

# Package ‘erah’

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**Type** Package

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**Title** Automated Spectral Deconvolution, Alignment, and Metabolite  
Identification in GC/MS-Based Untargeted Metabolomics

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**Description** Automated compound deconvolution, alignment across samples, and identification of metabolites by spectral library matching in Gas Chromatography - Mass spectrometry (GC-MS) untargeted metabolomics. Outputs a table with compound names, matching scores and the integrated area of the compound for each sample. Package implementation is described in Domingo-Almenara et al. (2016) <[doi:10.1021/acs.analchem.6b02927](https://doi.org/10.1021/acs.analchem.6b02927)>.

**License** GPL (>= 2)

**URL** <https://metsyslab.com/>, <http://xdomingoal.github.io/erah-devel/>

**BugReports** <https://github.com/xdomingoal/erah-devel/issues>

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alignComp	<i>Alignment of compounds</i>
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---

**Description**

Alignment of GC-MS deconvolved compounds

**Usage**

```
alignComp(Experiment, alParameters, blocks.size=NULL)

## S4 method for signature 'MetaboSet'
alignComp(Experiment, alParameters, blocks.size = NULL)
```

**Arguments**

Experiment	A 'MetaboSet' S4 object containing the experiment data previously created by newExp and deconvolved by deconvolveComp.
alParameters	The software alignment parameters object previously created by setAlPar
blocks.size	For experiment of more than 1000 samples, and depending on the computer, alignment can be conducted by block segmentation. See details.

**Details**

See eRah vignette for more details. To open the vignette, execute the following code in R: vignette("eRahManual", package="erah")

For experiments containing more than 100 (Windows) or 1000 (Mac or Linux) samples (numbers depending on the computer resources and sample type). In those cases alignment can be conducted by block segmentation. For an experiment of e.g. 1000 samples, the block.size can be set to 100, so the alignment will perform as multiple (ten) 100-samples experiments, to later align them into a single experiment.

This parameter is designed to solve the typical problem that appear when aligning under Windows operating system: "Error: cannot allocate vector of size XX Gb". Such a problem will not appear with Mac or Linux, but several hours of computation are expected when aligning a large number of samples. Using block segmentation provides a greatly improved run-time performance.

**Value**

The function returns an updated S4 'MetaboSet' class, where the GC-MS samples have been now aligned.

**Author(s)**

Xavier Domingo-Almenara. xavier.domingo@urv.cat

## References

[1] Xavier Domingo-Almenara, et al., eRah: A Computational Tool Integrating Spectral Deconvolution and Alignment with Quantification and Identification of Metabolites in GC-MS-Based Metabolomics. Analytical Chemistry (2016). DOI: 10.1021/acs.analchem.6b02927

## See Also

[newExp](#) [setDecPar](#) [deconvolveComp](#)

---

alignList	<i>Alignment list</i>
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---

## Description

The list of aligned metabolites and their relative quantification for each sample in a given experiment

## Usage

```
alignList(object, by.area = TRUE)

## S4 method for signature 'MetaboSet'
alignList(object, by.area = TRUE)
```

## Arguments

object	A 'MetaboSet' S4 object containing the experiment data. The experiment has to be previously deconvolved, aligned and (optionally) identified.
by.area	if TRUE (default), eRah outputs quantification by the area of the deconvolved chromatographic peak of each compound. If FALSE, eRah outputs the intensity of the deconvolved chromatographic peak.

## Details

Returns an alignment table containing the list of aligned metabolites and their relative quantification for each sample in a given experiment.

## Value

alignList returns a data frame object:

AlignID	The unique Tag for found metabolite by eRah. Each metabolite found by eRah for a given experiment has an unique AlignID tag number.
Factor	the Factor tag name. Each metabolite has an unique 'Factor' name to enhance visual interpretation.
tmean	The mean compound retention time.
FoundIn	The number of samples in which the compound has been detected (the number of samples where the compound area is non-zero).

**Quantification** As many columns as samples and as many rows as metabolites, where each column name has the name of each sample.

### See Also

[idList dataList](#)

---

compInfo

*Information of a Compound*

---

### Description

Displays basic information of a compound in the MS library.

### Usage

```
compInfo(comp.id, id.database = mslib)
```

### Arguments

comp.id	The DB.Id number of the compound.
id.database	The mass-spectra library to be compared with the empirical spectra. By default, the MassBank - Mass Bank of North America (MoNa) database are employed (mslib object).

### Details

Returns details on a given compound such as the synonyms, CAS, KEGG, retention index, among others.

### See Also

[findComp](#)

### Examples

```
# finding proline
findComp("proline")

# we see that proline 2TMS has the DB.Id number 42, then:
compInfo(42)
```

computeRIerror

*computeRIerror*

---

**Description**

This function uses RI of mslib database and RT of the identified compounds to discriminate proper compound identification.

