

# Package ‘rawDiag’

April 28, 2025

**Type** Package

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

**Version** 1.4.0

**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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 Tobias Kockmann [aut]

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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>

---

.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

---

|                         |                                |
|-------------------------|--------------------------------|
| <code>.cycleTime</code> | <i>Calculate MS Cycle Time</i> |
|-------------------------|--------------------------------|

---

**Description**

calculates the lock mass deviations along RT.

**Usage**

```
.cycleTime(x)
```

**Arguments**

|   |                                                                                                  |
|---|--------------------------------------------------------------------------------------------------|
| x | a data.frame object adhering to the specified criteria for the <code>is.rawDiag</code> 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

---

|                          |                                                |
|--------------------------|------------------------------------------------|
| <code>.fillNAgaps</code> | <i>Fill NA values with last previous value</i> |
|--------------------------|------------------------------------------------|

---

**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> |
|------------|------------------------------------------------------|

---

Description

Checks Bioconductor installation instructions

Usage

```
checkRawrr()
```

Value

TRUE if everything is installed correctly

---

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

---

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 | <i>Charge State Overview Plot</i> |
|-----------------|-----------------------------------|

---

**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`*Cycle Load Plot*

---

### 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

|                     |                                                                                                               |
|---------------------|---------------------------------------------------------------------------------------------------------------|
| <code>x</code>      | a <code>data.frame</code> object adhering to the specified criteria for the <code>is.rawDiag</code> function. |
| <code>method</code> | 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> |
|---------------|------------------------|

---

**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 is.rawDiag 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> |
|-------------------|----------------------------|

---

**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 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() |> rawDiag::plotInjectionTime()
```

---

plotLockMassCorrection

*Lock Mass Correction Plot*

---

**Description**

Lock Mass Correction Plot

**Usage**

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

**Arguments**

- |        |                                                                                                               |
|--------|---------------------------------------------------------------------------------------------------------------|
| x      | a <code>data.frame</code> 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 | <i>Mass Distribution Plot</i> |
|----------------------|-------------------------------|

---

## 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 is.rawDiag 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 | <i>mZ Distribution Plot of Ms2 Scans</i> |
|--------------------|------------------------------------------|

---

**Description**

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

**Usage**

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

**Arguments**

|        |                                                                                                               |
|--------|---------------------------------------------------------------------------------------------------------------|
| x      | a <code>data.frame</code> 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
rawDiag::plotMzDistribution(S)
```

---

|                      |                                                           |
|----------------------|-----------------------------------------------------------|
| plotPrecursorHeatmap | <i>Precursor Mass versus StartTime MS2 based hexagons</i> |
|----------------------|-----------------------------------------------------------|

---

**Description**

Precursor Mass versus StartTime MS2 based hexagons

**Usage**

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

**Arguments**

|        |                                                                                                               |
|--------|---------------------------------------------------------------------------------------------------------------|
| x      | a <code>data.frame</code> 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'.                        |
| 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> |
|--------------|------------------------|

---

**Description**

Plotting the elapsed scan time for each individual scan event.

**Usage**

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

**Arguments**

|        |                                                                                                               |
|--------|---------------------------------------------------------------------------------------------------------------|
| x      | a <code>data.frame</code> 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**

```
## 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> |
|---------------|-----------------------------|

---

**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> |
|-----------|--------------------------------|

---

**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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