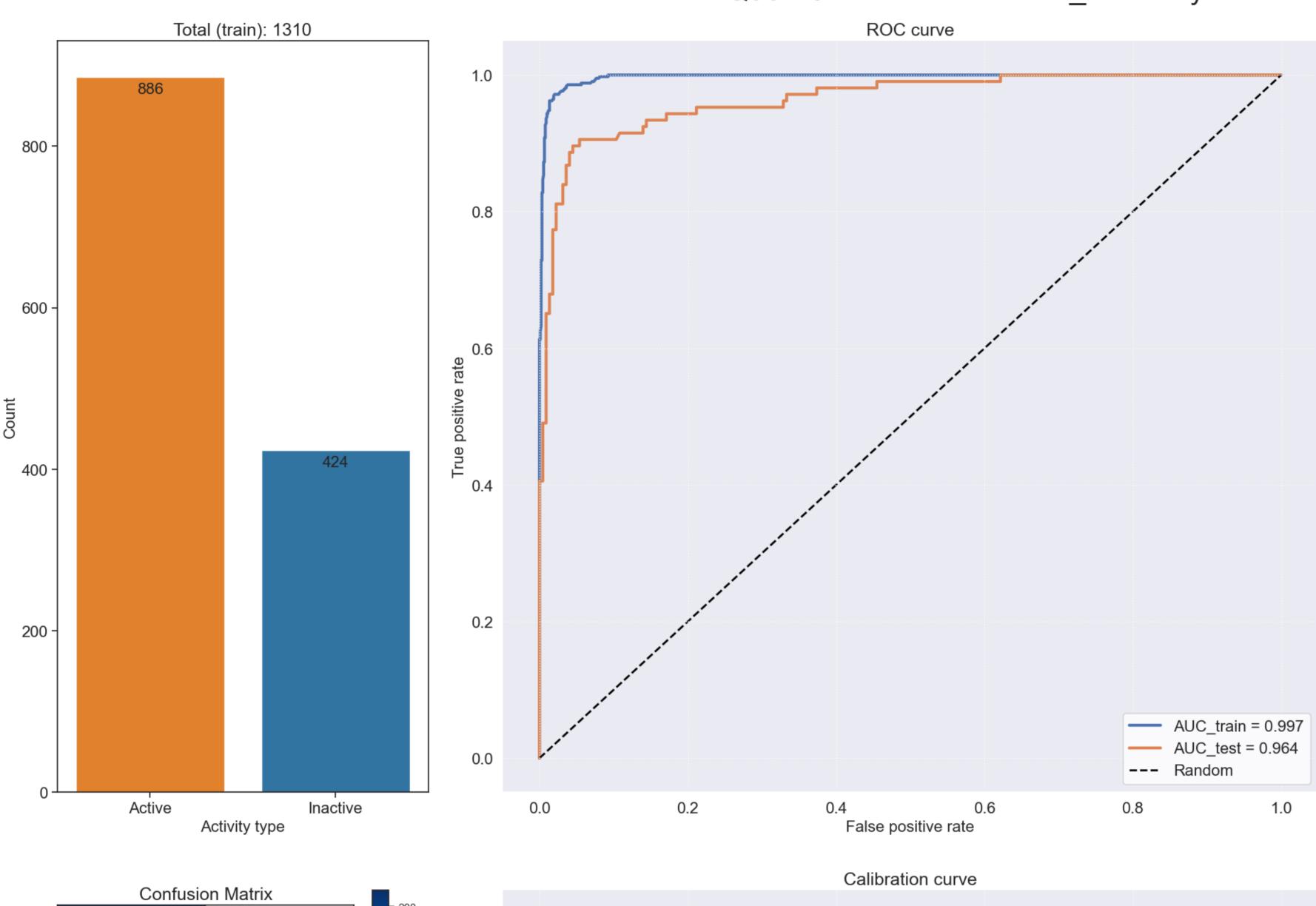
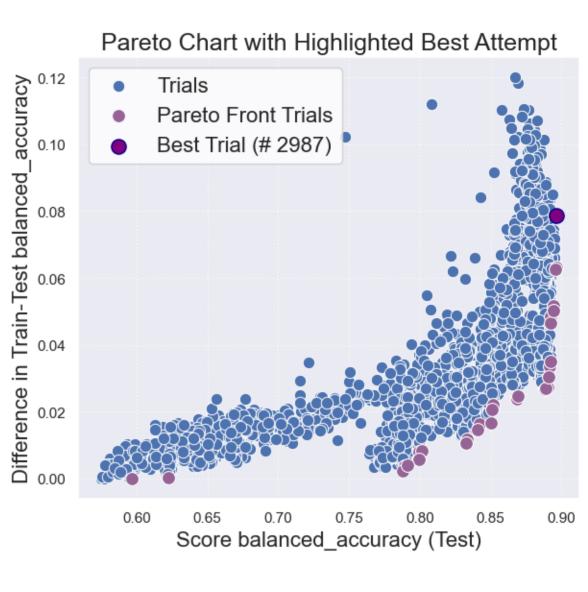
