Package 'rawReadeR'

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Type Package

Title Read Thermo .RAW files in R

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Description A series of C++ functions are used to access the Thermo MSFileReader.dll. Each C++ function is designed for single file and single scan input; corresponding R functions and system calls are used as multi scan and multi file wrappers to the C++ functions, via the pre-compiled binary executables.

License GPL (>= 3)

URL https://github.com/wilsontom/rawReadeR

BugReports https://github.com/wilsontom/rawReadeR/issues

LazyData TRUE

RoxygenNote 5.0.1

R topics documented:

compileAll *Compile .cpp files to executables (.exe)*

Description

Wrapper function which compiles all `.cpp` files into executables (`.exe`). The Microsoft Visual Studio `vcvars323.bat` file is used to set include paths and environment variables, so that this function can be simply executed in the Windows `cmd` line from an R session, as opposed to manually compiling all `.cpp` files through the Visual Studio C++ Developers Command Prompt. See https://github.com/wilsontom/rawReadeR/blob/master/README.md for futher details on installation.

Usage

```
compileAll(filepath)
```

Arguments

`filepath`	the filepath of the `rawReadeR` source directory.

Author(s)

Tom Wilson <tpw2@aber.ac.uk>

Examples

```
## Not run:
 options(VSPATH = "<path_to_visual_studio_vcvars32.bat>")
 source("rawReadeR/R/compileAll.R")
 compileAll("C:/rawReadeR")

## End(Not run)
```

getBValues *Get B Value*

Description

Get the FT-MS conversion parameter `B` for each scan in a given range

Usage

```
getBValues(filename, scans = c())
```

Arguments

filename	a .raw file
scans	a numeric vector of scan numbers to extract

Value

a numeric vector of the B value for each scan

Author(s)

Tom Wilson <tpw2@aber.ac.uk>

Examples

```
## Not run:
getBValues(QC.raw, scans = c(2:24)

## End(Not run)
```

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getCValues *Get C Value*

Description

Get the FT-MS conversion parameter C for each scan in a given range

Usage

```
getCValues(filename, scans = c())
```

Arguments

filename	a .raw file
scans	a numeric vector of scan numbers to extract

Value

a numeric vector of the C value for each scan

Author(s)

Tom Wilson <tpw2@aber.ac.uk>

Examples

```
## Not run:
getCValues(QC.raw, scans = c(2:24)

## End(Not run)
```

`getITtime` *Get Ion Injection Time*

Description

Get the ion injection time (IT) for each scan in a given range

Usage

```
getITtime(filename, scans = c())
```

Arguments

`filename`	a `.raw` file
`scans`	a numeric vector of scan numbers to extract

Value

a numeric vector of the ion injection time for each scan

Author(s)

Tom Wilson <tpw2@aber.ac.uk>

Examples

```
## Not run:
getITtime(QC.raw, scans = c(2:24)

## End(Not run)
```

getMzInt *Get Mass and Intensity*

Description

Get the profile data (m/z and intensity) across a given scan range

Usage

```
getMzInt(filename, scans = c())
```

Arguments

filename	a .raw file
scans	a numeric vector of scan numbers to extract

Value

a list of matrices for m/z and intensity.

Author(s)

Tom Wilson <tpw2@aber.ac.uk>

Examples

```
## Not run:
getMzInt(QC.raw, scans = c(2:24)

## End(Not run)
```

getMzIntNoise *Get Mass, Intensity and Noise*

Description

Get the profile data (m/z, intensity and noise) across a given scan range

Usage

```
getMzIntNoise(filename, scans = c())
```

Arguments

filename	a .raw file
scans	a numeric vector of scan numbers to extract

Value

a list of matrices for m/z, intensity and noise

Author(s)

Tom Wilson <tpw2@aber.ac.uk>

Examples

```
## Not run:
getMzIntNoise(QC.raw, scans = c(2:24)

## End(Not run)
```

`getResComp` *Get Resolution Compensation*

Description

Get the Resolution mass compensation (ppm) for each scan in a given range

Usage

```
getResComp(filename, scans = c())
```

Arguments

`filename`	a `.raw` file
`scans`	a numeric vector of scan numbers to extract

Value

a numeric vector of the resolution compensation for each scan

Author(s)

Tom Wilson <tpw2@aber.ac.uk>

Examples

```
## Not run:
getResComp(QC.raw, scans = c(2:24)

## End(Not run)
```

getRFComp *Get RF Compensation*

Description

Get the RF mass compensation (ppm) for each scan in a given range

Usage

```
getRFComp(filename, scans = c())
```

Arguments

filename	a .raw file
scans	a numeric vector of scan numbers to extract

Value

a numeric vector of the RF compensation for each scan

Author(s)

Tom Wilson <tpw2@aber.ac.uk>

Examples

```
## Not run:
getRFComp(QC.raw, scans = c(2:24)

## End(Not run)
```

getSpaceComp *Get Space Charge Compensation*

Description

Get the space charge mass compensation (ppm) for each scan in a given range

Usage

```
getSpaceComp(filename, scans = c())
```

Arguments

filename	a .raw file
scans	a numeric vector of scan numbers to extract

Value

a numeric vector of the space charge compensation for each scan

Author(s)

Tom Wilson <tpw2@aber.ac.uk>

Examples

```
## Not run:
getSpaceComp(QC.raw, scans = c(2:24)

## End(Not run)
```

`testPackage` *Package Testing*

Description

Run some basic tests to ensure there have been no problems during compilation

Usage

```
testPackage(scans = c(1:5))
```

Arguments

`scans`	a numeric vector of scan numbers to extract

Author(s)

Tom Wilson <tpw2@aber.ac.uk>

Examples

```
## Not run:
testPackage(scans = c(1:5))

## End(Not run)
```

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