

Isobar for developers

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September 29, 2011

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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	reporterNames	reporterMasses
Class:	ProteinGroup	character	numeric
Name:	isotopeImpurities	log	assayData
Class:	matrix	matrix	AssayData
Name:	phenoData	featureData	experimentData
Class:	AnnotatedDataFrame	AnnotatedDataFrame	MIAME

```

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

```

MSMS isobarically tagged proteomics data consists of spectrum 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

Bottom-up MSMS proteomics experiments identify peptides which are 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 format¹

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"

`NoiseModel` objects model the technical variance observed in the spectrum-level ratios of a certain experimental setup.

¹IBSpectra 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:

```
> toLatex(sessionInfo())
```

- R version 2.12.1 (2010-12-16), i386-pc-mingw32
- Locale: LC_COLLATE=C, LC_CTYPE=German_Austria.1252, LC_MONETARY=German_Austria.1252, LC_NUMERIC=C, LC_TIME=German_Austria.1252
- Base packages: base, datasets, grDevices, graphics, grid, methods, stats, utils
- Other packages: Biobase 2.10.0, biomaRt 2.6.0, distr 2.2.3, ggplot2 0.8.8, isobar 0.2.4, plyr 1.2.1, proto 0.3-8, reshape 0.8.3, sfsmisc 1.0-14, startupmsg 0.7
- Loaded via a namespace (and not attached): RCurl 1.5-0.1, XML 3.2-0.2, tools 2.12.1