Package 'IDSL.SUFA'

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Type Package

Title Simplified UFA

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Description A simplified version of the 'IDSL.UFA' package to calculate isotopic profiles and adduct formulas from molecular formulas with no dependency on other R packages for online tools and educational mass spectrometry courses. The 'IDSL.SUFA' package also provides an ancillary module to process user-defined adduct formulas.

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URL https://github.com/idslme/idsl.sufa

BugReports https://github.com/idslme/idsl.sufa/issues

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`element_sorter` *Element Sorter*

Description

This module sorts 84 non-labeled and 14 labeled elements in the periodic table for molecular formula deconvolution and isotopic profile calculation.

Usage

```
element_sorter(ElementList = "all", alphabeticalOrder = TRUE)
```

Arguments

`ElementList`	A string vector of elements needed for isotopic profile calculation. The default value for this parameter is a vector string of entire elements.
`alphabeticalOrder`	'TRUE' should be used to sort the elements for elemental deconvolution (default value), 'FALSE' should be used to keep the input order.

Value

`Elements`	A string vector of elements (alphabetically sorted or unsorted)
`massAbundanceList`	A list of isotopic mass and abundance of elements.
`Valence`	A vector of electron valences.

Examples

```
EL_mass_abundance_val <- element_sorter()
```

`formula_adduct_calculator` *Formula Adduct Calculator*

Description

This function takes a formula and a vector of ionization pathways and returns the adduct formulas.

Usage

```
formula_adduct_calculator(molecular_formula, IonPathway)
```

Arguments

molecular_formula	molecular formula
IonPathway	An ionization pathway. Pathways should be like [Coeff*M+ADD1-DED1+...] where "Coeff" should be an integer between 1-9 and ADD1 and DED1 may be ionization pathways. ex: 'IonPathway <- c("[M]+", "[M+H]+", "[2M-Cl]-", "[3M+CO2-H2O+Na-KO2+HCl-NH4]-")'

Value

A vector of adduct formulas

Examples

```
molecular_formula = "C15H10O7"
IonPathway = c("[M]+","[M+H]","[M+H2O+H]","[M+Na]")
Formula_adducts <- formula_adduct_calculator(molecular_formula, IonPathway)
```

---

formula_vector_generator

Molecular Formula Vector Generator

Description

This function convert a molecular formulas into a numerical vector

Usage

```
formula_vector_generator(molecular_formula, Elements, LElements = length(Elements),
allowedRedundantElements = FALSE)
```

Arguments

molecular_formula	molecular formula
Elements	a string vector of elements. This value must be driven from the 'element_sorter' function.
LElements	number of elements. To speed up loop calculations, consider calculating the number of elements outside of the loop.
allowedRedundantElements	'TRUE' should be used to deconvolute molecular formulas with redundant elements (e.g. CO2CH3O), and 'FALSE' should be used to skip such complex molecular formulas.(default value)

Value

a numerical vector for the molecular formula. This function returns a vector of -Inf values when the molecular formula has elements not listed in the 'Elements' string vector.

Examples

```
molecular_formula <- "[13]C2C12H2Br5Cl3O"
Elements_molecular_formula <- c("[13]C", "C", "H", "O", "Br", "Cl")
EL <- element_sorter(ElementList = Elements_molecular_formula, alphabeticalOrder = TRUE)
Elements <- EL[["Elements"]]
LElements <- length(Elements)
##
mol_vec <- formula_vector_generator(molecular_formula, Elements, LElements)
##
regenerated_molecular_formula <- SUFA_hill_molecular_formula_printer(Elements, mol_vec)
```

---

ionization_pathway_deconvoluter

Ionization Pathway Deconvoluter

Description

This function deconvolutes ionization pathways into a coefficient and a numerical vector to simplify prediction ionization pathways.

