

# Package ‘ASICS’

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**Type** Package

**Title** Automatic Statistical Identification in Complex Spectra

**Version** 2.27.0

**Description** With a set of pure metabolite reference spectra, ASICS quantifies concentration of metabolites in a complex spectrum. The identification of metabolites is performed by fitting a mixture model to the spectra of the library with a sparse penalty. The method and its statistical properties are described in Tardivel et al. (2017) <doi:10.1007/s11306-017-1244-5>.

**Depends** R (>= 3.5)

**Imports** BiocParallel, ggplot2, glmnet, grDevices, gridExtra, methods, mvtnorm, PepsNMR, plyr, quadprog, ropls, stats, SummarizedExperiment, utils, Matrix, zoo

**License** GPL (>= 2)

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'AnalysisResults-class.R' 'PureLibrary-class.R' 'alignment.R'  
'analysis\_on\_quantification.R' 'concentration\_optimisation.R'  
'data.R' 'library\_transformation.R' 'load\_data.R'  
'plotAlignment.R' 'plot\_spectrum.R' 'simulation.R'  
'user\_guide.R' 'utils.R'

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Contents

|                                          |           |
|------------------------------------------|-----------|
| accessors-methods . . . . .              | 2         |
| alignSpectra . . . . .                   | 4         |
| AnalysisResults-class . . . . .          | 5         |
| ASICS . . . . .                          | 6         |
| ASICSResults-class . . . . .             | 8         |
| ASICSUsersGuide . . . . .                | 9         |
| binning . . . . .                        | 9         |
| combineAndSubset-methods . . . . .       | 11        |
| createPureLibrary . . . . .              | 12        |
| createSpectra . . . . .                  | 13        |
| formatForAnalysis . . . . .              | 13        |
| importSpectra . . . . .                  | 15        |
| importSpectraBruker . . . . .            | 16        |
| kruskalWallis . . . . .                  | 18        |
| normaliseSpectra . . . . .               | 19        |
| oplsda . . . . .                         | 20        |
| pca . . . . .                            | 21        |
| plotAlignment . . . . .                  | 22        |
| PureLibrary-class . . . . .              | 23        |
| pure_library . . . . .                   | 24        |
| simulate_spectra . . . . .               | 24        |
| Spectra-class . . . . .                  | 25        |
| summary-methods . . . . .                | 26        |
| visualisation-methods-analyses . . . . . | 27        |
| visualisation-methods-spectra . . . . .  | 28        |
| <b>Index</b>                             | <b>30</b> |

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|                   |                  |
|-------------------|------------------|
| accessors-methods | <i>Accessors</i> |
|-------------------|------------------|

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Description

List of available accessors for each slot of all S4 classes present in the package.

**Usage**

```
## S4 method for signature 'Spectra'
getSampleName(object)

## S4 method for signature 'Spectra'
getPpmGrid(object)

## S4 method for signature 'Spectra'
getSpectra(object)

## S4 method for signature 'Spectra'
getNormMethod(object)

## S4 method for signature 'Spectra'
getNormParams(object)

## S4 method for signature 'ASICSResults'
getReconstructedSpectra(object)

## S4 method for signature 'ASICSResults'
getQuantification(object)

## S4 method for signature 'ASICSResults'
getDeformedLibrary(object)

## S4 method for signature 'AnalysisResults'
getTypeAnalysis(object)

## S4 method for signature 'AnalysisResults'
getTypeData(object)

## S4 method for signature 'AnalysisResults'
getDataset(object)

## S4 method for signature 'AnalysisResults'
getResults(object)

## S4 method for signature 'AnalysisResults'
getBestModel(object)

## S4 method for signature 'AnalysisResults'
getCVError(object)

## S4 method for signature 'AnalysisResults'
getMeanByGroup(object)

## S4 method for signature 'PureLibrary'
getNbProtons(object)
```

**Arguments**

object                    An object of class [Spectra](#), [PureLibrary](#), [ASICSResults](#) or [AnalysisResults](#).

**Value**

The wanted accessor

**Examples**

```
# Import data and create object
current_path <- file.path(system.file("extdata", package = "ASICS"),
                           "spectra_example.txt")
spectra_data <- read.table(current_path, header = TRUE, row.names = 1)
spectra_obj <- createSpectra(spectra_data)

# Sample names
getSampleName(spectra_obj)
# Spectra
getSpectra(spectra_obj)
```

---

|              |                  |
|--------------|------------------|
| alignSpectra | <i>Alignment</i> |
|--------------|------------------|

---

**Description**

Align spectra of a data frame by a method based on the CluPA algorithm (Vu et al., (2011))

**Usage**

```
alignSpectra(
  spectra,
  reference = NULL,
  max.shift = 0.02,
  ncores = 1,
  verbose = TRUE
)
```

**Arguments**

|           |                                                                                                                                                                              |
|-----------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| spectra   | Data frame with spectra in columns and chemical shift in rows. Colnames of this data frame correspond to pure metabolite names and rownames to chemical shift grid (in ppm). |
| reference | Index of the reference spectrum used for the alignment. Default to NULL, <i>i.e.</i> the reference spectrum is automatically detected.                                       |
| max.shift | Maximum shift allowed for the alignment. Default to 0.002.                                                                                                                   |
| ncores    | Number of cores used in parallel evaluation. Default to 1.                                                                                                                   |
| verbose   | A boolean value to allow print out process information.                                                                                                                      |

**Value**

A data frame with aligned spectra in columns and chemical shifts (in ppm) in rows.

**References**

Vu, T. N., Valkenborg, D., Smets, K., Verwaest, K. A., Dommissie, R., Lemiere, F., ... & Laukens, K. (2011). An integrated workflow for robust alignment and simplified quantitative analysis of NMR spectrometry data. *BMC Bioinformatics*, **12**(1), 405.

**Examples**

```
current_path <- system.file("extdata", package = "ASICS")
spectra_data <- importSpectra(name.dir = current_path,
                             name.file = "spectra_example.txt", type.import = "txt")
spectra_align <- alignSpectra(spectra_data)
```

---

AnalysisResults-class    Class [AnalysisResults](#)

---

**Description**

Objects of class [AnalysisResults](#) contains results of analyses performed with the functions [pca](#), [oplsda](#) and [kruskalWallis](#).

**Slots**

`type.analysis` Name of the analysis (e.g., "PCA", "OPLS-DA", ...).

`type.data` Type of data used for the analyses (e.g., "quantification", "buckets"...).

`dataset` The object of type [SummarizedExperiment](#) used for the analysis.

