

Package ‘enviPat’

October 21, 2022

Type Package

Title Isotope Pattern, Profile and Centroid Calculation for Mass Spectrometry

Version 2.6

Date 2022-10-21

Author Martin Loos, Christian Gerber

Maintainer Martin Loos <mloos@envibee.ch>

Description Fast and very memory-efficient calculation of isotope patterns, subsequent convolution to theoretical envelopes (profiles) plus valley detection and centroidization or intensoid calculation. Batch processing, resolution interpolation, wrapper, adduct calculations and molecular formula parsing.

Loos, M., Gerber, C., Corona, F., Hollender, J., Singer, H. (2015) <[doi:10.1021/acs.analchem.5b00941](https://doi.org/10.1021/acs.analchem.5b00941)>.

License GPL-2

BugReports <https://github.com/blosloos/enviPat/issues>

URL <https://www.envipat.eawag.ch/>,
<https://pubs.acs.org/doi/abs/10.1021/acs.analchem.5b00941>

NeedsCompilation yes

Repository CRAN

Date/Publication 2022-10-21 12:55:12 UTC

R topics documented:

| | |
|---------------------------|---|
| enviPat-package | 2 |
| adducts | 3 |
| check_chemform | 4 |
| check_ded | 6 |
| check_several | 7 |
| chemforms | 8 |
| envelope | 9 |

| | |
|---------------------------|----|
| getR | 11 |
| isopattern | 12 |
| isotopes | 15 |
| isowrap | 16 |
| mergeform | 17 |
| multiform | 18 |
| resolution_list | 19 |
| subform | 21 |
| vdetect | 22 |

| | |
|--------------|-----------|
| Index | 24 |
|--------------|-----------|

| | |
|-----------------|--|
| enviPat-package | <i>Calculation of isotope patterns, stick profiles (envelopes) and centroids/intensoids for mass spectrometry.</i> |
|-----------------|--|

Description

Fast and memory-efficient calculation of isotope patterns (fine structures) for up to very large molecules, based on three different algorithms. Subsequent convolution of isotope patterns with a peak shape function to theoretical envelopes (profiles). Based on envelopes, valley detection and centroidization/intensoid calculation. Allows for batch processing of chemical formulas and interpolation of measurement resolutions. Includes a wrapper combining all of the above functionalities.

Furthermore, includes (1) a check for consistency of chemical formulas, (2) a check for molecules with overlapping isotope patterns, (3) a list of all stable isotopes, (4) a list of different resolution data sets for Thermo Orbitrap and QExactive high-resolution mass spectrometers and (5) a list of adducts formed during electrospray ionization (ESI).

A web-based GUI for enviPat is freely available under <https://www.envipat.eawag.ch>.

Details

| | |
|-----------|------------|
| Package: | enviPat |
| Type: | Package |
| Version: | 1.0 |
| Date: | 2013-03-05 |
| License: | GPL-2 |
| LazyLoad: | yes |

Author(s)

Martin Loos, Christian Gerber

Maintainer: Martin Loos <martin.loos@alumni.ethz.ch>

References

Loos, M., Gerber, C., Corona, F., Hollender, J., Singer, H. (2015). Accelerated isotope fine structure calculation using pruned transition trees, *Analytical Chemistry* 87(11), 5738-5744.

<https://pubs.acs.org/doi/abs/10.1021/acs.analchem.5b00941>

See Also

[check_chemform](#) [getR](#) [isopattern](#) [envelope](#) [vdetect](#) [isowrap](#) [check_several](#)
[isotopes](#) [resolution_list](#) [chemforms](#)
[adducts](#) [check_ded](#) [mergeform](#) [subform](#) [multiform](#)

adducts

Adduct list

Description

List of common adducts observed for ESI-MS measurements in soft positive and negative ionization modes.

Usage

```
data(adducts)
```

Format

A data frame with 47 observations on the following 6 variables.

