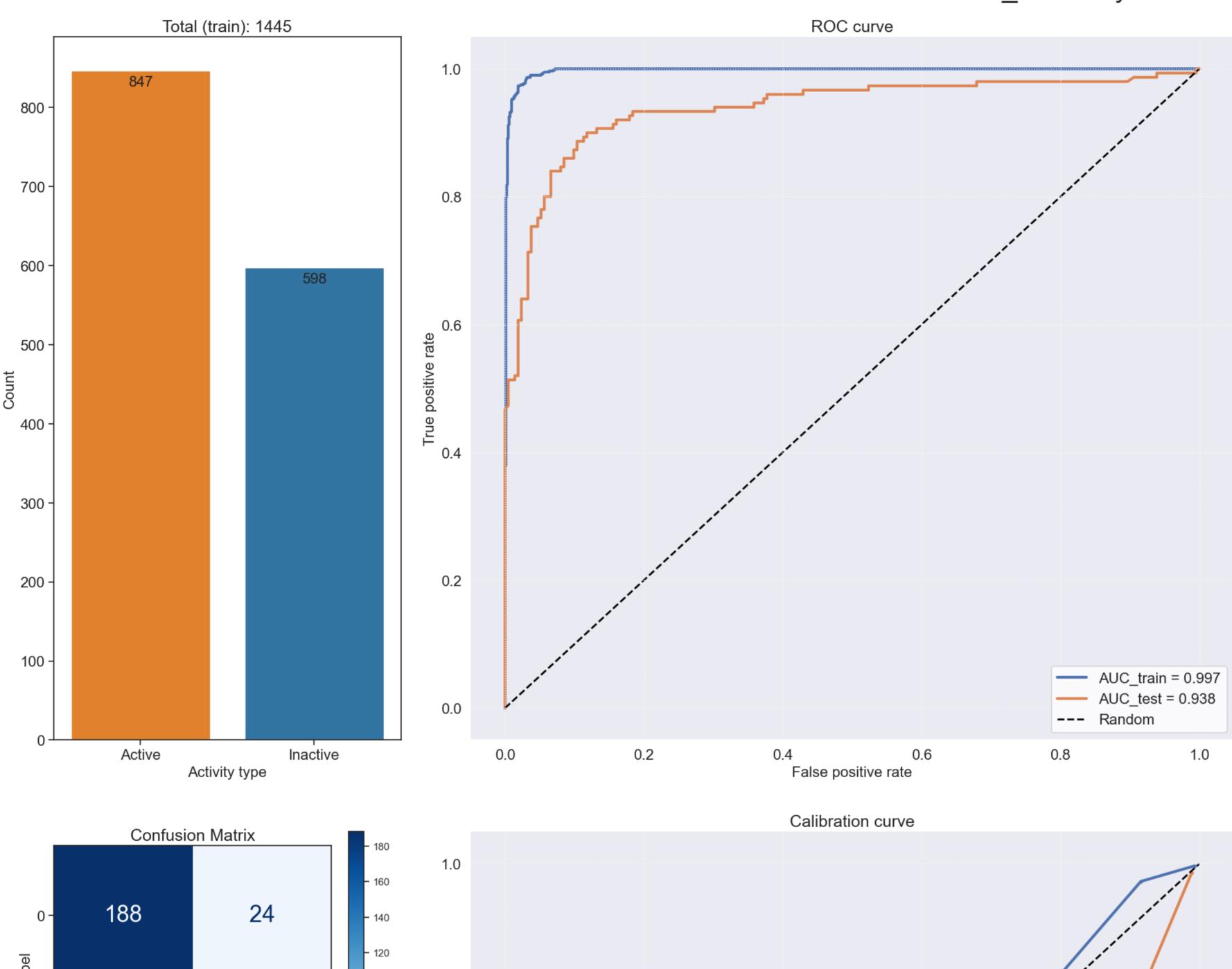
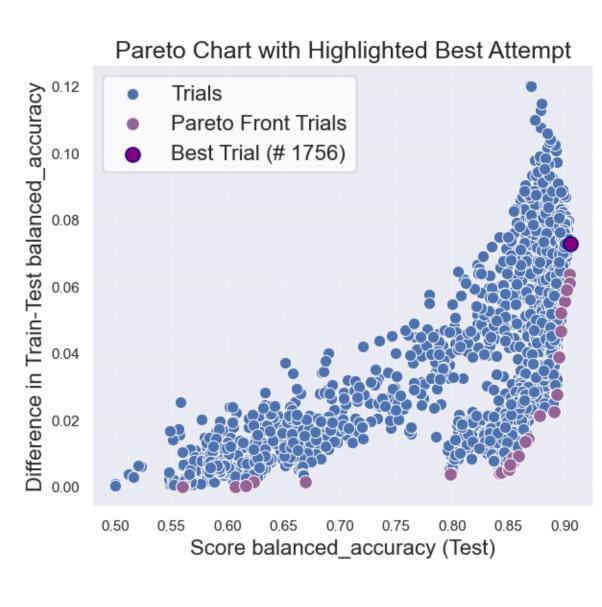
## Protein: P03956 - metric: balanced\_accuracy





