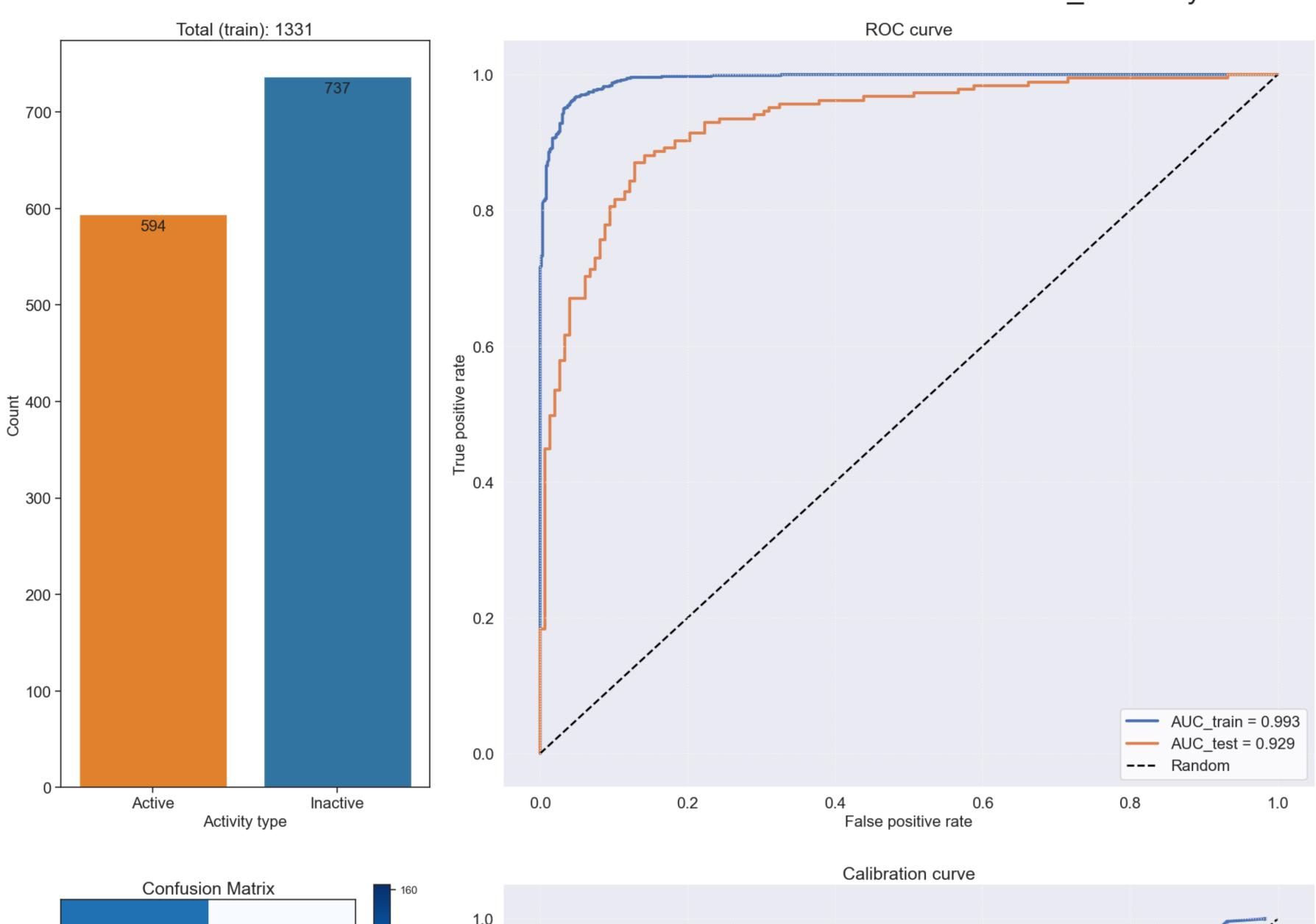
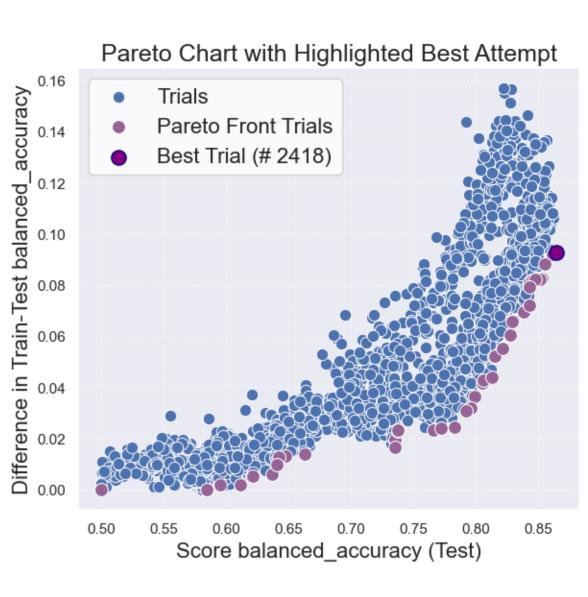
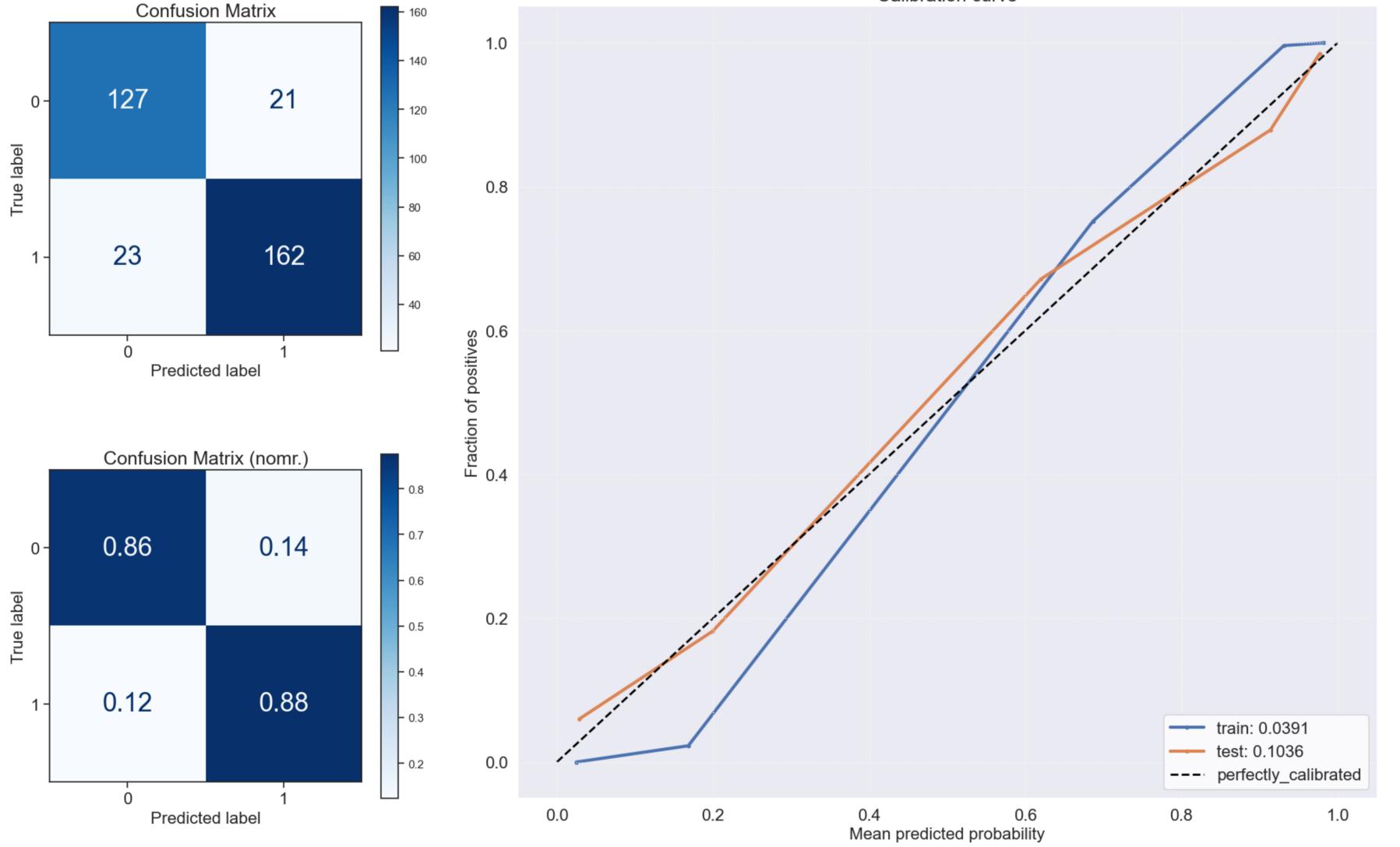
Protein: P11229 - metric: balanced_accuracy





