neg_cluster_based_classifier

October 25, 2023

```
[ ]: import numpy as np
     import pandas as pd
     import data_lib
     import plot_lib
     import transform_lib
     import decision_lib
     from sklearn import cluster

     np.random.seed(200)
```

```
[ ]: # print available data summary
     _ = data_lib.explore_datasets(datafolder="../Data",verbose=True)
     print(data_lib.LABELS_LIST)
```

```
--------------------------------------------------------------------------------
--------------
-- The following 4 groups were found
-- They contain 40 datasets
-- The first printed entity is the key to the returned dictionary
-----------------------------------
Group: ../Data/6P-positive-dilution-series-2-labelled/droplet-level-data/RawData
po-di-se-2-A4, files: 13                po-di-se-2-C4, files: 13
po-di-se-2-A1, files: 13
po-di-se-2-B1, files: 13                po-di-se-2-D1, files: 13
po-di-se-2-B4, files: 13
po-di-se-2-C1, files: 13                po-di-se-2-D4, files: 13
-----------------------------------
Group: ../Data/6P-positive-dilution-series-1-labelled/droplet-level-data/RawData
po-di-se-1-D4, files: 13                po-di-se-1-A4, files: 13
po-di-se-1-A1, files: 13
po-di-se-1-D1, files: 13                po-di-se-1-B1, files: 13
po-di-se-1-C1, files: 13
po-di-se-1-B4, files: 13                po-di-se-1-C4, files: 13
-----------------------------------
Group: ../Data/6P-positive-dilution-series-labelled/droplet-level-data/RawData
po-di-se-B8, files: 13                  po-di-se-A8, files: 13
po-di-se-C8, files: 13
po-di-se-D8, files: 13
```

```
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Group: ../Data/6P-wastewater-samples-labelled/droplet-level-data/RawData
wa-sa-A2, files: 13                     wa-sa-B4, files: 13
wa-sa-C5, files: 13
wa-sa-C4, files: 13                     wa-sa-B3, files: 13
wa-sa-B2, files: 13
wa-sa-A5, files: 13                     wa-sa-A3, files: 13
wa-sa-C2, files: 13
wa-sa-C3, files: 13                     wa-sa-D3, files: 13
wa-sa-D4, files: 13
wa-sa-B1, files: 13                     wa-sa-A4, files: 13
wa-sa-A1, files: 13
wa-sa-D2, files: 13                     wa-sa-D5, files: 13
wa-sa-C1, files: 13
wa-sa-B5, files: 13                     wa-sa-D1, files: 13
-----------------------------------
['IAV-M_POS', 'IAV-M_NEG', 'IBV-M_POS', 'IBV-M_NEG', 'MHV_POS', 'MHV_NEG', 'RSV-
N_POS', 'RSV-N_NEG', 'SARS-N1_POS', 'SARS-N1_NEG', 'SARS-N2_POS', 'SARS-N2_NEG']
```

0.0.1 Get samples for negative control

[ ]:

```
# negative control
#df_negative_control = data_lib.load_dataset([],["po-di-se-1-D1",␣
 ↪"po-di-se-1-D4", "po-di-se-2-D1", "po-di-se-2-D4", "po-di-se-D8"])
df_negative_control = data_lib.load_dataset([],["wa-sa-D3", "wa-sa-D5"])
np_negative_control = df_negative_control.to_numpy()
df_y_negative_control = pd.DataFrame(np.zeros(df_negative_control.shape[0]))
```

[ ]:

```
# compute transformation on waste water
df_wa = data_lib.load_dataset(None, [
                                     #"wa-sa-A2", "wa-sa-B4",
                                     #"wa-sa-C5", "wa-sa-C4",
                                     "wa-sa-B3", "wa-sa-B2",
                                     #"wa-sa-A5", "wa-sa-A3",
                                     #"wa-sa-C2", "wa-sa-C3",
                                     #"wa-sa-D3", "wa-sa-D4",
                                     #"wa-sa-B1", "wa-sa-A4",
                                     #"wa-sa-A1", "wa-sa-D2",
                                     #"wa-sa-D5", "wa-sa-C1",
                                     ])
np_wa = df_wa.to_numpy(copy=True)[:,:6]
ZCA_whitener = transform_lib.WhitenTransformer(transform_lib.Whitenings.ZCA_COR)
```