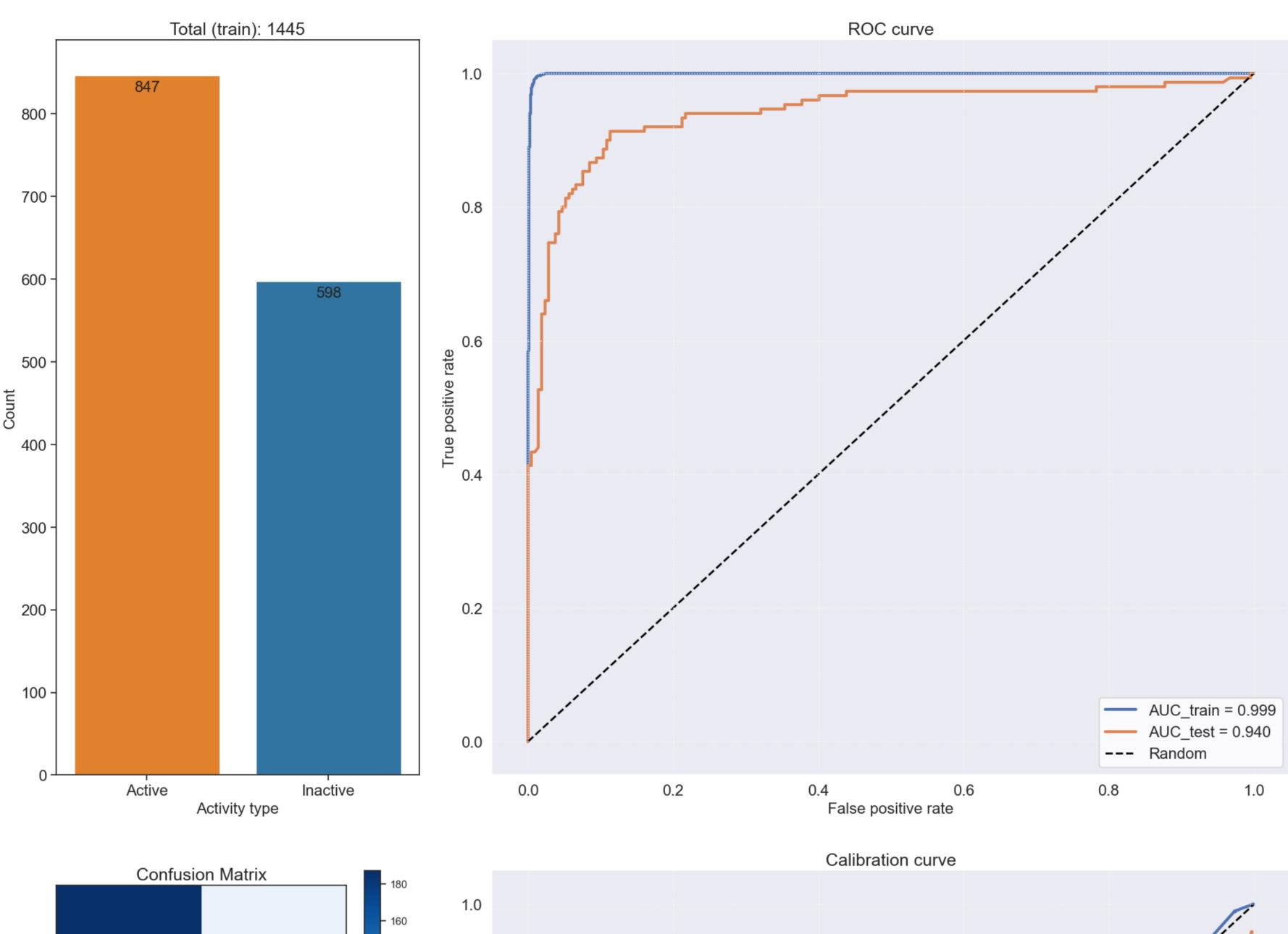
XGBoost Parameters	Value
alpha	3.7614
colsample_bytree	0.6484
gamma	0.1875
lambda	2.4389
learning_rate	0.0529
max_depth	4.0
min_child_weight	2.0
n_estimators	871.0
reg_alpha	0.1215
reg_lambda	0.6168
scale_pos_weight	1.67
subsample	0.7283