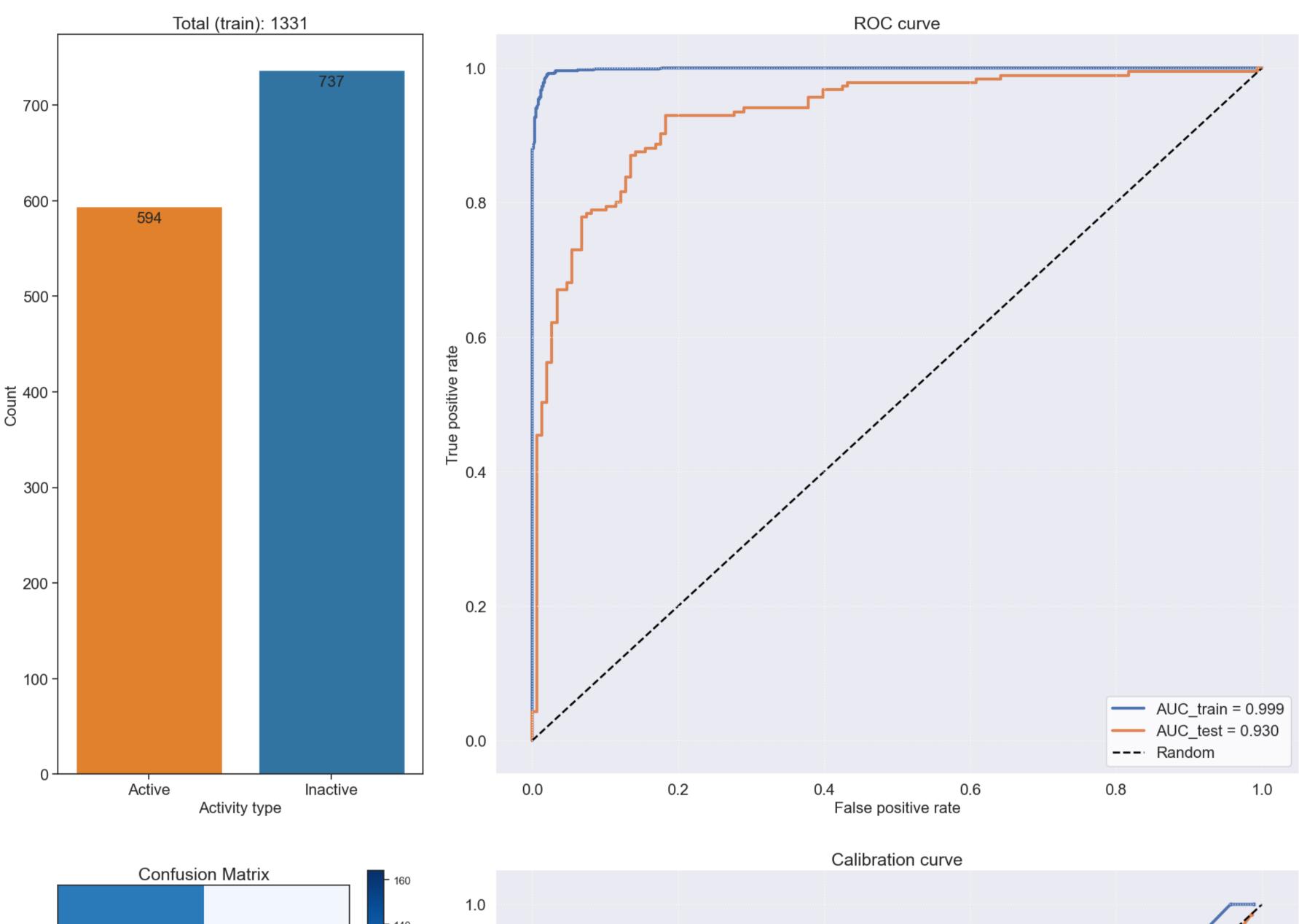
XGBoost Parameters	Value
alpha	1.092
colsample_bytree	0.6135
gamma	0.2494
lambda	3.9321
learning_rate	0.0881
max_depth	10.0
min_child_weight	2.0
n_estimators	141.0
reg_alpha	0.0437
reg_lambda	0.5096
scale_pos_weight	1.1157
subsample	0.5673

