

# Package ‘ChemoSpec’

June 7, 2023

**Type** Package

**Title** Exploratory Chemometrics for Spectroscopy

**Version** 6.1.9

**Date** 2023-06-06

**Description** A collection of functions for top-down exploratory data analysis of spectral data including nuclear magnetic resonance (NMR), infrared (IR), Raman, X-ray fluorescence (XRF) and other similar types of spectroscopy. Includes functions for plotting and inspecting spectra, peak alignment, hierarchical cluster analysis (HCA), principal components analysis (PCA) and model-based clustering. Robust methods appropriate for this type of high-dimensional data are available. ChemoSpec is designed for structured experiments, such as metabolomics investigations, where the samples fall into treatment and control groups. Graphical output is formatted consistently for publication quality plots. ChemoSpec is intended to be very user friendly and to help you get usable results quickly. A vignette covering typical operations is available.

**License** GPL-3

**Depends** R ( $\geq 3.5$ ), ChemoSpecUtils ( $\geq 1.0$ )

**Imports** plyr, stats, utils, grDevices, reshape2, readJDX ( $\geq 0.6$ ), patchwork, ggplot2, plotly, magrittr

**Suggests** IDPmisc, knitr, js, NbClust, lattice, baseline, mclust, pls, R.utils, RColorBrewer, seriation, MASS, grid, pcaPP, jsonlite, signal, speaq, tinytest, elasticnet, irlba, rmarkdown, bookdown, chemometrics, hyperSpec, amap, robustbase, gsubfn, roxut

**URL** <https://bryanhanson.github.io/ChemoSpec/>

**BugReports** <https://github.com/bryanhanson/ChemoSpec/issues>

**ByteCompile** TRUE

**VignetteBuilder** knitr

**Encoding** UTF-8

**RoxygenNote** 7.2.3

**NeedsCompilation** no

**Author** Bryan A. Hanson [aut, cre] (<<https://orcid.org/0000-0003-3536-8246>>),  
 Mike Bostock [cph, ctb] (author of the d3.js library used by  
 plotSpectraJS, <http://d3js.org>),  
 Matt Keinsley [ctb] (author of initial AOV-PCA code),  
 Tejasvi Gupta [ctb] (author of ggplot2 and plotly graphics)

**Maintainer** Bryan A. Hanson <[hanson@depauw.edu](mailto:hanson@depauw.edu)>

**Repository** CRAN

**Date/Publication** 2023-06-07 11:00:02 UTC

## R topics documented:

ChemoSpec-package . . . . .	3
aovPCALoadings . . . . .	4
aovPCAScores . . . . .	5
aov_pcaSpectra . . . . .	6
averageReplicates . . . . .	8
baselineSpectra . . . . .	9
binSpectra . . . . .	10
check4Gaps . . . . .	11
chkGraphicsOpt . . . . .	11
chkSpectra . . . . .	11
clupaSpectra . . . . .	12
colorSymbol . . . . .	13
conColScheme . . . . .	13
cv_pcaSpectra . . . . .	13
c_pcaSpectra . . . . .	15
evalClusters . . . . .	16
files2SpectraObject . . . . .	17
hcaScores . . . . .	21
hcaSpectra . . . . .	22
hmapSpectra . . . . .	23
hypTestScores . . . . .	24
irlba_pcaSpectra . . . . .	26
mclust3dSpectra . . . . .	27
mclustSpectra . . . . .	29
metMUD1 . . . . .	30
normSpectra . . . . .	31
pcaDiag . . . . .	33
plot2Loadings . . . . .	35
plot3dScores . . . . .	36
plotLoadings . . . . .	37
plotScores . . . . .	38
plotScree . . . . .	38
plotSpectra . . . . .	39
plotSpectraDist . . . . .	40

plotSpectraJS . . . . .	42
removeFreq . . . . .	43
removeGroup . . . . .	43
removeSample . . . . .	44
reviewAllSpectra . . . . .	44
rowDist . . . . .	45
r_pcaSpectra . . . . .	45
sampleDist . . . . .	46
sgfSpectra . . . . .	47
Spectra . . . . .	48
splitSpectraGroups . . . . .	49
sPlotSpectra . . . . .	50
SrE.IR . . . . .	51
sumGroups . . . . .	52
sumSpectra . . . . .	52
surveySpectra . . . . .	53
s_pcaSpectra . . . . .	54
updateGroups . . . . .	56
<b>Index</b>	<b>57</b>

## Description

A collection of functions for top-down exploratory data analysis of spectral data obtained via nuclear magnetic resonance (NMR), infrared (IR) or Raman spectroscopy. Includes functions for plotting and inspecting spectra, peak alignment, hierarchical cluster analysis (HCA), principal components analysis (PCA) and model-based clustering. Robust methods appropriate for this type of high-dimensional data are available. ChemoSpec is designed with metabolomics data sets in mind, where the samples fall into groups such as treatment and control. Graphical output is formatted consistently for publication quality plots. ChemoSpec is intended to be very user friendly and help you get usable results quickly. A vignette covering typical operations is available.

## Author(s)

Bryan A. Hanson (DePauw University), Tejasvi Gupta & Matthew J. Keinsley.

Maintainer: Bryan A. Hanson <hanson@depauw.edu>

## See Also

Additional documentation at <https://bryanhanson.github.io/ChemoSpec/>

---

`aovPCALoadings`*Plot aovPCAscores Loadings of a Spectra Object*

---

**Description**

Uses the results from [aovPCAscores](#) to plot the corresponding loadings.

**Usage**

```
aovPCALoadings(spectra, PCA, submat = 1, loads = 1, ref = 1, ...)
```

**Arguments**

<code>spectra</code>	An object of S3 class <a href="#">Spectra()</a> .
<code>PCA</code>	List of pca results created by <a href="#">aov_pcaSpectra</a> .
<code>submat</code>	Integer. Selects list element <code>submat</code> from <code>PCA</code> which is a list of PCA results, each corresponding to the computation in <a href="#">aov_pcaSpectra</a> .
<code>loads</code>	An integer vector giving the loadings to plot.
<code>ref</code>	An integer specifying the reference spectrum to plot, which appears at the bottom of the plot.
<code>...</code>	Parameters to be passed to the plotting routines. <i>Applies to base graphics only.</i>

**Value**

The returned value depends on the graphics option selected (see [GraphicsOptions\(\)](#)).

- `base`: None. Side effect is a plot.
- `ggplot2`: The plot is displayed, and a `ggplot2` object is returned if the value is assigned. The plot can be modified in the usual `ggplot2` manner.

**Author(s)**

Bryan A. Hanson (DePauw University), Matthew J. Keinsley.

**References**

Pinto, Bosc, Nocairi, Barros, and Rutledge. "Using ANOVA-PCA for Discriminant Analysis: ..." *Analytica Chimica Acta* 629.1-2 (2008): 47-55.

Harrington, Vieira, Espinoza, Nien, Romero, and Yergey. "Analysis of Variance–Principal Component Analysis: ..." *Analytica Chimica Acta* 544.1-2 (2005): 118-27.

**See Also**

An example using this function can be seen in [aov\\_pcaSpectra](#). See also [plotLoadings](#). Additional documentation at <https://bryanhanson.github.io/ChemoSpec/>

**Description**

Uses the results from [aov\\_pcaSpectra](#) to plot the scores. Argument `submat` is used to select PCA results from among those stored in argument `PCA`.

**Usage**

```
aovPCAscores(
  spectra,
  so,
  submat = 1,
  ellipse = "none",
  tol = "none",
  use.sym = FALSE,
  leg.loc = "topright",
  ...
)
```

**Arguments**

<code>spectra</code>	An object of S3 class <a href="#">Spectra()</a> .
<code>so</code>	List of <code>pca</code> results created by <a href="#">aov_pcaSpectra</a> .
<code>submat</code>	Integer. Selects list element <code>submat</code> from <code>PCA</code> which is a list of PCA results, each corresponding to the computation in <a href="#">aov_pcaSpectra</a> .
<code>ellipse</code>	A character vector specifying the type of ellipses to be plotted. One of <code>c("both", "none", "cls", "rob")</code> . <code>cls</code> specifies classical confidence ellipses, <code>rob</code> specifies robust confidence ellipses. An ellipse is drawn for each group unless there are three or fewer samples in the group.
<code>tol</code>	A number describing the fraction of points to be labeled. <code>tol = 1.0</code> labels all the points; <code>tol = 0.05</code> labels <i>approximately</i> the most extreme 5 percent. Set to 'none' to completely suppress labels. Note that a simple approach based upon quantiles is used, assumes that both <code>x</code> and <code>y</code> are each normally distributed, and treats <code>x</code> and <code>y</code> separately. Thus, this is not a formal treatment of outliers, just a means of labeling points. Groups are lumped together for the computation.
<code>use.sym</code>	A logical; if <code>TRUE</code> , the color scheme is set to black and the points plotted with symbols. Applies only to <a href="#">Spectra</a> objects.
<code>leg.loc</code>	Character; if "none" no legend will be drawn. Otherwise, any string acceptable to <a href="#">legend</a> .
<code>...</code>	Additional parameters to be passed to <a href="#">plotScores</a> . For example, you can plot confidence ellipses this way. Note that ellipses are drawn based on the groups in <code>spectra\$groups</code> , but the separation done by <a href="#">aov_pcaSpectra</a> is based on argument <code>fac</code> . These may not correspond, but you can edit <code>spectra\$groups</code> to match if necessary.

## Value

The returned value depends on the graphics option selected (see `ChemoSpecUtils::GraphicsOptions()`).

- **base** A data frame or list containing the data plotted. Assign the value and run `str()` or `names()` on it to see what it contains. Side effect is a plot.
- **ggplot2** The plot is displayed, and a `ggplot2` plot object is returned if the value is assigned. The plot can be modified in the usual `ggplot2` manner. If you want the plotted values, you can access them via the base graphics mode.

## Author(s)

Bryan A. Hanson (DePauw University), Matthew J. Keinsley.

## References

Pinto, Bosc, Nocairi, Barros, and Rutledge. "Using ANOVA-PCA for Discriminant Analysis: ..." *Analytica Chimica Acta* 629.1-2 (2008): 47-55.

Harrington, Vieira, Espinoza, Nien, Romero, and Yergey. "Analysis of Variance-Principal Component Analysis: ..." *Analytica Chimica Acta* 544.1-2 (2005): 118-27.

## See Also

The use of this function can be seen in `aov_pcaSpectra`. See also `plotScores`. Additional documentation at <https://bryanhanson.github.io/ChemoSpec/>

---

aov\_pcaSpectra

*ANOVA-PCA Analysis of Spectra Data*

---

## Description

ANOVA-PCA is a combination of both methods developed by Harrington. The data is partitioned into submatrices corresponding to each experimental factor, which are then subjected to PCA separately after adding the residual error back. If the effect of a factor is large compared to the residual error, separation along the 1st PC in the score plot should be evident. With this method, the significance of a factor can be visually determined (ANOVA-PCA is not blind to group membership). ANOVA-PCA with only one factor is the same as standard PCA and gives no additional separation.

## Usage

```
aov_pcaSpectra(spectra, fac, type = "class", choice = NULL, showNames = TRUE)
```

## Arguments

spectra	An object of S3 class <code>Spectra()</code> .
fac	A vector of character strings giving the factors to be used in the analysis. These should be elements of <code>Spectra</code> . Note that there should be 2 or more factors, because ANOVA-PCA on one factor is the same as standard PCA. See the example.
type	Either classical ("cls") or robust ("rob"); Results in either <code>c_pcaSpectra</code> or <code>r_pcaSpectra</code> being called on the <code>Spectra</code> object.
choice	The type of scaling to be performed. See <code>c_pcaSpectra</code> and <code>r_pcaSpectra</code> for details.
showNames	Logical. Show the names of the submatrices in the console.

## Value

A list of PCA results, one for each computed submatrix.

## Author(s)

Bryan A. Hanson (DePauw University), Matthew J. Keinsley.

## References

Pinto, Bosc, Nocairi, Barros, and Rutledge. "Using ANOVA-PCA for Discriminant Analysis: ..." *Analytica Chimica Acta* 629.1-2 (2008): 47-55.

Harrington, Vieira, Espinoza, Nien, Romero, and Yergey. "Analysis of Variance-Principal Component Analysis: ..." *Analytica Chimica Acta* 544.1-2 (2005): 118-27.

