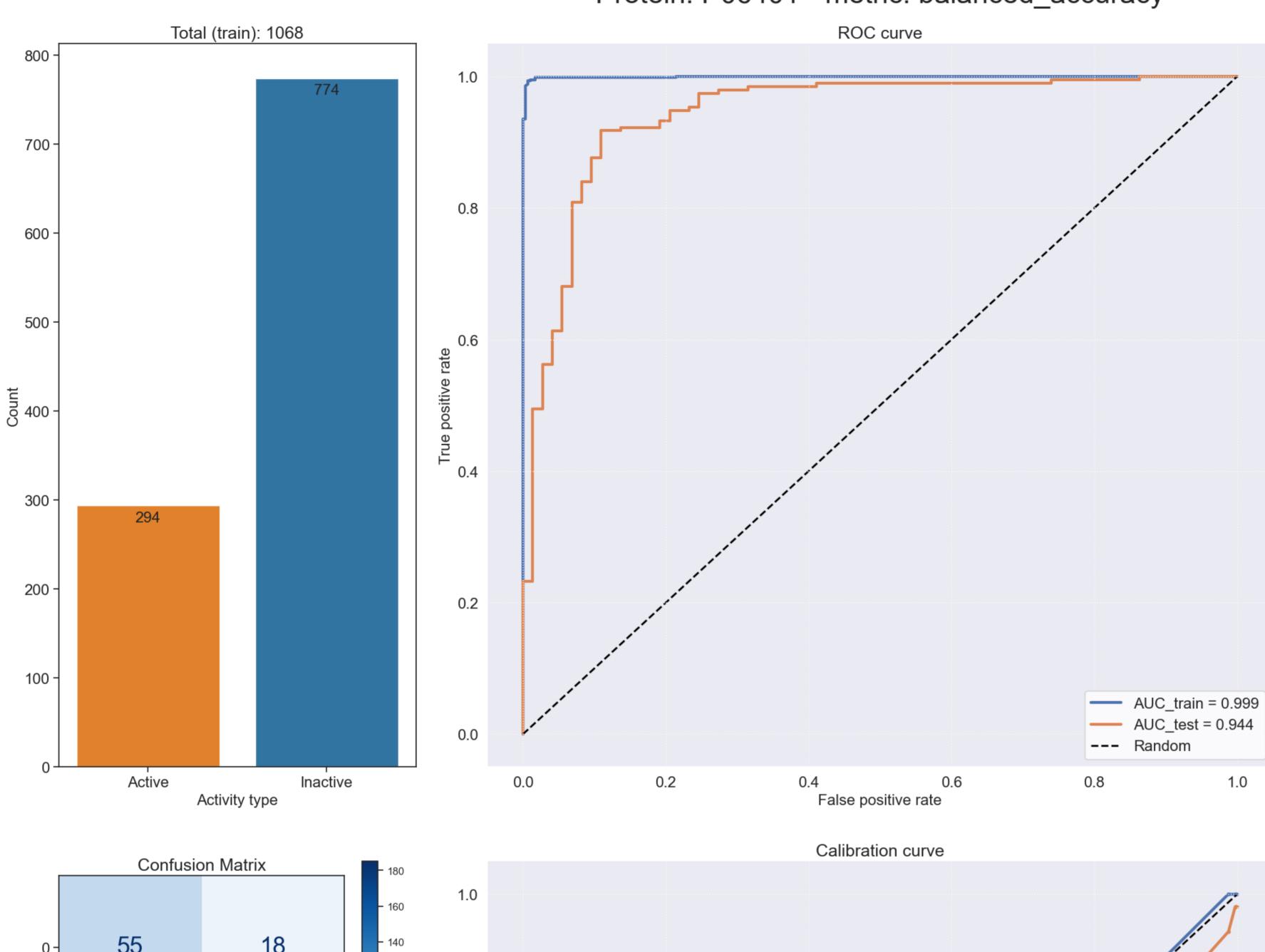
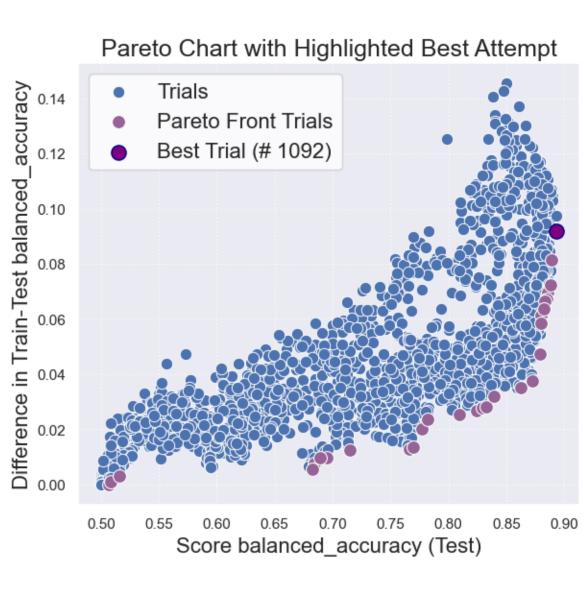
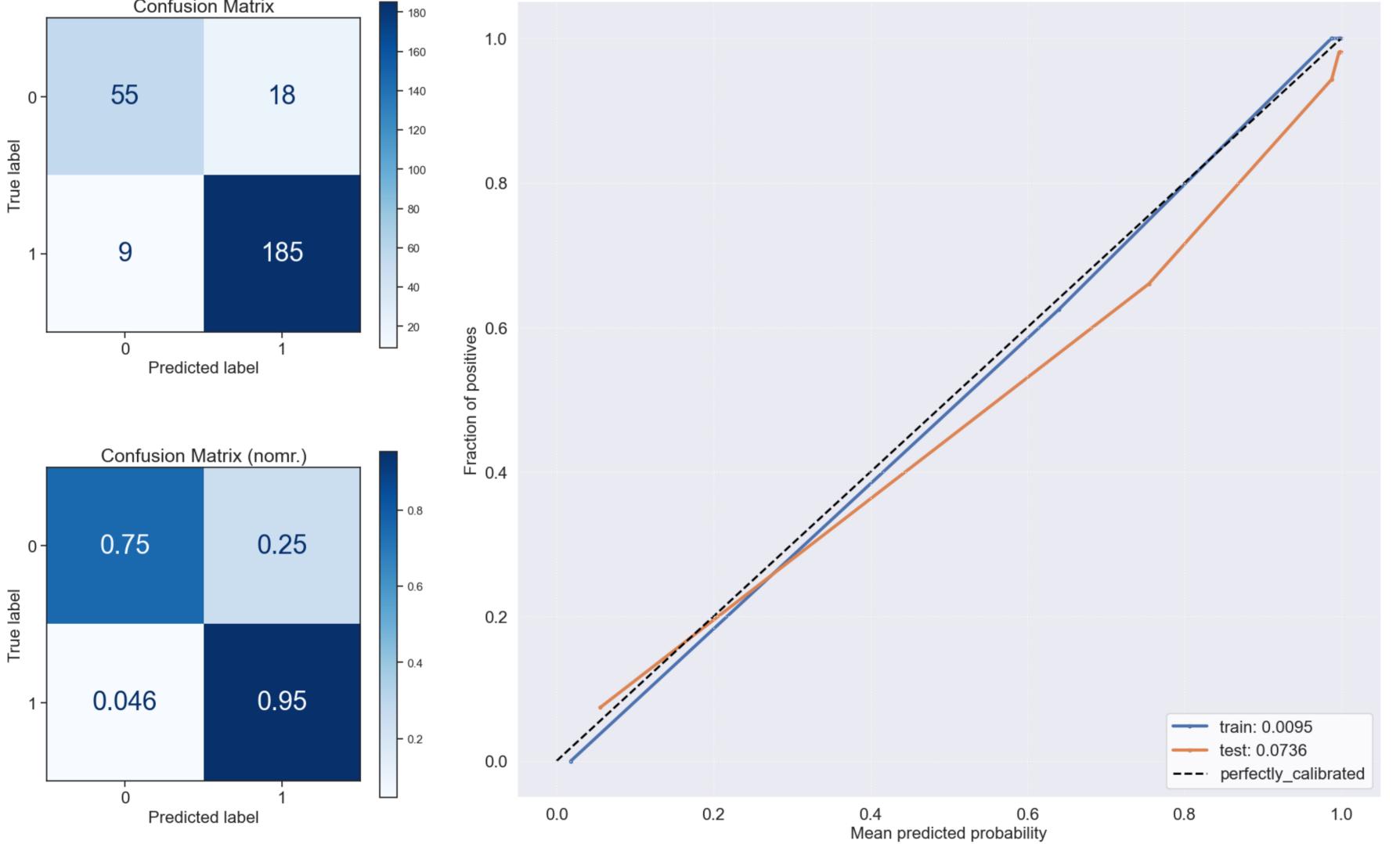
Protein: P06401 - metric: balanced_accuracy





