

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), Rcpp

LinkingTo Rcpp

Suggests RUnit

SystemRequirements None

License GPL-2

StagedInstalll no

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

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

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| | |
|--------------|----------------------------------|
| addMolecules | <i>Add/subtract sum formulae</i> |
|--------------|----------------------------------|

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, 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>

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 | <i>Calculate mass and isotope information for a molecule given as sum formula</i> |
|-------------|---|

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.

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 nitrogen rule check |
| isotopes | a list of isotopes |

getMass, getFormula and getScore: return the mass of the molecule as string or real value

Author(s)

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References

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

Examples

```
# For Ethanol:  
getMolecule("C2H6O")
```

| | |
|------------------|---|
| initializeCHNOPS | <i>Initialize (a subset of) elements of the periodic system of elements (PSE)</i> |
|------------------|---|

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.

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: `citation("Rdisop")`
Isotope patterns obtained through wikipedia.org

See Also

[getMolecule](#)

Examples

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

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