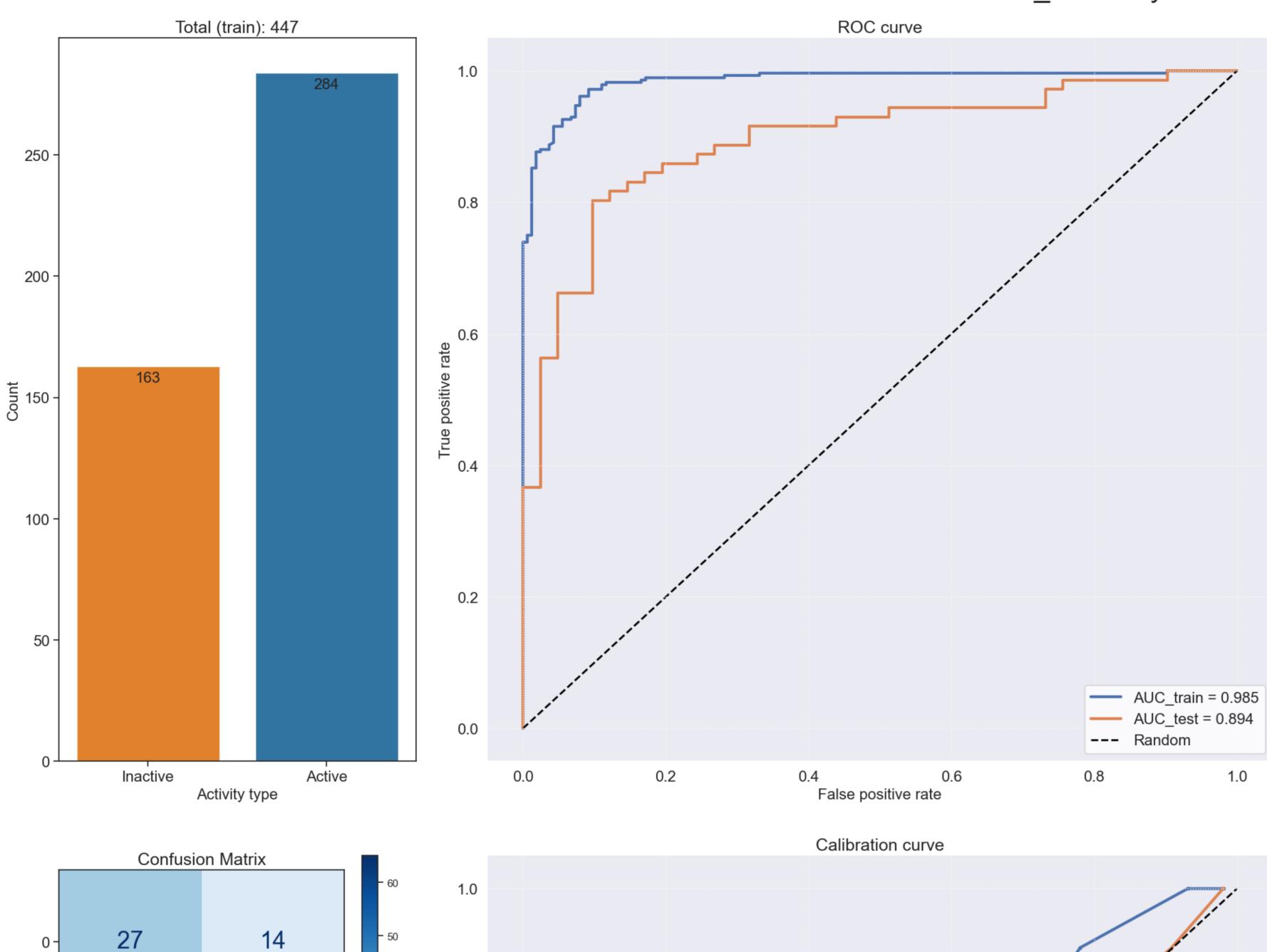
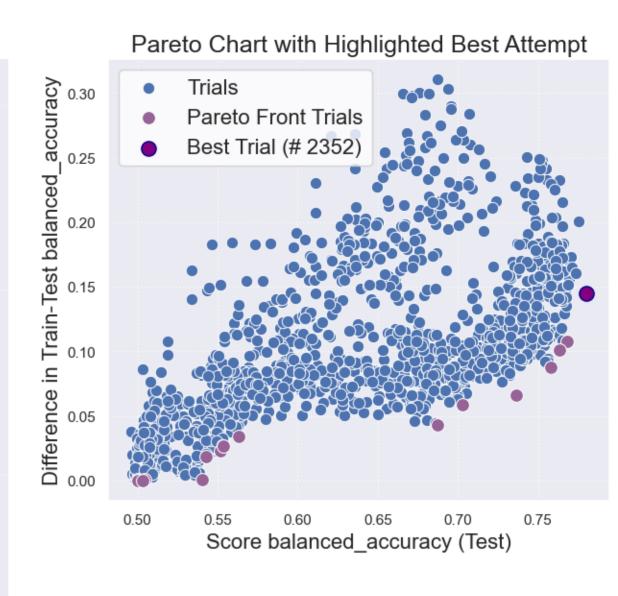
Protein: P49840 - metric: balanced_accuracy