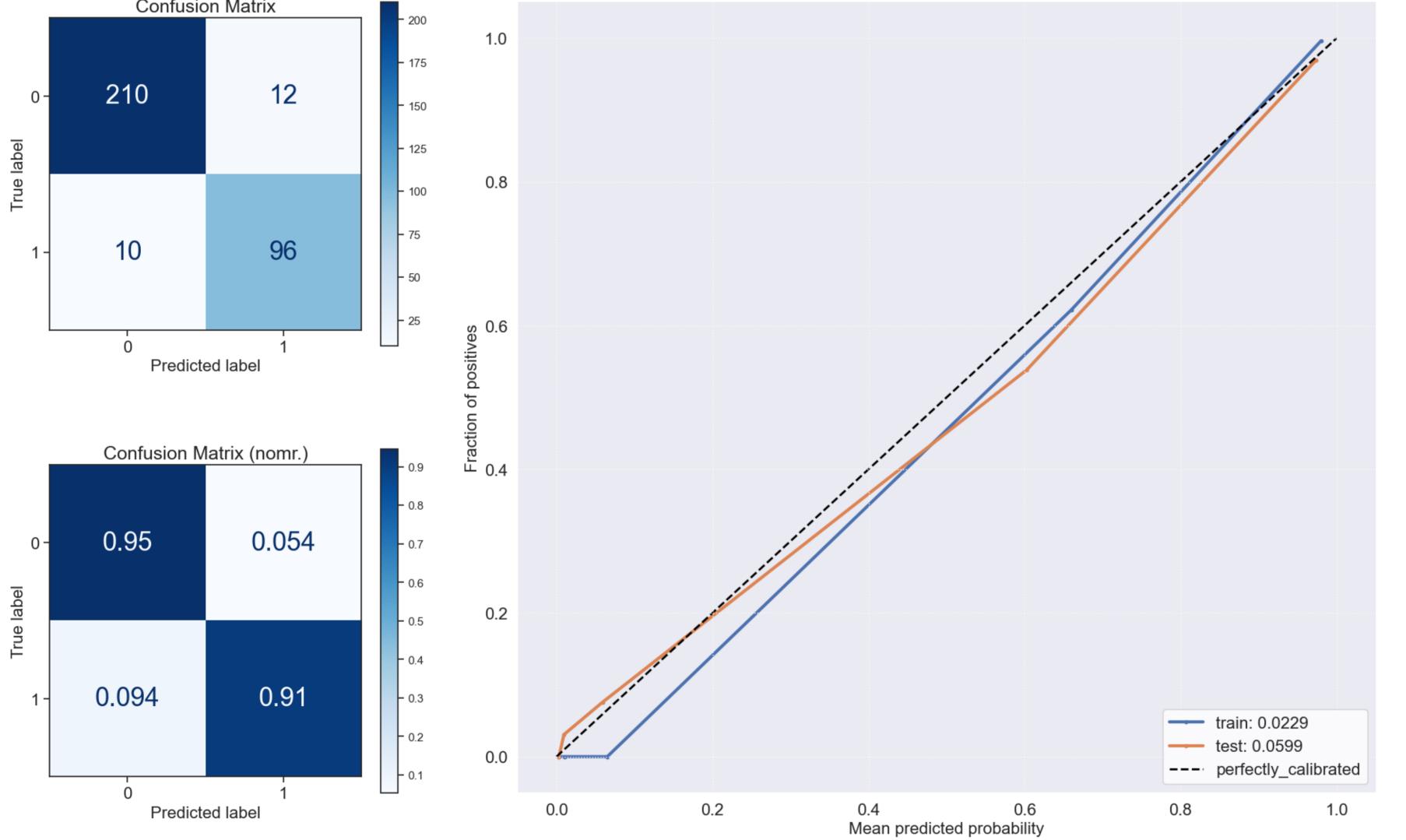
## Protein: Q96BI3 - metric: balanced\_accuracy