`results` Results of the analysis. Can be a data frame for test results or an object of class [opls](#) from [ropls](#) for PCA and OPLS-DA.

`best.model` Best model (only for OPLS-DA analyses).

`cv.error` Cross validation error (only for OPLS-DA analyses).

`mean.by.group` Data frame with means by group and a variable indicating if there is a significant difference between groups for tests and if the VIP associated to the variable is superior to the given threshold for OPLS-DA.

**Methods**

Multiple methods can be applied on [AnalysisResults](#) objects.

- As usual for S4 object, show and summary methods are available, see [Object summary](#)
- All slots have an accessor `get_slot` name, see [Accessors](#)
- All results contained in an object can be represent in a plot, see [Visualisation methods](#)

**Description**

Quantification of 1D <sup>1</sup>H NMR spectra with ASICS method using a library of pure metabolite spectra. The method is presented in Tardivel et al. (2017).

**Usage**

```
ASICS(
  spectra_obj,
  exclusion_areas = matrix(c(4.5, 5.1), ncol = 2),
  max.shift = 0.02,
  pure.library = NULL,
  noise.thres = 0.02,
  joint.align = TRUE,
  threshold.noise = NULL,
  combine = NULL,
  add.noise = 0.15,
  mult.noise = 0.172,
  quantif.method = c("FWER", "Lasso", "both"),
  clean.thres = 1,
  ref.spectrum = NULL,
  seed = 1234,
  ncores = 1,
  verbose = TRUE
)
```

**Arguments**

|                              |                                                                                                                                                                                                        |
|------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>spectra_obj</code>     | An object of class <a href="#">Spectra</a> obtained with the function <a href="#">createSpectra</a> .                                                                                                  |
| <code>exclusion_areas</code> | Definition domain of spectra that has to be excluded for the quantification (ppm). By default, the water region is excluded (4.5-5.1 ppm).                                                             |
| <code>max.shift</code>       | Maximum chemical shift allowed (in ppm). Default to 0.02.                                                                                                                                              |
| <code>pure.library</code>    | An object of class <a href="#">PureLibrary</a> containing the reference spectra (pure metabolite spectra). If NULL, the library included in the package (that contains 191 reference spectra) is used. |
| <code>noise.thres</code>     | Threshold for signal noise. Default to 0.02.                                                                                                                                                           |
| <code>joint.align</code>     | Logical. If TRUE, information from all spectra is taken into account to align individual library.                                                                                                      |
| <code>threshold.noise</code> | DEPRECATED, use <code>noise.thres</code> instead.                                                                                                                                                      |
| <code>combine</code>         | DEPRECATED, use <code>joint.align</code> instead.                                                                                                                                                      |

|                                    |                                                                                                                                                                                                                                                                                                                                                      |
|------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>add.noise, mult.noise</code> | additive and multiplicative noises. To set these noises, you can compute the standard deviation in a noisy area for <code>add.noise</code> or the standard deviation in a peak area for <code>mult.noise</code> when several spectra of the same sample are available. By default, <code>add.noise = 0.15</code> and <code>mult.noise = 0.172</code> |
| <code>quantif.method</code>        | either "FWER" to perform an independent quantification (the method available in ASICS since the beginning), "Lasso" to perform a joint quantification (all the spectra together) or "both" to perform a joint quantification after the FWER selection of the independent quantification. More details can be founded in the user's guide.            |
| <code>clean.thres</code>           | if <code>quantif.method == "both"</code> the percentage of spectra in which the metabolite needs to be identified by the FWER selection. Default to 1, <i>i.e.</i> metabolite is quantified if it was identified in at least 1% of the spectra.                                                                                                      |
| <code>ref.spectrum</code>          | index of the reference spectrum used for the alignment. Default to NULL, <i>i.e.</i> the reference spectrum is automatically detected.                                                                                                                                                                                                               |
| <code>seed</code>                  | Random seed to control randomness in the algorithm (used in the estimation of the significativity of a given metabolite concentration).                                                                                                                                                                                                              |
| <code>ncores</code>                | Number of cores used in parallel evaluation. Default to 1.                                                                                                                                                                                                                                                                                           |
| <code>verbose</code>               | A Boolean value to allow print out process information.                                                                                                                                                                                                                                                                                              |

**Value**

An object of type [ASICSResults](#) containing the quantification results.

**Note**

Since version 2.3.1 small changes were applied in order to improve the speed of metabolite selection algorithm, which can slightly impact outputs of the method.

**References**

Tardivel P., Canlet C., Lefort G., Tremblay-Franco M., Debrauwer L., Concordet D., Servien R. (2017). ASICS: an automatic method for identification and quantification of metabolites in complex 1D 1H NMR spectra. *Metabolomics*, **13**(10): 109. <https://doi.org/10.1007/s11306-017-1244-5>

**See Also**

[ASICSResults](#) [pure\\_library](#) [createSpectra](#)

**Examples**

```
# Import data and create object
current_path <- system.file("extdata", package = "ASICS")
spectra_data <- importSpectra(name.dir = current_path,
                             name.file = "spectra_example.txt", type.import = "txt")
spectra_obj <- createSpectra(spectra_data)

# Estimation of relative quantifications
to_exclude <- matrix(c(4.5, 10), ncol = 2)
```

```
resASICS <- ASICS(spectra_obj, exclusion.areas = to_exclude,  
                  joint.align = FALSE, quantif.method = "FWER")
```

---

|                    |                           |
|--------------------|---------------------------|
| ASICSResults-class | Class <i>ASICSResults</i> |
|--------------------|---------------------------|

---

## Description

Objects of class [ASICSResults](#) contains results of ASICS quantification method for a set of spectra. This object is an extension of the class [Spectra](#), with additional slots for quantification results, reconstructed spectra and deformed library.

## Slots

`sample.name` Character vector of sample names.

`ppm.grid` Numeric vector of a unique grid (definition domain) for all spectra (in ppm).

`spectra` Numeric matrix of original spectra. Columns contain the spectra and are in the same order than `sample.name`. Rows correspond to points of `ppm.grid`.

`reconstructed.spectra` Numeric matrix of reconstructed spectra (in columns) with estimated concentrations. Columns are in the same order than `sample.name` and rows correspond to points of `ppm.grid`.

`quantification` Data-frame with identified metabolites and their relative concentrations.

`deformed.library` A data frame containing the deformed library of each sample.

## Methods

Multiple methods can be applied to [Spectra](#) objects.

