Package 'AlpsNMR'

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Type Package

Title Automated spectraL Processing System for NMR

Version 3.2.3

Encoding UTF-8

Description Reads Bruker NMR data directories both zipped and unzipped.
It provides automated and efficient signal processing for untargeted
NMR metabolomics.
It is able to interpolate the samples, detect outliers, exclude regions,
normalize, detect peaks, align the spectra, integrate peaks, manage metadata and
visualize the spectra.
After spectra proccessing, it can apply multivariate analysis on extracted data.
Efficient plotting with 1-D data is also available.
Basic reading of 1D ACD/Labs exported JDX samples is also available.

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LazyData FALSE

Depends R (>= 4.0), dplyr (>= 0.7.5), future (>= 1.10.0), magrittr (>= 1.5)

Imports utils, graphics, stats, grDevices, signal (>= 0.7-6), assertthat (>= 0.2.0), rlang (>= 0.3.0.1), stringr (>= 1.3.1), tibble(>= 1.3.4), tidyr (>= 1.0.0), readxl (>= 1.1.0), plyr (>= 1.8.4), purrr (>= 0.2.5), glue (>= 1.2.0), reshape2 (>= 1.4.3), GGally (>= 1.4.0), mixOmics (>= 6.3.2), matrixStats (>= 0.54.0), writexl (>= 1.0), fs (>= 1.2.6), rmarkdown (>= 1.10), speaq (>= 2.4.0), htmltools (>= 0.3.6), ggrepel (>= 0.8.0), pcaPP (>= 1.9-73), furrr (>= 0.1.0), ggplot2 (>= 3.1.0), baseline (>= 1.2-1), zip (>= 2.0.4), tidyselect (>= 0.2.5), vctrs (>= 0.3.0), BiocParallel, SummarizedExperiment, S4Vectors

Suggests DT (>= 0.5), testthat (>= 2.0.0), plotly (>= 4.7.1), ChemoSpec, knitr

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Roxygen list(markdown = TRUE)

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R topics documented:

`AlpsNMR-package` *AlpsNMR: Automated spectraL Processing System for NMR*

Description

AlpsNMR allows you to import NMR spectra into R and provides automated and efficient signal processing for untargeted NMR metabolomics.

Details

The following functions can be combined with the pipe. They create or modify the nmr_dataset object.

- `nmr_read_samples_dir()` or `nmr_read_samples()`
- `nmr_interpolate_1D()`
- `nmr_exclude_region()`
- `nmr_normalize()`

- plot()

There are also functions to extract the metadata and submit the samples to irods, see the example below.

The nmr_dataset object is essentially a list, so it is easy to access its components for further analysis.

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Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
my_nmr_dataset <- dataset %>%
  nmr_interpolate_1D(axis = c(0.4, 10)) %>%
  nmr_exclude_region(exclude = list(water = c(4.6, 5))) %>%
  nmr_normalize(method = "pqn") %>%
  plot
```

AUC_model *Deprecated function Extracts AUC value*

Description

The function extracts the AUC value from the middle MUVR model

Usage

```
AUC_model(MVObj)
```

Arguments

MVObj	a MUVR model

Value

the AUC value of the middle model

Examples

```
message("Deprecated. MUVR is not compatible with Bioconductor,
use bp_kfold_VIP_analysis method instead")
```

---

bp_kfold_VIP_analysis *K-fold bootstrap and permutation over PLS-VIP*

Description

Bootstrap and permutation over PLS-VIP on AlpsNMR can be performed on both nmr_dataset_1D full spectra as well as nmr_dataset_peak_table peak tables.

Usage

```
bp_kfold_VIP_analysis(dataset, y_column, k = 4, ncomp = 3, nbootstrap = 300)
```

Arguments

dataset	An nmr_dataset_family object
y_column	A string with the name of the y column (present in the metadata of the dataset)
k	Number of folds, recomended between 4 to 10
ncomp	number of components for the bootstrap models
nbootstrap	number of bootstrap dataset

Details

Use of the bootstrap and permutation methods for a more robust variable importance in the projection metric for partial least squares regression, in a k-fold cross validation

Value

A list with the following elements:

- `important_vips`: A list with the important vips selected
- `relevant_vips`: List of vips with some relevance
- `wilcoxon_vips`: List of vips that pass a wilcoxon test
- `vip_means`: Means of the vips scores
- `vip_score_plot`: plot of the vips scores
- `kfold_resuls`: results of the k bp_VIP_analysis
- `kfold_index`: list of index of partitions of the folds

Examples

```
# Data analysis for a table of integrated peaks

## Generate an artificial nmr_dataset_peak_table:
### Generate artificial metadata:
num_samples <- 64 # use an even number in this example
num_peaks <- 20
metadata <- data.frame(
    NMRExperiment = as.character(1:num_samples),
    Condition = rep(c("A", "B"), times = num_samples/2),
    stringsAsFactors = FALSE
)

### The matrix with peaks
peak_means <- runif(n = num_peaks, min = 300, max = 600)
peak_sd <- runif(n = num_peaks, min = 30, max = 60)
peak_matrix <- mapply(function(mu, sd) rnorm(num_samples, mu, sd),
                                            mu = peak_means, sd = peak_sd)
colnames(peak_matrix) <- paste0("Peak", 1:num_peaks)
rownames(peak_matrix) <- paste0("Sample", 1:num_samples)

## Artificial differences depending on the condition:
peak_matrix[metadata$Condition == "A", "Peak2"] <-
    peak_matrix[metadata$Condition == "A", "Peak2"] + 70

peak_matrix[metadata$Condition == "A", "Peak6"] <-
    peak_matrix[metadata$Condition == "A", "Peak6"] - 60

### The nmr_dataset_peak_table
peak_table <- new_nmr_dataset_peak_table(
    peak_table = peak_matrix,
    metadata = list(external = metadata)
)

## We will use bootstrap and permutation method for VIPs selection
## in a a k-fold cross validation
bp_results <- bp_kfold_VIP_analysis(peak_table, # Data to be analized
                           y_column = "Condition", # Label
                           k = 3,
                           nbootstrap = 10)

message("Selected VIPs are: ", bp_results$importarn_vips)
```

---

bp_VIP_analysis *Bootstrap and permutation over PLS-VIP*

Description

Bootstrap and permutation over PLS-VIP on AlpsNMR can be performed on both nmr_dataset_1D full spectra as well as nmr_dataset_peak_table peak tables.

Usage

```
bp_VIP_analysis(dataset, train_index, y_column, ncomp, nbootstrap = 300)
```

Arguments

dataset	An nmr_dataset_family object
train_index	set of index used to generate the bootstrap datasets
y_column	A string with the name of the y column (present in the metadata of the dataset)
ncomp	number of components used in the plsda models
nbootstrap	number of bootstrap dataset

Details

Use of the bootstrap and permutation methods for a more robust variable importance in the projection metric for partial least squares regression

Value

A list with the following elements:

- `important_vips`: A list with the important vips selected
- `relevant_vips`: List of vips with some relevance
- `pls_vip`: Pls-VIPs of every bootstrap
- `pls_vip_perm`: Pls-VIPs of every bootstrap with permuted variables
- `pls_vip_means`: Pls-VIPs normaliced differences means
- `pls_vip_score_diff`: Differences of `pls_vip` and `pls_vip_perm`
- `pls_models`: pls models of the diferent bootstraps
- `pls_perm_models`: pls permuted models of the diferent bootstraps
- `classif_rate`: classification rate of the bootstrap models
- `general_model`: pls model trained with all train data
- `general_CR`: classification rate of the `general_model`
- `vips_model`: pls model trained with vips selection over all train data
- `vips_CR`: classification rate of the `vips_model`
- `error`: error spected in a t distribution
- `lower_bound`: lower bound of the confidence interval
- `upper_bound`: upper bound of the confidence interval

Examples

```
# Data analysis for a table of integrated peaks

## Generate an artificial nmr_dataset_peak_table:
### Generate artificial metadata:
num_samples <- 32 # use an even number in this example
num_peaks <- 20
metadata <- data.frame(
    NMRExperiment = as.character(1:num_samples),
    Condition = rep(c("A", "B"), times = num_samples/2),
    stringsAsFactors = FALSE
)

### The matrix with peaks
peak_means <- runif(n = num_peaks, min = 300, max = 600)
peak_sd <- runif(n = num_peaks, min = 30, max = 60)
peak_matrix <- mapply(function(mu, sd) rnorm(num_samples, mu, sd),
                                            mu = peak_means, sd = peak_sd)
colnames(peak_matrix) <- paste0("Peak", 1:num_peaks)

## Artificial differences depending on the condition:
peak_matrix[metadata$Condition == "A", "Peak2"] <-
    peak_matrix[metadata$Condition == "A", "Peak2"] + 70

peak_matrix[metadata$Condition == "A", "Peak6"] <-
    peak_matrix[metadata$Condition == "A", "Peak6"] - 60

### The nmr_dataset_peak_table
peak_table <- new_nmr_dataset_peak_table(
    peak_table = peak_matrix,
    metadata = list(external = metadata)
)

## We will use a double cross validation, splitting the samples with random
## subsampling both in the external and internal validation.
## The classification model will be a PLSDA, exploring at maximum 3 latent
## variables.
## The best model will be selected based on the area under the ROC curve
methodology <- plsda_auroc_vip_method(ncomp = 3)
model <- nmr_data_analysis(
    peak_table,
    y_column = "Condition",
    identity_column = NULL,
    external_val = list(iterations = 1, test_size = 0.25),
    internal_val = list(iterations = 3, test_size = 0.25),
    data_analysis_method = methodology
)
## Area under ROC for each outer cross-validation iteration:
model$outer_cv_results_digested$auroc

## The number of components for the bootstrap models is selected
ncomps <- model$outer_cv_results$`1`$model$ncomp
```

```
train_index <- model$train_test_partitions$outer$`1`$outer_train

# Bootstrap and permutation for VIP selection
bp_VIPS <- bp_VIP_analysis(peak_table, # Data to be analized
                           train_index,
                           y_column = "Condition",
                           ncomp = ncomps,
                           nbootstrap = 10)
```

`computes_peak_width_ppm` *Peak width estimation for integration*

Description

Estimates the peak width (ppm width) to perform peak integration using `nmr_integrate_peak_positions`. for this purpose, the full width at half maximum of a peak from alanine doublet is considered.

Usage

```
computes_peak_width_ppm(nmr_dataset)
```

Arguments

`nmr_dataset`	An nmr_dataset_1D.

Value

Numerical. A peak width (ppm) that may be set in `nmr_integrate_peak_positions`

See Also

Other peak integration functions: Pipelines, `nmr_identify_regions_blood()`, `nmr_identify_regions_cell()`, `nmr_identify_regions_urine()`, `nmr_integrate_regions()`, `validate_nmr_dataset_peak_table()`

Other nmr_dataset_1D functions: `[.nmr_dataset_1D()`, `file_lister()`, `files_to_rDolphin()`, `format.nmr_dataset_1D()`, `is.nmr_dataset_1D()`, `load_and_save_functions`, `new_nmr_dataset_1D()`, `nmr_align_find_ref()`, `nmr_baseline_removal()`, `nmr_baseline_threshold()`, `nmr_exclude_region()`, `nmr_integrate_regions()`, `nmr_interpolate_1D()`, `nmr_meta_add()`, `nmr_meta_export()`, `nmr_meta_get_column()`, `nmr_meta_get()`, `nmr_normalize()`, `nmr_pca_build_model()`, `nmr_pca_outliers_filter()`, `nmr_pca_outliers_plot()`, `nmr_pca_outliers_robust()`, `nmr_pca_outliers()`, `nmr_ppm_resolution()`, `plot.nmr_dataset_1D()`, `plot_webgl()`, `print.nmr_dataset_1D()`, `rdCV_PLS_RF_ML()`, `rdCV_PLS_RF()`, `save_files_to_rDolphin()`, `to_ChemoSpec()`, `validate_nmr_dataset_peak_table()`, `validate_nmr_dataset()`

confusion_matrix *Deprecated function Confusion matrix of the MUVR model*

Description

After creating a model with the rdCV_PLS_RF function, you can run confusion_matrix on the model to make a confusion matrix from MUVR. This gives information about the model performance (e.g. classification rate).

Usage

```
confusion_matrix(MVObj, model = "mid")
```

Arguments

MVObj	a MUVR model
model	What type of model to plot ('min', 'mid' or 'max'). Defaults to 'mid'.

Value

A confusion matrix of the model comparing actual vs predicted class

Examples

```
message("Deprecated. MUVR is not compatible with Bioconductor,
use bp_kfold_VIP_analysis method instead")
```

files_to_rDolphin *Files to rDoplhin*

Description

The rDolphin family functions are introduced to perform automatic targeted metabolite profiling. Therefore, ensure that you interpolated from -0.1 ppm in order to consider the TSP/DSS signal at 0.0 ppm. The function generates a list with the files required by to_rDolphin function. Then, it is required to save them with the save_files_to_rDolphin. to_rDolphin function will read the generated "parameters.csv" file. function.

Usage

```
files_to_rDolphin(nmr_dataset, biological_origin)
```

Arguments

nmr_dataset	An nmr_dataset object
biological_origin	String specify the type of sample (blood, urine, cell)

Value

a list containing:

- `meta_rDolphin`: metadata in rDolphin format,
- `NMR_spectra`: spectra matrix
- `ROI`: ROI template
- `Parameters`: parameters file

See Also

Other import/export functions: Pipelines, load_and_save_functions, nmr_data(), nmr_meta_export(), nmr_read_bruker_fid(), nmr_read_samples(), nmr_zip_bruker_samples(), save_files_to_rDolphin(), save_profiling_output(), to_ChemoSpec()

Other nmr_dataset_1D functions: [.nmr_dataset_1D(), computes_peak_width_ppm(), file_lister(), format.nmr_dataset_1D(), is.nmr_dataset_1D(), load_and_save_functions, new_nmr_dataset_1D(), nmr_align_find_ref(), nmr_baseline_removal(), nmr_baseline_threshold(), nmr_exclude_region(), nmr_integrate_regions(), nmr_interpolate_1D(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get(), nmr_normalize(), nmr_pca_build_model(), nmr_pca_outliers_filter(), nmr_pca_outliers_plot(), nmr_pca_outliers_robust(), nmr_pca_outliers(), nmr_ppm_resolution(), plot.nmr_dataset_1D(), plot_webgl(), print.nmr_dataset_1D(), rdCV_PLS_RF_ML(), rdCV_PLS_RF(), save_files_to_rDolphin(), to_ChemoSpec(), validate_nmr_dataset_peak_table(), validate_nmr_dataset()

Examples

```
## Not run:
# Set the directory in which rDolphin files will be saved
output_dir_10_rDolphin <- file.path(your_path, "10-rDolphin")
fs::dir_create(output_dir_10_rDolphin)

# Generate the files (for plasma/serum)
files_rDolphin = files_to_rDolphin(nmr_dataset_0_10_ppm, blood)

# Save the files
save_files_to_rDolphin(files_rDolphin, output_dir_10_rDolphin)

# Build the rDolphin object. Do not forget to set the directory
setwd(output_dir_10_rDolphin)
rDolphin_object = to_rDolphin("Parameters.csv")

# Visualize your spectra
rDolphin_plot(rDolphin_object)

# Run the main profiling function (it takes a while)
targeted_profiling = Automatic_targeted_profiling(rDolphin_object)

# Save results
save_profiling_output(targeted_profiling, output_dir_10_rDolphin)

save_profiling_plots(output_dir_10_rDolphin, targeted_profiling$final_output,
targeted_profiling$reproducibility_data)
```

```
#Additionally, you can run some stats
intensities = targeted_profiling$final_output$intensity
group = as.factor(rDolphin_object$Metadata$type)
model_PLS <- rdCV_PLS_RF(X = intensities, Y = group)

## End(Not run)
```

`file_lister` *NMR file lister*

Description

The function lists samples from the chosen folder required to import and create a nmr_dataset_1D object. The function is based on the `fs::dir_ls()` function.

Usage

```
file_lister(dataset_path_nmr, glob)
```

Arguments

`dataset_path_nmr`	A character vector of the path where samples are.
`glob`	A wildcard or globbing pattern common for the samples to be read, for example ending with *0 (spectra acquired by a NOESY sequence often end by 0: 10, 20, 30...) or *s (for example, samples from the tutorial in this package) passed on to `grep()` to filter paths.

Value

lists of samples from the chosen folder

See Also

Other nmr_dataset_1D functions: `[.nmr_dataset_1D()`, `computes_peak_width_ppm()`, `files_to_rDolphin()`, `format.nmr_dataset_1D()`, `is.nmr_dataset_1D()`, `load_and_save_functions`, `new_nmr_dataset_1D()`, `nmr_align_find_ref()`, `nmr_baseline_removal()`, `nmr_baseline_threshold()`, `nmr_exclude_region()`, `nmr_integrate_regions()`, `nmr_interpolate_1D()`, `nmr_meta_add()`, `nmr_meta_export()`, `nmr_meta_get_column()`, `nmr_meta_get()`, `nmr_normalize()`, `nmr_pca_build_model()`, `nmr_pca_outliers_filter()`, `nmr_pca_outliers_plot()`, `nmr_pca_outliers_robust()`, `nmr_pca_outliers()`, `nmr_ppm_resolution()`, `plot.nmr_dataset_1D()`, `plot_webgl()`, `print.nmr_dataset_1D()`, `rdCV_PLS_RF_ML()`, `rdCV_PLS_RF()`, `save_files_to_rDolphin()`, `to_ChemoSpec()`, `validate_nmr_dataset_peak_table()`, `validate_nmr_dataset()`

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
lists_of_samples <- file_lister(dir_to_demo_dataset, "*0")
```

`filter.nmr_dataset_family` *Keep samples based on metadata column criteria*

Description

Keep samples based on metadata column criteria

Usage

```
## S3 method for class 'nmr_dataset_family'
filter(.data, ...)
```

Arguments

`.data`	An nmr_dataset_family object
`...`	conditions, as in dplyr

Value

The same object, with the matching rows

See Also

Other subsetting functions: `[.nmr_dataset_1D()`, `[.nmr_dataset_peak_table()`, `[.nmr_dataset()`, `nmr_pca_outliers_filter()`

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
dataset_1D <- nmr_interpolate_1D(dataset, axis = c(min = -0.5, max = 10, by = 2.3E-4))

## example 1
sample_10 <- filter(dataset_1D, NMRExperiment == "10")

## example 2
#test_samples <- dataset_1D %>% filter(nmr_peak_table$metadata$external$Group == "placebo")
```

`format.nmr_dataset` *Format for nmr_dataset*

Description

Format for nmr_dataset

Usage

```
## S3 method for class 'nmr_dataset'
format(x, ...)
```

Arguments

`x`	an nmr_dataset object
`...`	for future use

Value

Format for nmr_dataset

See Also

Other class helper functions: `format.nmr_dataset_1D()`, `format.nmr_dataset_peak_table()`, `is.nmr_dataset_1D()`, `is.nmr_dataset_peak_table()`, `new_nmr_dataset_1D()`, `new_nmr_dataset_peak_table()`, `new_nmr_dataset()`, `print.nmr_dataset_1D()`, `print.nmr_dataset_peak_table()`, `print.nmr_dataset()`, `validate_nmr_dataset_family()`, `validate_nmr_dataset_peak_table()`, `validate_nmr_dataset()`

Other nmr_dataset functions: `[.nmr_dataset()`, `load_and_save_functions`, `new_nmr_dataset()`, `nmr_interpolate_1D()`, `nmr_meta_add()`, `nmr_meta_export()`, `nmr_meta_get_column()`, `nmr_meta_get()`, `nmr_ppm_resolution()`, `nmr_read_samples()`, `print.nmr_dataset()`, `validate_nmr_dataset()`

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
format(dataset)
```

`format.nmr_dataset_1D` *format for nmr_dataset_1D*

Description

format for nmr_dataset_1D

Usage

```
## S3 method for class 'nmr_dataset_1D'
format(x, ...)
```

Arguments

x	an nmr_dataset_1D object
...	for future use

Value

format for nmr_dataset_1D

See Also

Other class helper functions: format.nmr_dataset_peak_table(), format.nmr_dataset(), is.nmr_dataset_1D(), is.nmr_dataset_peak_table(), new_nmr_dataset_1D(), new_nmr_dataset_peak_table(), new_nmr_dataset(), print.nmr_dataset_1D(), print.nmr_dataset_peak_table(), print.nmr_dataset(), validate_nmr_dataset_famil validate_nmr_dataset_peak_table(), validate_nmr_dataset()

Other nmr_dataset_1D functions: [.nmr_dataset_1D(), computes_peak_width_ppm(), file_lister(), files_to_rDolphin(), is.nmr_dataset_1D(), load_and_save_functions, new_nmr_dataset_1D(), nmr_align_find_ref(), nmr_baseline_removal(), nmr_baseline_threshold(), nmr_exclude_region(), nmr_integrate_regions(), nmr_interpolate_1D(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get(), nmr_normalize(), nmr_pca_build_model(), nmr_pca_outliers_filter(), nmr_pca_outliers_plot(), nmr_pca_outliers_robust(), nmr_pca_outliers(), nmr_ppm_resolution(), plot.nmr_dataset_1D(), plot_webgl(), print.nmr_dataset_1D(), rdCV_PLS_RF_ML(), rdCV_PLS_RF(), save_files_to_rDolphin(), to_ChemoSpec(), validate_nmr_dataset_peak_table(), validate_nmr_dataset()

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
dataset_1D <- nmr_interpolate_1D(dataset, axis = c(min = -0.5, max = 10, by = 2.3E-4))
format(dataset_1D)
```

format.nmr_dataset_peak_table *Format for nmr_dataset_peak_table*

Description

Format for nmr_dataset_peak_table

Usage

```
## S3 method for class 'nmr_dataset_peak_table'
format(x, ...)
```

Arguments

x	an nmr_dataset_peak_table object
...	for future use

Value

Format for nmr_dataset_peak_table

See Also

Other nmr_dataset_peak_table functions: [.nmr_dataset_peak_table(), is.nmr_dataset_peak_table(), load_and_save_functions, new_nmr_dataset_peak_table(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get(), print.nmr_dataset_peak_table(), validate_nmr_dataset_peak_table(

Other class helper functions: format.nmr_dataset_1D(), format.nmr_dataset(), is.nmr_dataset_1D(), is.nmr_dataset_peak_table(), new_nmr_dataset_1D(), new_nmr_dataset_peak_table(), new_nmr_dataset(), print.nmr_dataset_1D(), print.nmr_dataset_peak_table(), print.nmr_dataset(), validate_nmr_dataset_famil validate_nmr_dataset_peak_table(), validate_nmr_dataset()

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
dataset_1D <- nmr_interpolate_1D(dataset, axis = c(min = -0.5, max = 10, by = 2.3E-4))
meta <- file.path(dir_to_demo_dataset, "dummy_metadata.xlsx")
metadata <- readxl::read_excel(meta, sheet = 1)
dataset_1D <- nmr_meta_add(dataset_1D, metadata = metadata, by = "NMRExperiment")
metadata <- list(external = dataset_1D[["metadata"]][["external"]])
peak_table <- nmr_data(dataset_1D)
new <- new_nmr_dataset_peak_table(peak_table, metadata)
format(new)
```

hmdb *The Human Metabolome DataBase multiplet table*

Description

The Human Metabolome DataBase multiplet table

References

https://hmdb.ca/

HMDB_blood *The Human Metabolome DataBase multiplet table: blood metabolites normally found in NMR-based metabolomics*

