Package: MetaboAnalystR (via r-universe)

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Title An R Package for Comprehensive Analysis of Metabolomics Data

Version 4.0.0

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BugReports https://github.com/xia-lab/MetaboAnalystR/issues

Description This package contains the R functions and libraries underlying the popular MetaboAnalyst web server, including 500 functions for data processing, normalization, statistical analysis, metabolite set enrichment analysis, metabolic pathway analysis, and biomarker analysis. The package is synchronized with the web server. After installing and loading the package, users will be able to reproduce the same results from their local computers using the corresponding R command history downloaded from MetaboAnalyst, to achieve maximum flexibility and reproducibility.

Depends R (>= 4.0), methods

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Encoding UTF-8

RoxygenNote 7.2.3

Imports RBGL, RColorBrewer, RSQLite, Cairo, Rcpp (>= 1.0.5), ggplot2, BiocParallel, progress, Rserve, rlang, jsonlite, plyr, purrr, data.table, vctrs, qs, pROC, caret, crmn, dplyr, edgeR, fgsea, glasso, gplots, igraph, impute, pcaMethods, plotly, scales, MSnbase, tibble, siggenes, lattice, MASS

Suggests graph, htmltools, pls, ellipse, scatterplot3d, randomForest, caTools, e1071, som, RJSONIO, rjson, ROCR, globaltest, GlobalAncova, Rgraphviz, preprocessCore, genefilter, pheatmap, sva, limma, fitdistrplus, lars, Hmisc, magrittr, xtable, KEGGgraph, metap, entropy, rsm, httr, knitr, rmarkdown, devtools, testthat, visNetwork, ggraph, RSclient, car, gdata, huge, ppcor, ctc, OptiLCMS

VignetteBuilder knitr

LinkingTo Rcpp

Config/pak/sysreqs libcairo2-dev libglpk-dev make libicu-dev libxml2-dev libnetcdf-dev libssl-dev

Repository https://mojaveazure.r-universe.dev

RemoteUrl https://github.com/xia-lab/MetaboAnalystR

RemoteRef HEAD

RemoteSha a2a0e4877fd94c613544e8302de5a28645480c93

Contents

.do.CVTest.LRmodel *Calculate ROC performance with CV An internal function called by PerformCV.test*

Description

Calculate ROC performance with CV

Usage

```
.do.CVTest.LRmodel(data.in, fmla.in, kfold = 10, run.stepwise = FALSE)
```

Arguments

data.in	Input matrix of data
fmla.in	Input for generalized linear model
kfold	Numeric
run.stepwise	Logistic Regression

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

.get.my.lib *Read RDS files from the internet*

Description

Function downloads the required file and reads it only if not already in working directory. Need to specify the file URL and the destfile.

Usage

```
.get.my.lib(filenm, sub.dir = NULL)
```

Arguments

filenm	Input the name of the file to download
sub.dir	sub.dir

.readDataTable *Read data table*

Description

Function to read in a data table. First, it will try to use fread, however, it has issues with some windows 10 files. In such case, use the slower read.table method.

Usage

```
.readDataTable(fileName, save.copy = TRUE)
```

Arguments

fileName	Input filename

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

AddErrMsg *Adds an error message*

Description

The error message will be printed in all cases. Used in higher functions.

Usage

```
AddErrMsg(msg)
```

Arguments

msg	Error message to print

`analyze.lipids` *Lipid analysis pipeliner*

Description

Lipid analysis pipeliner

Usage

```
analyze.lipids(inFile, iso = "y")
```

Arguments

`inFile`	Input the file to read in
`iso`	Default is set to "y"

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`ANOVA.Anal` *Perform ANOVA analysis*

Description

ANOVA analysis

Usage

```
ANOVA.Anal(mSetObj=NA, nonpar=FALSE, thresh=0.05, all_results=FALSE)
```

Arguments

`mSetObj`	Input the name of the created mSetObj (see InitDataObjects)
`nonpar`	Logical, use a non-parametric test (T) or not (F)
`thresh`	Numeric, from 0 to 1, indicate the p-value threshold
`all_results`	Logical, if TRUE, it will output the ANOVA results for all compounds

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

ANOVA2.Anal *Perform Two-way ANOVA*

Description

Perform Two-way ANOVA

Usage

```
ANOVA2.Anal(mSetObj=NA, thresh=0.05, p.cor="fdr",
type="time0")
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
thresh	Input the p-value threshold
p.cor	Select method for p-value correction, bonferroni, holm or fdr
type	Select b to perform between-subjects ANOVA, and w for within-subjects ANOVA

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

aof *ANOVA*

Description

Perform anova and only return p values and MSres (for Fisher's LSD)

Usage

```
aof(x, cls)
```

Arguments

x	Input the data to perform ANOVA
cls	Input class labels

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

aov.1wayrep *Perform Two-way ANOVA*

Description

Perform Two-way ANOVA Perform repeated measure one-way anova

Usage

```
aov.1wayrep(x)
```

Arguments

x	Input the data
time.fac	Input the time factor

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

aov.2way *Perform Two-way ANOVA*

Description

Perform Two-way ANOVA Perform two-way anova

Usage

```
aov.2way(x)
```

Arguments

x	Input data to perform 2-way ANOVA

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

aov.mixed *Perform Two-way ANOVA*

Description

Perform Two-way ANOVA Perform within-subjects anova

Usage

```
aov.mixed(x)
```

Arguments

x	Input the data
time.fac	Input the time factor

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

ASCAfun.res *Function to perform ASCA*

Description

Perform ASCA

Usage

```
ASCAfun.res(X, Fac)
```

Arguments

X	Input list of compounds
Fac	Numeric McGill University, Canada License: GNU GPL (>= 2)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca>

ASCAfun1 *Function to perform ASCA Adapted from online R script with performance tuning*

Description

Perform ASCA

Usage

```
ASCAfun1(X, Design, Fac)
```

Arguments

X	Numeric, number of compounds
Design	Number of levels in the factor
Fac	Numeric, the factor

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

ASCAfun2 *Function to perform ASCA*

Description

Perform ASCA

Usage

```
ASCAfun2(X, Desa, Desb, Fac)
```

Arguments

X	Numeric, number of compounds
Desa	Number of levels in the factor TIME
Desb	Number of levels in the other factor
Fac	Numeric, the factor

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

calculateConcISO *Calculate Concentration ISO*

Description

Assuming independent random distribution of FA, the most probable frequency will be the product of the each component. Note: the data is concentration, we need to get frequncies - percentage w.r.t the total nmol. the result is the saved as separate files for each lipid class data for each FA class, first col is sample name

Usage

```
calculateConcISO(dat, cls.name, cls.num, min.file, prob.file)
```

Arguments

dat	Input the data
cls.name	Input the class names
cls.num	Input the number of classes
min.file	Input the min file
prob.file	Input the prob file

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CalculateFeatureRanking *Calculates feature importance*

Description

Perform calculation of feature importance (AUC, p value, fold change)

Usage

```
CalculateFeatureRanking(mSetObj=NA, clust.num=5)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
clust.num	Numeric, input the number of clusters for cluster-analysis

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CalculateGlobalTestScore *Quantitative enrichment analysis with globaltest*

Description

Various enrichment analysis algorithms

Usage

```
CalculateGlobalTestScore(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CalculateHyperScore *Over-representation analysis using hypergeometric tests*

Description

Over-representation analysis using hypergeometric tests The probability is calculated from obtaining equal or higher number of hits using 1-phyper. Since phyper is a cumulative probability, to get P(X>=hit.num) => P(X>(hit.num-1))

Usage

```
CalculateHyperScore(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CalculateImpVarCutoff *Calculate the Important Variable Cutoff*

Description

This function calculates the all important features based on a specfic cutoff.

Usage

```
CalculateImpVarCutoff(mSetObj, spe.thresh, lev.thresh)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
spe.thresh	alpha threshold, less is better, default less than 5 percentile based chi-square note: spe and leverage are vectors, not a single value, but a list to store the result note: the last model is Model.res, no spe Calculate leverage cutoff based on permutation Calculate the reference distribution of leverages note: leverage.perm is a list with each member in a 3 column matrix
lev.thresh	leverage threshold, the higher better, default more than 95 percentile of permuted leverage

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CalculateOraScore *Calculate ORA score*

Description

Calculate the over representation analysis score

Usage

```
CalculateOraScore(mSetObj=NA, nodeImp, method)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
nodeImp	Indicate the pathway topology analysis, "rbc" for relative-betweeness centrality, and "dgr" for out-degree centrality.
method	is "fisher" or "hyperg"

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CalculatePairwiseDiff *Calculate Pairwise Differences*

Description

Mat are log normalized, diff will be ratio. Used in higher functions.

Usage

```
CalculatePairwiseDiff(mat)
```

Arguments

mat	Input matrix of data to calculate pair-wise differences.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CalculateQeaScore *Calculate quantitative enrichment score*

Description

Calculate quantitative enrichment score

Usage

```
CalculateQeaScore(mSetObj=NA, nodeImp, method)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
nodeImp	Indicate the pathway topology analysis, "rbc" for relative-betweeness centrality, and "dgr" for out-degree centrality.
method	Indicate the pathway enrichment analysis, global test is "gt" and global ancova is "ga".

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CalculateSSP *Single sample profiling to compare with*

Description

reference concentrations stored in the library

Usage

```
CalculateSSP(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CentroidCheck *CentroidCheck*

Description

CentroidCheck function used to check centroid or not

Usage

```
CentroidCheck(filename)
```

Arguments

filename	filename to check

Author(s)

Zhiqiang Pang

CheckMetaDataConsistency *Check if data are ready for meta-analysis*

Description

This function determines if all annotated data are ready for meta-analysis

Usage

```
CheckMetaDataConsistency(mSetObj = NA, combat = TRUE)
```

Arguments

mSetObj	Input name of the created mSet Object
combat	Adjust for batch effects, logical variable: TRUE = adjust for batch effects using an empirical Bayes framework (R package sva), FALSE = no batch effect adjustment.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CleanData *Perform data cleaning*

Description

Cleans data and removes -Inf, Inf, NA, negative and 0s.

Usage

```
CleanData(bdata, removeNA = T, removeNeg = T, removeConst = T)
```

Arguments

bdata	Input data to clean
removeNA	Logical, T to remove NAs, F to not.
removeNeg	Logical, T to remove negative numbers, F to not.
removeConst	Logical, T to remove samples/features with 0s, F to not.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CleanDataMatrix *Clean the data matrix*

Description

Function used in higher functinos to clean data matrix

Usage

```
CleanDataMatrix(ndata)
```

Arguments

ndata	Input the data to be cleaned

CleanNumber *Replace infinite numbers*

Description

Replace -Inf, Inf to 99999 and -99999

Usage

```
CleanNumber(bdata)
```

Arguments

bdata	Input matrix to clean numbers

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

ClearStrings *Remove spaces*

Description

Remove from, within, leading and trailing spaces

Usage

```
ClearStrings(query)
```

Arguments

query	Input the query to clear

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

ComputeAverageCurve *Compute average ROC curve*

Description

Compute the average ROC curve

Usage

```
ComputeAverageCurve(perf, avg.method)
```

Arguments

perf	Input the average
avg.method	Input the name of the method to compute the average curve

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

computeConc *Lipid analysis*

Description

The upper limit for each combination is considered to be the minimal of the fatty acid concentration (nmol fatty acid/gram of sample) X is the lopomics data obtained above the result is the saved as separate files for each lipid class

Usage

```
computeConc(X, iso = "y")
```

Arguments

X	Input the data
iso	Default is set to "y"

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

ComputeHighLow *Compute the 95 percent interval for threshold ROC*

Description

Computes the 95 percent interval only for the y-axis. Utility function, called upon by higher functions

Usage

```
ComputeHighLow(perf)
```

Arguments

perf	Input the performance

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`ContainMissing` *Check for missing data*

Description

ContainMissing is used to check if any missing data exists in the uploaded file.

Usage

```
ContainMissing(mSetObj=NA)
```

Arguments

`mSetObj`	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`Convert2AnalObject` *Convert2AnalObject This function is used to convert mSet object from raw spectra processing for the following analysis.*

Description

Convert2AnalObject This function is used to convert mSet object from raw spectra processing for the following analysis.

Usage

```
Convert2AnalObject(mSet, data.type, anal.type, paired = FALSE)
```

Arguments

`mSet`	mSet from raw spectral processing pipeline, OptiLCMS
`data.type`	data type, should be 'spec'
`anal.type`	analysis type, should be 'raw'
`paired`	data is paired or not, use FALSE by default

Convert2Mummichog *Convert mSetObj to proper format for MS Peaks to Pathways module*

Description

Following t-test analysis or effect size calculation, this functions converts the results from the mSetObj to the proper format for mummichog analysis.

Usage

```
Convert2Mummichog(
  mSetObj = NA,
  rt = FALSE,
  rds.file = FALSE,
  rt.type = "seconds",
  test = "tt",
  mode = NA
)
```

Arguments

mSetObj	Input the name of the created mSetObj.
rt	Logical, whether or not to include retention time information.
rds.file	Logical, if true, the "annotated_peaklist.rds" must be in the current working directory to get corresponding retention time information for the features. If not, the retention time information will be taken from the feature names. Feature names must be formatted so that the mz and retention time for a single peak is separated by two underscores. For instance, m/z of 410.2148 and retention time of 42.46914 seconds must be formatted as 410.2148__42.46914.
rt.type	Character, input whether retention time is in seconds (default as RT using MetaboAnalystR is seconds) or minutes (as from MZmine).
test	Character, input what statistical values to include in the mummichog input. For p-values and t-scores only from t-test, use "tt". For log2FC from the fold-change analsis, use "fc". For effect-sizes, use "es". For, p-values, fold-changes and effect sizes, use "all". For multiple groups, use 'aov'.
mode	ion mode, positive or negative

Author(s)

Jasmine Chong, Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`Convert2MummichogMetaPath` *Convert mSetObj to proper format for MS Peaks to Pathways module*

Description

Following t-test analysis or effect size calculation, this functions converts the results from the mSetObj to the proper format for mummichog analysis.

Usage

```
Convert2MummichogMetaPath(
  mSetObj = NA,
  rt = FALSE,
  rds.file = FALSE,
  rt.type = "seconds",
  test = "tt",
  mode = NA
)
```

Arguments

`mSetObj`	Input the name of the created mSetObj.
`rt`	Logical, whether or not to include retention time information.
`rds.file`	Logical, if true, the "annotated_peaklist.rds" must be in the current working directory to get corresponding retention time information for the features. If not, the retention time information will be taken from the feature names. Feature names must be formatted so that the mz and retention time for a single peak is separated by two underscores. For instance, m/z of 410.2148 and retention time of 42.46914 seconds must be formatted as 410.2148__42.46914.
`rt.type`	Character, input whether retention time is in seconds (default as RT using MetaboAnalystR is seconds) or minutes (as from MZmine).
`test`	Character, input what statistical values to include in the mummichog input. For p-values and t-scores only from t-test, use "tt". For log2FC from the fold-change analsis, use "fc". For effect-sizes, use "es". For, p-values, fold-changes and effect sizes, use "all".
`mode`	ion mode, positive or negative

Author(s)

Jasmine Chong, Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`CovariateScatter.Anal` *CovariateScatter.Anal*

Description

CovariateScatter.Anal

Usage

```
CovariateScatter.Anal(
  mSetObj,
  imgName = "NA",
  format = "png",
  analysis.var,
  ref = NULL,
  block = "NA",
  thresh = 0.05,
  pval.type = "fdr",
  contrast.cls = "anova"
)
```

Arguments

`mSetObj`	mSetObj object
`imgName`	image name
`format`	image format
`analysis.var`	variable of analysis
`ref`	reference group
`block`	block name
`thresh`	threshold
`pval.type`	pvalue type (raw or fdr)
`contrast.cls`	contrast group

`CreateAnalNullMsg` *Create null message for analysis Creates a message for the Sweave report*

Description

Creates a message stating that no analyses were performed on your data.

Usage

```
CreateAnalNullMsg()
```

CreateANOVAdoc *Create report of analyses*

Description

Report generation using Sweave Create ANOVA document

Usage

```
CreateANOVAdoc(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateAOV2doc *Create report of analyses*

Description

Report generation using Sweave ANOVA

Usage

```
CreateAOV2doc(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateASCAdoc *Create report of analyses*

Description

Report generation using Sweave Random Forest ASCA

Usage

```
CreateASCAdoc(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateBiomarkerInputDoc *Create biomarker analysis report: Data Input*

Description

Report generation using Sweave Power analysis report, data input documentation.

Usage

```
CreateBiomarkerInputDoc(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

`CreateBiomarkerIntr` *Create biomarker analysis report: Introduction*

Description

Report generation using Sweave Biomarker analysis report introduction

Usage

```
CreateBiomarkerIntr()
```

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

`CreateBiomarkerOverview` *Create biomarker analysis report: Overview*

Description

Report generation using Sweave Power analysis report overview

Usage

```
CreateBiomarkerOverview()
```

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

`CreateBiomarkerRatioOverview` *Create biomarker analysis report: Normalization, ratio*

Description

Report generation using Sweave Biomarker analysis, ratio option

Usage

```
CreateBiomarkerRatioOverview(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

CreateBiomarkerRnwReport *Create report of analyses (Biomarker)*

Description

Report generation using Sweave Puts together the analysis report

Usage

```
CreateBiomarkerRnwReport(mSetObj, usrName)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
usrName	Input the name of the user

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

CreateCorAnalysis *Create report of analyses*

Description

Report generation using Sweave Correlation and Partial Correlation Analysis

Usage

```
CreateCorAnalysis(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jessica Ewald <jessica.ewald@mail.mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateCorHeatmap *Create report of analyses*

Description

Report generation using Sweave For Correlation Heatmap

Usage

```
CreateCorHeatmap(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jessica Ewald <jessica.ewald@mail.mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateCorrDoc *Create report of analyses*

Description

Report generation using Sweave Create correlation document

Usage

```
CreateCorrDoc(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateCovAdj *Create report of analyses*

Description

Report generation using Sweave Covariate Adjustment

Usage

```
CreateCovAdj(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jessica Ewald <jessica.ewald@mail.mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

createCVset *Separate data set using k-fold cross validation (CV)*

Description

Separate data set with k-fold CV, used in higher function

Usage

```
createCVset(groupN, kfold, rseed)
```

Arguments

groupN	Input the size of the group
kfold	Input the number of cross-validations
rseed	Input the random seed

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateEBAMdoc *Create report of analyses*

Description

Report generation using Sweave Create EBAM document Note: the search for delta (SAM) and a0 (EBAM) will not be plotted it is only exploration, and may cause potential inconsistentcies.

Usage

```
CreateEBAMdoc(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateEnrichAnalDoc *Create report of analyses (Met Enrichment)*

Description

Report generation using Sweave Metabolite enrichment analysis report, analysis

Usage

```
CreateEnrichAnalDoc()
```

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateEnrichInputDoc *Create report of analyses (Met Enrichment)*

Description

Report generation using Sweave Metabolite enrichment analysis report data input

Usage

```
CreateEnrichInputDoc(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateEnrichIntr *Create report of analyses (Met Enrichment)*

Description

Report generation using Sweave Metabolite enrichment analysis report introduction

Usage

```
CreateEnrichIntr()
```

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateEnrichORAdoc *Create report of analyses (Met Enrichment)*

Description

Report generation using Sweave Metabolite enrichment analysis report, over representation analysis (ORA)

Usage

```
CreateEnrichORAdoc(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateEnrichOverview *Create report of analyses (Met Enrichment)*

Description

Report generation using Sweave Metabolite enrichment analysis report overview

Usage

```
CreateEnrichOverview()
```

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateEnrichProcessDoc *Create report of analyses (Met Enrichment)*

Description

Report generation using Sweave Metabolite enrichment analysis report enrichment process

Usage

```
CreateEnrichProcessDoc(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateEnrichQEAdoc *Create report of analyses (Met Enrichment)*

Description

Report generation using Sweave Metabolite enrichment analysis report Quantitative enrichment analysis

Usage

```
CreateEnrichQEAdoc(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateEnrichRnwReport *Create report of analyses (Met Enrichment)*

Description

Report generation using Sweave Metabolite enrichment analysis report

Usage

```
CreateEnrichRnwReport(mSetObj, usrName)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
usrName	Input the name of the user

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateEnrichSSPdoc *Create report of analyses (Met Enrichment)*

Description

Report generation using Sweave Metabolite enrichment analysis report Single sampling profiling

Usage

```
CreateEnrichSSPdoc(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateFooter *Create report of analyses (Met Enrichment)*

Description

Report generation using Sweave Metabolite enrichment analysis report footer

Usage

```
CreateFooter()
```

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateGraph *Create igraph from the edgelist saved from graph DB and decompose into subnets*

Description

Function for the network explorer module, prepares user's data for network exploration.

Usage

```
CreateGraph(mSetObj = NA)
```

Arguments

mSetObj	Input name of the created mSet Object

CreateGSEAAnalTable *Create Mummichog report of analyses*

Description

Report generation using Sweave Function to create a summary table of mummichog analysis

Report generation using Sweave Function to create a summary table of mummichog analysis

Usage

```
CreateGSEAAnalTable(mSetObj = NA)
```

CreateGSEAAnalTable(mSetObj = NA)

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

CreateHCdoc *Create report of analyses*

Description

Report generation using Sweave Create hierarchical clustering document

Usage

```
CreateHCdoc(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateIntegMatchingTable *CreateIntegMatchingTable*

Description

CreateIntegMatchingTable

Usage

```
CreateIntegMatchingTable(mSetObj = NA)
```

Arguments

mSetObj	mSetObj Object

CreateIntegPathwayAnalysisRnwReport

Create report of analyses (IntegPathwayAnalysis)

Description

Report generation using Sweave Puts together the analysis report

Usage

```
CreateIntegPathwayAnalysisRnwReport(mSetObj, usrName)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
usrName	Input the name of the user

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

CreateIntegratedPathwayAnalInputDoc

Create integrated pathway report: Data Input

Description

Report generation using Sweave integrated pathway report, data input documentation.

Usage

```
CreateIntegratedPathwayAnalInputDoc(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jasmine Chong McGill University, viewingCanada License: GNU GPL (>= 2)

`CreateIntegratedPathwayAnalIntr` *Create integrated pathway analysis report: Introduction*

Description

Report generation using Sweave Integrated pathwayr analysis report introduction

Usage

```
CreateIntegratedPathwayAnalIntr()
```

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

`CreateIntegratedPathwayDoc` *Create integrated pathway analysis report*

Description

Report generation using Sweave Biomarker analysis report, ROC Curve Based Model Creation and Evaluation

Usage

```
CreateIntegratedPathwayDoc(mSetObj = NA)
```

Arguments

`mSetObj`	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

CreateIntegratedPathwayGeneMapTable

Create a x-table for gene name mapping

Description

Report generation using Sweave Function to create a table for gene name mapping

Usage

```
CreateIntegratedPathwayGeneMapTable(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

CreateIntegratedPathwayNameMapTable

Create a x-table for compound name mapping

Description

Report generation using Sweave Function to create a table for compound name mapping

Usage

```
CreateIntegratedPathwayNameMapTable(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

CreateIntegratedPathwayResultsTable *Create a x-table for pathway results*

Description

Report generation using Sweave Function to create a table for pathway results

Usage

```
CreateIntegratedPathwayResultsTable(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

CreateiPCAdoc *Create report of analyses*

Description

Report generation using Sweave For Interactive PCA

Usage

```
CreateiPCAdoc(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateKMdoc *Create report of analyses*

Description

Report generation using Sweave Create Kmeans partitional clustering document

Usage

```
CreateKMdoc(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateLadder *R-code for R-SVM*

Description

use leave-one-out / Nfold or bootstrape to permute data for external CV build SVM model and use mean-balanced weight to sort genes on training set and recursive elimination of least important genes

Usage

```
CreateLadder(Ntotal, Nmin = 5)
```

Arguments

Ntotal	Total number
Nmin	Minimum number, default set to 5

Author(s)

Dr. Xin Lu, Research Scientist Biostatistics Department, Harvard School of Public Health create a decreasing ladder for recursive feature elimination

CreateMappingResultTable *Creates the mapping result table*

Description

Creates the mapping result table

Usage

```
CreateMappingResultTable(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

CreateMBdoc *Create report of analyses*

Description

Report generation using Sweave Multivariate Bayes

Usage

```
CreateMBdoc(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateMetaAnalTable *Create Mummichog report of analyses*

Description

Report generation using Sweave Function to create a summary table of mummichog analysis

Report generation using Sweave Function to create a summary table of mummichog analysis

Usage

```
CreateMetaAnalTable(mSetObj = NA)
```


```
CreateMetaAnalTable(mSetObj = NA)
```


Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

CreateMetaAnalysisDEdoc *Create MetaAnalysis analysis report: Data Normalization*

Description

Report generation using Sweave Meta-Analysis, data normalization documentation.

Usage

```
CreateMetaAnalysisDEdoc(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

`CreateMetaAnalysisInputDoc`

Create MetaAnalysis analysis report: Data Input

Description

Report generation using Sweave Power analysis report, data input documentation.

Usage

```
CreateMetaAnalysisInputDoc(mSetObj = NA)
```

Arguments

`mSetObj`	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

`CreateMetaAnalysisIntr`

Create MetaAnalysis analysis report: Introduction

Description

Report generation using Sweave MetaAnalysis analysis report introduction

Usage

```
CreateMetaAnalysisIntr()
```

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

`CreateMetaAnalysisNORMdoc` *Create MetaAnalysis analysis report: Data Normalization*

Description

Report generation using Sweave Meta-Analysis, data normalization documentation.

Usage

```
CreateMetaAnalysisNORMdoc(mSetObj = NA)
```

Arguments

`mSetObj`	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

`CreateMetaAnalysisOutput` *Create MetaAnalysis analysis report: Data Normalization*

Description

Report generation using Sweave MetaAnalysis analysis, data normalization documentation.

