Package 'eSEM'

December 20, 2023

Type Package

Title Enzyme activity inference from Structural Equation Modeling

Version 1.0

Date 2023-09-13

Author Dehui Kong

Maintainer Dehui Kong <dkong3@uthsc.edu>

Imports lavaan(>= 0.6-11), tidyr(>= 1.2.0), stringr(>= 1.4.0), dplyr(>= 1.0.9), psych(>= 2.2.5), devtools(>= 2.4.5), EFAtools(>= 0.4.1)

Description eSEM is used to infer enzyme activity.

Depends R (>= 3.5.0)

License GPL-3

Encoding UTF-8

LazyData true

RoxygenNote 7.2.3

Suggests knitr, rmarkdown

VignetteBuilder knitr

R topics documented:

aceAdjacency *aceAdjacency*

Description

This script is used to build HUMAN HAT-substrate adjacency matrix.

Usage

```
aceAdjacency(databaseACE)
```

Arguments

databaseACE	Default database or customized database input.

catchActRaw *catchResults*

Description

Catch Activity and Affinity. Activity contains Raw-Activity, Mean-Center, Z-scaled.

Usage

```
catchActRaw(x)
```

Arguments

x	The results from modeling fitting.
rawData	Input raw data (quantitative phospho-proteomics / ubiqutin-proteomics data)

eSEM *eSEM*

Description

Infer enzyme activity from phosphoralation, ubiquitination, acetylation

Usage

```
eSEM(
  input = NULL,
  datatype = NULL,
  organism = NULL,
  enzyme.organism = NULL,
  database = NULL,
  cor.off = 0.95,
  kmo.off = 0,
  enzyList = NULL,
  input.log2.norm = FALSE,
  whole.log2.trans = FALSE,
  whole.proteome = NULL,
  motif = NULL,
  output.folder = getwd()
)
```

Arguments

input	Dataframe. Your quantitative ubiquiti-proteomics, phospho-proteomic and acetyl-proteomics data.
datatype	Factor. Data type: ubiquitination or phosphoralation or acetylation; ("ubi", "psp", "ace")
organism	Vector. Substrate species; (“human”, “mouse”, “rat”)
enzyme.organism	Vector. Enzyme species; (“human”, “mouse”, “rat”)
database	Dataframe. Customized database input. Default is NULL using internal database.
cor.off	Numeric. Set up correlation cutoff value 0-1 to remove high collinear variables. Default is 0.95.
kmo.off	Numeric. Set up KMO cutoff value 0-1. Default is 0.
enzyList	Vector. Program only calculate the enzyme in the enzyList. Default is to output ALL enzyme activities and affinities.
input.log2.norm	Logical. FALSE or TRUE. Need program to do log2 transforming of the input file or not. Default is FALSE.
whole.log2.trans	Logical. FALSE or TRUE. Need program to do log2 transforming of the whole proteome or not. (Ignore if -whole.proteome is missing). Default is FALSE.
whole.proteome	Dataframe. Set up whole proteome used to normalize phosphor-proteome or ubiquitin-proteome whole proteome. Default is NULL.
motif	Matrix. Added kinase-subatrate relationships from motif discovery.
output.folder	Character. Character vector of location to save files if desired. Default is current directory.

Details

You can use eSEM package to get enzyme activity.

Value

List

Examples

```
result <- eSEM(input = input_ubi_example,
               datatype = "ubi",
               organism = "human",
               input.log2.norm = T)


result <- eSEM(input = input_psp_example,
               datatype = "psp",
               organism = "mouse",
               enzyme.organism = c("human", "mouse", "rat"),
               cor.off = 0.8,
               input.log2.norm = TRUE,
               whole.log2.trans = TRUE,
               motif = motif_example,
               whole.proteome = wholeProteome_example)


result <- eSEM(input = input_ace_example,
               datatype = "ace",
               organism = "human",
               input.log2.norm = FALSE)
```

---

getFa *Build MEME input*

Description

script to extract MEME input .fa file

Usage

```
getFa(ss = NULL, es = NULL, filePath)
```

Arguments

ss	Vector; Substrate species; ("mouse", "rat", "human")
es	Vector; Kinase species; ("mouse", "rat", "human")
filePath	The path is used to save .fa files. Recommend to create a new folder to save all .fa.files.

Examples

```
getFa(ss = "human", es = c("human", "mouse", "rat"), filePath = getwd())
```

`inputTransformPSP` *inputTransform*

Description

This script is used to log2 transform AND/OR whole proteome normalize input data.