Name Adduct name

calc Equation for calculating adduct m/z from uncharged non-adduct molecular mass M ($m/z = M/z + X$)

Charge z

Mult 1/z

Mass X

Ion_mode Ionization mode (positive or negative)

Formula_add Adduct chemical formula to be added

Formula_ded Adduct chemical formula to be subtracted

Multi Factor to multiply chemical formula with

Details

The correct way to calculate the isotopic pattern of a specific adduct is the following. First, multiply the chemical formula of the molecule by the times it appears in the final adduct; [multiform](#). Second, add the chemical formula of any adduct to that of the molecule; [mergeform](#). Third, subtract the chemical formula of any deduct from that of the molecule; [check_ded](#) & [subform](#). Finally, calculate the isotopic fine structure using the correct charge argument in [isopattern](#).

Note

Chemical formulas must conform to what is described in [check_chemform](#).

Source

<https://fiehnlab.ucdavis.edu/staff/kind/Metabolomics/MS-Adduct-Calculator/>

References

Huang N., Siegel M.M., Kruppa G.H., Laukien F.H., J. Am. Soc. Mass. Spectrom. 1999, 10. Automation of a Fourier transform ion cyclotron resonance mass spectrometer for acquisition, analysis, and e-mailing of high-resolution exact-mass electrospray ionization mass spectral data

See Also

[multiform](#) [mergeform](#) [check_ded](#) [subform](#)

Examples

```
# example of M+H adduct batch calculation
data(adducts)
data(isotopes)
data(chemforms)
# (1) check formulas for consistency - recommended
checked_chemforms <-check_chemform(isotopes, chemforms)
# (2) multiply, see column 4 of adducts
chemforms <-multiform(checked_chemforms[,2],1)
# (3) add adduct - see column 7 of adducts
chemforms<-mergeform(chemforms,"H1")
# (4) calculate fine structure
patterns <- isopattern(isotopes, chemforms)
```

check_chemform

Check chemical formulas

Description

Checks chemical formulas (=a vector of character strings) for consistency with usage in [isopattern](#); calculation of the molecular mass.

Usage

```
check_chemform(isotopes,chemforms,get_sorted=FALSE,get_list=FALSE)
```

Arguments

| | |
|------------|---|
| isotopes | isotopes |
| chemforms | Vector of character strings with chemical formulas |
| get_sorted | Should elements in each formula be sorted according to their order in isotopes? |
| get_list | Return list with vectors of elementwise atom counts contained in each chemical formula? |

Details

Default checks if (1) a chemical formula contains only letters, numbers and square or round brackets, (2) elements can be found in [isotopes](#) and (3) letters and round brackets are all followed by a number of counts. Where (3) are missing, they are set to 1.

(2) must consist of an upper case letter, possibly followed by lower case letters; to refer to individual isotopes (e.g., from isotope labelling of a molecule, e.g., N5 vs. [15]N2N3), square brackets may precede the capital letter. Any other symbols which may be part of a chemical formula (e.g., charges (+), dashes, asterisks, ...) are not permissible.

The molecular mass will be calculated from isotope masses and abundances listed in [isotopes](#).

Value

Dataframe with 3 columns for `get_list=FALSE`:

| | |
|-------------------|---------------------------------------|
| warning | Correct chemical formula, FALSE/TRUE? |
| new_formula | Chemical formula |
| monoisotopic_mass | Monoisotopic mass |

Or list containing vector of elements for `get_list=TRUE`.

Note

Highly recommended for usage with [isopattern](#)

Author(s)

Martin Loos, Christian Gerber

See Also

[isopattern](#) [isotopes](#)

Examples

```
# Check package data set of chemical formulas #####
data(chemforms);
data(isotopes);
checked<-check_chemform(isotopes,chemforms);
```

```
checked;

# Check for some senseless molecular formulas #####
chemforms<-c("C900C14H49", "082394", "C8G500Zn9", "Br1", "6DBr9889");
data(isotopes);
checked<-check_chemform(isotopes, chemforms);
checked;

# Molecular mass with and without isotope labelling #####
chemforms<-c("C10H5N4O5", "[13]C2C8D2H3[15]N2N2[18]O2O3");
data(isotopes);
checked<-check_chemform(isotopes, chemforms);
checked;
```

| | |
|-----------|---|
| check_ded | <i>Check if a chemical formula is subset in another one</i> |
|-----------|---|

Description

Check if a chemical formula is contained in another chemical formula

Usage

```
check_ded(formulas, deduct)
```

Arguments

| | |
|----------|--|
| formulas | Vector with the containing chemical formula(s) |
| deduct | Chemical formula to be contained ("deduct") |

Value

Returns a vector with length of input formulas, with TRUE if deduct is not contained and FALSE otherwise.

