

Package ‘AQuality’

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Description The functions proposed in this package allows to evaluate the process of measurement of the chemical components of water numerically or graphically. TSSS() and ICHS functions are useful to control the quality of measurements of chemical components of a sample of water. If one or more measurements include an error, the generated graph will indicate it with a position of the point that represents the sample outside the confidence interval. The function CI allows to evaluate the possibility of contamination of a water sample after being obtained.

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 AQuality-package

Water and Measurements Quality

Description

The package allows you to evaluate graphically the quality of measurements of water components

Details

The package includes two functions: TSSS() and ICHS(). The TSSS() function allows evaluating the quality of a set of measurement of water components, which correlate with total soluble solids. On the other hand, the ICHS() function allows evaluating the quality of a set of measurement of water components, which correlate with conductivity. The function CI allows to evaluate the possibility of contamination of a water sample after being obtained.

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 CI

Contamination Index

Description

Calculate an index that allows to estimate the possibility of microbiological contamination of a water sample after being obtained.

Usage

```
CI(sample, data)
```

Arguments

sample	Code of the sample whose quality you want to know.
data	Data.frame containing code of the database samples, and the concentration of the following chemical components: phosphate, nitrate, nitrite, tkm, ammonium, chemical demand of oxygen (dco), biological demand of oxygen (dbo) and organic matter.

Details

The CI() function performs the calculation of a score whose value allows to estimate the possibility of microbiological contamination of a water sample after being obtained.

Value

The CI() function returns a number (score). If $\text{score} \geq 0$ and $\text{score} \leq 2$, the sample is not contaminable. If $\text{score} > 2$ and $\text{score} \leq 4$, the sample is hardly contaminable. If $\text{score} > 4$ and $\text{score} \leq 6$, the sample is possibly contaminable. If $\text{score} > 6$ and $\text{score} \leq 8$, the sample is easily contaminable.

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dataCI

Data Sets~~

Description

Data.frame with data for testing the CI() (Contamination Index) function. Column 1: sample identification code. Column 2: onwards: measurement of chemical components of water used to calculate CI, expressed in ppm.

Usage

```
data("dataCI")
```

Format

A data frame with 6 observations on the following 9 variables.

code a character vector

phosphate a numeric vector

nitrate a numeric vector

nitrite a numeric vector

ammonium a numeric vector

dqo a numeric vector

tkn a numeric vector

organicmatter a character vector

dbo a numeric vector

Examples

```
# Including data.frame: dataCI in workspace.
data("dataCI")
# Column names of data.frame: dataCI
names(dataCI)
# Data set type of columns of data.frame: dataCI.
str(dataCI)
# Calculation of CI for the sample A1
#The following code should calculate the CI for the sample A1 included in dataCI, which
```

```
# is not acceptable as drinking water and is possibly contaminable.
CI("A1",dataCI)
#The following code should calculate the CI for the sample A2 included in dataCI, which
#is acceptable as drinking water and is hardly contaminable.
CI("A3",dataCI)
```

dataICHS

Data Sets

Description

Data.frame with data for testing the ICHS() (Ionic Charge Summation) function. Column 1: sample identification code. Column 2: measurement of water conductivity. Column3 onwards: measurement of ionic chemical components of water expressed in milliequivalent per litre.

Usage

```
data("dataICHS")
```

Format

A data frame with 411 observations on the following 14 variables.

```
codigo a character vector
conductividad a numeric vector
cargacloruro a numeric vector
cargacarbonato a numeric vector
cargabicarbonato a numeric vector
cargafosfato a numeric vector
carganitrato a numeric vector
carganitrito a numeric vector
cargafloruro a numeric vector
cargaarcenico a numeric vector
cargaamonio a numeric vector
cargasulfato a numeric vector
cargasodio a numeric vector
cargacalcio a numeric vector
```

Examples

```

# Including data.frame: data in workspace.
data("dataICHS")
# Column names of data.frame: data
names(dataICHS)
# Data set type of columns of data.frame: data.
str(dataICHS)
# Visualization of sample A45
#The following code should display a graphic with all samples in green dots and sample
# A45 as red big dot
ICHS("A45",dataICHS)

```

dataTSSS

Data Sets~~

Description

Data.frame with data for testing the TSSS() (total soluble solids summation) function. Column 1: sample identification code. Column 2: measurement of total soluble solids. Column3 onwards: measurement of chemical components of water expressed in the same units as column 2.