Description

The Human Metabolome DataBase multiplet table: blood metabolites normally found in NMR-based metabolomics

References

https://hmdb.ca/

HMDB_cell *The Human Metabolome DataBase multiplet table: cell metabolites normally found in NMR-based metabolomics*

Description

The Human Metabolome DataBase multiplet table: cell metabolites normally found in NMR-based metabolomics

References

https://hmdb.ca/

HMDB_urine — *The Human Metabolome DataBase multiplet table: urine metabolites normally found in NMR-based metabolomics*

Description

The Human Metabolome DataBase multiplet table: urine metabolites normally found in NMR-based metabolomics

References

https://hmdb.ca/

is.nmr_dataset — *Object is of nmr_dataset class*

Description

Object is of nmr_dataset class

Usage

```
is.nmr_dataset(x)
```

Arguments

x	An object

Value

TRUE if the object is an nmr_dataset, FALSE otherwise

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
is(dataset)
```

`is.nmr_dataset_1D` *Object is of nmr_dataset_1D class*

Description

Object is of nmr_dataset_1D class

Usage

```
is.nmr_dataset_1D(x)
```

Arguments

x	an nmr_dataset_1D object

Value

TRUE if the object is an nmr_dataset_1D, FALSE otherwise

See Also

Other class helper functions: format.nmr_dataset_1D(), format.nmr_dataset_peak_table(), format.nmr_dataset(), is.nmr_dataset_peak_table(), new_nmr_dataset_1D(), new_nmr_dataset_peak_table(), new_nmr_dataset(), print.nmr_dataset_1D(), print.nmr_dataset_peak_table(), print.nmr_dataset(), validate_nmr_dataset_family(), validate_nmr_dataset_peak_table(), validate_nmr_dataset()

Other nmr_dataset_1D functions: [.nmr_dataset_1D(), computes_peak_width_ppm(), file_lister(), files_to_rDolphin(), format.nmr_dataset_1D(), load_and_save_functions, new_nmr_dataset_1D(), nmr_align_find_ref(), nmr_baseline_removal(), nmr_baseline_threshold(), nmr_exclude_region(), nmr_integrate_regions(), nmr_interpolate_1D(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get(), nmr_normalize(), nmr_pca_build_model(), nmr_pca_outliers_filter(), nmr_pca_outliers_plot(), nmr_pca_outliers_robust(), nmr_pca_outliers(), nmr_ppm_resolution(), plot.nmr_dataset_1D(), plot_webgl(), print.nmr_dataset_1D(), rdCV_PLS_RF_ML(), rdCV_PLS_RF(), save_files_to_rDolphin(), to_ChemoSpec(), validate_nmr_dataset_peak_table(), validate_nmr_dataset()

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
dataset_1D <- nmr_interpolate_1D(dataset, axis = c(min = -0.5, max = 10, by = 2.3E-4))
result <- is(dataset_1D)
```

`is.nmr_dataset_peak_table` *Object is of nmr_dataset_peak_table class*

Description

Object is of nmr_dataset_peak_table class

Usage

```
is.nmr_dataset_peak_table(x)
```

Arguments

x	an nmr_dataset_peak_table object

Value

TRUE if the object is an nmr_dataset_peak_table, FALSE otherwise

See Also

Other nmr_dataset_peak_table functions: [.nmr_dataset_peak_table(), format.nmr_dataset_peak_table(), load_and_save_functions, new_nmr_dataset_peak_table(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get(), print.nmr_dataset_peak_table(), validate_nmr_dataset_peak_table(

Other class helper functions: format.nmr_dataset_1D(), format.nmr_dataset_peak_table(), format.nmr_dataset(), is.nmr_dataset_1D(), new_nmr_dataset_1D(), new_nmr_dataset_peak_table(), new_nmr_dataset(), print.nmr_dataset_1D(), print.nmr_dataset_peak_table(), print.nmr_dataset(), validate_nmr_dataset_family(), validate_nmr_dataset_peak_table(), validate_nmr_dataset()

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
dataset_1D <- nmr_interpolate_1D(dataset, axis = c(min = -0.5, max = 10, by = 2.3E-4))
meta <- file.path(dir_to_demo_dataset, "dummy_metadata.xlsx")
metadata <- readxl::read_excel(meta, sheet = 1)
dataset_1D <- nmr_meta_add(dataset_1D, metadata = metadata, by = "NMRExperiment")
metadata <- list(external = dataset_1D[["metadata"]][["external"]])
peak_table <- nmr_data(dataset_1D)
new <- new_nmr_dataset_peak_table(peak_table, metadata)
is(new)
```

load_and_save_functions *nmr_dataset_load*

Description

nmr_dataset_load

nmr_dataset_save

Usage

```
nmr_dataset_load(file_name)

nmr_dataset_save(nmr_dataset, file_name, ...)
```

Arguments

file_name	The file name to load or save to
nmr_dataset	An object from the nmr_dataset_family
...	Additional arguments passed to saveRDS.

Value

Functions to load and save nmr_dataset objects

load nmr dataset

save nmr dataset

See Also

Other nmr_dataset functions: [.nmr_dataset(), format.nmr_dataset(), new_nmr_dataset(), nmr_interpolate_1D(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get(), nmr_ppm_resolution(), nmr_read_samples(), print.nmr_dataset(), validate_nmr_dataset()

Other nmr_dataset_1D functions: [.nmr_dataset_1D(), computes_peak_width_ppm(), file_lister(), files_to_rDolphin(), format.nmr_dataset_1D(), is.nmr_dataset_1D(), new_nmr_dataset_1D(), nmr_align_find_ref(), nmr_baseline_removal(), nmr_baseline_threshold(), nmr_exclude_region(), nmr_integrate_regions(), nmr_interpolate_1D(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get(), nmr_normalize(), nmr_pca_build_model(), nmr_pca_outliers_filter(), nmr_pca_outliers_plot(), nmr_pca_outliers_robust(), nmr_pca_outliers(), nmr_ppm_resolution(), plot.nmr_dataset_1D(), plot_webgl(), print.nmr_dataset_1D(), rdCV_PLS_RF_ML(), rdCV_PLS_RF(), save_files_to_rDolphin(), to_ChemoSpec(), validate_nmr_dataset_peak_table(), validate_nmr_dataset()

Other nmr_dataset_peak_table functions: [.nmr_dataset_peak_table(), format.nmr_dataset_peak_table(), is.nmr_dataset_peak_table(), new_nmr_dataset_peak_table(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get(), print.nmr_dataset_peak_table(), validate_nmr_dataset_peak_table(

Other import/export functions: Pipelines, files_to_rDolphin(), nmr_data(), nmr_meta_export(), nmr_read_bruker_fid(), nmr_read_samples(), nmr_zip_bruker_samples(), save_files_to_rDolphin(), save_profiling_output(), to_ChemoSpec()

Examples

```
# dataset <- nmr_dataset_load("test")
nmr_dataset <- nmr_dataset_load(system.file("extdata", "nmr_dataset.rds", package = "AlpsNMR"))

dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
# nmr_dataset_save(dataset, "test")
```

`models_stability_plot_bootstrap` *Models stability plot*

Description

Plot stability among models of the external cross validation

Usage

```
models_stability_plot_bootstrap(bp_results)
```

Arguments

`bp_results`	bp_kfold_VIP_analysis results

Value

A plot of models stability

Examples

```
# Data analysis for a table of integrated peaks

## Generate an artificial nmr_dataset_peak_table:
### Generate artificial metadata:
num_samples <- 64 # use an even number in this example
num_peaks <- 20
metadata <- data.frame(
    NMRExperiment = as.character(1:num_samples),
    Condition = rep(c("A", "B"), times = num_samples/2),
    stringsAsFactors = FALSE
)

### The matrix with peaks
peak_means <- runif(n = num_peaks, min = 300, max = 600)
peak_sd <- runif(n = num_peaks, min = 30, max = 60)
peak_matrix <- mapply(function(mu, sd) rnorm(num_samples, mu, sd),
                                            mu = peak_means, sd = peak_sd)
colnames(peak_matrix) <- paste0("Peak", 1:num_peaks)
```

```
## Artificial differences depending on the condition:
peak_matrix[metadata$Condition == "A", "Peak2"] <-
    peak_matrix[metadata$Condition == "A", "Peak2"] + 70

peak_matrix[metadata$Condition == "A", "Peak6"] <-
    peak_matrix[metadata$Condition == "A", "Peak6"] - 60

### The nmr_dataset_peak_table
peak_table <- new_nmr_dataset_peak_table(
    peak_table = peak_matrix,
    metadata = list(external = metadata)
)

## We will use bootstrap and permutation method for VIPs selection
## in a a k-fold cross validation
#bp_results <- bp_kfold_VIP_analysis(peak_table, # Data to be analized
#                            y_column = "Condition", # Label
#                            k = 3,
#                            nbootstrap = 10)

#message("Selected VIPs are: ", bp_results$importarn_vips)

#models_stability_plot_bootstrap(bp_results)
```

`models_stability_plot_plsda` *Models stability plot*

Description

Plot stability among models of the external cross validation

Usage

```
models_stability_plot_plsda(model)
```

Arguments

`model`	A nmr_data_analysis_model

Value

A plot of models stability

Examples

```
# Data analysis for a table of integrated peaks

## Generate an artificial nmr_dataset_peak_table:
### Generate artificial metadata:
num_samples <- 32 # use an even number in this example
num_peaks <- 20
metadata <- data.frame(
    NMRExperiment = as.character(1:num_samples),
    Condition = rep(c("A", "B"), times = num_samples/2),
    stringsAsFactors = FALSE
)

### The matrix with peaks
peak_means <- runif(n = num_peaks, min = 300, max = 600)
peak_sd <- runif(n = num_peaks, min = 30, max = 60)
peak_matrix <- mapply(function(mu, sd) rnorm(num_samples, mu, sd),
                                            mu = peak_means, sd = peak_sd)
colnames(peak_matrix) <- paste0("Peak", 1:num_peaks)

## Artificial differences depending on the condition:
peak_matrix[metadata$Condition == "A", "Peak2"] <-
    peak_matrix[metadata$Condition == "A", "Peak2"] + 70

peak_matrix[metadata$Condition == "A", "Peak6"] <-
    peak_matrix[metadata$Condition == "A", "Peak6"] - 60

### The nmr_dataset_peak_table
peak_table <- new_nmr_dataset_peak_table(
    peak_table = peak_matrix,
    metadata = list(external = metadata)
)

methodology <- plsda_auroc_vip_method(ncomp = 3)
model <- nmr_data_analysis(
    peak_table,
    y_column = "Condition",
    identity_column = NULL,
    external_val = list(iterations = 3, test_size = 0.25),
    internal_val = list(iterations = 3, test_size = 0.25),
    data_analysis_method = methodology
)

#models_stability_plot_plsda(model)
```

`model_VIP` *Deprecated function Model VIP values*

Description

Once, the MVObj is created and validated, this function extracts autoselected ranked variables from the model (MUVR object). See `rdCV_PLS_RF` function.

Usage

```
model_VIP(MVObj)
```

Arguments

`MVObj`	a MUVR model

Value

a data frame with the order, name and average rank of selected variables

Examples

```
message("Deprecated. MUVR is not compatible with Bioconductor,
use bp_kfold_VIP_analysis method instead")
```

`MUVR_model_plot` *Deprecated function Model plot*

Description

Plot the model (a `MUVR` object) obtained from `rdCV_PLS_RF` function. For more information about the multivariate modelling with minimally biased variable selection (MUVR) from the `MUVR` package, see Shi et al., 2018 (DOI: 10.1093/bioinformatics/bty710).

Usage

```
MUVR_model_plot(MVObj, model = "mid", factCols, sampLabels, ylim = NULL)
```

Arguments

`MVObj`	a MUVR model
`model`	What type of model to plot ('min', 'mid' or 'max'). Defaults to 'mid'.
`factCols`	An optional vector with colors for the factor levels (in the same order as the levels).
`sampLabels`	Sample labels (optional; implemented for classification)
`ylim`	Optional for imposing y-limits for regression and classification analysis

Value

A plot with the model performance

Examples

```
message("MUVR is not compatible with Bioconductor,
use bp_kfold_VIP_analysis method instead")
```

`new_nmr_dataset` *Create an nmr_dataset object*

Description

Create an nmr_dataset object

Usage

```
new_nmr_dataset(metadata, data_fields, axis)
```

Arguments

`metadata`	A named list of data frames
`data_fields`	A named list. Check the examples
`axis`	A list. Check the examples

Value

Create an nmr_dataset object

Create an nmr_dataset object

See Also

Other class helper functions: `format.nmr_dataset_1D()`, `format.nmr_dataset_peak_table()`, `format.nmr_dataset()`, `is.nmr_dataset_1D()`, `is.nmr_dataset_peak_table()`, `new_nmr_dataset_1D()`, `new_nmr_dataset_peak_table()`, `print.nmr_dataset_1D()`, `print.nmr_dataset_peak_table()`, `print.nmr_dataset()`, `validate_nmr_dataset_family()`, `validate_nmr_dataset_peak_table()`, `validate_nmr_dataset()`

Other nmr_dataset functions: `[.nmr_dataset()`, `format.nmr_dataset()`, `load_and_save_functions`, `nmr_interpolate_1D()`, `nmr_meta_add()`, `nmr_meta_export()`, `nmr_meta_get_column()`, `nmr_meta_get()`, `nmr_ppm_resolution()`, `nmr_read_samples()`, `print.nmr_dataset()`, `validate_nmr_dataset()`

Examples

```
#
metadata_1D <- list(external = data.frame(NMRExperiment = c("10", "20")))
# Sample 10 and Sample 20 can have different lengths (due to different setups)
data_fields_1D <- list(data_1r = list(runif(16), runif(32)))
# Each sample has its own axis list, with one element (because this example is 1D)
axis_1D <- list(list(1:16), list(1:32))
my_1D_data <- new_nmr_dataset(metadata_1D, data_fields_1D, axis_1D)
```

```
# Example for 2D samples
metadata_2D <- list(external = data.frame(NMRExperiment = c("11", "21")))
data_fields_2D <- list(data_2rr = list(matrix(runif(16*3), nrow=16, ncol=3),
                        runif(32*3), nrow=32, ncol=3))
# Each sample has its own axis list, with one element (because this example is 1D)
axis_2D <- list(list(1:16, 1:3), list(1:32, 1:3))
my_2D_data <- new_nmr_dataset(metadata_2D, data_fields_2D, axis_2D)
```

`new_nmr_dataset_1D` *Creates a new 1D nmr_dataset object from scratch*

Description

Creates a new 1D nmr_dataset object from scratch

Usage

```
new_nmr_dataset_1D(ppm_axis, data_1r, metadata)
```

Arguments

`ppm_axis`	A numeric vector with the ppm values for the columns of data_1r
`data_1r`	A numeric matrix with one NMR spectrum on each row
`metadata`	A list of data frames with at least the `NMRExperiment` column

Value

Creates a new 1D nmr_dataset object from scratch

See Also

Other class helper functions: `format.nmr_dataset_1D()`, `format.nmr_dataset_peak_table()`, `format.nmr_dataset()`, `is.nmr_dataset_1D()`, `is.nmr_dataset_peak_table()`, `new_nmr_dataset_peak_table()`, `new_nmr_dataset()`, `print.nmr_dataset_1D()`, `print.nmr_dataset_peak_table()`, `print.nmr_dataset()`, `validate_nmr_dataset_family()`, `validate_nmr_dataset_peak_table()`, `validate_nmr_dataset()`

Other nmr_dataset_1D functions: `[.nmr_dataset_1D()`, `computes_peak_width_ppm()`, `file_lister()`, `files_to_rDolphin()`, `format.nmr_dataset_1D()`, `is.nmr_dataset_1D()`, `load_and_save_functions`, `nmr_align_find_ref()`, `nmr_baseline_removal()`, `nmr_baseline_threshold()`, `nmr_exclude_region()`, `nmr_integrate_regions()`, `nmr_interpolate_1D()`, `nmr_meta_add()`, `nmr_meta_export()`, `nmr_meta_get_column()`, `nmr_meta_get()`, `nmr_normalize()`, `nmr_pca_build_model()`, `nmr_pca_outliers_filter()`, `nmr_pca_outliers_plot()`, `nmr_pca_outliers_robust()`, `nmr_pca_outliers()`, `nmr_ppm_resolution()`, `plot.nmr_dataset_1D()`, `plot_webgl()`, `print.nmr_dataset_1D()`, `rdCV_PLS_RF_ML()`, `rdCV_PLS_RF()`, `save_files_to_rDolphin()`, `to_ChemoSpec()`, `validate_nmr_dataset_peak_table()`, `validate_nmr_dataset()`

Examples

```
# Create a random spectra matrix
nsamp <- 12
npoints <- 20
dummy_ppm_axis <- seq(from = 0.2, to = 10, length.out = npoints)
dummy_spectra_matrix <- matrix(runif(nsamp*npoints), nrow = nsamp, ncol = npoints)
metadata <- list(external = data.frame(NMRExperiment = paste0("Sample", 1:12),
                                       DummyClass = c("a", "b"),
                                       stringsAsFactors = FALSE))
dummy_nmr_dataset_1D <- new_nmr_dataset_1D(ppm_axis = dummy_ppm_axis,
                                           data_1r = dummy_spectra_matrix,
                                           metadata = metadata)
```

---

new_nmr_dataset_peak_table

Creates a new nmr_dataset_peak_table object from scratch

Description

Creates a new nmr_dataset_peak_table object from scratch

Usage

```
new_nmr_dataset_peak_table(peak_table, metadata)
```

Arguments

peak_table	A numeric matrix with one NMR spectrum on each row
metadata	A list of data frames with at least the NMRExperiment column

Value

Creates a new nmr_dataset_peak_table object from scratch

See Also

Other nmr_dataset_peak_table functions: [.nmr_dataset_peak_table(), format.nmr_dataset_peak_table(), is.nmr_dataset_peak_table(), load_and_save_functions, nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get(), print.nmr_dataset_peak_table(), validate_nmr_dataset_peak_table(

Other class helper functions: format.nmr_dataset_1D(), format.nmr_dataset_peak_table(), format.nmr_dataset(), is.nmr_dataset_1D(), is.nmr_dataset_peak_table(), new_nmr_dataset_1D(), new_nmr_dataset(), print.nmr_dataset_1D(), print.nmr_dataset_peak_table(), print.nmr_dataset(), validate_nmr_dataset_family(), validate_nmr_dataset_peak_table(), validate_nmr_dataset()

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
dataset_1D <- nmr_interpolate_1D(dataset, axis = c(min = -0.5, max = 10, by = 2.3E-4))
meta <- file.path(dir_to_demo_dataset, "dummy_metadata.xlsx")
metadata <- readxl::read_excel(meta, sheet = 1)
dataset_1D <- nmr_meta_add(dataset_1D, metadata = metadata, by = "NMRExperiment")
metadata <- list(external = dataset_1D[["metadata"]][["external"]])
peak_table <- nmr_data(dataset_1D)
new <- new_nmr_dataset_peak_table(peak_table, metadata)
```

---

nmr_align_find_ref *Find alignment reference*

Description

Find alignment reference

Usage

```
nmr_align_find_ref(nmr_dataset, peak_data)
```

Arguments

nmr_dataset	An nmr_dataset_1D
peak_data	The detected peak data given by nmr_detect_peaks.

Value

The NMRExperiment of the reference sample

See Also

Other alignment functions: Pipelines, validate_nmr_dataset_peak_table()

Other peak alignment functions: validate_nmr_dataset_peak_table()

Other nmr_dataset_1D functions: [.nmr_dataset_1D(), computes_peak_width_ppm(), file_lister(), files_to_rDolphin(), format.nmr_dataset_1D(), is.nmr_dataset_1D(), load_and_save_functions, new_nmr_dataset_1D(), nmr_baseline_removal(), nmr_baseline_threshold(), nmr_exclude_region(), nmr_integrate_regions(), nmr_interpolate_1D(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get(), nmr_normalize(), nmr_pca_build_model(), nmr_pca_outliers_filter(), nmr_pca_outliers_plot(), nmr_pca_outliers_robust(), nmr_pca_outliers(), nmr_ppm_resolution(), plot.nmr_dataset_1D(), plot_webgl(), print.nmr_dataset_1D(), rdCV_PLS_RF_ML(), rdCV_PLS_RF(), save_files_to_rDolphin(), to_ChemoSpec(), validate_nmr_dataset_peak_table(), validate_nmr_dataset()

`nmr_baseline_removal` *Baseline Removal NMR*

Description

Removes the baseline on an nmr_dataset_1D object, using baseline::baseline.als.

Usage

```
nmr_baseline_removal(nmr_dataset, lambda = 6, p = 0.05, maxit = 20)
```

Arguments

`nmr_dataset`	An nmr_dataset_1D.
`lambda`	2nd derivative constraint
`p`	Weighting of positive residuals
`maxit`	Maximum number of iterations

Value

The same nmr_dataset_1D object after baseline removal.