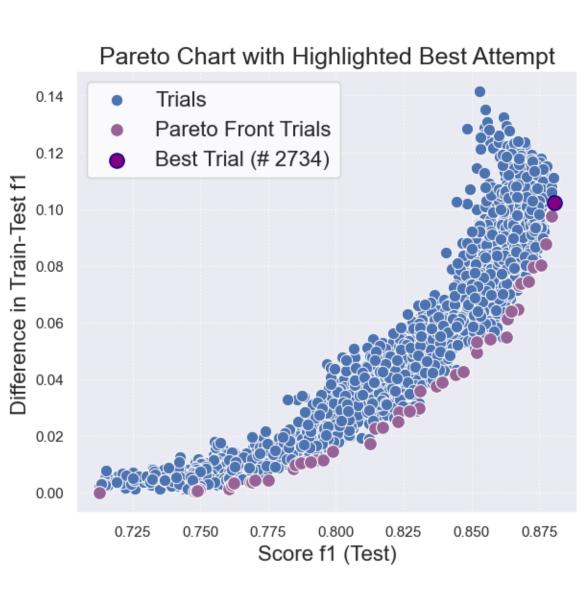


		Active/Inact	ive probability		
12		ve zone		Active zone	inactive (148) decoy (333)
10		0.4	0.6	0.8	
	0.2		pability	0.0	1.0

