

photobiologyInOut Version 0.4.13

User Guide

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1 Introduction

```
# this may be needed in some geographic locations as some Windows TZ strings are
# not recognized by all versions of R
Sys.setenv(TZ = 'UTC')
library(photobiology)
library(photobiologyWavebands)
library(photobiologyInOut)
library(lubridate)
library(ggplot2)
library(ggmap)
library(ggspectra)
library(hyperSpec)
library(colorSpec)
library(pavo)
library(readr)
```

```
options(tibble.print_max = 5,
        tibble.print_min = 3,
        photobiology.strict.range = NA_integer_)
```

This package defines functions for importing spectral data from different instruments, simulation models, and for data exchange with R packages ‘hyperSpec’ and ‘pavo’ (Table 1).

All functions attempt to decode and store as metadata as much of the information present in file headers as possible. In most cases, the unchanged header of the file is stored as is as a comment in the constructed objects.

It should be remembered, though, that this package has been developed based on the example files I had access to. Files from the same instruments with different hardware configurations, different firmware versions, or even settings may differ substantially. In many cases the output is produced by software in a host computer rather than by the instrument itself, adding further uncertainties and possible differences due to for example the operating system of the host computer. A further complication is that in some cases the format of dates, times and numbers depends on the locale settings in use at the time of data acquisition, or analysis. For all those reasons, do expect to have to do some debugging, and most importantly always validate the imported data against the original file (remembering to run a new validation each time there is a software or firmware update) or update of this package as I test each version before release only with the example files I have available, which are not many.

Table 1: Functions for importing measured and simulated spectral data.

R function	Instrument	Program	class of value
read_oo_ssirrad()	Ocean Optics spectrom.	SpectraSuite	source_spct
read_oo_ssdata()	Ocean Optics spectrom.	SpectraSuite	raw_spct
read_oo_jazirrad()	Ocean Optics Jaz	<i>instrument</i>	source_spct
read_oo_jazdata()	Ocean Optics Jaz	<i>instrument</i>	raw_spct
read_oo_pidata()	Ocean Optics spectrom.	STS DK (Raspbian)	raw_spct
read_avaspec_csv()	Avantes spectrom.	<i>instrument</i>	source_spct
read_macam_file()	Macam	<i>instrument</i>	source_spct
read_licor_file()	LI-COR LI-1800	PC1800 (MS-DOS)	source_spct
read_licor_file()	LI-COR LI-1800	PC1800 (MS-DOS)	filter_spct
read_licor_file()	LI-COR LI-1800	PC1800 (MS-DOS)	reflector_spct
read_m_licor_file()	LI-COR LI-1800	PC1800 (MS-DOS)	source_mspct
read_m_licor_file()	LI-COR LI-1800	PC1800 (MS-DOS)	filter_mspct
read_m_licor_file()	LI-COR LI-1800	PC1800 (MS-DOS)	reflector_mspct
R function	Simulation model	Version	class of value
read_tuv_usrout()	TUV (S. Madronich)	version 5.0	source_spct
read_uvspec_disort()	libRadtran	irradiance	source_spct
read_uvspec_vesa()	(T. & V. Kotilainen)	irradiance	source_spct
read_fmi_cum()	(A. Lindfors)	daily cumulated	source_spct
read_m_fmi_cum()	(A. Lindfors)	daily cumulated	source_mspct
R function	Data repository	Version	class of value
read_FReD_csv()	Floral Reflectance db.	2017-03-19	reflector_spct
read_ASTER_txt()	ASTER spectral lib.	version 2.0 ASCII	reflector_spct
R function	R package	Function	class of value
hyperSpec2mspct()	'hyperSpec'	import	source_mspct
mspct2hyperSpec()	'hyperSpec'	export	hyperSpec
rspec2mspct()	'pavo'	import	source_mspct

2 Examples

In the examples we use function `system-file` to reliably locate the example files included in the package. For reproducing the examples with these files, this call is needed. When using user's files only the path as a character string needs to be passed as argument.

2.1 Ocean Optics Jaz

2.1.1 Raw detector counts

Reading a raw data file generated by Ocean Optics' Jaz spectrometer. The light source was the Jaz PX pulsed Xenon light module.

The first few lines of the file look like this, with W for wavelength, D for dark, R for reference, S for sample and P for processed (all spectral data values are raw detector counts):

```
Jaz Data File
+++++
```

```

Date: Mon Apr 25 12:49:11 2016
User: jaz
Dark Spectrum Present: Yes
Reference Spectrum Present: Yes
Processed Spectrum Present: Yes
Spectrometers: JAZA3098
Integration Time (usec): 748000 (JAZA3098)
Spectra Averaged: 1 (JAZA3098)
Boxcar Smoothing: 0 (JAZA3098)
Correct for Electrical Dark: No (JAZA3098)
Strobe/Lamp Enabled: Yes (JAZA3098)
Correct for Detector Non-linearity: No (JAZA3098)
Correct for Stray Light: No (JAZA3098)
Number of Pixels in Processed Spectrum: 2048
>>>>Begin Processed Spectral Data<<<<
W D R S P
190.313904 0.000000 0.000000 0.000000 0.000000
190.695511 0.000000 0.000000 0.000000 0.000000
191.077087 1138.953125 1123.134277 1102.795898 228.570541
191.458633 1184.149658 1227.086426 1059.859131 -289.473419
191.840149 1175.110352 1193.188965 1132.173584 -237.500336
...

```

```

jaz.raw.file <-
  system.file("extdata", "spectrum.jaz",
             package = "photobiologyInOut", mustWork = TRUE)
jazraw.spct <- read_oo_jazdata(file = jaz.raw.file)

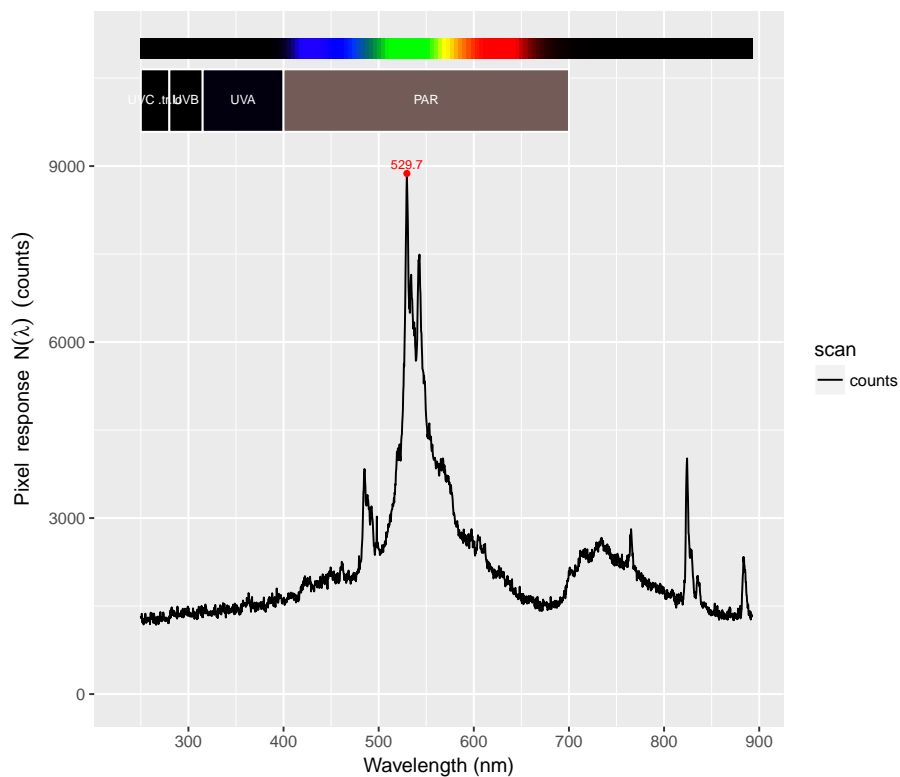
## Parsed with column specification:
## cols(
##   W = col_double(),
##   D = col_double(),
##   R = col_double(),
##   S = col_double(),
##   P = col_double()
## )

jazraw.spct <- trim_wl(jazraw.spct, range = c(250, 900))

```

Plotting the spectrum.

```
plot(jazraw.spct)
```



The metadata stored in attributes can be accessed with functions. It is clear, that not all settings can be recovered from the file. However, we store the record with all the fields which would have been filled if the data had been acquired directly from R using package 'ooacquire'.

```
getWhenMeasured(jazraw.spct)

## [1] "2016-04-25 12:49:02 UTC"
```

```
getInstrDesc(jazraw.spct)

## Data acquired with 'Jaz' s.n. JAZA3098
## grating 'NA', slit 'NA'
```

```
getInstrSettings(jazraw.spct)

## integ. time (s): NA
## total time (s): NA
## counts @ peak (% of max): NA
```

2.1.2 Spectral energy irradiance

Reading an "Absolute Irradiance File" (sic) generated by Ocean Optics' Jaz spectrometer results in a `source_spct` object. In this example, the light source measured was a 'white' fluorescent tube.

The first few lines of the file look like this:

```
Jaz Absolute Irradiance File
+++++
Date: Tue Feb 03 09:44:41 2015
User: jaz
Dark Spectrum Present: Yes
Processed Spectrum Present: Yes
Spectrometers: JAZA1065
Integration Time (usec): 193000 (JAZA1065)
Spectra Averaged: 3 (JAZA1065)
Boxcar Smoothing: 5 (JAZA1065)
Correct for Electrical Dark: Yes (JAZA1065)
Strobe/Lamp Enabled: No (JAZA1065)
Correct for Detector Non-linearity: Yes (JAZA1065)
Correct for Stray Light: No (JAZA1065)
Number of Pixels in Processed Spectrum: 2048
Fiber (micron): 3900
Collection Area: 0.119459
Int. Sphere: No
>>>>Begin Processed Spectral Data<<<<
W D S P
188.825226 0.000000 0.000000 0.000000
189.284851 0.000000 0.000000 0.000000
189.744415 -89.659378 -90.917900 -0.000000
190.203964 -106.165916 -96.419785 0.000000
...
```