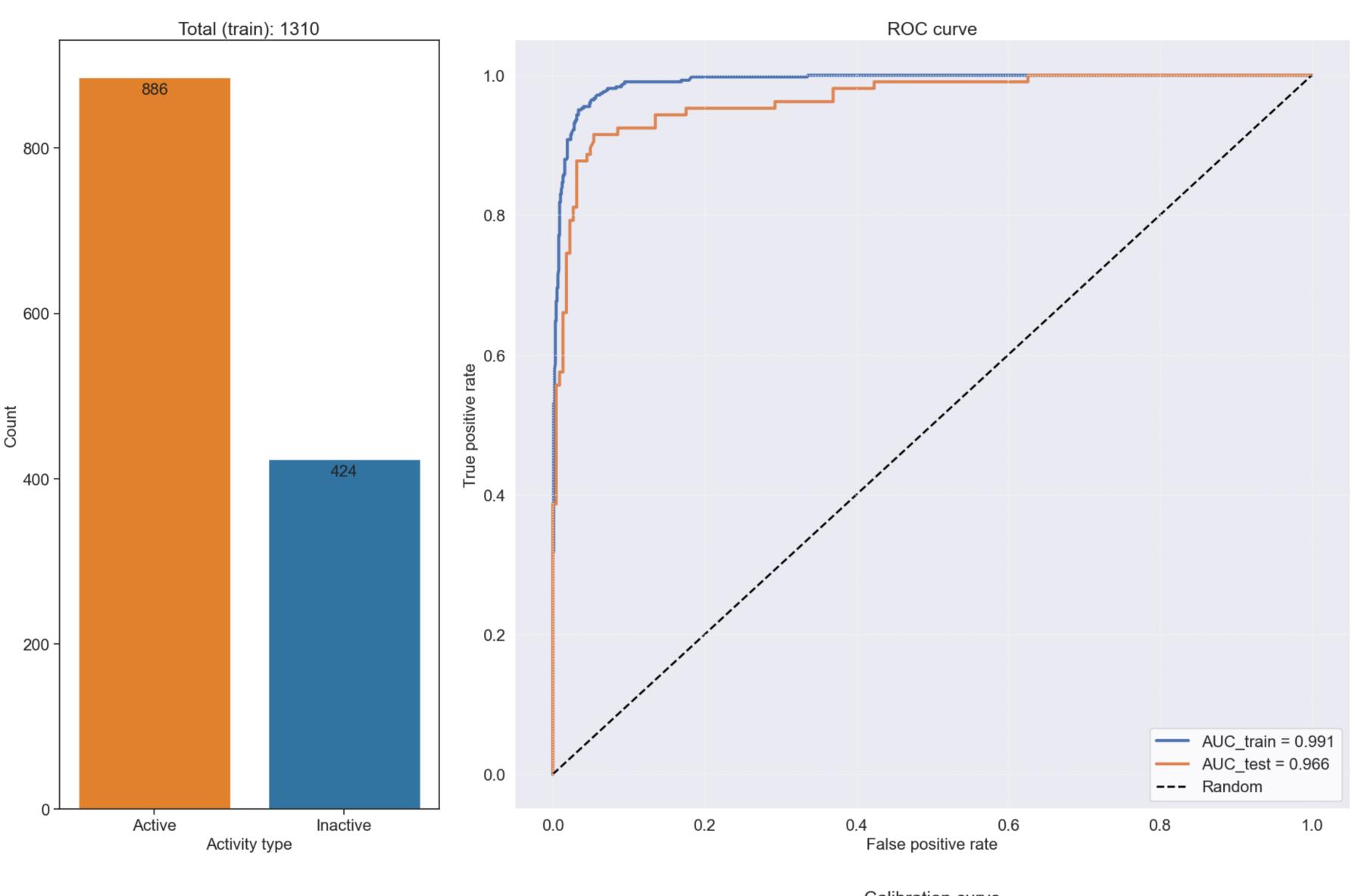
XGBoost Parameters	Value
alpha	2.171
colsample_bytree	0.6674
gamma	0.7971
lambda	1.075
learning_rate	0.1643
max_depth	8.0
min_child_weight	1.0
n_estimators	393.0
reg_alpha	0.8448
reg_lambda	0.2158
scale_pos_weight	1.7997
subsample	0.7801

