# Package 'ASEB'

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Title Predict Acetylated Lysine Sites

**Version** 1.50.0

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Description

ASEB is an R package to predict lysine sites that can be acetylated by a specific KAT-family.

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**Depends** R ( $\geq$  2.8.0), methods

Imports graphics, methods, utils

**License** GPL (>= 3)

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```
asebProteins
```

#### Description

This function is used to predict all lysine sites on a specific protein that can be acetylated by a specific KAT-family.

#### Usage

asebProteins(backgroundSites, prodefinedSites, testProteins, outputFile=NULL, permutationTimes=10
## S4 method for signature 'character, character, character'

asebProteins(backgroundSites, prodefinedSites, testProteins, outputFile=NULL, permutationTimes=10
## S4 method for signature 'SequenceInfo,SequenceInfo'

```
asebProteins(backgroundSites, prodefinedSites, testProteins, outputFile=NULL, permutationTimes=10
```

# Arguments

backgroundSites

SequenceInfo object or file name (character(1)) for background peptides set.

prodefinedSites

SequenceInfo object or file name (character(1)) for KAT special peptides set.

testProteins SequenceInfo object or file name (character(1)) for query Proteins set.

outputFile file name for output (character(1)).

permutationTimes

permutation times (integer(1)), default and recommended: 10000.

# Details

This function is used to predict lysine sites that can be acetylated by a specific KAT-family. The whole process is similar with the GSEA method (permuting gene sets). Please see the references for details.

The first three arguments of method asebProteins can be SequenceInfo objects or file names. If these arguments are SequenceInfo objects, this method returns a list to the users besides an output file. Otherwise, this method processes the FASTA format files directly and outputs all results to a file. In this case, this method can process huge number of sites each time without loading any sequences to R workspace.

# Value

The output file contains enrichment scores and P-values for each query site. The asebProteins, SequenceInfo, seque

| results   | contains enrichment scores and P-values for each query site. |
|-----------|--------------------------------------------------------------|
| curveInfo | contains information for enrichment score curves.            |

#### asebSites

#### Note

The acetylated lysine sites and their surrounding amino acids (8 on each side) are treated as acetylated peptides.

Example for peptides sequence : "KEHDDIFDKLKEAVKEE". All input file should follow FASTA format.

#### References

Subramanian, A. et al. (2005) Gene set enrichment analysis: a knowledge-based approach for interpreting genome-wide expression profiles. *Proc Natl Acad Sci U S A*, **102**, 15545-15550.

Mootha, V.K. et al. (2003) PGC-1alpha-responsive genes involved in oxidative phosphorylation are coordinately downregulated in human diabetes. *Nat Genet*, **34**, 267-273.

Guttman, M. et al. (2009) Chromatin signature reveals over a thousand highly conserved large non-coding RNAs in mammals. *Nature*, **458**, 223-227.

Li, T.T. et al. Characterization and prediction of lysine (K)-acetyl-transferase (KAT) specific acetylation sites. *Mol Cell Proteomics*, in press.

#### See Also

SequenceInfo, readSequence, asebSites, drawStat, drawEScurve.

#### Examples

```
backgroundSites <- readSequence(system.file("extdata", "background_sites.fa", package="ASEB"))
prodefinedSites <- readSequence(system.file("extdata", "predefined_sites.fa", package="ASEB"))
testProteins <- readSequence(system.file("extdata", "proteins_to_test.fa", package="ASEB"))
resultList <- asebProteins(backgroundSites, prodefinedSites, testProteins, permutationTimes=100)
resultList$results[1:2,]</pre>
```

```
asebSites
```

prediction of lysine sites that can be acetylated

#### Description

This function is used to predict lysine sites that can be acetylated by a specific KAT-family.

#### Usage

