

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(path = find.package("faahKO"))
```

The object `faahkoISA` 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(isa = faahkoISA,
+                                 assay.filename = 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(isa = faahkoISA,
+                     assay.filename = assay.filename,
+                     col.name = "Derived Spectral Data File",
+                     values = "faahkoDSDF.txt" )
```

An object of class "ISATab"

Slot "path":

```
[1] "/home/verou004/R/x86_64-pc-linux-gnu-library/3.4/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
 69 Study Protocol Type
 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
 88 Study Person Fax
 89 Study Person Address
 90 Study Person Affiliation
 91 Study Person Roles
 92 Study Person Roles Term Accession Number
 93 Study Person Roles Term Source REF

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37 Enzymes regulate biological processes through the conversion of specific substrates to product

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LC-MS analysis was performed using an Agilent 1100 LC-MSD SL instrument. For the LC analysis,

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The analysis of the resulting total ion chromatogram was performed manually by generating extr

	V6	V7
1	<NA>	<NA>
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4	v 1.26	<NA>
5	Phenotypic qualities (properties) ArrayExpress Experimental Factor Ontology	
6	<NA>	<NA>
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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	K01 KO
2	216	sample collection	K02 KO
3	216	sample collection	K03 KO
4	216	sample collection	K04 KO
5	216	sample collection	K05 KO
6	216	sample collection	K06 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	
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.filenames":
[1] "a_metabolite.txt"

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

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

	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
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
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
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
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	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`\$a_metabolite.txt

	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.technology.types.per.study":

\$`Global metabolite profiling of faah(-/-) mice`

[1] "mass spectrometry"

Slot "assay.measurement.types":

[1] "metabolite profiling"

Slot "assay.measurement.types.per.study":

\$`Global metabolite profiling of faah(-/-) mice`

[1] "metabolite profiling"

Slot "data_filenames":

\$a_metabolite.txt

	Raw Spectral Data File	Derived Spectral Data File
1	./cdf/K0/ko15.CDF	faahkoDSDF.txt
2	./cdf/K0/ko16.CDF	faahkoDSDF.txt
3	./cdf/K0/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":

\$K01

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

\$K02

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

\$K03

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

\$K04

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

\$K05

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

\$K06

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

\$WT1

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

\$WT2

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

\$WT3

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

\$WT4

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



```
$WT5  
[1] "a_metabolite.txt"
```

```
$WT6  
[1] "a_metabolite.txt"
```

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

```
$a_metabolite.txt
```

	Sample Name	Raw Spectral Data File
1	K01	./cdf/K0/ko15.CDF
2	K02	./cdf/K0/ko16.CDF
3	K03	./cdf/K0/ko18.CDF
4	K04	./cdf/K0/ko19.CDF
5	K05	./cdf/K0/ko21.CDF
6	K06	./cdf/K0/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":
```

```
$a_metabolite.txt
```

	Sample Name	MS Assay Name
1	K01	lc-ms-1
2	K02	lc-ms-2
3	K03	lc-ms-3
4	K04	lc-ms-4
5	K05	lc-ms-5
6	K06	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":
```

