

Package ‘eemR’

October 13, 2022

Type Package

Title Tools for Pre-Processing Emission-Excitation-Matrix (EEM)
Fluorescence Data

Version 1.0.1

Description Provides various tools for preprocessing Emission-Excitation-Matrix (EEM) for Parallel Factor Analysis (PARAFAC). Different methods are also provided to calculate common metrics such as humification index and fluorescence index.

License GPL (>= 2)

BugReports <https://github.com/PMassicotte/eemR/issues>

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

Depends R (>= 3.2.1)

LazyData TRUE

Imports stringr, dplyr, R.matlab, pracma, stats, rlist, viridis,
purrr, assertthat

RoxygenNote 6.1.1

Suggests cdom, magrittr, testthat, knitr, rmarkdown, ggplot2, plot3D,
extrafont, tidyr, shiny, DT, MBA

VignetteBuilder knitr

Encoding UTF-8

NeedsCompilation no

Author Philippe Massicotte [aut, cre]

Maintainer Philippe Massicotte <pmassicotte@hotmail.com>

Repository CRAN

Date/Publication 2019-06-26 13:50:03 UTC

R topics documented:

absorbance	2
eem	3
eem_bind	3
eem_biological_index	4
eem_coble_peaks	5
eem_cut	6
eem_export_matlab	7
eem_extract	8
eem_extract_blank	9
eem_fluorescence_index	10
eem_humification_index	11
eem_inner_filter_effect	12
eem_names	13
eem_names<-	14
eem_peaks	15
eem_raman_normalisation	16
eem_read	18
eem_remove_blank	19
eem_remove_scattering	21
eem_set_wavelengths	22
plot.eemlist	23
print.eemlist	23
summary.eemlist	24
Index	26

absorbance	<i>CDOM absorbance data.</i>
------------	------------------------------

Description

Simple absorbance spectra used to test package's functions.

Usage

```
data("absorbance")
```

Format

A data frame with 711 rows and 4 variables

Details

- wavelength. Wavelengths used for measurements (190-900 nm.)
- absorbance

Examples

```

data("absorbance")

plot(absorbance$wavelength, absorbance$sample1,
     type = "l",
     xlab = "Wavelengths", ylab = "Absorbance per meter"
)
lines(absorbance$wavelength, absorbance$sample2, col = "blue")
lines(absorbance$wavelength, absorbance$sample3, col = "red")

```

eem

eem constructor

Description

eem constructor

Usage

```
eem(data)
```

Arguments

data A list containing "file", "x", "em", "ex".

Value

An object of class eem containing:

- sample The file name of the eem.
- x A matrix with fluorescence values.
- em Emission vector of wavelengths.
- ex Excitation vector of wavelengths.

eem_bind

Bind eem or eemlist

Description

Function to bind EEMs that have been loaded from different folders or have been processed differently.

Usage

```
eem_bind(...)
```

Arguments

... One or more object of class `eemlist`.

Value

An object of `eemlist`.

Examples

```
file <- system.file("extdata/cary/scans_day_1/", "sample1.csv", package = "eemR")
eem <- eem_read(file, import_function = "cary")

eem <- eem_bind(eem, eem)
```

`eem_biological_index` *Calculate the biological fluorescence index (BIX)*

Description

The biological fluorescence index (BIX) is calculated by dividing the fluorescence at excitation 310 nm and emission at 380 nm ($ex = 310$, $em = 380$) by that at excitation 310 nm and emission at 430 nm ($ex = 310$, $em = 430$).

Usage

```
eem_biological_index(eem, verbose = TRUE)
```

Arguments

`eem` An object of class `eemlist`.
`verbose` Logical determining if additional messages should be printed.

Value

An object of class `eemlist`.
A data frame containing the biological index (BIX) for each `eem`.

Interpolation

Different excitation and emission wavelengths are often used to measure EEMs. Hence, it is possible to have mismatches between measured wavelengths and wavelengths used to calculate specific metrics. In these circumstances, EEMs are interpolated using the `interp2` function from the `parcma` library. A message warning the user will be prompted if data interpolation is performed.

