Package 'polyPK'

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Type Package

Title The Pharmacokinetics (PK) of Multi-Component Drugs Using a Metabolomics Approach

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Description

Poly-PK strategy is a new strategy of pharmacokinetic analysis of multi-component drugs (Guoxiang Xie, Tianlu Chen, Wei Jia, et al. (2012)<doi:10.1021/pr300318m>; Ke Lan, Guoxiang Xie and Wei Jia. (2013)<doi:10.1155/2013/819147>). This package is the first implementation of the Poly-PK strategy with 10 easy-to-use functions.

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Encoding UTF-8

LazyData TRUE

Imports imputeLCMD,plyr,sqldf,gplots,corrplot,circlize,mixOmics,pkr,Hmisc,ropls

Depends impute,pcaMethods,xlsx

Suggests knitr, rmarkdown

VignetteBuilder knitr

NeedsCompilation no

Repository CRAN

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R topics documented:

A *Test data of differential metabolites*

Description

The test data for examples at function ScatPlot.PKs,CorrPlot,HeatMap The data is a resulting matrix of function GetDiffData.

Usage

```
data("A")
```

Details

nothing

Source

GetDiffData

References

1. Ke Lan,Wei Jia,et al.An Integrated Metabolomics and Pharmacokinetics Strategy for Multi-Component Drug Evaluation.(2010)Current Drug Metabolism.

2. Guoxiang Xie,Wei Jia,et al.Metabolic Fate of Tea Polyphenols in Humans.(2012)Journal of Proteome Research.

3. Ke Lan,Wei Jia,et al.Towards Polypharmacokinetics:Pharmacokinetics of Multicomponent Drug and Herbal Medicines Using a Metabolomics Approach.(2013)Evidence-Based Complementary and Alternative Medicine.

4. Wei Jia,Tai-ping Fan,et al.The polypharmacokinetics of herbal medicines.(2015) Science.

5. Guoxiang Xie,Wei Jia,et al.Poly-pharmacokinetic study of a multicomponent herbal medicine in healthy Chinese volunteers.(2017)Clinical Pharmacology&Therapeutics.

Examples

```
data(A)
```

B *Test data of endogenous metabolites*

Description

The data B is an example of the endogenous metabolites, which can be an input argument of GetSecdAbso,CorrPlot,HeatMap etc.

Usage

```
data("B")
```

Details

nothing

Source

GetEndo

References

1. Ke Lan,Wei Jia,et al.An Integrated Metabolomics and Pharmacokinetics Strategy for Multi-Component Drug Evaluation.(2010)Current Drug Metabolism.

2. Guoxiang Xie,Wei Jia,et al.Metabolic Fate of Tea Polyphenols in Humans.(2012)Journal of Proteome Research.

3. Ke Lan,Wei Jia,et al.Towards Polypharmacokinetics:Pharmacokinetics of Multicomponent Drug and Herbal Medicines Using a Metabolomics Approach.(2013)Evidence-Based Complementary and Alternative Medicine.

4. Wei Jia,Tai-ping Fan,et al.The polypharmacokinetics of herbal medicines.(2015) Science.

5. Guoxiang Xie,Wei Jia,et al.Poly-pharmacokinetic study of a multicomponent herbal medicine in healthy Chinese volunteers.(2017)Clinical Pharmacology&Therapeutics.

Examples

```
data(B)
```

C *Test data of absorbed drug metabolites*

Description

The data C is an example of the absorbed drug metabolites, which can be an input argument of GetSecdAbso,CorrPlot,HeatMap etc.

Usage

```
data("C")
```

Details

nothing

Source

GetAbso

References

nothing

Examples

```
data(C)
```

CorrPlot *Plot the correlation diagram of two datasets*

Description

A function to calculate the correlation coefficients and plot the correlation diagram (8 types) of two input datasets.

