Package 'BRAIN'

November 11, 2026

Type Package

Title Baffling Recursive Algorithm for Isotope distributioN calculations

Version 1.58.0

Date 2018-08-08

Author Piotr Dittwald, with contributions of Dirk Valkenborg and Jurgen Claesen

Maintainer Piotr Dittwald <piotr.dittwald@mimuw.edu.pl>

Depends R (>= 2.8.1), PolynomF, Biostrings, lattice

Description Package for calculating aggregated isotopic distribution and exact center-masses for chemical substances (in this version composed of C, H, N, O and S). This is an implementation of the BRAIN algorithm described in the paper by J. Claesen, P. Dittwald, T. Burzykowski and D. Valkenborg.

License GPL-2

biocViews ImmunoOncology, MassSpectrometry, Proteomics

git_url https://git.bioconductor.org/packages/BRAIN

git_branch RELEASE_3_23

git_last_commit 210790a

git_last_commit_date 2026-04-28

Repository Bioconductor 3.23

Date/Publication 2026-11-11

Contents

BRAIN-package 2
calculateAverageMass 3
calculateIsotopicProbabilities 4
calculateMonoisotopicMass 5
calculateNrPeaks 6
getAtomsFromSeq 7

useBRAIN 8
useBRAIN2 10

Index **12**

`BRAIN-package` *Implementation of BRAIN (Baffling Recursive Algorithm for Isotope distributioN calculations)*

Description

This package implements BRAIN (Baffling Recursive Algorithm for Isotope distributioN calculations) is described in full details by Claesen et al. [Clae] (see also application note [Ditt]). The algorithm uses an algebraic approach (Viete's formulas, Newton identities [Macd]) which is especially useful for large molecules due to its advantageous scaling properties. This version of the package provides functions for calculating the aggregated isotopic distribution and center-masses masses for each aggregated isotopic variant for chemical components built from carbon, hydrogen, oxygen, nitrogen and sulfur (e.g. peptides). The natural abundances and molecular masses for stable isotopes of C, H, N, O, S are taken from IUPAC 1997 [Rosm]. Also, some heuristics to faster compute isotopic distribution are applied [Ditt2].

Details

Package:	BRAIN
Type:	Package
Version:	1.5.0
Date:	2018-08-02
License:	GPL-2
LazyLoad:	yes

Author(s)

Piotr Dittwald with contribution of Dirk Valkenborg and Jurgen Claesen

Maintainer: Piotr Dittwald <piotr.dittwald@mimuw.edu.pl>

References

[Clae] Claesen J., Dittwald P., Burzykowski T. and Valkenborg D. An efficient method to calculate the aggregated isotopic distribution and exact center-masses. JASMS, 2012, doi:10.1007/s13361-011-0326-2

[Ditt] Dittwald P., Claesen J., Burzykowski T., Valkenborg D., Gambin A. BRAIN: a universal tool for high-throughput calculations of the isotopic distribution for mass spectrometry. Anal Chem., 2013, doi: 10.1021/ac303439m

[Ditt2] Dittwald P., Valkenborg D. BRAIN 2.0: time and memory complexity improvements in the algorithm for calculating the isotope distribution. JASMS, 2014, doi: 10.1007/s13361-013-0796-5.

[Macd] Macdonald I.G., Symmetric functions and Hall polynomials / by I. G. Macdonald. Clarendon Press; Oxford University Press, Oxford : New York, 1979.

[Rosm] K.J.R. Rosman and P.D.P. Taylor. Isotopic compositions of the elements 1997. Pure and Applied Chemistry, 70(1):217-235, 1998.

Examples

```
nrPeaks = 1000
aC <-  list(C=23832, H=37816, N=6528, O=7031, S=170)  # Human dynein heavy chain
res <- useBRAIN(aC = aC, nrPeaks = nrPeaks)
iso <- res$isoDistr
masses <- res$masses
mono <- res$monoisotopicMass
avgMass <- res$avgMass
```

---

calculateAverageMass *Function computing theoretical average masses.*

Description

Function computing the theoretical average masses for chemical components composed of carbon, hydrogen, oxygen, nitrogen and sulfur (e.g. peptides).