[ ]:

```
# fix clustering algorithm
cluster_engine = cluster.DBSCAN(eps = 1000, min_samples = 1, n_jobs=8)
```

```
# initialize desion maker based on negative control cluster and defined some␣
 ↪settings
neg_cluster_based_classifier = decision_lib.
 ↪NegativeClusterBasedClassifier(negative_cluster=np_negative_control,
                                            cluster_algorithm=cluster_engine,
                                            aggressiveness=[7,17, 30, 15, 15,␣
 ↪19],
                                            whitening_transformer=ZCA_whitener,
                                           ␣
 ↪prediction_axis=['SARS-N2_POS','SARS-N1_POS','IBV-M_POS','RSV-N_POS','IAV-M_POS','MHV_POS']
                                            )

# fit the whitening transformer and compute thresholds for negative control␣
 ↪culster
neg_cluster_based_classifier.fit(np_wa)

# predict does not scale well due to clustering inside
df_predictions = neg_cluster_based_classifier.predict(np_wa,␣
 ↪cluster_on_transformed=False)
```

1 Validation

1.1 Get some (not very usefull) stats

Most points are simply negatives

[ ]:

```
neg_cluster_based_classifier.validate_labels(df_wa.iloc[:,6:])
```

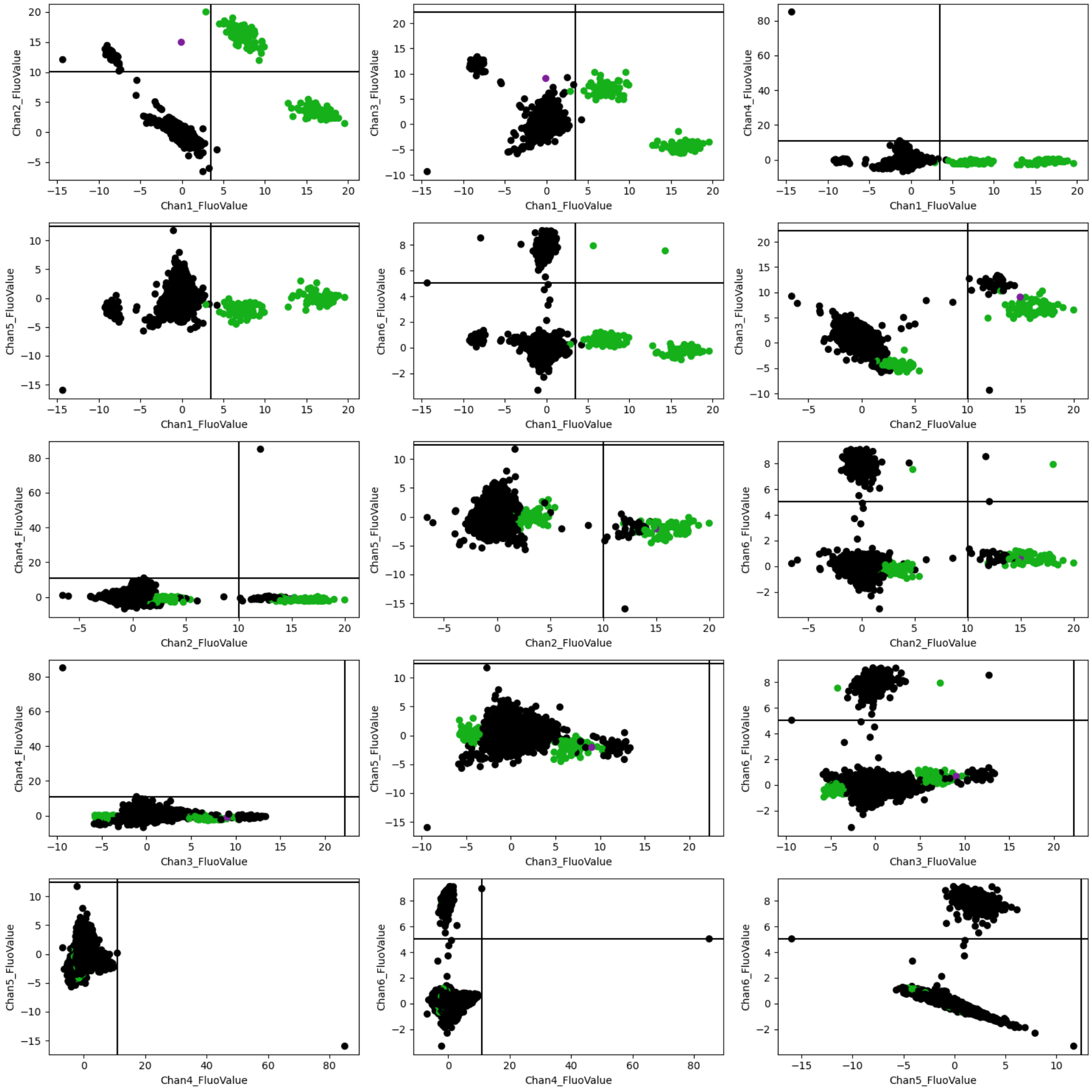
```
Total error rate: 0.006953408955661146
Total error per class:
    SARS-N2_POS  SARS-N1_POS  IBV-M_POS  RSV-N_POS  IAV-M_POS   MHV_POS
0        0.0039     0.002747    0.01431        0.0   0.002719  0.018045


False negative rate: 0.003483570911954004
False negative rate per class:
    SARS-N2_POS  SARS-N1_POS  IBV-M_POS  RSV-N_POS  IAV-M_POS   MHV_POS
0           0.0          0.0    0.01431        0.0   0.002719  0.003873


False positive rate: 0.003469838043707142
False negative rate per class:
    SARS-N2_POS  SARS-N1_POS  IBV-M_POS  RSV-N_POS  IAV-M_POS   MHV_POS
0        0.0039     0.002747        0.0        0.0        0.0  0.014172
```