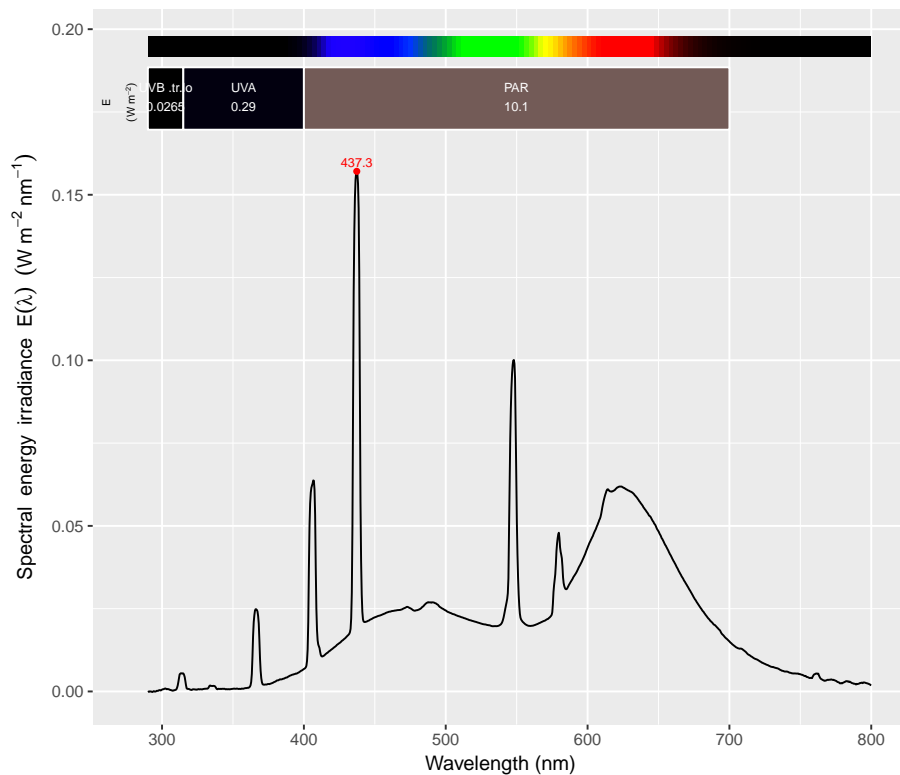
```
jaz.s.irrad.file <-
  system.file("extdata", "spectrum.JazIrrad",
             package = "photobiologyInOut", mustWork = TRUE)
jaz.spct <- read_oo_jazirrad(file = jaz.s.irrad.file)

## Parsed with column specification:
## cols(
##   W = col_double(),
##   D = col_double(),
##   S = col_double(),
##   P = col_double()
## )

jaz0.spct <- jaz.spct
jaz.spct <- trim_wl(jaz.spct, range = c(290, 800))
```

Plotting the spectrum.

```
plot(jaz.spct)
```

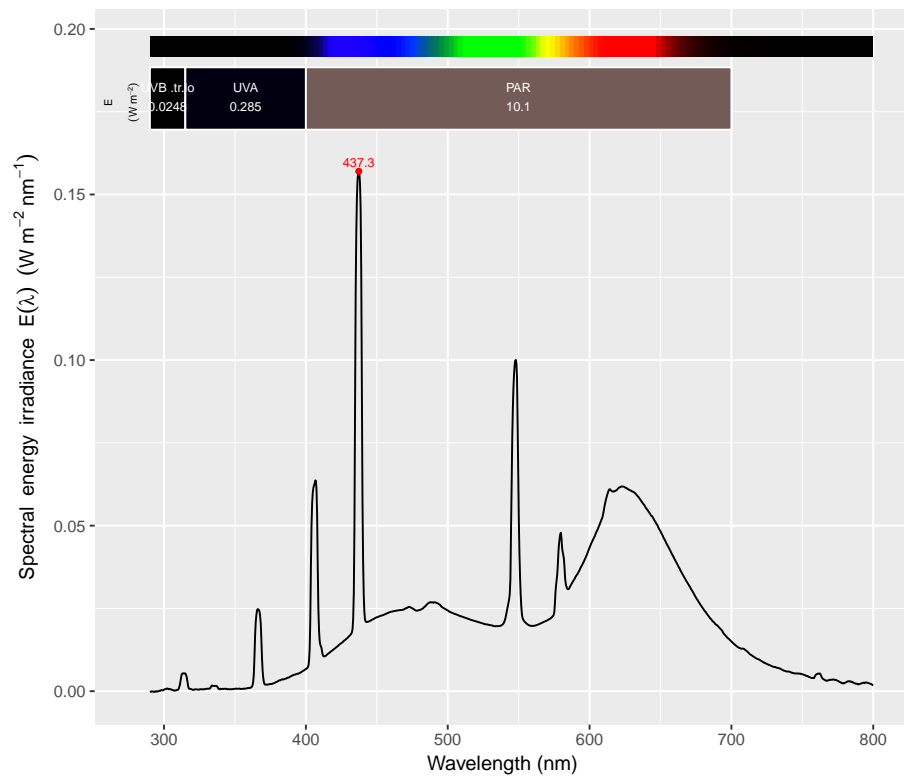


2.1.3 Cleaning spectral data

We can see that the data have problems. We get a warning because the data include negative values for spectral irradiance. We will use some methods from package 'photobiology' to correct the problem. As the data are noisy we cannot just shift the scale so that the most negative value becomes zero. Neither can we replace all negative values with zeros, as this would create bias.

In the following code chunk we will use a region of the spectrum in which spectral irradiance is known to be equal to zero as reference to shift the scale zero. Afterwards we discard data “known” to be zero, and for which the instrument calibration is not valid, and finally we plot the spectrum.

```
jaz.spct <- fshift(jaz0.spct, range = c(255, 290), f = "mean")
jaz.spct <- trim_wl(jaz.spct, range = c(290, 800))
plot(jaz.spct)
```

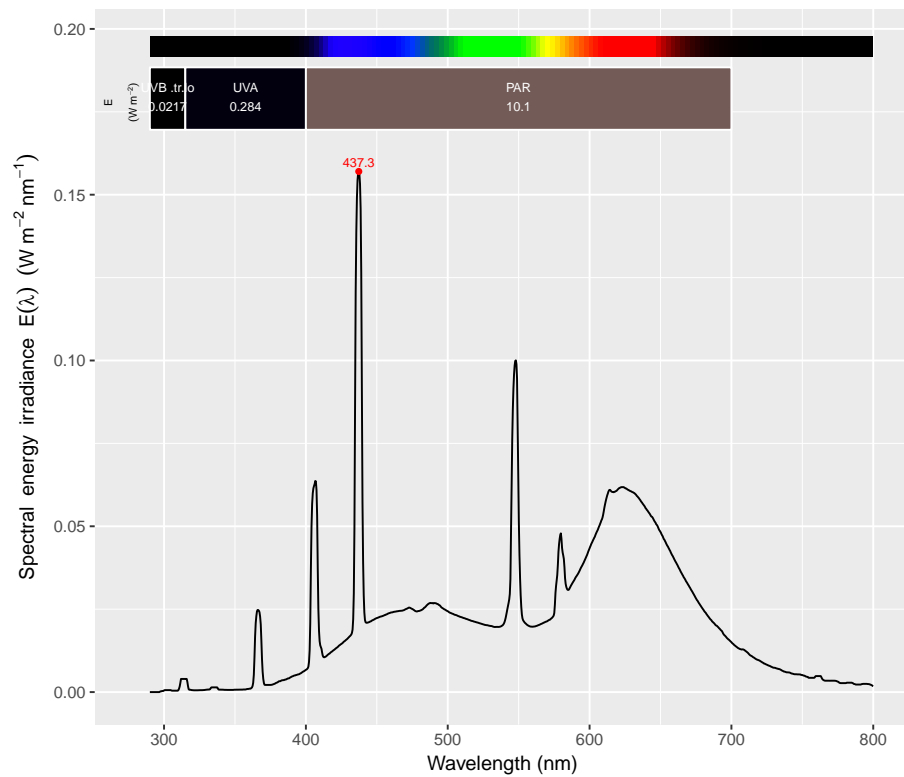


We can next try to smooth the spectrum as it is very noisy outside the visible region.

```
jaz.spct <- smooth_spct(jaz.spct)

## Warning in smooth_spct.source_spct(jaz.spct): 314 'bad' estimates in spectral irradiance

plot(jaz.spct)
```

Photon and energy irradiances.

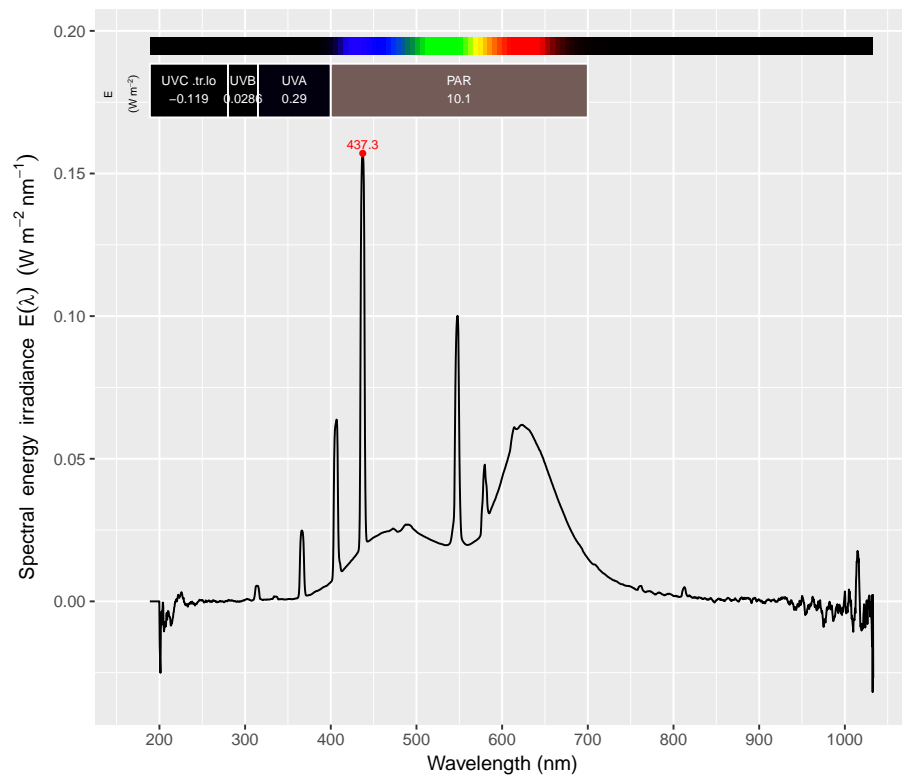
```
e_irrad(jaz.spct, PAR()) # W m-2

##      PAR
## 10.10459
## attr("time.unit")
## [1] "second"
## attr("radiation.unit")
## [1] "energy irradiance total"
```