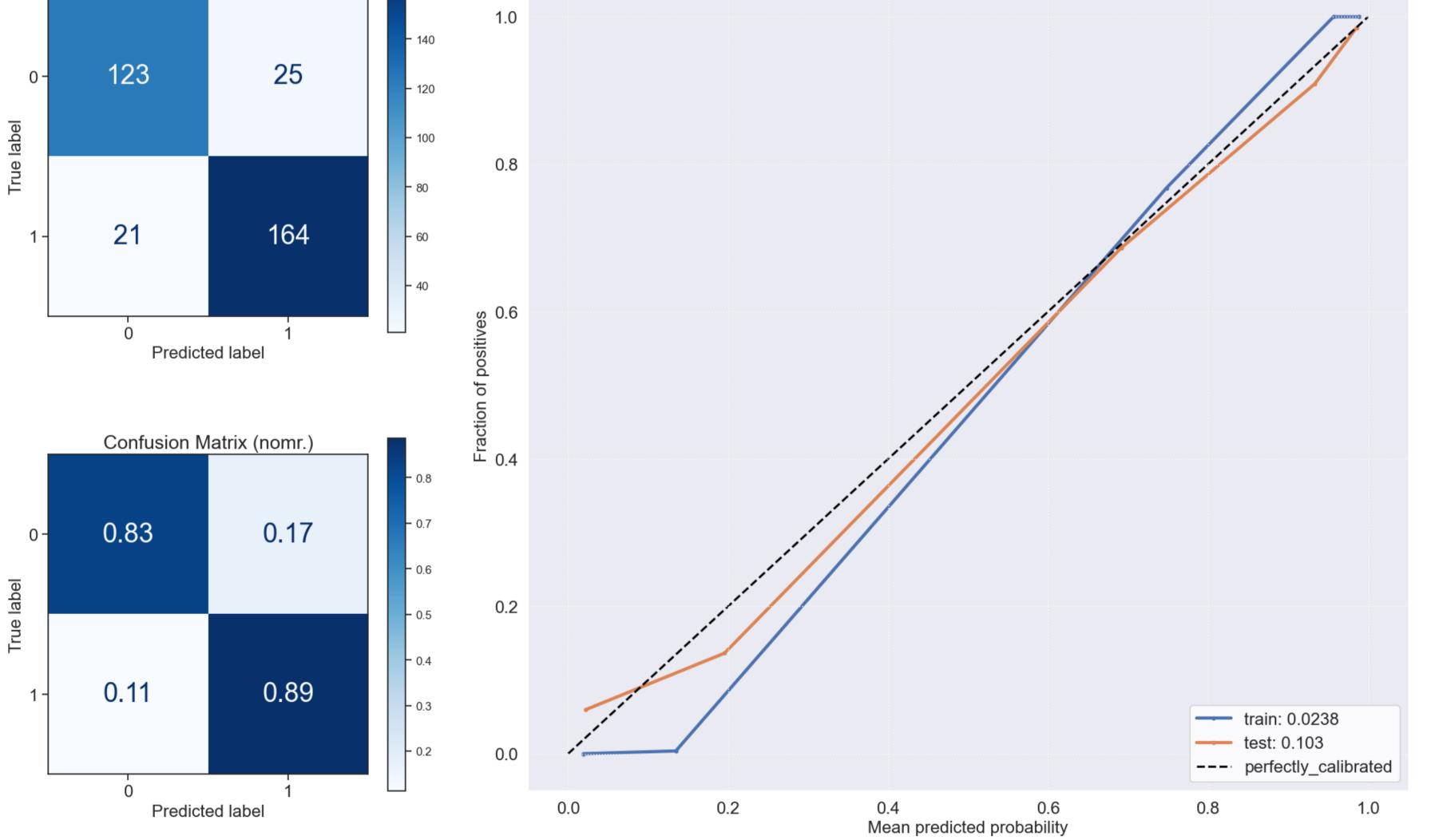
Metric	Train	Test
AUC	0.9933	0.9289
accuracy	0.9579	0.8679
balanced accuracy	0.9565	0.8669
recall_(sens)	0.9701	0.8757
specificity	0.9428	0.8581
precision	0.9546	0.8852
f1_score	0.9579	0.868

Protein: P11229 - metric: f1





XGBoost Parameters	Value
alpha	4.0424
colsample_bytree	0.9126
gamma	0.3539
lambda	2.0536
learning_rate	0.0615
max_depth	8.0
min_child_weight	1.0
n_estimators	438.0
reg_alpha	0.3836
reg_lambda	0.8124
scale_pos_weight	1.3947
subsample	0.9572

