

Risa: Building R objects from local ISA-Tab files

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1 Introduction

The Risa package is part of the ISA infrastructure software suite (<http://isa-tools.org>). It provides functionality to read ISA-Tab datasets, described in the following section. 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>.

2 ISA-Tab format

The Investigation / Study / Assay (ISA) Tab-delimited (Tab) 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 (<http://isa-tools.org>). In particular, ISA-Tab has been developed for - but not limited to - experiments using genomics, transcriptomics, proteomics or metabol/nomics techniques (the 'omics').

ISA-Tab uses three types of file to capture the experimental metadata:

- *Investigation file*
- *Study file*
- *Assay file* (with associated data files).

The Investigation file contains an overall description of an experiment while all experimental steps are described in the Study and in the Assay file(s). For each Investigation file there may be one or more Study files; for each Study file there may be one or more Assay files.

2.1 Investigation file

In this file, information is reported on a per-column basis and the fields are organized and divided in sections. The Investigation file is intended to meet three needs:

- to define key entities, such as factors, protocols, parameters, which may be referenced in the other files;
- to relate Assay files to Study files; and optionally,
- to relate each Study file to an Investigation (when two or more Study files need to be grouped). The declarative sections cover general information such as contacts, protocols and equipment, and also - where applicable - the description of terminologies (controlled vocabularies or ontologies) and other annotation resources that were used.

2.2 Study file

In this file, information is structured on a per-row basis with the first row being used for column headers. The Study file contains contextualizing information for one or more assays, for example; the subjects studied; their source(s); the sampling methodology; their characteristics; and any treatments or manipulations performed to prepare the specimens.

2.3 Assay file

In this file, as for the Study file, fields are organized on a per-row basis with the first row being used for column headers. The Assay file represents a portion of the experimental graph (i.e., one part of the overall structure of the workflow); each Assay file must contain assays of the same type, defined by the type of measurement (i.e. gene expression) and the technology employed (i.e. DNA microarray). Assay-related information includes protocols, additional information relating to the execution of those protocols and references to data files (whether raw or processed).

For easy transfer, ISA-Tab files and associated data files can be packaged into an ISAArchive, using a standalone Java application named ISAcreator (<http://isatab.sourceforge.net>). In order to facilitate identification of ISA-Tab components in an ISAArchive, specific extensions have been created as follows:

- *i_iname.txt* for identifying the Investigation file
- *s_sname.txt* for identifying Study file (s)
- *a_aname.txt* for identifying Assay file (s)

where 'iname', 'sname', 'aname' are the user-given names for the investigation, study/ies, assay(s), respectively.

3 The Risa package

The Risa package is used to build R objects from an ISA archive or dataset. The output is a list of objects containing, for example, the investigation, studies and assays filenames, the contents of their files, the list of samples, among other things.

These objects can then be used by downstream Bioconductor packages for data analysis and visualization (i.e, xcms). The package currently includes the function `processAssayXcmsSet` that, for a specific mass spectrometry assay, builds an `xcmsSet` object.

3.1 Building an R object from a local ISA dataset

If you have your own ISA archive, you can use the function `readISAtab` to convert it into an R object. The arguments for the function `readISAtab` are:

- `path` the name of the directory containing ISAtab files. The default is the working directory.
- `verbose` a boolean indicating to show messages for the different steps, if TRUE, or not to show them, if FALSE

As an example, we can use the *faahKO* dataset, whose version 1.2.11 contains an ISA dataset describing the experiment. First, it is required to load the *Risa* package, and the *faahKO* package must have been installed.

```
> library(Risa)
> require(faahKO)
```

Then, we read the ISA-Tab data set from the *faahKO* package:

```
> faahkoISA <- readISAtab(find.package("faahKO"))
```

The object `fahkoISA` belongs to the *ISAtab* class, and contains the following elements:

- `path` - the path of the ISA-Tab dataset,
- `investigation.filename` - the name of the Investigation file
- `investigation.file` - a data frame with the contents of the Investigation file
- `study.identifiers` - the list of study identifiers
- `study filenames` - the names of the study files
- `study.files` - a list of data frames with the contents of the study files
- `assay filenames` - the names of the assay files
- `assay filenames.per.study` - the names of the assay files according to the study they belong to
- `assay.files` - a list of data frames with the contents of the assay files
- `assay.files.per.study` - a list of data frames with the contents of the assay files divided per study they belong to
- `assay.technology.types` - a list with the technology types corresponding to each assay
- `assay.measurement.types` - a list with the measurement types corresponding to each assay
- `data filenames` - a list with the names of the data files
- `samples` - a list with the names of the samples
- `samples.per.assay.filename` - the samples classified according to the assay filename they belong to
- `assay filenames.per.sample` - the names of the assay files classified per sample name
- `sample.to.rawdatafile` - the association between samples and raw data files
- `sample.to.assayname` - the association between samples and assay names
- `rawdatafile.to.sample` - the association between raw data files and samples
- `assayname.to.sample` - the association between assay names and samples

Additionally, the ISA dataset could be compressed in a `.zip` file. If that is the case, the function `readISAtab` can be used, passing the `zipfile` as parameter. The only condition is that the ISA-Tab files are contained directly into the zip file, i.e. not inside additional folders.