- As usual for S4 object, show and summary methods are available, see [Object summary](#)
- All slots have an accessor `get_slot` name, see [Accessors](#)
- Two objects can be combined or a subset can be extracted, see [Combine and subset methods](#)
- All spectra contained in an object can be represented in a plot, see [Visualisation methods](#)

## See Also

[Spectra](#)

---

ASICSUsersGuide

View ASICS User's Guide

---

### Description

Open the ASICS User's Guide (with default browser)

### Usage

```
ASICSUsersGuide(view = TRUE)
```

### Arguments

`view` Logical. If TRUE, the user's guide will be opened with system default browser.

### Details

The function `vignette("ASICS")` will find the short ASICS vignette that describes the main functions and how to obtain the ASICS User's Guide.

The User's Guide is not itself a true vignette because it is not automatically generated during the package build process.

If the operating system is not Windows, then the HTML viewer used is the one given by `Sys.getenv("R_BROWSER")`. The HTML viewer can be changed using `Sys.setenv(R_BROWSER = )`.

### Value

Character string giving the file location. If `view = TRUE`, the HTML viewer is started and the User's Guide is opened, as a side effect.

### Examples

```
# To get the location
ASICSUsersGuide(view = FALSE)

# To open in a HTML viewer
## Not run: ASICSUsersGuide()
```

---

binning

Binning/Bucketing of NMR spectra

---

### Description

Apply a binning function on a spectrum.

**Usage**

```
binning(
  spectra,
  bin = 0.01,
  exclusion.areas = matrix(c(4.5, 5.1), ncol = 2),
  normalisation = TRUE,
  low.lim = 0.5,
  high.lim = 10,
  ncores = 1,
  verbose = TRUE,
  ...
)
```

**Arguments**

|                                |                                                                                                                                                                      |
|--------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>spectra</code>           | Data frame with spectra in columns and chemical shifts in rows. Colnames of this data frame correspond to sample names and rownames to chemical shift grid (in ppm). |
| <code>bin</code>               | Numeric value specifying the bin width.                                                                                                                              |
| <code>exclusion.areas</code>   | Definition domain of spectra that have to be excluded of the analysis (ppm). By default, the water region is excluded (4.5-5.1 ppm).                                 |
| <code>normalisation</code>     | Logical. If TRUE a normalisation is applied for each spectrum (see <a href="#">normaliseSpectra</a> for details). Default to TRUE.                                   |
| <code>low.lim, high.lim</code> | low and high chemical shift limits for the output bins (default values : <code>low.lim = 0.5</code> and <code>high.lim = 10</code> ).                                |
| <code>ncores</code>            | Number of cores used in parallel evaluation. Default to 1.                                                                                                           |
| <code>verbose</code>           | A boolean value to allow print out process information.                                                                                                              |
| <code>...</code>               | Further arguments to be passed to the function <a href="#">normaliseSpectra</a>                                                                                      |

**Value**

A data frame with normalised spectra in columns and buckets in rows (bucket names correspond to the center of the bucket).

**Examples**

```
current_path <- system.file("extdata", package = "ASICS")
spectra_data <- importSpectra(name.dir = current_path,
                             name.file = "spectra_example.txt", type.import = "txt")
spectra_bin <- binning(spectra_data, bin = 0.01, type.norm = "pqn")
```

---

`combineAndSubset-methods`*Combine or subset functions*

---

## Description

Methods available to combine multiple objects or to extract a subset of one object in ASICS package.

## Usage

```
## S4 method for signature 'Spectra,ANY,ANY,ANY'
x[i]

## S4 method for signature 'Spectra'
c(x, ...)

## S4 method for signature 'ASICSResults,ANY,ANY,ANY'
x[i]

## S4 method for signature 'ASICSResults'
c(x, ...)

## S4 method for signature 'PureLibrary,ANY,ANY,ANY'
x[i]

## S4 method for signature 'PureLibrary'
c(x, ...)
```

## Arguments

|                  |                                                                                                            |
|------------------|------------------------------------------------------------------------------------------------------------|
| <code>x</code>   | An object of class <a href="#">Spectra</a> , <a href="#">PureLibrary</a> or <a href="#">ASICSResults</a> . |
| <code>i</code>   | vector of indices specifying which elements to extract                                                     |
| <code>...</code> | objects to be concatenated                                                                                 |

## Value

A [Spectra](#) object containing a part of the original object or combining other [Spectra](#) objects

## Examples

```
# Import data and create object
current_path <- file.path(system.file("extdata", package = "ASICS"),
                           "spectra_example.txt")
spectra_data <- read.table(current_path, header = TRUE, row.names = 1)
spectra_obj <- createSpectra(spectra_data)
```



---

|               |                                |
|---------------|--------------------------------|
| createSpectra | Create a <i>Spectra</i> object |
|---------------|--------------------------------|

---

### Description

Create a new spectra object used for quantification.

### Usage

```
createSpectra(spectra, norm.method = NULL, norm.params = NULL)
```

### Arguments

|             |                                                                                                                                                                               |
|-------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| spectra     | Data frame with spectra in columns and chemical shifts in rows. Colnames of this data frame correspond to pure metabolite names and rownames to chemical shift grid (in ppm). |
| norm.method | Character specifying the normalisation method to use on spectra ONLY if the <a href="#">importSpectra</a> function was not used.                                              |
| norm.params | List containing normalisation parameteres (see <a href="#">normaliseSpectra</a> for details) ONLY if the <a href="#">importSpectra</a> function was not used.                 |

### Value

A [Spectra](#) object with spectra to quantify.

### See Also

[Spectra](#)

### Examples

```
current_path <- system.file("extdata", "example_spectra", package = "ASICS")
spectra_data <- importSpectraBruker(current_path)
spectra_obj <- createSpectra(spectra_data)
```

---

|                   |                          |
|-------------------|--------------------------|
| formatForAnalysis | Format data for analysis |
|-------------------|--------------------------|

---

### Description

Create an object of class [SummarizedExperiment](#) to use in functions [pca](#), [oplsda](#) or [kruskalWallis](#).

**Usage**

```
formatForAnalysis(
  data,
  design = NULL,
  feature_info = NULL,
  zero.threshold = 100,
  zero.group = NULL,
  outliers = NULL
)
```

**Arguments**

|                             |                                                                                                                                                                                                                      |
|-----------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>data</code>           | A data frame containing omics dataset with samples in columns and features of interest in rows (metabolites/buckets...).                                                                                             |
| <code>design</code>         | A data frame describing the columns of data with at least two columns, the first one corresponding to the column names of data. Default to NULL (in which case, the column names of data are used for study design). |
| <code>feature_info</code>   | A data frame describing the rows of data with at least two columns, the first one corresponding to the row names of data. Default to NULL (in which case, the row names of data are used for feature information).   |
| <code>zero.threshold</code> | Remove features having a proportion of zeros larger than or equal to <code>zero.threshold</code> . Default to 100.                                                                                                   |
| <code>zero.group</code>     | Variable name of design data frame specifying the group variable used to remove features with a proportion of zeros larger than or equal to <code>zero.threshold</code> within the group. Default to NULL, no group. |
| <code>outliers</code>       | Names of the outliers (samples) to remove.                                                                                                                                                                           |

**Value**

An object of type `SummarizedExperiment` with metabolite data given as buckets or quantified metabolites.