All in one statement.

```
plot(read_oo_jazirrad(file = jaz.s.irrad.file))

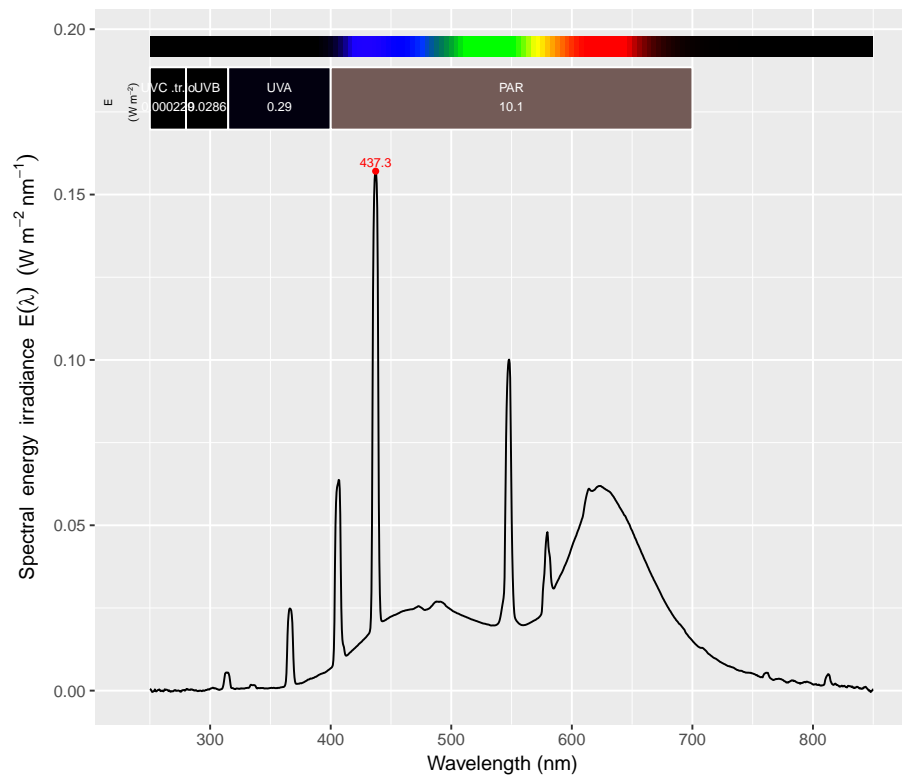
## Parsed with column specification:
## cols(
##   W = col_double(),
##   D = col_double(),
##   S = col_double(),
##   P = col_double()
## )
```



As above but limiting the wavelength range plotted.

```
plot(read_oo_jazirrad(file = jaz.s.irrad.file),
     range = c(250,850))

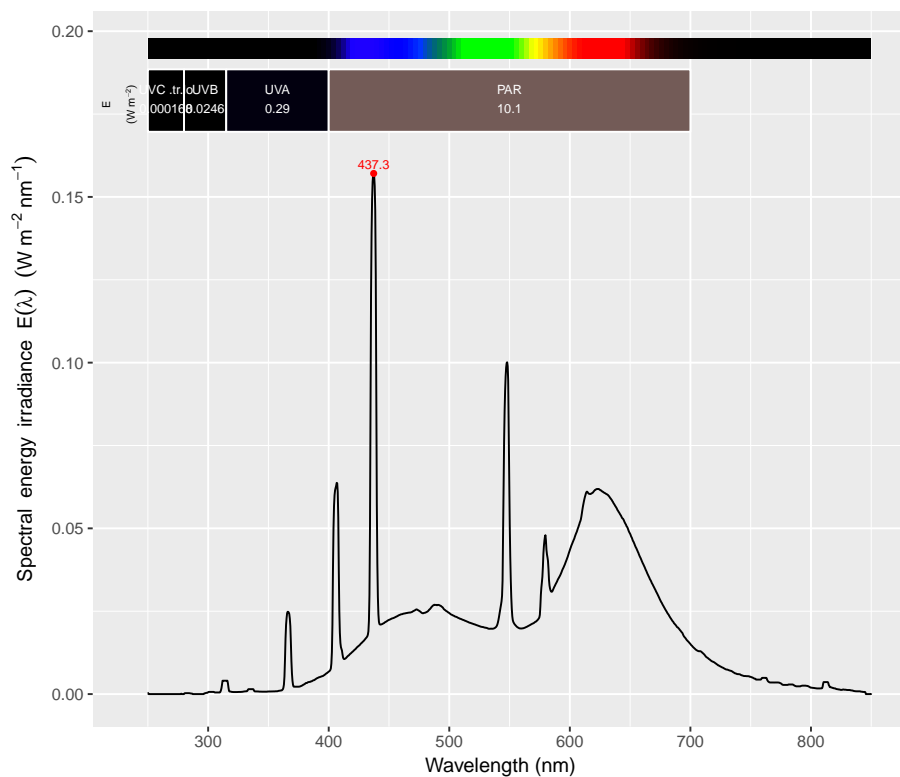
## Parsed with column specification:
## cols(
##   W = col_double(),
##   D = col_double(),
##   S = col_double(),
##   P = col_double()
## )
```



Adding our custom “adaptive” smoothing.

```
plot(smooth_spct(read_oo_jazirrad(file = jaz.s.irrad.file)),
     range = c(250,850))

## Parsed with column specification:
## cols(
##   W = col_double(),
##   D = col_double(),
##   S = col_double(),
##   P = col_double()
## )
## Warning in smooth_spct.source_spct(read_oo_jazirrad(file = jaz.s.irrad.file)): 714
## 'bad' estimates in spectral irradiance
```



2.2 Other modular spectrometers from Ocean Optics

Now a file from an Ocean Optics' Q6500 spectrometer, with data processed with the Spectra Suite software.

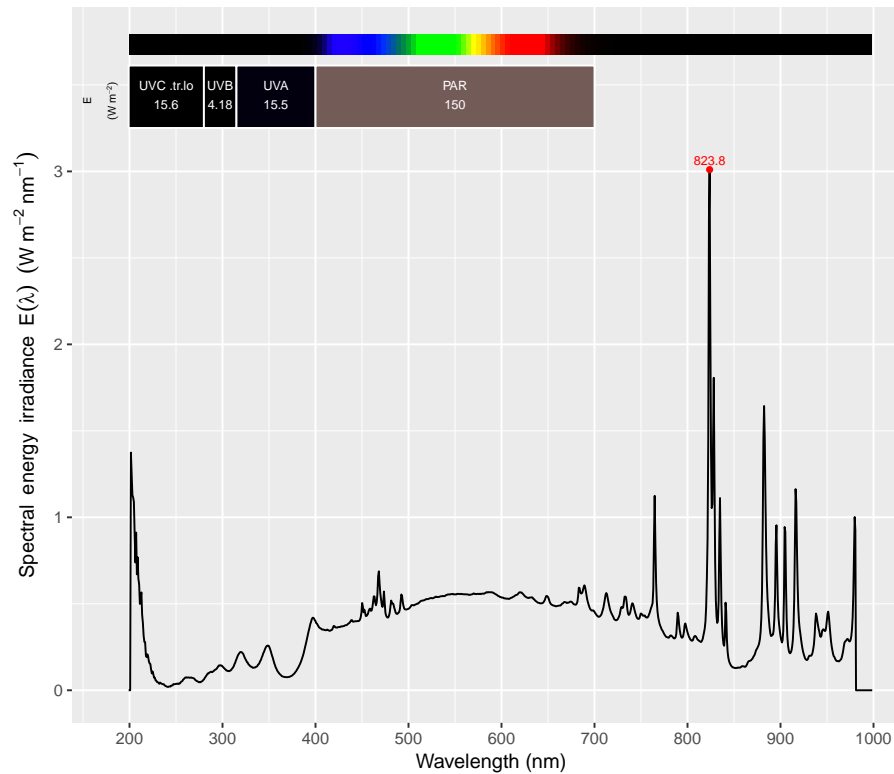
Format of the header is similar, but not identical. The first few lines of the file look like this:

```
SpectraSuite Data File
+++++
Date: Mon May 06 15:13:40 CEST 2013
User: User
Dark Spectrum Present: Yes
Reference Spectrum Present: No
Number of Sampled Component Spectra: 1
Spectrometers: QEB1523
Integration Time (usec): 100000 (QEB1523)
Spectra Averaged: 1 (QEB1523)
Boxcar Smoothing: 0 (QEB1523)
Correct for Electrical Dark: No (QEB1523)
Strobe/Lamp Enabled: No (QEB1523)
Correct for Detector Non-linearity: No (QEB1523)
Correct for Stray Light: Yes (QEB1523)
Number of Pixels in Processed Spectrum: 1044
>>>>Begin Processed Spectral Data<<<<
199.08 0.0000E00
```

```
199.89 0.0000E00
200.70 0.0000E00
...
```

```
q.raw.file <-
  system.file("extdata", "spectrum.SSIrrad",
              package = "photobiologyInOut", mustWork = TRUE)
plot(read_oo_ssirrad(file = q.raw.file))

## Parsed with column specification:
## cols(
##   w.length = col_double(),
##   s.e.irrad = col_double()
## )
```

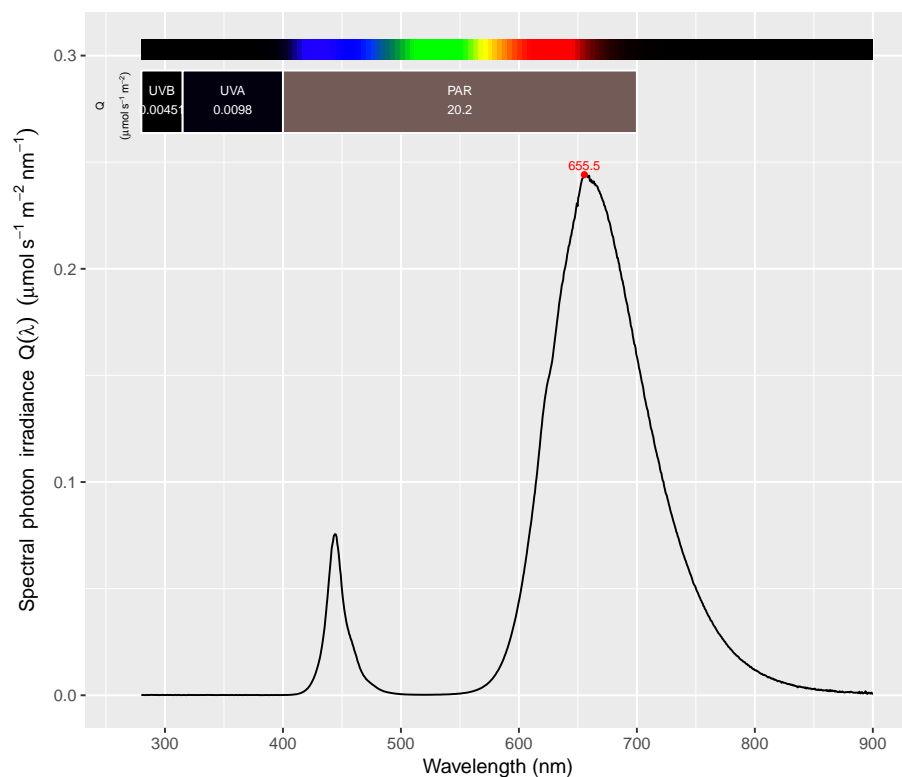


2.3 Modular spectrometers from Avantes

Avantes' two column .csv files can also be imported.

```
ava.raw.file <-
  system.file("extdata", "spectrum-avaspec.csv",
              package = "photobiologyInOut", mustWork = TRUE)
plot(read_avaspec_csv(file = ava.raw.file),
     range = c(280, 900), unit.out = "photon")
```

```
## Parsed with column specification:
## cols(
##   w.length = col_double(),
##   s.e.irrad = col_double()
## )
```



2.4 Scanning spectrometer from Macam

Macam's single column DTA files can also be imported.