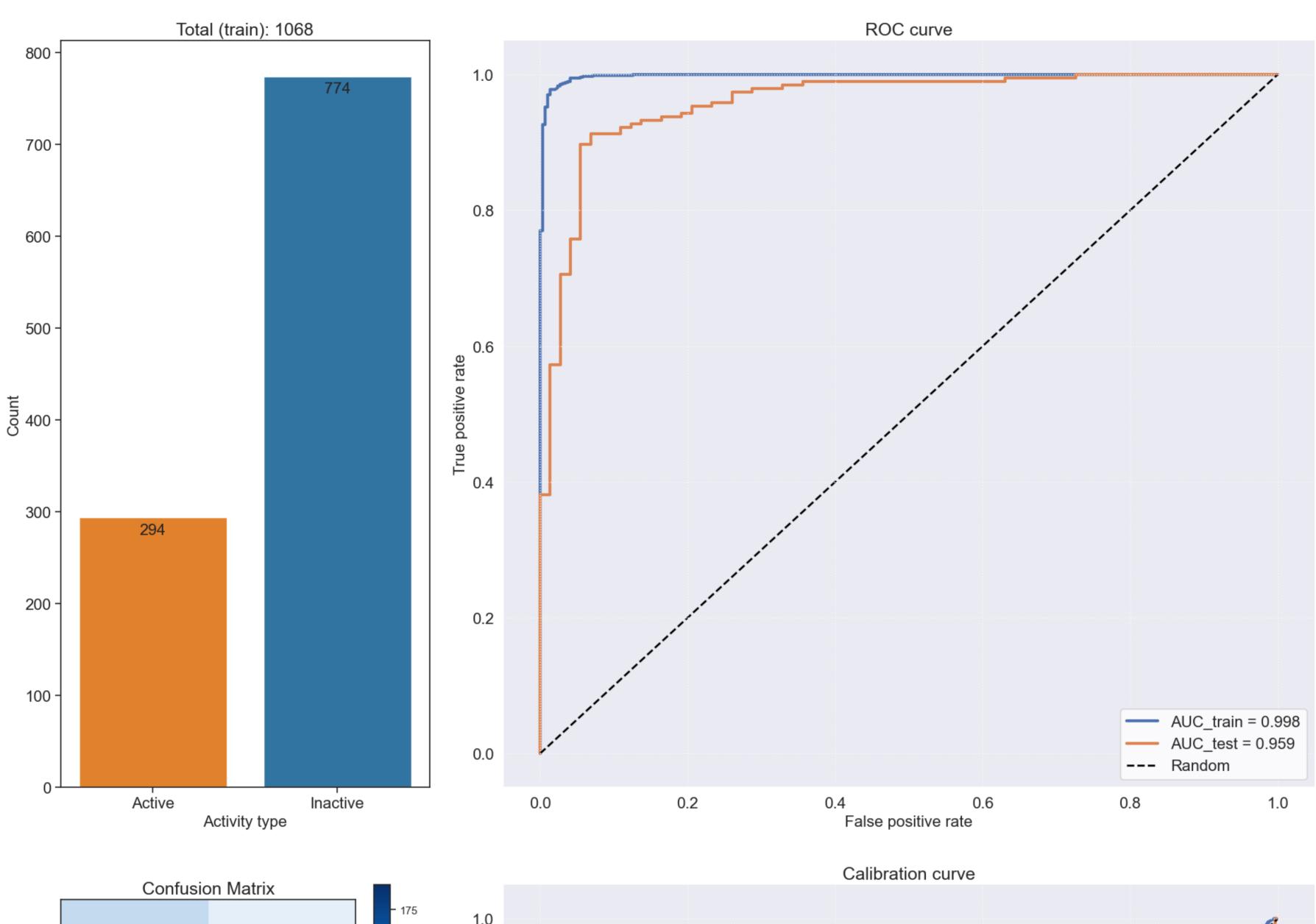
XGBoost Parameters	Value
alpha	3.5312
colsample_bytree	0.9969
gamma	0.4624
lambda	0.7795
learning_rate	0.3921
max_depth	4.0
min_child_weight	2.0
n_estimators	522.0
reg_alpha	0.4258
reg_lambda	0.5107
scale_pos_weight	1.2457
subsample	0.7686