References

Huguet, A., Vacher, L., Relexans, S., Saubusse, S., Froidefond, J. M., & Parlanti, E. (2009). Properties of fluorescent dissolved organic matter in the Gironde Estuary. *Organic Geochemistry*, 40(6), 706-719.

<http://doi.org/10.1016/j.orggeochem.2009.03.002>

See Also

[interp2](#)

Examples

```
file <- system.file("extdata/cary/scans_day_1/", package = "eemR")
eem <- eem_read(file, import_function = "cary")

eem_biological_index(eem)
```

eem_coble_peaks	<i>Extract fluorescence peaks</i>
-----------------	-----------------------------------

Description

Extract fluorescence peaks

Usage

```
eem_coble_peaks(eem, verbose = TRUE)
```

Arguments

eem	An object of class <code>eemlist</code> .
verbose	Logical determining if additional messages should be printed.

Details

According to Coble (1996), peaks are defined as follow:

Peak B: ex = 275 nm, em = 310 nm

Peak T: ex = 275 nm, em = 340 nm

Peak A: ex = 260 nm, em = 380:460 nm

Peak M: ex = 312 nm, em = 380:420 nm

peak C: ex = 350 nm, em = 420:480 nm

Given that peaks A, M and C are not defined at fix emission wavelength, the maximum fluorescence value in the region is extracted.

Value

An object of class `eemlist`.

A data frame containing peaks B, T, A, M and C for each eem. See details for more information.

Interpolation

Different excitation and emission wavelengths are often used to measure EEMs. Hence, it is possible to have mismatches between measured wavelengths and wavelengths used to calculate specific metrics. In these circumstances, EEMs are interpolated using the `interp2` function from the `parcma` library. A message warning the user will be prompted if data interpolation is performed.

References

Coble, P. G. (1996). Characterization of marine and terrestrial DOM in seawater using excitation-emission matrix spectroscopy. *Marine Chemistry*, 51(4), 325-346.

[http://doi.org/10.1016/0304-4203\(95\)00062-3](http://doi.org/10.1016/0304-4203(95)00062-3)

See Also

[interp2](#)

Examples

```
file <- system.file("extdata/cary/scans_day_1/", "sample1.csv", package = "eemR")
eem <- eem_read(file, import_function = "cary")

eem_coble_peaks(eem)
```

eem_cut

Cut emission and/or excitation wavelengths from EEMs

Description

Cut emission and/or excitation wavelengths from EEMs

Usage

```
eem_cut(eem, ex, em, exact = TRUE, fill_with_na = FALSE)
```

Arguments

<code>eem</code>	An object of class <code>eemlist</code> .
<code>ex</code>	A numeric vector of excitation wavelengths to be removed.
<code>em</code>	A numeric vector of emission wavelengths to be removed.
<code>exact</code>	Logical. If TRUE, only wavelengths matching <code>em</code> and/or <code>ex</code> will be removed. If FALSE, all wavelengths in the range of <code>em</code> and/or <code>ex</code> will be removed.
<code>fill_with_na</code>	Logical. If TRUE, fluorescence values at specified wavelengths will be replaced with NA. If FALSE, these values will be removed.

Value

An object of class eemlist.

Examples

```
# Open the fluorescence eem
file <- system.file("extdata/cary/scans_day_1/", "sample1.csv", package = "eemR")

eem <- eem_read(file, import_function = "cary")
plot(eem)

# Cut few excitation wavelengths
eem <- eem_cut(eem, ex = c(220, 225, 230, 230))
plot(eem)

eem <- eem_read(file, import_function = "cary")
eem <- eem_cut(eem, em = 350:400, fill_with_na = TRUE)
plot(eem)
```

eem_export_matlab *Export EEMs to Matlab*

Description

Export EEMs to Matlab

Usage

```
eem_export_matlab(file, ...)
```

Arguments

<code>file</code>	The .mat file name where to export the structure.
<code>...</code>	One or more object of class eemlist.