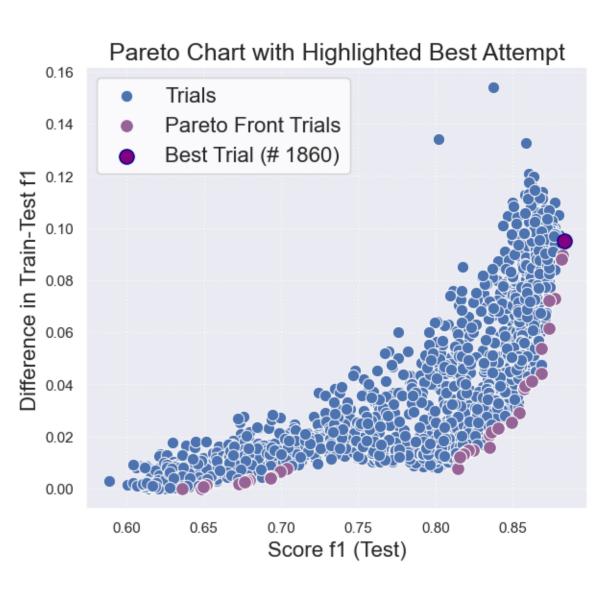
	Contusio	on Matrix	100							
True label	188	24	- 180 - 160 - 140 - 120	1.0					Jan de la companya de	
1-	16 0 Predicte	134 ed label	- 100 - 80 - 60 - 40 - 20	f positives 9.0						
label		latrix (nomr.)  0.11	- 0.8 - 0.7 - 0.6	Fraction of positives 5.0		, , o o o o o o o o o o o o o o o o o o				
True label	0.11	0.89	- 0.5 - 0.4 - 0.3 - 0.2	0.0					test: 0	0.0215 0.0898 ctly_calibrated
	0 Predicte	1 ed label			0.0	0.2	0.4 Mean predicted	0.6 d probability	0.8	1.0

			Active/Inact	ive probability			
40		Inactive zone			Active z	type active (150) inactive (212 decoy (362)	
30							_
Percent 05							
10							
0		<u></u>					
o o	0.0	0.2	0.4 Prot	0.6 pability	0.8	8 1.0	

Metric	Train	Test
AUC	0.9973	0.9378
accuracy	0.9758	0.8895
balanced accuracy	0.9771	0.8901
recall_(sens)	0.9849	0.8933
specificity	0.9693	0.8868
precision	0.9577	0.8481
f1_score	0.9758	0.8899

## Protein: P03956 - metric: f1





XGBoost Parameters	Value
alpha	1.55
colsample_bytree	0.7758
gamma	0.4821
lambda	2.4773
learning_rate	0.0452
max_depth	9.0
min_child_weight	3.0
n_estimators	947.0
reg_alpha	0.1012
reg_lambda	0.0049
scale_pos_weight	4.3661
subsample	0.7912