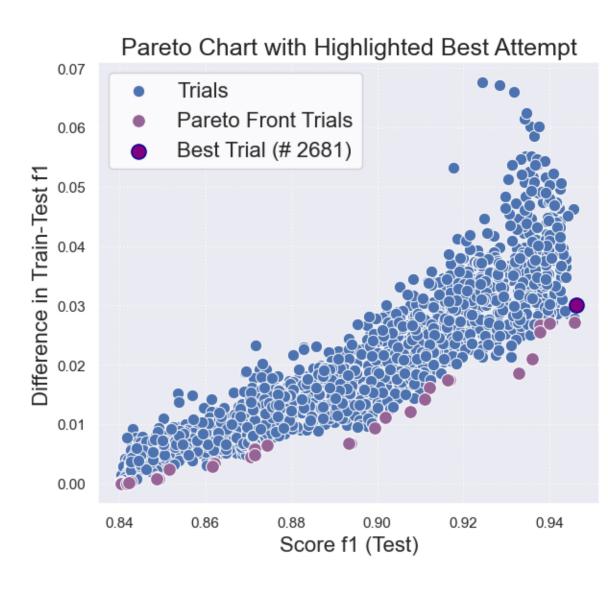


7.0			Active/Inacti	ve probability		
70		Inactive zone			Active zone	type active (194) inactive (73)
60						decoy (267)
50						
ent 40						
Percent						
20						
10						
0 —	0.0	0.2	0.4	0.6 ability	0.8	1.0
			1100	ability		

