Package 'ProtGenerics'

April 9, 2025

Title Generic infrastructure for Bioconductor mass spectrometry packages
Description S4 generic functions and classes needed by Bioconductor proteomics packages.
Version 1.39.2
Author Laurent Gatto <laurent.gatto@uclouvain.be>, Johannes Rainer <johannes.rainer@eurac.edu></johannes.rainer@eurac.edu></laurent.gatto@uclouvain.be>
Maintainer Laurent Gatto <laurent.gatto@uclouvain.be></laurent.gatto@uclouvain.be>
biocViews Infrastructure, Proteomics, MassSpectrometry
<pre>URL https://github.com/RforMassSpectrometry/ProtGenerics</pre>
Depends methods
Suggests testthat
License Artistic-2.0
NeedsCompilation no
RoxygenNote 7.3.2
git_url https://git.bioconductor.org/packages/ProtGenerics
git_branch devel
git_last_commit 0103c31
git_last_commit_date 2025-01-15
Repository Bioconductor 3.21
Date/Publication 2025-04-08
Contents
backendInitialize extractByIndex filterFeatures filterSpectra Param peaksData

2 backendInitialize

Index	1	0
	ProtGenerics	7
	ProcessingStep	6
	processing Queue	5

backendInitialize

General backend methods

Description

These methods are used for implementations of *backends* e.g. for Spectra or Chromatograms object to initialize the backend, merge backends or extract specific information from them. See the respective help pages (e.g. in the Spectra or Chromatograms packages) for information on the actual implementations of these methods.

Usage

```
backendInitialize(object, ...)
isReadOnly(object)
setBackend(object, backend, ...)
backendMerge(object, ...)
backendBpparam(object, ...)
backendParallelFactor(object, ...)
supportsSetBackend(object, ...)
```

Arguments

object The *backend* object.

Optional parameters.

backend A *backend* object.

extractByIndex 3

extractByIndex	Extracting elements by index	

Description

The extractByIndex() method allows to subset an object (or extract elements from it) by providing their integer indices.

Usage

```
extractByIndex(object, i)
```

Arguments

object The object to subset/from which to extract elements.

i integer with the indices.

filterFeatures	Filter features	

Description

Implementations of this generic filter function are supposed to filter *features* in object based on a filter criteria defined by parameter filter.

Usage

```
filterFeatures(object, filter, ...)
```

Arguments

object	The object to filter.
filter	The filtering criteria on which object should be filtered.
	Optional parameters.

4 Param

filterSpectra Filter Spectra

Description

Implementations of this generic filter function are supposed to filter *spectra* (e.g. within a Spectra object) based on filter criteria defined with parameter filter.

Usage

```
filterSpectra(object, filter, ...)
```

Arguments

object The object to filter.

filter The filtering criteria based on which object should be filtered.

Optional parameters.

Generic parameter class

Description

Param

The 'Param' class is a virtual class which can be used as *base* class from which *parameter* classes can inherit.

The methods implemented for the 'Param' class are:

- 'as.list': coerces the 'Param' class to a 'list' with list elements representing the object's slot values, names the slot names. *Hidden* slots (i.e. those with a name starting with '.') are not returned. In addition, a 'Param' class can be coerced to a 'list' using 'as(object, "list")'.
- 'show': prints the content of the 'Param' object (i.e. the individual slots and their value).

Usage

```
## S4 method for signature 'Param'
as.list(x, ...)
## S4 method for signature 'Param'
show(object)
```

Arguments

```
x 'Param' object.
... ignored.
object 'Param' object.
```

peaksData 5

Author(s)

Johannes Rainer

peaksData Get or set MS peak data

Description

These methods get or set mass spectrometry (MS) peaks data, which can be m/z, intensity or retention time values. See the respective help pages (e.g. in the Spectra or Chromatograms packages) for information on the actual implementations of these methods.

Usage

```
peaksData(object, ...)
peaksData(object) <- value
peaksVariables(object, ...)</pre>
```

Arguments

object A data object.
... Optional parameters.
value Replacement for peaks data.

processingQueue

Processing Queue

Description

These methods are related to the *processing queue* implemented in the [Spectra](https://github.com/RforMassSpectrometry and [Chromatograms](https://github.com/RforMassSpectrometry/Chromatograms) packages.

