

# Package: QFeaturesGUI (via r-universe)

June 5, 2026

**Title** A suite of shiny apps to use the main functionalities of the QFeatures package

**Version** 0.1.1

**Date** 2024-04-23

**Description** ``QFeaturesGUI is a suite of shiny apps that serve as graphical interfaces for the QFeatures package. Currently, the package contains the following shiny apps: 'importQFeatures'."

**biocViews** Software, ShinyApps, GUI, Proteomics

**URL** <https://rformassspectrometry.github.io/QFeaturesGUI/>,  
<https://github.com/rformassspectrometry/QFeaturesGUI>

**BugReports** <https://github.com/rformassspectrometry/QFeaturesGUI/issues>

**License** MIT + file LICENSE

**Encoding** UTF-8

**LazyData** false

**Imports** QFeatures, shiny, DT, shinydashboard, shinydashboardPlus, shinyalert, SummarizedExperiment, utils, htmltools, impute, pcaMethods, plotly, MultiAssayExperiment, RColorBrewer, methods, shinyFeedback, viridisLite, stats, SingleCellExperiment, ggplot2, tidyr, shinyjs, rmarkdown, tibble, dplyr, matrixStats, MsCoreUtils, waiter

**Depends** R (>= 4.3.0)

**Suggests** knitr, BiocStyle, testthat (>= 3.0.0)

**Roxygen** list(markdown = TRUE)

**VignetteBuilder** knitr

**Config/testthat/edition** 3

**Config/roxygen2/version** 8.0.0

**Config/pak/sysreqs** cmake libglpk-dev make libicu-dev libuv1-dev libxml2-dev libssl-dev zlib1g-dev

**Repository** <https://rformassspectrometry.r-universe.dev>

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importQFeatures	<i>A shiny app to import QFeatures objects.</i>
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## Description

importQFeatures is a simple graphical interface to import bulk and single-cell proteomics data. The app uses the [readQFeatures](#) function from the QFeatures package to convert simple tables (single or multiple, CSV or TSV) to a QFeatures object. The app allows users to convert tables to a QFeatures object.

## Usage

```
importQFeatures(colData = NULL, assayData = NULL, maxSize = 1000)
```

## Arguments

colData	A data frame that contains the sample table.
assayData	A data frame that contains the input table.
maxSize	An integer that changes the shiny.maxRequestSize value, in MB.

## Value

The "importQFeatures" Shiny app object.

## Examples

```
library(QFeaturesGUI)

data("sampleTable")
data("inputTable")
app <- importQFeatures(colData = sampleTable, assayData = inputTable, maxSize = 100)

if (interactive()) {
  shiny::runApp(app)
}
```

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`inputTable`*Example MaxQuant/SCoPE2 output*

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**Description**

A data.frame with 1088 observations and 139 variables, as produced by reading a MaxQuant output file with `read.delim()`.

- Sequence: a character vector
- Length: a numeric vector
- Modifications: a character vector
- Modified.sequence: a character vector
- Deamidation..N..Probabilities: a character vector
- Oxidation..M..Probabilities: a character vector
- Deamidation..N..Score.Diffs: a character vector
- Oxidation..M..Score.Diffs: a character vector
- Acetyl..Protein.N.term.: a numeric vector
- Deamidation..N.: a numeric vector
- Oxidation..M.: a numeric vector
- Missed.cleavages: a numeric vector
- Proteins: a character vector
- Leading.proteins: a character vector
- protein: a character vector
- Gene.names: a character vector
- Protein.names: a character vector
- Type: a character vector
- Set: a character vector
- MS.MS.m.z: a numeric vector
- Charge: a numeric vector
- m.z: a numeric vector
- Mass: a numeric vector
- Resolution: a numeric vector
- Uncalibrated...Calibrated.m.z..ppm.: a numeric vector
- Uncalibrated...Calibrated.m.z..Da.: a numeric vector
- Mass.error..ppm.: a numeric vector
- Mass.error..Da.: a numeric vector
- Uncalibrated.mass.error..ppm.: a numeric vector
- Uncalibrated.mass.error..Da.: a numeric vector