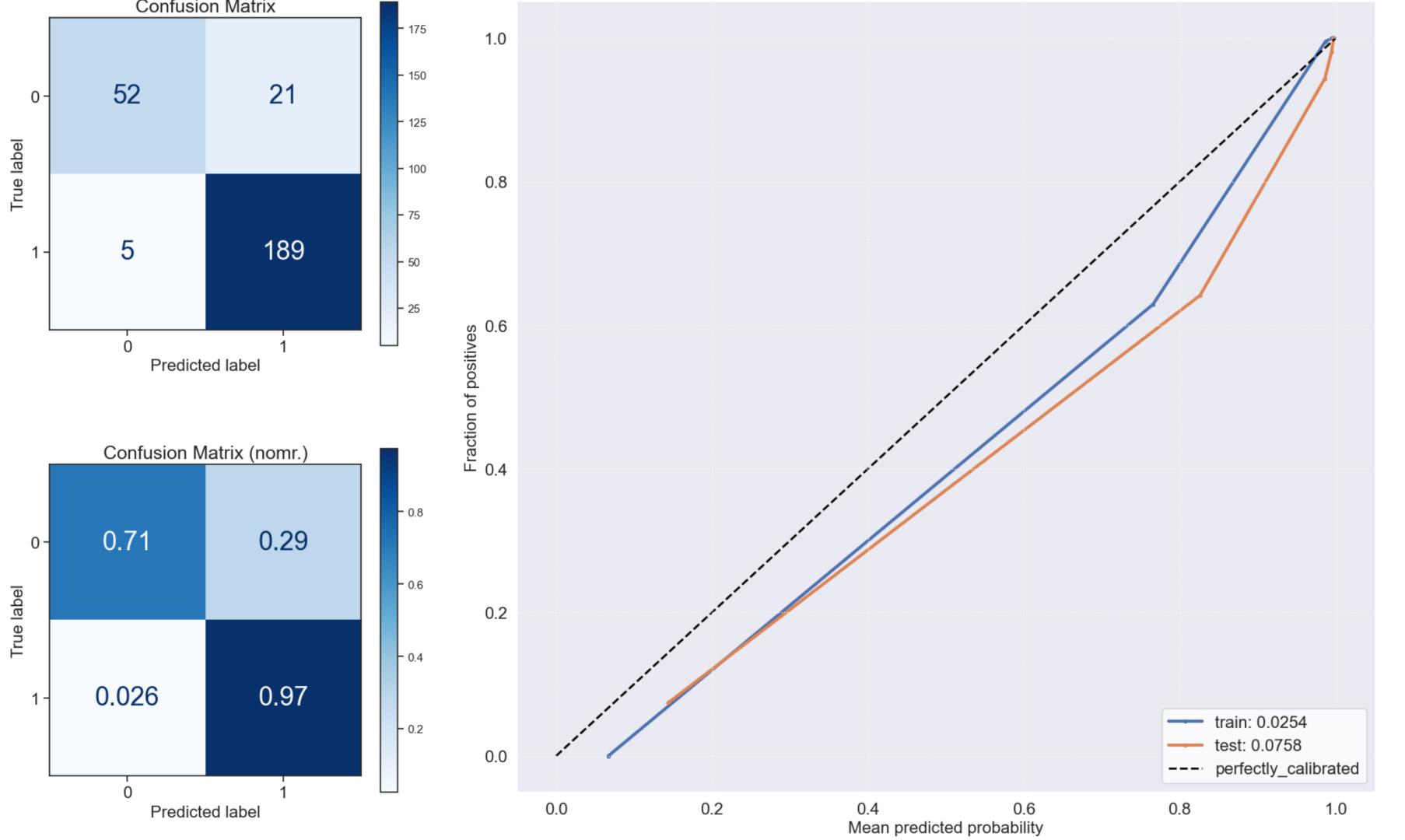
Metric	Train	Test
AUC	0.9994	0.9439
accuracy	0.9916	0.8989
balanced accuracy	0.9857	0.8535
recall_(sens)	0.9987	0.9536
specificity	0.9728	0.7534
precision	0.9898	0.9113
f1_score	0.9915	0.8967

Protein: P06401 - metric: f1





XGBoost Parameters	Value
alpha	2.5781
colsample_bytree	0.5842
gamma	0.9916
lambda	2.1106
learning_rate	0.024
max_depth	10.0
min_child_weight	1.0
n_estimators	599.0
reg_alpha	0.6739
reg_lambda	0.7337
scale_pos_weight	3.9049
subsample	0.6847

