

# Rdisop

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addMolecules      *Add/subtract sum formulae*

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## 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.

## 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**

```
# For proton-Adduct of Ethanol:
subMolecules("C2H7O", "H")
```

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decomposeIsotopes *Mass Decomposition of Isotope Patterns*

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**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)
decomposeIsotopes(masses, intensities, ppm=2.0, mzabs=0.0001, elements=NULL, fil
isotopeScore(molecule, masses, intensities, elements = NULL, filter = NULL, z =
```

**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
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.

**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

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

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getMolecule	<i>Calculate mass and isotope information for a molecule given as sum formula</i>
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## Description

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

## Usage

```
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

## 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**

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

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```
initializeCHNOPS    Initialize (a subset of) elements of the periodic system of elements (PSE)
```

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**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

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**

[getMolecule](#)

**Examples**

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

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RcppVersion

*Rcpp Version and License Information*

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**Description**

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

**Usage**

```
RcppVersion()
```

**Author(s)**

Dominick Samperi

**Examples**

```
RcppVersion()
```

# Index

## \*Topic **methods**

addMolecules, [1](#)  
decomposeIsotopes, [2](#)  
getMolecule, [3](#)  
initializeCHNOPS, [4](#)

## \*Topic **models**

RcppVersion, [5](#)

addMolecules, [1](#)

decomposeIsotopes, [2](#)  
decomposeMass, [3](#)  
decomposeMass  
(*decomposeIsotopes*), [2](#)

getFormula (*getMolecule*), [3](#)  
getIsotope (*getMolecule*), [3](#)  
getMass (*getMolecule*), [3](#)  
getMolecule, [3,5](#)  
getScore (*getMolecule*), [3](#)  
getValid (*getMolecule*), [3](#)

initializeCharges  
(*initializeCHNOPS*), [4](#)  
initializeCHNOPS, [4](#)  
initializeCHNOPSMgKCaFe  
(*initializeCHNOPS*), [4](#)  
initializeCHNOPSNaK  
(*initializeCHNOPS*), [4](#)  
initializeElements  
(*initializeCHNOPS*), [4](#)  
initializePSE (*initializeCHNOPS*),  
[4](#)  
isotopeScore (*decomposeIsotopes*),  
[2](#)

RcppVersion, [5](#)

subMolecules (*addMolecules*), [1](#)