

Package ‘cdom’

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Type Package

Title R Functions to Model CDOM Spectra

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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>

Encoding UTF-8

License GPL (>= 2)

Depends R (>= 3.0)

LazyData TRUE

Imports minpack.lm, ggplot2, tidyr, broom, purrr

RoxygenNote 7.3.3

Suggests eemR

NeedsCompilation no

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cdom_exponential	<i>Fit an exponential model to CDOM data.</i>
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Description

Fit an exponential model to CDOM data.

Usage

```
cdom_exponential(wl, absorbance, wl0 = 350, startwl, endwl)
```

Arguments

<code>wl</code>	The wavelength vector.
<code>absorbance</code>	The absorbance vector.
<code>wl0</code>	The reference wavelength (ex.: 350).
<code>startwl</code>	The starting wavelength (ex.: 240).
<code>endwl</code>	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_exponential(spectra$wavelength, spectra$spc1, 350, 190, 900)

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>
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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

[doi:10.4319/lo.2008.53.3.0955](https://doi.org/10.4319/lo.2008.53.3.0955)

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

[doi:10.4319/lo.2009.54.2.0590](https://doi.org/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")
```

coef.exponential_fit *Extract Model Coefficients from a CDOM exponential fit*

Description

Extract Model Coefficients from a CDOM exponential fit

Usage

```
## S3 method for class 'exponential_fit'  
coef(object, ...)
```

Arguments

object An object returned by cdom_exponential.
... other arguments.

Value

A numerical vector with estimated coefficients.

Examples

```
data(spectra)  
  
fit <- cdom_exponential(spectra$wavelength, spectra$spc1, 350, 190, 900)  
coef(fit)
```

plot.exponential_fit *Plot a Fitted CDOM Exponential Curve*

Description

Plot a Fitted CDOM Exponential Curve

Usage

```
## S3 method for class 'exponential_fit'  
plot(x, ...)
```

Arguments

x An object returned by cdom_exponential.
... other arguments.

Value

A ggplot2 object.

Examples

```
library(ggplot2)

data(spectra)

fit <- cdom_exponential(spectra$wavelength, spectra$spc1, 350, 190, 900)
p <- plot(fit)
p
p + ggtitle("My super fit")
```

predict.exponential_fit

Predict method for CDOM exponential fit

Description

Predict method for CDOM exponential fit

Usage

```
## S3 method for class 'exponential_fit'
predict(object, ...)
```

Arguments

object	An object returned by cdom_exponential.
...	other arguments.

Value

A numerical vector with predicted values.

Examples

```
data(spectra)

fit <- cdom_exponential(spectra$wavelength, spectra$spc1, 350, 190, 900)
predict(fit)
```

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)
```

summary.exponential_fit
Summary of a CDOM exponential fit

Description

Summary of a CDOM exponential fit

Usage

```
## S3 method for class 'exponential_fit'
summary(object, ...)
```

Arguments

object An object returned by `cdom_exponential`.
... other arguments.

Value

A numerical vector with estimated coefficients.

Examples

```
data(spectra)
```

```
fit <- cdom_exponential(spectra$wavelength, spectra$spc1, 350, 190, 900)  
summary(fit)
```

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