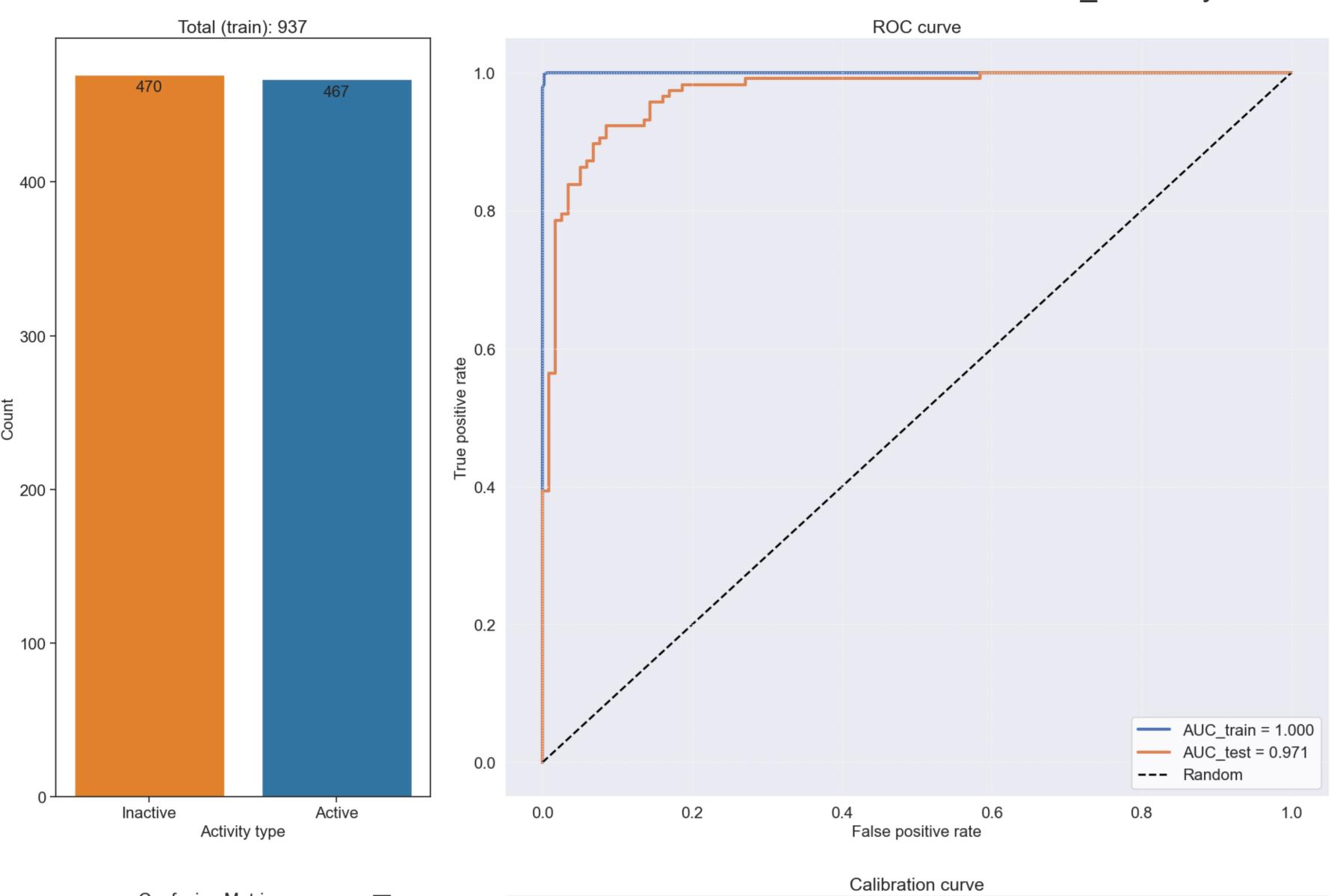
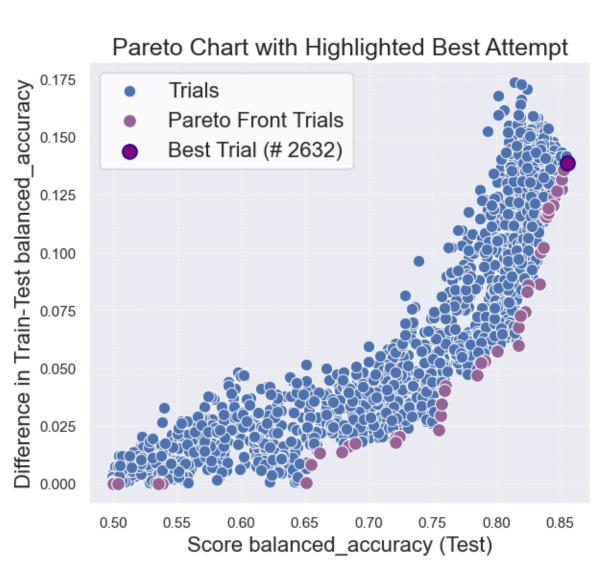