## See Also

The output of this function is used in used in `aovPCAscores` and `aovPCAloadings`. Additional documentation at <https://bryanhanson.github.io/ChemoSpec/>

## Examples

```
## Not run:
# This example assumes the graphics output is set to ggplot2 (see ?GraphicsOptions).
library("ggplot2")
data(metMUD2)

# Original factor encoding:
levels(metMUD2$groups)

# Split those original levels into 2 new ones (re-code them)
new.grps <- list(geneBb = c("B", "b"), geneCc = c("C", "c"))
mM3 <- splitSpectraGroups(metMUD2, new.grps)

# run aov_pcaSpectra
PCAs <- aov_pcaSpectra(mM3, fac = c("geneBb", "geneCc"))
```

```

p1 <- aovPCAscores(mM3, PCAs, submat = 1, ellipse = "cls")
p1 <- p1 + ggtitle("aovPCA: B vs b")
p1

p2 <- aovPCAscores(mM3, PCAs, submat = 2)
p2 <- p2 + ggtitle("aovPCA: C vs c")
p2

p3 <- aovPCAscores(mM3, PCAs, submat = 3)
p3 <- p3 + ggtitle("aovPCA: Interaction Term")
p3

p4 <- aovPCALoadings(spectra = mM3, PCA = PCAs)
p4 <- p4 + ggtitle("aov_pcaSpectra: Bb Loadings")
p4

## End(Not run)

```

---

averageReplicates      *Average Replicates in a Spectra Object*

---

## Description

Average the replicates in a [Spectra](#) object and return a new Spectra object with fewer samples. One should probably not do this until each individual sample has been visualized for quality control, in case it is a potential outlier.

## Usage

```
averageReplicates(spectra, uniq)
```

## Arguments

spectra	An object of S3 class <a href="#">Spectra()</a> .
uniq	Character. A character vector containing strings representing unique sample identifiers. The sample names will be searched for these strings, and all samples matching a given string will be averaged and put into a new Spectra object. For example, consider the case where samples are named S_1_01, S_1_02, ..., S_2_01, S_2_02, ... where _01 and so forth signifies replicates of a particular sample. With <code>uniq = c("S_1", "S_2")</code> all S_1 replicates will be averaged and all S_2 replicates will be averaged. N.B. the strings will be used as regex pattern and grepped.

## Value

An object of S3 class [Spectra](#).



**Author(s)**

Bryan A. Hanson (DePauw University).

**Examples**

```
data(SrE.IR)
averaged <- averageReplicates(SrE.IR, uniq = c("EPO", "OO", "adSrE", "pSrE"))
sumSpectra(SrE.IR)
sumSpectra(averaged)
```

---

baselineSpectra      *Baseline Correction of a Spectra Object*

---

**Description**

This function mostly wraps functions in package **baseline** which carries out a variety of baseline correction routines. A simple linear correction method is also available.

**Usage**

```
baselineSpectra(spectra, int = TRUE, retC = FALSE, show = 1, ...)
```

**Arguments**

spectra	An object of S3 class <a href="#">Spectra()</a> .
int	Logical; if TRUE, do the correction interactively using widgets. No results are saved. Use this for inspection and exploration only.
retC	Logical: shall the baseline-corrected spectra be returned in the Spectra object?
show	Integer. A vector giving the sample numbers for which you wish to see the results of the baseline correction. By "sample numbers" we mean the rows in the spectra\$data matrix. To find a specific sample type spectra\$names to see which row contains that sample. To see all samples, use show = 1:nrow(spectra\$data) where spectra is the name of your particular Spectra object.
...	Other arguments passed downstream. The relevant ones can be found in <a href="#">baseline</a> . Be sure to pay attention to argument method as you will probably want to use it. You can also use method = "linear" for a simple linear fit, see Details.

**Details**

In plots using methods from the baseline package, the x axis ticks give the data point index, not the original values from your data. Note that you cannot zoom the non-interactive display of corrected spectra because the underlying function hardwires the display. Try the interactive version instead (int = TRUE), or use [plotSpectra](#) on the corrected data. In addition to the methods provided by baseline, you can also use method = "linear". This correction is handled locally, and is very simple: a line is drawn from the first data point to the last, and this becomes the new baseline. This is most suitable for cases in which the baseline rises or falls steadily, as is often seen in chromatograms.

**Value**

If `int = TRUE`, an interactive plot is created. If `int = FALSE` and `retC = FALSE`, an object of class `baseline` is returned (see [baseline-class](#)). If `int = FALSE` and `retC = TRUE`, a `Spectra` object containing the corrected spectra is returned. In these latter two cases plots are also drawn.

**Author(s)**

Bryan A. Hanson (DePauw University).

**See Also**

Additional documentation at <https://bryanhanson.github.io/ChemoSpec/>

**Examples**

```
# You need to install package "baseline" for this example
if (requireNamespace("baseline", quietly = TRUE)) {
  data(SrE.IR)
  temp <- baselineSpectra(SrE.IR, int = FALSE, method = "modpolyfit")
}
```

---

binSpectra

*Bin or Bucket a Spectra Object*

---

**Description**

This function will bin a `Spectra` object by averaging every `bin.ratio` frequency values, and summing the corresponding intensity values. The net effect is a smoothed and smaller data set. If there are gaps in the frequency axis, each data chunk is processed separately. Note: some folks refer to binning as bucketing.

**Usage**

```
binSpectra(spectra, bin.ratio)
```

**Arguments**

<code>spectra</code>	An object of S3 class <code>Spectra()</code> .
<code>bin.ratio</code>	An integer giving the binning ratio, that is, the number of points to be grouped together into one subset of data.

**Details**

If the frequency range is not divisible by `bin.ratio` to give a whole number, data points are removed from the beginning of the frequency data until it is, and the number of data points removed is reported at the console. If there are gaps in the data where frequencies have been removed, each continuous piece is sent out and binned separately (by `binSpectra`).

**Value**

An object of S3 class [Spectra](#).

**Author(s)**

Bryan A. Hanson (DePauw University).

**See Also**

Additional documentation at <https://bryanhanson.github.io/ChemoSpec/>

**Examples**

```
data(metMUD1)
sumSpectra(metMUD1)
res <- binSpectra(metMUD1, bin.ratio = 4)
sumSpectra(res)
```

---

check4Gaps	<i>Check for Discontinuities (Gaps) in a Vector &amp; Optionally Make a Plot</i>
------------	--

---

**Description**

This function is used by ChemoSpec and ChemoSpec2D, but is formally part of ChemoSpecUtils. You can access full documentation via [check4Gaps](#).

---

chkGraphicsOpt	<i>Check the Graphics Output Option/Mode</i>
----------------	--

---

**Description**

This function is used by ChemoSpec and ChemoSpec2D, but is formally part of ChemoSpecUtils. You can access full documentation via [chkGraphicsOpt](#).

---

chkSpectra	<i>Verify the Integrity of a Spectra or Spectra2D Object</i>
------------	--

---

**Description**

This function is used by ChemoSpec and ChemoSpec2D, but is formally part of ChemoSpecUtils. You can access full documentation via [chkSpectra](#).

---

`clupaSpectra`*Hierarchical Cluster-Based Peak Alignment on a Spectra Object*

---

### Description

This function is a wrapper to several functions in the **speaq** package. It implements the CluPA algorithm described in the reference.

### Usage

```
clupaSpectra(spectra, bT = NULL, ...)
```

### Arguments

<code>spectra</code>	An object of S3 class <code>Spectra()</code> .
<code>bT</code>	Numeric. The baseline threshold. Defaults to five percent of the range of the data, in <code>spectra\$data</code> . Passed to <code>detectSpecPeaks</code> .
<code>...</code>	Other arguments to be passed to the underlying functions.

### Value

A modified `Spectra` object.

### Author(s)

Bryan A. Hanson (DePauw University).

### References

Vu TN, Valkenborg D, Smets K, Verwaest KA, Dommissie R, Lemiere F, Verschoren A, Goethals B, Laukens K. "An integrated workflow for robust alignment and simplified quantitative analysis of NMR spectrometry data" BMC Bioinformatics vol. 12 pg. 405 (2011).

### See Also

Additional documentation at <https://bryanhanson.github.io/ChemoSpec/>

### Examples

```
# You need to install package speaq for this example
# This example assumes the graphics output is set to ggplot2 (see ?GraphicsOptions).
if (requireNamespace("speaq", quietly = TRUE)) {
  library("ggplot2")
  data(alignMUD)

  p1 <- plotSpectra(alignMUD, which = 1:20, lab.pos = 4.5, offset = 0.1,
    yrange = c(0, 5000), amp = 500)
  p1 <- p1 + ggtitle("Misaligned NMR Spectra") +
```

```
    coord_cartesian(xlim = c(1.5, 1.8), ylim = c(0, 1900))
  p1

  aMUD <- clupaSpectra(alignMUD)

  p2 <- plotSpectra(aMUD, which = 1:20, lab.pos = 4.5, offset = 0.1,
    yrange = c(0, 5000), amp = 500)
  p2 <- p2 + ggtitle("Aligned NMR Spectra") +
    coord_cartesian(xlim = c(1.5, 1.8), ylim = c(0, 1900))
  p2
}
```

---

**colorSymbol***Color and Symbols in ChemoSpec and ChemoSpec2D*

---

**Description**

This help page serves both ChemoSpec and ChemoSpec2D, but is formally part of ChemoSpecUtils. You can access full documentation via [colorSymbol](#).

---

**conColScheme***Change the Color Scheme of a Spectra or Spectra2D Object*

---

**Description**

This help page serves both ChemoSpec and ChemoSpec2D, but is formally part of ChemoSpecUtils. You can access full documentation via [conColScheme](#).

---

**cv\_pcaSpectra***Cross-Validation of Classical PCA Results for a Spectra Object*

---

**Description**

This function carries out classical PCA on the data in a [Spectra](#) object using a cross-validation method. A simple re-write of Peter Filzmoser's [pcaCV](#) method with some small plotting changes.

**Usage**

```

cv_pcaSpectra(
  spectra,
  pcs,
  choice = "noscale",
  repl = 50,
  segments = 4,
  segment.type = c("random", "consecutive", "interleaved"),
  length.seg,
  trace = FALSE,
  ...
)

```

**Arguments**

spectra	An object of S3 class <code>Spectra()</code> .
pcs	As per <code>pcaCV</code> where it is called <code>amax</code> ; an integer giving the number of PC scores to include.
choice	A character string indicating the choice of scaling. One of <code>c("noscale", "autoscale", "Pareto")</code> .
repl	As per <code>pcaCV</code> ; the number of replicates to perform.
segments	As per <code>pcaCV</code> .
segment.type	As per <code>pcaCV</code> .
length.seg	As per <code>pcaCV</code> .
trace	As per <code>pcaCV</code> .
...	Parameters to be passed to the plotting routines.

**Value**

Invisibly, a list as described in `pcaCV`. Side effect is a plot.

**Author(s)**

Bryan A. Hanson, DePauw University. Derived from `pcaCV`.

**References**

K. Varmuza and P. Filzmoser *Introduction to Multivariate Statistical Analysis in Chemometrics*, CRC Press, 2009.

**See Also**

`pcaCV` for the underlying function. Additional documentation at <https://bryanhanson.github.io/ChemoSpec/>

## Examples

```
# You need to install package "pls" for this example
if (requireNamespace("pls", quietly = TRUE)) {
  data(SrE.IR)
  pca <- cv_pcaSpectra(SrE.IR, pcs = 5)
}
```

---

c\_pcaSpectra

*Classical PCA of Spectra Objects*

---

## Description

A wrapper which carries out classical PCA analysis on a [Spectra](#) object. The user can select various options for scaling. There is no normalization by rows - do this manually using [normSpectra](#). There is an option to control centering, but this is mainly for compatibility with the [aov\\_pcaSpectra](#) series of functions. Centering the data should always be done in PCA and it is the default here.

## Usage

```
c_pcaSpectra(spectra, choice = "noscale", cent = TRUE)
```

## Arguments

spectra	An object of S3 class <a href="#">Spectra()</a> .
choice	A character string indicating the choice of scaling. One of <code>c("noscale", "autoscale", "Pareto")</code> . "autoscale" is called "standard normal variate" or "correlation matrix PCA" in some literature.
cent	Logical: whether or not to center the data. Always center the data unless you know it to be already centered.

