Package 'IDSL.NPA'

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Type Package

Title Nominal Peak Analysis (NPA)

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Depends R (>= 4.0)

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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R topics documented:

`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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