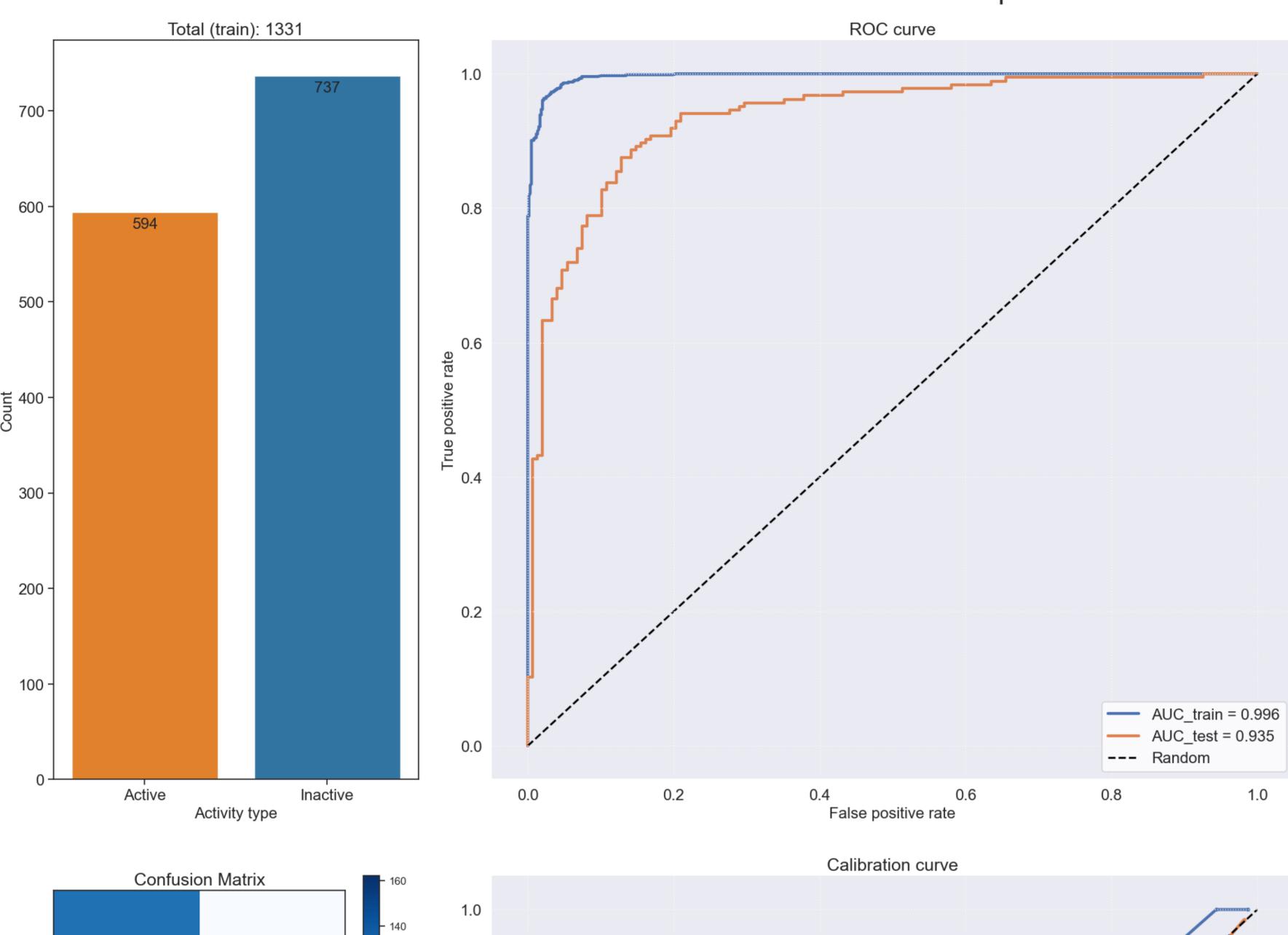


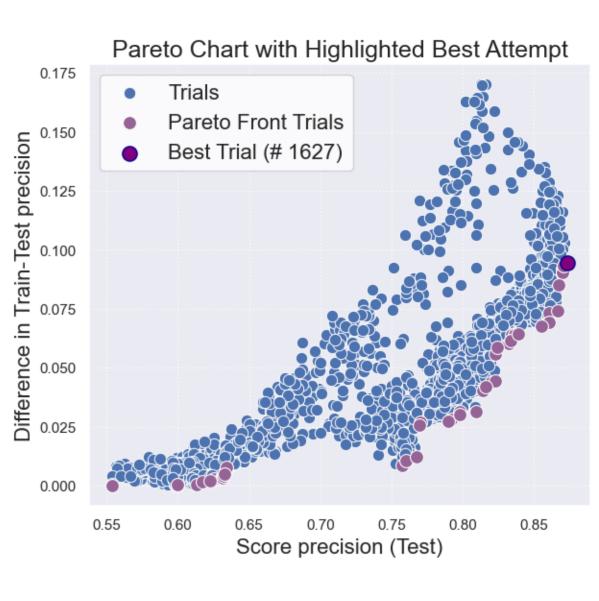
17.5		ctive zone		Activ	e zone	type active (185) inactive (148)
15.0						decoy (333)
12.5						
Dercent						П
7.5-						
5.0						
2.5				h 44 p		
0.0	.0 0.	2 0.	4 Probability	0.6	0.8	1.0