**Usage**

```
computeRIerror(  
  Experiment,  
  id.database = mslib,  
  reference.list,  
  ri.error.type = c("relative", "absolute"),  
  plot.results = TRUE  
)
```

**Arguments**

Experiment	S4 object with experiment Data, Metadata and Results. Results of experiment are used to extract RT and Compound DB Id.
id.database	Name of the preloaded database, in this case the regular db used by erah mslib
reference.list	List with the compounds and their attributes (AlignId...)
ri.error.type	Specify whether absolute or relative RI error is to be computed.
plot.results	Shows the RI/RT graphic (True by default)

**Details**

See eRah vignette for more details. To open the vignette, execute the following code in R: `vignette("eRahManual", package="erah")`

**Author(s)**

Xavier Domingo-Almenara. [xavier.domingo@urv.cat](mailto:xavier.domingo@urv.cat)

**References**

[1] Xavier Domingo-Almenara, et al., eRah: A Computational Tool Integrating Spectral Deconvolution and Alignment with Quantification and Identification of Metabolites in GC-MS-Based Metabolomics. Analytical Chemistry (2016). DOI: 10.1021/acs.analchem.6b02927

**See Also**

[showRTRICurve](#)

## Examples

```
## Not run:
ex <- computeRIerror(
  ex,
  mslib,
  reference.list=list(AlignID = c(45,67,92,120)),
  ri.error.type = "relative"
)

## End(Not run)
```

---

createdt

*Creating Experiment Tables*

---

## Description

eRah requires an instrumental and (optionally) phenotype .csv file for starting/creating a new eRah project/experiment. This function automatically creates the Phenoytpe and Instrumental data .csv files.

## Usage

```
createdt(path)
```

## Arguments

path	the path where the experiment-folder is (where the experiment samples are stored).
------	--

## Details

The experiment has to been organized as follows: all the samples related to each class have to be stored in the same folder (one folder = one class), and all the class-folders in one folder, which is the experiment folder.

Two things have to be considered at this step: .csv files are different when created by American and European computers, so errors may raise due to that fact. Also, the folder containing the samples, must contain only folders. If the folder contains files (for example, already created .csv files), eRah will prompt an error.

See eRah vignette for more details. To open the vignette, execute the following code in R: `vignette("eRahManual", package="erah")`

## See Also

[newExp](#)

**Examples**

```
## Not run:
# Store all the raw data files in one different folder per class,
# and all the class-folders in one folder, which is the experiment
# folder. Then execute

createdt(path)

# where path is the experiment folder path.
# The experiment can be now started by:

ex <- newExp(instrumental="path/DEMO_inst.csv",
phenotype="path/DEMO_pheno.csv", info="DEMO Experiment")

## End(Not run)
```

---

```
createInstrumentalTable
```

*Create Instrumental Table*

---

**Description**

Create table containing instrumental information such as sample IDs and file names.

**Usage**

```
createInstrumentalTable(files)
```

**Arguments**

files                      File paths to experiment samples.

**Details**

Creates instrumental information table based on experiment sample file paths. Columns containing further information can also be added to this.

**See Also**

[newExp](#) [createPhenoTable](#)

**Examples**

```
## Not run:
library(gcspikelite)

files <- list.files(system.file('data',package = 'gcspikelite'),full.names = TRUE)
files <- files[sapply(files,grep1,pattern = 'CDF')]
```



```
instrumental <- createInstrumentalTable(files)

## End(Not run)
```

---

createPhenoTable	<i>Create Phenotype Table</i>
------------------	-------------------------------

---

## Description

Create table containing sample meta information such as as sample ID and class.

## Usage

```
createPhenoTable(files, cls)
```

## Arguments

files	File paths to experiment samples.
cls	Character vector containing sample classes.

## Details

Creates phenotype information table based on experiment sample file paths and sample classes. Columns containing further information can also be added to this.

## See Also

[newExp createInstrumentalTable](#)

## Examples

```
## Not run:
library(gcspikelite)
data(targets)

files <- list.files(system.file('data',package = 'gcspikelite'),full.names = TRUE)
files <- files[sapply(files,grep1,pattern = 'CDF')]

phenotype <- createPhenoTable(files,as.character(targets$Group[order(targets$FileName)]))

## End(Not run)
```

dataList

*Data list***Description**

The final eRah list of aligned and identified metabolites and their relative quantification for each sample in a given experiment

**Usage**

```
dataList(Experiment, id.database = mslib, by.area = TRUE)
```

```
## S4 method for signature 'MetaboSet'
```

```
dataList(Experiment, id.database = mslib, by.area = TRUE)
```

**Arguments**

Experiment	A 'MetaboSet' S4 object containing the experiment data. The experiment has to be previously deconvolved, aligned and identified.
id.database	The mass-spectra library to be compared with the empirical spectra. By default, the MassBank - Mass Bank of North America (MoNa) database are employed (mslib object).
by.area	if TRUE (default), eRah outputs quantification by the area of the deconvolved chromatographic peak of each compound. If FALSE, eRah outputs the intensity of the deconvolved chromatographic peak.

**Details**

Returns an identification and alignment table containing the list of aligned and identified metabolites (names) and their relative quantification for each sample in a given experiment.

**Value**

alignList returns an S3 object:

AlignID	The unique Tag for found metabolite by eRah. Each metabolite found by eRah for a given experiment has an unique AlignID tag number.
tmean	The mean compound retention time.
FoundIn	The number of samples in which the compound has been detected (the number of samples where the compound area is non-zero).
Name.X	the name of the Xst/nd/rd... hit. idList return as many X (hits) as n.putative selected with <a href="#">identifyComp</a> .
MatchFactor.X	The match factor/score of spectral similarity (spectral correlation).
DB.Id.X	The identification number of the library. Each metbolite in the reference library has a different DB.Id number.

CAS.X	the CAS number of each identified metabolite.
Quantification	As many columns as samples and as many rows as metabolites, where each column name has the name of each sample.