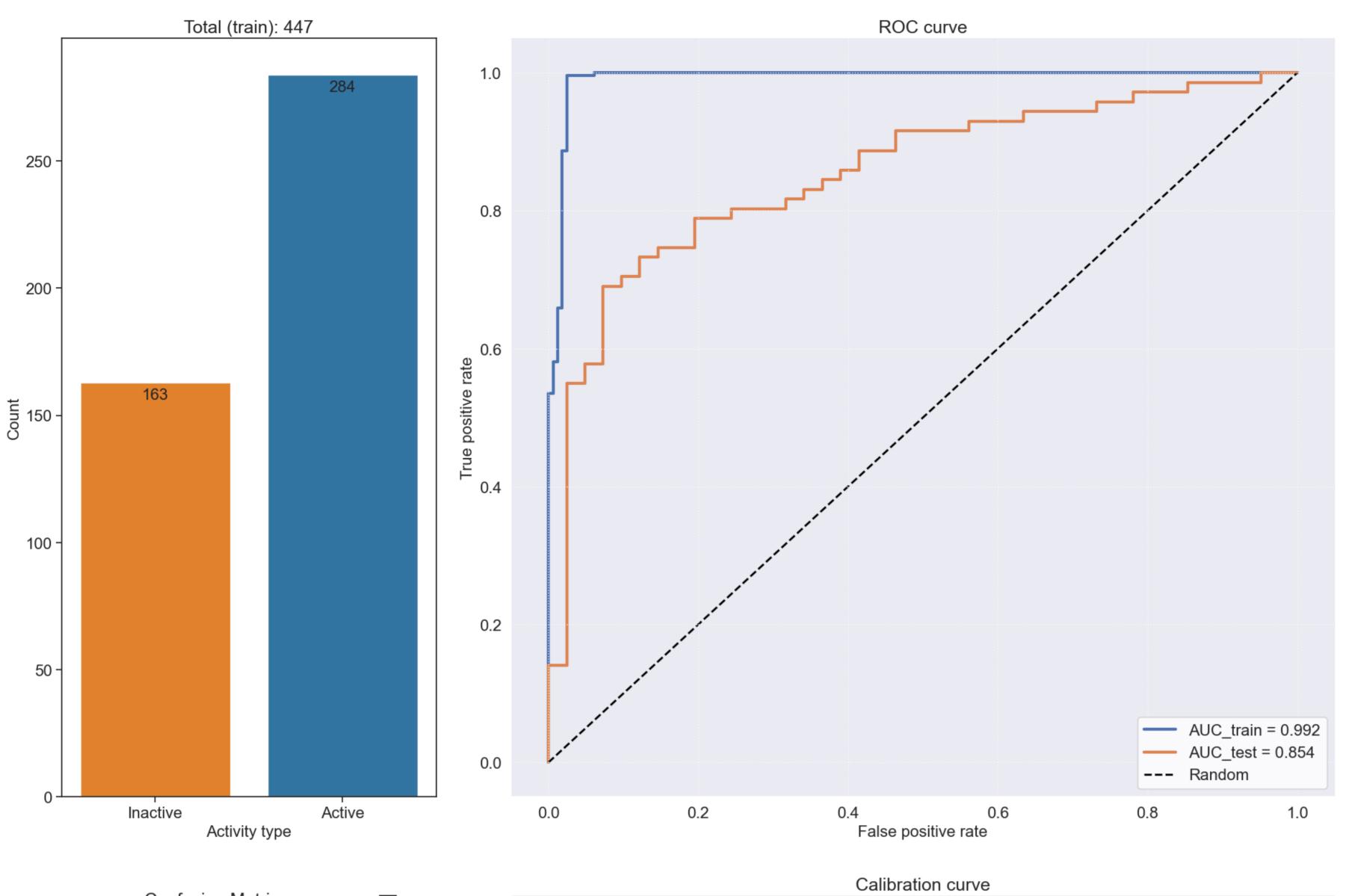
XGBoost Parameters	Value
alpha	1.4636
colsample_bytree	0.7369
gamma	0.1861
lambda	1.1632
learning_rate	0.0551
max_depth	8.0
min_child_weight	7.0
n_estimators	659.0
reg_alpha	0.2735
reg_lambda	0.478
scale_pos_weight	1.0154
subsample	0.9331

