Package 'Rdisop'

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Title Decomposition of Isotopic Patterns

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Description In high resolution mass spectrometry (HR-MS), the measured masses can be decomposed into potential element combinations (chemical sum formulas). Where additional mass/intensity information of respective isotopic peaks is available, decomposition can take this information into account to better rank the potential candidate sum formulas. To compare measured mass/intensity information with the theoretical distribution of candidate sum formulas, the latter needs to be calculated.
This package implements fast algorithms to address both tasks, the calculation of isotopic distributions for arbitrary sum formulas (assuming a HR-MS resolution of roughly 30,000), and the ranked list of sum formulas fitting an observed peak or isotopic peak set.

Depends R (>= 2.0.0), Rcpp

LinkingTo Rcpp

Suggests knitr, rmarkdown, RUnit, testthat (>= 3.0.0)

SystemRequirements None

License GPL-2

StagedInstalll no

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

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

biocViews ImmunoOncology, MassSpectrometry, Metabolomics

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Contents

`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

The input vector formula1 either amended or reduced by formula2.

Examples

```
# Remove the proton-Adduct from 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

```
decomposeIsotopes(
  masses,
  intensities,
  ppm = 2,
  mzabs = 1e-04,
  elements = NULL,
  filter = NULL,
  z = 0,
  maxisotopes = 10,
  minElements = "C0",
  maxElements = "C999999"
)

decomposeMass(
  mass,
  ppm = 2,
  mzabs = 1e-04,
  elements = NULL,
  filter = NULL,
  z = 0,
  maxisotopes = 10,
  minElements = "C0",
  maxElements = "C999999"
)

isotopeScore(
  molecule,
  masses,
  intensities,
  elements = NULL,
  filter = NULL,
  z = 0
)
```

Arguments

`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).

elements	List of allowed chemical elements, defaults to CHNOPS.
filter	NYI, will be a selection of DU, DBE and Nitrogen rules.
z	Charge z of m/z peaks for calculation of real mass, keep z=0 for auto-detection.
maxisotopes	Maximum number of isotopes shown in the resulting molecules.
minElements	Molecular formulas, which contain lower and upper boundaries of allowed formula respectively.
maxElements	Molecular formulas, which contain lower and upper boundaries of allowed formula respectively.
mass	A single mass (or m/z value).
molecule	An initialized molecule as returned by getMolecule() or the decomposeMass() and decomposeIsotope() functions.

Details

Sum formulas are calculated which explain the given mass or isotope pattern.

Value

A list of molecules, which contain the sub-lists ‘formulas‘ potential formulae, 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 citation("Rdisop")

Examples

```
# Glutamate:
decomposeIsotopes(c(147.0529, 148.0563), c(100.0, 5.56))
```

---

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)

getIsotope(molecule, index)

getFormula(molecule)

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 for the resulting molecule.
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()` will parse the sum formula and calculate the theoretical exact monoisotopic mass and the isotope distribution. For a given element, return the different mass values. Since of version 1-65-3, if a charge is specified, the exact mass of the molecule will be reduced or increased by n-times the electron mass (depending on the sign). Also, isotopic masses will additionally be devided by the charge specified to reflect what would be measured in HR-MS.

Value

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.

Author(s)

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References

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

Examples

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

`initializeElements` *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

```
initializeElements(names)

.getElement(name, elements = NULL)

initializeCHNOPS()

initializeCHNOPSMgKCaFe()

initializeCHNOPSNaK()

initializePSE()

initializeCharges()
```

Arguments

`names`	Vector of element names within PSE.
`name`	Chemical element name (abbr.).
`elements`	Character vector of chemical element names.

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 function ‘initializeCharges‘ is special, since it allows to parse charges as shown in examples.

Author(s)

Steffen Neumann <sneumann@IPB-Halle.DE>

References

For a description of the underlying IMS see citation("Rdisop"). Isotope patterns were obtained through wikipedia.org

Examples

```
initializeCHNOPS()
getMolecule("H3O+", elements=c(initializeCHNOPS(),initializeCharges()))
```

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