Note

Might be used prior to subtracting a "deduct" chemical formula from that of a molecule when including adducts in the calculation of isotopic patterns. Chemical formulas must conform to what is described in [check_chemform](#).

Author(s)

Martin Loos

See Also

[adducts](#)

Examples

```
formulas<-c("C8H4Cl2", "C10H16O2", "C3H10")
deduct<-c("C4H10")
check_ded(formulas, deduct)
```

| | |
|---------------|---|
| check_several | <i>Check for overlapping molecules.</i> |
|---------------|---|

Description

Check for molecules overlapping in m/z, based on isotope fine structures from [isopattern](#) or on centroids/intensoids from [envelope](#).

Usage

```
check_several(pattern, dmz, ppm = TRUE)
```

Arguments

| | |
|---------|--|
| pattern | Output from isopattern or from envelope . |
| dmz | m/z window. In combination with ppm=TRUE set as ppm or with ppm=FALSE set as absolute m/z. |
| ppm | Should m/z window be set in ppm (TRUE) or absolute m/z (FALSE)? |

Details

Overlaps in m/z among molecules are screened for within the m/z tolerance defined by the arguments dmz and ppm.

Value

Dataframe with 4 columns, with number of rows equal to the length of argument pattern

| | |
|-------------|---|
| compound | Chemical formula of the compound |
| warning | Overlap detected? |
| to? | If overlap: with which other compound(s)? Refers to row number, recycled for peak_number. |
| peak_number | If overlap: with which peak(s) of the other compound(s)? Refers to peak number. |

Author(s)

Martin Loos, Christian Gerber

See Also

[isopattern envelope](#)

Examples

```
data(isotopes)
data(chemforms)
pattern<-isopattern(
  isotopes,
  chemforms,
  threshold=0.1,
  plotit=TRUE,
  charge=FALSE,
  emass=0.00054858,
  algo=1
)
check_several(pattern,dmz=0.001,ppm=FALSE)
```

chemforms

Set of exemplary chemical formulas for small molecules.

Description

Vector with character strings of exemplary chemical formulas (pesticides, pharmaceuticals)

Usage

```
data(chemforms)
```

Format

Vector with character strings

Examples

```
data(chemforms)
chemforms
```


envelope

*Isotope pattern envelope calculation***Description**

Convolute an isotope pattern from `isopattern` with a peak shape function (Gaussian or Cauchy-Lorentz function) to its theoretical envelope (profile), at a given measurement resolution. The envelope is represented by sticks, i.e. measurement abundances at discrete m/z intervals.

Usage

```
envelope(pattern, ppm = FALSE, dmz = "get", frac = 1/4, env = "Gaussian",
resolution = 5e+05, plotit = FALSE, verbose = TRUE)
```

Arguments

| | |
|-------------------------|--|
| <code>pattern</code> | List of isotope pattern(s) as generated by <code>isopattern</code> . |
| <code>ppm</code> | Should stick discretization be set in ppm (TRUE) or absolute m/z (FALSE)? Only checked if <code>dmz</code> is not set to "get"; check details section. |
| <code>dmz</code> | Stick discretization. Set to "get" to derive discretization from argument <code>resolution</code> or set a numerical value in combination with <code>ppm</code> to use as ppm or absolute m/z . Check details section. |
| <code>frac</code> | Used if <code>dmz</code> is set to "get". Check details section. |
| <code>env</code> | Peak shape function; either "Gaussian" or "CauchyLorentz". |
| <code>resolution</code> | Single resolution value or vector of resolutions with length equal to the number of entries in list <code>pattern</code> . Check resolution definition in the details section. |
| <code>plotit</code> | Should results be plotted, TRUE/FALSE ? |
| <code>verbose</code> | Verbose, TRUE/FALSE? |

Details

The theoretical profiles are represented by sticks, i.e. abundances at discrete m/z intervals. While the profile width is set by argument `resolution`, the mass discretization between adjacent sticks can be set in two different ways.

