

# Package ‘MassSpecWavelet’

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**Title** Peak Detection for Mass Spectrometry data using wavelet-based algorithms

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**Description** Peak Detection in Mass Spectrometry data is one of the important preprocessing steps. The performance of peak detection affects subsequent processes, including protein identification, profile alignment and biomarker identification. Using Continuous Wavelet Transform (CWT), this package provides a reliable algorithm for peak detection that does not require any type of smoothing or previous baseline correction method, providing more consistent results for different spectra. See <doi:10.1093/bioinformatics/btl355> for further details.

**URL** <https://github.com/zeehio/MassSpecWavelet>

**BugReports** <http://github.com/zeehio/MassSpecWavelet/issues>

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---

MassSpecWavelet-package

*Peak detection of mass spectrum by Wavelet transform based methods*

---

## Description

MassSpecWavelet R package is aimed to detect peaks on Mass Spectrometry (MS) data using Continuous Wavelet Transform (CWT).

## Author(s)

Pan Du, Simon Lin

## References

Du, P., Kibbe, W.A. and Lin, S.M. (2006) Improved peak detection in mass spectrum by incorporating continuous wavelet transform-based pattern matching, *Bioinformatics*, 22, 2059-2065.

## See Also

Useful links:

- <https://github.com/zeehio/MassSpecWavelet>
- Report bugs at <http://github.com/zeehio/MassSpecWavelet/issues>

## Examples

```
data(exampleMS)
SNR.Th <- 3
peakInfo <- peakDetectionCWT(exampleMS, SNR.Th = SNR.Th)
majorPeakInfo <- peakInfo$majorPeakInfo
peakIndex <- majorPeakInfo$peakIndex
plotPeak(exampleMS, peakIndex, main = paste("Identified peaks with SNR >", SNR.Th))
```

---

cwt

*Continuous Wavelet Transform (CWT)*

---

## Description

CWT(Continuous Wavelet Transform) with Mexican Hat wavelet (by default) to match the peaks in Mass Spectrometry spectrum

## Usage

```
cwt(ms, scales = 1, wavelet = "mexh")
```

## Arguments

ms	Mass Spectrometry spectrum (a vector of MS intensities)
scales	a vector represents the scales at which to perform CWT. See the Details section. Additionally, a prepared_wavelets object is also accepted (see <a href="#">prepareWavelets()</a> ).
wavelet	The wavelet base, Mexican Hat by default. User can provide wavelet $\Psi(x)$ as a form of two row matrix. The first row is the $x$ value, and the second row is $\Psi(x)$ corresponding to $x$ .

## Details

The default mother wavelet is a Mexican Hat evaluated in the  $[-8, 8]$  range using 1024 points (a step of roughly  $1/64$ ):

$$\psi(x) = \frac{2}{\sqrt{3}}\pi^{-0.25}(1-x^2)\exp(-x^2/2)$$

The  $\sigma$  of the mother Mexican Hat is of one  $x$  unit.

The scaled wavelet is a downsampled version of the mother wavelet. The scale determines how many samples per  $x$  unit are taken. For instance, with the default Mexican Hat wavelet, a `scales = 2` will evaluate the  $[-8, 8]$  range sampling twice per  $x$  unit, this is with a step of 0.5. This generates a 33 points long scaled wavelet. Choosing this type of scaling is convenient because the scaled wavelet becomes a wavelet of  $\sigma = \text{'scales'}$  points. Using the default wavelet, a `scales` smaller than 1 will show sampling issues, while a `scales` larger than 64 will resample points from the original mother wavelet. If you need to use `scales` larger than 64, consider providing your own mother wavelet. See the examples.

According to [doi:10.1063/1.3505103](https://doi.org/10.1063/1.3505103), if your spectrum has a gaussian peak shape of variance  $m^2$  points then the `scales` range should cover  $[1, 1.9m]$ . If your spectrum has a Lorentzian peak shape of half-width-half-maximum  $L$  points then the `scales` range should cover  $[1, 2.9L]$ . They also suggest using a  $\log_{1.18}$  spacing. Take these values as suggestions for your analysis.

## Value

The return is the 2-D CWT coefficient matrix, with column names as the scale. Each column is the CWT coefficients at that scale. If the `scales` are too big for the given signal, the returned matrix may include less columns than the given `scales`.