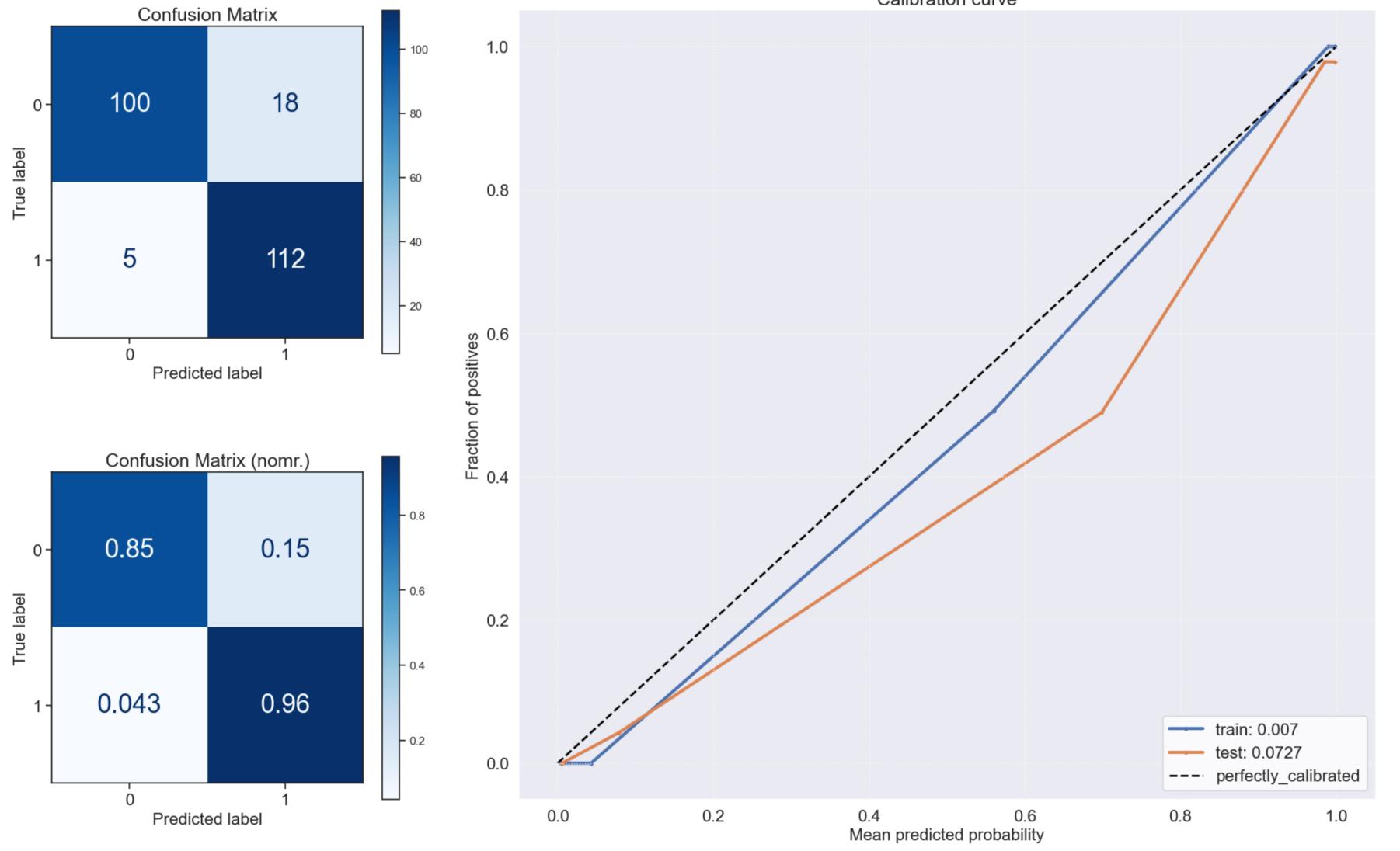
Protein: Q92769 - metric: balanced_accuracy





