

# Package ‘rawDiag’

April 9, 2025

**Type** Package

**Title** Brings Orbitrap Mass Spectrometry Data to Life; Fast and Colorful

**Version** 1.3.4

**Depends** R (>= 4.4)

**Imports** dplyr, ggplot2 (>= 3.4), grDevices, hexbin, htmltools, BiocManager, BiocParallel, rawrr (>= 1.15.5), rlang, reshape2, scales, shiny (>= 1.5), stats, utils

**Suggests** BiocStyle (>= 2.28), ExperimentHub, tartare, knitr, testthat

**Description** Optimizing methods for liquid chromatography coupled to mass spectrometry (LC-MS) poses a nontrivial challenge. The rawDiag package facilitates rational method optimization by generating MS operator-tailored diagnostic plots of scan-level metadata. The package is designed for use on the R shell or as a Shiny application on the Orbitrap instrument PC.

**License** GPL-3

**URL** <https://github.com/fgcz/rawDiag/>

**BugReports** <https://github.com/fgcz/rawDiag/issues>

**Encoding** UTF-8

**NeedsCompilation** no

**RoxygenNote** 7.3.2

**VignetteBuilder** knitr

**biocViews** MassSpectrometry, Proteomics, Metabolomics, Infrastructure, Software, ShinyApps

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**git\_branch** devel

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rawDiag-package	<i>rawDiag: Brings Orbitrap Mass Spectrometry Data to Life; Fast and Colorful</i>
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## Description

Optimizing methods for liquid chromatography coupled to mass spectrometry (LC-MS) poses a nontrivial challenge. The rawDiag package facilitates rational method optimization by generating MS operator-tailored diagnostic plots of scan-level metadata. The package is designed for use on the R shell or as a Shiny application on the Orbitrap instrument PC.

### Author(s)

**Maintainer:** Christian Panse <cp@fgcz.ethz.ch> ([ORCID](#))

Authors:

- Christian Trachsel <Christian.Trachsel@fgcz.ethz.ch>
- Tobias Kockmann <Tobias.Kockmann@fgcz.ethz.ch>

### See Also

Useful links:

- <https://github.com/fgcz/rawDiag/>
- Report bugs at <https://github.com/fgcz/rawDiag/issues>

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`.calculatioMasterScan` *Calculate Master Scan Number*

---

### Description

calculates the MS1 master scan number of an MS2 scan and populates the MasterScanNumber with it

### Usage

```
.calculatioMasterScan(x)
```

### Arguments

x a data.frame object adhering to the specified criteria for the `is.rawDiag` function.

### Value

a data.frame containing a MasterScanNumber column.

### Author(s)

Christian Trachsel

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`.cycleTime`*Calculate MS Cycle Time*

---

**Description**

calculates the lock mass deviations along RT.

**Usage**`.cycleTime(x)`**Arguments**

`x` a `data.frame` object adhering to the specified criteria for the `is.rawDiag` function.

**Value**

calculates the time of all ms cycles and the 95 the cycle time is defined as the time between two consecutive MS1 scans

**Note**

TODO: quantile part needed? If no MS1 scan is present? E.g., DIA take lowest window as cycle indicator?

**Author(s)**

Christian Trachsel (2017), Christian Panse (20231201) refactored

---

`.fillNAgaps`*Fill NA values with last previous value*

---

**Description**

Fill NA values with last previous value

**Usage**`.fillNAgaps(x)`**Arguments**

`x` a vector of values

**Value**

a vector with any NA values replaced with the last previous actual value

**Author(s)**

Christian Trachsel

**Examples**

```
c(NA, 1, 2, 3, NA, 4, 5, NA, NA, NA, 6) |>
  rawDiag:::.fillNAGaps()
```

---

buildRawDiagShinyApp *Build the rawDiag shiny application*

---

**Description**

Build the rawDiag shiny application

**Usage**

```
buildRawDiagShinyApp(rawDir = (dirname(rawrr::sampleFilePath())))
```

**Arguments**

rawDir            A directory containing the input raw files, default is set to the \$HOME/Downloads directory.