1.2 Plot the predictions

- Black = True negative prediction
- Green = True positive prediciton
- Purple = False negative
- Red = False positive

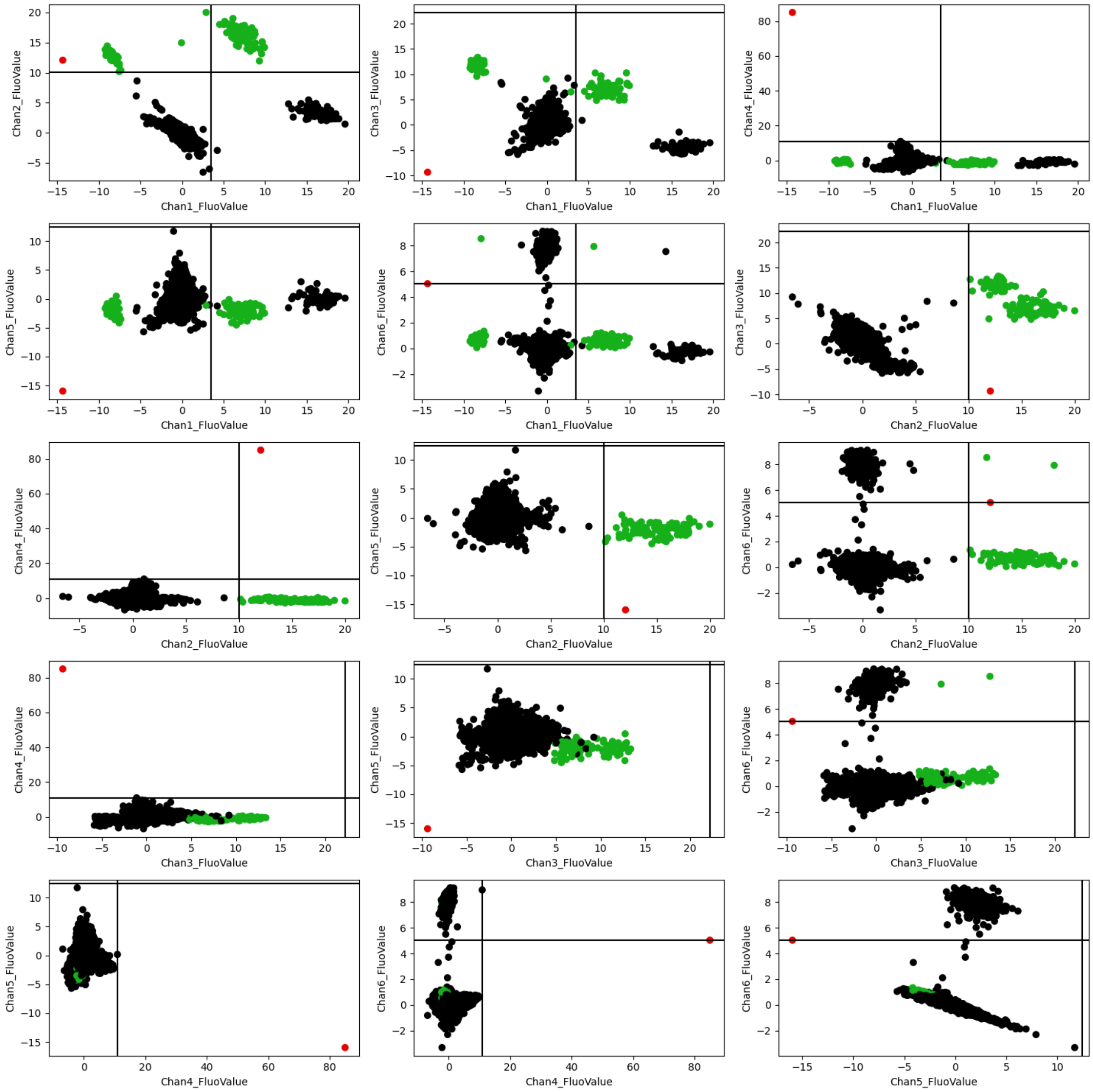
Plot SARS-N2_POS associated with channel 1

```
[ ]: plot_lib.pairwise_plots_pred_true_thresh(pd.
      ↪DataFrame(data=neg_cluster_based_classifier.X_transformed, columns=df_wa.
      ↪iloc[:,:6].columns),
                                                  df_predictions["SARS-N2_POS"],
                                                  df_wa.loc[:,"SARS-N2_POS"],
                                                  ␣
      ↪axis_thresh=neg_cluster_based_classifier.axis_threshholds)
```



