

# *isobar* for developers

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## 1 Introduction

This documents highlights the structure of the S4 classes and methods in the `isobar` package.

```
> library(isobar)
```

## 2 Classes

### 2.1 IBSpectra

```
> getClass("IBSpectra")
```

Virtual Class "IBSpectra" [package "isobar"]

Slots:

Name:	proteinGroup	reporterTagNames	reporterTagMasses
Class:	ProteinGroup	character	numeric

Name:	isotopeImpurities	log	assayData
Class:	matrix	matrix	AssayData

Name:	phenoData	featureData	experimentData
Class:	AnnotatedDataFrame	AnnotatedDataFrame	MIAxE

```

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

```

Known Subclasses:

```

Class "iTRAQspectra", directly
Class "TMTspectra", directly
Class "iTRAQ4plexspectra", by class "iTRAQspectra", distance 2
Class "iTRAQ8plexspectra", by class "iTRAQspectra", distance 2
Class "TMT2plexspectra", by class "TMTspectra", distance 2
Class "TMT6plexspectra", by class "TMTspectra", distance 2
Class "TMT6plexspectra2", by class "TMTspectra", distance 2
Class "TMT10plexspectra", by class "TMTspectra", distance 2

```

identifications and quantitative values. Spectrums are identified as stemming from distinct peptides, and quantitative information of each spectrum are extracted from a certain  $m/z$  region.

IBSpectra class holds this qualitative and quantitative information. It is a virtual class. It extends `eSet` from Biobase to store meta-information of spectrum identifications and quantitative information ( $m/z$  and `intensity`) of reporter tags. `eSet` is extended by slots for protein grouping, tag names, tag masses and isotope impurity correction matrix.

`ProteinGroup` objects store the mapping and grouping of peptide level identifications to protein identifications.

IBSpectra is a virtual class. Currently used isobaric tagging kits iTRAQ 4plex and 8plex, and TMT 2plex and 6plex are implemented in the `iTRAQ4plexspectra`, `iTRAQ8plexspectra`, `TMT2plexspectra`, `TMT6plexspectr` and `TMT10plexspectr`, respectively. These are subclasses of `iTRAQspectra` and `TMTspectra`, resp. which in turn are virtual subclasses of `IBSpectra`.

## 2.2 ProteinGroup

```
> getClass("ProteinGroup")
```

```
Class "ProteinGroup" [package "isobar"]
```

Slots:

```

Name:          spectrumToPeptide      spectrumId
Class:         character              data.frame

```

```

Name:          peptideSpecificity      peptideNProtein
Class:         data.frame              matrix

```

Name:	indistinguishableProteins	proteinGroupTable
Class:	character	data.frame

Name:	overlappingProteins	isoformToGeneProduct
Class:	matrix	data.frame

Name:	proteinInfo	peptideInfo
Class:	data.frame	data.frame

Name:	.__classVersion__
Class:	Versions

Extends:

Class "VersionedBiobase", directly

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

mapped back to proteins. This mapping leads to protein groups, which explain the observed peptides according to the parsimony law.

A `ProteinGroup` object is generated when a `IBSpectra` object is created by `readIBSpectra`. Protein to peptide to spectrum mapping is extracted from a suitable identification format<sup>1</sup>

## 2.3 NoiseModel

```
> getClass("NoiseModel")
```

Virtual Class "NoiseModel" [package "isobar"]

Slots:

Name:	na.region	low.intensity	f	parameter
Class:	numeric	numeric	function	numeric

Name:	.__classVersion__
Class:	Versions

Extends:

Class "VersionedBiobase", directly

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

Known Subclasses: "ExponentialNoANoiseModel", "ExponentialNoiseModel", "InverseNoiseModel", "InverseNoANoiseModel", "GeneralNoiseModel"

in the spectrum-level ratios of a certain experimental setup.

---

<sup>1</sup>IBSpectra CSV, and MzIdentML format. Mascot DAT and Phenyx pidres.xml format converters to IBSpectra format are provided.

### 3 Session Information

The version number of R and packages loaded for generating the vignette were:

- R version 3.4.0 (2017-04-21), x86\_64-apple-darwin15.6.0
- Locale: C/en\_US.UTF-8/en\_US.UTF-8/C/en\_US.UTF-8/en\_US.UTF-8
- Running under: OS X El Capitan 10.11.6
- Matrix products: default
- BLAS:  
/Library/Frameworks/R.framework/Versions/3.4/Resources/lib/libRblas.0.dylib
- LAPACK:  
/Library/Frameworks/R.framework/Versions/3.4/Resources/lib/libRlapack.dylib
- Base packages: base, datasets, grDevices, graphics, methods, parallel, stats, utils
- Other packages: Biobase 2.36.0, BiocGenerics 0.22.0, isobar 1.22.0
- Loaded via a namespace (and not attached): AnnotationDbi 1.38.0, DBI 0.6-1, IRanges 2.10.0, MASS 7.3-47, RCurl 1.95-4.8, RSQLite 1.1-2, Rcpp 0.12.10, S4Vectors 0.14.0, SweaveListingUtils 0.7.7, XML 3.98-1.6, biomaRt 2.32.0, bitops 1.0-6, colorspace 1.3-2, compiler 3.4.0, digest 0.6.12, distr 2.6.2, ggplot2 2.2.1, grid 3.4.0, gtable 0.2.0, lazyeval 0.2.0, memoise 1.1.0, munsell 0.4.3, plyr 1.8.4, scales 0.4.1, sfsmisc 1.1-0, startupmsg 0.9.4, stats4 3.4.0, tibble 1.3.0, tools 3.4.0