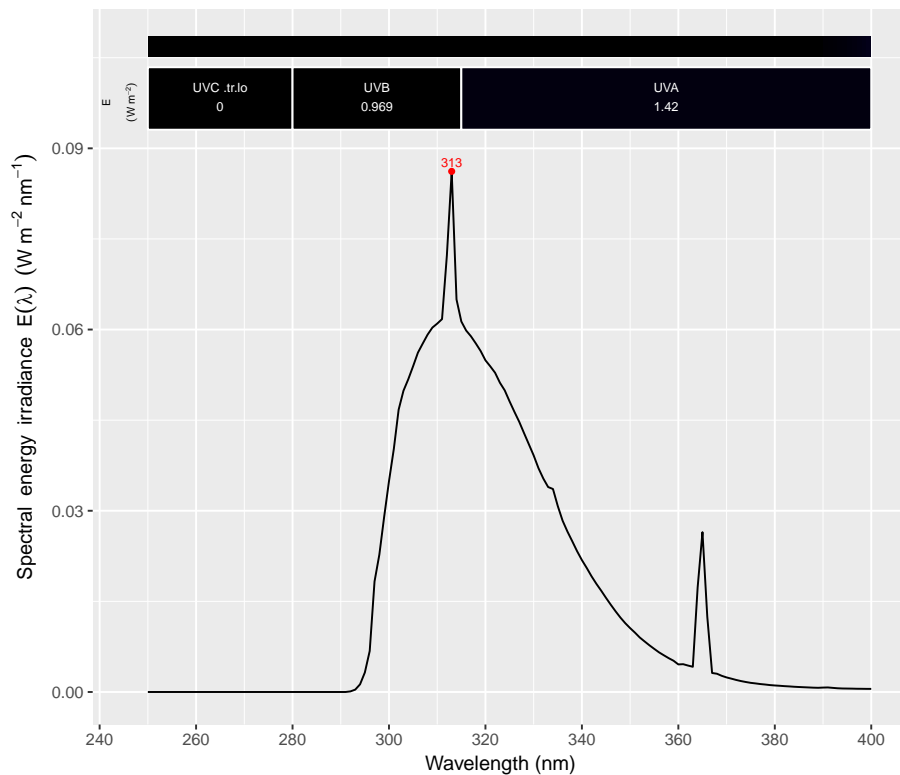
The first few lines of the file look like this with all data in a single column with alternate rows for wavelengths (in nm) and irradiances, and a very terse header:

```
@19/5/1997
@17:44:58
#No Title
2.500000000E+02
0.000000000E+00
2.510000000E+02
0.000000000E+00
2.520000000E+02
0.000000000E+00
...
```

```

macam.raw.file <-
  system.file("extdata", "spectrum.DTA",
              package = "photobiologyInOut", mustWork = TRUE)
plot(read_macam_dta(file = macam.raw.file))

```



2.5 LI-1800 scanning spectrometer from LI-COR

And a spectral photon irradiance output file generated by LI-COR's PC1800 program for the LI-1800 spectroradiometer.

The output has a relatively detailed header, but it lacks year information. Files can contain either energy or photon based spectral irradiances, and this is signalled in the header. In this example photon (= quantum) spectral irradiance is returned. The first few lines of the file look like this:

```

"FILE:FL2"
"REM: TLD 36W/865      (QNTM)"
"LIMS: 300- 900NM"
"INT:  1NM"
"DATE:08/23 16:32"
"MIN:  300NM 1.518E-04"
"MAX:  546NM 7.491E-01"
300  1.518E-04
301  3.355E-04
302  2.197E-04

```

```
303 3.240E-04
...
```

Function `read_licor_prn` will automatically detect whether the data is energy or photon based.

```
licor.file <-
  system.file("extdata", "spectrum.PRN",
              package = "photobiologyInOut", mustWork = TRUE)
licor.spct <- read_licor_prn(file = licor.file)
```

In all cases as much information as possible is decoded, and the data file headers are preserved as comments in the `source.spct` objects.

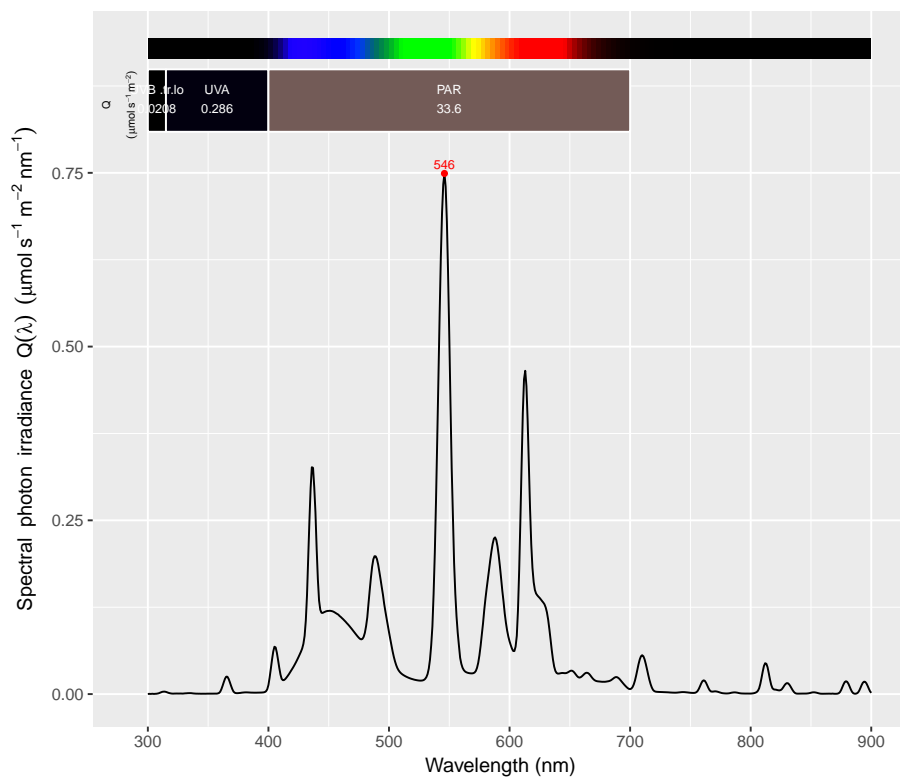
```
licor.spct

## Object: source_spct [601 x 2]
## Wavelength range 300 to 900 nm, step 1 nm
## Label: File: spectrum.PRN
## Measured on 0000-08-23 16:32:00 UTC
## Time unit 1s
##
## # A tibble: 601 × 2
##   w.length s.q.irrad
##   <dbl>    <dbl>
## 1      300 1.518e-10
## 2      301 3.355e-10
## 3      302 2.197e-10
## # ... with 598 more rows

cat(comment(licor.spct))

## LICOR LI-1800 file 'spectrum.PRN' imported on 2017-03-20 01:10:22 UTC
## "FILE:FL2"
## "REM: TLD 36W/865 (QNTM)"
## "LIMS: 300- 900NM"
## "INT: 1NM"
## "DATE:08/23 16:32"
## "MIN: 300NM 1.518E-04"
## "MAX: 546NM 7.491E-01"

plot(licor.spct, unit.out = "photon")
```

It is also possible to use the same function to import reflectance, and transmittance spectra acquired by the LI-1800.

And a spectral reflectance output file generated by LI-COR's PC1800 program for the LI-1800 spectroradiometer is used next.

The first few lines of the file look like this:

```
"FILE:RGD1"
"REM: REFL GREEN AD 1 "
"LIMS: 350- 800NM"
"INT: 2NM"
"DATE:05/30 13:50"
"MIN: 358NM 4.628E-02"
"MAX: 776NM 4.693E-01"
350 5.135E-02
352 4.713E-02
354 5.324E-02
356 4.740E-02
...
```

Function `read_licor_prn` cannot automatically detect the spectral quantity in the file, and when the irradiance default is not correct, users need to override it with an explicit argument for parameter `s.qty`.

```
licor.file <-
  system.file("extdata", "reflectance.PRN",
```

```

package = "photobiologyInOut", mustWork = TRUE)
licor.spct <- read_licor_prn(file = licor.file, s.qty = "Rfr")

```

In all cases as much information as possible is decoded, and the data file headers are preserved as comments in the source.spct objects.

```

licor.spct

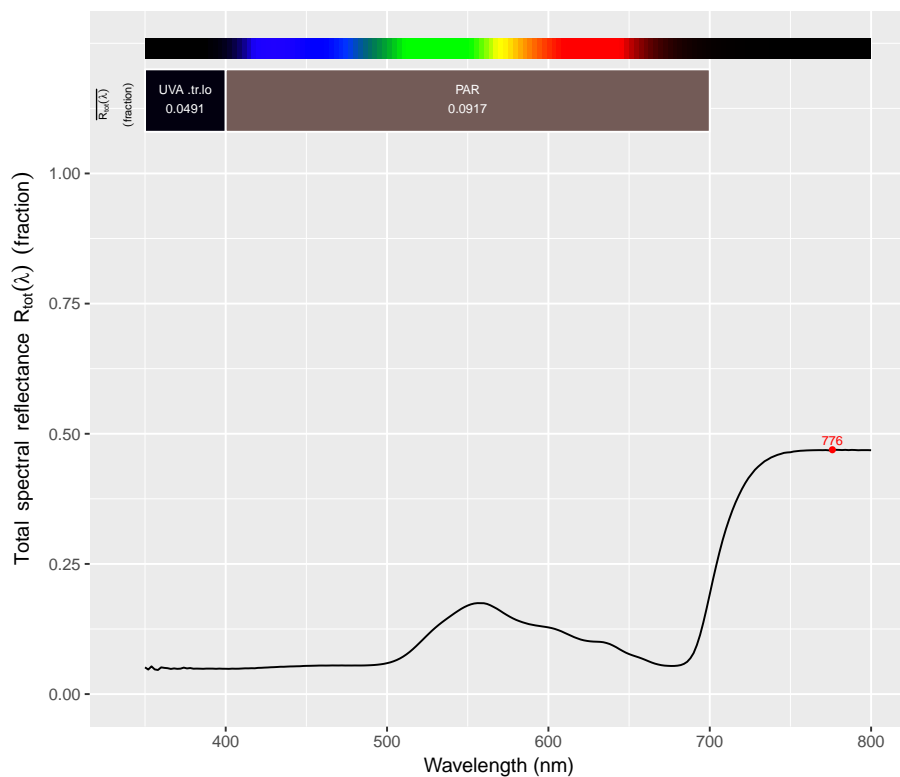
## Object: reflector_spct [226 x 2]
## Wavelength range 350 to 800 nm, step 2 nm
## Label: File: reflectance.PRN
## Measured on 0000-05-30 13:50:00 UTC
##
## # A tibble: 226 × 2
##   w.length      Rfr
##   <dbl>    <dbl>
## 1      350 0.05135
## 2      352 0.04713
## 3      354 0.05324
## # ... with 223 more rows

cat(comment(licor.spct))

## LICOR LI-1800 file 'reflectance.PRN' imported on 2017-03-20 01:10:23 UTC
## "FILE:RGD1"
## "REM: REFL GREEN AD 1 "
## "LIMS: 350- 800NM"
## "INT:  2NM"
## "DATE:05/30 13:50"
## "MIN:  358NM  4.628E-02"
## "MAX:  776NM  4.693E-01"

plot(licor.spct)