In this case, the parameters for the function `readISAtab` will be:

- `zipfile` a zip archive containing ISAtab files.
- `path` the name of the directory in which the files from the zip archive will be extracted. The default is the working directory.
- `verbose` a boolean indicating to show messages for the different steps, if `TRUE`, or not to show them, if `FALSE`

Building xcmsSets for mass spectrometry assays

The function `processAssayXcmsSet` allows to build an `xcmsSet` (object defined in the `xcms` package) from the information in an assay file.

The parameters for this function are:

- `isa`: an ISA object, as retrieved by the function `readISATab`
- `assay.filename` the name of the assay file with information about the relevant assay
- ... extra arguments that can be passed down to the `xcmsSet` function from the `xcms` package

Using the *faahKO* package as an example, we select the name of assay file, and use the `processAssayXcmsSet` to build a object of type *xcmsSet*:

```
> assay.filename <- faahkoISA["assay.names"][1]
> faahkoXset <- processAssayXcmsSet(faahkoISA, assay.filename)
```

Augmenting the ISA-Tab dataset after analysis

The *Risa* package also provides the functionality to augment the original ISA-Tab dataset with more information after analysis.

The function `updateAssayMetadata` allows to modify the metadata in a particular assay file. The arguments are:

- `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)

To continue with our example using the *faahKO* data package, we will assume that the results of analysis are stored in the file *faahkoDSDf.txt*. Then, we will update the ISA-Tab dataset adding the result file into the 'Derived Spectral Data File' column of the assay file.

```
> updateAssayMetadata(faahkoISA, assay.filename, "Derived Spectral Data File", "faahkoDSDf.txt")
```

An object of class "ISATab"

Slot "path":

```
[1] "/github/workspace/pkglib/faahKO"
```

Slot "investigation.filename":

```
[1] "i_Investigation.txt"
```

Slot "investigation.file":

```

V1
1 ONTOLOGY SOURCE REFERENCE
2 Term Source Name
3 Term Source File
4 Term Source Version
5 Term Source Description
6 INVESTIGATION
7 Investigation Identifier
```

8 Investigation Title
9 Investigation Description
10 Investigation Submission Date
11 Investigation Public Release Date
12 Comment [Created with configuration]
13 Comment [Last Opened With Configuration]
14 INVESTIGATION PUBLICATIONS
15 Investigation PubMed ID
16 Investigation Publication DOI
17 Investigation Publication Author List
18 Investigation Publication Title
19 Investigation Publication Status
20 Investigation Publication Status Term Accession Number
21 Investigation Publication Status Term Source REF
22 INVESTIGATION CONTACTS
23 Investigation Person Last Name
24 Investigation Person First Name
25 Investigation Person Mid Initials
26 Investigation Person Email
27 Investigation Person Phone
28 Investigation Person Fax
29 Investigation Person Address
30 Investigation Person Affiliation
31 Investigation Person Roles
32 Investigation Person Roles Term Accession Number
33 Investigation Person Roles Term Source REF
34 STUDY
35 Study Identifier
36 Study Title
37 Study Description
38 Study Submission Date
39 Study Public Release Date
40 Study File Name
41 STUDY DESIGN DESCRIPTORS
42 Study Design Type
43 Study Design Type Term Accession Number
44 Study Design Type Term Source REF
45 STUDY PUBLICATIONS
46 Study PubMed ID
47 Study Publication DOI
48 Study Publication Author List
49 Study Publication Title
50 Study Publication Status
51 Study Publication Status Term Accession Number
52 Study Publication Status Term Source REF
53 STUDY FACTORS
54 Study Factor Name
55 Study Factor Type
56 Study Factor Type Term Accession Number
57 Study Factor Type Term Source REF
58 STUDY ASSAYS
59 Study Assay Measurement Type
60 Study Assay Measurement Type Term Source REF
61 Study Assay Measurement Type Term Accession Number

62 Study Assay Technology Type
63 Study Assay Technology Type Term Source REF
64 Study Assay Technology Type Term Accession Number
65 Study Assay Technology Platform
66 Study Assay File Name
67 STUDY PROTOCOLS
68 Study Protocol Name
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70 Study Protocol Type Term Accession Number
71 Study Protocol Type Term Source REF
72 Study Protocol Description
73 Study Protocol URI
74 Study Protocol Version
75 Study Protocol Parameters Name
76 Study Protocol Parameters Name Term Accession Number
77 Study Protocol Parameters Name Term Source REF
78 Study Protocol Components Name
79 Study Protocol Components Type
80 Study Protocol Components Type Term Accession Number
81 Study Protocol Components Type Term Source REF
82 STUDY CONTACTS
83 Study Person Last Name
84 Study Person First Name
85 Study Person Mid Initials
86 Study Person Email
87 Study Person Phone
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The analysis of the resulting total ion chromatogram was performed manually by gen

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Phenotypic qualities (properties) ArrayExpress Experimental Factor Ontology

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Slot "investigation.identifier":
[1] ""

Slot "study.identifiers":
[1] "Global metabolite profiling of faah(-/-) mice"

Slot "study.titles":
[1] "Global metabolite profiling of faah(-/-) mice"

Slot "study.descriptions":
[1] "Enzymes regulate biological processes through the conversion of specific substrates"

Slot "study.contacts":
[1] " "

Slot "study.contacts.affiliations":
[1] ""

Slot "study_filenames":
Global metabolite profiling of faah(-/-) mice
"s_Proteomic_profiling_of_yeast_TFs.txt"