Usage

```
CorrPlot(dataset1,dataset2,cor.method = "spearman", filepath,
                 fig.form = "heatmap", design = FALSE)
```

Arguments

dataset1	The first dataset (data frame with required format). The first row should be column names. The first and the second column of the first row should be "Name" and "ID", and you can set 2 more tags at the third and the fourth column of the first row, such as "m.z" and "RT.min." or anything you like. From the fifth column till the end, sample indexes or names are expected. The first row of the data frame should be the gender information."1"means male, and "2" means female. The second row of the data frame should be the group information. The first column of the second row should be "group", and you can add group indexes of the data from the fifth column at the second row. The format of group number should be "0"(pre-dose). "1","2","3","4"...(post-dose). The third row of the data frame should be the information of timepoints. Please see the demo data for detailed format. This variable maybe the results of GetEndo,GetAbso,GetSecdAbso.
dataset2	The second dataset (data frame with required format). The form of dataset2 is the same as the form of dataset1. This variable maybe the results of GetEndo,GetAbso,GetSecdAbso.
cor.method	A character string indicating which correlation analysis ("pearson", "kendall", or "spearman") is to be used. Default: "spearman".
filepath	A character string indicating the path where the results may be saved in.
fig.form	The form of the correlation diagram. figure.fig.form=c("heatmap","bubble","ordered.bubble","chord","sq Default: "heatmap".
design	(optional) a study design dataset(data frame with required format).Use data(design) to see the detailed format. Default:"FALSE".

Details

nothing

Value

A folder named “CorrelationResults” containing three folders: "CorrelationResults(all)", "CorrelationResults(female)" and "CorrelationResults(male)". Each folder with three files will be created automatically.

p-value.xlsx: The p values of the correlation analysis.

r-value.xlsx: The r values of the correlation analysis.

correlation-matrix-HeatMap.pdf/correlation-matrix-ChordDiagram.pdf/ (ordered-)correlogram-square.pdf /(ordered-)correlogram-pie.pdf /correlation-matrix(-ordered)-BubbleDiagram.pdf: A PDF file which contains the selected form of correlation diagram.If the study design is given by right format, the time points of meals and sleeps will be described at the bottom of the picture.

Note

nothing

Author(s)

Mengci Li, Shouli Wang, Guoxiang Xie, Tianlu Chen and Wei Jia

References

nothing

See Also

ScatPlot:plot the PCA or PLS score figures and trajectories on input data.

HeatMap: plot heatmap of the input data.

Examples

```
##---- Should be DIRECTLY executable !! ----
data("B")
data("C")
CorrPlot(B,C,filepath=getwd(),fig.form="heatmap",design=FALSE)
##----the result is saved in your current working directory of the R process
```

DataPre *Preprocess the input data*

Description

Preprocess the input data. Variables with a lot of zeros and outliers may be removed. Missing values may be imputed and filled. Data may be transformed by logarithm transformation.

Usage

```
DataPre(tes,mv="min",rz=80,sv=TRUE,log=FALSE,filepath=getwd())
```

Arguments

tes	The data under pretreatment (data frame with required format). The first row should be column names. The first and the second column of the first row should be "Name" and "ID", and you can set 2 more tags at the third and the fourth column of the first row, such as "m.z" and "RT.min." or anything you like. From the fifth column till the end, sample indexes or names are expected. The first row of the data frame should be the gender information."1"means male, and "2" means female. The second row of the data frame should be the group information. The first column of the second row should be "group", and you can add group indexes of the data from the fifth column at the second row. The format of group number should be "0"(pre-dose). "1","2","3","4"...(post-dose). The third row of the data frame should be the information of timepoints. Please see the demo data for detailed format.

rz	The percentage of zeros for variable elimination (Default:80). Variables with zero numbers higher than rz
mv	The method of missing values imputation (Default: "min"). mv=c ("min", "knn", "qrilc").
sv	A logical value indicating whether to remove the outliers (Default: TRUE). The data which distance to the mean is bigger than 1.5 times of the difference value between lower quartile and upper quartile, should be identified as an outlier. And it will be replaced by the mean value of corresponding row.
log	A logical value indicating whether to take the logarithm on the data (Default: FALSE).
filepath	A character string indicating the path where the results may be saved in.

Details

nothing

Value

A data frame of the prepocessed data

A folder named "preprocessed-data" containing a file of the prepocessed datasets will be created automatically. The file's name is "preprocessed-data.xlsx".

