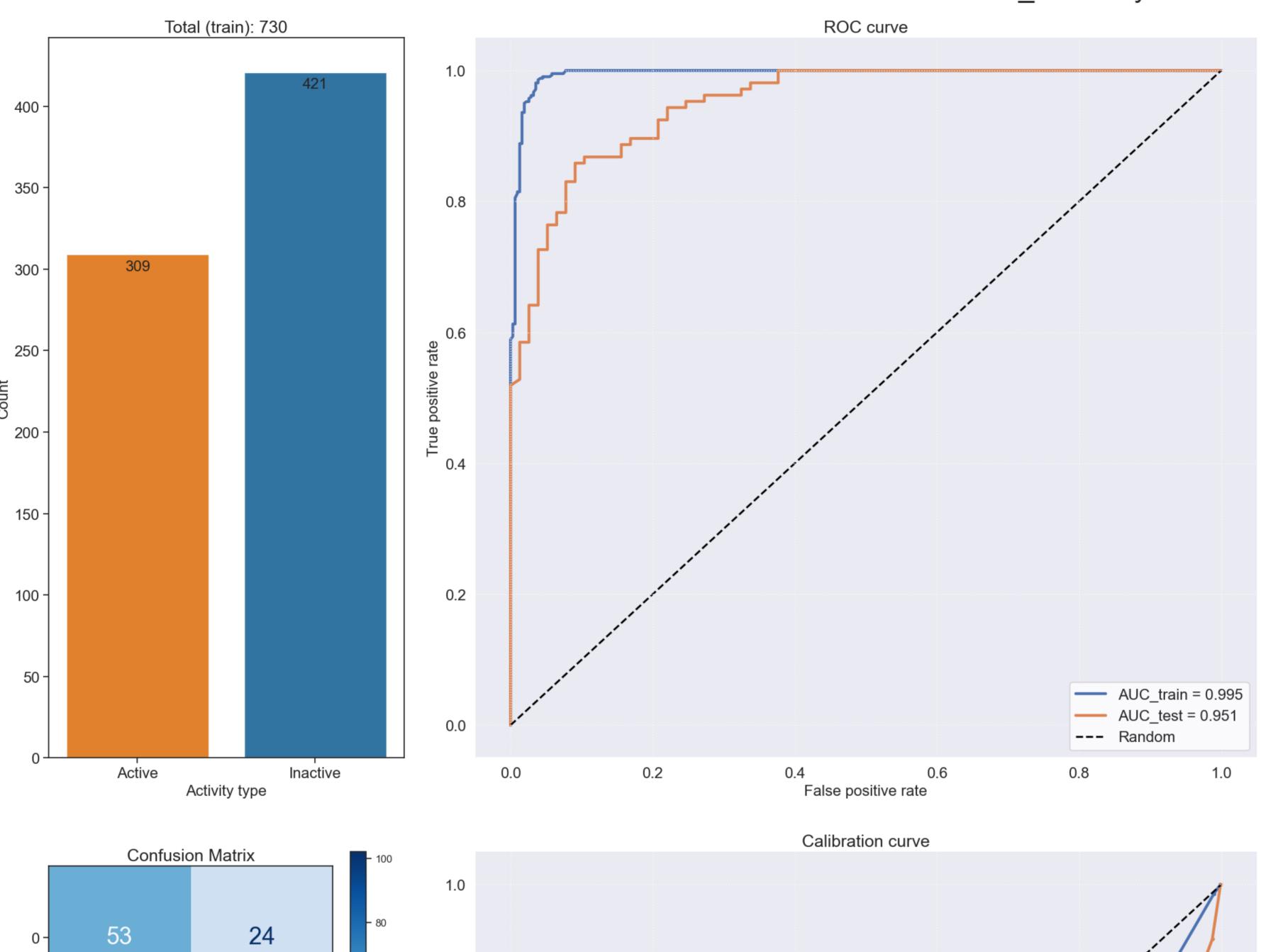
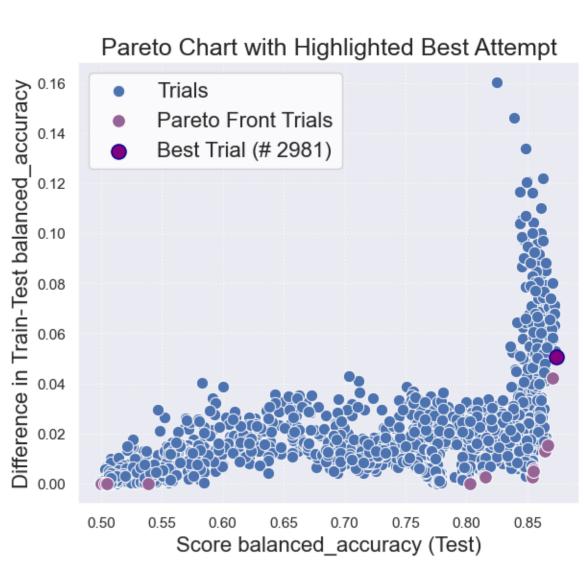
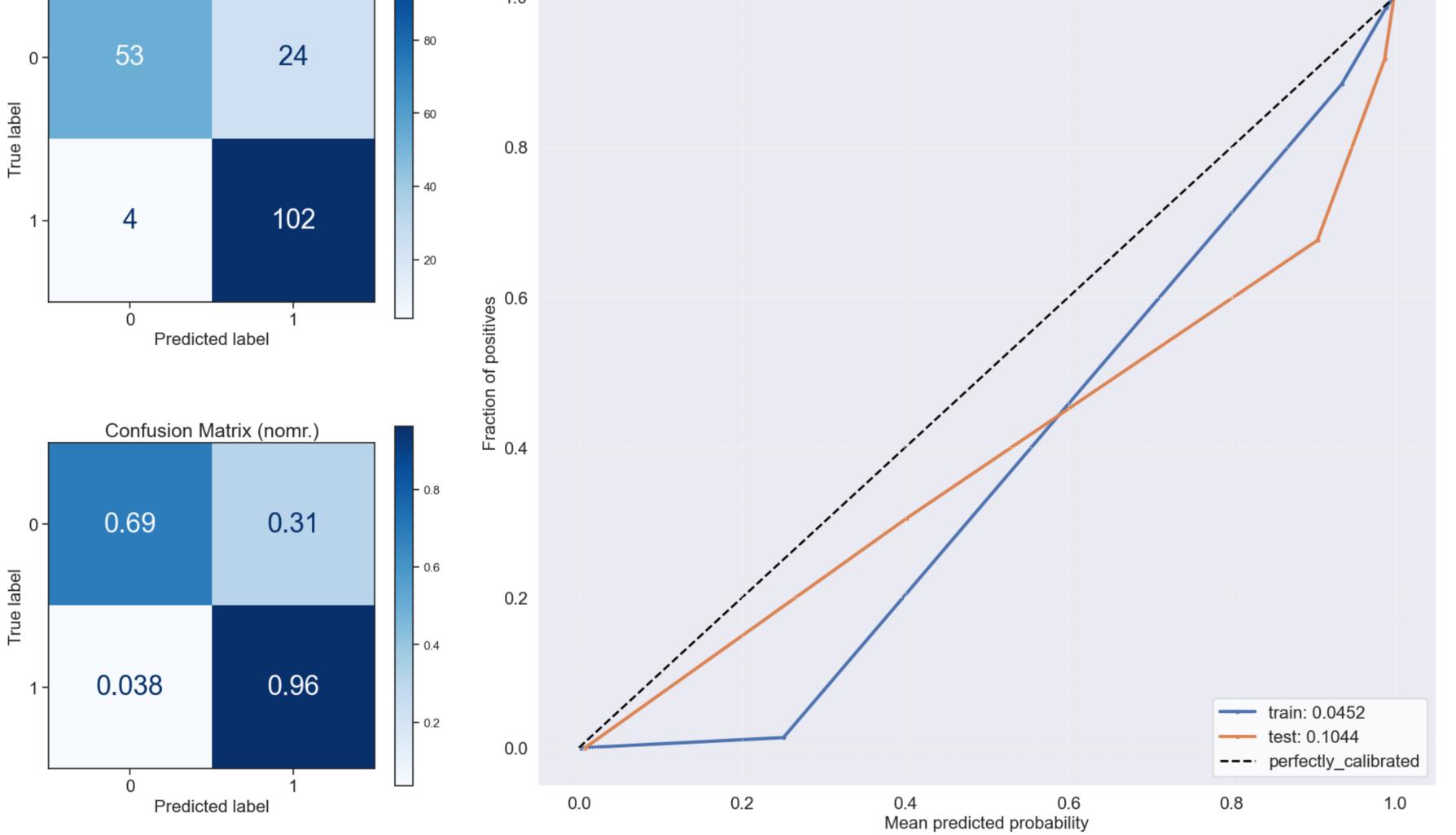
Protein: P11597 - metric: balanced_accuracy





