# Package 'RcometsAnalytics'

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Type Package
Title Comets Analytics for consortium based metabolomic analyses
<b>Version</b> 2.9.0.27
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<b>Description</b> This R package support all cohort-specific analyses of the COMETS consortium. Data are not saved in the system but output must be downloaded and submitted for meta-analyses. This package can be used in several ways: supports the CBIIT implementation of comets-analytics, local shiny based add-in called shinycomets, or console based analysis. See example vignette. The version of the package is noted as: level 1 and 2 reflect the comets-analytics version, 3rd level reflects the number of major revision and 4th level for bug fixes.
<b>Depends</b> R (>= $3.5.0$ )
Imports readxl, rio, dplyr, plyr, plotly, tidyr, heatmaply, stringr, data.table, caret, subselect, broom, psych, MASS, ppcor, survival
Suggests Hmisc, knitr, testthat, rmarkdown, RaMP
VignetteBuilder knitr
License GPL-3
RoxygenNote 7.3.1
NeedsCompilation no
<pre>URL http://comets-analytics.org/</pre>
<pre>BugReports https://github.com/CBIIT/nci-webtools-comets-analytics/issues</pre>
R topics documented:
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RcometsAnalytics-package

RcometsAnalytics R package

# Description

This R package supports all cohort-specific analyses of the COMETS consortium https://www.comets-analytics.org/. Data are not saved in the system but output must be downloaded and submitted for meta-analyses.

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## **Details**

```
Functions for analysis:
runModel (correlation, glm, lm, coxph, or clogit)
runAllModels (run models in batch mode from models sheet)
Functions for graphics:
plotVar (metabolite variance distribution plot)
plotMinvalues (distribution of minimum or missing values)
showHeatmap (heat map of metabolite correlations)
showHClust (interactive heat map with hierarchical clustering)
Functions for saving results to files:
OutputCSVResults (write to .csv file)
OutputXLSResults (write to excel file)
OutputListToExcel (write list of data frames to excel file with multiple sheets)
Functions for meta-analysis:
runMeta (run a single meta-analysis)
runAllMeta (run multiple meta-analyses)
meta_calc (main calculation function for meta-analysis)
```

checkIntegrity

Checks integrity of sheets in the user input CSV file

## **Description**

Checks integrity of sheets in the user input CSV file

# Usage

```
checkIntegrity(
  dta.metab,
  dta.smetab,
  dta.sdata,
  dta.vmap,
  dta.models,
  dict_metabnames,
  dta.op
)
```

## **Arguments**

```
dta.metab dta.metab
dta.smetab dta.smetab
dta.sdata dta.sdata
dta.vmap dta.vmap
dta.models dta.models
dict_metabnames
dta.op dta.op
```

4 chemClassEnrichment

chemClassEnrichment Chemical Class Enrichment

## **Description**

**Chemical Class Enrichment** 

# Usage

```
chemClassEnrichment(df, metabdata, db.version = NULL, pvalue.adj = 0.05)
```

# **Arguments**

df The "Effects" data frame returned from function runModel

metabdata Return object from readCOMETSinput

db.version The RaMP SQLite database version to use. The default is the most recent ver-

sion.

pvalue.adj The maximum BH-adjusted p-value for a metabolite to be included in the anal-

ysis.

#### **Details**

The **RaMP** R package must be installed prior to calling this function. An attempt to load RaMP will be done through the requireNamespace function.

The set of all possible metbolite id types are: LIPIDMAPS, pubchem, hmdb, chemspider, chebi, CAS, wikidata, swisslipids, kegg, lipidbank, plantfa, and kegg\_glycan. The **METABOLITES** sheet in the input Excel file will need to have at least one of the above id types as a column (case-insensitive). If the **METABOLITES** sheet contains more than one id type, then the metabolite ids passed into chemicalClassEnrichment depends on the order of the id type columns. For example, if the **METABOLITES** sheet contains columns HMDB (column F) and pubchem (column C), then the metbolite ids will taken from the pubchem column and any missing ids from the pubchem column will be assigned from the HMDB column.

#### Value

A data frame

# **Examples**

```
dir <- system.file("extdata", package="RcometsAnalytics", mustWork=TRUE)
csvfile <- file.path(dir, "cometsInputAge.xlsx")
exmetabdata <- readCOMETSinput(csvfile)
modeldata <- getModelData(exmetabdata,exposures="age", modelspec="Interactive",
outcomes=c("lactose","lactate"))
obj <- runModel(modeldata,exmetabdata, cohortLabel="DPP")
# ret <- chemClassEnrichment(obj$Effects, exmetabdata, pvalue.adj=1)</pre>
```

clogit.options 5

clogit.options

options list for clogit

# **Description**

A list of 2:

- method One of: "exact", "approximate", "efron", "breslow". The default is "exact".
- weights A variable name to specify weights. The default is NULL.

# **Examples**

```
model.options <- list(method="efron", weights="weightVarInData")</pre>
```

correlation.options

options list for model="correlation"

# **Description**

A list of 1:

• method Correlation method to use. It must be one of "spearman", "pearson", "kendall". The default value is "spearman".

# **Examples**

```
model.options <- list(method="pearson")</pre>
```

coxph.options

options list for coxph

# **Description**

A list of 6:

- ties One of: "efron", "breslow", "exact". The default is "efron".
- robust TRUE or FALSE for computing a robust covariance matrix). The default is FALSE.
- weights A variable name to specify weights. The default is NULL.
- singular.ok See coxph. The default is TRUE.
- Surv. type See the type option in Surv. The default is NULL.

# **Examples**

```
model.options <- list(robust=TRUE, weights="weightVarInData")</pre>
```

6 Effects

Effects Effects table

## **Description**

The Effects data frame contains the estimates for each exposure, and will contain multiple rows for categorical exposure variables. Depending on the model run and options specified, all the below names may not appear in the data frame.

