

# Package ‘rawReader’

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**Type** Package

**Title** Read Thermo .RAW files in R

**Version** 0.1.1

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**Description** R/C++ API to the Thermo MSFileReader.dll

**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 . . . . .	2
getBValues . . . . .	2
getCValues . . . . .	3
getITime . . . . .	4
getMzInt . . . . .	5
getMzIntNoise . . . . .	5
getResComp . . . . .	6
getRFComp . . . . .	7
getSpaceComp . . . . .	7
scanFilter . . . . .	8
testPackage . . . . .	9

<b>Index</b>	<b>10</b>
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compileAll	<i>Compile .cpp files to executables (.exe)</i>
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### Description

Wrapper function which compiles all .cpp files into executables (.exe). The Microsoft Visual Studio vcvars32.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/wilsonsom/rawReader/blob/master/README.md> for further 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)
```

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getBValues	<i>Get B Value</i>
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### 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	<i>Get C Value</i>
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**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*

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**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)
```

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getMzInt	<i>Get Mass and Intensity</i>
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**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)
```

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getMzIntNoise	<i>Get Mass, Intensity and Noise</i>
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**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)
```

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getResComp

*Get Resolution Compensation*

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**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)
```

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scanFilter

*Get Filter*

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**Description**

Get the scan filter for each scan in a given range

**Usage**

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

**Arguments**

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

**Value**

a character vector of the scan filter for each scan

**Author(s)**

Tom Wilson <tpw2@aber.ac.uk>

**Examples**

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



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testPackage	<i>Package Testing</i>
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**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)
```

# Index

`compileAll`, [2](#)

`getBValues`, [2](#)

`getCValues`, [3](#)

`getITtime`, [4](#)

`getMzInt`, [5](#)

`getMzIntNoise`, [5](#)

`getResComp`, [6](#)

`getRFComp`, [7](#)

`getSpaceComp`, [7](#)

`scanFilter`, [8](#)

`testPackage`, [9](#)