

Isobar for developers

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February 29, 2012

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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 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"

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:

¹IBSpectra 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), 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 2.14.0, ggplot2 0.9.0, isobar 1.1.1, plyr 1.7.1
- Loaded via a namespace (and not attached): MASS 7.3-17, RColorBrewer 1.0-5,
RCurl 1.91-1.1, XML 3.9-4.1, biomaRt 2.10.0, colorspace 1.1-1, dichromat 1.2-4,
digest 0.5.1, distr 2.3.3, grid 2.14.1, memoise 0.1, munsell 0.3, proto 0.3-9.2,
reshape2 1.2.1, scales 0.2.0, sfsmisc 1.0-19, startupmsg 0.7.2, stringr 0.6, tools 2.14.1