Package 'msconverteR'

July 12, 2019

Type Package

Title Convert vendor specific mass spectrometry files to mzML

Version 0.1.0

Description Use the pwiz docker container to convert vendor specific mass spectrometry files to .mzML from within the R console on Linux systems.

License GPL (>= 3)

Imports stevedore, stringr, crayon, clisymbols

Encoding UTF-8

LazyData true

RoxygenNote 6.1.1

Roxygen list(markdown = TRUE)

Suggests testthat

NeedsCompilation no

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R topics documented:

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convert_files	*Covert Files*

Description

Convert vendor specific mass spectrometry files to the open .mzML format. This functions makes a `system` call to docker in order to convert files. Conversion arguments should be supplied to the `args` parameter exactly as they would be for `msconvert` but omitting the `--filter` prefix.

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Usage

```
convert_files(files, outpath = NULL, args = c("peakPicking true1-",
  "polarity positive"))
```

Arguments

`files`	the absolute filepath vendor specific files to be converted
`outpath`	an optional filepath where `.mzML` files will be saved to. If `NULL` then `.mzML` files are saved to the same location as input files.
`args`	a character vector of `msconvert` arguments.

Details

For example to convert a file with vendor specific centroiding only;

`convert_files(rawFiles,outpath = NULL,args = 'peakPicking true1-')`

To only retain positive mode data;

`convert_files(rawFiles,outpath = NULL,args = c('peakPicking true1-','polarity positive'))`

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get_pwiz_container	*Get Proteowizard (pwiz) Docker Container*

Description

Pull the pwiz docker container (`chambm/pwiz-skyline-i-agree-to-the-vendor-licenses:latest`) from Docker Hub.

Usage

```
get_pwiz_container()
```

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