Usage

```
calculateAverageMass(aC)
```

Arguments

aC	List with fields C, H, N, O, S of integer non-negative values (if any field is ommited, then its value is set to 0).

Details

Mass is calculated in Daltons.

Value

Average mass (numeric)

Author(s)

Piotr Dittwald <piotr.dittwald@mimuw.edu.pl>

References

[Clae] Claesen J., Dittwald P., Burzykowski T. and Valkenborg D. An efficient method to calculate the aggregated isotopic distribution and exact center-masses. JASMS, 2012, doi:10.1007/s13361-011-0326-2

See Also

useBRAIN

Examples

```
aC <-  list(C=23832, H=37816, N=6528, O=7031, S=170)  # Human dynein heavy chain
res <- calculateAverageMass(aC = aC)
```

`calculateIsotopicProbabilities`

Function computing probabilities of aggregated isotopic variants using BRAIN algorithm.

Description

Function computing probabilities of aggregated isotopic variants for chemical components built from carbon, hydrogen, oxygen, nitrogen and sulfur (e.g. peptides).

Usage

```
calculateIsotopicProbabilities(aC, stopOption = "nrPeaks",
nrPeaks, coverage, abundantEstim)
```

Arguments

`aC`	List with fields C, H, N, O, S of integer non-negative values (if any field is ommited, then its value is set to 0).
`stopOption`	one of the following strings: "nrPeaks" (default), "coverage", "abundantEstim"
`nrPeaks`	Integer indicating the number of consecutive isotopic variants to be calculated, starting from the monoisotopic one. This value can always be provided, even if <stopOption> is not a default setting. In the latter case it is a hard stopping criterion.
`coverage`	Scalar indicating the value of the cumulative aggregated distribution. The calculations will be stopped after reaching this value.
`abundantEstim`	Integer indicating the number of consecutive isotopic variants to be calculated, starting from one after the most abundant one. All consecutive isotopic variants before the most abundant peak are also returned.

Details

Remember that the isotopic variants starts from the monoisotopic one. In case of large chemical molecules, first masses may have very low abundance values for the lower mass aggregated values. A sufficient number of peaks should be calculated to reach most abundant isotopic variant.

Value

Probabilities of aggregated isotopic variants (numeric vector)

Note

If also masses associated with the aggregated isotopic variants are needed, then the function useBRAIN should be used.

Author(s)

Piotr Dittwald <piotr.dittwald@mimuw.edu.pl>

References

[Clae] Claesen J., Dittwald P., Burzykowski T. and Valkenborg D. An efficient method to calculate the aggregated isotopic distribution and exact center-masses. JASMS, 2012, doi:10.1007/s13361-011-0326-2

See Also

useBRAIN

Examples

```
  nrPeaks = 1000
  aC <-  list(C=23832, H=37816, N=6528, O=7031, S=170)  # Human dynein heavy chain
  res <- calculateIsotopicProbabilities(aC = aC, stopOption="nrPeaks",
nrPeaks = nrPeaks)
```

---

calculateMonoisotopicMass

Function computing theoretical monoisotopic masses.

Description

Function computing the theoretical monoisotopic masses for chemical components composed of carbon, hydrogen, oxygen, nitrogen and sulfur (e.g. peptides).

Usage

```
calculateMonoisotopicMass(aC)
```

Arguments

aC	List with fields C, H, N, O, S of integer non-negative values (if any field is ommited, then its value is set to 0).

Details

Mass is calculated in Daltons.

Value

Monoisotopic mass (numeric)

Author(s)

Piotr Dittwald <piotr.dittwald@mimuw.edu.pl>

References

[Clae] Claesen J., Dittwald P., Burzykowski T. and Valkenborg D. An efficient method to calculate the aggregated isotopic distribution and exact center-masses. JASMS, 2012, doi:10.1007/s13361-011-0326-2

See Also

useBRAIN

Examples

```
aC <-  list(C=23832, H=37816, N=6528, O=7031, S=170)  # Human dynein heavy chain
res <- calculateMonoisotopicMass(aC = aC)
```

---

calculateNrPeaks *Function computing heuristically the required number of consecutive aggregated isotopic variants.*

Description

Function computing heuristically the required number of consecutive aggregated isotopic variants (starting from the monoisotopic mass).

