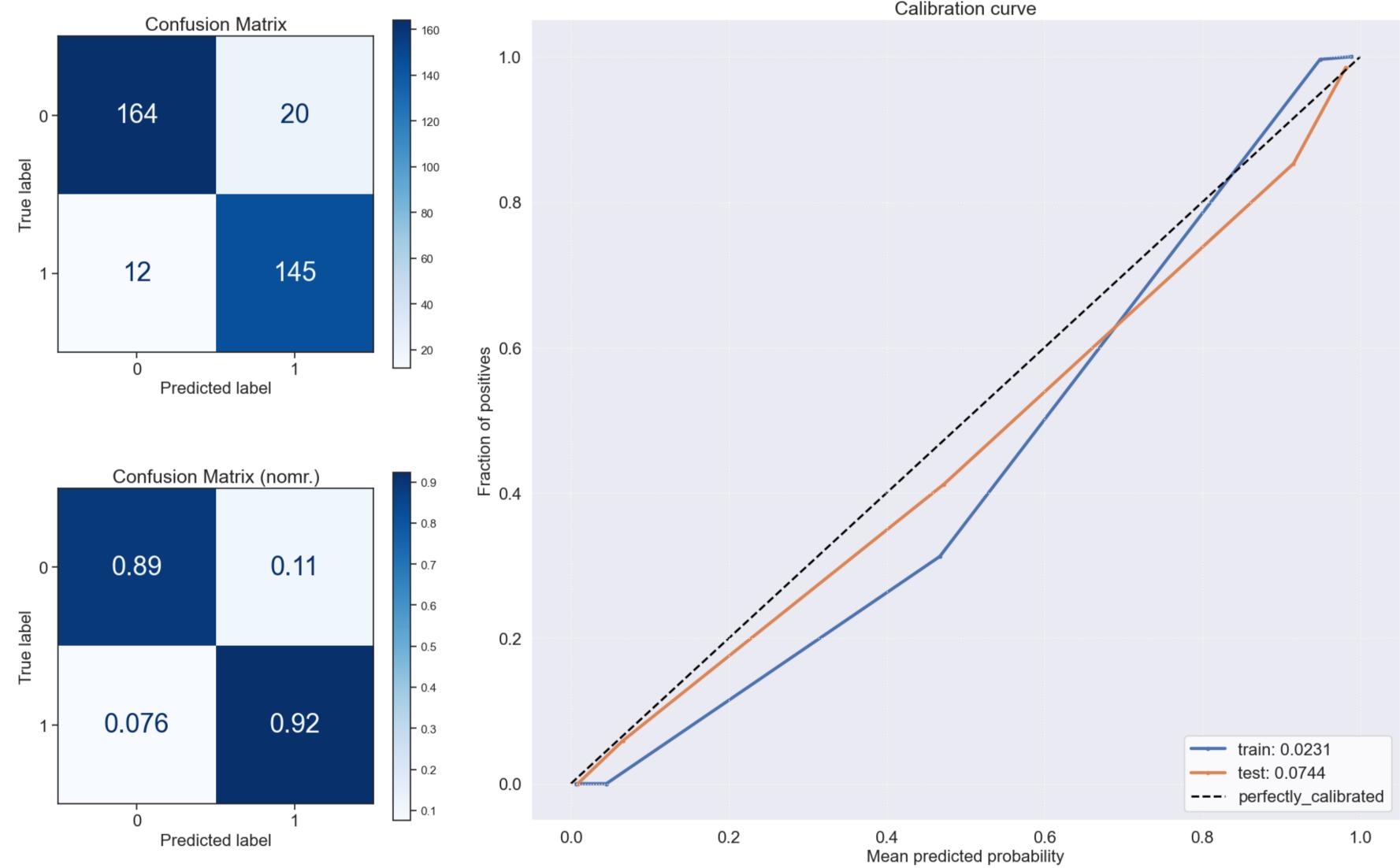
		Active/Inactiv	e probability		
35	Illactive zone			Active zone	type active (157) inactive (184) decoy (341)
25					
Percent 15					
10 -					
0 —					
	0.0 0.2	0.4 Proba	0.6 ability	0.8	1.0

Metric	Train	Test
AUC	0.9984	0.962
accuracy	0.9677	0.915
balanced accuracy	0.97	0.9179
recall_(sens)	1.0	0.9554
specificity	0.94	0.8804
precision	0.9345	0.8721
f1_score	0.9677	0.9151

Protein: Q99720 - metric: SoftVotingXGBoostEnsemble







30 		tive zone		inac	ve (157) tive (184) oy (341)
00					П
10					
0-0	.0 0.2	0.4	0.6	.8	1.0

Active/Inactive probability

Metric	Train	Test
AUC	0.9986	0.9645
accuracy	0.9743	0.9062
balanced accuracy	0.976	0.9074
recall_(sens)	0.9984	0.9236
specificity	0.9536	0.8913
precision	0.9486	0.8788
f1_score	0.9743	0.9063