Usage

```
inputTransformPSP(
  input_raw,
  input_log2_trans = FALSE,
  whole_log2_trans = FALSE,
  whole_proteome = NULL
)
```

Arguments

`input_raw`	Input raw data (quantitative phospho-proteomics/ubiquitin-proteomics data)
`input_log2_trans`	FALSE or TRUE. Need program to do log2 transforming of the input file or not. Default is FALSE.
`whole_log2_trans`	Need program to do log2 transforming of the whole proteome or not. Ignore if -whole.proteome is missing. Default is FALSE.
`whole_proteome`	Set up whole proteome used to normalize phospho-proteomics/ubiquitin-proteomics data by whole proteome. Default is NULL.

`mastInput` *Build MAST input*

Description

Script to extract MAST input FASTA file.

Usage

```
mastInput(input, savePath = getwd())
```

Arguments

input	The same quantitative phosphoproteomics data as eSEM() input file.
savePath	The path to save built MAST input file. Default is the current directory.

Examples

```
mastInput(input = input_psp_example)
```

---

motifEx *motifEx*

Description

This script is used to extract kinase-substrate relationships from motif scanning and build motif_input file for KSEM().

Usage

```
motifEx(mastFile, savePath = getwd())
```

Arguments

mastFile	The output file "extract_result.txt" from Step: 03step_ExtractMASTresult.sh.
savePath	Path to save motif_input.txt file. Default is current directory.

---

pspAdjacency *pspAdjacency*

Description

This script is used to build kinase-substrate adjacency matrix with only PSP database.

Usage

```
pspAdjacency(sp, ep, databasePSP)
```

Arguments

sp	Substrate species; ("mouse", "rat", "human").
ep	Enzyme species; ("mouse", "rat", "human").
databasePSP	Default database or customized database input.

pspMotifAdjacency *pspMotifAdjacency*

Description

This script is used to build enzyme-substrate adjacency matrix with PSP database + Motif.

Usage

```
pspMotifAdjacency(sp, ep, databasePSP, motif.ref)
```

Arguments

sp	Substrate species; ("mouse", "rat", "human").
ep	Enzyme species; ("mouse", "rat", "human").
databasePSP	Default database or customized database input.
motif.ref	Added enzyme-subatrate relationships from motif discovery. Same as KSEM -motif parameter.

singleEnzymeAff *singleEnzymeAff*

Description

Get single enzyme affinity.

Usage

```
singleEnzymeAff(enzyme, input, adj, cor.off, kmo.off)
```

Arguments

enzyme	Single enzyme name.
input	Normalized and transformed phospho-proteomics / ubiqutin-proteomics data.
adj	Adjacency matrix.
cor.off	Set up correlation cutoff value 0-1 to remove high collinear variables. Default is 0.95.
kmo.off	Set up KMO cutoff value 0-1. Default is 0.

singleHatAct *singleHatAct*

Description

Get single HAT activity.

Usage

```
singleHatAct(HAT, input, adj, cor.off, kmo.off)
```

Arguments

HAT	Single HAT name.
input	Normalized and transformed acetyl-proteomics data.
adj	Adjacency matrix.
cor.off	Set up correlation cutoff value 0-1 to remove high collinear variables. Default is 0.95.
kmo.off	Set up KMO cutoff value 0-1. Default is 0.

singleKinaseAct *singleKinaseAct*

Description

Get single kinase activity.

Usage

```
singleKinaseAct(kinase, input, adj, cor.off, kmo.off)
```

Arguments

kinase	Single kinase name.
input	Normalized and transformed phosphoproteomics data.
adj	Adjacency matrix.
cor.off	Set up correlation cutoff value 0-1 to remove high collinear variables. Default is 0.95.
kmo.off	Set up KMO cutoff value 0-1. Default is 0.

singleLigaseAct *singleLigaseAct*

Description

Get single ligase activity.

Usage

```
singleLigaseAct(ligase, input, adj, cor.off, kmo.off)
```

Arguments

ligase	Single ligase name.
input	Normalized and transformed ubiquiti-proteomics data.
adj	Adjacency matrix.
cor.off	Set up correlation cutoff value 0-1 to remove high collinear variables. Default is 0.95.
kmo.off	Set up KMO cutoff value 0-1. Default is 0.

ubiAdjacency *ubiAdjacency*

Description

This script is used to build ligase-substrate adjacency matrix with only PSP database.

Usage

```
ubiAdjacency(sp, databaseUBI)
```

Arguments

sp	Substrate species; ("mouse", "rat", "human").
databaseUBI	Default database or customized database input.