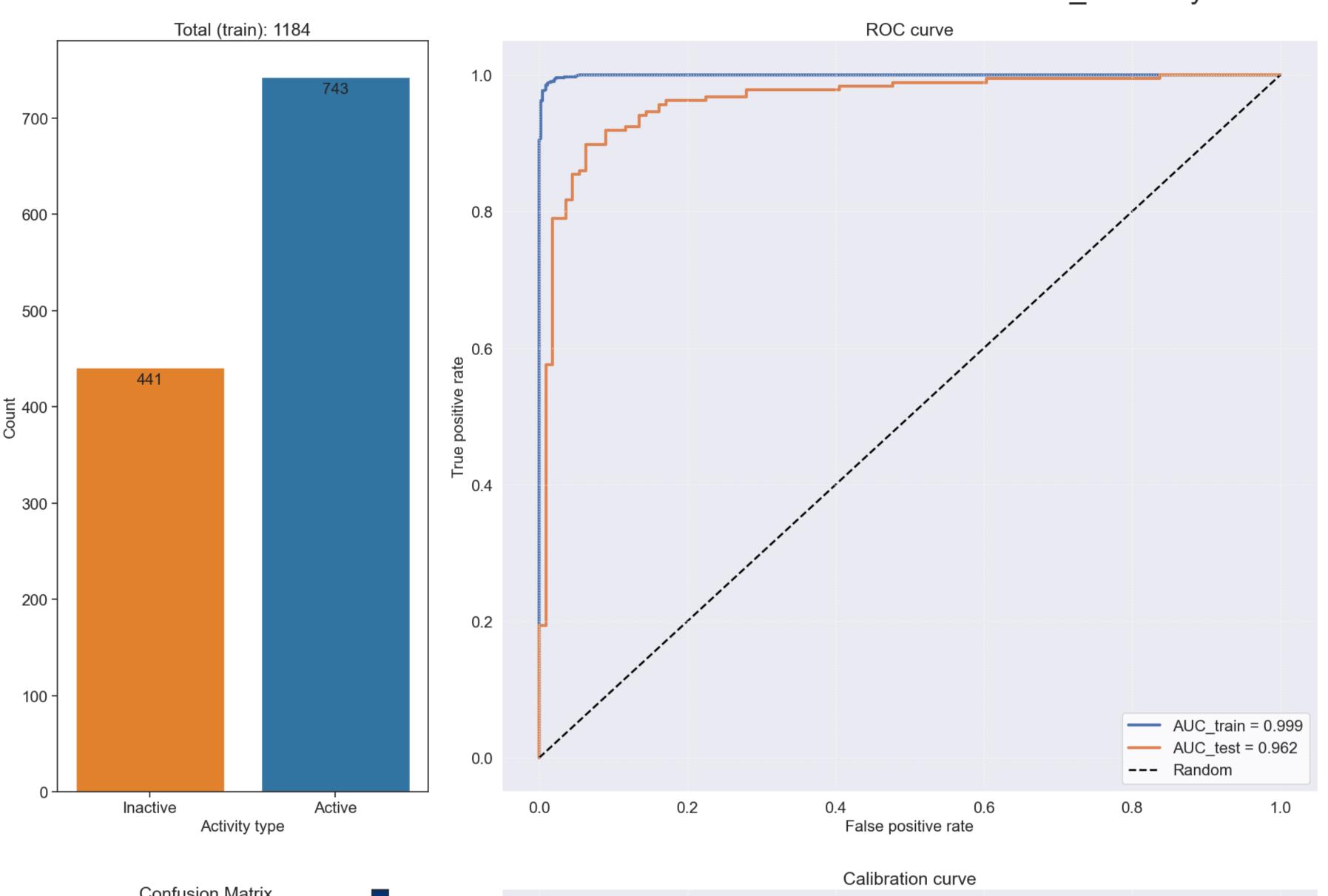
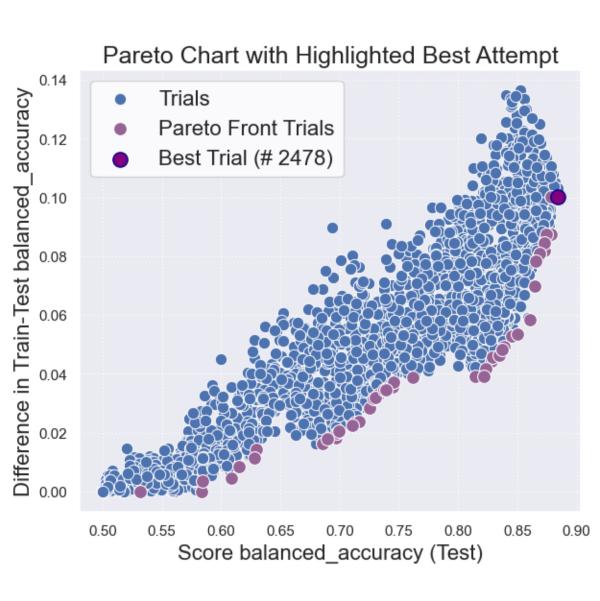
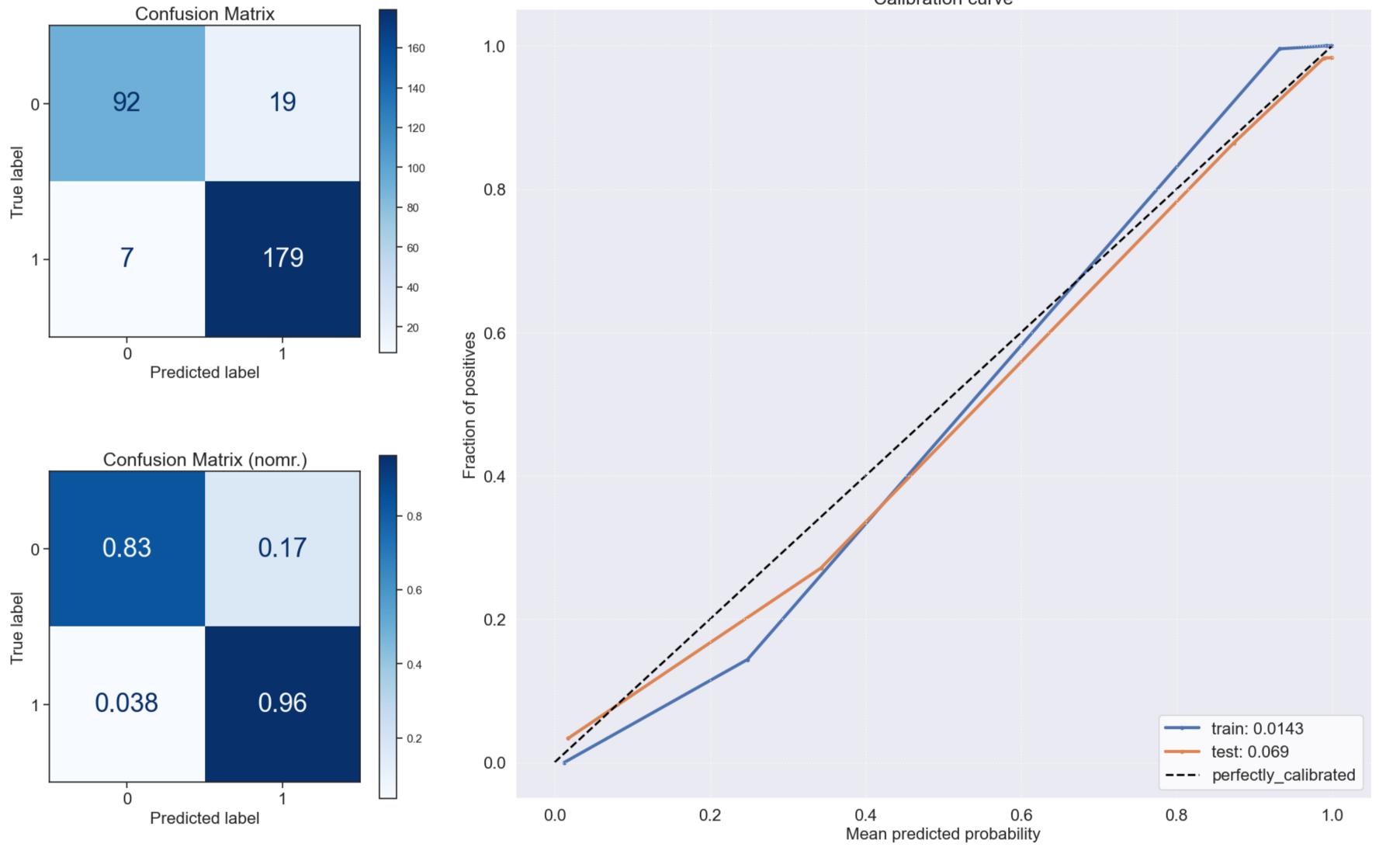
Protein: P08172 - metric: balanced_accuracy





