Package 'Inquilab'

January 20, 2025

Type Package

Title Dissipation Kinetics Analysis, Half Life Period, Rate Constant, Plots

Version 0.1.0

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Description For environmental chemists, ecologists, researchers and agricultural scientists to understand the dissipation kinetics, calculate the half-life periods and rate constants of compounds, pesticides, contaminants in different matrices.

License GPL

Encoding UTF-8

NeedsCompilation no

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Repository CRAN

Date/Publication 2024-03-12 09:20:06 UTC

Contents

`first_order_kinetics` *Calculate First Order Kinetics Parameters*

Description

This function calculates the rate constant, half-life, and provides a summary of the first-order dissipation kinetics of pesticides, including the intercept, R^2 value, and statistical measures of the fitted model.

Usage

```
first_order_kinetics(t, c)
```

Arguments

`t`	Numeric vector, time points.
`c`	Numeric vector, concentrations corresponding to each time point.

Details

The function performs a logarithmic transformation on the concentration values to fit a linear model which corresponds to the first-order kinetics equation. A negative of the slope of this model gives the rate constant, and the half-life is calculated using the natural logarithm of 2 divided by the rate constant.

Value

A list containing the following components:

`rate constant`	The calculated rate constant for the first-order kinetics.
`half life`	The calculated half-life based on the rate constant.
`summary`	A summary object providing statistical measures of the fitted model, including the intercept, R^2 value, among others.

See Also

`lm`, for details on the linear models used within.

Examples

```
t <- c(0, 5, 10, 15, 20, 25)
c <- c(100, 80, 60, 40, 20, 10)
first_order_kinetics(t, c)
```

plot_first_order_kinetics

Plot for First Order Kinetics

Description

This function plots the actual and predicted concentrations based on first-order kinetics.

Usage

```
plot_first_order_kinetics(t, c, kinetic_model)
```

Arguments

t	Numeric vector of time points.
c	Numeric vector of concentrations corresponding to each time point.
kinetic_model	Model object, result of lm function fitting log(c) ~ t.

Value

This function generates a plot of the actual vs. predicted concentrations based on the provided kinetic model and data points. The plot is rendered directly to the active plotting device.

Examples

```
t <- c(0, 5, 10, 15, 20, 25)
c <- c(100, 80, 60, 40, 20, 10)
model <- lm(log(c) ~ t)
plot_first_order_kinetics(t, c, model)
```

plot_second_order_kinetics

Plot for Second Order Kinetics

Description

This function plots the actual and transformed (1/c) concentrations based on second-order kinetics.

Usage

```
plot_second_order_kinetics(t, c, kinetic_model)
```

Arguments

t	Numeric vector, time points.
c	Numeric vector, concentrations corresponding to each time point.
kinetic_model	Model object, result of lm function fitting 1/c ~ t.

Value

This function generates a plot of the actual vs. predicted concentrations based on the provided kinetic model and data points. The plot is rendered directly to the active plotting device.

Examples

```
t <- c(0, 5, 10, 15, 20, 25)
c <- c(100, 80, 60, 40, 20, 10)
model <- lm(1/c ~ t)
plot_second_order_kinetics(t, c, model)
```

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second_order_kinetics *Calculate Second Order Kinetics Parameters*

Description

This function calculates the rate constant and half-life based on second-order dissipation kinetics of pesticides, and provides a summary of the kinetic model including intercept, R-squared value, and other statistical measures.

Usage

```
second_order_kinetics(t, c)
```

Arguments

t	Numeric vector, time points.
c	Numeric vector, concentrations corresponding to each time point.

Details

The function first checks if the concentration values are greater than zero and if the length of the time and concentration vectors are equal. It then transforms the concentration data for second-order kinetics analysis and fits a linear model to the transformed data. From the fitted model, it calculates the rate constant and the half-life of the reaction. Finally, it provides a summary of the kinetic model, including the intercept, R-squared value, and other statistical measures.

Value

A list containing the following components:

rate constant	The calculated rate constant for the first-order kinetics.
half life	The calculated half-life based on the rate constant and initial concentration.
summary	A summary object providing statistical measures of the fitted model, including the intercept, R^2 value, among others.

See Also

lm, for details on the linear models used within.

Examples

```
t <- c(0, 5, 10, 15, 20, 25)
c <- c(100, 80, 60, 40, 20, 10)
second_order_kinetics(t, c)
```

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