## Author(s)

Pan Du, Simon Lin

## Examples

```
data(exampleMS)
scales <- seq(1, 64, 3)
wCoefs <- cwt(exampleMS[5000:11000], scales = scales, wavelet = "mexh")

## Plot the 2-D CWT coefficients as image (It may take a while!)
xTickInterval <- 1000
image(5000:11000, scales, wCoefs,
      col = terrain.colors(256), axes = FALSE,
      xlab = "m/z index", ylab = "CWT coefficient scale", main = "CWT coefficients"
)
axis(1, at = seq(5000, 11000, by = xTickInterval))
axis(2, at = c(1, seq(10, 64, by = 10)))
box()

## Provide a larger wavelet:
scales <- c(seq(1, 64, 3), seq(72, 128, 8))
psi_xval <- seq(-8, 8, length.out = 4096)
```

```

psi <- (2 / sqrt(3) * pi^(-0.25)) * (1 - psi_xval^2) * exp(-psi_xval^2 / 2)
wCoefs <- cwt(exampleMS[5000:11000], scales = scales, wavelet = rbind(psi_xval, psi))
xTickInterval <- 1000
image(5000:11000, scales, wCoefs,
      col = terrain.colors(256), axes = FALSE,
      xlab = "m/z index", ylab = "CWT coefficient scale", main = "CWT coefficients"
)
axis(1, at = seq(5000, 11000, by = xTickInterval))
axis(2, at = c(1, seq(10, 128, by = 10)))
box()

## Custom log1.18 spaced scales:
get_scales <- function(scale_min, scale_max, num_scales) {
  (seq(0, 1, length.out = num_scales)^1.18) * (scale_max - scale_min) + scale_min
}
scales <- get_scales(scale_min = 1, scale_max = 64, num_scales = 32)
print(scales)
# For detecting a gaussian peak of 10 points:
gaussian_peak_sigma <- 10 # points
scales <- get_scales(scale_min = 1, scale_max = 1.9 * gaussian_peak_sigma, num_scales = 32)
print(scales)
# For detecting a lorentzian peak of 10 points:
lorentzian_peak_gamma <- 10 # points
scales <- get_scales(scale_min = 1, scale_max = 2.9 * lorentzian_peak_gamma, num_scales = 32)
print(scales)

```

---

exampleMS

*An example mass spectrum*

---

## Description

An example mass spectrum from CAMDA 2006. All-in-1 Protein Standard II (CIPHERGEN Cat. \# C100-0007) were measured on CIPHERGEN NP20 chips. There are 7 polypeptides in the sample with m/z values of 7034, 12230, 16951, 29023, 46671, 66433, 147300.

## Format

A numeric vector represents the mass spectrum with equal sample intervals.

## Source

CAMDA, CAMDA 2006 Competition Data Set. 2006, <http://camda.duke.edu>.

---

extendLength                      *Extend the length of a signal or matrix*

---

### Description

Extend the length of a signal or matrix by row

### Usage

```
extendLength(  
  x,  
  addLength = NULL,  
  method = c("reflection", "open", "circular"),  
  direction = c("right", "left", "both")  
)
```

### Arguments

x	a vector or matrix with column with each column as a signal
addLength	the length to be extended
method	three methods available, c("reflection", "open", "circular"). By default, it is "reflection".
direction	three options available: c("right", "left", "both")

### Value

The extended vector or matrix.

### Author(s)

Pan Du

### See Also

[extendNBase\(\)](#)

### Examples

```
a = matrix(rnorm(9), 3)  
extendLength(a, 3, direction='right')
```

---

extendNBase	<i>Extend the row number of a matrix as the exponential of base N</i>
-------------	-----------------------------------------------------------------------

---

### Description

Extend the data as the exponential of base N by increasing row number.

### Usage

```
extendNBase(x, nLevel = 1, base = 2, ...)
```

### Arguments

x	data matrix
nLevel	the level of DWT decomposition. Basically, it is equivalent to changing the 'base' as $\text{base}^{\text{nLevel}}$
base	the base, 2 by default
...	other parameters of used by <a href="#">extendLength()</a>

### Details

The method 'open' is padding the the matrix with the last row.

### Value

Return a extended matrix

### Author(s)

Pan Du

### See Also

[extendLength\(\)](#)

### Examples

```
a <- matrix(rnorm(9), 3)
MassSpecWavelet:::extendNBase(a)
```

---

`findLocalMaxWinSize`     *Find local maxima and return the size of the window where they are maximum.*

---

### Description

Compared to the rest of the package, this is a rather experimental function. If you plan to use it or are interested in it, please open an issue at <https://github.com/zeehio/MassSpecWavelet/issues> to show your interest.

### Usage

```
findLocalMaxWinSize(x, capWinSize = NA)
```

### Arguments

`x`                     A numeric vector.