Usage

```
CreateMetaAnalysisOutput(mSetObj = NA)
```

Arguments

`mSetObj`	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

`CreateMetaAnalysisOverview`
Create MetaAnalysis analysis report: Overview

Description

Report generation using Sweave Power analysis report overview

Usage

```
CreateMetaAnalysisOverview()
```

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

`CreateMetaAnalysisRnwReport`
Create report of analyses (Meta-Analysis)

Description

Report generation using Sweave Puts together the analysis report

Usage

```
CreateMetaAnalysisRnwReport(mSetObj, usrName)
```

Arguments

`mSetObj`	Input the name of the created mSetObj (see InitDataObjects)
`usrName`	Input the name of the user

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

CreateMetaMummichogInputDoc
Create analysis report: Functional Meta-Analysis Data Input

Description

Report generation using Sweave Mummichog analysis report, data input documentation.

Usage

```
CreateMetaMummichogInputDoc(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

CreateMetaMummichogIntro
Create analysis report: Functional Meta-Analysis Introduction

Description

Report generation using Sweave Mummichog analysis report introduction

Usage

```
CreateMetaMummichogIntro()
```

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

CreateMetaMummichogResults *Create analysis report: Functional Meta-Analysis Results*

Description

Report generation using Sweave Mummichog analysis report overview

Usage

```
CreateMetaMummichogResults(mSetObj)
```

Arguments

mSetObj	mSetObj

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

CreateMetaOverview *Create report of analyses*

Description

Report generation using Sweave For Metadata Overview

Usage

```
CreateMetaOverview(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jessica Ewald <jessica.ewald@mail.mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateMetaPathRnwReport *Create report of analyses (Biomarker)*

Description

Report generation using Sweave Puts together the analysis report

Usage

```
CreateMetaPathRnwReport(mSetObj, usrName)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
usrName	Input the name of the user

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

CreateMetaTable *Create MetaAnalysis table of results*

Description

Report generation using Sweave Function to create a table containing meta-analysis results.

Usage

```
CreateMetaTable(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

`CreateModelBiomarkersDoc`

Create biomarker analysis report: ROC Curve Based Model Creation and Evaluation

---

Description

Report generation using Sweave Biomarker analysis report, ROC Curve Based Model Creation and Evaluation

Usage

```
CreateModelBiomarkersDoc(mSetObj = NA)
```

Arguments

`mSetObj`	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

`CreateMultiBiomarkersDoc`

Create biomarker analysis report: Multivariate Biomarker Analysis

---

Description

Report generation using Sweave Biomarker analysis report, Multivariate Biomarker Analysis

Usage

```
CreateMultiBiomarkersDoc(mSetObj = NA)
```

Arguments

`mSetObj`	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

`CreateMummichogAnalTable`
Create Mummichog report of analyses

Description

Report generation using Sweave Function to create a summary table of mummichog analysis

Report generation using Sweave Function to create a summary table of mummichog analysis

Usage

```
CreateMummichogAnalTable(mSetObj = NA)
```


```
CreateMummichogAnalTable(mSetObj = NA)
```


Arguments

`mSetObj`	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

`CreateMummichogAnalysisDoc`
Create mummichog analysis report

Description

Report generation using Sweave Mummichog analysis report

Report generation using Sweave Mummichog analysis report

Usage

```
CreateMummichogAnalysisDoc(mSetObj = NA)
```


```
CreateMummichogAnalysisDoc(mSetObj = NA)
```


Arguments

`mSetObj`	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

CreateMummichogInputDoc

Create Mummichog analysis report: Data Input

Description

Report generation using Sweave Mummichog analysis report, data input documentation.

Report generation using Sweave Mummichog analysis report, data input documentation.

Usage

```
CreateMummichogInputDoc(mSetObj = NA)
```


```
CreateMummichogInputDoc(mSetObj = NA)
```


Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

CreateMummichogIntro *Create mummichog analysis report: Introduction*

Description

Report generation using Sweave Mummichog analysis report introduction

Report generation using Sweave Mummichog analysis report introduction

Usage

```
CreateMummichogIntro()
```


```
CreateMummichogIntro()
```


Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

CreateMummichogLibs *Create Mummichog Libraries from KEGG*

Description

Function to create mummichog libraries from MetaboAnalyst pathway libraries (metpa). Outputs the RDS files in the current working directory. RDS files are saved using the KEGG organism code.

Usage

```
CreateMummichogLibs(folder, kegg_compounds)
```

Arguments

folder	Input the path of the folder containing the metpa rda files.
kegg_compounds	Input the name of the KEGG dictionary containing the KEGG compound IDs, KEGG compopund names, and molecular weight.

CreateMummichogMetaAnalPathTable *Create analysis report: Functional Meta-Analysis Results Table*

Description

Report generation using Sweave Function to create a summary table of mummichog analysis

Usage

```
CreateMummichogMetaAnalPathTable(mSetObj)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

CreateMummichogMetaAnalReport

Create analysis report: Functional Meta-Analysis

Description

Report generation using Sweave Functional Meta-Analysis Report

Usage

```
CreateMummichogMetaAnalReport(mSetObj)
```

Arguments

mSetObj	mSetObj

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

CreateMummichogOverview

Create Mummichog analysis report: Overview

Description

Report generation using Sweave Mummichog analysis report overview

Report generation using Sweave Mummichog analysis report overview

Usage

```
CreateMummichogOverview()

CreateMummichogOverview()
```

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

CreateMummichogRnwReport

Create report of analyses (Biomarker)

Description

Report generation using Sweave Puts together the analysis report

Usage

```
CreateMummichogRnwReport(mSetObj, usrName)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
usrName	Input the name of the user

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

CreateNetworkExplorerDoc

Create integrated pathway analysis report

Description

Report generation using Sweave Biomarker analysis report, ROC Curve Based Model Creation and Evaluation

Usage

```
CreateNetworkExplorerDoc(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

CreateNetworkExplorerInputDoc

Create network explorer: Data Input

Description

Report generation using Sweave network explorer report, data input documentation.

Usage

```
CreateNetworkExplorerInputDoc(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jasmine Chong McGill University, viewingCanada License: GNU GPL (>= 2)

CreateNetworkExplorerIntr

Create integrated pathway analysis report: Introduction

Description

Report generation using Sweave Network explorer report introduction

Usage

```
CreateNetworkExplorerIntr()
```

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

CreateNetworkExplorerOverview
Create network explorer report: Overview

Description

Report generation using Sweave for the network explorer report overview

Usage

```
CreateNetworkExplorerOverview()
```

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

CreateNetworkExplorerRnwReport
Create report of analyses (Network Explorer)

Description

Report generation using Sweave Puts together the analysis report

Usage

```
CreateNetworkExplorerRnwReport(mSetObj, usrName)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
usrName	Input the name of the user

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

CreateNetworkGeneMapTable

Create a x-table for gene name mapping

Description

Report generation using Sweave Function to create a table for gene name mapping

Usage

```
CreateNetworkGeneMapTable(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

CreateNetworkNameMapTable

Create a x-table for compound name mapping

Description

Report generation using Sweave Function to create a table for compound name mapping

Usage

```
CreateNetworkNameMapTable(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

CreateNORMdoc *Create report of analyses*

Description

Report generation using Sweave Create normalization document

Usage

```
CreateNORMdoc(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateOPLSDAdoc *Create report of analyses*

Description

Report generation using Sweave Create OPLSDA document

Usage

```
CreateOPLSDAdoc(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreatePathAnalDoc *Create report of analyses (Met Pathway)*

Description

Report generation using Sweave Metabolomic pathway analysis Create pathway analysis doc

Usage

```
CreatePathAnalDoc(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreatePathInputDoc *Create report of analyses (Met Pathway)*

Description

Report generation using Sweave Metabolomic pathway analysis Create data input doc

Usage

```
CreatePathInputDoc()
```

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreatePathIntr *Create report of analyses (Met Pathway)*

Description

Report generation using Sweave Metabolomic pathway analysis Introduction

Usage

```
CreatePathIntr()
```

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreatePathProcessDoc *Create report of analyses (Met Pathway)*

Description

Report generation using Sweave Metabolomic pathway analysis Create MetPA process

Usage

```
CreatePathProcessDoc(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreatePathResultDoc *Create report of analyses (Met Pathway)*

Description

Report generation using Sweave Metabolomic pathway analysis Create MetPA results doc

Usage

```
CreatePathResultDoc(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreatePathRnwReport *Create report of analyses (Met Pathway)*

Description

Report generation using Sweave Metabolomic pathway analysis write .Rnw file template

Usage

```
CreatePathRnwReport(mSetObj, usrName)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
usrName	Input the name of the user

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`CreatePCAdoc` *Create report of analyses*

Description

Report generation using Sweave Create PCA document

Usage

```
CreatePCAdoc(mSetObj = NA)
```

Arguments

`mSetObj`	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`CreatePLSdoc` *Create report of analyses*

Description

Report generation using Sweave Create PLS document

Usage

```
CreatePLSdoc(mSetObj = NA)
```

Arguments

`mSetObj`	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreatePowerAnalDoc *Create power analysis report: Power Analysis*

Description

Report generation using Sweave Power analysis report, analysis

Usage

```
CreatePowerAnalDoc(mSetObj)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreatePowerInputDoc *Create power analysis report: Data Input*

Description

Report generation using Sweave Power analysis report, data input documentation.

Usage

```
CreatePowerInputDoc(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

CreatePowerIntr *Create power analysis report: Introduction*

Description

Report generation using Sweave Power analysis report introduction

Usage

```
CreatePowerIntr()
```

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

CreatePowerOverview *Create power analysis report: Overview*

Description

Report generation using Sweave Power analysis report overview

Usage

```
CreatePowerOverview()
```

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

CreatePowerParametersDoc *Create power analysis report: Power Parameter Selection*

Description

Report generation using Sweave Power analysis report, parameter selection

Usage

```
CreatePowerParametersDoc(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreatePowerRnwReport *Create report of analyses (Power)*

Description

Report generation using Sweave Put together the analysis report

Usage

```
CreatePowerRnwReport(mSetObj, usrName)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
usrName	Input the name of the user

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

CreateRandomForest *Create report of analyses*

Description

Report generation using Sweave Random Forest

Usage

```
CreateRandomForest(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jessica Ewald <jessica.ewald@mail.mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateRatioTable *Create report of analyses*

Description

Report generation using Sweave Function to create a summary table for biomarker analysis: included metabolite ratios

Usage

```
CreateRatioTable(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

CreateRawAnalysisRnwReport *Create report for raw spectra module*

Description

Report generation using Sweave Write .Rnw file template

Usage

```
CreateRawAnalysisRnwReport(mSetObj, usrName)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
usrName	Input the name of the user

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateRFdoc *Create report of analyses*

Description

Report generation using Sweave Create Random Forest document

Usage

```
CreateRFdoc(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateRHistAppendix *Create report of analyses*

Description

Report generation using Sweave Create footer

Usage

```
CreateRHistAppendix()
```

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateROCLabelsTable *Create a x-table for newly classified samples*

Description

Report generation using Sweave Function to create a table for newly classified samples

Usage

```
CreateROCLabelsTable(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

CreateSAMdoc *Create report of analyses*

Description

Report generation using Sweave Create SAM document

Usage

```
CreateSAMdoc(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateSemiTransColors *Create semitransparant colors*

Description

Create semitransparant colors for a given class label

Usage

```
CreateSemiTransColors(cls)
```

Arguments

cls	Input class labels

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateSOMdoc *Create report of analyses*

Description

Report generation using Sweave Create SOM partitional clustering document

Usage

```
CreateSOMdoc(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateSPLSDAdoc *Create report of analyses*

Description

Report generation using Sweave Create sPLS-DA document

Usage

```
CreateSPLSDAdoc(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateStatIntr *Create report of analyses*

Description

Report generation using Sweave Create header

Usage

```
CreateStatIntr()
```

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateStatIOdoc *Create report of analyses*

Description

Report generation using Sweave Read and process raw data

Usage

```
CreateStatIOdoc(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateStatRnwReport *Create report for statistical analysis module*

Description

Report generation using Sweave Write .Rnw file template

Usage

```
CreateStatRnwReport(mSetObj, usrName)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
usrName	Input the name of the user

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateSummaryTable *Create report of analyses*

Description

Report generation using Sweave Create a summary table for each type of uploaded data csv table has 5 col: sampleID, feature #, zero, missing #

Usage

```
CreateSummaryTable(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateSVMdoc *Create report of analyses*

Description

Report generation using Sweave Create R-SVM document

Usage

```
CreateSVMdoc(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`CreateTimeSeriesAnalNullMsg` *Create null analysis message for time-series sweave report*

Description

Creates empty time-series analysis message

Usage

```
CreateTimeSeriesAnalNullMsg()
```

`CreateTimeSeriesIOdoc` *Create report of analyses (Met Pathway)*

Description

Report generation using Sweave Metabolomic pathway analysis, time-series Read and process the raw data

Usage

```
CreateTimeSeriesIOdoc(mSetObj = NA)
```

Arguments

`mSetObj`	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateTimeSeriesRnwReport

Create report of analyses (Met Pathway)

Description

Report generation using Sweave Metabolomic pathway analysis Create timeseries .Rnw file template

Usage

```
CreateTimeSeriesRnwReport(mSetObj, usrName)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
usrName	Input the name of the user

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateUnivarBiomarkersDoc

Create power analysis report: Biomarker Univariate Analysis

Description

Report generation using Sweave Biomarker analysis report, Univariate Analysis

Usage

```
CreateUnivarBiomarkersDoc(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

CreateUNIVdoc *Create report of analyses*

Description

Report generation using Sweave Create univariate analyses document

Usage

```
CreateUNIVdoc(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

CreateUnivROCTable *Create summary table for univariate ROC analysis*

Description

Report generation using Sweave Function to create a summary table for univariate biomarker analysis

Usage

```
CreateUnivROCTable()
```

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

CreateVennMetaTable *Create MetaAnalysis table of results for Venn Diagram*

Description

Report generation using Sweave Function to create a table containing meta-analysis results.

Usage

```
CreateVennMetaTable(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

CrossReferencing *Various functions for mapping b/w names & database identifiers Given a list of compound names or ids, find matched name or ids from selected databases*

Description

Given a list of compound names or ids find matched name or IDs from selected databases

Usage

```
CrossReferencing(
  mSetObj = NA,
  q.type,
  hmdb = T,
  pubchem = T,
  chebi = F,
  kegg = T,
  metlin = F,
  lipid = F
)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects).
q.type	Input the query type, "name" for compound names, "hmdb" for HMDB IDs, "kegg" for KEGG IDs, "pubchem" for PubChem CIDs, "chebi" for ChEBI IDs, "metlin" for METLIN IDs, and "hmdb_kegg" for a both KEGG and HMDB IDs.
hmdb	Logical, T to cross reference to HMDB, F to not.
pubchem	Logical, T to cross reference to PubChem, F to not.
chebi	Logical, T to cross reference to CheBI, F to not.
kegg	Logical, T to cross reference to KEGG, F to not.
metlin	Logical, T to cross reference to MetLin, F to not.
lipid	Logical, if features are lipids (T), a different database will be used for compound matching.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

---

descendMin *Perform utilities for peak grouping*

Description

Perform various utilities for peak grouping

Usage

```
descendMin(y, istart = which.max(y))
```

Arguments

y	Input peaks
istart	Performs which.max on y

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

doCompoundMapping *Perform compound mapping*

Description

Perform compound mapping

Usage

```
doCompoundMapping(cmpd.vec, q.type)
```

Arguments

cmpd.vec	Input compound vector
q.type	Query type

doGeneIDMapping *Convert different gene IDs into entrez IDs for downstream analysis*

Description

Gene ID mapping, gene annotation, compound mapping, KEGG mapping

Usage

```
doGeneIDMapping(q.vec, org, type)
```

Arguments

q.vec	Input the query
org	Input the organism type
type	Input the type of data to annotate

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada

doKEGG2NameMapping *Perform KEGG to compound name mapping*

Description

Perform KEGG to compound name mapping

Usage

```
doKEGG2NameMapping(kegg.vec)
```

Arguments

kegg.vec	Input vector of KEGG compounds

doKOFiltering *Utility function*

Description

Returns matched KO in the same order (NA if no match)

Usage

```
doKOFiltering(ko.vec, type)
```

Arguments

ko.vec	Input the vector containing KOs
type	Input the type

doLogisticRegMdl *Develop a Logistic Regression Model with all of the combined k-fold CV subsets*

Description

Develop a Logistic Regression Model with all of the combined k-fold CV subsets

Usage

```
doLogisticRegMdl(x.train, y.train, x.test, y.test)
```

Arguments

x.train	Input the X training set
y.train	Input the Y training set
x.test	Input the X test set
y.test	Input the Y test set

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

EBAM.Init *For EBAM analysis*

Description

deteriming a0, only applicable for z.ebam (default)

Usage

```
EBAM.Init(
  mSetObj = NA,
  isPaired,
  isVarEq,
  nonPar,
  A0 = -99,
  delta,
  imgA0,
  imgSig,
  dpi = 72
)
```

Arguments

mSetObj	Input name of the created mSet Object
isPaired	Logical
isVarEq	Logical
nonPar	nonPar
A0	A0
delta	delta
imgA0	imgA0
imgSig	imgSig
dpi	dpi value of images

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

FC.Anal *Fold change analysis, unpaired*

Description

Perform fold change analysis, method can be mean or median

Usage

```
FC.Anal(mSetObj, fc.thresh=2, cmp.type = 0, paired=FALSE)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
fc.thresh	Fold-change threshold, numeric input
cmp.type	Comparison type, 0 for group 1 minus group 2, and 1 for group 1 minus group 2
paired	Logical, TRUE or FALSE

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

FeatureCorrelation *Pattern hunter*

Description

Calculate correlation of all other feature to a given feature name

Usage

```
FeatureCorrelation(mSetObj = NA, dist.name, varName)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
dist.name	Input the name of the distance measure
varName	Input the variable name

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

FilterVariable *Methods for non-specific filtering of variables*

Description

This is a function that filters the dataset, dependent on the user-specified method for filtering. The function applies a filtering method, ranks the variables within the dataset, and removes variables based on its rank. The final dataset should contain no more than than 5000 variables for effective computing.

Usage

```
FilterVariable(mSetObj=NA, filter, qcFilter, rsd)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
qc.filter	Filter the variables based on QC samples - True (T), or use non-QC based filtering - False (F).
rsd	Define the relative standard deviation cut-off. Variables with a RSD greater than this number will be removed from the dataset. It is only necessary to specify this argument if qc.filter is True (T). Otherwise, it will not be used in the function.
var.filter	Select the filter option, "rsd" which is the relative standard deviation, "nrsd" which is the non-parametric relative standard deviation, "mean" which is the mean, "sd" which is the standard deviation, "mad" which is the median absolute deviation, or "iqr" which is the interquantile range.
var.cutoff	var.cutoff value
int.filter	int.filter value
int.cutoff	int.cutoff value, numeric
filter.cutoff	percent to be filtered, for example, 5 (5%)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

findEqualGreaterM *Perform utilities for peak grouping*

Description

Perform various utilities for peak grouping

Usage

```
findEqualGreaterM(x, values)
```

Arguments

x	Input the data
values	Input the values

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

FisherLSD *Fisher for ANOVA*

Description

Perform Fisher LSD for ANOVA, used in higher function

Usage

```
FisherLSD(aov.obj, thresh)
```

Arguments

aov.obj	Input the anova object
thresh	Numeric, input the alpha threshold

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GeneratePeakList *GeneratePeakList*

Description

GeneratePeakList is used to generate the peak summary list for result page

Usage

```
GeneratePeakList(userPath)
```

Arguments

userPath	userPath

Author(s)

Zhiqiang Pang

Get.asca.tss *Function for ASCA permutation*

Description

Dummy is used only for the purpose to maintain lapply API this is used for permutation on ANOVA paritions, not on the SCA/PCA part, so the number of selected components is not applicable in this step

Usage

```
Get.asca.tss(dummy, perm = T)
```

Arguments

dummy	Dummy variable
perm	Logical, TRUE by default

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

Get.bwss — *Compute within group and between group sum of squares (BSS/WSS) for each row of a matrix which may have NA*

Description

Columns have labels, x is a numeric vector, cl is consecutive integers

Usage

```
Get.bwss(x, cl)
```

Arguments

x	Numeric vector
cl	Columns

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

Get.ConcRef — *Get the concentration reference*

Description

Get the concentration reference

Usage

```
Get.ConcRef(mSetObj = NA, cmpd.nm)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
cmpd.nm	Input the compound name

Get.Leverage *Fast leverage calculation for permutation purpose*

Description

note, the leverage combines all components the importance feature is for the factor not per components

Usage

```
Get.Leverage(XKw, Fac)
```

Arguments

XKw	Features
Fac	Factor

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

Get.pAUC *Calculate partial area under ROC curve*

Description

Calculate partial area under ROC curve

Usage

```
Get.pAUC(x, y, focus, cutoff)
```

Arguments

x	Input X
y	Input Y
focus	Method
cutoff	Numeric

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

Get.pred *Get predicted class probability*

Description

Get predicted class probability, used in higher function

Usage

```
Get.pred(x.train, y.train, x.test, y.test, clsMethod = "pls")
```

Arguments

x.train	Training X
y.train	Training Y
x.test	Test X
y.test	Test Y
clsMethod	Method to predict class, by default it is PLS

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

Get.rpart.summary *Get the text description of a recursive partitioning (rpart) result*

Description

x must be an rpart object

Usage

```
Get.rpart.summary(x)
```

Arguments

x	An Rpart object

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

Get.VIP *Calculate variable importance of projection (VIP) score for PLS object*

Description

Users give a pls object ('oscorespls'=T), function calculates VIP score usually one VIP for each component, return is the average of all VIP

Usage

```
Get.VIP(pls.obj, comp = 2)
```

Arguments

pls.obj	Input the PLS object
comp	Numeric, input the number of components, by default it is 2

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetAbundanceLabel *Determine value label for plotting*

Description

Concentration or intensity data type

Usage

```
GetAbundanceLabel(data.type)
```

Arguments

data.type	Input concentration or intensity data

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetAccuracyInfo *Export biomarker accuracy information*

Description

Export biomarker accuracy information

Usage

```
GetAccuracyInfo(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

GetAllDataNames *Get all meta-analysis name data*

Description

Get all meta-analysis name data

Usage

```
GetAllDataNames()
```

GetAllKMClusterMembers *K-means analysis - cluster*

Description

K-means analysis - cluster

Usage

```
GetAllKMClusterMembers(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

GetAllSOMClusterMembers *SOM analysis*

Description

Get members for given cluster index, return a character string

Usage

```
GetAllSOMClusterMembers(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetCandidateList *Get all candidate compound names for a given index*

Description

Returns 3 coloumns - inx, name, score

Usage

```
GetCandidateList(mSetObj = NA, lipid)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
lipid	Logical

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetCircleInfo *Export information about selected circle*

Description

Export information about selected circle

Usage

```
GetCircleInfo(mSetObj = NA)
```

Arguments

mSetObj	Input name of the created mSet Object

GetCIs *Get confidence intervals*

Description

For non-parametric tests, use quantiles, use normal (1.96*std.err) if parametric

Usage

```
GetCIs(data, param = F)
```

Arguments

data	Input data matrix
param	Logical, False by default

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetCMD *Retrieve last command from the Rhistory.R file*

Description

Fetches the last command from the Rhistory.R file

Usage

```
GetCMD(regexp)
```

Arguments

regexp	Retrieve last command from Rhistory file

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetCompoundDetails *Function to get adduct details from a specified compound*

Description

Function to get adduct details from a specified compound. The results will be both printed in the console as well as saved as a csv file. Note that performing this function multiple times will overwrite previous queries.

Usage

```
GetCompoundDetails(mSetObj = NA, cmpd.id)
```

Arguments

mSetObj	Input the name of the created mSetObj object.
cmpd.id	Input the name of the selected compound.