On the one hand, discretization can be given as a numerical value, either in ppm or absolute m/z . To do so, set argument `dmz` to a numerical value and specify with argument `ppm` if this value is stating the discretization in ppm or as absolute m/z .

On the other hand, discretization can be derived from the measurement resolution (R) set by argument `resolution`. To do so, set `dmz` to "get", which leads to argument `ppm` being ignored. In this case, the stick discretization is retrieved from $(dm/z)*frac$, with $(dm/z) = (m/z)/R =$ peak width at half maximum.

Value

List with length equal to length of list `pattern`, with equal names of list entries. Each entry in that list contains the sticks of the envelope in two columns:

| | |
|------------------------|------------------------------|
| <code>m/z</code> | Stick <code>m/z</code> |
| <code>abundance</code> | Stick <code>abundance</code> |

Note

The resolution R is defined as $R=(m/z)/(dm/z)$, with dm/z = peak width at half maximum, cp. [resolution_list](#).

Author(s)

Martin Loos, Christian Gerber

References

Li, L., Kresh, J., Karabacak, N., Cobb, J., Agar, J. and Hong, P. (2008). A Hierarchical Algorithm for Calculating the Isotopic Fine Structures of Molecules. *Journal of the American Society for Mass Spectrometry*, 19, 1867–1874.

See Also

[isopattern](#) [getR](#) [vdetect](#)

Examples

```
#####  
# batch of chemforms #####  
data(isotopes)  
data(chemforms)  
chemforms<-chemforms[1:5]  
  
pattern<-isopattern(  
  isotopes,  
  chemforms,  
  threshold=0.1,  
  plotit=TRUE,  
  charge=FALSE,  
  emass=0.00054858,  
  algo=2  
)  
  
profiles<-envelope(  
  pattern,  
  ppm=FALSE,  
  dmz=0.0001,  
  frac=1/4,  
  env="Gaussian",
```

```
    resolution=1E6,  
    plotit=TRUE  
  )  
#####
```

getR

Interpolation of MS measurement resolution

Description

Given a set of MS measurement resolutions (R) as a function of measurement mass (m/z), [getR](#) interpolates R for any given molecular mass(es) calculated by [check_chemform](#) using [smooth.spline](#).

Usage

```
getR(checked, resmass, nknots = 13, spar = 0.1, plotit = TRUE)
```

Arguments

| | |
|---------|--|
| checked | Dataframe produced by check_chemform . |
| resmass | Dataframe with two columns, resolution and mass; such as the list entries in resolution_list . |
| nknots | Integer number of knots to use for the smoothing spline. Default = 6. See also smooth.spline . |
| spar | Smoothing parameter, (0,1]. See also smooth.spline . |
| plotit | Plot results, TRUE/FALSE ? |

Value

Vector with resolutions.

Note

[check_chemform](#) gives molecular masses (m/z) for z=+/-1 only. If z>1 or z<-1 is required, molecular mass entries in argument checked have to be divided accordingly to be consistent.

Author(s)

Martin Loos, Christian Gerber

See Also

[smooth.spline](#) [check_chemform](#) [resolution_list](#)

Examples

```

data(resolution_list)
resmass<-resolution_list[[4]]
data(isotopes)
data(chemforms)
checked<-check_chemform(isotopes,chemforms)
resolution<-getR(checked,resmass,nknots=13,spar=0.1,plotit=TRUE)

# same for z=-2:
checked<-check_chemform(isotopes,chemforms)
checked[,3]<-(checked[,3]/abs(-2))
resolution<-getR(checked,resmass,nknots=13,spar=0.1,plotit=TRUE)

```

 isopattern

Isotope pattern calculation

Description

The function calculates the isotopologues ("isotope fine structure") of a given chemical formula or a set of chemical formulas (batch calculation) with fast and memory efficient transition tree algorithms, which can handle relative pruning thresholds. Returns accurate masses, probabilities and isotopic compositions of individual isotopologues. The isotopes of elements can be defined by the user.