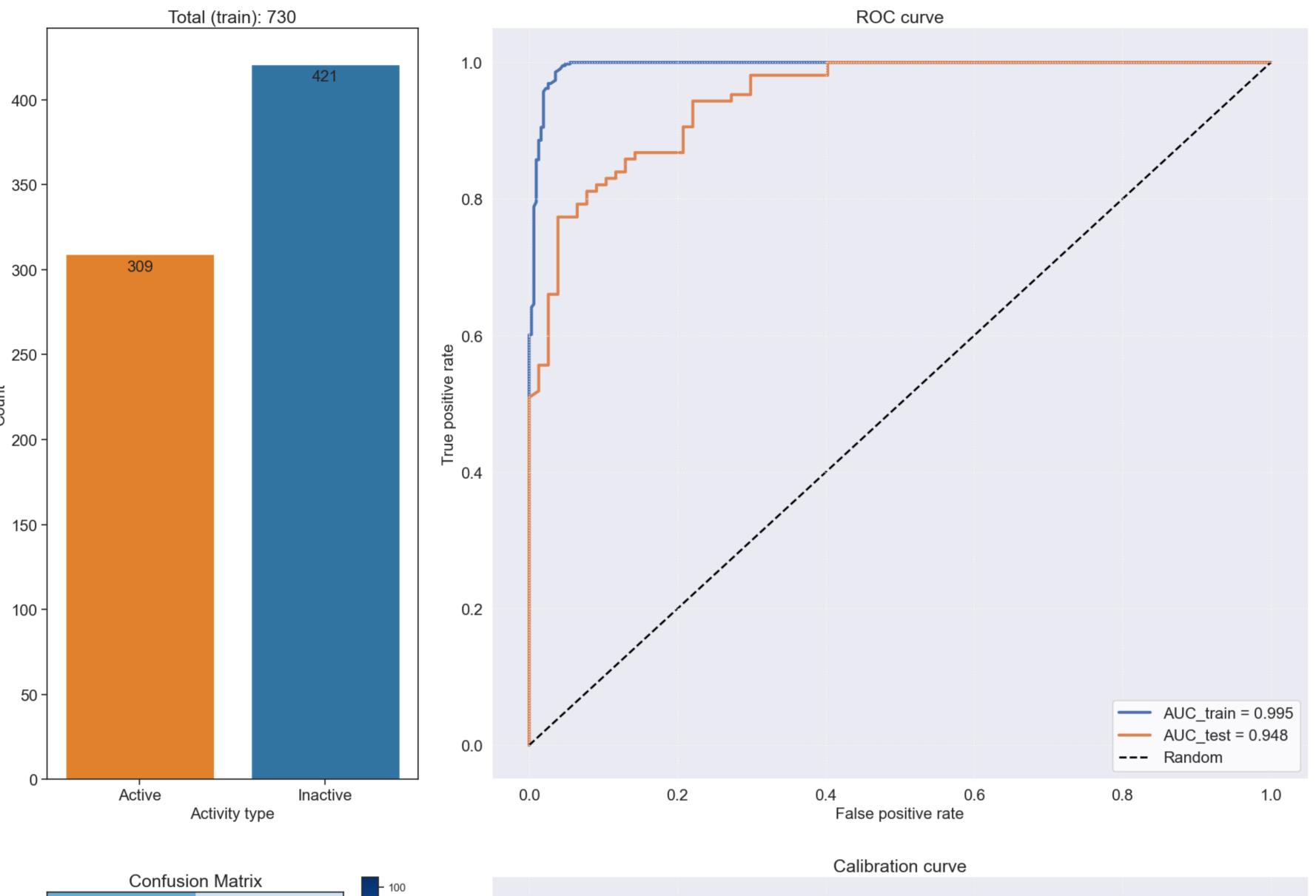
XGBoost Parameters	Value
alpha	2.6251
colsample_bytree	0.9862
gamma	0.9359
lambda	4.0148
learning_rate	0.0691
max_depth	7.0
min_child_weight	4.0
n_estimators	826.0
reg_alpha	0.6913
reg_lambda	0.1062
scale_pos_weight	5.5977
subsample	0.6914