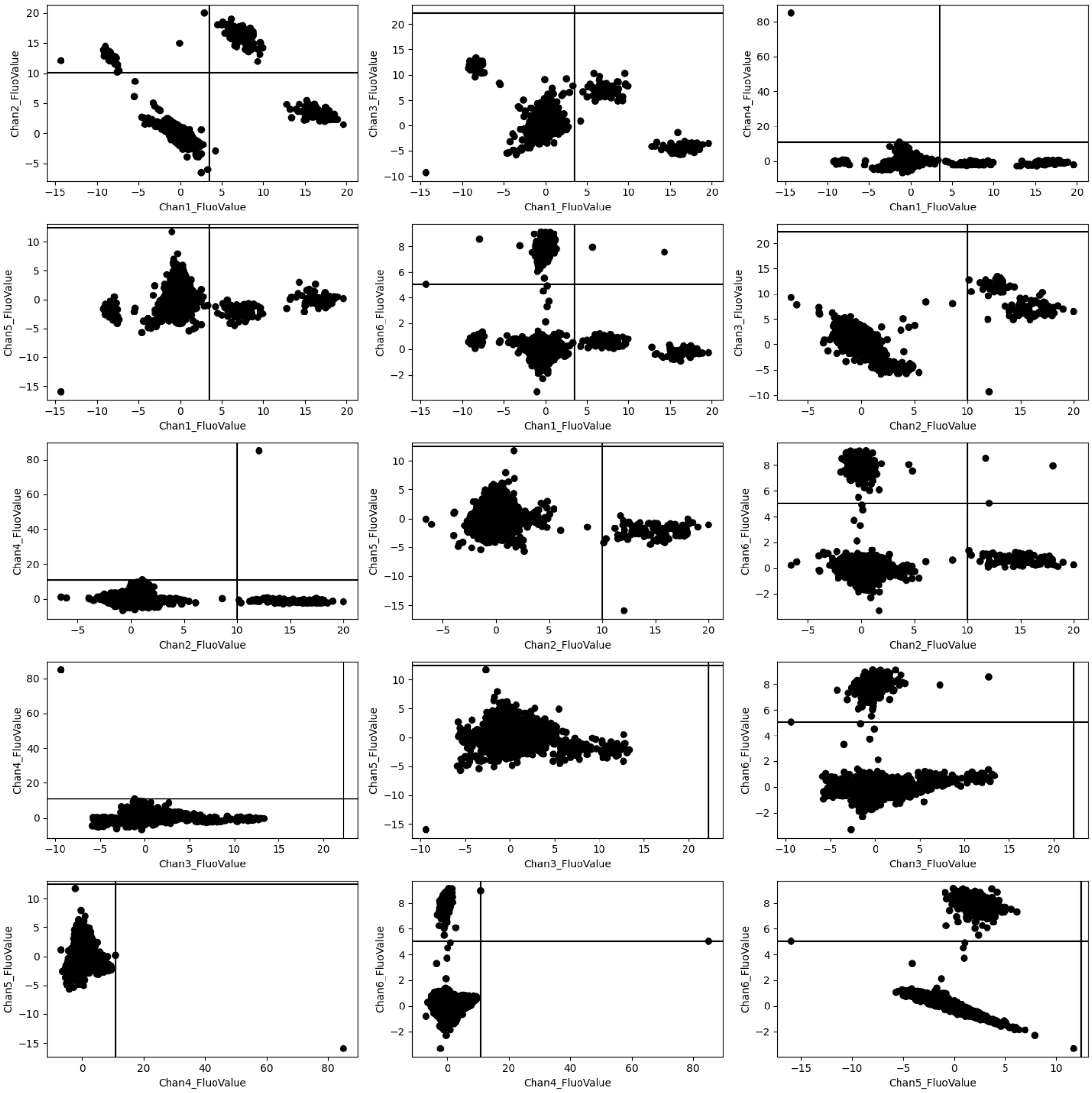
Plot SARS-N1_POS associated with cannel 2