Slot "study.files":
\$`Global metabolite profiling of faah(-/-) mice`

	Source Name	Characteristics[NEWT:Organism LC]	Term	Source	REF
1	Saghantelian_1	Mus musculus (Mouse)			NEWT
2	Saghantelian_2	Mus musculus (Mouse)			NEWT
3	Saghantelian_3	Mus musculus (Mouse)			NEWT
4	Saghantelian_4	Mus musculus (Mouse)			NEWT
5	Saghantelian_5	Mus musculus (Mouse)			NEWT
6	Saghantelian_6	Mus musculus (Mouse)			NEWT
7	Saghantelian_7	Mus musculus (Mouse)			NEWT
8	Saghantelian_8	Mus musculus (Mouse)			NEWT
9	Saghantelian_9	Mus musculus (Mouse)			NEWT
10	Saghantelian_10	Mus musculus (Mouse)			NEWT
11	Saghantelian_11	Mus musculus (Mouse)			NEWT
12	Saghantelian_12	Mus musculus (Mouse)			NEWT

	Term	Accession Number	Characteristics[tissue]	Term	Source	REF
1		10090	spinal cord			MA
2		10090	spinal cord			MA
3		10090	spinal cord			MA
4		10090	spinal cord			MA
5		10090	spinal cord			MA
6		10090	spinal cord			MA
7		10090	spinal cord			MA
8		10090	spinal cord			MA
9		10090	spinal cord			MA
10		10090	spinal cord			MA
11		10090	spinal cord			MA
12		10090	spinal cord			MA

Term Accession Number Protocol REF Sample Name Factor Value[Genotype]

1	216 sample collection	KO1	KO
2	216 sample collection	KO2	KO
3	216 sample collection	KO3	KO
4	216 sample collection	KO4	KO
5	216 sample collection	KO5	KO
6	216 sample collection	KO6	KO
7	216 sample collection	WT1	WT
8	216 sample collection	WT2	WT
9	216 sample collection	WT3	WT
10	216 sample collection	WT4	WT
11	216 sample collection	WT5	WT
12	216 sample collection	WT6	WT

Term	Source	REF	Term	Accession	Number
1		NA			NA
2		NA			NA
3		NA			NA
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6		NA			NA
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11		NA			NA
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```
Slot "assay.fileNames":
  V2
  "a_metabolite.txt"
```

```
Slot "assay.fileNames.per.study":
$`Global metabolite profiling of faah(-/-) mice`
$`Global metabolite profiling of faah(-/-) mice`[[1]]
[1] "a_metabolite.txt"
```

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Slot "assay.files":
$a_metabolite.txt
```

Sample	Name	Protocol	REF	Extract	Name	Protocol	REF	Labeled	Extract	Name
1	KO1	extraction		KO1	labeling					NA
2	KO2	extraction		KO2	labeling					NA
3	KO3	extraction		KO3	labeling					NA
4	KO4	extraction		KO4	labeling					NA
5	KO5	extraction		KO5	labeling					NA
6	KO6	extraction		KO6	labeling					NA
7	WT1	extraction		WT1	labeling					NA
8	WT2	extraction		WT2	labeling					NA
9	WT3	extraction		WT3	labeling					NA
10	WT4	extraction		WT4	labeling					NA
11	WT5	extraction		WT5	labeling					NA
12	WT6	extraction		WT6	labeling					NA

Label Term Source REF Term Accession Number Protocol REF

1	NA		NA		NA	mass spectrometry
2	NA		NA		NA	mass spectrometry
3	NA		NA		NA	mass spectrometry
4	NA		NA		NA	mass spectrometry
5	NA		NA		NA	mass spectrometry
6	NA		NA		NA	mass spectrometry
7	NA		NA		NA	mass spectrometry
8	NA		NA		NA	mass spectrometry
9	NA		NA		NA	mass spectrometry
10	NA		NA		NA	mass spectrometry
11	NA		NA		NA	mass spectrometry
12	NA		NA		NA	mass spectrometry
	Parameter Value[instrument]	Term	Source	REF	Term	Accession Number
1	Agilent 1100 LC-MSD SL			NA		NA
2	Agilent 1100 LC-MSD SL			NA		NA
3	Agilent 1100 LC-MSD SL			NA		NA
4	Agilent 1100 LC-MSD SL			NA		NA
5	Agilent 1100 LC-MSD SL			NA		NA
6	Agilent 1100 LC-MSD SL			NA		NA
7	Agilent 1100 LC-MSD SL			NA		NA
8	Agilent 1100 LC-MSD SL			NA		NA
9	Agilent 1100 LC-MSD SL			NA		NA
10	Agilent 1100 LC-MSD SL			NA		NA
11	Agilent 1100 LC-MSD SL			NA		NA
12	Agilent 1100 LC-MSD SL			NA		NA
	Parameter Value[ion source]	Term	Source	REF	Term	Accession Number
1	electrospray ionization			MS		1000073
2	electrospray ionization			MS		1000073
3	electrospray ionization			MS		1000073
4	electrospray ionization			MS		1000073
5	electrospray ionization			MS		1000073
6	electrospray ionization			MS		1000073
7	electrospray ionization			MS		1000073
8	electrospray ionization			MS		1000073
9	electrospray ionization			MS		1000073
10	electrospray ionization			MS		1000073
11	electrospray ionization			MS		1000073
12	electrospray ionization			MS		1000073
	Parameter Value[detector]	Term	Source	REF	Term	Accession Number
1				NA		NA
2				NA		NA
3				NA		NA
4				NA		NA
5				NA		NA
6				NA		NA
7				NA		NA
8				NA		NA
9				NA		NA
10				NA		NA
11				NA		NA
12				NA		NA
	Parameter Value[ionization mode]	Term	Source	REF	Term	Accession Number
1		positive mode		NA		NA
2		positive mode		NA		NA