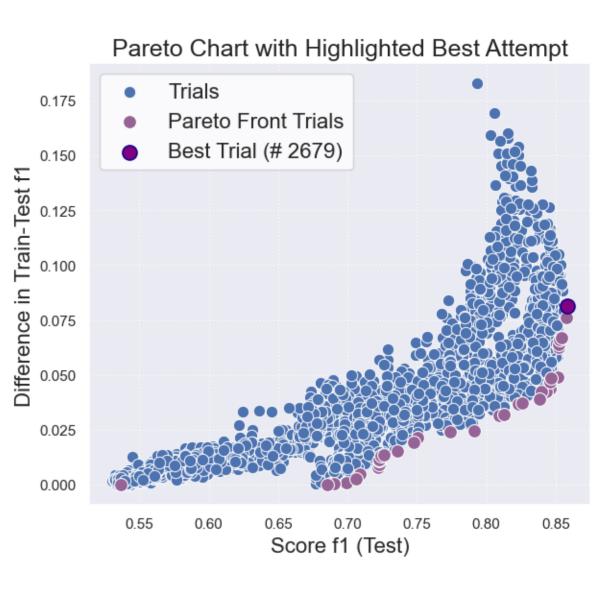


			Active/Inacti	ve probability		
50 -·····		Inactive zone			Active zone	type active (106) inactive (222) decoy (328)
± 30						
Percent						
10						
0 —	0.0	0.2	0.4 Prob	0.6 ability	0.8	1.0

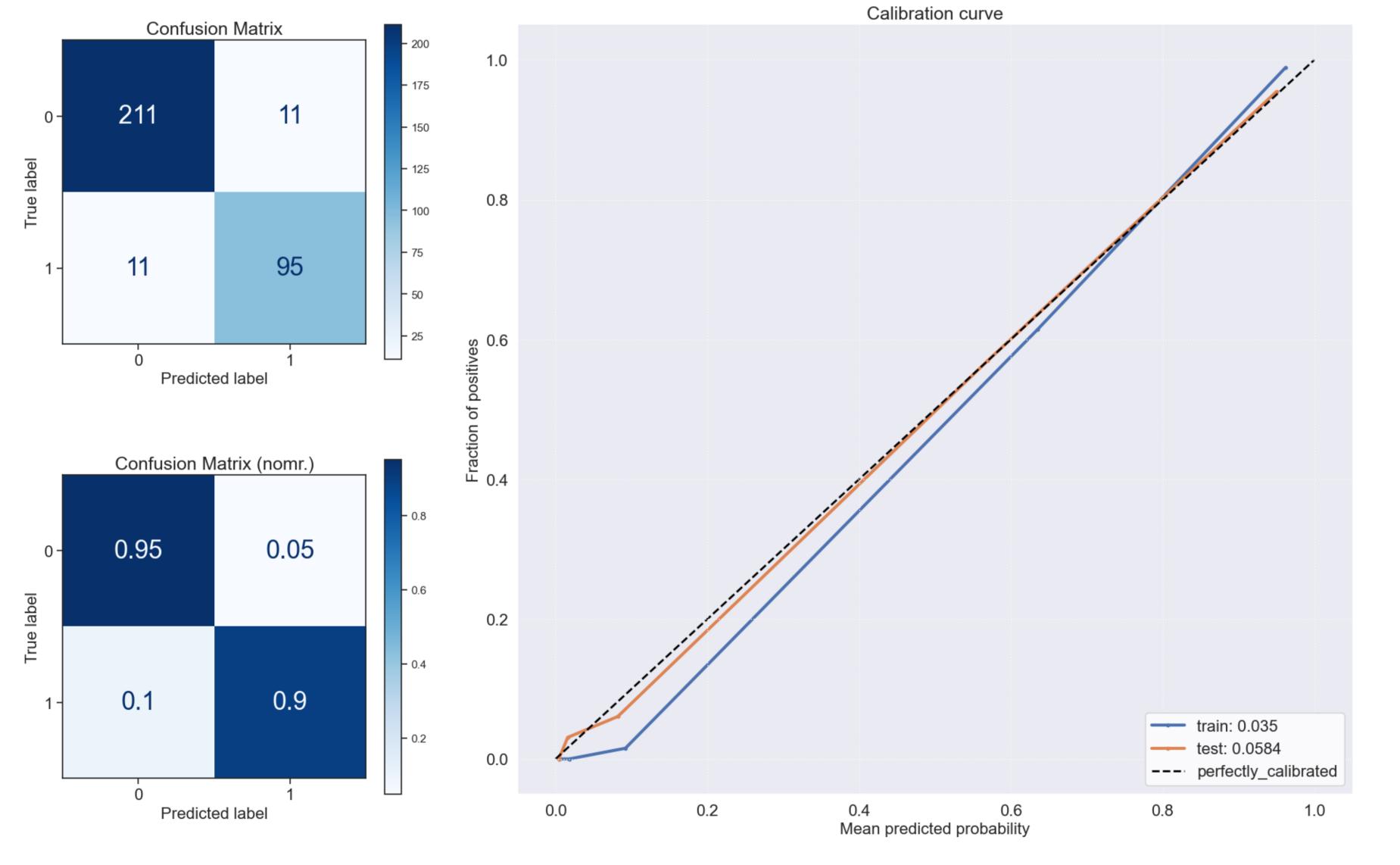
Metric	Train	Test
AUC	0.9967	0.9644
accuracy	0.9702	0.9329
balanced accuracy	0.9731	0.9258
recall_(sens)	0.9811	0.9057
specificity	0.965	0.9459
precision	0.9306	0.8889
f1_score	0.9704	0.9331

