Package 'Rdisop'

October 9, 2013

Title Decomposition of Isotopic Patterns

Version 1.20.0

Date 2012-11-30

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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, Rcpp

LinkingTo RcppClassic, Rcpp

Suggests RUnit

SystemRequirements None

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URL http://msbi.ipb-halle.de/

biocViews MassSpectrometry

R topics documented:

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`	Abolute 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` *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.

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 neutrogen 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` *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.

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(initializeC`

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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