Usage

```

isopattern(isotopes, chemforms, threshold = 0.001, charge = FALSE,
emass = 0.00054857990924, plotit = FALSE, algo=1, rel_to = 0, verbose = TRUE,
return_iso_calc_amount = FALSE)

```

Arguments

| | |
|------------------------|---|
| isotopes | Dataframe listing all relevant isotopes, such as isotopes . |
| chemforms | Vector with character strings of chemical formulas, such as data set chemforms or the second column in the value of check_chemform . |
| threshold | Probability below which isotope peaks can be omitted, as specified by argument <code>rel_to</code> . Set to 0 if all peaks shall be calculated. |
| charge | z in m/z. Either a single integer or a vector of integers with length equal to that of argument <code>chemforms</code> . Set to FALSE for omitting any charge calculations. |
| emass | Electrone mass; only relevant if charge is not set to FALSE. |
| plotit | Should results be plotted, TRUE/FALSE? |
| algo | Which algorithm to use? Type 1 or 2. See details. |
| rel_to | Probability definition, numeric 0, 1, 2, 3 or 4? See details. |
| verbose | Verbose, TRUE/FALSE? |
| return_iso_calc_amount | Ignore; number of intermediate isotopologues. |

Details

Isotope pattern calculation can be done by choosing one of two algorithms, set by argument `algo`. Both algorithms use transition tree updates to derive the exact mass and probability of a new isotopologue from existing ones, by steps of single isotope replacements. These transition tree approaches are memory-efficient and fast for a wide range of molecular formulas and are able to reproduce the isotope fine structure of molecules. The latter must often be pruned during calculation, c.p. argument `rel_to`.

`algo=1` grows transition trees within element-wise sub-molecules, whereas `algo==2` grows them in larger sub-molecules of two elements, if available. The latter approach can be slightly more efficient for very large or very complex molecules. The sub-isotopologues within sub-molecules are finally combined to the isotopologues of the full molecule. In contrast, intermediate counts of sub-isotopologues instead of fine structures are returned for `return_iso_calc_amount==TRUE`

`rel_to` offers 5 possibilities of how probabilities are defined and pruned, each affecting the `threshold` argument differently. Default option `rel_to=0` prunes and returns probabilities relative to the most intense isotope peak; `threshold` states a percentage of the intensity of this latter peak. Similarly, option `rel_to=1` normalizes relative to the peak consisting of the most abundant isotopes for each element, which is often the monoisotopic one. Option `rel_to=2` prunes and returns absolute probabilities; `threshold` is not a percentage but an absolute cutoff. Options `rel_to=3` and `rel_to=4` prune relative to the most intense and "monoisotopic" peak, respectively. Although `threshold` is a percentage, both options return absolute probabilities.

Value

List with length equal to length of vector `chemforms`; names of entries in list = chemical formula in `chemform`. Each entry in that list contains information on individual isotopologues (rows) with columns:

| | |
|------------------------------------|---|
| <code>m/z</code> | First column; <code>m/z</code> of an isotope peak. |
| <code>abundance</code> | Second column; abundance of an isotope peak. Probabilities are set relative to the most abundant peak of the isotope pattern. |
| <code>12C, 13C, 1H, 2H, ...</code> | Third to all other columns; atom counts of individual isotopes for an isotope peak. |

warning

Too low values for `threshold` may lead to unnecessary calculation of low probable isotope peaks - to the extent that not enough memory is available for either of the two algorithms.

Note

It is highly recommended to check argument `chemforms` with `check_chemform` prior to running `isopattern`; argument `chemforms` must conform to chemical formulas as defined in `check_chemform`. Element names must be followed by numbers (atom counts of that element), i.e. `C1H4` is a valid argument whereas `CH4` is not. Otherwise, numbers may only be used in square brackets to denote individual isotopes defined in the element name column of `iso_list`, such as `[14]C` or `[18]O`. For example, `[13]C2C35H67N1O13` is the molecular formula of erythromycin labeled at two C-positions with `[13]C`; `C37H67N1O13` is the molecular formula of the unlabeled compound.

For correct adduct isotope pattern calculations, please check [adducts](#).

Author(s)

Martin Loos, Christian Gerber

References

Loos, M., Gerber, C., Corona, F., Hollender, J., Singer, H. (2015). Accelerated isotope fine structure calculation using pruned transition trees, *Analytical Chemistry* 87(11), 5738-5744.

