

Isobar for developers

Florian P. Breitwieser, Jacques Colinge

February 27, 2012

Contents

1	Introduction	1
2	Classes	1
2.1	IBSpectra	1
2.2	ProteinGroup	2
2.3	NoiseModel	3
3	Session Information	3

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), 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 2.14.0, 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, XML 3.9-4, 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 0.1.0, sfsmisc 1.0-19, startupmsg 0.7.2, stringr 0.6, tools 2.14.1