**See Also**

[idList](#) [alignList](#)

---

deconvolveComp	<i>Deconvolution of compounds in samples</i>
----------------	--

---

**Description**

Deconvolution of GC-MS data

**Usage**

```
deconvolveComp(  
  Experiment,  
  decParameters,  
  samples.to.process = NULL,  
  down.sample = FALSE,  
  virtualScansPerSecond = NULL  
)  
  
## S4 method for signature 'MetaboSet'  
deconvolveComp(  
  Experiment,  
  decParameters,  
  samples.to.process = NULL,  
  down.sample = FALSE,  
  virtualScansPerSecond = NULL  
)
```

**Arguments**

Experiment	A 'MetaboSet' S4 object containing the experiment data previously created by <code>newExp</code> .
decParameters	The software deconvolution parameters object previously created by <code>setDecPar</code>
<code>samples.to.process</code>	Vector indicating which samples are to be processed.
<code>down.sample</code>	If TRUE, chromatograms are down sampled to define one peak with 10 scan points (according to the minimum peak width). This is to process longer chromatograms with wider peak widths (more than 20 seconds peak width and small scans per second values). See details.

**virtualScansPerSecond**

A virtual scans per second. If chromatograms are downsampled (for example, for a 1 mean peak width a 1 scans per second sampling frequency was used), eRah could not perform as expected. In these cases, the BEST solution is to re-acquire the samples. However, by selecting a different (virtual) scans per second frequency, eRah can upsample the data and process it more effectively.

**Details**

See eRah vignette for more details. To open the vignette, execute the following code in R: `vignette("eRahManual", package="erah")`

eRah uses multivariate methods which run-time performance depend on the amount of data to be analyzed. When peaks are wider and the #' scans per second is also a small value, the number of points (scans) that define a peak might be too many, leading eRah to a poor run#' -time performance. To solve that, use `down.sample=TRUE` to allow eRah to define a peak with 10 seconds, and analyze the data more #' efficiently.

**Value**

The function returns an updated S4 'MetaboSet' class, where the GC-MS samples have been now deconvolved.

**Author(s)**

Xavier Domingo-Almenara. [xavier.domingo@urv.cat](mailto:xavier.domingo@urv.cat)

**References**

[1] Xavier Domingo-Almenara, et al., eRah: A Computational Tool Integrating Spectral Deconvolution and Alignment with Quantification and Identification of Metabolites in GC-MS-Based Metabolomics. *Analytical Chemistry* (2016). DOI: 10.1021/acs.analchem.6b02927

**See Also**

[newExp setAlPar](#)

**Examples**

```
## Not run:
# Deconvolve data from a created experiment by \code{\link{newExp}}.
# ex <- newExp(instrumental="path")

# The following will set eRah for analyzing the chromatograms
# from minutes 5 to 15, and without taking into account the masses
# 35:69,73:75,147:149, with a minimum peak width of 0.7 seconds.

ex.dec.par <- setDecPar(min.peak.width=0.7, min.peak.height=5000,
                        noise.threshold=500, avoid.processing.mz=c(35:69,73:75,147:149),
                        analysis.time=c(5,15))

# An now deconvolve the compounds in the samples:
```

```
# ex <- deconvolveComp(ex, decParameters=ex.dec.par)

## End(Not run)
```

---

eRah_DB-class	<i>Class "eRah_DB"</i>
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---

### Description

The eRah\_DB class contains the slots for storing and accessing a MS library.

### Slots

name The name of the stored library  
 version The version of the stored library (and which is the database identifier, should be unique and used to check if is the database used in other experiments)  
 info Character vector containing complementary information about the library.  
 database A list of S3 objects, which each object contains the information on a different compound.

### Author(s)

Xavier Domingo-Almenara.

---

expClasses	<i>expClasses-method</i>
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---

### Description

The classes of a given experiment.

### Usage

```
expClasses(object)

## S4 method for signature 'MetaboSet'
expClasses(object)
```

### Arguments

object A 'MetaboSet' S4 object containing the experiment.

### Details

Returns the classes details of the experiment.

### See Also

metaData phenoData

---

export2CEF	<i>Export spectra to CEF</i>
------------	------------------------------

---

**Description**

Export spectra to CEF format for comparison with the NIST library through MassHunter interface.

**Usage**

```
export2CEF(Experiment, export.id = NULL,
           id.database = mslib, store.path = getwd())
```

**Arguments**

Experiment	A 'MetaboSet' S4 object containing the experiment.
export.id	If NULL, all the spectra in the experiment will be exported. Otherwise, only the AlignID in export.id will be exported
id.database	The mass-spectra library used in the experiment.
store.path	The path where the converted files are to be exported.

---

export2MSP	<i>Export spectra to MSP</i>
------------	------------------------------

---

**Description**

Export spectra to MSP format for comparison with the NIST library.

**Usage**

```
export2MSP(
  Experiment,
  export.id = NULL,
  id.database = mslib,
  store.path = getwd(),
  alg.version = 1
)
```

**Arguments**

Experiment	A 'MetaboSet' S4 object containing the experiment.
export.id	If NULL, all the spectra in the experiment will be exported. Otherwise, only the AlignID in export.id will be exported
id.database	The mass-spectra library used in the experiment.
store.path	The path where the converted files are to be exported.

alg.version	Different algorithm implementations. Users have to chose what version works with their NIST MSearch or other software version. By default, alg.version is set to 1. If it not works, try setting alg.version to 2 ;).
-------------	---

---

findComp	<i>Find a compound</i>
----------	------------------------

---

## Description

Finds compounds in the MS library by Name, CAS or chemical formula.