**Examples**

```
# Import quantification results
if (require("ASICSdata", quietly = TRUE)) {
  quantif_path <- system.file("extdata", "results_ASICS.txt",
                             package = "ASICSdata")
  quantification <- read.table(quantif_path, header = TRUE, row.names = 1)

  # Import design
  design <- read.table(system.file("extdata", "design_diabete_example.txt",
                                  package = "ASICSdata"), header = TRUE)

  # Create object for analysis and remove features with more than 25% of
  # zeros
  analysis_obj <- formatForAnalysis(quantification,
                                    design = design,
```

```

                                zero.threshold = 25,
                                zero.group = "condition")
    }

```

---

|               |                                   |
|---------------|-----------------------------------|
| importSpectra | <i>Import metabolomic spectra</i> |
|---------------|-----------------------------------|

---

## Description

Import spectra from text or CSV, fid or 1r (preprocessed spectrum) files. (optional) Spectra are baseline corrected, aligned and normalised during the importation.

## Usage

```

importSpectra(
  name.dir = NULL,
  name.file = NULL,
  type.import,
  baseline.correction = FALSE,
  alignment = FALSE,
  normalisation = TRUE,
  ncores = 1,
  verbose = TRUE,
  ...
)

```

## Arguments

|                     |                                                                                                                                                                                                                                                                                                    |
|---------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| name.dir            | Path of the folder containing the spectra. Each subfolder contains the fid or the 1r (preprocessed spectrum) files of this sample if type = "fid" or type = "1r".                                                                                                                                  |
| name.file           | Name of the txt or csv file containing the spectra in columns (spectrum names in the first line and ppm grid in the first column).                                                                                                                                                                 |
| type.import         | Type of import. Either "txt", "csv", "fid" or "1r".                                                                                                                                                                                                                                                |
| baseline.correction | Logical. If TRUE a baseline correction is applied for each spectrum. Default to FALSE.                                                                                                                                                                                                             |
| alignment           | Logical. If TRUE a peak alignment is applied between all spectra. Default to FALSE.                                                                                                                                                                                                                |
| normalisation       | Logical. If TRUE a normalisation is applied for each spectrum (see <a href="#">normaliseSpectra</a> for details). Default to TRUE.                                                                                                                                                                 |
| ncores              | Number of cores used in parallel evaluation. Default to 1.                                                                                                                                                                                                                                         |
| verbose             | A boolean value to allow print out process information.                                                                                                                                                                                                                                            |
| ...                 | Further arguments to be passed to the functions <a href="#">read.table</a> , <a href="#">importSpectraBruker</a> , <a href="#">Normalization</a> (PepsNMR-package), <a href="#">alignSpectra</a> or <a href="#">normaliseSpectra</a> for specifying the parameters of the algorithm, if necessary. |

## Details

Some preprocessing steps are included during the importation. First, spectra are baseline corrected if `baseline.correction = TRUE`. Then, all spectrum definition domains are aligned to a unique one (either the one specified in `ppm.grid` or the grid of the default library). Finally, all spectra are normalised if `normalisation = TRUE` and aligned if `alignment = TRUE`.

## Value

A data frame with spectra in columns and chemical shifts (in ppm) in rows.

## References

Wang, K.C., Wang, S.Y., Kuo, C.H., Tseng Y.J. (2013). Distribution-based classification method for baseline correction of metabolomic 1D proton nuclear magnetic resonance spectra. *Analytical Chemistry*, **85**(2), 1231-1239.

## See Also

[importSpectraBruker](#) [normaliseSpectra](#) [alignSpectra](#)

## Examples

```
## Import from txt file
current_path <- system.file("extdata", package = "ASICS")
spectra_data <- importSpectra(name.dir = current_path,
                             name.file = "spectra_example.txt", type.import = "txt")

## Import from fid file
current_path <- system.file("extdata", "example_spectra", package = "ASICS")
spectra_data <- importSpectra(name.dir = current_path, type.import = "fid",
                             subdirs = TRUE, dirs.names = TRUE)

## Import from txt file
current_path <- system.file("extdata", "example_spectra", package = "ASICS")
spectra_data <- importSpectra(name.dir = current_path, type.import = "1r")
```

---

|                     |                                                                  |
|---------------------|------------------------------------------------------------------|
| importSpectraBruker | <i>Import preprocessed metabolomic spectra from Bruker files</i> |
|---------------------|------------------------------------------------------------------|

---

## Description

Import preprocessed spectra from Bruker files contained in a single folder. This folder contains one subfolder for each sample. (optional) Spectra are baseline corrected, aligned and normalised by the area under the curve during the importation.

## Usage

```
importSpectraBruker(  
  name.dir,  
  which.spectra = "first",  
  ppm.grid = NULL,  
  sample.names = NULL,  
  ncores = 1,  
  verbose = TRUE  
)
```

## Arguments

|               |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
|---------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| name.dir      | Path of the folder containing one subfolder by sample. Each subfolder contains the Bruker files of this sample.                                                                                                                                                                                                                                                                                                                                                                                  |
| which.spectra | If there is no folder with experiment number (all_spectra/<spectrum_name>/pdata/...) set which.spectra to NULL. Else if there is more than one spectrum by sample (all_spectra/<spectrum_name>/<experiment_number>/pdata/...), which is the spectrum to import (either always the first one with which.spectra = "first", always the last one with which.spectra = "last" or a vector of length the number of spectra that specifies the number of each spectrum to import). Default to "first". |
| ppm.grid      | Numeric vector of a unique grid (definition domain) for all spectra (in ppm). Default to NULL (in which case, the default grid of the pure library is used).                                                                                                                                                                                                                                                                                                                                     |
| sample.names  | Character vector of sample names. Default to NULL (in which case, folder names are used).                                                                                                                                                                                                                                                                                                                                                                                                        |
| ncores        | Number of cores used in parallel evaluation. Default to 1.                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| verbose       | A boolean value to allow print out process information.                                                                                                                                                                                                                                                                                                                                                                                                                                          |

## Value

A data frame with spectra in columns and chemical shifts (in ppm) in rows.