3	positive mode	NA	NA
4	positive mode	NA	NA
5	positive mode	NA	NA
6	positive mode	NA	NA
7	positive mode	NA	NA
8	positive mode	NA	NA
9	positive mode	NA	NA
10	positive mode	NA	NA
11	positive mode	NA	NA
12	positive mode	NA	NA

	MS Assay Name	Raw Spectral Data File	Protocol	REF	Normalization	Name
1	lc-ms-1	./cdf/KO/ko15.CDF		NA		NA
2	lc-ms-2	./cdf/KO/ko16.CDF		NA		NA
3	lc-ms-3	./cdf/KO/ko18.CDF		NA		NA
4	lc-ms-4	./cdf/KO/ko19.CDF		NA		NA
5	lc-ms-5	./cdf/KO/ko21.CDF		NA		NA
6	lc-ms-6	./cdf/KO/ko22.CDF		NA		NA
7	lc-ms-7	./cdf/WT/wt15.CDF		NA		NA
8	lc-ms-8	./cdf/WT/wt16.CDF		NA		NA
9	lc-ms-9	./cdf/WT/wt18.CDF		NA		NA
10	lc-ms-10	./cdf/WT/wt19.CDF		NA		NA
11	lc-ms-11	./cdf/WT/wt21.CDF		NA		NA
12	lc-ms-12	./cdf/WT/wt22.CDF		NA		NA

	Data Transformation Name	Derived Spectral Data File	Factor Value[Genotype]
1	NA	faahkoDSDF.txt	KO
2	NA	faahkoDSDF.txt	KO
3	NA	faahkoDSDF.txt	KO
4	NA	faahkoDSDF.txt	KO
5	NA	faahkoDSDF.txt	KO
6	NA	faahkoDSDF.txt	KO
7	NA	faahkoDSDF.txt	WT
8	NA	faahkoDSDF.txt	WT
9	NA	faahkoDSDF.txt	WT
10	NA	faahkoDSDF.txt	WT
11	NA	faahkoDSDF.txt	WT
12	NA	faahkoDSDF.txt	WT

	Term Source	REF	Term Accession Number
1		NA	NA
2		NA	NA
3		NA	NA
4		NA	NA
5		NA	NA
6		NA	NA
7		NA	NA
8		NA	NA
9		NA	NA
10		NA	NA
11		NA	NA
12		NA	NA

```
Slot "assay.files.per.study":
$`Global metabolite profiling of faah(-/-) mice`
$`Global metabolite profiling of faah(-/-) mice`[[1]]
```

	Sample Name	Protocol	REF	Extract Name	Protocol	REF	Labeled Extract Name
1	K01	extraction		K01	labeling		NA
2	K02	extraction		K02	labeling		NA
3	K03	extraction		K03	labeling		NA
4	K04	extraction		K04	labeling		NA
5	K05	extraction		K05	labeling		NA
6	K06	extraction		K06	labeling		NA
7	WT1	extraction		WT1	labeling		NA
8	WT2	extraction		WT2	labeling		NA
9	WT3	extraction		WT3	labeling		NA
10	WT4	extraction		WT4	labeling		NA
11	WT5	extraction		WT5	labeling		NA
12	WT6	extraction		WT6	labeling		NA

	Label	Term	Source	REF	Term	Accession Number	Protocol	REF
1	NA			NA		NA	mass spectrometry	
2	NA			NA		NA	mass spectrometry	
3	NA			NA		NA	mass spectrometry	
4	NA			NA		NA	mass spectrometry	
5	NA			NA		NA	mass spectrometry	
6	NA			NA		NA	mass spectrometry	
7	NA			NA		NA	mass spectrometry	
8	NA			NA		NA	mass spectrometry	
9	NA			NA		NA	mass spectrometry	
10	NA			NA		NA	mass spectrometry	
11	NA			NA		NA	mass spectrometry	
12	NA			NA		NA	mass spectrometry	

	Parameter Value[instrument]	Term	Source	REF	Term	Accession Number
1	Agilent 1100	LC-MSD	SL	NA		NA
2	Agilent 1100	LC-MSD	SL	NA		NA
3	Agilent 1100	LC-MSD	SL	NA		NA
4	Agilent 1100	LC-MSD	SL	NA		NA
5	Agilent 1100	LC-MSD	SL	NA		NA
6	Agilent 1100	LC-MSD	SL	NA		NA
7	Agilent 1100	LC-MSD	SL	NA		NA
8	Agilent 1100	LC-MSD	SL	NA		NA
9	Agilent 1100	LC-MSD	SL	NA		NA
10	Agilent 1100	LC-MSD	SL	NA		NA
11	Agilent 1100	LC-MSD	SL	NA		NA
12	Agilent 1100	LC-MSD	SL	NA		NA

