

MSnbase development

Laurent Gatto*

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Abstract

This vignette describes the classes implemented in *MSnbase* package. It is intended as a starting point for developers or users who would like to learn more or further develop/extend *pSet*.

Keywords: Mass Spectrometry (MS), proteomics, infrastructure.

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*lg390@cam.ac.uk

Foreword

MSnbase is under active developed; current functionality is evolving and new features will be added. This software is free and open-source software. If you use it, please support the project by citing it in publications:

Laurent Gatto and Kathryn S. Lilley. *MSnbase - an R/Bioconductor package for isobaric tagged mass spectrometry data visualization, processing and quantitation*. *Bioinformatics* 28, 288-289 (2011).

Questions and bugs

You are welcome to contact me directly about *MSnbase*. For bugs, typos, suggestions or other questions, please file an issue in our tracking system¹ providing as much information as possible, a reproducible example and the output of `sessionInfo()`.

If you wish to reach a broader audience for general questions about proteomics analysis using R, you may want to use the Bioconductor support site: <https://support.bioconductor.org/>.

1 Introduction

This document is not a replacement for the individual manual pages, that document the slots of the *MSnbase* classes. It is a centralised high-level description of the package design.

MSnbase aims at being compatible with the *Biobase* infrastructure [1]. Many meta data structures that are used in *eSet* and associated classes are also used here. As such, knowledge of the *Biobase development and the new eSet vignette*² would be beneficial.

The initial goal is to use the *MSnbase* infrastructure for labelled quantitation using reporter ions (iTRAQ [2] and TMT [3]). Spectral counting should be trivial to apply with current features, as long as identification data is at hand. Currently, no effort is invested to streamline label-free quantitative proteomics, although some effort has been done to keep the infrastructure flexible enough to accommodate more designs.

2 MSnbase classes

All classes have a `...classVersion...` slot, of class *Versioned* from the *Biobase* package. This slot documents the class version for any instance to be used for debugging and object update purposes. Any

¹<https://github.com/lgatto/MSnbase/issues>

²The vignette can directly be accessed with `vignette("BiobaseDevelopment", package="Biobase")` once *Biobase* is loaded.

change in a class implementation should trigger a version change.

2.1 pSet: a virtual class for raw mass spectrometry data and meta data

This virtual class is the main container for mass spectrometry data, i.e spectra, and meta data. It is based on the *eSet* implementation for genomic data. The main difference with *eSet* is that the *assayData* slot is an environment containing any number of *Spectrum* instances (see section 2.6).

One new slot is introduced, namely *processingData*, that contains one *MSnProcess* instance (see section 2.4). and the *experimentData* slot is now expected to contain *MIAPe* data (see section 2.5). The annotation slot has not been implemented, as no prior feature annotation is known in shotgun proteomics.

```
getClass("pSet")
Virtual Class "pSet" [package "MSnbase"]

Slots:

Name:          assayData          phenoData
Class:         environment NAnnotatedDataFrame

Name:          featureData        experimentData
Class:  AnnotatedDataFrame        MIAxE

Name:          protocolData       processingData
Class:  AnnotatedDataFrame        MSnProcess

Name:          .cache             .__classVersion__
Class:         environment        Versions

Extends: "Versioned"

Known Subclasses: "MSnExp"
```

Future work Currently, few setters have been implemented.

2.2 MSnExp: a class for MS experiments

MSnExp extends *pSet* to store MS experiments. It does not add any new slots to *pSet*. Accessors and setters are all inherited from *pSet* and new ones should be implemented for *pSet*. Methods that manipulate actual data in experiments are implemented for *MSnExp* objects.

```
getClass("MSnExp")
Class "MSnExp" [package "MSnbase"]

Slots:

Name:          assayData          phenoData
Class:         environment NAnnotatedDataFrame

Name:          featureData        experimentData
Class:         AnnotatedDataFrame MIAxE

Name:          protocolData       processingData
Class:         AnnotatedDataFrame MSnProcess

Name:          .cache             .__classVersion__
Class:         environment        Versions

Extends:
Class "pSet", directly
Class "Versioned", by class "pSet", distance 2
```

2.3 MSnSet: a class for quantitative proteomics data

This class stores quantitation data and meta data after running `quantify` on an *MSnExp* object or by creating an *MSnSet* instance from an external file, as described in the `MSnbase-io` vignette and in `?readMSnSet`, `readMzTabData`, etc. The quantitative data is in form of a $m \times n$ matrix, where m is the number of features/spectra originally in the *MSnExp* used as parameter in `quantify` and n is the number of reporter ions (see section 2.7). If read from an external file, n corresponds to the number of features (protein groups, proteins, peptides, spectra) in the file and m is the number of columns with quantitative data (samples) in the file.