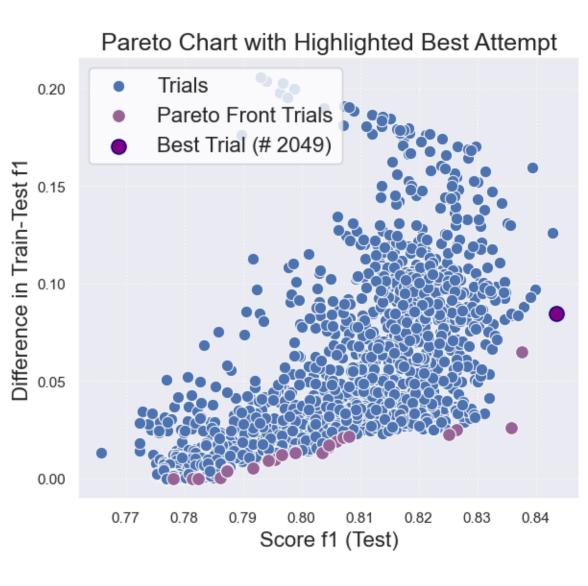
			- 60	1.0						
0 -	27	14	- 50							
label			- 40							
True			- 30	0.8						
1-	6	65	- 20							
	0	1	- 10	6.0 silves						
	Predicte	ed label		of positives 9.0						
	Confusion M	latrix (nomr.)	0.9	Fraction 6.0						
			- 0.8	L 0.4		,,,				
0 -	0.66	0.34	- 0.7			, property				
True label			- 0.6 - 0.5	0.2						
True			- 0.4		, para a la compania de la compania					
1-	0.085	0.92	- 0.3						train: 0.	.0576
			- 0.2	0.0					test: 0.7	
	0 Predicte	1 ed label	0.1		0.0	0.2	0.4 Mean predicted pr	0.6 obability	0.8	1.0

		Ac	tive/Inactive	probability		
4.4	Ina					inactive (41) decoy (112)
12						
± 10						
Percent 8 01						
6	пПппп		П			
4		_		П		
2						
0						
0	0.0 0.	2 0	.4	0.6	0.8	1.0
			Probabil	ity		