- 'addProcessing()' adds a processing step to the processing queue.
- 'applyProcessing()' execute the processing queue replacing the original data in 'object' with the processed one.
- 'processingChunkSize()' and 'processingChunkSize()<-' are supposed to get and set the number of elements (e.g. spectra) for which the data is loaded into memory and processed at a time.
- 'processingChunkFactor()': defines a 'factor' that can be used to split 'object' into chunks defined by the length of 'object' and its 'processingChunkSize()'.

6 ProcessingStep

Usage

```
processingChunkSize(object, ...)
processingChunkSize(object, ...) <- value
addProcessing(object, ...)
applyProcessing(object, ...)
processingChunkFactor(object, ...)</pre>
```

Arguments

object The object with the processing queue.
... Additional parameters to be defined.
value The replacement value.

ProcessingStep

Processing step

Description

Class containing the function and arguments to be applied in a lazy-execution framework.

Objects of this class are created using the ProcessingStep() function. The processing step is executed with the executeProcessingStep() function.

Usage

```
ProcessingStep(FUN = character(), ARGS = list())
## S4 method for signature 'ProcessingStep'
show(object)
executeProcessingStep(object, ...)
```

Arguments

FUN function or character representing a function name.

ARGS list of arguments to be passed along to FUN.

object ProcessingStep object.

... optional additional arguments to be passed along.

ProtGenerics 7

Details

This object contains all relevant information of a data analysis processing step, i.e. the function and all of its arguments to be applied to the data. This object is mainly used to record possible processing steps of a Spectra or OnDiskMSnExp object (from the Spectra and MSnbase packages, respectively).

Value

The ProcessingStep function returns and object of type ProcessingStep.

Author(s)

Johannes Rainer

Examples

```
## Create a simple processing step object
ps <- ProcessingStep(sum)
executeProcessingStep(ps, 1:10)</pre>
```

ProtGenerics

S4 generic functions for Bioconductor proteomics infrastructure

Description

These generic functions provide basic interfaces to operations on and data access to proteomics and mass spectrometry infrastructure in the Bioconductor project.

For the details, please consult the respective methods' manual pages.

Usage

```
psms(object, ...)
peaks(object, ...)
modifications(object, ...)
database(object, ...)
rtime(object, ...)
tic(object, ...)
spectra(object, ...)
intensity(object, ...)
mz(object, ...)
peptides(object, ...)
proteins(object, ...)
accessions(object, ...)
scans(object, ...)
mass(object, ...)
```

8 ProtGenerics

```
ions(object, ...)
chromatograms(object, ...)
chromatogram(object, ...)
isCentroided(object, ...)
writeMSData(object, file, ...)
## and many more
```

Arguments

object Object of class for which methods are defined.

file for writeMSData

: the name of the file to which the data should be exported.

... Further arguments, possibly used by downstream methods.

Details

When should one define a generics?:

Generics are appropriate for functions that have *generic* names, i.e. names that occur in multiple circumstances, (with different input classes, most often defined in different packages) or, when (multiple) dispatching is better handled by the generics mechanism rather than the developer. The dispatching mechanism will then automatically call the appropriate method and save the user from explicitly calling package::method or the developer to handle the multiple input types cases. When no such conflict exists or is unlikely to happen (for example when the name of the function is specific to a package or domain, or for class slots accessors and replacement methods), the usage of a generic is arguably questionable, and in most of these cases, simple, straightforward functions would be perfectly valid.

When to define a generic in ProtGenerics?:

ProtGenerics is not meant to be the central package for generics, nor should it stop developers from defining the generics they need. It is a means to centralise generics that are defined in different packages (for example mzR::psms and mzID::psms, or IRanges::score and mzR::score, now BioGenerics::score) or generics that live in a rather big package (say mzR) on which one wouldn't want to depend just for the sake of that generics' definition.

