

tpp.R documentation

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init

Function: generates files essential for TPP to run

Parameter	Description	Default Value
frame	A data frame consisting of the protein quantifications and quality scores	None
identifierColumn	A number indicating the column where the identifier of the protein is stored	None
coverageColumn	A number indicating the column where the percent coverage is stored	None
numPeptidesColumn	A number indicating the column where the number of peptides is stored	None
qpsmColumn	A number indicating the column where the qpsm values are stored	None
vehicle1Columns	A numeric vector indicating the columns where the vehicle quantifications are located	None
treatment1Columns	A numeric vector indicating the columns where the treatment quantifications are located	None
vehicle2Columns	A numeric vector indicating the columns where the parallel vehicle quantifications are located	NULL
treatment2Columns	A numeric vector indicating the columns where the parallel treatment quantifications are located	NULL
experimentNames	A character vector indicating the names of each experiment, where <i>experimentNames[1]</i> is the name of the <i>vehicle1Columns</i> quantifications, <i>experimentNames[2]</i> is the name of the <i>treatment1Columns</i> quantifications, <i>experimentNames[3]</i> is the name of the <i>vehicle2Columns</i> quantifications, and <i>experimentNames[4]</i> is the name of the <i>treatment2Columns</i> quantifications	c("Vehicle1", "Treatment1", "Vehicle2", "Treatment2")
temperatures	A numeric vector indicating the temperatures of each quantification point	None
tagNames	A character vector indicating the names of the MS tags used at each temperature point, where <i>tagNames[i]</i> corresponds with <i>experimentNames[i]</i>	None
resultPath	Path to where the output files will be stored	getwd()

Files Generated	File Type	Description
config	.csv	Configuration table used by TPP
vehicle1	.csv	Table representing <i>vehicle1Columns</i> consisting of qpsm values and relative protein amounts
treatment1	.csv	Table representing <i>treatment1Columns</i> consisting of qpsm values and relative protein amounts
vehicle2	.csv	Table representing <i>vehicle2Columns</i> consisting of qpsm values and relative protein amounts
treatment2	.csv	Table representing <i>treatment2Columns</i> consisting of qpsm values and relative protein amounts

analyze

Function: analyzes the data frames provided by *init*

Parameter	Description	Default Value
configPath	Path to the configuration file	"config.csv"
vehicle1Path	Path to the table representing <i>init</i> 's <i>vehicle1Columns</i>	"vehicle1.csv"
treatment1Path	Path to the table representing <i>init</i> 's <i>treatment1Columns</i>	"treatment1.csv"
vehicle2Path	Path to the table representing <i>init</i> 's <i>vehicle2Columns</i>	NULL
treatment2Path	Path to the table representing <i>init</i> 's <i>treatment2Columns</i>	NULL
experimentNames	A character vector indicating the names of each experiment, where <i>experimentNames</i> [1] is the name of the <i>vehicle1Path</i> quantifications, <i>experimentNames</i> [2] is the name of the <i>treatment1Path</i> quantifications, <i>experimentNames</i> [3] is the name of the <i>vehicle2Path</i> quantifications, and <i>experimentNames</i> [4] is the name of the <i>treatment2Path</i> quantifications	c("Vehicle1", "Treatment1", "Vehicle2", "Treatment2")
resultPath	Path to where the output files will be stored	getwd()

Files Generated	File Type	Description
results_TPP_TR	.xlsx	Results table generated by TPP that lists normalized quantifications, curve parameters, and quality variables
results	.csv	A copy of <i>results_TPP_TR</i> in .csv format
QCplots	.pdf	Contains the normalization curve and other graphs describing the data
dataObj	folder	Contains workspaces at different breakpoints during TPP's analysis

getSignificant

Function: get a list of proteins that are of high quality and show significant shifts

Parameter	Description	Default Value
resultPath	Path to the results table generated by <i>analyze</i>	"results.csv"
experimentNames	A character vector indicating the names of each experiment, where <i>experimentNames</i> [1] is the name of the <i>vehicle1Path</i> quantifications, <i>experimentNames</i> [2] is the name of the <i>treatment1Path</i> quantifications, <i>experimentNames</i> [3] is the name of the <i>vehicle2Path</i> quantifications, and <i>experimentNames</i> [4] is the name of the <i>treatment2Path</i> quantifications	c("Vehicle1", "Treatment1", "Vehicle2", "Treatment2")

Output Type	Description
Character vector	Results table generated by TPP that lists normalized quantifications, curve parameters, and quality variables

plotCurves

Function: plots curves for a specified list of proteins

Parameter	Description	Default Value
configPath	Path to the configuration file	"config.csv"
vehicle1Path	Path to the table representing <i>init's vehicle1Columns</i>	"vehicle1.csv"
treatment1Path	Path to the table representing <i>init's treatment1Columns</i>	"treatment1.csv"
vehicle2Path	Path to the table representing <i>init's vehicle2Columns</i>	NULL
treatment2Path	Path to the table representing <i>init's treatment2Columns</i>	NULL
experimentNames	A character vector indicating the names of each experiment, where <i>experimentNames[1]</i> is the name of the <i>vehicle1Path</i> quantifications, <i>experimentNames[2]</i> is the name of the <i>treatment1Path</i> quantifications, <i>experimentNames[3]</i> is the name of the <i>vehicle2Path</i> quantifications, and <i>experimentNames[4]</i> is the name of the <i>treatment2Path</i> quantifications	c("Vehicle1", "Treatment1", "Vehicle2", "Treatment2")
resultPath	Path to where the output files will be stored	getwd()
proteinList	List of protein identifiers to be fitted with curves and plotted	None

Files Generated	File Type	Description
Melting_Curves	folder	Contains plots for proteins in <i>proteinList</i>

poissonFit

Function: uses a poisson model to fit curves and analyze quantifications

Parameter	Description	Default Value
frame	A data frame consisting of the protein quantifications	None
identifierColumn	A number indicating the column where the identifier of the protein is stored	None
vehicleColumns	A numeric vector indicating the columns where the vehicle quantifications are located	None
treatmentColumns	A numeric vector indicating the columns where the treatment quantifications are located	None
temperatures	A numeric vector indicating the temperatures of each quantification point	None
resultPath	Path to where the output files will be stored	getwd()

Files Generated	File Type	Description
results	.csv	Results table that lists curve parameters and quality variables
Melting_Curves	folder	Contains plots for proteins in <i>proteinList</i>