

Package ‘Risa’

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Title Converting experimental metadata from ISA-tab into Bioconductor data structures

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Depends R (>= 2.0.9), Biobase (>= 2.4.0), methods, Rcpp (>= 0.9.13)

Imports xcms

Suggests faahKO (>= 1.2.11)

Description The Investigation / Study / Assay (ISA) tab-delimited format is a general purpose framework with which to collect and communicate complex metadata (i.e. sample characteristics, technologies used, type of measurements made) from experiments employing a combination of technologies, spanning from traditional approaches to high-throughput techniques. Risa allows to access metadata/data in ISA-Tab format and build Bioconductor data structures. Currently, data generated from microarray, flow cytometry and metabolomics-based (i.e. mass spectrometry) assays are supported. The package is extendable and efforts are undergoing to support metadata associated to proteomics assays.

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biocViews Annotation, DataImport, MassSpectrometry

URL <<http://isatab.sourceforge.net/>>

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ISAtab-class	<i>Class "ISAtab", a class for maintaing ISAtab information</i>
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Description

This class maintains informatino from an ISAtab dataset, including an investigation file, one or more study files, and one or more assay files for each study file.

Objects from the Class

Objects can be created by calls of the form `new("ISAtab", ...)`.

Slots

path: Object of class "character", it represents the path of the ISA-Tab dataset

investigation.filename: Object of class "character", it represents the name of the Investigation file

investigation.file: Object of class "data.frame", it is a data frame with the contents of the Investigation file

study.identifiers: Object of class "factor", it is the list of study identifiers

study.fileNames: Object of class "character", the names of the study files

study.files: Object of class "list", a list of data frames wiht the contents of the study files

assay.fileNames: Object of class "character", the names of the assay files

assay.fileNames.per.study: Object of class "list", the names of the assay files according to the study they belong to

assay.files: Object of class "list", a list of data frames with the contents of the assay files

assay.files.per.study: Object of class "list", a list of data frames with the contents of the assay files divided per study they belong to

assay.technology.types: Object of class "character", a list with the technology types corresponding to each assay

assay.measurement.types: Object of class "character", a list with the names of the data files

data.fileNames: Object of class "list", a list with the names of the samples

samples: Object of class "character"

samples.per.study: Object of class "list",

samples.per.assay.filename: Object of class "list",the samples classified according to the assay filename they belong to

assay.fileNames.per.sample: Object of class "character", the names of the assay files classified per sample name

sample.to.rawdatafile: Object of class "list", a list of data frames with samples associated with raw data files

sample.to.assayname: Object of class "list", maintains the association between samples and assay names

rawdatafile.to.sample: Object of class "list", maintains the association raw data file and samples

assayname.to.sample: Object of class "list", maintains the associations between assay names and samples

Methods

[signature(x = "ISAtab"): ...

Note

No notes yet.

Author(s)

Alejandra Gonzalez-Beltran, <isatools@googlegroups.com>

References

Risa is a component of the ISA software infrastructure <http://isa-tools.org/>. The source code and latest version can be found in the GitHub repository <https://github.com/ISA-tools/Risa>. Please, submit all 'bugs' and feature requests through <https://github.com/ISA-tools/Risa/issues>.

See Also

ISAtab-methods

Examples

```
showClass("ISAtab")
```

processAssayXcmsSet *Build an xcmsSet object given a mass spectrometry assay*

Description

processAssayXcmsSet reads a ISA-tab file.

Usage

```
processAssayXcmsSet(isa, assay.filename, ...)
```

Arguments

isa	an ISA object, as retrieved by the function readISAtab
assay.filename	a boolean indicating to show messages for the different steps, if TRUE, or not to show them, if FALSE
...	extra arguments that can be pass down to the xcmsSet function from the xcms package

Value

the xcmsSet object built from the assay metadata and data files

Author(s)

Steffen Neumann, Alejandra Gonzalez-Beltran / Maintainer: Alejandra Gonzalez-Beltran <isatools@googlegroups.com>

See Also

readISAtab

Examples

```
faahkoISA = readISAtab(find.package("faahKO"))
assay.filename <- faahkoISA["assay.filenames"][[1]]
xset = processAssayXcmsSet(faahkoISA, assay.filename)
```

readISAtab

Reads an ISAtab dataset into an R object.