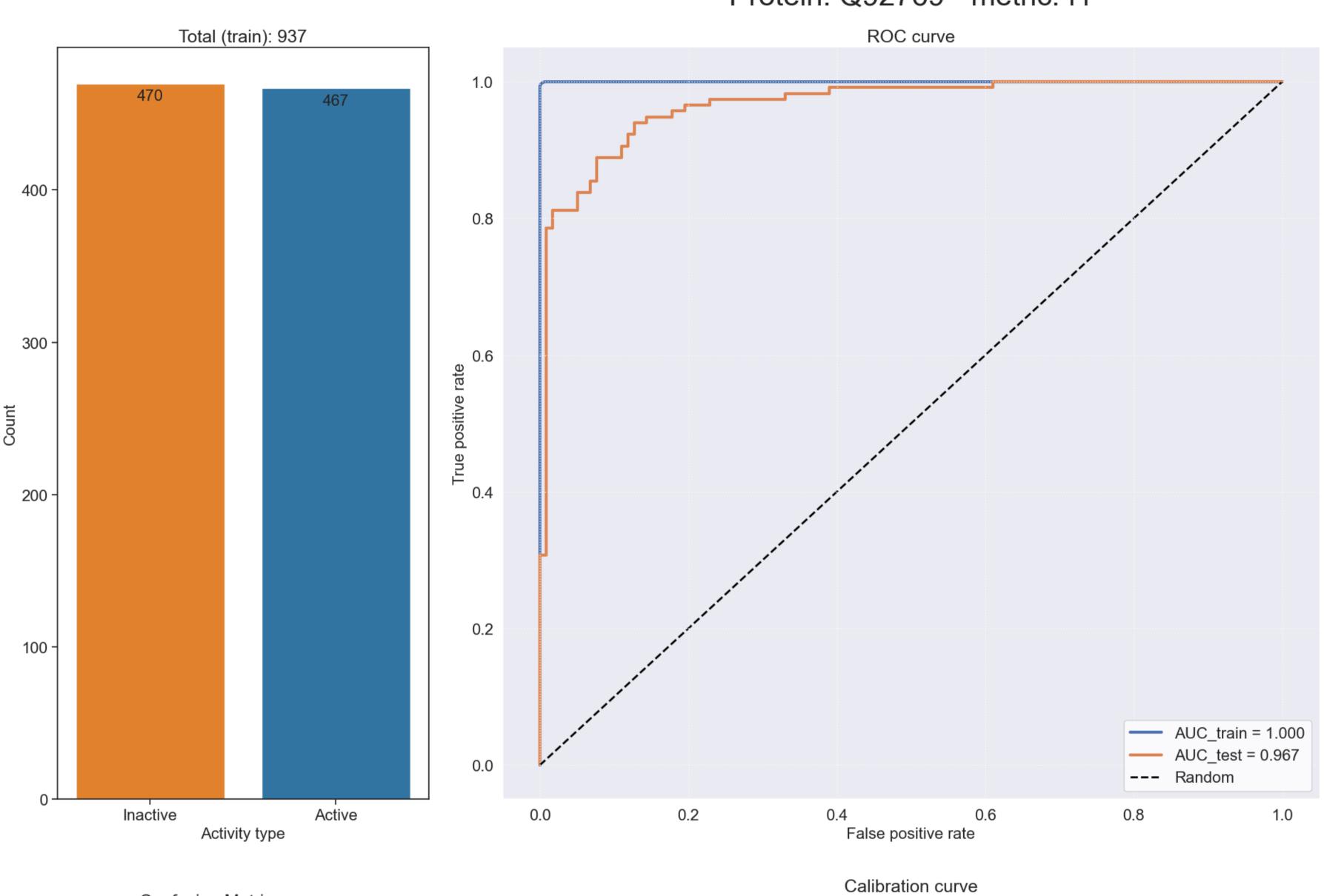
XGBoost Parameters	Value
alpha	4.482
colsample_bytree	0.9916
gamma	0.1757
lambda	4.469
learning_rate	0.1561
max_depth	10.0
min_child_weight	3.0
n_estimators	967.0
reg_alpha	0.0328
reg_lambda	0.0118
scale_pos_weight	3.2947
subsample	0.961