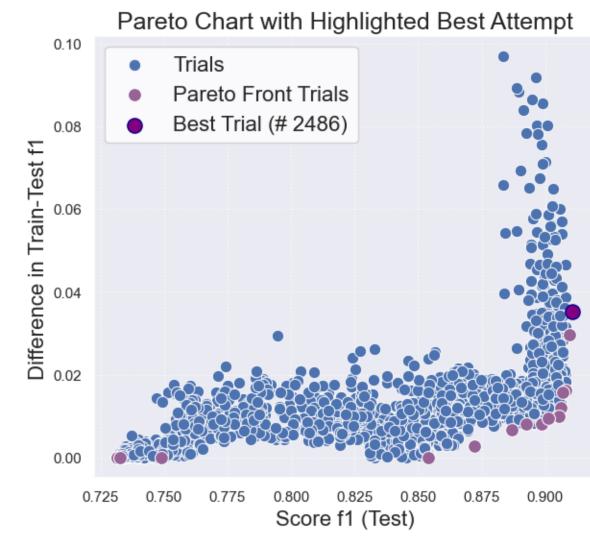


	Activ	/e/Inactive probability	
50	Inactive zone	Active z	type active (106) inactive (77) decoy (183)
Percent 08 08			
20			
0 —	0.0 0.2 0.4	0.6 0. Probability	8 1.0