## Details

The scale choice `autoscale` scales the columns by their standard deviation. `Pareto` scales by the square root of the standard deviation.

## Value

An object of class `prcomp`, modified to include a list element called `$method`, a character string describing the pre-processing carried out and the type of PCA performed (used to annotate plots).

## Author(s)

Bryan A. Hanson (DePauw University).

## References

K. Varmuza and P. Filzmoser *Introduction to Multivariate Statistical Analysis in Chemometrics*, CRC Press, 2009.

## See Also

`prcomp` for the underlying function, `s_pcaSpectra` for sparse PCA calculations, `r_pcaSpectra` for robust PCA calculations, `irlba_pcaSpectra` for PCA via the IRLBA algorithm. Additional documentation at <https://bryanhanson.github.io/ChemoSpec/>

For displaying the results, `ChemoSpecUtils::plotScree()`, `ChemoSpecUtils::plotScores()`, `plotLoadings()`, `plot2Loadings()`, `sPlotSpectra()`.

## Examples

```
## Not run:
# This example assumes the graphics output is set to ggplot2 (see ?GraphicsOptions).
library("ggplot2")
data(metMUD1)
pca <- c_pcaSpectra(metMUD1)

p1 <- plotScree(pca)
p1

p2 <- plotScores(metMUD1, pca, pcs = c(1, 2), ellipse = "cls", tol = 0.05)
p2 <- p2 + ggtitle("Scores: metMUD1 NMR Data")
p2

p3 <- plotLoadings(metMUD1, pca, loads = 1:2, ref = 1)
p3 <- p3 + ggtitle("Loadings: metMUD1 NMR Data")
p3

## End(Not run)
```

---

evalClusters

*Evaluate or Compare the Quality of Clusters Quantitatively*

---

## Description

This function is a wrapper for `NbClust` in package **NbClust**. It can be used to quantitatively compare different clustering options.

## Usage

```
evalClusters(spectra, ...)
```



## Arguments

spectra An object of S3 class [Spectra\(\)](#).  
... Other parameters to be passed to the function. In particular, NbClust package will need some parameters. See the example.

## Value

A list giving the results, as described in [NbClust](#).

## Author(s)

Bryan A. Hanson (DePauw University).

## References

M. Charrad et. al. "NbClust: An R Package for Determining the Relevant Number of Clusters in a Data Set." J. Stat. Soft. vol. 61 no. 6 October 2014.

## See Also

[hclust](#) for the underlying base function. [hcaSpectra](#) for HCA analysis of a [Spectra](#) object. [hcaScores](#) for HCA analysis of PCA scores from a [Spectra](#) object. Additional documentation at <https://bryanhanson.github.io/ChemoSpec/>

## Examples

```
## Not run:  
data(metMUD2)  
res <- evalClusters(metMUD2, min.nc = 2, max.nc = 5, method = "average", index = "k1")  
  
## End(Not run)
```

---

files2SpectraObject *Import Data into a Spectra Object*

---

## Description

These functions import data into a [Spectra](#) object. For "csv-like" files they use [read.table](#), so they are very flexible in regard to file formatting. **Be sure to see the ...argument below for important details you need to provide.** files2SpectraObject can also read JCAMP-DX files and will do so if fileExt is any of "dx", "DX", "jdx" or "JDX".

**Usage**

```

files2SpectraObject(
  gr.crit = NULL,
  gr.cols = "auto",
  freq.unit = "no frequency unit provided",
  int.unit = "no intensity unit provided",
  descrip = "no description provided",
  fileExt = "\\.(csv|CSV)$",
  out.file = "mydata",
  debug = FALSE,
  ...
)

matrix2SpectraObject(
  gr.crit = NULL,
  gr.cols = c("auto"),
  freq.unit = "no frequency unit provided",
  int.unit = "no intensity unit provided",
  descrip = "no description provided",
  in.file = NULL,
  out.file = "mydata",
  chk = TRUE,
  ...
)

```

**Arguments**

- |                        |  |
|------------------------|--|
| <code>gr.crit</code>   | Group Criteria. A vector of character strings which will be searched for among the file/sample names in order to assign an individual spectrum to group membership. This is done using <code>grep</code> , so characters like "." (period/dot) do not have their literal meaning (see below). Warnings are issued if there are file/sample names that don't match entries in <code>gr.crit</code> or there are entries in <code>gr.crit</code> that don't match any file names.  |
| <code>gr.cols</code>   | Group Colors. See <a href="#">colorSymbol</a> for some options. One of the following: <ul style="list-style-type: none"> <li>• Legacy behavior and the default: The word "auto", in which case up to 8 colors will be automatically assigned from package <code>RColorBrewer</code> Set1.</li> <li>• "Col7". A unique set of up to 7 colorblind-friendly colors is used.</li> <li>• "Col8". A unique set of up to 8 colors is used.</li> <li>• "Col12". A mostly paired set of up to 12 colors is used.</li> <li>• A vector of acceptable color designations with the same length as <code>gr.crit</code>.</li> </ul> Colors will be assigned one for one, so the first element of <code>gr.crit</code> is assigned the first element of <code>gr.col</code> and so forth. For <code>Col12</code> you should pay careful attention to the order of <code>gr.crit</code> in order to match up colors. |
| <code>freq.unit</code> | A character string giving the units of the x-axis (frequency or wavelength).   |
| <code>int.unit</code>  | A character string giving the units of the y-axis (some sort of intensity).  |

descrip	A character string describing the data set that will be stored. This string is used in some plots so it is recommended that its length be less than about 40 characters.
fileExt	A character string giving the extension of the files to be processed. regex strings can be used. For instance, the default finds files with either ".csv" or ".CSV" as the extension. Matching is done via a grep process, which is greedy. See also the "Advanced Tricks" section.
out.file	A file name. The completed object of S3 class <code>Spectra</code> will be written to this file.
debug	Logical. Applies to <code>files2SpectraObject</code> only. Set to TRUE for troubleshooting when an error is thrown during import. In addition, values of 1-5 will work when importing a JCAMP-DX file via <code>fileExt = "\.jdx"</code> etc. These will be passed through to the <code>readJDX</code> function. See there for much more info on importing JCAMP-DX files.
...	Arguments to be passed to <code>read.table</code> , <code>list.files</code> or <code>readJDX</code> ; see the "Advanced Tricks" section. For <code>read.table</code> , <b>You MUST supply values for sep, dec and header consistent with your file structure, unless they are the same as the defaults for read.table.</b>
in.file	Character. Applies to <code>matrix2SpectraObject</code> only. Input file name, including extension. Can be a vector of file names.
chk	Logical. Applies to <code>matrix2SpectraObject</code> only. Should the Spectra object be checked for integrity? If you are having trouble importing your data, set this to FALSE and do <code>str(your object)</code> to troubleshoot.

### Value

A object of class `Spectra`. An *unnamed* object of S3 class `Spectra` is also written to `out.file`. To read it back into the workspace, use `new.name <- loadObject(out.file)` (`loadObject` is package **R.utils**).

### Functions

- `files2SpectraObject()`: Import data from separate csv files
- `matrix2SpectraObject()`: Import a matrix of data

### files2SpectraObject

`files2SpectraObject` acts on all files in the current working directory with the specified `fileExt` so there should be no extra files of that type hanging around (except see next paragraph). The first column should contain the frequency values and the second column the intensity values. The files may have a header or not (supply `header = TRUE/FALSE` as necessary). The frequency column is assumed to be the same in all files.

If `fileExt` contains any of "dx", "DX", "jdx" or "JDX", then the files will be processed by `readJDX`. Consider setting `debug = TRUE`, or `debug = 1` etc for this format, as there are many options for JCAMP, and many are untested. See `readJDX` for options and known limitations.

### matrix2SpectraObject

This function takes one or more csv-like files, containing frequencies in the first column, and samples in additional columns, and processes it into a [Spectra](#) object. The file MUST have a header row which includes the sample names. There need not be a header for the first (frequency) column. If more than one file given, they must all have the same frequency entries.

### gr.crit and Sample Name Gotchas

The matching of `gr.crit` against the sample file names (in `files2SpectraObject`) or column headers/sample names (in `codematrix2SpectraObject`) is done one at a time, in order, using `grep`. While powerful, this has the potential to lead to some "gotchas" in certain cases, noted below.

Your file system may allow file/sample names which R will not like, and will cause confusing behavior. File/sample names become variables in `ChemoSpec`, and R does not like things like "-" (minus sign or hyphen) in file/sample names. A hyphen is converted to a period (".") if found, which is fine for a variable name. However, a period in `gr.crit` is interpreted from the `grep` point of view, namely a period matches any single character. At this point, things may behave very differently than one might hope. See [make.names](#) for allowed characters in R variables and make sure your file/sample names comply.

The entries in `gr.crit` must be mutually exclusive. For example, if you have files with names like "Control\_1" and "Sample\_1" and use `gr.crit = c("Control", "Sample")` groups will be assigned as you would expect. But, if you have file names like "Control\_1\_Shade" and "Sample\_1\_Sun" you can't use `gr.crit = c("Control", "Sample", "Sun", "Shade")` because each criteria is grepped in order, and the "Sun/Shade" phrases, being last, will form the basis for your groups. Because this is a `grep` process, you can get around this by using regular expressions in your `gr.crit` argument to specify the desired groups in a mutually exclusive manner. In this second example, you could use `gr.crit = c("Control(.*)Sun", "Control(.*)Shade", "Sample(.*)Sun", "Sample(.*)Shade")` to have your groups assigned based upon both phrases in the file names.

To summarize, `gr.crit` is used as a `grep` pattern, and the file/sample names are the target. Make sure your file/sample names comply with [make.names](#).

Finally, samples whose names are not matched using `gr.crit` are still incorporated into the [Spectra](#) object, but they are not assigned a group or color. Therefore they don't plot, but they do take up space in a plot! A warning is issued in these cases, since one wouldn't normally want a spectrum to be orphaned this way.

All these problems can generally be identified by running [sumSpectra](#) once the data is imported.

### Advanced Tricks

The `...` argument can be used to pass any argument to `read.table` or `list.files`. This includes the possibility of passing arguments that will cause trouble later, for instance `na.strings` in `read.table`. While one might successfully read in data with NA, it will eventually cause problems. The intent of this feature is to allow one to recurse a directory tree containing the data, and/or to specify a starting point other than the current working directory. So for instance if the current working directory is not the directory containing the data files, you can use `path = "my_path"` to point to the desired top-level directory, and `recursive = TRUE` to work your way through a set of sub-directories. In addition, if you are reading in JCAMP-DX files, you can pass arguments to `readJDX` via `...`, e.g. `SOFC = FALSE`. Finally, while argument `fileExt` appears to be a file extension (from its

name and the description elsewhere), it's actually just a grep pattern that you can apply to any part of the file name if you know how to construct the proper pattern.

### Author(s)

Bryan A. Hanson (DePauw University).

### See Also

Additional documentation at <https://bryanhanson.github.io/ChemoSpec/>, as well as [updateGroups](#).

### Examples

```
## Not run:
# This example assumes the graphics output is set to ggplot2 (see ?GraphicsOptions).
library("ggplot2")

wd <- getwd() # save current location
setwd(tempdir())

# Grab an included file & move to a temporary directory
tf <- system.file("extdata/PCRF.jdx", package = "ChemoSpec")
chk <- file.copy(from = tf, to = basename(tf))

# Now read in the file, summarize and plot
spec <- files2SpectraObject(
  gr.crit = "PCRF", freq.unit = "ppm", int.unit = "intensity",
  descrip = "test import", fileExt = "\\*.jdx")
sumSpectra(spec)
p <- plotSpectra(spec, lab.pos = 3.5, main = "Reduced Fat Potato Chip")
p <- p + ggtitle("Reduced Fat Potato Chip")
p

setwd(wd) # restore working directory

## End(Not run)
```

---

hcaScores

*HCA on PCA/MIA/PARAFAC scores from a Spectra or Spectra2D Object*

---

### Description

This function is used by ChemoSpec and ChemoSpec2D, but is formally part of ChemoSpecUtils. You can access full documentation via [hcaScores](#).