Usage

```
calculateNrPeaks(aC)
```

Arguments

aC	List with fields C, H, N, O, S of integer non-negative values (if any field is ommited, then its value is set to 0).

Details

This function uses following rule of thumb: the difference between the theoretical monoisotopic mass and the theoretical average mass is computed and multiplied by two. Subsequently, the obtained number is rounded to the nearest integer greater than or equal to the multiplied difference. For small molecules, the minimal number of returned variants is five.

Value

Integer number not lower than 5.

Author(s)

Jurgen Claesen <jurgen.claesen@uhasselt.be>

References

[Clae] Claesen J., Dittwald P., Burzykowski T. and Valkenborg D. An efficient method to calculate the aggregated isotopic distribution and exact center-masses. JASMS, 2012, doi:10.1007/s13361-011-0326-2

See Also

useBRAIN

Examples

```
aC <-  list(C=23832, H=37816, N=6528, O=7031, S=170)  # Human dynein heavy chain
res <- calculateNrPeaks(aC = aC)
```

`getAtomsFromSeq` *Function computing an atomic composition from amono acid sequence.*

Description

Function computing an atomic composition from (naturally occuring) amino acid sequence.

Usage

```
getAtomsFromSeq(seq)
```

Arguments

`seq`	The character vector of AAString (see Biostrings package) with amino acid sequence. It should contain only letters "A", "R", "N", "D", "C", "E", "Q", "G", "H", "I", "L", "K", "M", "F", "P", "S", "T", "W", "Y", "V" (1-letter symbols of 20 naturally occuring amino acids).

Details

The atomic composition is just a summaric atomic composition of all amino acids composing the sequence minus (n-1) times the water molecule, where n is a length of given amino acid sequence.

Value

Named list with the following fields with number of correcponding atoms (integer non-negative values):

- C,
- H,
- N,
- O,
- S

Author(s)

Piotr Dittwald <piotr.dittwald@mimuw.edu.pl>

Examples

```
seq1 <-  "AACD"
aC1 <- getAtomsFromSeq(seq = seq1)
seq2 <-  AAString("ACCD")
aC2 <- getAtomsFromSeq(seq = seq2)
```

---

useBRAIN *Function computing probabilities of aggregated isotopic variants and their center-masses using BRAIN algorithm.*

Description

Function computing probabilities of isotopic variants and their aggregated masses for chemical components composed of carbon, hydrogen, oxygen, nitrogen and sulfur (e.g. peptides). Additionally the function returns also the monoisotopic mass and the average mass of given chemical component.

Usage

```
useBRAIN(aC, stopOption = "nrPeaks", nrPeaks, coverage, abundantEstim)
```

Arguments

aC	List with fields C, H, N, O, S of integer non-negative values (if any field is ommited, then its value is set to 0).
stopOption	one of the following strings: "nrPeaks" (default), "coverage", "abundantEstim"
nrPeaks	Integer indicating the number of consecutive isotopic variants to be calculated, starting from the monoisotopic one. This value can always be provided, even if <stop.option> is not a default setting. In the latter case it is a hard stopping criterion.
coverage	Scalar indicating the value of the cumulative aggregated distribution. The calculations will be stopped after reaching this value.
abundantEstim	Integer indicating the number of consecutive isotopic variants to be calculated, starting from one after the most abundant one. All consecutive isotopic variants before the most abundant peak are also returned.

Details

Function uses recursive formulae based on algebraic Newton-Girard identity (see [Clae]).