Note

nothing

Author(s)

Mengci Li, Shouli Wang, Guoxiang Xie, Tianlu Chen and Wei Jia

References

Hastie, Botstein, et al. Imputing Missing Data for Gene Expression Arrays, Stanford University Statistics Department Technical report (1999)

See Also

nothing

Examples

```
data("preData")
DataPre(preData)
##The result will be saved at your current working directory of the R process.
```

design *Test data of study design*

Description

Given the information of meal times and sleep times and so on.Please use data(design) to see the format.

Usage

```
data("design")
```

Examples

```
data(design)
## maybe str(design) ; plot(design) ...
```

drugData *The drug constitutes dataset (data frame)*

Description

An example of drug metabolites data,which is the input of GetAbso,Simi

Usage

```
data("drugData")
```

Details

nothing

Source

nothing

References

nothing

Examples

```
data(drugData)
```

GetAbso *Get the absorbed drug constitutes from the differential compounds*

Description

A function to get the absorbed drug constitutes by similarity analysis on the list of differential compounds and the list of drug constitutes.

Usage

```
GetAbso(drug,A,simidata, sim = 80, filepath=getwd(),design=FALSE)
```

Arguments

drug	The drug constitutes dataset (data frame)
A	The differential compounds which is derived from the GetDiffData function.
simidata	The same compounds of drug and pre-dose metabolome data, which is derived from Simi.
sim	The parameter (percentage) for similarity analysis. Default: 80.
filepath	A character string indicating the path where the results may be saved in.
design	(optional) a study design dataset(data frame with required format).Use data(design) to see the detailed format. Default:"FALSE".

Details

nothing

Value

A data frame of the list and data of absorbed drug constitutes.

A folder named "AbsorbedDrugMetabolites" containing a file named "AbsorbedDrugMetabolites.xlsx" will be created automatically which is the list and data of absorbed drug constitutes. And the foreground color of the same compounds produced by Simi will be marked with light blue. If the study design is given by right fromat, the meal times and sleep times will be marked as yellow and grey.

Note

nothing

Author(s)

Mengci Li, Shouli Wang, Guoxiang Xie, Tianlu Chen and Wei Jia

References

1. Ke Lan, Wei Jia, et al. An Integrated Metabolomics and Pharmacokinetics Strategy for Multi-Component Drug Evaluation. (2010) Current Drug Metabolism.

2. Guoxiang Xie, Wei Jia, et al. Metabolic Fate of Tea Polyphenols in Humans. (2012) Journal of Proteome Research.

3. Ke Lan, Wei Jia, et al. Towards Polypharmacokinetics: Pharmacokinetics of Multicomponent Drug and Herbal Medicines Using a Metabolomics Approach. (2013) Evidence-Based Complementary and Alternative Medicine.

4. Wei Jia, Tai-ping Fan, et al. The polypharmacokinetics of herbal medicines. (2015) Science.

5. Guoxiang Xie, Wei Jia, et al. Poly-pharmacokinetic study of a multicomponent herbal medicine in healthy Chinese volunteers. (2017) Clinical Pharmacology&Therapeutics.

See Also

GetDiffData GetEndo GetSecdAbso Simi

Examples

```
##---- Should be DIRECTLY executable !! ----

data("drugData")
data("A")
data("simidata")
#data("design")
GetAbso(drugData, A,simidata, sim = 80, filepath=getwd(),design=FALSE)
##the result is saved in your current working directory of the R process,which
##is the input (C) of function GetSecdAbso
```

`GetDiffData` *Get the differential compounds across all the time points*

Description

A function to get all the differential compounds between the pre-dose and every post-dose datasets.