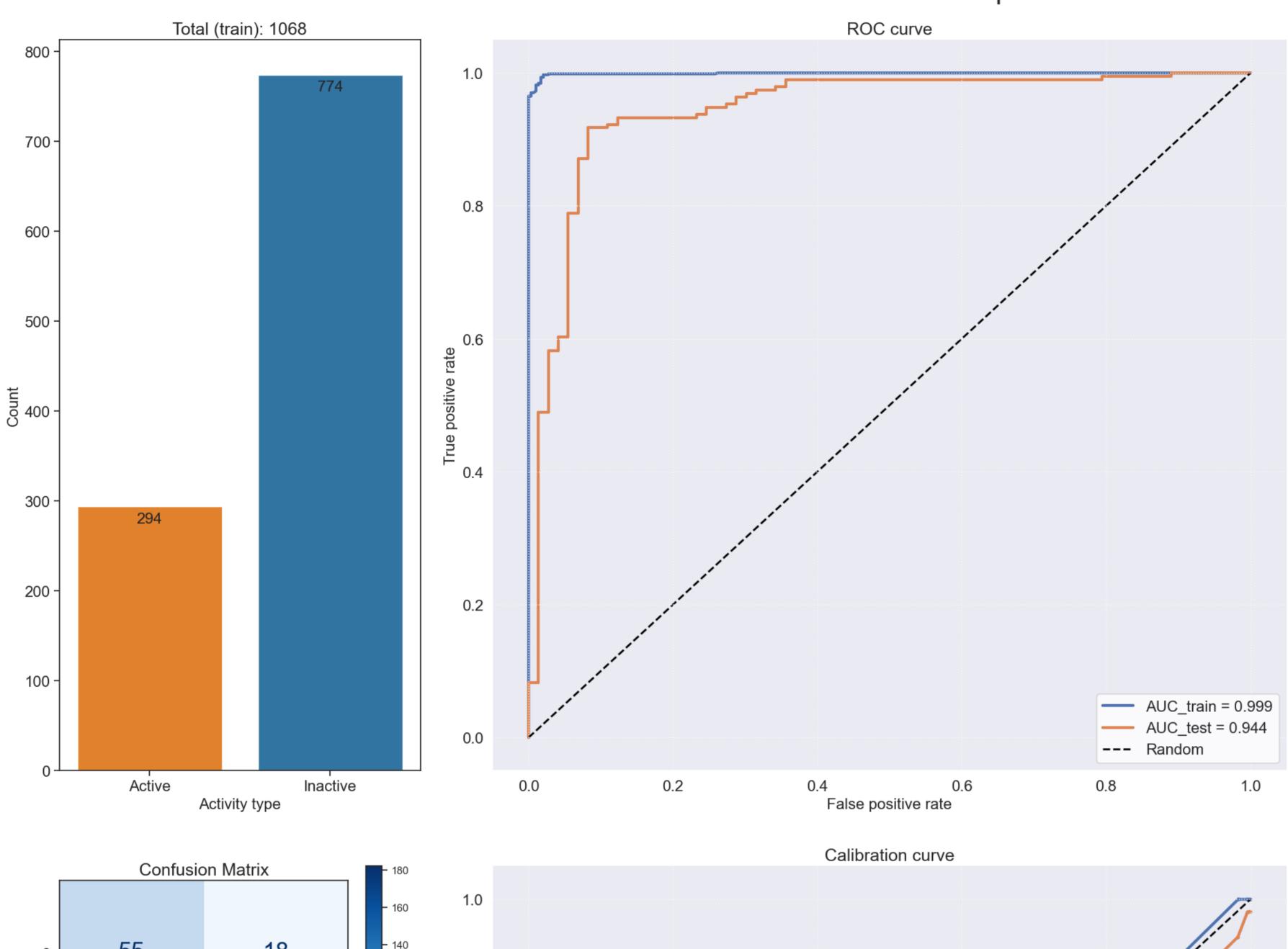


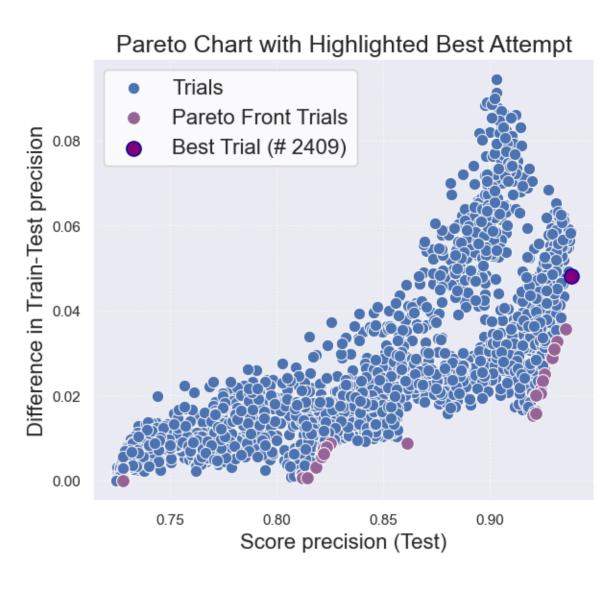
		Inactive zone				decoy (267)
50						
🛶 /						
Percent						
20						
40						
0		, <u></u>			┍┩ ┱╌┸ ╒ ┱┖╌┸ ╒ ┩	
J	0.0	0.2	0.4 Proba	0.6 ability	0.8	1.0