- corr The correlation between term and the outcome
- estimate The regression coefficient of term
- estimate.lower The lower confidence limit for term
- estimate.upper The upper confidence limit for term
- exp.estimate The exponentiated regression coefficient of term
- exp.estimate.lower The exponentiated lower confidence limit for term
- exp.estimate.upper The exponentiated upper confidence limit for term
- exp.std.error The standard error of exp.estimate from the delta method
- exposurespec Exposure variable
- model Model label from getModelData
- model\_number Model number used in runAllModels
- outcomespec Outcome variable
- pvalue The p-value of the test
- pvalue.adj Adjusted p-values for exposure variables only
- run Run number that can be used to link with the ModelSummary table
- statistic The test statistic for term
- std.error The standard error of estimate
- stratavar Stratum variable(s)
- strata Stratum level(s)
- term Variable in the model

# **Details**

Missing values will appear if a model did not converge, produced an error, or not run because of too many missing values in the outcome. Adjusted p-values are only computed for models with a single outcome variable or single exposure variable.

Errors\_Warnings 7

Errors_Warnings	Errors and Warnings table

## **Description**

Columns in the Errors\_Warnings table.

- type WARNING or ERROR
- object The object that produced the warning or error. This is typically a variable or a particular stratum.
- · message Message describing the warning or error
- model Model label from getModelData
- model\_number Model number used in runAllModels

## **Details**

The kinds of warnings and errors stored in this matrix are ones that apply to all models or all outcomes for an exposure variable. An error message for a particular exposure-outcome pair will be stored in the message column of the ModelSummary table.

file.list

list to describe or transform a file for meta-analysis

# Description

A list of 20:

- file The complete path to the file. Must be specified.
- cohort The name of the cohort. Use this option to set or change the name of the cohort. Must be specified for files not obtained from version 3.0 of RcometsAnalytics.
- sep The file delimiter. For example "," for csv files, "\t" for tab-delimited files. The default is NULL.
- correlation 0 or 1 for correlation results. The default is 0, so that the file is assumed to be from a non-correlation model.
- estimate.col Column name for the beta estimate or correlation. The default value is "estimate".
- se.col Column name for the standard error. Needed for non-correlation models. The default value is "std.error".
- nobs.col Column name for the number of subjects. If such a column does not exist in the file, set nobs to a value. The default is "nobs".
- nobs Number of observations. Must be specified if nobs.col is not specified. The default is NULL.
- outcome.col Column name for the outcome. If such a column does not exist in the file, then set outcome.name. The default is "outcome uid".
- outcome.name The name of the outcome variable. Must be specified if outcome.col is not specified. No default.

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• exposure.col Column name for the exposure. If such a column does not exist in the file, then set exposure.name. The default is "exposure\_uid".

- exposure.name The name of the exposure variable. Must be specified if exposure.col is not specified. No default.
- stratavar.col Column name for the stratification variable. The default is NULL.
- strata.col Column name for the stratification values. The default is NULL.
- strata.name The name of the stratification variable. Use this option to change the name of the stratification variable or to add a stratification variable to the file. When adding a stratification variable, set strata.value also. The default is NULL.
- strata.value The constant value of the stratification. The default is NULL.
- model.col Column name for the model. The default is NULL.
- model.name The name of the model. Use this option to change or add the model name to the results. The default is NULL.
- change.col.values A list of sublists, where each sublist has elements "col", "old", and "new". Use this option to change the values of a (exposure or stratification) column to new values. For example, list(list(col="smoke", old=c("never", "current", "former"), new=c(0, 1, 2))) will change the values "never" to 0, "current" to 1, and "former" to 2 in the "smoke" column. The default is NULL.
- where Vector of strings with a variable name, a comparison operator (e.g. "<", ">=", "<=", ">=", "!=", "="), and a value. The strings are combined by the logical AND (&) operator. For example, where = c("study = A", "age > 50") uses all subjects with age > 50 and in study A. This option would primarily be used if the file contained results from multiple cohorts and each cohort needed to be included in the meta-analysis.
- new.ref.value The new reference value for a categorical. exposure variable. This option will update the Effects data frame based on the new reference value. Note that the updated p-values will be based on a Wald test regardless of the original test. This option is applied before the option change.col.values. This option is only for results files from non-correlation models obtained using version 3.0 of RcometsAnalytics. The default is NULL.

## **Details**

For any type of file, the parameter file must be specified. For files not obtained from version 3.0 of RcometsAnalytics, other parameters may need to be specified. This list can be used with the functions runMeta and meta\_transform.

# **Examples**

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Function that subsets input data based on "where variable"

# Description

Function that subsets input data based on "where variable"

# Usage

```
filterCOMETSinput(readData, where = NULL)
```

# **Arguments**

readData list from readComets or readData\$subjdata

where users can specify which subjects to perform the analysis by specifying this pa-

rameter. 'where' expects a vector with a variable name, a comparison operator ("<", ">", "=","<=",">="), and a value. For example, "where = c("Gender=Female")".

# Value

filtered list

fixData

Fixes input data (e.g. takes care of factors, and other data frame conversions)

# **Description**

Fixes input data (e.g. takes care of factors, and other data frame conversions)

# Usage

```
fixData(dta, compbl = FALSE)
```

# Arguments

dta any data frame

compbl compress multiple blank spaces to single blank space for all character or factor

variables in the dataset

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getModelData

Prepares data for the models to be run as specified in the input. Can be run in interactive or batch mode. Each model is checked for validity (correlation between predictors, zero variance, etc.).

# Description

Prepares data for the models to be run as specified in the input. Can be run in interactive or batch mode. Each model is checked for validity (correlation between predictors, zero variance, etc.).

# Usage

```
getModelData(
  readData,
  modelspec = "Batch",
  modlabel = "",
  outcomes = "All metabolites",
  exposures = "",
  adjvars = NULL,
  strvars = NULL,
  wgtvar = NULL,
  offvar = NULL,
  timevar = NULL,
  groupvar = NULL,
  where = NULL,
  exposurerefs = NULL
)
```

# **Arguments**

readData	List from readCOMETSinput
modelspec	How model is specified (Interactive or Batch). The default is Batch
modlabel	If batch, chosen model specified by batch mode (the MODEL column in the Models sheet). If interactive, then the model label.
outcomes	If Interactive, a vector of outcome variables (see details), the default is All metabolites)
exposures	If Interactive, a vector of exposure variables (see details)
adjvars	If Interactive, a vector adjustment covariates (see details)
strvars	If Interactive, stratification covariates (see details)
wgtvar	If Interactive, a variable of weights (see details)
offvar	If Interactive, an offset variable (see details)
timevar	If Interactive, time variable(s) for survival models (see details)
groupvar	If Interactive, a group variable for conditional logistic models (see details)
where	users can specify which subjects to perform the analysis on by specifying this parameter. 'where' expects a vector of strings with a variable name, a comparison operator (e.g. "<", ">=", ">=", "!=", "="), and a value. For example, where = c("age>50", "bmi > 22") uses all subjects with age > 50 AND bmi > 22. Note that when running in Batch mode, rules in the WHERE column of the Models sheet must be separated by a comma.

