

Risa: Building R objects from local ISA-Tab files

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November 6, 2019

1 Introduction

The Risa package is part of the ISA infrastructure software suite (<http://isa-tools.org>). It provides functionality to read ISA-Tab datasets, described in the following section. The source code and latest version can be found in the GitHub repository <https://github.com/ISA-tools/Risa>. Please, submit all 'bugs' and feature requests through <https://github.com/ISA-tools/Risa/issues>.

2 ISA-Tab format

The Investigation / Study / Assay (ISA) Tab-delimited (Tab) format is a general purpose framework with which to collect and communicate complex metadata (i.e. sample characteristics, technologies used, type of measurements made) from experiments employing a combination of technologies (<http://isa-tools.org>). In particular, ISA-Tab has been developed for - but not limited to - experiments using genomics, transcriptomics, proteomics or metabol/nomics techniques (the 'omics').

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

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

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

2.1 Investigation file

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

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

2.2 Study file

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

2.3 Assay file

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

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

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

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

3 The Risa package

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

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

3.1 Building an R object from a local ISA dataset

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

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

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

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

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

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

The object `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] "/Library/Frameworks/R.framework/Versions/4.0/Resources/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 |

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| 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 |
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| 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 |
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| 88 | Study Person Fax |
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| 90 | Study Person Affiliation |
| 91 | Study Person Roles |
| 92 | Study Person Roles Term Accession Number |
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37 Enzymes regulate biological processes through the conversion of specific substrates to product

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

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Phenotypic qualities (properties) ArrayExpress Experimental Factor Ontology

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

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

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

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

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 | |
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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 |
| 3 | | | NA | | | NA |
| 4 | | | NA | | | NA |
| 5 | | | NA | | | NA |
| 6 | | | NA | | | NA |
| 7 | | | 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 |
|-------|------|--------|-----|------|-----------|--------|----------|-----|
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|----|----|----|----------------------|
| 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 |

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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 |
| 8 | positive mode | NA | NA |
| 9 | positive mode | NA | NA |
| 10 | positive mode | NA | NA |
| 11 | positive mode | NA | NA |
| 12 | positive mode | NA | NA |

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Slot "assay.names":

\$a_metabolite.txt

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

Slot "assay.technology.types":

[1] "mass spectrometry"

Slot "assay.measurement.types":

[1] "metabolite profiling"

Slot "data.filenames":

\$a_metabolite.txt

| | Raw Spectral Data File | Derived Spectral Data File |
|----|------------------------|----------------------------|
| 1 | ./cdf/K0/ko15.CDF | faahkoDSDF.txt |
| 2 | ./cdf/K0/ko16.CDF | faahkoDSDF.txt |
| 3 | ./cdf/K0/ko18.CDF | faahkoDSDF.txt |
| 4 | ./cdf/K0/ko19.CDF | faahkoDSDF.txt |
| 5 | ./cdf/K0/ko21.CDF | faahkoDSDF.txt |
| 6 | ./cdf/K0/ko22.CDF | faahkoDSDF.txt |
| 7 | ./cdf/WT/WT15.CDF | faahkoDSDF.txt |
| 8 | ./cdf/WT/WT16.CDF | faahkoDSDF.txt |
| 9 | ./cdf/WT/WT18.CDF | faahkoDSDF.txt |
| 10 | ./cdf/WT/WT19.CDF | faahkoDSDF.txt |
| 11 | ./cdf/WT/WT21.CDF | faahkoDSDF.txt |
| 12 | ./cdf/WT/WT22.CDF | faahkoDSDF.txt |

Slot "samples":

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

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

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

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

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

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

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

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

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

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

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

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



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

```
[[10]]  
[[10]][[1]]  
[1] "a_metabolite.txt"
```

```
[[11]]  
[[11]][[1]]  
[1] "a_metabolite.txt"
```

```
[[12]]  
[[12]][[1]]  
[1] "a_metabolite.txt"
```

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

```
[[1]]  
  Sample Name Raw Spectral Data File  
1      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/KO/ko15.CDF      K01
2      ./cdf/KO/ko16.CDF      K02
3      ./cdf/KO/ko18.CDF      K03
4      ./cdf/KO/ko19.CDF      K04
5      ./cdf/KO/ko21.CDF      K05
6      ./cdf/KO/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
```

```
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] "K01" "K02" "K03" "K04" "K05" "K06"
```

```
[[1]][[2]]
```

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

```

Slot "assay.tabs":
[[1]]
An object of class "MSAssayTab"
Slot "path":
[1] "/Library/Frameworks/R.framework/Versions/4.0/Resources/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 Under development (unstable) (2019-11-03 r77362), x86_64-apple-darwin15.6.0
- Locale: C/en_US.UTF-8/en_US.UTF-8/C/en_US.UTF-8/en_US.UTF-8
- Running under: OS X El Capitan 10.11.6
- Matrix products: default
- BLAS:

/Library/Frameworks/R.framework/Versions/4.0/Resources/lib/libRblas.0.dylib
- LAPACK:

/Library/Frameworks/R.framework/Versions/4.0/Resources/lib/libRlapack.dylib
- Base packages: base, datasets, grDevices, graphics, methods, parallel, stats, stats4, utils
- Other packages: Biobase 2.47.0, BiocGenerics 0.33.0, BiocParallel 1.21.0, MSnbase 2.13.0, ProtGenerics 1.19.0, Rcpp 1.0.2, Risa 1.29.0, S4Vectors 0.25.0, affy 1.65.1, biocViews 1.55.1, faahKO 1.27.0, mzR 2.21.0, xcms 3.9.0
- Loaded via a namespace (and not attached): BiocManager 1.30.9, DEoptimR 1.0-8, IRanges 2.21.1, MALDIquant 1.19.3, MASS 7.3-51.4, MassSpecWavelet 1.53.0, Matrix 1.2-17, R6 2.4.0, RANN 2.6.1, RBGL 1.63.1, RColorBrewer 1.1-2, RCurl 1.95-4.12, RUnit 0.4.32, XML 3.98-1.20, affyio 1.57.0, assertthat 0.2.1, bitops 1.0-6, codetools 0.2-16, colorspace 1.4-1, compiler 4.0.0, crayon 1.3.4, digest 0.6.22, doParallel 1.0.15, dplyr 0.8.3, foreach 1.4.7, ggplot2 3.2.1, glue 1.3.1, graph 1.65.0, grid 4.0.0, gtable 0.3.0, impute 1.61.0, iterators 1.0.12, lattice 0.20-38, lazyeval 0.2.2, limma 3.43.0, magrittr 1.5, multtest 2.43.0, munsell 0.5.0, mzID 1.25.0, ncd4 1.17, pcaMethods 1.79.1, pillar 1.4.2, pkgconfig 2.0.3,

plyr 1.8.4, preprocessCore 1.49.0, purrr 0.3.3, rlang 0.4.1, robustbase 0.93-5, scales 1.0.0, splines 4.0.0, survival 3.1-6, tibble 2.1.3, tidyselect 0.2.5, tools 4.0.0, vsn 3.55.0, zlibbioc 1.33.0

Further information

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