`capWinSize`          the maximum window size to report. NA means unlimited.

### Value

An integer vector `y` of the same length as `x`. `y[i]` will be the size of the largest window on `x` containing `x[i]` where:

- `x[i]` is a local maximum or a center of a plateau
- `x[i]` is not at a window border Optionally, if `capWinSize` is a positive integer, the maximum window size is capped to that value, to increase performance. Use this in case you just want to check if there exists a window of that size. @export @examples `x <- c(1, 2, 3, 2, 1)`  
`findLocalMaxWinSize(x)`

---

`getLocalMaximumCWT`     *Identify the local maximum of each column in 2-D CWT coefficients matrix*

---

### Description

Identify the local maximum of each column in 2-D CWT coefficients matrix by using a slide window. The size of slide window linearly changes from the coarse scale (bigger window size) to detail scale. The scale of CWT increases with the column index.



**Usage**

```
getLocalMaximumCWT(  
  wCoefs,  
  minWinSize = 5,  
  amp.Th = 0,  
  isAmpThreshRelative = FALSE,  
  exclude0scaleAmpThresh = FALSE  
)
```

**Arguments**

<code>wCoefs</code>	2-D CWT coefficients, each column corresponding to CWT coefficient at one scale. The column name is the scale.
<code>minWinSize</code>	The minimum slide window size used.
<code>amp.Th</code>	The minimum peak amplitude.
<code>isAmpThreshRelative</code>	Whether <code>amp.Th</code> is given relative to <code>max(wCoefs)</code> .
<code>exclude0scaleAmpThresh</code>	When computing the relative <code>amp.Th</code> , if this is set to TRUE, the <code>amp.Th</code> will exclude the zero-th scale from the <code>max(wCoefs)</code> . The zero-th scale corresponds to the original signal, that may have a much larger baseline than the wavelet coefficients and can distort the threshold calculation. The default is FALSE to preserve backwards compatibility.

**Value**

return a matrix with same dimension as CWT coefficient matrix, `wCoefs`. The local maxima are marked as 1, others are 0.

**Author(s)**

Pan Du

**See Also**

[localMaximum\(\)](#)

**Examples**

```
data(exampleMS)  
scales <- seq(1, 64, 3)  
wCoefs <- cwt(exampleMS[5000:11000], scales = scales, wavelet = "mexh")  
  
localMax <- getLocalMaximumCWT(wCoefs)  
plotLocalMax(localMax)
```

---

`getRidge`*Identify ridges based on the local maximum matrix*

---

### Description

Identify ridges by connecting the local maximum of 2-D CWT coefficients from the coarse scale to detail scale. The local maximum matrix is returned from `getLocalMaximumCWT()`

### Usage

```
getRidge(  
  localMax,  
  iInit = ncol(localMax),  
  step = -1,  
  iFinal = 1,  
  minWinSize = 5,  
  gapTh = 3,  
  skip = NULL,  
  scaleToWinSize = "doubleodd"  
)
```

### Arguments

<code>localMax</code>	The local maximum matrix is returned from <code>getLocalMaximumCWT()</code> with 1 represents maximum, others are 0.
<code>iInit</code>	The start column to search ridge. By default, it starts from the coarsest scale level.
<code>step</code>	Search step. -1 by default, which means searching from coarse scale to detail scale column by column.
<code>iFinal</code>	The final column index of search ridge.
<code>minWinSize</code>	The minimum slide window size used.
<code>gapTh</code>	The gap allowed during searching for ridge. 3 by default.
<code>skip</code>	The column to be skipped during search.
<code>scaleToWinSize</code>	How scales should be mapped to window sizes. Traditionally, <code>MassSpecWavelet</code> used the "doubleodd" mapping ( <code>winSize &lt;- 2*scale+1</code> ). <code>xcms</code> switched this mapping to "halve" ( <code>winSize &lt;- floor(scale/2)</code> ). Besides "doubleodd" and "halve" this parameter can also be a custom function of the scale.

### Value

Return a list of ridge. As some ridges may end at the scale larger than 1, in order to keep the uniqueness of the ridge names, we combined the smallest scale of the ridge and m/z index of the peak at that scale together to name the ridges. For example the ridge name "1\\_653" means the peak ridge ends at the CWT scale 1 with m/z index 653 at scale 1.

**Author(s)**

Pan Du, Simon Lin

**References**

Du, P., Kibbe, W.A. and Lin, S.M. (2006) Improved peak detection in mass spectrum by incorporating continuous wavelet transform-based pattern matching, *Bioinformatics*, 22, 2059-2065.