GetConvertFullPath *Perform utilities for cropping images*

Description

Obtain the full path to convert (from imagemagik) for cropping images

Usage

```
GetConvertFullPath()
```

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

getDataFromTextArea *Transform two column text to data matrix*

Description

Transform two column input text to data matrix (single column data frame)

Usage

```
getDataFromTextArea(txtInput, sep.type = "space")
```

Arguments

txtInput	Input text
sep.type	Indicate the seperator type for input text. Default set to "space"

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetExtendRange *Extend axis*

Description

Extends the axis range to both ends vec is the values for that axis unit is the width to extend, 10 will increase by 1/10 of the range

Usage

```
GetExtendRange(vec, unit = 10)
```

Arguments

vec	Input the vector
unit	Numeric

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetFC *Used by higher functions to calculate fold change*

Description

Utility method to calculate FC, used in higher function

Usage

```
GetFC(mSetObj = NA, paired = FALSE, cmpType)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
paired	Logical, true of false
cmpType	Numeric, 0 or 1

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetFeatureNumbers *Numbers for subset selection*

Description

Return a series of number for subsets selection

Usage

```
GetFeatureNumbers(feat.len)
```

Arguments

feat.len	Input the feature length

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetFinalNameMap *Return the final (after user selection) map as dataframe*

Description

Returns three columns: original name, HMDB name and KEGG ID, for enrichment and pathway analysis, respectively

Usage

```
GetFinalNameMap(mSetObj = NA, lipid = FALSE)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
lipid	Logical

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetFisherPvalue *Get fisher p-values*

Description

Get fisher p-values

Usage

```
GetFisherPvalue(numSigMembers, numSigAll, numMembers, numAllMembers)
```

Arguments

numSigMembers	Number of significant members
numSigAll	Number of all significant features
numMembers	Number of members
numAllMembers	Number of all members

GetGroupNames *Get all group names*

Description

Get all group names

Usage

```
GetGroupNames(mSetObj = NA, exp.fac = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
exp.fac	exp.fac

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetHTMLMetSet *Given a metset inx, return hmtl highlighted metset cmpds and references*

Description

Given a metset inx, return hmtl highlighted metset cmpds and references

Usage

```
GetHTMLMetSet(mSetObj = NA, msetNm)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
msetNm	Input the name of the metabolite set

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetHTMLPathSet *Given a metset inx, return hmtl highlighted pathway cmpds*

Description

Given a metset inx, return hmtl highlighted pathway cmpds

Usage

```
GetHTMLPathSet(mSetObj = NA, msetNm)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
msetNm	Input the name of the metabolite set

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetImpFeatureMat *Get important feature matrix*

Description

feat.outp is a list that contains the ranked features in each cross validation (CV) and returns a two column matrix, col 1 = median ranking and col 2 = mean importance measure

Usage

```
GetImpFeatureMat(mSetObj = NA, feat.outp, bestFeatNum)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
feat.outp	Input the list that contains the ranked features in each cross validation (CV) and returns a two column matrix, col 1 = median ranking and col 2 = mean importance measure
bestFeatNum	Numeric

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetKEGGNodeInfo *Retrieves KEGG node information*

Description

Retrieves KEGG node information

Usage

```
GetKEGGNodeInfo(pathName, g, width, height, usr = par("usr"))
```

Arguments

pathName	Input the path Name
g	Input data
width	Input the width
height	Input the height
usr	Input the user

GetKMClusterMembers *K-means analysis - cluster*

Description

Get the cluster members for given index add HTML color to the names based on its group membership

Usage

```
GetKMClusterMembers(mSetObj = NA, i)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
i	Input the cluster index

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetLassoFreqs *Compute lasso frequency*

Description

Not part of default, need to perform function to compute lasso frequency msg: There are more than 500 variables and n<m You may wish to restart and set use.Gram=FALSE

Usage

```
GetLassoFreqs(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetLimmaResTable *Get result table from eBayes fit object*

Description

Get result table from eBayes fit object

Usage

```
GetLimmaResTable(fit.obj)
```

Arguments

fit.obj	eBayes fit object to parse to a table

GetMapTable *Get mapping table*

Description

Return results from compound name mapping in a table

Usage

```
GetMapTable(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

GetMaxPCAComp *For plotting PCA, selects max top 9 components*

Description

Rotate PCA analysis

Usage

```
GetMaxPCAComp(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetMeanROC *Compute data points on the ROC curve*

Description

perf is the performance object from ROCR

Usage

```
GetMeanROC(perf)
```

Arguments

perf	Performance object from ROCR

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetMetaResultMatrix *Single.type return logFC or p value for individual data analysis*

Description

Single.type return logFC or p value for individual data analysis

Usage

```
GetMetaResultMatrix(mSetObj = NA, single.type = "fc")
```

Arguments

mSetObj	Input name of the created mSet Object
single.type	Default is "fc"

GetMetSetName *Given a metset inx, give its name*

Description

Given a metset inx, give its name

Usage

```
GetMetSetName(mSetObj = NA, msetInx)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
msetInx	Input the index of the metabolite set

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetMsetLibCheckMsg *Get the library check messages*

Description

Get the library check messages

Usage

```
GetMsetLibCheckMsg(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

`GetMsetNames` *Return the selected metset library to java for display*

Description

Return the selected metset library to java for display

Usage

```
GetMsetNames(mSetObj = NA)
```

Arguments

`mSetObj`	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`GetMummichogPathSetDetails` *Function to get compound details from a specified pathway*

Description

Function to get compound details from a specified pathway. The results will be both printed in the console as well as saved as a csv file. Note that performing this function multiple times will overwrite previous queries. Significant compounds will be indicated with an asterisk.

Usage

```
GetMummichogPathSetDetails(mSetObj = NA, msetNm)
```

Arguments

`mSetObj`	Input the name of the created mSetObj object.
`msetNm`	Input the name of the pathway

GetNetworkGeneMappingResultTable *Exports Gene-Mapping result into a table*

Description

Exports Gene-Mapping result into a table

Usage

```
GetNetworkGeneMappingResultTable(mSetObj = NA)
```

Arguments

mSetObj	Input name of the created mSet Object

GetNewSampleNames *Obtain sample names and their class labels*

Description

Obtain sample names and their class labels

Usage

```
GetNewSampleNames(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetNMDRStudy *Function to retrieve dataset from the Metabolomics Workbench.*

Description

This function uses the httr R package to make an API call to the Metabolomics Workbench to download and save a dataset based on the Study ID into the current working directory.

Usage

```
GetNMDRStudy(mSetObj=NA, StudyID)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects).
StudyID	Input the StudyID of the study from the Metabolomics Workbench. Use the ListNMDRStudies function to obtain a list of all available studies from the Metabolomics Workbench.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca>, Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

GetORA.pathNames *Export pathway names from ORA analysis*

Description

Export pathway names from ORA analysis

Usage

```
GetORA.pathNames(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

GetORA.smpdbIDs *Only for human pathways (SMPDB)*

Description

Only for human pathways + ath, eco, mmu & sce

Usage

```
GetORA.smpdbIDs(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetORATable *Get ORA table*

Description

Get ORA table

Usage

```
GetORATable(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

GetQEA.keggIDs *Only for human pathways (KEGG)*

Description

Only for human pathways + ath, eco, mmu & sce

Usage

```
GetQEA.keggIDs(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetQEA.pathNames *Export pathway names from QEA analysis*

Description

Export pathway names from QEA analysis

Usage

```
GetQEA.pathNames(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

GetQEATable *QEA table*

Description

QEA table

Usage

```
GetQEATable(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

GetRCommandHistory *Export R Command History*

Description

Export R Command History

Usage

```
GetRCommandHistory(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

GetRFConf.Table *Classification performance table for random forest analysis*

Description

Classification performance table for random forest analysis

Usage

```
GetRFConf.Table(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

GetRFConfMat *Random Forest Confusion Matrix*

Description

Return double confusion matrix

Usage

```
GetRFConfMat(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetRFOOB *Random Forest OOB*

Description

Get the OOB error for the last signif

Usage

```
GetRFOOB(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetRFSigMat *Random Forest Significance matrix*

Description

Significance measure, double brackets

Usage

```
GetRFSigMat(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetROC.coords *Return ROC corodinates with confidence intervals*

Description

Return ROC corodinates with confidence intervals

Usage

```
GetROC.coords(mSetObj = NA, fld.nm, val, plot = TRUE, imgNm)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
fld.nm	The kind of input coordinate
val	The coordinates to look for
plot	Logical, by default set to TRUE
imgNm	Input the image name

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetROCLassoFreq *Get p-values from lasso*

Description

Get p-values from lasso

Usage

```
GetROCLassoFreq(data, cls)
```

Arguments

data	Input data
cls	Input class labels

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetROCTtestP *Get p-values for ROC*

Description

ROC p-vaues, used in higher function

Usage

```
GetROCTtestP(data, cls)
```

Arguments

data	Input data
cls	Input class labels

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetSampleSizeLadder *Retrieve sample size ladder*

Description

Return sample size ladder, used in higher functions

Usage

```
GetSampleSizeLadder(maxNum)
```

Arguments

maxNum	Numeric

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetSigTable *Create Latex table*

Description

generate Latex table

Usage

```
GetSigTable(mat, method, data.type)
```

Arguments

mat	Input matrix
method	Input method to create table
data.type	Input the data type

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetSigTable.Anova *Sig Table for Anova*

Description

Sig Table for Anova

Usage

```
GetSigTable.Anova(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

GetSigTable.Aov2 *Sig table for AOV2*

Description

Sig table for AOV2

Usage

```
GetSigTable.Aov2(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

GetSigTable.ASCA *Table of features well modelled by ASCA*

Description

Table of features well modelled by ASCA

Usage

```
GetSigTable.ASCA(mSetObj = NA, nm)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
nm	Input the name of the well modelled features

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetSigTable.Corr *Sig table for Correlation Analysis*

Description

Sig table for Correlation Analysis

Usage

```
GetSigTable.Corr(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

GetSigTable.Dose *Sig Table for Anova*

Description

Sig Table for Anova

Usage

```
GetSigTable.Dose(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

GetSigTable.EBAM *Sig table for EBAM*

Description

Sig table for EBAM

Usage

```
GetSigTable.EBAM(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

GetSigTable.FC *Sig Table for Fold-Change Analysis*

Description

Sig Table for Fold-Change Analysis

Usage

```
GetSigTable.FC(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

GetSigTable.MB *Sig table for MB analysis*

Description

Sig table for MB analysis

Usage

```
GetSigTable.MB(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

GetSigTable.RF *Sig table for random forest analysis*

Description

Sig table for random forest analysis

Usage

```
GetSigTable.RF(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

GetSigTable.SAM *Sig table for SAM*

Description

Sig table for SAM

Usage

```
GetSigTable.SAM(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

GetSigTable.SVM *Sig table for SVM*

Description

Sig table for SVM

Usage

```
GetSigTable.SVM(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

GetSigTable.TT *Sig Table for T-test Analysis*

Description

Sig Table for T-test Analysis

Usage

```
GetSigTable.TT(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

GetSigTable.Volcano *Sig table for Volcano Analysis*

Description

Sig table for Volcano Analysis

Usage

```
GetSigTable.Volcano(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

GetSOMClusterMembers *SOM analysis*

Description

Get members for given cluster index, return a character string

Usage

```
GetSOMClusterMembers(mSetObj = NA, i, j)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
i	Index of X
j	Index of Y

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetSSPTable — *Replace the last column of the ssp.mat with the final selection from users*

Description

Replace the last column of the ssp.mat with the final selection from users

Usage

```
GetSSPTable(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetSuggestedSAMDelta — *For SAM analysis*

Description

obtain a default delta with reasonable number of sig features and decent FDR

Usage

```
GetSuggestedSAMDelta(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetSVMSigMat *Recursive Support Vector Machine (R-SVM) Significance Measure*

Description

Return significance measure, double[][]

Usage

```
GetSVMSigMat(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetTopInx *Volcano indices*

Description

Get indices of top n largest/smallest number

Usage

```
GetTopInx(vec, n, dec = T)
```

Arguments

vec	Vector containing volcano indices
n	Numeric
dec	Logical, default set to TRUE

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetTrainTestSplitMat *Make random partitions*

Description

Make random partitions, returns matrices indicating whether the observation is in train/test for each run note: try to get a balanced sampling for each group (classification) or each quantile (regression). This is very useful for unbalanced data

Usage

```
GetTrainTestSplitMat(y, propTraining = 2/3, nRuns = 30)
```

Arguments

y	Input the data
propTraining	By default set to 2/3
nRuns	By default set to 30

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetTtestRes *Retrieve T-test p-values*

Description

Utility method to get p values

Usage

```
GetTtestRes(mSetObj = NA, paired = FALSE, equal.var = TRUE, nonpar = F)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
paired	Default set to FALSE
equal.var	Default set to TRUE
nonpar	Use non-parametric tests, default is set to FALSE

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetTTSigMat *T-test matrix*

Description

Return a double matrix with 2 columns - p values and lod

Usage

```
GetTTSigMat(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetUnivReport *Utility method to perform the univariate analysis automatically*

Description

The approach is computationally expensive,and fails more often get around: make it lazy unless users request, otherwise the default t-test will also be affected

Usage

```
GetUnivReport(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetVariableLabel *Determine variable label for plotting*

Description

Determine data type, binned spectra, nmr peak, or ms peak

Usage

```
GetVariableLabel(data.type)
```

Arguments

data.type	Input the data type

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GetXYCluster *Determine row/column number for plotting*

Description

Determine the number of rows and columns for a given total number of plots (used by Kmeans and SOM plots)

Usage

```
GetXYCluster(total)
```

Arguments

total	Input the total

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

GroupPeakList *Group peak list*

Description

Group peaks from the peak list based on position using the XCMS grouping algorithm (align peaks wrt, rt, and mz). For NMR peaks, need to change ppm -> mz and add dummy rt. If the data is 2-column MS, first need to add dummy rt. If the data is 3-column MS, the data can be used directly. The default mzwid for MS is 0.25 m/z, and for NMR is 0.03 ppm. The default bw is 30 for LCMS, and 5 for GCMS.

Usage

```
GroupPeakList(mSetObj=NA, mzwid, bw, minfrac, minsamp, max)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
mzwid	define the width of overlapping m/z slices to use for creating peak density chromatograms and grouping peaks across samples
bw	define the bandwidth (standard deviation or half width at half maximum) of gaussian smoothing kernel to apply to the peak density chromatogram
minfrac	define the minimum fraction of samples necessary in at least one of the sample groups for it to be a valid group
minsamp	define the minimum number of samples necessary in at least one of the sample groups for it to be a valid group
max	define the maximum number of groups to identify in a single m/z slice

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

heckbert *Heckbert algorithm*

Description

function to calculate tick mark based on Heckbert algorithm available in the "labeling" package implemented by Justin Talbot adapted from the imagemap package Heckbert's labeling algorithm Heckbert, P. S. (1990) Nice numbers for graph labels, Graphics Gems I, Academic Press Professional, Inc.

Usage

```
heckbert(dmin, dmax, m)
```

Arguments

dmin	Heckbert
dmax	Heckbert
m	Heckbert

Author(s)

Justin Talbot <jtalbot@stanford.edu>

HMDBID2KEGGID *Given a vector of HMDBIDs, return a vector of KEGG IDs*

Description

This function, when given a vector of HMDBIDs, returns a vector of KEGG ID. HMDB standing for the Human Metabolome Database.

Usage

```
HMDBID2KEGGID(ids)
```

Arguments

ids	Input the vector of HMDB Ids

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

HMDBID2Name *Given a vector of HMDBIDs, return a vector of HMDB compound names*

Description

This function, when given a vector of HMDBIDs, return a vector of HMDB compound names. HMDB standing for the Human Metabolome Database.

Usage

```
HMDBID2Name(ids)
```

Arguments

ids	Input the vector of HMDB Ids

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`ImputeMissingVar` *Data processing: Replace missing variables*

Description

Replace missing variables by min/mean/median/KNN/BPCA/PPCA/svdImpute.

Usage

```
ImputeMissingVar(mSetObj, method)
```

Arguments

`mSetObj`	Input the name of the created mSetObj (see InitDataObjects)
`method`	Select the option to replace missing variables, either replacement based on the minimum ("min), the mean ("mean"), or the median ("median") value of each feature columns, or several options to impute the missing values, using k-nearest neighbour ("KNN"), probabilistic PCA ("PPCA"), Bayesian PCA ("BPCA") method, or Singular Value Decomposition ("svdImpute")

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`InitDataObjects` *Constructs a dataSet object for storing data*

Description

This functions handles the construction of a mSetObj object for storing data for further processing and analysis. It is necessary to utilize this function to specify to MetaboAnalystR the type of data and the type of analysis you will perform.

Usage

```
InitDataObjects(data.type, anal.type, paired=FALSE)
```

Arguments

data.type	The type of data, either list (Compound lists), conc (Compound concentration data), specbin (Binned spectra data), pktable (Peak intensity table), nmrpeak (NMR peak lists), mspeak (MS peak lists), or msspec (MS spectra data)
anal.type	Indicate the analysis module to be performed: stat, pathora, pathqea, msetora, msetssp, msetqea, mf, cmpdmap, smpmap, or pathinteg
paired	indicate if the data is paired or not. Logical, default set to FALSE

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

InitializaPlan *InitializePlan*

Description

this function is used to initialize a plan before submit job to spring daemon

Usage

```
InitializaPlan()
```

Author(s)

Zhiqiang Pang

InitMSObjects *InitMSObjects*

Description

InitMSObjects

Usage

```
InitMSObjects(data.type = NULL, anal.type = NULL, paired = FALSE)
```

Arguments

data.type	should be "raw"
anal.type	should be "spec"
paired	should be "FALSE"

InitPowerAnal *Function for power analysis*

Description

Perform power analysis, requires the SSPA R package.

Usage

```
InitPowerAnal(mSetObj, clsOpts)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
clsOpts	For data with >2 groups, specify the two classes on which to perform power analysis, otherwise for data with 2 groups, "NA" will automatically select the 2 groups.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

InitStatAnalMode *Introduction for statistical analysis module report Initialize Statistical Analysis Report*

Description

Introduction for statistical analysis module report Initialize Statistical Analysis Report

Usage

```
InitStatAnalMode()
```

InitTimeSeriesAnal *Create report of analyses (Met Pathway)*

Description

Report generation using Sweave Metabolomic pathway analysis, time-series analysis

Usage

```
InitTimeSeriesAnal()
```

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

iPCA.Anal *Perform PCA analysis, prepare file for interactive liveGraphics3D*

Description

Perform PCA analysis, prepares a JSON file for interactive liveGraphics3D, as well as interactive 3D PCA score and loading plots using the plotly R package. These plots are saved in the created mSetObj; to view these, type "mSetObj$imgSet$time$score3d" to view the interactive score plot, and "mSetObj$imgSet$time$load3d" to view the interactive loading plot.

Usage

```
iPCA.Anal(mSetObj, fileNm, metaCol, metaShape)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
fileNm	select a file name

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

isEmptyMatrix *Sig table matrix is empty*

Description

Test if a sig table matrix is empty

Usage

```
isEmptyMatrix(mat)
```

Arguments

mat	Matrix to test if empty

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

IsSmallSmplSize *Check if the sample size is small*

Description

Returns whether or not the sanity check found that there were too many groups in the dataset containing too few samples. It will return a 0 if the data passes the check, or will return a 1 if the data does not.

Usage

```
IsSmallSmplSize(mSetObj=NA)
```

Arguments

mSetObj	Input name of the created mSet Object

KEGGID2HMDBID *Given a vector of KEGGIDs, return a vector of HMDB ID*

Description

This functionn, when given a vector of KEGGIDs, returns a vector of HMDB IDs. HMDB standing for the Human Metabolome Database.

Usage

```
KEGGID2HMDBID(ids)
```

Arguments

ids	Vector of KEGG ids

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

KEGGID2Name *Given a vector containing KEGGIDs, returns a vector of KEGG compound names*

Description

This function, given a vector containing KEGGIDs, returns a vector of KEGG compound names.

Usage

```
KEGGID2Name(ids)
```

Arguments

ids	Vector of KEGG ids

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

KEGGPATHID2SMPDBIDs *Given a vector containing KEGG pathway IDs, return a vector containing SMPDB IDs (only for hsa)*

Description

This function, when given a vector of KEGG pathway IDs, return a vector of SMPDB IDs (only for hsa). SMPDB standing for the Small Molecule Pathway Database, and hsa standing for human serum albumin.

Usage

```
KEGGPATHID2SMPDBIDs(ids)
```

Arguments

ids	Vector of KEGG pathway IDs

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

Kmeans.Anal *K-means analysis*

Description

Perform K-means analysis

Usage

```
Kmeans.Anal(mSetObj = NA, clust.num)
```

Arguments

mSetObj	Input name of the created mSet Object
clust.num	Numeric, input the number of clusters for K-means analysis

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

kwtest *Kruskal-Wallis*

Description

Perform Kruskal-Wallis Test

Usage

```
kwtest(x, cls)
```

Arguments

x	Input data to perform Kruskal-Wallis
cls	Input class labels

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

ListNMDRStudies *Function to retrieve all available datasets from the Metabolomics Workbench.*

Description

This function uses the httr R package to make an API call to the Metabolomics Workbench to retrieve a table of all compatible datasets.

Usage

```
ListNMDRStudies(mSetObj=NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects).

Author(s)

Jeff Xia <jeff.xia@mcgill.ca>, Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

LoadKEGGKO_lib *Utility function for PerformKOEnrichAnalysis_KO01100*

Description

Utility function for PerformKOEnrichAnalysis_KO01100

Usage

```
LoadKEGGKO_lib(category)
```

Arguments

category	Module or pathway

LogNorm *Column-wise Normalization*

Description

Column-wise norm methods, when x is a column Options for log, zero mean and unit variance, and several zero mean and variance/SE

Usage

```
LogNorm(x, min.val)
```

Arguments

x	Input data
min.val	Input minimum value

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada

make_cpdlist *Utility function to create compound lists for permutation analysis*

Description

From a vector of m/z features, this function outputs a vector of compounds.

Usage

```
make_cpdlist(mSetObj=NA, input_mzs)
```

Arguments

mSetObj	Input the name of the created mSetObj
input_mzs	The vector of randomly drawn m/z features.

Author(s)

Jasmine Chong, Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

make_ecpdlist *Utility function to create compound lists for permutation analysis*

Description

From a vector of m/z features, this function outputs a vector of compounds.

Usage

```
make_ecpdlist(mSetObj=NA, input_mzs)
```

Arguments

mSetObj	Input the name of the created mSetObj
input_mzs	The vector of randomly drawn m/z features.

Author(s)

Jasmine Chong, Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

map *sPLS-DA Map*

Description

map variable for (s)plsda

Usage

```
map(Y)
```

Arguments

Y	Input data

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

MapCmpd2KEGGNodes *Utility function for PrepareKeggQueryJson*

Description

Utility function for PrepareKeggQueryJson

Usage

```
MapCmpd2KEGGNodes(cmpds, net = "ko01100")
```

Arguments

cmpds	Input the compounds
net	Input the network name

MapKO2KEGGEdges *Utility function for PrepareKeggQueryJson*

Description

Utility function for PrepareKeggQueryJson

Usage

```
MapKO2KEGGEdges(kos, net = "ko01100")
```

Arguments

kos	Input the KOs
net	Input the name of the network

Match.Pattern *Match pattern for correlation analysis*

Description

Match pattern for correlation analysis

Usage

```
Match.Pattern(mSetObj = NA, dist.name = "pearson", pattern = NULL)
```

Arguments

mSetObj	Input the name of the created mSetObj
dist.name	Input the distance method, default is set to pearson
pattern	Set the pattern, default is set to NULL

`melt` *melt Convert an object into a molten data frame. This function is from reshape2 package.*

Description

This the generic melt function. See the following functions for the details about different data structures:

Usage

```
melt(data, ..., na.rm = FALSE, value.name = "value")
```

Arguments

`data`	Data set to melt
`...`	further arguments passed to or from other methods.
`na.rm`	Should NA values be removed from the data set? This will convert explicit missings to implicit missings.
`value.name`	name of variable used to store values

`MergeDatasets` *Utility function for PrepareKeggQueryJson*

Description

Utility function for PrepareKeggQueryJson

Usage

```
MergeDatasets(dataSet1, dataSet2)
```

Arguments

`dataSet1`	Input the first dataset
`dataSet2`	Input the second dataset

`MergeDuplicates` *Merge duplicated columns or rows by their mean*

Description

dim 1 => row, dim 2 => column

Usage

```
MergeDuplicates(data, dim = 2)
```

Arguments

`data`	Input the data
`dim`	Numeric, input the dimensions, default is set to 2

`MetaboAnalystR` *MetaboAnalystR: A package for computating the notorious bar statistic.*

Description

The MetaboAnalystR package provides a pipeline for metabolomics processing.

MetaboAnalystR functions

The MetaboAnalystR functions ...

`MetaboliteMappingExact` *Mapping from different metabolite IDs*

Description

For compound names to other ids, can do exact or approximate matches For other IDs, except HMDB ID, all others may return multiple/non-unique hits Multiple hits or non-unique hits will allow users to manually select

Usage

```
MetaboliteMappingExact(mSetObj = NA, q.type, lipid = F)
```

Arguments

mSetObj	Input the name of the created mSetObj.
q.type	Inpute the query-type, "name" for compound names, "hmdb" for HMDB IDs, "kegg" for KEGG IDs, "pubchem" for PubChem CIDs, "chebi" for ChEBI IDs, "metlin" for METLIN IDs, and "hmdb_kegg" for a both KEGG and HMDB IDs.
lipid	Boolean, if features are lipids, a different database will be used for compound matching.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

MetaPathNormalization *MetaPathNormalization*

Description

MetaPathNormalization

Usage

```
MetaPathNormalization(
  mSetObj = NA,
  sampleNor,
  tranform,
  scale = "NULL",
  name,
  name2
)
```

Arguments

mSetObj	mSetObj
sampleNor	sample Normalization option
tranform	sample transformation option
scale	sample scale option
name	file name 1 with absolute path
name2	file name 2 with absolute path or "null"

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> Zhiqiang Pang<zhiqiang.pang@mail.mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`multi.stat` *Get multiple category statistics*

Description

Get multiple category statistics

Usage

```
multi.stat(pred, resp)
```

Arguments

`pred`	Input predictions
`resp`	Input responses

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`my.lsd.test` *Calculate Fisher's Least Significant Difference (LSD)*

Description

Adapted from the 'agricolae' package

Usage

```
my.lsd.test(y, trt, alpha = 0.05)
```

Arguments

`y`	Input Y
`trt`	Input trt
`alpha`	Numeric, default is 0.05

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

my.parse.peaklist *my.parse.peaklist*

Description

Read peak list files. This function reads peak list files and fills the data into a dataSet object. For NMR peak lists, the input should be formatted as two-columns containing numeric values (ppm, int). Further, this function will change ppm to mz, and add a dummy 'rt'. For MS peak data, the lists can be formatted as two-columns (mz, int), in which case the function will add a dummy 'rt', or the lists can be formatted as three-columns (mz, rt, int).