[ ]:
```
plot_lib.pairwise_plots_pred_true_thresh(pd.
↪DataFrame(data=neg_cluster_based_classifier.X_transformed, columns=df_wa.
↪iloc[:,:6].columns),
                                            df_predictions["SARS-N1_POS"],
                                            df_wa.loc[:,"SARS-N1_POS"],
                                            axis_thresh=neg_cluster_based_classifier.
↪axis_threshholds
                                            )
```



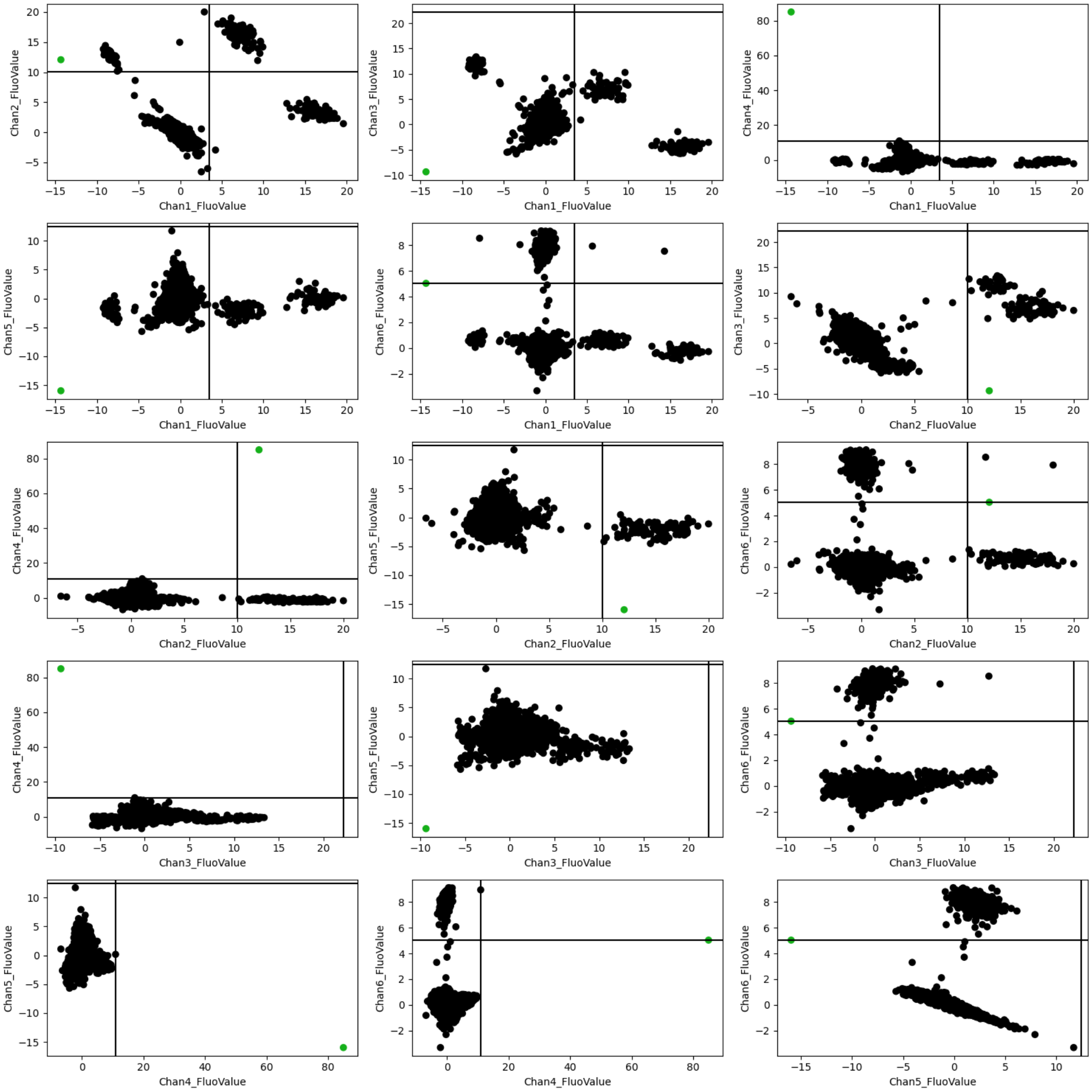
Plot IBV-M_POS associated with cannel 3

```
[ ]: plot_lib.pairwise_plots_pred_true_thresh(pd.
     ↪DataFrame(data=neg_cluster_based_classifier.X_transformed, columns=df_wa.
     ↪iloc[:,:6].columns),
                                                df_predictions["IBV-M_POS"],
                                                df_wa.loc[:,"IBV-M_POS"],
                                                ␣
     ↪axis_thresh=neg_cluster_based_classifier.axis_threshholds,
                                                )
```