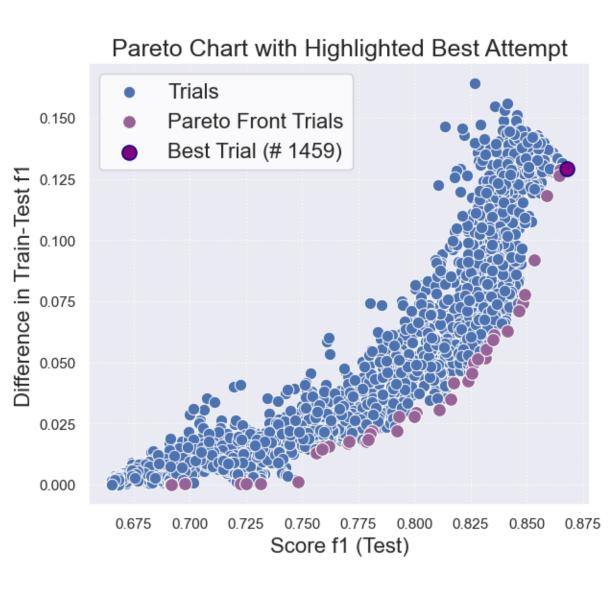


60	Active/Inactive probability						
50		Inactive zone			Active 2	zone type active inactive decoy	e (117) ve (118)
40						decoy	(234)
Percent 08							
20							
10							
0 —	0.0	0.2	0.4	0.6	6 0.	.8	1.0
			Prob	ability			

Metric	Train	Test
AUC	1.0	0.9709
accuracy	0.9947	0.9021
balanced accuracy	0.9947	0.9024
recall_(sens)	1.0	0.9573
specificity	0.9894	0.8475
precision	0.9894	0.8615
f1_score	0.9947	0.9019

Protein: Q92769 - metric: f1





XGBoost Parameters	Value
alpha	3.3427
colsample_bytree	0.7303
gamma	0.0242
lambda	3.928
learning_rate	0.1492
max_depth	8.0
min_child_weight	1.0
n_estimators	376.0
reg_alpha	0.3282
reg_lambda	0.5551
scale_pos_weight	3.4607
subsample	0.7906

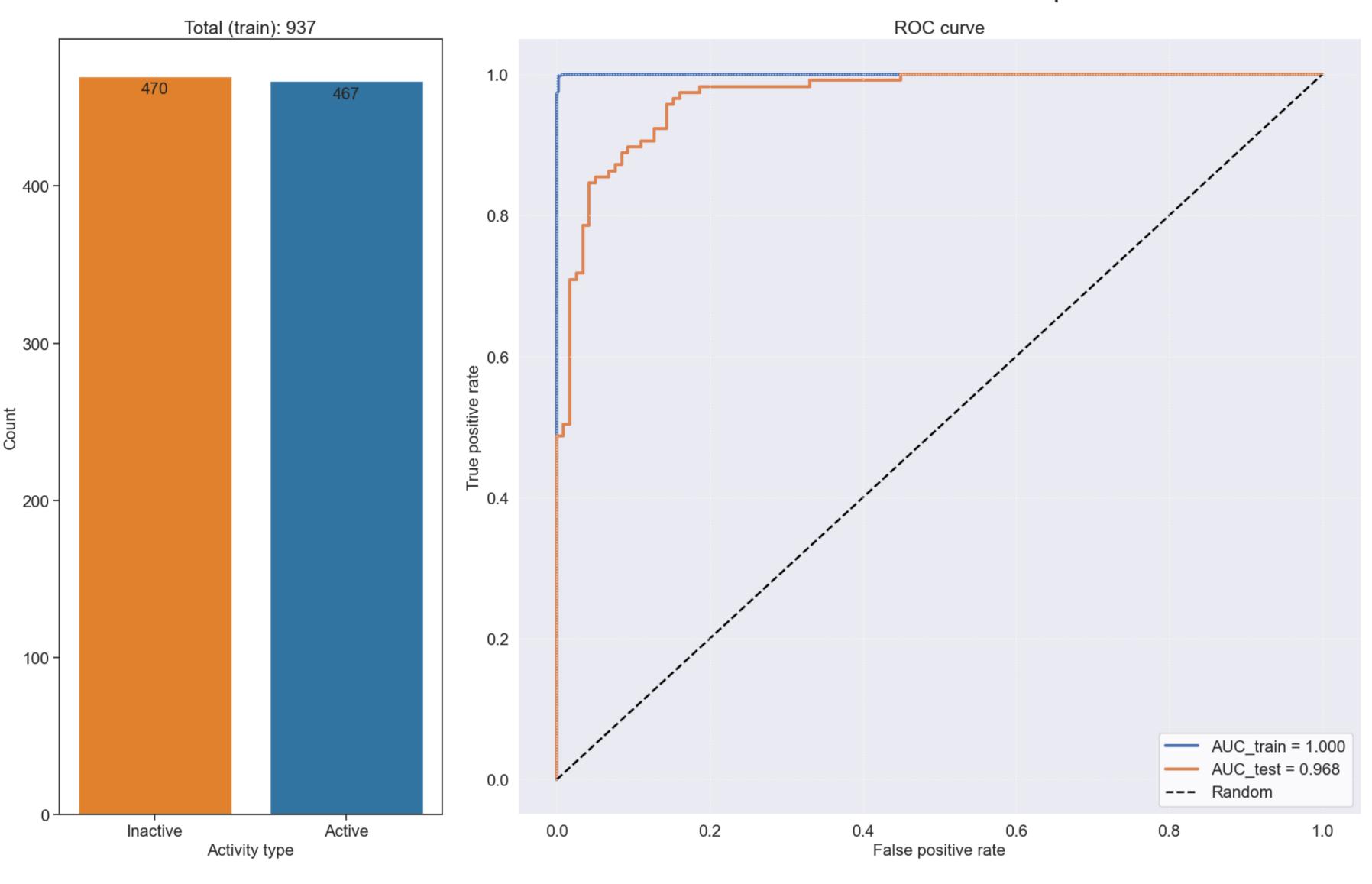
label O	97	21	- 100 - 80 - 60	1.0						
True label	5	112	- 40 - 20	0.8						
L	0 Predicte	1 ed label		Fraction of positives 0.0			2000			
	Confusion M	latrix (nomr.)	1	Fractio 60						
True label	0.82	0.18	- 0.8 - 0.6	0.2						
True	0.043	0.96	- 0.4 - 0.2	0.0					train: 0.08	
	0 Predicte	1 ed label			0.0	0.2	0.4 Mean predicte	0.6 ed probability	0.8	1.0