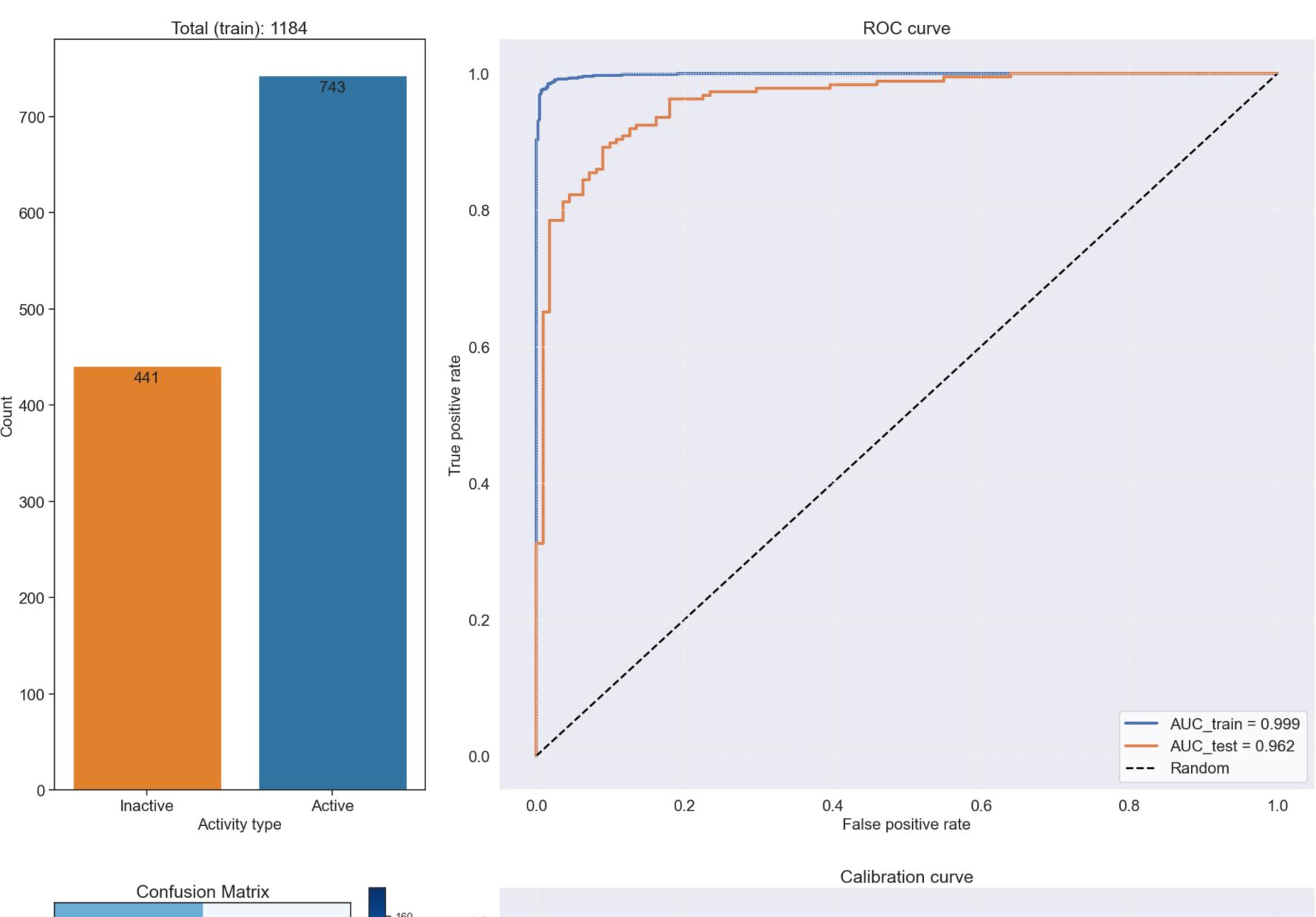
XGBoost Parameters	Value
alpha	0.1883
colsample_bytree	0.6155
gamma	0.0447
lambda	1.7216
learning_rate	0.0918
max_depth	4.0
min_child_weight	2.0
n_estimators	813.0
reg_alpha	0.5241
reg_lambda	0.0037
scale_pos_weight	1.4757
subsample	0.5729