## Protein: Q96BI3 - metric: f1





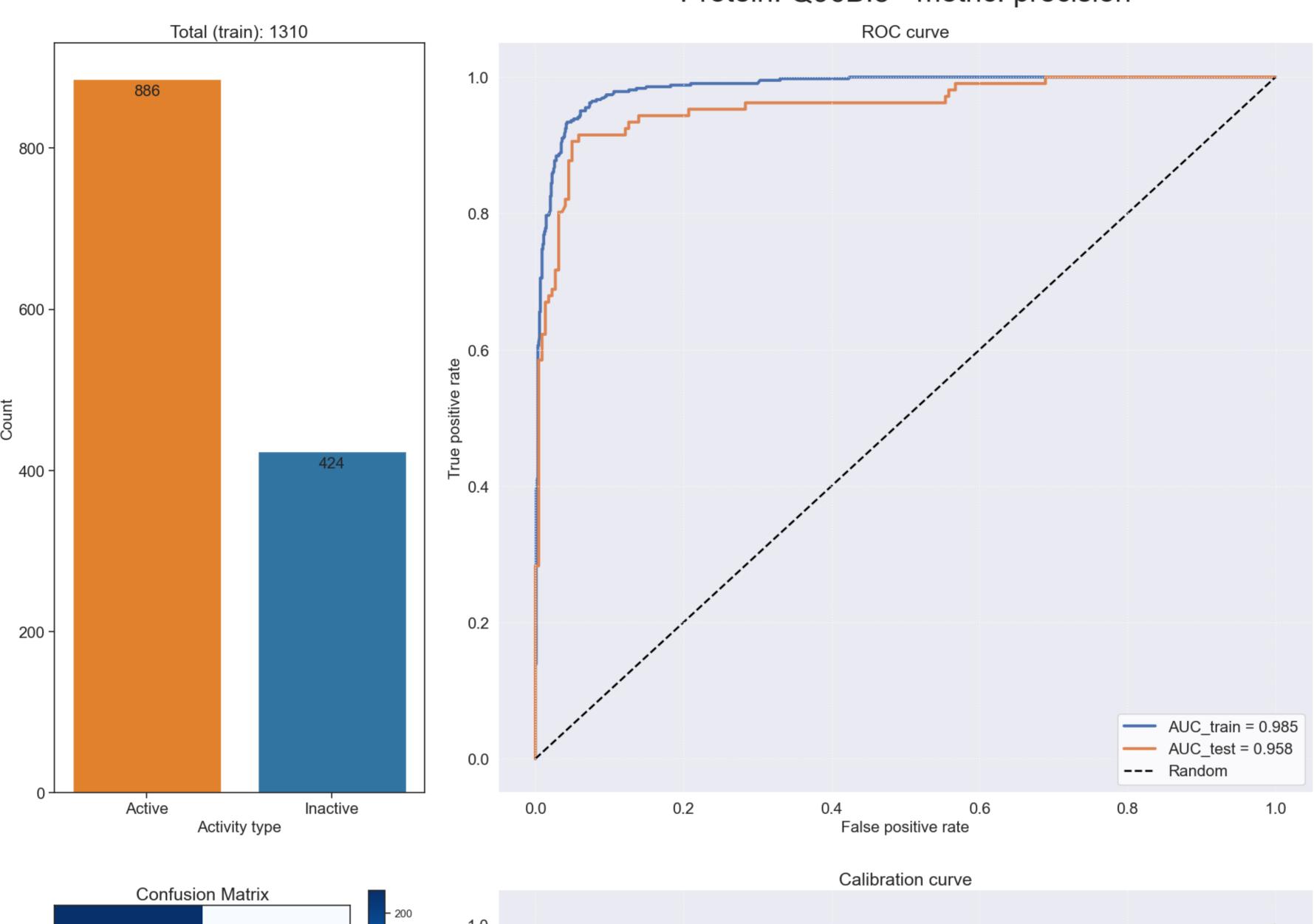
XGBoost Parameters	Value
alpha	3.3087
colsample_bytree	0.6138
gamma	0.1929
lambda	2.3324
learning_rate	0.0266
max_depth	4.0
min_child_weight	2.0
n_estimators	956.0
reg_alpha	0.7398
reg_lambda	0.939
scale_pos_weight	1.5073
subsample	0.5977

