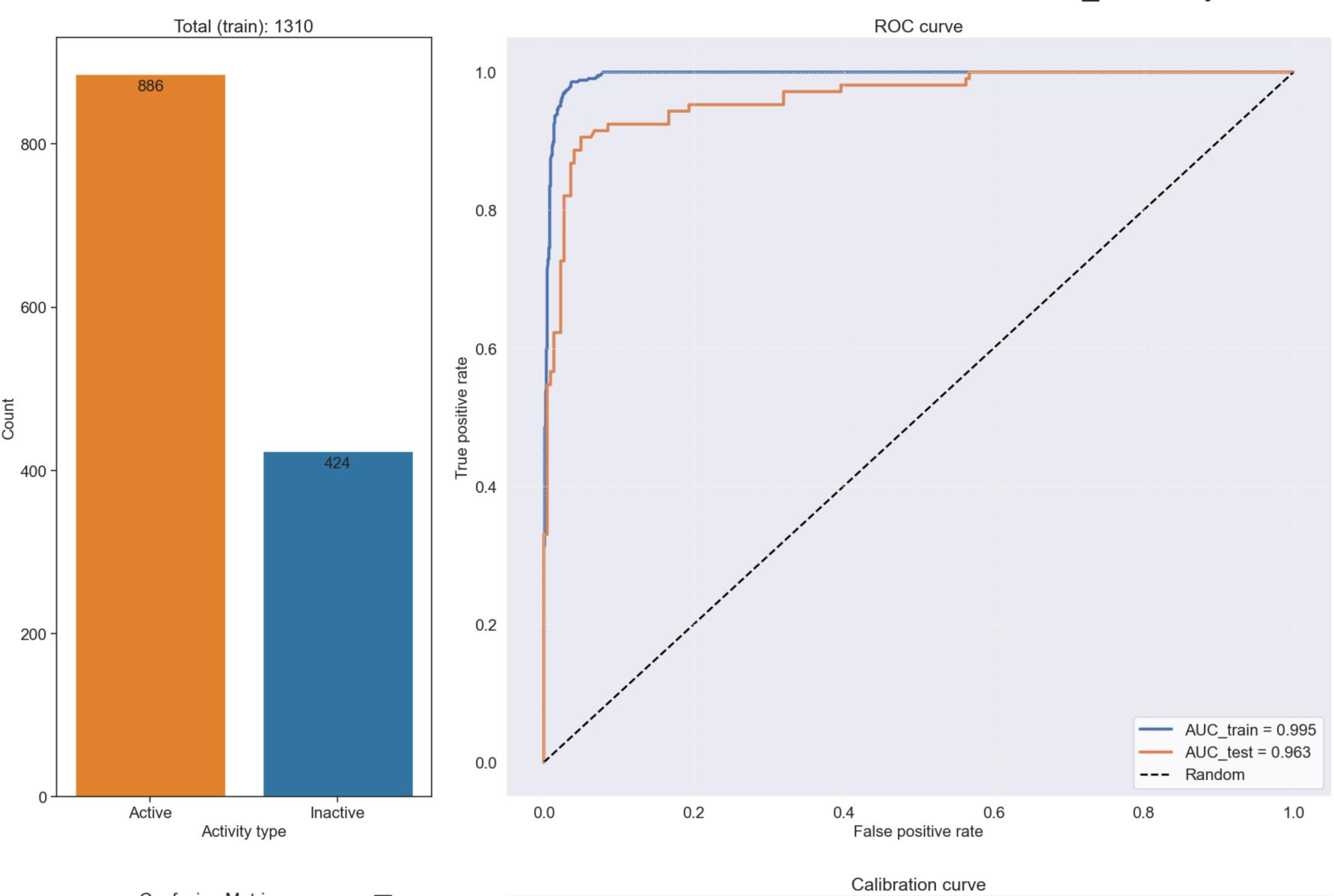
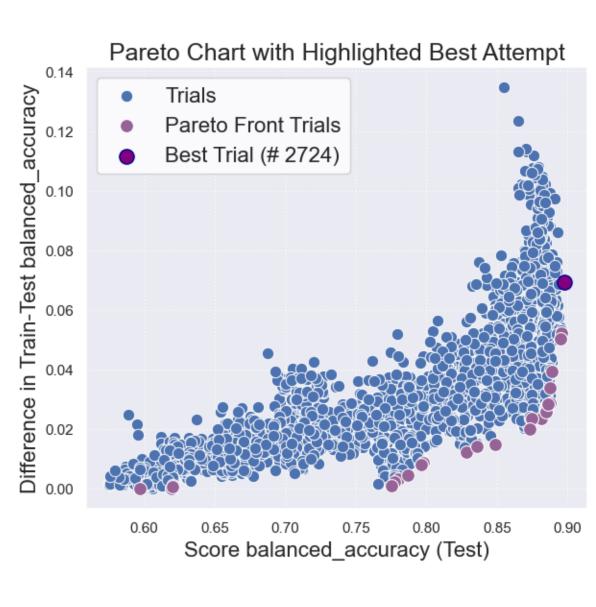
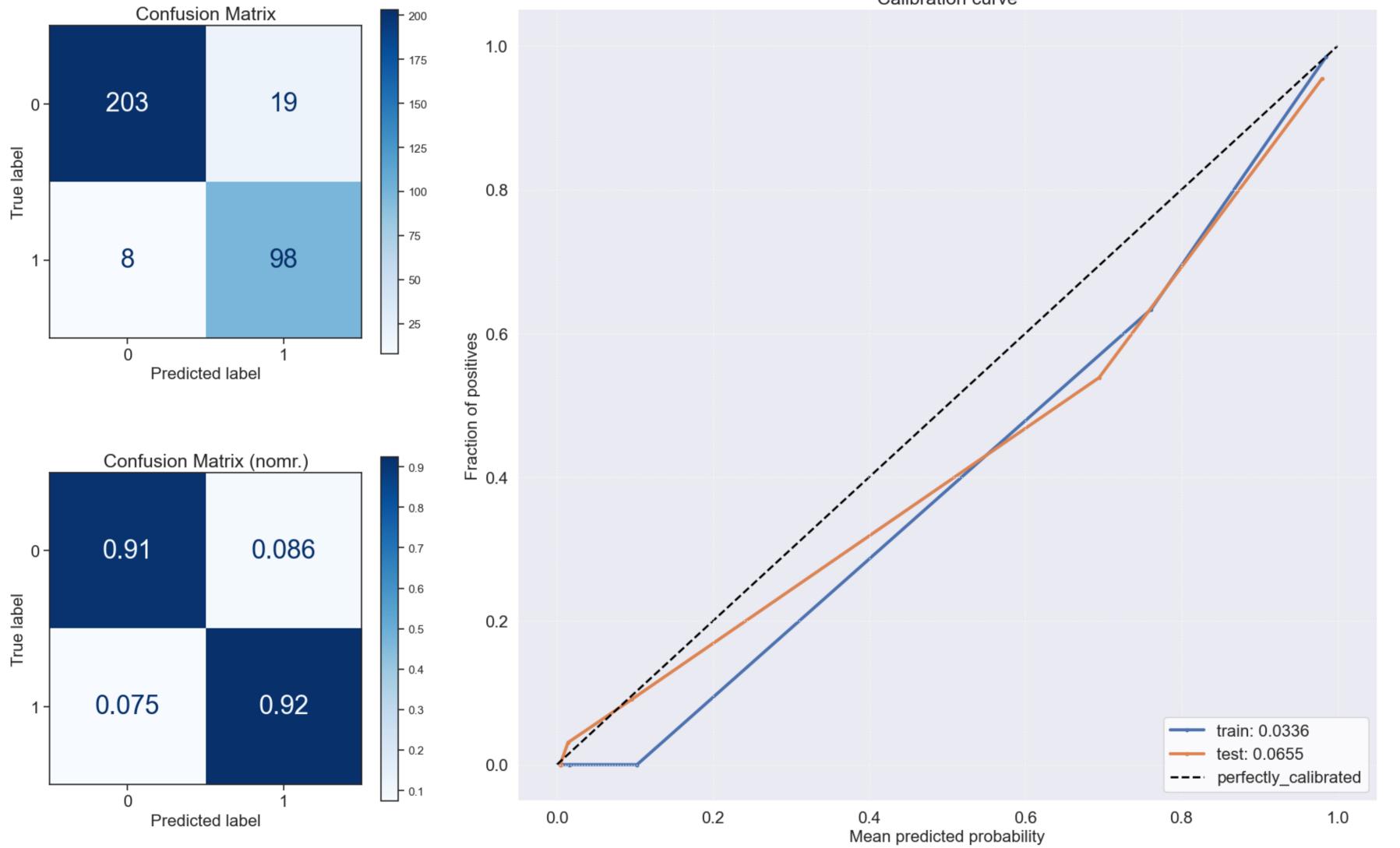
## Protein: Q92542 - metric: balanced\_accuracy