---

`hcaSpectra`*Plot HCA Results of a Spectra Object*

---

**Description**

A wrapper which carries out HCA and plots a dendrogram colored by the information in a `Spectra` object. Many methods for computing the clusters and distances are available.

**Usage**

```
hcaSpectra(  
  spectra,  
  c.method = "complete",  
  d.method = "euclidean",  
  use.sym = FALSE,  
  leg.loc = "topright",  
  ...  
)
```

**Arguments**

<code>spectra</code>	An object of S3 class <code>Spectra()</code> .
<code>c.method</code>	A character string describing the clustering method; must be acceptable to <code>hclust</code> .
<code>d.method</code>	A character string describing the distance calculation method; must be acceptable as a method in <code>rowDist</code> .
<code>use.sym</code>	A logical; if true, use no color and use lower-case letters to indicate group membership.
<code>leg.loc</code>	Character; if "none" no legend will be drawn. Otherwise, any string acceptable to <code>legend</code> .
<code>...</code>	Other parameters to be passed to the plotting functions.

**Value**

A list, containing an object of class `hclust` and an object of class `dendrogram`. The side effect is a plot.

**Author(s)**

Bryan A. Hanson (DePauw University).

**See Also**

`hclust` for the underlying function. `hcaScores` for similar analysis of PCA scores from a `Spectra` object. Additional documentation at <https://bryanhanson.github.io/ChemoSpec/>

## Examples

```
# You need to install package "amap" for this example
if (requireNamespace("amap", quietly = TRUE)) {
  data(SrE.IR)
  myt <- expression(bolditalic(Serenoa) ~ bolditalic(repens) ~ bold(IR ~ Spectra))
  res <- hcaSpectra(SrE.IR, main = myt)
}
```

---

hmapSpectra

*Serialized Heat Map for a Spectra Object*

---

## Description

Creates a heat map with marginal dendrograms using seriation procedures. Heirchical cluster analysis is followed by re-ordering the clusters in a coordinated way across each dimension (controlled by argument `method`, see [hmap](#)). The vignette for package **seriation** has more details.

## Usage

```
hmapSpectra(spectra, ...)
```

## Arguments

<code>spectra</code>	An object of S3 class <code>Spectra()</code> .
<code>...</code>	Additional arguments to be passed downstream. A great deal of control is available - check <a href="#">hmap</a> for details. Most of the control actually derives from the <code>heatmap</code> function in package <b>stats</b> . See the examples.

## Value

A list as described in [hmap](#). Side effect is a plot.

## Note

The underlying `stats::heatmap` function does certain things automatically for the user. For instance, if you pass a vector of names to argument `row_labels` it is automatically reordered using the `rowInd` vector that is computed. The user does not need to do the reordering. Another example is the labeling of the columns. The labels are automatically turned 90 degrees, and not every column is labeled to keep things readable.

## Interpretation

Looking at the 2nd `hmapSpectra` example, and keeping in mind the nature of the sample (see [SrE.IR](#)), the most similar samples based on the ester peaks (~1740), are in the lower right corner of the heatmap. These are the two outlier samples, composed of triglycerides which contain the ester functional group (and no detectable carboxylic acid). The most similar samples based on the

carboxylic acid peaks (~1710) are in the upper left corner. These samples are mostly from the "pure" extract group, according to the manufacturer's label. These samples have a modest to low amount of the ester functional group, which indicates dilution (or adulteration if you like). In fact, the first two samples (NP\_adSrE and NR\_pSrE) are the two samples with the smallest ester peaks (see first plot in the examples). This suggests that NP\_adSrE was diluted only a little with added olive oil.

### Author(s)

Bryan A. Hanson (DePauw University).

### See Also

[hmap](#) which will get you to the package (there is no package index page); the vignette is a good place to begin (`browseVignettes("seriation")`). Additional documentation at <https://bryanhanson.github.io/ChemoSpec/>

### Examples

```
# You need to install package "seriation" for this example
if (requireNamespace("seriation", quietly = TRUE)) {
  data(SrE.IR)

  # Let's look just at the carbonyl region
  IR <- removeFreq(SrE.IR, rem.freq = SrE.IR$freq > 1775 | SrE.IR$freq < 1660)
  p <- plotSpectra(IR, which = 1:16, lab.pos = 1800)

  # Defaults, except for color scheme:
  res <- hmapSpectra(IR, col = heat.colors(5))

  # Label samples and frequencies by passing arguments to stats:heatmap
  # Also make a few other nice plot adjustments
  res <- hmapSpectra(IR,
    col = heat.colors(5),
    row_labels = IR$names, col_labels = as.character(round(IR$freq)),
    margins = c(4, 6)
  )
}
```

---

hypTestScores

*Conduct MANOVA using PCA Scores and Factors in a Spectra Object*

---

### Description

This function provides a convenient interface for carrying out manova using the scores from PCA and the factors (groups) stored in a [Spectra](#) object. The function will do anova as well, if you only provide one vector of scores, though this is probably of limited use. A [Spectra](#) object contains group information stored in its `spectra$groups` element, but you can also use [splitSpectraGroups](#) to generate additional groups/factors that might be more useful than the original.



**Usage**

```
hypTestScores(spectra, pca, pcs = 1:3, fac = NULL, ...)
```

**Arguments**

spectra	An object of S3 class <code>Spectra()</code> .
pca	An object of class <code>prcomp</code> .
pcs	An integer vector giving the PCA scores to use as the response in the manova analysis.
fac	A character vector giving the factors to be used in the manova. They will be searched for within the <code>Spectra</code> object.
...	Additional arguments to be passed downstream, in this case to <code>aov</code> . Untested.

**Details**

This function is an extraordinarily thin wrapper which helps the user to avoid writing a very tedious formula specification.

**Value**

The results of the analysis print to the console unless assigned. If assigned, the object class is one of several described in `aov` depending upon the data passed to it.

**Author(s)**

Bryan A. Hanson (DePauw University).

**See Also**

`splitSpectraGroups` which can be used to create additional factor elements in the `Spectra` object, which can then be used with this function. Additional documentation at <https://bryanhanson.github.io/ChemoSpec/>

**Examples**

```
data(metMUD2)

# Original factor encoding:
levels(metMUD2$groups)

# Split those original levels into 2 new ones (re-code them)
new.grps <- list(geneBb = c("B", "b"), geneCc = c("C", "c"))
mM3 <- splitSpectraGroups(metMUD2, new.grps)

# Now do the PCA and anova, with 3 ways to see the results
pca <- c_pcaSpectra(mM3)
res <- hypTestScores(mM3, pca, fac = c("geneBb", "geneCc"))
res
```

```
summary(res)
summary.aov(res)

# You can also call this function on the existing groups:
res <- hypTestScores(metMUD2, pca, fac = "groups")
```

---

irlba\_pcaSpectra      *IRLBA PCA of Spectra Objects*

---

### Description

A wrapper which carries out IRLBA PCA analysis on a [Spectra](#) object. The user can select various options for scaling. There is no normalization by rows - do this manually using [normSpectra](#). The data can be supplied already centered if desired.

### Usage

```
irlba_pcaSpectra(spectra, choice = "noscale", n = 3, center = TRUE, ...)
```

### Arguments

spectra	An object of S3 class <a href="#">Spectra()</a> .
choice	A character string indicating the choice of scaling. One of <code>c("noscale", "autoscale", "Pareto")</code> . "autoscale" is called "standard normal variate" or "correlation matrix PCA" in some literature.
n	Integer. The number of components desired.
center	Logical. Should the data be centered? Data must be centered for PCA, either before arriving here or via this argument.
...	Other parameters to be passed to <a href="#">irlba</a> .

### Details

The scale choice `autoscale` scales the columns by their standard deviation. `Pareto` scales by the square root of the standard deviation.

### Value

A modified object of class `prcomp` and `computed_via_irlba`, which includes a list element called `$method`, a character string describing the pre-processing carried out and the type of PCA performed (used to annotate plots).

### Author(s)

Bryan A. Hanson (DePauw University).

## References

J. Baglama and L. Reichel, "Augmented Implicitly Restarted Lanczos Bidiagonalization Methods" *SIAM J. Sci. Comput.* (2005).

## See Also

[prcomp\\_irlba](#) for the underlying function, [c\\_pcaSpectra](#) for classical PCA calculations, [r\\_pcaSpectra](#) for robust PCA calculations, [s\\_pcaSpectra](#) for sparse PCA calculations. Additional documentation at <https://bryanhanson.github.io/ChemoSpec/>

For displaying the results, [ChemoSpecUtils::plotScree\(\)](#), [ChemoSpecUtils::plotScores\(\)](#), [plotLoadings\(\)](#), [plot2Loadings\(\)](#), [sPlotSpectra\(\)](#).

## Examples

```
## Not run:
# This example assumes the graphics output is set to ggplot2 (see ?GraphicsOptions).
library("ggplot2")
data(SrE.NMR)
pca <- irlba_pcaSpectra(SrE.NMR)

p1 <- plotScree(pca)
p1

p2 <- plotScores(SrE.NMR, pca, pcs = c(1, 2), ellipse = "cls", tol = 0.05)
p2 <- p2 + ggtitle("Scores: SrE NMR Data")
p2

p3 <- plotLoadings(SrE.NMR, pca, loads = 1:2, ref = 1)
p3 <- p3 + ggtitle("Loadings: SrE NMR Data")
p3

## End(Not run)
```

## Description

This function conducts an mclust analysis of the PCA results of a [Spectra](#) object and displays the results in 3D. Classical or robust confidence ellipses can be added if desired. Improperly classified data points can be marked. The interactive plot is made via plotly and appears in a browser window. Note that the confidence ellipses computed here are generated independently of the Mclust results - they do not correspond to the ellipses seen in 2D plots from Mclust.

**Usage**

```
mclust3dSpectra(  
  spectra,  
  pca,  
  pcs = 1:3,  
  ellipse = TRUE,  
  rob = FALSE,  
  cl = 0.95,  
  frac.pts.used = 0.8,  
  truth = NULL,  
  ...  
)
```

**Arguments**

spectra	An object of S3 class <code>Spectra()</code> .
pca	An object of class <code>prcomp</code> .
pcs	An integer vector describing which PCs to use.
ellipse	Logical indicating if confidence ellipses should be drawn.
rob	Logical; if <code>ellipse = TRUE</code> , indicates that robust confidence ellipses should be drawn. If <code>FALSE</code> , classical confidence ellipses are drawn.
cl	A number indicating the confidence interval for the ellipse.
frac.pts.used	If <code>ellipse = TRUE</code> and <code>rob = TRUE</code> , a number indicating the fraction of the data points to be considered "good" and thus used to compute the robust confidence ellipse.
truth	A character vector indicating the known group membership for each row of the PC scores. Generally this would be <code>spectra\$groups</code> .
...	Arguments to be passed to <code>mclust</code> .

**Value**

The `mclust` model is returned invisibly, and a plot is produced.

**Author(s)**

Bryan A. Hanson (DePauw University).

**See Also**

`Mclust` for background on the method. Additional documentation at <https://bryanhanson.github.io/ChemoSpec/>

**Examples**

```
## Not run:
require(mclust)
data(metMUD1)
pca <- c_pcaSpectra(metMUD1)
mclust3dSpectra(metMUD1, pca)

# show mis-classified points
mclust3dSpectra(metMUD1, pca, truth = metMUD1$groups)

## End(Not run)
```

---

mclustSpectra

*mclust Analysis of a Spectra Object PCA Results*


---

**Description**

This function is a wrapper for the Mclust function and associated plotting functions.

**Usage**

```
mclustSpectra(
  spectra,
  pca,
  pcs = c(1:3),
  dims = c(1, 2),
  plot = c("BIC", "proj", "errors"),
  use.sym = FALSE,
  ...
)
```

**Arguments**

spectra	An object of S3 class <code>Spectra()</code> .
pca	An object of class <code>prcomp</code> .
pcs	An integer vector describing which PCs to use.
dims	A integer vector giving the PCA dimensions to use.
plot	A character string indicating what plot to make. Options are <code>c("BIC", "proj", "error")</code> ; see <code>Mclust</code> for details.
use.sym	Logical; if true, the color scheme is changed to black and symbols are used for plotting.
...	Other parameters to be passed downstream.

**Value**

The Mclust model is returned invisibly, and a plot is made.