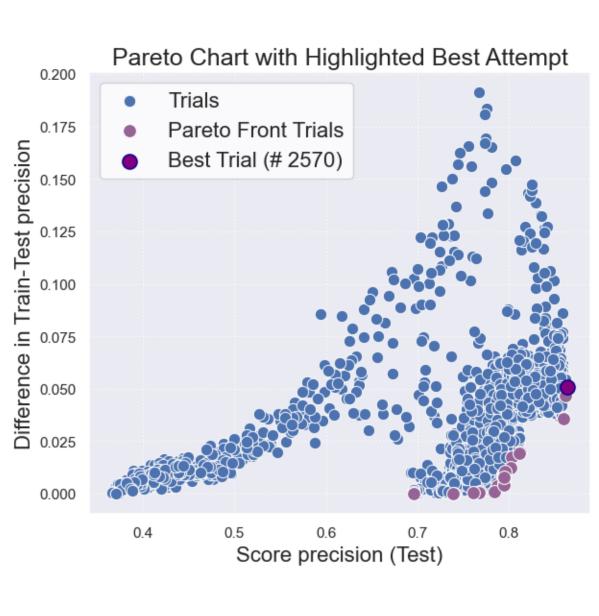


		Α	ctive/Inactive	probability		
35	lr	nactive zone			Active zone	type active (106) inactive (222)
30						decoy (328)
25						
- 20						
10						
5				_		
0 —	0.0	0.2	0.4	0.6	0.8	1.0
			Probab	ility		

Metric	Train	Test
AUC	0.991	0.9662
accuracy	0.958	0.9329
balanced accuracy	0.9567	0.9233
recall_(sens)	0.9528	0.8962
specificity	0.9605	0.9505
precision	0.9203	0.8962
f1_score	0.9582	0.9329

## Protein: Q96BI3 - metric: precision





XGBoost Parameters	Value
alpha	3.7239
colsample_bytree	0.9359
gamma	0.6023
lambda	3.6493
learning_rate	0.0075
max_depth	9.0
min_child_weight	3.0
n_estimators	790.0
reg_alpha	0.418
reg_lambda	0.8922
scale_pos_weight	1.1008
subsample	0.6974