Usage

```
ionization_pathway_deconvoluter(IonPathways, Elements)
```

Arguments

IonPathways	A vector of ionization pathways. Pathways should be like [Coeff*M+ADD1-DED1+...] where "Coeff" should be an integer between 1-9 and ADD1 and DED1 may be ionization pathways. ex: 'IonPathways <- c("[M]+", "[M+H]+", "[2M-Cl]-", "[3M+CO2-H2O+Na-KO2+HCl-NH4]-")'
Elements	A vector string of the used elements

Value

A list of adduct calculation values for each ionization pathway.

Examples

```
Elements <- element_sorter()[["Elements"]]
IonPathways <- c("[M]+", "[M+H]+", "[2M-Cl]-", "[3M+CO2-H2O+2Na-KO2+HCl-2NH4]-")
Ion_DC <- ionization_pathway_deconvoluter(IonPathways, Elements)
```

`isotopic_profile_calculator` *Isotopic Profile Calculator*

Description

This function was designed to calculate isotopic profile distributions for small molecules with masses <= 1200 Da. Nonetheless, this function may suit more complicated tasks with complex biological compounds. Details of the equations used in this function are available in the reference[1]. In this function, neighboring isotopologues are merged using the satellite clustering merging (SCM) method described in the reference[2].

Usage

```
isotopic_profile_calculator(MoleFormVec, massAbundanceList, peak_spacing,
intensity_cutoff, UFA_IP_memeory_variables = c(1e30, 1e-12, 100))
```

Arguments

`MoleFormVec`	A numerical vector of the molecular formula
`massAbundanceList`	A list of isotopic mass and abundance of elements obtained from the 'element_sorter' function
`peak_spacing`	A maximum space between two isotopologues in Da
`intensity_cutoff`	A minimum intensity threshold for isotopic profiles in percentage
`UFA_IP_memeory_variables`	A vector of three variables. Default values are c(1e30, 1e-12, 100) to manage memory usage. UFA_IP_memeory_variables[1] is used to control the overall size of isotopic combinations. UFA_IP_memeory_variables[2] indicates the minimum relative abundance (RA calculated by eq(1) in the reference [1]) of an isotopologue to include in the isotopic profile calculations. UFA_IP_memeory_variables[3] is the maximum elapsed time to calculate the isotopic profile on the 'setTimeLimit' function of base R.

Value

A matrix of isotopic profile. The first and second column represents the mass and intensity profiles, respectively.

References

[1] Fakouri Baygi, S., Crimmins, B.S., Hopke, P.K. Holsen, T.M. (2016). Comprehensive emerging chemical discovery: novel polyfluorinated compounds in Lake Michigan trout. *Environmental Science and Technology*, 50(17), 9460-9468, doi:10.1021/acs.est.6b01349.

[2] Fakouri Baygi, S., Fernando, S., Hopke, P.K., Holsen, T.M. and Crimmins, B.S. (2019). Automated Isotopic Profile Deconvolution for High Resolution Mass Spectrometric Data (APGC-QToF) from Biological Matrices. *Analytical chemistry*, 91(24), 15509-15517, doi:10.1021/acs.analchem.9b03335.

See Also

https://ipc.idsl.me/

Examples

```
EL <- element_sorter(alphabeticalOrder = TRUE)
Elements <- EL[["Elements"]]
massAbundanceList <- EL[["massAbundanceList"]]
peak_spacing <- 0.005 # mDa
intensity_cutoff <- 1 # (in percentage)
MoleFormVec <- formula_vector_generator("C8H10N4O2", Elements)
IP <- isotopic_profile_calculator(MoleFormVec, massAbundanceList, peak_spacing,
intensity_cutoff)
```

---

isotopic_profile_molecular_formula_feeder

Isotopic Profile Molecular Formula Feeder

Description

A function to calculate isotopic profiles from a molecular formulas

Usage

```
isotopic_profile_molecular_formula_feeder(molecular_formula, peak_spacing = 0,
intensity_cutoff = 1, IonPathway = "[M]", UFA_IP_memeory_variables = c(1e30, 1e-12, 100),
plotProfile = TRUE, allowedVerbose = TRUE)
```

Arguments

`molecular_formula`
: A molecular formulas

`peak_spacing`
: A maximum space between isotopologues in Da to merge neighboring isotopologues.

