

Package ‘SIPETool’

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Type Package

Title SIFT-MS and CPET Data Processor

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Description Processor for selected ion flow tube mass spectrometer (SIFT-MS) output file from breath analysis. It allows the filtering of the SIFT output file (i.e., variation over time of the target analyte concentration) and the following analysis for the determination of: maximum, average, and standard deviation value of target concentration measured at each exhalation, and the respiratory rate over the measurement. Additionally, it is possible to align the SIFT-MS data with other on-line techniques such as cardio pulmonary exercise test (CPET) for a comprehensive characterization of breath samples.

License GPL-3

Encoding UTF-8

LazyData true

Imports Convolutioner

RoxygenNote 7.2.3

NeedsCompilation no

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CPET_time	<i>SIPETool example files</i>
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Description

Raw and filtered output from SIFT-MS, and CPET system. Four different files are available:
raw_sift -> raw data from SIFT-MS
CPET_time -> data from CPET system for time alignment
SIFT_time -> filtered data from SIFT-MS for time alignment
SIFT_filtered -> raw data from SIFT-MS filtered using SIFT_output_filter

data_indexer	<i>data indexer</i>
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Description

This function takes as input a vector and return the data index according to the selected time frame

Usage

```
data_indexer(dat, time_frame_index = NA)
```

Arguments

dat	input vector
time_frame_index	custom data range from the time column

Value

a vector indexed according to the specified time frame

Examples

```
data_indexer(c(1:10,10:1,1:10,10:1,1:10,10:1,1:10,10:1,1:10,10:1))
```

normalizer	<i>Data normalizer</i>
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Description

This function takes as input a vector and returns it normalized between a specified range

Usage

```
normalizer(dat, norm_range = c(0, 1))
```

Arguments

dat	the vector to normalize
norm_range	the range used for normalization

Value

vector normalized between norm_range

Examples

```
normalizer(c(1:10,10:1,1:10,10:1,1:10,10:1,1:10,10:1,1:10,10:1))
```

raw_SIFT	<i>SIPETool example files</i>
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Description

Raw and filtered output from SIFT-MS, and CPET system. Four different files are available:
raw_SIFT -> raw data from SIFT-MS CPET_time -> data from CPET system for time alignment
SIFT_time -> filtered data from SIFT-MS for time alignment SIFT_filtered -> raw data from SIFT-MS filtered using SIFT_output_filter

SIFT_filtered	<i>SIPETool example files</i>
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Description

Raw and filtered output from SIFT-MS, and CPET system. Four different files are available:
raw_sift -> raw data from SIFT-MS CPET_time -> data from CPET system for time alignment
SIFT_time -> filtered data from SIFT-MS for time alignment SIFT_filtered -> raw data from SIFT-MS filtered using SIFT_output_filter

SIFT_output_filter *SIFT output filter*

Description

This function takes as input the output file generated by the SIFT-MS and returns a .csv containing the TIME and the concentrations data selected by the user

Usage

```
SIFT_output_filter(  
  setdir = getwd(),  
  input_name = file.choose(),  
  output_name,  
  n_parameters = 2,  
  param_names = c("Isoprene", "Acetone"),  
  out_file = TRUE  
)
```

Arguments

setdir	allow the selection of the working directory
input_name	allow the selection of the input file
output_name	name of the .csv output file
n_parameters	number of analytes
param_names	vector with name of the analytes
out_file	flag for the export of a csv file

Value

Filtered data and optional csv from SIFT input

Examples

```
data(raw_SIFT)  
SIFT_output_filter(input_name = raw_SIFT, output_name = "testfile", out_file = FALSE)
```

SIFT_time	<i>SIPETool example files</i>
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Description

Raw and filtered output from SIFT-MS, and CPET system. Four different files are available:
raw_sift -> raw data from SIFT-MS CPET_time -> data from CPET system for time alignment
SIFT_time -> filtered data from SIFT-MS for time alignment SIFT_filtered -> raw data from SIFT-MS filtered using SIFT_output_filter

sign_detect	<i>Sign detection</i>
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Description

This function takes as input a vector and returns the sign of each element

Usage

```
sign_detect(dat)
```

Arguments

dat the vector to be used

Value

vector with the signs of each element of the original matrix

Examples

```
sign_detect(c(1:10,10:1,1:10,10:1,1:10,10:1,1:10,10:1,1:10,10:1))
```

`tidal_analyzer`*Tidal analyzer*

Description

This function takes as input a csv file containing a time column and data columns and returns the position of the end tids for each data column maximazing the sincronization between data. This function was originally devised for the analysis of the end tids coming from exhaled breath analyzed through SIFT-MS technology

Usage

```
tidal_analyzer(  
  setdir = getwd(),  
  input_name = file.choose(),  
  output_name,  
  starting_threshold = 0.03,  
  time_frame = NA,  
  out_file = TRUE  
)
```

Arguments

<code>setdir</code>	working directory
<code>input_name</code>	csv file
<code>output_name</code>	name of the output file
<code>starting_threshold</code>	initial value for the dynamic threshold
<code>time_frame</code>	custom data range from the time column
<code>out_file</code>	flag for the export of a csv file

Value

csv containing the end tids, their maximum, average, frequency, and timing

Examples

```
data(SIFT_filtered)  
tidal_analyzer(input_name = head(SIFT_filtered, n = 100), output_name = "out", out_file = FALSE)
```

tidal_finder	<i>Tidal_finder</i>
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Description

This function takes as input a matrix and returns for each column the end tids depending of the threshold set. It is possible to set a custom time frame for the search of the tids. Note: a minimum amount of 45 points are necessary.

Usage

```
tidal_finder(  
  dat,  
  height_threshold = 0.2,  
  refine = FALSE,  
  time_frame_index = NA  
)
```

Arguments

dat	the input matrix
height_threshold	the minimum height of the tidal
refine	refine the dataset
time_frame_index	custom time frame

Value

matrix with the tids for each column

Examples

```
tidal_finder(c(1:10,10:1,1:10,10:1,1:10,10:1,1:10,10:1,1:10,10:1))
```

time_filter	<i>Time_alignment</i>
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Description

This function takes as input two data set containing a time vector and a data vector and return the two data sets aligned. This is done by reducing the dimensions of the data set with higher points. The first data set is the one coming from the CPET-ESE and the second one from the SIFT-MS

Usage

```
time_filter(Cy = file.choose(), sift = file.choose())
```

Arguments

Cy	CPET-ESE output file
sift	SIFT-MS refined file

Value

A plot and the SIFT-MS data file resized for the alignment with the CPET-ESE file

Examples

```
data(SIFT_time)
data(CPET_time)
time_filter(CPET_time, SIFT_time)
```

trend

Trend finder

Description

This function takes as input a vector and returns the trend of each column expressed as the difference between two consecutive elements

Usage

```
trend(dat)
```

Arguments

dat	the vector to analyze
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Value

vector containing the trend of the each column

Examples

```
trend(c(1:10,10:1,1:10,10:1,1:10,10:1,1:10,10:1,1:10,10:1))
```

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