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exposurerefs If Interactive, a vector of exposure reference levels for categorical exposure variables. If specified, then this vector must have the same length as exposures.

#### **Details**

All metabolite variables specified should be listed in the metabolite\_name column of the Metabolites sheet of the Excel file. All non-metabolite variables should be listed in the VARREFERENCE column of the VarMap sheet. The wgtvar, offvar, and timevar are only used for specific models. See the model option in options.

## Value

a list comprising:

1: subset data: gdta

2: exposure variables: ccovs

3: outcome variables: rcovs

4: adjustment variables: acovs

5: stratification variable: scovs

6: model specification: modspec

7: model label: modlab

8: whether all metabolites vs all metabolites is run: allvsall

9: weight variables: wgtcov 10: offset variables: offcov

## **Examples**

```
dir <- system.file("extdata", package="RcometsAnalytics", mustWork=TRUE)
csvfile <- file.path(dir, "cometsInputAge.xlsx")
exmetabdata <- readCOMETSinput(csvfile)
modeldata <- getModelData(exmetabdata,modlabel="1 Age")</pre>
```

glm.options

options list for glm

# **Description**

A list of 6:

- family One of: "binomial", "gaussian", "Gamma", "inverse.gaussian", "poisson", "quasi", "quasibinomial", "quasipoisson". The default is "gaussian".
- link NULL or a string for the link function to use (see family). The default is to use the canonical link for family.
- $\bullet$  weights A variable name to specify weights. The default is NULL.
- offset A variable name to specify an offset. The default is NULL.
- control See glm. The default is glm. control.
- singular.ok See glm. The default is TRUE.

## **Examples**

```
model.options <- list(family="binomial", weights="weightVarInData")</pre>
```

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Harmonize	Harmonizes metabolites by looking up metabolites names from user input and finding the corresponding COMETS harmonized name.
	inpui ana jinaing ine corresponding COME13 narmonizea name.

# Description

Harmonizes metabolites by looking up metabolites names from user input and finding the corresponding COMETS harmonized name.

# Usage

```
Harmonize(dtalist)
```

# **Arguments**

dtalist

results of reading a CSV data sheet (with read\_excel)

lm.options

options list for lm

# **Description**

A list of 4:

- weights A variable name to specify weights. The default is NULL.
- offset A variable name to specify an offset. The default is NULL.
- tol See 1m. The default is 1e-7.
- singular.ok See lm. The default is TRUE.

# **Examples**

```
model.options <- list(weights="weightVarInData")</pre>
```

 ${\tt mergeResultsFiles}$ 

This function will combine output files assumed to be from the same cohort and same model.

# **Description**

This function will combine output files assumed to be from the same cohort and same model.

# Usage

```
mergeResultsFiles(filevec, out.file, op = NULL)
```

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## **Arguments**

filevec	Character vector of files that contain the output files from runModel or runAllModels. Valid file extensions are ".xlsx", and ".rda".
out.file	NULL or a file to save the results. The file extension must be either ".xlsx", or ".rda".
ор	A list containing the options to use or NULL. The options are precedence and check.consistency with default values of "nobs" and TRUE respectively (see details). The default is NULL.

#### **Details**

This function will merge output files containing results from the same model and same cohort. Within a file, metabolites with missing results (estimate and std.error) will be excluded. The files can have different and overlapping metabolites. When there is an overlapping metabolite among the files, the option precedence="nobs" will choose the file with the largest number of subjects for that metabolite. With precedence="data", the first file in filevec that contains the metabolite will be chosen. The option check.consistency will check for the same outcome, exposure, and stratification variable names across the files.

#### Value

List of data frames containing the merged results

metaOutputColumns
-------------------

# **Description**

The Results data frame contains the estimates from the meta-analyses. Depending on the model run and options specified, all the below names may not appear in the data frame returned from runMeta.

- outcome\_uid The harmonized outcome variable
- exposure\_uid The harmonized exposure variable
- term For a continuous exposure, this will be the same as exposure\_uid. For a categorical exposure, it will be the dummy variable for the exposure.
- n. cohort The number of included cohorts for the estimates.
- n. sub Total number of subjects.
- fixed.pvalue P-value for the fixed-effects model.
- random.pvalue P-value for the random-effects model.
- fixed.estimate Estimate for the fixed-effects model.
- fixed.std.error Estimated standard error of fixed.estimate. This will not appear for correlation models.
- random.estimate Estimate for the random-effects model.
- random.std.error Estimated standard error of random.estimate. This will not appear for correlation models.
- fixed.estimate.L Lower 95 percent confidence limit for fixed.estimate.
- fixed.estimate.U Upper 95 percent confidence limit for fixed.estimate.

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- random.estimate.L Lower 95 percent confidence limit for random.estimate.
- random.estimate.U Upper 95 percent confidence limit for random.estimate.
- het.pvalue P-value for Cochran's Q test of heterogeneity.
- stratavar Stratum variable(s)
- strata Stratum level(s)
- strata.fixed.het.pvalue P-value for Cochran's Q test of heterogeneity across the strata using the fixed-effects meta-analysis estimates.
- strata.fixed.het.df Degrees of freedom for the above test.
- strata.random.het.pvalue P-value for Cochran's Q test of heterogeneity across the strata using the random-effects meta-analysis estimates.
- strata.random.het.df Degrees of freedom for the above test.

The Duplicates data frame contains the meta-analysis results for duplicated metabolites. It contains the same columns as the Results data frame plus the columns run, outcomespec, and exposurespec which are useful for differentiating the duplicated metabolites.

## **Details**

Correlation models will not contain columns for fixed.std.error and random.std.error. Instead, there will be columns for lower and upper confidence limits of fixed.estimate and random.estimate. The meta-analysis options add.cohort.names and add.cohort.cols will also add cohort specific columns to the output (see meta\_options).

meta\_calc

Main function that performs the meta-analysis calculations.

# **Description**

Main function that performs the meta-analysis calculations.