**See Also**

[getLocalMaximumCWT\(\)](#), [identifyMajorPeaks\(\)](#)

**Examples**

```
data(exampleMS)
scales <- seq(1, 64, 3)
wCoefs <- cwt(exampleMS[5000:11000], scales = scales, wavelet = "mexh")

localMax <- getLocalMaximumCWT(wCoefs)
ridgeList <- getRidge(localMax)
plotRidgeList(ridgeList)
```

---

getRidgeLength

*Estimate the length of the ridge*

---

**Description**

Estimate the length of the ridge line, which is composed of local maxima at adjacent CWT scales. The ridge line is cut off at the end point, whose amplitude divided by the maximum ridge amplitude is larger than the cutoff amplitude ratio threshold (0.5 by default).

**Usage**

```
getRidgeLength(ridgeList, Th = 0.5)
```

**Arguments**

ridgeList	a list of identified ridges
Th	the cutoff amplitude ratio (the amplitude divided by the maximum amplitude of the ridge) threshold of the ridge line end.

**Value**

a vector of estimated ridge length

**Author(s)**

Pan Du

**Examples**

```
stopifnot(getRidgeLength(list(c(5,4,3,2,1), c(5,3,1))) == c(3,2))
```

---

getRidgeValue	<i>Get the CWT coefficient values corresponding to the peak ridge</i>
---------------	-----------------------------------------------------------------------

---

**Description**

Get the CWT coefficient values corresponding to the peak ridge

**Usage**

```
getRidgeValue(ridgeList, wCoefs, skip = 0)
```

**Arguments**

ridgeList	a list of ridge lines
wCoefs	2-D CWT coefficients
skip	the CWT scale level to be skipped, by default the 0 scale level (raw spectrum) is skipped.

**Value**

A list of ridge values corresponding to the input ridgeList.

**Author(s)**

Pan Du

---

identifyMajorPeaks	<i>Identify peaks based on the ridges in 2-D CWT coefficient matrix</i>
--------------------	-------------------------------------------------------------------------

---

**Description**

Identify the peaks based on the ridge list (returned by `getRidge()`) in 2-D CWT coefficient matrix and estimated Signal to Noise Ratio (SNR)

**Usage**

```

identifyMajorPeaks(
  ms,
  ridgeList,
  wCoefs,
  scales = as.numeric(colnames(wCoefs)),
  SNR.Th = 3,
  peakScaleRange = 5,
  ridgeLength = 32,
  nearbyPeak = FALSE,
  nearbyWinSize = ifelse(nearbyPeak, 150, 100),
  winSize.noise = 500,
  SNR.method = "quantile",
  minNoiseLevel = 0.001,
  excludeBoundariesSize = nearbyWinSize/2
)

```

**Arguments**

<code>ms</code>	the mass spectrometry spectrum
<code>ridgeList</code>	returned by <code>getRidge()</code>
<code>wCoefs</code>	2-D CWT coefficients
<code>scales</code>	scales of CWT, by default it is the colnames of <code>wCoefs</code>
<code>SNR.Th</code>	threshold of SNR
<code>peakScaleRange</code>	the CWT scale range of the peak.
<code>ridgeLength</code>	the maximum ridge scale of the major peaks.
<code>nearbyPeak</code>	determine whether to include the small peaks close to large major peaks
<code>nearbyWinSize</code>	the window size to determine the nearby peaks. Only effective when <code>nearbyPeak</code> is true.
<code>winSize.noise</code>	the local window size to estimate the noise level.
<code>SNR.method</code>	method to estimate noise level. Currently, only 95 percentage quantile is supported.
<code>minNoiseLevel</code>	the minimum noise level used in calculating SNR, i.e., if the estimated noise level is less than "minNoiseLevel", it will use "minNoiseLevel" instead. If the noise level is less than 0.5, it will be treated as the ratio to the maximum amplitude of the spectrum.
<code>excludeBoundariesSize</code>	number of points at each boundary of the <code>ms</code> signal that will be excluded in search for peaks to avoid boundary effects.

**Details**

The determination of the peaks is based on three rules: Rule 1: The maximum ridge scale of the peak should larger than a certain threshold Rule 1.1: Based on the scale of the peak (corresponding to the maximum value of the peak ridge) should be within certain range Rule 2: Based on the peak SNR Rule 3: The peak should not appear at the boundaries of the signal.