- Max.intensity.m.z.0: a numeric vector
- Retention.time: a numeric vector
- Retention.length: a numeric vector
- Calibrated.retention.time: a numeric vector
- Calibrated.retention.time.start: a numeric vector
- Calibrated.retention.time.finish: a numeric vector
- Retention.time.calibration: a numeric vector
- Match.time.difference: a logical vector
- Match.m.z.difference: a logical vector
- Match.q.value: a logical vector
- Match.score: a logical vector
- Number.of.data.points: a numeric vector
- Number.of.scans: a numeric vector
- Number.of.isotopic.peaks: a numeric vector
- PIF: a numeric vector
- Fraction.of.total.spectrum: a numeric vector
- Base.peak.fraction: a numeric vector
- PEP: a numeric vector
- MS.MS.count: a numeric vector
- MS.MS.scan.number: a numeric vector
- Score: a numeric vector
- Delta.score: a numeric vector
- Combinatorics: a numeric vector
- Intensity: a numeric vector
- Reporter.intensity.corrected.0: a numeric vector
- Reporter.intensity.corrected.1: a numeric vector
- Reporter.intensity.corrected.2: a numeric vector
- Reporter.intensity.corrected.3: a numeric vector
- Reporter.intensity.corrected.4: a numeric vector
- Reporter.intensity.corrected.5: a numeric vector
- Reporter.intensity.corrected.6: a numeric vector
- Reporter.intensity.corrected.7: a numeric vector
- Reporter.intensity.corrected.8: a numeric vector
- Reporter.intensity.corrected.9: a numeric vector
- Reporter.intensity.corrected.10: a numeric vector
- RI1: a numeric vector
- RI2: a numeric vector

- RI3: a numeric vector
- RI4: a numeric vector
- RI5: a numeric vector
- RI6: a numeric vector
- RI7: a numeric vector
- RI8: a numeric vector
- RI9: a numeric vector
- RI10: a numeric vector
- RI11: a numeric vector
- Reporter.intensity.count.0: a numeric vector
- Reporter.intensity.count.1: a numeric vector
- Reporter.intensity.count.2: a numeric vector
- Reporter.intensity.count.3: a numeric vector
- Reporter.intensity.count.4: a numeric vector
- Reporter.intensity.count.5: a numeric vector
- Reporter.intensity.count.6: a numeric vector
- Reporter.intensity.count.7: a numeric vector
- Reporter.intensity.count.8: a numeric vector
- Reporter.intensity.count.9: a numeric vector
- Reporter.intensity.count.10: a numeric vector
- Reporter.PIF: a logical vector
- Reporter.fraction: a logical vector
- Reverse: a character vector
- Potential.contaminant: a logical vector
- id: a numeric vector
- Protein.group.IDs: a character vector
- Peptide.ID: a numeric vector
- Mod..peptide.ID: a numeric vector
- MS.MS.IDs: a character vector
- Best.MS.MS: a numeric vector
- AIF.MS.MS.IDs: a logical vector
- Deamidation..N..site.IDs: a numeric vector
- Oxidation..M..site.IDs: a logical vector
- remove: a logical vector
- dart\_PEP: a numeric vector
- dart\_qval: a numeric vector
- razor\_protein\_fdr: a numeric vector

- Deamidation..NQ..Probabilities: a logical vector
- Deamidation..NQ..Score.Diffs: a logical vector
- Deamidation..NQ.: a logical vector
- Reporter.intensity.corrected.11: a logical vector
- Reporter.intensity.corrected.12: a logical vector
- Reporter.intensity.corrected.13: a logical vector
- Reporter.intensity.corrected.14: a logical vector
- Reporter.intensity.corrected.15: a logical vector
- Reporter.intensity.corrected.16: a logical vector
- RI12: a logical vector
- RI13: a logical vector
- RI14: a logical vector
- RI15: a logical vector
- RI16: a logical vector
- Reporter.intensity.count.11: a logical vector
- Reporter.intensity.count.12: a logical vector
- Reporter.intensity.count.13: a logical vector
- Reporter.intensity.count.14: a logical vector
- Reporter.intensity.count.15: a logical vector
- Reporter.intensity.count.16: a logical vector
- Deamidation..NQ..site.IDs: a logical vector
- input\_id: a logical vector
- rt\_minus: a logical vector
- rt\_plus: a logical vector
- mu: a logical vector
- muij: a logical vector
- sigmaij: a logical vector
- pep\_new: a logical vector
- exp\_id: a logical vector
- peptide\_id: a logical vector
- stan\_peptide\_id: a logical vector
- exclude: a logical vector
- residual: a logical vector
- participated: a logical vector
- peptide: a character vector

**Usage**

```
data("inputTable")
```

## Format

An object of class `data.frame` with 1361 rows and 149 columns.