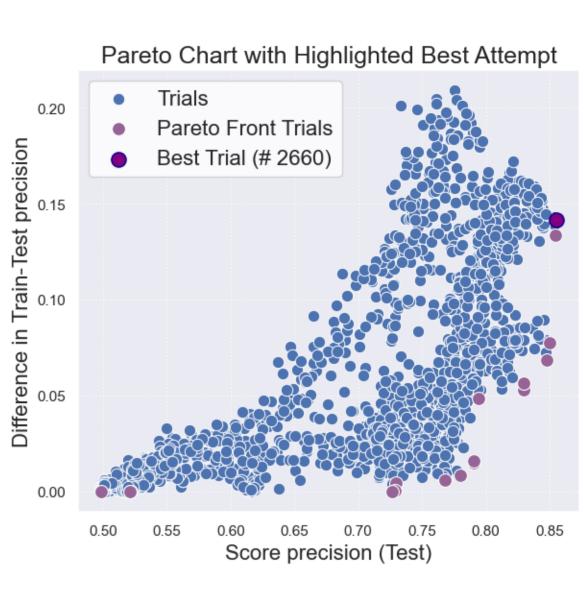
	Active/Inactive probability						
60 50		Inactive zone				type active (117) inactive (118) decoy (234)	
40							
Percent 80							
20							
0 —	0.0	0.2	0.4	0.6	0.8	1.0	
			Prob	ability			

