addMolecules

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 mimick simple chemical reactions. No chemical checks are performed.
decomposeIsotopes

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)
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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, z=0)
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

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

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)
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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

**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**

```r
getMolecule(formula, elements = NULL, z = 0)
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
- **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
initializeCHNOPS

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 neutron 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:
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()
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)

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References

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

See Also

getMolecule

Examples

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