## Usage

```
findComp(name = NULL, id.database = mslib, CAS = NULL, chem.form = NULL)
```

## Arguments

name	The name of the compound to be found.
id.database	The mass-spectra library to be compared with the empirical spectra. By default, the MassBank - Mass Bank of North America (MoNa) database are employed (mslib object).
CAS	The CAS number of the compound to be found.
chem.form	The chemical formula of the compound to be found.

## Value

findComp returns an S3 object:

DB.Id	The identification number of the library. Each metbolite in the reference library has a different DB.Id number.
Compound Name	Compound Name.
CAS	CAS number
Formula	Chemical Formula.

## See Also

[compInfo](#)

## Examples

```
# finding proline

findComp("proline")

# be careful, exact matches are not supported,
# as well as different names like these cases:
```

```
findComp("L-proline (2TMS)")
```

```
findComp("proline 2")
```

---

identifyComp	<i>Identification of compounds</i>
--------------	------------------------------------

---

### Description

Identification of compounds. Each empirical spectrum is compared against a ms library.

### Usage

```
identifyComp(Experiment, id.database = mslib, mz.range = NULL, n.putative = 3)

## S4 method for signature 'MetaboSet'
identifyComp(Experiment, id.database = mslib, mz.range = NULL, n.putative = 3)
```

### Arguments

Experiment	A 'MetaboSet' S4 object containing the experiment data previously created by newExp, deconvolved by deconvolveComp and optionally aligned by alignComp.
id.database	The mass-spectra library to be compared with the empirical spectra. By default, the MassBank-[2] - Mass Bank of North America (MoNa) database are employed.
mz.range	The same as in alignComp. If specified already in alignComp, then there is no need to specify it again. If not, it has to be specified.
n.putative	The number of hits (compound candidate names) to be returned for each spectrum found.

### Value

The function returns an updated S4 'MetaboSet' class, where the GC-MS samples have been now aligned.

### Author(s)

Xavier Domingo-Almenara. xavier.domingo@urv.cat



## References

- [1] Xavier Domingo-Almenara, et al., eRah: A Computational Tool Integrating Spectral Deconvolution and Alignment with Quantification and Identification of Metabolites in GC-MS-Based Metabolomics. *Analytical Chemistry* (2016). DOI: 10.1021/acs.analchem.6b02927
- [2] MassBank: A public repository for sharing mass spectral data for life sciences, H. Horai, M. Arita, S. Kanaya, Y. Nihei, T. Ikeda, K. Suwa, Y. Ojima, K. Tanaka, S. Tanaka, K. Aoshima, Y. Oda, Y. Kakazu, M. Kusano, T. Tohge, F. Matsuda, Y. Sawada, M. Yokota Hirai, H. Nakanishi, K. Ikeda, N. Akimoto, T. Maoka, H. Takahashi, T. Ara, N. Sakurai, H. Suzuki, D. Shibata, S. Neumann, T. Iida, K. Tanaka, K. Funatsu, F. Matsuura, T. Soga, R. Taguchi, K. Saito and T. Nishioka, *J. Mass Spectrom.*, 45 (2010) 703-714.

## See Also

[newExp](#) [alignComp](#) [setAlPar](#) [setDecPar](#)

---

idList

*Identification list*

---

## Description

The list of identified metabolites in a given experiment

## Usage

```
idList(object, id.database = mslib)

## S4 method for signature 'MetaboSet'
idList(object, id.database = mslib)
```

## Arguments

object	A 'MetaboSet' S4 object containing the experiment data. The experiment has to be previously deconvolved, aligned and identified.
id.database	The mass-spectra library to be compared with the empirical spectra. By default, the MassBank - Mass Bank of North America (MoNa) database are employed (mslib object).

## Details

Returns an identification table containing the names, match scores, and other variables for a given experiment.

**Value**

idList returns an S3 object:

AlignID	The unique Tag for found metabolite by eRah. Each metabolite found by eRah for a given experiment has an unique AlignID tag number.
tmean	The mean compound retention time.
Name.X	the name of the Xst/nd/rd... hit. idList return as many X (hits) as n.putative selected with <a href="#">identifyComp</a> .
FoundIn	The number of samples in which the compound has been detected (the number of samples where the compound area is non-zero).
MatchFactor.X	The match factor/score of spectral similarity (spectral correlation).
DB.Id.X	The identification number of the library. Each metbolite in the reference library has a different DB.Id number.
CAS.X	the CAS number of each identified metabolite.

**See Also**

[alignList](#) [dataList](#)

---

importGMD

---

*Import MSP files from GMD to R*


---

**Description**

Import the Golm Metabolome Database.

**Usage**

```
importGMD(filename, DB.name, DB.version, DB.info,
type = c("VAR5.ALK", "VAR5.FAME", "MDN35.ALK", "MDN35.FAME"))
```

**Arguments**

filename	The filepath containing the GMD database file.
DB.name	The name of the database (each user may chose its own name)
DB.version	The version of the database (each user may chose its own version)
DB.info	Some info about the database for further reference
type	The type of RI to be imported from the database

**Details**

For more details, please see the eRah manual

---

`importMSP`*Import MSP files to R*

---

**Description**

Import MS libraries in MSP format to eRah DB format.