Usage

```
my.parse.peaklist(mSetObj = NA, foldername = "upload")
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects).
foldername	Name of the folder containing the NMR or MS peak list files to read.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

Normalization *Normalization*

Description

This function performs row-wise normalization, transformation, and scaling of your metabolomic data.

Usage

```
Normalization(mSetObj, rowNorm, transNorm, scaleNorm, ref=NULL, ratio=FALSE, ratioNum=20)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
rowNorm	Select the option for row-wise normalization, "QuantileNorm" for Quantile Normalization, "CompNorm" for Normalization by a reference feature, "SumNorm" for Normalization to constant sum, "MedianNorm" for Normalization to sample median, and "SpecNorm" for Normalization by a sample-specific factor.
transNorm	Select option to transform the data, "LogNorm" for Log Normalization, and "CrNorm" for Cubic Root Transformation.

scaleNorm	Select option for scaling the data, "MeanCenter" for Mean Centering, "AutoNorm" for Autoscaling, "ParetoNorm" for Pareto Scaling, amd "RangeNorm" for Range Scaling.
ref	Input the name of the reference sample or the reference feature, use " " around the name.
ratio	This option is only for biomarker analysis.
ratioNum	Relevant only for biomarker analysis.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca>, Jasmine Chong McGill University, Canada

---

OPLSDA.Permut *Perform OPLS-DA permutation*

Description

Orthogonal PLS-DA (from ropls) perform permutation, using training classification accuracy as indicator, for two or multi-groups

Usage

```
OPLSDA.Permut(mSetObj = NA, num = 100)
```

Arguments

mSetObj	Input name of the created mSet Object
num	Input the number of permutations, default is set to 100.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

OPLSR.Anal *Perform OPLS-DA*

Description

Orthogonal PLS-DA (from ropls) Add reg (regression i.e. if class order matters)

Usage

```
OPLSR.Anal(mSetObj = NA, reg = FALSE)
```

Arguments

mSetObj	Input name of the created mSet Object
reg	Logical

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

---

parseFisher *Return only the signicant comparison names*

Description

Return only the signicant comparison names, used in higher function

Usage

```
parseFisher(fisher, cut.off)
```

Arguments

fisher	Input fisher object
cut.off	Numeric, set cut-off

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

---

parseTukey *Return only the signicant comparison names*

Description

Return only the signicant comparison names, used in higher function

Usage

```
parseTukey(tukey, cut.off)
```

Arguments

tukey	Input tukey output
cut.off	Input numeric cut-off

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PCA.Anal *Perform PCA analysis*

Description

Perform PCA analysis, obtain variance explained, store item to PCA object

Usage

```
PCA.Anal(mSetObj = NA)
```

Arguments

mSetObj	Input name of the created mSet Object McGill University, Canada License: GNU GPL (>= 2)

Author(s)

Jeff Xia<jeff.xia@mcgill.ca>

PCA.Flip *Rotate PCA analysis*

Description

Rotate PCA analysis

Usage

```
PCA.Flip(mSetObj = NA, axisOpt)
```

Arguments

mSetObj	Input name of the created mSet Object
axisOpt	Input the axis option

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PCA.GENES *Obtain principal components into a matrix that has more variables than individuals*

Description

X is a matrix that has as columns the compounds that were considered as variables in the PCA analysis. First we center the matrix by columns (Xoff) and then we obtain the eigenvalues and the eigenvectors of the matrix Xoff use the equivalences between the loadings and scores to obtain the solution

Usage

```
PCA.GENES(X)
```

Arguments

X	Input matrix that has as columns the compounds that were considered as variables in the PCA analysis

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

Perform.ASCA *Perform ASCA*

Description

The ASCA algorithm was adapted from the ASCA-genes method (analysis of variance (ANOVA) simultaneous component analysis) by Maria Jose Nueda (mj.nueda@ua.es) and Ana Conesa (aconesa@ivia.es)

Usage

```
Perform.ASCA(mSetObj = NA, a = 1, b = 2, x = 2, res = 2)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
a	specify the number of components for facA
b	specify the number of components for facB
x	specify the number of components for interaction AB
res	specify the number of model residuals type is string, indicating the type of analysis "abc" separately "aab" facA joins with AB "bab" facB joins with AB

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

Perform.ASCA.permute *Perform ASCA model validation by permutation*

Description

Perform ASCA model validation by permutation we use Manly's unrestricted permutation of observations which esentially permutes the data over all cells in the designed experiment, then calculates the score for each main factor or interaction components. This will get the null distribution for all effects in one go

Usage

```
Perform.ASCA.permute(mSetObj=NA, perm.num)
```

Arguments

mSetObj	Input name of the created mSet Object
perm.num	Select the number of permutations, default is 20

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

Perform.Permut *Perform permutation tests only for ROC Tester*

Description

Perform permutation tests for the ROC Curve Based Model Creation and Evaluation module

Usage

```
Perform.Permut(mSetObj=NA, perf.measure, perm.num, propTraining = 2/3)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
perf.measure	Input the performance measure to rate the performance of the model, either the area under the ROC curve ("auroc") or the predictive accuracy ("accu")
perm.num	Input the number of permutations to perform
propTraining	Numeric, input the fraction of samples to set aside for training. Default is set to 2/3.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

Perform.permutation *Permutation*

Description

Perform permutation, options to change number of cores used

Usage

```
Perform.permutation(perm.num, fun)
```

Arguments

perm.num	Numeric, input the number of permutations to perform
fun	Dummy function

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

Perform.UnivROC *Perform Classical Univariate ROC*

Description

Perform Classical Univariate ROC

Usage

```
Perform.UnivROC(mSetObj=NA, feat.nm, version,
format="png", dpi=72, isAUC, isOpt, optMethod, isPartial, measure, cutoff)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
feat.nm	Input the name of the feature to perform univariate ROC analysis
version	image version mark, can be any character
format	Select the image format, png, of pdf.
dpi	Input the dpi. If the image format is pdf, users need not define the dpi. For png images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.

isAUC	Logical, select T to compute the 95 percent confidence interval band and "F" to not
isOpt	Logical, show the optimal cutoff, T to show it and F to not
optMethod	Select the optimal cutoff by using either closest.topleft for closest to top-left corner or youden for farthest to the diagonal line (Youden)
isPartial	Logical, input T to calculate a partial ROC curve, and F to not
measure	Select the parameter to limit the calculation of the partial ROC curve, se for the X-axis (maximum false-positive rate) and sp for the Y-axis, representing the minimum true positive-rate
cutoff	Input the threshold to limit the calculation of the partial ROC curve, the number must be between 0 and 1.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PerformAdductMapping *PerformAdductMapping*

Description

This function reads in the user's adduct list and saves it as a matrix.

Usage

```
PerformAdductMapping(mSetObj = NA, add.mode)
```

Arguments

mSetObj	Input the name of the created mSetObj object
add.mode	Adduct mode, positive or negative

Author(s)

Jasmine Chong, Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PerformApproxMatch *Perform approximate compound matches*

Description

Given a query, perform approximate compound matching

Usage

```
PerformApproxMatch(mSetObj = NA, q, lipid)
```

Arguments

mSetObj	Input the name of the created mSetObj.
q	Input the q vector.
lipid	lipid, logical

PerformBatchCorrection *Batch Effect Correction*

Description

This function is designed to perform the batch effect correction

Usage

```
PerformBatchCorrection(
  mSetObj = NA,
  imgName = NULL,
  Method = NULL,
  center = NULL
)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input the name of the plot to create
Method	Batch effect correction method, default is "auto". Specific method, including "Combat", "WaveICA","EigenMS","QC_RLSC","ANCOVA","RUV_random","RUV_2","RUV_s","RUV and "CCMN".
center	The center point of the batch effect correction, based on "QC" or "", which means correct to minimize the distance between batches.

Author(s)

Zhiqiang Pang, Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PerformCmpdMapping *Perform compound mapping for integrative analysis methods*

Description

Perform compound mapping

Usage

```
PerformCmpdMapping(mSetObj = NA, cmpdIDs, org, idType)
```

Arguments

mSetObj	Input name of the created mSet Object
cmpdIDs	Input the list of compound IDs
org	Input the organism code
idType	Input the ID type

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PerformCurrencyMapping *Map currency metabolites to KEGG & BioCyc*

Description

This function maps the user selected list of compounds to its corresponding KEGG IDs and BioCyc IDs

Usage

```
PerformCurrencyMapping(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj object

Author(s)

Jasmine Chong, Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PerformCV.explore *Perform Monte-Carlo Cross Validation (MCCV)*

Description

Classification MCCV, aims to find the best feature subsets using default model parameters

Usage

```
PerformCV.explore(mSetObj, cls.method, rank.method="auroc", lvNum=2, propTraining=2/3)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
cls.method	Select the classification method, "rf" for random forest classification, "pls" for PLS-DA, and "svm" for support vector machine
rank.method	Select the ranking method, "rf" for random forest mean decrease accuracy, "fisher" for Fisher's univariate ranking based on area under the curve "auroc" for univariate ranking based on area under the curve, "tt" for T-test univariate ranking based on area under the curve, "pls" for partial least squares, and "svm" for support vector machine
lvNum	Input the number of latent variables to include in the analyis, only for PLS-DA classification
propTraining	Input the proportion of samples to use for training

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PerformCV.test *Perform MCCV for manually selected features*

Description

MCCV for manually selected features (no additional feature selection)

Usage

```
PerformCV.test(mSetObj, method, lvNum, propTraining=2/3, nRuns=100)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
method	Select the classification method, "rf" for random forest classification, "pls" for PLS-DA, and "svm" for support vector machine
lvNum	Input the number of latent variables to include in the analyis, only for PLS-DA classification
propTraining	Input the proportion of samples to use for training, by default it is 2/3
nRuns	Input the number of MCCV runs, by default it is 100

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PerformDataInspect *PerformDataInspect*

Description

PerformDataInspect is used to plot 2D/3D structure of the MS data

Usage

```
PerformDataInspect(
  datapath = NULL,
  rt.range = c(0, 0),
  mz.range = c(0, 0),
  dimension = "3D",
  res = 100
)
```

Arguments

datapath	data file path
rt.range	retention time range, unit is seconds
mz.range	m/z range
dimension	view dimension, canbe "2D" or "3D"
res	resolution number, higher of the number means higher resolution

Author(s)

Zhiqiang Pang

`PerformDataTrimming` *Perform ROI Extraction from raw MS data (PerformDataTrimming)*

Description

This function performs the raw data trimming. This function will output an trimmed MSnExp file to memory or hardisk according to the choice of users must provide the data path for 'datapath', and optionally provide other corresponding parameters.

Usage

```
PerformDataTrimming(
  datapath,
  mode = "ssm",
  write = FALSE,
  mz,
  mzdiff,
  rt,
  rtdiff,
  rt.idx = 1/15,
  rmConts = TRUE,
  plot = TRUE,
  running.controller = NULL
)
```

Arguments

`datapath`	Character, the path of the raw MS data files' or folder's path (.mzXML, .CDF and .mzML) for parameters training.
`mode`	Character, mode for data trimming to select the chraracteristic peaks. Default is 'ssm'. Users could select random trimed according to mz value (mz_random) or RT value (rt_random). Besides, specific peaks at certain mz (mz_specific) or RT (rt_specific) could also be extracted. 'none' will not trim the data.
`write`	Logical, if true, will write the trimmed data to the directory 'trimmed' folder in the datapath. The data in memory will be kept.
`mz`	Numeric, mz value(s) for specific selection. Positive values means including (the values indicted) and negative value means excluding/removing.
`mzdiff`	Numeric, the deviation (ppm) of mz value(s).
`rt`	Numeric, rt value for specific selection. Positive values means including and negative value means excluding.
`rtdiff`	Numeric, the deviation (seconds) of rt value(s).
`rt.idx`	Numeric, the relative rt (retention time) range, from 0 to 1. 1 means all retention time will be retained, while 0 means none. Default is 1/15. If default rt.idx produce too few peaks, please consider increasing this value.

rmConts	LOgical, whether to exclude/remove the potential contamination for parameters optimization. Default is TRUE.
plot	Logical, if TRUE, will plot the chromatogram of the trimmed data.
running.controller	The resuming pipeline running controller. Optional. Don't need to define by hand.

Value

will return an mSet objects with extracted ROI

Author(s)

Zhiqiang Pang <zhiqiang.pang@mail.mcgill.ca> Jeff Xia <jeff.xia@mcgill.ca> Mcgill University License: GNU GPL (>= 2)

PerformDetailMatch *Perform detailed name match*

Description

Given a query, perform compound matching.

Usage

```
PerformDetailMatch(mSetObj = NA, q)
```

Arguments

mSetObj	Input name of the created mSet Object.
q	Input the query.

PerformEachDEAnal *Performs differential expression analysis on individual data*

Description

This function performs DE analysis on individual data using the common matrix, which will be used/compared in later steps of the analysis (according to the p-value). The DE for each feature may be adjusted using the p-value.

Usage

```
PerformEachDEAnal(mSetObj = NA)
```

Arguments

mSetObj	Input name of the created mSet Object

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PerformGeneMapping *Perform integrated gene mapping*

Description

Used for the pathinteg module

Usage

```
PerformGeneMapping(mSetObj = NA, geneIDs, org, idType)
```

Arguments

mSetObj	Input name of the created mSet Object
geneIDs	Input the list of gene IDs
org	Input the organism code
idType	Input the ID type

PerformIndNormalization *Perform normalization for individually-uploaded datasets for meta-analysis*

Description

This function performs normalization of individuall-uploaded datasets prior to meta-analysis.

Usage

```
PerformIndNormalization(mSetObj = NA, dataName, norm.opt, auto.opt)
```

Arguments

mSetObj	Input name of the created mSet Object
dataName	Input the name of the individual dataset for normalization.
norm.opt	Performs log2 normalization "log", or no normalization "none".
auto.opt	Performs auto-scaling of data (1), or no (0).

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`PerformIntegPathwayAnalysis`
Perform integrative pathway analysis

Description

used for integrative analysis as well as general pathways analysis for meta-analysis results

Usage

```
PerformIntegPathwayAnalysis(mSetObj, topo="dc", enrich="hyper",
libOpt="integ", integOpt="query")
```

Arguments

`mSetObj`	Input name of the created mSet Object
`topo`	Select the mode for topology analysis: Degree Centrality ("dc") measures the number of links that connect to a node (representing either a gene or metabolite) within a pathway; Closeness Centrality ("cc") measures the overall distance from a given node to all other nodes in a pathway; Betweenness Centrality ("bc")measures the number of shortest paths from all nodes to all the others that pass through a given node within a pathway.
`enrich`	Method to perform over-representation analysis (ORA) based on either hypergenometrics analysis ("hyper") or Fisher's exact method ("fisher").
`libOpt`	Select the different modes of pathways, either the gene-metabolite mode ("integ") which allows for joint-analysis and visualization of both significant genes and metabolites or the gene-centric ("genetic") and metabolite-centric mode ("metab") which allows users to identify enriched pathways driven by significant genes or metabolites, respectively.
`integOpt`	integOpt,default is "query"

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PerformKOEnrichAnalysis_KO01100

Performs KO enrichment analysis based on the KO01100 map

Description

This function performs KO enrichment analysis based on the KO01100 map and saves the .JSON file

Usage

```
PerformKOEnrichAnalysis_KO01100(mSetObj = NA, category, file.nm)
```

Arguments

mSetObj	Input name of the created mSet Object
category	Input the option to perform enrichment analysis, "pathway"
file.nm	Input name of file to save

Author(s)

Othman Soufan, Jeff Xia <jeff.xia@mcgill.ca>, othman.soufan@mcgill.ca McGill University, Canada License: GNU GPL (>= 2)

PerformKOEnrichAnalysis_List

Utility function for PerformKOEnrichAnalysis_KO01100

Description

Please note: only return hits in map KO01100

Usage

```
PerformKOEnrichAnalysis_List(mSetObj, file.nm)
```

Arguments

mSetObj	mSetObj object
file.nm	Input the file name

`PerformLimmaDE` *Perform differential expression analysis using Limma for individually-uploaded data.*

Description

This function performs DE analysis of individually-uploaded data prior to meta-analysis.

Usage

```
PerformLimmaDE(mSetObj = NA, dataName, p.lvl = 0.1, fc.lvl = 0)
```

Arguments

`mSetObj`	Input name of the created mSet Object
`dataName`	Input the name of the individual dataset for normalization.
`p.lvl`	Numeric, input the p-value (FDR) cutoff.
`fc.lvl`	Numeric, input the fold-change (FC) cutoff.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`PerformMapping_ko01100` *Utility function for PrepareKeggQueryJson geneIDs is text one string, need to make to vector*

Description

Utility function for PrepareKeggQueryJson geneIDs is text one string, need to make to vector

Usage

```
PerformMapping_ko01100(inputIDs, type)
```

Arguments

`inputIDs`	Input list of IDs
`type`	Input the type of IDs

performMB *Timecourse analysis*

Description

Adapted from the timecourse package by Yu Chuan Tai This method is only applicable for time-series, not for general case two/multiple factor analysis

Usage

```
performMB(mSetObj, topPerc)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
topPerc	select the cut-off, default is 10

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PerformMetaMerge *Meta-Analysis Method: Direct merging of datasets*

Description

This function is one of three methods to perform meta-analysis. Direct merging of individual data into a mega-dataset results in an analysis of that mega-dataset as if the individual data were derived from the same experiment. This method thereby ignores any inherent bias and heterogeneity between the different data. Because of this, there exists several confounders such as different experimental protocols, technical platforms, and raw data processing procedures that can mask true underlying differences. It is therefore highly suggested that this approach be used only when individual data are very similar (i.e. from the same lab, same platform, without batch effects)."

Usage

```
PerformMetaMerge(mSetObj = NA, BHth = 0.05)
```

Arguments

mSetObj	Input name of the created mSet Object.
BHth	Numeric input to set the significance level. By default it is 0.05.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PerformMetaPSEA *PerformMetaPSEA Function to perform peak set enrichment meta-analysis at either the empirical compound, compound level or pathway level.*

Description

This is the main function that performs either the mummichog algorithm, GSEA, or both for peak set enrichment meta-analysis.

Usage

```
PerformMetaPSEA(
  mSetObj = NA,
  lib,
  libVersion,
  minLib = 3,
  permNum = 100,
  metaLevel = "pathway",
  combine.level = "pvalue",
  pval.method = "fisher",
  es.method = "fixed",
  rank.metric = "mean",
  mutual.feats = TRUE,
  pooled_cutoff = 0.05
)
```

Arguments

mSetObj	Input the name of the created mSetObj object.
lib	Input the name of the organism library, default is hsa_mfn.
libVersion	Input the version of the KEGG pathway libraries ("current" or "old").
minLib	numeric, default is 3
permNum	Numeric, input the number of permutations to perform. Default is 100.
metaLevel	Character, input whether the meta-analysis is at the empirical compound ("ec"), compound ("cpd"), or pathway level ("pathway").
combine.level	Character, input whether to combine p-values or pool the peaks.
pval.method	Character, input the method to perform p-value combination.
es.method	Character, input the method to perform effect-size meta-analysis.
rank.metric	Character, input how to calculate pre-ranking metric. "mean" to use the average, "min" to use the lowest score, "max" to use the highest score.
mutual.feats	mutual.feats, logical
pooled_cutoff	pooled_cutoff, numeric

Author(s)

Jasmine Chong, Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`PerformMirrorPlotting` *PerformMirrorPlotting*

Description

PerformMirrorPlotting

Usage

```
PerformMirrorPlotting(
  mSetObj = NA,
  fragDB_path = NA,
  peak_idx,
  sub_idx,
  interactive = T,
  ppm,
  dpi,
  format,
  width,
  height
)
```

Arguments

`mSetObj`	mSetObj
`fragDB_path`	Fragmentation database path
`peak_idx`	peak_idx
`sub_idx`	sub_idx
`interactive`	interactive or not
`ppm`	ppm
`dpi`	dpi
`format`	format
`width`	width
`height`	height
`featurelabel`	featurelabel
`imageNM`	imageNM

PerformMirrorPlottingWeb
PerformMirrorPlottingWeb

Description

PerformMirrorPlottingWeb

Usage

```
PerformMirrorPlottingWeb(
  mSetObj = NA,
  fragDB_path,
  featurelabel,
  result_num,
  sub_idx,
  ppm,
  imageNM,
  dpi,
  format,
  width,
  height
)
```

Arguments

mSetObj	mSetObj
fragDB_path	Fragmentation database path
featurelabel	featurelabel
result_num	result_num
sub_idx	sub_idx
ppm	ppm
imageNM	imageNM
dpi	dpi
format	format
width	width
height	height

PerformMS1ResultsFormatting

PerformMS1ResultsFormatting This function is used to format the results from other tools into the generic format of MetaboAnalystR Currently,we are supporting the compatibility for four commonly used open-source tools: MS-DIAL, MZmine, Asari and XCMS online The first parameter file_path should be a valid file of the result. User need to specify the type in the 2nd argument, type. This argument can be msdial, mzmine, asari and xcms Please note, if your original data does not contain meta information, you need to manually add them in the generated "metaboanalyst_input.csv" file The formatted file is 'sample in columns'.

Description

PerformMS1ResultsFormatting This function is used to format the results from other tools into the generic format of MetaboAnalystR Currently,we are supporting the compatibility for four commonly used open-source tools: MS-DIAL, MZmine, Asari and XCMS online The first parameter file_path should be a valid file of the result. User need to specify the type in the 2nd argument, type. This argument can be msdial, mzmine, asari and xcms Please note, if your original data does not contain meta information, you need to manually add them in the generated "metaboanalyst_input.csv" file The formatted file is 'sample in columns'.

Usage

```
PerformMS1ResultsFormatting(file_path, type, meta_data = NA)
```

Arguments

file_path	
type	
meta_data	this is path to a table containing two columns, the first column is the sample names and second column is the group information

PerformMS2ResultsFormatting

PerformMS2ResultsFormatting This function is used to format the results from other tools into the generic format of MetaboAnalystR for functional analysis Currently,we are supporting the compatibility for four commonly used open-source tools: MS-FINDER, and SIRIUS The first parameter file_path should be a valid file of the result. User need to specify the type in the 2nd argument, type. This argument can be msfinder, or sirius The 3rd column

Description

PerformMS2ResultsFormatting This function is used to format the results from other tools into the generic format of MetaboAnalystR for functional analysis Currently,we are supporting the compatibility for four commonly used open-source tools: MS-FINDER, and SIRIUS The first parameter file_path should be a valid file of the result. User need to specify the type in the 2nd argument, type. This argument can be msfinder, or sirius The 3rd column

Usage

```
PerformMS2ResultsFormatting(file_path, type, MS1_features_list = NA)
```

Arguments

file_path	file path of NS2 file
type	type, can be msfinder or sirius
MS1_features_list	this is feature list used functional analysis

---

`performMS2searchBatch` *performMS2searchBatch*

Description

performMS2searchBatch

Usage

```
performMS2searchBatch(
  mSetObj = NA,
  ppm1 = 10,
  ppm2 = 25,
  dbpath = "",
  frgdbpath = "",
  database = "all",
  similarity_meth = 0,
  precMZ = NA,
  sim_cutoff = 30,
  ionMode = "positive",
  unit1 = "ppm",
  unit2 = "ppm",
  ncores = 1
)
```

Arguments

mSetObj	mSetObj
ppm1	ppm value for ms1
ppm2	ppm value for ms2
dbpath	database path
frgdbpath	fragmentation database path
database	database option
similarity_meth	similarity computing method
precMZ	mz of precursor
sim_cutoff	filtration cutoff of similarity score. will be enabled soon.
ionMode	ion mode, for ESI+, is should be 1. for ESI-, it should be 0
unit1	ppm or da for ms1 matching
unit2	ppm or da for ms2
ncores	number of cpu cores used to search

Author(s)

Zhiqiang Pang

---

performMS2searchSingle

performMS2searchSingle

Description

performMS2searchSingle

Usage

```
performMS2searchSingle(
  mSetObj = NA,
  ppm1 = 10,
  ppm2 = 25,
  dbpath = "",
  frgdbpath = "",
  database = "all",
  similarity_meth = 0,
  precMZ = NA,
  sim_cutoff = 30,
  ionMode = "positive",
  unit1 = "ppm",
  unit2 = "ppm"
)
```

Arguments

mSetObj	mSetObj
ppm1	ppm value for ms1
ppm2	ppm value for ms2
dbpath	database path
frgdbpath	fragmentation database path
database	database option
similarity_meth	similarity computing method
precMZ	mz of precursor
sim_cutoff	filtration cutoff of similarity score. will be enabled soon.
ionMode	ion mode, for ESI+, is should be 1. for ESI-, it should be 0
unit1	ppm or da for ms1 matching
unit2	ppm or da for ms2

PerformMultiMatch *Perform multiple name matches*

Description

Given a query, performs compound name matching.

Usage

```
PerformMultiMatch(mSetObj = NA, q, lipid)
```

Arguments

mSetObj	Input name of the created mSet Object.
q	Input the query.
lipid	lipid, logical

`PerformParamsOptimization` *Perform Parameters Optimization*

Description

This function is used to optimize the critical parameters of peak picking and alignment for the following data processing. It utilizes the trimed data and the internal instrument-specific parameters. Parallel computing will be performed. The number of cores user want to use could be specified.

Usage

```
PerformParamsOptimization(
  mSet,
  param = NULL,
  method = "DoE",
  ncore = 4,
  running.controller = NULL
)
```

Arguments

`mSet`	mSet object, usually generated by 'PerformROIExtraction' or 'PerformDataTrimming' here.
`param`	List, Parameters defined by 'SetPeakParam' function.
`method`	Character, method of parameters optimization, including "DoE' only. Default is "DoE". Other method is under development.
`ncore`	Numeric, CPU threads number used to perform the parallel based optimization. If thers is memory issue, please reduce the 'ncore' used here. For default, 2/3 CPU threads of total will be used.
`running.controller`	The resuming pipeline running controller. Optional. Don't need to define by hand.