See Also

baseline::baseline.als

Other nmr_dataset_1D functions: `[.nmr_dataset_1D()`, `computes_peak_width_ppm()`, `file_lister()`, `files_to_rDolphin()`, `format.nmr_dataset_1D()`, `is.nmr_dataset_1D()`, `load_and_save_functions`, `new_nmr_dataset_1D()`, `nmr_align_find_ref()`, `nmr_baseline_threshold()`, `nmr_exclude_region()`, `nmr_integrate_regions()`, `nmr_interpolate_1D()`, `nmr_meta_add()`, `nmr_meta_export()`, `nmr_meta_get_column()`, `nmr_meta_get()`, `nmr_normalize()`, `nmr_pca_build_model()`, `nmr_pca_outliers_filter()`, `nmr_pca_outliers_plot()`, `nmr_pca_outliers_robust()`, `nmr_pca_outliers()`, `nmr_ppm_resolution()`, `plot.nmr_dataset_1D()`, `plot_webgl()`, `print.nmr_dataset_1D()`, `rdCV_PLS_RF_ML()`, `rdCV_PLS_RF()`, `save_files_to_rDolphin()`, `to_ChemoSpec()`, `validate_nmr_dataset_peak_table()`, `validate_nmr_dataset()`

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
dataset_1D <- nmr_interpolate_1D(dataset, axis = c(min = -0.5, max = 10, by = 2.3E-4))
dataset_no_base_line <- nmr_baseline_removal(dataset_1D, lambda = 6, p = 0.01)
```

`nmr_baseline_threshold` *Threshold estimation for peak detection*

Description

Estimates the threshold value for peak detection on an nmr_dataset_1D object. This is performed computing the mean and the standard deviation of each spectrum beyond 9.5 ppm. The threshold is then averaged of means and adding 3 times the mean of the standard deviations

Usage

```
nmr_baseline_threshold(nmr_dataset)
```

Arguments

`nmr_dataset`	An nmr_dataset_1D.

Value

Numerical. A threshold value in intensity below that no peak is detected.

See Also

Other peak detection functions: `Pipelines`, `nmr_identify_regions_blood()`, `nmr_identify_regions_cell()`, `nmr_identify_regions_urine()`, `nmr_integrate_regions()`, `regions_from_peak_table()`, `validate_nmr_dataset_peak_table()`

Other nmr_dataset_1D functions: `[.nmr_dataset_1D()`, `computes_peak_width_ppm()`, `file_lister()`, `files_to_rDolphin()`, `format.nmr_dataset_1D()`, `is.nmr_dataset_1D()`, `load_and_save_functions`, `new_nmr_dataset_1D()`, `nmr_align_find_ref()`, `nmr_baseline_removal()`, `nmr_exclude_region()`, `nmr_integrate_regions()`, `nmr_interpolate_1D()`, `nmr_meta_add()`, `nmr_meta_export()`, `nmr_meta_get_column()`, `nmr_meta_get()`, `nmr_normalize()`, `nmr_pca_build_model()`, `nmr_pca_outliers_filter()`, `nmr_pca_outliers_plot()`, `nmr_pca_outliers_robust()`, `nmr_pca_outliers()`, `nmr_ppm_resolution()`, `plot.nmr_dataset_1D()`, `plot_webgl()`, `print.nmr_dataset_1D()`, `rdCV_PLS_RF_ML()`, `rdCV_PLS_RF()`, `save_files_to_rDolphin()`, `to_ChemoSpec()`, `validate_nmr_dataset_peak_table()`, `validate_nmr_dataset()`

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
dataset_1D <- nmr_interpolate_1D(dataset, axis = c(min = -0.5, max = 10, by = 2.3E-4))
bl_threshold <- nmr_baseline_threshold(dataset_1D)
```

nmr_batman *Batman helpers*

Description

Batman helpers

Usage

```
nmr_batman_write_options(
  bopts,
  batman_dir = "BatmanInput",
  filename = "batmanOptions.txt"
)

nmr_batman_export_dataset(
  nmr_dataset,
  batman_dir = "BatmanInput",
  filename = "NMRdata.txt"
)

nmr_batman_multi_data_user_hmdb(
  batman_dir = "BatmanInput",
  filename = "multi_data_user.csv"
)

nmr_batman_multi_data_user(
  multiplet_table,
  batman_dir = "BatmanInput",
  filename = "multi_data_user.csv"
)

nmr_batman_metabolites_list(
  metabolite_names,
  batman_dir = "BatmanInput",
  filename = "metabolitesList.csv"
)
```

Arguments

bopts	Batman options
batman_dir	Batman input directorye
filename	Filename to use, inside batman_dir
nmr_dataset	An nmr_dataset_1D object
multiplet_table	A data frame, like the hmdb dataset

metabolite_names
: A character vector of the metabolite names to consider

Value

These are helper functions to make Batman tests easier

See Also

Other batman functions: `nmr_batman_options()`

Examples

```
bopts <- nmr_batman_options()
# nmr_batman_write_options(bopts)

dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
dataset_1D <- nmr_interpolate_1D(dataset, axis = c(min = -0.5, max = 10, by = 2.3E-4))
#nmr_batman_export_dataset(dataset_1D)

message("Use of multi_data_user_hmdb")
#multi_data_user_hmdb <- nmr_batman_multi_data_user_hmdb()
hmdb <- NULL
#utils::data("hmdb", package = "AlpsNMR", envir = environment())
#hmdb <- nmr_batman_multi_data_user(hmbd)

metabolite_names <- c("alanine", "glucose")
#metabolite_names <- nmr_batman_metabolites_list(metabolite_names)
```

---

nmr_batman_options *Batman Options helper*

Description

Batman Options helper

Usage

```
nmr_batman_options(
  ppmRange = matrix(c(3, 3.1, 3.6, 3.7, 3.9, 4, 4, 4.1, 6.95, 7.05, 7.6, 7.7, 7.8,
    7.9), ncol = 2, byrow = TRUE),
  specNo = "1",
  paraProc = 4L,
  negThresh = -0.5,
  scaleFac = 1e+06,
  downSamp = 1,
  hiresFlag = 1,
```

```
  randSeed = 100025L,
  nItBurnin = 200L,
  nItPostBurnin = 5000L,
  multFile = 2L,
  thinning = 50L,
  cfeFlag = 0,
  nItRerun = 5000L,
  startTemp = 1000,
  specFreq = 600,
  a = 1e-05,
  b = 1e-09,
  muMean = 1.1,
  muVar = 0.2,
  muVar_prop = 0.002,
  nuMVar = 0.0025,
  nuMVarProp = 0.1,
  tauMean = -0.05,
  tauPrec = 2,
  rdelta = 0.02,
  csFlag = 0
)
```

Arguments

ppmRange	Range of ppm to process
specNo	Index of spectra to process
paraProc	Number of cores to use
negThresh	Truncation threshold for negative intensities
scaleFac	Divide each spectrum by this number
downSamp	Decimate each spectrum by this factor
hiresFlag	Keep High Resolution deconvolved spectra
randSeed	A random seed
nItBurnin	Number of burn-in iterations
nItPostBurnin	Number of iterations after burn-in
multFile	Multiplet file (integer)
thinning	Save MCMC state every thinning iterations
cfeFlag	Same concentration for all spectra (fixed effect)
nItRerun	Number of iterations for a batman rerun
startTemp	Start temperature
specFreq	NMR Spectrometer frequency
a	Shape parameter for the gamma distribution (used for lambda, the precision)
b	Rate distribution parameter for the gamma distribution (used for lambda, the precision)

muMean	Peak width mean in ln(Hz)
muVar	Peak width variance in ln(Hz)
muVar_prop	Peak width proposed variance in ln(Hz)
nuMVar	Peak width metabolite variance in ln(Hz)
nuMVarProp	Peak width metabolite proposed variance in ln(Hz)
tauMean	mean of the prior on tau
tauPrec	inverse of variance of prior on tau
rdelta	Truncation of the prior on peak shift (ppm)
csFlag	Specify chemical shift for each multiplet in each spectrum? (chemShiftperSpectra.csv file)

Value

A batman_options object with the Batman Options

See Also

Other batman functions: nmr_batman

Examples

```
bopts <- nmr_batman_options()
```

---

nmr_data *Set/Return the full spectra matrix*

Description

Set/Return the full spectra matrix

Usage

```
nmr_data(nmr_dataset, ...)

nmr_data(nmr_dataset) <- value

## S3 replacement method for class 'nmr_dataset_1D'
nmr_data(nmr_dataset) <- value
```

Arguments

nmr_dataset	An object from the nmr_dataset_family to get the raw data from
...	Unused and left for future compatibility
value	A matrix

Value

a matrix

The given nmr_dataset

See Also

Other import/export functions: Pipelines, files_to_rDolphin(), load_and_save_functions, nmr_meta_export(), nmr_read_bruker_fid(), nmr_read_samples(), nmr_zip_bruker_samples(), save_files_to_rDolphin(), save_profiling_output(), to_ChemoSpec()

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
dataset_1D <- nmr_interpolate_1D(dataset, axis = c(min = -0.5, max = 10, by = 2.3E-4))
dataset_data <- nmr_data(dataset_1D)
```

---

nmr_dataset *nmr_dataset (S3 class)*

Description

An nmr_dataset represents a set of NMR samples. It is defined as an S3 class, and it can be treated as a regular list.

Details

It currently has the following elements:

- metadata: A list of data frames. Each data frame contains metadata of a given area (acquisition parameters, preprocessing parameters, general sample information...)
- axis: A list with length equal to the dimensionality of the data. For 1D spectra it is a list with a numeric vector
- data_*: Data arrays with the actual spectra. The first index represents the sample, the rest of the indices match the length of each axis. Typically data_1r is a matrix with one sample on each row and the chemical shifts in the columns.
- num_samples: The number of samples in the dataset

See Also

Functions to save and load these objects

Other AlpsNMR dataset objects: nmr_dataset_1D, nmr_dataset_family

nmr_dataset_1D *nmr_dataset_1D (S3 class)*

Description

An `nmr_dataset_1D` represents a set of 1D interpolated NMR samples. It is defined as an S3 class, and it can be treated as a regular list.

Details

It currently has the following elements:

- `metadata`: A list of data frames. Each data frame contains metadata of a given area (acquisition parameters, preprocessing parameters, general sample information...)
- `axis`: A numeric vector with the chemical shift axis in ppm.
- `data_1r`: A matrix with one sample on each row and the chemical shifts in the columns.

See Also

Other AlpsNMR dataset objects: `nmr_dataset_family`, `nmr_dataset`

nmr_dataset_family *nmr_dataset like objects (S3 classes)*

Description

The AlpsNMR package defines and uses several objects to manage NMR Data.

Details

These objects share some structure and functions, so it makes sense to have an abstract class to ensure that the shared structures are compatible

See Also

Functions to save and load these objects

Other AlpsNMR dataset objects: `nmr_dataset_1D`, `nmr_dataset`

nmr_dataset_peak_table

nmr_dataset_peak_table (S3 class)

Description

An nmr_dataset_peak_table represents a peak table with metadata. It is defined as an S3 class, and it can be treated as a regular list.

Details

- metadata: A list of data frames. Each data frame contains metadata. Usually the list only has one data frame named "external".
- peak_table: A matrix with one sample on each row and the peaks in the columns

nmr_dataset_peak_table_to_SummarizedExperiment

Export nmr_dataset_peak_table to SummarizedExperiment

Description

Export nmr_dataset_peak_table to SummarizedExperiment

Usage

```
nmr_dataset_peak_table_to_SummarizedExperiment(nmr_peak_table)
```

Arguments

nmr_peak_table	An nmr_dataset_peak_table object

Value

SummarizedExperiment object (unmodified)

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
dataset_1D <- nmr_interpolate_1D(dataset, axis = c(min = -0.5, max = 10, by = 2.3E-4))
meta <- file.path(dir_to_demo_dataset, "dummy_metadata.xlsx")
metadata <- readxl::read_excel(meta, sheet = 1)
dataset_1D <- nmr_meta_add(dataset_1D, metadata = metadata, by = "NMRExperiment")
metadata <- list(external = dataset_1D[["metadata"]][["external"]])
peak_table <- nmr_data(dataset_1D)
nmr_peak_table <- new_nmr_dataset_peak_table(peak_table, metadata)
se <- nmr_dataset_peak_table_to_SummarizedExperiment(nmr_peak_table)
```

nmr_data_1r_to_SummarizedExperiment *Export 1D NMR data to SummarizedExperiment*

Description

Export 1D NMR data to SummarizedExperiment

Usage

```
nmr_data_1r_to_SummarizedExperiment(nmr_dataset)
```

Arguments

nmr_dataset	An nmr_dataset_1D object

Value

SummarizedExperiment An SummarizedExperiment object (unmodified)

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
dataset_1D <- nmr_interpolate_1D(dataset, axis = c(min = -0.5, max = 10, by = 2.3E-4))
se <- nmr_data_1r_to_SummarizedExperiment(dataset_1D)
```

nmr_data_analysis *Data analysis*

Description

Data analysis on AlpsNMR can be performed on both nmr_dataset_1D full spectra as well as nmr_dataset_peak_table peak tables.

Usage

```
nmr_data_analysis(
  dataset,
  y_column,
  identity_column,
  external_val,
  internal_val,
  data_analysis_method
)
```

Arguments

`dataset`	An nmr_dataset_family object
`y_column`	A string with the name of the y column (present in the metadata of the dataset)
`identity_column`	`NULL` or a string with the name of the identity column (present in the metadata of the dataset).
`external_val, internal_val`	A list with two elements: `iterations` and `test_size`. See random_subsampling for further details
`data_analysis_method`	An nmr_data_analysis_method object

Details

The workflow consists of a double cross validation strategy using random subsampling for splitting into train and test sets. The classification model and the metric to choose the best model can be customized (see `new_nmr_data_analysis_method()`), but for now only a PLSDA classification model with a best area under ROC curve metric is implemented (see the examples here and plsda_auroc_vip_method)

Value

A list with the following elements:

- `train_test_partitions`: A list with the indices used in train and test on each of the cross-validation iterations
- `inner_cv_results`: The output returned by `train_evaluate_model` on each inner cross-validation
- `inner_cv_results_digested`: The output returned by `choose_best_inner`.
- `outer_cv_results`: The output returned by `train_evaluate_model` on each outer cross-validation
- `outer_cv_results_digested`: The output returned by `train_evaluate_model_digest_outer`.

Examples

```
# Data analysis for a table of integrated peaks

## Generate an artificial nmr_dataset_peak_table:
### Generate artificial metadata:
num_samples <- 32 # use an even number in this example
num_peaks <- 20
metadata <- data.frame(
    NMRExperiment = as.character(1:num_samples),
    Condition = rep(c("A", "B"), times = num_samples/2),
    stringsAsFactors = FALSE
)

### The matrix with peaks
```

```
peak_means <- runif(n = num_peaks, min = 300, max = 600)
peak_sd <- runif(n = num_peaks, min = 30, max = 60)
peak_matrix <- mapply(function(mu, sd) rnorm(num_samples, mu, sd),
                                            mu = peak_means, sd = peak_sd)
colnames(peak_matrix) <- paste0("Peak", 1:num_peaks)

## Artificial differences depending on the condition:
peak_matrix[metadata$Condition == "A", "Peak2"] <-
    peak_matrix[metadata$Condition == "A", "Peak2"] + 70

peak_matrix[metadata$Condition == "A", "Peak6"] <-
    peak_matrix[metadata$Condition == "A", "Peak6"] - 60

### The nmr_dataset_peak_table
peak_table <- new_nmr_dataset_peak_table(
    peak_table = peak_matrix,
    metadata = list(external = metadata)
)

## We will use a double cross validation, splitting the samples with random
## subsampling both in the external and internal validation.
## The classification model will be a PLSDA, exploring at maximum 3 latent
## variables.
## The best model will be selected based on the area under the ROC curve
methodology <- plsda_auroc_vip_method(ncomp = 3)
model <- nmr_data_analysis(
    peak_table,
    y_column = "Condition",
    identity_column = NULL,
    external_val = list(iterations = 3, test_size = 0.25),
    internal_val = list(iterations = 3, test_size = 0.25),
    data_analysis_method = methodology
)
## Area under ROC for each outer cross-validation iteration:
model$outer_cv_results_digested$auroc
## Rank Product of the Variable Importance in the Projection
## (Lower means more important)
sort(model$outer_cv_results_digested$vip_rankproducts)
```

`nmr_data_analysis_method` *Create method for NMR data analysis*

Description

Create method for NMR data analysis

Usage

```
new_nmr_data_analysis_method(
  train_evaluate_model,
  train_evaluate_model_params_inner,
  choose_best_inner,
  train_evaluate_model_params_outer,
  train_evaluate_model_digest_outer
)
```

Arguments

`train_evaluate_model`

A function. The `train_evaluate_model` must have the following signature:

```
function(x_train, y_train, identity_train, x_test, y_test, identity_test, ...)
```

The `x_train` and `y_train` (and their test counterparts) are self-explanatory.

The `identity_` arguments are expected to be factors. They can be used for instance with a callback that uses mixOmics::plsda in a `multilevel` approach for longitudinal studies. In those studies the `identity` would be an identifier of the subject.

The `...` arguments are free to be defined for each `train_evaluate_model`.

`train_evaluate_model_params_inner, train_evaluate_model_params_outer`

A list with additional arguments to pass to `train_evaluate_model` either in the inner cv loop or in the outer cv loop.

`choose_best_inner`

A function with a single argument:

```
function(inner_cv_results)
```

The argument is a list of `train_evaluate_model` outputs. The return value of must be a list with at least an element named `train_evaluate_model_args`. `train_evaluate_model_args` must be a named list.

- Each element must be named as one of the `train_evaluate_model` arguments.
- Each element must be a vector as long as the number of outer cross-validations.
- The values of each vector must be the values that the `train_evaluate_model` argument must take on each outer cross-validation iteration Additional list elements can be returned and will be given back to the user

`train_evaluate_model_digest_outer`

A function with a single argument:

function(outer_cv_results)

The argument is a list of `train_evaluate_model` outputs in outer cross-validation. The return value is returned by `nmr_data_analysis`

Value

An object encapsulating the method dependent functions that can be used with nmr_data_analysis

Examples

```
help(new_nmr_data_analysis_method)
```

`nmr_exclude_region` *Exclude region from samples*

Description

Excludes a given region (for instance to remove the water peak)

Usage

```
nmr_exclude_region(samples, exclude = list(water = c(4.7, 5)))

## S3 method for class 'nmr_dataset_1D'
nmr_exclude_region(samples, exclude = list(water = c(4.7, 5)))
```

Arguments

`samples`	An object
`exclude`	A list with regions to be removed Typically: `exclude = list(water = c(4.7,5.0))`

Value

The same object, with the regions excluded

See Also

Other nmr_dataset_1D functions: `[.nmr_dataset_1D()`, `computes_peak_width_ppm()`, `file_lister()`, `files_to_rDolphin()`, `format.nmr_dataset_1D()`, `is.nmr_dataset_1D()`, `load_and_save_functions`, `new_nmr_dataset_1D()`, `nmr_align_find_ref()`, `nmr_baseline_removal()`, `nmr_baseline_threshold()`, `nmr_integrate_regions()`, `nmr_interpolate_1D()`, `nmr_meta_add()`, `nmr_meta_export()`, `nmr_meta_get_column()`, `nmr_meta_get()`, `nmr_normalize()`, `nmr_pca_build_model()`, `nmr_pca_outliers_filter()`, `nmr_pca_outliers_plot()`, `nmr_pca_outliers_robust()`, `nmr_pca_outliers()`, `nmr_ppm_resolution()`, `plot.nmr_dataset_1D()`, `plot_webgl()`, `print.nmr_dataset_1D()`, `rdCV_PLS_RF_ML()`, `rdCV_PLS_RF()`, `save_files_to_rDolphin()`, `to_ChemoSpec()`, `validate_nmr_dataset_peak_table()`, `validate_nmr_dataset()`

Examples

```
nmr_dataset <- nmr_dataset_load(system.file("extdata", "nmr_dataset.rds", package = "AlpsNMR"))
exclude_regions <- list(water = c(5.1, 4.5))
nmr_dataset <- nmr_exclude_region(nmr_dataset, exclude = exclude_regions)

nmr_dataset <- nmr_dataset_load(system.file("extdata", "nmr_dataset.rds", package = "AlpsNMR"))
exclude_regions <- list(water = c(5.1, 4.5))
nmr_dataset <- nmr_exclude_region(nmr_dataset, exclude = exclude_regions)
```

nmr_export_data_1r *Export 1D NMR data to a CSV file*

Description

Export 1D NMR data to a CSV file

Usage

```
nmr_export_data_1r(nmr_dataset, filename)
```

Arguments

nmr_dataset	An nmr_dataset_1D object
filename	The csv filename

Value

The nmr_dataset object (unmodified)

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
dataset_1D <- nmr_interpolate_1D(dataset, axis = c(min = -0.5, max = 10, by = 2.3E-4))
#nmr_export_data_1r(dataset_1D, "exported_nmr_dataset")
```

nmr_identify_regions_blood *NMR peak identification (plasma/serum samples)*

Description

Identify given regions and return a data frame with plausible assignations in human plasma/serum samples.

Usage

```
nmr_identify_regions_blood(
  ppm_to_assign,
  num_proposed_compounds = 3,
  verbose = FALSE
)
```

Arguments

ppm_to_assign	A vector with the ppm regions to assign
num_proposed_compounds	set the number of proposed metabolites sorted by the number times reported in the HMDB: HMDB_blood.
verbose	Logical value. Set it to TRUE to print additional information

Value

a data frame with plausible assignations.

See Also

Other peak detection functions: Pipelines, nmr_baseline_threshold(), nmr_identify_regions_cell(), nmr_identify_regions_urine(), nmr_integrate_regions(), regions_from_peak_table(), validate_nmr_dataset_peak_table()

Other peak integration functions: Pipelines, computes_peak_width_ppm(), nmr_identify_regions_cell(), nmr_identify_regions_urine(), nmr_integrate_regions(), validate_nmr_dataset_peak_table()

Examples

```
# We identify regions from from the corresponding ppm storaged in a vector.
ppm_to_assign <- c(4.060960203, 3.048970634,2.405935596,
3.24146865,0.990616851,1.002075066,0.955325548)
identification <- nmr_identify_regions_blood (ppm_to_assign)
```

---

nmr_identify_regions_cell

NMR peak identification (cell samples)

Description

Identify given regions and return a data frame with plausible assignations in cell samples.

Usage

```
nmr_identify_regions_cell(
  ppm_to_assign,
  num_proposed_compounds = 3,
  verbose = FALSE
)
```

Arguments

ppm_to_assign	A vector with the ppm regions to assign
num_proposed_compounds	set the number of proposed metabolites in HMDB_cell.
verbose	Logical value. Set it to TRUE to print additional information

Value

a data frame with plausible assignations.

See Also

Other peak detection functions: Pipelines, nmr_baseline_threshold(), nmr_identify_regions_blood(), nmr_identify_regions_urine(), nmr_integrate_regions(), regions_from_peak_table(), validate_nmr_dataset_peak_table()

Other peak integration functions: Pipelines, computes_peak_width_ppm(), nmr_identify_regions_blood(), nmr_identify_regions_urine(), nmr_integrate_regions(), validate_nmr_dataset_peak_table()

Examples

```
# We identify regions from from the corresponding ppm storaged in a vector.
ppm_to_assign <- c(4.060960203, 3.048970634,2.405935596,
3.24146865,0.990616851,1.002075066,0.955325548)
identification <- nmr_identify_regions_cell (ppm_to_assign, num_proposed_compounds = 3)
```

---

nmr_identify_regions_urine

NMR peak identification (urine samples)

Description

Identify given regions and return a data frame with plausible assignations in human urine samples. The data frame contains the column "Bouatra_2013" showing if the proposed metabolite was reported in this publication as regular urinary metabolite.