## See Also

[normaliseSpectra](#) [alignSpectra](#)

## Examples

```
current_path <- system.file("extdata", "example_spectra", package = "ASICS")  
spectra_data <- importSpectraBruker(current_path)
```

kruskalWallis

*Kruskal-Wallis rank sum tests on a [SummarizedExperiment](#) object***Description**

Perform Kruskal-Wallis tests on a [SummarizedExperiment](#) object obtained with the [formatForAnalysis](#) function

**Usage**

```
kruskalWallis(
  analysis_data,
  condition,
  alpha = 0.05,
  type.data = "quantifications",
  ...
)
```

**Arguments**

|               |                                                                                                                                                                                   |
|---------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| analysis_data | A <a href="#">SummarizedExperiment</a> object obtained with the <a href="#">formatForAnalysis</a> function.                                                                       |
| condition     | The name of the design variable (two level factor) specifying the group of each sample.                                                                                           |
| alpha         | Cutoff for adjusted p-values. Default to 0.05.                                                                                                                                    |
| type.data     | Type of data used for the analyses ( <i>e.g.</i> ,                                                                                                                                |
| ...           | Arguments to be passed to <a href="#">p.adjust</a> such as the correction method to use with the method argument. "quantifications", "buckets"...). Default to "quantifications". |

**Value**

A S4 object of class [AnalysisResults](#) containing test results.

**See Also**

[AnalysisResults](#)

**Examples**

```
# Import quantification results
if (require("ASICSdata", quietly = TRUE)) {
  quantif_path <- system.file("extdata", "results_ASICS.txt",
                             package = "ASICSdata")
  quantification <- read.table(quantif_path, header = TRUE, row.names = 1)

  # Import design
```

```

design <- read.table(system.file("extdata", "design_diabete_example.txt",
                             package = "ASICSdata"), header = TRUE)
design$condition <- factor(design$condition)

# Create object for analysis and remove features with more than 25% of
# zeros
analysis_obj <- formatForAnalysis(quantification,
                                zero.threshold = 25, design = design)
res_tests <- kruskalWallis(analysis_obj, "condition", method = "BH")
}

```

---

|                  |                      |
|------------------|----------------------|
| normaliseSpectra | <i>Normalisation</i> |
|------------------|----------------------|

---

## Description

Normalise a data frame of spectra to a constant sum (CS) or with a method of PepsNMR package (see [Normalization](#)).

## Usage

```
normaliseSpectra(spectra, type.norm = "CS", verbose = TRUE, ...)
```

## Arguments

|           |                                                                                                                                                                               |
|-----------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| spectra   | Data frame with spectra in columns and chemical shifts in rows. Colnames of this data frame correspond to pure metabolite names and rownames to chemical shift grid (in ppm). |
| type.norm | Type of normalisation : "CS", "mean", "pqn", "median", "firstquartile" or "peak". Default to "CS".                                                                            |
| verbose   | A boolean value to allow print out process information.                                                                                                                       |
| ...       | other arguments to be passed to <a href="#">Normalization</a>                                                                                                                 |

## Value

A data frame with normalised spectra in columns and chemical shifts (in ppm) in rows.

## Examples

```

current_path <- system.file("extdata", package = "ASICS")
spectra_data <- importSpectra(name.dir = current_path,
                             name.file = "spectra_example.txt", type.import = "txt")
spectra_norm <- normaliseSpectra(spectra_data, type.norm = "pqn")

```

---

|        |                                                                                                                                     |
|--------|-------------------------------------------------------------------------------------------------------------------------------------|
| oplsda | <i>Orthogonal projections to latent structures discriminant analysis (OPLS-DA) on a <a href="#">SummarizedExperiment</a> object</i> |
|--------|-------------------------------------------------------------------------------------------------------------------------------------|

---

## Description

Perform an OPLS-DA with the function of the [ropls](#) package on a [SummarizedExperiment](#) object obtained with the [formatForAnalysis](#) function

## Usage

```
oplsda(
  analysis_data,
  condition,
  cross.val = 1,
  thres.VIP = 1,
  type.data = "quantifications",
  seed = 12345,
  ...
)
```

## Arguments

|               |                                                                                                                                   |
|---------------|-----------------------------------------------------------------------------------------------------------------------------------|
| analysis_data | A <a href="#">SummarizedExperiment</a> object obtained with the <a href="#">formatForAnalysis</a> function.                       |
| condition     | The name of the design variable (two level factor) specifying the response to be explained.                                       |
| cross.val     | Number of cross validation folds.                                                                                                 |
| thres.VIP     | A number specifying the VIP threshold used to identify influential variables.                                                     |
| type.data     | Type of data used for the analyses ( <i>e.g.</i> , "quantifications", "buckets"...). Default to "quantifications".                |
| seed          | Random seed to control randomness of cross validation folds.                                                                      |
| ...           | Further arguments to be passed to the function <a href="#">opls</a> for specifying the parameters of the algorithm, if necessary. |

## Value

A S4 object of class [AnalysisResults](#) containing OPLS-DA results.

## References

Trygg, J. and Wold, S. (2002). Orthogonal projections to latent structures (O-PLS). *Journal of Chemometrics*, **16**(3), 119–128.

Thevenot, E.A., Roux, A., Xu, Y., Ezan, E., Junot, C. 2015. Analysis of the human adult urinary metabolome variations with age, body mass index and gender by implementing a comprehensive workflow for univariate and OPLS statistical analyses. *Journal of Proteome Research*. **14**:3322-3335.