Active/Inactive probability

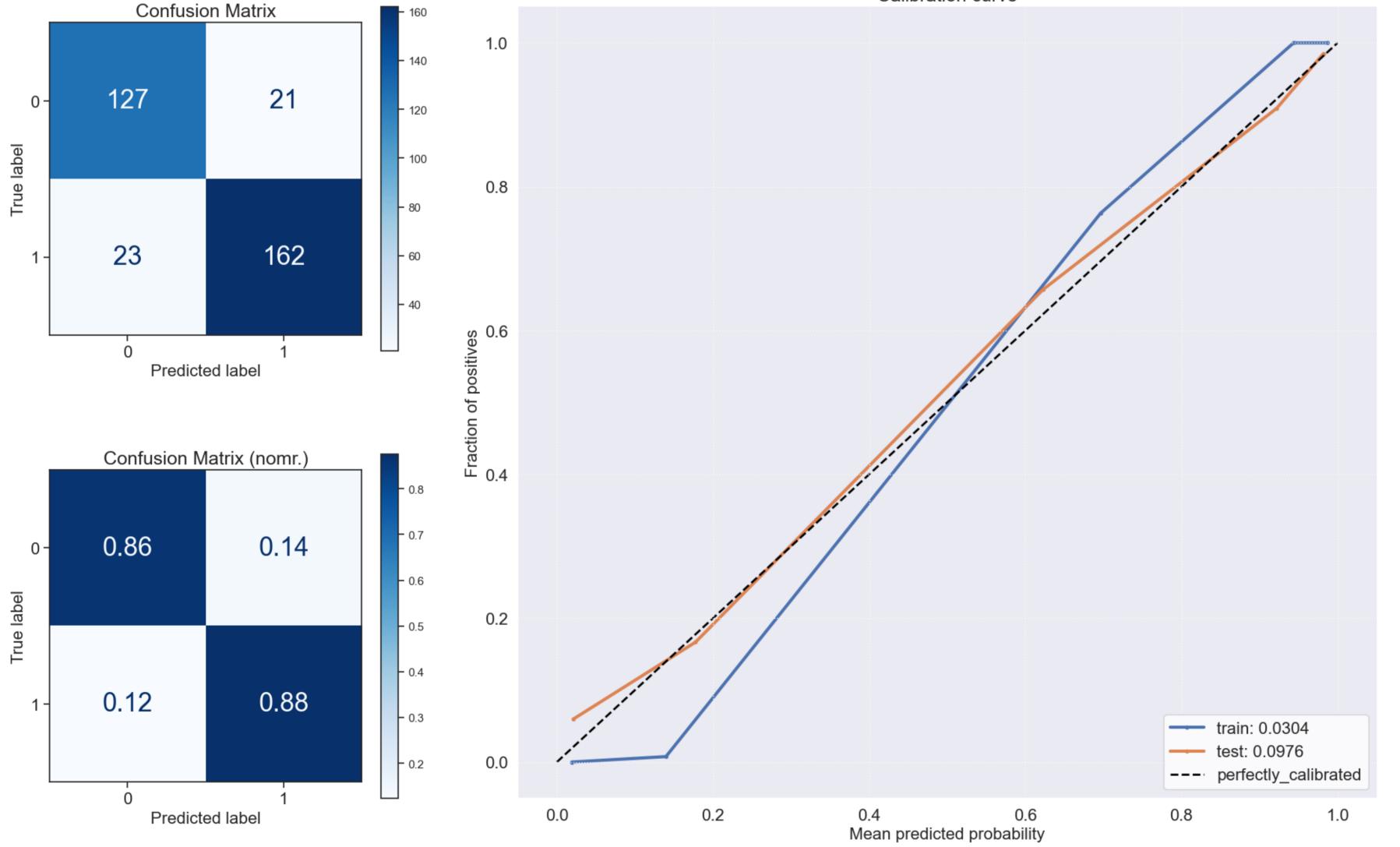
Metric	Train	Test
AUC	0.9986	0.9295
accuracy	0.9782	0.8619
balanced accuracy	0.9761	0.8588
recall_(sens)	0.9959	0.8865
specificity	0.9562	0.8311
precision	0.9658	0.8677
f1_score	0.9782	0.8617