Value

Named list with the following fields:

- isoDistrProbabilities of aggregated isotopic variants (numeric vector)
- massesAggregated masses for isotopic variants (numeric vector)
- monoisotopicMassMonoisotopic mass (numeric)
- avgMassAverage mass - weighted average of the isotopic variants contributing to the most abundant aggregated variant (numeric)

Note

Remember that the isotopic variants starts from monoisotopic one. For large chemical molecules, first masses may have very low abundances. So sufficient number of peaks should be calculated to reach most abundant isotopic variant.

If only isotopic probabilities are needed, then the function calculateIsotopicProbabilities should be used.

Author(s)

Piotr Dittwald <piotr.dittwald@mimuw.edu.pl>

References

[Clae] Claesen J., Dittwald P., Burzykowski T. and Valkenborg D. An efficient method to calculate the aggregated isotopic distribution and exact center-masses. JASMS, 2012, doi:10.1007/s13361-011-0326-2

See Also

calculateIsotopicProbabilities

Examples

```
nrPeaks = 1000
aC <-  list(C=23832, H=37816, N=6528, O=7031, S=170)  # Human dynein heavy chain
res <-  useBRAIN(aC = aC, stopOption="nrPeaks", nrPeaks = nrPeaks)
```

---

useBRAIN2 *Function computing probabilities of aggregated isotopic variants using heuristics.*

Description

Function computing probabilities of isotopic variants using heuristics, for chemical components composed of carbon, hydrogen, oxygen, nitrogen and sulfur (e.g. peptides). Additionally the function returns also the monoisotopic mass and the average mass of given chemical component.

Usage

```
useBRAIN2(aC, stopOption = "nrPeaks", nrPeaks, approxStart = 1, approxParam = NULL))
```

Arguments

aC	List with fields C, H, N, O, S of integer non-negative values (if any field is ommited, then its value is set to 0).
stopOption	only option "nrPeaks" allowed
nrPeaks	Integer indicating the number of consecutive isotopic variants to be calculated, starting from the monoisotopic one. This value can always be provided, even if <stop.option> is not a default setting. In the latter case it is a hard stopping criterion.
approxStart	Integer indicating the number of first isotopic peak to be calculated
approxParam	Integer indicating the length of recurrence (see RCL in [Ditt2])

Details

Function uses RCL and LSP heuristics from [Ditt2].

Value

Named list with the following fields:

- isoDistrProbabilities of aggregated isotopic variants (numeric vector)

Note

Remember that the isotopic variants starts from monoisotopic one. For large chemical molecules, first masses may have very low abundances. So sufficient number of peaks should be calculated to reach most abundant isotopic variant.

If only isotopic probabilities are needed, then the function calculateIsotopicProbabilities should be used.

Author(s)

Piotr Dittwald <piotr.dittwald@mimuw.edu.pl>

References

[Ditt2] Dittwald P., Valkenborg D. BRAIN 2.0: time and memory complexity improvements in the algorithm for calculating the isotope distribution. JASMS, 2014, doi: 10.1007/s13361-013-0796-5.

See Also

calculateIsotopicProbabilities

Examples

```
nrPeaks = 1000
aC <-  list(C=23832, H=37816, N=6528, O=7031, S=170)  # Human dynein heavy chain
res <-  useBRAIN(aC = aC, stopOption="nrPeaks", nrPeaks = nrPeaks)
res2 <-  useBRAIN2(aC = aC, stopOption="nrPeaks", nrPeaks = nrPeaks, approxStart = 10)
old = res$iso[10:109]/res$iso[11:110]
new  = res2$iso[1:100]/res2$iso[2:101]
max(old - new)
max((old - new)/old)
res3 <-  useBRAIN2(aC = aC, stopOption="nrPeaks", nrPeaks = nrPeaks, approx=TRUE, approxParam = 10)
max(res3$iso - res$iso)
```

Index

∗ **package**
BRAIN-package, 2

BRAIN *(*BRAIN-package*)*, 2
BRAIN-package, 2

calculateAverageMass, 3
calculateIsotopicProbabilities, 4, *10, 11*
calculateMonoisotopicMass, 5
calculateNrPeaks, 6

getAtomsFromSeq, 7

useBRAIN, *4–7*, 8
useBRAIN2, 10