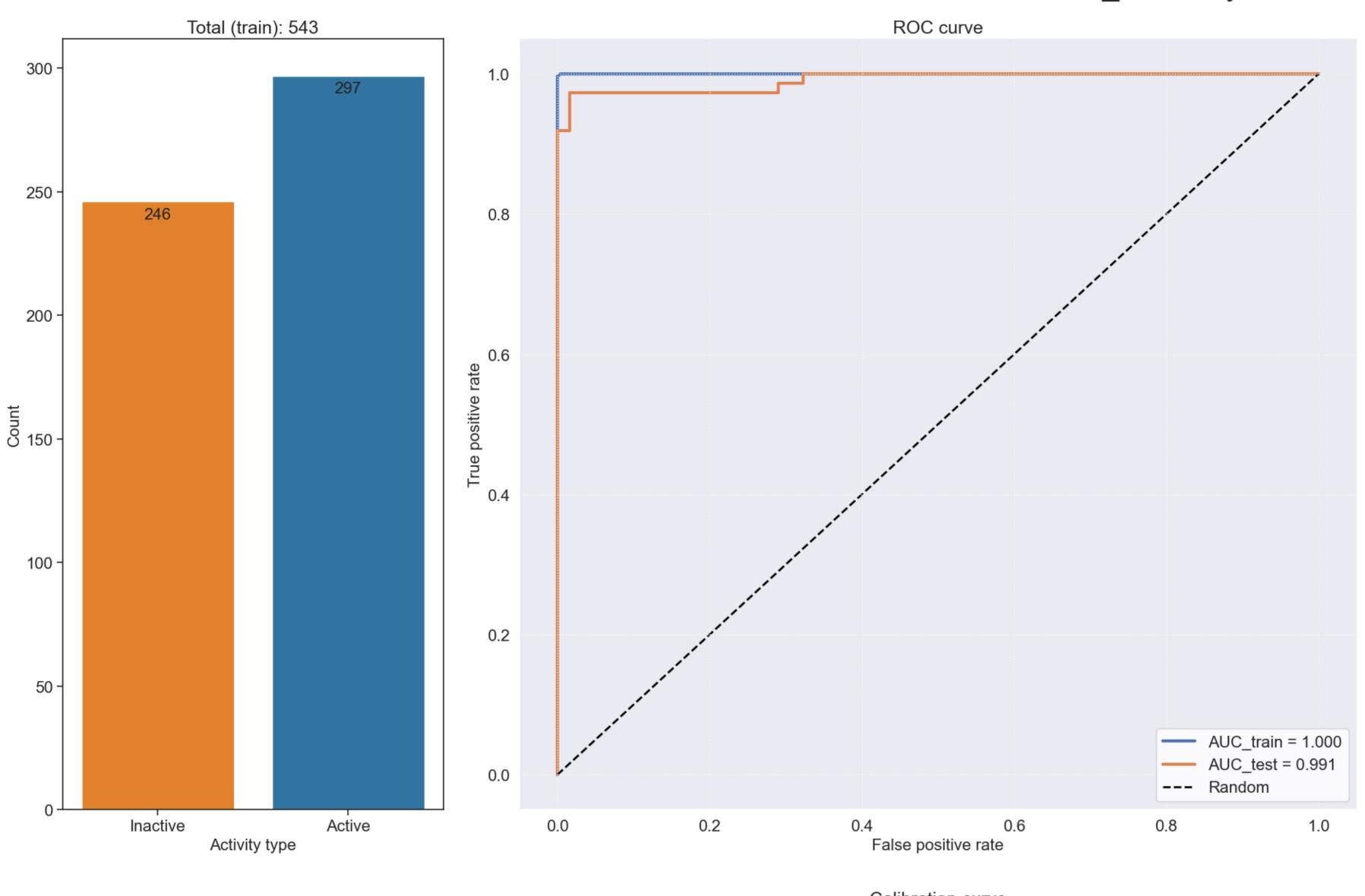
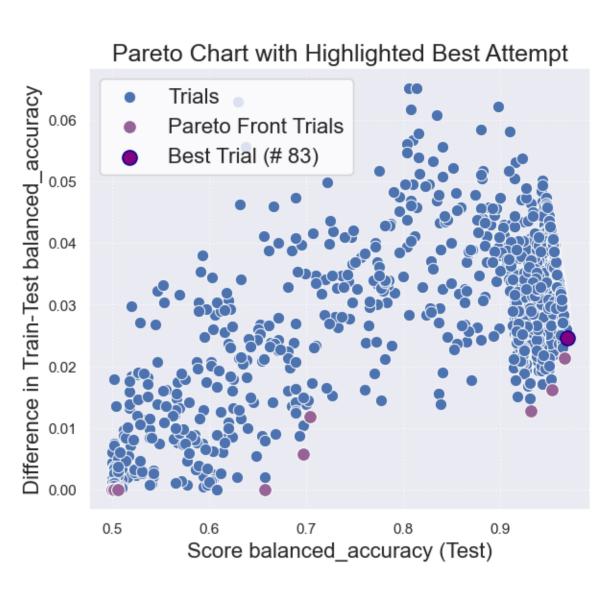
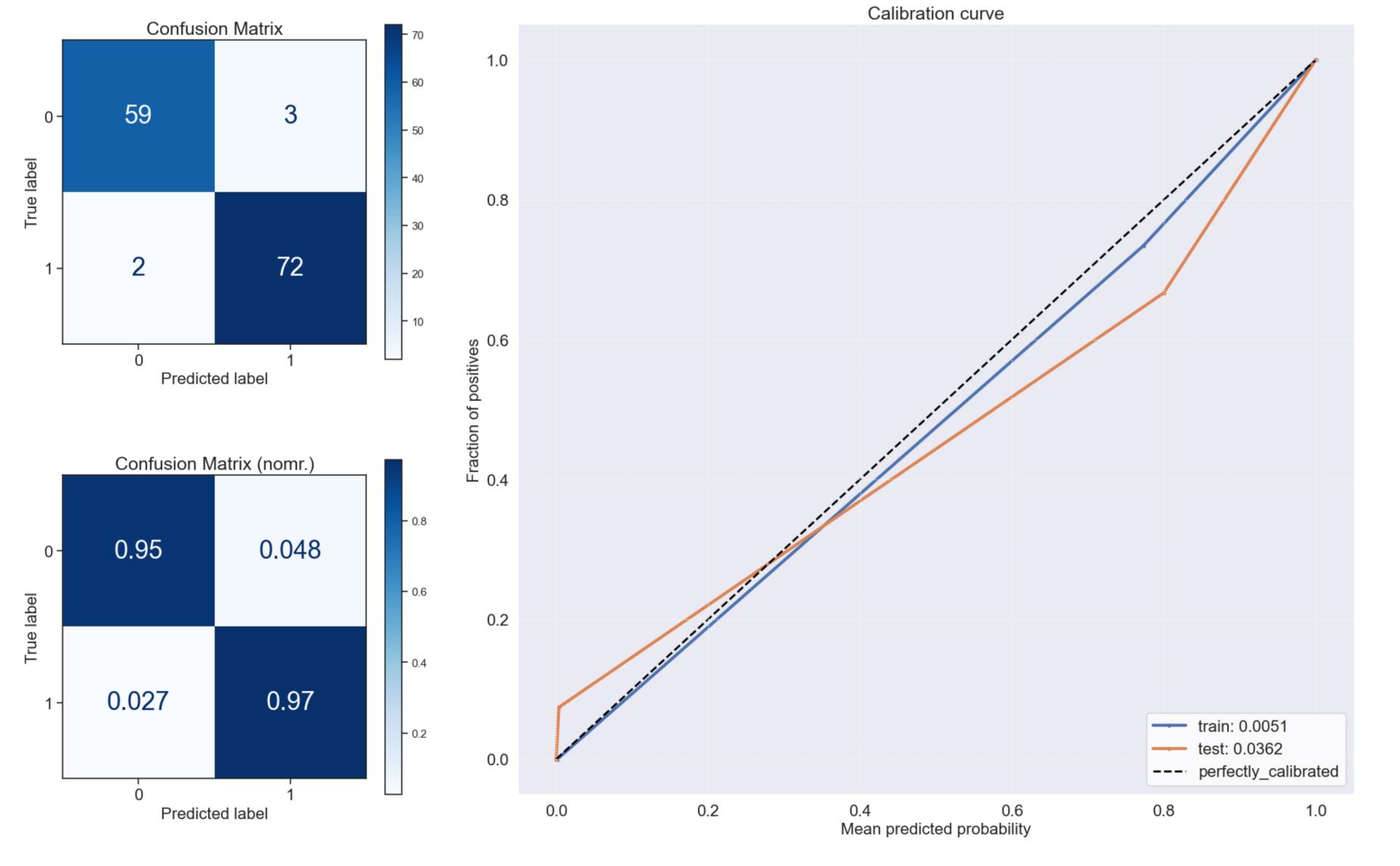
Protein: P01375 - metric: balanced_accuracy