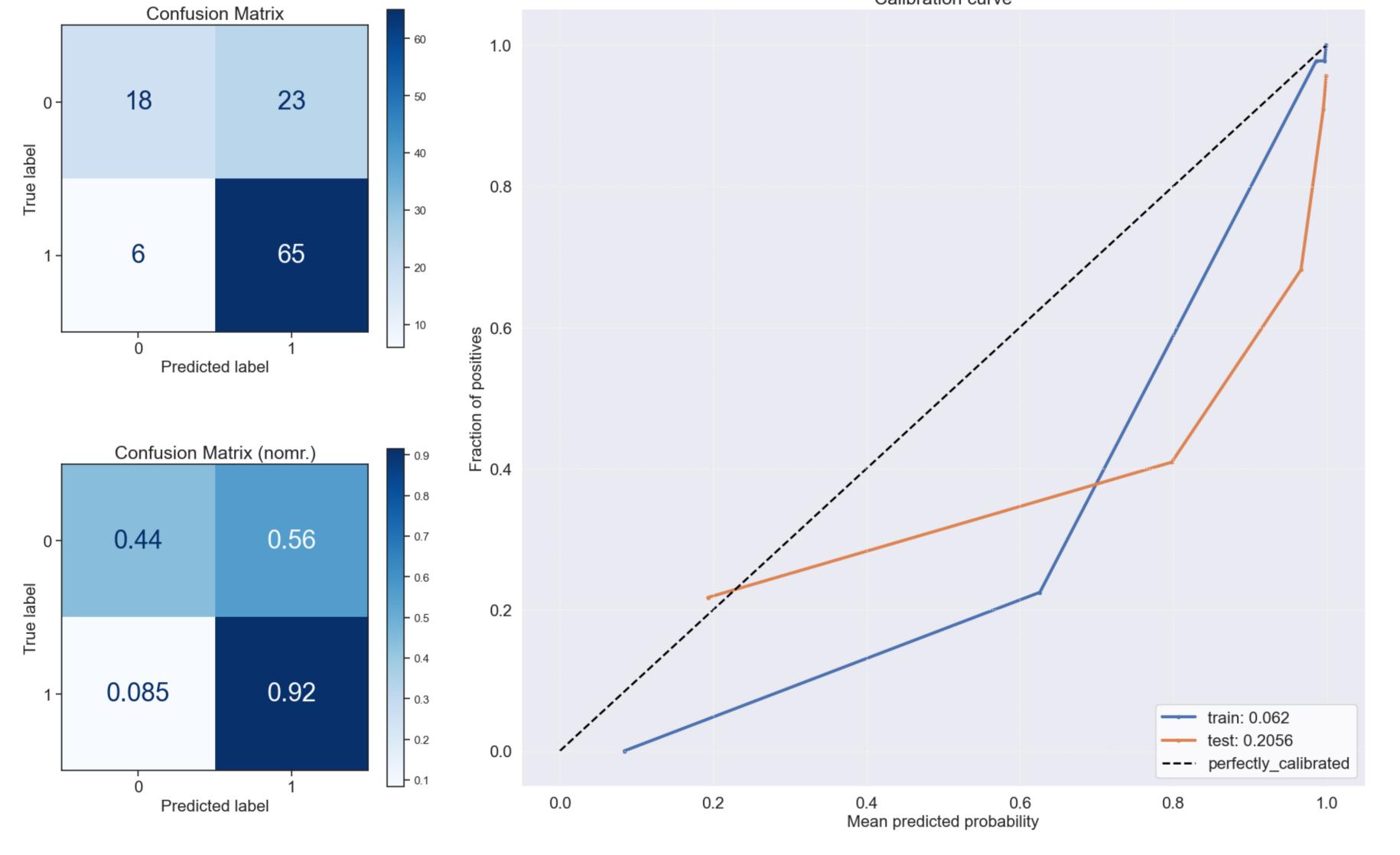
Metric	Train	Test
AUC	0.9848	0.8942
accuracy	0.9396	0.8214
balanced accuracy	0.9355	0.787
recall_(sens)	0.9507	0.9155
specificity	0.9202	0.6585
precision	0.9541	0.8228
f1_score	0.9396	0.8165