Usage

```
nmr_identify_regions_urine(
  ppm_to_assign,
  num_proposed_compounds = 5,
  verbose = FALSE
)
```

Arguments

ppm_to_assign	A vector with the ppm regions to assign
num_proposed_compounds	set the number of proposed metabolites sorted by the number times reported in the HMDB: HMDB_urine.
verbose	Logical value. Set it to TRUE to print additional information

Value

a data frame with plausible assignations.

See Also

Other peak detection functions: Pipelines, nmr_baseline_threshold(), nmr_identify_regions_blood(), nmr_identify_regions_cell(), nmr_integrate_regions(), regions_from_peak_table(), validate_nmr_dataset_p

Other peak integration functions: Pipelines, computes_peak_width_ppm(), nmr_identify_regions_blood(), nmr_identify_regions_cell(), nmr_integrate_regions(), validate_nmr_dataset_peak_table()

Examples

```
# We identify regions from from the corresponding ppm storaged in a vector.
ppm_to_assign <- c(4.060960203, 3.048970634,2.405935596,
3.24146865,0.990616851,1.002075066,0.955325548)
identification <- nmr_identify_regions_urine (ppm_to_assign, num_proposed_compounds = 5)
```

---

nmr_integrate_regions *Integrate regions*

Description

Integrate given regions and return a data frame with them

Usage

```
nmr_integrate_regions(samples, regions, ...)

## S3 method for class 'nmr_dataset_1D'
nmr_integrate_regions(
  samples,
  regions,
  fix_baseline = TRUE,
  excluded_regions_as_zero = FALSE,
  set_negative_areas_to_zero = FALSE,
  ...
)
```

Arguments

samples	A nmr_dataset object
regions	A named list. Each element of the list is a region, given as a named numeric vector of length two with the range to integrate. The name of the region will be the name of the column
...	Keep for compatibility
fix_baseline	A logical. If TRUE it removes the baseline. See details below
excluded_regions_as_zero	A logical. It determines the behaviour of the integration when integrating regions that have been excluded. If TRUE, it will treat those regions as zero. If FALSE (the default) it will return NA values.

If `fix_baseline` is `TRUE`, then the region boundaries are used to estimate a baseline. The baseline is estimated "connecting the boundaries with a straight line". Only when the spectrum is above the baseline the area is integrated (negative contributions due to the baseline estimation are ignored).

`set_negative_areas_to_zero`
: A logical. Ignored if `fix_baseline` is `FALSE`. When set to `TRUE` negative areas are set to zero.

Value

An nmr_dataset_peak_table object

See Also

Other peak detection functions: `Pipelines`, `nmr_baseline_threshold()`, `nmr_identify_regions_blood()`, `nmr_identify_regions_cell()`, `nmr_identify_regions_urine()`, `regions_from_peak_table()`, `validate_nmr_dataset_peak_table()`

Other peak integration functions: `Pipelines`, `computes_peak_width_ppm()`, `nmr_identify_regions_blood()`, `nmr_identify_regions_cell()`, `nmr_identify_regions_urine()`, `validate_nmr_dataset_peak_table()`

Other nmr_dataset_1D functions: `[.nmr_dataset_1D()`, `computes_peak_width_ppm()`, `file_lister()`, `files_to_rDolphin()`, `format.nmr_dataset_1D()`, `is.nmr_dataset_1D()`, `load_and_save_functions`, `new_nmr_dataset_1D()`, `nmr_align_find_ref()`, `nmr_baseline_removal()`, `nmr_baseline_threshold()`, `nmr_exclude_region()`, `nmr_interpolate_1D()`, `nmr_meta_add()`, `nmr_meta_export()`, `nmr_meta_get_column()`, `nmr_meta_get()`, `nmr_normalize()`, `nmr_pca_build_model()`, `nmr_pca_outliers_filter()`, `nmr_pca_outliers_plot()`, `nmr_pca_outliers_robust()`, `nmr_pca_outliers()`, `nmr_ppm_resolution()`, `plot.nmr_dataset_1D()`, `plot_webgl()`, `print.nmr_dataset_1D()`, `rdCV_PLS_RF_ML()`, `rdCV_PLS_RF()`, `save_files_to_rDolphin()`, `to_ChemoSpec()`, `validate_nmr_dataset_peak_table()`, `validate_nmr_dataset()`

Examples

```
#Creating a dataset
dataset <- new_nmr_dataset_1D(ppm_axis = 1:10,
                              data_1r = matrix(sample(0:99,replace = TRUE), nrow = 10),
                            metadata = list(external = data.frame(NMRExperiment = c("10",
                              "20", "30", "40", "50", "60", "70", "80", "90", "100"))))

# Integrating selected regions
peak_table_integration = nmr_integrate_regions(
                                    samples = dataset,
                                    regions = list(ppm = c(2,5)),
                                    fix_baseline = TRUE)

#Creating a dataset
dataset <- new_nmr_dataset_1D(ppm_axis = 1:10,
                              data_1r = matrix(sample(0:99,replace = TRUE), nrow = 10),
                            metadata = list(external = data.frame(NMRExperiment = c("10",
                               "20", "30", "40", "50", "60", "70", "80", "90", "100"))))

# Integrating selected regions
peak_table_integration = nmr_integrate_regions(
```

```
samples = dataset,
regions = list(ppm = c(2,5)),
fix_baseline = TRUE)
```

`nmr_interpolate_1D` *Interpolate a set of 1D NMR Spectra*

Description

Interpolate a set of 1D NMR Spectra

Usage

```
nmr_interpolate_1D(samples, axis = c(min = 0.2, max = 10, by = 8e-04))

## S3 method for class 'nmr_dataset'
nmr_interpolate_1D(samples, axis = c(min = 0.2, max = 10, by = 8e-04))
```

Arguments

`samples`	An NMR dataset
`axis`	The ppm axis range and optionally the ppm step

Value

Interpolate a set of 1D NMR Spectra

See Also

Other nmr_dataset functions: `[.nmr_dataset()`, `format.nmr_dataset()`, `load_and_save_functions`, `new_nmr_dataset()`, `nmr_meta_add()`, `nmr_meta_export()`, `nmr_meta_get_column()`, `nmr_meta_get()`, `nmr_ppm_resolution()`, `nmr_read_samples()`, `print.nmr_dataset()`, `validate_nmr_dataset()`

Other nmr_dataset_1D functions: `[.nmr_dataset_1D()`, `computes_peak_width_ppm()`, `file_lister()`, `files_to_rDolphin()`, `format.nmr_dataset_1D()`, `is.nmr_dataset_1D()`, `load_and_save_functions`, `new_nmr_dataset_1D()`, `nmr_align_find_ref()`, `nmr_baseline_removal()`, `nmr_baseline_threshold()`, `nmr_exclude_region()`, `nmr_integrate_regions()`, `nmr_meta_add()`, `nmr_meta_export()`, `nmr_meta_get_column()`, `nmr_meta_get()`, `nmr_normalize()`, `nmr_pca_build_model()`, `nmr_pca_outliers_filter()`, `nmr_pca_outliers_plot()`, `nmr_pca_outliers_robust()`, `nmr_pca_outliers()`, `nmr_ppm_resolution()`, `plot.nmr_dataset_1D()`, `plot_webgl()`, `print.nmr_dataset_1D()`, `rdCV_PLS_RF_ML()`, `rdCV_PLS_RF()`, `save_files_to_rDolphin()`, `to_ChemoSpec()`, `validate_nmr_dataset_peak_table()`, `validate_nmr_dataset()`

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
dataset_1D <- nmr_interpolate_1D(dataset, axis = c(min = -0.5, max = 10, by = 2.3E-4))

dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
dataset_1D <- nmr_interpolate_1D(dataset, axis = c(min = -0.5, max = 10, by = 2.3E-4))
```

---

nmr_meta_add *Add metadata to an nmr_dataset object*

Description

This is useful to add metadata to datasets that can be later used for plotting spectra or further analysis (PCA...).

Usage

```
nmr_meta_add(nmr_data, metadata, by = "NMRExperiment")

nmr_meta_add_tidy_excel(nmr_data, excel_file)
```

Arguments

nmr_data	an nmr_dataset_family object
metadata	A data frame with metadata to add
by	A column name of both the nmr_data$metadata$external and the metadata data.frame. If you want to merge two columns with different headers you can use a named character vector c("NMRExperiment" = "ExperimentNMR") where the left side is the column name of the nmr_data$metadata$external and the right side is the column name of the metadata data frame.
excel_file	Path to a tidy Excel file name. The Excel can consist of multiple sheets, that are added sequentially. The first column of the first sheet MUST be named as one of the metadata already present in the dataset, typically will be "NMRExperiment". The rest of the columns of the first sheet can be named at will. Similary, the first column of the second sheet must be named as one of the metadata already present in the dataset, typically "NMRExperiment" or any of the columns of the first sheet. The rest of the columns of the second sheet can be named at will. See the package vignette for an example.

Value

The nmr_dataset_family object with the added metadata

See Also

Other metadata functions: Pipelines, nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get()

Other nmr_dataset functions: [.nmr_dataset(), format.nmr_dataset(), load_and_save_functions, new_nmr_dataset(), nmr_interpolate_1D(), nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get(), nmr_ppm_resolution(), nmr_read_samples(), print.nmr_dataset(), validate_nmr_dataset()

Other nmr_dataset_1D functions: [.nmr_dataset_1D(), computes_peak_width_ppm(), file_lister(), files_to_rDolphin(), format.nmr_dataset_1D(), is.nmr_dataset_1D(), load_and_save_functions, new_nmr_dataset_1D(), nmr_align_find_ref(), nmr_baseline_removal(), nmr_baseline_threshold(), nmr_exclude_region(), nmr_integrate_regions(), nmr_interpolate_1D(), nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get(), nmr_normalize(), nmr_pca_build_model(), nmr_pca_outliers_filter(), nmr_pca_outliers_plot(), nmr_pca_outliers_robust(), nmr_pca_outliers(), nmr_ppm_resolution(), plot.nmr_dataset_1D(), plot_webgl(), print.nmr_dataset_1D(), rdCV_PLS_RF_ML(), rdCV_PLS_RF(), save_files_to_rDolphin(), to_ChemoSpec(), validate_nmr_dataset_peak_table(), validate_nmr_dataset()

Other nmr_dataset_peak_table functions: [.nmr_dataset_peak_table(), format.nmr_dataset_peak_table(), is.nmr_dataset_peak_table(), load_and_save_functions, new_nmr_dataset_peak_table(), nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get(), print.nmr_dataset_peak_table(), validate_nmr_dataset_peak_table()

Examples

```
# Load a demo dataset with four samples:
dataset <- system.file("dataset-demo", package = "AlpsNMR")
nmr_dataset <- nmr_read_samples_dir(dataset)

# At first we just have the NMRExperiment column
nmr_meta_get(nmr_dataset, groups = "external")
# Get a table with NMRExperiment -> SubjectID
dummy_metadata <- system.file("dataset-demo", "dummy_metadata.xlsx", package = "AlpsNMR")
NMRExp_SubjID <- readxl::read_excel(dummy_metadata, sheet = 1)

NMRExp_SubjID
# We can link the SubjectID column of the first excel into the dataset
nmr_dataset <- nmr_meta_add(nmr_dataset, NMRExp_SubjID, by = "NMRExperiment")
nmr_meta_get(nmr_dataset, groups = "external")
# The second excel can use the SubjectID:
SubjID_Age <- readxl::read_excel(dummy_metadata, sheet = 2)
SubjID_Age
# Add the metadata by its SubjectID:
nmr_dataset <- nmr_meta_add(nmr_dataset, SubjID_Age, by = "SubjectID")
# The final loaded metadata:
nmr_meta_get(nmr_dataset, groups = "external")

# Read a tidy excel file:

dataset <- system.file("dataset-demo", package = "AlpsNMR")
nmr_dataset <- nmr_read_samples_dir(dataset)

# At first we just have the NMRExperiment column
nmr_meta_get(nmr_dataset, groups = "external")
# Get a table with NMRExperiment -> SubjectID
```

```
dummy_metadata <- system.file("dataset-demo", "dummy_metadata.xlsx", package = "AlpsNMR")

nmr_dataset <-nmr_meta_add_tidy_excel(nmr_dataset, dummy_metadata)
# Updated Metadata:
nmr_meta_get(nmr_dataset, groups = "external")
```

`nmr_meta_export` *Export Metadata to an Excel file*

Description

Export Metadata to an Excel file

Usage

```
nmr_meta_export(
  nmr_dataset,
  xlsx_file,
  groups = c("info", "orig", "title", "external")
)
```

Arguments

`nmr_dataset`	An nmr_dataset_family object
`xlsx_file`	"The .xlsx excel file"
`groups`	A character vector. Use `"external"` for the external metadata or the default for a more generic solution

Value

The Excel file name

See Also

Other metadata functions: `Pipelines`, `nmr_meta_add()`, `nmr_meta_get_column()`, `nmr_meta_get()`

Other nmr_dataset functions: `[.nmr_dataset()`, `format.nmr_dataset()`, `load_and_save_functions`, `new_nmr_dataset()`, `nmr_interpolate_1D()`, `nmr_meta_add()`, `nmr_meta_get_column()`, `nmr_meta_get()`, `nmr_ppm_resolution()`, `nmr_read_samples()`, `print.nmr_dataset()`, `validate_nmr_dataset()`

Other nmr_dataset_1D functions: `[.nmr_dataset_1D()`, `computes_peak_width_ppm()`, `file_lister()`, `files_to_rDolphin()`, `format.nmr_dataset_1D()`, `is.nmr_dataset_1D()`, `load_and_save_functions`, `new_nmr_dataset_1D()`, `nmr_align_find_ref()`, `nmr_baseline_removal()`, `nmr_baseline_threshold()`, `nmr_exclude_region()`, `nmr_integrate_regions()`, `nmr_interpolate_1D()`, `nmr_meta_add()`, `nmr_meta_get_column()`, `nmr_meta_get()`, `nmr_normalize()`, `nmr_pca_build_model()`, `nmr_pca_outliers_filter()`, `nmr_pca_outliers_plot()`, `nmr_pca_outliers_robust()`, `nmr_pca_outliers()`, `nmr_ppm_resolution()`, `plot.nmr_dataset_1D()`, `plot_webgl()`, `print.nmr_dataset_1D()`, `rdCV_PLS_RF_ML()`, `rdCV_PLS_RF()`, `save_files_to_rDolphin()`, `to_ChemoSpec()`, `validate_nmr_dataset_peak_table()`, `validate_nmr_dataset()`

Other nmr_dataset_peak_table functions: [.nmr_dataset_peak_table(), format.nmr_dataset_peak_table(), is.nmr_dataset_peak_table(), load_and_save_functions, new_nmr_dataset_peak_table(), nmr_meta_add(), nmr_meta_get_column(), nmr_meta_get(), print.nmr_dataset_peak_table(), validate_nmr_dataset_peak_table()

Other import/export functions: Pipelines, files_to_rDolphin(), load_and_save_functions, nmr_data(), nmr_read_bruker_fid(), nmr_read_samples(), nmr_zip_bruker_samples(), save_files_to_rDolphin(save_profiling_output(), to_ChemoSpec()

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
#nmr_meta_export(dataset, "metadata.xlsx")
```

---

nmr_meta_get *Get metadata*

Description

Get metadata

Usage

```
nmr_meta_get(samples, columns = NULL, groups = NULL)
```

Arguments

samples	a nmr_dataset_family object
columns	Columns to get. By default gets all the columns.
groups	Groups to get. Groups are predefined of columns. Typically "external" for metadata added with nmr_meta_add. Both groups and columns can't be given simultaneously.

Value

a data frame with the injection metadata

See Also

Other metadata functions: Pipelines, nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column()

Other nmr_dataset functions: [.nmr_dataset(), format.nmr_dataset(), load_and_save_functions, new_nmr_dataset(), nmr_interpolate_1D(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(), nmr_ppm_resolution(), nmr_read_samples(), print.nmr_dataset(), validate_nmr_dataset()

Other nmr_dataset_1D functions: [.nmr_dataset_1D(), computes_peak_width_ppm(), file_lister(), files_to_rDolphin(), format.nmr_dataset_1D(), is.nmr_dataset_1D(), load_and_save_functions,

new_nmr_dataset_1D(), nmr_align_find_ref(), nmr_baseline_removal(), nmr_baseline_threshold(), nmr_exclude_region(), nmr_integrate_regions(), nmr_interpolate_1D(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(), nmr_normalize(), nmr_pca_build_model(), nmr_pca_outliers_filte nmr_pca_outliers_plot(), nmr_pca_outliers_robust(), nmr_pca_outliers(), nmr_ppm_resolution(), plot.nmr_dataset_1D(), plot_webgl(), print.nmr_dataset_1D(), rdCV_PLS_RF_ML(), rdCV_PLS_RF(), save_files_to_rDolphin(), to_ChemoSpec(), validate_nmr_dataset_peak_table(), validate_nmr_dataset()

Other nmr_dataset_peak_table functions: [.nmr_dataset_peak_table(), format.nmr_dataset_peak_table(), is.nmr_dataset_peak_table(), load_and_save_functions, new_nmr_dataset_peak_table(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(), print.nmr_dataset_peak_table(), validate_nmr_dataset_peak_table()

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
metadata <- nmr_meta_get(dataset)
```

---

nmr_meta_get_column *Get a single metadata column*

Description

Get a single metadata column

Usage

```
nmr_meta_get_column(samples, column = "NMRExperiment")
```

Arguments

samples	a nmr_dataset_family object
column	A column to get

Value

A vector with the column

See Also

Other metadata functions: Pipelines, nmr_meta_add(), nmr_meta_export(), nmr_meta_get()

Other nmr_dataset functions: [.nmr_dataset(), format.nmr_dataset(), load_and_save_functions, new_nmr_dataset(), nmr_interpolate_1D(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get(), nmr_ppm_resolution(), nmr_read_samples(), print.nmr_dataset(), validate_nmr_dataset()

Other nmr_dataset_1D functions: [.nmr_dataset_1D(), computes_peak_width_ppm(), file_lister(), files_to_rDolphin(), format.nmr_dataset_1D(), is.nmr_dataset_1D(), load_and_save_functions, new_nmr_dataset_1D(), nmr_align_find_ref(), nmr_baseline_removal(), nmr_baseline_threshold(),

nmr_exclude_region(), nmr_integrate_regions(), nmr_interpolate_1D(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get(), nmr_normalize(), nmr_pca_build_model(), nmr_pca_outliers_filter(), nmr_pca_outliers_plot(), nmr_pca_outliers_robust(), nmr_pca_outliers(), nmr_ppm_resolution(), plot.nmr_dataset_1D(), plot_webgl(), print.nmr_dataset_1D(), rdCV_PLS_RF_ML(), rdCV_PLS_RF(), save_files_to_rDolphin(), to_ChemoSpec(), validate_nmr_dataset_peak_table(), validate_nmr_dataset()

Other nmr_dataset_peak_table functions: [.nmr_dataset_peak_table(), format.nmr_dataset_peak_table(), is.nmr_dataset_peak_table(), load_and_save_functions, new_nmr_dataset_peak_table(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get(), print.nmr_dataset_peak_table(), validate_nmr_dataset_peak_table()

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
metadata_column <- nmr_meta_get_column(dataset)
```

---

nmr_normalize *Normalize nmr_dataset_1D samples*

Description

The nmr_normalize function is used to normalize all the samples according to a given criteria.

Usage

```
nmr_normalize(
  samples,
  method = c("area", "max", "value", "region", "pqn", "none"),
  ...
)

nmr_normalize_extra_info(samples)
```

Arguments

samples	A nmr_dataset_1D object
method	The criteria to be used for normalization - area: Normalize to the total area - max: Normalize to the maximum intensity - value: Normalize each sample to a user defined value - region: Integrate a region and normalize each sample to that region - pqn: Use Probabalistic Quotient Normalization for normalization - none: Do not normalize at all
...	Method dependent arguments: - method == "value": - value: A numeric vector with the normalization values to use - method == "region": - ppm_range: A chemical shift region to integrate - . . . : Other arguments passed on to nmr_integrate_regions

Details

The nmr_normalize_extra_info function is used to extract additional information after the normalization. Typically, we want to know what was the actual normalization factor applied to each sample. The extra information includes a plot, representing the dispersion of the normalization factor for each sample.

Value

The nmr_dataset_1D object, with the samples normalized. Further information for diagnostic of the normalization process is also saved and can be extracted by calling nmr_normalize_extra_info() afterwards.

See Also

Other nmr_dataset_1D functions: [.nmr_dataset_1D(), computes_peak_width_ppm(), file_lister(), files_to_rDolphin(), format.nmr_dataset_1D(), is.nmr_dataset_1D(), load_and_save_functions, new_nmr_dataset_1D(), nmr_align_find_ref(), nmr_baseline_removal(), nmr_baseline_threshold(), nmr_exclude_region(), nmr_integrate_regions(), nmr_interpolate_1D(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get(), nmr_pca_build_model(), nmr_pca_outliers_filter nmr_pca_outliers_plot(), nmr_pca_outliers_robust(), nmr_pca_outliers(), nmr_ppm_resolution(), plot.nmr_dataset_1D(), plot_webgl(), print.nmr_dataset_1D(), rdCV_PLS_RF_ML(), rdCV_PLS_RF(), save_files_to_rDolphin(), to_ChemoSpec(), validate_nmr_dataset_peak_table(), validate_nmr_dataset()

Examples

```
nmr_dataset <- nmr_dataset_load(system.file("extdata", "nmr_dataset.rds", package = "AlpsNMR"))
nmr_dataset <- nmr_normalize(nmr_dataset, method = "area")
norm_dataset <- nmr_normalize(nmr_dataset)
norm_dataset$plot
nmr_dataset <- nmr_dataset_load(system.file("extdata", "nmr_dataset.rds", package = "AlpsNMR"))
nmr_dataset <- nmr_normalize(nmr_dataset, method = "area")
norm_extra_info <- nmr_normalize_extra_info(nmr_dataset)
norm_extra_info$plot
```

---

nmr_pca_build_model *Build a PCA on for an nmr_dataset*

Description

This function builds a PCA model with all the NMR spectra. Regions with zero values (excluded regions) or near-zero variance regions are automatically excluded from the analysis.