Active/Inactive probability

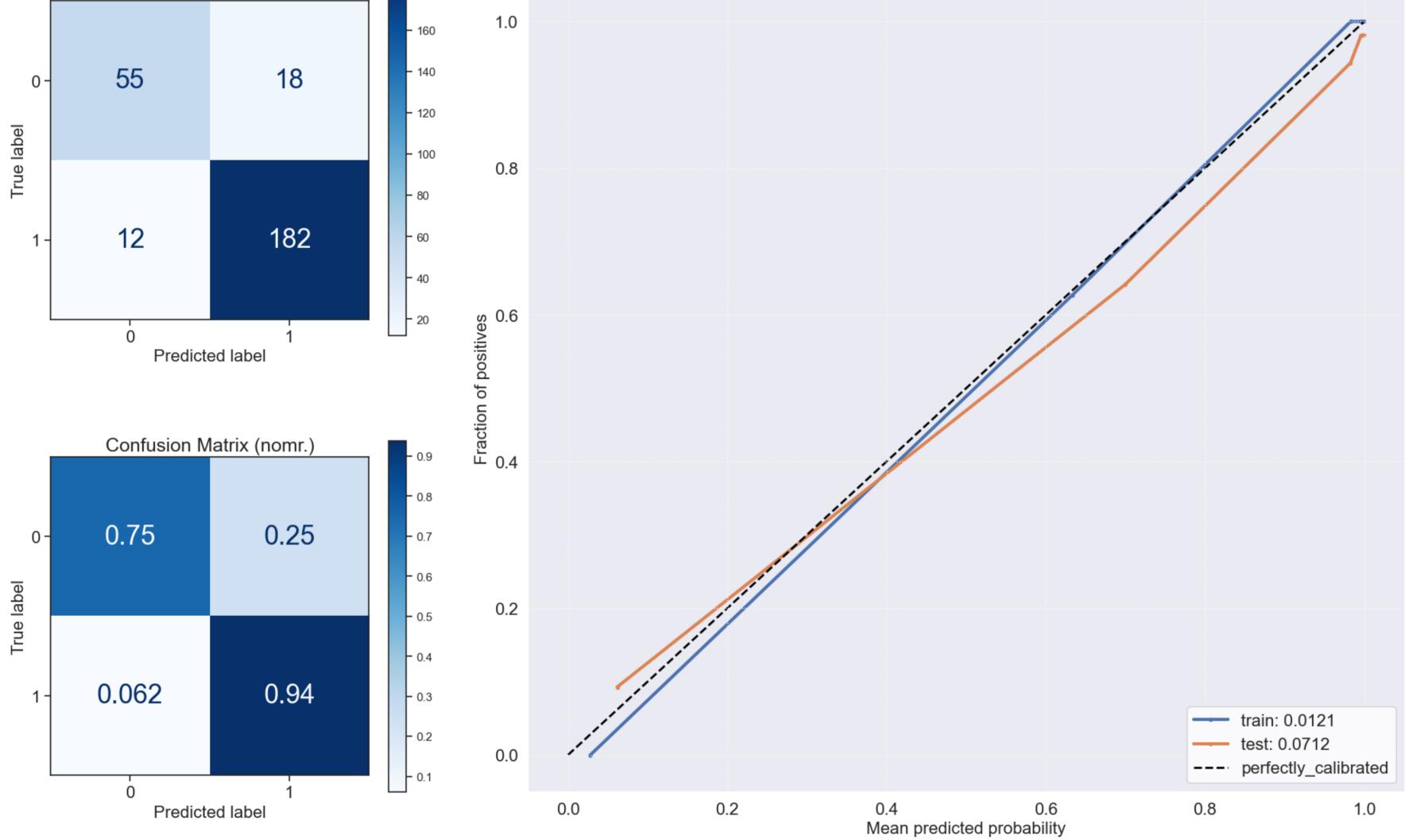
Metric	Train	Test
AUC	0.9981	0.9593
accuracy	0.9644	0.9026
balanced accuracy	0.9354	0.8433
recall_(sens)	1.0	0.9742
specificity	0.8707	0.7123
precision	0.9532	0.9
f1_score	0.9636	0.8986

