

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 ISArchive, using a standalone Java application named ISAcreeator (<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. 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 `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(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] "F:/biocbuild/bbs-3.16-bioc/R/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
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

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

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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 |
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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]

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|----|-----------------------|-----|----|
| 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 |
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| 4 | | NA | | NA |
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| 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
```

| | 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 |
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| 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 |
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| 7 | electrospray ionization | | MS | 1000073 |
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| 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 |

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|----|---------------|----|----|
| 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 |
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| 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 | 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 | 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] "KO1" "KO2" "KO3" "KO4" "KO5" "KO6" "WT1" "WT2" "WT3" "WT4" "WT5" "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]]
[[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] "F:/biocbuild/bbs-3.16-bioc/R/library/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 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 | | KO |
| 2 | | NA | | KO |
| 3 | | NA | | KO |
| 4 | | NA | | KO |
| 5 | | NA | | KO |
| 6 | | NA | | KO |
| 7 | | NA | | WT |
| 8 | | NA | | WT |
| 9 | | NA | | WT |
| 10 | | NA | | WT |
| 11 | | NA | | WT |
| 12 | | 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 4.2.1 (2022-06-23 ucrt), x86_64-w64-mingw32
- Locale: LC_COLLATE=C, LC_CTYPE=English_United States.utf8, LC_MONETARY=English_United States.utf8, LC_NUMERIC=C, LC_TIME=English_United States.utf8
- Running under: Windows Server x64 (build 20348)
- Matrix products: default
- Base packages: base, datasets, grDevices, graphics, methods, stats, stats4, utils
- Other packages: Biobase 2.58.0, BiocGenerics 0.44.0, BiocParallel 1.32.0, MSnbase 2.24.0, ProtGenerics 1.30.0, Rcpp 1.0.9, Risa 1.40.0, S4Vectors 0.36.0, affy 1.76.0, biocViews 1.66.0, faahKO 1.37.0, mzR 2.32.0, xcms 3.20.0
- Loaded via a namespace (and not attached): BiocManager 1.30.19, DBI 1.1.3, DEoptimR 1.0-11, DelayedArray 0.24.0, GenomeInfoDb 1.34.0, GenomeInfoDbData 1.2.9, GenomicRanges 1.50.0, IRanges 2.32.0, MALDIquant 1.21, MASS 7.3-58.1, MassSpecWavelet 1.64.0, Matrix 1.5-1, MatrixGenerics 1.10.0, MsCoreUtils 1.10.0, MsFeatures 1.6.0, R6 2.5.1, RANN 2.6.1, RBGL 1.74.0, RColorBrewer 1.1-3, RCurl 1.98-1.9, RUnit 0.4.32, SummarizedExperiment 1.28.0, XML 3.99-0.12, XVector 0.38.0, affyio 1.68.0, assertthat 0.2.1, bitops 1.0-7, cli 3.4.1, clue 0.3-62, cluster 2.1.4, codetools 0.2-18, colorspace 2.0-3, compiler 4.2.1, digest 0.6.30, doParallel 1.0.17, dplyr 1.0.10, fansi 1.0.3, foreach 1.5.2, generics 0.1.3, ggplot2 3.3.6, glue 1.6.2, graph 1.76.0, grid 4.2.1, gtable 0.3.1, impute 1.72.0, iterators 1.0.14, lattice 0.20-45, lifecycle 1.0.3, limma 3.54.0, magrittr 2.0.3, matrixStats 0.62.0, munsell 0.5.0, mzID 1.36.0, ncd4 1.19, parallel 4.2.1, pcaMethods 1.90.0, pillar 1.8.1, pkgconfig 2.0.3, plyr 1.8.7, preprocessCore 1.60.0, rlang 1.0.6, robustbase 0.95-0, scales 1.2.1, snow 0.4-4, tibble 3.1.8, tidyselect 1.2.0, tools 4.2.1, utf8 1.2.2, vctrs 0.5.0, vsn 3.66.0, zlibbioc 1.44.0

Further information

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