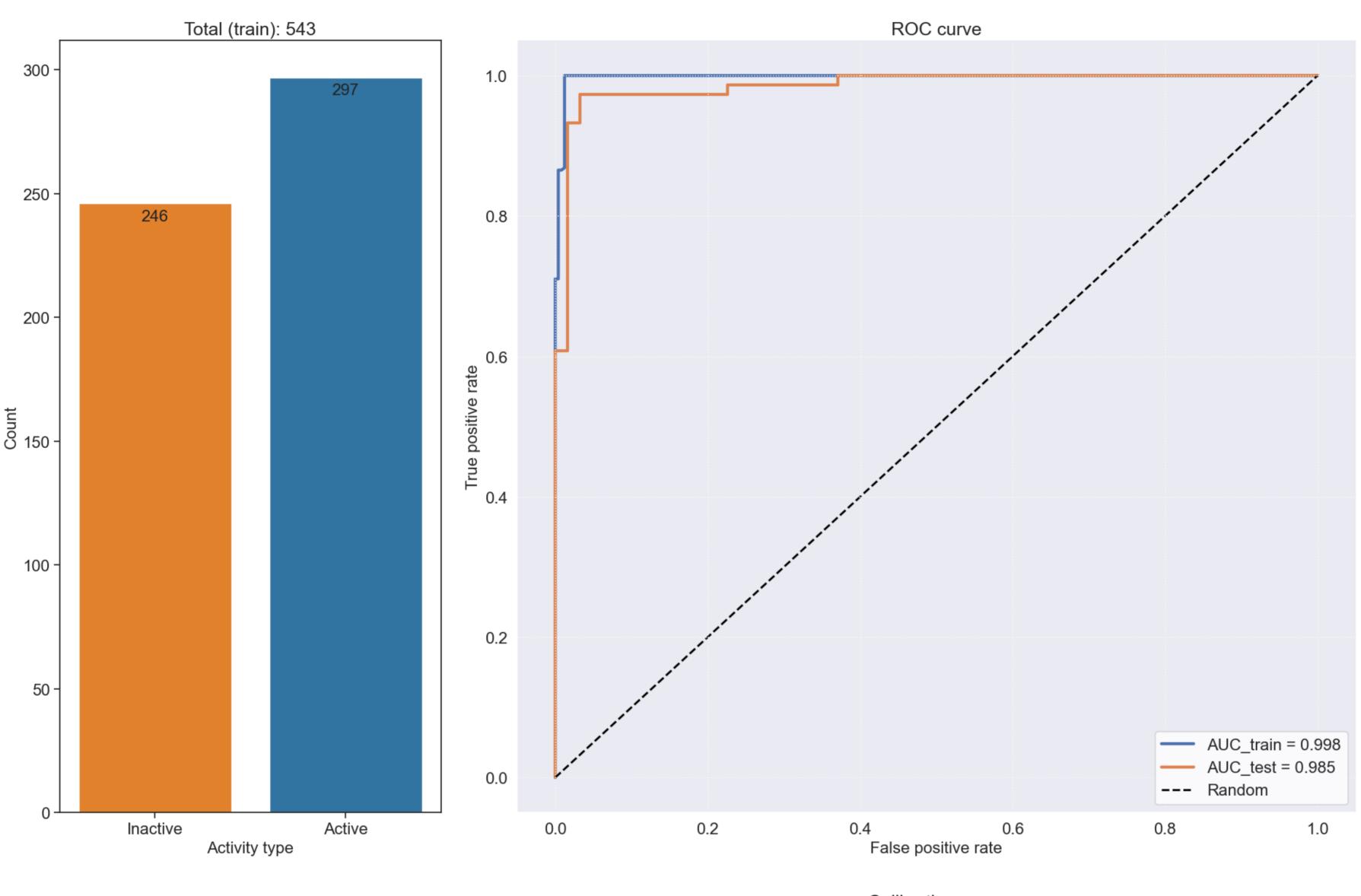
XGBoost Parameters	Value
alpha	1.0303
colsample_bytree	0.8763
gamma	0.1703
lambda	1.0852
learning_rate	0.1909
max_depth	9.0
min_child_weight	1.0
n_estimators	986.0
reg_alpha	0.4337
reg_lambda	0.2819
scale_pos_weight	30.4816
subsample	0.5495