	Parameter Value[ion source]	Term	Source	REF	Term	Accession Number
1	electrospray	ionization		MS		1000073
2	electrospray	ionization		MS		1000073
3	electrospray	ionization		MS		1000073
4	electrospray	ionization		MS		1000073
5	electrospray	ionization		MS		1000073
6	electrospray	ionization		MS		1000073
7	electrospray	ionization		MS		1000073
8	electrospray	ionization		MS		1000073
9	electrospray	ionization		MS		1000073
10	electrospray	ionization		MS		1000073
11	electrospray	ionization		MS		1000073
12	electrospray	ionization		MS		1000073

	Parameter Value[detector]	Term	Source	REF	Term	Accession Number
1			NA		NA	NA

2	NA	NA	NA
3	NA	NA	NA
4	NA	NA	NA
5	NA	NA	NA
6	NA	NA	NA
7	NA	NA	NA
8	NA	NA	NA
9	NA	NA	NA
10	NA	NA	NA
11	NA	NA	NA
12	NA	NA	NA

	Parameter Value	[ionization mode]	Term	Source	REF	Term	Accession	Number
1		positive mode			NA			NA
2		positive mode			NA			NA
3		positive mode			NA			NA
4		positive mode			NA			NA
5		positive mode			NA			NA
6		positive mode			NA			NA
7		positive mode			NA			NA
8		positive mode			NA			NA
9		positive mode			NA			NA
10		positive mode			NA			NA
11		positive mode			NA			NA
12		positive mode			NA			NA

	MS Assay Name	Raw	Spectral Data File	Protocol	REF	Normalization	Name
1	lc-ms-1		./cdf/KO/ko15.CDF		NA		NA
2	lc-ms-2		./cdf/KO/ko16.CDF		NA		NA
3	lc-ms-3		./cdf/KO/ko18.CDF		NA		NA
4	lc-ms-4		./cdf/KO/ko19.CDF		NA		NA
5	lc-ms-5		./cdf/KO/ko21.CDF		NA		NA
6	lc-ms-6		./cdf/KO/ko22.CDF		NA		NA
7	lc-ms-7		./cdf/WT/wt15.CDF		NA		NA
8	lc-ms-8		./cdf/WT/wt16.CDF		NA		NA
9	lc-ms-9		./cdf/WT/wt18.CDF		NA		NA
10	lc-ms-10		./cdf/WT/wt19.CDF		NA		NA
11	lc-ms-11		./cdf/WT/wt21.CDF		NA		NA
12	lc-ms-12		./cdf/WT/wt22.CDF		NA		NA

	Data Transformation Name	Derived	Spectral Data File	Factor	Value	[Genotype]
1		NA		NA		KO
2		NA		NA		KO
3		NA		NA		KO
4		NA		NA		KO
5		NA		NA		KO
6		NA		NA		KO
7		NA		NA		WT
8		NA		NA		WT
9		NA		NA		WT
10		NA		NA		WT
11		NA		NA		WT
12		NA		NA		WT

	Term	Source	REF	Term	Accession	Number
1			NA		NA	
2			NA		NA	
3			NA		NA	

4	NA	NA
5	NA	NA
6	NA	NA
7	NA	NA
8	NA	NA
9	NA	NA
10	NA	NA
11	NA	NA
12	NA	NA

Slot "assay.names":

\$a_metabolite.txt

	MS Assay Name
1	lc-ms-1
2	lc-ms-2
3	lc-ms-3
4	lc-ms-4
5	lc-ms-5
6	lc-ms-6
7	lc-ms-7
8	lc-ms-8
9	lc-ms-9
10	lc-ms-10
11	lc-ms-11
12	lc-ms-12

Slot "assay.technology.types":

[1] "mass spectrometry"

Slot "assay.measurement.types":

[1] "metabolite profiling"

Slot "data.filenames":

\$a_metabolite.txt

	Raw Spectral Data File	Derived Spectral Data File
1	./cdf/KO/ko15.CDF	faahkoDSDF.txt
2	./cdf/KO/ko16.CDF	faahkoDSDF.txt
3	./cdf/KO/ko18.CDF	faahkoDSDF.txt
4	./cdf/KO/ko19.CDF	faahkoDSDF.txt
5	./cdf/KO/ko21.CDF	faahkoDSDF.txt
6	./cdf/KO/ko22.CDF	faahkoDSDF.txt
7	./cdf/WT/wt15.CDF	faahkoDSDF.txt
8	./cdf/WT/wt16.CDF	faahkoDSDF.txt
9	./cdf/WT/wt18.CDF	faahkoDSDF.txt
10	./cdf/WT/wt19.CDF	faahkoDSDF.txt
11	./cdf/WT/wt21.CDF	faahkoDSDF.txt
12	./cdf/WT/wt22.CDF	faahkoDSDF.txt

Slot "samples":