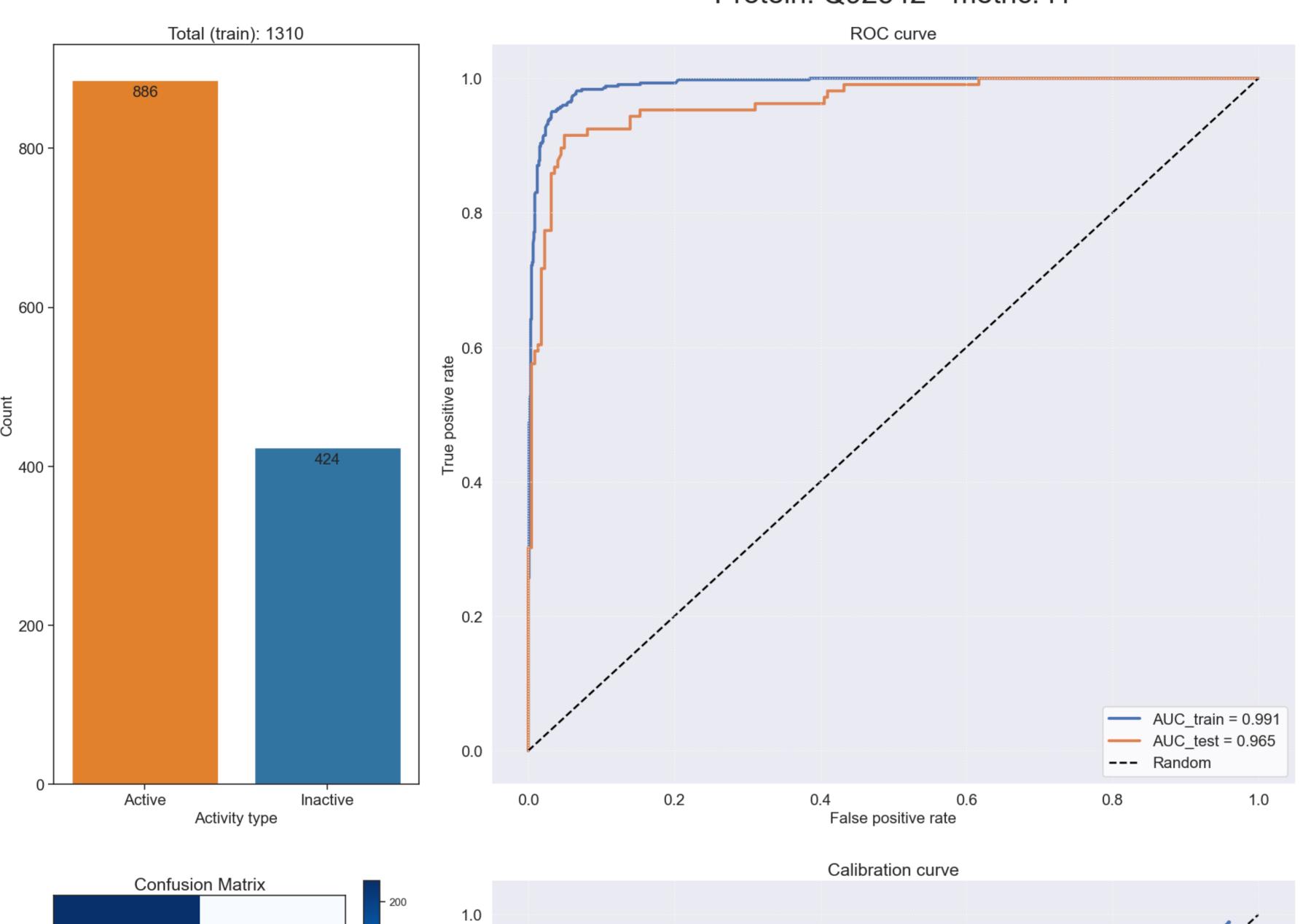
XGBoost Parameters	Value
alpha	4.8201
colsample_bytree	0.6671
gamma	0.5052
lambda	3.7264
learning_rate	0.0149
max_depth	8.0
min_child_weight	4.0
n_estimators	908.0
reg_alpha	0.3932
reg_lambda	0.0035
scale_pos_weight	4.0441
subsample	0.7835

