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:

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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

Author(s)
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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`: Molecular formulas, which contain lower and upper boundaries of allowed formula respectively
- `maxElements`: 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>
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)
geMass(molecule)
geFormula(molecule)
geIsotope(molecule, index)
geScore(molecule)
geValid(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

<table>
<thead>
<tr>
<th>Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>formula</td>
<td>repeated sum formula</td>
</tr>
<tr>
<td>mass</td>
<td>exact monoisotopic mass of molecule</td>
</tr>
<tr>
<td>score</td>
<td>probability, for given molecules a dummy value which is always 1.0</td>
</tr>
<tr>
<td>valid</td>
<td>result of neutron rule check</td>
</tr>
<tr>
<td>isotopes</td>
<td>a list of isotopes</td>
</tr>
</tbody>
</table>

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()
initializeCHNOPS(MgKCaFe())
initializePSE()
initializeElements(names)
```

**Arguments**

<table>
<thead>
<tr>
<th>Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>names</td>
<td>vector of element names within PSE</td>
</tr>
</tbody>
</table>

**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**

```r
# For Ethanol:
elements <- initializeCHNOPS()
```
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