Details

The function exports EEMs into PARAFAC-ready Matlab .mat file usable by the **drEEM** toolbox.

Value

A structure named OriginalData is created and contains:

nSample The number of eems.
nEx The number of excitation wavelengths.
nEm The number of emission wavelengths.
Ex A vector containing excitation wavelengths.

Em A vector containing emission wavelengths.

X A 3D matrix (nSample X nEx X nEm) containing EEMs.

sample_name The list of sample names (i.e. file names) of the imported EEMs.

Known bug in export

eemR uses R.Matlab to export the the fluorescence data into a matfile. However, there is currently a bug in the latter package that require the user to reshape the exported data once in Matlab. This can be done using the following command: `load('OriginalData.mat'); OriginalData.X = reshape(OriginalData.X, OriginalData.nSample, OriginalData.nEm, OriginalData.nEx)`

Examples

```
file <- system.file("extdata/cary/", package = "eemR")
eem <- eem_read(file, recursive = TRUE, import_function = "cary")

export_to <- paste(tempfile(), ".mat", sep = "")
eem_export_matlab(export_to, eem)
```

eem_extract	<i>Extract EEM samples</i>
-------------	----------------------------

Description

Extract EEM samples

Usage

```
eem_extract(eem, sample, keep = FALSE, ignore_case = FALSE,
            verbose = TRUE)
```

Arguments

eem	An object of class eemlist.
sample	Either numeric or character vector. See details for more information.
keep	logical. If TRUE, the specified sample will be returned. If FALSE, they will be removed.
ignore_case	Logical, should sample name case should be ignored (TRUE) or not (FALSE). Default is FALSE.
verbose	Logical determining if removed/extracted eems should be printed on screen.

Details

sample argument can be either numeric or character vector. If it is numeric, samples at specified index will be removed.

If sample is character, regular expression will be used and all sample names that have a partial or complete match with the expression will be removed. See examples for more details.

Value

An object of class eemlist.

Examples

```
folder <- system.file("extdata/cary/scans_day_1", package = "eemR")
eems <- eem_read(folder, import_function = "cary")

eems

# Remove first and third samples
eem_extract(eems, c(1, 3))

# Remove everything except first and third samples
eem_extract(eems, c(1, 3), keep = TRUE)

# Remove all samples containing "3" in their names.
eem_extract(eems, "3")

# Remove all samples containing either character "s" or character "2" in their names.
eem_extract(eems, c("s", "2"))

# Remove all samples containing "blank" or "nano"
eem_extract(eems, c("blank", "nano"))
```

eem_extract_blank	<i>Extract blank EEM</i>
-------------------	--------------------------

Description

Extract blank EEM

Usage

```
eem_extract_blank(eem, average = TRUE)
```

Arguments

eem	An object of class eemlist.
average	Logical. If TRUE blank EEMs will be averaged

Value

An object of class eemlist.

`eem_fluorescence_index`*Calculate the fluorescence index (FI)*

Description

Calculate the fluorescence index (FI)

Usage

```
eem_fluorescence_index(eem, verbose = TRUE)
```

Arguments

<code>eem</code>	An object of class <code>eemlist</code> .
<code>verbose</code>	Logical determining if additional messages should be printed.

Value

An object of class `eemlist`.

A data frame containing fluorescence index (FI) for each eem.

Interpolation

Different excitation and emission wavelengths are often used to measure EEMs. Hence, it is possible to have mismatches between measured wavelengths and wavelengths used to calculate specific metrics. In these circumstances, EEMs are interpolated using the `interp2` function from the `parcma` library. A message warning the user will be prompted if data interpolation is performed.