Usage

```
GetDiffData(preData,postData,simidata,mv,rz,sv,log,t,r.adj,filepath,design)
```

Arguments

`preData`	The original pre-dose dataset (data frame) with an indicator of gender variable at the first row, grouping variable at the second row, and time points at the third row.
`postData`	The original post-dose dataset (data frame) with an indicator of gender variable at the first row, grouping variable at the second row, and time points at the third row.

simidata	The same compounds of drug and pre-dose metabolome data, which is derived from Simi.
rz	The percentage of zeros for variable elimination(Default:80)
mv	The method of missing values imputation (Default:"min"). mv=c("min","knn","qrilc")
sv	A logical value indicating whether to remove the outliers (Default:TRUE). The data which distance to the mean is bigger than 1.5 times of the difference value between lower quartile and upper quartile, should be identified as an outlier. And it will be replaced by the mean value of corresponding row.
log	A logical value indicating whether to take the logarithm on the datasets (Default: FALSE)
t	The method for differential compounds identification. C ("Ttest", "MWtest"). Default: "Ttest". Compounds with p values less than 0.05 were taken as differential ones.
r.adj	The methods for p values adjustment. r.adj=c("holm", "fdr"). Default: "fdr".
filepath	A character string indicating the path where the results may be saved in.
design	(optional) a study design dataset(data frame with required format).Use data(design) to see the detailed format.Default:"FALSE"

Details

nothing

Value

A	A list of all the differential compounds, with preprocessed data. The compounds were listed in weight rank order calculated by the SAM (Significance analysis of microarrays) method (see reference 6).
A_pre	A list of all the differential compounds, with original data. The compounds were listed in weight rank order calculated by the SAM (Significance analysis of microarrays) method (see reference 6).
p	The p values of differential compounds. The dimension of p is i*j, if there are i compounds exist in both pre-dose and post-dose data sets and there are j post-dose time points.
p_adj	The adjusted p values of differential compounds. The dimension of p_adj is the same as p.

A folder named "DifferentialMetabolites" containing four files of the above 4 datasets will be created automatically.

The name of the file is: "p-value.xlsx", "p-value(adjusted).xlsx", "DifferentialMetabolites(preprocessed).xlsx" and "DifferentialMetabolites(raw).xlsx" respectively.

And the foreground color of the same compounds produced by Simi will be marked with light blue.If the study design is given by right fromat, the meal times and sleep times will be marked as yellow and grey.

Note

nothing

Author(s)

Mengci Li, Shouli Wang, Guoxiang Xie, Tianlu Chen and Wei Jia

References

1. Ke Lan, Wei Jia, et al. An Integrated Metabolomics and Pharmacokinetics Strategy for Multi-Component Drug Evaluation. (2010) Current Drug Metabolism.

2. Guoxiang Xie, Wei Jia, et al. Metabolic Fate of Tea Polyphenols in Humans. (2012) Journal of Proteome Research.

3. Ke Lan, Wei Jia, et al. Towards Polypharmacokinetics:Pharmacokinetics of Multicomponent Drug and Herbal Medicines Using a Metabolomics Approach. (2013) Evidence-Based Complementary and Alternative Medicine.

4. Wei Jia, Tai-ping Fan, et al. The polypharmacokinetics of herbal medicines. (2015) Science.

5. Guoxiang Xie, Wei Jia, et al. Poly-pharmacokinetic study of a multicomponent herbal medicine in healthy Chinese volunteers. (2017) Clinical Pharmacology&Therapeutics.

6. Virginia Goss Tusher, Robert Tibshirani,et al. Significance analysis of microarrays applied to the ionizing radiation response. (2001) PNAS.

See Also

GetEndo GetAbso GetSecdAbso Simi

Examples

```
##---- Should be DIRECTLY executable !! ----
## Not run: data("preData")
data("postData")
data("simidata")
data("design")

GetDiffData(preData,postData,simidata,filepath=getwd(),design=FALSE)

## End(Not run)
##the result will be saved in your current working directory of the R process.
```

`GetEndo` *Get the altered endogenous metabolites from the differential compounds*

Description

A function to get the altered endogenous metabolites by similarity analysis on the list of differential compounds and the list of pre-dose compounds.

Usage

```
GetEndo(pre,A,simidata,sim=80,filepath,design)
```

Arguments

pre	The pre-dose dataset (data frame).
A	The differential compounds which is derived from the GetDiffData function.
simidata	The same compounds of drug and pre-dose metabolome data, which is derived from Simi.
sim	The parameter (percentage) for similarity analysis. Default: 80.
filepath	A character string indicating the path where the results may be saved in.
design	(optional) a study design dataset(data frame with required format).Use data(design) to see the detailed format. Default:"FALSE"

Details

nothing

Value

A data frame which is the list and data of altered endogenous metabolites.