**Value**

returns the rawDiag shiny apps

**Note**

launch the shiny application by embracing your command line while expecting the raw file in \$HOME/Downloads

- MacOSX and Linux: R -q -e "library(rawDiag); buildRawDiagShinyApp() |> shiny::runApp(launch.browse"
- Microsoft Windows: R.exe -e "library(rawDiag); buildRawDiagShinyApp() |> shiny::runApp(launch.browse"

**Author(s)**

Christian Trachsel (2017), Christian Panse (2023)

**References**

- rawDiag: [doi:10.1021/acs.jproteome.8b00173](https://doi.org/10.1021/acs.jproteome.8b00173),
- rawrr: [doi:10.1021/acs.jproteome.0c00866](https://doi.org/10.1021/acs.jproteome.0c00866)

**Examples**

```

rawrr::sampleFilePath() |>
  dirname() |>
  rawDiag::buildRawDiagShinyApp() |>
  shiny::runApp()

# or use your 'Download' folder
(Sys.getenv('HOME') |>
  file.path("Downloads")) |>
  rawDiag::buildRawDiagShinyApp() |>
  shiny::runApp()

```

---

checkRawrr	<i>Checks Bioconductor installation instructions</i>
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**Description**

Checks Bioconductor installation instructions

**Usage**

```
checkRawrr()
```

**Value**

TRUE if everything is installed correctly

---

is.rawDiag	<i>Is an Object an rawDiag Object?</i>
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---

**Description**

Is an Object an rawDiag Object?

**Usage**

```
is.rawDiag(object)
```

**Arguments**

object            any R object.

**Value**

a boolean

**Author(s)**

Christian Panse 2018

**Examples**

```
rawrr::sampleFilePath() |> rawDiag::readRaw() |> rawDiag::is.rawDiag()
```

---

plotChargeState      *Charge State Overview Plot*

---

**Description**

graphs the number of occurrences of all selected precursor charge states.

**Usage**

```
plotChargeState(x, method = "trellis")
```

**Arguments**

x	a data.frame object adhering to the specified criteria for the is.rawDiag function.
method	specifying the plot method 'trellis'   'violin'   'overlay'. The default is 'trellis'.

**Value**

a `ggplot` object.

**Author(s)**

Christian Trachsel (2017), Christian Panse (2023)

**References**

- rawDiag: [doi:10.1021/acs.jproteome.8b00173](https://doi.org/10.1021/acs.jproteome.8b00173),
- rawrr: [doi:10.1021/acs.jproteome.0c00866](https://doi.org/10.1021/acs.jproteome.0c00866)

**Examples**

```
rawrr::sampleFilePath() |> rawDiag::readRaw() -> S  
S |> rawDiag::plotLockMassCorrection()
```

---

plotCycleLoad	<i>Cycle Load Plot</i>
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---

### Description

plotting the number of MS2 per MS1 (the duty cycle) scan versus retention time. The deepskyblue colored loess curve shows the trend.

### Usage

```
plotCycleLoad(x, method = "trellis")
```

### Arguments

x	a data.frame object adhering to the specified criteria for the <code>is.rawDiag</code> function.
method	specifying the plot method 'trellis'   'violin'   'overlay'. The default is 'trellis'.

### Value

a `ggplot` object.

### Author(s)

Christian Trachsel (2017), Christian Panse (2023)

### References

- rawDiag: [doi:10.1021/acs.jproteome.8b00173](https://doi.org/10.1021/acs.jproteome.8b00173),
- rawrr: [doi:10.1021/acs.jproteome.0c00866](https://doi.org/10.1021/acs.jproteome.0c00866)

### Examples

```
rawrr::sampleFilePath() |> rawDiag::readRaw() -> S  
S |> rawDiag::plotCycleLoad()
```



---

plotCycleTime	<i>Plot Cycle Time</i>
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---

### Description

graphs the time difference between two consecutive MS1 scans (cycle time) with respect to RT (scatter plots) or its density (violin). A smooth curve graphs the trend. The 95th percentile is indicated by a red dashed line.

### Usage

```
plotCycleTime(x, method = "trellis")
```

### Arguments

x	a data.frame object adhering to the specified criteria for the <code>is.rawDiag</code> function.
method	specifying the plot method 'trellis'   'violin'   'overlay'. The default is 'trellis'.

### Value

a [ggplot](#) object.

### Examples

```
rawrr::sampleFilePath() |> rawDiag::readRaw() |> rawDiag::plotCycleTime()
```

---

plotInjectionTime	<i>Plot Injection Time</i>
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---

### Description

shows the injection time density of each mass spectrometry file as a violin plot. The higher the maximum number of MS2 scans is in the method, the more the density is shifted towards the maximum injection time value.