```



3 Data from loggers

3.1 Campbell Scientific

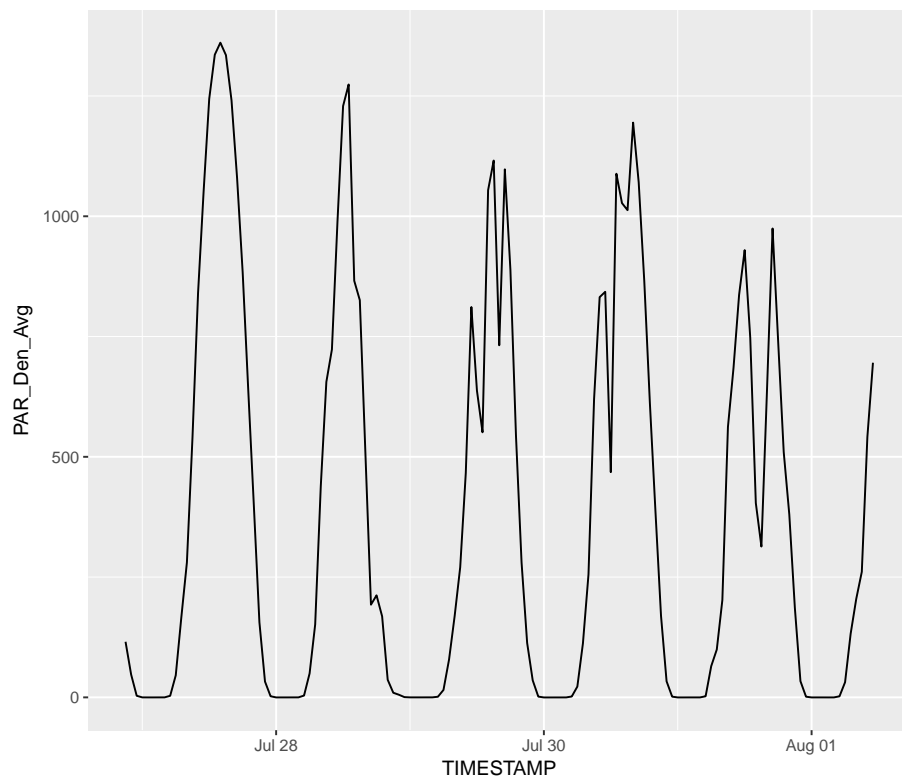
The functions in the package have been tested with a very recent datalogger model, the CR6, and using current versions of programs PC400 and PC200W to download the data. The currently used format of .DAT files is easy to decode and one function can automatically detect the number and type of columns and the number of rows. All information is preserved in the returned `tibble::tibble` object, which is derived from `data.frame`.

```
cs.day.file <-
  system.file("extdata", "cr6-day.dat",
    package = "photobiologyInOut", mustWork = TRUE)
day.dat <- read_csi_dat(file = cs.day.file)
day.dat

## # A tibble: 2 × 33
##   TIMESTAMP RECORD PAR_Den_Avg PAR_BF_tot_Avg
##   <dtm>    <int>    <dbl>      <dbl>
## 1 2016-07-27      0    20.86722    401.0677
## 2 2016-07-28      1   526.48310    591.7202
```

```
## # ... with 29 more variables: PAR_BF_diff_Avg <dbl>,
## #   PAR_Den_Min <dbl>, PAR_Den_TMn <dtm>,
## #   PAR_Den_Max <dbl>, PAR_Den_TMx <dtm>,
## #   PAR_BF_tot_Min <dbl>, PAR_BF_tot_TMn <dtm>,
## #   PAR_BF_tot_Max <dbl>, PAR_BF_tot_TMx <dtm>,
## #   PAR_BF_diff_Min <dbl>, PAR_BF_diff_TMn <dtm>,
## #   PAR_BF_diff_Max <dbl>, PAR_BF_diff_TMx <dtm>,
## #   AirTemp_Avg <dbl>, AirDewPoint_Avg <dbl>,
## #   AirPressure_Avg <dbl>, AirTemp_Min <dbl>,
## #   AirTemp_TMn <dtm>, AirTemp_Max <dbl>,
## #   AirTemp_TMx <dtm>, AirDewPoint_Min <dbl>,
## #   AirDewPoint_TMn <dtm>, AirDewPoint_Max <dbl>,
## #   AirDewPoint_TMx <dtm>, AirPressure_Min <dbl>,
## #   AirPressure_TMn <dtm>, AirPressure_Max <dbl>,
## #   AirPressure_TMx <dtm>, BattV_Min <dbl>
```

```
cs.hour.file <-
  system.file("extdata", "cr6-hour.dat",
    package = "photobiologyInOut", mustWork = TRUE)
hour.dat <- read_csi_dat(file = cs.hour.file)
ggplot(hour.dat, aes(TIMESTAMP, PAR_Den_Avg)) + geom_line()
```



4 Output from simulation models

4.1 TUV

The output from the TUV model can be imported either by editing it before import, or by making a simple edit to the output routine of TUV. This function is known to work with TUV version 5.0 output. The output from TUV can contain a variable number of spectra in “parallel” columns, which are *melted* into a single column, with a factor with letter as levels, a numeric variable with the zenith angle and a POSIXct column with times. A date needs to be always supplied as the output file from TUV has only time of day information.

```
tuv.file <-
  system.file("extdata", "usrout.txt",
             package = "photobiologyInOut", mustWork = TRUE)
tuv.spct <- read_tuv_usrout(file = tuv.file,
                          date = ymd("2014-03-21"))
summary(subset(tuv.spct, spct.idx == "A"))

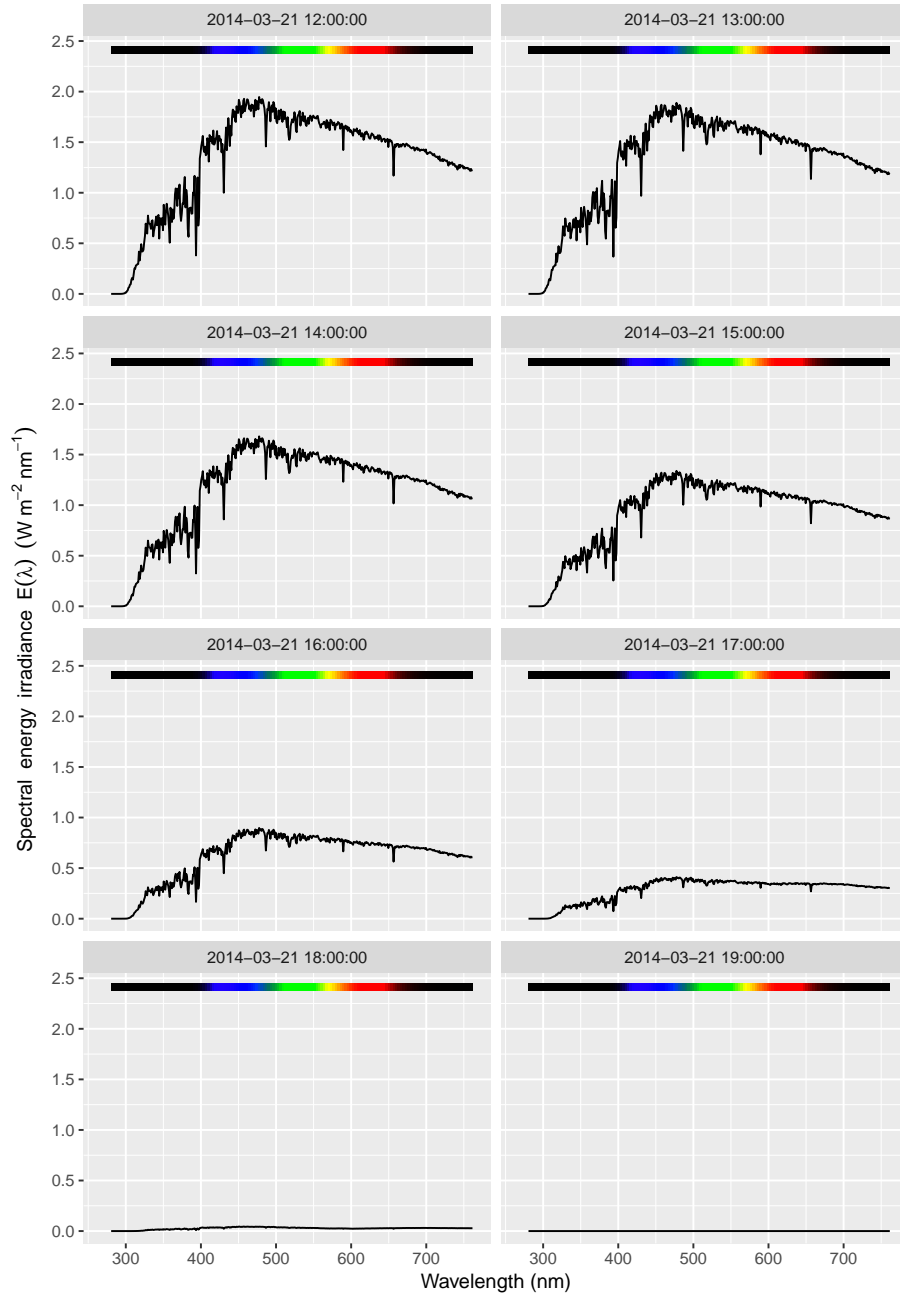
## Summary of object: source_spct [482 x 5]
## containing 8 spectra in long form
## Wavelength range 280.5 to 761.5 nm, step 1 nm
## Time unit is
##
##      w.length      spct.idx      s.e.irrad
## Min.    :280.5    A      :482    Min.    :0.000
## 1st Qu.:400.8    B      : 0    1st Qu.:1.216
## Median :521.0    C      : 0    Median :1.483
## Mean   :521.0    D      : 0    Mean   :1.322
## 3rd Qu.:641.2    E      : 0    3rd Qu.:1.680
## Max.   :761.5    F      : 0    Max.   :1.947
##
##      (Other): 0
##
##      angle      date
## Min.    :1.829    Min.    :2014-03-21 12:00:00
## 1st Qu.:1.829    1st Qu.:2014-03-21 12:00:00
## Median :1.829    Median :2014-03-21 12:00:00
## Mean   :1.829    Mean   :2014-03-21 12:00:00
## 3rd Qu.:1.829    3rd Qu.:2014-03-21 12:00:00
## Max.   :1.829    Max.   :2014-03-21 12:00:00
##
tuv.spct

## Object: source_spct [3,856 x 5]
## containing 8 spectra in long form
## Wavelength range 280.5 to 761.5 nm, step 1 nm
## Label: TUV spectral simulation File: usrout.txt
## Measured on 2014-03-21 12:00:00 UTC
## Measured on 2014-03-21 13:00:00 UTC
## Measured on 2014-03-21 14:00:00 UTC
## Measured on 2014-03-21 15:00:00 UTC
## Measured on 2014-03-21 16:00:00 UTC
## Measured on 2014-03-21 17:00:00 UTC
## Measured on 2014-03-21 18:00:00 UTC
## Measured on 2014-03-21 19:00:00 UTC
```

```
## Time unit is
##
## # A tibble: 3,856 × 5
##   w.length spct.idx s.e.irrad angle
##   <dbl>   <fctr>   <dbl> <dbl>
## 1    280.5         A 3.041e-15 1.829
## 2    281.5         A 1.164e-13 1.829
## 3    282.5         A 1.824e-12 1.829
## # ... with 3,853 more rows, and 1 more variables:
## #   date <dtm>
```