**Usage**

```
importMSP(filename, DB.name, DB.version, DB.info)
```

**Arguments**

<code>filename</code>	The filepath containing the MSP library file.
<code>DB.name</code>	The name of the database (each user may chose its own name)
<code>DB.version</code>	The version of the database (each user may chose its own version)
<code>DB.info</code>	Some info about the database for further reference

**Details**

The MSP input file should look like:

—  
Name: Metabolite\_name

Formula: H2O

MW: 666

ExactMass: 666.266106

CAS#: 11-22-3

DB#: 1

Comments: Metabolite\_name reference standard

Num Peaks: XX

53 1; 54 2; 55 5; 56 2; 57 2;

58 14; 59 18; 60 1000; 61 2; 67 1;

Name: Metabolite\_name\_2

Formula: H2O2

MW: 999

ExactMass: 999.266106

CAS#: 22-33-4

DB#: 2

Comments: Metabolite\_name\_"" reference standard

Num Peaks: XX

66 10; 67 1000; 155 560; 156 800; 157 2;  
158 14; 159 1; 160 100; 161 2; 167 1;

\_\_\_\_\_

OR

\_\_\_\_\_

Name: Metabolite\_name

Formula: H2O

MW: 666

ExactMass: 666.266106

CASNO: 11-22-3

DB#: 1

Comment: Metabolite\_name reference standard

Num peaks: XX

53 1

54 2

55 5

Name: Metabolite\_name\_2

Formula: H2O2

MW: 999

ExactMass: 999.266106

CASNO: 22-33-4

DB#: 2

Comment: Metabolite\_name\_"" reference standard

Num Peaks: XX

66 10

67 1000

155 560

\_\_\_\_\_

Or combinations of both.

For more details, please see the eRah manual.

---

MetaboSet-class	Class "MetaboSet"
-----------------	-------------------

---

### Description

The MetaboSet class is a single generic class valid for all sorts of metabolomic studies regardless of the experimental platform, the statistical processing and the annotation stage. It is the core operation class of eRah.

### Details

MetaboSet

### Slots

**Info** Slot Info stores the general information of the experiment and the experimental platform used in the analysis of the biological samples.

**Data** Slot Data contains either the raw data or the path of the files. It also contains the list of the selected features (deconvolved compounds). In the subslot Parameters it is saved the information regarding the feature selector algorithm (type, parameters, version...) and the experimental platform used.

**MetaData** Slot MetaData has two slots. In the Instrumental slot it is saved a data frame with some mandatory fields (filename, date, time, sampleID) and optional fields related to the experimental platform (Column ID, Column Type, Ioniser,...). Slot Phenotypic contains a data frame with the sample and experimental information (phenotypes, longitudinal data,...).

**Results** In the Results slot it is saved the information related to the statistical and identification results. The slot Parameters contains all the values of the parameters used in the identification and statistical functions. Slot Identification has the results of the identification process as well as the identification or/and annotation steps. The results of the statistical functions are saved in the Statistics slot.

### Author(s)

Xavier Domingo-Almenara, Arnald Alonso and Francesc Fernandez-Albert.

---

metaData	<i>metaData-method</i>
----------	------------------------

---

### Description

Displays the Experiment metadata

**Usage**

```
metaData(object)

## S4 method for signature 'MetaboSet'
metaData(object)
```

**Arguments**

object                    A 'MetaboSet' S4 object containing the experiment.

**See Also**

[phenoData](#)

---

mslib	<i>MassBank Spectral Library</i>
-------	----------------------------------

---

**Description**

The default mass spectral library of eRah, which is the MassBank repository.

**Usage**

```
data(mslib)
```

**Format**

An object of class eRah\_DB of length 1.

**Details**

This is the eRah default MS library, and automatically loaded with the eRah package. It contains almost 500 MS spectra. For details, see reference below.

**Author(s)**

The TOF-MS spectra were contributed by Kazusa DNA Research Institute, the Engineering Department of Osaka University and Plant Science Center of RIKEN.

MassBank (<http://www.massbank.jp/>)

**References**

[1] MassBank: A public repository for sharing mass spectral data for life sciences, H. Horai, M. Arita, S. Kanaya, Y. Nihei, T. Ikeda, K. Suwa, Y. Ojima, K. Tanaka, S. Tanaka, K. Aoshima, Y. Oda, Y. Kakazu, M. Kusano, T. Tohge, F. Matsuda, Y. Sawada, M. Yokota Hirai, H. Nakanishi, K. Ikeda, N. Akimoto, T. Maoka, H. Takahashi, T. Ara, N. Sakurai, H. Suzuki, D. Shibata, S. Neumann, T. Iida, K. Tanaka, K. Funatsu, F. Matsuura, T. Soga, R. Taguchi, K. Saito and T. Nishioka, J. Mass Spectrom., 45, 703-714 (2010)

**See Also**[compInfo](#)

---

newExp	<i>New Experiment</i>
--------	-----------------------

---

**Description**

Sets a new experiment for eRah

**Usage**

```
newExp(instrumental, phenotype = NULL, info = character())
```

**Arguments**

instrumental	A data.frame containing the sample instrumental information.
phenotype	(optional) A data.frame containing sample phenotype information.
info	Experiment description

**Details**

See eRah vignette for more details. To open the vignette, execute the following code in R: `vignette("eRahManual", package="erah")`

**Value**

newExp returns an S4 object of the class 'MetaboSet'.

**Author(s)**

Xavier Domingo-Almenara. [xavier.domingo@urv.cat](mailto:xavier.domingo@urv.cat)

**References**

[1] Xavier Domingo-Almenara, et al., eRah: A Computational Tool Integrating Spectral Deconvolution and Alignment with Quantification and Identification of Metabolites in GC-MS-Based Metabolomics. *Analytical Chemistry* (2016). DOI: 10.1021/acs.analchem.6b02927

**See Also**

[createInstrumentalTable](#) [createPhenoTable](#) [setDecPar](#) [setAlPar](#)

## Examples

```
## Not run:
library(gcspikelite)
data(targets)

files <- list.files(system.file('data',package = 'gcspikelite'),full.names = TRUE)
files <- files[sapply(files,grep1,pattern = 'CDF')]

instrumental <- createInstrumentalTable(files)
phenotype <- createPhenoTable(files,as.character(targets$Group[order(targets$FileName)]))

ex <- newExp(instrumental = instrumental,
phenotype = phenotype, info = "DEMO Experiment")

## End(Not run)
```

---

phenoData

*phenoData-method*

---

## Description

Displays the Experiment phenotypic data (if included).

