

isobar for developers

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Contents

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
Class "TMT6plexspectra2", by class "TMTspectra", distance 2
Class "TMT10plexspectra", 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`, `TMT6plexspectra` and `TMT10plexspectra`, 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", "GeneralNoiseModel"

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:

- R version 3.2.4 (2016-03-10), x86_64-apple-darwin13.4.0
- Locale: C/en_US.UTF-8/en_US.UTF-8/C/en_US.UTF-8/en_US.UTF-8

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

- Base packages: base, datasets, grDevices, graphics, methods, parallel, stats, utils
- Other packages: Biobase 2.30.0, BiocGenerics 0.16.1, isobar 1.16.1
- Loaded via a namespace (and not attached): Rcpp 0.12.3, SweaveListingUtils 0.6.2, distr 2.5.3, plyr 1.8.3, sfsmisc 1.1-0, startupmsg 0.9, tools 3.2.4