## Usage

```
meta_calc(beta, se)
```

# **Arguments**

beta matrix or vector of betas. If a matrix, then the rows represent the metabolites and the columns represent the cohorts.

se matrix or vector of the standard errors for beta. This object must be in the same

order and have the same dimension as beta.

# Value

List containing the results from fixed-effect and random-effect meta-analyses along with Cochran's Q test for heterogeneity.

meta\_opfile 15

meta_opfile	Options file for meta-analyses	

## **Description**

An Excel file containing models and options for the runAllMeta function

#### **Details**

The file can contain sheets **META\_MODELS** and **META\_TYPES**. Each sheet is optional. The **META\_MODELS** sheet should have a column called MODEL containing the models that the user wants to run meta-analyses for. If the **MODELS** sheet is not given then meta-analyses for all models will be run. This sheet can also have an optional column called META\_TYPE that links to the META\_TYPE column in the **META\_TYPES** sheet to define the options for each meta-analysis model. The **META\_TYPES** sheet should contain columns META\_TYPE, OPTION, and VALUE. See the example file in /inst/extdata/cometsMetaInput.xlsx. If the **META\_TYPES** sheet is not specified, then the default values for all meta-analysis options will be used.

meta_options	Meta-analysis options	
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## **Description**

A list of options for the runMeta function

## **Details**

- min.n.cohort Minimum number of cohorts to include when meta-analyzing each metabolite. The default is 2.
- min.nsub.cohort Minimum number of subjects in a cohort for a metabolite to be included from that cohort. The default is 25.
- min.nsub.total Minimum number of subjects in all cohorts for a metabolite to be metaanalyzed. The default is 50.
- cohorts.include Character vector of cohorts to include. The default is NULL.
- cohorts.exclude Character vector of cohorts to exclude. The default is NULL.
- output.type Type of output file, either "xlsx" for an Excel worksheet or "rda" for an R object file created with the save() function. The default is "xlsx".
- strata.exclude.het.test A list of stratification levels to be excluded from the test for heterogeneity. This list has the form list(var1=vec1, var2=vec2, ...), where var1, var2, ... are stratification variables, and vec1, vec2, ... are vectors of stratification levels to be removed from the test. The default is NULL.
- stopOnFileError TRUE or FALSE to stop processing when a problem with any one of the input files is encountered. If FALSE, then the files containing errors will be removed from the analysis. The default is TRUE.
- cohorts.indep Vector of cohort names that correspond to multiple input files, where each file will be treated as an independent cohort.

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• cohorts.merge Vector of cohort names where each of these cohorts have multiple files that will be merged together. This will take the union of all metabolites in the files. A metabolite that occurs in multiple files will be chosen from the file with the maximum sample size for that metabolite.

- add.cohort.names TRUE or FALSE to add binary columns (one for each cohort) to the data frame of results to show which cohorts contributed to the meta-analysis The value will be 1 if the cohort contributed to the result or 0 if the cohort did not. The default is TRUE.
- add.cohort.cols Vector of column names to add to the output for each cohort. These must be column names from the ModelSummary or Effects tables in the meta-analysis input files. For example, if add.cohort.cols = "pvalue", then the p-values from each cohort will be added to the output, and the columns will be of the form <cohort name>.pvalue. A missing value will appear if the cohort did not contribute to the result. The default is NULL.

meta\_transform

Function for transforming a set of results data

## **Description**

Function for transforming a set of results data

# Usage

```
meta_transform(file.obj, out.file = NULL)
```

## **Arguments**

file.obj list of type file.list

out.file NULL or the name of an output file to save the results. The file extension must

be ".xlsx" or ".rda".

#### **Details**

This function will transform or update a file of model results so that the results can be used for a meta-analysis. The types of changes that can be made are:

- 1. Column values can be modified. For example, if the smoking status values 'never', 'current', and 'former' need to be changed to 0, 1, 2.
- 2. A column with a constant value can be added. For example, a column with the number of subjects used in the analysis can be added. Or for instance, for a file from an all-female study, a stratification column containing the value 'female' can be added.
- 3. The file can be subsetted if it contains results from multiple models or multiple cohorts.
- 4. The results can be updated to reflect a different reference value of a categorical exposure variable.
- 5. The name of the cohort can be renamed.
- 6. The name of the model can be renamed.

## Value

A list of objects with names ModelSummary, Effects, Errors\_Warnings, Table1, Info.

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|--|

# **Description**

The ModelSummary data frame contains one row of model summary results for each exposure/outcome combination. Depending on the model run and options specified, all the below names may not appear in the data frame.

- · adjspec Original adjustment variables specified
- adjvars Adjustment variables included in the model
- adjvars.removed Adjustment variables removed from the model
- adj\_uid Adjustment variable universal ids
- · adj.r.squared Adjusted R-squared
- · aic Akaike information criterion
- bic Bayesian information criterion
- cohort String passed into runModel
- converged TRUE or FALSE for model convergence
- deviance Deviance of the fitted model
- df.null NULL model degrees of freedom
- df.residual Residual degrees of freedom
- exposure Exposure variable
- exposure\_uid Exposure universal id
- exposurespec Exposure variable
- loglik Log-likelihood of the fitted model
- message Error message produced from the modeling function
- model Model label from getModelData
- model\_function Model function used in runModel
- model\_number Model number used in runAllModels
- nobs Number of observations used
- null.deviance Deviance of the NULL model
- outcome Outcome variable
- outcomespec Outcome variable
- outcome\_uid Outcome universal id
- run Run number that can be used to link with the Effects table
- runmode "Batch" or "Interactive"
- r. squared R-squared, the fraction of variance explained by the model
- sigma Square root of the estimated variance of the random error
- stratavar Stratum variable(s)
- strata Stratum level(s)
- term Variable in the model

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• wald.pvalue P-value from the Wald test of the exposure variable. Note that this test may be a multi-df test if the exposure is categorical.

- wald.pvalue.adj Adjusted p-values of wald.pvalue for exposure variables only
- exposure.covariances String of exposure reference level, dummy variable names and covariances for a categorical exposure variable in a non-correlation model. This covariances can be used for changing the reference level of the categorical exposure variable. The string has the form: "reflv1,v2,...,vmlcov(v1,v2),cov(v1,v3),cov(v2,v3),cov(v1,v4),...,cov(vm-1, vm)", where ref is the reference level and v1, v2, ..., vm are the dummy variable names.