References

<http://doi.wiley.com/10.4319/lo.2001.46.1.0038>

See Also

[interp2](#)

Examples

```
file <- system.file("extdata/cary/scans_day_1/", "sample1.csv", package = "eemR")
eem <- eem_read(file, import_function = "cary")

eem_fluorescence_index(eem)
```

`eem_humification_index`*Calculate the fluorescence humification index (HIX)*

Description

The fluorescence humification index (HIX), which compares two broad aromatic dominated fluorescence maxima, is calculated at 254 nm excitation by dividing the sum of fluorescence intensities between emission 435 to 480 nm by the the sum of fluorescence intensities between 300 to 345 nm.

Usage

```
eem_humification_index(eem, scale = FALSE, verbose = TRUE)
```

Arguments

<code>eem</code>	An object of class <code>eemlist</code> .
<code>scale</code>	Logical indicating if HIX should be scaled, default is <code>FALSE</code> . See details for more information.
<code>verbose</code>	Logical determining if additional messages should be printed.

Value

An object of class `eemlist`.

A data frame containing the humification index (HIX) for each eem.

Interpolation

Different excitation and emission wavelengths are often used to measure EEMs. Hence, it is possible to have mismatches between measured wavelengths and wavelengths used to calculate specific metrics. In these circumstances, EEMs are interpolated using the `interp2` function from the `parcma` library. A message warning the user will be prompted if data interpolation is performed.

References

Ohno, T. (2002). Fluorescence Inner-Filtering Correction for Determining the Humification Index of Dissolved Organic Matter. *Environmental Science & Technology*, 36(4), 742-746.

<http://doi.org/10.1021/es0155276>

See Also

[interp2](#)

Examples

```
file <- system.file("extdata/cary/scans_day_1/", package = "eemR")
eem <- eem_read(file, import_function = "cary")

eem_humification_index(eem)
```

eem_inner_filter_effect

Inner-filter effect correction

Description

Inner-filter effect correction

Usage

```
eem_inner_filter_effect(eem, absorbance, pathlength = 1)
```

Arguments

eem	An object of class <code>eemlist</code> .
absorbance	A data frame with: wavelength A numeric vector containing wavelengths. ... One or more numeric vectors containing absorbance spectra.
pathlength	A numeric value indicating the pathlength (in cm) of the cuvette used for absorbance measurement. Default is 1 (1cm).

Details

The inner-filter effect correction procedure is assuming that fluorescence has been measured in 1 cm cuvette. Hence, absorbance will be converted per cm. Note that absorbance spectra should be provided (i.e. not absorption).

Value

An object of class `eemlist`.

An object of class `eem` containing:

- `sample` The file name of the eem.
- `x` A matrix with fluorescence values.
- `em` Emission vector of wavelengths.
- `ex` Excitation vector of wavelengths.

Names matching

The names of absorbance variables are expected to match those of the eems. If the appropriate absorbance spectrum is not found, an uncorrected eem will be returned and a warning message will be printed.

Sample dilution

Kothawala et al. 2013 have shown that a 2-fold dilution was required for sample presenting total absorbance > 1.5 in a 1 cm cuvette. Accordingly, a message will warn the user if total absorbance is greater than this threshold.

References

Parker, C. a., & Barnes, W. J. (1957). Some experiments with spectrofluorometers and filter fluorimeters. *The Analyst*, 82(978), 606. <http://doi.org/10.1039/an9578200606>

Kothawala, D. N., Murphy, K. R., Stedmon, C. A., Weyhenmeyer, G. A., & Tranvik, L. J. (2013). Inner filter correction of dissolved organic matter fluorescence. *Limnology and Oceanography: Methods*, 11(12), 616-630. <http://doi.org/10.4319/lom.2013.11.616>

Examples

```
library(eemR)
data("absorbance")

folder <- system.file("extdata/cary/scans_day_1", package = "eemR")
eems <- eem_read(folder, import_function = "cary")
eems <- eem_extract(eems, "nano") # Remove the blank sample

# Remove scattering (1st order)
eems <- eem_remove_scattering(eems, "rayleigh")

eems_corrected <- eem_inner_filter_effect(eems, absorbance = absorbance, pathlength = 1)

op <- par(mfrow = c(2, 1))
plot(eems, which = 1)
plot(eems_corrected, which = 1)
par(op)
```

eem_names

The names of an eem or eemlist objects

Description

The names of an eem or eemlist objects

Usage

```
eem_names(eem)
```

Arguments

eem An object of class eemlist.