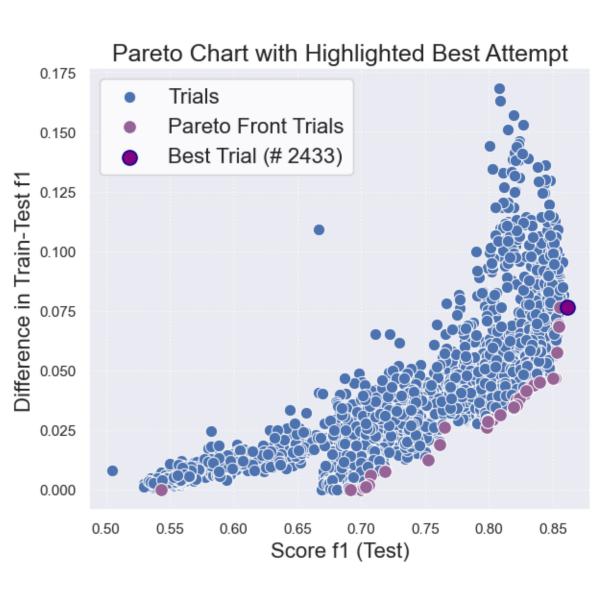


			Active/Inactive	e probabilit	ty		
35	I	nactive zone			Active :		type active (106) inactive (222) decoy (328)
30							
Percent - 05							П
15							
10							
5							
0-	0.0	0.2	0.4 Proba	0.6 ability	0	0.8	1.0