Protein: P49840 - metric: f1





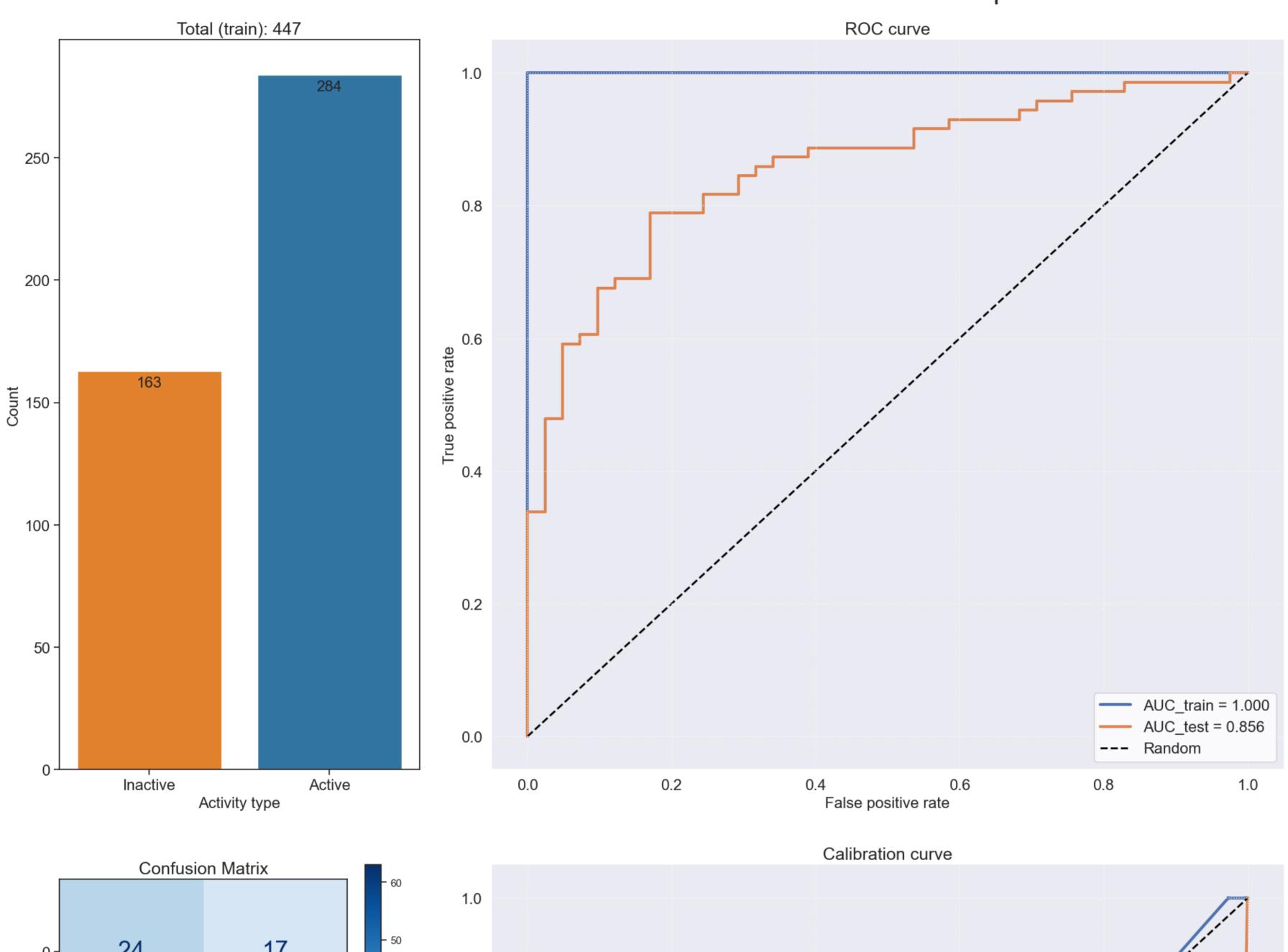
XGBoost Parameters	Value
alpha	2.9313
colsample_bytree	0.7897
gamma	0.4848
lambda	4.0272
learning_rate	0.3476
max_depth	9.0
min_child_weight	9.0
n_estimators	508.0
reg_alpha	0.9157
reg_lambda	0.4859
scale_pos_weight	22.7098
subsample	0.6109

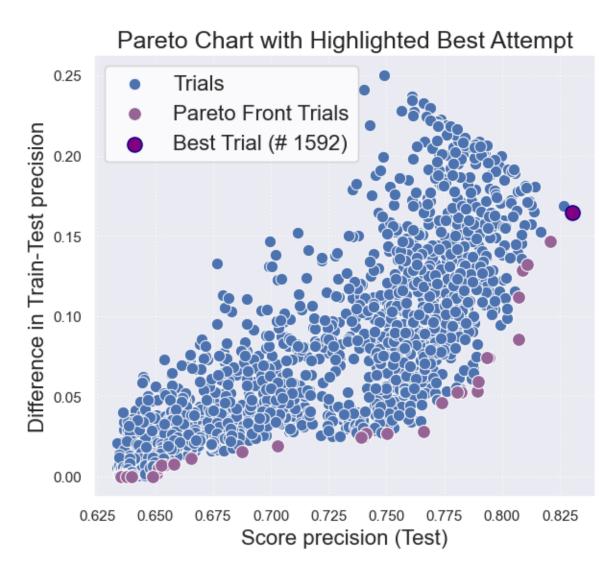


60				Inactive proba			
		Inactive zone				Active zone	type active (71) inactive (41)
40							
Percent 08							
20							
0-	0.0	0.2	0.4		0.6	0.8	1.0
		5.2	0.1	Probability	5.5	0.0	