Details

PerformParamsOptimization

Value

will a parameter object can be used for following processing

Author(s)

Zhiqiang Pang <zhiqiang.pang@mail.mcgill.ca> Jeff Xia <jeff.xia@mcgill.ca> Mcgill University

PerformPeakProfiling *PerformPeakProfiling*

Description

PerformPeakProfiling

Usage

```
PerformPeakProfiling(mSet, Params, plotSettings, ncore)
```

Arguments

mSet	mSet
Params	Params
plotSettings	plotSettings
ncore	number of cores

PerformPowerProfiling *Perform power profiling*

Description

Perform power profiling of data

Usage

```
PerformPowerProfiling(mSetObj=NA, fdr.lvl, smplSize)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
fdr.lvl	Specify the false-discovery rate level.
smplSize	Specify the maximum sample size, the number must be between 60-1000.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PerformPSEA *Function to perform peak set enrichment analysis*

Description

This is the main function that performs either the mummichog algorithm, GSEA, or both for peak set enrichment analysis.

Usage

```
PerformPSEA(mSetObj=NA, lib, libVersion, minLib, permNum = 100)
```

Arguments

mSetObj	Input the name of the created mSetObj object.
lib	Input the name of the organism library, default is hsa_mfn.
libVersion	Input the version of the KEGG pathway libraries ("current" or "old").
minLib	Numeric, input the minimum number of metabolites needed to consider the pathway or metabolite set.
permNum	Numeric, input the number of permutations to perform. Default is 100.

Author(s)

Jasmine Chong, Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PerformPvalCombination

Meta-Analysis Method: Combining p-values

Description

This function is one of three methods to perform meta-analysis. Here, p-values are combined using either the Fisher's method or the Stouffer's method.

Usage

```
PerformPvalCombination(mSetObj = NA, method = "stouffer", BHth = 0.05)
```

Arguments

mSetObj	Input name of the created mSet Object.
method	Method of p-value combination. By default it is "stouffer", else it is "fisher".
BHth	Numeric input to set the significance level. By default it is 0.05.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`PerformROIExtraction` *Perform ROI Extraction from raw MS data (PerformDataTrimming)*

Description

This function performs the raw data trimming. This function will output an trimmed MSnExp file to memory or hardisk according to the choice of users must provide the data path for 'datapath', and optionally provide other corresponding parameters.

Usage

```
PerformROIExtraction(
  datapath,
  mode = "ssm",
  write = FALSE,
  mz,
  mzdiff,
  rt,
  rtdiff,
  rt.idx = 1/15,
  rmConts = TRUE,
  plot = TRUE,
  running.controller = NULL
)
```

Arguments

`datapath`	Character, the path of the raw MS data files' or folder's path (.mzXML, .CDF and .mzML) for parameters training.
`mode`	Character, mode for data trimming to select the chraracteristic peaks. Default is 'ssm'. Users could select random trimed according to mz value (mz_random) or RT value (rt_random). Besides, specific peaks at certain mz (mz_specific) or RT (rt_specific) could also be extracted. 'none' will not trim the data.
`write`	Logical, if true, will write the trimmed data to the directory 'trimmed' folder in the datapath. The data in memory will be kept.
`mz`	Numeric, mz value(s) for specific selection. Positive values means including (the values indicted) and negative value means excluding/removing.
`mzdiff`	Numeric, the deviation (ppm) of mz value(s).
`rt`	Numeric, rt value for specific selection. Positive values means including and negative value means excluding.
`rtdiff`	Numeric, the deviation (seconds) of rt value(s).

rt.idx	Numeric, the relative rt (retention time) range, from 0 to 1. 1 means all retention time will be retained, while 0 means none. Default is 1/15. If default rt.idx produce too few peaks, please consider increasing this value.
rmConts	LOgical, whether to exclude/remove the potential contamination for parameters optimization. Default is TRUE.
plot	Logical, if TRUE, will plot the chromatogram of the trimmed data.
running.controller	The resuming pipeline running controller. Optional. Don't need to define by hand.

Value

will return an mSet objects with extracted ROI

Author(s)

Zhiqiang Pang <zhiqiang.pang@mail.mcgill.ca> Jeff Xia <jeff.xia@mcgill.ca> Mcgill University License: GNU GPL (>= 2)

PerformSignalDriftCorrection

Signal Drift Correction

Description

This function is designed to perform the signal drift correction. Batch effect and signal drift correction will be performed with QC-RLSC method in this function.

Usage

```
PerformSignalDriftCorrection(mSetObj = NA, imgName = NULL)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input the name of the plot to create

Author(s)

Zhiqiang Pang, Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PerformVoteCounting *Meta-Analysis Method: Vote Counting*

Description

This function is one of three methods to perform meta-analysis. Here, significant features are selected based on a selected criteria (i.e. an adjusted p-value <0.05 and the same direction of FC) for each dataset. The votes are then calculated for each feature by counting the total of number of times a feature is significant across all included datasets. However, this method is statistically inefficient and should be considered the last resort in situations where other methods to perform meta-analysis cannot be applied.

Usage

```
PerformVoteCounting(mSetObj = NA, BHth = 0.05, minVote)
```

Arguments

mSetObj	Input name of the created mSet Object.
BHth	Numeric input to set the significance level. By default it is 0.05.
minVote	Numeric input to set the minimum vote-count.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

Plot.Permutation *Plot results of permutation tests*

Description

Plot results of permutation tests

Usage

```
Plot.Permutation(mSetObj=NA, imgName, format="png", dpi=72)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
imgName	Input a name for the plot
format	elect the image format, "png", of "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`Plot.sampletrend` *Sample Trend Scatter*

Description

Scatter sample trend comparison between all sample of different batches

Usage

```
Plot.sampletrend(
  mSetObj,
  imgName,
  format = "png",
  dpi = 72,
  width = NA,
  method
)
```

Arguments

`mSetObj`	Input name of the created mSet Object
`imgName`	Input a name for the plot
`format`	Select the image format, "png", or "pdf".
`dpi`	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 600.
`width`	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.
`method`	method of correction

Author(s)

Zhiqiang Pang <zhiqiang.pang@mail.mcgill.ca>, Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotAccuracy *Plot classification performance using different features for Multi-Biomarker*

Description

Plot of the accuracy of classification with an increasing number of features.

Usage

```
PlotAccuracy(mSetObj=NA, imgName, format="png", dpi=72)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
imgName	Input a name for the plot
format	Select the image format, "png", of "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotANOVA *Plot ANOVA*

Description

Plot ANOVA

Usage

```
PlotANOVA(mSetObj=NA, imgName, format="png", dpi=72, width=NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotANOVA2 *Plot Venn diagram of ANOVA results*

Description

Plot Venn diagram of ANOVA results

Usage

```
PlotANOVA2(mSetObj, imgName, format="png", dpi=72, width=NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotASCA.Permutation *Plot ASCA permutation*

Description

Plot plsda classification performance using different components

Usage

```
PlotASCA.Permutation(mSetObj=NA, imgName, format="png", dpi=72, width=NA)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotAscaImpVar *Plot the important variables for each factor*

Description

Plot the important variables for each factor

Usage

```
PlotAscaImpVar(mSetObj=NA, imgName, format, dpi, width=NA, type)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.
type	select model a, b, or ab

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotASCAInteraction *Plot ASCA interaction plots*

Description

Plot ASCA interaction plots

Usage

```
PlotASCAInteraction(mSetObj=NA, imgName, format="png", dpi=72, colorBW=FALSE, width=NA)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
colorBW	Logical, use black and white (TRUE) or colors (FALSE)
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotASCAModel *Plot score plots of each ASCA model for component 1 against time*

Description

Plot score plots of each ASCA model for component 1 against time

Usage

```
PlotASCAModel(mSetObj=NA, imgName, format="png", dpi=72, width=NA, type, colorBW=FALSE)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
imgName	Input a name for the ASCA score plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.
type	select model a or b
colorBW	Logical, use black/white coloring (T) or not (F)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotASCAModelScree *Plot scree plots for each model in ASCA*

Description

Plot scree plots for each model in ASCA

Usage

```
PlotASCAModelScree(mSetObj, imgName, format="png", dpi=72, width=NA)
```

Arguments

mSetObj	Input name of the created mSet Object.
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`PlotClustPCA` *Plot K-means summary PCA plot*

Description

Plot K-means summary PCA plot

Usage

```
PlotClustPCA(
  mSetObj,
  imgName,
  format = "png",
  dpi = 72,
  width = NA,
  colpal = "default",
  anal = "km",
  labels = "T"
)
```

Arguments

`mSetObj`	Input name of the created mSet Object
`imgName`	Input a name for the plot
`format`	Select the image format, "png", or "pdf".
`dpi`	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
`width`	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.
`colpal`	palete of color
`anal`	analysis type
`labels`	labels to show, default is "T"

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`PlotCmpdSummary` *Plot compound summary change to use dataSet$proc instead of dataSet$orig in case of too many NAs*

Description

Plot compound summary change to use dataSet$proc instead of dataSet$orig in case of too many NAs

Usage

```
PlotCmpdSummary(
  mSetObj = NA,
  cmpdNm,
  meta = "NA",
  meta2 = "NA",
  count = 0,
  format = "png",
  dpi = 72,
  width = NA
)
```

Arguments

`mSetObj`	Input the name of the created mSetObj (see InitDataObjects)
`cmpdNm`	Input the name of the compound to plot
`meta`	meta is "NA"
`meta2`	only applicable for multifac module, secondary factor
`count`	img count number
`format`	Input the format of the image to create
`dpi`	Input the dpi of the image to create
`width`	Input the width of the image to create

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotCmpdView *Plot Compound View*

Description

Plots a bar-graph of selected compound over groups

Usage

```
PlotCmpdView(mSetObj=NA, cmpdNm, format="png", dpi=72, width=NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
cmpdNm	Input a name for the compound
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotConcRange *Plot the compound concentration data compared to the reference concentration range*

Description

Plot the compound concentration data compared to the reference concentration range

Usage

```
PlotConcRange(mSetObj, nm, format="png", dpi=72, width=NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
nm	of the input compound
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotCorr *Pattern hunter, correlation plot*

Description

Plot correlation

Usage

```
PlotCorr(
  mSetObj = NA,
  imgName,
  searchType = "feature",
  format = "png",
  dpi = 72,
  width = NA
)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
searchType	searchType, default is "feature"
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`PlotCorrHeatMap` *Pattern hunter, corr heatmap*

Description

Plot correlation heatmap

Usage

```
PlotCorrHeatMap(
  mSetObj = NA,
  imgName,
  format = "png",
  dpi = 72,
  width = NA,
  target,
  cor.method,
  colors,
  fix.col,
  no.clst,
  fz,
  unit,
  corrCutoff = 0
)
```

Arguments

`mSetObj`	Input name of the created mSet Object.
`imgName`	Input the name of the image to create
`format`	Select the image format, "png", or "pdf".
`dpi`	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
`width`	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.
`target`	Input "row" to select features, or "col" to select samples.
`cor.method`	Indicate the correlation method, 'pearson', 'spearman', or 'kendall'.
`colors`	Indicate the colors for the heatmap, "bwm" for default, "gbr" for red/green, "heat" for heat colors, "topo" for topo colors, and "gray" for gray scale.
`fix.col`	Logical, fix colors (TRUE) or not (FALSE).

no.clst	Logical, indicate if the correlations should be clustered (TRUE) or not (FALSE).
corrCutoff	set corrCutoff McGill University, Canada License: GNU GPL (>= 2)
viewOpt	Indicate "overview" to get an overview of the heatmap, and "detail" to get a detailed view of the heatmap.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca>

PlotDetailROC *Plot detailed ROC*

Description

Plot detailed ROC

Usage

```
PlotDetailROC(mSetObj = NA, imgName, thresh, sp, se, dpi = 72, format = "png")
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
imgName	Input a name for the plot
thresh	Input the threshold
sp	Specificity
se	Sensitivity
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
format	Select the image format, "png", or "pdf".

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotEBAM.Cmpd *Plot EBAM*

Description

Plot EBAM

Usage

```
PlotEBAM.Cmpd(mSetObj=NA, imgName, format, dpi, width)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotEnrichDotPlot *Plot MSEA Dot Plot*

Description

Dot plot of enrichment analysis results.

Usage

```
PlotEnrichDotPlot(
  mSetObj = NA,
  enrichType = "ora",
  imgName,
  format = "png",
  dpi = 72,
  width = NA
)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
enrichType	Input whether the enrichment analysis was over-respresentation analysis (ora) or quantitative enrichment analysis (qea).
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotEnrichNet.Overview

PlotEnrichNet.Overview

Description

Used in higher functions, the color is based on p values

Usage

```
PlotEnrichNet.Overview(folds, pvals, layoutOpt = layout.fruchterman.reingold)
```

Arguments

folds	Input fold-change for bar plot
pvals	Input p-values for bar plot
layoutOpt	Input the layout option, default is set to layout.fruchterman.reingold

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotEnrichPieChart *Create a pie chart for compound classes*

Description

This function creates a pie-chart for compound classes in the enrichment analysis if the library is based on chemical ontologies.

Usage

```
PlotEnrichPieChart(
  mSetObj = NA,
  enrichType,
  imgName,
  format = "png",
  dpi = 72,
  width = 8,
  maxClass = 15,
  colPal = "Set1"
)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
enrichType	enrichType
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Numeric, input the width, the default is 8.
maxClass	Numeric, input the maximum number of lipid classes to include in the pie-chart. By default this is set to 15.
colPal	Character, input the preferred R Color Brewer palette to be used for the pie chart. By default this is set to "Set1".

PlotFC *Plot fold change*

Description

Plot fold change analysis

Usage

```
PlotFC(mSetObj=NA, imgName, format="png", dpi=72, width=NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotHCTree *Plot Dendrogram*

Description

Dendogram

Usage

```
PlotHCTree(
  mSetObj = NA,
  imgName,
  format = "png",
  dpi = 72,
  width = NA,
  smplDist,
  clstDist
)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.
smplDist	Method to calculate sample distance
clstDist	Method to calculate clustering distance

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotHeatMap *Create Heat Map Plot*

Description

Plot a heatmap based on results from t-tests/ANOVA, VIP or randomforest

Usage

```
PlotHeatMap(
  mSetObj = NA,
  imgName,
  format = "png",
  dpi = 72,
  width = NA,
  dataOpt,
  scaleOpt,
  smplDist,
  clstDist,
  palette,
  fzCol,
  fzRow,
  fzAnno,
  annoPer,
  unitCol,
  unitRow,
  rowV = T,
  colV = T,
```

```
  var.inx = NULL,
  border = T,
  grp.ave = F,
  show.legend = T,
  show.annot.legend = T,
  showColnm = T,
  showRownm = T,
  maxFeature = 2000
)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.
dataOpt	Set data options
scaleOpt	Set the image scale
smplDist	Input the sample distance method
clstDist	Input the clustering distance method
palette	Input color palette choice
rowV	Default is set to T
colV	Default is set to T
var.inx	Default is set to NA
border	Indicate whether or not to show cell-borders, default is set to T
grp.ave	Logical, default is set to F
viewOpt	Set heatmap options, default is set to "detail"
metadata	metadata

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotHeatMap2 *Plot heatmap visualization for time-series data*

Description

Plot heatmap visualization for time-series data

Usage

```
PlotHeatMap2(
  mSetObj = NA,
  imgName,
  dataOpt = "norm",
  scaleOpt = "row",
  format = "png",
  dpi = 72,
  width = NA,
  smplDist = "pearson",
  clstDist = "average",
  colorGradient = "npj",
  fzCol,
  fzRow,
  fzAnno,
  annoPer,
  unitCol,
  unitRow,
  rankingMethod = "mean",
  topFeature = 2000,
  useTopFeature = F,
  drawBorder = T,
  show.legend = T,
  show.annot.legend = T,
  showColnm = T,
  showRownm = F,
  maxFeature = 2000
)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
imgName	Input a name for the plot
dataOpt	dataOpt, default is "norm"
scaleOpt	scaleOpt
format	Select the image format, "png", or "pdf".

dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.
smplDist	Select distance measure: euclidean, pearson, or minkowski
clstDist	Select clustering algorithm: ward, average, complete, single
colorGradient	Select heatmap colors: bwm, gray
rankingMethod	rankingMethod
topFeature	topFeature
useTopFeature	Use significant features only: F or T (default false)
drawBorder	Show cell borders: F or T (default F)
viewOpt	Select overview or detailed view: overview or detail
includeRowNames	includeRowNames, logical

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`PlotImpBiomarkers` *Plot selected compounds by their percentage frequency*

Description

Plot the important variables of single biomarker model ranked by order of importance

Usage

```
PlotImpBiomarkers(mSetObj=NA, imgName, format="png", dpi=72,
mdl.inx, measure = "freq", feat.num = 15)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
imgName	Input a name for the plot
format	elect the image format, "png", of "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
mdl.inx	Model index, -1 selects the model with the best AUC, input 1-6 to view the important features of one of the top six models
measure	Choose to rank features by the frequency of being selected "freq", or the mean importance measure "mean"
feat.num	Input the number of features to include in the plot, by default it is 15.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`PlotImpVar` *Plot PLS important variables,*

Description

Plot PLS important variables, BHan: added bgcolor parameter for B/W color

Usage

```
PlotImpVar(mSetObj = NA, imp.vec, xlbl, feat.num = 15, color.BW = FALSE)
```

Arguments

`mSetObj`	Input name of the created mSet Object
`imp.vec`	Input the vector of important variables
`xlbl`	Input the x-label
`feat.num`	Numeric, set the feature numbers, default is set to 15
`color.BW`	Use black-white for plot (T) or colors (F)

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`PlotImpVarMeta` *Plot PLS important variables,*

Description

Plot PLS important variables, BHan: added bgcolor parameter for B/W color

Usage

```
PlotImpVarMeta(
  mSetObj = NA,
  imp.vec,
  xlbl,
  feat.num = 15,
  color.BW = FALSE,
  type = "meta"
)
```

Arguments

mSetObj	Input name of the created mSet Object
imp.vec	Input the vector of important variables
xlbl	Input the x-label
feat.num	Numeric, set the feature numbers, default is set to 15
color.BW	Use black-white for plot (T) or colors (F)
type	type, default is "type"

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotInmexGraph *Plot an igraph object and return the node information (position and labels)*

Description

Plot an igraph object and return the node information (position and labels) Used in a higher function

Usage

```
PlotInmexGraph(
  mSetObj,
  pathName,
  g,
  width = NA,
  height = NA,
  bg.color = NULL,
  line.color = NULL,
  format = "png",
  dpi = NULL
)
```

Arguments

mSetObj	Input name of the created mSet Object
pathName	Input the pathway name
g	Input the graph
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.
height	Input the height of the graph to create
bg.color	Set the background color, default is set to NULL

line.color	Set the line color, default is set to NULL
format	image format
dpi	dpi of the image

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotInmexPath *Plot integrated methods pathway analysis*

Description

Only update the background info for matched node

Usage

```
PlotInmexPath(
  mSetObj = NA,
  pathName,
  width = NA,
  height = NA,
  format = "png",
  dpi = NULL
)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
pathName	Input the Name of the pathway to plot.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.
height	Input the height of the image to create.
format	format of the image
dpi	dpi, dpi of the image

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotKEGGPath *Plot metabolome pathway*

Description

Plot KEGG pathway graph

Usage

```
PlotKEGGPath(
  mSetObj = NA,
  pathName,
  width = NA,
  height = NA,
  format = "png",
  dpi = NULL
)
```

Arguments

mSetObj	Input name of the created mSet Object
pathName	Input the name of the selected pathway
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.
height	Input the height of the created plot.
format	format of the image.
dpi	dpi of the image.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotKmeans *Plot K-means analysis*

Description

Plot K-means analysis

Usage

```
PlotKmeans(
  mSetObj = NA,
  imgName,
  format = "png",
  dpi = 72,
  width = NA,
  colpal = "default",
  facet = FALSE
)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.
colpal	Character, input "default" to use the default ggplot color scheme or "colblind" to use the color-blind friendly palette.
facet	logical, TRUE to plot in multiple facets

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotMBTimeProfile *Plot MB Time Profile*

Description

Plot MB Time Profile

Usage

```
PlotMBTimeProfile(
  mSetObj = NA,
  cmpdNm,
  version,
  format = "png",
  dpi = 72,
  width = NA
)
```

Arguments

mSetObj	Input name of the created mSet Object
cmpdNm	Input the name of the compound
version	image mark
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotMetaCorrHeatmap *Generate correlation heatmap for metadata*

Description

Plot correlation coefficients between metadata

Usage

```
PlotMetaCorrHeatmap(
  mSetObj = NA,
  cor.opt = "pearson",
  imgName,
  format = "png",
  dpi = 96,
  width = NA
)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
cor.opt	Meethod for computing correlation coefficient

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotMetaHeatmap *Generate heatmaps for metadata table*

Description

Plot a heatmap showing clustering patterns among the metadata

Usage

```
PlotMetaHeatmap(
  mSetObj = NA,
  clustSelOpt = "both",
  smplDist = "pearson",
  clstDist = "average",
  colorGradient = "bwm",
  includeRowNames = T,
  imgName,
  format = "png",
  dpi = 96,
  width = NA
)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
viewOpt	high-level summary or plotting the names inside cell

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotMetpaPath *Plot KEGG pathway*

Description

Plot KEGG pathway

Usage

```
PlotMetpaPath(
  mSetObj = NA,
  pathName,
  width = NA,
  height = NA,
```

```
  format = "png",
  dpi = NULL
)
```

Arguments

mSetObj	Input name of the created mSet Object
pathName	Input the name of the selected KEGG pathway
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.
height	height value for the image.
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

---

plotMirror *plotMirror*

Description

plotMirror

Usage

```
plotMirror(
  mSetObj = NA,
  featureidx = 1,
  precMZ,
  ppm,
  imageNM = "",
  dpi = 300,
  format = "png",
  width = 8,
  height = 8,
  cutoff_relative = 5
)
```

Arguments

mSetObj	mSetObj
featureidx	index of feature
precMZ	mz of precursor
ppm	ppm for ms2 fragment matching mz error
imageNM	image name
dpi	dpi of images
format	format of images
width	width of images
height	height of images
cutoff_relative	cutoff of relative intensity to filter out

Author(s)

Zhiqiang Pang

PlotMSEA.Overview *Plot MSEA overview*

Description

Barplot height is enrichment fold change color is based on p values, used in higher functions

Usage

```
PlotMSEA.Overview(folds, pvals)
```

Arguments

folds	Input the fold-change values
pvals	Input the p-values

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

plotMSfeature *plotMSfeature*

Description

plotMSfeature is used to plot MS feature stats for different groups

Usage

```
plotMSfeature(FeatureNM, format = "png", dpi = 72, width = NA)
```

Arguments

FeatureNM	FeatureNM
format	format
dpi	dpi
width	width

Author(s)

Zhiqiang Pang

PlotMultiFacCmpdSummary *Plot compound summary for multi-linear regression tool*

Description

Plot compound summary for multi-linear regression tool

Usage

```
PlotMultiFacCmpdSummary(
  mSetObj = NA,
  cmpdNm,
  meta,
  meta2,
  version,
  format = "png",
  dpi = 72,
  width = NA
)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
cmpdNm	Input the name of the compound to plot
meta	Input the metadata to visualize
version	version
format	Input the format of the image to create
dpi	Input the dpi of the image to create
width	Input the width of the image to create

Author(s)

Jessica Ewald<jessica.ewald@mcgill.ca> McGill University, Canada License: GPL-3 License

---

PlotNormSummary *Two plot summary plot: Feature View of before and after normalization*

Description

For each plot, the top is a box plot, bottom is a density plot

Usage

```
PlotNormSummary(mSetObj, imgName, format, dpi, width)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca>, Jasmine Chong McGill University, Canada

PlotOPLS.Imp *PlotOPLS.Imp OPLS VIP plotting function*

Description

PlotOPLS.Imp OPLS VIP plotting function

Usage

```
PlotOPLS.Imp(
  mSetObj = NA,
  imgName,
  format = "png",
  dpi = 72,
  width = NA,
  type = "vip",
  feat.nm = "tscore",
  feat.num = 15,
  color.BW = FALSE
)
```

Arguments

mSetObj	mSetObj objects generated from last step
imgName	image name
format	image format, can be "png", "jpg", "tiff", "pdf" and "svg"
dpi	numeric, dpi number
width	numeric, width number
type	analysis type, can be "vip" only
feat.nm	feature name, should be "tscore" for now
feat.num	feature number
color.BW	color information

PlotOPLS.MDL *Plot OPLS*

Description

Plot OPLS

Usage

```
PlotOPLS.MDL(mSetObj = NA, imgName, format = "png", dpi = 72, width = NA)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.

PlotOPLS.Permutation *Plot OPLS-DA permutation*

Description

Orthogonal PLS-DA (from ropls) perform permutation, using training classification accuracy as indicator, for two or multi-groups

Usage

```
PlotOPLS.Permutation(
  mSetObj = NA,
  imgName,
  format = "png",
  dpi = 72,
  width = NA
)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotOPLS.Splot *S-plot for OPLS-DA*

Description

Orthogonal PLS-DA (from ropls) S-plot for important features from OPLS-DA

Usage

```
PlotOPLS.Splot(
  mSetObj = NA,
  imgName,
  plotType = "all",
  format = "png",
  dpi = 72,
  width = NA
)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
plotType	plotType for the image, can be "all" or "custom"
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotOPLS2DScore *Create OPLS-DA score plot*

Description

Orthogonal PLS-DA (from ropls) score plot

Usage

```
PlotOPLS2DScore(
  mSetObj = NA,
  imgName,
  format = "png",
  dpi = 72,
  width = NA,
  inx1,
  inx2,
  reg = 0.95,
  show = 1,
  grey.scale = 0,
  cex.opt = "na"
)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.
inx1	Numeric, indicate the number of the principal component for the x-axis of the loading plot.
inx2	Numeric, indicate the number of the principal component for the y-axis of the loading plot.
reg	Numeric
show	Show variable labels, 1 or O
grey.scale	Numeric, indicate grey-scale, 0 for no, and 1 for yes

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotORA *Plot over-representation analysis (ORA)*

Description

Plot over-representation analysis (ORA)

Usage

```
PlotORA(mSetObj=NA, imgName, imgOpt, format="png", dpi=72, width=NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
imgName	Input a name for the plot
imgOpt	"net"
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotPathSummary *Plot a scatterplot (circle) overview of the matched pathways*

Description

x axis is the pathway impact factor y axis is the p value (from ORA or globaltest) return the circle information

Usage

```
PlotPathSummary(
  mSetObj = NA,
  show.grid,
  imgName,
  format = "png",
  dpi = 72,
  width = NA,
  xlim = NA,
  ylim = NA
)
```

Arguments

mSetObj	Input name of the created mSet Object
show.grid	logical, show grid or not
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5.
xlim	limit of x axis
ylim	limit of y axis

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotPathwayMetaAnalysis

PlotPathwayMetaAnalysis

Description

Function to create summary plot of MS Peaks to Paths meta-analysis at the pathway level. This function creates a summary plot of the MS Peaks to Paths meta-analysis at the pathway level. The plot can either be a heatmap or a network, both of which can be made interactive. NETWORK: The size of the nodes in the network correspond to the number of studies in which that pathway was significant. The color of the nodes correspond to the meta-p-value for each pathway, with (default coloring) red being the most significant and yellow the least.

Usage