## Usage

```
phenoData(object)

## S4 method for signature 'MetaboSet'
phenoData(object)
```

## Arguments

object            A 'MetaboSet' S4 object containing the experiment.

## See Also

[metaData](#)



---

plotAlign	<i>Plotting chromatographic profile with and without alignment</i>
-----------	--

---

### Description

Plots the chromatophic profiles of the compounds found by eRah. Similarly to plotProfile, but with two sub-windows, showing the chromatophic profiles before and after alignment.

### Usage

```
plotAlign(Experiment, AlignId, per.class = T, xlim = NULL)

## S4 method for signature 'MetaboSet'
plotAlign(Experiment, AlignId, per.class = T, xlim = NULL)
```

### Arguments

Experiment	A 'MetaboSet' S4 object containing the experiment after being deconvolved, aligned and (optionally) identified.
AlignId	the Id identifier for the compound to be shown.
per.class	logical. if TRUE the profiles are shown one color per class, if FALSE one color per sample.
xlim	x axis (retention time) limits (see <a href="#">plot.default</a> ).

### Author(s)

Xavier Domingo-Almenara. [xavier.domingo@urv.cat](mailto:xavier.domingo@urv.cat)

### See Also

[plotSpectra](#) [plotProfile](#)

---

plotChr	<i>Plotting sample chromatogram</i>
---------	-------------------------------------

---

### Description

Plot the sample chromatogram

**Usage**

```
plotChr(
  Experiment,
  N.sample = 1,
  type = c("BIC", "TIC", "EIC"),
  xlim = NULL,
  mz = NULL
)

## S4 method for signature 'MetaboSet'
plotChr(
  Experiment,
  N.sample = 1,
  type = c("BIC", "TIC", "EIC"),
  xlim = NULL,
  mz = NULL
)
```

**Arguments**

Experiment	A 'MetaboSet' S4 object containing the experiment.
N.sample	Integer. The number of the sample to query.
type	The type of plotting, Base Ion Chromatogram (BIC), Total Ion Chromatogram (TIC), or Extracted Ion Chromatogram (EIC).
xlim	The range in minutes, separated by comas: c(rt.min, rt.max) of the limits of plotting. By default, all the chromatogram is plotted.
mz	Just when EIC is selected. The range separated by comas: c(mz.min, mz.max) or a vector of numbers: c(50,67,80), of the masses to be plotted.

**See Also**

[sampleInfo](#)

**Examples**

```
## Not run:
plotChr(Experiment, 1, "BIC")

# Plots from minute 5 to 7.
plotChr(Experiment, 1, "TIC", xlim=c(5,7))

# Plots from minute 5 to 7, and only the masses from 50 to 70.
plotChr(Experiment, 1, "EIC", mz=50:70 xlim=c(5,7))

# Plots the EIC from minute 7 to 7.5, and only the masses 50, 54 and 70.
plotChr(Experiment, 1, "EIC", xlim=c(7,7.5), mz=c(50,54,70))

## End(Not run)
```

---

plotProfile	<i>Plotting chromatographic profile</i>
-------------	---

---

**Description**

Plots the chromatophic profiles of the compounds found by eRah.

**Usage**

```
plotProfile(Experiment, AlignId, per.class = T, xlim = NULL, cols=NULL)

## S4 method for signature 'MetaboSet'
plotProfile(Experiment, AlignId, per.class = T, xlim = NULL, cols = NULL)
```

**Arguments**

Experiment	A 'MetaboSet' S4 object containing the experiment after being deconvolved, aligned and (optionally) identified.
AlignId	the Id identificator for the compound to be shown.
per.class	logical. if TRUE (by default) the profiles are shown one color per class, if FALSE one color per sample.
xlim	x axis (retention time) limits (see <a href="#">plot.default</a> ).
cols	vector of colors. Colors are used cyclically.

**Author(s)**

Xavier Domingo-Almenara. [xavier.domingo@urv.cat](mailto:xavier.domingo@urv.cat)

**See Also**

[plotSpectra](#) [plotAlign](#)

---

plotSpectra	<i>Plotting Spectra</i>
-------------	-------------------------

---

**Description**

Plots the empirical spectra found by eRah, and allows comparing it with the reference spectra.

**Usage**

```
plotSpectra(Experiment, AlignId, n.putative = 1,
  compare = T, id.database = mslib, comp.db = NULL,
  return.spectra = F, draw.color = "purple", xlim = NULL)

## S4 method for signature 'MetaboSet'
plotSpectra(
  Experiment,
  AlignId,
  n.putative = 1,
  compare = T,
  id.database = mslib,
  comp.db = NULL,
  return.spectra = F,
  draw.color = "purple",
  xlim = NULL
)
```

**Arguments**

Experiment	A 'MetaboSet' S4 object containing the experiment after being deconvolved, aligned and (optionally) identified.
AlignId	the Id identifier for the compound to be shown.
n.putative	The hit number (position) to be returned when comparing the empirical spectrum with the reference. See details
compare	logical. If TRUE, then the reference spectrum from the library is shown for comparison.
id.database	The mass-spectra library to be compared with the empirical spectra. By default, the MassBank-[2] - Mass Bank of North America (MoNa) database are employed.
comp.db	If you want to compare the empirical spectrum with another spectrum from the database, select the comp.db number from the database.
return.spectra	logical. If TRUE, the function returns the empirical spectrum for the selected compound
draw.color	Selects the color for the reference spectrum (see <a href="#">colors</a> ).
xlim	x axis (mass - m/z) limits (see <a href="#">plot.default</a> ).