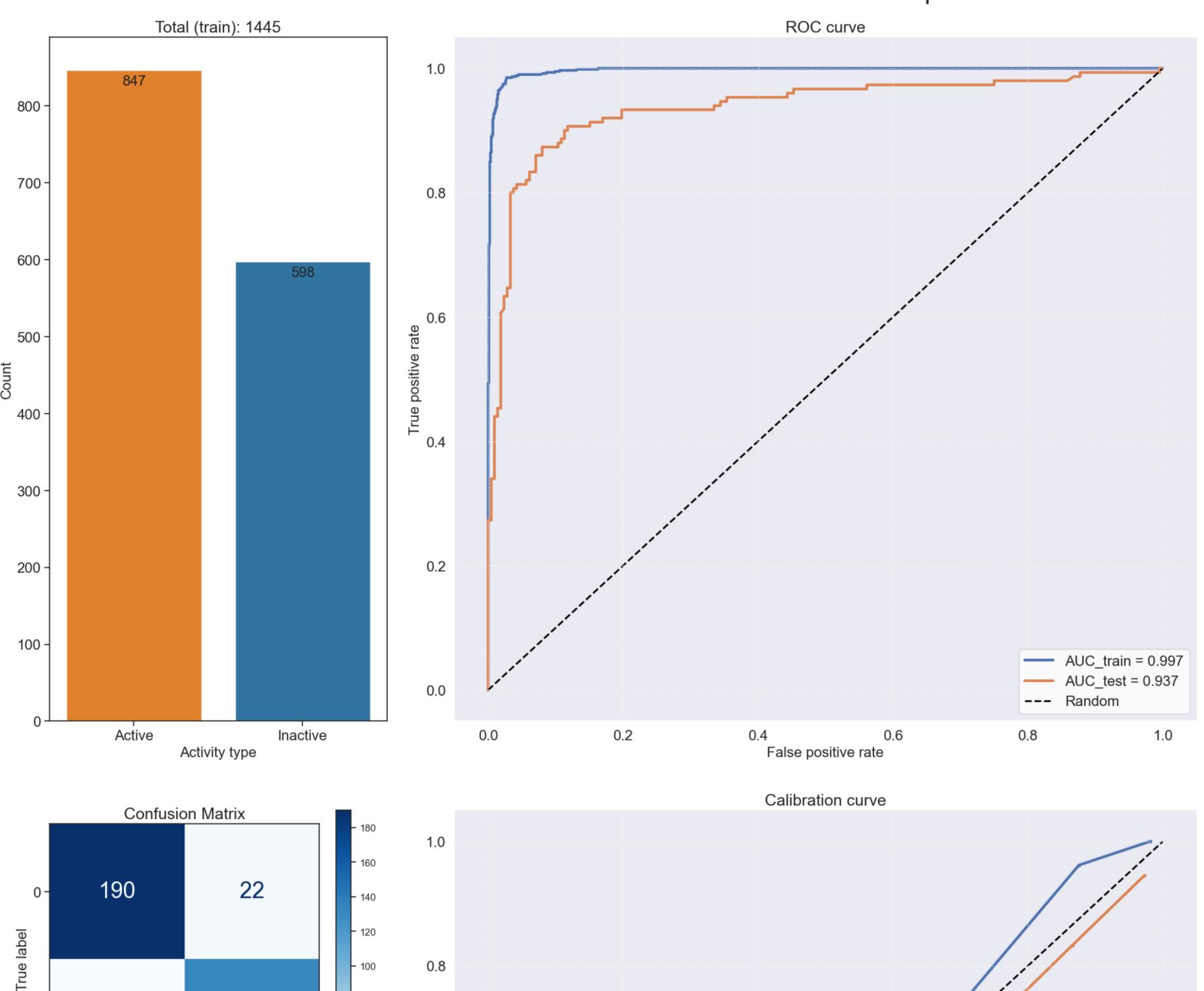
	Comadic	711 IVIGUIX	1 180							
abel O	187	25	- 160 - 140 - 120	1.0						
True label	0 Predicte	137	- 100 - 80 - 60 - 40 - 20	0.0 and the second seco						
label	Confusion M		- 0.9 - 0.8 - 0.7 - 0.6	Fraction of 8.0		, or				
True lal	0.087	0.91	- 0.5 - 0.4 - 0.3 - 0.2 - 0.1	0.2					train: 0	
	0 Predicte	1 ed label	v.1		0.0	0.2	0.4 Mean predicted	0.6 probability	0.8	1.0