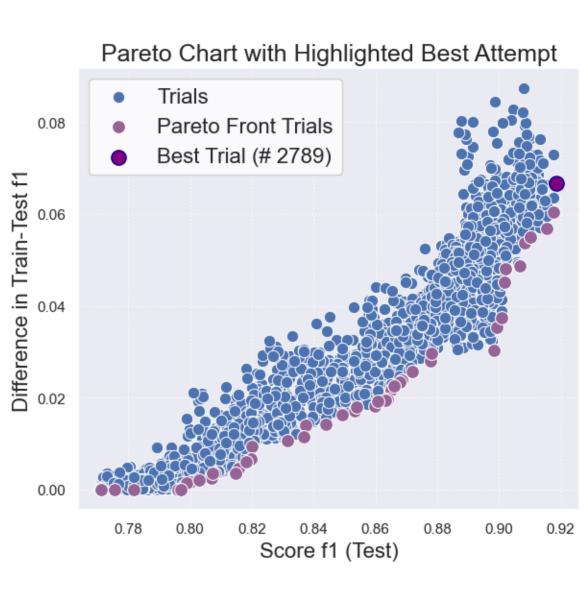


	Active/Inactive probability						
		Inactive zone			Active	type active (18 inactive (28 decoy (28	(111)
40							
10							
Ü	0.0	0.2	0.4 Proba	0.6 ability	0.	.8 1.0)

