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 funcitonality to read ISA-Tab datasets, described in the following section.

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 ISArchive, using a standalone Java application named ISAcreator (http://isatab.sourceforge.net). In order to facilitate identification of ISA-Tab components in an ISArchive, 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 wiht 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.filenames"][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 Assingment 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
```

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```
> 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 <- groupCorr(an,
> #                graphMethod="lpc",
> #                calcIso = TRUE,
> #                calcCiS = TRUE,
> #                calcCaS = TRUE,
> #                cor_eic_th=0.5)
>
> 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(1),
+                    smallmolecule_abundance_sub = character(1),
+                    smallmolecule_abundance_stdev_sub = character(1),
+                    smallmolecule_abundance_std_error_sub = character(1),
+                    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/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
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```
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
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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
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77          Study Protocol Parameters Name Term Source REF
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81       Study Protocol Components Type Term Source REF
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84                              Study Person First Name
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86                                   Study Person Email
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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	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
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":
                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] "KO1" "KO2" "KO3" "KO4" "KO5" "KO6" "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          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
```

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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
                                           "KO1"
 Global metabolite profiling of faah(-/-) mice2
                                           "KO2"
 Global metabolite profiling of faah(-/-) mice3
                                           "KO3"
 Global metabolite profiling of faah(-/-) mice4
                                           "KO4"
 Global metabolite profiling of faah(-/-) mice5
                                           "KO5"
 Global metabolite profiling of faah(-/-) mice6
                                           "KO6"
 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] "KO1" "KO2" "KO3" "KO4" "KO5" "KO6" "WT1" "WT2" "WT3" "WT4" "WT5" "WT6"



Slot "samples.per.assay.filename":
$a_metabolite.txt
 [1] "KO1" "KO2" "KO3" "KO4" "KO5" "KO6" "WT1" "WT2" "WT3" "WT4" "WT5" "WT6"



Slot "assay.filenames.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          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
```

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://isatools.org.