Protein: P11229 - metric: precision





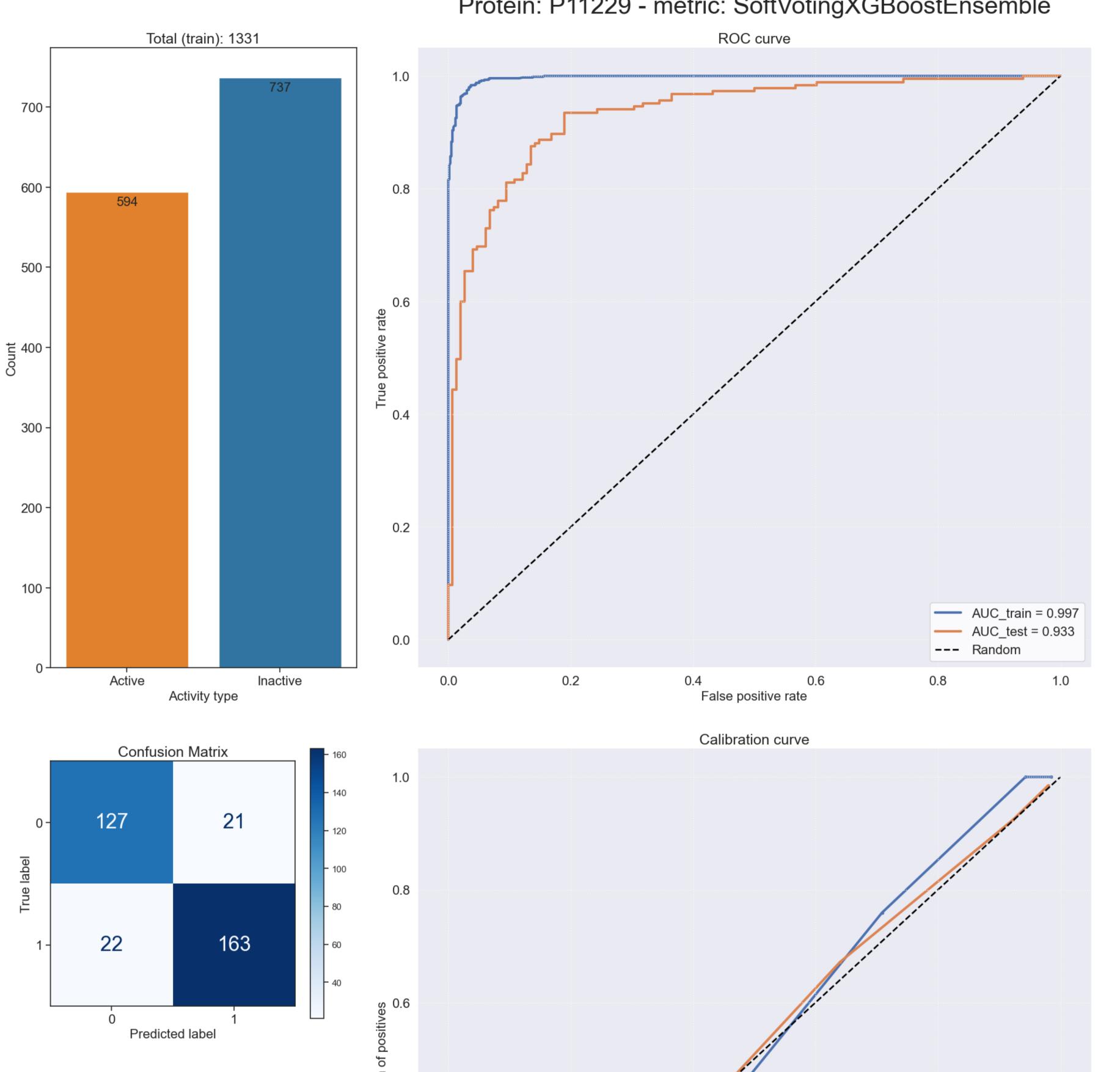
XGBoost Parameters	Value
alpha	2.1987
colsample_bytree	0.6549
gamma	0.2291
lambda	0.6975
learning_rate	0.0247
max_depth	10.0
min_child_weight	3.0
n_estimators	904.0
reg_alpha	0.352
reg_lambda	0.9731
scale_pos_weight	1.0746
subsample	0.7356