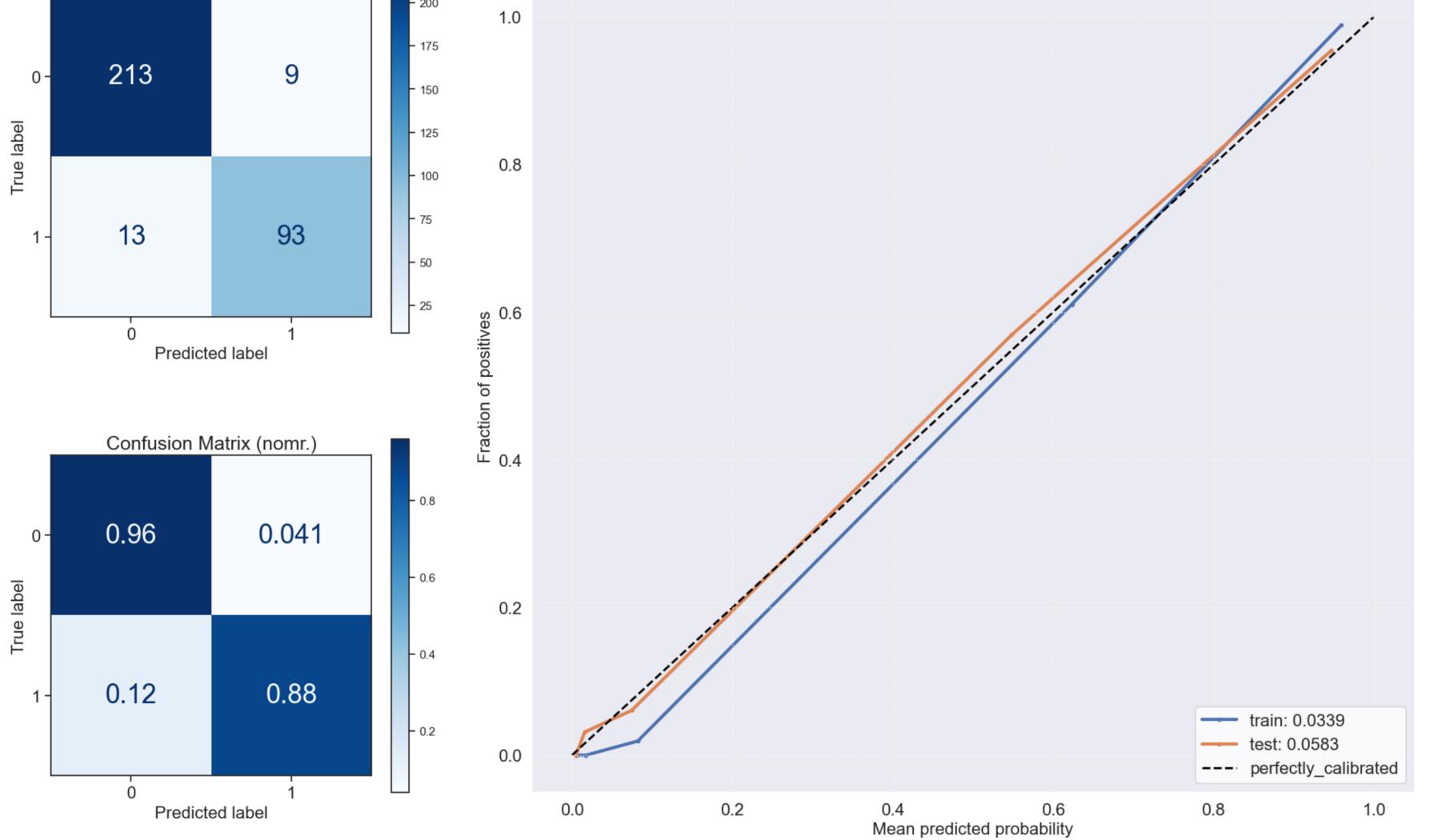
Metric	Train	Test
AUC	0.9947	0.963
accuracy	0.955	0.9177
balanced accuracy	0.9642	0.9195
recall_(sens)	0.9906	0.9245
specificity	0.9379	0.9144
precision	0.8842	0.8376
f1_score	0.9556	0.9187