**Author(s)**

Bryan A. Hanson (DePauw University).

**See Also**

[Mclust](#) for background on the method. Additional documentation at <https://bryanhanson.github.io/ChemoSpec/>

**Examples**

```
## Not run:
require("mclust")
data(metMUD1)
cls <- c_pcaSpectra(metMUD1, choice = "autoscale")

p <- plotScores(metMUD1, cls)

mclustSpectra(metMUD1, cls, plot = "BIC")
mclustSpectra(metMUD1, cls, plot = "proj")
mclustSpectra(metMUD1, cls, plot = "errors", truth = metMUD1$groups)

## End(Not run)
```

---

metMUD1

*Made Up NMR Data Sets*

---

**Description**

These data sets are simulated 300 MHz NMR spectra. They are designed mainly to illustrate certain chemometric methods and are small enough that they process quickly.

**Format**

The data is stored as a [Spectra](#) object.

**Details**

alignMUD is a series of mis-aligned spectra of a single small organic molecule.

metMUD1 is composed of 20 samples, each a mixture of four typical small organic compounds (we'll leave it to the reader as an exercise to deduce the spin systems!). These compounds are present in varying random amounts. Ten of the samples are control samples, and ten are treatment samples. Thus you can run PCA and other methods on this data set, and expect to see a separation. This data set is normalized.

metMUD2 also consists of 20 samples of mixtures of the same four compounds. However, the concentrations of some of the compounds are correlated with other compounds, both positively and negatively, and some concentrations are random. metMUD2 is divided into different sample groups which correspond conceptually to two genes, each active or knocked out. This data set is designed to be similar to a metabolomics data set in which the concentrations of some compounds co-vary, and others are independent. This data set is normalized.

### Author(s)

Bryan A. Hanson (DePauw University).

### Source

Created using various tools. Contact the author for a script if interested.

### See Also

Additional documentation at <https://bryanhanson.github.io/ChemoSpec/>

### Examples

```
data(metMUD1)
sumSpectra(metMUD1)
#
data(metMUD2)
sumSpectra(metMUD2)
```

---

normSpectra

*Normalize a Spectra Object*

---

### Description

This function carries out normalization of the spectra in a [Spectra](#) object. There are currently four options:

- "PQN" carries out "Probabilistic Quotient Normalization" as described in the reference. This is probably the best option for many data sets. However, please be careful if your sample has protein in it, PQN is potentially biased. See the references.
- "TotInt" normalizes by total intensity. In this case, the y-data of a [Spectra](#) object is normalized by dividing each y-value by the sum of the y-values in a given spectrum. Thus each spectrum sums to 1. This method assumes that the total concentration of all substances giving peaks does not vary across samples which may not be true.
- "Range" allows one to do something similar to "TotInt" but rather than using the sum of the entire spectrum as the denominator, only the sum of the given range is used. This would be appropriate if there was an internal standard in the spectrum which was free of interference, and one wanted to normalize relative to it.
- "zeroOne" scales each spectrum separately to a  $[0 \dots 1]$  scale. This is sometimes useful for visual comparison of chromatograms but is inappropriate for spectral data sets.

**Usage**

```
normSpectra(spectra, method = "PQN", RangeExpress = NULL)
```

**Arguments**

spectra	An object of S3 class <code>Spectra()</code> .
method	One of <code>c("PQN", "TotInt", "Range", "zero2one")</code> giving the method for normalization.
RangeExpress	A vector of logicals (must be of length( <code>Spectra\$freq</code> )). This vector should be TRUE for the frequency range you want to serve as the basis for norming, and FALSE otherwise. The entire spectrum will be divided by the sum of the TRUE range. See the examples.

**Value**

An object of S3 class `Spectra()`.

**Author(s)**

Bryan A. Hanson (DePauw University).

**References**

- Probabilistic Quotient Normalization is reported in F. Dieterle et al. *Analytical Chemistry* vol. 78 pages 4281-4290 (2006).
- The exact same mathematics are called "median fold change normalization" by Nicholson's group, reported in K. A. Veselkov et. al. *Analytical Chemistry* vol. 83 pages 5864-5872 (2011).
- Corriea et al. "1H NMR Signals from Urine Excreted Protein are a Source of Bias in Probabilistic Quotient Normalization" *Analytical Chemistry* vol. 94 pages 6919-6923 (2022).

**See Also**

Additional documentation at <https://bryanhanson.github.io/ChemoSpec/>

**Examples**

```
# This example assumes the graphics output is set to ggplot2 (see ?GraphicsOptions).
library("ggplot2")
data(SrE.IR)

# Reference spectrum before normalization
p1 <- plotSpectra(SrE.IR) + ggtitle("Original Spectrum")
p1

# Default PQN normalization
res1 <- normSpectra(SrE.IR)
p2 <- plotSpectra(res1) + ggtitle("PQN Normalization")
p2
```



```

# Norm over carbonyl region
RE <- SrE.IR$freq > 1650 & SrE.IR$freq < 1800
res2 <- normSpectra(SrE.IR, method = "Range", RangeExpress = RE)
p3 <- plotSpectra(res2) + ggtitle("Normalized to Carbonyl Peaks")
p3

# Check numerically
rowSums(res2$data[, RE]) # compare to rowSums(SrE.IR$data[,RE])

```

pcaDiag

*Outlier Diagnostic Plots for PCA of a Spectra Object***Description**

A function to carry diagnostics on the PCA results for a [Spectra](#) object. Basically a wrapper to Filzmoser's [pcaDiagplot](#) which colors everything according to the scheme stored in the [Spectra](#) object. Works with PCA results of either class `prcomp` or class `princomp`. Works with either classical or robust PCA results.

**Usage**

```

pcaDiag(
  spectra,
  pca,
  pcs = 3,
  quantile = 0.975,
  plot = c("OD", "SD"),
  use.sym = FALSE,
  ...
)

```

**Arguments**

<code>spectra</code>	An object of S3 class <a href="#">Spectra()</a> .
<code>pca</code>	An object of class <code>prcomp</code> modified to include a character string ( <code>\$method</code> ) describing the pre-processing carried out and the type of PCA performed.
<code>pcs</code>	As per <a href="#">pcaDiagplot</a> . The number of principal components to include.
<code>quantile</code>	As per <a href="#">pcaDiagplot</a> . The significance criteria to use as a cutoff.
<code>plot</code>	A character string, indicating whether to plot the score distances or orthogonal distances, or both. Options are <code>c("OD", "SD")</code> .
<code>use.sym</code>	logical; if true, the color scheme is change to black and symbols are used for plotting.
<code>...</code>	Parameters to be passed to the plotting routines. <i>Applies to base graphics only.</i>

## Details

If both plots are desired, the output should be directed to a file rather than the screen. Otherwise, the 2nd plot overwrites the 1st in the active graphics window. Alternatively, just call the function twice, once specifying OD and once specifying SD.

## Value

The returned value depends on the graphics option selected (see `ChemoSpecUtils::GraphicsOptions()`).

- **base** A data frame or list containing the data plotted. Assign the value and run `str()` or `names()` on it to see what it contains. Side effect is a plot.
- **ggplot2** The plot is displayed, and a `ggplot2` plot object is returned if the value is assigned. The plot can be modified in the usual `ggplot2` manner. If you want the plotted values, you can access them via the base graphics mode.

## Author(s)

Bryan A. Hanson (DePauw University), Tejasvi Gupta.

## References

K. Varmuza and P. Filzmoser *Introduction to Multivariate Statistical Analysis in Chemometrics*, CRC Press, 2009.

## See Also

`pcaDiagplot` in package `chemometrics` for the underlying function. Additional documentation at <https://bryanhanson.github.io/ChemoSpec/>

## Examples

```
# This example assumes the graphics output is set to ggplot2 (see ?GraphicsOptions).
library("ggplot2")
data(SrE.IR)
pca <- c_pcaSpectra(SrE.IR, choice = "noscale")
p1 <- pcaDiag(SrE.IR, pca, pcs = 2, plot = "OD") + ggtitle("OD Plot")
p1
p2 <- pcaDiag(SrE.IR, pca, pcs = 2, plot = "SD") + ggtitle("SD Plot")
p2
```

---

`plot2Loadings`*Plot PCA Loadings from a Spectra Object Against Each Other*

---

### Description

Plots two PCA loadings specified by the user, and labels selected (extreme) points. Typically used to determine which variables (frequencies) are co-varying, although in spectroscopy most peaks are represented by several variables and hence there is a lot of co-varying going on. Also useful to determine which variables are contributing the most to the clustering on a score plot.

### Usage

```
plot2Loadings(spectra, pca, loads = c(1, 2), tol = 0.05, ...)
```

### Arguments

<code>spectra</code>	An object of S3 class <code>Spectra()</code> .
<code>pca</code>	An object of class <code>prcomp</code> , modified to include a list element called <code>\$method</code> , a character string describing the pre-processing carried out and the type of PCA performed (it appears on the plot). This is automatically provided if <code>ChemoSpec</code> functions <code>c_pcaSpectra</code> or <code>r_pcaSpectra</code> were used to create <code>pca</code> .
<code>loads</code>	A vector of two integers specifying which loading vectors to plot.
<code>tol</code>	A number describing the fraction of points to be labeled. <code>tol = 1.0</code> labels all the points; <code>tol = 0.05</code> labels <i>approximately</i> the most extreme 5 percent. Set to 'none' to completely suppress labels. Note that a simple approach based upon quantiles is used, assumes that both x and y are each normally distributed, and treats x and y separately. Thus, this is not a formal treatment of outliers, just a means of labeling points. Groups are lumped together for the computation.
<code>...</code>	Parameters to be passed to the plotting routines. <i>Applies to base graphics only.</i>

### Value

The returned value depends on the graphics option selected (see `GraphicsOptions()`).

- `base`: None. Side effect is a plot.
- `ggplot2`: The plot is displayed, and a `ggplot2` object is returned if the value is assigned. The plot can be modified in the usual `ggplot2` manner.

### Author(s)

Bryan A. Hanson (DePauw University), Tejasvi Gupta.

### See Also

See `plotLoadings` to plot one loading against the original variable (frequency) axis. See `sPlotSpectra` for a different approach. Additional documentation at <https://bryanhanson.github.io/ChemoSpec/>

## Examples

```
# This example assumes the graphics output is set to ggplot2 (see ?GraphicsOptions).
library("ggplot2")
data(SrE.IR)
pca <- c_pcaSpectra(SrE.IR)
myt <- expression(bolditalic(Serenoa) ~ bolditalic(repens) ~ bold(IR ~ Spectra))
p <- res <- plot2Loadings(SrE.IR, pca, loads = c(1, 2), tol = 0.001)
p <- p + ggtitle(myt)
p
```

---

plot3dScores

*3D PCA Score Plot for a Spectra Object*

---

## Description

Creates an interactive 3D plot of PCA scores from the analysis of a [Spectra](#) object, color coded according to the scheme stored in the object. The plot is created by `plotly` and appears in a browser window.

## Usage

```
plot3dScores(
  spectra,
  pca,
  pcs = c(1:3),
  ellipse = TRUE,
  rob = FALSE,
  cl = 0.95,
  frac.pts.used = 0.8
)
```

## Arguments

<code>spectra</code>	An object of S3 class <a href="#">Spectra()</a> .
<code>pca</code>	An object of class <a href="#">prcomp</a> .
<code>pcs</code>	A vector of three integers specifying the PCA scores to plot.
<code>ellipse</code>	Logical indicating if confidence ellipses should be drawn.
<code>rob</code>	Logical; if <code>ellipse = TRUE</code> , indicates that robust confidence ellipses should be drawn. If <code>FALSE</code> , classical confidence ellipses are drawn.
<code>cl</code>	A number indicating the confidence interval for the ellipse.
<code>frac.pts.used</code>	If <code>ellipse = TRUE</code> and <code>rob = TRUE</code> , a number indicating the fraction of the data points to be considered "good" and thus used to compute the robust confidence ellipse.

**Value**

None. Side effect is a plot in a browser window.

**Author(s)**

Bryan A. Hanson (DePauw University).

**See Also**

Additional documentation at <https://bryanhanson.github.io/ChemoSpec/>

**Examples**

```
if (interactive()) {  
  data(metMUD1)  
  pca <- c_pcaSpectra(metMUD1, choice = "noscale")  
  p <- plot3dScores(metMUD1, pca)  
  p  
}
```

---

plotLoadings

*Plot PCA Loadings for a Spectra Object*

---

**Description**

Creates a multi-panel plot of loadings along with a reference spectrum.

