

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/PMassicotte/cdom/issues>

URL <https://github.com/PMassicotte/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

$$y = a0 + e^{(-S(x-\lambda_0))} + K$$

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	<i>Calculate the slope ratio (SR) from an absorption spectra.</i>
------------------	---

Description

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

Usage

```
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

http://www.aslo.org/lo/toc/vol_53/issue_3/0955.html

Examples

```
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	<i>CDOM absorption data.</i>
---------	------------------------------

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](#)