**Value**

Return a list with following elements:

peakIndex	the m/z indexes of the identified peaks
peakCenterIndex	the m/z indexes of peak centers, which correspond to the maximum on the ridge. peakCenterIndex includes all the peaks, not just the identified major peaks.
peakCenterValue	the CWT coefficients (the maximum on the ridge) corresponding to peakCenterIndex
peakSNR	the SNR of the peak, which is the ratio of peakCenterValue and noise level
peakScale	the estimated scale of the peak, which corresponds to the peakCenterIndex
potentialPeakIndex	the m/z indexes of all potential peaks, which satisfy all requirements of a peak without considering its SNR. Useful, if you want to change to a lower SNR threshold later.
allPeakIndex	the m/z indexes of all the peaks, whose order is the same as peakCenterIndex, peakCenterValue, peakSNR and peakScale.

All of these return elements have peak names, which are the same as the corresponding peak ridges. see [getRidge\(\)](#) for details.

**Author(s)**

Pan Du, Simon Lin

**References**

Du, P., Kibbe, W.A. and Lin, S.M. (2006) Improved peak detection in mass spectrum by incorporating continuous wavelet transform-based pattern matching, *Bioinformatics*, 22, 2059-2065.

**See Also**

[peakDetectionCWT\(\)](#), [tuneInPeakInfo\(\)](#)

**Examples**

```
data(exampleMS)
scales <- seq(1, 64, 3)
wCoefs <- cwt(exampleMS, scales = scales, wavelet = "mexh")

localMax <- getLocalMaximumCWT(wCoefs)
ridgeList <- getRidge(localMax)

SNR.Th <- 3
majorPeakInfo <- identifyMajorPeaks(exampleMS, ridgeList, wCoefs, SNR.Th = SNR.Th)
## Plot the identified peaks
peakIndex <- majorPeakInfo$peakIndex
plotPeak(exampleMS, peakIndex, main = paste("Identified peaks with SNR >", SNR.Th))
```

---

localMaximum	<i>Identify local maximum within a slide window.</i>
--------------	------------------------------------------------------

---

### Description

The simplest local maximum detection using a sliding window searches for maxima in a window of a given size, and slides that window across the signal, shifting it one position at a time.

### Usage

```
localMaximum(x, winSize = 5)
```

### Arguments

x	a vector represents a signal profile
winSize	the slide window size, 5 by default.

### Details

The default implementation found here shifts the window by half of its size instead of by one position at a time. This makes the implementation faster, at the expense of not being able to detect peaks that are too close to each other, if they appear in some positions with respect to the windows.

Additionally, this implementation removes all instances of peaks found at a distance less than the window size

Experimentally, we are exploring other algorithms for local maxima detection. These algorithms can be chosen setting the "MassSpecWavelet.localMaximum.algorithm" option. See the "Finding local maxima" vignette for further details.

### Value

Return a vector with the same length of the input x. The position of local maximum is set as 1L, 0L else where.

### Author(s)

Pan Du and Sergio Oller

### See Also

[getLocalMaximumCWT\(\)](#)

**Examples**

```
x <- rnorm(200)
lmax <- localMaximum(x, 5)
maxInd <- which(lmax > 0)
plot(x, type = "l")
points(maxInd, x[maxInd], col = "red")
```

---

mexh

*The mexican hat function*

---

**Description**

$$\psi(x) = \frac{2}{\sqrt{3}}\pi^{-0.25}(1-x^2)\exp(-x^2/2)$$

**Usage**

```
mexh(x)
```

**Arguments**

x where to evaluate the mexican hat

**Value**

A vector of the same length as x with the corresponding values

**Examples**

```
x <- seq(-8, 8, length.out = 256)
mexh(x)
```

---

mzInd2vRange

*Match m/z index to m/z value with a certain error range*

---

**Description**

Match m/z index to m/z value with a certain error range

**Usage**

```
mzInd2vRange(mzInd, error = 0.003)
```



**Arguments**

mzInd            a vector of m/z index  
error            error range

**Value**

return a vector of sorted m/z values

**Author(s)**

Pan Du

**See Also**

[mzV2indRange\(\)](#)

---

mzV2indRange            *Match m/z value to m/z index with a certain error range*

---

**Description**

Match m/z value to m/z index with a certain error range

**Usage**

```
mzV2indRange(mzV, error = 0.003)
```

**Arguments**

mzV            a vector of m/z value  
error            error range

**Value**

return a vector of sorted m/z indexes

**Author(s)**

Pan Du

**See Also**

[mzInd2vRange\(\)](#)

---

peakDetectionCWT      *The main function of peak detection by CWT based pattern matching*

