Package ‘deisotoper’
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Type Package
Title Detection of Isotope Pattern of a Mass Spectrometric Measurement
Version 0.0.7
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Suggests DiagrammeR, lattice, roxygen2, protViz (>= 0.4.0), shiny, testthat, knitr, rmarkdown
SystemRequirements Java (>= 8.0)
Description Provides a low-level interface for a deisotoper container implemented in the 'Java' programming language and means of S3 helper functions for plotting and debugging isotopes of mass spectrometric data. The deisotoper algorithm detects and aggregates peaks which belong to the same isotopic cluster of a given mass spectrum.
License GPL-3
URL https://github.com/protViz/deisotoper/
BugReports https://github.com/protViz/deisotoper/issues
deisotoper.R
LazyData true
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\texttt{deisotope}  \hspace{1cm}  \textit{Deisotope a Mass Spectrum}

Description

Deisotope a Mass Spectrum

Usage

\texttt{deisotope(deisotoper, massspectrum, algorithm = \textquote{features-based})}

Arguments

\begin{itemize}
  \item \texttt{deisotoper} \hspace{1cm} \texttt{a \textit{deisotoper} object.}
  \item \texttt{massspectrum} \hspace{1cm} \texttt{a list of numeric vectors mz and intensity where mz is ordered and mz and intensity have the same length.}
  \item \texttt{algorithm} \hspace{1cm} \texttt{the supported deisotope algorithms, default is method=\textquote{features-based}.}
\end{itemize}

Author(s)

Lucas Schmidt, Christian Panse, Witold E. Wolski

References

\begin{itemize}
  \item Features-Based Deisotoping Method for Tandem Mass Spectra, \texttt{http://dx.doi.org/10.1155/2011/210805}.
\end{itemize}

See Also

\texttt{deisotoper}

Examples

\begin{verbatim}
x <- list(mz = c(1, 2, 2.5, 3), intensity = rep(1, 4), pepmass=600, charge=2)
xd <- deisotope(dtoper <- deisotoper(), x)
plot.deisotoper(x, xd)
summary(dtoper)
\end{verbatim}
**deisotoper**  

**Construct a Deisotoper Object**

**Description**

deisotoper returns a deisotoper object.  
deisotope detects and aggregates peaks which belong to the same isotopic cluster of a given mass spectrum.

**Usage**

deisotoper(amino_acid_masses = list(A = 71.03711, R = 156.10111, N = 114.04293, D = 115.02694, C = 103.00919, E = 129.04259, Q = 128.05858, G = 57.02146, H = 137.05891, I = 113.08406, L = 113.08406, K = 128.09496, M = 131.04049, F = 147.06841, P = 97.05276, S = 87.03203, T = 101.04768, W = 186.07931, Y = 163.06333, V = 99.06841), F1 = 0.8, F2 = 0.5, F3 = 0.1, F4 = 0.1, F5 = 0.1, delta = 0.003, errortolerance = 0.3, distance = 1.00048, noise = 0, decharge = FALSE, modus = "first", comment = "")

**Arguments**

- **amino_acid_masses**
  
  List of amino acid masses used for scoring.

- **F1**
  
  F1 multiplier used for scoring.

- **F2**
  
  F2 multiplier used for scoring.

- **F3**
  
  F3 multiplier used for scoring.

- **F4**
  
  F4 multiplier used for scoring.

- **F5**
  
  F5 multiplier used for scoring.

- **delta**
  
  Delta value used for clustering.

- **errortolerance**
  
  Error tolerance used for scoring.

- **distance**
  
  Distance between two peaks used by clustering.

- **noise**
  
  Noise value for noise filtering (in percent).

- **decharge**
  
  De- and activates decharging.

- **modus**
  
  Modus of aggregation ('first' or 'highest').

- **comment**
  
  Default is empty word.

**Details**

Input: a peak peaked mass spectrum.

The algorithm: The deisotoper algorithm detects and aggregates peaks which belong to the same isotopic cluster of a given mass spectrum.

Output:
Value
deisotoper as list of JavaRef

Author(s)
Lucas Schmidt, Christian Panse

References

See Also
deisotope

Examples

```r
# EXAMPLE 1
# standart configured deisotoper
dtoper <- deisotoper()

# return the configuration of dtoper
cfg <- config.deisotoper(dtoper)

# example data
intensity = c(378322, 32496.6, 85689.6, 64440.3, 49645.2, 25102.5, 32516.2, 83497.2, 74653.1, 37228, 196053, 83826.4, 112718, 114812, 88089.5, 61521.3, 220054, 58888.5, 280334, 122311, 14953.2, 26959.6, 24854, 27122.9, 86216.1, 63360.3, 358968, 47393.5, 37893.2, 16532.9, 17259, 37250.4, 33679.8, 21243.6, 17854.9, 51232.4, 12738.8, 19515.4, 31560.1, 48772.3, 66481.2, 23353.6, 11994, 15211, 9883.29, 14753.7, 17384.7, 51575.9, 10917.6, 40518.3, 15107.3, 62106.4, 72496.1, 9430.4, 10289.3, 34831.3, 41981.1, 1700, 2500, 12000, 9000, 4000, 0)
```
# deisotope the data
xd <- deisotope(dtoper, x)
summary.deisotoper(dtoper)

# plot the example data and the deisotoped data
op <- par(mfrow=c(2,2))
plot.deisotoper(x, xd)
plot.deisotoper(x, xd, xlim=c(275,285))
plot.deisotoper(x, xd, xlim=c(790,795))
plot.deisotoper(x, xd, xlim=c(901,910))
par(op)

# return the annotated spectrum of the above deisotoped data
print.deisotoper(dtoper)

# EXAMPLE 2
# standart configured deisotoper with changed delta and decharging
dtoper2 <- deisotoper(delta = 0.005, decharge = TRUE)

# return the configuration of dtoper2
config2 <- config.deisotoper(dtoper2)

## Not run:
# return the GraphViz dot graphs of the above deisotoped data
xdot <- dot.deisotoper(dtoper)

# draws the isotopic cluster graphs in the browser (html)
if(require(DiagrammeR)){
  lapply(xdot, DiagrammeR::grViz)
}

## End(Not run)

findNN  

**find index of nearest neighbor.**
Description

Given a vector of sorted double values vec of size n and a vector of m query objects q, findNN determines for each element q[i] in q the nearest neighbor index o so that the following remains true:
there is no element k with 1 ≤ k ≤ n and k is not o so that
abs(vec[k] - q[i]) < abs(vec[o] - q[i]).

The internal algorithm of findNN is implemented as binary search. findNN has $O(m \cdot \log(n))$ time complexity.

Usage

findNN(q, vec)

Arguments

q a double vector which can be considered as query objects.
vec a sorted double vector which can be considered as a data base.

Value

an integer vector

Author(s)

Lucas Schmidt, Christian Panse

See Also

protViz::findNN's cplusplus implementation.

Examples

(NNidx <- findNN(q<-c(1, 1.0001, 1.24, 1.26), DB<-seq(1,5,by=0.25)))
(NNidx <- c(1,1,2,2))

# should be 0
unique(DB[findNN(DB, DB)] - DB)
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