Protein: P06401 - metric: precision



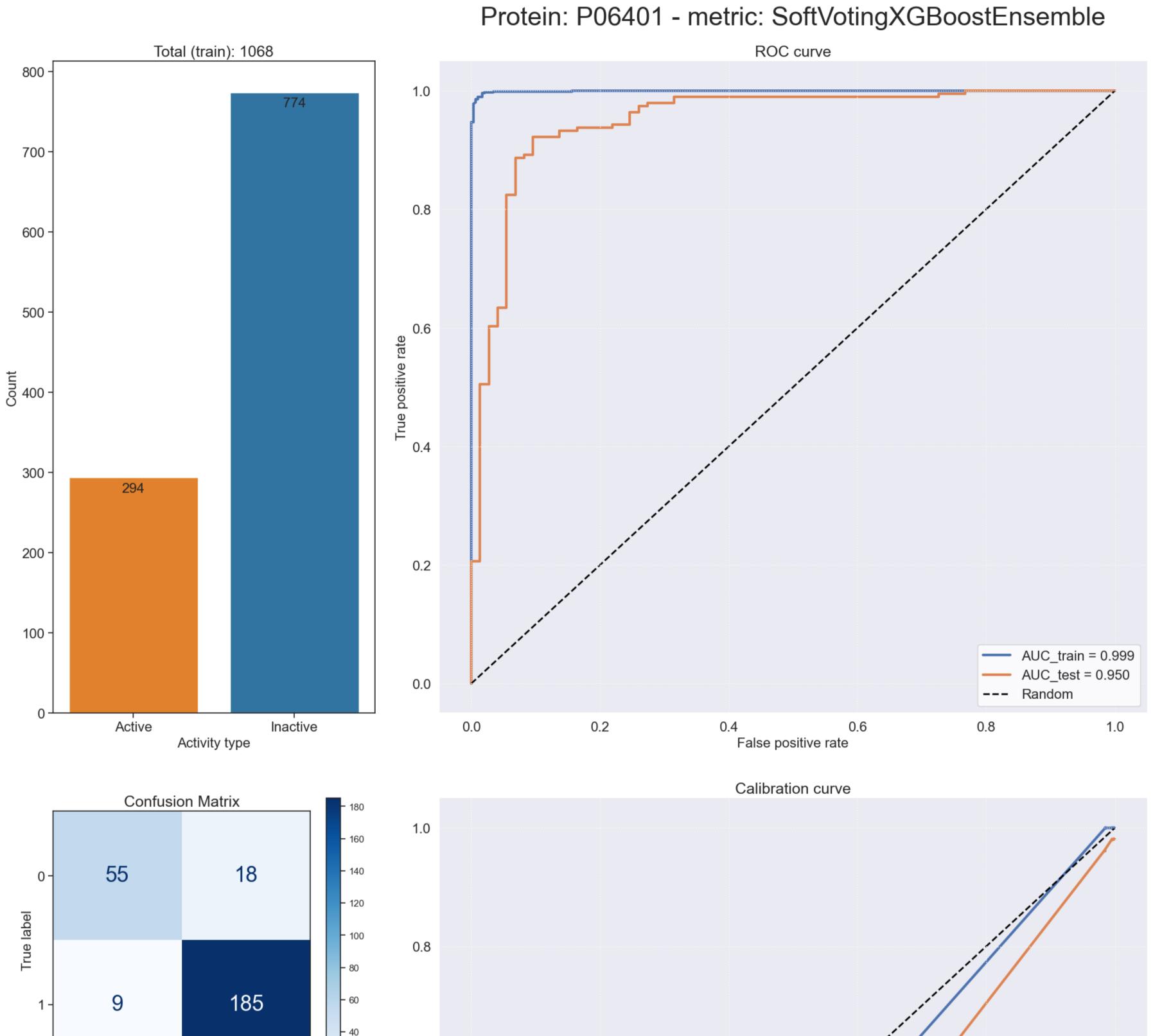


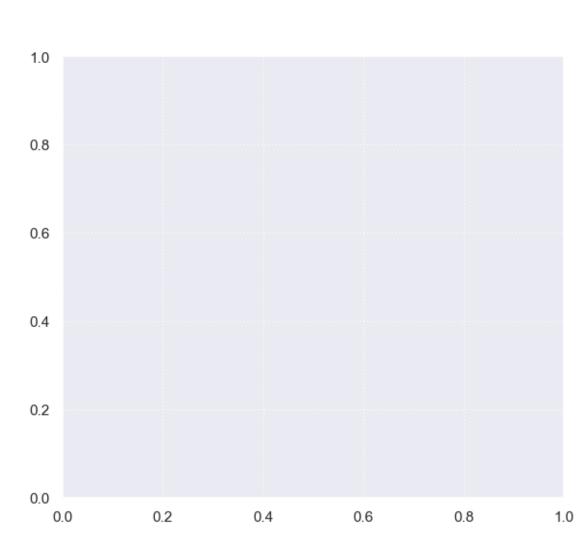
XGBoost Parameters	Value
alpha	1.9326
colsample_bytree	0.9025
gamma	0.5518
lambda	3.2674
learning_rate	0.1727
max_depth	7.0
min_child_weight	3.0
n_estimators	689.0
reg_alpha	0.0601
reg_lambda	0.4639
scale_pos_weight	1.1332
subsample	0.7843