A folder named "EndogenousMetabolites" containing a file named "EndogenousMetabolites.xlsx" will be created automatically which is the list and data of altered endogenous metabolites. And the foreground color of the same compounds produced by Simi will be marked with light blue. If the study design is given by right format, the meal times and sleep times will be marked as yellow and grey.

Note

nothing

Author(s)

Mengci Li, Shouli Wang, Guoxiang Xie, Tianlu Chen and Wei Jia

References

1. Ke Lan, Wei Jia, et al. An Integrated Metabolomics and Pharmacokinetics Strategy for Multi-Component Drug Evaluation. (2010) Current Drug Metabolism.

2. Guoxiang Xie, Wei Jia, et al. Metabolic Fate of Tea Polyphenols in Humans. (2012) Journal of Proteome Research.

3. Ke Lan, Wei Jia, et al. Towards Polypharmacokinetics:Pharmacokinetics of Multicomponent Drug and Herbal Medicines Using a Metabolomics Approach. (2013) Evidence-Based Complementary and Alternative Medicine.

4. Wei Jia, Tai-ping Fan,et al. The polypharmacokinetics of herbal medicines. (2015) Science.

5. Guoxiang Xie, Wei Jia, et al. Poly-pharmacokinetic study of a multicomponent herbal medicine in healthy Chinese volunteers. (2017) Clinical Pharmacology&Therapeutics.

See Also

GetDiffData GetAbso GetSecdAbso Simi

Examples

```
##---- Should be DIRECTLY executable !! ----
data("preData")
 data("A")
 data("simidata")
data("design")
 GetEndo(preData,A,simidata,sim=80,filepath=getwd(),design=FALSE)
##----the result is saved at your current working directory of the R process
##----which is the input (B) of function GetSecdAbso
```

`GetSecdAbso` *Get the secondary metabolites of the absorbed drug constitutes*

Description

A function to get secondary metabolites of the absorbed drug constitutes.

Usage

```
GetSecdAbso(A,B,C,simidata,sim=80,filepath,design)
```

Arguments

`A`	The differential compounds dataset which is derived from the GetDiffData function.
`B`	The altered endogenous metabolites dataset which is derived from the GetEndo function.
`C`	The absorbed drug constitutes dataset which is derived from the GetAbso function.
`simidata`	The same compounds of drug and pre-dose metabolome data, which is derived from Simi.
`sim`	The parameter (percentage) for similarity analysis. Default: 80.
`filepath`	A character string indicating the path where the results may be saved in.
`design`	(optional) a study design dataset(data frame with required format).Use data(design) to see the detailed format. Default:"FALSE".

Details

nothing

Value

A folder named "SecondAbsorbedMetabolites" containing a file named "SecondAbsorbedMetabolites.xlsx" will be created automatically which is the list and data of secondary metabolites of the absorbed drug constitutes. And the foreground color of the same compounds produced by Simi will be marked with light blue. If the study design is given by right from, the meal times and sleep times will be marked as yellow and grey.

Note

The list of absorbed drug compounds was obtained by excluding compounds in B and C from that of A.

Author(s)

Mengci Li, Shouli Wang, Guoxiang Xie, Tianlu Chen and Wei Jia

References

1. Ke Lan, Wei Jia, et al. An Integrated Metabolomics and Pharmacokinetics Strategy for Multi-Component Drug Evaluation. (2010) Current Drug Metabolism.

2. Guoxiang Xie, Wei Jia, et al. Metabolic Fate of Tea Polyphenols in Humans. (2012) Journal of Proteome Research.

3. Ke Lan, Wei Jia, et al. Towards Polypharmacokinetics: Pharmacokinetics of Multicomponent Drug and Herbal Medicines Using a Metabolomics Approach. (2013) Evidence-Based Complementary and Alternative Medicine.