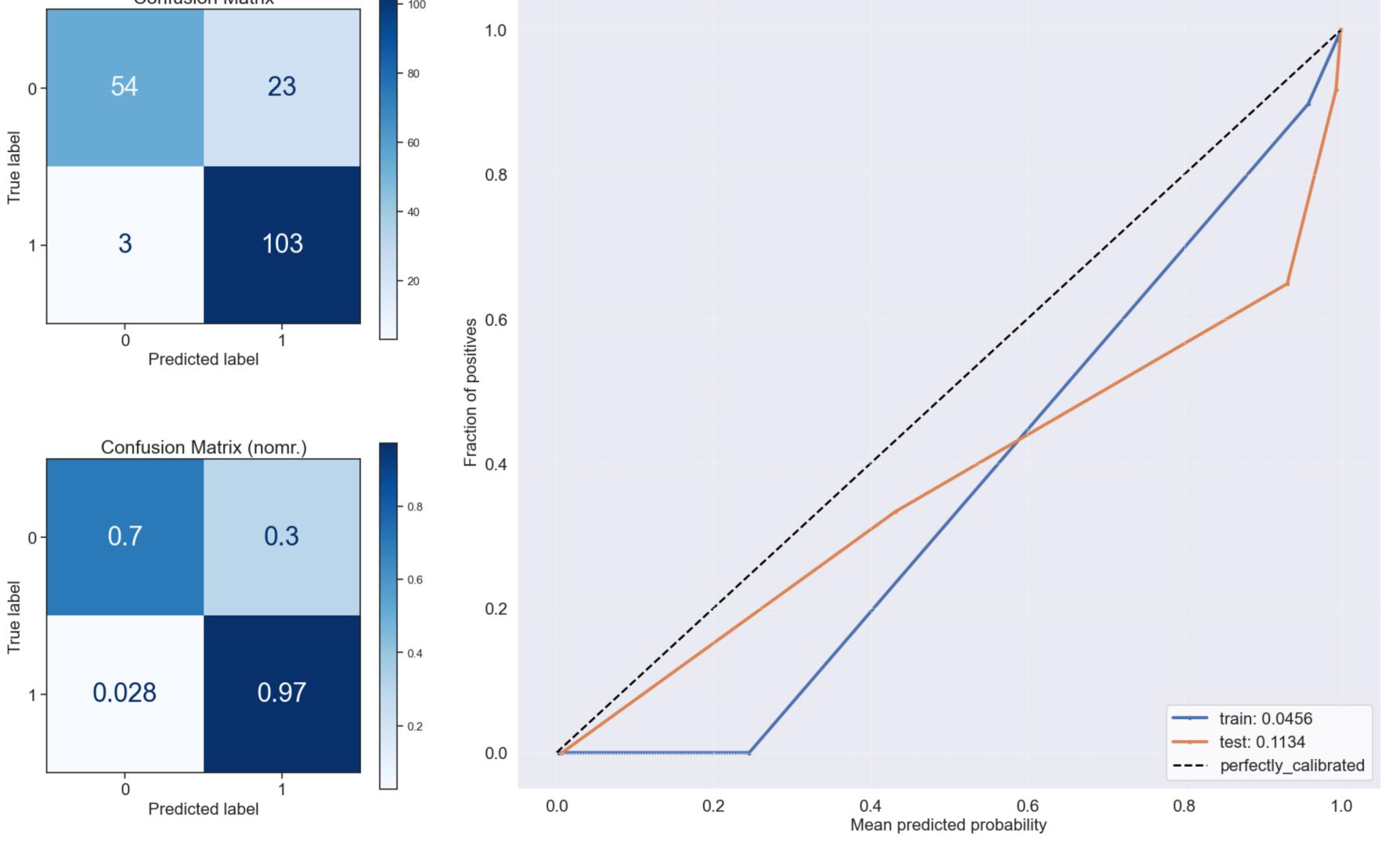
Metric	Train	Test
AUC	0.9946	0.9512
accuracy	0.937	0.847
balanced accuracy	0.9256	0.8253
recall_(sens)	1.0	0.9623
specificity	0.8511	0.6883
precision	0.9015	0.8095
f1_score	0.9361	0.8422

