

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 TMT6plexspectr, 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 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.

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:

- R version 2.15.1 (2012-06-22), 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, 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