Package: msconverteR (via r-universe)

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Type Package

Title Convert vendor specific mass spectrometry files to mzML

Version 0.1.2

Author Tom Wilson [aut, cre]

Maintainer Tom Wilson <`tpw2@aber.ac.uk`>

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 7.3.2

Roxygen list(markdown = TRUE)

Suggests testthat, withr

Config/pak/sysreqs libicu-dev libssl-dev

Repository https://aberhrml.r-universe.dev

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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'))`

When converting multiple files, all input files must be located in the same directory so they can be mounted into the container together.

`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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