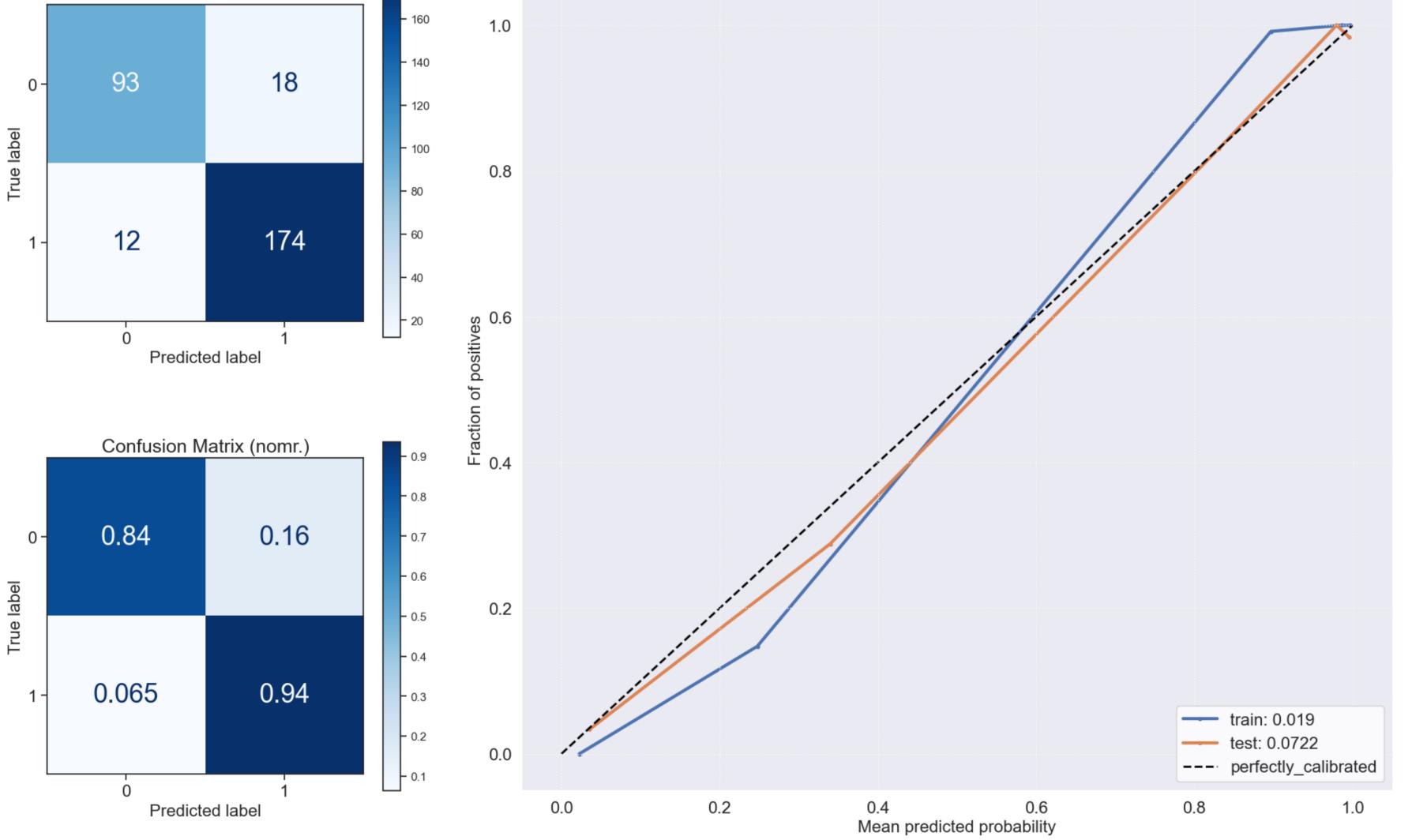
Metric	Train	Test
AUC	0.9994	0.9625
accuracy	0.9873	0.9125
balanced accuracy	0.9844	0.8956
recall_(sens)	0.996	0.9624
specificity	0.9728	0.8288
precision	0.984	0.904
f1_score	0.9873	0.9113