Usage

```
nmr_pca_build_model(
  nmr_dataset,
  ncomp = NULL,
  center = TRUE,
```

```
  scale = FALSE,
  ...
)

## S3 method for class 'nmr_dataset_1D'
nmr_pca_build_model(
  nmr_dataset,
  ncomp = NULL,
  center = TRUE,
  scale = FALSE,
  ...
)
```

Arguments

nmr_dataset	a nmr_dataset_1D object
ncomp	Integer, if data is complete ncomp decides the number of components and associated eigenvalues to display from the pcasvd algorithm and if the data has missing values, ncomp gives the number of components to keep to perform the reconstitution of the data using the NIPALS algorithm. If NULL, function sets ncomp = min(nrow(X),ncol(X))
center	(Default=TRUE) Logical, whether the variables should be shifted to be zero centered. Only set to FALSE if data have already been centered. Alternatively, a vector of length equal the number of columns of X can be supplied. The value is passed to scale. If the data contain missing values, columns should be centered for reliable results.
scale	(Default=FALSE) Logical indicating whether the variables should be scaled to have unit variance before the analysis takes place. The default is FALSE for consistency with prcomp function, but in general scaling is advisable. Alternatively, a vector of length equal the number of columns of X can be supplied. The value is passed to scale.
...	Additional arguments passed on to mixOmics::pca

Value

A PCA model as given by mixOmics::pca with two additional attributes:

- nmr_data_axis containing the full ppm axis
- nmr_included with the data points included in the model These attributes are used internally by AlpsNMR to create loading plots

See Also

Other PCA related functions: nmr_pca_outliers_filter(), nmr_pca_outliers_plot(), nmr_pca_outliers_robust(), nmr_pca_outliers(), nmr_pca_plots

Other nmr_dataset_1D functions: [.nmr_dataset_1D(), computes_peak_width_ppm(), file_lister(), files_to_rDolphin(), format.nmr_dataset_1D(), is.nmr_dataset_1D(), load_and_save_functions, new_nmr_dataset_1D(), nmr_align_find_ref(), nmr_baseline_removal(), nmr_baseline_threshold(),

nmr_exclude_region(), nmr_integrate_regions(), nmr_interpolate_1D(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get(), nmr_normalize(), nmr_pca_outliers_filter(), nmr_pca_outliers_plot(), nmr_pca_outliers_robust(), nmr_pca_outliers(), nmr_ppm_resolution(), plot.nmr_dataset_1D(), plot_webgl(), print.nmr_dataset_1D(), rdCV_PLS_RF_ML(), rdCV_PLS_RF(), save_files_to_rDolphin(), to_ChemoSpec(), validate_nmr_dataset_peak_table(), validate_nmr_dataset()

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
dataset_1D <- nmr_interpolate_1D(dataset, axis = c(min = -0.5, max = 10, by = 2.3E-4))
model <- nmr_pca_build_model(dataset_1D)

dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
dataset_1D <- nmr_interpolate_1D(dataset, axis = c(min = -0.5, max = 10, by = 2.3E-4))
model <- nmr_pca_build_model(dataset_1D)
```

---

nmr_pca_outliers *Compute PCA residuals and score distance for each sample*

Description

Compute PCA residuals and score distance for each sample

Usage

```
nmr_pca_outliers(
  nmr_dataset,
  pca_model,
  ncomp = NULL,
  quantile_critical = 0.975
)
```

Arguments

nmr_dataset	An nmr_dataset_1D object
pca_model	A pca model returned by nmr_pca_build_model
ncomp	Number of components to use. Use NULL for 90% of the variance
quantile_critical	critical quantile

Value

A list with:

- outlier_info: A data frame with the NMRExperiment, the Q residuals and T scores
- ncomp: Number of components used to compute Q and T
- Tscore_critical, QResidual_critical: Critical values, given a quantile, for both Q and T.

See Also

Other PCA related functions: nmr_pca_build_model(), nmr_pca_outliers_filter(), nmr_pca_outliers_plot(), nmr_pca_outliers_robust(), nmr_pca_plots

Other outlier detection functions: Pipelines, nmr_pca_outliers_filter(), nmr_pca_outliers_plot(), nmr_pca_outliers_robust()

Other nmr_dataset_1D functions: [.nmr_dataset_1D(), computes_peak_width_ppm(), file_lister(), files_to_rDolphin(), format.nmr_dataset_1D(), is.nmr_dataset_1D(), load_and_save_functions, new_nmr_dataset_1D(), nmr_align_find_ref(), nmr_baseline_removal(), nmr_baseline_threshold(), nmr_exclude_region(), nmr_integrate_regions(), nmr_interpolate_1D(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get(), nmr_normalize(), nmr_pca_build_model(), nmr_pca_outliers_filter(), nmr_pca_outliers_plot(), nmr_pca_outliers_robust(), nmr_ppm_resolution(), plot.nmr_dataset_1D(), plot_webgl(), print.nmr_dataset_1D(), rdCV_PLS_RF_ML(), rdCV_PLS_RF(), save_files_to_rDolphin(), to_ChemoSpec(), validate_nmr_dataset_peak_table(), validate_nmr_dataset()

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
dataset_1D <- nmr_interpolate_1D(dataset, axis = c(min = -0.5, max = 10, by = 2.3E-4))
model <- nmr_pca_build_model(dataset_1D)
outliers_info <- nmr_pca_outliers(dataset_1D, model)
```

---

nmr_pca_outliers_filter

Exclude outliers

Description

Exclude outliers

Usage

```
nmr_pca_outliers_filter(nmr_dataset, pca_outliers)
```

Arguments

nmr_dataset	An nmr_dataset_1D object
pca_outliers	The output from nmr_pca_outliers()

Value

An nmr_dataset_1D without the detected outliers

See Also

Other PCA related functions: nmr_pca_build_model(), nmr_pca_outliers_plot(), nmr_pca_outliers_robust(), nmr_pca_outliers(), nmr_pca_plots

Other outlier detection functions: Pipelines, nmr_pca_outliers_plot(), nmr_pca_outliers_robust(), nmr_pca_outliers()

Other nmr_dataset_1D functions: [.nmr_dataset_1D(), computes_peak_width_ppm(), file_lister(), files_to_rDolphin(), format.nmr_dataset_1D(), is.nmr_dataset_1D(), load_and_save_functions, new_nmr_dataset_1D(), nmr_align_find_ref(), nmr_baseline_removal(), nmr_baseline_threshold(), nmr_exclude_region(), nmr_integrate_regions(), nmr_interpolate_1D(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get(), nmr_normalize(), nmr_pca_build_model(), nmr_pca_outliers_plot(), nmr_pca_outliers_robust(), nmr_pca_outliers(), nmr_ppm_resolution(), plot.nmr_dataset_1D(), plot_webgl(), print.nmr_dataset_1D(), rdCV_PLS_RF_ML(), rdCV_PLS_RF(), save_files_to_rDolphin(), to_ChemoSpec(), validate_nmr_dataset_peak_table(), validate_nmr_dataset()

Other subsetting functions: [.nmr_dataset_1D(), [.nmr_dataset_peak_table(), [.nmr_dataset(), filter.nmr_dataset_family()

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
dataset_1D <- nmr_interpolate_1D(dataset, axis = c(min = -0.5, max = 10, by = 2.3E-4))
model <- nmr_pca_build_model(dataset_1D)
outliers_info <- nmr_pca_outliers(dataset_1D, model)
dataset_whitout_outliers <- nmr_pca_outliers_filter(dataset_1D, outliers_info)
```

---

nmr_pca_outliers_plot *Plot for outlier detection diagnostic*

Description

Plot for outlier detection diagnostic

Usage

```
nmr_pca_outliers_plot(nmr_dataset, pca_outliers, ...)
```

Arguments

nmr_dataset	An nmr_dataset_1D object
pca_outliers	The output from nmr_pca_outliers()
...	Additional parameters passed on to ggplot2::aes_string()

Value

A plot for the outlier detection

See Also

Other PCA related functions: nmr_pca_build_model(), nmr_pca_outliers_filter(), nmr_pca_outliers_robust(), nmr_pca_outliers(), nmr_pca_plots

Other outlier detection functions: Pipelines, nmr_pca_outliers_filter(), nmr_pca_outliers_robust(), nmr_pca_outliers()

Other nmr_dataset_1D functions: [.nmr_dataset_1D(), computes_peak_width_ppm(), file_lister(), files_to_rDolphin(), format.nmr_dataset_1D(), is.nmr_dataset_1D(), load_and_save_functions, new_nmr_dataset_1D(), nmr_align_find_ref(), nmr_baseline_removal(), nmr_baseline_threshold(), nmr_exclude_region(), nmr_integrate_regions(), nmr_interpolate_1D(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get(), nmr_normalize(), nmr_pca_build_model(), nmr_pca_outliers_filter(), nmr_pca_outliers_robust(), nmr_pca_outliers(), nmr_ppm_resolution(), plot.nmr_dataset_1D(), plot_webgl(), print.nmr_dataset_1D(), rdCV_PLS_RF_ML(), rdCV_PLS_RF(), save_files_to_rDolphin(), to_ChemoSpec(), validate_nmr_dataset_peak_table(), validate_nmr_dataset()

Examples

```
#dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
#dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
#dataset_1D <- nmr_interpolate_1D(dataset, axis = c(min = -0.5, max = 10, by = 2.3E-4))
#model <- nmr_pca_build_model(dataset_1D)
#outliers_info <- nmr_pca_outliers(dataset_1D, model)
#nmr_pca_outliers_plot(dataset_1D, outliers_info)
```

---

nmr_pca_outliers_robust

Outlier detection through robust PCA

Description

Outlier detection through robust PCA

Usage

```
nmr_pca_outliers_robust(nmr_dataset, ncomp = 5)
```

Arguments

nmr_dataset	An nmr_dataset_1D object
ncomp	Number of rPCA components to use We have observed that the statistical test used as a threshold for outlier detection usually flags as outliers too many samples, due possibly to a lack of gaussianity As a workaround, a heuristic method has been implemented: We know that in the Q residuals vs T scores plot from nmr_pca_outliers_plot() outliers are on the right or on the top of the plot, and quite separated from non-outlier samples.

To determine the critical value, both for Q and T, we find the biggest gap between samples in the plot and use as critical value the center of the gap.

This approach seems to work well when there are outliers, but it fails when there isn't any outlier. For that case, the gap would be placed anywhere and that is not desirable as many samples would be incorrectly flagged. The second assumption that we use is that no more than 10\ the samples may pass our critical value. If more than 10\ pass the critical value, then we assume that our heuristics are not reasonable and we don't set any critical limit.

Value

A list similar to nmr_pca_outliers

See Also

Other PCA related functions: nmr_pca_build_model(), nmr_pca_outliers_filter(), nmr_pca_outliers_plot(), nmr_pca_outliers(), nmr_pca_plots

Other outlier detection functions: Pipelines, nmr_pca_outliers_filter(), nmr_pca_outliers_plot(), nmr_pca_outliers()

Other nmr_dataset_1D functions: [.nmr_dataset_1D(), computes_peak_width_ppm(), file_lister(), files_to_rDolphin(), format.nmr_dataset_1D(), is.nmr_dataset_1D(), load_and_save_functions, new_nmr_dataset_1D(), nmr_align_find_ref(), nmr_baseline_removal(), nmr_baseline_threshold(), nmr_exclude_region(), nmr_integrate_regions(), nmr_interpolate_1D(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get(), nmr_normalize(), nmr_pca_build_model(), nmr_pca_outliers_filter(), nmr_pca_outliers_plot(), nmr_pca_outliers(), nmr_ppm_resolution(), plot.nmr_dataset_1D(), plot_webgl(), print.nmr_dataset_1D(), rdCV_PLS_RF_ML(), rdCV_PLS_RF(), save_files_to_rDolphin(), to_ChemoSpec(), validate_nmr_dataset_peak_table(), validate_nmr_dataset()

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
dataset_1D <- nmr_interpolate_1D(dataset, axis = c(min = -0.5, max = 10, by = 2.3E-4))
outliers_info <- nmr_pca_outliers_robust(dataset_1D)
```

---

nmr_pca_plots *Plotting functions for PCA*

Description

Plotting functions for PCA

Usage

```
nmr_pca_plot_variance(pca_model)

nmr_pca_scoreplot(nmr_dataset, pca_model, comp = seq_len(2), ...)

nmr_pca_loadingplot(pca_model, comp)
```

Arguments

pca_model	A PCA model trained with nmr_pca_build_model
nmr_dataset	an nmr_dataset_1D object
comp	Components to represent
...	Additional aesthetics passed on to ggplot2::aes (use bare unquoted names)

Value

Plot of PCA

See Also

Other PCA related functions: nmr_pca_build_model(), nmr_pca_outliers_filter(), nmr_pca_outliers_plot(), nmr_pca_outliers_robust(), nmr_pca_outliers()

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
dataset_1D <- nmr_interpolate_1D(dataset, axis = c(min = -0.5, max = 10, by = 2.3E-4))
model <- nmr_pca_build_model(dataset_1D)
nmr_pca_plot_variance(model)

dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
dataset_1D <- nmr_interpolate_1D(dataset, axis = c(min = -0.5, max = 10, by = 2.3E-4))
model <- nmr_pca_build_model(dataset_1D)
nmr_pca_scoreplot(dataset_1D, model)

dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
dataset_1D <- nmr_interpolate_1D(dataset, axis = c(min = -0.5, max = 10, by = 2.3E-4))
model <- nmr_pca_build_model(dataset_1D)
nmr_pca_loadingplot(model, 1)
```

`nmr_ppm_resolution` *PPM resolution of the spectra*

Description

The function gets the ppm resolution of the dataset using the median of the difference of data points.

Usage

```
nmr_ppm_resolution(nmr_dataset)

## S3 method for class 'nmr_dataset'
nmr_ppm_resolution(nmr_dataset)

## S3 method for class 'nmr_dataset_1D'
nmr_ppm_resolution(nmr_dataset)
```

Arguments

`nmr_dataset`	An object containing NMR samples

Value

Numeric (the ppm resolution, measured in ppms)

See Also

Other nmr_dataset functions: `[.nmr_dataset()`, `format.nmr_dataset()`, `load_and_save_functions`, `new_nmr_dataset()`, `nmr_interpolate_1D()`, `nmr_meta_add()`, `nmr_meta_export()`, `nmr_meta_get_column()`, `nmr_meta_get()`, `nmr_read_samples()`, `print.nmr_dataset()`, `validate_nmr_dataset()`

Other nmr_dataset_1D functions: `[.nmr_dataset_1D()`, `computes_peak_width_ppm()`, `file_lister()`, `files_to_rDolphin()`, `format.nmr_dataset_1D()`, `is.nmr_dataset_1D()`, `load_and_save_functions`, `new_nmr_dataset_1D()`, `nmr_align_find_ref()`, `nmr_baseline_removal()`, `nmr_baseline_threshold()`, `nmr_exclude_region()`, `nmr_integrate_regions()`, `nmr_interpolate_1D()`, `nmr_meta_add()`, `nmr_meta_export()`, `nmr_meta_get_column()`, `nmr_meta_get()`, `nmr_normalize()`, `nmr_pca_build_model()`, `nmr_pca_outliers_filter()`, `nmr_pca_outliers_plot()`, `nmr_pca_outliers_robust()`, `nmr_pca_outliers()`, `plot.nmr_dataset_1D()`, `plot_webgl()`, `print.nmr_dataset_1D()`, `rdCV_PLS_RF_ML()`, `rdCV_PLS_RF()`, `save_files_to_rDolphin()`, `to_ChemoSpec()`, `validate_nmr_dataset_peak_table()`, `validate_nmr_dataset()`

Examples

```
nmr_dataset <- nmr_dataset_load(system.file("extdata", "nmr_dataset.rds", package = "AlpsNMR"))
nmr_ppm_resolution(nmr_dataset)
message("the ppm resolution of this dataset is ", nmr_ppm_resolution(nmr_dataset), " ppm")

nmr_dataset <- nmr_dataset_load(system.file("extdata", "nmr_dataset.rds", package = "AlpsNMR"))
nmr_ppm_resolution(nmr_dataset)
message("the ppm resolution of this dataset is ", nmr_ppm_resolution(nmr_dataset), " ppm")
```

```
nmr_dataset <- nmr_dataset_load(system.file("extdata", "nmr_dataset.rds", package = "AlpsNMR"))
nmr_ppm_resolution(nmr_dataset)
message("the ppm resolution of this dataset is ", nmr_ppm_resolution(nmr_dataset), " ppm")
```

`nmr_read_bruker_fid` *Read Free Induction Decay file*

Description

Reads an FID file. This is a very simple function.

Usage

```
nmr_read_bruker_fid(sample_name, endian = "little")
```

Arguments

`sample_name`	A single sample name
`endian`	Endianness of the fid file ("little" by default, use "big" if acqus$BYTORDA == 1)

Value

A numeric vector with the free induction decay values

See Also

Other import/export functions: `Pipelines`, `files_to_rDolphin()`, `load_and_save_functions`, `nmr_data()`, `nmr_meta_export()`, `nmr_read_samples()`, `nmr_zip_bruker_samples()`, `save_files_to_rDolphin()`, `save_profiling_output()`, `to_ChemoSpec()`

Examples

```
fid <- nmr_read_bruker_fid("sample.fid")
```

`nmr_read_samples` *Read NMR samples*

Description

These functions load samples from files and return a nmr_dataset.

Usage

```
nmr_read_samples_dir(
  samples_dir,
  format = "bruker",
  pulse_sequence = NULL,
  metadata_only = FALSE,
  ...
)

nmr_read_samples(
  sample_names,
  format = "bruker",
  pulse_sequence = NULL,
  metadata_only = FALSE,
  ...
)
```

Arguments

`samples_dir`	A directory that contains multiple samples
`format`	Either "bruker" or "jdx"
`pulse_sequence`	If it is set to a pulse sequence ("NOESY", "JRES", "CPMG"...) it will only load the samples that match that pulse sequence.
`metadata_only`	A logical, to load only metadata (default: `FALSE`)
`...`	Arguments passed to `read_bruker_sample()` for data loading
`sample_names`	A character vector with file or directory names.

Value

a nmr_dataset object

See Also

Other nmr_dataset functions: `[.nmr_dataset()`, `format.nmr_dataset()`, `load_and_save_functions`, `new_nmr_dataset()`, `nmr_interpolate_1D()`, `nmr_meta_add()`, `nmr_meta_export()`, `nmr_meta_get_column()`, `nmr_meta_get()`, `nmr_ppm_resolution()`, `print.nmr_dataset()`, `validate_nmr_dataset()`

Other import/export functions: `Pipelines`, `files_to_rDolphin()`, `load_and_save_functions`, `nmr_data()`, `nmr_meta_export()`, `nmr_read_bruker_fid()`, `nmr_zip_bruker_samples()`, `save_files_to_rDolphin()`, `save_profiling_output()`, `to_ChemoSpec()`

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)

dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
zip_files <- fs::dir_ls(dir_to_demo_dataset, glob = "*.zip")
dataset <- nmr_read_samples(sample_names = zip_files)
```

---

nmr_zip_bruker_samples

Create one zip file for each brucker sample path

Description

Create one zip file for each brucker sample path

Usage

```
nmr_zip_bruker_samples(path, workdir, overwrite = FALSE, ...)
```

Arguments

path	Character vector with sample directories
workdir	Directory to store zip files
overwrite	Should existing zip files be overwritten?
...	Passed to utils::zip

Value

A character vector of the same length as path, with the zip file names

See Also

Other import/export functions: Pipelines, files_to_rDolphin(), load_and_save_functions, nmr_data(), nmr_meta_export(), nmr_read_bruker_fid(), nmr_read_samples(), save_files_to_rDolphin(), save_profiling_output(), to_ChemoSpec()

Examples

```
outpaths <- nmr_zip_bruker_samples(".", getwd())
```

Parameters_blood *to rDolphin*

Description

Parameters for blood (plasma/serum) samples profiling

Details

The template `Parameters_blood` contains the chosen normalization approach (by default, PQN), the Spectometer Frequency (by default, 600.04MHz), alignment (by default, TSP 0.00 ppm), bucket resolution (by default, 0.00023)

References

github.com/danielcanueto/rDolphin

Parameters_cell *Parameters for cell samples profiling*

Description

The template `Parameters_cell` contains the chosen normalization approach (by default, PQN), the Spectometer Frequency (by default, 600.04MHz), alignment (by default, TSP 0.00 ppm), bucket resolution (by default, 0.00023)

References

github.com/danielcanueto/rDolphin

Parameters_urine *Parameters for urine samples profiling*

Description

The template `Parameters_urine` contains the chosen normalization approach (by default, PQN), the Spectometer Frequency (by default, 600.04MHz), alignment (by default, TSP 0.00 ppm), bucket resolution (by default, 0.00023)

References

github.com/danielcanueto/rDolphin

`permutation_test_model` *Permutation test*

Description

Make permutations with data and default settings from an nmr_data_analysis_method

Usage

```
permutation_test_model(
  dataset,
  y_column,
  identity_column,
  external_val,
  internal_val,
  data_analysis_method,
  nPerm = 50
)
```

Arguments

`dataset`	An nmr_dataset_family object
`y_column`	A string with the name of the y column (present in the metadata of the dataset)
`identity_column`	`NULL` or a string with the name of the identity column (present in the metadata of the dataset).
`external_val`	A list with two elements: `iterations` and `test_size`. See random_subsampling for further details
`internal_val`	A list with two elements: `iterations` and `test_size`. See random_subsampling for further details
`data_analysis_method`	An nmr_data_analysis_method object
`nPerm`	number of permutations

Value

A permutation matrix with permuted values

Examples

```
# Data analysis for a table of integrated peaks

## Generate an artificial nmr_dataset_peak_table:
### Generate artificial metadata:
num_samples <- 32 # use an even number in this example
```

```
num_peaks <- 20
metadata <- data.frame(
    NMRExperiment = as.character(1:num_samples),
    Condition = rep(c("A", "B"), times = num_samples/2),
    stringsAsFactors = FALSE
)

### The matrix with peaks
peak_means <- runif(n = num_peaks, min = 300, max = 600)
peak_sd <- runif(n = num_peaks, min = 30, max = 60)
peak_matrix <- mapply(function(mu, sd) rnorm(num_samples, mu, sd),
                                            mu = peak_means, sd = peak_sd)
colnames(peak_matrix) <- paste0("Peak", 1:num_peaks)

## Artificial differences depending on the condition:
peak_matrix[metadata$Condition == "A", "Peak2"] <-
    peak_matrix[metadata$Condition == "A", "Peak2"] + 70

peak_matrix[metadata$Condition == "A", "Peak6"] <-
    peak_matrix[metadata$Condition == "A", "Peak6"] - 60

### The nmr_dataset_peak_table
peak_table <- new_nmr_dataset_peak_table(
    peak_table = peak_matrix,
    metadata = list(external = metadata)
)

methodology <- plsda_auroc_vip_method(ncomp = 3)
model <- nmr_data_analysis(
    peak_table,
    y_column = "Condition",
    identity_column = NULL,
    external_val = list(iterations = 3, test_size = 0.25),
    internal_val = list(iterations = 3, test_size = 0.25),
    data_analysis_method = methodology
)

p = permutation_test_model(peak_table,
                           y_column = "Condition",
                           identity_column = NULL,
                           external_val = list(iterations = 3, test_size = 0.25),
                           internal_val = list(iterations = 3, test_size = 0.25),
                           data_analysis_method = methodology,
                           nPerm = 10)
```