## **Details**

Missing values will appear if a model did not converge, produced an error, or not run because of too many missing values in the outcome. Adjusted p-values are only computed for models with a single outcome variable or single exposure variable.

options

options list

## **Description**

A list of 19:

- check.cor.cutoff Cutoff value to remove highly correlated columns in the design matrix. The default value is 0.97.
- check.cor.method Correlation method to remove highly correlated columns in the design matrix. It must be one of "spearman", "pearson", "kendall". The default value is "spearman".
- check.design TRUE or FALSE to check the design matrix for linearly dependent columns, highly correlated columns, or for being ill-conditioned whenever it is updated. The default is TRUE.
- check.illCond TRUE or FALSE to check for an ill-conditioned design matrix. The default is TRUE.
- check.nsubjects Minimum number of subjects. The default is 25.
- max.npairwise The maximum number of metabolites to process the "all pairwise correlations" model. The default is 1000.
- max.nstrata The maximum number of strata for a stratified analysis. The default is 10.
- model String for the model function. Currently, it must be one of "correlation", "lm", "glm", "coxph", or "clogit". The default is "correlation".
- model.options List of options specific for the model. See correlation.options, glm.options, lm.options, coxph.options and clogit.options for options specific to model="correlation", "lm", "glm", "coxph", "clogit" respectively. The default is NULL.
- output.ci\_alpha Confidence interval level for estimated from glm models. This option must be a number >= 0 and < 1, where 0 is for not creating confidence intervals. The default value is 0.95.
- output.Effects A string to define the terms output in the returned Effects and ModelSummary data frames. Currently, it must be "exposure" or "all". If set to "all", then summary statistics for the exposure and adjustment variables will be output. Otherwise, only summary statistics for the exposure will be output. This option is ignored with model = "correlation". The default is "exposure".

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• output.exp\_parms TRUE, FALSE or NULL to exponentiate parameter estimates. Standard errors are obtained from the delta method. The default is NULL, so that estimates from logistic regression and survival models will be exponentiated, and not otherwise.

- output.metab.cols Character vector of column names in the METABOLITES sheet to be output in the ModelSummary and Effects data frames. Metabolite ids are matched first using the outcomespec column and then using the exposurespec column. The default is "metabolite name".
- output. ModelSummary A string to defines the columns output in the returned ModelSummary data frame. Currently, it must be "anova" or "all". This option is ignored with model = "correlation". The default is "anova".
- output.type "rda" or "xlsx" to define the type of output file(s) when runAllModels is called. See output.common.cols and output.merge.

  The default is "xlsx".
- method.adjPvalue Method for adjusted p-values. It must be one of: "holm", "hochberg", "hommel", "bonferroni", "BH", "BY", "fdr", "none". Adjusted p-values are only computed for models with a single outcome variable or a single exposure variable. The default is 'fdr'.
- chemEnrich 0 or 1 to run a chemical class enrichment (0=no, 1=yes) using RaMP. The default is 0.
- chemEnrich.adjPvalue The BH-adjusted p-value cutoff to select metabolites for chemical class enrichment. The default is 0.05.

#### **Details**

Before any analysis is performed, an initial design matrix is constructed using the above options as follows:

- 1. Adjustment variables with less than two distinct non-missing values, or with less than check.nsubjects non-missing values are removed.
- 2. The design matrix is created from the remaining adjustment variables and any linearly dependent columns are removed.
- 3. If check.cor.cutoff > 0, then highly correlated columns are removed by computing the correlation matrix cor\_matrix = cor(design\_matrix, method=check.cor.method).
- 4. If check.illCond is TRUE, then the function subselect::trim.matrix is applied to the correlation matrix to determine if additional columns will be removed.

If check.design is TRUE, then steps 2-4 are repeated each time an exposure variable is added to the design matrix or when rows of the design matrix are removed due to missing values in an outcome variable.

# **Examples**

```
# Logistic regression with all default options
model.op <- list(family="binomial")
op <- list(model="glm", model.options=model.op)
# Compute Pearson correlations requiring at least 100 subjects
model.op <- list(method="pearson")
op <- list(model="correlation", check.nsubjects=100, model.options=model.op)</pre>
```

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OutputCSVResults

Create output CSV file

## **Description**

Create output CSV file

## Usage

```
OutputCSVResults(filename, dataf, cohort = "")
```

## **Arguments**

filename name of CSV file and can include path dataf correlation output (from function runCorr())

cohort cohort name

#### Value

the filename of the CSV file with results named with cohort

## **Examples**

```
## Not run:
dir <- system.file("extdata", package="RcometsAnalytics", mustWork=TRUE)
csvfile <- file.path(dir, "cometsInputAge.xlsx")
exmetabdata <- readCOMETSinput(csvfile)
modeldata <- getModelData(exmetabdata,exposures="age",modlabel="1 Age",
outcomes=c("lactose","lactate"))
corrmatrix <-runCorr(modeldata,exmetabdata,"DPP")
# Get correlation results
OutputCSVResults(filename="corr",dataf=corrmatrix,cohort="DPP")
# Get harmonization results
OutputCSVResults(filename="harmonization",dataf=exmetabdata$metab,cohort="DPP")
## End(Not run)</pre>
```

OutputListToExcel

Create an excel xlsx file from a list of data frames

# **Description**

Create an excel xlsx file from a list of data frames

# Usage

```
OutputListToExcel(filename, obj)
```

## **Arguments**

filename Name of file and can include path. It must have a ".xlsx" extension.

obj List of data frames or matrices

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OutputXLSResults

Create output XLSX file

# **Description**

Create output XLSX file

## Usage

```
OutputXLSResults(filename, datal, cohort = "")
```

# **Arguments**

filename name of file and can include path

data list to output (each item on list outputs to a worksheet)

cohort cohort name

#### Value

the filename of the XLSX file with results named with cohort

# **Examples**

```
dir <- system.file("extdata", package="RcometsAnalytics", mustWork=TRUE)
csvfile <- file.path(dir, "cometsInputAge.xlsx")
exmetabdata <- readCOMETSinput(csvfile)
modeldata <- getModelData(exmetabdata,exposures="age",modlabel="1 Age",
outcomes=c("lactose","lactate"))
# Get descriptive data
descdata <-runDescrip(exmetabdata)
OutputXLSResults(filename="corr",datal=descdata,cohort="DPP")</pre>
```

plotMinvalues

Plot the distribution of minimum or missing values for each metabolite

# **Description**

Plot the distribution of minimum or missing values for each metabolite

# Usage

```
plotMinvalues(
  cometsdata,
  title = NULL,
  xlabel = NULL,
  ylabel = "Frequency",
  xylabelsize = 12,
  titlesize = 16,
  missing = FALSE
)
```