Protein: P08172 - metric: f1





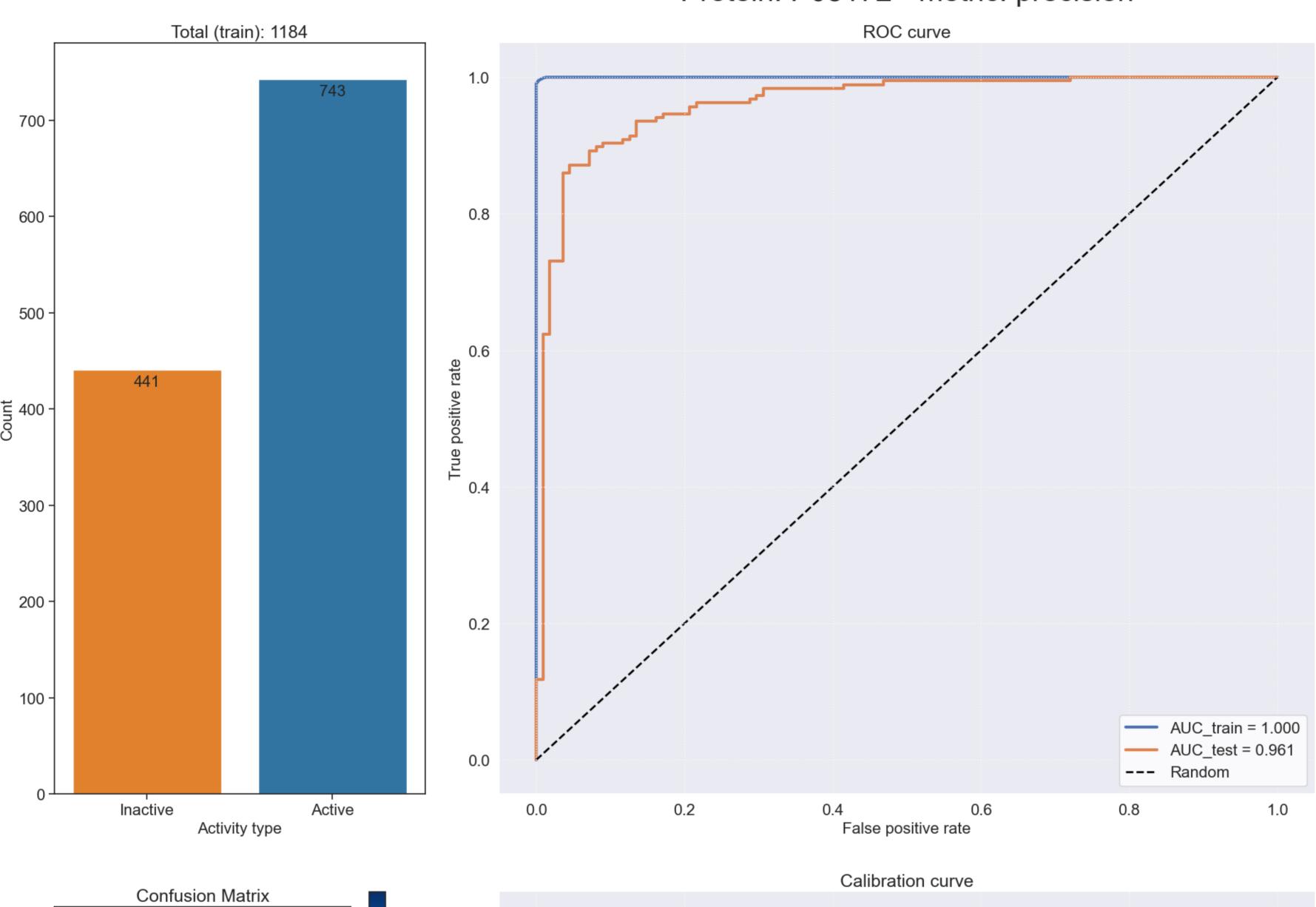
XGBoost Parameters	Value
alpha	3.6221
colsample_bytree	0.5853
gamma	0.3378
lambda	4.5761
learning_rate	0.0693
max_depth	9.0
min_child_weight	1.0
n_estimators	489.0
reg_alpha	0.9535
reg_lambda	0.6018
scale_pos_weight	1.0993
subsample	0.5869

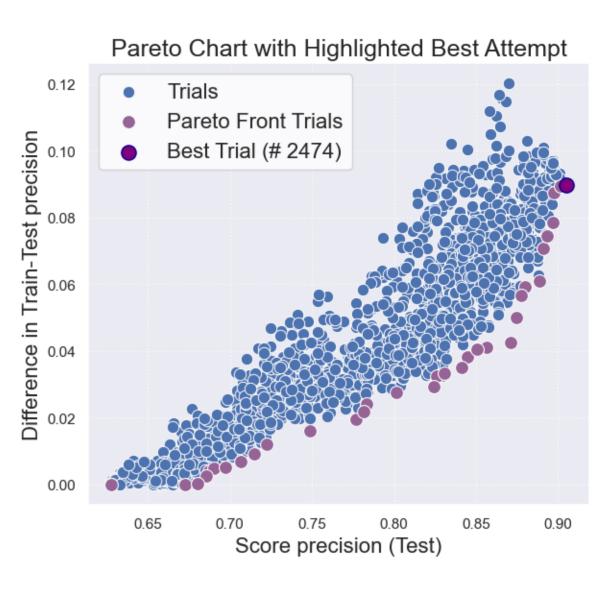


	Active/Inactive probability						
40	Ina	ctive zone			Active :	zone	type active (186) inactive (111)
30							decoy (297)
ercent							
10							
10							
0	0.0 0.	2 0.	4 Probak	0.0 pility	6 0	.8	1.0

