Package 'msconverteR'

September 22, 2021

Type Package

Title Convert vendor specific mass spectrometry files to mzML

Version 0.1.2

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 7.1.1

Roxygen list(markdown = TRUE)

Suggests testthat

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.

Usage

```
convert_files(files, outpath = NULL, msconvert_args = c(), docker_args = c())
```

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.
`msconvert_args`	a character vector of arguments to pass to `msconvert`.
`docker_args`	additional arguments to pass to docker run

Details

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

`convert_files(rawFiles,outpath = NULL,msconvert_args = 'peakPicking true 1-')`

To only retain positive mode data;

`convert_files(rawFiles,outpath = NULL,msconvert_args = c('peakPicking true 1-','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()
```

Index