`permutation_test_plot` *Permutation test plot*

Description

Plot permutation test using actual model and permutated models

Usage

```
permutation_test_plot(
  nmr_data_analysis_model,
  permMatrix,
  xlab = "AUCs",
  xlim,
  ylim = NULL,
  breaks = "Sturges",
  main = "Permutation test"
)
```

Arguments

nmr_data_analysis_model	A nmr_data_analysis_model
permMatrix	A permutation fitness outcome from permutation_test_model
xlab	optional xlabel
xlim	optional x-range
ylim	otional y-range
breaks	optional custom histogram breaks (defaults to 'sturges')
main	optional plot title (or TRUE for autoname)

Value

A plot with the comparison between the actual model versus the permuted models

Examples

```
# Data analysis for a table of integrated peaks

## Generate an artificial nmr_dataset_peak_table:
### Generate artificial metadata:
num_samples <- 32 # use an even number in this example
num_peaks <- 20
metadata <- data.frame(
    NMRExperiment = as.character(1:num_samples),
    Condition = rep(c("A", "B"), times = num_samples/2),
    stringsAsFactors = FALSE
)

### The matrix with peaks
peak_means <- runif(n = num_peaks, min = 300, max = 600)
peak_sd <- runif(n = num_peaks, min = 30, max = 60)
peak_matrix <- mapply(function(mu, sd) rnorm(num_samples, mu, sd),
                                            mu = peak_means, sd = peak_sd)
colnames(peak_matrix) <- paste0("Peak", 1:num_peaks)

## Artificial differences depending on the condition:
peak_matrix[metadata$Condition == "A", "Peak2"] <-
```

```
    peak_matrix[metadata$Condition == "A", "Peak2"] + 70

peak_matrix[metadata$Condition == "A", "Peak6"] <-
    peak_matrix[metadata$Condition == "A", "Peak6"] - 60

### The nmr_dataset_peak_table
peak_table <- new_nmr_dataset_peak_table(
    peak_table = peak_matrix,
    metadata = list(external = metadata)
)

methodology <- plsda_auroc_vip_method(ncomp = 3)
model <- nmr_data_analysis(
    peak_table,
    y_column = "Condition",
    identity_column = NULL,
    external_val = list(iterations = 3, test_size = 0.25),
    internal_val = list(iterations = 3, test_size = 0.25),
    data_analysis_method = methodology
)

p = permutation_test_model(peak_table,
                           y_column = "Condition",
                           identity_column = NULL,
                           external_val = list(iterations = 3, test_size = 0.25),
                           internal_val = list(iterations = 3, test_size = 0.25),
                           data_analysis_method = methodology,
                           nPerm = 10)

permutation_test_plot(model, p)
```

`Pipelines` *Pipelines*

Description

Uses nmr_pca_outliers_robust to perform the detection of outliers

Normalize the full spectra to the internal calibrant region, then exclude that region and finally perform PQN normalization.

Usage

```
pipe_load_samples(samples_dir, glob = "*0", output_dir = NULL)

pipe_add_metadata(nmr_dataset_rds, excel_file, output_dir)

pipe_interpolate_1D(nmr_dataset_rds, axis, output_dir)
```

```
pipe_exclude_regions(nmr_dataset_rds, exclude, output_dir)

pipe_outlier_detection(nmr_dataset_rds, output_dir)

pipe_filter_samples(nmr_dataset_rds, conditions, output_dir)

pipe_peakdet_align(
  nmr_dataset_rds,
  nDivRange_ppm = 0.1,
  scales = seq(1, 16, 2),
  baselineThresh = 0.01,
  SNR.Th = -1,
  maxShift_ppm = 0.0015,
  acceptLostPeak = FALSE,
  output_dir = NULL
)

pipe_peak_integration(
  nmr_dataset_rds,
  peak_det_align_dir,
  peak_width_ppm,
  output_dir
)

pipe_normalization(
  nmr_dataset_rds,
  internal_calibrant = NULL,
  output_dir = NULL
)
```

Arguments

samples_dir	The directory where the samples are
glob	A wildcard aka globbing pattern (e.g. *.csv) passed on to grep() to filter paths.
output_dir	The output directory for this pipe element
nmr_dataset_rds	The nmr_dataset.rds file name coming from previous nodes
excel_file	An excel file name. See details for the requirements The excel file can have one or more sheets. The excel sheets need to be as simple as possible: One header column on the first row and values below. Each of the sheets contain metadata that has to be integrated. The merge (technically a left join) is done using the first column of each sheet as key. In practical terms this means that the first sheet of the excel file MUST start with an "NMRExperiment" column, and as many additional columns to add (e.g. FluidXBarcode, SampleCollectionDate, TimePoint and SubjectID). The second sheet can have as the first column any of the already added columns, for instance the "SubjectID", and any additional columns (e.g. Gender, Age).

The first column on each sheet, named the key column, MUST have unique values. For instance, a sheet starting with "SubjectID" MUST specify each subject ID only once (without repetitions).

`axis` The ppm axis range and optionally the ppm step

`exclude` A list with regions to be removed Typically: `exclude = list(water = c(4.7,5.0))`

`conditions` A character vector with conditions to filter metadata. The `conditions` parameter should be a character vector of valid R logical conditions. Some examples:

- conditions <- 'Gender == "Female"'
- conditions <- 'Cohort == "Chuv"'
- conditions <- 'TimePoint %in% c("T0", "T31")'
- conditions <- c(Cohort == "Chuv", 'TimePoint %in% c("T0", "T31")')

Only samples fullfilling all the given conditions are kept in further analysis.

`nDivRange_ppm` Segment size, in ppms, to divide the spectra and search for peaks.

`scales` The parameter of peakDetectionCWT function of MassSpecWavelet package, look it up in the original function.

`baselineThresh` It will remove all peaks under an intensity set by baselineThresh. If you set it to 'NULL', nmr_detect_peaks will automatically compute an aproximate value considering baseline between 9.5 and 10.0 ppm (automatically calculation using `baselineThresh = NULL` will not work if spectra were not interpolated up to 10.0 ppm)

`SNR.Th` The parameter of peakDetectionCWT function of MassSpecWavelet package, look it up in the original function. If you set -1, the function will itself recompute this value.

`maxShift_ppm` The maximum shift allowed, in ppm

`acceptLostPeak` This is an option for users, TRUE is the default value. If the users believe that all the peaks in the peak list are true positive, change it to FALSE.

`peak_det_align_dir`
Output directory from pipe_peakdet_align

`peak_width_ppm` A peak width in ppm

`internal_calibrant`
A ppm range where the internal calibrant is, or `NULL`.

Details

If there is no internal calibrant, only the PQN normalization is done.

Value

This function saves the result to the output directory

This function saves the result to the output directory

This function saves the result to the output directory

This function saves the result to the output directory

This function saves the result to the output directory

Pipeline: Filter samples according to metadata conditions

Pipeline: Peak detection and Alignment

Pipeline: Peak integration

Pipe: Full spectra normalization

See Also

Other import/export functions: files_to_rDolphin(), load_and_save_functions, nmr_data(), nmr_meta_export(), nmr_read_bruker_fid(), nmr_read_samples(), nmr_zip_bruker_samples(), save_files_to_rDolphin(), save_profiling_output(), to_ChemoSpec()

Other metadata functions: nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get()

Other outlier detection functions: nmr_pca_outliers_filter(), nmr_pca_outliers_plot(), nmr_pca_outliers_robust(), nmr_pca_outliers()

Other peak detection functions: nmr_baseline_threshold(), nmr_identify_regions_blood(), nmr_identify_regions_cell(), nmr_identify_regions_urine(), nmr_integrate_regions(), regions_from_peak_table(), validate_nmr_dataset_peak_table()

Other alignment functions: nmr_align_find_ref(), validate_nmr_dataset_peak_table()

Other peak integration functions: computes_peak_width_ppm(), nmr_identify_regions_blood(), nmr_identify_regions_cell(), nmr_identify_regions_urine(), nmr_integrate_regions(), validate_nmr_dataset_peak_table()

Examples

```
## Example of pipeline usage
## There are differet ways of load the dataset
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
#excel_file <- system.file("dataset-demo",
#                          "dummy_metadata.xlsx",
#                          package = "AlpsNMR")
#output_dir <- tempdir()

## Load samples with pipes
#pipe_load_samples(dir_to_demo_dataset,
#                  glob = "*.zip",
#                  output_dir = "../pipe_output")

## Another way to load it
#nmr_dataset <- nmr_read_samples_dir(dir_to_demo_dataset)

## Saving the dataset in a .rds file
#nmr_dataset_rds <- tempfile(fileext = ".rds")
#nmr_dataset_save(nmr_dataset, nmr_dataset_rds)

## Interpolation
#pipe_interpolate_1D(nmr_dataset_rds,
#                    axis = c(min = -0.5, max = 10, by = 2.3E-4),
#                    output_dir)

## Get the new path, based in output_dir
```

```
#nmr_dataset_rds <- paste(output_dir, "\", "nmr_dataset.rds", sep = "", collapse = NULL)

## Adding metadata to samples
#pipe_add_metadata(nmr_dataset_rds = nmr_dataset_rds, output_dir = output_dir,
#                  excel_file = excel_file)

## Filtering samples
#conditions <- 'SubjectID == "Ana"'
#pipe_filter_samples(nmr_dataset_rds, conditions, output_dir)

## Outlier detection
#pipe_outlier_detection(nmr_dataset_rds, output_dir)

## Exclude regions
#exclude_regions <- list(water = c(5.1, 4.5))
#pipe_exclude_regions(nmr_dataset_rds, exclude_regions, output_dir)

## peak aling
#pipe_peakdet_align(nmr_dataset_rds, output_dir = output_dir)

## peak integration
#pipe_peak_integration(nmr_dataset_rds,
#                      peak_det_align_dir = output_dir,
#                      peak_width_ppm = 0.006, output_dir)

## Normalization
#pipe_normalization(nmr_dataset_rds, output_dir = output_dir)
```

`plot.nmr_dataset_1D` *Plot an nmr_dataset_1D*

Description

Plot an nmr_dataset_1D

Usage

```
## S3 method for class 'nmr_dataset_1D'
plot(
  x,
  NMRExperiment = NULL,
  chemshift_range = NULL,
  interactive = FALSE,
  quantile_plot = NULL,
  quantile_colors = NULL,
  ...
)
```

Arguments

x	a nmr_dataset_1D object
NMRExperiment	A character vector with the NMRExperiments to include. Use "all" to include all experiments.
chemshift_range	range of the chemical shifts to be included. Can be of length 3 to include the resolution in the third element (e.g. c(0.2,0.8,0.005))
interactive	if TRUE return an interactive plotly plot, otherwise return a ggplot one.
quantile_plot	If TRUE plot the 10\ If two numbers between 0 and 1 are given then a custom percentile can be plotted
quantile_colors	A vector with the colors for each of the quantiles
...	arguments passed to ggplot2::aes_string.

Value

The plot

See Also

Other plotting functions: plot_interactive()

Other nmr_dataset_1D functions: [.nmr_dataset_1D(), computes_peak_width_ppm(), file_lister(), files_to_rDolphin(), format.nmr_dataset_1D(), is.nmr_dataset_1D(), load_and_save_functions, new_nmr_dataset_1D(), nmr_align_find_ref(), nmr_baseline_removal(), nmr_baseline_threshold(), nmr_exclude_region(), nmr_integrate_regions(), nmr_interpolate_1D(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get(), nmr_normalize(), nmr_pca_build_model(), nmr_pca_outliers_filter(), nmr_pca_outliers_plot(), nmr_pca_outliers_robust(), nmr_pca_outliers(), nmr_ppm_resolution(), plot_webgl(), print.nmr_dataset_1D(), rdCV_PLS_RF_ML(), rdCV_PLS_RF(), save_files_to_rDolphin(), to_ChemoSpec(), validate_nmr_dataset_peak_table(), validate_nmr_dataset()

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
#dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
#dataset_1D <- nmr_interpolate_1D(dataset, axis = c(min = -0.5, max = 10, by = 2.3E-4))
#plot(dataset_1D)
```

---

plot_bootstrap_multimodel

Bootstrap plot predictions

Description

Bootstrap plot predictions

Usage

```
plot_bootstrap_multimodel(bp_results, dataset, y_column, plot = TRUE)
```

Arguments

bp_results	bp_kfold_VIP_analysis results
dataset	An nmr_dataset_family object
y_column	A string with the name of the y column (present in the metadata of the dataset)
plot	A boolean that indicate if results are plotted or not

Value

A plot of the results or a ggplot object

Examples

```
# Data analysis for a table of integrated peaks

## Generate an artificial nmr_dataset_peak_table:
### Generate artificial metadata:
num_samples <- 64 # use an even number in this example
num_peaks <- 20
metadata <- data.frame(
    NMRExperiment = as.character(1:num_samples),
    Condition = rep(c("A", "B"), times = num_samples/2),
    stringsAsFactors = FALSE
)

### The matrix with peaks
peak_means <- runif(n = num_peaks, min = 300, max = 600)
peak_sd <- runif(n = num_peaks, min = 30, max = 60)
peak_matrix <- mapply(function(mu, sd) rnorm(num_samples, mu, sd),
                                            mu = peak_means, sd = peak_sd)
colnames(peak_matrix) <- paste0("Peak", 1:num_peaks)

## Artificial differences depending on the condition:
peak_matrix[metadata$Condition == "A", "Peak2"] <-
    peak_matrix[metadata$Condition == "A", "Peak2"] + 70

peak_matrix[metadata$Condition == "A", "Peak6"] <-
    peak_matrix[metadata$Condition == "A", "Peak6"] - 60

### The nmr_dataset_peak_table
peak_table <- new_nmr_dataset_peak_table(
    peak_table = peak_matrix,
    metadata = list(external = metadata)
)

## We will use bootstrap and permutation method for VIPs selection
## in a a k-fold cross validation
#bp_results <- bp_kfold_VIP_analysis(peak_table, # Data to be analized
```

```
#                           y_column = "Condition", # Label
#                           k = 3,
#                           nbootstrap = 10)

#message("Selected VIPs are: ", bp_results$importarn_vips)

#plot_bootstrap_multimodel(bp_results, peak_table, "Condition")
```

`plot_interactive` *Plots in WebGL*

Description

Plots in WebGL

Usage

```
plot_interactive(plt, html_filename)
```

Arguments

`plt`	A plot created with plotly or ggplot2
`html_filename`	The file name where the plot will be saved

Value

The html_filename

See Also

Other plotting functions: `plot.nmr_dataset_1D()`

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
dataset_1D <- nmr_interpolate_1D(dataset, axis = c(min = -0.5, max = 10, by = 2.3E-4))
# plot <- plot(dataset_1D)
# html_plot_interactive <- plot_interactive(plot, "html_plot_interactive.html")
```

`plot_plsda_multimodel` *Multi PLDSA model plot predictions*

Description

Multi PLDSA model plot predictions

Usage

```
plot_plsda_multimodel(model, plot = TRUE)
```

Arguments

`model`	A nmr_data_analysis_model
`plot`	A boolean that indicate if results are plotted or not

Value

A plot of the results or a ggplot object

Examples

```
#' # Data analysis for a table of integrated peaks

## Generate an artificial nmr_dataset_peak_table:
### Generate artificial metadata:
num_samples <- 32 # use an even number in this example
num_peaks <- 20
metadata <- data.frame(
    NMRExperiment = as.character(1:num_samples),
    Condition = rep(c("A", "B"), times = num_samples/2),
    stringsAsFactors = FALSE
)

### The matrix with peaks
peak_means <- runif(n = num_peaks, min = 300, max = 600)
peak_sd <- runif(n = num_peaks, min = 30, max = 60)
peak_matrix <- mapply(function(mu, sd) rnorm(num_samples, mu, sd),
                                        mu = peak_means, sd = peak_sd)
colnames(peak_matrix) <- paste0("Peak", 1:num_peaks)

## Artificial differences depending on the condition:
peak_matrix[metadata$Condition == "A", "Peak2"] <-
    peak_matrix[metadata$Condition == "A", "Peak2"] + 70

peak_matrix[metadata$Condition == "A", "Peak6"] <-
    peak_matrix[metadata$Condition == "A", "Peak6"] - 60

### The nmr_dataset_peak_table
```

```
peak_table <- new_nmr_dataset_peak_table(
    peak_table = peak_matrix,
    metadata = list(external = metadata)
)

## We will use a double cross validation, splitting the samples with random
## subsampling both in the external and internal validation.
## The classification model will be a PLSDA, exploring at maximum 3 latent
## variables.
## The best model will be selected based on the area under the ROC curve
methodology <- plsda_auroc_vip_method(ncomp = 1)
model <- nmr_data_analysis(
    peak_table,
    y_column = "Condition",
    identity_column = NULL,
    external_val = list(iterations = 2, test_size = 0.25),
    internal_val = list(iterations = 2, test_size = 0.25),
    data_analysis_method = methodology
)

#plot_plsda_multimodel(model)
```

`plot_plsda_samples` *Plot PLSDA predictions*

Description

Plot PLSDA predictions

Usage

```
plot_plsda_samples(model, newdata = NULL, plot = TRUE)
```

Arguments

`model`	A plsda model
`newdata`	newdata to predict, if not included model$X_test will be used
`plot`	A boolean that indicate if results are plotted or not

Value

A plot of the samples or a ggplot object

Examples

```
#' # Data analysis for a table of integrated peaks

## Generate an artificial nmr_dataset_peak_table:
### Generate artificial metadata:
num_samples <- 32 # use an even number in this example
num_peaks <- 20
metadata <- data.frame(
    NMRExperiment = as.character(1:num_samples),
    Condition = rep(c("A", "B"), times = num_samples/2),
    stringsAsFactors = FALSE
)

### The matrix with peaks
peak_means <- runif(n = num_peaks, min = 300, max = 600)
peak_sd <- runif(n = num_peaks, min = 30, max = 60)
peak_matrix <- mapply(function(mu, sd) rnorm(num_samples, mu, sd),
                                            mu = peak_means, sd = peak_sd)
colnames(peak_matrix) <- paste0("Peak", 1:num_peaks)

## Artificial differences depending on the condition:
peak_matrix[metadata$Condition == "A", "Peak2"] <-
    peak_matrix[metadata$Condition == "A", "Peak2"] + 70

peak_matrix[metadata$Condition == "A", "Peak6"] <-
    peak_matrix[metadata$Condition == "A", "Peak6"] - 60

### The nmr_dataset_peak_table
peak_table <- new_nmr_dataset_peak_table(
    peak_table = peak_matrix,
    metadata = list(external = metadata)
)

## We will use a double cross validation, splitting the samples with random
## subsampling both in the external and internal validation.
## The classification model will be a PLSDA, exploring at maximum 3 latent
## variables.
## The best model will be selected based on the area under the ROC curve
methodology <- plsda_auroc_vip_method(ncomp = 1)
model <- nmr_data_analysis(
    peak_table,
    y_column = "Condition",
    identity_column = NULL,
    external_val = list(iterations = 1, test_size = 0.25),
    internal_val = list(iterations = 1, test_size = 0.25),
    data_analysis_method = methodology
)

#plot_plsda_samples(model$outer_cv_results[[1]]$model)
```

plot_vip_scores *Plot vip scores of bootstrap*

Description

Plot vip scores of bootstrap

Usage

```
plot_vip_scores(vip_means, error, nbootstrap, plot = TRUE)
```

Arguments

vip_means	vips means values of bootstraps
error	error tolerated, calculated in the bootstrap
nbootstrap	number of bootstraps realiced
plot	A boolean that indicate if results are plotted or not

Value

A plot of the results or a ggplot object

Examples

```
# Data analysis for a table of integrated peaks

## Generate an artificial nmr_dataset_peak_table:
### Generate artificial metadata:
num_samples <- 64 # use an even number in this example
num_peaks <- 20
metadata <- data.frame(
    NMRExperiment = as.character(1:num_samples),
    Condition = rep(c("A", "B"), times = num_samples/2),
    stringsAsFactors = FALSE
)

### The matrix with peaks
peak_means <- runif(n = num_peaks, min = 300, max = 600)
peak_sd <- runif(n = num_peaks, min = 30, max = 60)
peak_matrix <- mapply(function(mu, sd) rnorm(num_samples, mu, sd),
                                            mu = peak_means, sd = peak_sd)
colnames(peak_matrix) <- paste0("Peak", 1:num_peaks)

## Artificial differences depending on the condition:
peak_matrix[metadata$Condition == "A", "Peak2"] <-
    peak_matrix[metadata$Condition == "A", "Peak2"] + 70

peak_matrix[metadata$Condition == "A", "Peak6"] <-
```

```
    peak_matrix[metadata$Condition == "A", "Peak6"] - 60

### The nmr_dataset_peak_table
peak_table <- new_nmr_dataset_peak_table(
    peak_table = peak_matrix,
    metadata = list(external = metadata)
)

## We will use bootstrap and permutation method for VIPs selection
## in a a k-fold cross validation
#bp_results <- bp_kfold_VIP_analysis(peak_table, # Data to be analized
#                            y_column = "Condition", # Label
#                            k = 3,
#                            nbootstrap = 10)

#message("Selected VIPs are: ", bp_results$importarn_vips)

#plot_vip_scores(bp_results$kfold_results[[1]]$vip_means,
#                bp_results$kfold_results[[1]]$error[1],
#                nbootstrap = 10)
```

`plot_webgl` *Plot a dataset into a HTML file*

Description

Uses WebGL for performance

Usage

```
plot_webgl(nmr_dataset, html_filename, ...)
```

Arguments

`nmr_dataset`	An nmr_dataset_1D
`html_filename`	The output HTML filename to be created
`...`	Arguments passed on to `plot.nmr_dataset_1D`
	`x` a nmr_dataset_1D object
	`chemshift_range` range of the chemical shifts to be included. Can be of length 3 to include the resolution in the third element (e.g. `c(0.2,0.8,0.005)`)
	`NMRExperiment` A character vector with the NMRExperiments to include. Use "all" to include all experiments.
	`quantile_plot` If `TRUE` plot the 10\ If two numbers between 0 and 1 are given then a custom percentile can be plotted
	`quantile_colors` A vector with the colors for each of the quantiles
	`interactive` if `TRUE` return an interactive plotly plot, otherwise return a ggplot one.

