Rdisop
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RcppVersion  Rcpp Version and License Information

Description
RcppVersion displays the version of Rcpp/RcppTemplate that was used to build this package.

Usage
RcppVersion()

Author(s)
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Examples
RcppVersion()

addMolecules  Add/subtract sum formulae

Description
Simple arithmetic modifications of sum formulae.

Usage
addMolecules(formula1, formula2, elements = NULL)
subMolecules(formula1, formula2, elements = NULL)

Arguments
formula1  Sum formula
formula2  Sum formula
elements  list of allowed chemical elements, defaults to full periodic system of elements
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 mass of molecule
- score: dummy value, always 1.0
- isotopes: a list of isotopes

Author(s)

Steffen Neumann <sneumann@IPB-Halle.DE>

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

```r
decomposeMass(mass, ppm=2.0, mzabs=0.0001, elements=NULL, filter=NULL, z=0)
decomposeIsotopes(masses, intensities, ppm=2.0, mzabs=0.0001, elements=NULL, filter=NULL)
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
- **elements**: list of allowed chemical elements, defaults to CHNOPS
- **filter**: NYI, will be a selection of DU, DBE and Nitrogen rules
- **molecule**: a molecule as obtained from getMolecule() or decomposeMass / decomposeIsotopes
getMolecule

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 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: WABI Paper

See Also

decomposeMass

Examples

```r
# For Glutamate:
decomposeIsotopes(c(147.0529,148.0563), c(100.0,5.561173))
```

getMolecule  

---

**Description**

Parse the sum formula and calculate the theoretical exact mass and the isotope distribution.

**Usage**

```r
getMolecule(formula, elements = NULL, z = 0)
getMass(molecule)
getFormula(molecule)
getIsotope(molecule, index)
getScore(molecule)
getValid(molecule)
```
initializeCHNOPS

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
- **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 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 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)

Steffen Neumann <sneumann@IPB-Halle.DE>

References

For a description of the underlying IMS see: WABI Paper

Examples

```r
# For Ethanol:
getcMolecule("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()
initializeCHNOPS(MgKCaFe())
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

formula repeated sum formula
mass exact mass of molecule
isotopes a list of isotopes

The initializeCharges() is special, since it allows to parse charges such as getMolecule("H3O+",
elements=c(initializeCHNOPS(),initializeCharges()))

Author(s)

Steffen Neumann <sneumann@IPB-Halle.DE>

References

For a description of the underlying IMS see: WABI Paper
Isotope patterns obtained through wikipedia.org

See Also

getcMolecule

Examples

# For Ethanol:
elements <- initializeCHNOPS()
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