---

## Description

This function is a wrapper of `cwt()`, `getLocalMaximumCWT()`, `getRidge()`, `identifyMajorPeaks()`

## Usage

```
peakDetectionCWT(
  ms,
  scales = c(1, seq(2, 30, 2), seq(32, 64, 4)),
  SNR.Th = 3,
  nearbyPeak = TRUE,
  peakScaleRange = 5,
  amp.Th = 0.01,
  minNoiseLevel = amp.Th/SNR.Th,
  ridgeLength = 24,
  peakThr = NULL,
  tuneIn = FALSE,
  ...,
  exclude0scaleAmpThresh = FALSE,
  getRidgeParams = list(gapTh = 3, skip = 2)
)
```

## Arguments

<code>ms</code>	the mass spectrometry spectrum
<code>scales</code>	Scales of CWT. See <code>cwt()</code> for details. Additionally, a <code>prepared_wavelets</code> object is also accepted (see <code>prepareWavelets()</code> ).
<code>SNR.Th</code>	SNR (Signal to Noise Ratio) threshold
<code>nearbyPeak</code>	Determine whether to include the nearby small peaks of major peaks. TRUE by default
<code>peakScaleRange</code>	the scale range of the peak. larger than 5 by default.
<code>amp.Th</code>	the minimum required relative amplitude of the peak (ratio to the maximum of CWT coefficients)
<code>minNoiseLevel</code>	the minimum noise level used in computing the SNR
<code>ridgeLength</code>	the minimum highest scale of the peak in 2-D CWT coefficient matrix
<code>peakThr</code>	Minimal absolute intensity (above the baseline) of peaks to be picked. If this value is provided, then the smoothing function <code>signal::sgolayfilt()</code> will be called to estimate the local intensity.(added based on the suggestion and code of Steffen Neumann)

tuneIn	determine whether to tune in the parameter estimation of the detected peaks. If TRUE, peak detection is run again on a segment of the spectrum with more detailed scales. This tuning happens with the default wavelet and settings so it may not be that useful to you if you are using custom wavelets or thresholds.
...	other parameters used by <code>identifyMajorPeaks()</code> . Additionally, <code>f1</code> (filter length, with a default value of 1001) and <code>forder</code> (filter order, with a default value of 2) are set and passed to <code>signal::sgolayfilt()</code> when <code>peakThr</code> is given.
exclude0scaleAmpThresh	When computing the relative <code>amp.Th</code> , if this is set to TRUE, the <code>amp.Th</code> will exclude the zero-th scale from the <code>max(wCoefs)</code> . The zero-th scale corresponds to the original signal, that may have a much larger baseline than the wavelet coefficients and can distort the threshold calculation. The default is FALSE to preserve backwards compatibility.
getRidgeParams	A list with parameters for <code>getRidge()</code> .

**Value**

majorPeakInfo	return of <code>identifyMajorPeaks()</code>
ridgeList	return of <code>getRidge()</code>
localMax	return of <code>getLocalMaximumCWT()</code>
wCoefs	2-D CWT coefficient matrix, see <code>cwt()</code> for details.

**Author(s)**

Pan Du, Simon Lin

**References**

Du, P., Kibbe, W.A. and Lin, S.M. (2006) Improved peak detection in mass spectrum by incorporating continuous wavelet transform-based pattern matching, *Bioinformatics*, 22, 2059-2065.

**See Also**

`cwt()`, `getLocalMaximumCWT()`, `getRidge()`, `identifyMajorPeaks()`

**Examples**

```
data(exampleMS)

# Detect peaks with prepared wavelets:
prep_wav <- prepareWavelets(length(exampleMS))
SNR.Th <- 3
peakInfo <- peakDetectionCWT(exampleMS, prep_wav, SNR.Th = SNR.Th, exclude0scaleAmpThresh=TRUE)
peakIndex <- peakInfo$majorPeakInfo$peakIndex
plotPeak(exampleMS, peakIndex, main = paste("Identified peaks with SNR >", SNR.Th))

SNR.Th <- 3
peakInfo <- peakDetectionCWT(exampleMS, SNR.Th = SNR.Th)
majorPeakInfo <- peakInfo$majorPeakInfo
```

```
peakIndex <- majorPeakInfo$peakIndex
plotPeak(exampleMS, peakIndex, main = paste("Identified peaks with SNR >", SNR.Th))

## In some cases, users may want to add peak filtering based on the absolute peak amplitude
peakInfo <- peakDetectionCWT(exampleMS, SNR.Th = SNR.Th, peakThr = 500)
majorPeakInfo <- peakInfo$majorPeakInfo
peakIndex <- majorPeakInfo$peakIndex
plotPeak(exampleMS, peakIndex, main = paste("Identified peaks with SNR >", SNR.Th))
```