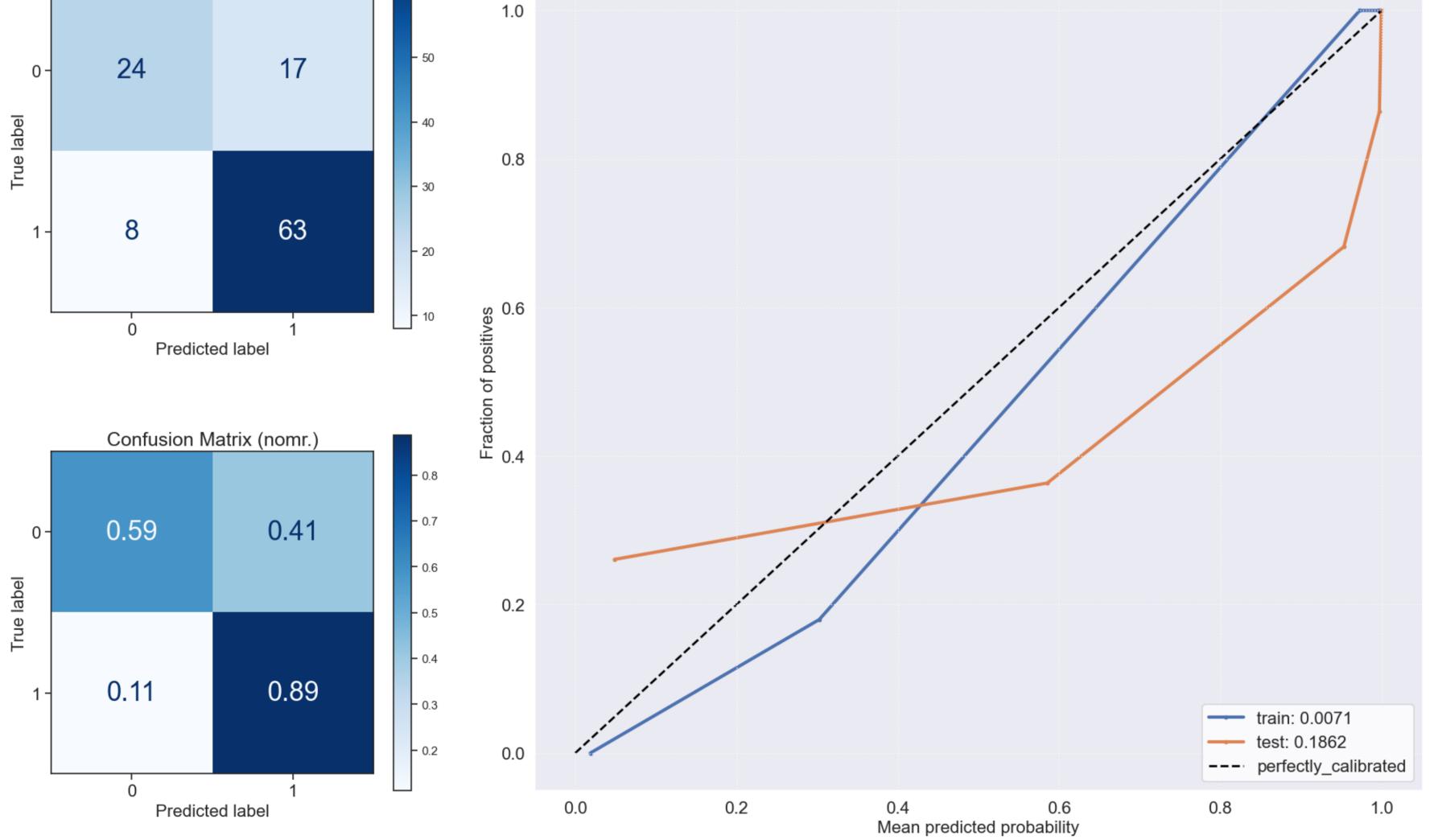
Metric	Train	Test
AUC	0.9917	0.8537
accuracy	0.9128	0.7411
balanced accuracy	0.8804	0.6773
recall_(sens)	1.0	0.9155
specificity	0.7607	0.439
precision	0.8793	0.7386
f1_score	0.9096	0.7211