This prompted to keep a similar implementation as the *ExpressionSet* class, while adding the proteomics-specific annotation slot introduced in the *pSet* class, namely `processingData` for objects of class *MSnProcess* (see section 2.4).

```
getClass("MSnSet")
Class "MSnSet" [package "MSnbase"]

Slots:

Name:          experimentData     processingData          qual
Class:         MIAPE              MSnProcess             data.frame
```

```

Name:          assayData          phenoData          featureData
Class:         AssayData AnnotatedDataFrame AnnotatedDataFrame

Name:          annotation          protocolData  .__classVersion__
Class:         character AnnotatedDataFrame          Versions

Extends:
Class "eSet", directly
Class "VersionedBiobase", by class "eSet", distance 2
Class "Versioned", by class "eSet", distance 3

```

The *MSnSet* class extends the virtual *eSet* class to provide compatibility for *ExpressionSet*-like behaviour. The experiment meta-data in *experimentData* is also of class *MIAPE* (see section 2.5). The annotation slot, inherited from *eSet* is not used. As a result, it is easy to convert *ExpressionSet* data from/to *MSnSet* objects with the coercion method `as`.

```

data(itraqdata)
class(msnset)

[1] "MSnSet"
attr("package")
[1] "MSnbase"

class(as(msnset, "ExpressionSet"))

[1] "ExpressionSet"
attr("package")
[1] "Biobase"

data(sample.ExpressionSet)
class(sample.ExpressionSet)

[1] "ExpressionSet"
attr("package")
[1] "Biobase"

class(as(sample.ExpressionSet, "MSnSet"))

[1] "MSnSet"
attr("package")
[1] "MSnbase"

```

2.4 MSnProcess: a class for logging processing meta data

This class aims at recording specific manipulations applied to *MSnExp* or *MSnSet* instances. The processing slot is a character vector that describes major processing. Most other slots are of class `logical` that indicate whether the data has been centroided, smoothed, ...although many of the

functionality is not implemented yet. Any new processing that is implemented should be documented and logged here.

It also documents the raw data file from which the data originates (files slot) and the *MSnbase* version that was in use when the *MSnProcess* instance, and hence the *MSnExp/MSnSet* objects, were originally created.

```
getClass("MSnProcess")
Class "MSnProcess" [package "MSnbase"]

Slots:

Name:          files          processing          merged
Class:         character      character          logical

Name:          cleaned        removedPeaks        smoothed
Class:         logical        character          logical

Name:          trimmed        normalised          MSnbaseVersion
Class:         numeric        logical            character

Name:  __classVersion__
Class:  Versions

Extends: "Versioned"
```

2.5 MIAPE: Minimum Information About a Proteomics Experiment

The Minimum Information About a Proteomics Experiment [4, 5] *MIAPE* class describes the experiment, including contact details, information about the mass spectrometer and control and analysis software.

```
getClass("MIAPE")
Class "MIAPE" [package "MSnbase"]

Slots:

Name:          title          url
Class:         character      character

Name:          abstract        pubMedIds
Class:         character      character

Name:          samples          preprocessing
Class:         list            list
```

```
Name:          other          dateStamp
Class:         list           character

Name:          name           lab
Class:         character      character

Name:          contact        email
Class:         character      character

Name:          instrumentModel instrumentManufacturer
Class:         character      character

Name: instrumentCustomisations softwareName
Class:         character      character

Name:          softwareVersion switchingCriteria
Class:         character      character

Name:          isolationWidth  parameterFile
Class:         numeric        character

Name:          ionSource       ionSourceDetails
Class:         character       character

Name:          analyser        analyserDetails
Class:         character       character

Name:          collisionGas     collisionPressure
Class:         character       numeric

Name:          collisionEnergy  detectorType
Class:         character       character

Name:          detectorSensitivity .__classVersion__
Class:         character       Versions
```

