binspec

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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

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classifier_accuracies

Classifier Accuracies

Description

Find the best classifier using leave-one-out cross validation (svm) and out-of-bag error (random forests). Returns a vector of classification accuracies

Usage

```
classifier_accuracies(peaks, labels, minpeaks)
```

Arguments

peaks	Boolean matrix of mass spectra rows with m/z columns, indicating if an m/z value corresponds to a peak.
labels	The correct classifications of the peaks.
minpeaks	How many "true" values must show up for a given m/z value for it to be considered a feature.

`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

`round_df` *Round data frame*

Description

Round all m/z and intensity values to integers.

Usage

```
round_df(df)
```

Arguments

`df`   Data frame

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