Confusion Matrix

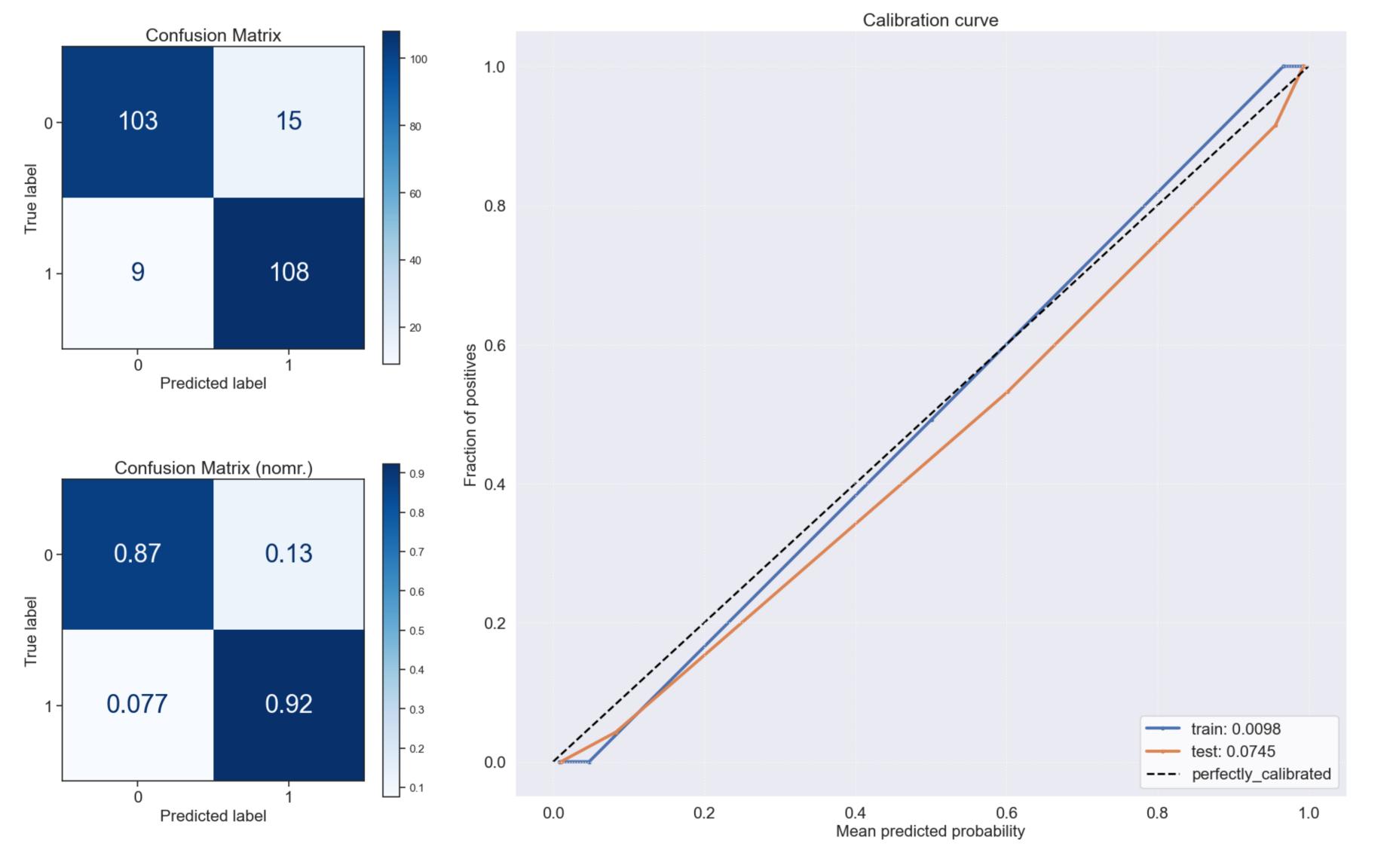
Metric	Train	Test
AUC	1.0	0.9666
accuracy	0.9968	0.8894
balanced accuracy	0.9968	0.8896
recall_(sens)	1.0	0.9573
specificity	0.9936	0.822
precision	0.9936	0.8421
f1_score	0.9968	0.8889