Value

An object of class eemlist.

A character vector containing the names of the EEMs.

Examples

```
file <- system.file("extdata/cary/", package = "eemR")
eem <- eem_read(file, recursive = TRUE, import_function = "cary")

eem_names(eem)
```

eem_names<- *Set the sample names of an eem or eemlist objects*

Description

Set the sample names of an eem or eemlist objects

Usage

```
eem_names(x) <- value
```

Arguments

x An object of class eem or eemlist.

value A character vector with new sample names. Must be equal in length to the number of samples in the eem or eemlist.

Value

An eem or eemlist.

Examples

```
folder <- system.file("extdata/cary/scans_day_1", package = "eemR")
eems <- eem_read(folder, import_function = "cary")

eem_names(eems)
eem_names(eems) <- c("a", "b", "c", "d")
eem_names(eems)
```

eem_peaks	<i>Extract fluorescence peaks</i>
-----------	-----------------------------------

Description

Extract fluorescence peaks

Usage

```
eem_peaks(eem, ex, em, verbose = TRUE)
```

Arguments

eem	An object of class <code>eemlist</code> .
ex	A numeric vector with excitation wavelengths.
em	A numeric vector with emission wavelengths.
verbose	Logical determining if additional messages should be printed.

Value

An object of class `eemlist`.

A data frame containing excitation and emission peak values. See details for more information.

Interpolation

Different excitation and emission wavelengths are often used to measure EEMs. Hence, it is possible to have mismatches between measured wavelengths and wavelengths used to calculate specific metrics. In these circumstances, EEMs are interpolated using the [interp2](#) function from the `parcma` library. A message warning the user will be prompted if data interpolation is performed.

See Also

[interp2](#)

Examples

```
file <- system.file("extdata/cary/scans_day_1/", "sample1.csv", package = "eemR")
eem <- eem_read(file, import_function = "cary")

eem_peaks(eem, ex = c(250, 350), em = c(300, 400))
```

eem_raman_normalisation

Fluorescence Intensity Calibration Using the Raman Scatter Peak of Water

Description

Normalize fluorescence intensities to the standard scale of Raman Units (R.U).

Usage

```
eem_raman_normalisation(eem, blank = NA)
```

Arguments

eem	An object of class <code>eemlist</code> .
blank	An object of class <code>eemlist</code> .

Details

The function will first try to use the provided `blank`. If the `blank` is omitted, the function will then try to extract the `blank` from the `eemlist` object. This is done by looking for sample names containing one of these complete or partial strings (ignoring case):

1. nano
2. miliq
3. milliq
4. mq
5. blank

Note that if `blank` is omitted, the function will group the `eemlist` based on file location and will assume that there is a `blank` sample in each folder. In that context, the `blank` will be used on each sample in the same folder. If more than one `blank` is found they will be averaged (a message will be printed if this appends).

Consider the following example where there are two folders that could represent scans performed on two different days 'scans_day_1' and 'scans_day_2'.

```
scans_day_1
    nano.csv
    sample1.csv
    sample2.csv
    sample3.csv
scans_day_2
    blank.csv
    s1.csv
    s2.csv
    s3.csv
```


In each folder there are three samples and one blank files. In that context, 'eem_remove_blank()' will use the blank 'nano.csv' from 'sample1.csv', 'sample2.csv' and 'sample3.csv'. The same strategy will be used for files in folder 'scans_day_2' but with blank named 'blank.csv'.

Note that the blanks eem are not returned by the function.

The normalization procedure consists in dividing all fluorescence intensities by the area (integral) of the Raman peak. The peak is located at excitation of 350 nm. ($ex = 370$) between 371 nm. and 428 nm in emission ($371 \leq em \leq 428$). Note that the data is interpolated to make sure that fluorescence at $em = 350$ exist.

