

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.

```
> library(Risa)
> library(xcms)
> library(CAMERA)
> library(faahKO)

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

The object `isaobject` 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`
- `sample.to.assayname`
- `rawdatafile.to.sample`
- `assayname.to.sample`

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` a boolean indicating to show messages for the different steps, if TRUE, or not to show them, if FALSE
- ... extra arguments that can be passed down to the `xcmsSet` function from the `xcms` package

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

ko15: 250:38 300:103 350:226 400:338 450:431 500:529 550:674 600:847
ko16: 250:43 300:128 350:275 400:394 450:500 500:637 550:835 600:1027
ko18: 250:25 300:93 350:227 400:337 450:411 500:498 550:640 600:758
ko19: 250:19 300:67 350:169 400:258 450:301 500:373 550:488 600:580
ko21: 250:24 300:60 350:166 400:254 450:315 500:391 550:501 600:582
ko22: 250:31 300:71 350:183 400:280 450:338 500:422 550:532 600:604
wt15: 250:41 300:105 350:212 400:319 450:416 500:533 550:684 600:838
wt16: 250:27 300:107 350:232 400:347 450:440 500:549 550:712 600:905
wt18: 250:24 300:87 350:200 400:293 450:351 500:426 550:548 600:661
wt19: 250:22 300:65 350:161 400:243 450:293 500:358 550:483 600:561
wt21: 250:28 300:69 350:157 400:229 450:282 500:364 550:493 600:592
wt22: 250:30 300:81 350:188 400:280 450:356 500:473 550:618 600:765
```

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 use the *xcms* and *CAMERA* packages and follow a typical workflow for the analysis of mass spectrometry in metabolomics. Finally, we will update the ISA-Tab dataset adding the result file into the "Metabolite Assignment File" column of the assay file.

```
> faahkoXset <- group(faahkoXset, minfrac=0.75, bw=2)

262 325 387 450 512 575

> retcor(faahkoXset, plottype="mdevden")
```

Retention Time Correction Groups: 43

```

> faahkoXset <- fillPeaks(faahkoXset)

ko15 ko16 ko18 ko19 ko21 ko22 wt15 wt16 wt18 wt19 wt21 wt22

> an <- xsAnnotate(faahkoXset,
+                 sample=seq(1,length(sampnames(faahkoXset))),
+                 nSlaves=2)

Run cleanParallel after processing to remove the spawned slave processes!

> an <- groupFWHM(an)

Start grouping after retention time.
Created 34 pseudospectra.

> an <- findIsotopes(an) # optional but recommended.

Generating peak matrix!
Run isotope peak annotation
% finished: 10 30 40 50 60 70 80 90 100
Found isotopes: 15

> an <- findAdducts(an,
+                 polarity="positive")

Generating peak matrix for peak annotation!

Calculating possible adducts in 34 Groups...
% finished: 10 30 40 50 60 70 80 90 100

> pl <- getPeaklist(an)
> l <- nrow(pl)
> charge <- sapply(an@isotopes, function(x) {ifelse( length(x) > 0, x$charge, NA) })
> abundance <- groupval(an@xcmsSet, value="into")
> maf <- data.frame(identifier = character(l),
+                 chemical_formula = character(l),
+                 description = character(l),
+                 mass_to_charge = pl$mz,
+                 fragmentation = character(l),
+                 charge = charge,
+                 retention_time = pl$rt,
+                 taxid = character(l),
+                 species = character(l),
+                 database = character(l),
+                 database_version = character(l),
+                 reliability = character(l),
+                 uri = character(l),
+                 search_engine = character(l),
+                 search_engine_score = character(l),
+                 modifications = character(l),
+                 smallmolecule_abundance_sub = character(l),
+                 smallmolecule_abundance_stdev_sub = character(l),
+                 smallmolecule_abundance_std_error_sub = character(l),
+                 abundance, stringsAsFactors=FALSE)
> maf_character <- apply(maf, 2, as.character)
> ##