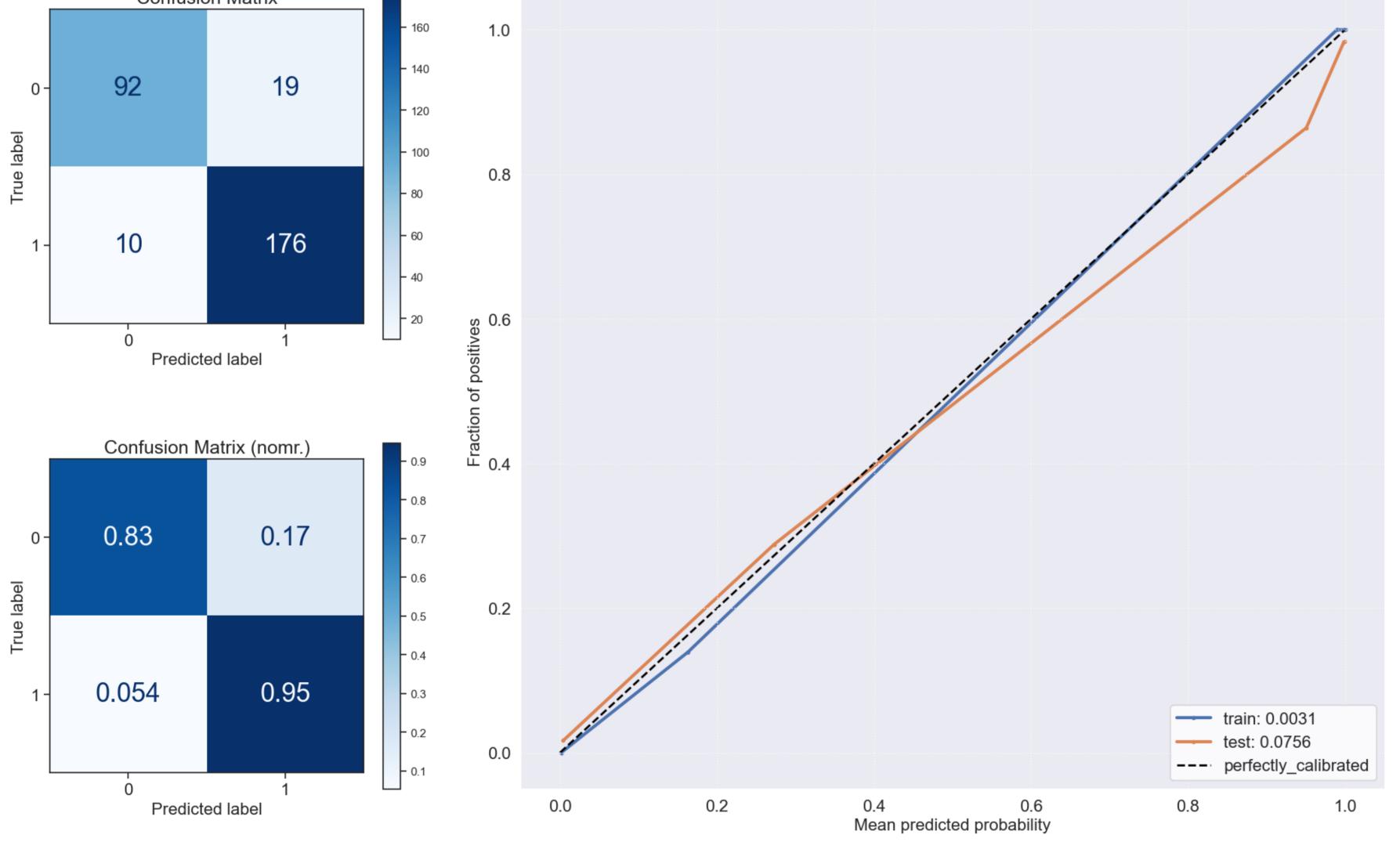
Metric	Train	Test
AUC	0.9987	0.9621
accuracy	0.984	0.899
balanced accuracy	0.9812	0.8867
recall_(sens)	0.9919	0.9355
specificity	0.9705	0.8378
precision	0.9827	0.9062
f1_score	0.9839	0.8984

