Package 'IDSL.UFAx'

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Type Package

Title Exhaustive Chemical Enumeration for United Formula Annotation

Version 1.8

Depends R (>= 4.0)

Imports IDSL.IPA (>= 2.6), IDSL.UFA (>= 1.8), doParallel, foreach, readxl, RcppAlgos

Author Sadjad Fakouri-Baygi [cre, aut] (<https://orcid.org/0000-0002-6864-6911>), Dinesh Barupal [aut] (<https://orcid.org/0000-0002-9954-8628>)

Maintainer Sadjad Fakouri-Baygi <sadjad.fakouri-baygi@mssm.edu>

Description A pipeline to annotate a number of peaks from the IDSL.IPA peaklists using an exhaustive chemical enumeration-based approach. This package can perform elemental composition calculations using the following 15 elements : C, B, Br, Cl, K, S, Si, N, H, As, F, I, Na, O, and P.

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

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

Encoding UTF-8

Archs i386, x64

NeedsCompilation no

Repository CRAN

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R topics documented:

UFAx_workflow *UFAx Workflow*

Description

This function runs the exhaustive chemical enumeration part of the IDSL.UFAx pipeline.

Usage

```
UFAx_workflow(spreadsheet)
```

Arguments

spreadsheet	IDSL.UFAx parameter spreadsheet

Value

The MolecularFormulaAnnotationTable is saved in the assigned folder in the parameter spreadsheet.

Note

You should load the IDSL.UFA package to run the IDSL.UFAx functions.

Examples

```
library(IDSL.UFA) # You should load the IDSL.UFA package to run the IDSL.UFAx functions.
library(IDSL.UFAx)
s_path <- system.file("extdata", package = "IDSL.UFAx")
SSh1 <- paste0(s_path,"/UFAx_parameters.xlsx")
temp_wd <- tempdir() # update this address
temp_wd_zip <- paste0(temp_wd,"/003.mzML_UFAx_testfiles.zip")
spreadsheet <- readxl::read_xlsx(SSh1)
download.file(
  paste0("https://github.com/idslme/IDSL.UFAx/blob/main/UFAx_educational_files/",
         "003.mzML_UFAx_testfiles.zip?raw=true"), destfile = temp_wd_zip, mode = "wb")
unzip(temp_wd_zip, exdir = temp_wd)
spreadsheet[1, 4] <- temp_wd
spreadsheet[3, 4] <- temp_wd
spreadsheet[6, 4] <- temp_wd
spreadsheet[5, 4] <- "seq(1, 100, 1)" # peak IDs to process
UFAx_results <- UFAx_workflow(spreadsheet)
```

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