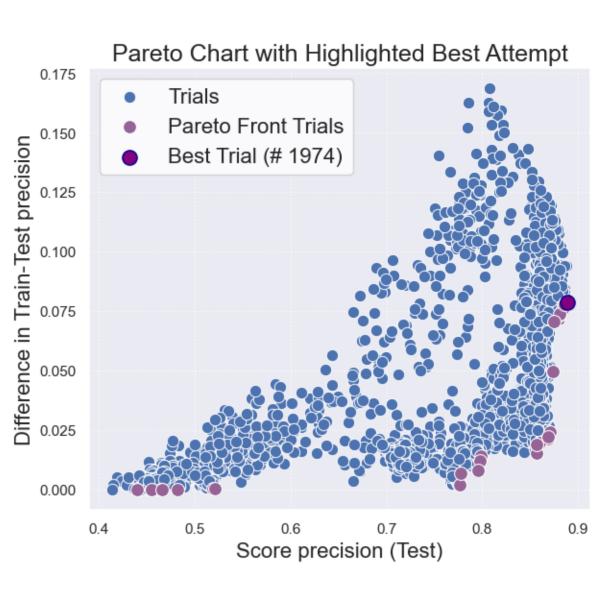
50		Inactive zone			Active zone	type active (150) inactive (212)
40						
Percent						
<u>20</u>						
10						
0 —		0.2	0.4	0.6	0.8	10
	0.0	0.2	0.4 Probab		0.0	1.0

Active/Inactive probability

Metric	Train	Test
AUC	0.9992	0.9397
accuracy	0.9799	0.895
balanced accuracy	0.9829	0.8977
recall_(sens)	1.0	0.9133
specificity	0.9658	0.8821
precision	0.9537	0.8457
f1_score	0.98	0.8955

## Protein: P03956 - metric: precision





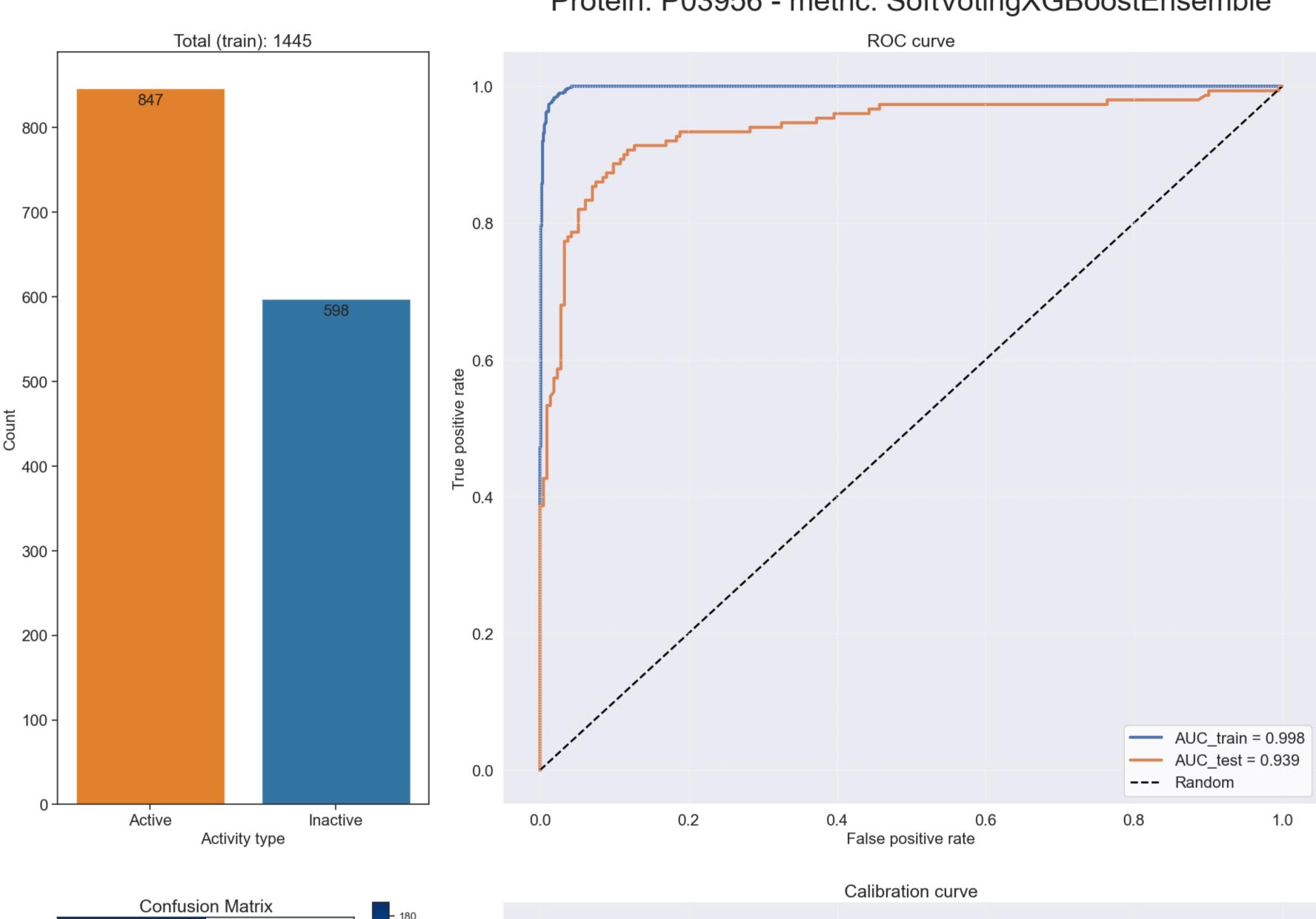
XGBoost Parameters	Value
alpha	0.2074
colsample_bytree	0.736
gamma	0.4446
lambda	3.969
learning_rate	0.0084
max_depth	10.0
min_child_weight	1.0
n_estimators	826.0
reg_alpha	0.1849
reg_lambda	0.0799
scale_pos_weight	1.2361
subsample	0.6487