Extends:

Class "MIAxE", directly

Class "Versioned", by class "MIAxE", distance 2

2.6 Spectrum et al.: classes for MS spectra

Spectrum is a virtual class that defines common attributes to all types of spectra. MS1 and MS2 specific attributes are defined in the *Spectrum1* and *Spectrum2* classes, that directly extend *Spectrum*.

```
getClass("Spectrum")
```

```
Virtual Class "Spectrum" [package "MSnbase"]
```

```
Slots:
```

```
Name:          msLevel          peaksCount          rt
Class:         integer           integer             numeric
```

```
Name:    acquisitionNum    scanIndex    tic
Class:   integer           integer       numeric
```

```
Name:          mz          intensity    fromFile
Class:         numeric      numeric       integer
```

```
Name:    centroided  __classVersion__
Class:   logical     Versions
```

```
Extends: "Versioned"
```

```
Known Subclasses: "Spectrum2", "Spectrum1"
```

```
getClass("Spectrum1")
```

```
Class "Spectrum1" [package "MSnbase"]
```

```
Slots:
```

```
Name:          polarity          msLevel    peaksCount
Class:         integer           integer     integer
```

```
Name:          rt    acquisitionNum    scanIndex
Class:         numeric    integer       integer
```

```
Name:          tic          mz    intensity
Class:         numeric    numeric    numeric
```

```
Name:    fromFile    centroided  __classVersion__
Class:   integer     logical       Versions
```

```
Extends:
```



```
Class "Spectrum", directly
Class "Versioned", by class "Spectrum", distance 2
```

```
getClass("Spectrum2")
```

```
Class "Spectrum2" [package "MSnbase"]
```

```
Slots:
```

```
Name:          merged          precScanNum          precursorMz
Class:          numeric          integer          numeric
```

```
Name: precursorIntensity precursorCharge collisionEnergy
Class:          numeric          integer          numeric
```

```
Name:          msLevel          peaksCount          rt
Class:          integer          integer          numeric
```

```
Name:          acquisitionNum scanIndex          tic
Class:          integer          integer          numeric
```

```
Name:          mz          intensity          fromFile
Class:          numeric          numeric          integer
```

```
Name:          centroided  .__classVersion__
Class:          logical          Versions
```

```
Extends:
```

```
Class "Spectrum", directly
```

```
Class "Versioned", by class "Spectrum", distance 2
```

2.7 ReporterIons: a class for isobaric tags

The iTRAQ and TMT (or any other peak of interest) are implemented *ReporterIons* instances, that essentially defines an expected MZ position for the peak and a width around this value as well a names for the reporters.

```
getClass("ReporterIons")
```

```
Class "ReporterIons" [package "MSnbase"]
```

```
Slots:
```

```
Name:          name          reporterNames          description
Class:          character          character          character
```

```

Name:          mz          col          width
Class:         numeric     character  numeric

Name:  .__classVersion__
Class:  Versions

Extends: "Versioned"

```

2.8 NAnnotatedDataFrame: multiplexed AnnotatedDataFrames

The simple expansion of the *AnnotatedDataFrame* classes adds the `multiplex` and `multiLabel` slots to document the number and names of multiplexed samples.

```

getClass("NAnnotatedDataFrame")

Class "NAnnotatedDataFrame" [package "MSnbase"]

Slots:

Name:          multiplex      multiLabels      varMetadata
Class:         numeric       character        data.frame

Name:          data          dimLabels .__classVersion__
Class:         data.frame    character        Versions

Extends:
Class "AnnotatedDataFrame", directly
Class "Versioned", by class "AnnotatedDataFrame", distance 2

```

2.9 Other classes

Lists of MSnSet instances

3 Miscellaneous

Unit tests *MSnbase* implements unit tests with the *testthat* package.

