

Package ‘IDSL.MXP’

September 27, 2022

Type Package

Title Parser for mzML, mzXML, and netCDF Files (Mass Spectrometry Data)

Version 1.6

Depends R (>= 4.0)

Imports xml2, RNetCDF, base64enc

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 tiny parser to extract mass spectra data and metadata table of MS acquisition properties from mzML, mzXML and netCDF mass spectrometry files.

License MIT + file LICENSE

URL <https://ipa.idsl.me/mxp>, <https://github.com/idslme/idsl.mxp>
<https://colab.research.google.com/drive/1gXwwuI1zzDHykKfodLSQQt5rwTuFEMpD>

BugReports <https://github.com/idslme/idsl.mxp/issues>

Encoding UTF-8

Archs i386, x64

NeedsCompilation no

Repository CRAN

Date/Publication 2022-09-27 07:10:02 UTC

R topics documented:

getNetCDF	2
getScanTable	2
getSpectra	3
MXP_locate_regex	4
peak2list	5

Index	7
--------------	----------

getNetCDF	<i>getNetCDF</i>
-----------	------------------

Description

This function returns a list of two data objects needed for the mass spectrometry data processing.

Usage

```
getNetCDF(MSfile)
```

Arguments

MSfile	name of the mass spectrometry file with .cdf extension
--------	--

Value

scanTable	a dataframe of different scan properties including 'seqNum', 'msLevel', 'polarity', 'peaksCount', 'totIonCurrent', 'retentionTime', 'basePeakMZ', 'basePeakIntensity', 'collisionEnergy', 'lowMZ', 'highMZ', 'precursorScanNum', 'precursorMZ', 'precursorCharge', 'precursorIntensity', 'injectionTime', 'filterString', 'scanType', 'centroided', 'isolationWindowTargetMZ', 'isolationWindowLowerOffset', 'isolationWindowUpperOffset', 'scanWindowLowerLimit', and 'scanWindowUpperLimit'.
spectralList	a list of matrices of m/z and intensity values for each chromatogram scan

Note

'retentionTime' column in the 'scanTable' object is presented in minute.

getScanTable	<i>getScanTable</i>
--------------	---------------------

Description

This function creates a scanTable from chromatogram scans of the mass spectrometry data.

Usage

```
getScanTable(xmlData, msFormat)
```

Arguments

xmlData	A structured data of the mass spectrometry data created by the 'read_xml' function.
msFormat	format extension of the mass spectrometry file c("mzML", "mzXML")

Value

a dataframe of different scan properties including 'seqNum', 'msLevel', 'polarity', 'peaksCount', 'totIonCurrent', 'retentionTime', 'basePeakMZ', 'basePeakIntensity', 'collisionEnergy', 'lowMZ', 'highMZ', 'precursorScanNum', 'precursorMZ', 'precursorCharge', 'precursorIntensity', 'injectionTime', 'filterString', 'scanType', 'centroided', 'isolationWindowTargetMZ', 'isolationWindowLowerOffset', 'isolationWindowUpperOffset', 'scanWindowLowerLimit', and 'scanWindowUpperLimit'. 'scanType' is only provided for the mzXML data format.

Note

'retentionTime' column is presented in minute.

Examples

```
temp_wd <- tempdir()
temp_wd_zip <- paste0(temp_wd, "/idsl_ipa_test_files.zip")
download.file(paste0("https://github.com/idslme/IDSL_IPA/blob/main/",
"IPA_educational_files/idsl_ipa_test_files.zip?raw=true"),
destfile = temp_wd_zip, mode = "wb")
unzip(temp_wd_zip, exdir = temp_wd)
xmlData <- xml2::read_xml(paste0(path = temp_wd, "/", MSfile = "003.mzML"))
scanTable <- getScanTable(xmlData, msFormat = "mzML")
```

getSpectra

getSpectra

Description

This function creates a spectralList for the chromatogram scans of the mass spectrometry data.

Usage

```
getSpectra(xmlData, msFormat)
```

Arguments

xmlData	a structured data of the mass spectrometry data created by the 'read_xml' function.
msFormat	format extension of the mass spectrometry file c("mzML", "mzXML")

Value

a list of matrices of m/z and intensity values for each chromatogram scan

Examples

```
temp_wd <- tempdir()
temp_wd_zip <- paste0(temp_wd, "/idsl_ipa_test_files.zip")
download.file(paste0("https://github.com/idslme/IDSL_IPA/blob/main/",
"IPA_educational_files/idsl_ipa_test_files.zip?raw=true"),
destfile = temp_wd_zip, mode = "wb")
unzip(temp_wd_zip, exdir = temp_wd)
xmlData <- xml2::read_xml(paste0(path = temp_wd, "/", MSfile = "003.mzML"))
spectralList <- getSpectra(xmlData, msFormat = "mzML")
```

MXP_locate_regex	<i>MXP Locate regex</i>
------------------	-------------------------

Description

Locate indices of the pattern in the string

Usage

```
MXP_locate_regex(string, pattern)
```

Arguments

string	a string as character
pattern	a pattern to screen

Details

This function returns 'NA' 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 <- MXP_locate_regex(string, pattern)
```

peak2list	<i>Peak to List (The main function)</i>
-----------	---

Description

This function returns a list of two data objects required for the mass spectrometry data processing.

Usage

```
peak2list(path = getwd(), MSfileName = "")
```

Arguments

path	address of the mass spectrometry file
MSfileName	name of the mass spectrometry file with .mzML or .mzXML extensions

Details

<https://ipa.idsl.me/mxp>

Value

scanTable	a dataframe of different scan properties including 'seqNum', 'msLevel', 'polarity', 'peaksCount', 'totIonCurrent', 'retentionTime', 'basePeakMZ', 'basePeakIntensity', 'collisionEnergy', 'lowMZ', 'highMZ', 'precursorScanNum', 'precursorMZ', 'precursorCharge', 'precursorIntensity', 'injectionTime', 'filterString', 'scanType', 'centroided', 'isolationWindowTargetMZ', 'isolationWindowLowerOffset', 'isolationWindowUpperOffset', 'scanWindowLowerLimit', and 'scanWindowUpperLimit'. 'scanType' is only provided for the mzXML data format.
spectralList	a list of matrices of m/z and intensity values for each chromatogram scan

Note

'retentionTime' column in the 'scanTable' object is presented in minute.

See Also

<https://colab.research.google.com/drive/1gXwwuI1zzDHykKfodLSQQt5rwTuFEMpD>

Examples

```
temp_wd <- tempdir()
temp_wd_zip <- paste0(temp_wd, "/idsl_ipa_test_files.zip")
download.file(paste0("https://github.com/idslme/IDSL_IPA/blob/main/",
"IPA_educational_files/idsl_ipa_test_files.zip?raw=true"),
destfile = temp_wd_zip, mode = "wb")
```

```
unzip(temp_wd_zip, exdir = temp_wd)
p2l <- peak2list(path = temp_wd, MSfileName = "003.mzML")
```

Index

[getNetCDF](#), 2

[getScanTable](#), 2

[getSpectra](#), 3

[MXP_locate_regex](#), 4

[peak2list](#), 5