Plot RSV-N_POS associated with cannel 4

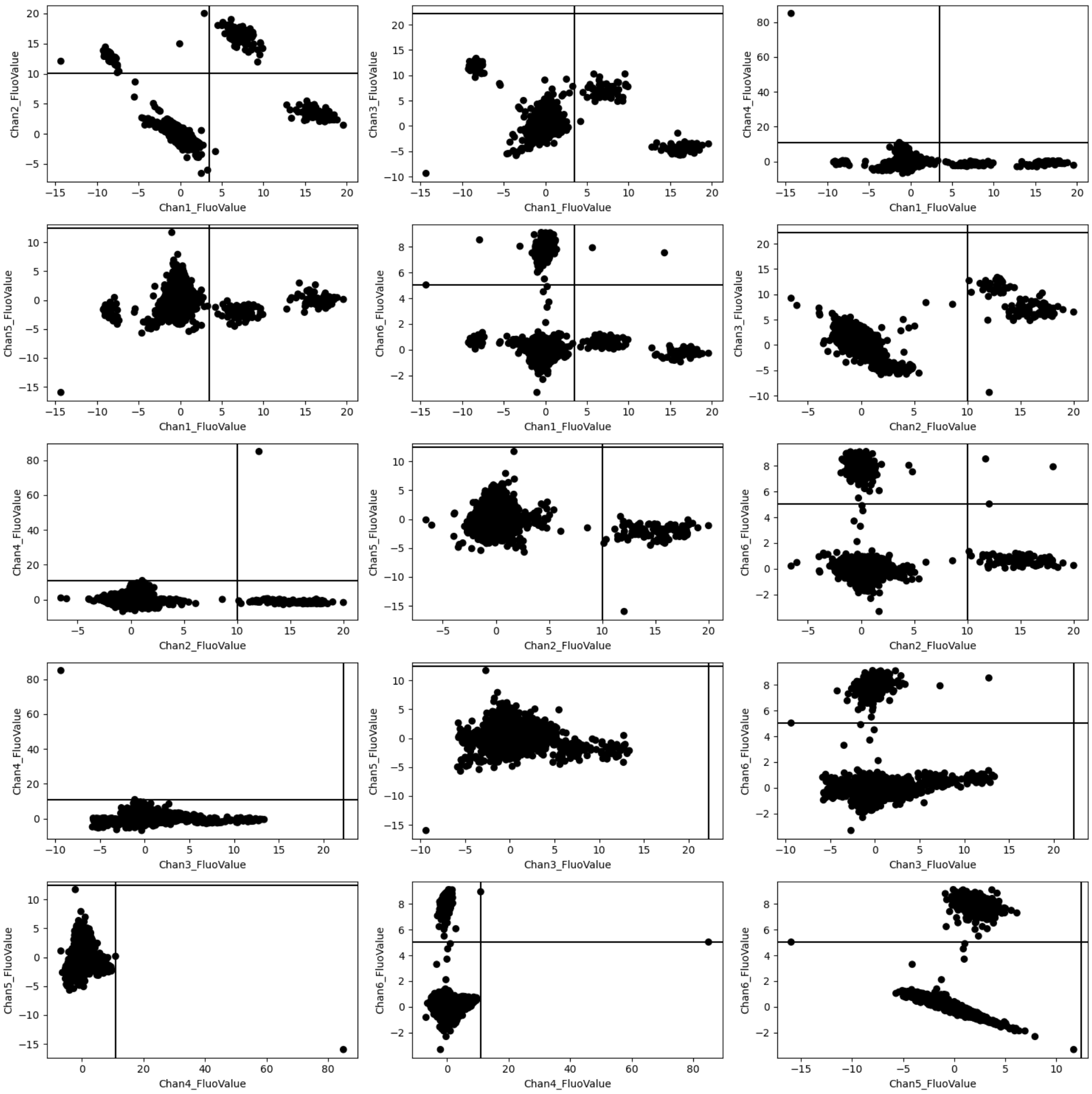
```
[ ]: plot_lib.pairwise_plots_pred_true_thresh(pd.
     ↪DataFrame(data=neg_cluster_based_classifier.X_transformed, columns=df_wa.
     ↪iloc[:,:6].columns),
                                                 df_predictions["RSV-N_POS"],
                                                 df_wa.loc[:,"RSV-N_POS"],
                                                ␣
     ↪axis_thresh=neg_cluster_based_classifier.axis_threshholds,
                                                 )
```