```

```

> ## These columns are defined by mzTab
> ##
>
> maf.std.colnames <- c("identifier", "chemical_formula", "description",
+ "mass_to_charge", "fragmentation", "charge", "retention_time",
+ "taxid", "species", "database", "database_version", "reliability",
+ "uri", "search_engine", "search_engine_score", "modifications",
+ "smallmolecule_abundance_sub", "smallmolecule_abundance_stdev_sub",
+ "smallmolecule_abundance_std_error_sub")
> a.samples <- faahkoISA["samples.per.assay.filename"][[ assay.filename ]]
> ##
> ## Plus the columns for the sample intensities
> ##
> all.colnames <- c(maf.std.colnames, a.samples)
> write.table(maf_character, file="faahko_maf2.csv",
+             row.names=FALSE, col.names=all.colnames, quote=TRUE, sep="\t", na="\"")
> updateAssayMetadata(faahkoISA, assay.filename, "Metabolite Assignment File", "faahko_maf2.csv" )

```

An object of class "ISAtab"

Slot "path":

```
[1] "/Users/agbeltran/Library/R/2.15-bioc-release/library/faahK0"
```

Slot "investigation.filename":

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

Slot "investigation.file":

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

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A 2:1:1 CHCl₃/MeOH/1% NaCl solution (8 mL per brain and 4 mL per spinal cord in 8 mL vials) wa

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Slot "study.identifiers":

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

24 Levels: 10.1021/bi0480335 15533037 16/11/2004 1796 ... v 1.26

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			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
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11			NA			NA
12			NA			NA

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"

Slot "assay.files":

\$a_metabolite.txt

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

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.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	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

Slot "samples":

Global metabolite profiling of faah(-/-) mice1
"K01"

Global metabolite profiling of faah(-/-) mice2
"K02"

Global metabolite profiling of faah(-/-) mice3
"K03"

```

Global metabolite profiling of faah(-/-) mice4
      "K04"
Global metabolite profiling of faah(-/-) mice5
      "K05"
Global metabolite profiling of faah(-/-) mice6
      "K06"
Global metabolite profiling of faah(-/-) mice7
      "WT1"
Global metabolite profiling of faah(-/-) mice8
      "WT2"
Global metabolite profiling of faah(-/-) mice9
      "WT3"
Global metabolite profiling of faah(-/-) mice10
      "WT4"
Global metabolite profiling of faah(-/-) mice11
      "WT5"
Global metabolite profiling of faah(-/-) mice12
      "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.names.per.sample":
  [1] "a_metabolite.txt" "a_metabolite.txt" "a_metabolite.txt" "a_metabolite.txt"
  [5] "a_metabolite.txt" "a_metabolite.txt" "a_metabolite.txt" "a_metabolite.txt"
  [9] "a_metabolite.txt" "a_metabolite.txt" "a_metabolite.txt" "a_metabolite.txt"

Slot "sample.to.rawdatafile":
[[1]]
  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":
[[1]]
  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":

[[1]]

	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":

[[1]]

	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

For more details in a similar workflow, 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`.


```
> write.assay.file(faahkoISA, assay.filename)
```

Session Info

```
> toLatex(sessionInfo())
```

- R version 2.15.1 (2012-06-22), x86_64-apple-darwin9.8.0
- Locale: C/en_US.UTF-8/C/C/C/C
- Base packages: base, datasets, grDevices, graphics, methods, stats, utils
- Other packages: Biobase 2.16.0, BiocGenerics 0.2.0, CAMERA 1.12.0, Rcpp 0.9.13, Risa 0.99.1, faahKO 1.2.11, mzR 1.2.2, xcms 1.32.0
- Loaded via a namespace (and not attached): Hmisc 3.9-3, RBGL 1.32.1, cluster 1.14.2, codetools 0.2-8, graph 1.34.0, grid 2.15.1, igraph 0.6-2, lattice 0.20-10, tools 2.15.1

Further information

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