**Usage**

```
plotLoadings(spectra, pca, loads = c(1), ref = 1, ...)
```

**Arguments**

spectra	An object of S3 class <code>Spectra()</code> .
pca	An object of class <code>prcomp</code> , modified to include a list element called <code>\$method</code> , a character string describing the pre-processing carried out and the type of PCA performed (it appears on the plot). This is automatically provided if <code>ChemoSpec</code> functions <code>c_pcaSpectra</code> or <code>r_pcaSpectra</code> were used to create <code>pca</code> .
loads	An integer vector giving the loadings to plot. More than 3 loadings creates a useless plot using the default graphics window.
ref	An integer specifying the reference spectrum to plot, which appears at the bottom of the plot.
...	Parameters to be passed to the plotting routines. <i>Applies to base graphics only.</i>

**Value**

The returned value depends on the graphics option selected (see [GraphicsOptions\(\)](#)).

- base: None. Side effect is a plot.
- ggplot2: The plot is displayed, and a ggplot2 object is returned if the value is assigned. The plot can be modified in the usual ggplot2 manner.

**Author(s)**

Bryan A. Hanson (DePauw University), Tejasvi Gupta.

**See Also**

[c\\_pcaSpectra](#) for an example. See [plot2Loadings](#) to plot two loadings against each other, and [sPlotSpectra](#) for an alternative approach. Additional documentation at <https://bryanhanson.github.io/ChemoSpec/>

---

plotScores	<i>Plot Scores from PCA, MIA or PARAFAC Analysis of a Spectra or Spectra2D Object</i>
------------	---

---

**Description**

This function is used by ChemoSpec and ChemoSpec2D, but is formally part of ChemoSpecUtils. You can access full documentation via [plotScores](#).

---

plotSree	<i>Scree Plots from PCA or MIA Analysis of a Spectra or Spectra2D Object</i>
----------	--

---

**Description**

This function is used by ChemoSpec and ChemoSpec2D, but is formally part of ChemoSpecUtils. You can access full documentation via [plotSree](#).

plotSpectra

*Plot Spectra Object***Description**

Plots the spectra stored in a [Spectra](#) object. Spectra may be plotted offset or stacked. The vertical scale is controlled by a combination of several parameters.

**Usage**

```
plotSpectra(
  spectra,
  which = c(1),
  yrange = range(spectra$data),
  offset = 0,
  amplify = 1,
  lab.pos = mean(spectra$freq),
  showGrid = TRUE,
  leg.loc = "none",
  ...
)
```

**Arguments**

spectra	An object of S3 class <a href="#">Spectra()</a> .
which	An integer vector specifying which spectra to plot, and the order.
yrange	A vector giving the limits of the y axis desired, for instance <code>c(0, 15)</code> . This parameter depends upon the range of values in the stored spectra and defaults to the height of the largest peak in the data set. Interacts with the next two arguments, as well as the number of spectra to be plotted as given in <code>which</code> . Trial and error is used to adjust all these arguments to produce the desired plot.
offset	A number specifying the vertical offset between spectra if more than one is plotted. Set to 0.0 to overlay the spectra.
amplify	A number specifying an amplification factor to be applied to all spectra. Useful for magnifying spectra so small features show up (though large peaks will then be clipped, unless you zoom on the x axis).
lab.pos	A number (in frequency units) giving the location of a label for each spectrum. Generally, pick an area that is clear in all spectra plotted. If no label is desired, set <code>lab.pos = "none"</code> .
showGrid	Logical. Places light gray vertical lines at each tick mark if TRUE.
leg.loc	Either a list with elements <code>x</code> and <code>y</code> , or a string like <code>'topright'</code> . Values in a list should be on <code>[0, 1]</code> , i.e. the lower left of the plot area is <code>0, 0</code> and the upper right is <code>1, 1</code> . Allowed string values are those described in <a href="#">graphics::legend()</a> under 'Details'. A value of <code>'none'</code> is acceptable as well.
...	Parameters to be passed to the plotting routines. <i>Applies to base graphics only.</i>

**Value**

The returned value depends on the graphics option selected (see [GraphicsOptions\(\)](#)).

- base: None. Side effect is a plot.
- ggplot2: The plot is displayed, and a ggplot2 object is returned if the value is assigned. The plot can be modified in the usual ggplot2 manner.

**Author(s)**

Bryan A. Hanson (DePauw University), Tejasvi Gupta.

**See Also**

[plotSpectraJS](#) for the interactive version. See [GraphicsOptions](#) for more information about the graphics options. Additional documentation at <https://bryanhanson.github.io/ChemoSpec/>

**Examples**

```
# This example assumes the graphics output is set to ggplot2 (see ?GraphicsOptions).
library("ggplot2")
data(metMUD1)

p1 <- plotSpectra(metMUD1, which = c(10, 11), yrange = c(0, 1.5),
  offset = 0.06, amplify = 10, lab.pos = 0.5)
p1 <- p1 + ggtitle("metMUD1 NMR Data")
p1

# Add a legend at x, y coords
p2 <- plotSpectra(metMUD1, which = c(10, 11), yrange = c(0, 1.5),
  offset = 0.06, amplify = 10, lab.pos = 0.5, leg.loc = list(x = 0.8, y = 0.8))
p2 <- p2 + ggtitle("metMUD1 NMR Data")
p2
```

---

plotSpectraDist	<i>Plot the Distance Between Spectra and a Reference Spectrum in a Spectra Object</i>
-----------------	---

---

**Description**

This function plots the distance between a reference spectrum and all other spectra in a [Spectra](#) object. Distance can be defined in a number of ways (see Arguments).

**Usage**

```
plotSpectraDist(spectra, method = "pearson", ref = 1, labels = TRUE, ...)
```



**Arguments**

spectra	An object of S3 class <code>Spectra()</code> .
method	Character. Any method acceptable to <code>rowDist</code> .
ref	Integer. The spectrum to be used as a reference.
labels	Logical. Shall the points be labeled?
...	Parameters to be passed to the plotting routines. <i>Applies to base graphics only.</i>

**Value**

The returned value depends on the graphics option selected (see `ChemoSpecUtils::GraphicsOptions()`).

- **base** A data frame or list containing the data plotted. Assign the value and run `str()` or `names()` on it to see what it contains. Side effect is a plot.
- **ggplot2** The plot is displayed, and a `ggplot2` plot object is returned if the value is assigned. The plot can be modified in the usual `ggplot2` manner. If you want the plotted values, you can access them via the base graphics mode.

**Author(s)**

Bryan A. Hanson (DePauw University), Tejasvi Gupta.

**See Also**

To compare all spectra simultaneously in a heatmap, see `sampleDist`. Additional documentation at <https://bryanhanson.github.io/ChemoSpec/>

**Examples**

```
# You need to install package "amap" to use this function
if (requireNamespace("amap", quietly = TRUE)) {
  # This example assumes the graphics output is set to ggplot2 (see ?GraphicsOptions).
  library("ggplot2")
  data(SrE.NMR)
  txt1 <- paste("Distance from", SrE.NMR$names[1])
  txt2 <- paste("Rank Distance from", SrE.NMR$names[1])
  p <- plotSpectraDist(SrE.NMR)
  p <- p + labs(title = txt1, xlab = txt2, ylab = txt2) +
    coord_cartesian(ylim = c(0, 1.1), xlim = c(0, 16))
  p
}
```

---

`plotSpectraJS`*Plot a Spectra Object Interactively*

---

### Description

This function uses the d3.js JavaScript library by Mike Bostock to plot a [Spectra](#) object interactively. This is most useful for data exploration. For high quality plots, consider [plotSpectra](#).

### Usage

```
plotSpectraJS(spectra, which = NULL, browser = NULL, minify = TRUE)
```

### Arguments

<code>spectra</code>	An object of S3 class <a href="#">Spectra()</a> .
<code>which</code>	Integer. If not NULL, specifies by number which spectra to plot. If greater control is needed, use <a href="#">removeSample</a> which is more flexible before calling this function.
<code>browser</code>	Character. Something that will make sense to your OS. Only necessary if you want to override your system specified browser as understood by R. See below for further details.
<code>minify</code>	Logical. Shall the JavaScript be minified? This improves performance. However, it requires package <code>js</code> which in turn requires package <code>V8</code> . The latter is not available on all platforms. Details may be available at <a href="https://github.com/jeroen/V8">https://github.com/jeroen/V8</a>

### Details

The spectral data are incorporated into the web page. Keep in mind that very large data sets, like NMR spectra with 32K points, will bog down the browser. In these cases, you may need to limit the number of samples in passed to this function. See [removeSample](#) or use argument `which`.

### Value

None; side effect is an interactive web page. The temporary directory containing the files that drive the web page is written to the console in case you wish to use those files. This directory is deleted when you quit R. If you wish to read the file, don't minify the code, it will be unreadable.

### Browser Choice

The browser is called by [browseURL](#), which in turn uses `options("browser")`. Exactly how this is handled is OS dependent.

### RStudio Viewer

If `browser` is NULL, you are using RStudio, and a viewer is specified, this will be called. You can stop this by with `options(viewer = NULL)`.

### Browser Choice (Mac)

On a Mac, the default browser is called by `/bin/sh/open` which in turn looks at which browser you have set in the system settings. You can override your default with `browser = "/usr/bin/open -a 'Google Chrome' "` for example.

### Browser Choice & Performance

You can check the performance of your browser at [peacekeeper.futuremark.com](http://peacekeeper.futuremark.com) The most relevant score is the rendering category.

### Author(s)

Bryan A. Hanson (DePauw University).

### See Also

[plotSpectra](#) for non-interactive plotting. Details about `d3.js` are at <https://d3js.org>. Additional documentation at <https://bryanhanson.github.io/ChemoSpec/>

### Examples

```
if (interactive()) {
  require("jsonlite")
  require("js")
  data(metMUD2)
  plotSpectraJS(metMUD2)
}
```

---

removeFreq

*Remove Frequencies from a Spectra or Spectra2D Object*

---

### Description

This function is used by ChemoSpec and ChemoSpec2D, but is formally part of ChemoSpecUtils. You can access full documentation via [removeFreq](#).

---

removeGroup

*Remove Groups from a Spectra or Spectra2D Object*

---

### Description

This function is used by ChemoSpec and ChemoSpec2D, but is formally part of ChemoSpecUtils. You can access full documentation via [removeGroup](#).

---

removeSample	<i>Remove Samples from a Spectra or Spectra2D Object</i>
--------------	--

---

### Description

This function is used by ChemoSpec and ChemoSpec2D, but is formally part of ChemoSpecUtils. You can access full documentation via [removeSample](#).

---

reviewAllSpectra	<i>Review All the Spectra in a Spectra Object</i>
------------------	---

---

### Description

Utility to review all spectra in a Spectra object. Output depends upon the graphics output choice.

**base:** Plots each spectrum one at a time, and waits for a return in the console before plotting the next spectrum. Use ESC to get out of the loop.

**ggplot2:** All the spectra are plotted in a single column.

### Usage

```
reviewAllSpectra(spectra, ...)
```

### Arguments

spectra	An object of S3 class <a href="#">Spectra()</a> .
...	Parameters to be passed to the plotting routines. <i>Applies to base graphics only.</i>

### Value

The returned value depends on the graphics option selected (see [GraphicsOptions\(\)](#)).

- base: None. Side effect is a plot.
- ggplot2: The plot is displayed, and a ggplot2 object is returned if the value is assigned. The plot can be modified in the usual ggplot2 manner.

### Author(s)

Bryan A. Hanson (DePauw University), Tejasvi Gupta.

### See Also

See [GraphicsOptions](#) for more information about the graphics options. Additional documentation at <https://bryanhanson.github.io/ChemoSpec/>

**Examples**

```
# Because there are 16 spectra in this data set, you probably want to
# expand the height of the graphics device to see the spectra clearly.
# This example assumes the graphics output is set to ggplot2 or plotly (see ?GraphicsOptions).
# If you do options(ChemoSpecGraphics == "plotly") you'll get the results
# in a web page, which is particularly convenient.
library("ggplot2")
data(metMUD1)
p <- reviewAllSpectra(metMUD1)
p
```

---

rowDist	<i>Compute Distance Between Rows of a Matrix</i>
---------	--

---

**Description**

This function is used by ChemoSpec and ChemoSpec2D, but is formally part of ChemoSpecUtils. You can access full documentation via [rowDist](#).