**Details**

When identification is applied (see [identifyComp](#)), the number of hits to be returned (n.putative) has to be selected. Therefore, here you can compare the empirical spectrum (found by eRah) with each n.putative hit returned (1, 2, ...) by (see [identifyComp](#)).

**Value**

plotSpectra returns an vector when return.spectra=TRUE.

x                      vector. Contains the empirical spectrum.

**Author(s)**

Xavier Domingo-Almenara. xavier.domingo@urv.cat

**References**

- [1] eRah: an R package for spectral deconvolution, alignment, and metabolite identification in GC/MS-based untargeted metabolomics. Xavier Domingo-Almenara, Alexandre Perera, Maria Vinaixa, Sara Samino, Xavier Correig, Jesus Brezmes, Oscar Yanes. (2016) Article in Press.
- [2] MassBank: A public repository for sharing mass spectral data for life sciences, H. Horai, M. Arita, S. Kanaya, Y. Nihei, T. Ikeda, K. Suwa, Y. Ojima, K. Tanaka, S. Tanaka, K. Aoshima, Y. Oda, Y. Kakazu, M. Kusano, T. Tohge, F. Matsuda, Y. Sawada, M. Yokota Hirai, H. Nakanishi, K. Ikeda, N. Akimoto, T. Maoka, H. Takahashi, T. Ara, N. Sakurai, H. Suzuki, D. Shibata, S. Neumann, T. Iida, K. Tanaka, K. Funatsu, F. Matsuura, T. Soga, R. Taguchi, K. Saito and T. Nishioka, J. Mass Spectrom., 45, 703-714 (2010)

**See Also**

[plotProfile](#) [plotAlign](#)

---

RawDataParameters-class

*Class "RawDataParameters"*

---

**Description**

The RawDataParameters class contains the slots for storing and accessing into a MS sample, and the essential parameters for performing its processing (deconvolution).

**Slots**

data The data matrix of the sample to be processed  
 min.mz The minimum adquired mz number  
 max.mz The maximum adquired mz number  
 start.time Starting time of adquisition  
 mz.resolution Mz resolution  
 scans.per.second Scans per second  
 avoid.processing.mz Which mz do not have to be processed  
 min.peak.width Minimum peak width (stored in scans)  
 min.peak.height Minimum peak height  
 noise.threshold The noise threshold  
 compression.coef Compression coefficient (parameter for Orthogonal Signal Deconvolution)

**Author(s)**

Xavier Domingo-Almenara.

---

recMissComp	<i>Missing compound recovery</i>
-------------	----------------------------------

---

### Description

Missing compounds recovery: fits a general model (all the compounds above a certain minimum number of samples) to all the samples.

### Usage

```
recMissComp(Experiment, min.samples, free.model = F)
```

```
## S4 method for signature 'MetaboSet'  
recMissComp(Experiment, min.samples, free.model = F)
```

### Arguments

Experiment	A 'MetaboSet' S4 object containing the experiment data previously created by newExp, deconvolved by deconvolveComp and aligned by alignComp.
min.samples	The minimum number of samples in which a compound has to appear to be considered for searching into the rest of the samples where this compound missing.
free.model	If TRUE, the spectra found in the samples where the compound is missing is used to get the final average spectra. (See details)

### Details

WARNING: If compounds were previously identified, they have to be identified again after applying the "recMissComp" function. This means that "identifyComp" function has to be executed always after "recMissComp" for identification of compounds, even if "identifyComp" has been previously applied before.

The free.model parameter is recommended to be always FALSE (except for carbon tracking applications). This is because the spectra of the samples where the compound is missing is usually affected by noise, and this could decrease the matching score for a certain compound.

### Value

The function returns an updated S4 'MetaboSet' class, where the GC-MS samples have been now aligned.

### Author(s)

Xavier Domingo-Almenara. xavier.domingo@urv.cat

### References

[1] Domingo-Almenara X, et al. Compound deconvolution in GC-MS-based metabolomics by blind source separation. Journal of Chromatography A (2015). Vol. 1409: 226-233. DOI: 10.1016/j.chroma.2015.07.044

**See Also**

[newExp](#) [alignComp](#) [setAlPar](#) [setDecPar](#)

---

sampleInfo	<i>Information of the samples</i>
------------	-----------------------------------

---

**Description**

Returns basic information on the samples.

**Usage**

```
sampleInfo(Experiment, N.sample = 1)

## S4 method for signature 'MetaboSet'
sampleInfo(Experiment, N.sample = 1)
```

**Arguments**

Experiment	A 'MetaboSet' S4 object containing the experiment.
N.sample	Integer. The number of the sample to query.

**Details**

Returns details on a given sample of the experiment, such as name, start time, end time, minium and maximum adquired m/z and scans per second.

**See Also**

[plotChr](#)

---

setAlPar	<i>Set Alignment Parameters</i>
----------	---------------------------------

---

**Description**

Setting alignment parameters for eRah.