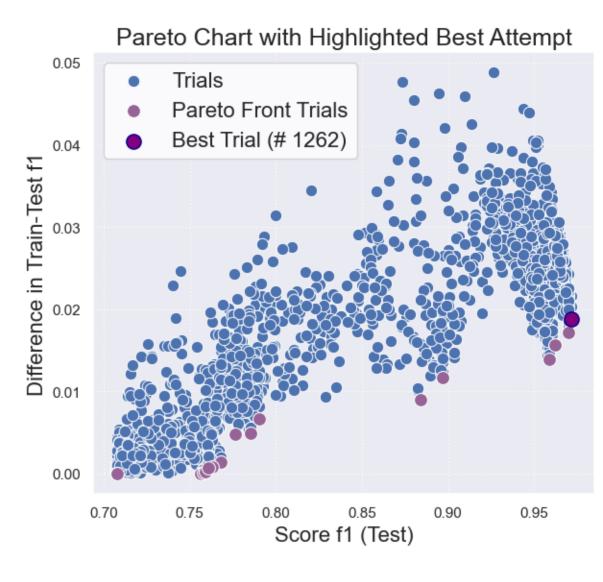


			Active/Inact	ive probability		
80		Inactive zone			Active zone	type active (74) inactive (62) decoy (136)
60						
Percent 00						
20						
0						
U	0.0	0.2	0.4 Prot	0.6 pability	0.8	1.0