Protein: P49840 - metric: precision



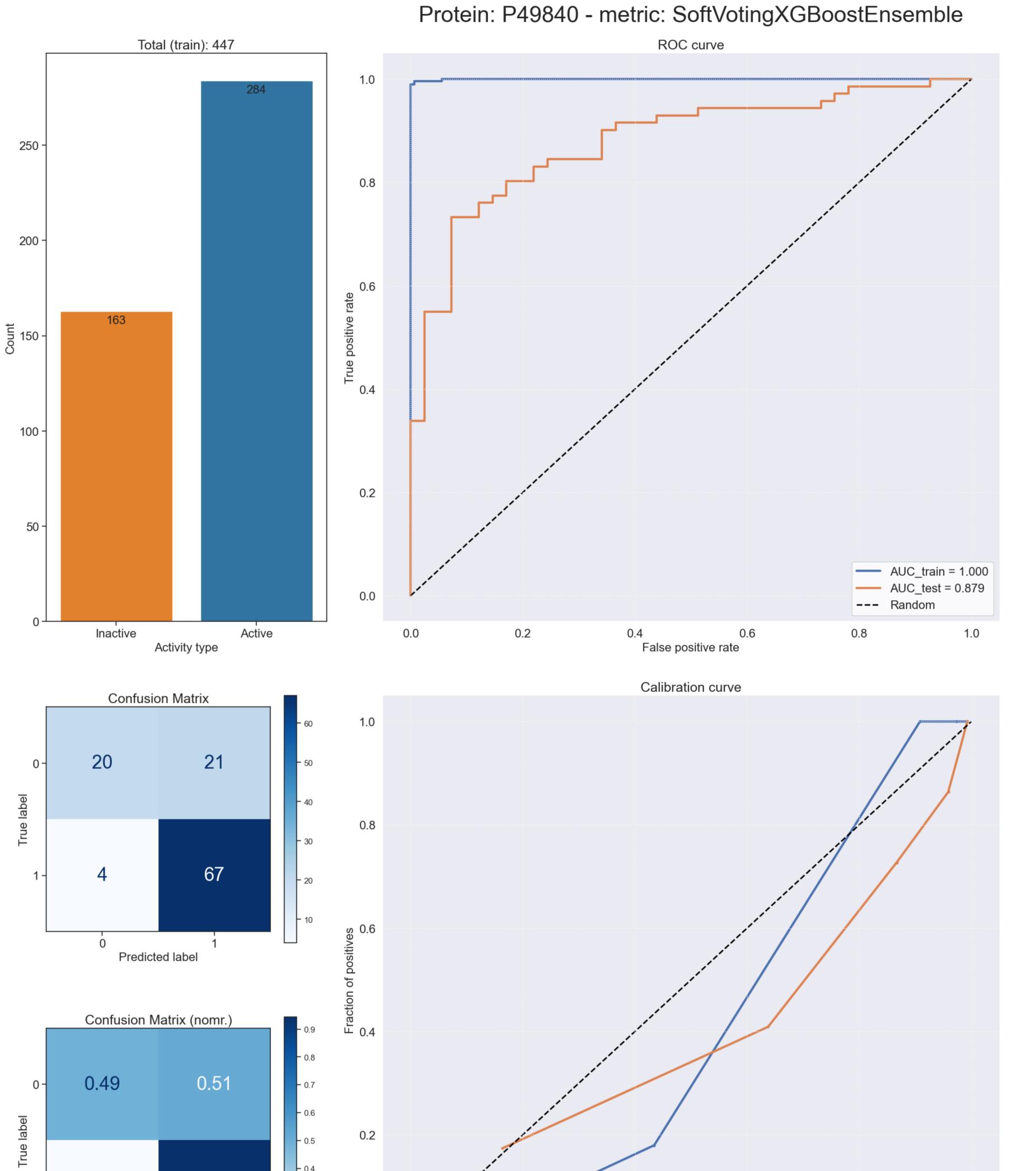


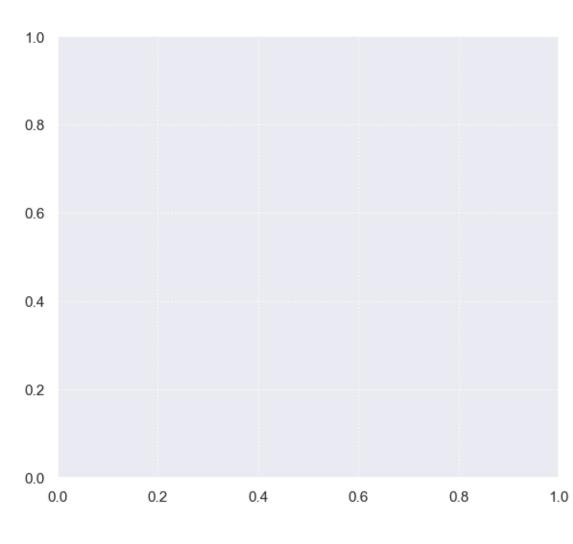
XGBoost Parameters	Value
alpha	1.9999
colsample_bytree	0.5388
gamma	0.2914
lambda	3.2909
learning_rate	0.865
max_depth	9.0
min_child_weight	2.0
n_estimators	742.0
reg_alpha	0.8004
reg_lambda	0.6208
scale_pos_weight	3.7381
subsample	0.6425