```
$a_metabolite.txt
```

	Raw Spectral Data File	Sample Name
1	./cdf/K0/ko15.CDF	K01
2	./cdf/K0/ko16.CDF	K02
3	./cdf/K0/ko18.CDF	K03
4	./cdf/K0/ko19.CDF	K04
5	./cdf/K0/ko21.CDF	K05
6	./cdf/K0/ko22.CDF	K06
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":

\$a_metabolite.txt

	MS Assay Name	Sample Name
1	lc-ms-1	K01
2	lc-ms-10	WT4
3	lc-ms-11	WT5
4	lc-ms-12	WT6
5	lc-ms-2	K02
6	lc-ms-3	K03
7	lc-ms-4	K04
8	lc-ms-5	K05
9	lc-ms-6	K06
10	lc-ms-7	WT1
11	lc-ms-8	WT2
12	lc-ms-9	WT3

Slot "factors":

\$`Global metabolite profiling of faah(-/-) mice`

\$`Global metabolite profiling of faah(-/-) mice`\$`Factor Value[Genotype]`

[1] KO KO KO KO KO KO WT WT WT WT WT WT

Levels: KO WT

Slot "treatments":

\$`Global metabolite profiling of faah(-/-) mice`

[1] KO WT

Levels: KO WT

Slot "groups":

\$`Global metabolite profiling of faah(-/-) mice`

\$`Global metabolite profiling of faah(-/-) mice`[[1]]

[1] "K01" "K02" "K03" "K04" "K05" "K06"

\$`Global metabolite profiling of faah(-/-) mice`[[2]]

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

Slot "assay.tabs":

[[1]]

An object of class "MSAssayTab"

Slot "path":

[1] "/home/verou004/R/x86_64-pc-linux-gnu-library/3.4/faahKO"

Slot "study.filename":

Global metabolite profiling of faah(-/-) mice

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

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

	MS Assay Name	Raw Spectral Data File	Protocol	REF	Normalization Name
1	lc-ms-1	./cdf/KO/ko15.CDF	NA	NA	NA
2	lc-ms-2	./cdf/KO/ko16.CDF	NA	NA	NA
3	lc-ms-3	./cdf/KO/ko18.CDF	NA	NA	NA
4	lc-ms-4	./cdf/KO/ko19.CDF	NA	NA	NA
5	lc-ms-5	./cdf/KO/ko21.CDF	NA	NA	NA
6	lc-ms-6	./cdf/KO/ko22.CDF	NA	NA	NA
7	lc-ms-7	./cdf/WT/wt15.CDF	NA	NA	NA
8	lc-ms-8	./cdf/WT/wt16.CDF	NA	NA	NA
9	lc-ms-9	./cdf/WT/wt18.CDF	NA	NA	NA
10	lc-ms-10	./cdf/WT/wt19.CDF	NA	NA	NA
11	lc-ms-11	./cdf/WT/wt21.CDF	NA	NA	NA
12	lc-ms-12	./cdf/WT/wt22.CDF	NA	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(isa = faahkoISA,
+             path = temp)
> # write.assay.file(isa = faahkoISA,
> #                 assay.filename = assay.filename,
> #                 path = temp)
```

Session Info

- R version 3.4.4 (2018-03-15), x86_64-pc-linux-gnu
- Locale: LC_CTYPE=C, LC_NUMERIC=C, LC_TIME=C, LC_COLLATE=C, LC_MONETARY=C, LC_MESSAGES=en_US.UTF-8, LC_PAPER=nl_NL.UTF-8, LC_NAME=C, LC_ADDRESS=C, LC_TELEPHONE=C, LC_MEASUREMENT=nl_NL.UTF-8, LC_IDENTIFICATION=C
- Running under: Ubuntu 14.04.3 LTS
- Matrix products: default
- BLAS: /usr/lib/libblas/libblas.so.3.0
- LAPACK: /usr/lib/lapack/liblapack.so.3.0
- Base packages: base, datasets, grDevices, graphics, methods, parallel, stats, utils
- Other packages: Biobase 2.38.0, BiocGenerics 0.24.0, BiocParallel 1.12.0, MSnbase 2.4.2, ProtGenerics 1.10.0, Rcpp 0.12.17, Risa 1.23.0, affy 1.56.0, biocViews 1.46.0, faahKO 1.18.0, mzR 2.12.0, xcms 3.0.2
- Loaded via a namespace (and not attached): BiocInstaller 1.28.0, IRanges 2.12.0, MALDIquant 1.17, MASS 7.3-50, MassSpecWavelet 1.44.0, Matrix 1.2-14, R6 2.2.2, RANN 2.5.1, RBGL 1.54.0, RColorBrewer 1.1-2, RCurl 1.95-4.10, RUnit 0.4.32, S4Vectors 0.16.0, XML 3.98-1.11, affyio 1.48.0, assertthat 0.2.0, backports 1.1.2, bitops 1.0-6, codetools 0.2-15, colorspace 1.3-2, commonmark 1.5, compiler 3.4.4, crayon 1.3.4, desc 1.2.0, devtools 1.13.5, digest 0.6.15, doParallel 1.0.11, foreach 1.4.4, ggplot2 2.2.1, graph 1.56.0, grid 3.4.4, gtable 0.2.0, impute 1.52.0, iterators 1.0.9, lattice 0.20-35, lazyeval 0.2.1, limma 3.34.9, magrittr 1.5, memoise 1.1.0, multtest 2.34.0, munsell 0.5.0, mzID 1.16.0, pcaMethods 1.70.0, pillar 1.2.3, plyr 1.8.4, preprocessCore 1.40.0, rlang 0.2.1, roxygen2 6.0.1, rprojroot 1.3-2, rstudioapi 0.7, scales 0.5.0, splines 3.4.4, stats4 3.4.4, stringi 1.2.3, stringr 1.3.1, survival 2.42-3, tibble 1.4.2, tools 3.4.4, vsn 3.46.0, withr 2.1.2, xml2 1.2.0, zlibbioc 1.24.0

Further information

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