binspec

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`ann_classify` *Artificial Neural Network*

Description

Build a ANN classifier and test it.

Usage

```
ann_classify(training_set, training_labels, test_set, test_labels)
```

`binary_peaks` *Find binary peaks*

Description

Find peaks in window of size 2*neighbors + 1 and label m/z integers within the error as peaks. Returns vector of peak m/z integers.

Usage

```
binary_peaks(df, neighbors, error = 0)
```

Arguments

`df`	Data frame of m/z and intensities
`neighbors`	Number of neighboring m/z values to compare on right and left
`error`	m/z Decimal error value

`combine_peaks` *Combine peak vectors*

Description

Create a binary matrix, each column represents and m/z value, and each row represents a mass spectra. The value indicates whether or not the m/z of this spectra is a peak.

Usage

```
combine_peaks(list_mz_peaks)
```

Arguments

`list_mz_peaks`
List of m/z peak vectors

`random_forest_classify` *Random Forest*

Description

Build a random forest classifier and test it. No need for test set because out-of-bag error measurement.

Usage

```
random_forest_classify(training_set, training_labels)
```

`round_df` *Round data frame*

Description

Round all m/z and intensity values to integers.

Usage

```
round_df(df)
```

Arguments

`df` Data frame

`svm_classify` *Support Vector Machine*

Description

Build a SVM classifier and test it.

Usage

```
svm_classify(training_set, training_labels, test_set, test_labels)
```

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