Value

An object of class `eemlist`.

An object of class `eem` containing:

- `sample` The file name of the eem.
- `x` A matrix with fluorescence values.
- `em` Emission vector of wavelengths.
- `ex` Excitation vector of wavelengths.

References

Lawaetz, A. J., & Stedmon, C. A. (2009). Fluorescence Intensity Calibration Using the Raman Scatter Peak of Water. *Applied Spectroscopy*, 63(8), 936-940.

<https://journals.sagepub.com/doi/10.1366/000370209788964548>

Murphy, K. R., Stedmon, C. a., Graeber, D., & Bro, R. (2013). Fluorescence spectroscopy and multi-way techniques. *PARAFAC. Analytical Methods*, 5(23), 6557.

<http://xlink.rsc.org/?DOI=c3ay41160e>

Examples

```
# Open the fluorescence eem
file <- system.file("extdata/cary/scans_day_1", "sample1.csv", package = "eemR")
eem <- eem_read(file, import_function = "cary")

plot(eem)

# Open the blank eem
file <- system.file("extdata/cary/scans_day_1", "nano.csv", package = "eemR")
blank <- eem_read(file, import_function = "cary")

# Do the normalisation
eem <- eem_raman_normalisation(eem, blank)

plot(eem)
```

eem_read

Read excitation-emission fluorescence matrix (eem)

Description

Read excitation-emission fluorescence matrix (eem)

Usage

```
eem_read(file, recursive = FALSE, import_function)
```

Arguments

file	File name or folder containing fluorescence file(s).
recursive	logical. Should the listing recurse into directories?
import_function	Either a character or a user-defined function to import a single eem. If a character, it should be one of "cary", "aqualog", "shimadzu", "fluoromax4". See <code>browseVignettes("eemR")</code> to learn how to create your own import function.

Details

At the moment, Cary Eclipse, Aqualog and Shimadzu EEMs are supported.

eemR will automatically try to determine from which spectrofluorometer the files originate and load the data accordingly. Note that EEMs are reshaped so $X[1, 1]$ represents the fluorescence intensity at $X[\min(\text{ex}), \min(\text{em})]$.

Value

If file is a single filename:

An object of class eem containing:

- sample The file name of the eem.
- x A matrix with fluorescence values.
- em Emission vector of wavelengths.
- ex Excitation vector of wavelengths.

If file is a folder, the function returns an object of class eemlist which is simply a list of eem.

Examples

```
file <- system.file("extdata/cary/scans_day_1/", package = "eemR")
eems <- eem_read(file, recursive = TRUE, import_function = "cary")
```

eem_remove_blank	<i>Blank correction</i>
------------------	-------------------------

Description

This function is used to remove blank from eems which can help to reduce the effect of scatter bands.

Usage

```
eem_remove_blank(eem, blank = NA)
```

Arguments

eem	An object of class <code>eemlist</code> .
blank	An object of class <code>eemlist</code> .

Details

The function will first try to use the provided `blank`. If the `blank` is omitted, the function will then try to extract the `blank` from the `eemlist` object. This is done by looking for sample names containing one of these complete or partial strings (ignoring case):

1. nano
2. miliq
3. milliq
4. mq
5. blank

Note that if `blank` is omitted, the function will group the `eemlist` based on file location and will assume that there is a blank sample in each folder. In that context, the `blank` will be used on each sample in the same folder. If more than one `blank` is found they will be averaged (a message will be printed if this appends).

Consider the following example where there are two folders that could represent scans performed on two different days 'scans_day_1' and 'scans_day_2'.

```
scans_day_1
    nano.csv
    sample1.csv
    sample2.csv
    sample3.csv
scans_day_2
    blank.csv
    s1.csv
    s2.csv
    s3.csv
```

In each folder there are three samples and one blank files. In that context, 'eem_remove_blank()' will use the blank 'nano.csv' from 'sample1.csv', 'sample2.csv' and 'sample3.csv'. The same strategy will be used for files in folder 'scans_day_2' but with blank named 'blank.csv'.