---

r_pcaSpectra	<i>Robust PCA of a Spectra Object</i>
--------------	---------------------------------------

---

**Description**

A wrapper which carries out robust PCA analysis on a [Spectra](#) object. The data are row- and column-centered, and the user can select various options for scaling.

**Usage**

```
r_pcaSpectra(spectra, choice = "noscale")
```

**Arguments**

spectra	An object of S3 class <a href="#">Spectra()</a> .
choice	A character vector describing the type of scaling to be carried out. One of <code>c("noscale", "mad")</code> .

**Value**

An object of classes `converted_from_princomp` and `princomp`. It includes a list element called `$method`, a character string describing the pre-processing carried out and the type of PCA performed (used to annotate plots).

**Author(s)**

Bryan A. Hanson (DePauw University).

**References**

K. Varmuza and P. Filzmoser *Introduction to Multivariate Statistical Analysis in Chemometrics*, CRC Press, 2009.

**See Also**

[PCAGrid](#) for the underlying function, [c\\_pcaSpectra](#) for classical PCA calculations, [s\\_pcaSpectra](#) for sparse PCA calculations, [irlba\\_pcaSpectra](#) for PCA via the IRLBA algorithm. Additional documentation at <https://bryanhanson.github.io/ChemoSpec/>

For displaying the results, [ChemoSpecUtils::plotScree\(\)](#), [ChemoSpecUtils::plotScores\(\)](#), [plotLoadings\(\)](#), [plot2Loadings\(\)](#), [sPlotSpectra\(\)](#).

<https://bryanhanson.github.io/ChemoSpec/>

**Examples**

```
## Not run:
# This example assumes the graphics output is set to ggplot2 (see ?GraphicsOptions).
library("ggplot2")
data(metMUD1)
pca <- r_pcaSpectra(metMUD1)

p1 <- plotScree(pca)
p1

p2 <- plotScores(metMUD1, pca, pcs = c(1, 2), ellipse = "cls", tol = 0.05)
p2 <- p2 + ggtitle("Scores: metMUD1 NMR Data")
p2

p3 <- plotLoadings(metMUD1, pca, loads = 1:2, ref = 1)
p3 <- p3 + ggtitle("Loadings: metMUD1 NMR Data")
p3

## End(Not run)
```

---

sampleDist

*Compute the Distances Between Samples in a Spectra or Spectra2D Object*

---

**Description**

This function is used by ChemoSpec and ChemoSpec2D, but is formally part of ChemoSpecUtils. You can access full documentation via [sampleDist](#).

**Description**

This function is a simple wrapper around the function `sgolayfilt`. It allows one to apply Savitzky-Golay filters to a `Spectra` object in a convenient way.

**Usage**

```
sgfSpectra(spectra, m = 0, ...)
```

**Arguments**

<code>spectra</code>	An object of S3 class <code>Spectra()</code> .
<code>m</code>	The desired m-th derivative. <code>m = 0</code> smooths the data (i.e. a rolling average), <code>m = 1</code> gives the first derivative etc.
<code>...</code>	Other parameters to be passed to <code>sgolayfilt</code> .

**Value**

A object of class `Spectra`.

**Author(s)**

Bryan A. Hanson (DePauw University).

**See Also**

Additional documentation at <https://bryanhanson.github.io/ChemoSpec/>

**Examples**

```
# You need to install package "signal" for this example
# This example assumes the graphics output is set to ggplot2 (see ?GraphicsOptions).
if (requireNamespace("signal", quietly = TRUE)) {
  library("ggplot2")
  library("patchwork")
  data(SrE.IR)
  myt1 <- expression(bolditalic(Serenoa) ~ bolditalic(repens) ~ bold(IR ~ Spectra))
  myt2 <- expression(bolditalic(Serenoa) ~ bolditalic(repens) ~ bold(IR ~ Spectra ~ (Smoothed)))

  p1 <- plotSpectra(SrE.IR)
  p1 <- p1 + ggtitle(myt1) + coord_cartesian(xlim = c(1900, 2100), ylim = c(0.0, 0.03))

  sgf <- sgfSpectra(SrE.IR)

  p2 <- plotSpectra(sgf)
```

```

p2 <- p2 + ggtitle(myt2) + coord_cartesian(xlim = c(1900, 2100), ylim = c(0.0, 0.03))

p3 <- p1/p2
p3
}

```

Spectra

*Spectra Objects***Description**

In ChemoSpec, spectral data sets are stored in an S3 class called `Spectra`, which contains a variety of information in addition to the spectra themselves. `Spectra` objects are created by [files2SpectraObject](#) or [matrix2SpectraObject](#).

**Structure**

The structure of a `Spectra` object is a list of 9 elements and an attribute as follows:

- **\$freq** (numeric) A common frequency (or wavelength) axis for all the spectra.
- **\$data** (numeric) The intensities for the spectra. A matrix of dimension no. samples x no. frequency points.
- **\$names** (character) The sample names for the spectra; length must be no. samples.
- **\$groups** (factor) The group classification of the samples; length must be no. samples.
- **\$colors** (character) The colors for each sample; length must be no. samples. Groups and colors correspond.
- **\$sym** (integer) As for colors, but symbols for plotting (if b/w is desired).
- **\$alt.sym** (character) Lower-case letters as alternate symbols for plotting.
- **\$unit** (character) Two entries, the first giving the x axis unit, the second the y axis unit.
- **\$desc** (character) A character string describing the data set. This appears on plots and therefore should probably be kept to 40 characters or less.
- attribute: character with value "Spectra" The S3 class designation.

**Author(s)**

Bryan A. Hanson (DePauw University).

**See Also**

[sumSpectra](#) to summarize a `Spectra` object. [sumGroups](#) to summarize group membership of a `Spectra` object. [chkSpectra](#) to verify the integrity of a `Spectra` object. [colorSymbol](#) for a discussion of color options. Finally, additional documentation at <https://bryanhanson.github.io/ChemoSpec/>



---

splitSpectraGroups      *Create New Groups from an Existing Spectra Object*

---

### Description

This function takes an existing [Spectra](#) object and uses your instructions to split the existing `spectra$groups` into new groups. The new groups are added to the existing [Spectra](#) object (a list) as new elements. This allows one to use different combinations of factors than were originally encoded in the [Spectra](#) object. The option also exists to replace the color scheme with one which corresponds to the new factors.

### Usage

```
splitSpectraGroups(spectra, inst = NULL, rep.cols = NULL, ...)
```

### Arguments

<code>spectra</code>	An object of S3 class <a href="#">Spectra()</a> .
<code>inst</code>	A list giving the name of the new element to be created from a set of target strings given in a character vector. See the example for the syntax.
<code>rep.cols</code>	Optional. A vector giving new colors which correspond to the levels of <code>inst</code> . Only possible if <code>inst</code> has only one element, as the possible combinations of levels and colors may get complicated.
<code>...</code>	Additional arguments to be passed downstream. Currently not used.

### Details

The items in the character vector are grepped among the existing `spectra$groups` entries; when found, they are placed in a new element of [Spectra](#). In the example, all `spectra$groups` entries containing "G" are coded as "G" in a new element called `spectra$env`, and any entries containing "T" are handled likewise. This amounts to a sort of recoding of factors (the example demonstrates this). Every entry in `spectra$groups` should be matched by one of the entries in the character vector. If not, you will get NA entries. Also, if the targets in the character vector are not unique, your results will reflect the order of the levels. Since this is a grep process, you can pass any valid grep string as the target.

If `rep.cols` is provided, these colors are mapped one for one onto the levels of the the first element of `inst`. This provides a different means of changing the sample color encoding than [conColScheme](#).

### Value

An object of S3 class [Spectra](#), modified to have additional elements as specified by `inst`.

### Author(s)

Bryan A. Hanson (DePauw University).

**See Also**

[conColScheme](https://bryanhanson.github.io/ChemoSpec/) Additional documentation at <https://bryanhanson.github.io/ChemoSpec/>

**Examples**

```
data(metMUD2)
levels(metMUD2$groups) # original factor encoding

# Split those original levels into 2 new ones (re-code them)
new.grps <- list(geneBb = c("B", "b"), geneCc = c("C", "c"))
res <- splitSpectraGroups(metMUD2, new.grps)
str(res) # note two new elements, "geneBb" and "geneCc"
sumSpectra(res) # reports on extra elements

# Note that if you want to use a newly created group in
# plotScores and other functions to drive the color scheme
# and labeling, you'll have to update the groups element:
res$groups <- as.factor(paste(res$geneBb, res$geneCc, sep = ""))
```

---

sPlotSpectra

*s-Plot of Spectra Data (Post PCA)*


---

**Description**

Produces a scatter plot of the correlation of the variables against their covariance for a chosen principal component. It allows visual identification of variables driving the separation and thus is a useful adjunct to traditional loading plots.

**Usage**

```
sPlotSpectra(spectra, pca, pc = 1, tol = 0.05, ...)
```

**Arguments**

spectra	An object of S3 class <a href="#">Spectra()</a> .
pca	The result of a pca calculation on <a href="#">Spectra</a> (i.e. the output from <a href="#">c_pcaSpectra</a> or <a href="#">r_pcaSpectra</a> ).
pc	An integer specifying the desired pc plot.
tol	A number describing the fraction of points to be labeled. <code>tol = 1.0</code> labels all the points; <code>tol = 0.05</code> labels <i>approximately</i> the most extreme 5 percent. Set to 'none' to completely suppress labels. Note that a simple approach based upon quantiles is used, assumes that both x and y are each normally distributed, and treats x and y separately. Thus, this is not a formal treatment of outliers, just a means of labeling points. Groups are lumped together for the computation.
...	Parameters to be passed to the plotting routines. <i>Applies to base graphics only.</i>

**Value**

The returned value depends on the graphics option selected (see `GraphicsOptions()`).

- `base`: None. Side effect is a plot.
- `ggplot2`: The plot is displayed, and a `ggplot2` object is returned if the value is assigned. The plot can be modified in the usual `ggplot2` manner.

**Author(s)**

Bryan A. Hanson (DePauw University), Tejasvi Gupta, Matthew J. Keinsley.

**References**

Wiklund, Johansson, Sjoström, Mellerowicz, Edlund, Shockcor, Gottfries, Moritz, and Trygg. "Visualization of GC/TOF-MS-Based Metabolomics Data for Identification of Biochemically Interesting Compounds Using OPLS Class Models" *Analytical Chemistry* Vol.80 no.1 pgs. 115-122 (2008).

**See Also**

Additional documentation at <https://bryanhanson.github.io/ChemoSpec/>

**Examples**

```
# This example assumes the graphics output is set to ggplot2 (see ?GraphicsOptions).
library("ggplot2")
data(SrE.IR)
pca <- c_pcaSpectra(SrE.IR)
myt <- expression(bolditalic(Serenoa) ~ bolditalic(repens) ~ bold(IR ~ Spectra))
p <- sPlotSpectra(spectra = SrE.IR, pca = pca, pc = 1, tol = 0.001)
p <- p + ggtitle(myt)
p
```

---

SrE.IR

*IR and NMR Spectra of Serenoa repens (Saw Palmetto) Oil Extracts and Reference Oils*

---

**Description**

A collection of 14 IR and NMR spectra of essential oil extracted from the palm *Serenoa repens* or Saw Palmetto, which is commonly used to treat BPH in men. The 14 spectra are of different retail samples, and are divided into two categories based upon the label description: `adSrE`, adulterated extract, and `pSrE`, pure extract. The adulterated samples typically have olive oil added to them, which is inactive towards BPH. There are two additional spectra included as references/outliers: evening primrose oil, labeled `EPO` in the data set, and olive oil, labeled `OO`. These latter two oils are mixtures of triglycerides for the most part, while the `SrE` samples are largely fatty acids. As a result, the spectra of these two groups are subtly different.

**Format**

The data are stored as a [Spectra](#) object.

**Source**

IR data collected in the author's laboratory. NMR data collected at Purdue University with the generosity and assistance of Prof. Dan Raftery and Mr. Tao Ye.