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## **Arguments**

cometsdata output of readCOMETSinput function title main title for the plot (default is "Distribution of the Number of Minimum Valxlabel x-axis label (default is "Number of minimum values") ylabel y-axis label (default is "Frequency") size of x and y labels (default=8) xylabelsize titlesize size of title (default, 20)

TRUE or FALSE to plot distribution of missing values (default=FALSE) missing

## Value

a distribution plot

# **Examples**

```
dir <- system.file("extdata", package="RcometsAnalytics", mustWork=TRUE)</pre>
csvfile <- file.path(dir, "cometsInputAge.xlsx")</pre>
exmetabdata <- readCOMETSinput(csvfile)</pre>
plotMinvalues(exmetabdata)
```

plotVar

Plot the variance distribution of transformed metabolite abundances

# Description

Plot the variance distribution of transformed metabolite abundances

# Usage

```
plotVar(
  cometsdata,
  title = "Distribution of Variance",
  titlesize = 16,
  xlabel = "Variance of transformed metabolite abundances",
  ylabel = "Frequency",
  xylabelsize = 12
)
```

# **Arguments**

```
output of readCOMETSinput function
cometsdata
title
                   main title for the plot (default is "Distribution of Variance")
titlesize
                   size of title (default, 20)
xlabel
                   x-axis label (default is "Variance of transformed metabolite abundances")
ylabel
                   y-axis label (default is "Frequency")
xylabelsize
                   size of x and y labels (default=8)
```

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## Value

```
a distribution plot
```

## **Examples**

```
dir <- system.file("extdata", package="RcometsAnalytics", mustWork=TRUE)
csvfile <- file.path(dir, "cometsInputAge.xlsx")
exmetabdata <- readCOMETSinput(csvfile)
plotVar(exmetabdata)</pre>
```

prdebug

debug by printing object with time time

# Description

debug by printing object with time time

#### Usage

```
prdebug(lab, x)
```

# **Arguments**

lab label of object x object

readCOMETSinput

Read in Excel file that contains metabolite data, covariate data, models, and model options.

# **Description**

Read in Excel file that contains metabolite data, covariate data, models, and model options.

# Usage

```
readCOMETSinput(file, mode = "Batch")
```

# **Arguments**

file

path of Excel file to be read in. This file must contain sheets with names **Metabolites**, **SubjectMetabolites**, **SubjectData**, **VarMap**, and optionally **Models**, **Model\_Types** (see details).

mode

How is this function being called (Interactive or Batch). When running in Batch mode, all models in the **Models** sheet must be valid; otherwise an error will be thrown. When running in Interactive mode, a warning will be given if the **Models** sheet contains errors. The default is Batch.

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#### **Details**

Additional information regarding each sheet in the input Excel file is given below.

#### Metabolites

A table with the columns METABID, METABOLITE\_NAME, and possibly other columns of information about the metabolites. The METABID column is used for harmonizing the metabolite names across different cohorts when meta-analyses are performed.

#### **SubjectMetabolites**

A table with the subject ids in the first column and metabolites as the other columns. Each cell must contain a numeric value or left empty (missing); otherwise an error will occur.

#### SubjectData

A table with the subject ids in the first column and covariates as the other columns. For continuous variables, each cell must contain a numeric value or left empty (missing); otherwise an error will occur.

#### VarMap

A table with at least the required columns VARREFERENCE, COHORTVARIABLE, VARTYPE, VARDEFINITION, and optionally ACCEPTED\_VALUES. The COHORTVARIABLE column must contain names that match the column names in the **SubjectData** table. These names will be renamed to their corresponding name in the VARREFERENCE column. The VARTYPE column should have values continuous or categorical for each row. The ACCEPTED\_VALUES column defines the allowed values that the variable should have, and an error will be thrown if the variable is outside of the accepted values. For a categorical variable, ACCEPTED\_VALUES should be a comma separated list of values such as '1, 2, 3'. For a continuous variable, ACCEPTED\_VALUES should be a range of the form: (a, b), (a, b], [a, b), or [a, b], where parentheses denote exclusion of the value, and brackets denote inclusion of the value. Use Inf or -Inf to denote infinity or minus infinity.

#### Models

A table where each row represents a model to be run, and with columns MODEL, OUTCOMES, EXPOSURE, ADJUSTMENT, STRATIFICATION, WHERE, and optionally MODEL\_TYPE, TIME, GROUP, and EXPOSURE\_REFERENCE. All variable names in this table must match variable names in the VARREFERENCE column of the VarMap sheet. The MODEL column is a label for the model. The OUTCOMES and EXPOSURE columns define the outcome and exposure variables for the model. Use All metabolites to specify that all metabolite variables are to be included as outcomes or exposures, otherwise use a space separated list of variable names. For any categorical exposure variable, the EXPOSURE\_REFERENCE column is required to specify the reference level. The reference level must match one of the ACCEPTED\_VALUES in the VarMap sheet. The ADJUSTMENT column contains a space separated list of covariate adjustment variables; use an empty cell for no covariate adjustment. The STRATIFICATION column is used for stratified analyses, with a space separated list of stratification variables. If more than one stratification variable is specified, then the strata are defined by all unique combinations of the stratification variables that appear in the data. The WHERE column is used to define a subset of subjects to include in the analysis, and has the form variable operator value, where operator can be one of the following >, <, >=, <= !=, =. An example WHERE condition is age > 50, which will include all subjects older than 50 in the analysis. Multiple WHERE conditions must be separated by a comma and are logically connected with the & operator. For example, the WHERE condition age > 50 , bmi >= 22 will include the subjects older than 50 AND with bmi >= 22. Values in the MODEL\_TYPE column must match with the MODEL\_TYPE column in the **Model Types** sheet. The TIME column is only required when survival models are run. This column can contain a single time variable or two time variables separated by a space. The GROUP column is only required when conditional logistic regression models are run. This column can contain only a single variable that defines the groups (sets, strata). This sheet is not required when running in interactive mode, but is required when running in batch mode.