Protein: Q92769 - metric: precision





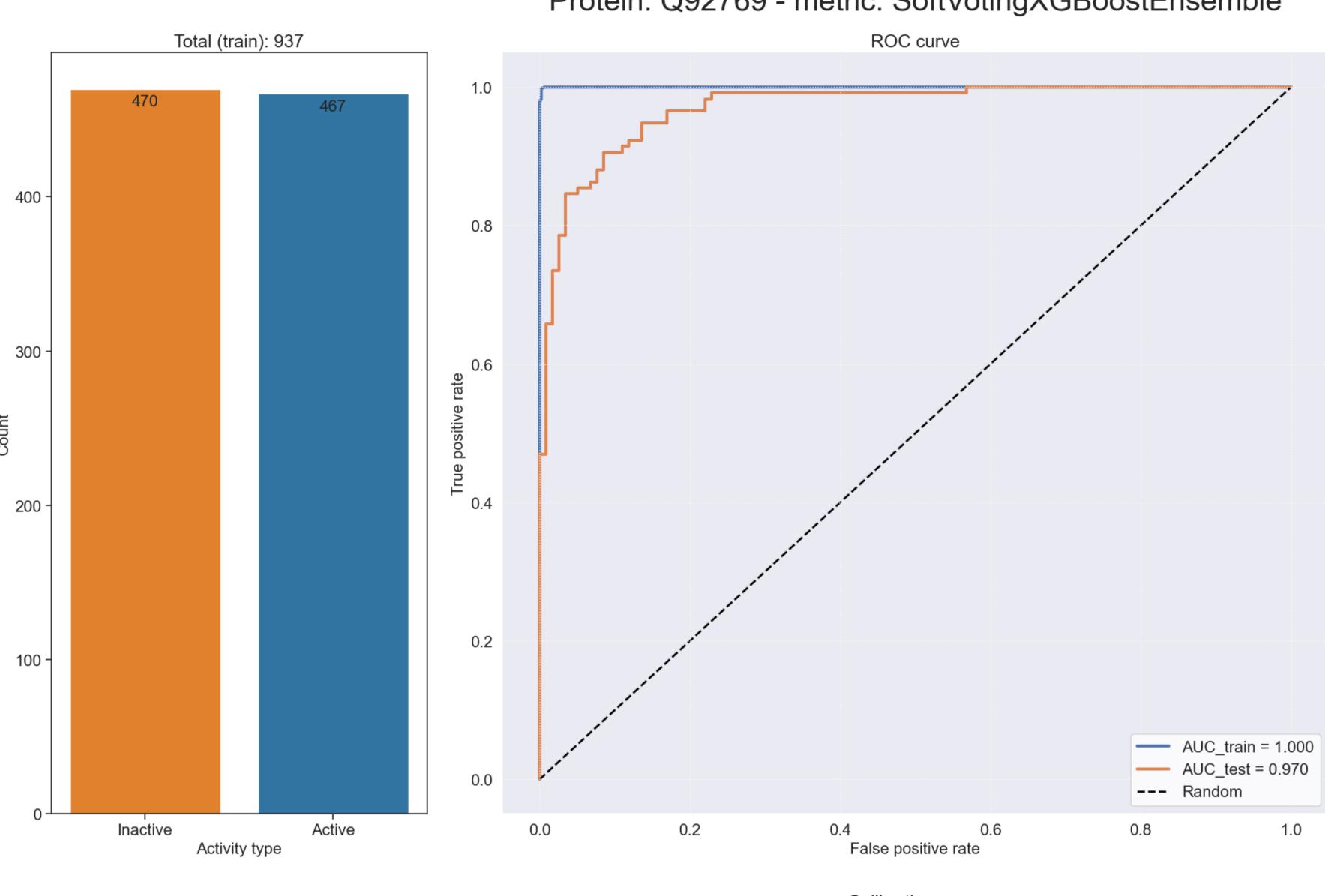
XGBoost Parameters	Value
alpha	3.7127
colsample_bytree	0.9009
gamma	0.0199
lambda	0.8909
learning_rate	0.0915
max_depth	8.0
min_child_weight	2.0
n_estimators	297.0
reg_alpha	0.055
reg_lambda	0.6621
scale_pos_weight	1.2134
subsample	0.9019