## Protein: Q92542 - metric: f1





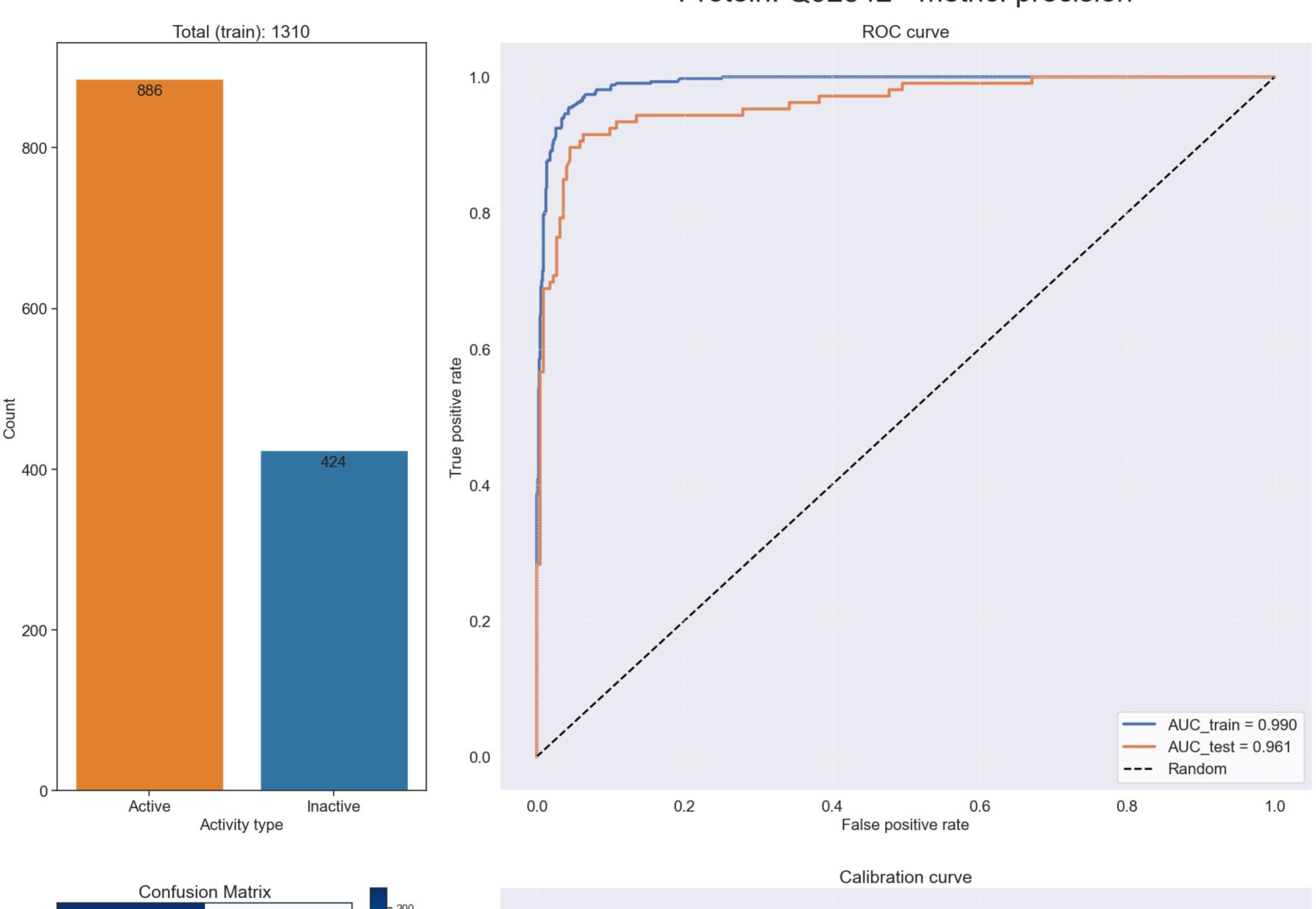
XGBoost Parameters	Value
alpha	1.327
colsample_bytree	0.5251
gamma	0.6341
lambda	1.0749
learning_rate	0.0326
max_depth	7.0
min_child_weight	2.0
n_estimators	448.0
reg_alpha	0.5642
reg_lambda	0.5788
scale_pos_weight	1.3519
subsample	0.5896

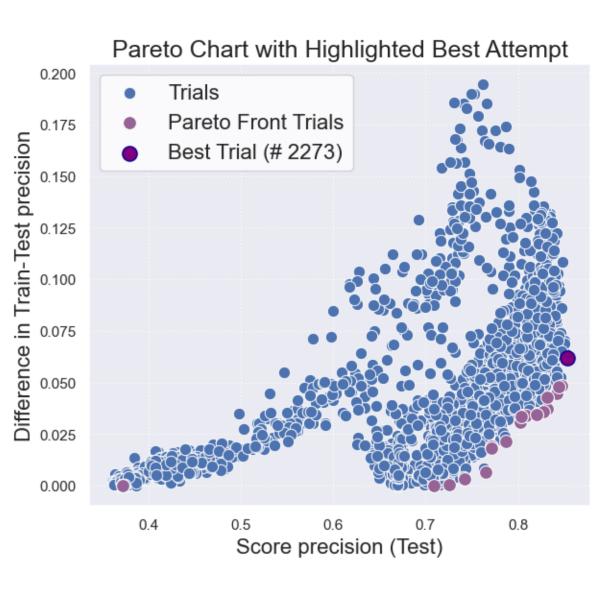


			Active/Inactive	probability		
35					Active zone	inactive (222) decoy (328)
25						
15						
5 0						
	0.0	0.2	0.4 Probabi	0.6 lity	0.8	1.0