# Model\_Types

A table where each row specifies an option and has columns MODEL\_TYPE, FUNCTION, OPTION, and VALUE. For an example sheet and additional information about this sheet, see the Excel file

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/extdata/cometsInput.xlsx. This sheet is optional, but is required when the **Models** sheet contains the column MODEL\_TYPE.

## Value

a list comprising of data and information needed for getModelData.

# **Examples**

```
dir <- system.file("extdata", package="RcometsAnalytics", mustWork=TRUE)
csvfile <- file.path(dir, "cometsInputAge.xlsx")
exmetabdata <- readCOMETSinput(csvfile)</pre>
```

runAllMeta This function allows users to run meta-analyses on all models or a subset of models

## **Description**

This function allows users to run meta-analyses on all models or a subset of models

## Usage

```
runAllMeta(filesFolders, out.dir, opfile = NULL)
```

# Arguments

filesFolders	Character vector of files and/or folders that contain the output files from runAllModels.
	Valid file extensions are ".xlsx", ".rda", ".zip", ".tar", and ".tar.gz". Zip and tar
	files must contain files with extensions ".xlsx" or ".rda". See details.
out.dir	Output directory to save the results for each model.
opfile	Excel file containing the models and options. See meta_opfile. The default is NULL.

## **Details**

```
The names of the files output from runAllModels will be of the form <model name>__<cohort name>__<date>.xlsx or <model name>__<cohort name>__<date>.rda.
```

These output files from runAllModels can be bundled together into zip or tar files. There is no file name requirement for the zip and tar files.

The steps used to obtain the initial set of files to include in the meta-analyses are:

- 1. Recursively list all files found in any folder of filesFolders.
- 2. Unzip or untar any zip or tar file.
- 3. Remove files that do not have a file name of the forms above.

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runAllModels	This function allows users to run all models that are provided in the "Models" sheet of the input Excel file.

# **Description**

This function allows users to run all models that are provided in the "Models" sheet of the input Excel file.

# Usage

```
runAllModels(readData, cohortLabel = "", writeTofile = TRUE)
```

# **Arguments**

readData list from readCOMETSinput

cohortLabel cohort label (e.g. DPP, NCI, Shanghai)

writeTofile TRUE/FALSE (whether or not to write results for each model into separate xlsx

files). Files are written to current directory. Default is TRUE.

#### Value

A list of return objects from runModel or runCorr. The ith element in this list is the output from the ith model run.

# **Examples**

```
## Not run:
dir <- system.file("extdata", package="RcometsAnalytics", mustWork=TRUE)
csvfile <- file.path(dir, "cometsInputAge.xlsx")
exmetabdata <- readCOMETSinput(csvfile)
allmodeloutput <- runAllModels(exmetabdata)
## End(Not run)</pre>
```

runCorr

Calculate correlations for input model.

# Description

Calculate correlations for input model.

# Usage

```
runCorr(modeldata, metabdata, cohort = "")
```

# **Arguments**

modeldata list from function getModelData

metabdata metabolite data list from readCOMETSinput cohort cohort label (e.g DPP, NCI, Shanghai)

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#### **Details**

This function is a special case of runModel with the option op\$model = "correlation", however for backwards compatibility, it returns a data frame as in the original version of the **COMETS** R package.

## Value

data frame with each row representing the correlation for each combination of outcomes and exposures represented as specified in the model (\*spec), label (\*lab), and universal id (\*\_uid) with additional columns for n, pvalue, method of model specification (Interactive or Batch), universal id for outcomes (outcome\_uid) and exposures (exposure\_uid) name of the cohort, adjustment (adjvars) and stratification (stratavar,strata) variables. Attribute of dataframe includes ptime for processing time of model run.

# **Examples**

```
dir <- system.file("extdata", package="RcometsAnalytics", mustWork=TRUE)
csvfile <- file.path(dir, "cometsInputAge.xlsx")
exmetabdata <- readCOMETSinput(csvfile)
modeldata <- getModelData(exmetabdata,exposures="age",modlabel="1 Age",
outcomes=c("lactose","lactate"), modelspec="Interactive")
corrmatrix <- runCorr(modeldata,exmetabdata, "DPP")</pre>
```

runDescrip

This function provides a description of the input data (for categorical data, the number of samples of each type; for continous data, the median and other statistics for each variable)

# **Description**

This function provides a description of the input data (for categorical data, the number of samples of each type; for continous data, the median and other statistics for each variable)

# Usage

```
runDescrip(readData)
```

# **Arguments**

readData list from readComets

## Value

a list with 2 data frames, continuous and categorical summaries. Type of variable is defined in varmap

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#### **Examples**

```
## Not run:
dir <- system.file("extdata", package="RcometsAnalytics", mustWork=TRUE)
csvfile <- file.path(dir, "cometsInputAge.xlsx")
exmetabdata <- readCOMETSinput(csvfile)
allmodeloutput <- runAllModels(exmetabdata)
# Get descriptive data
descdata <-runDescrip(exmetabdata)
OutputXLSResults(filename="corr",datal=descdata,cohort="DPP")
## End(Not run)</pre>
```

runMeta

This function allows users to run a single meta-analysis

## **Description**

This function allows users to run a single meta-analysis

# Usage

```
runMeta(file.obj, op = NULL)
```

# **Arguments**

file.obj

Character vector of file names or a list, where each element of the list is a file name or a list of type file.list. The files can be output files from runModel or runAllModels. If all the files are from runModel or runAllModels, file.obj can be a vector. A list is required if any of the files are not from runModel and runAllModels, or if any of the files requires changes.

ор

A list containing the options to use. See meta\_options. The default is NULL.

#### Value

List of data frames containing the results and information. See metaOutputColumns for of a description of columns in the results table.

runModel

Main function for running the models

# **Description**

Main function for running the models

# Usage

```
runModel(
  modeldata,
  metabdata,
  cohortLabel = "",
  op = NULL,
  writeTofile = FALSE
```

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## **Arguments**

modeldata list from function getModelData

metabdata metabolite data list from readCOMETSinput cohortLabel cohort label (e.g DPP, NCI, Shanghai)

op list of options when running in Interactive mode (see options).

writeTofile TRUE/FALSE (whether or not to write results to the current directory). Default

is FALSE.