**See Also**[AnalysisResults](#)**Examples**

```
# Import quantification results
if (require("ASICSdata", quietly = TRUE)) {
  quantif_path <- system.file("extdata", "results_ASICS.txt",
                             package = "ASICSdata")
  quantification <- read.table(quantif_path, header = TRUE, row.names = 1)

  # Import design
  design <- read.table(system.file("extdata", "design_diabete_example.txt",
                                  package = "ASICSdata"), header = TRUE)
  design$condition <- factor(design$condition)

  # Create object for analysis and remove features with more than 25% of
  # zeros
  analysis_obj <- formatForAnalysis(quantification,
                                   zero.threshold = 25, design = design)
  res_oplsda <- oplsda(analysis_obj, "condition", orthoI = 1)
}
```

pca

*Principal Component Analysis (PCA) on a [SummarizedExperiment](#) object*

**Description**

Perform a PCA with the function of the [ropls](#) package on a [SummarizedExperiment](#) object obtained from the [formatForAnalysis](#) function

**Usage**

```
pca(
  analysis_data,
  scale.unit = TRUE,
  type.data = "quantifications",
  condition = NULL
)
```

**Arguments**

|               |                                                                                                             |
|---------------|-------------------------------------------------------------------------------------------------------------|
| analysis_data | A <a href="#">SummarizedExperiment</a> object obtained from the <a href="#">formatForAnalysis</a> function. |
| scale.unit    | Logical. If TRUE, data are scaled to unit variance prior PCA.                                               |

|           |                                                                                                                                    |
|-----------|------------------------------------------------------------------------------------------------------------------------------------|
| type.data | Type of data used for the analysis (e.g., "quantifications", "buckets"...). Default to "quantifications".                          |
| condition | The name of the design variable (two level factor) specifying the groups, if one is available. Default to NULL, no group provided. |

**Value**

A S4 object of class [AnalysisResults](#) containing PCA results.

**See Also**

[AnalysisResults](#)

**Examples**

```
# Import quantification results
if (require("ASICSdata", quietly = TRUE)) {
  quantif_path <- system.file("extdata", "results_ASICS.txt",
                             package = "ASICSdata")
  quantification <- read.table(quantif_path, header = TRUE, row.names = 1)

  # Create object for analysis and remove features with more than 25% of
  # zeros
  analysis_obj <- formatForAnalysis(quantification, zero.threshold = 25)
  res_pca <- pca(analysis_obj)
}
```

---

|               |                  |
|---------------|------------------|
| plotAlignment | <i>Tile plot</i> |
|---------------|------------------|

---

**Description**

Tile plot of spectra to see if an alignment is needed or the result of an alignment.

**Usage**

```
plotAlignment(spectra_obj, xlim = c(0, 10))
```

**Arguments**

|             |                                                                                                       |
|-------------|-------------------------------------------------------------------------------------------------------|
| spectra_obj | An object of class <a href="#">Spectra</a> obtained with the function <a href="#">createSpectra</a> . |
| xlim        | Boundaries for x.                                                                                     |

**Value**

A [ggplot](#) plot of original and reconstructed spectra of one sample in the same figure for [ASICSResults](#) object. In addition, one pure metabolite spectrum (as provided in the reference library) and the deformed one can be superimposed to the plot.

**See Also**[alignSpectra](#)**Examples**

```
# Import data and create object
current_path <- system.file("extdata", "example_spectra", package = "ASICS")
spectra_data <- importSpectraBruker(current_path)
spectra_obj <- createSpectra(spectra_data)
plotAlignment(spectra_obj, xlim = c(3,4))
```

---

|                   |                          |
|-------------------|--------------------------|
| PureLibrary-class | <i>Class</i> PureLibrary |
|-------------------|--------------------------|

---

**Description**

Objects of class `PureLibrary` contain a set of pure metabolite NMR spectra, used as a reference for the quantification. This class is an extension of the class [Spectra](#), with an additional slot (number of protons for each metabolite) needed for spectrum quantification.

**Slots**

`nb.protons` Numeric vector of the number of protons of each pure metabolite spectra.

**Methods**

Multiple methods can be applied on [PureLibrary](#) objects.

- As usual for S4 object, show and summary methods are available, see [Object summary](#)
- All slots have an accessor `get_slot` name, see [Accessors](#)
- Two objects can be combined or a subset can be extracted, see [Combine and subset methods](#)
- All spectra contained in an object can be represented in a plot, see [Visualisation methods](#)

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

---

pure\_library

*Pure spectra library*

---

### Description

The 1D <sup>1</sup>H NMR spectra of 191 reference compounds were collected to build the default library of reference spectra. These compounds have been prepared and measured using a Bruker Avance III HD spectrometer in the MetaToul - AXIOM Site at Toulouse (France). For more details on the preparation, please see Tardivel et al. (2017).

### Format

A [PureLibrary](#) object with 4 entries:

**sample.name** names of the metabolites

**ppm.grid** common grid for all spectra

**spectra** data frame with each pure metabolite spectrum in column

**nb.protons** number of protons of each metabolite

### References

Tardivel P., Canlet C., Lefort G., Tremblay-Franco M., Debrauwer L., Concordet D., Servien R. (2017). ASICS: an automatic method for identification and quantification of metabolites in complex 1D <sup>1</sup>H NMR spectra. *Metabolomics*, **13**(10): 109. <https://doi.org/10.1007/s11306-017-1244-5>

---

simulate\_spectra

*Simulate a set of spectra*

---

### Description

Simulate a set of spectra based on the default library with shifts

### Usage

```
simulate_spectra(  
  n.spectra,  
  max.shift = 0.02,  
  metab.percent = 0.5,  
  metab.different = 4,  
  add.noise = 0.07,  
  mult.noise = 0.09  
)
```

**Arguments**

|                                    |                                                                                                                   |
|------------------------------------|-------------------------------------------------------------------------------------------------------------------|
| <code>n.spectra</code>             | Number of spectra to simulate.                                                                                    |
| <code>max.shift</code>             | Maximum shift allowed for artificial deformation of pure spectra (default to 0.02).                               |
| <code>metab.percent</code>         | Percentage of present metabolites in complex spectra (default to 0.5).                                            |
| <code>metab.different</code>       | Number of metabolites that are different between each complex spectra (default to 4).                             |
| <code>add.noise, mult.noise</code> | additive and multiplicative noises. By default, <code>add.noise = 0.15</code> and <code>mult.noise = 0.172</code> |

**Value**

A list with a data frame of simulated spectra in columns and a data frame of simulated quantifications.

**Examples**

```
spectra <- simulate_spectra(n.spectra = 10)
```

Spectra-class

Class *Spectra***Description**

Objects of class *Spectra* contain a set of NMR spectra. It includes preprocessed spectra and can be created with the function `createSpectra`.

**Slots**

|                          |                                                                                                                                                                        |
|--------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>sample.name</code> | Character vector of sample names.                                                                                                                                      |
| <code>ppm.grid</code>    | Numeric vector of a unique grid (definition domain) for all spectra (in ppm).                                                                                          |
| <code>spectra</code>     | Numeric matrix with all spectra in columns. Columns must be in the same order as for <code>sample.name</code> and rows correspond to points of <code>ppm.grid</code> . |
| <code>norm.method</code> | Character specifying the normalisation method to use on spectra                                                                                                        |
| <code>norm.params</code> | List containing normalisation parameters (see <code>normaliseSpectra</code> for details).                                                                              |

**Methods**

Multiple methods can be applied on *Spectra* objects.