4. Wei Jia, Tai-ping Fan, et al. The polypharmacokinetics of herbal medicines. (2015) Science.

5. Guoxiang Xie, Wei Jia, et al. Poly-pharmacokinetic study of a multicomponent herbal medicine in healthy Chinese volunteers. (2017) Clinical Pharmacology&Therapeutics.

See Also

GetDiffData GetAbso GetEndo Simi

Examples

```
##---- Should be DIRECTLY executable !! ----
##-- ==>  Define data, use random,
##--or do  help(data=index)  for the standard data sets.
data("A")
data("B")
data("C")
data("simidata")
data("design")
GetSecdAbso(A,B,C,simidata,sim=80,filepath=getwd(),design=FALSE)
```

HeatMap *Plot the heatmap of input data*

Description

A function to plot the heatmap and clusters of input data.

Usage

```
HeatMap(data,cluster="both",scale="row",filepath,design)
```

Arguments

data	The data under analysis (data.frame with required format) The first row should be column names. The first and the second column of the first row should be "Name" and "ID", and you can set 2 more tags at the third and the fourth column of the first row, such as "m.z" and "RT.min." or anything you like. From the fifth column till the end, sample indexes or names are expected. The first row of the data frame should be the gender information. "1" means male, and "2" means female. The second row of the data frame should be the group information. The first column of the second row should be "group", and you can add group indexes of the data from the fifth column at the second row. The format of group number should be "0"(pre-dose). "1","2","3","4"...(post-dose). The third row of the data frame should be the information of timepoints. Please see the demo data for detailed format.
cluster	A string indicating whether or in which direction the dendrograms should be drawn (“none”, “row”, “column” or “both”). Default:”both”.
scale	A character indicating whether the data should be centered and scaled before analysis and in which (“none”, “row” or “column”) direction. Default:"row".
filepath	A character string indicating the path where the results may be saved in.
design	(optional) a study design dataset(data frame with required format).Use data(design) to see the detailed format. Default:"FALSE".

Details

nothing

Value

A folder named “HeatMap” containing a PDF file (the heatmap figure) will be created automatically. If the study design is given by right format, the time points of meals and sleeps will be described at the bottom of the picture.

Note

nothing

Author(s)

Mengci Li, Shouli Wang, Guoxiang Xie, Tianlu Chen and Wei Jia

References

nothing

See Also

CorrPlot: plot the correlation diagram of two datasets.

ScatPlot: plot the PCA or PLS score figures and trajectories on input data.

Examples

```
##---- Should be DIRECTLY executable !! ----
##-- ==>  Define data, use random,
##--or do  help(data=index)  for the standard data sets.
data("B")
HeatMap(data=B,cluster="both",scale="row",filepath=getwd(),design=FALSE)
##the result is saved in your current working directory of the R process
```

PKs *Calculate the representative pharmacokinetics parameters and plot the time-intensity curves of specified compounds.*

Description

A function to calculate the 7 pharmacokinetics parameters (Tmax, Cmax, AUC, CL, Tlast, Tfirst, Cmin) and plot the time-intensity curves for specified compounds.

Usage

```
PKs(d.pk,d.point="mean",d.ebar="SE",filepath=getwd(),design=FALSE)
```

Arguments

d.pk	The data under analysis (data frame with required format) The first row should be column names. The first and the second column of the first row should be "Name" and "ID", and you can set 2 more tags at the third and the fourth column of the first row, such as "m.z" and "RT.min." or anything you like. From the fifth column till the end, sample indexes or names are expected. The first row of the data frame should be the gender information."1"means male, and "2" means female. The second row of the data frame should be the group information. The first column of the second row should be "group", and you can add group indexes of the data from the fifth column at the second row. The format of group number should be "0"(pre-dose). "1","2","3","4"...(post-dose). The third row of the data frame should be the information of timepoints. Please see the demo data for detailed format.
d.point	The value to calculate the pharmacokinetics parameters, and the value of points in the time-intensity curve. d.point=c ("mean","median"). Default:"mean".
d.ebar	The value of error bars. d.ebar=c ("SE","SD"). Defalut:"SE".
filepath	A character string indicating the path where the results may be saved in.
design	(optional) a study design dataset(data frame with required format). Use data(design) to see the detailed format. Default:"FALSE"

Details

nothing

Value

A list of metabolites and 7 pharmacokinetics parameters (Tmax,Cmax,AUC,CL,Tlast,Tfirst,Cmin) of specified compound.