[1] "K01" "K02" "K03" "K04" "K05" "K06" "WT1" "WT2" "WT3" "WT4" "WT5" "WT6"

```
Slot "samples.per.study":
$`Global metabolite profiling of faah(-/-) mice`
 [1] "K01" "K02" "K03" "K04" "K05" "K06" "WT1" "WT2" "WT3" "WT4" "WT5" "WT6"
```

```
Slot "samples.per.assay.filename":
$a_metabolite.txt
 [1] "K01" "K02" "K03" "K04" "K05" "K06" "WT1" "WT2" "WT3" "WT4" "WT5" "WT6"
```

```
Slot "assay.filenames.per.sample":
[[1]]
[[1]][[1]]
[1] "a_metabolite.txt"
```

```
[[2]]
[[2]][[1]]
[1] "a_metabolite.txt"
```

```
[[3]]
[[3]][[1]]
[1] "a_metabolite.txt"
```

```
[[4]]
[[4]][[1]]
[1] "a_metabolite.txt"
```

```
[[5]]
[[5]][[1]]
[1] "a_metabolite.txt"
```

```
[[6]]
[[6]][[1]]
[1] "a_metabolite.txt"
```

```
[[7]]
[[7]][[1]]
[1] "a_metabolite.txt"
```

```
[[8]]
[[8]][[1]]
[1] "a_metabolite.txt"
```

```
[[9]]
[[9]][[1]]
```



```
[1] "a_metabolite.txt"
```

```
[[10]]
```

```
[[10]][[1]]
```

```
[1] "a_metabolite.txt"
```

```
[[11]]
```

```
[[11]][[1]]
```

```
[1] "a_metabolite.txt"
```

```
[[12]]
```

```
[[12]][[1]]
```

```
[1] "a_metabolite.txt"
```

```
Slot "sample.to.rawdatafile":
```

```
[[1]]
```

	Sample Name	Raw Spectral Data File
1	KO1	./cdf/KO/ko15.CDF
2	KO2	./cdf/KO/ko16.CDF
3	KO3	./cdf/KO/ko18.CDF
4	KO4	./cdf/KO/ko19.CDF
5	KO5	./cdf/KO/ko21.CDF
6	KO6	./cdf/KO/ko22.CDF
7	WT1	./cdf/WT/wt15.CDF
8	WT2	./cdf/WT/wt16.CDF
9	WT3	./cdf/WT/wt18.CDF
10	WT4	./cdf/WT/wt19.CDF
11	WT5	./cdf/WT/wt21.CDF
12	WT6	./cdf/WT/wt22.CDF

```
Slot "sample.to.assayname":
```

```
[[1]]
```

	Sample Name	MS Assay Name
1	KO1	lc-ms-1
2	KO2	lc-ms-2
3	KO3	lc-ms-3
4	KO4	lc-ms-4
5	KO5	lc-ms-5
6	KO6	lc-ms-6
7	WT1	lc-ms-7
8	WT2	lc-ms-8
9	WT3	lc-ms-9
10	WT4	lc-ms-10
11	WT5	lc-ms-11
12	WT6	lc-ms-12

```
Slot "rawdatafile.to.sample":
```

```
[[1]]
  Raw Spectral Data File Sample Name
1      ./cdf/KO/ko15.CDF      KO1
2      ./cdf/KO/ko16.CDF      KO2
3      ./cdf/KO/ko18.CDF      KO3
4      ./cdf/KO/ko19.CDF      KO4
5      ./cdf/KO/ko21.CDF      KO5
6      ./cdf/KO/ko22.CDF      KO6
7      ./cdf/WT/wt15.CDF      WT1
8      ./cdf/WT/wt16.CDF      WT2
9      ./cdf/WT/wt18.CDF      WT3
10     ./cdf/WT/wt19.CDF      WT4
11     ./cdf/WT/wt21.CDF      WT5
12     ./cdf/WT/wt22.CDF      WT6
```

Slot "assayname.to.sample":

```
[[1]]
  MS Assay Name Sample Name
1      lc-ms-1      KO1
2      lc-ms-10     WT4
3      lc-ms-11     WT5
4      lc-ms-12     WT6
5      lc-ms-2      KO2
6      lc-ms-3      KO3
7      lc-ms-4      KO4
8      lc-ms-5      KO5
9      lc-ms-6      KO6
10     lc-ms-7      WT1
11     lc-ms-8      WT2
12     lc-ms-9      WT3
```

Slot "factors":

```
[[1]]
[[1]]$`Factor Value[Genotype]`
 [1] KO KO KO KO KO KO WT WT WT WT WT WT
Levels: KO WT
```

Slot "treatments":

```
$`Factor Value[Genotype]`
 [1] KO WT
Levels: KO WT
```

Slot "groups":

```
[[1]]
[[1]][[1]]
 [1] "KO1" "KO2" "KO3" "KO4" "KO5" "KO6"

[[1]][[2]]
 [1] "WT1" "WT2" "WT3" "WT4" "WT5" "WT6"
```

```

Slot "assay.tabs":
[[1]]
An object of class "MSAssayTab"
Slot "path":
[1] "/github/workspace/pkglib/faahKO"

Slot "study.filename":
[1] "s_Proteomic_profiling_of_yeast_TFs.txt"

Slot "study.identifier":
[1] "Global metabolite profiling of faah(-/-) mice"

Slot "assay.filename":
[1] "a_metabolite.txt"