<https://pubs.acs.org/doi/abs/10.1021/acs.analchem.5b00941>

<https://www.envipat.eawag.ch/index.php>

See Also

[isopattern](#) [chemforms](#) [check_chemform](#) [getR](#) [envelope](#) [vdetect](#) [check_several](#)

Examples

```
#####  
# batch of chemforms #####  
data(isotopes)  
data(chemforms)  
pattern<-isopattern(  
  isotopes,  
  chemforms,  
  threshold=0.1,  
  plotit=TRUE,  
  charge=FALSE,  
  emass=0.00054858,  
  algo=1  
)  
#####  
# Single chemical formula ##  
data(isotopes)  
pattern<-isopattern(  
  isotopes,  
  "C100H200S2C15",  
  threshold=0.1,  
  plotit=TRUE,  
  charge=FALSE,  
  emass=0.00054858,  
  algo=1  
)  
#####
```

isotopes

Stable isotopes

Description

Dataframe with stable isotopes.

Usage

```
data(isotopes)
```

Format

A data frame with 302 observations on the following 4 variables.

element Chemical element

isotope Stable isotopes of an element

mass Relative atomic mass

abundance Isotopic composition of an element

ratioC Maximum number of atoms of an element for one C-atom in a molecule, based on 99.99 % of case molecules.

Details

The ratioC-value stems from a database survey conducted by Kind&Fiehn (2007); to disable, set value to 0. The list serves as input into several package nontarget-functions. The first column of the data frame also contains names of specific isotopes used for labeled compounds.

Source

https://physics.nist.gov/cgi-bin/Compositions/stand_alone.pl

References

Kind, T. and Fiehn, O., 2007. Seven golden rules for heuristic filtering of molecular formulas obtained by accurate mass spectrometry. *BMC Bioinformatics*, 8:105.

Examples

```
data(isotopes)
```

| | |
|---------|--|
| isowrap | <i>Combined (batch) calculation of isotope pattern, envelope and centroids/intensoids/valleys on interpolated resolutions.</i> |
|---------|--|

Description

Wrapper combining the functions [getR](#), [isopattern](#), [envelope](#) and [vdetect](#).
 Uses chemical formulas from [check_chemform](#) as argument.

Usage

```
isowrap(isotopes, checked, resmass, resolution = FALSE, nknots = 6,
spar = 0.2, threshold = 0.1, charge = 1, emass = 0.00054858, algo=2,
ppm = FALSE, dmz = "get", frac = 1/4, env = "Gaussian",
detect = "centroid", plotit = FALSE)
```

Arguments

| | |
|------------|---|
| isotopes | Dataframe listing all relevant isotopes, such as isotopes . |
| checked | Output dataframe from check_chemform with correct chemical formulas. |
| resmass | For resolution interpolation: dataframe with two columns, resolution and mass; see getR . Otherwise, set to FALSE and use argument resolution to utilize a single resolution. |
| resolution | Single resolution value. Only used if argument resmass is set to FALSE. |
| nknots | Number of knots, see getR . Ignored if argument resmass set to FALSE. |
| spar | Smoothing parameter, see getR . Ignored if argument resmass set to FALSE. |
| threshold | Abundance below which isotope peaks are omitted, see isopattern . |
| charge | z in m/z, see isopattern . |
| emass | Electrone mass. Only relevant if charge is not set to FALSE, see isopattern . |
| algo | Which algorithm to use? Type 1 or 2. See details section in isopattern . |
| ppm | Set stick discretization, see details section of envelope . |
| dmz | Set stick discretization, see details section of envelope . |
| frac | Set stick discretization, see details section of envelope . |
| env | Peak shape function, see envelope . |
| detect | Return either "centroid", "intensoid" or "valley". See vdetect . |
| plotit | Should results be plotted, TRUE/FALSE? |

Value

List with length equal to length of list profiles, with equal names of list entries. Each entry in that list contains the centroids, intensoids or valley of the envelope in two columns:

| | |
|-----------|---|
| m/z | m/z |
| abundance | area(centroid) or abundance (intensoid, valley) |

Author(s)