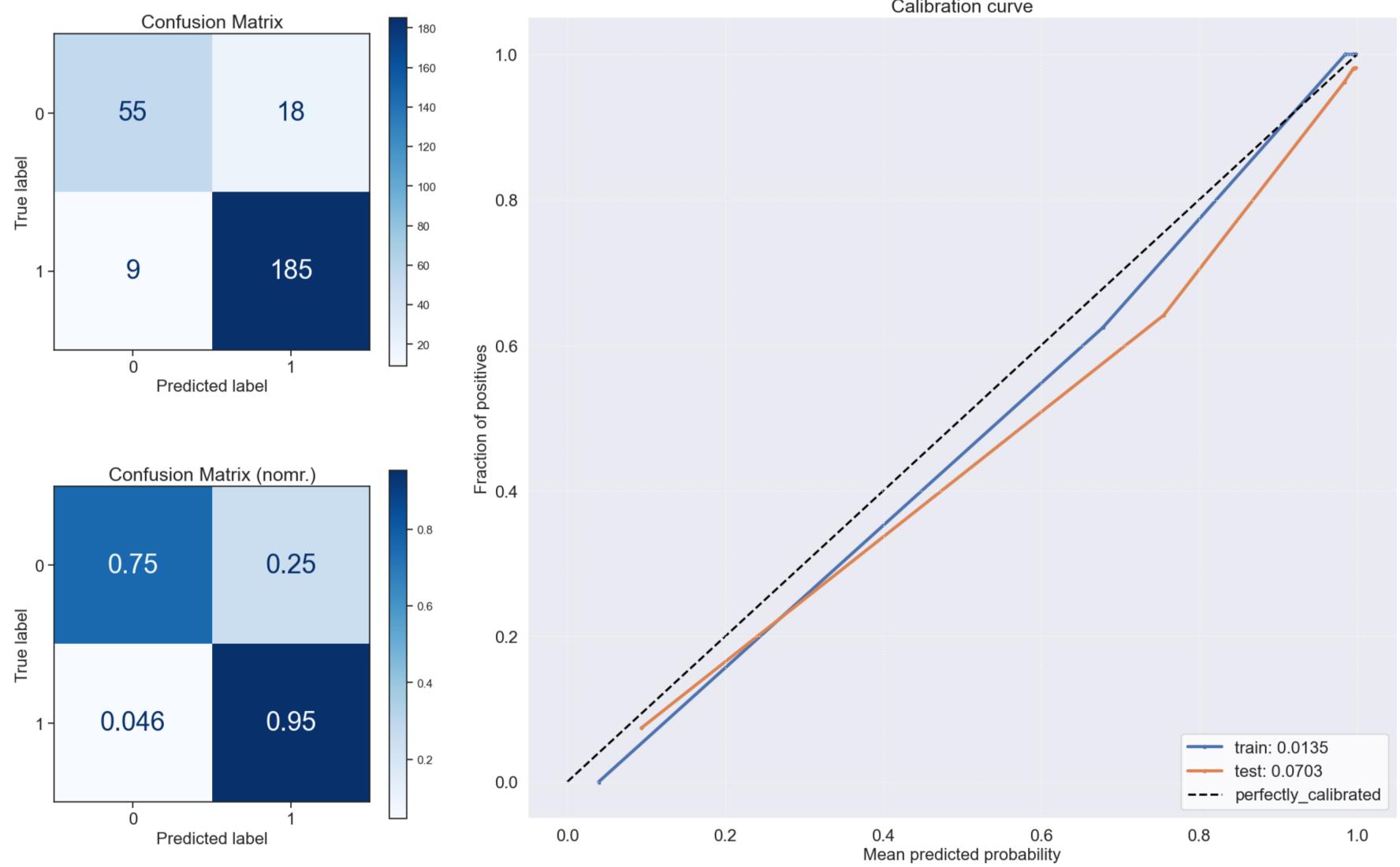


		Ac	tive/Inactive	e probability	/		
	In					zone	type active (194) inactive (73) decoy (267)
40							
Percent							
10							
0 —	0.0	0.2).4 Proba	0.6 bility	0.	.8	1.0

Metric	Train	Test
AUC	0.9992	0.9441
accuracy	0.9878	0.8876
balanced accuracy	0.9789	0.8458
recall_(sens)	0.9987	0.9381
specificity	0.9592	0.7534
precision	0.9847	0.91
f1_score	0.9878	0.8861







50		Inactive zone				inactive decoy ((73)
40							
rcent							
_							
10							
0							
	0.0	0.2	0.4 Proba	0.6 ability	0.8	1.0	0

Active/Inactive probability

Metric	Train	Test
AUC	0.9994	0.9504
accuracy	0.9878	0.8989
balanced accuracy	0.9789	0.8535
recall_(sens)	0.9987	0.9536
specificity	0.9592	0.7534
precision	0.9847	0.9113
f1_score	0.9878	0.8967