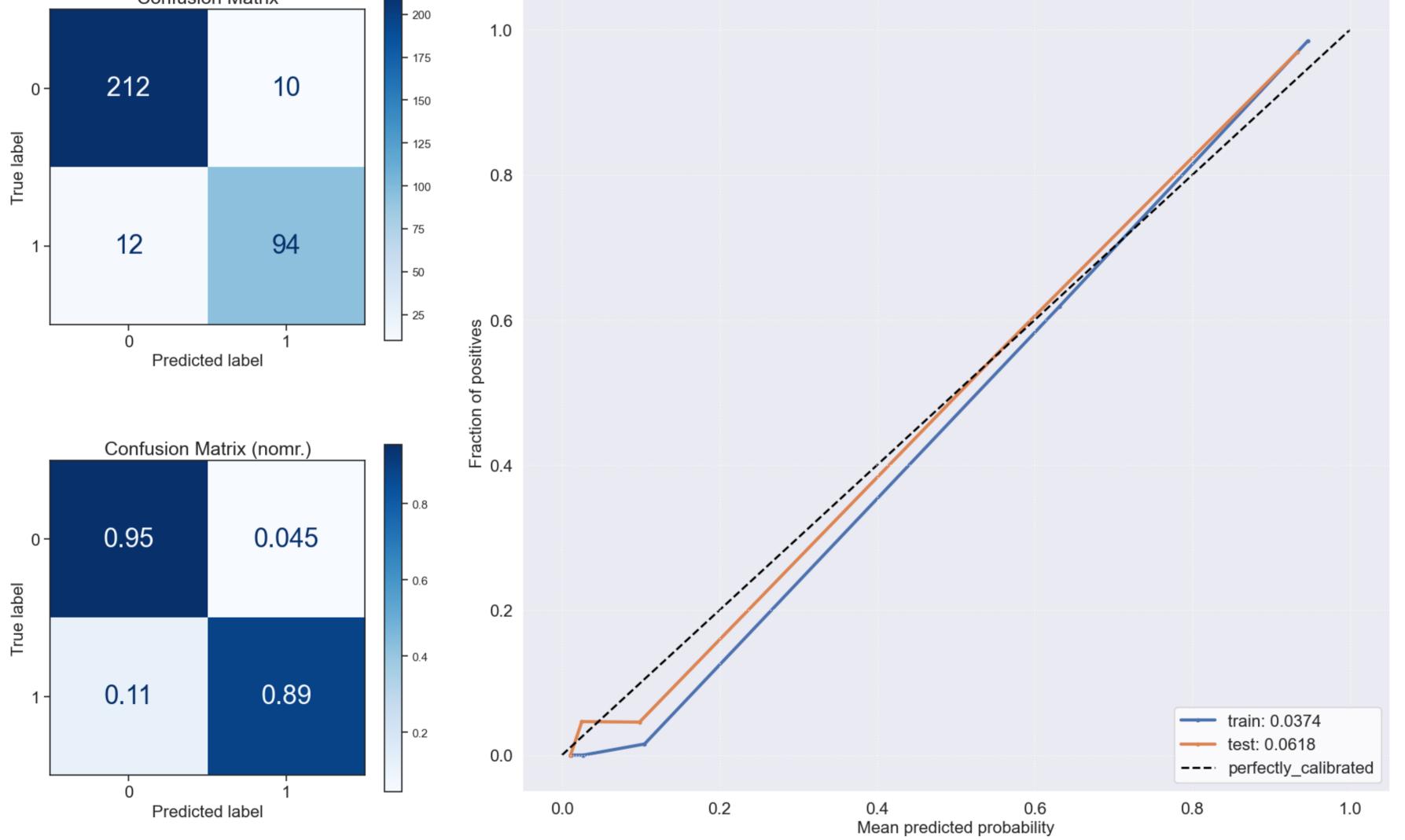
Metric	Train	Test
AUC	0.9909	0.9646
accuracy	0.9588	0.9329
balanced accuracy	0.9566	0.9184
recall_(sens)	0.9505	0.8774
specificity	0.9628	0.9595
precision	0.9243	0.9118
f1_score	0.9589	0.9326