Protein: P08172 - metric: precision





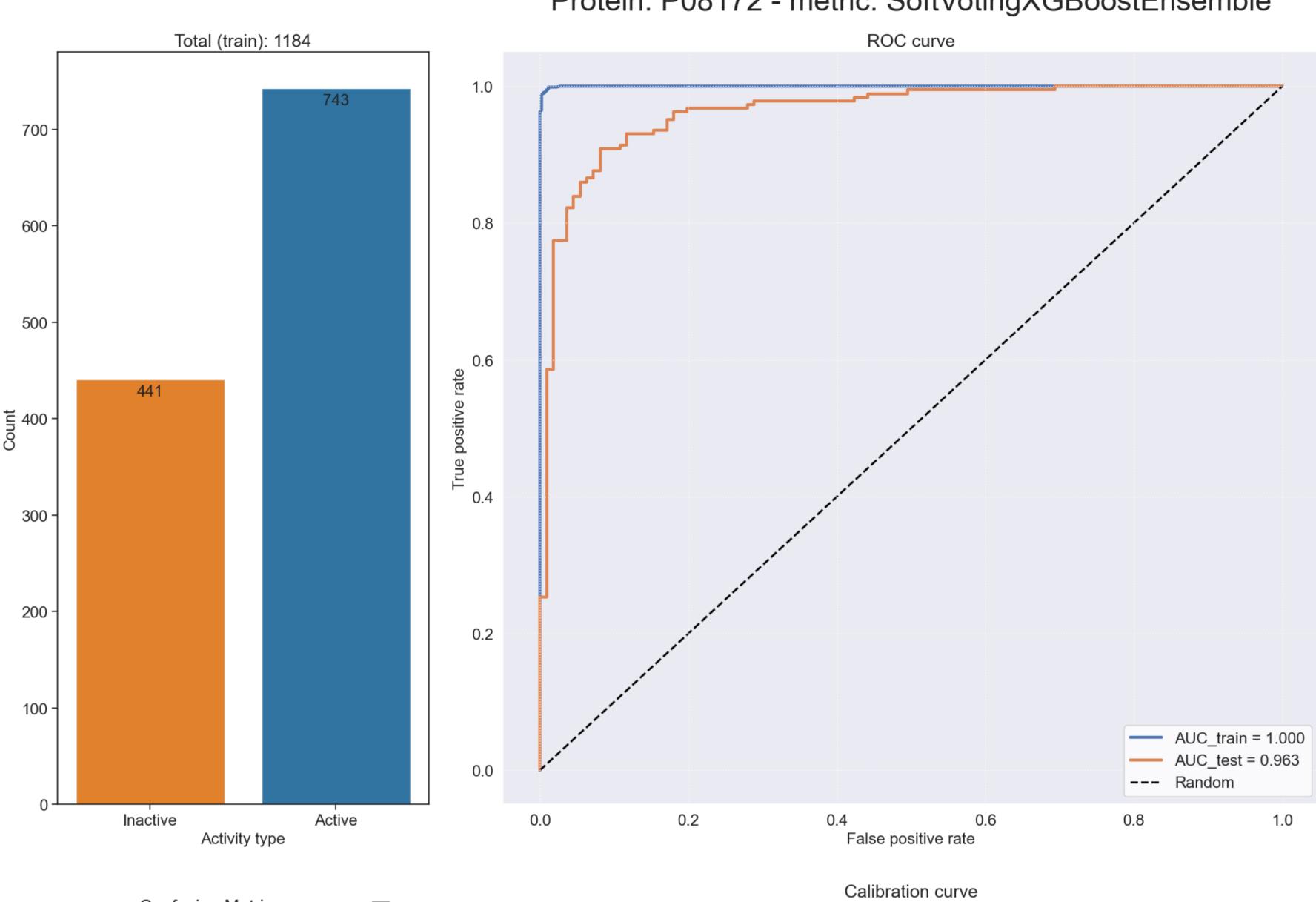
XGBoost Parameters	Value
alpha	3.4579
colsample_bytree	0.663
gamma	0.0304
lambda	2.3241
learning_rate	0.1026
max_depth	10.0
min_child_weight	1.0
n_estimators	745.0
reg_alpha	0.0116
reg_lambda	0.0886
scale_pos_weight	1.5341
subsample	0.8459