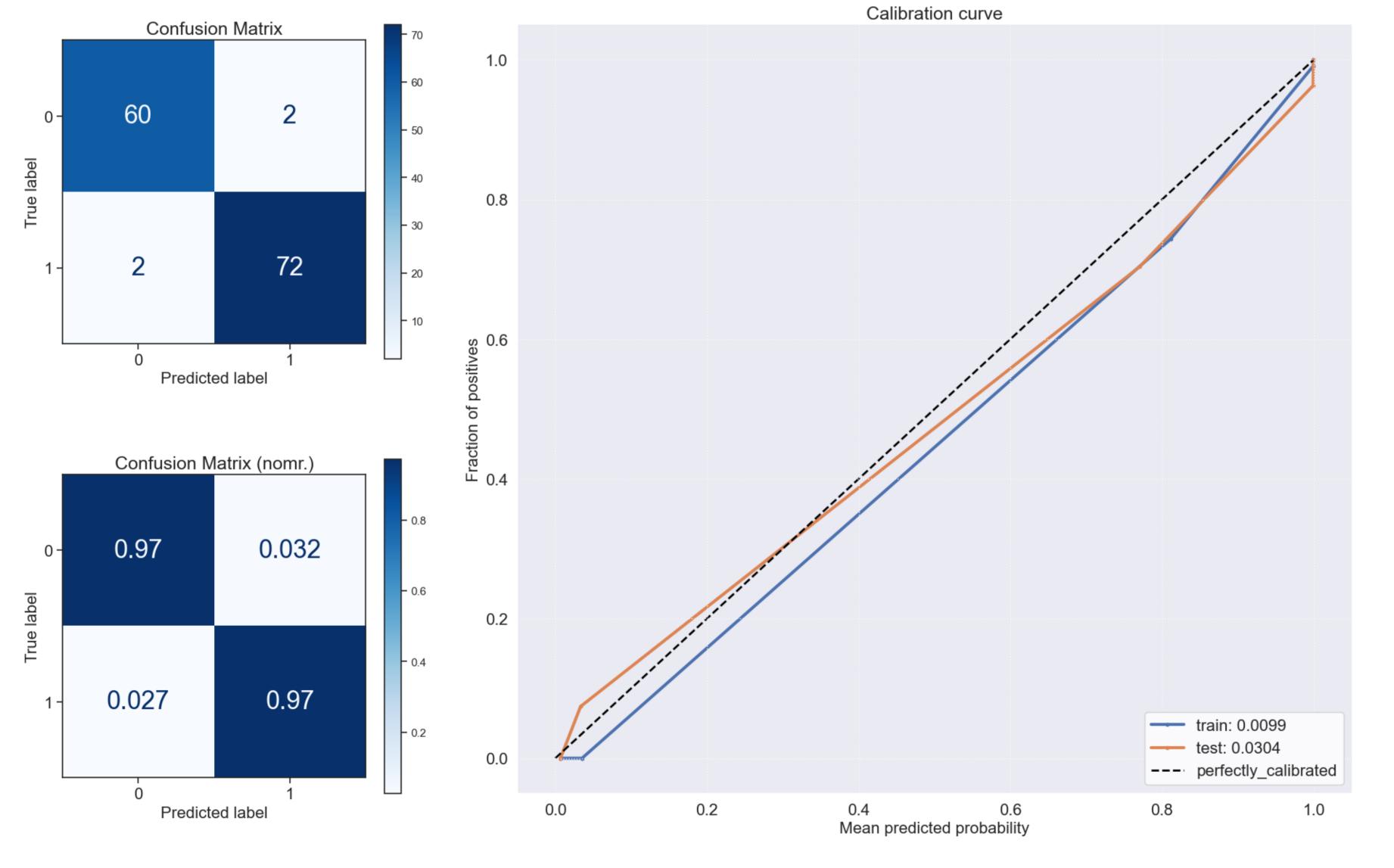
Metric	Train	Test
AUC	1.0	0.9908
accuracy	0.9945	0.9632
balanced accuracy	0.9939	0.9623
recall_(sens)	1.0	0.973
specificity	0.9878	0.9516
precision	0.99	0.96
f1_score	0.9945	0.9632