Martin Loos, Christian Gerber

See Also

[vdetect](#)

Examples

```
data(isotopes);
data(resolution_list);
data(chemforms);
chemforms<-chemforms[1:10];

checked<-check_chemform(
  isotopes,
  chemforms
);

resmass<-resolution_list[[1]]

centro<-isowrap(
  isotopes,
  checked,
  resmass=resolution_list[[4]],
  resolution=FALSE,
  nknots=4,
  spar=0.2,
  threshold=0.1,
  charge=1,
  emass=0.00054858,
  algo=2,
  ppm=FALSE,
  dmz="get", # retrieve dm from R=m/dm
  frac=1/4,
  env="Gaussian",
  detect="centroid",
  plotit=TRUE
)
```

mergeform

Combine chemical formulas

Description

Combine chemical formulas

Usage

```
mergeform(formula1, formula2)
```

Arguments

formula1 Vector of first chemical formula(s), character string(s)
formula2 Second chemical formula, single character string

Details

Useful for adduct calculations, check [adducts](#). Chemical formulas must conform to what is described in [check_chemform](#).

Value

Merged chemical formula(s), character string

Author(s)

Martin Loos

See Also

[adducts](#)

Examples

```
formula1<-c("C10[13]C2H10C110")  
formula2<-c("C2H5Na1")  
mergeform(formula1, formula2)
```

multiform

Multiply a chemical formula

Description

Multiply all atom numbers in a chemical formula by a factor

Usage

```
multiform(formula_in, fact)
```

Arguments

formula_in Chemical formula to be multiplied, vector of character strings
fact Factor to multiply with

Details

Useful for adduct calculations, check [adducts](#). Chemical formulas must conform to what is described in [check_chemform](#).

Value

Multiplied chemical formula, character string

Author(s)

Martin Loos

See Also

[adducts](#)

Examples

```
formula_in <- "C10[13]C2H10C110"  
multiform(formula_in, 3)
```

resolution_list

Resolutions (R) list for mass spectrometers

Description

List of different resolutions $R=f(m/z)$ for various (high-resolution) mass spectrometers. For each of the instruments, different resolution settings are available. Here, R is defined as $R=(m/z)/(dm/z)$, with dm/z = peak width at half maximum. Serves as input to [getR](#) to interpolate R from given molecular masses.

Usage

```
data(resolution_list)
```

Format

The format is: List with 29 data sets: Instrument_(massRange_instrumentMode_slicerMode)_Resolution@m/z
Elite/R240000@400
Elite/R120000@400
Elite/R60000@400
Elite/R30000@400
OrbitrapXL,Velos,VelosPro/R120000@400
OrbitrapXL,Velos,VelosPro/R60000@400
OrbitrapXL,Velos,VelosPro/R30000@400

OrbitrapXL,Velos,VelosPro/R15000@400
OrbitrapXL,Velos,VelosPro/R7500@400
Q-Exactive,ExactivePlus/280K@200
Q-Exactive,ExactivePlus/R140000@200
Q-Exactive,ExactivePlus/R70000@200
Q-Exactive,ExactivePlus/R35000@200
Q-Exactive,ExactivePlus/R17500@200
Exactive/R100000@200
Exactive/R50000@200
Exactive/R25000@200
Exactive/R12500@200
OTFusion,QExactiveHF/480000@200
OTFusion,QExactiveHF/240000@200
OTFusion,QExactiveHF/120000@200
OTFusion,QExactiveHF/60000@200
OTFusion,QExactiveHF/30000@200
OTFusion,QExactiveHF/15000@200
QTOF_XevoG2-S/R25000@200
Sciex_TripleTOF5600_R25000@200
Sciex_TripleTOF6600_R25000@200
Sciex_QTOFX500R_R25000@200
Agilent_low_extended_highSens_QTOF6550_R25000@200

Source

Data assembled from individual measurements.

Examples

```
data(resolution_list)
resolution_list
```

| | |
|---------|---|
| subform | <i>Subtract one chemical formula from another</i> |
|---------|---|

Description

Subtract one chemical formula from another

Usage

```
subform(formula1, formula2)
```

Arguments

| | |
|----------|-----------------------------------|
| formula1 | Chemical formula to subtract from |
| formula2 | Chemical formula to subtract |

Details

Useful for adduct calculations, check [adducts](#). Chemical formulas must conform to what is described in [check_chemform](#). Prior check if formula2 is contained in formula1 at all? See [check_ded](#).