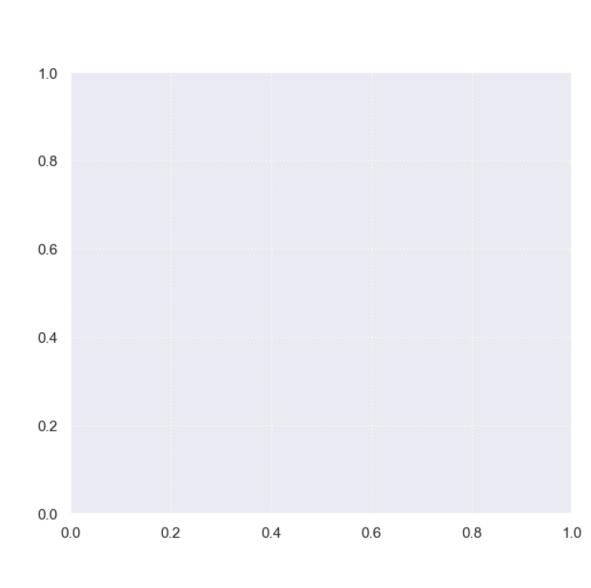
0 -	190	22	- 140								
abel			- 120								
True label			- 100 - 80	0.8							
1-	18	132	- 60								
			- 40	0.6							
	0 Predicte	1 ed label		positives 9.0			.1				
				ð							
	Confusion M	latrix (nomr.)	1	Fraction 5.0							
			- 0.8 - 0.7			مر					
0 -	0.9	0.1	- 0.7			por a de la companya					
True label			- 0.5	0.2							
Tru			- 0.4		, in the second						
1-	0.12	0.88	- 0.3							rain: 0.024	
	-	1	- 0.2	0.0	· · · · · · · · · · · · · · · · · · ·					est: 0.085 erfectly_calib	rated
	0 Predicte	ed label			0.0	0.2	0.4 Mean predicted pro	0.6 bability	0.8		1.0