Protein: P01375 - metric: f1





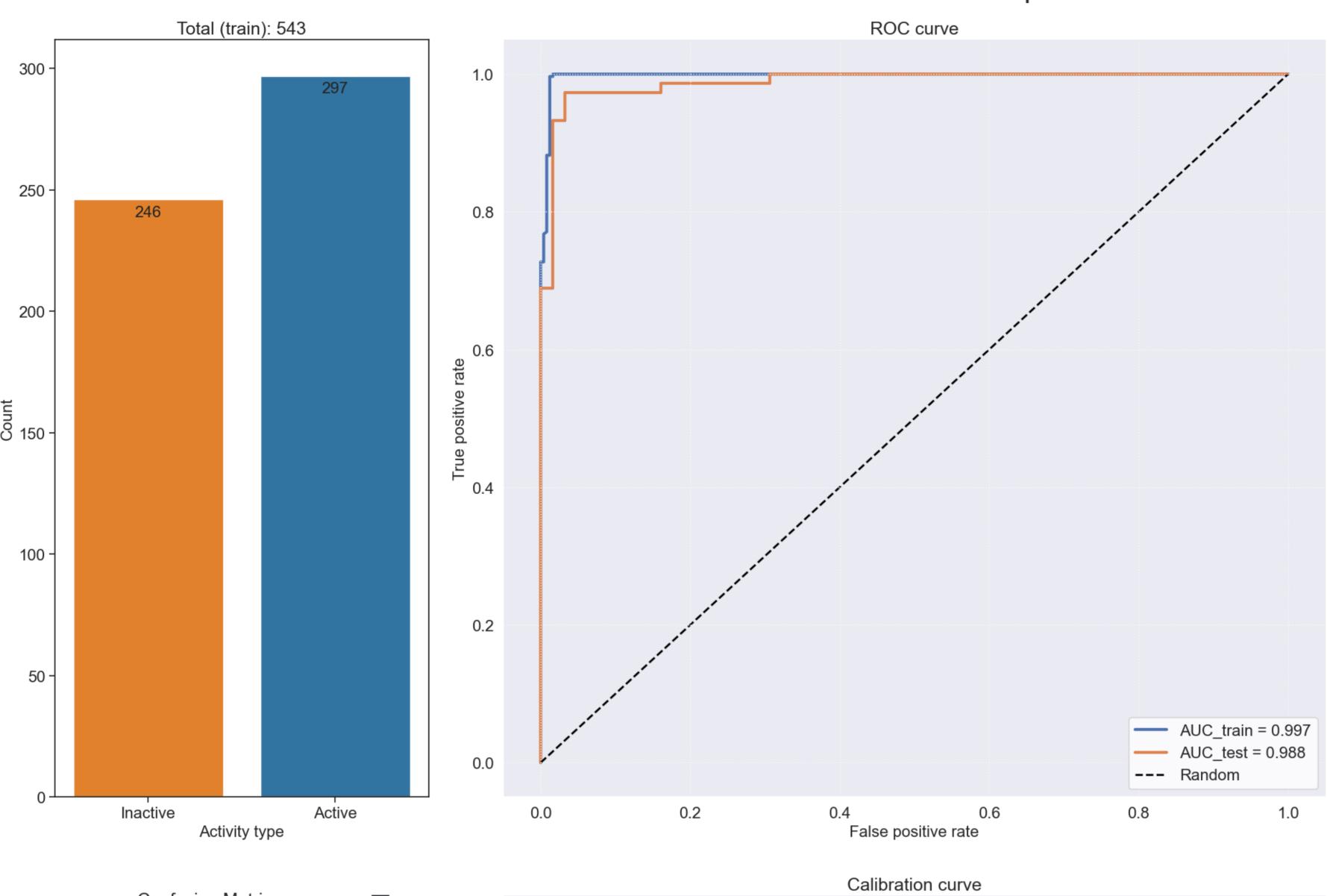
XGBoost Parameters	Value
alpha	4.4695
colsample_bytree	0.6179
gamma	0.5892
lambda	0.5344
learning_rate	0.017
max_depth	7.0
min_child_weight	2.0
n_estimators	993.0
reg_alpha	0.5356
reg_lambda	0.786
scale_pos_weight	15.0883
subsample	0.7535

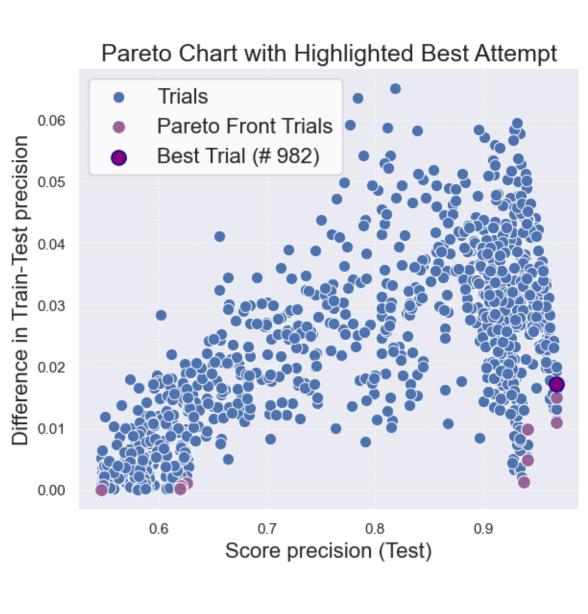


		Ac	tive/Inactive proba	bility		
80	Ina	ctive zone		Active	zone	type active (74) nactive (62)
00						decoy (136)
Percent O O						
20	1					
0 —						
O	0.0	.2 0	.4 Probability	0.6).8	1.0

