

# Package: msconverteR (via r-universe)

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**Type** Package

**Title** Convert vendor specific mass spectrometry files to mzML

**Version** 0.1.2

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**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://wilsontom.r-universe.dev>

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**RemoteUrl** <https://github.com/wilsontom/msconverteR>

**RemoteRef** HEAD

**RemoteSha** ea965cb36869844e474e61b9f407e9438e300e74

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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'))
```

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

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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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