```
PlotPathwayMetaAnalysis(
  mSetObj = NA,
  imgName,
  plotType = "heatmap",
  heatmap_colorType = "brewer",
  heatmap_palette = "RdYlBu",
  heatmap_interactive = FALSE,
  heatmap_square = TRUE,
  heatmap_allPaths = TRUE,
  heatmap_npaths = 25,
  heatmap_vertical = TRUE,
  heatmap_fontSize = 9,
  pvalCutoff = 0.05,
  overlap = 0.25,
  networkType = "static",
  layout = "kk",
  net_palette = "YlOrRd",
  netTextSize = 2.5,
  netPlotSize = 7.5,
  bubble_interactive = FALSE,
  bubbleMaxPaths = 15,
  bubble_colorType = "brewer",
  bubble_palette = "RdBu",
  bubbleFontSize = 9,
  bubblePlotSize = 7,
  format = "png",
  width = 7,
  height = 5,
  dpi = 300
)
```

Arguments

mSetObj	Input the name of the created mSetObj object.
imgName	name of image.
plotType	Use "heatmap" to create a heatmap summary, "network" to create a network summary, or "bubble" to create a bubble plot summary of the meta-analysis results.
heatmap_colorType	Character, "brewer" for R Color Brewer scales or "viridis" for viridis color scales. Used for creating the heatmap color scheme.
heatmap_palette	Character, input the preferred color palette according to R Color Brewer or viridis (e.g. "RdBu").
heatmap_interactive	Boolean. FALSE to create a non-interactive plot and TRUE for plotly generated interactive plot.

`heatmap_square` Boolean. TRUE for the heatmap to be squares versus rectangles (FALSE).

`heatmap_allPaths`
: Boolean. TRUE to use all paths when plotting the heatmap. FALSE to use a subset of paths, number defined in npaths.

`heatmap_npaths` Numeric. The number of pathways to subset the pathway results.

`heatmap_vertical`
: Boolean. TRUE, heatmap plot will be vertical. FALSE, heatmap plot will be horizontal.

`heatmap_fontSize`
: Numeric, input the preferred font size to be used in the heatmap plot.

`pvalCutoff` The size of the nodes in the network correspond to the number of studies in which that pathway was significant. This pvalCutoff (Numeric) is thus used to determine whether or not a pathway was found to be significant in each individual study.

`overlap` Numeric, this number is used to create edges between the nodes. By default it is set to 0.25, meaning that if 2 pathways (nodes) share 25 the same compounds/empirical compounds, they will be connected by a node.

`networkType` Character, "static" to create a static image or "interactive" to create an interactive network saved as an html in your working directory.

`layout` Character, layout from ggraph. "kk" for the spring-based algorithm by Kamada and Kawai as default. "drl" for force directed algorithm from the DrL toolbox. "lgl" for Large Graph Layout. "fr" for force-directed of Fruchterman and Reingold.

`net_palette` Character, input the color code for the nodes in the network. Default is "YlOrRd". Uses the hcl palettes from the grDevices. Use hcl.pals() to view the name of all available palettes.

`netTextSize` Numeric, input the preferred font size to be used in the network plot.

`netPlotSize` Numeric, input the preferred dimensions (in inches) of the network to be saved.

`bubble_interactive`
: logical

`bubbleMaxPaths` maximum number of pathways

`bubble_colorType`
: Character, "brewer" for R Color Brewer scales or "viridis" for viridis color scales. Used for creating the bubble plot color scheme.

`bubble_palette` Character, use two/three colors max if using R ColorBrewer palettes for pleasing looking plots.

`bubbleFontSize` font size of the bubble plot

`bubblePlotSize` plot size of the bubble plot

`format` format of the image

`width` width of the image

`height` height of the image

`dpi` dpi of the image

Author(s)

Jasmine Chong, Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`PlotPCA.overview` *Scatter plot colored by different batches*

Description

Scatter plot colored by different batches

Usage

```
PlotPCA.overview(
  mSetObj,
  imgName,
  format = "png",
  dpi = 72,
  width = NA,
  method
)
```

Arguments

`mSetObj`	Input name of the created mSet Object
`imgName`	Input a name for the plot
`format`	Select the image format, "png", or "pdf".
`dpi`	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 600.
`width`	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.
`method`	method of correction

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotPCA2DScore *Create 2D PCA score plot*

Description

Rotate PCA analysis

Usage

```
PlotPCA2DScore(mSetObj=NA, imgName, format="png",
dpi=72, width=NA, pcx, pcy, reg = 0.95, show=1, grey.scale = 0)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.
pcx	Specify the principal component on the x-axis
pcy	Specify the principal component on the y-axis
reg	Numeric, input a number between 0 and 1, 0.95 will display the 95 percent confidence regions, and 0 will not.
show	Display sample names, 1 = show names, 0 = do not show names.
grey.scale	Use grey-scale colors, 1 = grey-scale, 0 = not grey-scale.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotPCA3DLoading *PlotPCA3DLoading*

Description

PlotPCA3DLoading

Usage

```
PlotPCA3DLoading(mSetObj = NA, imgName, format = "json", inx1, inx2, inx3)
```

Arguments

mSetObj	mSetObj
imgName	imgName
format	format
inx1	inx1
inx2	inx2
inx3	inx3

PlotPCA3DScore *Create 3D PCA score plot*

Description

Rotate PCA analysis

Usage

```
PlotPCA3DScore(mSetObj=NA, imgName, format="json", inx1, inx2, inx3)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
inx1	Numeric, indicate the number of the principal component for the x-axis of the loading plot.
inx2	Numeric, indicate the number of the principal component for the y-axis of the loading plot.
inx3	Numeric, indicate the number of the principal component for the z-axis of the loading plot.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotPCA3DScoreImg *Create 3D PCA score plot*

Description

This function creates both a static 3D PCA score plot as well as an interactive 3D PCA score plot using the plotly R package. The 3D PCA score plot is stored in the mSetObj (mSetObj$imgSet$pca.3d). To view the plot, if your mSetObj is named mSet, type "mSet$imgSet$pca.3d" inro your R console, and the 3D plot will appear.

Usage

```
PlotPCA3DScoreImg(mSetObj=NA, imgName,
format="png", dpi=72, width=NA, inx1, inx2, inx3, angl)
```

Arguments

mSetObj	Input name of the created mSet Object.
imgName	Input a name for the plot.
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.
inx1	Numeric, indicate the number of the principal component for the x-axis of the loading plot.
inx2	Numeric, indicate the number of the principal component for the y-axis of the loading plot.
inx3	Numeric, indicate the number of the principal component for the z-axis of the loading plot.
angl	Input the angle

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotPCABiplot *Create PCA Biplot, set xpd = T to plot outside margin*

Description

Rotate PCA analysis

Usage

```
PlotPCABiplot(mSetObj=NA, imgName, format="png", dpi=72, width=NA, inx1, inx2)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.
inx1	Numeric, indicate the number of the principal component for the x-axis of the loading plot.
inx2	Numeric, indicate the number of the principal component for the y-axis of the loading plot.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotPCALoading *Plot PCA loadings and also set up the matrix for display*

Description

Rotate PCA analysis

Usage

```
PlotPCALoading(mSetObj=NA, imgName, format="png", dpi=72, width=NA, inx1, inx2)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.
inx1	Numeric, indicate the number of the principal component for the x-axis of the loading plot.
inx2	Numeric, indicate the number of the principal component for the y-axis of the loading plot.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotPCAPairSummary *Plot PCA pair summary, format image in png, tiff, pdf, ps, svg*

Description

Rotate PCA analysis

Usage

```
PlotPCAPairSummary(mSetObj=NA, imgName, format="png", dpi=72, width=NA, pc.num)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.
pc.num	Numeric, input a number to indicate the number of principal components to display in the pairwise score plot.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`PlotPCAScree` *Plot PCA scree plot*

Description

Rotate PCA analysis

Usage

```
PlotPCAScree(mSetObj=NA, imgName, format="png", dpi=72, width=NA, scree.num)
```

Arguments

`mSetObj`	Input name of the created mSet Object
`imgName`	Input a name for the plot
`format`	Select the image format, "png", or "pdf".
`dpi`	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
`width`	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.
`scree.num`	Numeric, input a number to indicate the number of principal components to display in the scree plot.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`PlotPeaks2Paths` *PlotPeaks2Paths*

Description

Plots either the original mummichog or GSEA results.

Usage

```
PlotPeaks2Paths(
  mSetObj = NA,
  imgName = "",
  format = "png",
  dpi = 72,
  width = 9,
  labels = "default",
  num_annot = 5,
  interactive = F
)
```

Arguments

mSetObj	Input the name of the created mSetObj object
imgName	Input a name for the plot
format	Character, input the format of the image to create.
dpi	Numeric, input the dpi of the image to create.
width	Numeric, input the width of the image to create.
labels	Character, indicate if the plot should be labeled. By default it is set to "default", and the 5 top-ranked pathways per each algorithm will be plotted. Users can adjust the number of pathways to be annotated per pathway using the "num_annot" parameter.
num_annot	number of annotations for top plotting

Author(s)

Jasmine Chong, Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotPLS.Classification

Plot PLS-DA classification performance using different components

---

Description

Plot plsda classification performance using different components

Usage

```
PlotPLS.Classification(
  mSetObj = NA,
  imgName,
  format = "png",
  dpi = 72,
  width = NA
)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotPLS.Imp *Plot PLS important features*

Description

Plot PLS important features, BHan: added bgcolor parameter for B/W color

Usage

```
PlotPLS.Imp(
  mSetObj = NA,
  imgName,
  format = "png",
  dpi = 72,
  width = NA,
  type,
  feat.nm,
  feat.num,
  color.BW = FALSE
)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.

width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.
type	Indicate the type variables of importance to use, "vip" to use VIp scores, or "type" for coefficients
feat.nm	Feature name
feat.num	Feature numbers
color.BW	Logical, true to use black and white, or false to not

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`PlotPLS.Permutation` *Plot PLS-DA classification performance using different components, permutation*

Description

Plot plsda classification performance using different components

Usage

```
PlotPLS.Permutation(
  mSetObj = NA,
  imgName,
  format = "png",
  dpi = 72,
  width = NA
)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotPLS2DScore *Plot PLS score plot*

Description

Plot PLS score plot

Usage

```
PlotPLS2DScore(
  mSetObj = NA,
  imgName,
  format = "png",
  dpi = 72,
  width = NA,
  inx1,
  inx2,
  reg = 0.95,
  show = 1,
  grey.scale = 0,
  cex.opt = "na"
)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.
inx1	Numeric, indicate the number of the principal component for the x-axis of the loading plot.
inx2	Numeric, indicate the number of the principal component for the y-axis of the loading plot.
reg	Numeric, default is 0.95
show	Show labels, 1 or 0
grey.scale	Numeric, use a grey scale (0) or not (1)

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotPLS3DLoading *PlotPLS3DLoading*

Description

PlotPLS3DLoading

Usage

```
PlotPLS3DLoading(mSetObj = NA, imgName, format = "json", inx1, inx2, inx3)
```

Arguments

mSetObj	mSetObj
imgName	imgName
format	format
inx1	inx1
inx2	inx2
inx3	inx3

PlotPLS3DScore *Plot PLS 3D score plot*

Description

Plot PLS 3D score plot

Usage

```
PlotPLS3DScore(mSetObj = NA, imgName, format = "json", inx1, inx2, inx3)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
inx1	Numeric, indicate the number of the principal component for the x-axis of the loading plot.
inx2	Numeric, indicate the number of the principal component for the y-axis of the loading plot.
inx3	Numeric, indicate the number of the principal component for the z-axis of the loading plot.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotPLS3DScoreImg *Plot PLS 3D score plot*

Description

This function creates two 3D PLS-DA score plots, the first is static for Analysis Report purposes, as well as an interactive 3D plot using the plotly R package. The 3D score plot is saved in the created mSetObj (mSetObj$imgSet$plsda.3d). To view the score plot, if the name of your mSetObj is mSet, enter "mSet$imgSet$plsda.3d" to view the interactive score plot.

Usage

```
PlotPLS3DScoreImg(
  mSetObj = NA,
  imgName,
  format = "png",
  dpi = 72,
  width = NA,
  inx1,
  inx2,
  inx3,
  angl
)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.
inx1	Numeric, indicate the number of the principal component for the x-axis of the loading plot.
inx2	Numeric, indicate the number of the principal component for the y-axis of the loading plot.
inx3	Numeric, indicate the number of the principal component for the z-axis of the loading plot.
angl	Input the angle

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotPLSLoading *Plot PLS loading plot, also set the loading matrix for display*

Description

Plot PLS loading plot, also set the loading matrix for display

Usage

```
PlotPLSLoading(
  mSetObj = NA,
  imgName,
  format = "png",
  dpi = 72,
  width = NA,
  inx1,
  inx2
)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.
inx1	Numeric, indicate the number of the principal component for the x-axis of the loading plot.
inx2	Numeric, indicate the number of the principal component for the y-axis of the loading plot.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotPLSPairSummary *Plot PLS pairwise summary*

Description

Plot PLS pairwise summary

Usage

```
PlotPLSPairSummary(
  mSetObj = NA,
  imgName,
  format = "png",
  dpi = 72,
  width = NA,
  pc.num
)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.
pc.num	Numeric, indicate the number of principal components

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotPowerProfile *Plot power profile*

Description

Plot power profile, specifying FDR level and sample size. It will return the image as well as the predicted power at various sample sizes.

Usage

```
PlotPowerProfile(mSetObj=NA, fdr.lvl, smplSize, imgName, format, dpi, width)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
fdr.lvl	Specify the false-discovery rate level.
smplSize	Specify the maximum sample size, the number must be between 60-1000.
imgName	Specify the name to save the image as.
format	Specify the format of the image to save it as, either "png" or "pdf".
dpi	Specify the dots-per-inch (dpi). By default it is 72, for publications the recommended dpi is 300.
width	Specify the width of the image. NA specifies a width of 9, 0 specifies a width of 7, otherwise input a chosen width.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotPowerStat *Plot power statistics*

Description

Create plot for power statistics

Usage

```
PlotPowerStat(mSetObj, imgName, format="png", dpi=72, width=NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
imgName	Specify the name to save the image as.
format	Specify the format of the image to save it as, either "png" or "pdf"
dpi	Specify the dots-per-inch (dpi). By default it is 72, for publications the recommended dpi is 300.
width	Specify the width of the image. NA or 0 specifies a width of 10, otherwise input a chosen width.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotProbView *Plot a summary view of the classification result*

Description

Plot of predicted class probabilities. On the x-axis is the proability, and the y-axis is the index of each predicted sample based on the probility. The samples are turned into separations at the x-axis. This plot can be created for multivariate ROC curve analysis using SVM, PLS, and RandomForest. Please note that sometimes, not all samples will be tested, instead they will be plotted at the 0.5 neutral line.

Usage

```
PlotProbView(mSetObj=NA, imgName, format="png", dpi=72, mdl.inx, show, showPred)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
imgName	Input a name for the plot
format	Select the image format, "png", of "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
mdl.inx	Model index, 0 means to compare all models, -1 means to use the best model, input 1-6 to plot a ROC curve for one of the top six models
show	1 or 0, if 1, label samples classified to the wrong groups
showPred	Show predicted samples

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotProbViewTest *Plot a summary view of the classification result of tester prediction*

Description

Plot of predicted class probabilities. On the x-axis is the proability, and the y-axis is the index of each predicted sample based on the probility. The samples are turned into separations at the x-axis. This plot can be created for multivariate ROC curve analysis using SVM, PLS, and RandomForest. Please note that sometimes, not all samples will be tested, instead they will be plotted at the 0.5 neutral line.

Usage

```
PlotProbViewTest(mSetObj=NA, imgName, format="png", dpi=72, mdl.inx, show, showPred)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
imgName	Input a name for the plot
format	Select the image format, "png", of "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
mdl.inx	Model index, 0 means to compare all models, -1 means to use the best model, input 1-6 to plot a ROC curve for one of the top six models
show	1 or 0, if 1, label samples classified to the wrong groups
showPred	Show predicted samples

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

---

plotProfile *Plot the variable across time points (x)*

Description

Colored by experimental conditions, used in higher function

Usage

```
plotProfile(mSetObj = NA, varName)
```

Arguments

mSetObj	Input name of the created mSet Object
varName	Input the name of the variable

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotPSEAIntegPaths *PlotPSEAIntegPaths*

Description

Plots both the original mummichog and the GSEA results by combining p-values using the Fisher's method (sumlog).

Usage

```
PlotPSEAIntegPaths(
  mSetObj = NA,
  imgName = "",
  format = "png",
  dpi = 72,
  width = 9,
  labels = "default",
  labels.x = 5,
  labels.y = 5,
  scale.axis = TRUE,
  interactive = F
)
```

Arguments

mSetObj	Input the name of the created mSetObj object
imgName	Input a name for the plot
format	Character, input the format of the image to create.
dpi	Numeric, input the dpi of the image to create.
width	Numeric, input the width of the image to create.
labels	Character, indicate if the plot should be labeled. By default it is set to "default", and the 5 top-ranked pathways per each algorithm will be plotted. Users can adjust the number of pathways to be annotated per pathway using the "labels.x" and "labels.y" parameters. Users can set this to "none" for no annotations, or "all" to annotate all pathways.
labels.x	Numeric, indicate the number of top-ranked pathways using the fGSEA algorithm to annotate on the plot.
labels.y	Numeric, indicate the number of top-ranked pathways using the original mummichog algorithm to annotate on the plot.
scale.axis	logical, TRUE to scale

Author(s)

Jasmine Chong, Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotQEA.MetSet *View individual compounds related to a given metabolite set*

Description

View individual compounds related to a given metabolite set Functions for various plots for enrichment analysis

Usage

```
PlotQEA.MetSet(mSetObj=NA, setNM, format="png", dpi=72, width=NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
setNM	Input the name of the metabolite set
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotQEA.Overview *Plot QEA overview*

Description

Plot QEA overview

Usage

```
PlotQEA.Overview(mSetObj=NA, imgName, imgOpt, format="png", dpi=72, width=NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
imgName	Input a name for the plot
imgOpt	"net"
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotRF.Classify *Plot Random Forest*

Description

Random Forest plot

Usage

```
PlotRF.Classify(mSetObj, imgName, format, dpi, width)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotRF.ClassifyMeta *Plot Random Forest*

Description

Random Forest plot

Usage

```
PlotRF.ClassifyMeta(mSetObj, imgName, format, dpi, width, type)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.
type	plotting type, default is "meta".

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotRF.Outlier *Plot Random Forest outliers*

Description

Random Forest plot of outliers

Usage

```
PlotRF.Outlier(mSetObj=NA, imgName, format="png", dpi=72, width=NA)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotRF.VIP *Plot Random Forest variable importance*

Description

Random Forest plot of variable importance ranked by MeanDecreaseAccuracy

Usage

```
PlotRF.VIP(mSetObj=NA, imgName, format, dpi, width)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotRF.VIPMeta *Plot Random Forest variable importance*

Description

Random Forest plot of variable importance ranked by MeanDecreaseAccuracy

Usage

```
PlotRF.VIPMeta(mSetObj=NA, imgName, format, dpi, width, type)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.
type	type of image

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotROC *Plot ROC*

Description

Pred and auroc are lists containing predictions and labels from different cross-validations

Usage

```
PlotROC(mSetObj=NA, imgName, format="png", dpi=72, mdl.inx,
avg.method, show.conf, show.holdout, focus="fpr", cutoff = 1.0)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
imgName	Input a name for the plot
format	Select the image format, "png", of "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
mdl.inx	Model index, 0 means to compare all models, input 1-6 to plot a ROC curve for one of the top six models
avg.method	Input the method to compute the average ROC curve, either "threshold", "vertical" or "horizontal"
show.conf	Logical, if 1, show confidence interval, if 0 do not show
show.holdout	Logical, if 1, show the ROC curve for hold-out validation, if 0 do not show
focus	"fpr"
cutoff	Input the threshold to limit the calculation of the ROC curve, the number must be between 0 and 1.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotROC.LRmodel *Plot ROC for the logistic regression model*

Description

Plot ROC for the logistic regression model

Usage

```
PlotROC.LRmodel(
  mSetObj = NA,
  imgName,
  format = "png",
  dpi = 72,
  show.conf = FALSE,
  sp.bin = 0.01
)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
show.conf	Logical, show confidence intervals
sp.bin	Numeric, default is set to 0.01.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotROCTest *Plot ROC for the ROC Curve Based Model Creation and Evaluation module*

Description

Plot the ROC curve of the biomarker model created using a user-selected subset of features. Pred and auroc are lists containing predictions and labels from different cross-validations.

Usage

```
PlotROCTest(mSetObj=NA, imgName, format="png",
dpi=72, mdl.inx, avg.method, show.conf, show.holdout, focus="fpr", cutoff = 1.0)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
imgName	Input a name for the plot
format	Select the image format, "png", of "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
mdl.inx	Model index, 0 means to compare all models, input 1-6 to plot a ROC curve for one of the top six models
avg.method	Input the method to compute the average ROC curve, either "threshold", "vertical" or "horizontal"
show.conf	Logical, if 1, show confidence interval, if 0 do not show
show.holdout	Logical, if 1, show the ROC curve for hold-out validation, if 0 do not show
focus	"fpr"
cutoff	Input the threshold to limit the calculation of the ROC curve, the number must be between 0 and 1.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`PlotRocUnivBoxPlot` *Plot a boxplot view of a selected compound*

Description

Plots a boxplot of the selected compound's concentration between the groups.

Usage

```
PlotRocUnivBoxPlot(
  mSetObj,
  feat.nm,
  version,
  format = "png",
  dpi = 72,
  isOpt,
  isQuery
)
```

Arguments

`mSetObj`	Input the name of the created mSetObj (see InitDataObjects)
`feat.nm`	Input the name of the selected compound.
`version`	version mark for image name
`format`	Select the image format, "png", of "pdf".
`dpi`	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
`isOpt`	logical
`isQuery`	logical

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotRSVM.Classification *Recursive Support Vector Machine (R-SVM) plot*

Description

Plot recursive SVM classification

Usage

```
PlotRSVM.Classification(mSetObj, imgName, format, dpi, width)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotRSVM.Cmpd *Recursive Support Vector Machine (R-SVM) plot of important variables*

Description

Plot recursive SVM variables of importance if too many, plot top 15

Usage

```
PlotRSVM.Cmpd(mSetObj=NA, imgName, format="png", dpi=72, width=NA)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotSAM.Cmpd *Plot SAM*

Description

Plot SAM with positive and negative metabolite sets

Usage

```
PlotSAM.Cmpd(mSetObj = NA, imgName, format = "png", dpi = 72, width = NA)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotSAM.FDR *Plot SAM Delta Plot*

Description

Plot SAM Delta Plot (FDR)

Usage

```
PlotSAM.FDR(mSetObj = NA, imgName, format = "png", dpi = 72, width = NA)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotSampleNormSummary *Two plot summary plot: Sample View of before and after normalization*

Description

For each plot, the top is a density plot and the bottom is a box plot.

Usage

```
PlotSampleNormSummary(mSetObj=NA, imgName, format="png", dpi=72, width=NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
imgName	Input a name for the plot
format	Select the image format, "png", of "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca>, Jasmine Chong McGill University, Canada

---

PlotSelectedFeature *Create a box-plot of a feature's expression pattern across the different datasets*

Description

This function plots a box-plot of the expression pattern of a user-selected feature across the different datasets included in meta-analysis.

Usage

```
PlotSelectedFeature(mSetObj = NA, gene.id, format = "png", dpi = 72)
```

Arguments

mSetObj	Input name of the created mSet Object.
gene.id	Input the name of the selected feature.
format	format, in "png" etc.
dpi	dpi value for the image.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotSigVar *Supporting function for plotting important variables for each factor*

Description

Supporting function for plotting important variables for each factor note, by control xpd to plot legend outside the plotting area without using layout

Usage

```
PlotSigVar(x, y, xline, yline, title)
```

Arguments

x	Input the X variable
y	Input the Y variable
xline	Input the xline
yline	Input the yline
title	Input the title

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

plotSingleTIC *plotSingleTIC*

Description

plotSingleTIC is used to plot single TIC

Usage

```
plotSingleTIC(filename, imageNumber, format = "png", dpi = 72, width = NA)
```

Arguments

filename	filename
imageNumber	imageNumber
format	format
dpi	dpi
width	width

Author(s)

Zhiqiang Pang

PlotSOM *SOM Plot*

Description

Plot SOM map for less than 20 clusters

Usage

```
PlotSOM(
  mSetObj = NA,
  imgName,
  format = "png",
  dpi = 72,
  width = NA,
  colpal = "default",
  facet = TRUE
)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.
colpal	Character, input "default" to use the default ggplot color scheme or "colblind" to use the color-blind friendly palette.
facet	logical

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotSPLS2DScore *Score Plot SPLS-DA*

Description

Sparse PLS-DA (from mixOmics) score plot

Usage

```
PlotSPLS2DScore(
  mSetObj = NA,
  imgName,
  format = "png",
  dpi = 72,
  width = NA,
  inx1,
  inx2,
  reg = 0.95,
  show = 1,
  grey.scale = 0,
  cex.opt = "na"
)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.
inx1	Numeric, indicate the number of the principal component for the x-axis of the loading plot.
inx2	Numeric, indicate the number of the principal component for the y-axis of the loading plot.
reg	Numeric, between 1 and 0
show	Numeric, 1 or 0
grey.scale	Numeric, use grey-scale, 0 for no, and 1 for yes.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotSPLS3DLoading *PlotSPLS3DLoading*

Description

PlotSPLS3DLoading

Usage

```
PlotSPLS3DLoading(mSetObj = NA, imgName, format = "json", inx1, inx2, inx3)
```

Arguments

mSetObj	mSetObj
imgName	imgName
format	format
inx1	inx1
inx2	inx2
inx3	inx3

PlotSPLS3DScore *3D SPLS-DA score plot*

Description

Sparse PLS-DA (from mixOmics) 3D score plot

Usage

```
PlotSPLS3DScore(
  mSetObj = NA,
  imgName,
  format = "json",
  inx1 = 1,
  inx2 = 2,
  inx3 = 3
)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
inx1	Numeric, indicate the number of the principal component for the x-axis of the loading plot.
inx2	Numeric, indicate the number of the principal component for the y-axis of the loading plot.
inx3	Numeric, indicate the number of the principal component for the z-axis of the loading plot.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotSPLS3DScoreImg *Plot sPLS-DA 3D score plot*

Description

This function creates two 3D sPLS-DA score plots, the first is static for Analysis Report purposes, as well as an interactive 3D plot using the plotly R package. The 3D score plot is saved in the created mSetObj (mSetObj$imgSet$splsda.3d). To view the score plot, if the name of your mSetObj is mSet, enter "mSet$imgSet$splsda.3d" to view the interactive score plot.