Note that the blanks eem are not returned by the function.

Note that blank correction should be performed before Raman normalization (eem_raman_normalisation()). An error will occur if trying to perform blank correction after Raman normalization.

Value

An object of class eemlist.

References

Murphy, K. R., Stedmon, C. a., Graeber, D., & Bro, R. (2013). Fluorescence spectroscopy and multi-way techniques. PARAFAC. Analytical Methods, 5(23), 6557. <http://doi.org/10.1039/c3ay41160e>
<http://xlink.rsc.org/?DOI=c3ay41160e>

Examples

```
## Example 1

# Open the fluorescence eem
file <- system.file("extdata/cary/scans_day_1", "sample1.csv", package = "eemR")
eem <- eem_read(file, import_function = "cary")

plot(eem)

# Open the blank eem
file <- system.file("extdata/cary/scans_day_1", "nano.csv", package = "eemR")
blank <- eem_read(file, import_function = "cary")

plot(blank)

# Remove the blank
eem <- eem_remove_blank(eem, blank)

plot(eem)

## Example 2

# Open the fluorescence eem
folder <- system.file("extdata/cary/scans_day_1", package = "eemR")
eems <- eem_read(folder, import_function = "cary")

plot(eems, which = 3)

# Open the blank eem
file <- system.file("extdata/cary/scans_day_1", "nano.csv", package = "eemR")
blank <- eem_read(file, import_function = "cary")
```

```
plot(blank)

# Remove the blank
eem <- eem_remove_blank(eems, blank)

plot(eems, which = 3)

# Automatic correction
folder <- system.file("extdata/cary/", package = "eemR")

# Look at the folder structure
list.files(folder, "*.csv", recursive = TRUE)

eems <- eem_read(folder, recursive = TRUE, import_function = "cary")
res <- eem_remove_blank(eems)
```

eem_remove_scattering *Remove Raman and Rayleigh scattering*

Description

Remove Raman and Rayleigh scattering

Usage

```
eem_remove_scattering(eem, type, order = 1, width = 10)
```

Arguments

eem	An object of class <code>eemlist</code> .
type	A string, either "raman" or "rayleigh".
order	A integer number, either 1 (first order) or 2 (second order).
width	Slit width in nm for the cut. Default is 10 nm.

Value

An object of class `eemlist`.

References

Lakowicz, J. R. (2006). Principles of Fluorescence Spectroscopy. Boston, MA: Springer US.#'

<http://doi.org/10.1007/978-0-387-46312-4>

Murphy, K. R., Stedmon, C. a., Graeber, D., & Bro, R. (2013). Fluorescence spectroscopy and multi-way techniques. PARAFAC. Analytical Methods, 5(23), 6557. <http://doi.org/10.1039/c3ay41160e#>

<http://xlink.rsc.org/?DOI=c3ay41160e>

Examples

```
# Open the fluorescence eem
file <- system.file("extdata/cary/scans_day_1", "sample1.csv", package = "eemR")
eem <- eem_read(file, import_function = "cary")

plot(eem)

# Remove the scattering
eem <- eem_remove_scattering(eem = eem, type = "raman", order = 1, width = 10)
eem <- eem_remove_scattering(eem = eem, type = "rayleigh", order = 1, width = 10)

plot(eem)
```

eem_set_wavelengths *Set Excitation and/or Emission wavelengths*

Description

This function allows to manually specify either excitation or emission vector of wavelengths in EEMs. This function is mostly used with spectrophotometers such as Shimadzu that do not include excitation wavelengths in fluorescence files.

Usage

```
eem_set_wavelengths(eem, ex, em)
```

Arguments

eem	An object of class <code>eemlist</code> .
ex	A numeric vector of excitation wavelengths.
em	A numeric vector of emission wavelengths.

Value

An object of class `eemlist`.