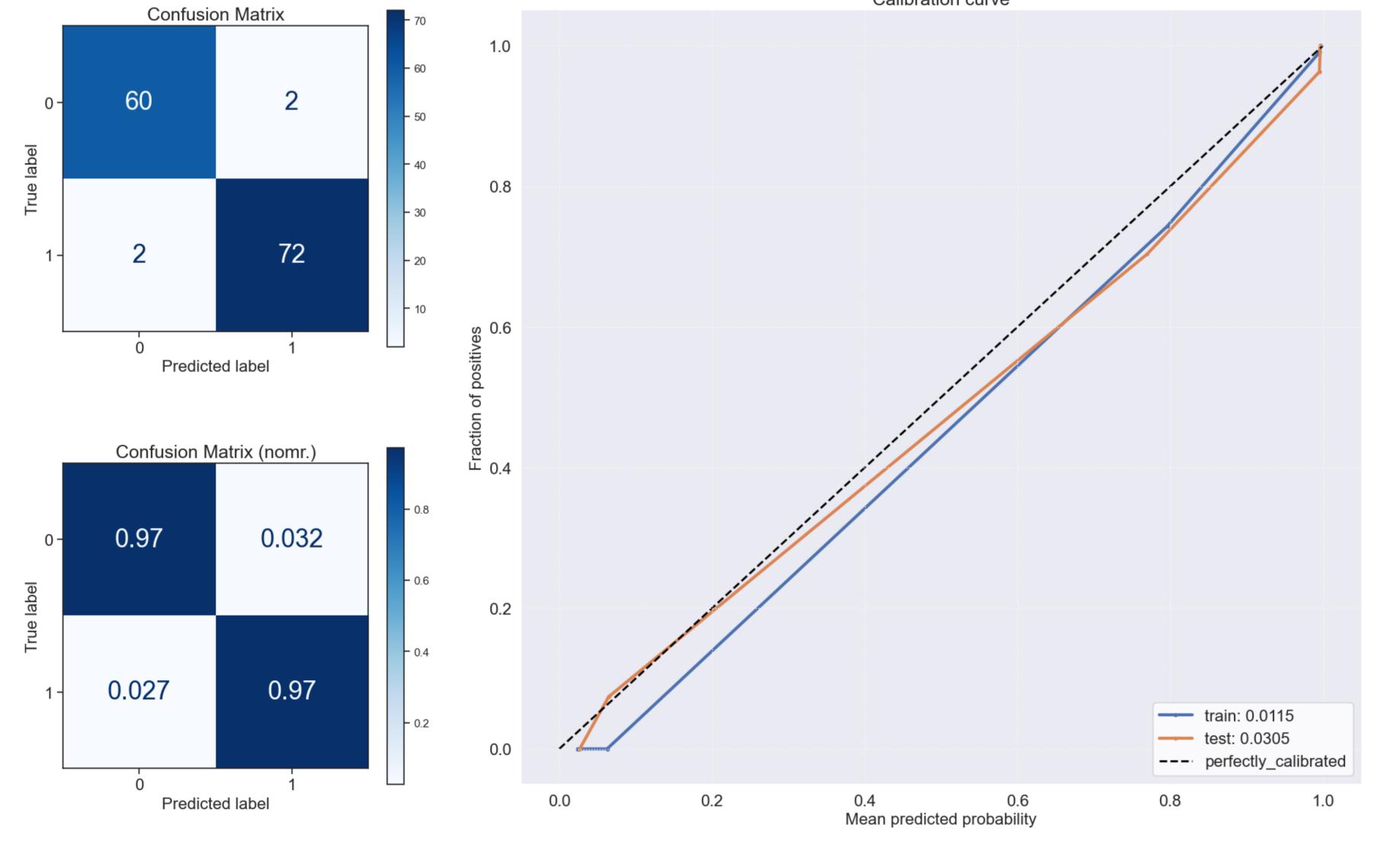
Metric	Train	Test
AUC	0.9977	0.9854
accuracy	0.9908	0.9706
balanced accuracy	0.9898	0.9704
recall_(sens)	1.0	0.973
specificity	0.9797	0.9677
precision	0.9834	0.973
f1_score	0.9908	0.9706

