

# 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      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"

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 2.15.1 (2012-06-22), i386-pc-mingw32
- Locale: LC\_COLLATE=C, LC\_CTYPE=English\_United States.1252, LC\_MONETARY=English\_United States.1252, LC\_NUMERIC=C, LC\_TIME=English\_United States.1252
- Base packages: base, datasets, grDevices, graphics, methods, stats, utils
- Other packages: Biobase 2.18.0, BiocGenerics 0.4.0, isobar 1.4.0, plyr 1.7.1
- Loaded via a namespace (and not attached): distr 2.3.3, sfsmisc 1.0-21, startupmsg 0.7.2, tools 2.15.1