Plot IAV-M_POS associated with cannel 5

```
[ ]:
```

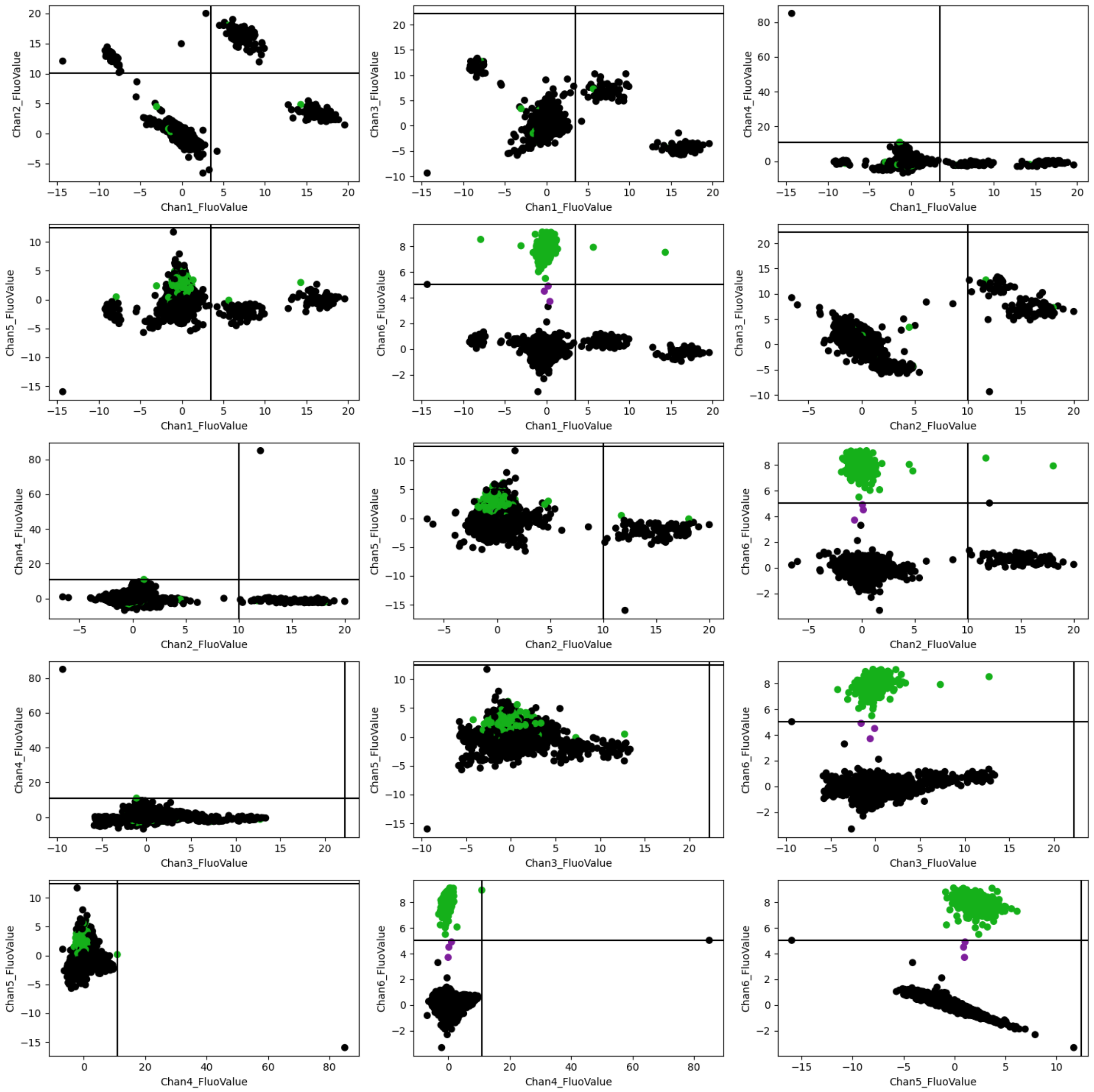
```
plot_lib.pairwise_plots_pred_true_thresh(pd.
 ↪DataFrame(data=neg_cluster_based_classifier.X_transformed, columns=df_wa.
 ↪iloc[:,:6].columns),
                                                  df_predictions["IAV-M_POS"],
                                                  df_wa.loc[:,"IAV-M_POS"],
                                                  ␣
 ↪axis_thresh=neg_cluster_based_classifier.axis_threshholds,
                                                  )
```



Plot MHV_POS associated with cannel 6

[ ]:

```
plot_lib.pairwise_plots_pred_true_thresh(pd.
↪DataFrame(data=neg_cluster_based_classifier.X_transformed, columns=df_wa.
↪iloc[:,:6].columns),
                                          df_predictions["MHV_POS"],
                                          df_wa.loc[:,"MHV_POS"],
                                          ␣
↪axis_thresh=neg_cluster_based_classifier.axis_threshholds,
                                          )
```


Chan2_FluoValue
Chan1_FluoValue
Chan3_FluoValue
Chan1_FluoValue
Chan4_FluoValue
Chan1_FluoValue
Chan5_FluoValue
Chan1_FluoValue
Chan6_FluoValue
Chan1_FluoValue
Chan3_FluoValue
Chan2_FluoValue
Chan4_FluoValue
Chan2_FluoValue
Chan5_FluoValue
Chan2_FluoValue
Chan6_FluoValue
Chan2_FluoValue
Chan4_FluoValue
Chan3_FluoValue
Chan5_FluoValue
Chan3_FluoValue
Chan6_FluoValue
Chan3_FluoValue
Chan5_FluoValue
Chan4_FluoValue
Chan6_FluoValue
Chan4_FluoValue
Chan6_FluoValue
Chan5_FluoValue