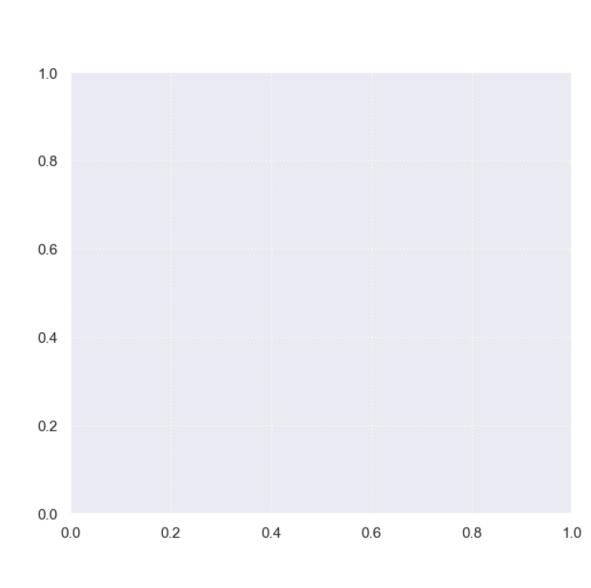


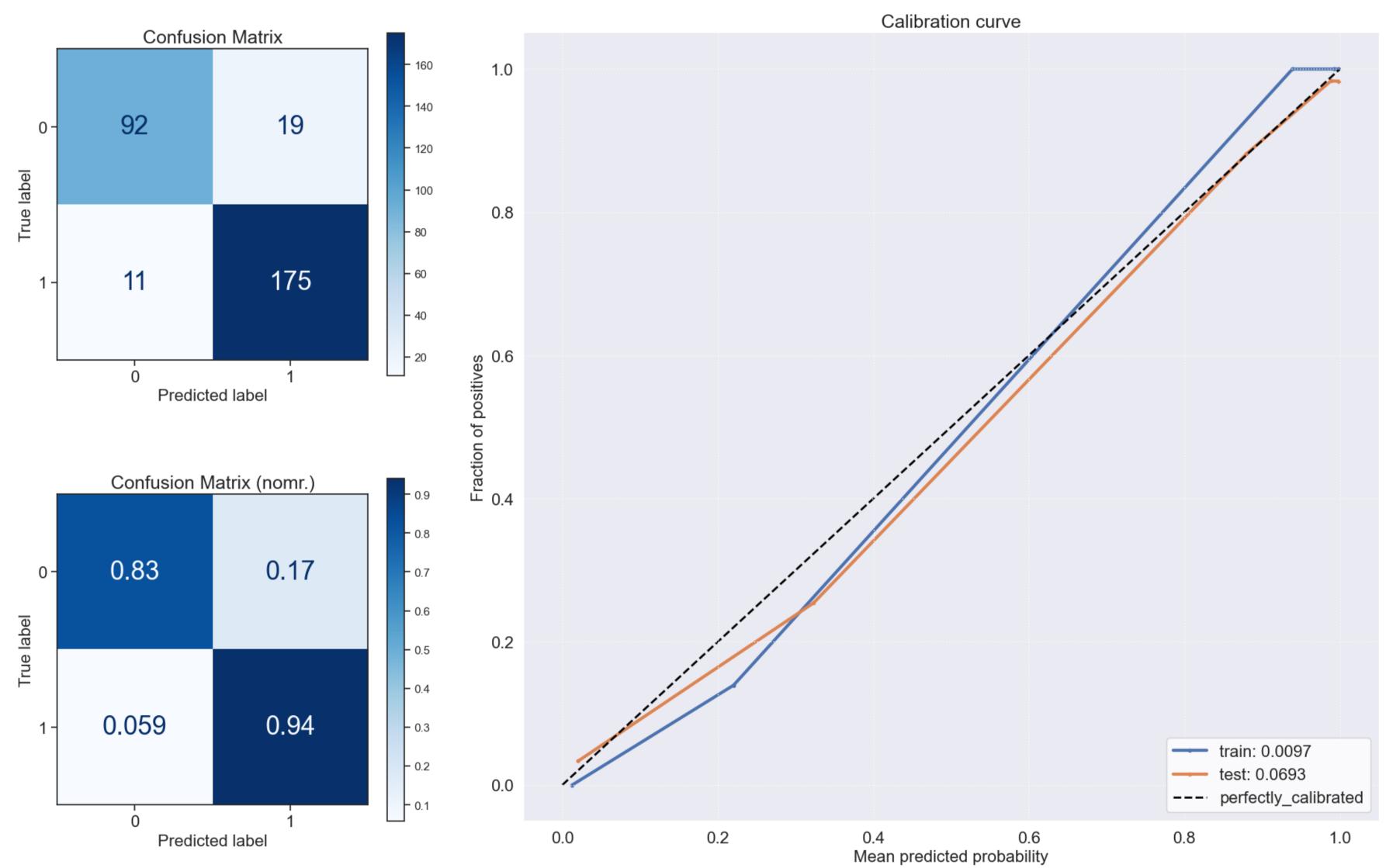
			Active/Inact	ive probability		
00		Inactive zone			Active zone	active (186) inactive (111) decoy (297)
50						
Percent 30						
20						
10						
	0.0	0.2	0.4 Prok	0.6 pability	0.8	1.0

Metric	Train	Test
AUC	1.0	0.9614
accuracy	0.9958	0.9024
balanced accuracy	0.9948	0.8875
recall_(sens)	0.9987	0.9462
specificity	0.9909	0.8288
precision	0.9946	0.9026
f1_score	0.9958	0.9014

Protein: P08172 - metric: SoftVotingXGBoostEnsemble







		Ac	tive/Inactive pr	obability		
50	Ina	ctive zone			Active zone	type active (186) inactive (111) decoy (297)
40						
Percent 08						
20						
10						
0—	0.0	.2 ().4 Probability	0.6	0.8	1.0

Metric	Train	Test
AUC	0.9998	0.9631
accuracy	0.9941	0.899
balanced accuracy	0.993	0.8848
recall_(sens)	0.9973	0.9409
specificity	0.9887	0.8288
precision	0.9933	0.9021
f1_score	0.9941	0.8982