## **Details**

This function will check for stratification variables, and if present run within each stratum. The design matrix is checked for validity (see options). When running in Batch mode, the options are obtained from the Options sheet in the excel file.

#### Value

A list of objects with names ModelSummary, Effects, Errors\_Warnings, Table1, Info.

Important: check the adjvars.removed column in the ModelSummary data frame to see if any adjustment variables were dropped from the model, and use caution interpreting results when variables are removed. The Errors\_Warnings object may also contain additional variables removed. Attribute of this list includes ptime for processing time of model run.

# **Examples**

```
dir <- system.file("extdata", package="RcometsAnalytics", mustWork=TRUE)
csvfile <- file.path(dir, "cometsInputAge.xlsx")
exmetabdata <- readCOMETSinput(csvfile)
modeldata <- getModelData(exmetabdata,exposures="age",modlabel="1 Age",
outcomes=c("lactose","lactate"))
obj <- runModel(modeldata,exmetabdata, cohortLabel="DPP")</pre>
```

showCorr

Function that returns top N lines of the runCorr output

## **Description**

Function that returns top N lines of the runCorr output

## Usage

```
showCorr(corr, nlines = 50)
```

# Arguments

corr returned object from runCorr

nlines number of lines to return (default 50)

# Value

first 50 lines of output

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#### **Examples**

```
dir <- system.file("extdata", package="RcometsAnalytics", mustWork=TRUE)
csvfile <- file.path(dir, "cometsInputAge.xlsx")
exmetabdata <- readCOMETSinput(csvfile)
modeldata <- getModelData(exmetabdata,modlabel="1 Age")
corrmatrix <- runCorr(modeldata,exmetabdata,"DPP")
showCorr(corrmatrix)</pre>
```

showHClust

Show interactive heatmap using heatmaply\_cor with hierarchical clustering

# **Description**

This function outputs a heatmap with hierarchical clustering. It thus requires you to have at least 2 outcome and 2 exposure variables in your models.

# Usage

```
showHClust(
  ccorrList,
  strata = NULL,
  clust = TRUE,
  colscale = "RdYlBu",
  showticklabels = TRUE
)
```

# **Arguments**

ccorrList correlation object (output of runCorr)

Strata Only valid if ccorrList is from a stratified analysis. If NULL, then results from

the first stratum will be used in the plot.

clust TRUE or FALSE to show hierarchical clustering. The default is TRUE.

colscale colorscale, can be custom or named ("Hots", "Greens", "Blues", "Greys", "Purples")

see RColorBrewer\_colors

showticklabels TRUE or FALSE to show axis labels. The default is TRUE.

## Value

a heatmap with outcomes as rows and exposures in columns.

#### References

For colorscale reference: RColorBrewer\_colors

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# **Examples**

```
dir <- system.file("extdata", package="RcometsAnalytics", mustWork=TRUE)
csvfile <- file.path(dir, "cometsInputAge.xlsx")
exmetabdata <- readCOMETSinput(csvfile)
modeldata <- getModelData(exmetabdata, modelspec="Interactive",
exposures=c("age","bmi_grp"))
corrmatrix <-runCorr(modeldata,exmetabdata,"DPP")
#showHClust(corrmatrix)</pre>
```

showHeatmap

Show interactive heatmap using plot\_ly

# **Description**

Show interactive heatmap using plot\_ly

# Usage

```
showHeatmap(
  ccorrList,
  strata = NULL,
  rowsortby = "estimate",
  plothgt = 700,
  plotwid = 800,
  colscale = "RdYlBu"
)
```

# **Arguments**

ccorrList	correlation object (output of runCorr)
strata	Only valid if ccorrList is from a stratified analysis. If NULL, then results from the first stratum will be used in the plot.
rowsortby	How row labels are sorted
plothgt	Plot height default 700
plotwid	Plot width default 800
colscale	<pre>colorscale, can be custom or named ("Hots", "Greens", "Blues", "Greys", "Purples") see https://plot.ly/ipython-notebooks/color-scales/</pre>

# Value

a heatmap with outcomes as rows and exposures in columns.

# References

For colorscale reference: https://plot.ly/ipython-notebooks/color-scales/

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#### **Examples**

```
## Not run:
dir <- system.file("extdata", package="RcometsAnalytics", mustWork=TRUE)
csvfile <- file.path(dir, "cometsInputAge.xlsx")
exmetabdata <- readCOMETSinput(csvfile)
modeldata <- getModelData(exmetabdata,modlabel="1 Age")
corrmatrix <-runCorr(modeldata,exmetabdata,"DPP")
showHeatmap(corrmatrix)
## End(Not run)</pre>
```

showModel

Function that displays the first N rows of each data frame in the the runModel output.

## **Description**

Function that displays the first N rows of each data frame in the the runModel output.

# Usage

```
showModel(obj, nlines = 10)
```

# **Arguments**

obj returned object from runModel
nlines number of lines to display (default 10)

## **Examples**

```
dir      <- system.file("extdata", package="RcometsAnalytics", mustWork=TRUE)
csvfile      <- file.path(dir, "cometsInputAge.xlsx")
exmetabdata <- readCOMETSinput(csvfile)
modeldata      <- getModelData(exmetabdata,modlabel="1 Age")
result            <- runModel(modeldata,exmetabdata, cohortLabel="DPP")
showModel(result)</pre>
```

Table1

Non-metabolite Variable Summary Table

# **Description**

Columns in Table1. Depending on the model run and options specified, all the below names may not appear in the data frame.

- · category Category for categorical variables only
- in.model How variable enters the model (outcome, exposure, adjustment, time, group, weight, offset)
- max Maximum value

Table1

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- mean Mean value
- median Median value
- min Minimum value
- n Number of non-missing observations
- n.missing Number of missing observations
- n.outcomeEqual0 Number of non-missing observations with outcome = 0
- n.outcomeEqual1 Number of non-missing observations with outcome = 1
- n.unique Number of unique non-missing observations
- quartile1 25th percentile
- quartile3 75th percentile
- stratavar Stratum variable(s)
- strata Stratum level(s)
- type Either continuous or categorical
- variable Variable name in the model

## **Details**

The columns max, mean, median, min, n.missing, n.unique, quartile1, and quartile3 are for continuous variables only.

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