Cmax: The peak plasma concentration of a drug after administration.

AUC: Area under the Drug Concentration Curve(0- infinite).

CL: The rate of clear.

Tlast: The last time.

Tfirst: Time to observe the first non-zero concentration.

Cmin: The least plasma concentration of a drug after administration.

A folder named "PKresluts" will also be created automatically which contains three folders:"PKresluts(all)","PKresluts(male) Each folder has two kinds of files (.xlsx and .PDF).

The file named “PK-parameters.xlsx” contains the pharmacokinetics parameters and the one or more *.PDF files show the time-intensity curves of specified metabolites. Each metabolite has one PDF file named "Time-Intensity-Curve of (its own name).pdf".If the study design is given by right format, the time points of meals and sleeps will be described at the bottom of the picture.

Note

nothing

Author(s)

Mengci Li, Shouli Wang, Guoxiang Xie, Tianlu Chen and Wei Jia

References

1. Veng Pedersen P. Mean time parameters in pharmacokinetics. Definition, computation and clinical implications. (1898) Clin Pharmacokinet.

2. Krishnaswami S, Wang T, et al. Single- and multiple-dose pharmacokinetics of tofacitinib in healthy Chinese volunteers. (2015) Clin Pharmacol Drug Dev.

See Also

nothing

Examples

```
data("C")
PKs(C,d.point="mean",d.ebar="SE",filepath=getwd(),design=FALSE)
####the result is saved in your current working directory of the R process
```

postData *The post-dose metabolites dataset (data frame)*

Description

The example data of post-dose metabolites,which can be an input argument of GetDiffData,GetEndo and DataPre.The first row should be column names. The first row of the data frame should be the gender information.The second row of the data frame should be the group information.The format of group number should be"1","2","3","4"...(post-dose).. The third row of the data frame should be the information of timepoints.

Usage

```
data("postData")
```

Details

nothing

Source

nothing

References

nothing

Examples

```
data(postData)
## maybe str(postData) ; plot(postData) ...
```

preData *The pre-dose metabolites dataset (data frame)*

Description

The example data of pre-dose metabolites,which can be an input argument of GetDiffData,GetEndoand DataPre.The first row should be column names. The first row of the data frame should be the gender information.The second row of the data frame should be the group information.The format of group number should be "0"(pre-dose). The third row of the data frame should be the information of timepoints.

Usage

```
data("preData")
```

Details

nothing

Source

nothing

References

nothing

Examples

```
data(preData)
## maybe str(preData) ; plot(preData) ...
```

`ScatPlot` *Plot the PCA or PLSDA score figures and trajectories on input data*

Description

A function to plot the PCA or PLSDA figures of input data.

Usage

```
ScatPlot(scat.data,scform="PCA",num.of.cp,fold,filepath,design)
```

Arguments

`scat.data`	The data under analysis (data frame with required format). The first row should be column names. The first and the second column of the first row should be "Name" and "ID", and you can set 2 more tags at the third and the fourth column of the first row, such as "m.z" and "RT.min." or anything you like. From the fifth column till the end, sample indexes or names are expected. The first row of the data frame should be the gender information. "1" means male, and "2" means female. The second row of the data frame should be the group information. The first column of the second row should be "group", and you can add group indexes of the data from the fifth column at the second row. The format of group number should be "0"(pre-dose). "1","2","3","4"...(post-dose). The third row of the data frame should be the information of timepoints. Please see the demo data for detailed format.
`scform`	The form of scat plot. scform=c ("PCA","PLSDA"). Default:"PCA".
`num.of.cp`	The number of components to decompose. Default:2.
`fold`	Integer: number of random permutations [default is 100 for single response models (without train/test partition)].
`filepath`	A character string indicating the path where the results may be saved in.
`design`	(optional) a study design dataset(data frame with required format).Use data(design) to see the detailed format. Default:"FALSE".