This function creates two 3D sPLS-DA score plots, the first is static for Analysis Report purposes, as well as an interactive 3D plot using the plotly R package. The 3D score plot is saved in the created mSetObj (mSetObj$imgSet$splsda.3d). To view the score plot, if the name of your mSetObj is mSet, enter "mSet$imgSet$splsda.3d" to view the interactive score plot.

Usage

```
PlotSPLS3DScoreImg(
  mSetObj = NA,
  imgName,
  format = "png",
  dpi = 72,
  width = NA,
  inx1,
  inx2,
  inx3,
  angl
)

PlotSPLS3DScoreImg(
  mSetObj = NA,
```

```
  imgName,
  format = "png",
  dpi = 72,
  width = NA,
  inx1,
  inx2,
  inx3,
  angl
)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.
inx1	Numeric, indicate the number of the principal component for the x-axis of the loading plot.
inx2	Numeric, indicate the number of the principal component for the y-axis of the loading plot.
inx3	Numeric, indicate the number of the principal component for the z-axis of the loading plot.
angl	Input the angle

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotSPLSDA.Classification

Create SPLS-DA classification plot

Description

Sparse PLS-DA (from mixOmics) plot of classification performance using different components

Usage

```
PlotSPLSDA.Classification(
  mSetObj = NA,
  imgName,
  format = "png",
  dpi = 72,
  width = NA
)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotSPLSLoading *Create SPLS-DA loading plot*

Description

Sparse PLS-DA (from mixOmics) loading plot

Usage

```
PlotSPLSLoading(
  mSetObj = NA,
  imgName,
  format = "png",
  dpi = 72,
  width = NA,
  inx,
  viewOpt = "detail"
)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.
inx	Input the model index
viewOpt	Detailed view "detail"

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotSPLSPairSummary *Plot SPLS-DA*

Description

Sparse PLS-DA (from mixOmics) pairwise summary plot

Usage

```
PlotSPLSPairSummary(
  mSetObj = NA,
  imgName,
  format = "png",
  dpi = 72,
  width = NA,
  pc.num
)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.

width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.
pc.num	Numeric, indicate the number of principle components

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotStaticCorrHeatMap *Create high resolution static HeatMap for download only*

Description

'@param #same as PlotCorrHeatMap

Usage

```
PlotStaticCorrHeatMap(
  mSetObj = NA,
  imgName,
  format = "png",
  dpi = 72,
  width = NA,
  target,
  cor.method,
  colors,
  viewOpt,
  fix.col,
  no.clst,
  corrCutoff = 0
)
```

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`PlotStaticHeatMap` *Create high resolution static HeatMap for download only*

Description

'@param #same as PlotHeatMap

Usage

```
PlotStaticHeatMap(
  mSetObj = NA,
  imgName,
  format = "png",
  dpi = 72,
  width = NA,
  dataOpt,
  scaleOpt,
  smplDist,
  clstDist,
  palette,
  fzCol,
  fzRow,
  viewOpt = "detail",
  rowV = T,
  colV = T,
  var.inx = NULL,
  border = T,
  grp.ave = F,
  show.legend = T,
  show.annot.legend = T,
  includeRowNames = T
)
```

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`PlotStaticHeatMap2` *Create high resolution static HeatMap for download only*

Description

'@param #same as PlotHeatMap2

Usage

```
PlotStaticHeatMap2(
  mSetObj = NA,
  imgName,
  dataOpt = "norm",
  scaleOpt = "row",
  format = "png",
  dpi = 72,
  width = NA,
  smplDist = "pearson",
  clstDist = "average",
  colorGradient = "bwm",
  fzCol,
  fzRow,
  viewOpt = "overview",
  rankingMethod = "mean",
  topFeature = 2000,
  useTopFeature = F,
  drawBorder = T,
  show.legend = T,
  show.annot.legend = T,
  includeRowNames = T
)
```

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotStaticMetaHeatmap *Create high resolution static HeatMap for download only*

Description

Plot a heatmap showing clustering patterns among the metadata

Usage

```
PlotStaticMetaHeatmap(
  mSetObj = NA,
  viewOpt = "detailed",
  clustSelOpt = "both",
  smplDist = "pearson",
  clstDist = "average",
  colorGradient = "bwm",
  includeRowNames = T,
  imgName,
  format = "png",
```

```
  dpi = 96,
  width = NA
)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
viewOpt	high-level summary or plotting the names inside cell

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotSubHeatMap *Create Sub Heat Map Plot*

Description

Plot a sub heatmap based on results from t-tests/ANOVA, VIP or randomforest

Usage

```
PlotSubHeatMap(
  mSetObj = NA,
  imgName,
  format = "png",
  dpi = 72,
  width = NA,
  dataOpt,
  scaleOpt,
  smplDist,
  clstDist,
  palette,
  fzCol,
  fzRow,
  fzAnno,
  annoPer,
  unitCol,
  unitRow,
  method.nm,
  top.num,
  rowV = T,
  colV = T,
  border = T,
  grp.ave = F,
  show.legend = T,
  show.annot.legend = T,
```

```
  showColnm = T,
  showRownm = T,
  viewOpt,
  download = F
)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.
dataOpt	Set data options
scaleOpt	Set the image scale
smplDist	Input the sample distance method
clstDist	Input the clustering distance method
palette	Input color palette choice
method.nm	Input the method for sub-heat map
top.num	Input the top number
rowV	Default is set to T
colV	Default is set to T
border	Indicate whether or not to show cell-borders, default is set to T
grp.ave	Logical, default is set to F
viewOpt	Set heatmap options, default is set to "detail"

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotTestAccuracy *Plot classification performance using different features for Biomarker Tester*

Description

Plot of the accuracy of classification with an increasing number of features.

Usage

```
PlotTestAccuracy(mSetObj=NA, imgName, format="png", dpi=72)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
imgName	Input a name for the plot
format	Select the image format, "png", of "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotTT *Plot t-test*

Description

Plot t-test

Usage

```
PlotTT(mSetObj=NA, imgName, format="png", dpi=72, width=NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
imgName	Input a name for the plot
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotVolcano *Create volcano plot*

Description

For labelling interesting points, it is defined by the following rules: need to be signficant (sig.inx) and or 2. top 5 p, or 2. top 5 left, or 3. top 5 right.

Usage

```
PlotVolcano(mSetObj=NA, imgName, plotLbl, plotTheme, format="png", dpi=72, width=NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
imgName	Input a name for the plot
plotLbl	Logical, plot labels, 1 for yes and 0 for no.
plotTheme	plotTheme, numeric, canbe 0, 1 or 2
format	Select the image format, "png", or "pdf".
dpi	Input the dpi. If the image format is "pdf", users need not define the dpi. For "png" images, the default dpi is 72. It is suggested that for high-resolution images, select a dpi of 300.
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PlotXIC *PlotXIC*

Description

PlotXIC is used to plot both MS XIC/EIC features of different group and samples

Usage

```
PlotXIC(featureNum, format = "png", dpi = 72, width = NA)
```

Arguments

featureNum	featureNum
format	format
dpi	dpi
width	width

Author(s)

Zhiqiang Pang

---

plot_dist *Batch Distance Plotting*

Description

Scatter sample trend comparison between all sample of different batches

Usage

```
plot_dist(mSetObj = NA, imgName = "dist", format = "png", width = NA, dpi = 72)
```

Arguments

mSetObj	mSetObj
imgName	imgName
format	format
width	width
dpi	dpi

PLSDA.CV *PLS-DA classification and feature selection*

Description

PLS-DA classification and feature selection

Usage

```
PLSDA.CV(
  mSetObj = NA,
  cvOpt = "loo",
  foldNum = 5,
  compNum = GetDefaultPLSCVComp(mSetObj),
  choice = "Q2",
  segments = 10
)
```

Arguments

mSetObj	Input name of the created mSet Object
compNum	GetDefaultPLSCVComp()
choice	Input the choice, by default it is Q2
methodName	Logical, by default set to TRUE

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PLSDA.Permut *Perform PLS-DA permutation*

Description

Perform PLS-DA permutation using training classification accuracy as indicator, for two or multi-groups

Usage

```
PLSDA.Permut(mSetObj = NA, num = 100, type = "accu")
```

Arguments

mSetObj	Input name of the created mSet Object
num	Numeric, input the number of permutations
type	Type of accuracy, if "accu" indicate prediction accuracy, else "sep" is separation distance

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PLSR.Anal — *PLS analysis using oscorespls (Orthogonal scores algorithm) so that VIP can be calculated note: the VIP is calculated only after PLSDA-CV is performed to determine the best # of comp. used for VIP*

Description

PLS analysis using oscorespls

Usage

```
PLSR.Anal(mSetObj = NA, reg = FALSE)
```

Arguments

mSetObj	Input name of the created mSet Object
reg	Logical

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

Predict.class — *Get predicted class probability*

Description

Get predicted class probability

Usage

```
Predict.class(x.train, y.train, x.test, clsMethod = "pls", lvNum, imp.out = F)
```

Arguments

x.train	Input the x training samples
y.train	Input the y training samples
x.test	Input the x testing samples
clsMethod	Se the classification method, default is set to pls
lvNum	Input the number of levels
imp.out	Logical, set to F by default

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PrepareIntegData *Prepare integrated data*

Description

Used for the pathinteg module.

Usage

```
PrepareIntegData(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

PrepareKeggQueryJson *Prepare user's query for mapping KEGG Global Metabolic Network*

Description

This function prepares the user's data for the KEGG Global Metabolic Network

Usage

```
PrepareKeggQueryJson(mSetObj = NA)
```

Arguments

mSetObj	Input name of the created mSet Object

Author(s)

Othman Soufan, Jeff Xia <jeff.xia@mcgill.ca>, othman.soufan@mcgill.ca McGill University, Canada License: GNU GPL (>= 2)

PrepareMetaPath *PrepareMetaPath*

Description

PrepareMetaPath

Usage

```
PrepareMetaPath(
  mSetObj = NA,
  mode = "negative",
  ppm = 30,
  version = "v2",
  pcutoff = 0.05,
  rt.type = "seconds",
  dataName,
  dataName2
)
```

Arguments

mSetObj	mSetObj
mode	ion mode, can be "positive" or "negative"
ppm	mass error, default is 30
version	mummichog version, can be "v1" or "v2"
pcutoff	p value cut-off, default is 0.05
rt.type	character, retention time type, can be "minutes" or "seconds"
dataName	file name 1 with absolute path
dataName2	file name 2 with absolute path or "null"

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> Zhiqiang Pang<zhiqiang.pang@mail.mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PrepareNetworkData *Prepare data for network exploration*

Description

Function for the network explorer module, prepares user's data for network exploration.

Usage

```
PrepareNetworkData(mSetObj = NA)
```

Arguments

mSetObj	Input name of the created mSet Object

PreparePDFReport *Create report of analyses*

Description

Report generation using Sweave Note: most analyses were already performed, only need to embed the results to the right place without rerunning the whole analysis through Sweave. Only some auxilliary info (i.e. time, version etc need to run in R through Sweave

Usage

```
PreparePDFReport(mSetObj = NA, usrName)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
usrName	Input the name of the user

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PreparePeakTable4PSEA *PreparePeakTable4PSEA*

Description

PreparePeakTable4PSEA

Usage

```
PreparePeakTable4PSEA(mSetObj = NA)
```

Arguments

mSetObj	mSet Objective from previous step

Author(s)

Zhiqiang Pang, Jeff Xia

PreparePermResult *Prepare report for permutation tests*

Description

Function to prepare a report for permutation tests, used in higher functions

Usage

```
PreparePermResult(perm.vec)
```

Arguments

perm.vec	Input permutation vector

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PreparePrenormData *Prepare data for normalization*

Description

Function should always be initialized (new or overwrite previous prenorm object).

Usage

```
PreparePrenormData(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

PrepareROCData *Prepare data for ROC analysis*

Description

Prepare data for ROC analysis

Usage

```
PrepareROCData(mSetObj = NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PrepareROCDetails *ROC with CI for AUC*

Description

ROC with CI for AUC

Usage

```
PrepareROCDetails(mSetObj = NA, feat.nm)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
feat.nm	Input the feature name

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

PrepareUpsetData *Prepare data for Upset diagram*

Description

Prepare data for Upset diagram

Usage

```
PrepareUpsetData(mSetObj = NA, fileNm)
```

Arguments

mSetObj	Input name of the created mSet Object
fileNm	json file name to save

processMSMSupload *processMSMSuploadd*

Description

processMSMSuploadd

Usage

```
processMSMSupload(mSetObj = NA, spectrum)
```

Arguments

mSetObj	mSetObj
spectrum	spectrum for uploading

Author(s)

Zhiqiang Pang

RankFeatures *Rank features based on different importance measures*

Description

Ranks features based on various importance measures, return imp.vec which contains the importance measures of unordered features

Usage

```
RankFeatures(x.in, y.in, method, lvNum)
```

Arguments

x.in	Input the X features
y.in	Input the Y features
method	Input the method
lvNum	Input the number of levels

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

Read.BatchDataBC *Data I/O for batch effect checking*

Description

Read multiple user uploaded CSV data one by one format: row, col

Usage

```
Read.BatchDataBC(mSetObj = NA, filePath, format, label, missingEstimate)
```

Arguments

mSetObj	Input name of the created mSet Object
filePath	Input the path to the batch files
format	Input the format of the batch files
label	Input the label-type of the files
missingEstimate	Approach to estimate the missing values

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

Read.BatchDataTB *Data I/O for batch effect checking*

Description

Read peak data tale. format: row, col

Usage

```
Read.BatchDataTB(mSetObj = NA, filePath, format, missingEstimate)
```

Arguments

mSetObj	Input name of the created mSet Object
filePath	Input the path to the batch files
format	Input the format of the batch files
missingEstimate	Approach to estimate the missing values

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`Read.mzTab` *Read an mzTab tab separated file from the passed in file. Adapted from: https://github.com/lifs-tools/rmzTab-m/blob/master/R/MzTabReader.r*

Description

Read an mzTab tab separated file from the passed in file. Adapted from: https://github.com/lifs-tools/rmzTab-m/blob/master/R/MzTabReader.r

Usage

```
Read.mzTab(mSetObj = NA, filename, identifier = "name")
```

Arguments

`mSetObj`	Input the name of the created mSetObj (see InitDataObjects).
`filename`	The name of the mzTab file to parse.
`identifier`	The identifier to be used when the table is parsed. Use "name" to use the chemical_name, "mass" to use the theoretical_neutral_mass and "sml_id" to use the SML_ID. If the number of missing name and mass entries is greater than 90 then the SML_ID will be used.

`Read.PeakList` *Read peak list files*

Description

This function reads peak list files and fills the data into a dataSet object. For NMR peak lists, the input should be formatted as two-columns containing numeric values (ppm, int). Further, this function will change ppm to mz, and add a dummy 'rt'. For MS peak data, the lists can be formatted as two-columns (mz, int), in which case the function will add a dummy 'rt', or the lists can be formatted as three-columns (mz, rt, int).

Usage

```
Read.PeakList(mSetObj=NA, foldername)
```

Arguments

`mSetObj`	Input the name of the created mSetObj (see InitDataObjects).
`foldername`	Name of the folder containing the NMR or MS peak list files to read.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

Read.PeakListData *Constructor to read uploaded user files into the mummichog object*

Description

This function handles reading in CSV or TXT files and filling in the mSet object for mummichog analysis. It makes sure that all necessary columns are present.

Usage

```
Read.PeakListData(mSetObj=NA, filename = NA, meta.anal = FALSE, method = "pvalue")
```

Arguments

mSetObj	Input the name of the created mSetObj.
filename	Input the path name for the CSV/TXT files to read.
meta.anal	Logical, TRUE if data will be used for meta-analysis.
method	Input the type of statistical scores included in the mummichog input. "pvalue" for p-values, "es" for effect-sizes, and "both" for both p-values and effect-sizes.

Author(s)

Jasmine Chong, Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

Read.SignalDriftData *Data I/O for signal drift checking*

Description

Read peak data tale. format: row, col

Usage

```
Read.SignalDriftData(mSetObj = NA, filePath, format)
```

Arguments

mSetObj	Input name of the created mSet Object
filePath	Input the path to the batch files
format	Input the format of the batch files

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

Read.TextData — *Read.TextData Constructor to read uploaded CSV or TXT files into the dataSet object*

Description

This function handles reading in CSV or TXT files and filling in the dataSet object created using "InitDataObjects".

Usage

```
Read.TextData(
  mSetObj = NA,
  filePath,
  format = "rowu",
  lbl.type = "disc",
  nmdr = FALSE
)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects).
filePath	Input the path name for the CSV/TXT files to read.
format	Specify if samples are paired and in rows (rowp), unpaired and in rows (rowu), in columns and paired (colp), or in columns and unpaired (colu).
lbl.type	Specify the data label type, either categorical (disc) or continuous (cont).
nmdr	Boolean. Default set to FALSE (data is uploaded by the user and not fetched through an API call to the Metabolomics Workbench).

Author(s)

Jeff Xia <jeff.xia@mcgill.ca>, Jasmine Chong McGill University, Canada License: GNU GPL (>= 2)

Read.TextDataTs — *Read.TextDataTs*

Description

Read.TextDataTs is used to read metabolomics data for co-vairiate analysis

Usage

```
Read.TextDataTs(mSetObj = NA, filePath, format = "rowu")
```

Arguments

mSetObj	metaboanalyst object, initialized by InitDataObjects("pktable", "mf", FALSE)
filePath	file path of data
format	format of data table, can be "rowu" or "colu"

ReadIndData *Read in individual data*

Description

This function determines reads in user's individual data for meta-analysis.

Usage

```
ReadIndData(mSetObj = NA, dataName, format = "colu")
```

Arguments

mSetObj	Input name of the created mSet Object
dataName	Name of inputted dataset.
format	Specify if samples are paired and in rows (rowp), unpaired and in rows (rowu), in columns and paired (colp), or in columns and unpaired (colu).

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

ReadMetaData *ReadMetaData*

Description

ReadMetaData

Usage

```
ReadMetaData(mSetObj = NA, metafilename)
```

Arguments

mSetObj	metaboanalyst object, initialized by InitDataObjects("pktable", "mf", FALSE)
metafilename	file path of data

ReadMetaPathTable *ReadMetaPathTable*

Description

ReadMetaPathTable

Usage

```
ReadMetaPathTable(mSetObj = NA, dataNM, dataFormat, dataType)
```

Arguments

mSetObj	mSetObj
dataNM	file name with absolute path
dataFormat	data format, can be colu or rowu
dataType	data type, usually "massPeaks"

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> Zhiqiang Pang<zhiqiang.pang@mail.mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

ReadMetaPathTableMix *ReadMetaPathTableMix*

Description

ReadMetaPathTableMix

Usage

```
ReadMetaPathTableMix(mSetObj = NA, dataNM, dataNM2, dataFormat, dataType)
```

Arguments

mSetObj	mSetObj
dataNM	file name 1 with absolute path (should be ESI+)
dataNM2	file name 2 with absolute path (should be ESI-)
dataFormat	data format, can be colu or rowu
dataType	data type, usually "massPeaks"

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> Zhiqiang Pang<zhiqiang.pang@mail.mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

ReadPairFile *Read paired peak or spectra files*

Description

This function reads paired peak lists or spectra files. The pair information is stored in a file where each line is a pair and names are separated by ":".

Usage

```
ReadPairFile(filePath = "pairs.txt")
```

Arguments

filePath	Set file path

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

RecordRCommand *Record R Commands*

Description

Record R Commands

Usage

```
RecordRCommand(mSetObj = NA, cmd)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
cmd	Commands

rectUnique *Perform utilities for peak grouping*

Description

Perform various utilities for peak grouping

Usage

```
rectUnique(m, order = seq(length = nrow(m)), xdiff = 0, ydiff = 0)
```

Arguments

m	Peaks
order	Performs seq(length = nrow(m))
xdiff	Default set to 0
ydiff	Default set to 0

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

RegisterData *Register data in R*

Description

When there are multiple datasets, record their name and save the inputted data as a .qs file to save memory. Note, the memory will only contain one mSetObj$dataSet object. By default the last one will be the most recent/current dataSet object. Users can switch which data to load into memory.

Usage

```
RegisterData(mSetObj = NA, dataSet)
```

Arguments

mSetObj	Input name of the created mSet Object
dataSet	Input dataset to be registered in R.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

RemoveCmpd *Remove selected compounds*

Description

Remove compounds

Usage

```
RemoveCmpd(mSetObj = NA, inx)
```

Arguments

mSetObj	Input name of the created mSet Object
inx	Input the index of compound to remove

RemoveData *Remove data object, the current dataSet will be the last one by default*

Description

Remove data object, the current dataSet will be the last one by default

Usage

```
RemoveData(dataName)
```

Arguments

dataName	Input name of data to remove

RemoveDuplicates *Given a data with duplicates, remove duplicates*

Description

Dups is the one with duplicates

Usage

```
RemoveDuplicates(data, lvlOpt = "mean", quiet = T)
```

Arguments

data	Input data to remove duplicates
lvlOpt	Set options, default is mean
quiet	Set to quiet, logical, default is T

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

RemoveFile *Remove file*

Description

Remove file

Usage

```
RemoveFile(fileName)
```

Arguments

fileName	Input name of file to remove

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

RemoveFolder *Remove folder*

Description

Remove folder

Usage

```
RemoveFolder(folderName)
```

Arguments

folderName	Input name of folder to remove

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

RemoveGene *Remove selected genes*

Description

Remove selected genes based on an index

Usage

```
RemoveGene(mSetObj = NA, inx)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
inx	Input compound index

RemoveMissingPercent *Data processing: remove variables with missing values*

Description

Remove variables based upon a user-defined percentage cut-off of missing values. If a user specifies a threshold of 20 in at least 20

Usage

```
RemoveMissingPercent(mSetObj, percent)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
percent	Input the percentage cut-off you wish to use. For instance, 50 percent is represented by percent=0.5.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

ReplaceMin *Replace missing or zero values*

Description

This function will replace zero/missing values by half of the smallest positive value in the original dataset. This method will be called after all missing value imputations are conducted. Also, it directly modifies the mSet$dataSet$proc if executed after normalization, or the mSet$dataSet$norm if before normalization.

Usage

```
ReplaceMin(mSetObj=NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

RerenderMetPAGraph *Redraw current graph for zooming or clipping then return a value*

Description

Redraw current graph for zooming or clipping then return a value

Usage

```
RerenderMetPAGraph(mSetObj = NA, imgName, width, height, zoom.factor = NA)
```

Arguments

mSetObj	Input name of the created mSet Object
imgName	Input the name of the plot
width	Input the width, there are 2 default widths, the first, width = NULL, is 10.5. The second default is width = 0, where the width is 7.2. Otherwise users can input their own width.
height	Input the height of the created plot.
zoom.factor	zoom factor, numeric

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

RF.Anal *Perform Random Forest Analysis*

Description

Perform Random Forest

Usage

```
RF.Anal(mSetObj = NA, treeNum = 500, tryNum = 7, randomOn = 1)
```

Arguments

mSetObj	Input name of the created mSet Object
treeNum	Input the number of trees to create, default is set to 500
tryNum	Set number of tries, default is 7
randomOn	Set random, default is 1

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

RF.AnalMeta *Perform Random Forest Analysis*

Description

Perform Random Forest

Usage

```
RF.AnalMeta(
  mSetObj = NA,
  treeNum = 500,
  tryNum = 7,
  randomOn = 1,
  selectedMeta
)
```

Arguments

mSetObj	Input name of the created mSet Object
treeNum	Input the number of trees to create, default is set to 500
tryNum	Set number of tries, default is 7
randomOn	Set random, default is 1
selectedMeta	selected Meta elements

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`ROCPredSamplesTable` *Create a table of newly classified samples*

Description

Function to create the table of newly classified samples

Usage

```
ROCPredSamplesTable(mSetObj = NA)
```

Arguments

`mSetObj`	Input the name of the created mSetObj (see InitDataObjects) Function to create the table of newly classified samples

---

`RSVM` *R-SVM core code*

Description

Core code to perform R-SVM

Usage

```
RSVM(x, y, ladder, CVtype, CVnum = 0)
```

Arguments

`x`	Row matrix of data
`y`	Class label: 1 / -1 for 2 classes
`ladder`	Input the ladder
`CVtype`	Integer (N fold CV), "LOO" leave-one-out CV, "bootstrape" bootstrape CV
`CVnum`	Number of CVs, LOO: defined as sample size, Nfold and bootstrape: user defined, default as sample size outputs a named list Error: a vector of CV error on each level SelFreq: a matrix for the frequency of each gene being selected in each level with each column corresponds to a level of selection and each row for a gene The top important gene in each level are those high-freqent ones

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

RSVM.Anal *Recursive Support Vector Machine (R-SVM)*

Description

recursive SVM for feature selection and classification

Usage

```
RSVM.Anal(mSetObj = NA, cvType)
```

Arguments

mSetObj	Input name of the created mSet Object
cvType	Cross-validation type

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

SaintyCheckMSPfile *SaintyCheckMSPfile*

Description

SaintyCheckMSPfile

Usage

```
SaintyCheckMSPfile(
  mSetObj = NA,
  filename = "",
  format_type = "mzmine",
  keepAllspec = FALSE
)
```

Arguments

mSetObj	mSetObj
filename	filename with path
format_type	format type, can be 'mzmine' or 'msdial'
keepAllspec	if you want to search all spectra from your local, turn keepAllspec to TRUE. it is FALSE by default.

Author(s)

Zhiqiang Pang

SAM.Anal *Perform Signifiance Analysis of Microarrays (SAM) analysis*

Description

Perform SAM

Usage

```
SAM.Anal(
  mSetObj = NA,
  method = "d.stat",
  paired = FALSE,
  varequal = TRUE,
  delta = 0,
  imgName,
  dpi = 72
)
```

Arguments

mSetObj	Input name of the created mSet Object
method	Method for SAM analysis, default is set to "d.stat", alternative is "wilc.stat"
paired	Logical, indicates if samples are paired or not. Default is set to FALSE
varequal	Logical, indicates if variance is equal. Default is set to TRUE
delta	numeric
imgName	image name, character
dpi	image dpi, integer

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

SanityCheckData *Sanity Check Data*

Description

SanityCheckData is used for data processing, and performs a basic sanity check of the uploaded content, ensuring that the data is suitable for further analysis. The function will return a message if the data has successfully passed the check and is deemed suitable for further analysis. If it fails, the function will return a 0. The function will perform the check directly onto the mSet$dataSet object, and must be performed immediately after reading in data. The sanity check function evaluates the accuracy of sample and class labels, data structure, deals with non-numeric values, removes columns that are constant across all samples (variance = 0), and by default replaces missing values with half of the original minimal positive value in your dataset.

Usage

```
SanityCheckData(mSetObj=NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

SanityCheckIndData *Sanity check of individual datasets for meta-analysis*

Description

Performs a sanity check on each-uploaded dataset for meta-analysis. Briefly, this function will exclude empty rows, check class labels, ensure only 2 groups are being compared within the dataset, ensure sample names are unique, remove low quality samples/features, and replace missing values.