`intensity_cutoff`
: A minimum intensity threshold for isotopic profiles in percentage.

`IonPathway`
: An ionization pathway. Pathways should be like [Coeff*M+ADD1-DED1+...] where "Coeff" should be an integer between 1-9 and ADD1 and DED1 may be ionization pathways. ex: 'IonPathway <- c("[M]+", "[M+H]+", "[2M-Cl]-", "[3M+CO2-H2O+Na-KO2+HCl-NH4]-")'

`UFA_IP_memeory_variables`
: A vector of three variables. Default values are c(1e30, 1e-12, 100) to manage memory usage. UFA_IP_memeory_variables[1] is used to control the overall size of isotopic combinations. UFA_IP_memeory_variables[2] indicates the minimum relative abundance (RA calculated by eq(1) in the reference [1]) of an isotopologue to include in the isotopic profile calculations. UFA_IP_memeory_variables[3] is the maximum elapsed time to calculate the isotopic profile on the 'setTimeLimit' function of base R.

plotProfile	c(TRUE, FALSE). A 'TRUE' plotProfile generates a spectra plot.
allowedVerbose	c(TRUE, FALSE). A 'TRUE' allowedVerbose provides messages about the flow of the function.

Value

A list of isotopic profiles

References

[1] Fakouri Baygi, S., Crimmins, B.S., Hopke, P.K. Holsen, T.M. (2016). Comprehensive emerging chemical discovery: novel polyfluorinated compounds in Lake Michigan trout. *Environmental Science and Technology*, 50(17), 9460-9468, doi:10.1021/acs.est.6b01349.

See Also

https://ipc.idsl.me/

Examples

```
molecular_formula <- "C12Cl10"
peak_spacing <- 0.005 # in Da for QToF instruments
# Use this piece of code for intensity cutoff to preserve significant isotopologues
intensity_cutoff <- 1
IonPathway <- "[M+H]+"
isotopic_profile <- isotopic_profile_molecular_formula_feeder(molecular_formula,
peak_spacing, intensity_cutoff, IonPathway)
```

SUFA_hill_molecular_formula_printer

Print Hill Molecular Formula

Description

This function produces molecular formulas from a list numerical vectors in the Hill notation system

Usage

```
SUFA_hill_molecular_formula_printer(Elements, MolVecMat)
```

Arguments

Elements	A vector string of the used elements.
MolVecMat	A matrix of numerical vectors of molecular formulas in each row.

Value

A vector of molecular formulas

Examples

```
Elements <- c("C", "H", "O", "N", "Br", "Cl")
MoleFormVec1 <- c(2, 6, 1, 0, 0, 0) # C2H6O
MoleFormVec2 <- c(8, 10, 2, 4, 0 ,0) # C8H10N4O2
MoleFormVec3 <- c(12, 2, 1, 0, 5, 3) # C12H2Br5Cl3O
MolVecMat <- rbind(MoleFormVec1, MoleFormVec2, MoleFormVec3)
H_MolF <- SUFA_hill_molecular_formula_printer(Elements, MolVecMat)
```

UFA_locate_regex *UFA Locate regex*

Description

Locate indices of the pattern in the string

Usage

```
UFA_locate_regex(string, pattern, ignore.case = FALSE, perl = FALSE, fixed = FALSE,
useBytes = FALSE)
```

Arguments

string	a string as character
pattern	a pattern to screen
ignore.case	ignore.case
perl	perl
fixed	fixed
useBytes	useBytes

Details

This function returns 'NULL' when no matches are detected for the pattern.

Value

A 2-column matrix of location indices. The first and second columns represent start and end positions, respectively.

Examples

```
pattern <- "Cl"
string <- "NaCl.5HCl"
Location_Cl <- UFA_locate_regex(string, pattern)
```

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