---

plotLocalMax

*Plot the local maximum matrix*

---

### Description

Plot the local maximum matrix of 2-D CWT coefficients returned by [getLocalMaximumCWT\(\)](#)

### Usage

```
plotLocalMax(
  localMax,
  wCoefs = NULL,
  range = c(1, nrow(localMax)),
  colorMap = "RYB",
  main = NULL,
  cex = 3,
  pch = ".",
  ...
)
```

### Arguments

localMax	local maximum matrix of 2-D CWT coefficients returned by <a href="#">getLocalMaximumCWT()</a>
wCoefs	2-D CWT coefficients
range	plot range of m/z index
colorMap	the colormap used in plotting the points
main	parameter of <a href="#">plot()</a>
cex	parameter of <a href="#">plot()</a>
pch	parameter of <a href="#">plot()</a>
...	other parameters of <a href="#">points()</a>

### Value

No value is returned; this function is called for its side effects (plot).

**Author(s)**

Pan Du

**See Also**[getLocalMaximumCWT\(\)](#)**Examples**

```
data(exampleMS)
scales <- seq(1, 64, 3)
wCoefs <- cwt(exampleMS[5000:11000], scales = scales, wavelet = "mexh")

localMax <- getLocalMaximumCWT(wCoefs)
plotLocalMax(localMax)
```

---

plotPeak

*Plot the identified peaks over the spectrum*

---

**Description**

Plot the identified peaks over the spectrum. The identified peaks are returned by [peakDetectionCWT\(\)](#) or [identifyMajorPeaks\(\)](#)

**Usage**

```
plotPeak(
  ms,
  peakIndex = NULL,
  mz = 1:length(ms),
  range = c(min(mz), max(mz)),
  method = c("p", "l"),
  main = NULL,
  log = "",
  ...
)
```

**Arguments**

ms	the MS spectrum
peakIndex	m/z indexes of the identified peaks
mz	m/z value correspond to m/z index
range	the plot range of m/z value
method	plot method of the identified peaks. method 'p' plot circles on the peaks; method 'l' add vertical lines over the peaks.

main            parameter of `plot()`  
log             parameter of `plot()`  
...             other parameters of `points()`

**Value**

No value is returned; this function is called for its side effects (plot).

**Author(s)**

Pan Du

**See Also**

[peakDetectionCWT\(\)](#), [identifyMajorPeaks\(\)](#)

**Examples**

```
data(exampleMS)
SNR.Th <- 3
peakInfo <- peakDetectionCWT(exampleMS, SNR.Th = SNR.Th)
majorPeakInfo <- peakInfo$majorPeakInfo
peakIndex <- majorPeakInfo$peakIndex
plotPeak(exampleMS, peakIndex, main = paste("Identified peaks with SNR >", SNR.Th))
```

---

plotRidgeList

*Plot the ridge list*

---

**Description**

Plot the ridge list returned by [getRidge\(\)](#)

**Usage**

```
plotRidgeList(
  ridgeList,
  wCoefs = NULL,
  range = NULL,
  colorMap = "RYB",
  main = NULL,
  pch = ".",
  cex = 3,
  ...
)
```

**Arguments**

ridgeList	returned by <a href="#">getRidge()</a>
wCoefs	2-D CWT coefficients
range	plot range of m/z index
colorMap	colorMap to plot the points of local maximum
main	parameter of <a href="#">plot()</a>
pch	parameter of <a href="#">plot()</a>
cex	parameter of <a href="#">plot()</a>
...	other parameters of <a href="#">points()</a>

**Value**

No value is returned; this function is called for its side effects (plot).

**Author(s)**

Pan Du

**See Also**

[getRidge\(\)](#)

**Examples**

```
data(exampleMS)
scales <- seq(1, 64, 3)
wCoefs <- cwt(exampleMS[5000:11000], scales = scales, wavelet = "mexh")

localMax <- getLocalMaximumCWT(wCoefs)
ridgeList <- getRidge(localMax)
plotRidgeList(ridgeList)
```

---

prepareWavelets

*Prepare daughter wavelets for faster CWT*

---

**Description**

Prepare daughter wavelets for faster CWT

**Usage**

```
prepareWavelets(
  mslength,
  scales = c(1, seq(2, 30, 2), seq(32, 64, 4)),
  wavelet = "mexh",
  wavelet_xlimit = 8,
  wavelet_length = 1024L,
  extendLengthScales = TRUE
)
```