The goal of ProtGenerics is to step in when namespace conflicts arise so as to to facilitate inter-operability of packages. In case such conflict appears due to multiple generics, we would (1) add these same definitions in ProtGenerics, (2) remove the definitions from the packages they stem from, which then (3) only need to import ProtGenerics. This would be very minor/straightforward changes for the developers and would resolve issues when they arise.

More generics can be added on request by opening an issue or sending a pull request on:

https://github.com/lgatto/ProtGenerics

Author(s)

Laurent Gatto

ProtGenerics 9

See Also

- The **BiocGenerics** package for S4 generic functions needed by many Bioconductor packages.
- showMethods for displaying a summary of the methods defined for a given generic function.
- selectMethod for getting the definition of a specific method.
- setGeneric and setMethod for defining generics and methods.

Examples

```
## List all the symbols defined in this package:
ls('package:ProtGenerics')

## Not run:
    ## What methods exists for 'peaks'
    showMethods("peaks")

    ## To look at one method in particular
    getMethod("peaks", "mzRpwiz")

## End(Not run)
```

Index

* methods	dataStorage (ProtGenerics), 7
ProtGenerics, 7	<pre>dataStorage<- (ProtGenerics), 7</pre>
	<pre>detectorType (ProtGenerics), 7</pre>
accessions (ProtGenerics), 7	
acquisitionNum (ProtGenerics), 7	estimatePrecursorIntensity
addProcessing(processingQueue), 5	(ProtGenerics), 7
adjacencyMatrix (ProtGenerics), 7	executeProcessingStep(ProcessingStep)
aggregateFeatures (ProtGenerics), 7	6
alignRt (ProtGenerics), 7	expemail (ProtGenerics), 7
analyser (ProtGenerics), 7	exptitle(ProtGenerics),7
analyserDetails (ProtGenerics), 7	extractByIndex, 3
analyzer (ProtGenerics), 7	
analyzerDetails (ProtGenerics), 7	<pre>filterAcquisitionNum(ProtGenerics), 7</pre>
applyProcessing(processingQueue), 5	filterDataOrigin(ProtGenerics),7
as.list,Param-method(Param),4	<pre>filterDataStorage (ProtGenerics), 7</pre>
	<pre>filterEmptySpectra(ProtGenerics), 7</pre>
<pre>backendBpparam(backendInitialize), 2</pre>	filterFeatures, 3
backendInitialize, 2	filterIntensity ($ProtGenerics$), 7
<pre>backendMerge (backendInitialize), 2</pre>	filterIsolationWindow(ProtGenerics),7
backendParallelFactor	filterMsLevel (ProtGenerics), 7
<pre>(backendInitialize), 2</pre>	filterMz(ProtGenerics),7
bin (ProtGenerics), 7	filterMzRange (ProtGenerics), 7
	filterMzValues (ProtGenerics), 7
<pre>calculateFragments (ProtGenerics), 7</pre>	filterNA(ProtGenerics),7
centroided (ProtGenerics), 7	filterPolarity (ProtGenerics), 7
<pre>centroided<- (ProtGenerics), 7</pre>	filterPrecursorCharge(ProtGenerics),7
characterOrFunction-class	filterPrecursorMz(ProtGenerics),7
(ProcessingStep), 6	filterPrecursorMzRange(ProtGenerics),
chromatogram (ProtGenerics), 7	filterPrecursorMzValues (ProtGenerics)
chromatograms (ProtGenerics), 7	7
collisionEnergy (ProtGenerics), 7	filterPrecursorScan ($ProtGenerics$), 7
<pre>collisionEnergy<- (ProtGenerics), 7</pre>	<pre>filterProductMz (ProtGenerics), 7</pre>
<pre>combineFeatures (ProtGenerics), 7</pre>	filterProductMzRange ($ProtGenerics$), 7
compareChromatograms (ProtGenerics), 7	filterProductMzValues(ProtGenerics), 7
<pre>compareSpectra(ProtGenerics), 7</pre>	filterRanges (ProtGenerics), 7
compounds (ProtGenerics), 7	<pre>filterRt (ProtGenerics), 7</pre>
	filterSpectra,4
database (ProtGenerics), 7	filterValues (ProtGenerics), 7
dataOrigin (ProtGenerics), 7	
dataOrigin<-(ProtGenerics).7	impute (ProtGenerics), 7

