Package 'IDSL.NPA'

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Type Package

Title Nominal Peak Analysis (NPA)

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Imports IDSL.MXP, IDSL.IPA, IDSL.FSA, readxl

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Description
A pipeline to process nominal mass spectrometry data to create .msp files for untargeted analyses.

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

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

Encoding UTF-8

Archs i386, x64

NeedsCompilation no

Repository CRAN

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Contents

IDSL.NPA_MSPgenerator *IDSL.NPA MSP Generator*

Description

This function creates standard .msp files that can also be used for Pepsearch.

Usage

```
IDSL.NPA_MSPgenerator(NPA_peaklist, number_processing_threads = 1)
```

Arguments

NPA_peaklist	A dataframe peaklist of co-detected peaks
number_processing_threads	Number of processing threads for multi-threaded processing

Value

A string of standard .msp file

IDSL.NPA_referenceMSPgenerator *IDSL.NPA Reference MSP Generator*

Description

This function creates reference standard .msp files.

Usage

```
IDSL.NPA_referenceMSPgenerator(NPA_peaklist, refNPAtable, selectedPeaks_IDref)
```

Arguments

NPA_peaklist	A dataframe peaklist of co-detected peaks
refNPAtable	reference NPA table
selectedPeaks_IDref	selectedPeaks_IDref

Value

A string of standard .msp file

IDSL.NPA_workflow *IDSL.NPA workflow*

Description

This function executes the NPA workflow.

Usage

```
IDSL.NPA_workflow(spreadsheet)
```

Arguments

spreadsheet	NPA spreadsheet

Value

This function organizes the IDSL.NPA file processing for better performance using the template spreadsheet.

IDSL.NPA_xlsxAnalyzer *IDSL.NPA workflow xlsx Analyzer*

Description

This function processes the spreadsheet of the NPA parameters to ensure the parameter inputs are consistent with the requirements of the IDSL.NPA pipeline.

Usage

```
IDSL.NPA_xlsxAnalyzer(spreadsheet)
```

Arguments

spreadsheet	'Start' tab of the parameter spreadsheet

Value

This function returns the NPA parameters to feed the 'IDSL.NPA_workflow' function.

NPA_fragmentationPeakDetection
NPA Fragmentation Peaks Detection

Description

This function detects fragmentation peaks for the NPA analysis

Usage

```
NPA_fragmentationPeakDetection(input_MS_path, MSfilename, smoothingWindow,
peakHeightThreshold, minSNRbaseline, RTtolerance, nSpline, topRatioPeakHeight,
minIonRangeDifference, minNumNPApeaks, pearsonRHOthreshold, outputNPAeic = NULL,
number_processing_threads = 1)
```

Arguments

input_MS_path	path to the MS files
MSfilename	MS file
smoothingWindow	number of scans for peak smoothing.
peakHeightThreshold	A minimum peak height threshold
minSNRbaseline	A minimum baseline S/N threshold
RTtolerance	retention time tolerance to detect common peaks
nSpline	number of points for further smoothing using a cubic spline smoothing method to add more points to calculate Pearson correlation rho values
topRatioPeakHeight	The top percentage of the chromatographic peak to calculate Pearson correlation rho values
minIonRangeDifference	Minimum distance (Da) between lowest and highest m/z to prevent clustering isotopic envelopes
minNumNPApeaks	Minumum number of ions in a NPA cluster
pearsonRHOthreshold	Minimum threshold for Pearson correlation rho values
outputNPAeic	When 'NULL' NPA EICs are not plotted. 'outputNPAeic' represents an address to save NPA EICs figures.
number_processing_threads	Number of processing threads for multi-threaded processing

Value

A dataframe peaklist of co-detected NPA analysis.

NPA_peakDeconvolution *NPA Peak Deconvolution*

Description

This function detects fragmentation peaks for the NPA analysis.

Usage

```
NPA_peakDeconvolution(input_MS_path, MSfilename, smoothingWindow,
peakHeightThreshold, minSNRbaseline, number_processing_threads = 1)
```

Arguments

input_MS_path	path to the MS files
MSfilename	MS file
smoothingWindow	number of scans for peak smoothing.
peakHeightThreshold	A minimum peak height threshold
minSNRbaseline	A minimum baseline S/N threshold
number_processing_threads	Number of processing threads for multi-threaded processing

Value

A dataframe peaklist of co-detected DIA analysis.

NPA_reference_xlsxAnalyzer *NPA reference xlsxAnalyzer*

Description

NPA reference xlsxAnalyzer

Usage

```
NPA_reference_xlsxAnalyzer(ref_xlsx_file, input_path_hrms = NULL, PARAM = NULL,
PARAM_ID = "", checkpoint_parameter = TRUE)
```

Arguments

ref_xlsx_file	ref_xlsx_file
input_path_hrms	input_path_hrms
PARAM	PARAM
PARAM_ID	PARAM_ID
checkpoint_parameter	checkpoint_parameter

Value

ref_table	ref_table
PARAM	PARAM
checkpoint_parameter	checkpoint_parameter

NPA_workflow *FSA NPA Workflow*

Description

This function runs the NPA analysis.

Usage

```
NPA_workflow(PARAM_NPA)
```

Arguments

PARAM_NPA	PARAM_NPA

Value

This function stores .Rdata and .csv data from dataframe peaklist of co-detected NPA analysis.

Examples

```
s_path <- system.file("extdata", package = "IDSL.NPA")
SSh1 <- paste0(s_path,"/NPA_parameters.xlsx")
## To see the results, use a known folder instead of the `tempdir()` command
temp_wd <- tempdir()
temp_wd_zip <- paste0(temp_wd, "/idsl.npa_testfile.zip")
spreadsheet <- readxl::read_xlsx(SSh1, sheet = "NPA")
PARAM_NPA <- cbind(spreadsheet[, 2], spreadsheet[, 4])
download.file(paste0("https://github.com/idslme/IDSL.NPA/blob/main/",
                     "NPA_educational_files/idsl.npa_testfile.zip?raw=true"),
              destfile = temp_wd_zip, mode = "wb")
```

```
unzip(temp_wd_zip, exdir = temp_wd)
PARAM_NPA[2, 2] <- "NO"
PARAM_NPA[4, 2] <- temp_wd
PARAM_NPA[8, 2] <- temp_wd
## To ensure `PARAM_NPA` is consistent with the `NPA_workflow`
PARAM_NPA <- NPA_xlsxAnalyzer(PARAM_NPA)
##
NPA_workflow(PARAM_NPA)
```

`NPA_xlsxAnalyzer` *xlsx Analyzer for NPA analysis*

Description

This function processes the spreadsheet of the NPA spreadsheet tab to ensure the parameter inputs are in agreement with requirements of the NPA analysis.

Usage

```
NPA_xlsxAnalyzer(spreadsheet)
```

Arguments

`spreadsheet`	NPA spreadsheet tab

Value

parameters to feed the ‘NPA_workflow‘ function.

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