## Details

The dataset is a subset of the SCoPE2 dataset (version 2, Specht et al. 2019, [BioRxiv](#)). The input file `evidence_unfiltered.csv` was downloaded from a [Google Drive repository](#). The MaxQuant evidence file was loaded and the data was cleaned (renaming columns, removing duplicate fields,...). MS runs that were selected in the `scp1` dataset (see `?scp1`) were kept along with a blank run. The data is stored as a `data.frame`.

## See Also

`readSCP()` from the `scp` package for an example on how `mqScpData` is parsed into a [QFeatures](#) object.

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processQFeatures      *Launch a Shiny application to process QFeatures objects*

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## Description

`processQFeatures()` launches an interactive Shiny application that allows users to visually configure and apply pre-processing workflows to a [QFeatures](#) object.

The input `qfeatures` can be provided either as an in-memory [QFeatures](#) object or as a path to an `.rds` file containing one.

## Usage

```
processQFeatures(  
  qfeatures,  
  initialSets = seq_along(qfeatures),  
  prefilledSteps = c("sampleFiltering", "featureFiltering", "missingValuesFeatures",  
    "missingValuesSamples", "normalisation", "aggregation", "join", "aggregation")  
)
```

## Arguments

<code>qfeatures</code>	A <a href="#">QFeatures</a> object to be processed, or a character string specifying the path to a <code>.rds</code> file containing a <a href="#">QFeatures</a> object.
<code>initialSets</code>	An integer, logical, or character vector specifying which assays (feature sets) should be used as the starting point for processing. Defaults to all assays in <code>qfeatures</code> .
<code>prefilledSteps</code>	A character vector specifying the initial workflow steps to display when the application launches. Steps must be provided using their internal identifiers (e.g. <code>"sampleFiltering"</code> , <code>"featureFiltering"</code> , <code>"normalisation"</code> ).

## Details

The application provides a drag-and-drop workflow builder that allows users to select, order, and configure processing steps such as filtering, normalization, and transformation. The configured workflow can then be applied to the selected assays.

## Value

The processQFeatures Shiny application.

## Examples

```
# the example should be launched with `ask = FALSE`

library(QFeatures)
library(QFeaturesGUI)

data("sampleTable")
data("inputTable")

qfeatures <- readQFeatures(
  inputTable,
  colData = sampleTable,
  runCol = "Raw.file"
)

app <- processQFeatures(
  qfeatures,
  initialSets = seq_along(qfeatures)
)

if (interactive()) {
  shiny::runApp(app)
}
```

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sampleTable

*Single-cell sample annotation*

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## Description

A data frame with 48 observations on the following 6 variables.

- Set: a character vector
- Channel: a character vector
- SampleType: a character vector
- lcbatch: a character vector
- sortday: a character vector
- digest: a character vector

**Usage**

```
data("sampleTable")
```

**Format**

An object of class `data.frame` with 64 rows and 6 columns.

**Details**

The dataset is a subset of the SCoPE2 dataset (version 2, Specht et al. 2019, [BioRxiv](#)). The input files `batch.csv` and `annotation.csv` were downloaded from a [Google Drive repository](#). The two files were loaded and the column names were adapted for consistency with `mqScpData` table (see `?mqScpData`). The two tables were filtered to contain only sets present in `mqScpData`. The tables were then merged based on the run ID, hence merging the sample annotation and the batch annotation. Finally, annotation for the blank run was added manually. The data is stored as a `data.frame`.

**See Also**

`readSCP()` from the `scp` package to see how this file is used.

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