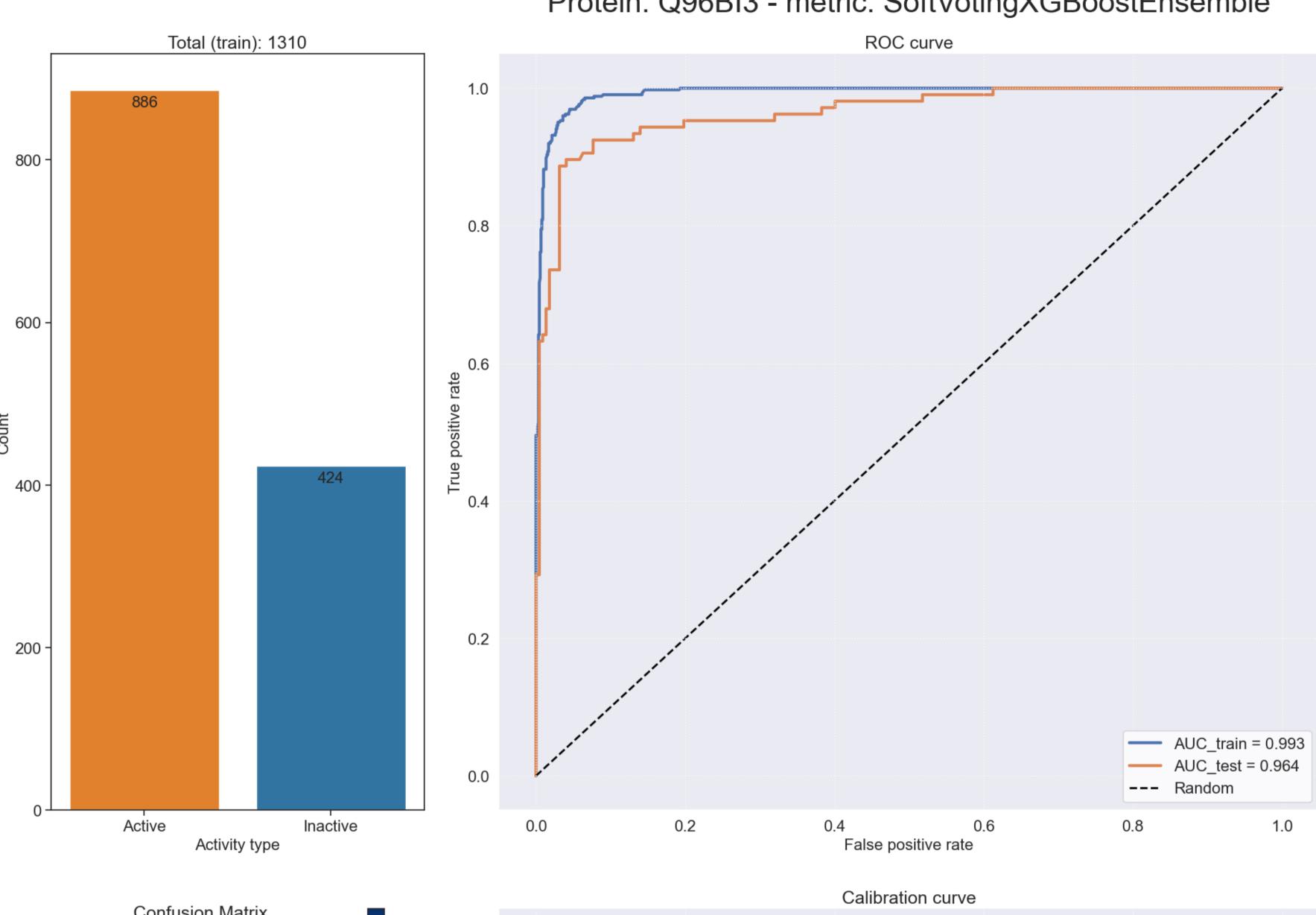
label O	214	8	- 175 - 150 - 125	1.0				A service of the serv
True label	21	85	- 100 - 75 - 50 - 25	0.8 0.8				
•	0 Predicte Confusion M			Fraction of positives 0.0				
True label		0.036	- 0.8 - 0.6	0.4				
True	0.2	0.8	- 0.4 - 0.2	0.0				train: 0.0446 test: 0.065 perfectly_calibrated
	0 Predicte	1 ed label			0.0	2 0.4	0.6	0.8 1.0