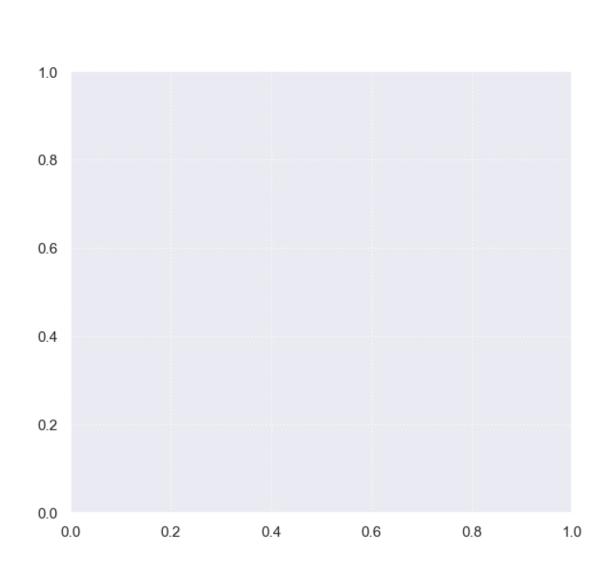


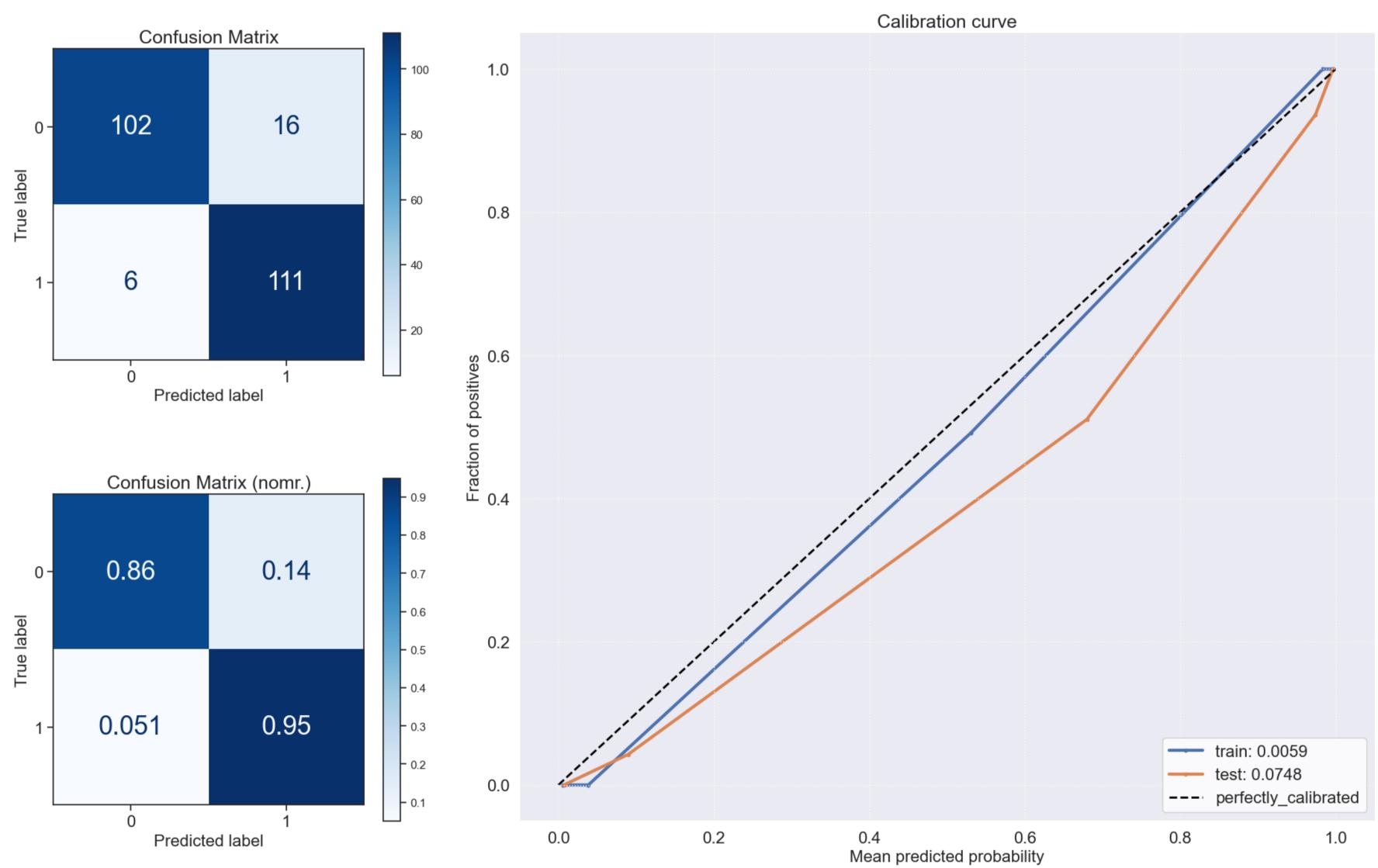
			tive/Inactive prob			
35	Ina	ctive zone			ctive zone	type active (117) inactive (118) decoy (234)
25						
Bercent						
10						
5						
0	0.0	2 0	4	0.6	0.8	1.0
	0.0		Probability	-	0.0	

Metric	Train	Test
AUC	0.9999	0.9684
accuracy	0.9979	0.8979
balanced accuracy	0.9979	0.898
recall_(sens)	0.9979	0.9231
specificity	0.9979	0.8729
precision	0.9979	0.878
f1_score	0.9979	0.8978

Protein: Q92769 - metric: SoftVotingXGBoostEnsemble







50		A	ctive/Inactiv	e probability	/		
40		active zone			Active 2	zone	type active (117) inactive (118) decoy (234)
ant 30							
Percent 00							
10						Г	
0 —	0.0	0.2	0.4 Proba	0.6	0	.8	1.0

Metric	Train	Test
AUC	1.0	0.9704
accuracy	0.9968	0.9064
balanced accuracy	0.9968	0.9066
recall_(sens)	1.0	0.9487
specificity	0.9936	0.8644
precision	0.9936	0.874
f1_score	0.9968	0.9062