Protein: P11597 - metric: f1





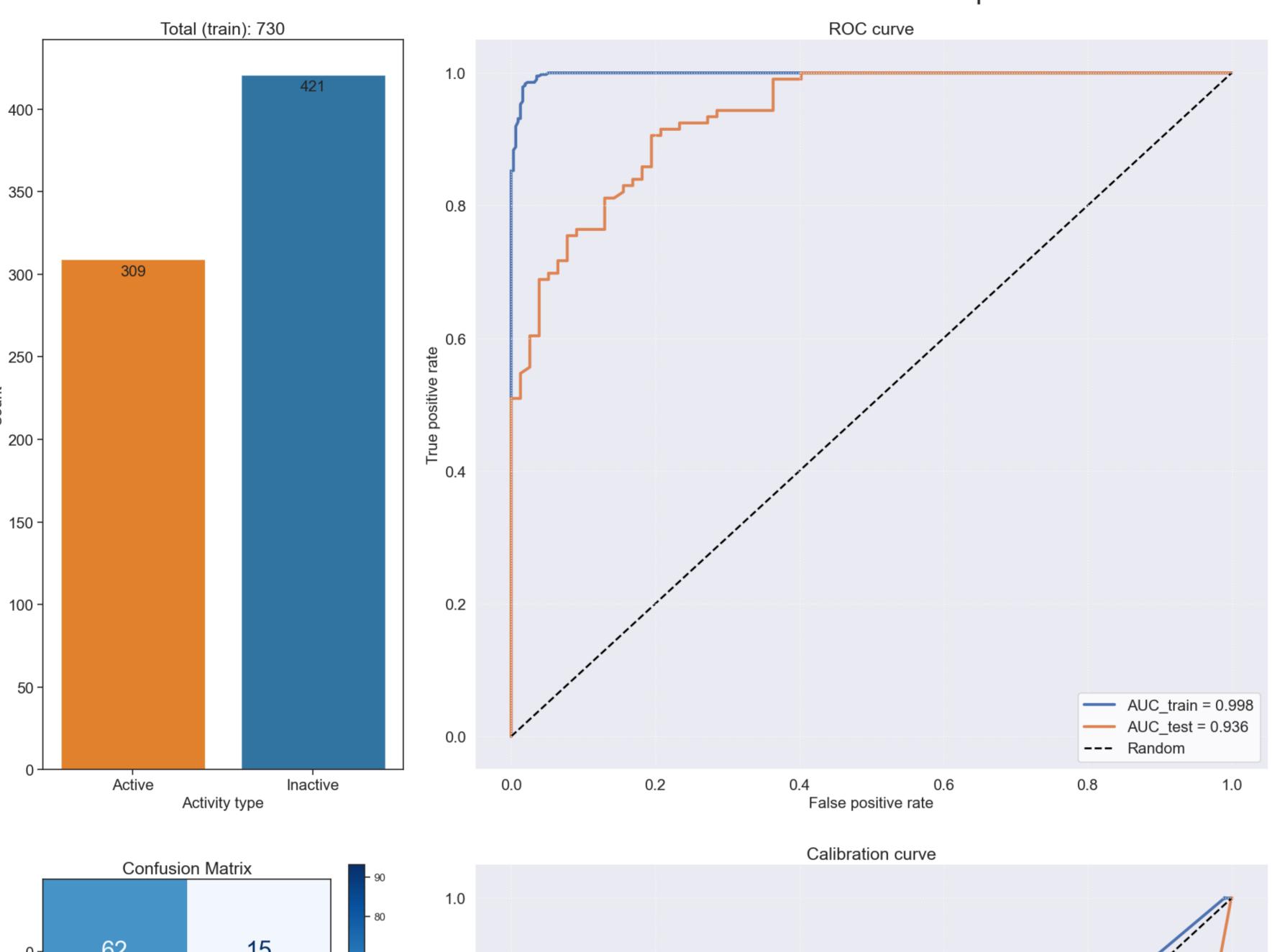
XGBoost Parameters	Value
alpha	3.9437
colsample_bytree	0.7166
gamma	0.8392
lambda	2.3878
learning_rate	0.0531
max_depth	8.0
min_child_weight	4.0
n_estimators	948.0
reg_alpha	0.4296
reg_lambda	0.2082
scale_pos_weight	9.4388
subsample	0.6211

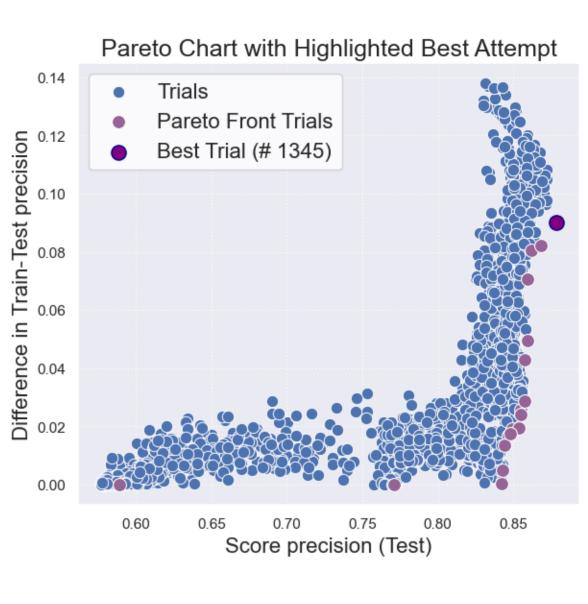


		Active/Inactive	orobability		
60	Inactive zon			Active zone	type active (106) inactive (77) decoy (183)
Percent 40					
20					
0 —	0.0 0.2	0.4 Probabili	0.6 ity	0.8	1.0

