Package ‘cdom’

August 29, 2016

Type Package
Title R Functions to Model CDOM Spectra
Version 0.1.0
Date 2016-02-22
Description Wrapper functions to model and extract various quantitative information from absorption spectra of chromophoric dissolved organic matter (CDOM).
BugReports https://github.com/PMassicot/cdom/issues
URL https://github.com/PMassicot/cdom
License GPL (>= 2)
Depends R (>= 3.0)
LazyData TRUE
Imports minpack.lm, ggplot2, tidyr, broom
RoxygenNote 5.0.1
Suggests eemR
NeedsCompilation no
Author Philippe Massicotte [aut, cre]
Maintainer Philippe Massicotte <pm@bios.au.dk>
Repository CRAN
Date/Publication 2016-03-04 08:39:29

R topics documented:

  cdom_fit_exponential .................................................. 2
  cdom_slope_ratio ...................................................... 3
  cdom_spectral_curve ................................................... 4
  spectra ................................................................. 5

Index 6
cdom_fit_exponential  
Fit an exponential model to CDOM data.

Description
Fit an exponential model to CDOM data.

Usage

cdom_fit_exponential(wl, absorbance, wl0 = 350, startwl, endwl)

Arguments

- **wl**  
The wavelength vector.
- **absorbance**  
The absorbance vector.
- **wl0**  
The reference wavelength (ex.: 350).
- **startwl**  
The starting wavelength (ex.: 240).
- **endwl**  
The ending wavelength (ex.: 600).

Details

\[ y = a_0 + e^{(-S(x-\lambda_0))} + K \]

Value

A list containing:

- **params** A data frame with values of fitted parameters.
- **r2** R2 of the nls model.
- **data** A data frame with fitted (predicted) values of the model.

The function will return NULL if the model did not converged.

Examples

# Fit an exponential model using the reference wavelength 350 between 190 and 900 nm.
data(spectra)
fit <- cdom_fit_exponential(spectra$wavelength, spectra$spc1, 350, 190, 900)
str(fit)
plot(spectra$wavelength, spectra$spc1)
lines(spectra$wavelength, fit$data$fitted, col = "red")
cdom_slope_ratio

Calculate the slope ratio (SR) from an absorption spectra.

Description

Calculate the slope ratio (SR) from an absorption spectra.

Usage

```r
cdom_slope_ratio(wl, absorbance)
```

Arguments

- `wl`: The wavelength vector.
- `absorbance`: The absorbance vector.

Details

Calculate the slope ratio (SR) as defined by Helms et al. (2008).

\[
SR = \frac{S_{275-295}}{S_{350-400}}
\]

Value

The value of the slope ratio.

References


Examples

```r
data("spectra")

cdom_slope_ratio(spectra$wavelength, spectra$spc1)
```
cdom_spectral_curve  

Calculate the spectral curve of CDOM spectra.

Description

Calculate the spectral curve of CDOM spectra has proposed by Loiselle et al. 2009.

Usage

cdom_spectral_curve(wl, absorbance, interval = 21, r2threshold = 0.8)

Arguments

wl        The wavelength vector.
absorbance The absorbance vector.
interval   The interval used to calculate each slope (default = 21 nm).
r2threshold The r2 threshold that determines if a slope is "valide". The default value is 0.8 meaning that the determination coefficient of the regression between log-transformed data and wavelength should be >= 0.8.

Value

A dataframe containing the centered wavelength, the calculated slope and the determination coefficient of the linear regression used to calculate the slope.

References

http://doi.wiley.com/10.4319/lo.2009.54.2.0590

Examples

data(spectra)
res <- cdom_spectral_curve(spectra$wavelength, spectra$spc2)
plot(res$wl, res$s, type = "l")
spectra

CDOM absorption data.

Description
Simple absorption spectra used to test package’s functions.

Usage
data(spectra)

Format
A data frame with 711 rows and 26 variables

Details
• wavelength. Wavelengths used for measurements (190-900 nm.)
• Absorption

Examples
library(ggplot2)
library(tidyr)
data("spectra")

spectra <- gather(spectra, sample, absorption, -wavelength)

ggplot(spectra, aes(x = wavelength, y = absorption, group = sample)) +
  geom_line(size = 0.1)
Index

*Topic datasets
  spectra, 5

cdom_fit_exponential, 2
cdom_slope_ratio, 3
cdom_spectral_curve, 4

spectra, 5