**Usage**

```
setAlPar(min.spectra.cor, max.time.dist,mz.range = c(70:600))
```

### Arguments

<code>min.spectra.cor</code>	Minimum spectral correlation value. From 0 (non similar) to 1 (very similar). This value sets how similar two or more compounds have to be considered for alignment between them.
<code>max.time.dist</code>	Maximum retention time distance. This value (in seconds) sets how far two or more compounds can be to be considered for alignment between them.
<code>mz.range</code>	The range of masses that is considered when comparing spectra.

### Author(s)

Xavier Domingo-Almenara. [xavier.domingo@urv.cat](mailto:xavier.domingo@urv.cat)

### References

[1] Xavier Domingo-Almenara, et al., eRah: A Computational Tool Integrating Spectral Deconvolution and Alignment with Quantification and Identification of Metabolites in GC-MS-Based Metabolomics. Analytical Chemistry (2016). DOI: 10.1021/acs.analchem.6b02927

### See Also

[newExp setDecPar alignComp](#)

### Examples

```
## Not run:  
# The following will set eRah for aligning compounds which are  
# at least 90 (per cent) similar, and which peaks are at a  
# maximum distance of 2 seconds. All the masses are considered when  
# computing the spectral similarity.  
  
ex.al.par <- setAlPar(min.spectra.cor=0.90, max.time.dist=2,  
mz.range=1:600)  
  
## End(Not run)
```

---

setDecPar

*Set Software Parameters*

---

### Description

Sets Software Parameters for eRah.



**Usage**

```
setDecPar(  
  min.peak.width,  
  min.peak.height = 2500,  
  noise.threshold = 500,  
  avoid.processing.mz = c(73:75, 147:149),  
  compression.coef = 2,  
  analysis.time = 0  
)
```

**Arguments**

min.peak.width	Minimum compound peak width (in seconds). This is a critical parameter that conditions the efficiency of eRah. Typically, this should be the half of the mean compound width.
min.peak.height	Minimum compound peak height
noise.threshold	Data above this threshold will be considered as noise
avoid.processing.mz	The masses that do not want to be considered for processing. Typically, in GC-MS those masses are 73,74,75,147,148 and 149, since they are they are ubiquitous mass fragments typically generated from compounds carrying a trimethylsilyl moiety.
compression.coef	Data is compressed when using the orthogonal signal deconvolution (OSD) algorithm according to this value. A level 2 of compression is recommended.
analysis.time	The chromatographic retention time window to process. If 0, all the chromatogram is processed.

**Details**

See eRah vignette for more details. To open the vignette, execute the following code in R: `vignette("eRahManual", package="erah")`

**Author(s)**

Xavier Domingo-Almenara. [xavier.domingo@urv.cat](mailto:xavier.domingo@urv.cat)

**References**

[1] Xavier Domingo-Almenara, et al., eRah: A Computational Tool Integrating Spectral Deconvolution and Alignment with Quantification and Identification of Metabolites in GC-MS-Based Metabolomics. *Analytical Chemistry* (2016). DOI: 10.1021/acs.analchem.6b02927

**See Also**

[newExp](#) [deconvolveComp](#) [alignComp](#) [setAlPar](#)

## Examples

```
## Not run:
# The following will set eRah for analyzing the chromatograms
# from minutes 5 to 15, and without taking into account the masses
# 35:69, 73:75, 147:149, with a minimum peak width of 0.7 seconds.
ex.dec.par <- setDecPar(min.peak.width = 0.7,
                        min.peak.height = 5000,
                        noise.threshold = 500,
                        avoid.processing.mz = c(35:69, 73:75, 147:149),
                        analysis.time = c(5, 15))

## End(Not run)
```

---

show, MetaboSet-method    *Show MetaboSet object*

---

## Description

Show MetaboSet object

## Usage

```
## S4 method for signature 'MetaboSet'
show(object)
```

## Arguments

object                      S4 object of class MetaboSet

## Details

show-MetaboSet

---

showRTRICurve                      *Show RT-RI curve*

---

## Description

This function uses RI of mslib database and RT of the identified compounds to discriminate proper compound identification.

**Usage**

```
showRTRICurve(  
  Experiment,  
  reference.list,  
  nAnchors = 4,  
  ri.thrs = "1R",  
  id.database = mslib  
)
```

**Arguments**

Experiment	S4 object with experiment Data, Metadata and Results. Results of experiment are used to extract RT and Compound DB Id.
reference.list	List with the compounds and their attributes (AlignId...)
nAnchors	The desired equivalent number of degrees of freedom for the smooth.spline function
ri.thrs	Retention Index threshold given by the user to discriminate between identification results
id.database	Name of the preloaded database (mslib by default, the regular db used by erah)

**Details**

See eRah vignette for more details. To open the vignette, execute the following code in R: `vignette("eRahManual", package="erah")`

**Author(s)**

Xavier Domingo-Almenara. [xavier.domingo@urv.cat](mailto:xavier.domingo@urv.cat)

**References**

[1] Xavier Domingo-Almenara, et al., eRah: A Computational Tool Integrating Spectral Deconvolution and Alignment with Quantification and Identification of Metabolites in GC-MS-Based Metabolomics. *Analytical Chemistry* (2016). DOI: 10.1021/acs.analchem.6b02927

**See Also**

[computeRIerror](#)

**Examples**

```
## Not run:  
# The following set erah to determine which identified compounds are in RI threshold  
RTRICurve <- showRTRICurve(ex, list, nAnchors=4, ri.thrs='1R')  
  
## End(Not run)
```

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