Value

the html filename created

See Also

Other nmr_dataset_1D functions: [.nmr_dataset_1D(), computes_peak_width_ppm(), file_lister(), files_to_rDolphin(), format.nmr_dataset_1D(), is.nmr_dataset_1D(), load_and_save_functions, new_nmr_dataset_1D(), nmr_align_find_ref(), nmr_baseline_removal(), nmr_baseline_threshold(), nmr_exclude_region(), nmr_integrate_regions(), nmr_interpolate_1D(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get(), nmr_normalize(), nmr_pca_build_model(), nmr_pca_outliers_filter(), nmr_pca_outliers_plot(), nmr_pca_outliers_robust(), nmr_pca_outliers(), nmr_ppm_resolution(), plot.nmr_dataset_1D(), print.nmr_dataset_1D(), rdCV_PLS_RF_ML(), rdCV_PLS_RF(), save_files_to_rDolphin(), to_ChemoSpec(), validate_nmr_dataset_peak_table(), validate_nmr_dataset()

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
#dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
#dataset_1D <- nmr_interpolate_1D(dataset, axis = c(min = -0.5, max = 10, by = 2.3E-4))
#html_plot <- plot_webgl(dataset_1D, "html_plot.html")
```

---

plsda_auroc_vip_compare

Compare PLSDA auroc VIP results

Description

Compare PLSDA auroc VIP results

Usage

```
plsda_auroc_vip_compare(...)
```

Arguments

...	Results of nmr_data_analysis to be combined. Give each result a name.

Value

A plot of the AUC for each method

Examples

```
# Data analysis for a table of integrated peaks

## Generate an artificial nmr_dataset_peak_table:
### Generate artificial metadata:
num_samples <- 32 # use an even number in this example
num_peaks <- 20
metadata <- data.frame(
    NMRExperiment = as.character(1:num_samples),
    Condition = rep(c("A", "B"), times = num_samples/2),
    stringsAsFactors = FALSE
)

### The matrix with peaks
peak_means <- runif(n = num_peaks, min = 300, max = 600)
peak_sd <- runif(n = num_peaks, min = 30, max = 60)
peak_matrix <- mapply(function(mu, sd) rnorm(num_samples, mu, sd),
                                            mu = peak_means, sd = peak_sd)
colnames(peak_matrix) <- paste0("Peak", 1:num_peaks)

## Artificial differences depending on the condition:
peak_matrix[metadata$Condition == "A", "Peak2"] <-
    peak_matrix[metadata$Condition == "A", "Peak2"] + 70

peak_matrix[metadata$Condition == "A", "Peak6"] <-
    peak_matrix[metadata$Condition == "A", "Peak6"] - 60

### The nmr_dataset_peak_table
peak_table <- new_nmr_dataset_peak_table(
    peak_table = peak_matrix,
    metadata = list(external = metadata)
)

## We will use a double cross validation, splitting the samples with random
## subsampling both in the external and internal validation.
## The classification model will be a PLSDA, exploring at maximum 3 latent
## variables.
## The best model will be selected based on the area under the ROC curve
methodology <- plsda_auroc_vip_method(ncomp = 1)
model1 <- nmr_data_analysis(
    peak_table,
    y_column = "Condition",
    identity_column = NULL,
    external_val = list(iterations = 1, test_size = 0.25),
    internal_val = list(iterations = 1, test_size = 0.25),
    data_analysis_method = methodology
)

methodology2 <- plsda_auroc_vip_method(ncomp = 2)
model2 <- nmr_data_analysis(
    peak_table,
    y_column = "Condition",
```

```
    identity_column = NULL,
    external_val = list(iterations = 1, test_size = 0.25),
    internal_val = list(iterations = 1, test_size = 0.25),
    data_analysis_method = methodology2
)

plsda_auroc_vip_compare(model1 = model1, model2 = model2)
```

`plsda_auroc_vip_method` *Method for nmr_data_analysis (PLSDA model with AUROC and VIP outputs)*

Description

Method for nmr_data_analysis (PLSDA model with AUROC and VIP outputs)

Usage

```
plsda_auroc_vip_method(ncomp, auc_increment_threshold = 0.05)
```

Arguments

`ncomp`	Max. number of latent variables to explore in the PLSDA analysis
`auc_increment_threshold`	Choose the number of latent variables when the AUC does not increment more than this threshold.

Value

Returns an object to be used with nmr_data_analysis to perform a (optionally multilevel) PLS-DA model, using the area under the ROC curve as figure of merit to determine the optimum number of latent variables.

Examples

```
method <- plsda_auroc_vip_method(3)
```

ppm_resolution *Unlisted PPM resolution*

Description

A wrapper to unlist the output from the function `nmr_ppm_resolution(nmr_dataset)` when no interpolation has been applied.

Usage

```
ppm_resolution(nmr_dataset)
```

Arguments

`nmr_dataset`	An object containing NMR samples

Value

A number (the ppm resolution, measured in ppms)

Numeric (the ppm resolution, measured in ppms)

Examples

```
nmr_dataset <- nmr_dataset_load(system.file("extdata", "nmr_dataset.rds", package = "AlpsNMR"))
nmr_ppm_resolution(nmr_dataset)
```

ppm_VIP_vector *Feature selection and validation in multivariate analysis*

Description

Numeric VIPs vector

Usage

```
ppm_VIP_vector(VIPs)
```

Arguments

`VIPs`	a dataframe from the model_VIP(MVObj) function. It requires a "ppms" variable

Details

The function extracts the VIPs vector (numeric) from the model_VIP(MVObj) function. It is not necessary if you have the ppm values in a numeric vector. This is needed in case that an automated pipeline is applied, connecting the output from model_VIP(MVObj) to `nmr_identify_regions` family functions.

Value

a numeric ppm vector ready to be identified with nmr_identify_regions_blood, nmr_identify_cell or nmr_identify_regions_urine

Examples

```
message("Deprecated. MUVR is not compatible with Bioconductor,
use bp_kfold_VIP_analysis method instead")
```

---

print.nmr_dataset *Print for nmr_dataset*

Description

Print for nmr_dataset

Usage

```
## S3 method for class 'nmr_dataset'
print(x, ...)
```

Arguments

x	an nmr_dataset object
...	for future use

Value

Print for nmr_dataset

See Also

Other class helper functions: format.nmr_dataset_1D(), format.nmr_dataset_peak_table(), format.nmr_dataset(), is.nmr_dataset_1D(), is.nmr_dataset_peak_table(), new_nmr_dataset_1D(), new_nmr_dataset_peak_table(), new_nmr_dataset(), print.nmr_dataset_1D(), print.nmr_dataset_peak_table(), validate_nmr_dataset_family(), validate_nmr_dataset_peak_table(), validate_nmr_dataset()

Other nmr_dataset functions: [.nmr_dataset(), format.nmr_dataset(), load_and_save_functions, new_nmr_dataset(), nmr_interpolate_1D(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get(), nmr_ppm_resolution(), nmr_read_samples(), validate_nmr_dataset()

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
print(dataset)
```

`print.nmr_dataset_1D` *print for nmr_dataset_1D*

Description

print for nmr_dataset_1D

Usage

```
## S3 method for class 'nmr_dataset_1D'
print(x, ...)
```

Arguments

x	an nmr_dataset_1D object
...	for future use

Value

print for nmr_dataset_1D

See Also

Other class helper functions: format.nmr_dataset_1D(), format.nmr_dataset_peak_table(), format.nmr_dataset(), is.nmr_dataset_1D(), is.nmr_dataset_peak_table(), new_nmr_dataset_1D(), new_nmr_dataset_peak_table(), new_nmr_dataset(), print.nmr_dataset_peak_table(), print.nmr_dataset(), validate_nmr_dataset_family(), validate_nmr_dataset_peak_table(), validate_nmr_dataset()

Other nmr_dataset_1D functions: [.nmr_dataset_1D(), computes_peak_width_ppm(), file_lister(), files_to_rDolphin(), format.nmr_dataset_1D(), is.nmr_dataset_1D(), load_and_save_functions, new_nmr_dataset_1D(), nmr_align_find_ref(), nmr_baseline_removal(), nmr_baseline_threshold(), nmr_exclude_region(), nmr_integrate_regions(), nmr_interpolate_1D(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get(), nmr_normalize(), nmr_pca_build_model(), nmr_pca_outliers_filter(), nmr_pca_outliers_plot(), nmr_pca_outliers_robust(), nmr_pca_outliers(), nmr_ppm_resolution(), plot.nmr_dataset_1D(), plot_webgl(), rdCV_PLS_RF_ML(), rdCV_PLS_RF(), save_files_to_rDolphin(), to_ChemoSpec(), validate_nmr_dataset_peak_table(), validate_nmr_dataset()

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
dataset_1D <- nmr_interpolate_1D(dataset, axis = c(min = -0.5, max = 10, by = 2.3E-4))
print(dataset_1D)
```

`print.nmr_dataset_peak_table` *print for nmr_dataset_peak_table*

Description

print for nmr_dataset_peak_table

Usage

```
## S3 method for class 'nmr_dataset_peak_table'
print(x, ...)
```

Arguments

x	an nmr_dataset_peak_table object
...	for future use

Value

print for nmr_dataset_peak_table

See Also

Other nmr_dataset_peak_table functions: [.nmr_dataset_peak_table(), format.nmr_dataset_peak_table(), is.nmr_dataset_peak_table(), load_and_save_functions, new_nmr_dataset_peak_table(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get(), validate_nmr_dataset_peak_tabl

Other class helper functions: format.nmr_dataset_1D(), format.nmr_dataset_peak_table(), format.nmr_dataset(), is.nmr_dataset_1D(), is.nmr_dataset_peak_table(), new_nmr_dataset_1D(), new_nmr_dataset_peak_table(), new_nmr_dataset(), print.nmr_dataset_1D(), print.nmr_dataset(), validate_nmr_dataset_family(), validate_nmr_dataset_peak_table(), validate_nmr_dataset()

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
dataset_1D <- nmr_interpolate_1D(dataset, axis = c(min = -0.5, max = 10, by = 2.3E-4))
meta <- file.path(dir_to_demo_dataset, "dummy_metadata.xlsx")
metadata <- readxl::read_excel(meta, sheet = 1)
dataset_1D <- nmr_meta_add(dataset_1D, metadata = metadata, by = "NMRExperiment")
metadata <- list(external = dataset_1D[["metadata"]][["external"]])
peak_table <- nmr_data(dataset_1D)
new <- new_nmr_dataset_peak_table(peak_table, metadata)
new
```

p_value_perm *Deprecated function p-Value from permutation test*

Description

The fucntion calculates the cumulative (1-tailed) probability of 'actual' belonging to 'h0' (`permutation_object` from the `permutation_test_model` function).

Usage

```
p_value_perm(model_actual, permutation_object)
```

Arguments

`model_actual`	The actual model performance (e.g. misclassifications or Q2)
`permutation_object`	Null hypothesis distribution from permutation test from `permutation_test_model` function

Value

The p-value indicating if there is significant differences between the model performance and the null hypothesis distribution from permutation test test

Examples

```
message("MUVR is not compatible with Bioconductor,
use bp_kfold_VIP_analysis method instead")
```

random_subsampling *Random subsampling*

Description

Random subsampling

Usage

```
random_subsampling(
  sample_idx,
  iterations = 10L,
  test_size = 0.25,
  keep_together = NULL,
  balance_in_train = NULL
)
```

Arguments

sample_idx	Typically a numeric vector with sample index to be separated. A character vector with sample IDs could also be used
iterations	An integer, the number of iterations in the random subsampling
test_size	A number between 0 and 1. The samples to be included in the test set on each interation.
keep_together	Either NULL or a factor with the same length as sample_idx. keep_together can be used to ensure that groups of samples are kept in together in all iterations (either on training or on test, but never split). A typical use case for this is when you have sample replicates and you want to keep all replicates together to prevent overoptimistic results (having one sample on the train subset and its replicate on the test subset would make the prediction easier to guess). Another use case for this is when you have a longitudinal study and you want to keep some subjects in the same train or test group, because you want to use some information in a longitudinal way (e.g. a multilevel plsda model).
balance_in_train	Either NULL or a factor with the same length as sample_idx. balance_in_train can be used to force that on each iteration, the train partition contains the same number of samples of the given factor levels. For instance, if we have a dataset with 40 samples of class "A" and 20 samples of class "B", using a test_size = 0.25, we can force to always have 16 samples of class "A" and 16 samples of class "B" in the training subset. This is beneficial to those algorithms that require that the training groups are balanced.

Value

A list of length equal to iterations. Each element of the list is a list with two entries (training and test) containing the sample_idx values that will belong to each subset.

Examples

```
random_subsampling(1:100, iterations = 4, test_size = 0.25)

subject_id <- c("Alice", "Bob", "Charlie", "Eve")
random_subsampling(1:4, iterations = 2, test_size = 0.25, keep_together = subject_id)
```

---

rdCV_PLS_RF *Deprecated function*

Description

Deprecated function

Usage

```
rdCV_PLS_RF(nmr_peak_table)
```

Arguments

nmr_peak_table an AlpsNMR integration object (2 classes)

Value

a MUVR model containing selection parameters, validation and fitness

References

Shi,L. et al. (2018) Variable selection and validation in multivariate modelling. Bioinformatics.

See Also

nmr_data_analysis Feature selection and validation in multivariate analysis

Statistical analysis and feature selection in a repeated double cross-validation frame based on the partial least squares (PLS) or random forest (RF) analyses using an algorithm for multivariate modelling with minimally biased variable selection (MUVR) from the MUVR package. If your work with a nmr_peak_table object from AlpsNMR, first you need to extract the X data from the main nmr_dataset object (e.g. your peak table) with the nmr_data function, otherwise you would try to set a list on the X. You also need to set the class from this object, or just set it from another Y vector.

Other nmr_dataset_1D functions: [.nmr_dataset_1D(), computes_peak_width_ppm(), file_lister(), files_to_rDolphin(), format.nmr_dataset_1D(), is.nmr_dataset_1D(), load_and_save_functions, new_nmr_dataset_1D(), nmr_align_find_ref(), nmr_baseline_removal(), nmr_baseline_threshold(), nmr_exclude_region(), nmr_integrate_regions(), nmr_interpolate_1D(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get(), nmr_normalize(), nmr_pca_build_model(), nmr_pca_outliers_filter(), nmr_pca_outliers_plot(), nmr_pca_outliers_robust(), nmr_pca_outliers(), nmr_ppm_resolution(), plot.nmr_dataset_1D(), plot_webgl(), print.nmr_dataset_1D(), rdCV_PLS_RF_ML(), save_files_to_rDolphin(), to_ChemoSpec(), validate_nmr_dataset_peak_table(), validate_nmr_dataset()

Examples

```
message("Deprecated. MUVR is not compatible with Bioconductor,
use bp_kfold_VIP_analysis method instead")
```

---

rdCV_PLS_RF_ML *Deprecated function Feature selection and validation in MULTILEVEL analysis*

Description

Statistical analysis and feature selection in a repeated double cross-validation frame based on the partial least squares (PLS) or random forest (RF) analyses using an algorithm for multivariate modelling with minimally biased variable selection (MUVR) from the MUVR package. The function rdCV_PLS_RF_ML allows the multilevel comparison, especially useful in crossover or longitudinal studies (2 timepoints) considering the same individual (it requires 2 samples of the same observation).

Usage

```
rdCV_PLS_RF_ML(nmr_peak_table)
```

Arguments

nmr_peak_table	an AlpsNMR integration object (2 classes)

Value

a MUVR model containing selection parameters, validation and fitness

References

Shi,L. et al. (2018) Variable selection and validation in multivariate modelling. Bioinformatics.

See Also

Other nmr_dataset_1D functions: [.nmr_dataset_1D(), computes_peak_width_ppm(), file_lister(), files_to_rDolphin(), format.nmr_dataset_1D(), is.nmr_dataset_1D(), load_and_save_functions, new_nmr_dataset_1D(), nmr_align_find_ref(), nmr_baseline_removal(), nmr_baseline_threshold(), nmr_exclude_region(), nmr_integrate_regions(), nmr_interpolate_1D(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get(), nmr_normalize(), nmr_pca_build_model(), nmr_pca_outliers_filter(), nmr_pca_outliers_plot(), nmr_pca_outliers_robust(), nmr_pca_outliers(), nmr_ppm_resolution(), plot.nmr_dataset_1D(), plot_webgl(), print.nmr_dataset_1D(), rdCV_PLS_RF(), save_files_to_rDolphin(), to_ChemoSpec(), validate_nmr_dataset_peak_table(), validate_nmr_dataset()

Examples

```
message("Deprecated. MUVR is not compatible with Bioconductor,
use bp_kfold_VIP_analysis method instead")
```

---

read_bruker_sample *Read a Bruker sample directory*

Description

Read a Bruker sample directory

Usage

```
read_bruker_sample(
  sample_path,
  pdata_file = NULL,
  pdata_path = "pdata/1",
  all_components = FALSE
)
```

Arguments

sample_path	A character path of the sample directory
pdata_file	File name of the binary NMR data to load. Usually "1r". If it is null it is autodetected and all files are loaded.
pdata_path	Path from sample_path to the preprocessed data
all_components	If FALSE load only the real component. Otherwise load all of them

Value

a list with all the bruker sample information

---

regions_from_peak_table

Build list of regions for peak integration

Description

Build list of regions for peak integration

Usage

```
regions_from_peak_table(peak_pos_ppm, peak_width_ppm)
```

Arguments

peak_pos_ppm	The peak positions, in ppm
peak_width_ppm	The peak widths (or a single peak width for all peaks)

Value

A list of regions suitable for nmr_integrate_regions

See Also

Other peak detection functions: Pipelines, nmr_baseline_threshold(), nmr_identify_regions_blood(), nmr_identify_regions_cell(), nmr_identify_regions_urine(), nmr_integrate_regions(), validate_nmr_dataset_peak_table()

ROI_blood *ROIs for blood (plasma/serum) samples*

Description

The template ROI_blood contains the targeted list of metabolites to be quantified (blood samples)

References

github.com/danielcanueto/rDolphin

ROI_cell *ROIs for cell samples*

Description

The template ROI_cell contains the targeted list of metabolites to be quantified (cell samples)

References

github.com/danielcanueto/rDolphin

ROI_urine *ROIs for urine samples*

Description

The template ROI_urine contains the targeted list of metabolites to be quantified (urine samples)

References

github.com/danielcanueto/rDolphin

`save_files_to_rDolphin` *Save files to rDoplhin*

Description

The function saves the CSV files required by to_rDolphin and Automatic_targeted_profiling functions for metabolite profiling.

Usage

```
save_files_to_rDolphin(files_rDolphin, output_directory)
```

Arguments

`files_rDolphin`	a list containing 4 elements from `files_to_rDolphin` • `meta_rDolphin`: metadata in rDolphin format, • `NMR_spectra`: spectra matrix • `ROI`: ROI template • `Parameters_blood`: parameters file
`output_directory`	a directory in which the CSV files are saved

Value

CSV files containing:

See Also

Other import/export functions: `Pipelines`, `files_to_rDolphin()`, `load_and_save_functions`, `nmr_data()`, `nmr_meta_export()`, `nmr_read_bruker_fid()`, `nmr_read_samples()`, `nmr_zip_bruker_samples()`, `save_profiling_output()`, `to_ChemoSpec()`

Other nmr_dataset_1D functions: `[.nmr_dataset_1D()`, `computes_peak_width_ppm()`, `file_lister()`, `files_to_rDolphin()`, `format.nmr_dataset_1D()`, `is.nmr_dataset_1D()`, `load_and_save_functions`, `new_nmr_dataset_1D()`, `nmr_align_find_ref()`, `nmr_baseline_removal()`, `nmr_baseline_threshold()`, `nmr_exclude_region()`, `nmr_integrate_regions()`, `nmr_interpolate_1D()`, `nmr_meta_add()`, `nmr_meta_export()`, `nmr_meta_get_column()`, `nmr_meta_get()`, `nmr_normalize()`, `nmr_pca_build_model()`, `nmr_pca_outliers_filter()`, `nmr_pca_outliers_plot()`, `nmr_pca_outliers_robust()`, `nmr_pca_outliers()`, `nmr_ppm_resolution()`, `plot.nmr_dataset_1D()`, `plot_webgl()`, `print.nmr_dataset_1D()`, `rdCV_PLS_RF_ML()`, `rdCV_PLS_RF()`, `to_ChemoSpec()`, `validate_nmr_dataset_peak_table()`, `validate_nmr_dataset()`

Other to_rDolphin_blood functions: `save_profiling_output()`

Examples

```
## Not run:
dataset <- system.file("dataset-demo", package = "AlpsNMR")
excel_file <- system.file("dataset-demo", "dummy_metadata.xlsx", package = "AlpsNMR")
nmr_dataset <- nmr_read_samples_dir(dataset)
files_rDolphin = files_to_rDolphin_blood(nmr_dataset)
output_directory = "."
save_files_to_rDolphin(files_rDolphin, output_directory)

## End(Not run)
```

`save_profiling_output` *Save rDoplhin output*

Description

The function saves the output from Automatic_targeted_profiling function in CSV format.

