

isobar for developers

Florian P. Breitwieser, Jacques Colinge

April 11, 2014

Contents

1	Introduction	1
2	Classes	1
2.1	IBSpectra	1
2.2	ProteinGroup	2
2.3	NoiseModel	3
3	Session Information	4

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`, `TMT6plexspectr` and `TMT10plexspectr`, 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.

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 3.1.0 RC (2014-04-02 r65358), x86_64-apple-darwin10.8.0
- Locale: en_US.UTF-8/en_US.UTF-8/en_US.UTF-8/C/en_US.UTF-8/en_US.UTF-8
- Base packages: base, datasets, graphics, grDevices, methods, parallel, stats, utils
- Other packages: Biobase 2.24.0, BiocGenerics 0.10.0, isobar 1.10.0, plyr 1.8.1
- Loaded via a namespace (and not attached): distr 2.5.2, Rcpp 0.11.1, sfsmisc 1.0-25, startupmsg 0.9, SweaveListingUtils 0.6.1, tools 3.1.0