Package 'IsoSpecR'

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Type Package

Title An R Interface to the IsoSpec Algorithm

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Description IsoSpec is a fine structure calculator used for obtaining the most probable masses of a chemical compound given the frequencies of the composing isotopes and their masses. It finds the smallest set of isotopologues with a given probability. The probability is assumed to be that of the product of multinomial distributions, each corresponding to one particular element and parametrized by the frequencies of finding these elements in nature. These numbers are supplied by IUPAC - the International Union of Pure and Applied Chemistry.

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URL http://matteolacki.github.io/IsoSpec/

Depends R (>= 3.0.0)

Imports Rcpp (>= 0.12.0)

LazyData no

LinkingTo Rcpp

NeedsCompilation yes

SystemRequirements C++11

RoxygenNote 5.0.1

Repository CRAN

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R topics documented:

IsoSpecify *Calculate the isotopic fine structure peaks.*

Description

IsoSpecify is a wrapper around Rinterface for the C++ implementation of the IsoSpec algorithm.

Usage

```
IsoSpecify(molecule, stopCondition, isotopes = NULL, fancy = FALSE,
  algo = 0, step = 0.25, tabSize = 1000)
```

Arguments

molecule	A named integer vector, e.g. c(C=2,H=6,O=1), containing the chemical formula of the substance of interest.
stopCondition	A numeric value between 0 and 1.
isotopes	A named list of isotopic information required for IsoStar, e.g. isotopicData$IsoSpecShortList. The names must be valid element symbols. Each enlisted object should be a data.frame containing columns element (specifying the symbol of the element), mass (specifying the mass of the isotope), abundance (specyfying the assumed frequency of finding that isotope).
fancy	Logical. If TRUE, then the algorithm's results are presented in a dataframe, sorted increasingly with mass. ATTENTION!!! Sorting by mass compromises linear operating time and should be avoided in large scale computations. Then again - who would use R for that?
algo	An integer: 0 - use standard IsoStar algoritm, where stopCondition specifies the probability of the optimal p-set, 1 - use a version of algorithm that uses priority queue. Slower than 0, but does not require sorting. 2 - use a threshold version of the algorithm, where stopCondition specifies the height of the pruned peaks. 3 - for the threshold version of IsoStar with stopCondition being the percentage of the highest peak below which isotopologues get pruned.
step	The percent of the the percentile of isotopologues in the current isolayer, specyfying the cutoff for the next isolayer. It has been optimised and better not change the default value.
tabSize	A technical parameter: the initial size of the C++ dynamic table containing the results. Better not change the default value.

Value

A list constaining the masses, logarithms of probability, and the tags of isotopes making up the molecule.

Examples

```
res <- IsoSpecify( molecule = c(C=10,H=22,O=1), stopCondition = .9999 )
```

`isotopicData` *Data on isotope masses, abundances and other.*

Description

A list of data frames or table data frames (dplyr like), containing different information on isotopes.

Usage

```
isotopicData
```

Format

A list of 6 tbl_df's or data frames, each constaining:

element The symbol of an element from Mendeleev's periodic table.

isotope String composed of the nucleon number and the symbol of element.

mass Isotope's Mass in Daltons.

abundance The abundance of the isotopes. In case of enviPat data abundances do not sum to one. In case of all other, they do.

ratioC As in enviPat reference manual: "Maximum number of atoms of an element for one C-atom in a molecule, based on 99.99 % of case molecules".

Source

R Package enviPat and Commission on Isotopic Abundances and Atomic Weights, CIAAW, http://www.ciaaw.org/index.htm.

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