Protein: P01375 - metric: precision





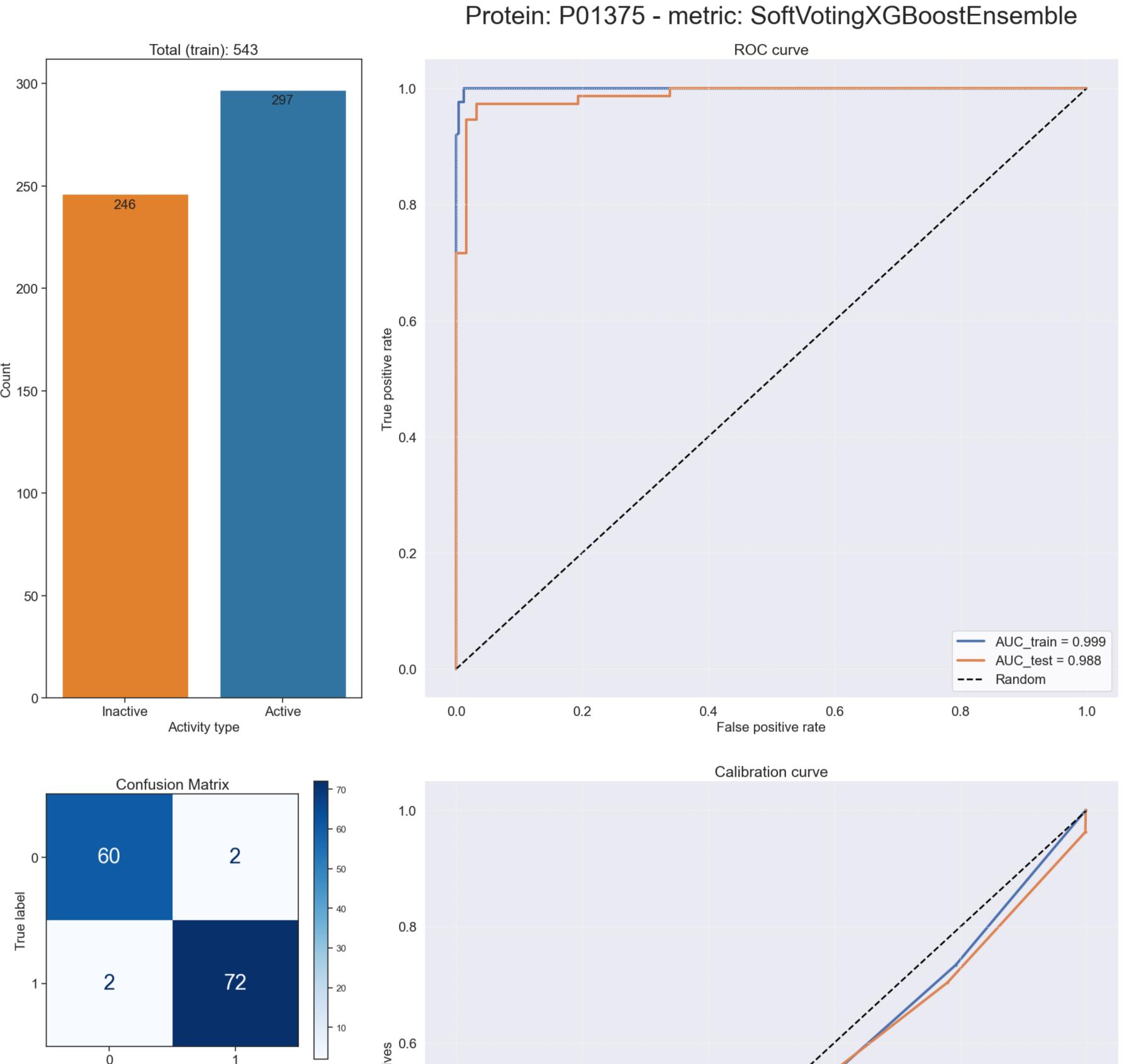
XGBoost Parameters	Value
alpha	0.8855
colsample_bytree	0.6752
gamma	0.8055
lambda	3.2973
learning_rate	0.0058
max_depth	8.0
min_child_weight	1.0
n_estimators	808.0
reg_alpha	0.8409
reg_lambda	0.1488
scale_pos_weight	6.8578
subsample	0.9205