Processing methods Methods that process raw data, i.e. spectra should be implemented for *Spectrum* objects first and then eapply'ed (or similar) to the `assayData` slot of an *MSnExp* instance in the specific method.

4 Session information

- R version 3.2.3 (2015-12-10), x86_64-pc-linux-gnu
- Locale: LC_CTYPE=en_US.UTF-8, LC_NUMERIC=C, LC_TIME=en_US.UTF-8, LC_COLLATE=C, LC_MONETARY=en_US.UTF-8, LC_MESSAGES=en_US.UTF-8, LC_PAPER=en_US.UTF-8, LC_NAME=C, LC_ADDRESS=C, LC_TELEPHONE=C, LC_MEASUREMENT=en_US.UTF-8, LC_IDENTIFICATION=C
- Base packages: base, datasets, grDevices, graphics, grid, methods, parallel, stats, stats4, utils
- Other packages: AnnotationDbi 1.32.3, Biobase 2.30.0, BiocGenerics 0.16.1, BiocParallel 1.4.3, IRanges 2.4.8, MLInterfaces 1.50.0, MSnbase 1.18.1, ProtGenerics 1.2.1, Rcpp 0.12.3, RcppClassic 0.9.6, Rdisop 1.30.0, S4Vectors 0.8.11, XML 3.98-1.3, annotate 1.48.0, cluster 2.0.3, ggplot2 2.0.0, gplots 2.17.0, knitr 1.12.3, mzR 2.4.0, pRoloc 1.10.1, pRolocdata 1.8.0, reshape2 1.4.1, zoo 1.7-12
- Loaded via a namespace (and not attached): BiocInstaller 1.20.1, BiocStyle 1.8.0, DBI 0.3.1, DEoptimR 1.0-4, FNN 1.1, KernSmooth 2.23-15, MALDIquant 1.14, MASS 7.3-45, Matrix 1.2-3, MatrixModels 0.4-1, R6 2.1.2, RColorBrewer 1.1-2, RCurl 1.95-4.7, RSQLite 1.0.0, SparseM 1.7, affy 1.48.0, affyio 1.40.0, assertthat 0.1, base64enc 0.1-3, biomaRt 2.26.1, bitops 1.0-6, caTools 1.17.1, car 2.1-1, caret 6.0-64, class 7.3-14, codetools 0.2-14, colorspace 1.2-6, digest 0.6.9, diptest 0.75-7, doParallel 1.0.10, dplyr 0.4.3, e1071 1.6-7, evaluate 0.8, flexmix 2.3-13, foreach 1.4.3, formatR 1.2.1, fpc 2.1-10, futile.logger 1.4.1, futile.options 1.0.0, gbm 2.1.1, gdata 2.17.0, genefilter 1.52.1, ggvis 0.4.2, gtable 0.1.2, gtools 3.5.0, highr 0.5.1, htmltools 0.3, htmlwidgets 0.5, httpuv 1.3.3, hwriter 1.3.2, impute 1.44.0, iterators 1.0.8, kernlab 0.9-23, labeling 0.3, lambda.r 1.1.7, lattice 0.20-33, limma 3.26.8, lme4 1.1-11, lpSolve 5.6.13, magrittr 1.5, mclust 5.1, mgcv 1.8-11, mime 0.4, minqa 1.2.4, mlbench 2.1-1, modeltools 0.2-21, munsell 0.4.3, mvtnorm 1.0-5, mzID 1.8.0, nlme 3.1-124, nloptr 1.0.4, nnet 7.3-12, pbkrtest 0.4-6, pcaMethods 1.60.0, pls 2.5-0, plyr 1.8.3, prabclus 2.2-6, preprocessCore 1.32.0, proxy 0.4-15, quantreg 5.21, randomForest 4.6-12, rda 1.0.2-2, rgl 0.95.1441, robustbase 0.92-5, rpart 4.1-10, sampling 2.7, scales 0.3.0, sfsmisc 1.1-0, shiny 0.13.1, splines 3.2.3, stringi 1.0-1, stringr 1.0.0, survival 2.38-3, threejs 0.2.1, tools 3.2.3, trimcluster 0.1-2, vsn 3.38.0, xtable 1.8-2, zlibbioc 1.16.0

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