## Protein: Q92542 - metric: precision





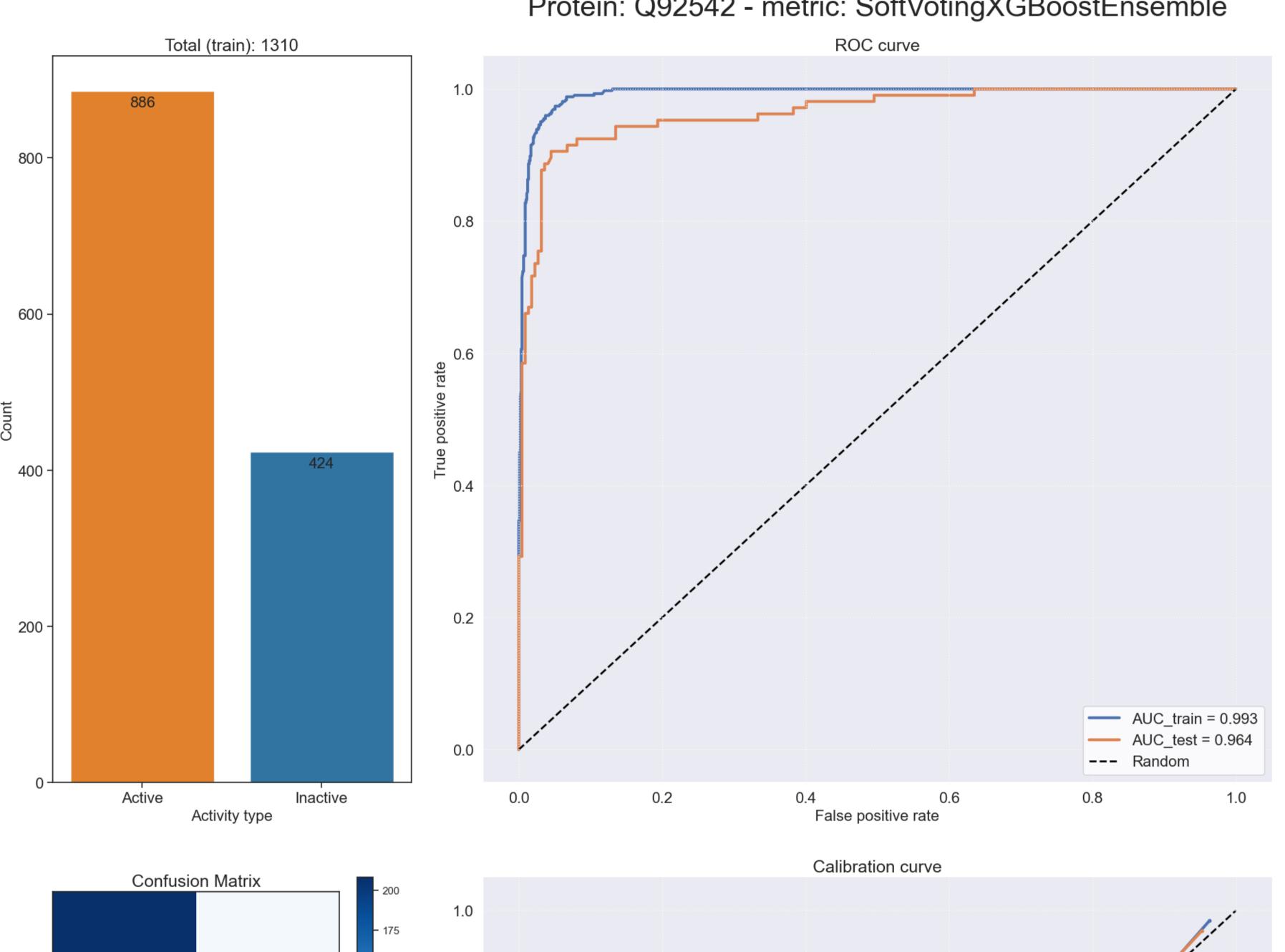
XGBoost Parameters	Value
alpha	3.9379
colsample_bytree	0.8561
gamma	0.9512
lambda	2.1628
learning_rate	0.0346
max_depth	9.0
min_child_weight	1.0
n_estimators	199.0
reg_alpha	0.6756
reg_lambda	0.993
scale_pos_weight	1.5361
subsample	0.5421

