

Package ‘msconverteR’

February 14, 2022

Type Package

Title Convert vendor specific mass spectrometry files to mzML

Version 0.1.3

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	<i>Covert Files</i>
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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'))
```

get_pwiz_container	<i>Get Proteowizard (pwiz) Docker Container</i>
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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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