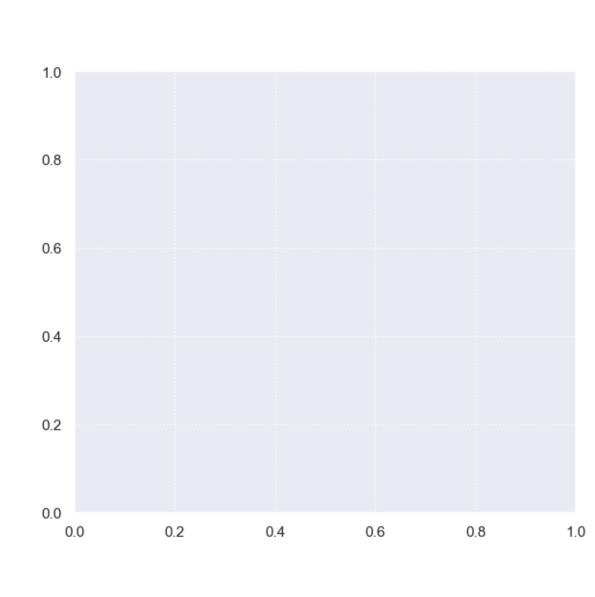
Mean predicted probability

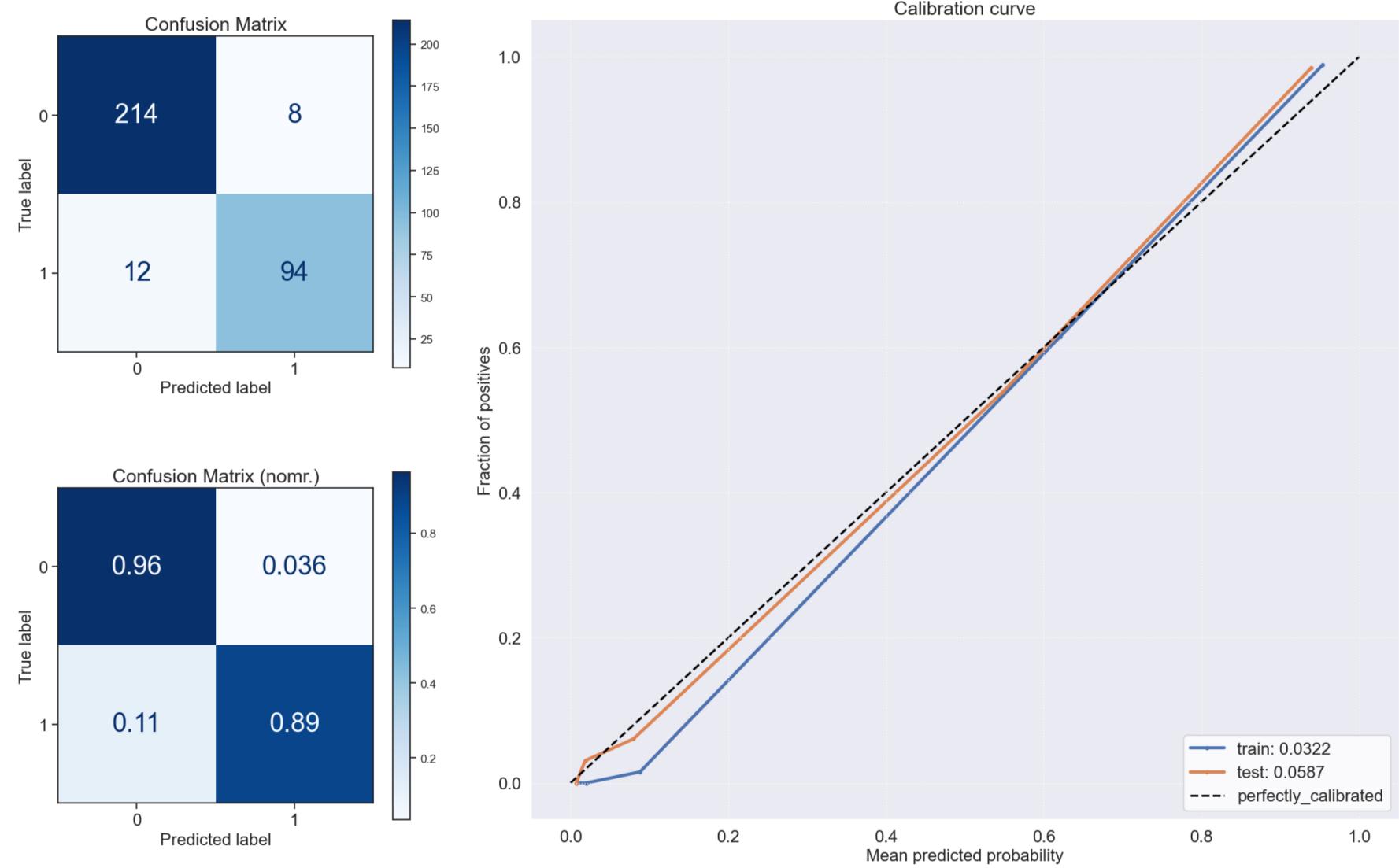
			Ac	tive/Inactiv	e probabi	lity		
20		Ina	ctive zone			Active :	zone	type active (106) inactive (222) decoy (328)
Percent 5	_							
10								
0	0.0		.2 0	4	-	6 0	.8	1.0
				Proba				

Metric	Train	Test
AUC	0.9852	0.958
accuracy	0.9473	0.9116
balanced accuracy	0.9408	0.8829
recall_(sens)	0.9222	0.8019
specificity	0.9594	0.964
precision	0.9157	0.914
f1_score	0.9474	0.91

## Protein: Q96BI3 - metric: SoftVotingXGBoostEnsemble







			Active/Inact	ve probability		
35		Inactive zor			Active zone	active (106) inactive (222)
25						
Percent 05						
10						ПС
5					n <u>_</u>	
0 —	0.0	0.2	0.4 Prok	0.6 pability	0.8	1.0

Metric	Train	Test
AUC	0.993	0.9642
accuracy	0.9603	0.939
balanced accuracy	0.9584	0.9254
recall_(sens)	0.9528	0.8868
specificity	0.9639	0.964
precision	0.9266	0.9216
f1_score	0.9604	0.9387