It is possible to extract individual spectra with `subset`, or as done here plot them in different panels.

```
plot(tuv.spct, annotations = c("colour_guide")) +
  facet_wrap(~date, ncol = 2)
```



The output is a single `source_spect` object that can be easily converted into a `source_mspect` object containing the individual spectra as members of the collection.

```

tuv.mspect <- subset2mspect(tuv.spct)
tuv.mspect

## Object: source_mspect [8 x 1]
## --- Member: A ---
## Object: source_spct [482 x 4]
## Wavelength range 280.5 to 761.5 nm, step 1 nm
## Label: TUV spectral simulation File: usROUT.txt
## Measured on 2014-03-21 12:00:00 UTC
## Measured on 2014-03-21 13:00:00 UTC
## Measured on 2014-03-21 14:00:00 UTC
## Measured on 2014-03-21 15:00:00 UTC
## Measured on 2014-03-21 16:00:00 UTC
## Measured on 2014-03-21 17:00:00 UTC
## Measured on 2014-03-21 18:00:00 UTC
## Measured on 2014-03-21 19:00:00 UTC
## Time unit is
##
## # A tibble: 482 x 4
##   w.length s.e.irrad angle      date
## *   <dbl>      <dbl> <dbl>    <dtm>
## 1   280.5 3.041e-15 1.829 2014-03-21 12:00:00
## 2   281.5 1.164e-13 1.829 2014-03-21 12:00:00
## 3   282.5 1.824e-12 1.829 2014-03-21 12:00:00
## # ... with 479 more rows
## --- Member: B ---
## Object: source_spct [482 x 4]
## Wavelength range 280.5 to 761.5 nm, step 1 nm
## Label: TUV spectral simulation File: usROUT.txt
## Measured on 2014-03-21 12:00:00 UTC
## Measured on 2014-03-21 13:00:00 UTC
## Measured on 2014-03-21 14:00:00 UTC
## Measured on 2014-03-21 15:00:00 UTC
## Measured on 2014-03-21 16:00:00 UTC
## Measured on 2014-03-21 17:00:00 UTC
## Measured on 2014-03-21 18:00:00 UTC
## Measured on 2014-03-21 19:00:00 UTC
## Time unit is
##
## # A tibble: 482 x 4
##   w.length s.e.irrad angle      date
## *   <dbl>      <dbl> <dbl>    <dtm>
## 1   280.5 1.314e-15 13.198 2014-03-21 13:00:00
## 2   281.5 5.415e-14 13.198 2014-03-21 13:00:00
## 3   282.5 9.039e-13 13.198 2014-03-21 13:00:00
## # ... with 479 more rows
## --- Member: C ---
## Object: source_spct [482 x 4]
## Wavelength range 280.5 to 761.5 nm, step 1 nm
## Label: TUV spectral simulation File: usROUT.txt
## Measured on 2014-03-21 12:00:00 UTC
## Measured on 2014-03-21 13:00:00 UTC
## Measured on 2014-03-21 14:00:00 UTC
## Measured on 2014-03-21 15:00:00 UTC
## Measured on 2014-03-21 16:00:00 UTC
## Measured on 2014-03-21 17:00:00 UTC
## Measured on 2014-03-21 18:00:00 UTC

```



```

## Measured on 2014-03-21 19:00:00 UTC
## Time unit 1s
##
## # A tibble: 482 × 4
##   w.length s.e.irrad angle      date
## *   <dbl>     <dbl> <dbl>    <dtm>
## 1    280.5 4.521e-17  28.2 2014-03-21 14:00:00
## 2    281.5 2.510e-15  28.2 2014-03-21 14:00:00
## 3    282.5 5.413e-14  28.2 2014-03-21 14:00:00
## # ... with 479 more rows
## --- Member: D ---
## Object: source_spct [482 x 4]
## Wavelength range 280.5 to 761.5 nm, step 1 nm
## Label: TUV spectral simulation File: usROUT.txt
## Measured on 2014-03-21 12:00:00 UTC
## Measured on 2014-03-21 13:00:00 UTC
## Measured on 2014-03-21 14:00:00 UTC
## Measured on 2014-03-21 15:00:00 UTC
## Measured on 2014-03-21 16:00:00 UTC
## Measured on 2014-03-21 17:00:00 UTC
## Measured on 2014-03-21 18:00:00 UTC
## Measured on 2014-03-21 19:00:00 UTC
## Time unit 1s
##
## # A tibble: 482 × 4
##   w.length s.e.irrad angle      date
## *   <dbl>     <dbl> <dbl>    <dtm>
## 1    280.5 3.075e-20 43.202 2014-03-21 15:00:00
## 2    281.5 3.273e-18 43.202 2014-03-21 15:00:00
## 3    282.5 1.234e-16 43.202 2014-03-21 15:00:00
## # ... with 479 more rows
## --- Member: E ---
## Object: source_spct [482 x 4]
## Wavelength range 280.5 to 761.5 nm, step 1 nm
## Label: TUV spectral simulation File: usROUT.txt
## Measured on 2014-03-21 12:00:00 UTC
## Measured on 2014-03-21 13:00:00 UTC
## Measured on 2014-03-21 14:00:00 UTC
## Measured on 2014-03-21 15:00:00 UTC
## Measured on 2014-03-21 16:00:00 UTC
## Measured on 2014-03-21 17:00:00 UTC
## Measured on 2014-03-21 18:00:00 UTC
## Measured on 2014-03-21 19:00:00 UTC
## Time unit 1s
##
## # A tibble: 482 × 4
##   w.length s.e.irrad angle      date
## *   <dbl>     <dbl> <dbl>    <dtm>
## 1    280.5 2.253e-26 58.205 2014-03-21 16:00:00
## 2    281.5 7.751e-24 58.205 2014-03-21 16:00:00
## 3    282.5 8.148e-22 58.205 2014-03-21 16:00:00
## # ... with 479 more rows
## --- Member: F ---
## Object: source_spct [482 x 4]
## Wavelength range 280.5 to 761.5 nm, step 1 nm
## Label: TUV spectral simulation File: usROUT.txt
## Measured on 2014-03-21 12:00:00 UTC

```

```

## Measured on 2014-03-21 13:00:00 UTC
## Measured on 2014-03-21 14:00:00 UTC
## Measured on 2014-03-21 15:00:00 UTC
## Measured on 2014-03-21 16:00:00 UTC
## Measured on 2014-03-21 17:00:00 UTC
## Measured on 2014-03-21 18:00:00 UTC
## Measured on 2014-03-21 19:00:00 UTC
## Time unit 1s
##
## # A tibble: 482 × 4
##   w.length s.e.irrad angle      date
## *   <dbl>      <dbl> <dbl>      <dtm>
## 1    280.5 1.929e-27 73.208 2014-03-21 17:00:00
## 2    281.5 5.710e-25 73.208 2014-03-21 17:00:00
## 3    282.5 5.202e-23 73.208 2014-03-21 17:00:00
## # ... with 479 more rows
## --- Member: G ---
## Object: source_spct [482 x 4]
## Wavelength range 280.5 to 761.5 nm, step 1 nm
## Label: TUV spectral simulation File: usrout.txt
## Measured on 2014-03-21 12:00:00 UTC
## Measured on 2014-03-21 13:00:00 UTC
## Measured on 2014-03-21 14:00:00 UTC
## Measured on 2014-03-21 15:00:00 UTC
## Measured on 2014-03-21 16:00:00 UTC
## Measured on 2014-03-21 17:00:00 UTC
## Measured on 2014-03-21 18:00:00 UTC
## Measured on 2014-03-21 19:00:00 UTC
## Time unit 1s
##
## # A tibble: 482 × 4
##   w.length s.e.irrad angle      date
## *   <dbl>      <dbl> <dbl>      <dtm>
## 1    280.5 4.721e-28 88.211 2014-03-21 18:00:00
## 2    281.5 1.385e-25 88.211 2014-03-21 18:00:00
## 3    282.5 1.250e-23 88.211 2014-03-21 18:00:00
## # ... with 479 more rows
## --- Member: H ---
## Object: source_spct [482 x 4]
## Wavelength range 280.5 to 761.5 nm, step 1 nm
## Label: TUV spectral simulation File: usrout.txt
## Measured on 2014-03-21 12:00:00 UTC
## Measured on 2014-03-21 13:00:00 UTC
## Measured on 2014-03-21 14:00:00 UTC
## Measured on 2014-03-21 15:00:00 UTC
## Measured on 2014-03-21 16:00:00 UTC
## Measured on 2014-03-21 17:00:00 UTC
## Measured on 2014-03-21 18:00:00 UTC
## Measured on 2014-03-21 19:00:00 UTC
## Time unit 1s
##
## # A tibble: 482 × 4
##   w.length s.e.irrad angle      date
## *   <dbl>      <dbl> <dbl>      <dtm>
## 1    280.5          0 103.213 2014-03-21 19:00:00
## 2    281.5          0 103.213 2014-03-21 19:00:00
## 3    282.5          0 103.213 2014-03-21 19:00:00

```

```
## # ... with 479 more rows
##
## --- END ---
```

With the default of `lubridate::today()` for date times are ‘mapped’ to the current local date using the time zone of the computer as visible to R.

```
tuv_nd.spct <- read_tuv_usrout(file = tuv.file)
tuv_nd.spct

## Object: source_spct [3,856 x 5]
## containing 8 spectra in long form
## Wavelength range 280.5 to 761.5 nm, step 1 nm
## Label: TUV spectral simulation File: usrout.txt
## Measured on 2017-03-20 12:00:00 UTC
## Measured on 2017-03-20 13:00:00 UTC
## Measured on 2017-03-20 14:00:00 UTC
## Measured on 2017-03-20 15:00:00 UTC
## Measured on 2017-03-20 16:00:00 UTC
## Measured on 2017-03-20 17:00:00 UTC
## Measured on 2017-03-20 18:00:00 UTC
## Measured on 2017-03-20 19:00:00 UTC
## Time unit 1s
##
## # A tibble: 3,856 × 5
##   w.length spct.idx s.e.irrad angle
##   <dbl>   <fctr>   <dbl> <dbl>
## 1    280.5         A 3.041e-15 1.829
## 2    281.5         A 1.164e-13 1.829
## 3    282.5         A 1.824e-12 1.829
## # ... with 3,853 more rows, and 1 more variables:
## #   date <dtm>
```

4.2 libRadtran

By default `libRadtran`’s `uvspec` writes only spectral irradiances to a text file as output. This is different from ‘TUV’ which by default includes an extensive header with the parameter settings used for the simulation. It is easy to read this simple output file with R’s functions. However, we provide functions, that simplify reading of the files. The output from `uvspec` varies depending on its input. The main source of differences is the solver routine used. We will provide a separate function for each solver.