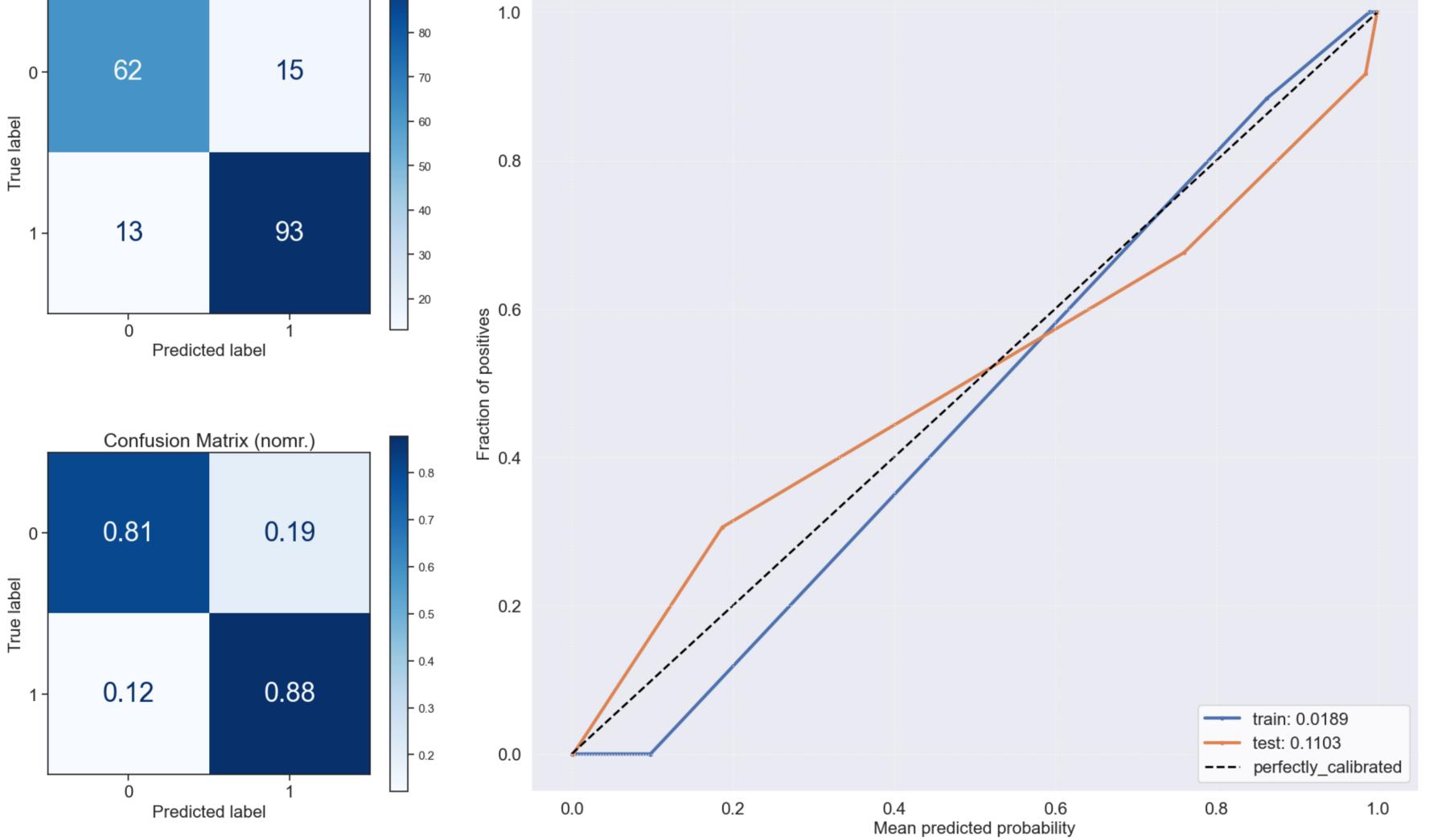
Metric	Train	Test
AUC	0.9951	0.9481
accuracy	0.937	0.8579
balanced accuracy	0.9256	0.8365
recall_(sens)	1.0	0.9717
specificity	0.8511	0.7013
precision	0.9015	0.8175
f1_score	0.9361	0.8534

