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

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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")`
- `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:
de分解Isotopes(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)
ge分解otope(molecule, index)
ge分解ore(molecule)
ge分解Valid(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.
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()
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.
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)

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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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