Description

Reads an ISAtab dataset given as a zip file or as a set of files in a specific folder, and builds an object from the ISAtab class.

Usage

```
readISAtab(path = getwd(), zipfile = NULL, verbose = FALSE)
```

Arguments

path	the name of the directory in which the ISAtab files are located (if the parameter zipfile is not provided or if it is equal to NULL), or the name of the directory where the zip file will be extracted (if the parameter zipfile is not NULL.) The default is the working directory.
zipfile	a zip archive containing ISAtab files. The default value is NULL.
verbose	a boolean indicating to show messages for the different steps, if TRUE, or not to show them, if FALSE

Value

The result is an object from the ISAtab class.

Author(s)

Alejandra Gonzalez-Beltran, Audrey Kauffmann / Maintainer: Alejandra Gonzalez-Beltran, ISA Team <isatools@googlegroups.com>

Examples

```

## Example for mass spectrometry dataset
temp = tempdir()
datafiles = c(file.path(system.file("cdf/KO", package="faahKO"), grep("CDF",dir(system.file("cdf/KO", package="
file.copy(datafiles, temp, recursive=TRUE)
isafiles = file.path(system.file(package="faahKO"), grep("txt",dir(system.file(package="faahKO")),value=TRUE))
file.copy(isafiles, temp, recursive=TRUE)
isaObject1 = readISAtab(path = temp)

## Example of readISAtab for a mass spectrometry experiment
isazip = system.file("extdata", "faahKO-metadata.zip", package="Risa")
isaObject2 = readISAtab(zipfile = isazip, path = file.path(system.file("extdata", package="Risa"), "ISAexample"), verbose=TRUE)

```

Risa

*Risa package overview***Description**

The Risa package builds R objects from ISA-tab format files and it is a component of the ISA software infrastructure <http://isa-tools.org/>. The source code and latest version can be found in the GitHub repository <https://github.com/ISA-tools/Risa>. Please, submit all 'bugs' and feature requests through <https://github.com/ISA-tools/Risa/issues>.

The Risa package contains the function `readISAtab` that can be used to read ISA-tab files from a local zip archive or from a local folder.

Author(s)

Alejandra Gonzalez-Beltran, Steffen Neumann, Audrey Kauffmann, Gabriella Rustici, Philippe Rocca-Serra, Eamonn Maguire, Susanna-Asunta Sansone. Maintainer: Alejandra Gonzalez-Beltran <isatools@googlegroups.com>

See Also

`readISAtab`, `processAssayXcmsSet`, `updateAssayMetadata`, `writeISAtab`

Examples

```

## Example of readISAtab for a mass spectrometry experiment from a zip file
isazip = system.file("extdata", "faahKO-metadata.zip", package="Risa")
isaset = readISAtab(zipfile = isazip, path = file.path(system.file("extdata", package="Risa"), "ISAexample"), verbose=TRUE)

require("faahKO")
## Example of readISAtab for mass spectrometry data
temp = tempdir()
datafiles = c(file.path(system.file("cdf/KO", package="faahKO"), grep("CDF",dir(system.file("cdf/KO", package="
file.copy(datafiles, temp, recursive=TRUE)
isafiles = file.path(system.file(package="faahKO"), grep("txt",dir(system.file(package="faahKO")),value=TRUE))
file.copy(isafiles, temp, recursive=TRUE)
isatab.object = readISAtab(path = temp)

```

updateAssayMetadata *Update metadata into the assay file*

Description

updateAssayMetadata Updates metadata into a particular assay file. See an example of use for a metabolite dataset at <https://github.com/sneumann/mtbls2>.

Usage

```
updateAssayMetadata(isa, assay.filename, col.name, values)
```

Arguments

isa	An isatab object, as retrieved by the readISAtab function.
assay.filename	the filename of the assay file to be augmented/modified
col.name	the name of the column of the assay file to be modified
values	the values to be added to the column of the assay file: it could be a single value, and in this case the value is repeated across the column, or it could be a list of values (whose length must match the number of rows of the assay file)

Value

The updated ISA-Tab object.