Protein: P11597 - metric: precision





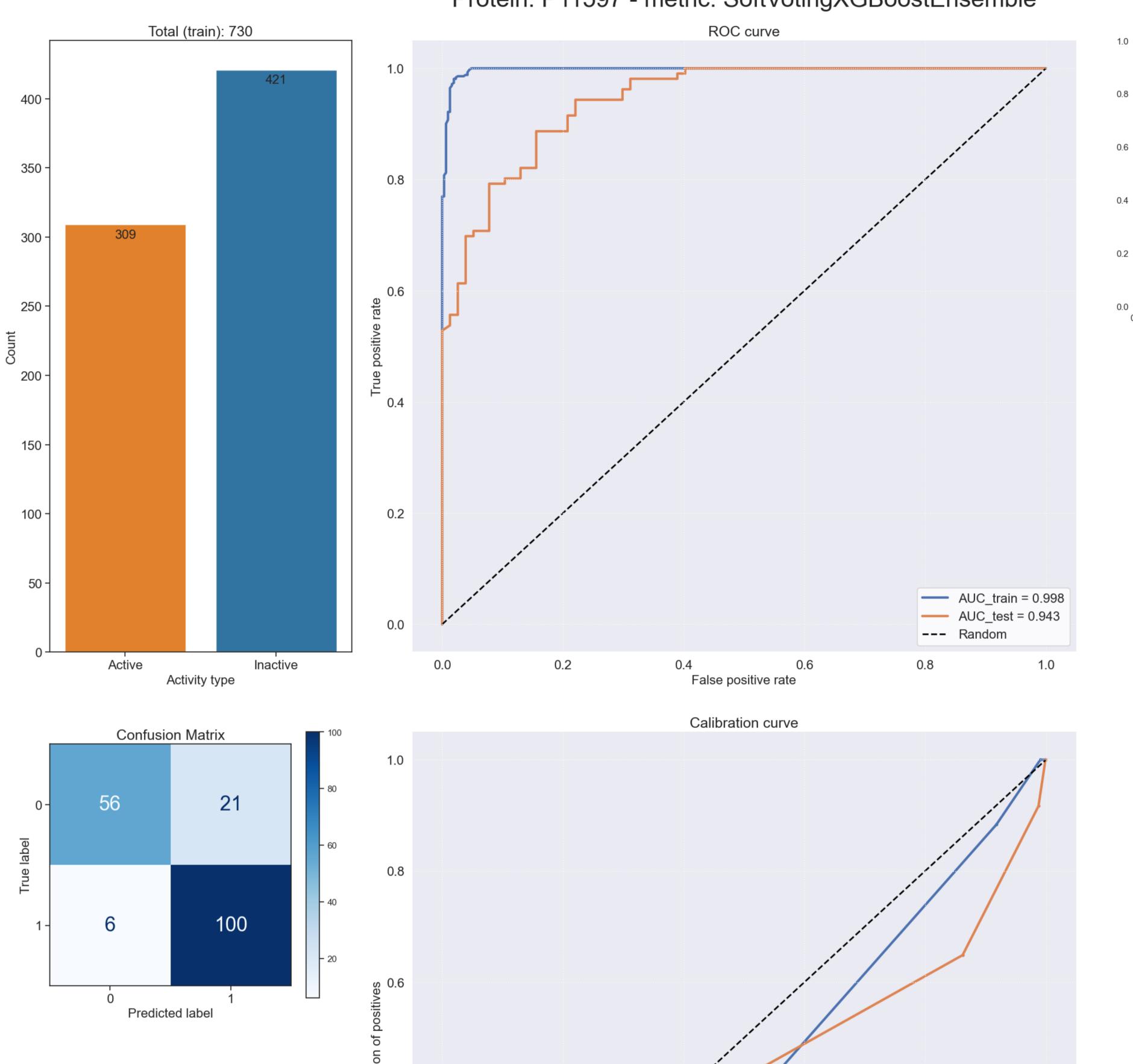
XGBoost Parameters	Value
alpha	4.8456
colsample_bytree	0.8572
gamma	0.9902
lambda	2.0947
learning_rate	0.4494
max_depth	6.0
min_child_weight	1.0
n_estimators	317.0
reg_alpha	0.1825
reg_lambda	0.9164
scale_pos_weight	1.6997
subsample	0.5311

