Package: slurmwiz (via r-universe)

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Type Package

Title Convert Raw Mass Spectrometry Files

Version 0.1.4

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Description Wrapper for converting raw mass spectrometry data files using the pwiz docker container through apptainer on a high performance computer (HPC) cluster running SLRUM workload manager.

License GPL (>= 3)

Imports yaml, glue

Suggests pkgload, testthat (>= 3.0.0), withr

Config/testthat/edition 3

Encoding UTF-8

RoxygenNote 7.3.2

Roxygen list(markdown = TRUE)

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

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RemoteUrl https://github.com/wilsontom/slurmwiz

RemoteRef HEAD

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Contents

`detect_file_type` *Detect File Type*

Description

Detect the main file type in a directory of raw files

Usage

```
detect_file_type(input)
```

Arguments

`input`	the absolute file path of the directory of raw files for conversion

Value

a character string of the file type for conversion

`slurm_convert` *Convert Raw Files using msconvert and SLURM*

Description

Convert raw mass spectrometry files using a combination of singularity, t

Usage

```
slurm_convert(input, output, format_out, conversion_args)
```

Arguments

`input`	the absolute file path of the directory of raw files for conversion
`output`	the absolute file path where converted data files will be saved to
`format_out`	a character string of `msconvert` format for conversioin.
`conversion_args`	a character string of `msconvert` arguments without the `--filter` prefix (ie, `peakPicking true 1-`)

Examples

```
## Not run:
slurm_convert(input = 'hpc/storage/my_raw_data', output = 'hpc/home/my_converted_data', format_out = 'mzML', conv

## End(Not run)
```

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