Package ‘Rdisop’

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**Title**  Decomposition of Isotopic Patterns

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**Author**  Anton Pervukhin <apervukh@minet.uni-jena.de>, Steffen Neumann <sneumann@ipb-halle.de>

**Maintainer**  Steffen Neumann <sneumann@ipb-halle.de>

**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

**R topics documented:**

- addMolecules 2
- decomposeIsotopes 3
- getMolecule 4
- initializeCHNOPS 5

**Index**  7
**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

**Author(s)**

Steffen Neumann <sneumann@IPB-Halle.DE>

**Examples**

```r
# For proton-Adduct of Ethanol:
subMolecules("C2H70", "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**

```r
decomposeMass(mass, ppm=2.0, mzabs=0.0001, elements=NULL, filter=NULL, z=0, maxisotopes = 10, minElements="C0", maxElements="C999999")
```

```r
decomposeIsotopes(masses, intensities, ppm=2.0, mzabs=0.0001, elements=NULL, filter=NULL, z=0, maxisotopes = 10, minElements="C0", maxElements="C999999")
```

```r
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)**

Steffen Neumann <sneumann@IPB-Halle.DE>
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
getMolecule(formula, elements = NULL, z = 0, maxisotopes = 10)
getMass(molecule)
getFormula(molecule)
getIsotope(molecule, index)
getScore(molecule)
getValid(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
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.
initializeCHNOPS

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

Author(s)

Steffen Neumann <sneumann@IPB-Halle.DE>

References

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

Examples

# 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.
initializeCHNOPS

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()))`.

Author(s)

Steffen Neumann <sneumann@IPB-Halle.DE>

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()
Index

*Topic* **methods**
  - addMolecules, 2
  - decomposeIsotopes, 3
  - getMolecule, 4
  - initializeCHNOPS, 5

addMolecules, 2

decomposeIsotopes, 3
decomposeMass, 4
decomposeMass (decomposeIsotopes), 3

getFormula (getMolecule), 4
getIsotope (getMolecule), 4
getMass (getMolecule), 4
getMolecule, 4, 6
getScore (getMolecule), 4
getValid (getMolecule), 4

initializeCharges (initializeCHNOPS), 5
initializeCHNOPS, 5
initializeCHNOPS\(\text{MgKCaFe}\) (initializeCHNOPS), 5
initializeCHNOPS\(\text{NaK}\) (initializeCHNOPS), 5
initializeElements (initializeCHNOPS), 5
initializePSE (initializeCHNOPS), 5
isotopeScore (decomposeIsotopes), 3

subMolecules (addMolecules), 2