INDEX 11

instrumentCustomisations	processingChunkFactor
(ProtGenerics), 7	(processingQueue), 5
<pre>instrumentManufacturer(ProtGenerics), 7</pre>	<pre>processingChunkSize(processingQueue), 5</pre>
<pre>instrumentModel (ProtGenerics), 7</pre>	<pre>processingChunkSize<-</pre>
intensity (ProtGenerics), 7	(processingQueue), 5
<pre>intensity<- (ProtGenerics), 7</pre>	<pre>processingData(ProtGenerics), 7</pre>
<pre>ionCount (ProtGenerics), 7</pre>	<pre>processingData<- (ProtGenerics), 7</pre>
ions (ProtGenerics), 7	processingQueue, 5
<pre>ionSource (ProtGenerics), 7</pre>	ProcessingStep, 6
<pre>ionSourceDetails (ProtGenerics), 7</pre>	ProcessingStep-class (ProcessingStep), 6
isCentroided (ProtGenerics), 7	productMz (ProtGenerics), 7
isolationWindowLowerMz (ProtGenerics), 7	productMz<- (ProtGenerics), 7
isolationWindowLowerMz<-	proteins (ProtGenerics), 7
(ProtGenerics), 7	ProtGenerics, 7
<pre>isolationWindowTargetMz (ProtGenerics),</pre>	ProtGenerics-package (ProtGenerics), 7
7	psms (ProtGenerics), 7
isolationWindowTargetMz<-	
(ProtGenerics), 7	quantify(ProtGenerics),7
<pre>isolationWindowUpperMz (ProtGenerics), 7</pre>	rtima (PratCanarias) 7
isolationWindowUpperMz<-	rtime (ProtGenerics), 7
(ProtGenerics), 7	rtime<- (ProtGenerics), 7
<pre>isReadOnly (backendInitialize), 2</pre>	<pre>scanIndex(ProtGenerics), 7</pre>
	scans (ProtGenerics), 7
mass (ProtGenerics), 7	selectMethod, 9
modifications (ProtGenerics), 7	setBackend(backendInitialize), 2
msInfo(ProtGenerics),7	setGeneric,9
msLevel(ProtGenerics), 7	setMethod, 9
msLevel<- (ProtGenerics), 7	show, Param-method (Param), 4
mz (ProtGenerics), 7	show, ProcessingStep-method
mz<- (ProtGenerics), 7	(ProcessingStep), 6
_	showMethods, 9
Param, 4	smooth (ProtGenerics), 7
Param-class (Param), 4	smoothed (ProtGenerics), 7
peaks (ProtGenerics), 7	<pre>smoothed<- (ProtGenerics), 7</pre>
peaks<- (ProtGenerics), 7	spectra (ProtGenerics), 7
peaksData, 5	spectra<- (ProtGenerics), 7
peaksData<- (peaksData), 5	spectraData (ProtGenerics), 7
peaksVariables (peaksData), 5	spectraData<- (ProtGenerics), 7
peptides (ProtGenerics), 7	spectraNames (ProtGenerics), 7
polarity (ProtGenerics), 7	spectraNames<- (ProtGenerics), 7
polarity<- (ProtGenerics), 7	spectrapply (ProtGenerics), 7
precAcquisitionNum (ProtGenerics), 7	spectraVariables (ProtGenerics), 7
precScanNum (ProtGenerics), 7	<pre>supportsSetBackend(backendInitialize),</pre>
precursorCharge (ProtGenerics), 7	2
precursorCharge<- (ProtGenerics), 7	
precursorIntensity (ProtGenerics), 7	tic(ProtGenerics),7
precursorIntensity<- (ProtGenerics), 7	tolerance (ProtGenerics), 7
precursorMz (ProtGenerics), 7	
precursorMz<- (ProtGenerics), 7	uniqueMsLevels (ProtGenerics). 7

12 INDEX

writeMSData(ProtGenerics), 7