Value

A unified and filtered peaklist

Author(s)

Martin Loos

See Also

[adducts](#), [check_ded](#)

Examples

```
formula1<-c("C10[13]C2H10C110")
formula2<-c("C2H5[13]C1")
subform(formula1, formula2)
```

vdetect *Valley detection and centroidization*

Description

Checks envelopes calculated by [envelope](#) for valleys and extracts centroids or intensoids.

Usage

```
vdetect(profiles,detect="centroid",plotit=TRUE,verbose=TRUE)
```

Arguments

| | |
|----------|---|
| profiles | List of stick profiles as generated by envelope . |
| detect | To return either "centroid", "intensoid" or "valley". |
| plotit | Should results be plotted, TRUE/FALSE? |
| verbose | Verbose, TRUE/FALSE? |

Value

List with length equal to length of list profiles, with equal names of list entries. Each entry in that list contains the centroids, intensoids or valleys of the envelope in two columns:

| | |
|-----------|--|
| m/z | m/z |
| abundance | Area (centroid) or abundance (intensoid, valley) |

definitions

Valley: local profile minimum, i.e. any envelope stick flanked by two other sticks of higher abundance.

Stick: see [envelope](#).

Centroid mass: intensity-weighted sum of the m/z of sticks between two valleys.

Centroid intensity: profile area between two valleys (mean of upper and lower sum of stick intensities), normalized to the maximum centroid area of the envelope.

Intensoid mass: m/z of the most intense stick between two valleys.

Intensoid intensity: intensity of the most intensive stick between two valleys, normalized to the most intense intensoid.

Note

Too low stick discretization leads to imprecision in valley, centroid and intensoid characteristics.

Author(s)

Martin Loos, Christian Gerber

See Also[isopattern envelope](#)**Examples**

```
#####  
# batch of chemforms #####  
data(isotopes)  
data(chemforms)  
chemforms<-chemforms[1:5]  
  
pattern<-isopattern(  
  isotopes,  
  chemforms,  
  threshold=0.1,  
  plotit=TRUE,  
  charge=FALSE,  
  emass=0.00054858,  
  algo=2  
)  
  
profiles<-envelope(  
  pattern,  
  ppm=FALSE,  
  dmz=0.0001,  
  frac=1/4,  
  env="Gaussian",  
  resolution=1E6,  
  plotit=TRUE  
)  
  
centro<-vdetect(  
  profiles,  
  detect="centroid",  
  plotit=TRUE  
)  
  
#####
```

Index

* datasets

adducts, [3](#)
chemforms, [8](#)
isotopes, [15](#)
resolution_list, [19](#)

* package

enviPat-package, [2](#)

adducts, [3](#), [3](#), [6](#), [14](#), [18](#), [19](#), [21](#)

check_chemform, [3](#), [4](#), [4](#), [6](#), [11–14](#), [16](#), [18](#), [19](#),
[21](#)

check_ded, [3](#), [4](#), [6](#), [21](#)

check_several, [3](#), [7](#), [14](#)

chemforms, [3](#), [8](#), [12](#), [14](#)

envelope, [3](#), [7](#), [8](#), [9](#), [14](#), [16](#), [22](#), [23](#)

enviPat (enviPat-package), [2](#)

enviPat-package, [2](#)

getR, [3](#), [10](#), [11](#), [11](#), [14](#), [16](#), [19](#)

isopattern, [3–5](#), [7–10](#), [12](#), [13](#), [14](#), [16](#), [23](#)

isotopes, [3](#), [5](#), [12](#), [15](#), [16](#)

isowrap, [3](#), [16](#)

mergeform, [3](#), [4](#), [17](#)

multiform, [3](#), [4](#), [18](#)

resolution_list, [3](#), [10](#), [11](#), [19](#)

smooth.spline, [11](#)

subform, [3](#), [4](#), [21](#)

vdetect, [3](#), [10](#), [14](#), [16](#), [17](#), [22](#)