Calibration of Quinine Fluorescence Emission Vignette for the Data Set `flu` of the R package `hyperSpec`

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This vignette gives an example how to

- write an import function for a spectrometer manufacturer's proprietary ASCII files,
- add further data columns to the spectra, and
- set up a linear calibration (ordinary and inverse least squares, respectively).

The data set `flu` in `hyperSpec` consists of 6 fluorescence emission spectra of quinine solutions. They were acquired during an student practicum and were kindly provided by M. Kammer.

The concentrations of the solutions range from 0.05 mg/l to 0.30 mg/l. Spectra were acquired with a Perkin Elmer LS50-B fluorescence spectrometer at 350 nm excitation.

In order to work with `hyperSpec`, the library needs to be loaded in `R`:

```
> library(hyperSpec)
```

Now we need to import the spectra. They are in Perkin Elmer's ASCII file format, one spectrum per file. The files are completely ASCII text, with the actual spectra starting at line 55.

The function should automatically read in all files specified by a pattern, such as `*.txt`. In order to gain some speed, the specrta matrix is preallocated after the first file is read, and the header lines are predefined instead of searching for the .

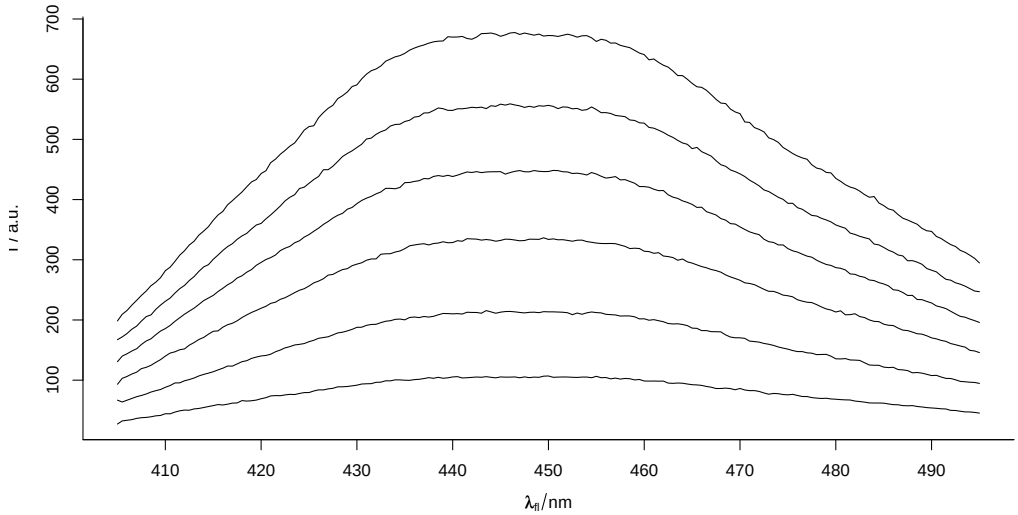
```
> read.PE <- function(files = "*.txt", skip = 54) {
+     files <- Sys.glob(files)
+     buffer <- matrix(scan(files[1], skip = skip), ncol = 2, byrow = TRUE)
+     wavelength <- buffer[, 1]
+     spc <- matrix(ncol = nrow(buffer), nrow = length(files))
+     spc[1, ] <- buffer[, 2]
+     for (f in seq(along = files)[-1]) {
+         buffer <- matrix(scan(files[f], skip = skip), ncol = 2, byrow = TRUE)
+         if (!all.equal(buffer[, 1], wavelength))
+             stop(paste(files[f], "has different wavelengh axis."))
+         spc[f, ] <- buffer[, 2]
+     }
+     new("hyperSpec", wavelength = wavelength, spc = spc, label = list(.wavelength = expression(lambda[fl]/nm),
+         spc = "I / a.u."))
+ }
> flu <- read.PE("*.txt")
```

Now the spectra are in a hyperSpec object and can be examined e.g. by

```
> flu
```

```
hyperSpec object
   6 spectra
   1 data columns
   181 data points / spectrum
wavelength: lambda[fl]/nm [numeric 181]  405.0 405.5 406.0 ... 494.0 494.5 495.0
data:  (6 rows x 1 columns)
   (1) spc: I / a.u. [AsIs matrix 6 x 181] range 27.15000 32.34467 33.37867 ... 676.6457 676.7353 677.4947
```

```
> plot(flu)
```



The calibration model needs the quinine concentrations for the spectra. This information can be stored together with the specta.

```
> flu$c <- seq(from = 0.05, to = 0.3, by = 0.05)
> labels(flu, "c") <- "c / (mg / l)"
> flu
hyperSpec object
   6 spectra
   2 data columns
   181 data points / spectrum
wavelength: lambda[fl]/nm [numeric 181]  405.0 405.5 406.0 ... 494.0 494.5 495.0
data:  (6 rows x 2 columns)
   (1) spc: I / a.u. [AsIs matrix 6 x 181] range 27.15000 32.34467 33.37867 ... 676.6457 676.7353 677.4947
   (2) c: c / (mg / l) [numeric 6] range 0.05 0.10 0.15 0.20 0.25 0.30
```

Now the `hyperSpec` object `flu` contains two data columns, holding the actual spectra and the respective concentrations.