

# Package ‘IDSL.UFAX’

April 5, 2023

**Type** Package

**Title** Exhaustive Chemical Enumeration for United Formula Annotation

**Version** 1.9.1

**Depends** R (>= 4.0)

**Imports** IDSL.IPA (>= 2.7), IDSL.UFA , readxl, RcppAlgos

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

**Maintainer** Dinesh Barupal <dinesh.barupal@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.

**License** MIT + file LICENSE

**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

**Date/Publication** 2023-04-05 19:03:34 UTC

## R topics documented:

UFAX_workflow . . . . .	2
<b>Index</b>	<b>3</b>

---

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.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)
```

# Index

UFax\_workflow, [2](#)