Package ‘Rdisop’

March 23, 2017

Title Decomposition of Isotopic Patterns

Version 1.34.0

Date 2015-12-08

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Description Identification of metabolites using high precision mass

spectrometry. MS Peaks are used to derive a ranked list

of sum formulae, alternatively for a given sum formula

the theoretical isotope distribution can be calculated
to search in MS peak lists.

Depends R (>= 2.0.0), RcppClassic

LinkingTo RcppClassic, Rcpp

Suggests RUnit

SystemRequirements None

License GPL-2

URL https://github.com/sneumann/Rdisop

BugReports https://github.com/sneumann/Rdisop/issues/new

biocViews MassSpectrometry, Metabolomics

NeedsCompilation yes

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Description

Simple arithmetic modifications of sum formulae.

Usage

```r
addMolecules(formula1, formula2, elements = NULL, maxisotopes = 10)
subMolecules(formula1, formula2, elements = NULL, maxisotopes = 10)
```

Arguments

- `formula1`: Sum formula
- `formula2`: Sum formula
- `elements`: list of allowed chemical elements, defaults to full periodic system of elements
- `maxisotopes`: maximum number of isotopes shown in the resulting molecules

Details

`addMolecules()` adds the second argument to the first. `subMolecules()` subtracts the second argument from the first.

This can be useful to revert e.g. adduct/fragment formation found in ESI mass spectrometry, or to mimic simple chemical reactions. No chemical checks are performed.

Value

A list with the elements

- `formula`: repeated sum formula
- `mass`: exact monoisotopic mass of molecule
- `score`: dummy value, always 1.0
- `isotopes`: a list of isotopes

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Examples

```r
# For proton-Adduct of Ethanol:
subMolecules("C2H7O", "H")
```
decomposeIsotopes  Mass Decomposition of Isotope Patterns

Description
Calculate the elementary compositions from an exact Mass or Isotope Pattern, obtained e.g.\ by FTICR or TOF mass spectrometers

Usage
decomposeMass(mass, ppm=2.0, mzabs=0.0001, elements=NULL, filter=NULL, z=0, maxisotopes = 10, minElements="C0", maxElements="C999999")
decomposeIsotopes(masses, intensities, ppm=2.0, mzabs=0.0001, elements=NULL, filter=NULL, z=0, maxisotopes = 10, minElements="C0", maxElements="C999999")
isotopeScore(molecule, masses, intensities, elements = NULL, filter = NULL, z = 0)

Arguments
mass  A single exact mass (or m/z value)
masses  A vector of masses (or m/z values) of an isotope cluster
intensities  Absolute or relative intensities of the masses peaks
ppm  allowed deviation of hypotheses from given mass
mzabs  absolute deviation in dalton (mzabs and ppm will be added)
z  charge z of m/z peaks for calculation of real mass. 0 is for auto-detection
maxisotopes  maximum number of isotopes shown in the resulting molecules
elements  list of allowed chemical elements, defaults to CHNOPS
minElements, maxElements  Molecular formulas, which contain lower and upper boundaries of allowed formula respectively
filter  NYI, will be a selection of DU, DBE and Nitrogen rules
molecule  a molecule as obtained from getMolecule() or decomposeMass / decomposeIsotopes

Details
Sum formulas are calculated which explain the given mass or isotope pattern.

Value
A list of molecules, which contain the sub-lists

formula  potential formulae
mass  exact monoisotopic mass of hypothesis
score  calculated score
isotopes  a list of isotopes

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getMolecule

References

For a description of the underlying IMS see: see citation("Rdisop")

See Also
decomposeMass

Examples

# For Glutamate:
decomposeIsotopes(c(147.0529,148.0563), c(100.0,5.561173))

getMolecule  

Calculate mass and isotope information for a molecule given as sum formula

Description

Parse the sum formula and calculate the theoretical exact mass and the isotope distribution.

Usage

ginemolecule(formula, elements = NULL, z = 0, maxisotopes = 10)
gemass(molecule)
gformula(molecule)
gisotope(molecule, index)
gscore(molecule)
gvalid(molecule)

Arguments

formula  Sum formula  
elements  list of allowed chemical elements, defaults to full periodic system of elements  
z  charge z of molecule for exact mass calculation  
maxisotopes  maximum number of isotopes shown in the resulting molecules  
molecule  an initialized molecule as returned by getMolecule() or the decomposeMass() and decomposeIsotope() functions  
index  return the n-th isotope mass/abundance pair of the molecule

Details

ginemolecule() Parse the sum formula and calculate the theoretical exact monoisotopic mass and the isotope distribution. For a given element, return the different mass values.
Value

getMolecule: A list with the elements

- formula: repeated sum formula
- mass: exact monoisotopic mass of molecule
- score: probability, for given molecules a dummy value which is always 1.0
- valid: result of neutron rule check
- isotopes: a list of isotopes

getMass, getFormula and getScore: return the mass of the molecule as string or real value

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References

For a description of the underlying IMS see: see citation("Rdisop")

Examples

```r
# For Ethanol:
getMolecule("C2H6O")
```

**initializeCHNOPS**  
(*Initialize (a subset of) elements of the periodic system of elements (PSE)*)

Description

Initialize the information about name, mass and isotopes. To reduce the number of decomposition hypotheses, subsets of elements can be created.

Usage

```r
initializeCHNOPS()
initializeCHNOPSMgKCaFe()
initializePSE()
initializeElements(names)
```

Arguments

- names: vector of element names within PSE

Details

These functions return full, pre-defined or user-defined (sub-) lists of elements.
Value

- name: repeated sum formula
- mass: nominal mass of molecule
- isotope: a list of isotopes

The initializeCharges() is special, since it allows to parse charges such as `getMolecule("H3O+", elements=c(initializeCHNOPS(),initializeCharges()))`

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References

For a description of the underlying IMS see: see citation("Rdisop")
Isotope patterns obtained through wikipedia.org

See Also

getMolecule

Examples

# For Ethanol:
elements <- initializeCHNOPS()
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