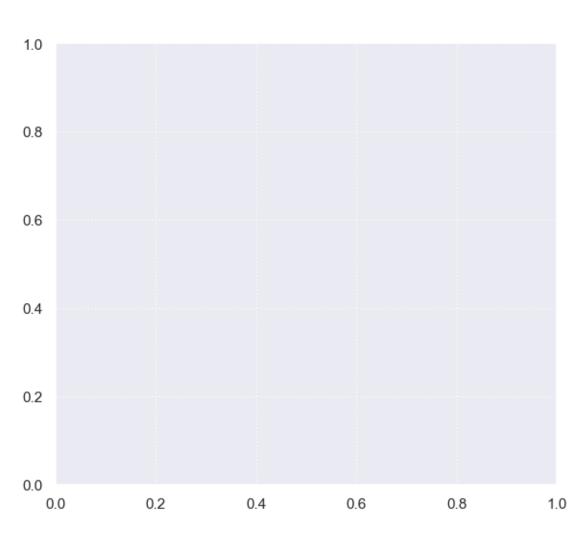


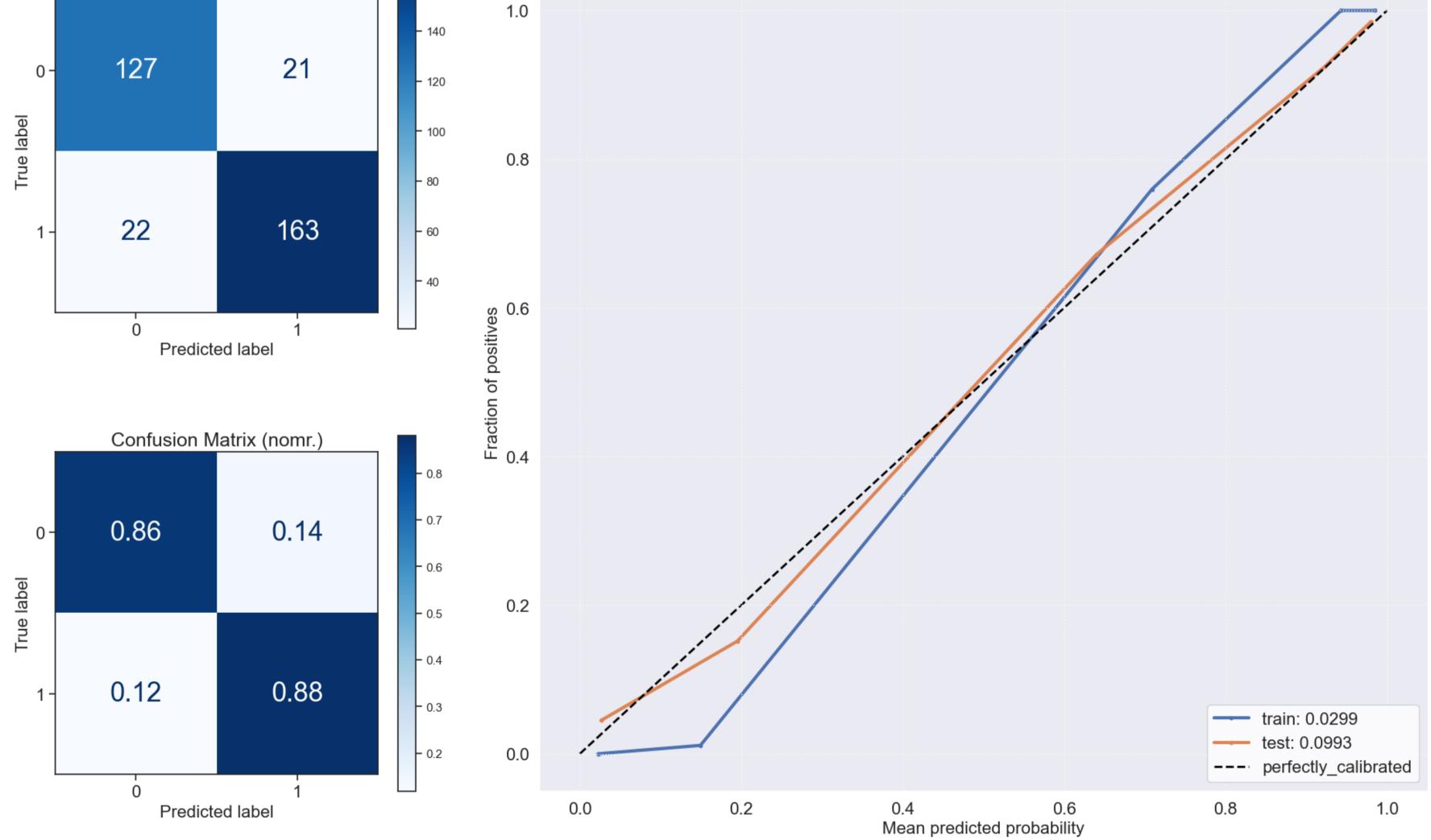
44			Active/Inactiv			
14		Inactive zon			Active zone	type active (185) inactive (148)
						decoy (333)
10						
Percent						
4						
2						
2						
0 —	0.0	0.2	0.4 Proba	0.6 bility	0.8	1.0

Metric	Train	Test
AUC	0.9964	0.9347
accuracy	0.9692	0.8679
balanced accuracy	0.9681	0.8669
recall_(sens)	0.9783	0.8757
specificity	0.9579	0.8581
precision	0.9665	0.8852
f1_score	0.9692	0.868

Protein: P11229 - metric: SoftVotingXGBoostEnsemble







				Active	e/Inactive	e probabili	ty			
1	4		inactive				Active	zone	type active (1) inactive (decoy (3)	(148)
ent 1	0									
Percent	6									
	2									
	0.	0	0.2	0.4	Probab	0.6 pility	0	.8	1.0)

Metric	Train	Test
AUC	0.997	0.9332
accuracy	0.973	0.8709
balanced accuracy	0.9712	0.8696
recall_(sens)	0.9878	0.8811
specificity	0.9545	0.8581
precision	0.9642	0.8859
f1_score	0.9729	0.8709