- As usual for S4 object, show and summary methods are available, see [Object summary](#)
- All slots have an accessor `get_slot` name, see [Accessors](#)
- Two objects can be combined or a subset can be extracted, see [Combine and subset methods](#)
- All spectra contained in an object can be represented in a plot, see [Visualisation methods](#)

---

summary-methods*Summary methods*

---

## Description

Methods available to summarize the various S4 objects of ASICS package.

## Usage

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

## S4 method for signature 'Spectra'
summary(object)

## S4 method for signature 'Spectra'
length(x)

## S4 method for signature 'Spectra'
dim(x)

## S4 method for signature 'ASICSResults'
show(object)

## S4 method for signature 'ASICSResults'
dim(x)

## S4 method for signature 'AnalysisResults'
show(object)

## S4 method for signature 'AnalysisResults'
summary(object)
```

## Arguments

|        |                                                                                                                                              |
|--------|----------------------------------------------------------------------------------------------------------------------------------------------|
| object | An object of class <a href="#">Spectra</a> , <a href="#">PureLibrary</a> , <a href="#">ASICSResults</a> or <a href="#">AnalysisResults</a> . |
| x      | An object of class <a href="#">Spectra</a> , <a href="#">PureLibrary</a> or <a href="#">ASICSResults</a> .                                   |

## Value

A summary of the object, its length or its dimensions.

## Examples

```
# Import data and create object
current_path <- file.path(system.file("extdata", package = "ASICS"),
                           "spectra_example.txt")
```

```
spectra_data <- read.table(current_path, header = TRUE, row.names = 1)
spectra_obj <- createSpectra(spectra_data)

# Summary
summary(spectra_obj)
# Length
length(spectra_obj)
# Dimensions
dim(spectra_obj)
```

---

visualisation-methods-analyses

*Visualisation methods*


---

## Description

Method available to plot results of analyses in ASICS package.

## Usage

```
## S4 method for signature 'AnalysisResults,ANY'
plot(
  x,
  y,
  ...,
  graph = c("default", "ind", "var", "eig", "boxplot", "buckets"),
  add.label = TRUE,
  n.label.var = 10,
  axes = c(1, 2),
  col.ind = NULL,
  xlim = c(0.5, 10),
  ylim = NULL
)
```

## Arguments

|             |                                                                                                                                                                                                                                                                                                                                                                                                                         |
|-------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| x           | An object of class <a href="#">AnalysisResults</a> .                                                                                                                                                                                                                                                                                                                                                                    |
| y           | Currently not used.                                                                                                                                                                                                                                                                                                                                                                                                     |
| ...         | Currently not used.                                                                                                                                                                                                                                                                                                                                                                                                     |
| graph       | A vector specifying what to plot. Allowed values are "eig" for the scree-graph (PCA), "ind" for plot of individuals (PCA and OPLS-DA), "var" for plot of variables (PCA and OPLS-DA), "boxplot" for boxplots of test results and "buckets" to show significant or influential buckets on the mean spectrum. Default value is "default" ( <i>i.e.</i> , c("ind", "var") for PCA and OPLS-DA and c("boxplot") for tests). |
| add.label   | If TRUE, labels are added on individual plot.                                                                                                                                                                                                                                                                                                                                                                           |
| n.label.var | An integer indicating the number of label to add on variable plot.                                                                                                                                                                                                                                                                                                                                                      |

|            |                                                                                                                          |
|------------|--------------------------------------------------------------------------------------------------------------------------|
| axes       | A numeric vector of length 2 specifying the dimensions to be plotted for individual and variable plots.                  |
| col.ind    | A character specifying the name of the design variable used to color the observations by groups for PCA individual plot. |
| xlim, ylim | Boundaries for x and y, respectively.                                                                                    |

### Value

- PCA: a [ggplot](#) plot that allows for the visualisation of PCA results (eigen values, individuals and variables)
- OPLS-DA: a [ggplot](#) plot that allows for the visualisation of OPLS-DA results (individuals and variables). If `cross.val > 1` in [oplsda](#), the best model is plotted.

### Examples

```
# Import quantification results
if (require("ASICSdata", quietly = TRUE)) {
  quantif_path <- system.file("extdata", "results_ASICS.txt",
                             package = "ASICSdata")
  quantification <- read.table(quantif_path, header = TRUE, row.names = 1)

  # Import design
  design <- read.table(system.file("extdata", "design_diabete_example.txt",
                                  package = "ASICSdata"), header = TRUE)
  design$condition <- factor(design$condition)

  # Create object for analysis and remove metabolites with more than 25% of
  # zeros
  analysis_obj <- formatForAnalysis(quantification,
                                    zero.threshold = 25, design = design)

  # Perform a PCA and plot results
  res_pca <- pca(analysis_obj)
  plot(res_pca)

  # Perform an OPLS-DA and plot results
  res_oplsda <- oplsda(analysis_obj, "condition", orthoI = 1)
  plot(res_oplsda)
}
```

---

visualisation-methods-spectra

*Visualisation methods*

---

### Description

Methods available to plot one object in ASICS package.

**Usage**

```
## S4 method for signature 'Spectra,ANY'
plot(x, y, xlim = c(0.5, 10), ylim = NULL, ...)

## S4 method for signature 'ASICSResults,ANY'
plot(
  x,
  y,
  idx = 1,
  xlim = c(0.5, 10),
  ylim = NULL,
  pure.library = NULL,
  add.metab = NULL,
  ...
)
```

**Arguments**

|              |                                                                                                                         |
|--------------|-------------------------------------------------------------------------------------------------------------------------|
| x            | An object of class <a href="#">Spectra</a> , <a href="#">PureLibrary</a> or <a href="#">ASICSResults</a> .              |
| y            | Currently not used.                                                                                                     |
| xlim, ylim   | Boundaries for x and y, respectively.                                                                                   |
| ...          | Currently not used.                                                                                                     |
| idx          | Index of the spectrum to plot. Default to 1.                                                                            |
| pure.library | Pure library used for the quantification. Default to NULL (in which case, the library included in the package is used). |
| add.metab    | Name of one metabolite to add to the plot. Default to NULL (in which case, no pure spectrum added to the plot).         |

**Value**

- A [ggplot](#) plot of all spectra (or of a subset) on the same figure for [Spectra](#) and [PureLibrary](#) objects.
- A [ggplot](#) plot of original and reconstructed spectra of one sample in the same figure for [ASICSResults](#) object. In addition, one pure metabolite spectrum (as provided in the reference library) and the deformed one can be superimposed to the plot.

**Examples**