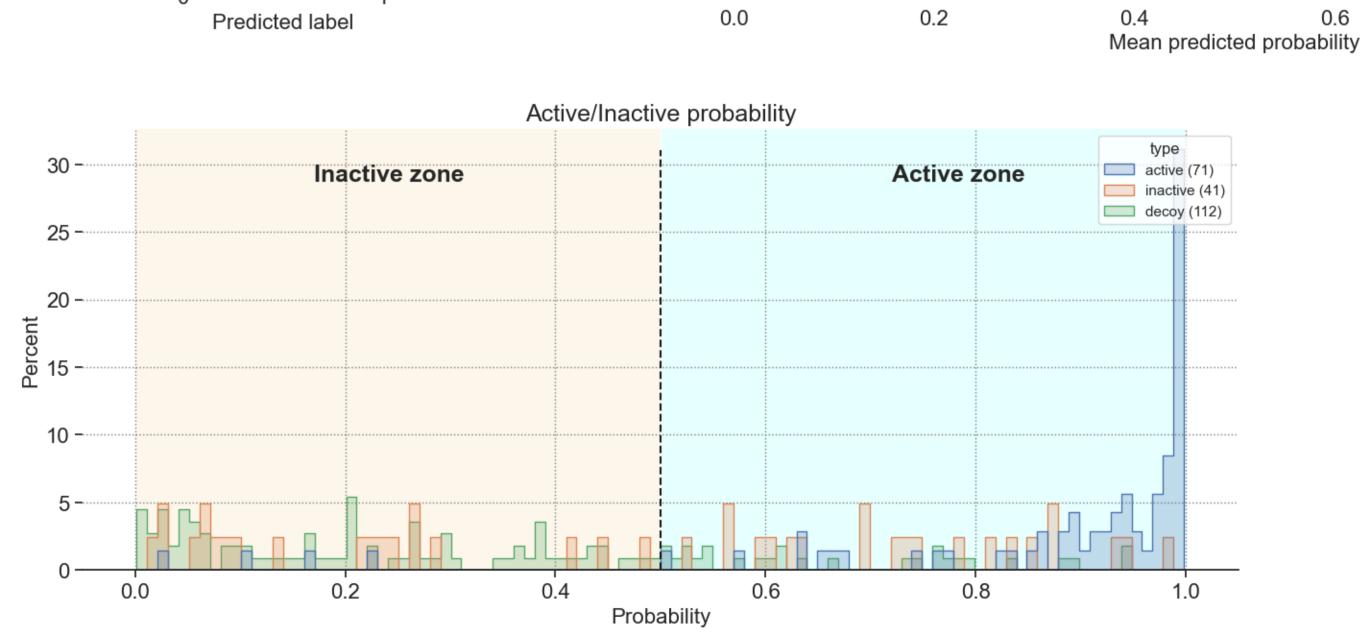


			Active/Inactive	e probability			
60	I.	nactive zone			Active z	one	type active (71) inactive (41) decoy (112)
50							
40							
Percent 8							
20							
10							
0—	0.0	0.2	0.4 Proba	0.6 ability	0.	8	1.0

Metric	Train	Test
AUC	1.0	0.8557
accuracy	0.9978	0.7768
balanced accuracy	0.9969	0.7363
recall_(sens)	1.0	0.8873
specificity	0.9939	0.5854
precision	0.9965	0.7875
f1_score	0.9978	0.7697







0.2

0.0

0.0

0.2

- 0.5

- 0.4

- 0.3

0.2

0.1

0.94

0.056

Predicted label

Metric	Train	Test
AUC	0.9998	0.8787
accuracy	0.9754	0.7768
balanced accuracy	0.9663	0.7157
recall_(sens)	1.0	0.9437
specificity	0.9325	0.4878
precision	0.9627	0.7614
f1_score	0.9752	0.7595

--- train: 0.0305

--- test: 0.1571

0.8

--- perfectly_calibrated

1.0