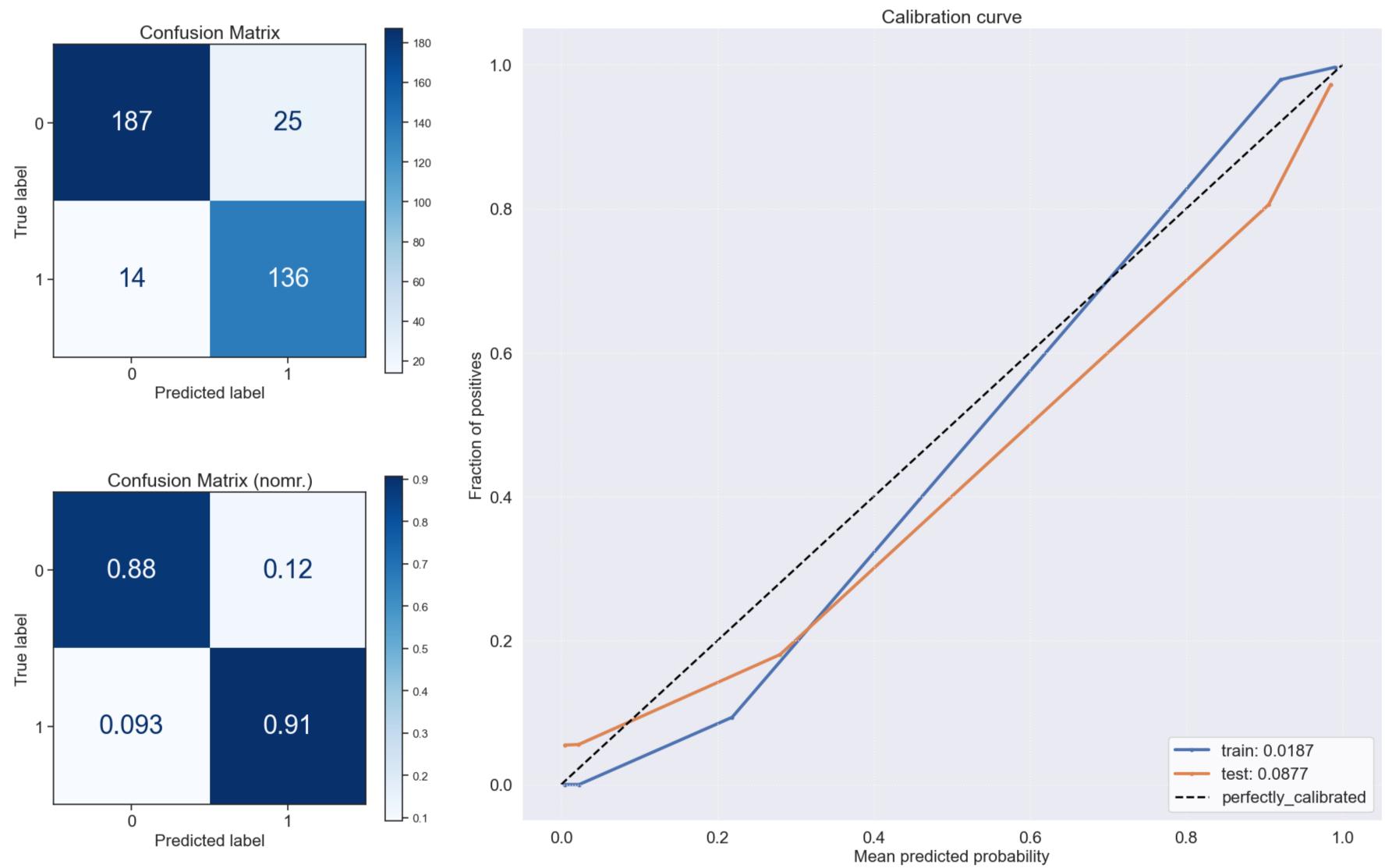
		Active/Inac	tive probability	
25 <del></del>	Ina	active zone	Active	type active (150) inactive (212) decoy (362)
15 10				
5 <b>-</b>	0.0 0	0.4 Pro	0.6 obability	0.8 1.0
ĺ		110		

Metric	Train	Test
AUC	0.9967	0.9366
accuracy	0.9744	0.8895
balanced accuracy	0.9745	0.8881
recall_(sens)	0.9749	0.88
specificity	0.974	0.8962
precision	0.9636	0.8571
f1_score	0.9744	0.8897

## Protein: P03956 - metric: SoftVotingXGBoostEnsemble







Active/Inactive probability							
					Active zone	inactive (212) decoy (362)	
25						П	
- 05							
10							
5							
Ü	0.0	0.2	0.4 Proba	0.6 ability	0.8	1.0	

Metric	Train	Test
AUC	0.9982	0.939
accuracy	0.9785	0.8923
balanced accuracy	0.9802	0.8944
recall_(sens)	0.99	0.9067
specificity	0.9705	0.8821
precision	0.9595	0.8447
f1_score	0.9786	0.8927