**See Also**

Additional documentation at <https://bryanhanson.github.io/ChemoSpec/>

**Examples**

```
data(SrE.IR)
sumSpectra(SrE.IR)
data(SrE.NMR)
sumSpectra(SrE.NMR)
```

---

sumGroups

*Summarize the Group Membership of a Spectra or Spectra2D Object*

---

**Description**

This function is used by ChemoSpec and ChemoSpec2D, but is formally part of ChemoSpecUtils. You can access full documentation via [sumGroups](#).

---

sumSpectra

*Summarize a Spectra or Spectra2D Object*

---

**Description**

This function is used by ChemoSpec and ChemoSpec2D, but is formally part of ChemoSpecUtils. You can access full documentation via [sumSpectra](#).

**Description**

Compute and plot various measures of central tendency and spread for a [Spectra](#) object. Several different measures/spreads are available. These are useful as an overview of where a data set varies the most.

**Usage**

```
surveySpectra(
  spectra,
  method = c("sd", "sem", "sem95", "mad", "iqr"),
  by.gr = TRUE,
  ...
)

surveySpectra2(
  spectra,
  method = c("sd", "sem", "sem95", "mad", "iqr"),
  lab.pos = 0.9 * max(spectra$freq),
  ...
)
```

**Arguments**

spectra	An object of S3 class <a href="#">Spectra()</a> .
method	Character. One of <code>c("sd", "sem", "sem95", "mad", "iqr")</code> .
by.gr	Logical, indicating if the analysis is to be done by group or not. Applies to <code>surveySpectra</code> only.
...	Parameters to be passed to the plotting routines. <i>Applies to base graphics only.</i>
lab.pos	Numeric, giving the frequency where the label should be drawn. Applies to <code>surveySpectra2</code> only.

**Details**

For `surveySpectra` the method choice works as follows: `sd` plots the mean spectrum +/- the standard deviation, `sem` plots the mean spectrum +/- the standard error of the mean, `sem95` plots the mean spectrum +/- the standard error at the 95 percent confidence interval, `mad` plots the median spectrum +/- the median absolute deviation, and finally, `iqr` plots the median spectrum + the upper hinge and - the lower hinge.

For `surveySpectra2`, the spectra are mean centered and plotted. Below that, the relative summary statistic is plotted, offset, but on the same scale.

**Value**

The returned value depends on the graphics option selected (see `GraphicsOptions()`).

- `base`: None. Side effect is a plot.
- `ggplot2`: The plot is displayed, and a `ggplot2` object is returned if the value is assigned. The plot can be modified in the usual `ggplot2` manner.

**Functions**

- `surveySpectra()`: Spectral survey emphasizing mean or median spectrum, optionally by group.
- `surveySpectra2()`: Spectral survey emphasizing variation among spectra.

**Author(s)**

Bryan A. Hanson (DePauw University), Tejasvi Gupta.

**See Also**

Additional documentation at <https://bryanhanson.github.io/ChemoSpec/>

**Examples**

```
# This example assumes the graphics output is set to ggplot2 (see ?GraphicsOptions).
library("ggplot2")
data(SrE.IR)
myt <- expression(bolditalic(Serenoa) ~ bolditalic(repens) ~ bold(Extract ~ IR ~ Spectra))

p1 <- surveySpectra(SrE.IR, method = "iqr")
p1 <- p1 + ggtitle(myt)
p1

p2 <- surveySpectra2(SrE.IR, method = "iqr")
p2 <- p2 + ggtitle(myt)
p2
```

**Description**

A wrapper which carries out sparse PCA analysis on a `Spectra` object. The user can select various options for scaling. There is no normalization by rows - do this manually using `normSpectra`. The data will be centered, as is required by PCA.

## Usage

```
s_pcaSpectra(spectra, choice = "noscale", K = 3, para = rep(0.5, K), ...)
```

## Arguments

spectra	An object of S3 class <code>Spectra()</code> .
choice	A character string indicating the choice of scaling. One of <code>c("noscale", "autoscale", "Pareto")</code> . "autoscale" is called "standard normal variate" or "correlation matrix PCA" in some literature.
K	Integer. The number of components desired.
para	A vector of length(K) giving the tuning parameters.
...	Other parameters to be passed to <code>arrayspc</code> .

## Details

The scale choice `autoscale` scales the columns by their standard deviation. `Pareto` scales by the square root of the standard deviation.

## Value

An object of class `prcomp` and `converted_from_arrayspc`, which includes a list element called `$method`, a character string describing the pre-processing carried out and the type of PCA performed (used to annotate plots). A check is carried out to see if the computation was successful and a warning issued if it failed.

## Author(s)

Bryan A. Hanson (DePauw University).

## References

H. Zou, T. Hastie and R. Tibshirani "Sparse Principal Components Analysis" *J. Comp. Stat. Graphics* vol. 15 no. 2 pgs. 265-286 (2006).

## See Also

`arrayspc` for the underlying function, `c_pcaSpectra` for classical PCA calculations, `r_pcaSpectra` for robust PCA calculations, `irlba_pcaSpectra` for PCA via the IRLBA algorithm. Additional documentation at <https://bryanhanson.github.io/ChemoSpec/>

For displaying the results, `ChemoSpecUtils::plotScree()`, `ChemoSpecUtils::plotScores()`, `plotLoadings()`, `plot2Loadings()`, `sPlotSpectra()`.

## Examples

```
## Not run:  
# This example assumes the graphics output is set to ggplot2 (see ?GraphicsOptions).  
library("ggplot2")  
data(SrE.NMR)
```

```
pca <- s_pcaSpectra(SrE.NMR)

p1 <- plotScree(pca)
p1

p2 <- plotScores(SrE.NMR, pca, pcs = c(1, 2), ellipse = "cls", tol = 0.05)
p2 <- p2 + ggtitle("Scores: SrE NMR Data")
p2

p3 <- plotLoadings(SrE.NMR, pca, loads = 1:2, ref = 1)
p3 <- p3 + ggtitle("Loadings: SrE NMR Data")
p3

## End(Not run)
```

---

updateGroups

*Update Group Names in a Spectra or Spectra2D Object*

---

### **Description**

This function is used by ChemoSpec and ChemoSpec2D, but is formally part of ChemoSpecUtils. You can access full documentation via [updateGroups](#).



# Index

- \* **classes**
  - Spectra, 48
- \* **cluster**
  - evalClusters, 16
  - hcaSpectra, 22
  - mclust3dSpectra, 27
  - mclustSpectra, 29
- \* **datasets**
  - metMUD1, 30
  - SrE. IR, 51
- \* **file**
  - files2SpectraObject, 17
- \* **hplot**
  - baselineSpectra, 9
  - plot2Loadings, 35
  - plot3dScores, 36
  - plotLoadings, 37
  - plotSpectra, 39
  - plotSpectraDist, 40
  - reviewAllSpectra, 44
  - sampleDist, 46
  - sPlotSpectra, 50
  - surveySpectra, 53
- \* **htest**
  - aov\_pcaSpectra, 6
  - aovPCAloadings, 4
  - aovPCAscores, 5
  - hypTestScores, 24
- \* **import**
  - files2SpectraObject, 17
- \* **manip**
  - binSpectra, 10
  - normSpectra, 31
- \* **multivariate**
  - aov\_pcaSpectra, 6
  - aovPCAloadings, 4
  - aovPCAscores, 5
  - c\_pcaSpectra, 15
  - ChemoSpec-package, 3
  - cv\_pcaSpectra, 13
  - evalClusters, 16
  - hcaSpectra, 22
  - hmapSpectra, 23
  - hypTestScores, 24
  - irlba\_pcaSpectra, 26
  - mclust3dSpectra, 27
  - mclustSpectra, 29
  - pcaDiag, 33
  - plot2Loadings, 35
  - plot3dScores, 36
  - plotLoadings, 37
  - plotSpectraDist, 40
  - r\_pcaSpectra, 45
  - s\_pcaSpectra, 54
  - sampleDist, 46
  - sgfSpectra, 47
- \* **package**
  - ChemoSpec-package, 3
- \* **plot**
  - plotSpectraJS, 42
- \* **robust**
  - r\_pcaSpectra, 45
- \* **utilities**
  - averageReplicates, 8
  - binSpectra, 10
  - clupaSpectra, 12
  - normSpectra, 31
  - sgfSpectra, 47
  - splitSpectraGroups, 49
- alignMUD (metMUD1), 30
- aov, 25
- aov\_pcaSpectra, 4–6, 6, 15
- aovPCAloadings, 4, 7
- aovPCAscores, 4, 5, 7
- arrayspc, 55
- averageReplicates, 8
- baseline, 9

- baselineSpectra, 9
- binSpectra, 10, 10
- browseURL, 42
- c\_pcaSpectra, 7, 15, 27, 35, 37, 38, 46, 50, 55
- check4Gaps, 11, 11
- ChemoSpec (ChemoSpec-package), 3
- ChemoSpec-package, 3
- ChemoSpecUtils::GraphicsOptions(), 6, 34, 41
- ChemoSpecUtils::plotScores(), 16, 27, 46, 55
- ChemoSpecUtils::plotScree(), 16, 27, 46, 55
- chkGraphicsOpt, 11, 11
- chkSpectra, 11, 11, 48
- clupaSpectra, 12
- colorSymbol, 13, 13, 18, 48
- conColScheme, 13, 13, 49, 50
- cv\_pcaSpectra, 13
- dendrogram, 22
- evalClusters, 16
- files2SpectraObject, 17, 48
- graphics::legend(), 39
- GraphicsOptions, 40, 44
- GraphicsOptions(), 4, 35, 38, 40, 44, 51, 54
- hcaScores, 17, 21, 21, 22
- hcaSpectra, 17, 22
- hclust, 17, 22
- hmap, 23, 24
- hmapSpectra, 23
- hypTestScores, 24
- irlba, 26
- irlba\_pcaSpectra, 16, 26, 46, 55
- legend, 5, 22
- list.files, 19
- make.names, 20
- matrix2SpectraObject, 48
- matrix2SpectraObject (files2SpectraObject), 17
- Mclust, 28, 30
- mclust3dSpectra, 27
- mclustSpectra, 29
- metMUD1, 30
- metMUD2 (metMUD1), 30
- NbClust, 17
- normSpectra, 15, 26, 31, 54
- pcaCV, 13, 14
- pcaDiag, 33
- pcaDiagplot, 33, 34
- PCAGrid, 46
- plot2Loadings, 35, 38
- plot2Loadings(), 16, 27, 46, 55
- plot3dScores, 36
- plotLoadings, 4, 35, 37
- plotLoadings(), 16, 27, 46, 55
- plotScores, 5, 6, 38, 38
- plotScree, 38, 38
- plotSpectra, 9, 39, 42, 43
- plotSpectraDist, 40
- plotSpectraJS, 40, 42
- prcomp, 15, 16, 25, 28, 29, 33, 35–37
- prcomp\_irlba, 27
- r\_pcaSpectra, 7, 16, 27, 35, 37, 45, 50, 55
- read.table, 17, 19
- readJDX, 19
- removeFreq, 43, 43
- removeGroup, 43, 43
- removeSample, 42, 44, 44
- reviewAllSpectra, 44
- rowDist, 22, 41, 45, 45
- s\_pcaSpectra, 16, 27, 46, 54
- sampleDist, 41, 46, 46
- sgfSpectra, 47
- sgolayfilt, 47
- Spectra, 5, 7, 8, 10–13, 15, 17, 19, 20, 22, 24–27, 30, 31, 33, 36, 39, 40, 42, 45, 47, 48, 49, 50, 52–54
- Spectra(), 4, 5, 7–10, 12, 14, 15, 17, 22, 23, 25, 26, 28, 29, 32, 33, 35–37, 39, 41, 42, 44, 45, 47, 49, 50, 53, 55
- splitSpectraGroups, 24, 25, 49
- sPlotSpectra, 35, 38, 50
- sPlotSpectra(), 16, 27, 46, 55
- SrE.IR, 23, 51
- SrE.NMR (SrE.IR), 51
- sumGroups, 48, 52, 52

sumSpectra, [20](#), [48](#), [52](#), [52](#)

surveySpectra, [53](#)

surveySpectra2 (surveySpectra), [53](#)

updateGroups, [21](#), [56](#), [56](#)