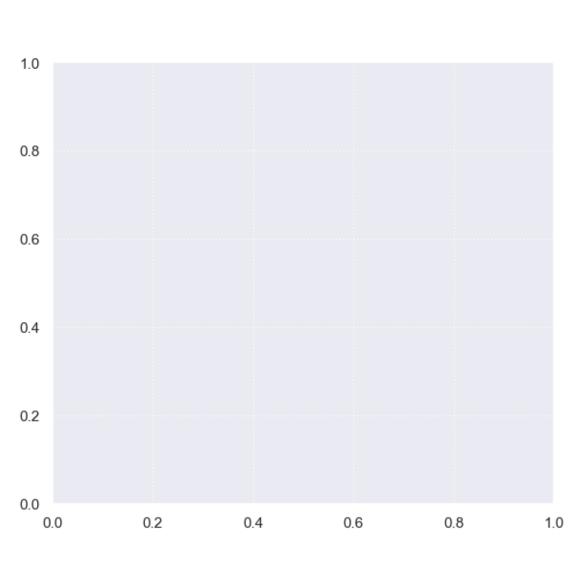


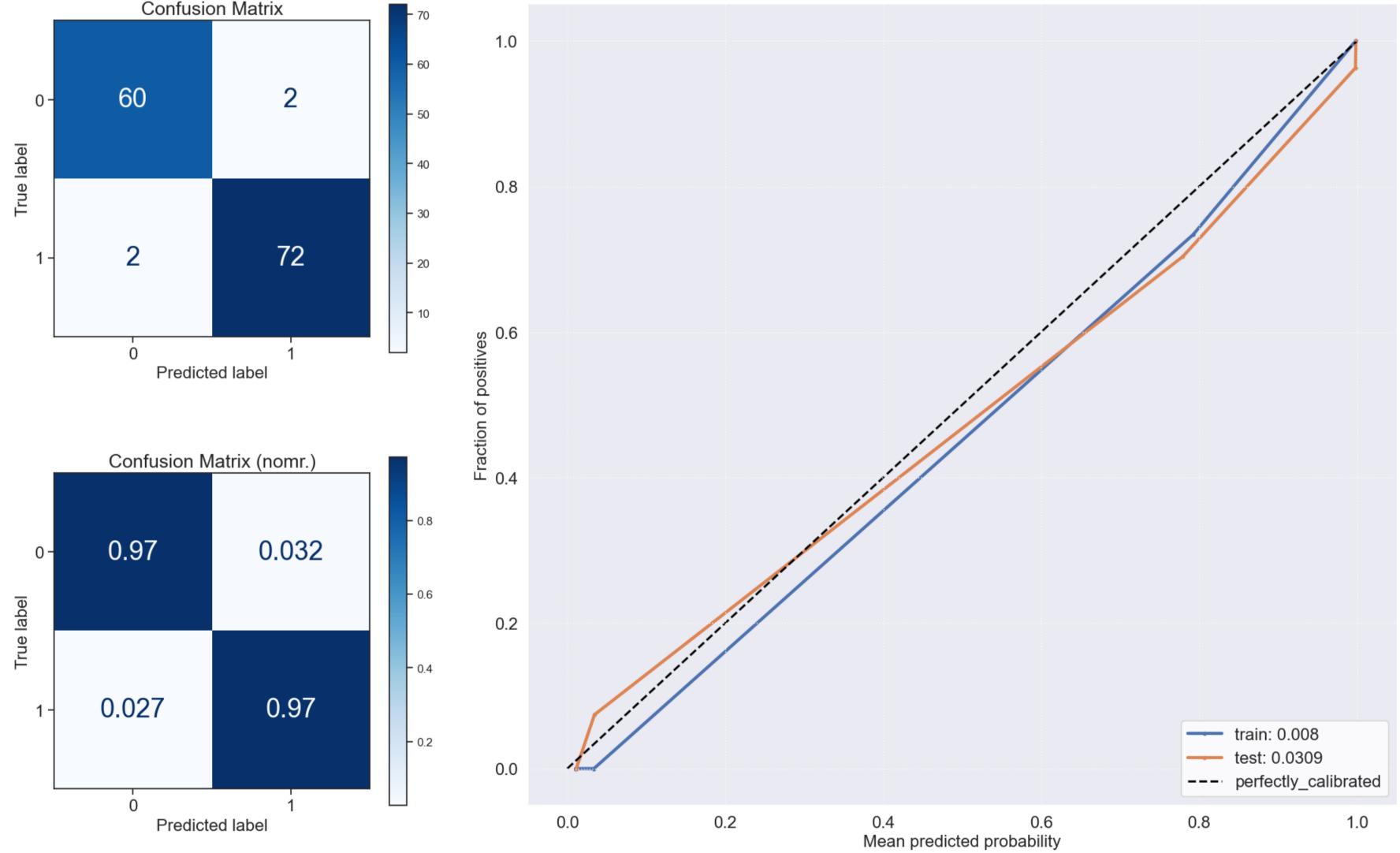
80	Ins	ctive zone		:	Active zone	type active (74)
70	IIIc					inactive (62)
. •						4000) (100)
60						
Percent 05						
30						
20					<u></u>	
10						
0	0.0 0	.2 0	.4	0.6	0.8	1.0
	Probability					

Active/Inactive probability

Metric	Train	Test
AUC	0.9975	0.9884
accuracy	0.9908	0.9706
balanced accuracy	0.9898	0.9704
recall_(sens)	1.0	0.973
specificity	0.9797	0.9677
precision	0.9834	0.973
f1_score	0.9908	0.9706







	Active/Inactive probability					
80		ctive zone			Active zone	type active (74) inactive (62)
60						decoy (136)
Percent 6 6						
	_					
20						
0 —	0.0 0.	.2 0.	.4 Probability	0.6	0.8	1.0

Metric	Train	Test
AUC	0.9995	0.9882
accuracy	0.9926	0.9706
balanced accuracy	0.9919	0.9704
recall_(sens)	1.0	0.973
specificity	0.9837	0.9677
precision	0.9867	0.973
f1_score	0.9926	0.9706