For reading this simple output, no special function is needed. We can use `read.table` from base R. Here we read a file with two columns with wavelengths and global spectral energy irradiance (named “eglo” in `libRadtran`) in $\text{mW m}^{-2} \text{nm}^{-1}$. The file was created with one of the ‘`uvspec`’ examples included with `libRadtran`, but reducing the output to two columns.

The first few lines of the file look like this:

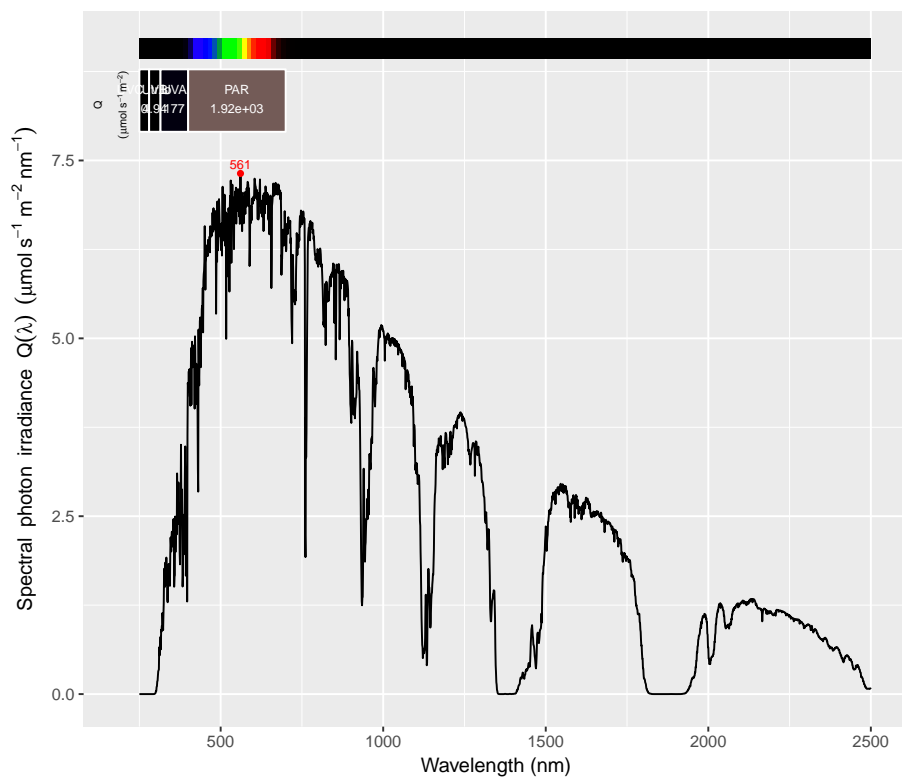
```
250.000 0.000000e+00
251.000 0.000000e+00
252.000 0.000000e+00
```

```
253.000 0.000000e+00
...
```

```
uvspec.2col.file <-
  system.file("extdata", "uvspec-plain-2col.dat",
              package = "photobiologyInOut", mustWork = TRUE)
lrt.df <- read.table(file = uvspec.2col.file,
                    col.names = c("w.length", "s.e.irrad"))
uvspec.01.spct <- source_spct(w.length = lrt.df$w.length,
                             s.e.irrad = lrt.df$s.e.irrad * 1e-3)
summary(uvspec.01.spct)

## Summary of object: source_spct [3,751 x 2]
## Wavelength range 250 to 4000 nm, step 1 nm
## Time unit 1s
##
##      w.length      s.e.irrad
## Min.      : 250    Min.      :0.000000
## 1st Qu.:1188    1st Qu.:0.003808
## Median :2125    Median :0.023999
## Mean      :2125    Mean      :0.244545
## 3rd Qu.:3062    3rd Qu.:0.264351
## Max.      :4000    Max.      :1.744596

cat(comment(uvspec.01.spct))
plot(uvspec.01.spct, range = c(250, 2500), unit.out = "photon")
```



An example using solver `disort` and our function `read_uvspec_disort()` follows.

The first few lines of the file look like this:

```
290.000 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
291.000 1.046525e-11 4.800521e-06 1.674293e-07 2.374267e-12 5.342789e-07 2.664720e-08
292.000 5.888299e-10 2.813865e-05 9.814190e-07 1.335888e-10 3.162808e-06 1.561977e-07
293.000 4.383296e-09 5.764524e-05 2.010660e-06 9.944455e-10 6.522616e-06 3.200065e-07
...
```

```
uvspec.disort.file <-
  system.file("extdata", "uvspec-disort.dat",
             package = "photobiologyInOut", mustWork = TRUE)
uvspec.02.spct <- read_uvspec_disort(uvspec.disort.file)
summary(uvspec.02.spct)

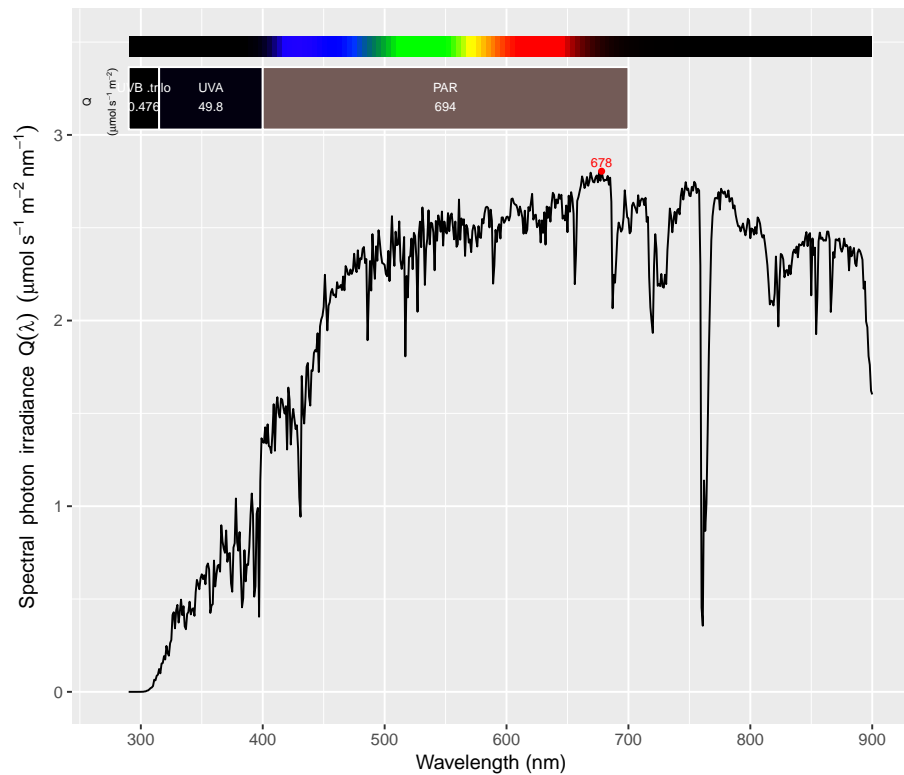
## Summary of object: source_spct [611 x 4]
## Wavelength range 290 to 900 nm, step 1 nm
## Label: libRadtran spectral simulation File: uvspec-disort.dat
## Time unit 1s
##
##      w.length      s.e.irrad.dir      s.e.irrad.diff
##  Min.   :290.0      Min.   :0.0000      Min.   :0.00000
##  1st Qu.:442.5      1st Qu.:0.2693      1st Qu.:0.01647
##  Median :595.0      Median :0.3781      Median :0.04204
```

```
## Mean :595.0 Mean :0.3269 Mean :0.06485
## 3rd Qu.:747.5 3rd Qu.:0.4440 3rd Qu.:0.11234
## Max. :900.0 Max. :0.4928 Max. :0.19479
## s.e.irrad
## Min. :0.0000
## 1st Qu.:0.3237
## Median :0.4236
## Mean :0.3918
## 3rd Qu.:0.5049
## Max. :0.6058

cat(comment(uvspec.02.spct))

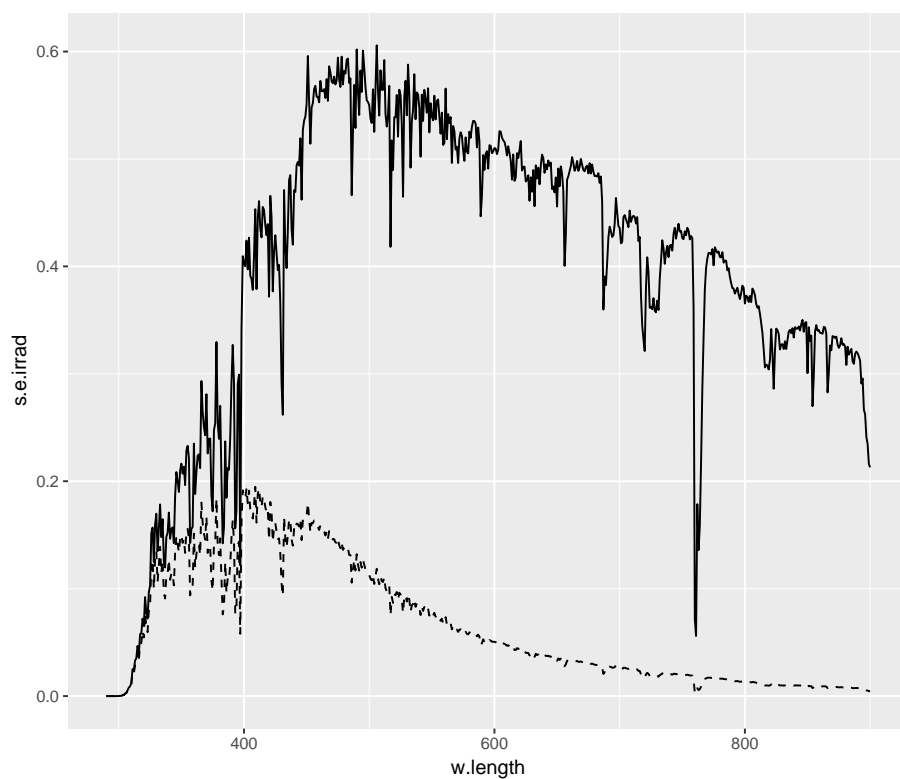
## libRadtran file 'uvspec-disort.dat' imported on 2017-03-20 01:10:28 UTC

plot(uvspec.02.spct, unit.out = "photon")
```