### Usage

```
plotInjectionTime(x, method = "trellis")
```

### Arguments

x	a data.frame object adhering to the specified criteria for the <code>is.rawDiag</code> function.
method	specifying the plot method 'trellis'   'violin'   'overlay'. The default is 'trellis'.

**Value**

a `ggplot` object.

**Author(s)**

Christian Trachsel (2017), Christian Panse (2023)

**References**

- rawDiag: [doi:10.1021/acs.jproteome.8b00173](https://doi.org/10.1021/acs.jproteome.8b00173),
- rawrr: [doi:10.1021/acs.jproteome.0c00866](https://doi.org/10.1021/acs.jproteome.0c00866)

**Examples**

```
rawrr::sampleFilePath() |> rawDiag::readRaw() |> rawDiag::plotInjectionTime()
```

---

plotLockMassCorrection

*Lock Mass Correction Plot*

---

**Description**

Lock Mass Correction Plot

**Usage**

```
plotLockMassCorrection(x, method = "trellis")
```

**Arguments**

x	a data.frame object adhering to the specified criteria for the <code>is.rawDiag</code> function.
method	specifying the plot method 'trellis'   'violin'   'overlay'. The default is 'trellis'.

**Value**

a `ggplot` object.

**Author(s)**

Christian Trachsel (2017), Christian Panse (2023)

**References**

- rawDiag: [doi:10.1021/acs.jproteome.8b00173](https://doi.org/10.1021/acs.jproteome.8b00173),
- rawrr: [doi:10.1021/acs.jproteome.0c00866](https://doi.org/10.1021/acs.jproteome.0c00866)

## Examples

```
rawrr::sampleFilePath() |>  
  rawDiag::readRaw() |>  
  rawDiag::plotLockMassCorrection()
```

---

plotMassDistribution *Mass Distribution Plot*

---

## Description

plots the mass frequency in dependency to the charge state

## Usage

```
plotMassDistribution(x, method = "trellis")
```

## Arguments

x	a data.frame object adhering to the specified criteria for the <code>is.rawDiag</code> function.
method	specifying the plot method 'trellis'   'violin'   'overlay'. The default is 'trellis'.

## Details

displays charge state resolved frequency of precursor masses.

## Value

a `ggplot` object.

## Author(s)

Christian Trachsel (2017), Christian Panse (2023)

## References

- rawDiag: [doi:10.1021/acs.jproteome.8b00173](https://doi.org/10.1021/acs.jproteome.8b00173),
- rawrr: [doi:10.1021/acs.jproteome.0c00866](https://doi.org/10.1021/acs.jproteome.0c00866)

## Examples

```
rawrr::sampleFilePath() |> rawDiag::readRaw() |> rawDiag::plotMassDistribution('overlay')
```

---

plotMzDistribution     *mZ Distribution Plot of Ms2 Scans*

---

### Description

draws precursor mass vs retention time for each MS2 scan in the raw file.

### Usage

```
plotMzDistribution(x, method = "trellis")
```

### Arguments

`x`                    a `data.frame` object adhering to the specified criteria for the `is.rawDiag` function.

`method`                specifying the plot method 'trellis' | 'violin' | 'overlay'. The default is 'trellis'.

### Value

a `ggplot` object.

### Author(s)

Christian Trachsel (2017), Christian Panse (2023)

### References

- `rawDiag`: [doi:10.1021/acs.jproteome.8b00173](https://doi.org/10.1021/acs.jproteome.8b00173),
- `rawrr`: [doi:10.1021/acs.jproteome.0c00866](https://doi.org/10.1021/acs.jproteome.0c00866)

### Examples

```
rawrr::sampleFilePath() |> rawDiag::readRaw() -> S  
rawDiag::plotMzDistribution(S)
```

---

plotPrecursorHeatmap     *Precursor Mass versus StartTime MS2 based hexagons*

---

### Description

Precursor Mass versus StartTime MS2 based hexagons

### Usage

```
plotPrecursorHeatmap(x, method = "overlay", bins = 80)
```

**Arguments**

x	a data.frame object adhering to the specified criteria for the is.rawDiag function.
method	specifying the plot method 'trellis'   'violin'   'overlay'. The default is 'trellis'.
bins	number of bins in both vertical and horizontal directions. default is 80.

**Value**

a `ggplot` object.

