Package ‘Rdisop’

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Title Decomposition of Isotopic Patterns

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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

R topics documented:

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

Index 7
addMolecules

`addMolecules` Add/subtract sum formulae

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")
de 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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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

gutmolecule(formula, elements = NULL, z = 0, maxisotopes = 10)
gtMass(molecule)
gtFormula(molecule)
gtIsotope(molecule, index)
gtScore(molecule)
gtValid(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

gutmolecule() 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
# 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()))`

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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**

```r
# 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