Author(s)

Alejandra Gonzalez-Beltran / Maintainer: Alejandra Gonzalez-Beltran, ISA Team <isatools@googlegroups.com>

See Also

readISAtab, <https://github.com/sneumann/mtbls2>

Examples

```
### This example shows how to add values to the column "Derived Spectral Data File", assuming that the results are stored in a file named "faahKO.txt"
faahkoISA = readISAtab(find.package("faahKO"))
assay.filename <- faahkoISA["assay.fileNames"][[1]]
updateAssayMetadata(faahkoISA, assay.filename, "Derived Spectral Data File", "faahkoDSDF.txt")
```

write.assay.file	<i>Write an Assay File from the ISA-Tab dataset</i>
------------------	---

Description

write.assay.file writes a specific assay file from the ISA-tab dataset into disk.

Usage

```
write.assay.file(isa, assay.filename, path = getwd())
```

Arguments

isa	the ISA-Tab object (as retrieved by the readISAtab function)
assay.filename	the name of the assay file to be written to disk
path	the output path in which the study file is going to be written, by default is the working directory

Author(s)

Alejandra Gonzalez-Beltran / Maintainer: Alejandra Gonzalez-Beltran, ISA Team <isatools@googlegroups.com>

See Also

write.ISAtab, write.investigation.file, write.study.file, readISAtab

Examples

```
### Example of writing the study file of faahKO ISA-Tab dataset into the temp directory
faahkoISA <- readISAtab(find.package("faahKO"))
temp = tempdir()
write.assay.file(faahkoISA, faahkoISA["assay.names"][1], temp)
```

write.investigation.file	<i>Writes the Investigation File of an ISA-Tab dataset</i>
--------------------------	--

Description

write.investigation.file reads a ISA-tab file.

Usage

```
write.investigation.file(isa, path = getwd())
```

Arguments

isa	the ISA-Tab object (as retrieved by the readISAtab function)
path	the output path in which the study file is going to be written, by default is the working directory

Author(s)

Alejandra Gonzalez-Beltran / Maintainer: Alejandra Gonzalez-Beltran, ISA Team <isatools@googlegroups.com>

See Also

write.ISAtab, write.study.file, write.assay.file, readISAtab

Examples

```
### Example of writing the study file of faahKO ISA-Tab dataset into the temp director
faahkoISA <- readISAtab(find.package("faahKO"))
temp = tempdir()
write.investigation.file(faahkoISA, temp)
```

write.ISAtab

Write an ISA-Tab dataset

Description

write.ISAtab writes a ISA-Tab dataset.

Usage

```
write.ISAtab(isa, path = getwd())
```

Arguments

isa	the ISA-Tab object as built with the function readISAtab.
path	the directory where the files are going to be written, by default is the working directory

Author(s)

Alejandra Gonzalez-Beltran / Maintainer: Alejandra Gonzalez-Beltran, ISA Team <isatools@googlegroups.com>

See Also

write.investigation.file, write.study.file, write.assay.file, readISAtab

Examples

```
### Example of writing the study file of faahKO ISA-Tab dataset into the temp director
faahkoISA <- readISAtab(system.file("extdata", "faahKO-metadata", package="Risa"))
temp = tempdir()
write.ISAtab(faahkoISA, temp)
```

`write.study.file`*Write a Study File of an ISA-Tab dataset*

Description

`write.study.file` writes a specific Study file from the ISA-tab dataset.

Usage

```
write.study.file(isa, study.filename, path = getwd())
```

Arguments

<code>isa</code>	the ISA-Tab object (as retrieved by the readISAtab function)
<code>study.filename</code>	the name of the study file to be written to disk
<code>path</code>	the output path in which the study file is going to be written, by default is the working directory

Author(s)

Alejandra Gonzalez-Beltran / Maintainer: Alejandra Gonzalez-Beltran, ISA Team <isatools@googlegroups.com>

See Also

`write.study.file`, `write.ISAtab`, `readISAtab`

Examples

```
### Example of writing the study file of faahKO ISA-Tab dataset into the temp director
faahkoISA <- readISAtab(find.package("faahKO"))
temp = tempdir()
write.study.file(faahkoISA, faahkoISA["study.filenames"][[1]], temp)
```

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