Examples

```
folder <- system.file("extdata/shimadzu", package = "eemR")

eem <- eem_read(folder, import_function = "shimadzu")
eem <- eem_set_wavelengths(eem, ex = seq(230, 450, by = 5))

plot(eem)
```

plot.eemlist	<i>Surface plot of eem</i>
--------------	----------------------------

Description

Surface plot of eem

Usage

```
## S3 method for class 'eemlist'  
plot(x, which = 1, interactive = FALSE,  
      show_peaks = FALSE, ...)
```

Arguments

x	An object of class eemlist.
which	An integer representing the index of eem to be plotted.
interactive	If TRUE a Shiny app will start to visualize EEMS.
show_peaks	Boolean indicating if Cobble's peaks should be displayed on the surface plot. Default is FALSE.
...	Extra arguments for image.plot.

Examples

```
folder <- system.file("extdata/cary/scans_day_1/", package = "eemR")  
eem <- eem_read(folder, import_function = "cary")  
  
plot(eem, which = 3)
```

print.eemlist	<i>Display summary of an eemlist object</i>
---------------	---

Description

Display summary of an eemlist object

Usage

```
## S3 method for class 'eemlist'  
print(x, ...)
```

Arguments

x	An object of class eemlist.
...	Extra arguments.

Value

A data frame containing summarized information on EEMs.

sample Character. Sample name of the EEM,
ex_min Numerical. Minimum excitation wavelength
ex_max Numerical. Maximum excitation wavelength
em_min Numerical. Minimum emission wavelength
em_max Numerical. Maximum emission wavelength
is_blank_corrected Logical. TRUE if the sample has been blank corrected.
is_scatter_corrected Logical. TRUE if scattering bands have been removed from the sample.
is_ife_corrected Logical. TRUE if the sample has been corrected for inner-filter effect.
is_raman_normalized Logical. TRUE if the sample has been Raman normalized.
manufacturer Character. The name of the manufacturer.

Examples

```
folder <- system.file("extdata/cary", package = "eemR")
eem <- eem_read(folder, recursive = TRUE, import_function = "cary")

print(eem)
```

summary.eemlist

Display summary of an eemlist object

Description

Display summary of an eemlist object

Usage

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

Arguments

object An object of class eemlist.
... Extra arguments.

Value

A data frame containing summarized information on EEMs.

sample Character. Sample name of the EEM,
ex_min Numerical. Minimum excitation wavelength
ex_max Numerical. Maximum excitation wavelength
em_min Numerical. Minimum emission wavelength
em_max Numerical. Maximum emission wavelength
is_blank_corrected Logical. TRUE if the sample has been blank corrected.
is_scatter_corrected Logical. TRUE if scattering bands have been removed from the sample.
is_ife_corrected Logical. TRUE if the sample has been corrected for inner-filter effect.
is_raman_normalized Logical. TRUE if the sample has been Raman normalized.
manufacturer Character. The name of the manufacturer.

Examples

```
folder <- system.file("extdata/cary", package = "eemR")
eem <- eem_read(folder, recursive = TRUE, import_function = "cary")

summary(eem)
```

Index

* datasets

absorbance, [2](#)

absorbance, [2](#)

eem, [3](#)

eem_bind, [3](#)

eem_biological_index, [4](#)

eem_coble_peaks, [5](#)

eem_cut, [6](#)

eem_export_matlab, [7](#)

eem_extract, [8](#)

eem_extract_blank, [9](#)

eem_fluorescence_index, [10](#)

eem_humification_index, [11](#)

eem_inner_filter_effect, [12](#)

eem_names, [13](#)

eem_names<-, [14](#)

eem_peaks, [15](#)

eem_raman_normalisation, [16](#)

eem_read, [18](#)

eem_remove_blank, [19](#)

eem_remove_scattering, [21](#)

eem_set_wavelengths, [22](#)

interp2, [4–6](#), [10](#), [11](#), [15](#)

plot.eemlist, [23](#)

print.eemlist, [23](#)

summary.eemlist, [24](#)