```
asebSites(backgroundSites, prodefinedSites, testSites, outputFile=NULL, permutationTimes=10000)
## S4 method for signature 'character, character, character'
asebSites(backgroundSites, prodefinedSites, testSites, outputFile=NULL, permutationTimes=10000)
## S4 method for signature 'SequenceInfo,SequenceInfo,SequenceInfo'
asebSites(backgroundSites, prodefinedSites, testSites, outputFile=NULL, permutationTimes=10000)
```

#### Arguments

backgroundSites

SequenceInfo object or file name (character(1)) for background peptides set.

prodefinedSites

SequenceInfo object or file name (character(1)) for KAT special peptides set.

asebSites

| testSites        | SequenceInfo object or file name (character(1)) for query peptides set. |  |  |  |  |  |  |
|------------------|-------------------------------------------------------------------------|--|--|--|--|--|--|
| outputFile       | file name for output (character(1)).                                    |  |  |  |  |  |  |
| permutationTimes |                                                                         |  |  |  |  |  |  |
|                  | permutation times (integer(1)), default and recommended: 10000.         |  |  |  |  |  |  |

#### Details

This function is used to predict lysine sites that can be acetylated by a specific KAT-family. It will give an enrichment score and a P-value for each query lysine site. The whole process is similar with the GSEA method (permuting gene sets). Please see the references for details.

The first three arguments of method asebSites can be SequenceInfo objects or file names. If these arguments are SequenceInfo objects, this method returns a list to the users besides an output file. Otherwise, this method processes the FASTA format files directly and outputs all results to a file. In this case, this method can process huge number of sites each time without loading any sequences to R workspace.

# Value

The output file contains enrichment scores and P-values for each query site. The asebSites, SequenceInfo, SequenceInfo also returns a list contains two data.frame objects: results and curveInfo.

| results   | contains enrichment scores and P-values for each query site. |
|-----------|--------------------------------------------------------------|
| curveInfo | contains information for enrichment score curves.            |

# Note

The acetylated lysine sites and their surrounding amino acids (8 on each side) are treated as acetylated peptides.

Example for peptides sequence : "KEHDDIFDKLKEAVKEE". All input file should follow FASTA format.

#### References

Subramanian, A. et al. (2005) Gene set enrichment analysis: a knowledge-based approach for interpreting genome-wide expression profiles. *Proc Natl Acad Sci U S A*, **102**, 15545-15550.

Mootha, V.K. et al. (2003) PGC-1alpha-responsive genes involved in oxidative phosphorylation are coordinately downregulated in human diabetes. *Nat Genet*, **34**, 267-273.

Guttman, M. et al. (2009) Chromatin signature reveals over a thousand highly conserved large non-coding RNAs in mammals. *Nature*, **458**, 223-227.

Li, T.T. et al. Characterization and prediction of lysine (K)-acetyl-transferase (KAT) specific acetylation sites. *Mol Cell Proteomics*, in press.

# See Also

SequenceInfo, readSequence, asebProteins, drawStat, drawEScurve.

#### drawEScurve

#### Examples

```
backgroundSites <- readSequence(system.file("extdata", "background_sites.fa", package="ASEB"))
prodefinedSites <- readSequence(system.file("extdata", "predefined_sites.fa", package="ASEB"))
testSites <- readSequence(system.file("extdata", "sites_to_test.fa", package="ASEB"))
resultList <- asebSites(backgroundSites, prodefinedSites, testSites, permutationTimes=100)
resultList$results[1:2,]</pre>
```

```
drawEScurve
```

draw Enriment Score curves for specific sites

#### Description

This function is used to draw Enriment Score curves for specific sites.

# Usage

```
drawEScurve(curveInfoDataFrame, sites=NULL, max_p_value=0.1, min_es=0.2, outputDir=NULL, figKind=0
## S4 method for signature 'data.frame'
drawEScurve(curveInfoDataFrame, sites=NULL, max_p_value=0.1, min_es=0.2, outputDir=NULL, figKind=0
```

#### Arguments

| curveInfoDataFrame     |                                                                                                                                                   |  |  |  |  |
|------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------|--|--|--|--|
|                        | data.frame object: contains curve information for sites, see example.                                                                             |  |  |  |  |
| sites                  | character vector: only draw curves for sites with ids appear in this vector. default: draw curves for all the sites appear in curveInfoDataFrame. |  |  |  |  |
| <pre>max_p_value</pre> | numeric(1), only draw curves for sites with p-value less than this value.                                                                         |  |  |  |  |
| min_es                 | numeric(1), only draw curves for sites with Enriment Score more than this value.                                                                  |  |  |  |  |
| outputDir              | character(1), output directory name for all the figures.                                                                                          |  |  |  |  |
| figKind                | character(1), fig format: "pdf" or "jpeg".                                                                                                        |  |  |  |  |

#### Details

This function is used to draw Enrichment Score curves for specific sites. These curves show running-sum process for calculating enrichment score. The data.frame object contains curve information is given by asebSites or asebProteins.

# See Also

SequenceInfo, readSequence, asebSites, asebProteins, drawStat.

#### Examples

