

# 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

```

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**, and **TMT6plexspectra**, 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      peptideSpecificity
Class:         character              data.frame

Name:          peptideNProtein indistinguishableProteins
Class:         matrix                character

Name:          proteinGroupTable      overlappingProteins

```

Class: data.frame matrix

Name: isoformToGeneProduct proteinInfo

Class: data.frame data.frame

Name: peptideInfo .\_\_classVersion\_\_

Class: data.frame 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"

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

## 3 Session Information

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

---

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

- R version 2.14.1 (2011-12-22), x86\_64-unknown-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=C, 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, stats, utils
- Other packages: Biobase 2.14.0, ggplot2 0.8.9, isobar 1.1.1, plyr 1.5, proto 0.3-9.2, reshape 0.8.4
- Loaded via a namespace (and not attached): RCurl 1.5-0, XML 3.2-0, biomaRt 2.6.0, distr 2.3.3, sfsmisc 1.0-14, startupmsg 0.7.1, tools 2.14.1