```
# Import data and create object
current_path <- system.file("extdata", "example_spectra", package = "ASICS")
spectra_data <- importSpectraBruker(current_path)
spectra_obj <- createSpectra(spectra_data)
spectra_obj <- createSpectra(spectra_data)

# Plot the spectra
plot(spectra_obj)
```

# Index

- [,ASICSResults,ANY,ANY,ANY-method  
(combineAndSubset-methods), 11
- [,PureLibrary,ANY,ANY,ANY-method  
(combineAndSubset-methods), 11
- [,Spectra,ANY,ANY,ANY-method  
(combineAndSubset-methods), 11
- [.ASICSResults  
(combineAndSubset-methods), 11
- [.PureLibrary  
(combineAndSubset-methods), 11
- [.Spectra (combineAndSubset-methods), 11
  
- Accessors, 5, 8, 23, 25
- accessors-methods, 2
- alignSpectra, 4, 15–17, 23
- AnalysisResults, 4, 5, 18, 20–22, 26, 27
- AnalysisResults-class, 5
- ASICS, 6
- ASICSResults, 4, 7, 8, 11, 22, 26, 29
- ASICSResults-class, 8
- ASICSUsersGuide, 9
  
- binning, 9
  
- c,ASICSResults-method  
(combineAndSubset-methods), 11
- c,PureLibrary-method  
(combineAndSubset-methods), 11
- c,Spectra-method  
(combineAndSubset-methods), 11
- c.ASICSResults  
(combineAndSubset-methods), 11
- c.PureLibrary  
(combineAndSubset-methods), 11
- c.Spectra (combineAndSubset-methods), 11
- Combine and subset methods, 8, 23, 25
- combineAndSubset-methods, 11
- createPureLibrary, 12
- createSpectra, 6, 7, 13, 22, 25
  
- dim,ASICSResults-method  
(summary-methods), 26
- dim,Spectra-method (summary-methods), 26
- dim.Spectra (summary-methods), 26
  
- formatForAnalysis, 13, 18, 20, 21
  
- getBestModel (accessors-methods), 2
- getBestModel,AnalysisResults-method  
(accessors-methods), 2
- getCError (accessors-methods), 2
- getCError,AnalysisResults-method  
(accessors-methods), 2
- getDataset (accessors-methods), 2
- getDataset,AnalysisResults-method  
(accessors-methods), 2
- getDeformedLibrary (accessors-methods),  
2
- getDeformedLibrary,ASICSResults-method  
(accessors-methods), 2
- getMeanByGroup (accessors-methods), 2
- getMeanByGroup,AnalysisResults-method  
(accessors-methods), 2
- getNbProtons (accessors-methods), 2
- getNbProtons,PureLibrary-method  
(accessors-methods), 2
- getNormMethod (accessors-methods), 2
- getNormMethod,Spectra-method  
(accessors-methods), 2
- getNormParams (accessors-methods), 2
- getNormParams,Spectra-method  
(accessors-methods), 2
- getPpmGrid (accessors-methods), 2
- getPpmGrid,Spectra-method  
(accessors-methods), 2
- getQuantification (accessors-methods), 2
- getQuantification,ASICSResults-method  
(accessors-methods), 2
- getReconstructedSpectra  
(accessors-methods), 2

- getReconstructedSpectra, ASICSResults-method (accessors-methods), [2](#)
- getResults (accessors-methods), [2](#)
- getResults, AnalysisResults-method (accessors-methods), [2](#)
- getSampleName (accessors-methods), [2](#)
- getSampleName, Spectra-method (accessors-methods), [2](#)
- getSpectra (accessors-methods), [2](#)
- getSpectra, Spectra-method (accessors-methods), [2](#)
- getTypeAnalysis (accessors-methods), [2](#)
- getTypeAnalysis, AnalysisResults-method (accessors-methods), [2](#)
- getTypeData (accessors-methods), [2](#)
- getTypeData, AnalysisResults-method (accessors-methods), [2](#)
- ggplot, [22](#), [28](#), [29](#)
- importSpectra, [13](#), [15](#)
- importSpectraBruker, [15](#), [16](#), [16](#)
- kruskalWallis, [5](#), [13](#), [18](#)
- length, Spectra-method (summary-methods), [26](#)
- length.Spectra (summary-methods), [26](#)
- normaliseSpectra, [10](#), [13](#), [15–17](#), [19](#), [25](#)
- Normalization, [15](#), [19](#)
- Object summary, [5](#), [8](#), [23](#), [25](#)
- opls, [5](#), [20](#)
- oplsda, [5](#), [13](#), [20](#), [28](#)
- p.adjust, [18](#)
- pca, [5](#), [13](#), [21](#)
- plot, AnalysisResults, ANY-method (visualisation-methods-analyses), [27](#)
- plot, ASICSResults, ANY-method (visualisation-methods-spectra), [28](#)
- plot, Spectra, ANY-method (visualisation-methods-spectra), [28](#)
- plot.AnalysisResults (visualisation-methods-analyses), [27](#)
- plot.ASICSResults (visualisation-methods-spectra), [28](#)
- plot.Spectra (visualisation-methods-spectra), [28](#)
- plotAlignment, [22](#)
- pure\_library, [7](#), [24](#)
- PureLibrary, [4](#), [6](#), [11](#), [12](#), [23](#), [24](#), [26](#), [29](#)
- PureLibrary-class, [23](#)
- read.table, [15](#)
- ropls, [5](#), [20](#), [21](#)
- show, AnalysisResults-method (summary-methods), [26](#)
- show, ASICSResults-method (summary-methods), [26](#)
- show, Spectra-method (summary-methods), [26](#)
- show.AnalysisResults (summary-methods), [26](#)
- show.ASICSResults (summary-methods), [26](#)
- show.Spectra (summary-methods), [26](#)
- simulate\_spectra, [24](#)
- Spectra, [4](#), [6](#), [8](#), [11](#), [13](#), [22](#), [23](#), [25](#), [26](#), [29](#)
- Spectra-class, [25](#)
- SummarizedExperiment, [5](#), [13](#), [14](#), [18](#), [20](#), [21](#)
- summary, AnalysisResults-method (summary-methods), [26](#)
- summary, Spectra-method (summary-methods), [26](#)
- summary-methods, [26](#)
- summary.AnalysisResults (summary-methods), [26](#)
- summary.Spectra (summary-methods), [26](#)
- Visualisation methods, [5](#), [8](#), [23](#), [25](#)
- visualisation-methods-analyses, [27](#)
- visualisation-methods-spectra, [28](#)