**Note**

TODO: define bin with dynamically as  $h = 2 \times \text{IQR} \times n^{-1/3}$  or number of bins  $(\text{max-min})/h$

**Author(s)**

Christian Trachsel (2017)

**References**

- rawDiag: [doi:10.1021/acs.jproteome.8b00173](https://doi.org/10.1021/acs.jproteome.8b00173),
- rawrr: [doi:10.1021/acs.jproteome.0c00866](https://doi.org/10.1021/acs.jproteome.0c00866)

**Examples**

```
rawrr::sampleFilePath() |> rawDiag::readRaw() |> rawDiag::plotPrecursorHeatmap()
```

---

plotScanTime	<i>Scan Event Plot</i>
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---

**Description**

Plotting the elapsed scan time for each individual scan event.

**Usage**

```
plotScanTime(x, method = "trellis")
```

**Arguments**

x	a data.frame object adhering to the specified criteria for the is.rawDiag function.
method	specifying the plot method 'trellis'   'violin'   'overlay'. The default is 'trellis'.

**Value**

a `ggplot` object.

**Author(s)**

Christian Trachsel (2017), Christian Panse (2023)

**References**

- rawDiag: [doi:10.1021/acs.jproteome.8b00173](https://doi.org/10.1021/acs.jproteome.8b00173),
- rawrr: [doi:10.1021/acs.jproteome.0c00866](https://doi.org/10.1021/acs.jproteome.0c00866)

**Examples**

```
## for debugging bioconductor check
if (Sys.info()['sysname'] %in% c("Darwin", "Linux")) {Sys.which('mono')}
rawrr::sampleFilePath() |> rawDiag::readRaw() -> S

rawDiag::checkRawrr()

S |> rawDiag::plotScanTime()
```

---

plotTicBasepeak

*Total Ion Count and Base Peak Plot*

---

**Description**

displays the Total Ion Count (TIC) and the Base Peak Chromatogram of a mass spectrometry measurement. Multiple files are handled by faceting based on rawfile name.

**Usage**

```
plotTicBasepeak(x, method = "trellis")
```

**Arguments**

**x** a data.frame object adhering to the specified criteria for the `is.rawDiag` function.

**method** specifying the plot method 'trellis' | 'violin' | 'overlay'. The default is 'trellis'.

**Value**

a ggplot2 object for graphing the TIC and the Base Peak chromatogram.

**Author(s)**

Christian Trachsel (2017), Christian Panse (20231130) refactored

**Examples**

```
rawrr::sampleFilePath() |> rawDiag::readRaw() |> rawDiag::plotTicBasepeak()
```

---

rawDiagServer	<i>rawDiag shiny module</i>
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---

**Description**

rawDiag shiny module

**Usage**

```
rawDiagServer(id, vals)
```

**Arguments**

id	An ID string that corresponds with the ID used to call the module's UI function.
vals	containing rawfile

**Value**

rawDiag shiny module server

**Examples**

```
shiny::shiny(rawDir = (rawrr::sampleFilePath() |> dirname()))
```

---

rawDiagUI	<i>rawDiag shiny module UI</i>
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---

**Description**

rawDiag shiny module UI

**Usage**

```
rawDiagUI(id)
```

**Arguments**

id	An ID string that corresponds with the ID used to call the module's UI function.
----	--

**Value**

a shiny UI module  
rawDiag shiny module UI

## Examples

```
rawDiag::shiny(rawDir = (rawrr::sampleFilePath() |> dirname()))
```

---

readRaw

*Reads selected raw file trailer information for rawDiag plot functions*

---

## Description

implements a wrapper function using the rawrr methods [readIndex](#), [readTrailer](#), and [readChromatogram](#) to read proprietary mass spectrometer generated data using third-party libraries.

## Usage

```
readRaw(  
  rawfile,  
  msgFUN = function(x) {  
    message(x)  
  }  
)
```

## Arguments

rawfile	the name of the raw file containing the mass spectrometry data from the Thermo Fisher Scientific instrument.
msgFUN	this function is used for logging information while composing the resulting data.frame. It can also be used for shiny progress bar. The default is using the message.

## Value

a data.frame containing the selected trailer information.

## Note

The set up procedure for the rawrr package needs to be run in order to use this package.

## Author(s)

Christian Panse (2016-2023)

## References

[doi:10.1021/acs.jproteome.8b00173](https://doi.org/10.1021/acs.jproteome.8b00173)



**Examples**

```
rawDiag::checkRawrr()  
rawrr::sampleFilePath() |>  
  rawDiag::readRaw()
```

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