```

```

Slot "assay.file":
  Sample Name Protocol REF Extract Name Protocol REF Labeled Extract Name
1          KO1  extraction          KO1  labeling          NA
2          KO2  extraction          KO2  labeling          NA
3          KO3  extraction          KO3  labeling          NA
4          KO4  extraction          KO4  labeling          NA
5          KO5  extraction          KO5  labeling          NA
6          KO6  extraction          KO6  labeling          NA
7          WT1  extraction          WT1  labeling          NA
8          WT2  extraction          WT2  labeling          NA
9          WT3  extraction          WT3  labeling          NA
10         WT4  extraction          WT4  labeling          NA
11         WT5  extraction          WT5  labeling          NA
12         WT6  extraction          WT6  labeling          NA

  Label Term Source REF Term Accession Number Protocol REF
1      NA      NA      NA      NA mass spectrometry
2      NA      NA      NA      NA mass spectrometry
3      NA      NA      NA      NA mass spectrometry
4      NA      NA      NA      NA mass spectrometry
5      NA      NA      NA      NA mass spectrometry
6      NA      NA      NA      NA mass spectrometry
7      NA      NA      NA      NA mass spectrometry
8      NA      NA      NA      NA mass spectrometry
9      NA      NA      NA      NA mass spectrometry
10     NA      NA      NA      NA mass spectrometry
11     NA      NA      NA      NA mass spectrometry
12     NA      NA      NA      NA mass spectrometry

  Parameter Value[instrument] Term Source REF Term Accession Number
1      Agilent 1100 LC-MSD SL      NA      NA
2      Agilent 1100 LC-MSD SL      NA      NA
3      Agilent 1100 LC-MSD SL      NA      NA
4      Agilent 1100 LC-MSD SL      NA      NA
5      Agilent 1100 LC-MSD SL      NA      NA
6      Agilent 1100 LC-MSD SL      NA      NA
7      Agilent 1100 LC-MSD SL      NA      NA
8      Agilent 1100 LC-MSD SL      NA      NA

```

9	Agilent 1100 LC-MSD SL			NA	NA
10	Agilent 1100 LC-MSD SL			NA	NA
11	Agilent 1100 LC-MSD SL			NA	NA
12	Agilent 1100 LC-MSD SL			NA	NA

	Parameter Value	[ion source]	Term	Source	REF	Term	Accession	Number
1	electrospray	ionization			MS		1000073	
2	electrospray	ionization			MS		1000073	
3	electrospray	ionization			MS		1000073	
4	electrospray	ionization			MS		1000073	
5	electrospray	ionization			MS		1000073	
6	electrospray	ionization			MS		1000073	
7	electrospray	ionization			MS		1000073	
8	electrospray	ionization			MS		1000073	
9	electrospray	ionization			MS		1000073	
10	electrospray	ionization			MS		1000073	
11	electrospray	ionization			MS		1000073	
12	electrospray	ionization			MS		1000073	

	Parameter Value	[detector]	Term	Source	REF	Term	Accession	Number
1		NA			NA		NA	
2		NA			NA		NA	
3		NA			NA		NA	
4		NA			NA		NA	
5		NA			NA		NA	
6		NA			NA		NA	
7		NA			NA		NA	
8		NA			NA		NA	
9		NA			NA		NA	
10		NA			NA		NA	
11		NA			NA		NA	
12		NA			NA		NA	

	Parameter Value	[ionization mode]	Term	Source	REF	Term	Accession	Number
1		positive mode			NA		NA	
2		positive mode			NA		NA	
3		positive mode			NA		NA	
4		positive mode			NA		NA	
5		positive mode			NA		NA	
6		positive mode			NA		NA	
7		positive mode			NA		NA	
8		positive mode			NA		NA	
9		positive mode			NA		NA	
10		positive mode			NA		NA	
11		positive mode			NA		NA	
12		positive mode			NA		NA	

	MS Assay Name	Raw	Spectral Data File	Protocol	REF	Normalization	Name
1	lc-ms-1		./cdf/KO/ko15.CDF		NA		NA
2	lc-ms-2		./cdf/KO/ko16.CDF		NA		NA
3	lc-ms-3		./cdf/KO/ko18.CDF		NA		NA
4	lc-ms-4		./cdf/KO/ko19.CDF		NA		NA
5	lc-ms-5		./cdf/KO/ko21.CDF		NA		NA
6	lc-ms-6		./cdf/KO/ko22.CDF		NA		NA
7	lc-ms-7		./cdf/WT/wt15.CDF		NA		NA
8	lc-ms-8		./cdf/WT/wt16.CDF		NA		NA
9	lc-ms-9		./cdf/WT/wt18.CDF		NA		NA
10	lc-ms-10		./cdf/WT/wt19.CDF		NA		NA

11	lc-ms-11	./cdf/WT/wt21.CDF	NA	NA
12	lc-ms-12	./cdf/WT/wt22.CDF	NA	NA
	Data Transformation Name	Derived Spectral Data File	Factor Value	[Genotype]
1		NA	NA	KO
2		NA	NA	KO
3		NA	NA	KO
4		NA	NA	KO
5		NA	NA	KO
6		NA	NA	KO
7		NA	NA	WT
8		NA	NA	WT
9		NA	NA	WT
10		NA	NA	WT
11		NA	NA	WT
12		NA	NA	WT

	Term Source REF	Term Accession Number
1	NA	NA
2	NA	NA
3	NA	NA
4	NA	NA
5	NA	NA
6	NA	NA
7	NA	NA
8	NA	NA
9	NA	NA
10	NA	NA
11	NA	NA
12	NA	NA

Slot "assay.technology.type":
[1] "mass spectrometry"

Slot "assay.measurement.type":
[1] "metabolite profiling"

Slot "assay.names":

	MS Assay Name
1	lc-ms-1
2	lc-ms-2
3	lc-ms-3
4	lc-ms-4
5	lc-ms-5
6	lc-ms-6
7	lc-ms-7
8	lc-ms-8
9	lc-ms-9
10	lc-ms-10
11	lc-ms-11
12	lc-ms-12

