Package 'lablaster'

October 13, 2022

Title Laser Ablation Blast Through Endpoint Detection

Version 0.0.1

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Description Imports a data frame containing a single time resolved laser ablation mass spectrometry analysis of a foraminifera (or other carbonate shell), then detects when the laser has burnt through the foraminifera test as a function of change in signal over time.

License LGPL (>= 3)

Encoding UTF-8

RoxygenNote 7.2.0

Imports magrittr, ggplot2, smooth, scales, stats, rlang

Depends R (>= 3.5.0)

LazyData true

R topics documented:

| coral6 | *Time resolved analysis by laser ablation inductively coupled plasma mass spectrometry of a branching coral, identified hereon as "coral6".* |

Description

A coral from Chris Standish.

Usage

```
coral6
```

Format

A data frame with 300 rows and 5 variables:

Time time stamp of each observation (in milliseconds)

Mg24 raw data for 24Mg

Ca43 raw data for 43Ca

Mn55 raw data for 55Mn

Sr86 raw data for 86Sr

| endPoint | *Detects when the laser blasts through the target sample in a laser ablation mass spectrometry time resolved analysis.* |

Description

This function imports a data frame containing a single time resolved laser ablation mass spectrometry analysis of a foraminifera (or other carbonate shell). It assumes that the first row contains the signal of the target sample and that background correction has already been applied.

Column names referencing the time stamps and target signal are specified as function arguments. Then the signal column is evaluated by smoothing the values using a moving average, then scaled between 0-1 and the rate of change over a number of observations.

The function identifies the maximum rate of signal change, locates the corresponding time stamp and then subtracts the time it took for the laser to blast through the target. The result (endTime) is the time stamp of the last observation while the laser is still focussed the desired target.

Usage

```
endPoint(
  df,
  dt = 10,
  smoothing = 5,
  timeCol = "Time",
  signalCol = "Ca44",
  profile = "FLASE",
  timeUnits = "seconds"
)
```

Arguments

df	A data frame containing a single time resolved analysis, with a column referencing time and another with the corresponding measured counts data.
dt	An integer that controls the number of observations (rows) are used in calculating a rolling lagged difference in 44Ca signal. Using a lower value for a faster blast through of chamber wall can improve end point sensitivity. Default = 10.
smoothing	Controls the length of the moving average filter to apply over the dt period. Default = 5.
timeCol	The column title in the data frame identifying the time stamp of the time resolved analysis. Default = "Time".
signalCol	The column title in the data frame identifying the numerical data used to identify the laser ablation blast through endpoint. This is often 44Ca but could be any column of numerical data that you want to detect the endpoint. Default = "Ca44".
profile	Logical. A visualisation of the endpoint detection mechanism as a ggplot2 object. To make this profile plot, set the argument to TRUE, otherwise set it to FALSE. Specifying to not make a plot can save a substantial amount of time. Default = "FALSE".
timeUnits	The units that the time resolved analysis is measured in. This is the units of the timeCol. This argument is a string and is only necessary if the argument profile = "TRUE". Default = "seconds".

Value

The function returns a data frame containing the columns:

- dfReturn$df contains a data frame with only the observations between the first data frame row and the endTime.
- dfReturn$startTime contains the earliest time in your TRA as a numerical value.
- df$Return$endTime contains the last time step while the laser is still focussed the desired target in your TRA before the as a numerical value.
- df$Return$profile contains a visualisation of your TRA identifying where the laser ablated through the carbonate shell as a ggplot object. This is only available if a profile was generated using profile = "TRUE".

Examples

```
endPoint(df = foram72shot3, dt = 10, smoothing = 5, timeCol = "Time",
 signalCol = "Ca44", profile = "TRUE",  timeUnits = "seconds")
endPoint(df = foram166shot7, dt = 8, smoothing = 7, timeCol = "Time",
 signalCol = "Ca44", profile = "FALSE",  timeUnits = "seconds")
endPoint(df = foram174shot4, dt = 10, smoothing = 5, timeCol = "Time",
 signalCol = "Ca43", profile = "TRUE",  timeUnits = "seconds")
endPoint(df = coral6, dt = 10, smoothing = 5, timeCol = "Time",
 signalCol = "Sr86", profile = "FALSE",  timeUnits = "milliseconds")
```

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foram166shot7	*Time resolved analysis by laser ablation inductively coupled plasma mass spectrometry of a planktonic foraminifera*

Description

The fifth from final chamber of Menardella exilis foraminifera 166, identified hereon as "foram166shot7".

Usage

```
foram166shot7
```

Format

A data frame with 144 rows and 8 variables:

Time time stamp of each observation (in seconds)

Mg24 raw data for 24Mg

Al27 raw data for 27Al

Ca43 raw data for 43Ca

Ca44 raw data for 44Ca

Mn55 raw data for 55Mn

Cu65 raw data for 65Cu

Sr88 raw data for 88Sr

foram174shot4	*Time resolved analysis by laser ablation inductively coupled plasma mass spectrometry of a planktonic foraminifera*

Description

An antepenultimate chamber of Menardella exilis foraminifera 174, identified hereon as "foram174shot4".

Usage

```
foram174shot4
```

Format

A data frame with 144 rows and 8 variables:

Time time stamp of each observation (in seconds)

Mg24 raw data for 24Mg

Al27 raw data for 27Al

Ca43 raw data for 43Ca

Ca44 raw data for 44Ca

Mn55 raw data for 55Mn

Cu65 raw data for 65Cu

Sr88 raw data for 88Sr

foram72shot3	*Time resolved analysis by laser ablation inductively coupled plasma mass spectrometry of a planktonic foraminifera*

Description

An antepenultimate chamber of Menardella exilis foraminifera 72, identified hereon as "foram72shot3".

Usage

```
foram72shot3
```

Format

A data frame with 144 rows and 8 variables:

Time time stamp of each observation (in seconds)

Mg24 raw data for 24Mg

Al27 raw data for 27Al

Ca43 raw data for 43Ca

Ca44 raw data for 44Ca

Mn55 raw data for 55Mn

Cu65 raw data for 65Cu

Sr88 raw data for 88Sr

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