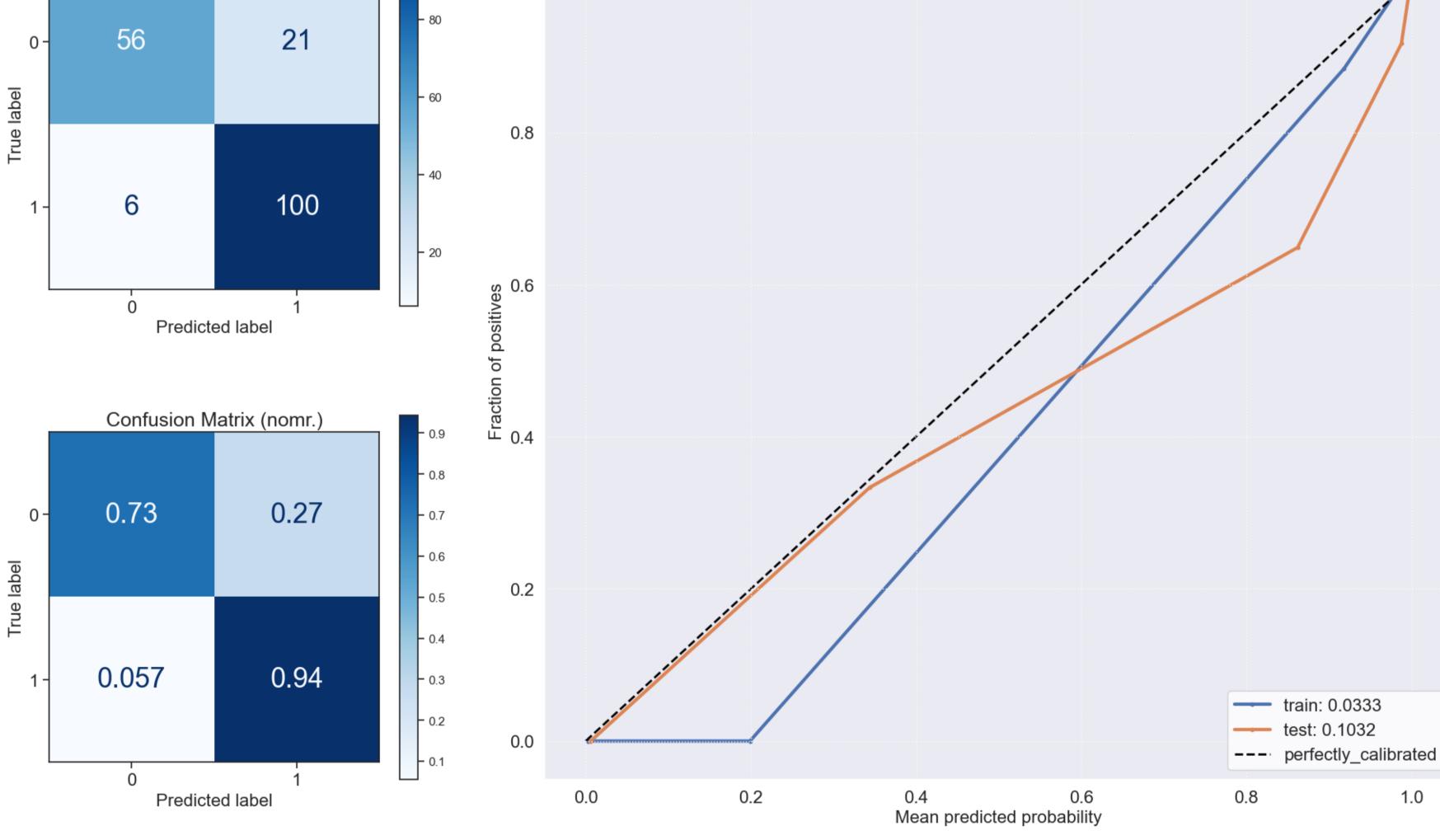


	Active/Inactive probability					
50		Inactive zone			Active zone	
40						decoy (183)
Percent						
20 						
10						
0 —						
	0.0	0.2	0.4 Prob	0.6 ability	0.8	1.0

Metric	Train	Test
AUC	0.9982	0.9357
accuracy	0.9781	0.847
balanced accuracy	0.9745	0.8413
recall_(sens)	0.9976	0.8774
specificity	0.9515	0.8052
precision	0.9655	0.8611
f1_score	0.978	0.8467

Protein: P11597 - metric: SoftVotingXGBoostEnsemble





		Active/Inactive	orobability		
50	Inactive zo	ne		Active zone	type active (106) inactive (77) decoy (183)
Percent 08					
20 					
0 —	0.0 0.2	0.4	0.6	0.8	1.0
		Probabili	ty		

Metric	Train	Test
AUC	0.9975	0.943
accuracy	0.9493	0.8525
balanced accuracy	0.9401	0.8353
recall_(sens)	1.0	0.9434
specificity	0.8803	0.7273
precision	0.9192	0.8264
f1_score	0.9488	0.8494

0.2

0.6

0.0