Usage

```
data("dataTSSS")
```

Format

A data frame with 411 observations on the following 16 variables.

```

codigo a character vector
solidostotales a numeric vector
cloruro a numeric vector
carbonato a numeric vector
bicarbonato a numeric vector
fosfato a numeric vector
nitrato a numeric vector
nitrito a numeric vector
fluoruro a numeric vector
arsenico a numeric vector
amonio a numeric vector
sulfato a numeric vector
sodio a numeric vector
tkn a numeric vector
calcio a numeric vector
magnesio a numeric vector

```

Examples

```
# Including data.frame: data in workspace.
data("dataTSSS")
# Column names of data.frame: data
names(dataTSSS)
# Data set type of columns of data.frame: data.
str(dataTSSS)
# Visualization of sample A45
#The following code should display a graphic with all samples in green dots and sample
# A45 as red big dot
TSSS("A45",dataTSSS)
```

 ICHS

Ionic Charge Summation

Description

Plots ionic charge summation as a function of conductivity.

Usage

```
ICHS(sample, data, confllevel = 0.95, pchdata = 19, coldata = "green", cexdata = 0.5,
  pchsample = 19, colsample = "red", cexsample = 3, xaxis = "CONDUCTIVITY",
  yaxis = "IONIC CHARGE SUMMATION", title = paste("Sample ", as.character(sample)),
  linetyprediction = 2, linewidthprediction = 1, linecolorprediction = 5)
```

Arguments

sample	Code of the sample whose quality you want to know.
data	Data.frame containing code of the database samples, conductivity, measurements of ionic water components.
confllevel	Significance level used in the predict function.
pchdata	Symbol used to graph all the data in the data.frame.
coldata	Color of the symbols of all the data in the data.frame.
cexdata	Symbol size of all data in the data frame.
pchsample	Symbol chosen to represent the point whose measurement quality is to be represented.
colsample	Color chosen to represent the point whose measurement quality is to be represented.
cexsample	Size of the symbol chosen to represent the point whose measurement quality is to be represented.
xaxis	X axis label.
yaxis	Y axis label.
title	Title of the graph including the code of the chosen sample.

linetyprediction
Linear model prediction line type.

linewidthprediction
Linear model prediction line thickness.

linecolorprediction
Linear model prediction line color.

Details

The `ICHS()` function performs a linear model using column 2 (conductivity) as the independent variable and the other components of water as dependent variables (columns 3 onwards). Based on the linear model, a data prediction interval is obtained with a certain confidence level (`conflvel`). Then, `ICHS()` graphs the values of the entire database and finally graphs as a point with different color, the sample whose measurement quality you want to observe.

Value

The `ICHS()` function returns a graph of the sum of ionic chemical components as a function of the measurement of conductivity for each sample. It contains the confidence interval indicated in a dotted line, and the sample under observation. If the point that represents the sample is within the region delimited by the lines of the confidence interval, it is presumed that there were no serious measurement errors of the components analyzed.

Author(s)

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TSSS

Total Soluble Solids Summation

Description

Plot total soluble solids summation as a function of total soluble solids measurement.

Usage

```
TSSS(sample, data, conflvel = 0.95, pchdata = 19, coldata = "green", cexdata = 0.5,
pchsample = 19, colsample = "red", cexsample = 3, xaxis = "TOTAL SOLUBLE SOLIDS",
yaxis = "MASS SUMMATION", title = paste("Sample ", as.character(sample)),
linetyprediction = 2, linewidthprediction = 1, linecolorprediction = 5)
```

Arguments

`sample` Code of the sample whose quality you want to know.

`data` Data.frame containing code of the database samples, total soluble solids, measurements of other water components.

`conflvel` Significance level used in the predict function.

<code>pchdata</code>	Symbol used to graph all the data in the data.frame.
<code>coldata</code>	Color of the symbols of all the data in the data.frame.
<code>cexdata</code>	Symbol size of all data in the data frame.
<code>pchsample</code>	Symbol chosen to represent the point whose measurement quality is to be represented.
<code>colsample</code>	Color chosen to represent the point whose measurement quality is to be represented.
<code>cexsample</code>	Size of the symbol chosen to represent the point whose measurement quality is to be represented.
<code>xaxis</code>	X axis label.
<code>yaxis</code>	Y axis label.
<code>title</code>	Title of the graph including the code of the chosen sample.
<code>linetyprediction</code>	Linear model prediction line type.
<code>linewidthprediction</code>	Linear model prediction line thickness.
<code>linecolorprediction</code>	Linear model prediction line color.

Details

The `TSSS()` function performs a linear model using column 2 (total soluble solids) as the dependent variable and the other components of water as independent variables (columns 3 onwards). Based on the linear model, a data prediction interval is obtained with a certain confidence level (`conflevel`). Then, `TSSS()` graphs the values of the entire database and finally graphs as a point with different color, the sample whose measurement quality you want to observe.

Value

The `TSSS()` function returns a graph of the sum of soluble solids as a function of the measurement of total soluble solids for each sample. It contains the confidence interval and the sample under observation indicated in a dotted line. If the point that represents the sample is within the region delimited by the lines of the confidence interval, it is presumed that there were no serious measurement errors of the components analyzed.

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