```
backgroundSites <- readSequence(system.file("extdata", "background_sites.fa", package="ASEB"))
prodefinedSites <- readSequence(system.file("extdata", "predefined_sites.fa", package="ASEB"))
testSites <- readSequence(system.file("extdata", "sites_to_test.fa", package="ASEB"))
resultList <- asebSites(backgroundSites, prodefinedSites, testSites, permutationTimes=100)
drawEScurve(resultList$curveInfo, max_p_value=0.1, min_es=0.1, outputDir=tempdir(), figKind="jpeg")
cat("see figures in output dir:", tempdir(),"\n")</pre>
```

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drawStat

#### Description

This function is used to show P-values and enrichment scores for all lysine sites on a specific protein.

# Usage

```
drawStat(curveInfoDataFrame, proteinIds=NULL, outputDir=NULL, figKind=c("pdf","jpeg"))
## S4 method for signature 'data.frame'
drawStat(curveInfoDataFrame, proteinIds=NULL, outputDir=NULL, figKind=c("pdf","jpeg"))
```

#### Arguments

curveInfoDataFrame

|            | data.frame object: contains curve information for all proteins, see example.                                                                            |
|------------|---------------------------------------------------------------------------------------------------------------------------------------------------------|
| proteinIds | character vector: only draw curves for proteins with ids appear in this vector. default: draw curves for all the proteins appear in curveInfoDataFrame. |
| outputDir  | character(1), output directory name for all the figures.                                                                                                |
| figKind    | character(1), fig format: "pdf" or "jpeg".                                                                                                              |

# Details

This function is used to draw P-values and enrichment scores for all lysine sites on a specific protein. The X-axis shows positions of all lysine sites on a specific protein, and Y-axis shows the enrichment scores  $(0\sim1)$  and P-values  $(0\sim1)$  for each lysine site. The data.frame object contains curve information is given by asebProteins.

#### See Also

SequenceInfo, readSequence, asebSites, asebProteins, drawEScurve.

#### Examples

```
backgroundSites <- readSequence(system.file("extdata", "background_sites.fa", package="ASEB"))
prodefinedSites <- readSequence(system.file("extdata", "predefined_sites.fa", package="ASEB"))
testProteins <- readSequence(system.file("extdata", "proteins_to_test.fa", package="ASEB"))
resultList <- asebProteins(backgroundSites, prodefinedSites, testProteins, permutationTimes=100)
#drawEScurve(resultList$curveInfo, max_p_value=0.5, min_es=0, outputDir=tempdir(), figKind="jpeg")
drawStat(resultList$curveInfo, outputDir=tempdir(), figKind="jpeg");
cat("see figures in output dir:", tempdir(), "\n")</pre>
```

readSequence

# Description

This function is used to read sequences from FASTA format file.

#### Usage

readSequence(file)

# Arguments

| file | character(1), file name for input.         |
|------|--------------------------------------------|
|      | The input file should follow FASTA format. |

# Details

This function return an object of SequenceInfo that contains sequences and identifiers from FASTA format input file.

# Value

A SequenceInfo object containing sequences and identifiers from input file.

# See Also

SequenceInfo, asebSites, asebProteins, drawStat, drawEScurve.

# Examples

```
ff <- system.file("extdata", "background_sites.fa", package="ASEB")
readSequence(ff)</pre>
```

SequenceInfo "SequenceInfo" class

# Description

This class is used to store sequences and identifiers for lysine sites or proteins.

# **Objects from the Class**

Objects from this class are created by constructor SequenceInfo, as outlined below.

# Slots

sequences: "character" containing sequences.

id: "character" containing identifiers.

# Methods

Constructor:

**SequenceInfo** signature(sequences = "character", id = "character"): Create a SequenceInfo object from sequences and their identifiers. The length of id must match that of sequences.

# See Also

readSequence, asebSites, asebProteins, drawStat, drawEScurve.

# Examples

showClass("SequenceInfo")

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