Usage

```
SanityCheckIndData(mSetObj = NA, dataName)
```

Arguments

mSetObj	Input name of the created mSet Object
dataName	Input name of the dataset to perform the sanity check.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

SanityCheckMeta *SanityCheckMeta#'*

Description

SanityCheckMeta#'

Usage

```
SanityCheckMeta(mSetObj = NA, init = 1)
```

Arguments

mSetObj	metaboanalyst object
init	can be 0 or 1

SanityCheckMetaPathTable *SanityCheckMetaPathTable*

Description

SanityCheckMetaPathTable

Usage

```
SanityCheckMetaPathTable(mSetObj = NA, dataName, dataName2)
```

Arguments

mSetObj	mSetObj
dataName	file name 1 with absolute path
dataName2	file name 2 with absolute path or "null"

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> Zhiqiang Pang<zhiqiang.pang@mail.mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

SanityCheckMummichogData *Sanity Check Data*

Description

SanityCheckData is used for data processing, and performs a basic sanity check of the uploaded data, ensuring that the data is suitable for further analysis. The function ensure that all parameters are properly set based on updated parameters.

Usage

```
SanityCheckMummichogData(mSetObj=NA)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects).

Author(s)

Jasmine Chong, Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

savePeakListMetaData *Function to save each mSetObj as a RDS file to be used later in PerformMetaPSEA. Should be called after SetPeakEnrichMethod/SetMummichogPval*

Description

Function to save each mSetObj as a RDS file to be used later in PerformMetaPSEA. Should be called after SetPeakEnrichMethod/SetMummichogPval

Usage

```
savePeakListMetaData(mSetObj = NA)
```

Arguments

mSetObj	mSetObj

SaveTransformedData *Save the processed data with class names*

Description

This function saves the processed data with class names as CSV files. Several files may be generated, the original data, processed data, peak normalized, and/or normalized data.

Usage

```
SaveTransformedData(mSetObj = NA)
```

Arguments

mSetObj	Input name of the created mSet Object

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

SearchByCompound *Search for compound from all member compounds of metabolite set*

Description

Search for compound from all member compounds of metabolite set

Usage

```
SearchByCompound(mSetObj = NA, query)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
query	Input the query to search

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

SearchByName *Given a metabolite set name, search its index*

Description

Given a metabolite set name, search its index

Usage

```
SearchByName(mSetObj = NA, query)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
query	Input the query to search

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

SearchMsetLibraries *Search metabolite set libraries*

Description

Search metabolite set libraries

Usage

```
SearchMsetLibraries(mSetObj = NA, query, type)
```

Arguments

mSetObj	Input name of the created mSet Object
query	Input the query to search
type	Input the data type (name or compound)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

SearchNetDB *Perform mapping of user's data to interaction network*

Description

This function performs mapping of user's data to the internal network to create a network from the seed nodes

Usage

```
SearchNetDB(
  mSetObj = NA,
  db.type,
  table.nm,
  require.exp = TRUE,
  min.score = 900
)
```

Arguments

mSetObj	Input name of the created mSet Object
db.type	Input the database type
table.nm	Input the organism code for the sqlite table (ppi). For chemical type, the table.nm is drugbank of ctd
require.exp	Logical, only used for the STRING database
min.score	Input the minimal score, only used for the STRING database

Author(s)

Othman Soufan, Jeff Xia <jeff.xia@mcgill.ca>, othman.soufan@mcgill.ca McGill University, Canada License: GNU GPL (>= 2)

SelectMultiData *Select one or more datasets for meta-analysis*

Description

This function selects one or more datasets to be used for meta-analysis. 1 is used to indicate that a dataset is selected and by default, all datasets will be selected for meta-analysis.

Usage

```
SelectMultiData(mSetObj = NA)
```

Arguments

mSetObj	Input name of the created mSet Object

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

SetAnalysisMode *Set biomarker analysis mode*

Description

ROC utilities

Usage

```
SetAnalysisMode(mSetObj, mode)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)s
mode	Input the selected mode for biomarker analysis, "univ" for univariate ROC curve analysis, "explore" for multivariate ROC curve analysis, and "test" for ROC curve based model creation and evaluation. McGill University, Canada License: GNU GPL (>= 2)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca>

SetCachexiaSetUsed *Set the cachexia set used*

Description

Set cachexia set used

Usage

```
SetCachexiaSetUsed(mSetObj = NA, used)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
used	Set data to be used

SetCandidate *Set matched name based on user selection from all potential hits*

Description

Note: to change object in the enclosing enviroment, use "«-"

Usage

```
SetCandidate(mSetObj = NA, query_nm, can_nm)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects).
query_nm	Input the query name.
can_nm	Input the candidate name.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

SetCurrentGroups *To choose from two groups*

Description

Choose two groups (when more than two groups uploaded)

Usage

```
SetCurrentGroups(mSetObj = NA, grps)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
grps	Input the groups

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

SetCurrentMsetLib *Set current user selected metset library for search*

Description

if enrichment analysis, also prepare lib by creating a list of metabolite sets

Usage

```
SetCurrentMsetLib(mSetObj=NA, libname, excludeNum)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
libname	Input user selected name of library, "self", "kegg_pathway", "smpdb_pathway", "blood", "urine", "csf", "snp", "predicted", "location", and "drug".
excludeNum	Users input the mimimum number compounds within selected metabolite sets (metabolitesets < excludeNum)

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`SetCustomData` *Set custom data*

Description

The "selected.cmpds" should be for extraction

Usage

```
SetCustomData(mSetObj = NA, selected.cmpds, selected.smpls)
```

Arguments

`mSetObj`	Input the name of the created mSetObj (see InitDataObjects)
`selected.cmpds`	Input the vector containing the compounds
`selected.smpls`	Input the vector containing the samples

`SetDataTypeOfMeta` *SetDataTypeOfMeta*

Description

SetDataTypeOfMeta

Usage

```
SetDataTypeOfMeta(mSetObj = NA)
```

Arguments

`mSetObj`	metaboanalyst object

SetDesignType *For two factor time series only*

Description

For two factor time series only

Usage

```
SetDesignType(mSetObj = NA, design)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
design	Input the design type

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

setInclusionDataSets *setInclusionDataSets#'*

Description

setInclusionDataSets#'

Usage

```
setInclusionDataSets(mSetObj = NA, datasVec)
```

Arguments

mSetObj	mSetObj
datasVec	a vector of all files

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> Zhiqiang Pang<zhiqiang.pang@mail.mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

Examples

```
#setInclusionDataSets(c("A1_pos.csv","B1_pos.csv","C1_pos.csv"));
```

SetKEGG.PathLib *Set KEGG pathway library*

Description

note, this process can be long, need to return a value to force Java to wait

Usage

```
SetKEGG.PathLib(mSetObj = NA, libNm, lib.version)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
libNm	lib name option KEGG pathway library or "v2018" for the KEGG pathway library version prior to November 2019.
lib.version	Input the KEGG pathway version. "current" for the latest

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

SetMetabolomeFilter *Set metabolome filter*

Description

Set metabolome filter

Usage

```
SetMetabolomeFilter(mSetObj = NA, TorF)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
TorF	Input metabolome filter

setMS2DBOpt *setMS2DBOpt*

Description

setMS2DBOpt

Usage

```
setMS2DBOpt(mSetObj = NA, DBoption = "regular")
```

Arguments

mSetObj	mSetObj object
DBoption	database option to define neutral loss or not, can be either 'regualr" or 'nl'.

Author(s)

Zhiqiang Pang

SetMummichogPval *Set the cutoff for mummichog analysis*

Description

Set the p-value cutoff for mummichog analysis.

Usage

```
SetMummichogPval(mSetObj = NA, cutoff)
```

Arguments

mSetObj	Input the name of the created mSetObj.
cutoff	cutoff value for mummichog running

Author(s)

Jasmine Chong, Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

SetMummichogPvalFromPercent *Set the cutoff for mummichog analysis*

Description

Set the p-value cutoff for mummichog analysis.

Usage

```
SetMummichogPvalFromPercent(mSetObj = NA, fraction)
```

Arguments

mSetObj	Input the name of the created mSetObj.
fraction	fraction value for mummichog running

Author(s)

Jasmine Chong, Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

SetOrganism *Set organism for further analysis*

Description

Set organism for further analysis

Set organism for further analysis

Usage

```
SetOrganism(mSetObj = NA, org)

SetOrganism(mSetObj = NA, org)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
org	Set organism ID

SetPeakEnrichMethod *Set the peak enrichment method for the MS Peaks to Paths module*

Description

This function sets the peak enrichment method.

Usage

```
SetPeakEnrichMethod(mSetObj = NA, algOpt, version = "v2")
```

Arguments

mSetObj	Input the name of the created mSetObj.
algOpt	algorithm option, can be "gsea", "mum" and "integ"
version	version of mummichog

Author(s)

Jasmine Chong, Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

SetPeakFormat *Set the peak format for the mummichog analysis*

Description

Set the peak format for mummichog analysis.

Usage

```
SetPeakFormat(mSetObj = NA, type = "mpt")
```

Arguments

mSetObj	mSetObj
type	Input the name of mummichog analysis type, usually 'mpt'.

Author(s)

Jasmine Chong, Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

SetPeakList.GroupValues *Set peak list group values*

Description

Set peak list group values

Usage

```
SetPeakList.GroupValues(mSetObj = NA)
```

Arguments

mSetObj	Input name of mSetObj, the data used is the nmr.xcmsSet object

SetPeakParam *SetPeakParam*

Description

SetPeakParam, used to set the peak param

Usage

```
SetPeakParam(
  platform = "general",
  Peak_method = "centWave",
  RT_method = "loess",
  mzdiff,
  snthresh,
  bw,
  ppm,
  min_peakwidth,
  max_peakwidth,
  noise,
  prefilter,
  value_of_prefilter,
  fwhm,
  steps,
  sigma,
  peakBinSize,
  max,
  criticalValue,
  consecMissedLimit,
```

```
  unions,
  checkBack,
  withWave,
  profStep,
  minFraction,
  minSamples,
  maxFeatures,
  mzCenterFun,
  integrate,
  extra,
  span,
  smooth,
  family,
  fitgauss,
  polarity,
  perc_fwhm,
  mz_abs_iso,
  max_charge,
  max_iso,
  corr_eic_th,
  mz_abs_add,
  adducts,
  rmConts,
  BlankSub
)
```

Arguments

platform	platform
Peak_method	Peak_method
RT_method	RT_method
mzdiff	mzdiff
snthresh	snthresh
bw	bw
ppm	ppm
min_peakwidth	min_peakwidth
max_peakwidth	max_peakwidth
noise	noise
prefilter	prefilter
value_of_prefilter	value_of_prefilter
fwhm	fwhm
steps	steps
sigma	sigma

peakBinSize	peakBinSize
max	max
criticalValue	criticalValue
consecMissedLimit	consecMissedLimit
unions	unions
checkBack	checkBack
withWave	withWave
profStep	profStep
minFraction	minFraction
minSamples	minSamples
maxFeatures	maxFeatures
mzCenterFun	mzCenterFun
integrate	integrate
extra	extra
span	span
smooth	smooth
family	family
fitgauss	fitgauss
polarity	polarity
perc_fwhm	perc_fwhm
mz_abs_iso	mz_abs_iso
max_charge	max_charge
max_iso	max_iso
corr_eic_th	corr_eic_th
mz_abs_add	mz_abs_add
adducts	adducts
rmConts	rmConts

Author(s)

Zhiqiang Pang

SetRTincluded *SetRTincluded*

Description

SetRTincluded

Usage

```
SetRTincluded(mSetObj = NA, rt = "no")
```

Arguments

mSetObj	mSetObj
rt	retention time types, "minutes", "seconds" or "no"

Value

mSetObj

SetSMPDB.PathLib *Set SMPDB pathway library*

Description

note, this process can be long, need to return a value to force Java to wait

Usage

```
SetSMPDB.PathLib(mSetObj = NA, libNm)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
libNm	Input library name

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

Setup.AdductData *Save adduct names for mapping*

Description

Save adduct names for mapping

Usage

```
Setup.AdductData(mSetObj = NA, qvec)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
qvec	Input the vector to query

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

Setup.BiofluidType *Save biofluid type for SSP*

Description

Save biofluid type for SSP

Usage

```
Setup.BiofluidType(mSetObj = NA, type)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
type	Input the biofluid type

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`Setup.ConcData` *Save concentration data*

Description

Save concentration data

Usage

```
Setup.ConcData(mSetObj = NA, conc)
```

Arguments

`mSetObj`	Input the name of the created mSetObj (see InitDataObjects)
`conc`	Input the concentration data

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`Setup.HMDBReferenceMetabolome` *Read user uploaded metabolome as a list of HMDB compound names*

Description

Read user uploaded metabolome as a list of HMDB compound names

Usage

```
Setup.HMDBReferenceMetabolome(mSetObj = NA, filePath)
```

Arguments

`mSetObj`	Input the name of the created mSetObj (see InitDataObjects)
`filePath`	Input the path to the user's list of HMDB compound names

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

Setup.KEGGReferenceMetabolome *Read user uploaded metabolome as a list of KEGG pathway ids*

Description

Read user uploaded metabolome as a list of KEGG pathway ids

Usage

```
Setup.KEGGReferenceMetabolome(mSetObj = NA, filePath)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
filePath	Input the path to the user's list of KEGG pathway ids

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

Setup.MapData *Save compound name for mapping*

Description

Save compound name for mapping

Usage

```
Setup.MapData(mSetObj = NA, qvec)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
qvec	Input the vector to query

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

Setup.UserMsetLibData *Read user upload metabolite set library file*

Description

Return two col csv file, first name, second cmpd list

Usage

```
Setup.UserMsetLibData(mSetObj = NA, filePath)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
filePath	Input the path to the user's uploaded metabolite set library

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

SetupKEGGLinks *Only works for human (hsa.rda) data*

Description

Only works for human (hsa.rda) data 2018 - works for ath, eco, mmu, sce

Usage

```
SetupKEGGLinks(smpdb.ids)
```

Arguments

smpdb.ids	Input the list of SMPD ids to add SMPDB links

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

SetupSMPDBLinks *Only works for human (hsa.rda) data*

Description

Only works for human (hsa.rda) data 2018 - works for ath, eco, mmu, sce

Usage

```
SetupSMPDBLinks(kegg.ids)
```

Arguments

kegg.ids	Input the list of KEGG ids to add SMPDB links

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

SOM.Anal *SOM analysis*

Description

SOM analysis

Usage

```
SOM.Anal(mSetObj = NA, x.dim, y.dim, initMethod, neigb = "gaussian")
```

Arguments

mSetObj	Input name of the created mSet Object
x.dim	Input X dimension for SOM analysis
y.dim	Input Y dimension for SOM analysis
initMethod	Input the method
neigb	Default is set to 'gaussian'

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`sparse.mint.block_iteration` *Perform Sparse Generalized Canonical Correlation (sgccak)*

Description

Runs sgccak() modified from RGCCA

Usage

```
sparse.mint.block_iteration(
  A,
  design,
  study = NULL,
  keepA.constraint = NULL,
  keepA = NULL,
  scheme = "horst",
  init = "svd",
  max.iter = 100,
  tol = 1e-06,
  verbose = TRUE,
  bias = FALSE,
  penalty = NULL
)
```

Arguments

`A`	Data
`design`	Set design
`study`	Default set to NULL
`keepA.constraint`	Default set to NULL
`keepA`	Default set to NULL
`scheme`	Scheme, default set to "horst"
`init`	Init mode, default set to "svd"
`max.iter`	Max number of iterations, numeric, default set to 100
`tol`	Tolerance, numeric, default set to 1e-06
`verbose`	Default set to TRUE
`bias`	Default set to FALSE
`penalty`	Default set to NULL

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

splsda *Perform sPLS-DA*

Description

Sparse PLS functions (adapted from mixOmics package for web-based usage) this function is a particular setting of internal_mint.block the formatting of the input is checked in internal_wrapper.mint

Usage

```
splsda(
  X,
  Y,
  ncomp = 2,
  mode = c("regression", "canonical", "invariant", "classic"),
  keepX,
  keepX.constraint = NULL,
  scale = TRUE,
  tol = 1e-06,
  max.iter = 100,
  near.zero.var = FALSE,
  logratio = "none",
  multilevel = NULL
)
```

Arguments

X	numeric matrix of predictors
Y	a factor or a class vector for the discrete outcome
ncomp	the number of components to include in the model. Default to 2.
mode	Default set to c("regression", "canonical", "invariant", "classic")
keepX	Number of X variables kept in the model on the last components (once all keepX.constraint[[i]] are used).
keepX.constraint	A list containing which variables of X are to be kept on each of the first PLS-components.
scale	Boleean. If scale = TRUE, each block is standardized to zero means and unit variances (default: TRUE).
tol	Convergence stopping value.
max.iter	integer, the maximum number of iterations.
near.zero.var	boolean, see the internal nearZeroVar function (should be set to TRUE in particular for data with many zero values). Setting this argument to FALSE (when appropriate) will speed up the computations
logratio	"None" by default, or "CLR"
multilevel	Designate multilevel design, "NULL" by default

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

`SPLSR.Anal` *Perform SPLS-DA*

Description

Sparse PLS-DA (from mixOmics)

Usage

```
SPLSR.Anal(
  mSetObj = NA,
  comp.num,
  var.num,
  compVarOpt,
  validOpt = "Mfold",
  foldNum = 5,
  doCV = FALSE
)
```

Arguments

`mSetObj`	Input name of the created mSet Object
`comp.num`	Input the number of computations to run
`var.num`	Input the number of variables
`compVarOpt`	Input the option to perform SPLS-DA
`validOpt`	INput the valid option

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

SumNorm *Row-wise Normalization*

Description

Row-wise norm methods, when x is a row. Normalize by a sum of each sample, assume constant sum (1000). Options for normalize by sum median, reference sample, reference reference (compound), or quantile normalization

Usage

```
SumNorm(x)
```

Arguments

x	Input data to normalize

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada

template.match *Pattern hunter*

Description

Run template on all the high region effect genes

Usage

```
template.match(x, template, dist.name)
```

Arguments

x	Input data
template	Input template
dist.name	Input distance method

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

Ttests.Anal *Perform t-test analysis*

Description

This function is used to perform t-test analysis.

Usage

```
Ttests.Anal(
  mSetObj = NA,
  nonpar = F,
  threshp = 0.05,
  paired = FALSE,
  equal.var = TRUE,
  pvalType = "fdr",
  all_results = FALSE
)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
nonpar	Logical, use a non-parametric test, T or F. False is default.
threshp	Numeric, enter the adjusted p-value (FDR) cutoff
paired	Logical, is data paired (T) or not (F).
equal.var	Logical, evaluates if the group variance is equal (T) or not (F).
pvalType	pvalType, can be "fdr" etc.
all_results	Logical, if TRUE, returns T-Test analysis results for all compounds.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

UnzipUploadedFile *Unzip .zip files*

Description

Unzips uploaded .zip files, removes the uploaded file, checks for success

Usage

```
UnzipUploadedFile(inPath, outPath, rmFile = T)
```

Arguments

inPath	Input the path of the zipped files
outPath	Input the path to directory where the unzipped files will be deposited
rmFile	Logical, input whether or not to remove files. Default set to T

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

UpdateData *Update data for filtering*

Description

Function to update the mSetObj after removing features or samples.

Usage

```
UpdateData(mSetObj = NA, order.group = FALSE)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)

UpdateEC_Rules *Update the mSetObj with user-selected parameters for MS Peaks to Pathways.*

Description

This functions handles updating the mSet object for mummichog analysis.

Usage

```
UpdateEC_Rules(mSetObj = NA, force_primary_ion, rt_tol)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects).
force_primary_ion	Character, if "yes", only mz features that match compounds with a primary ion are kept.
rt_tol	Numeric. Input the retention time tolerance used for determining ECs (in seconds).

Author(s)

Jasmine Chong, Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

UpdateGraphSettings *Update graph settings*

Description

Function to update the graph settings.

Usage

```
UpdateGraphSettings(mSetObj = NA, colVec, shapeVec)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
colVec	colVec
shapeVec	shapeVec

UpdateInstrumentParameters *Update the mSetObj with user-selected parameters for MS Peaks to Pathways.*

Description

This functions handles updating the mSet object for mummichog analysis. It is necessary to utilize this function to specify to the organism's pathways to use (libOpt), the mass-spec mode (msModeOpt) and mass-spec instrument (instrumentOpt).

Usage

```
UpdateInstrumentParameters(mSetObj=NA, instrumentOpt,
msModeOpt, force_primary_ion, rt_frac, rt_tol)
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects).
instrumentOpt	Numeric. Define the mass-spec instrument used to perform untargeted metabolomics.
msModeOpt	Character. Define the mass-spec mode of the instrument used to perform untargeted metabolomics.
force_primary_ion	Character, if "yes", only mz features that match compounds with a primary ion are kept.
rt_frac	rt_frac.
rt_tol	rt_tol.

Author(s)

Jasmine Chong, Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

UpdateIntegPathwayAnalysis

Update integrative pathway analysis for new input list

Description

used for integrative analysis as well as general pathways analysis for meta-analysis results

Usage

```
UpdateIntegPathwayAnalysis(mSetObj=NA, qids, file.nm,
topo="dc", enrich="hyper", libOpt="integ")
```

Arguments

mSetObj	Input name of the created mSet Object
qids	Input the query IDs
file.nm	Input the name of the file
topo	Select the mode for topology analysis: Degree Centrality ("dc") measures the number of links that connect to a node (representing either a gene or metabolite) within a pathway; Closeness Centrality ("cc") measures the overall distance from a given node to all other nodes in a pathway; Betweenness Centrality ("bc")measures the number of shortest paths from all nodes to all the others that pass through a given node within a pathway.
enrich	Method to perform over-representation analysis (ORA) based on either hypergenometrics analysis ("hyper") or Fisher's exact method ("fisher").
libOpt	Select the different modes of pathways, either the gene-metabolite mode ("integ") which allows for joint-analysis and visualization of both significant genes and metabolites or the gene-centric ("genetic") and metabolite-centric mode ("metab") which allows users to identify enriched pathways driven by significant genes or metabolites, respectively.

Author(s)

Jeff Xia <jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

UpdateOPLS.Splot *Update OPLS loadings*

Description

Update the OPLS loadings

Usage

```
UpdateOPLS.Splot(mSetObj = NA, plotType)
```

Arguments

mSetObj	Input name of the created mSet Object
plotType	Set annotation type, "all" to label all variables and "none" to label no variables.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

UpdatePCA.Loading *Update PCA loadings*

Description

Update the PCA loadings

Usage

```
UpdatePCA.Loading(mSetObj = NA, plotType)
```

Arguments

mSetObj	Input name of the created mSet Object
plotType	Set annotation type, "all" to label all variables and "none" to label no variables.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

UpdatePLS.Loading *Update PLS loadings*

Description

Update the PLS loadings

Usage

```
UpdatePLS.Loading(mSetObj = NA, plotType)
```

Arguments

mSetObj	Input name of the created mSet Object
plotType	Set annotation type, "all" to label all variables and "none" to label no variables.

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

usr2png *Perform utilities for MetPa*

Description

Convert user coords (as used in current plot) to pixels in a png adapted from the imagemap package

Usage

```
usr2png(xy, im)
```

Arguments

xy	Input coordinates
im	Input coordinates

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

Volcano.Anal *Perform Volcano Analysis*

Description

Perform volcano analysis

Usage

```
Volcano.Anal(mSetObj=NA, paired=FALSE, fcthresh,
cmpType, nonpar=F, threshp, equal.var=TRUE, pval.type="raw")
```

Arguments

mSetObj	Input the name of the created mSetObj (see InitDataObjects)
paired	Logical, T if data is paired, F if data is not.
fcthresh	Numeric, input the fold change threshold
cmpType	Comparison type, 0 indicates group 1 vs group 2, and 1 indicates group 2 vs group 1
nonpar	Logical, indicate if a non-parametric test should be used (T or F)
threshp	Numeric, indicate the p-value threshold
equal.var	Logical, indicates if the group variance is equal (T) or unequal (F)
pval.type	To indicate raw p-values, use "raw". To indicate FDR-adjusted p-values, use "fdr".

Author(s)

Jeff Xia<jeff.xia@mcgill.ca> McGill University, Canada License: GNU GPL (>= 2)

XSet2MSet *Converts xset object from XCMS to mSet object for MetaboAnalyst*

Description

This function converts processed raw LC/MS data from XCMS to a usable data object (mSet) for MetaboAnalyst. The immediate next step following using this function is to perform a SanityCheck, and then further data processing and analysis can continue.

Usage

```
XSet2MSet(xset, dataType, analType, paired = F, format, lbl.type)
```

Arguments

xset	The name of the xcmsSet object created.
dataType	The type of data, either list (Compound lists), conc (Compound concentration data), specbin (Binned spectra data), pktable (Peak intensity table), nmrpeak (NMR peak lists), mspeak (MS peak lists), or msspec (MS spectra data).
analType	Indicate the analysis module to be performed: stat, pathora, pathqea, msetora, msetssp, msetqea, mf, cmpdmap, smpmap, or pathinteg.
paired	Logical, is data paired (T) or not (F).
format	Specify if samples are paired and in rows (rowp), unpaired and in rows (rowu), in columns and paired (colp), or in columns and unpaired (colu).
lbl.type	Specify the data label type, either categorical (disc) or continuous (cont).

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