Package ‘Rdisop’

March 26, 2024

Title  Decomposition of Isotopic Patterns

Version  1.62.0

Date  2023-02-12

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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), Rcpp

LinkingTo  Rcpp

Suggests  RUnit

SystemRequirements  None

License  GPL-2

StagedInstall  no

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

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

biocViews  ImmunoOncology, MassSpectrometry, Metabolomics

git_url  https://git.bioconductor.org/packages/Rdisop

git_branch  RELEASE_3_18

git_last_commit  ad6fa13

git_last_commit_date  2023-10-24

Repository  Bioconductor 3.18

Date/Publication  2024-03-25
addMolecules

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addMolecules

Add/subtract sum formulae

Description

Simple arithmetic modifications of sum formulae.

Usage

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 mimick 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

# 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

Author(s)

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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

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

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

`getMolecule()` 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 neutrogen 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

initializeCHNOPS()
initializeCHNOPS(MgKCaFe())
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

A list with the elements

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

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initializeCHNOPS

Examples

# For Ethanol:
elements <- initializeCHNOPS()
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