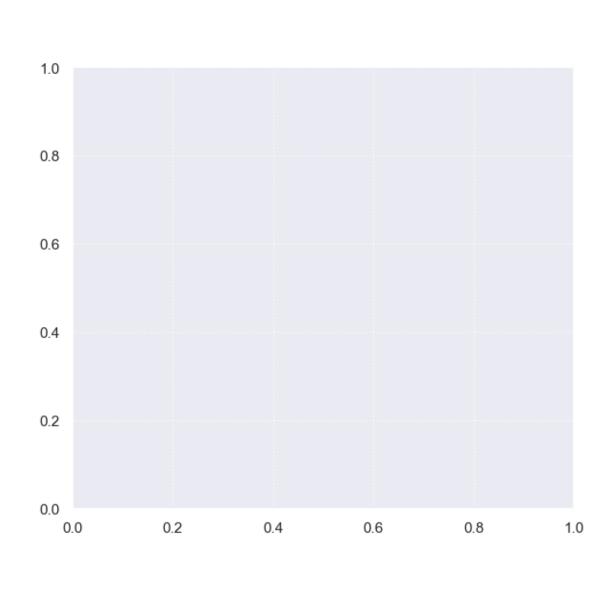


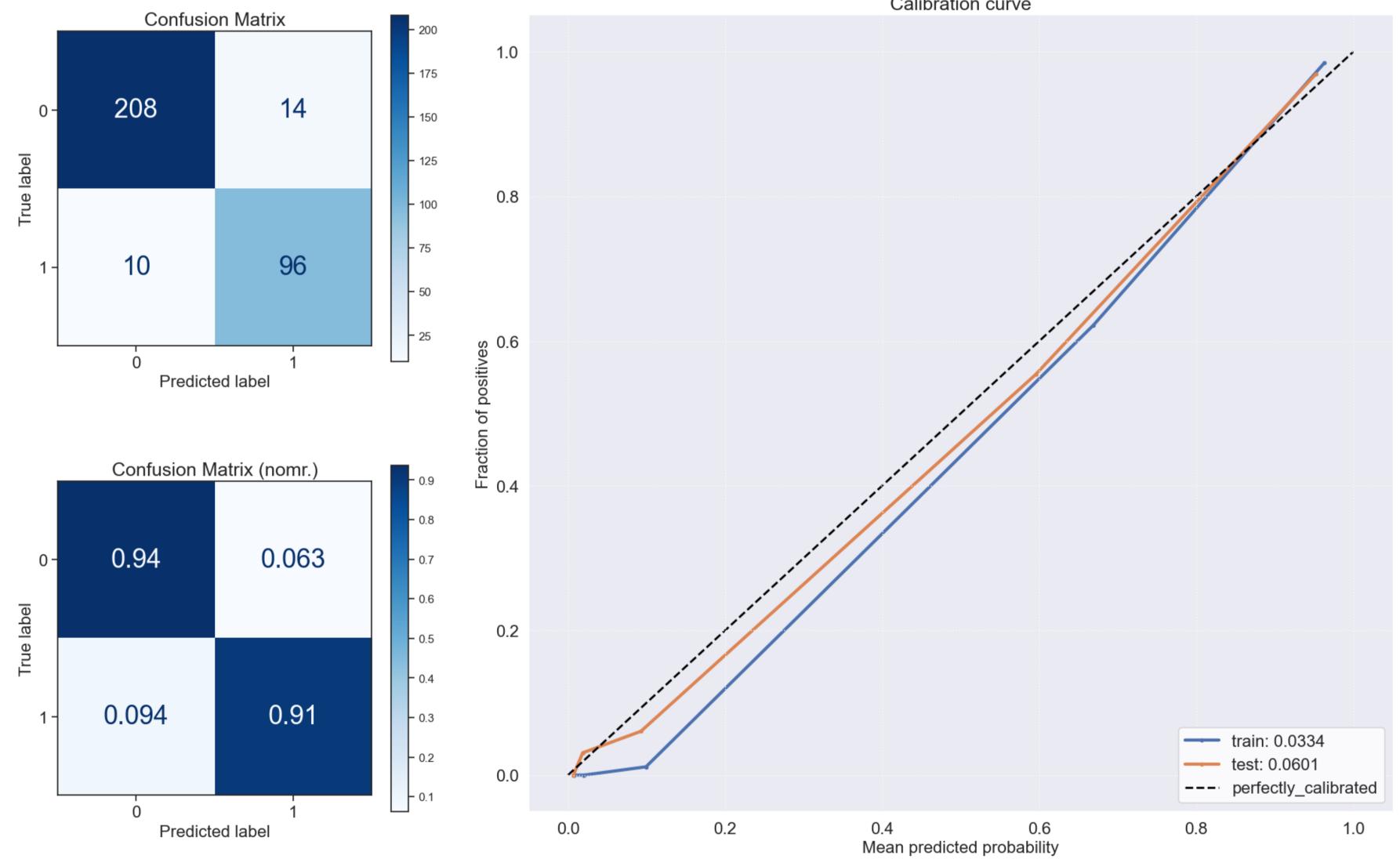
	Active/Inactive probability					
30		ctive zone			Active zone	type active (106) inactive (222)
25						decoy (328)
20						
Percent						
10 <del></del>						
0						
0	.0 0.	2 0	).4 Drahahilit	0.6	0.8	1.0
			Probabilit	У		

Metric	Train	Test
AUC	0.9904	0.9614
accuracy	0.9534	0.9329
balanced accuracy	0.9514	0.9209
recall_(sens)	0.9458	0.8868
specificity	0.9571	0.955
precision	0.9134	0.9038
f1_score	0.9536	0.9328

## Protein: Q92542 - metric: SoftVotingXGBoostEnsemble







			Active/Inactive	ve probabilit	У		
35		Inactive zone			Active z	zone	type active (106) inactive (222) decoy (328)
25							
Dercent 20							
10							
5 <del></del>							
0	0.0	0.2	0.4 Prob	0.6 ability	0.	.8	1.0

Metric	Train	Test
AUC	0.9928	0.9641
accuracy	0.9565	0.9268
balanced accuracy	0.9598	0.9213
recall_(sens)	0.9693	0.9057
specificity	0.9503	0.9369
precision	0.9033	0.8727
f1_score	0.9569	0.9272