**Arguments**

mslength	Length of the signal to transform
scales	a vector represents the scales at which to perform CWT. See the Details section. Additionally, a prepared_wavelets object is also accepted (see <a href="#">prepareWavelets()</a> ).
wavelet	The wavelet base, Mexican Hat by default. User can provide wavelet $\Psi(x)$ as a form of two row matrix. The first row is the $x$ value, and the second row is $\Psi(x)$ corresponding to $x$ .
wavelet_xlimit	The mother wavelet will be evaluated between these limits. Ignored if wavelet is a matrix.
wavelet_length	The number of points of the mother wavelet. Ignored if wavelet is a matrix
extendLengthScales	A logical value. If the signal is too short, we may need to pad it to convolve it with larger daughter wavelets. Set this to TRUE to let scales be used to determine the padding length. It's set to FALSE by default to preserve backwards compatibility.

**Value**

A prepared\_wavelets object.

**See Also**

cwt

**Examples**

```
x <- runif(2000)
scales <- c(1, 2, 4, 8)
prep_wavelets <- prepareWavelets(length(x), scales = scales)
wCoefs <- cwt(x, prep_wavelets)
```



---

smoothDWT                      *smooth (denoise) the spectrum by DWT (Discrete Wavelet Transform)*

---

### Description

Smooth (denoise) the spectrum by DWT (Discrete Wavelet Transform)

### Usage

```
smoothDWT(  
  ms,  
  nLevel = 6,  
  wf = "la8",  
  localNoiseTh = seq(1, 0, by = -0.2),  
  localWinSize = 500,  
  globalNoiseTh = 0.75,  
  smoothMethod = c("soft", "hard"),  
  method = c("dwt", "modwt")  
)
```

### Arguments

ms	a vector representing the mass spectrum
nLevel	the level of DWT decomposition
wf	the name of wavelet for DWT
localNoiseTh	local noise level threshold
localWinSize	local window size for estimate local noise threshold
globalNoiseTh	global noise level threshold
smoothMethod	the method used for denoising. 'hard' means keeping the dwt coefficients higher than the threshold unchanged; "soft" means the dwt coefficients higher than the threshold were subtracted by the threshold.
method	'dwt' or 'modwt' used for decomposition

### Value

return the smoothed mass spectrum with the 'detail' component of DWT as an attribute 'detail'.

### Author(s)

Pan Du

---

tuneInPeakInfo	<i>Tune in the peak information: peak position and peak scale</i>
----------------	-------------------------------------------------------------------

---

### Description

Based on the identified peak position, more precise estimation of the peak information, i.e., peak position and peak scale, can be got by this function. The basic idea is to cut the segment of spectrum near the identified peaks, and then do similar procedures as [peakDetectionCWT\(\)](#), but with more detailed scales around the estimated peak scale.

### Usage

```
tuneInPeakInfo(
  ms,
  majorPeakInfo = NULL,
  peakIndex = NULL,
  peakScale = NULL,
  maxScale = 128,
  ...
)
```

### Arguments

ms	the mass spectrometry spectrum
majorPeakInfo	return of <a href="#">identifyMajorPeaks()</a>
peakIndex	the m/z index of the identified peaks
peakScale	the scales of the identified peaks
maxScale	the maximum scale allowed for the peak
...	other parameters of used by <a href="#">getLocalMaximumCWT()</a> , <a href="#">getRidge()</a> , <a href="#">identifyMajorPeaks()</a>

### Details

The majorPeakInfo or peakIndex and peakScale must be provided.

### Value

peakCenterIndex	the updated peak center m/z index
peakScale	the updated peak scale
peakValue	the corresponding peak value

### Author(s)

Pan Du

**References**

Du, P., Kibbe, W.A. and Lin, S.M. (2006) Improved peak detection in mass spectrum by incorporating continuous wavelet transform-based pattern matching, *Bioinformatics*, 22, 2059-2065.

**See Also**

[peakDetectionCWT\(\)](#)

**Examples**

```
data(exampleMS)
SNR.Th <- 3
peakInfo <- peakDetectionCWT(exampleMS, SNR.Th = SNR.Th)
majorPeakInfo <- peakInfo$majorPeakInfo
betterPeakInfo <- tuneInPeakInfo(exampleMS, majorPeakInfo)
plot(500:length(exampleMS), exampleMS[500:length(exampleMS)], type = "l", log = "x")
abline(v = betterPeakInfo$peakCenterIndex, col = "red")
```

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