Usage

```
save_profiling_output(targeted_profiling, output_directory)
```

Arguments

`targeted_profiling`	A list from Automatic_targeted_profiling function
`output_directory`	a directory in which the CSV files are saved

Value

rDolphin output from Automatic_targeted_profiling function:

- metabolites_intensity
- metabolites_quantification
- ROI_profiles_used
- chemical_shift
- fitting_error
- half_bandwidth
- signal_area_ratio

See Also

Other import/export functions: `Pipelines`, `files_to_rDolphin()`, `load_and_save_functions`, `nmr_data()`, `nmr_meta_export()`, `nmr_read_bruker_fid()`, `nmr_read_samples()`, `nmr_zip_bruker_samples()`, `save_files_to_rDolphin()`, `to_ChemoSpec()`

Other to_rDolphin_blood functions: `save_files_to_rDolphin()`

Examples

```
## Not run:
rDolphin_object = to_rDolphin(parameters)
targeted_profiling = Automatic_targeted_profiling(rDolphin)
save_profiling_output(targeted_profiling, output_directory)

## End(Not run)
```

SummarizedExperiment_to_nmr_dataset_peak_table

Import SummarizedExperiment as mr_dataset_peak_table

Description

Import SummarizedExperiment as mr_dataset_peak_table

Usage

```
SummarizedExperiment_to_nmr_dataset_peak_table(se)
```

Arguments

se	An SummarizedExperiment object

Value

nmr_dataset_peak_table An nmr_dataset_peak_table object (unmodified)

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
dataset_1D <- nmr_interpolate_1D(dataset, axis = c(min = -0.5, max = 10, by = 2.3E-4))
meta <- file.path(dir_to_demo_dataset, "dummy_metadata.xlsx")
metadata <- readxl::read_excel(meta, sheet = 1)
dataset_1D <- nmr_meta_add(dataset_1D, metadata = metadata, by = "NMRExperiment")
metadata <- list(external = dataset_1D[["metadata"]][["external"]])
peak_table <- nmr_data(dataset_1D)
nmr_peak_table <- new_nmr_dataset_peak_table(peak_table, metadata)
se <- nmr_dataset_peak_table_to_SummarizedExperiment(nmr_peak_table)
nmr_peak_table <- SummarizedExperiment_to_nmr_dataset_peak_table(se)
```

SummarizedExperiment_to_nmr_data_1r *Import SummarizedExperiment as 1D NMR data*

Description

Import SummarizedExperiment as 1D NMR data

Usage

```
SummarizedExperiment_to_nmr_data_1r(se)
```

Arguments

se	An SummarizedExperiment object

Value

nmr_dataset An nmr_dataset_1D object (unmodified)

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
dataset_1D <- nmr_interpolate_1D(dataset, axis = c(min = -0.5, max = 10, by = 2.3E-4))
se <- nmr_data_1r_to_SummarizedExperiment(dataset_1D)
dataset_1D <- SummarizedExperiment_to_nmr_data_1r(se)
```

to_ChemoSpec *Convert to ChemoSpec Spectra class*

Description

Convert to ChemoSpec Spectra class

Usage

```
to_ChemoSpec(nmr_dataset, desc = "A nmr_dataset")
```

Arguments

nmr_dataset	An nmr_dataset_1D object
desc	a description for the dataset

Value

A Spectra object from the ChemoSpec package

See Also

Other import/export functions: Pipelines, files_to_rDolphin(), load_and_save_functions, nmr_data(), nmr_meta_export(), nmr_read_bruker_fid(), nmr_read_samples(), nmr_zip_bruker_samples(), save_files_to_rDolphin(), save_profiling_output()

Other nmr_dataset_1D functions: [.nmr_dataset_1D(), computes_peak_width_ppm(), file_lister(), files_to_rDolphin(), format.nmr_dataset_1D(), is.nmr_dataset_1D(), load_and_save_functions, new_nmr_dataset_1D(), nmr_align_find_ref(), nmr_baseline_removal(), nmr_baseline_threshold(), nmr_exclude_region(), nmr_integrate_regions(), nmr_interpolate_1D(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get(), nmr_normalize(), nmr_pca_build_model(), nmr_pca_outliers_filter(), nmr_pca_outliers_plot(), nmr_pca_outliers_robust(), nmr_pca_outliers(), nmr_ppm_resolution(), plot.nmr_dataset_1D(), plot_webgl(), print.nmr_dataset_1D(), rdCV_PLS_RF_ML(), rdCV_PLS_RF(), save_files_to_rDolphin(), validate_nmr_dataset_peak_table(), validate_nmr_dataset()

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
dataset_1D <- nmr_interpolate_1D(dataset, axis = c(min = -0.5, max = 10, by = 2.3E-4))
chemo_spectra <- to_ChemoSpec(dataset_1D)
```

---

validate_nmr_dataset *Validate nmr_dataset objects*

Description

Validate nmr_dataset objects

Validate 1D nmr datasets

Usage

```
validate_nmr_dataset(samples)

validate_nmr_dataset_1D(nmr_dataset_1D)
```

Arguments

samples	An nmr_dataset object
nmr_dataset_1D	An nmr_dataset_1D object

Value

Validate nmr_dataset objects

The nmr_dataset_1D unchanged

This function is useful for its side-effects. Stopping in case of error

See Also

Other class helper functions: format.nmr_dataset_1D(), format.nmr_dataset_peak_table(), format.nmr_dataset(), is.nmr_dataset_1D(), is.nmr_dataset_peak_table(), new_nmr_dataset_1D(), new_nmr_dataset_peak_table(), new_nmr_dataset(), print.nmr_dataset_1D(), print.nmr_dataset_peak_table() print.nmr_dataset(), validate_nmr_dataset_family(), validate_nmr_dataset_peak_table()

Other nmr_dataset functions: [.nmr_dataset(), format.nmr_dataset(), load_and_save_functions, new_nmr_dataset(), nmr_interpolate_1D(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get(), nmr_ppm_resolution(), nmr_read_samples(), print.nmr_dataset()

Other class helper functions: format.nmr_dataset_1D(), format.nmr_dataset_peak_table(), format.nmr_dataset(), is.nmr_dataset_1D(), is.nmr_dataset_peak_table(), new_nmr_dataset_1D(), new_nmr_dataset_peak_table(), new_nmr_dataset(), print.nmr_dataset_1D(), print.nmr_dataset_peak_table() print.nmr_dataset(), validate_nmr_dataset_family(), validate_nmr_dataset_peak_table()

Other nmr_dataset_1D functions: [.nmr_dataset_1D(), computes_peak_width_ppm(), file_lister(), files_to_rDolphin(), format.nmr_dataset_1D(), is.nmr_dataset_1D(), load_and_save_functions, new_nmr_dataset_1D(), nmr_align_find_ref(), nmr_baseline_removal(), nmr_baseline_threshold(), nmr_exclude_region(), nmr_integrate_regions(), nmr_interpolate_1D(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get(), nmr_normalize(), nmr_pca_build_model(), nmr_pca_outliers_filter(), nmr_pca_outliers_plot(), nmr_pca_outliers_robust(), nmr_pca_outliers(), nmr_ppm_resolution(), plot.nmr_dataset_1D(), plot_webgl(), print.nmr_dataset_1D(), rdCV_PLS_RF_ML(), rdCV_PLS_RF(), save_files_to_rDolphin(), to_ChemoSpec(), validate_nmr_dataset_peak_tab

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
validate_nmr_dataset(dataset)

dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
dataset_1D <- nmr_interpolate_1D(dataset, axis = c(min = -0.5, max = 10, by = 2.3E-4))
dataset_1D_validated <- validate_nmr_dataset_1D(dataset_1D)
```

---

validate_nmr_dataset_family

Validate nmr_dataset_family objects

Description

Validate nmr_dataset_family objects

Usage

```
validate_nmr_dataset_family(nmr_dataset_family)
```

Arguments

nmr_dataset_family
: An nmr_dataset_family object

Value

The nmr_dataset_family unchanged

This function is useful for its side-effects: Stopping in case of error

See Also

Other class helper functions: format.nmr_dataset_1D(), format.nmr_dataset_peak_table(), format.nmr_dataset(), is.nmr_dataset_1D(), is.nmr_dataset_peak_table(), new_nmr_dataset_1D(), new_nmr_dataset_peak_table(), new_nmr_dataset(), print.nmr_dataset_1D(), print.nmr_dataset_peak_table(), print.nmr_dataset(), validate_nmr_dataset_peak_table(), validate_nmr_dataset()

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
dataset_1D <- nmr_interpolate_1D(dataset, axis = c(min = -0.5, max = 10, by = 2.3E-4))
validate_nmr_dataset_family(dataset_1D)
```

---

validate_nmr_dataset_peak_table

Validate nmr_dataset_peak_table objects

Description

The function detects peaks on an nmr_dataset_1D object, using speaq::detectSpecPeaks. detectSpecPeaks divides the whole spectra into smaller segments and uses MassSpecWavelet::peakDetectionCWT for peak detection.

This function is based on speaq::dohCluster.

The function allows the integration of a given ppm vector with a specific width.

Usage

```
validate_nmr_dataset_peak_table(nmr_dataset_peak_table)

nmr_detect_peaks(
  nmr_dataset,
  nDivRange_ppm = 0.1,
  scales = seq(1, 16, 2),
  baselineThresh = NULL,
  SNR.Th = 3
)
```

```
nmr_detect_peaks_plot(nmr_dataset, peak_data, NMRExperiment, ...)

nmr_detect_peaks_tune_snr(
  ds,
  NMRExperiment = NULL,
  SNR_thresholds = seq(from = 2, to = 6, by = 0.1)
)

nmr_align(
  nmr_dataset,
  peak_data,
  NMRExp_ref = NULL,
  maxShift_ppm = 0.0015,
  acceptLostPeak = FALSE
)

nmr_integrate_peak_positions(
  samples,
  peak_pos_ppm,
  peak_width_ppm = 0.006,
  ...
)

get_integration_with_metadata(integration_object)
```

Arguments

nmr_dataset_peak_table	An nmr_dataset_peak_table object
nmr_dataset	An nmr_dataset_1D
nDivRange_ppm	Segment size, in ppms, to divide the spectra and search for peaks.
scales	The parameter of peakDetectionCWT function of MassSpecWavelet package, look it up in the original function.
baselineThresh	It will remove all peaks under an intensity set by baselineThresh. If you set it to 'NULL', nmr_detect_peaks will automatically compute an aproximate value considering baseline between 9.5 and 10.0 ppm (automatically calculation using baselineThresh = NULL will not work if spectra were not interpolated up to 10.0 ppm)
SNR.Th	The parameter of peakDetectionCWT function of MassSpecWavelet package, look it up in the original function. If you set -1, the function will itself re-compute this value.
peak_data	The detected peak data given by nmr_detect_peaks.
NMRExperiment	A string with the single NMRExperiment used explore the SNR thresholds. If not given, use the first one.
...	Arguments passed on to nmr_integrate_regions

	`regions` A named list. Each element of the list is a region, given as a named numeric vector of length two with the range to integrate. The name of the region will be the name of the column
`ds`	An nmr_dataset_1D dataset
`SNR_thresholds`	A numeric vector with the SNR thresholds to explore
`NMRExp_ref`	NMRExperiment of the reference to use for alignment
`maxShift_ppm`	The maximum shift allowed, in ppm
`acceptLostPeak`	This is an option for users, TRUE is the default value. If the users believe that all the peaks in the peak list are true positive, change it to FALSE.
`samples`	A nmr_dataset object
`peak_pos_ppm`	The peak positions, in ppm
`peak_width_ppm`	The peak widths (or a single peak width for all peaks)
`integration_object`	A nmr_dataset object

Value

The nmr_dataset_peak_table unchanged

This function is useful for its side-effects: Stopping in case of error

A data frame with the NMRExperiment, the sample index, the position in ppm and index and the peak intensity

Plot peak detection results

A list with the following elements:

- `peaks_detected`: A data frame with the columns from the nmr_detect_peaks output and an additional column `SNR_threshold` with the threshold used on each row.
- `num_peaks_per_region`: A summary of the `peaks_detected` table, with the number of peaks detected on each chemical shift region
- `plot_num_peaks_per_region`: A visual representation of `num_peaks_per_region`
- `plot_spectrum_and_detections`: A visual representation of the spectrum and the peaks detected with each SNR threshold. Use plotly::ggplotly or plot_interactive on this to zoom and explore the results.

An nmr_dataset_1D, with the spectra aligned

Integrate peak positions

Get integrals with metadata from integrate peak positions

integration dataframe

Parallelization

This function accepts parallellization with future strategies. You can use `plan(multiprocess)` or `plan(sequential)` before calling this function to determine if it should be parallellized or not.

See Also

nmr_align for peak alignment with the detected peak table

Other nmr_dataset_peak_table functions: [.nmr_dataset_peak_table(), format.nmr_dataset_peak_table(), is.nmr_dataset_peak_table(), load_and_save_functions, new_nmr_dataset_peak_table(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get(), print.nmr_dataset_peak_table()

Other class helper functions: format.nmr_dataset_1D(), format.nmr_dataset_peak_table(), format.nmr_dataset(), is.nmr_dataset_1D(), is.nmr_dataset_peak_table(), new_nmr_dataset_1D(), new_nmr_dataset_peak_table(), new_nmr_dataset(), print.nmr_dataset_1D(), print.nmr_dataset_peak_table(), print.nmr_dataset(), validate_nmr_dataset_family(), validate_nmr_dataset()

Other peak detection functions: Pipelines, nmr_baseline_threshold(), nmr_identify_regions_blood(), nmr_identify_regions_cell(), nmr_identify_regions_urine(), nmr_integrate_regions(), regions_from_peak_table()

Other nmr_dataset_1D functions: [.nmr_dataset_1D(), computes_peak_width_ppm(), file_lister(), files_to_rDolphin(), format.nmr_dataset_1D(), is.nmr_dataset_1D(), load_and_save_functions, new_nmr_dataset_1D(), nmr_align_find_ref(), nmr_baseline_removal(), nmr_baseline_threshold(), nmr_exclude_region(), nmr_integrate_regions(), nmr_interpolate_1D(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get(), nmr_normalize(), nmr_pca_build_model(), nmr_pca_outliers_filter(), nmr_pca_outliers_plot(), nmr_pca_outliers_robust(), nmr_pca_outliers(), nmr_ppm_resolution(), plot.nmr_dataset_1D(), plot_webgl(), print.nmr_dataset_1D(), rdCV_PLS_RF_ML(), rdCV_PLS_RF(), save_files_to_rDolphin(), to_ChemoSpec(), validate_nmr_dataset()

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Other alignment functions: Pipelines, nmr_align_find_ref()

Other peak alignment functions: nmr_align_find_ref()

Other nmr_dataset_1D functions: [.nmr_dataset_1D(), computes_peak_width_ppm(), file_lister(), files_to_rDolphin(), format.nmr_dataset_1D(), is.nmr_dataset_1D(), load_and_save_functions, new_nmr_dataset_1D(), nmr_align_find_ref(), nmr_baseline_removal(), nmr_baseline_threshold(), nmr_exclude_region(), nmr_integrate_regions(), nmr_interpolate_1D(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get(), nmr_normalize(), nmr_pca_build_model(), nmr_pca_outliers_filter(), nmr_pca_outliers_plot(), nmr_pca_outliers_robust(), nmr_pca_outliers(), nmr_ppm_resolution(), plot.nmr_dataset_1D(), plot_webgl(), print.nmr_dataset_1D(), rdCV_PLS_RF_ML(), rdCV_PLS_RF(), save_files_to_rDolphin(), to_ChemoSpec(), validate_nmr_dataset()

Other peak integration functions: Pipelines, computes_peak_width_ppm(), nmr_identify_regions_blood(), nmr_identify_regions_cell(), nmr_identify_regions_urine(), nmr_integrate_regions()

Other nmr_dataset_1D functions: [.nmr_dataset_1D(), computes_peak_width_ppm(), file_lister(), files_to_rDolphin(), format.nmr_dataset_1D(), is.nmr_dataset_1D(), load_and_save_functions, new_nmr_dataset_1D(), nmr_align_find_ref(), nmr_baseline_removal(), nmr_baseline_threshold(), nmr_exclude_region(), nmr_integrate_regions(), nmr_interpolate_1D(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get(), nmr_normalize(), nmr_pca_build_model(), nmr_pca_outliers_filter(), nmr_pca_outliers_plot(), nmr_pca_outliers_robust(), nmr_pca_outliers(), nmr_ppm_resolution(), plot.nmr_dataset_1D(), plot_webgl(), print.nmr_dataset_1D(), rdCV_PLS_RF_ML(), rdCV_PLS_RF(), save_files_to_rDolphin(), to_ChemoSpec(), validate_nmr_dataset()

Other peak integration functions: Pipelines, computes_peak_width_ppm(), nmr_identify_regions_blood(), nmr_identify_regions_cell(), nmr_identify_regions_urine(), nmr_integrate_regions()

Other nmr_dataset_1D functions: [.nmr_dataset_1D(), computes_peak_width_ppm(), file_lister(), files_to_rDolphin(), format.nmr_dataset_1D(), is.nmr_dataset_1D(), load_and_save_functions, new_nmr_dataset_1D(), nmr_align_find_ref(), nmr_baseline_removal(), nmr_baseline_threshold(), nmr_exclude_region(), nmr_integrate_regions(), nmr_interpolate_1D(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get(), nmr_normalize(), nmr_pca_build_model(), nmr_pca_outliers_filter(), nmr_pca_outliers_plot(), nmr_pca_outliers_robust(), nmr_pca_outliers(), nmr_ppm_resolution(), plot.nmr_dataset_1D(), plot_webgl(), print.nmr_dataset_1D(), rdCV_PLS_RF_ML(), rdCV_PLS_RF(), save_files_to_rDolphin(), to_ChemoSpec(), validate_nmr_dataset()

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
nmr_dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
dataset_1D <- nmr_interpolate_1D(nmr_dataset, axis = c(min = -0.5, max = 10, by = 2.3E-4))

sample_10 <- filter(dataset_1D, NMRExperiment == "10")

# 1.Peak detection in the dataset.
peak_data <- nmr_detect_peaks(dataset_1D,
                              nDivRange_ppm = 0.1, # Size of detection segments
                              scales = seq(1, 16, 2),
                              baselineThresh = 0, # Minimum peak intensity
                              SNR.Th = 4) # Signal to noise ratio

#nmr_detect_peaks_plot(sample_10, peak_data, "NMRExp_ref")
```

```
peaks_detected <- nmr_detect_peaks_tune_snr(sample_10,
                                            SNR_thresholds = seq(from = 2,
                                            to = 3, by = 0.5))


# 2.Find the reference spectrum to align with.
NMRExp_ref <- nmr_align_find_ref(dataset_1D, peak_data)

# 3.Spectra alignment using the ref spectrum and a maximum alignment shift
nmr_dataset <- nmr_align(dataset_1D, # the dataset
                         peak_data, # detected peaks
                         NMRExp_ref = NMRExp_ref, # ref spectrum
                         maxShift_ppm = 0.0015, # max alignment shift
                         acceptLostPeak = FALSE) # lost peaks

# 4.PEAK INTEGRATION (please, consider previous normalization step).
# First we take the peak table from the reference spectrum
peak_data_ref <- filter(peak_data, NMRExperiment == NMRExp_ref)

# Then we integrate spectra considering the peaks from the ref spectrum
nmr_peak_table <- nmr_integrate_peak_positions(
                      samples = nmr_dataset,
                      peak_pos_ppm = peak_data_ref$ppm,
                      peak_width_ppm = NULL)

validate_nmr_dataset_peak_table(nmr_peak_table)

#If you wanted the final peak table before machine learning you can run
nmr_peak_table_completed <- get_integration_with_metadata(nmr_peak_table)
```

`[.nmr_dataset` *Extract parts of an nmr_dataset*

Description

Extract parts of an nmr_dataset

Usage

```
## S3 method for class 'nmr_dataset'
x[i]
```

Arguments

`x`	an nmr_dataset object
`i`	indices of the samples to keep

Value

an nmr_dataset with the extracted samples

See Also

Other subsetting functions: [.nmr_dataset_1D(), [.nmr_dataset_peak_table(), filter.nmr_dataset_family(), nmr_pca_outliers_filter()

Other nmr_dataset functions: format.nmr_dataset(), load_and_save_functions, new_nmr_dataset(), nmr_interpolate_1D(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get(), nmr_ppm_resolution(), nmr_read_samples(), print.nmr_dataset(), validate_nmr_dataset()

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
dataset2 <- dataset[1:3] # get the first 3 samples
```

[.nmr_dataset_1D *Extract parts of an nmr_dataset_1D*

Description

Extract parts of an nmr_dataset_1D

Usage

```
## S3 method for class 'nmr_dataset_1D'
x[i]
```

Arguments

x	an nmr_dataset_1D object
i	indices of the samples to keep

Value

an nmr_dataset_1D with the extracted samples

See Also

Other subsetting functions: [.nmr_dataset_peak_table(), [.nmr_dataset(), filter.nmr_dataset_family(), nmr_pca_outliers_filter()

Other nmr_dataset_1D functions: computes_peak_width_ppm(), file_lister(), files_to_rDolphin(), format.nmr_dataset_1D(), is.nmr_dataset_1D(), load_and_save_functions, new_nmr_dataset_1D(), nmr_align_find_ref(), nmr_baseline_removal(), nmr_baseline_threshold(), nmr_exclude_region(), nmr_integrate_regions(), nmr_interpolate_1D(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(),

nmr_meta_get(), nmr_normalize(), nmr_pca_build_model(), nmr_pca_outliers_filter(), nmr_pca_outliers_plot(), nmr_pca_outliers_robust(), nmr_pca_outliers(), nmr_ppm_resolution(), plot.nmr_dataset_1D(), plot_webgl(), print.nmr_dataset_1D(), rdCV_PLS_RF_ML(), rdCV_PLS_RF(), save_files_to_rDolphin(), to_ChemoSpec(), validate_nmr_dataset_peak_table(), validate_nmr_dataset()

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
dataset_1D <- nmr_interpolate_1D(dataset, axis = c(min = -0.5, max = 10, by = 2.3E-4))
dataset_1D[0]
```

[.nmr_dataset_peak_table

Extract parts of an nmr_dataset_peak_table

Description

Extract parts of an nmr_dataset_peak_table

Usage

```
## S3 method for class 'nmr_dataset_peak_table'
x[i]
```

Arguments

x	an nmr_dataset_peak_table object
i	indices of the samples to keep

Value

an nmr_dataset_peak_table with the extracted samples

See Also

Other subsetting functions: [.nmr_dataset_1D(), [.nmr_dataset(), filter.nmr_dataset_family(), nmr_pca_outliers_filter()

Other nmr_dataset_peak_table functions: format.nmr_dataset_peak_table(), is.nmr_dataset_peak_table(), load_and_save_functions, new_nmr_dataset_peak_table(), nmr_meta_add(), nmr_meta_export(), nmr_meta_get_column(), nmr_meta_get(), print.nmr_dataset_peak_table(), validate_nmr_dataset_peak_table(

Examples

```
dir_to_demo_dataset <- system.file("dataset-demo", package = "AlpsNMR")
dataset <- nmr_read_samples_dir(dir_to_demo_dataset)
dataset_1D <- nmr_interpolate_1D(dataset, axis = c(min = -0.5, max = 10, by = 2.3E-4))
meta <- file.path(dir_to_demo_dataset, "dummy_metadata.xlsx")
metadata <- readxl::read_excel(meta, sheet = 1)
dataset_1D <- nmr_meta_add(dataset_1D, metadata = metadata, by = "NMRExperiment")
metadata <- list(external = dataset_1D[["metadata"]][["external"]])
peak_table <- nmr_data(dataset_1D)
new <- new_nmr_dataset_peak_table(peak_table, metadata)
new[0]
```

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