Slot "data_filenames":

	Raw Spectral Data File	Derived Spectral Data File
1	./cdf/KO/ko15.CDF	NA
2	./cdf/KO/ko16.CDF	NA

```

3      ./cdf/KO/ko18.CDF      NA
4      ./cdf/KO/ko19.CDF      NA
5      ./cdf/KO/ko21.CDF      NA
6      ./cdf/KO/ko22.CDF      NA
7      ./cdf/WT/wt15.CDF      NA
8      ./cdf/WT/wt16.CDF      NA
9      ./cdf/WT/wt18.CDF      NA
10     ./cdf/WT/wt19.CDF      NA
11     ./cdf/WT/wt21.CDF      NA
12     ./cdf/WT/wt22.CDF      NA

```

For an example for a real use case, please refer to <https://github.com/sneumann/mtbls2/>.

Writing ISA-Tab datasets

The Risa package offers functions to write the whole ISA-Tab dataset or part of it back to disk. These functions are `write.ISAtab`, `write.investigation.file`, `write.study.file`, `write.assay.file`.

So, after updating the assay file as indicated above, we can save it back to disk, using the following command:

```

> temp = tempdir()
> write.ISAtab(faahkoISA, temp)
> #write.assay.file(faahkoISA, assay.filename, temp)

```

Session Info

```

> toLatex(sessionInfo())

```

- R version 4.4.1 (2024-06-14), x86_64-pc-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=en_US.UTF-8, LC_NAME=C, LC_ADDRESS=C, LC_TELEPHONE=C, LC_MEASUREMENT=en_US.UTF-8, LC_IDENTIFICATION=C
- Time zone: Etc/UTC
- TZcode source: system (glibc)
- Running under: Ubuntu 24.04 LTS
- Matrix products: default
- BLAS: /usr/lib/x86_64-linux-gnu/openblas-pthread/libblas.so.3
- LAPACK: /usr/lib/x86_64-linux-gnu/openblas-pthread/libopenblas-p-r0.3.26.so; LAPACK version3.12.0
- Base packages: base, datasets, grDevices, graphics, methods, stats, utils
- Other packages: Biobase 2.65.0, BiocGenerics 0.51.0, BiocParallel 1.39.0, Rcpp 1.0.12, Risa 1.47.0, affy 1.83.0, biocViews 1.73.0, faahKO 1.45.0, xcms 4.3.1

- Loaded via a namespace (and not attached): AnnotationFilter 1.29.0, BiocManager 1.30.23, DBI 1.2.3, DelayedArray 0.31.3, GenomeInfoDb 1.41.1, GenomeInfoDbData 1.2.12, GenomicRanges 1.57.1, IRanges 2.39.0, MALDIquant 1.22.2, MASS 7.3-61, MSnbase 2.31.1, MassSpecWavelet 1.71.0, Matrix 1.7-0, MatrixGenerics 1.17.0, MetaboCoreUtils 1.13.0, MsCoreUtils 1.17.0, MsExperiment 1.7.0, MsFeatures 1.13.0, MultiAssayExperiment 1.31.3, PSMATCH 1.9.0, ProtGenerics 1.37.0, QFeatures 1.15.1, R6 2.5.1, RBGL 1.81.0, RColorBrewer 1.1-3, RCurl 1.98-1.14, RUnit 0.4.33, S4Arrays 1.5.2, S4Vectors 0.43.0, SparseArray 1.5.10, Spectra 1.15.3, SummarizedExperiment 1.35.1, UCSC.utils 1.1.0, XML 3.99-0.17, XVector 0.45.0, abind 1.4-5, affyio 1.75.0, bitops 1.0-7, buildtools 1.0.0, cli 3.6.3, clue 0.3-65, cluster 2.1.6, codetools 0.2-20, colorspace 2.1-0, compiler 4.4.1, crayon 1.5.3, digest 0.6.36, doParallel 1.0.17, dplyr 1.1.4, fansi 1.0.6, foreach 1.5.2, fs 1.6.4, generics 0.1.3, ggplot2 3.5.1, glue 1.7.0, graph 1.83.0, grid 4.4.1, gtable 0.3.5, hms 1.1.3, httr 1.4.7, igraph 2.0.3, impute 1.79.0, iterators 1.0.14, jsonlite 1.8.8, knitr 1.47, lattice 0.22-6, lazyeval 0.2.2, lifecycle 1.0.4, limma 3.61.2, magrittr 2.0.3, maketools 1.3.0, matrixStats 1.3.0, munsell 0.5.1, mzID 1.43.0, mzR 2.39.0, ncd4 1.22, parallel 4.4.1, pcaMethods 1.97.0, pillar 1.9.0, pkgconfig 2.0.3, plyr 1.8.9, preprocessCore 1.67.0, prettyunits 1.2.0, progress 1.2.3, purrr 1.0.2, reshape2 1.4.4, rlang 1.1.4, scales 1.3.0, statmod 1.5.0, stats4 4.4.1, stringi 1.8.4, stringr 1.5.1, sys 3.4.2, tibble 3.2.1, tidyr 1.3.1, tidyselect 1.2.1, tools 4.4.1, utf8 1.2.4, vctrs 0.6.5, vsn 3.73.0, xfun 0.45, zlibbioc 1.51.1

Further information

For further information about the ISA software infrastructure, please visit our website <http://isa-tools.org>.