Details

nothing

Value

A folder named "PCAresults" or "PLSDAresluts" with three folders: "PCA/PLSDA(all)", "PCA/PLSDA(male)" and "PCA/PLSDA(female)". In each folder, 4 (for PCA) or 6 (for PLSDA) files will be created automatically.

PCA(PLSDA)-loading.xlsx: The loading values of PCA (PLSDA) analysis.

PCA(PLSDA)-score.xlsx: The score values of PCA (PLSDA) analysis.

PCA(PLSDA)-scorePlot.pdf: A 2 dimensional scores plot of PCA (PLSDA) analysis. If the study design is given, the time points of meals and sleeps will be described at the bottom of the picture.

PCA(PLSDA)-scorePlot(track).pdf: A trajectory plot derived from the PCA (PLSDA) scores plot in which samples of a group will be represented by one point (the center of the group) and will be connected by lines in time ascending order. If the study design is given, the time points of meals and sleeps will be described at the bottom of the picture.

ErrorRate.xlsx (only in "PLSDAresluts"): For PLS-DA models, "ScatPlot" produces a matrix of overall error rate estimation. The dimensions of the matrix correspond to the components in the model and to the prediction method used, respectively.

PermutationPlot.pdf (only in "PLSDAresluts"): Scatter plot of true and permutated R2Ys and Q2Ys.

Note

nothing

Author(s)

Mengci Li, Shouli Wang, Guoxiang Xie, Tianlu Chen and Wei Jia

References

nothing

See Also

CorrPlot: plot the correlation diagram of two datasets.

HeatMap: plot heatmap of the input data.

Examples

```
## Not run: data("A")
ScatPlot(scat.data=A,scform="PCA",num.of.cp=2,filepath=getwd(),design=FALSE)
## End(Not run)
##----the result is saved in your current working directory of the R process
```

Simi *Get the same compounds in two datasets*

Description

A function which can get the same compounds in two datasets.Especially the same compounds of drug and pre-dose metabolome data.

Arguments

data1	The pre-dose dataset (data frame with required format).The first row should be column names. The first and the second column of the first row should be "Name" and "ID", and you can set 2 more tags at the third and the fourth column of the first row, such as "m.z" and "RT.min." or anything you like. From the fifth column till the end, sample indexes or names are expected. The first row of the data frame should be the gender information."1"means male,and "2" means female.The second row of the data frame should be the group information.The first column of the second row should be "group", and you can add group indexes of the data from the fifth column at the second row. The format of group number should be "0"(pre-dose). "1","2","3","4"...(post-dose). The third row of the data frame should be the information of timepoints.Please see the demo data for detailed format.
data2	The drug constitutes dataset (data frame)
filepath	A character string indicating the path where the results may be saved in.

Details

The results can be an input argument "simidata" of GetDiffData ,GetEndo,GetAbso,GetSecdAbso

Value

A list :

`repetitive rates in data1`
: The repetitive rates of same compounds in first metabolites dataset

`repetitive rates in data2`
: The repetitive rates of same compounds in second metabolites dataset

`similar metabolites`
: IDs of same compounds(matrix),which can be an input argument of GetDiffData ,GetEndo,GetAbso,GetSecdAbso

And a folder named "SimilarData" containing a file named "Similar-data.xlsx" will be created automatically, which is the same compounds dataset.

Author(s)

Mengci Li, Shouli Wang, Guoxiang Xie, Tianlu Chen, Wei Jia

See Also

GetDiffData GetEndo GetAbso GetSecdAbso

Examples

```
##---- Should be DIRECTLY executable !! ----
## Not run: data(preData)
data(drugData)
Simi(data1<-preData,data2<-drugData,filepath=getwd())
## End(Not run)
```

`simidata` *Test data of same compounds.*

Description

The same compounds of drug and pre-dose metabolome data,which can be an input argument of GetDiffData,GetEndo,GetAbso and GetSecdAbso

Usage

```
data("simidata")
```

Source

Simi

Examples

```
data(simidata)
## maybe str(simidata) ; plot(simidata) ...
```

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