# 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.
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CPET\_time

SIPETool example files

#### **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 allignment SIFT\_time -> raw data from SIFT-MS for time allignment SIFT\_filtered -> raw data from SIFT-MS filtered using SIFT\_output\_filter

data\_indexer

data indexer

#### **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

```
data_indexer(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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normalizer

Data normalizer

#### **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

SIPETool example files

#### **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 allignment SIFT\_time -> filtered data from SIFT-MS for time allignment SIFT\_filtered -> raw data from SIFT-MS filtered using SIFT\_output\_filter

SIFT\_filtered

SIPETool example files

#### **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 allignment SIFT\_time -> filtered data from SIFT-MS for time allignment SIFT\_filtered -> raw data from SIFT-MS filtered using SIFT\_output\_filter

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```
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**

```
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

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

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 ${\tt SIFT\_time}$ 

SIPETool example files

# 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 allignment SIFT\_time -> raw data from SIFT-MS for time allignment SIFT\_filtered -> raw data from SIFT-MS filtered using SIFT\_output\_filter

sign\_detect

Sign detection

# 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

```
sign_detect(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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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 tidals for each data column maximazing the syncronization between data. This function was originally devised for the analysis of the end tidals 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**

#### Value

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

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

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tidal\_finder

Tidal finder

#### **Description**

This function takes as input a matrix and returns for each column the end tidals depending of the threshold set. It is possible to set a custom time frame for the search of the tidals. 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 tidals 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

Time\_alignment

#### **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

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#### **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

# Value

vector containing the trend of the each column

```
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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