The data contains also estimates of diffuse and direct spectral irradiance. Here we plot the total energy irradiance with a solid line and the diffuse component with a dashed line.

```
ggplot(uvspec.02.spct) +
  geom_line() +
  geom_line(aes(y = s.e.irrad.diff), linetype = "dashed")
```



The uvspec file used to generate the spectrum read above is:

```
data_files_path uvspec_home/data/
atmosphere_file uvspec_home/data/atmmod/afglms.dat
source solar uvspec_home/data/solar_flux/kurudz_1.0nm.dat
rte_solver disort
mol_abs_param lowtran
deltam on
number_of_streams 6
wavelength 290 900
day_of_year 287
altitude 0.012
albedo_library IGBP
brdf_rpv_type 5
mol_modify 03 288 DU
mol_modify H2O 10 MM
sza 69.4662
sur_temperature 273
```

If we plan to save and reuse the spectral object, it is recommended to append the input file to the comment.

```
uvspec.disort.inp.file <-
  system.file("extdata", "uvspec-disort.inp",
             package = "photobiologyInOut", mustWork = TRUE)
comment(uvspec.02.spct) <- paste(comment(uvspec.02.spct),
```

```

                                read_file(uvspec.disort.inp.file),
                                sep = "\n\n")
cat(comment(uvspec.02.spct))

## libRadtran file 'uvspec-disort.dat' imported on 2017-03-20 01:10:28 UTC
##
## data_files_path uvspec_home/data/

## atmosphere_file uvspec_home/data/atmmod/afglms.dat

## source solar uvspec_home/data/solar_flux/kurudz_1.0nm.dat

## rte_solver disort

## mol_abs_param lowtran

## deltam on

## number_of_streams 6

## wavelength 290 900

## day_of_year 287

## altitude 0.012

## albedo_library IGBP

## brdf_rpv_type 5

## mol_modify 03 288 DU

## mol_modify H2O 10 MM

## sza 69.4662

## sur_temperature 273

```

We give two additional examples, which will most likely need some adjustment by users, as these are for output from libRadtran post-processed to add additional information. These are included in the package because myself and collaborators use these formats heavily. In fact users could develop shell scripts or Perl scripts using the same output format.

4.3 Output enriched with time and date data

In this case the file to be read is similar as above, but including separate columns for direct and diffuse components of the spectral energy irradiance. In addition two columns, one with date strings in ISO format and one with times have been added. The file instead of containing a single spectrum, contains several spectra in long form.

The first few lines of the file look like this:

```
290.000 2015-05-19 11_00_00 0.000000e+00 0.000000e+00
```



```

291.000 2015-05-19 11_00_00 0.000000e+00 0.000000e+00
292.000 2015-05-19 11_00_00 0.000000e+00 0.000000e+00
293.000 2015-05-19 11_00_00 1.893645e-05 3.439497e-05
294.000 2015-05-19 11_00_00 1.648530e-04 2.764368e-04
...

```

A function is included for reading data saved in a text file in this format. It also automatically converts $\text{mW m}^{-2} \text{nm}^{-1}$ into $\text{W m}^{-2} \text{nm}^{-1}$.

```

uvspec.multi.file <-
  system.file("extdata", "uvspec-multi.dat",
             package = "photobiologyInOut", mustWork = TRUE)
lbr.multi.spct <- read_uvspec_disort_vesa(uvspec.multi.file)
print(lbr.multi.spct, n = 5)

## Object: source_spct [3,055 x 5]
## containing 5 spectra in long form
## Wavelength range 290 to 900 nm, step 1 nm
## Label: libRadtran spectral simulation File: uvspec-multi.dat
## Measured on 2015-05-19 11:00:00 UTC
## Measured on 2015-05-19 11:01:00 UTC
## Measured on 2015-05-19 11:02:00 UTC
## Measured on 2015-05-19 11:03:00 UTC
## Measured on 2015-05-19 11:04:00 UTC
## Time unit 1s
##
## # A tibble: 3,055 × 5
##   w.length      datetime s.e.irrad.dir
##   <dbl>          <dtm>    <dbl>
## 1     290 2015-05-19 11:00:00 0.000000e+00
## 2     291 2015-05-19 11:00:00 0.000000e+00
## 3     292 2015-05-19 11:00:00 0.000000e+00
## 4     293 2015-05-19 11:00:00 1.893645e-11
## 5     294 2015-05-19 11:00:00 1.648530e-10
## # ... with 3,050 more rows, and 2 more variables:
## #   s.e.irrad.diff <dbl>, s.e.irrad <dbl>

```

4.4 Scripts developed by Anders Lindfors

Functions `read_fmi_cum` and `read_m_fmi_cum` can be used to read text files output by a simulation model of solar spectral irradiance. The model was developed at the Finnish Meteorological Institute (FMI) by Dr. Anders Lindfors and collaborators and uses functions from 'libRadtran' as its engine, but saves some additional metadata to the output file.

The first few lines of the file look like this:

```

# date number_of_scans start_scan stop_scan max_time_gap max_sza_gap warnings
# 20140821 15 3:30:00 17:30:00 60 7.4
# wavelength exposure(J/m2/nm)
2900 0.00000000e+00
2910 2.93132235e-05
2920 7.23526379e-04
...

```

We can read an individual file into a `source_spct` object while adding some metadata read from the file header. In this case values are for daily global spectral energy exposures rather than irradiances. Wavelengths are expressed in Angstroms instead of nanometres.

```
fmi.file <-
  system.file("extdata", "2014-08-21_cum.hel",
             package = "photobiologyInOut", mustWork = TRUE)
z.spct <- read_fmi_cum(fmi.file)
class_spct(z.spct)

## [1] "source_spct" "generic_spct"

getWhenMeasured(z.spct)

## [1] "2017-03-20 01:09:54 UTC"

z.spct

## Object: source_spct [511 x 2]
## Wavelength range 290 to 800 nm, step 1 nm
## Label: File: 2014-08-21_cum.hel
## Measured on 2017-03-20 01:09:54 UTC
## Time unit 86400s (~1 days)
##
## # A tibble: 511 × 2
##   w.length      s.e.irrad
##   <dbl>         <dbl>
## 1      290 0.000000e+00
## 2      291 2.931322e-05
## 3      292 7.235264e-04
## # ... with 508 more rows
```

With function `read_m_fmi_cum` with an “m” in the name we can read several files each containing a single spectrum. The returned object is a collection of source spectra.

```
fmi.files <-
  system.file("extdata", c("2014-08-21_cum.hel", "2014-08-21_cum.hel"),
             package = "photobiologyInOut", mustWork = TRUE)
z.mspct <- read_m_fmi_cum(fmi.files)
class(z.mspct)

## [1] "source_mspct" "generic_mspct" "list"

getWhenMeasured(z.mspct)

## # A tibble: 1 × 2
##       spct.idx      when.measured
##       <fctr>         <dtm>
## 1 2014_08_21_cum.hel 2017-03-20 01:09:54

z.mspct

## Object: source_mspct [1 x 1]
```

```
## --- Member: 2014_08_21_cum.hel ---
## Object: source_spct [511 x 2]
## Wavelength range 290 to 800 nm, step 1 nm
## Label: File: 2014-08-21_cum.hel
## Measured on 2017-03-20 01:09:54 UTC
## Time unit 86400s (~1 days)
##
## # A tibble: 511 × 2
##   w.length   s.e.irrad
##   <dbl>       <dbl>
## 1     290 0.000000e+00
## 2     291 2.931322e-05
## 3     292 7.235264e-04
## # ... with 508 more rows
##
## --- END ---
```

Above we gave the names of the files explicitly, but as we show here, one can build on-the-fly a list of file names matching some pattern. The example below is not run, as the location of example files may vary. The string "." should be replaced with the path to the folder where the files to be read are located.

```
fmi.files <- list.files(".", "*cum.hel")
fmi.files <- paste(".", fmi.files, sep = ".")
z1.mspct <- read_m_fmi_cum(fmi.files)
class(z1.mspct)
getWhenMeasured(z1.mspct)
z1.mspct
```

One also add a geocode at the time of import (or later).

```
z2.mspct <-
  read_m_fmi_cum(fmi.files,
    geocode = geocode("Kumpula, Helsinki, Finland",
      source = "google"))
class(z2.mspct)

## [1] "source_mspct" "generic_mspct" "list"

getWhenMeasured(z2.mspct)

## # A tibble: 1 × 2
##   spct.idx   when.measured
##   <fctr>       <dtm>
## 1 2014_08_21_cum.hel 2017-03-20 01:09:54

getWhereMeasured(z2.mspct)

## # A tibble: 1 × 3
##   spct.idx   lon   lat
##   <fctr>   <dbl> <dbl>
## 1 2014_08_21_cum.hel 24.96474 60.20911

z2.mspct
```

```
## Object: source_mspct [1 x 1]
## --- Member: 2014_08_21_cum.hel ---
## Object: source_spct [511 x 2]
## Wavelength range 290 to 800 nm, step 1 nm
## Label: File: 2014-08-21_cum.hel
## Measured on 2017-03-20 01:09:54 UTC
## Measured at 60.2091078 N, 24.9647354 E
## Time unit 86400s (~1 days)
##
## # A tibble: 511 x 2
##   w.length      s.e.irrad
##   <dbl>          <dbl>
## 1      290 0.000000e+00
## 2      291 2.931322e-05
## 3      292 7.235264e-04
## # ... with 508 more rows
##
## --- END ---
```

5 Online public repositories of spectral data

5.1 FReD Floral Reflectance Database

The files downloaded from FReD do not contain a header, but the first column indicates the flower ID.

```
157, 300, 0.0627119
157, 301, 0.0654036
157, 302, 0.0677941
157, 303, 0.0670396
...
```

```
fred.file <-
  system.file("extdata", "FReDflowerID_157.csv",
             package = "photobiologyInOut", mustWork = TRUE)
fred.spct <- read_FReD_csv(file = fred.file,
                        label = "Gazania heterochaeta",
                        geocode = data.frame(lat = -28.8751, lon = 17.2293))

## Parsed with column specification:
## cols(
##   flower.id = col_integer(),
##   w.length = col_integer(),
##   Rfr = col_double()
## )
```

In this case as there is no metadata present in the file, it needs to be supplied by the user.

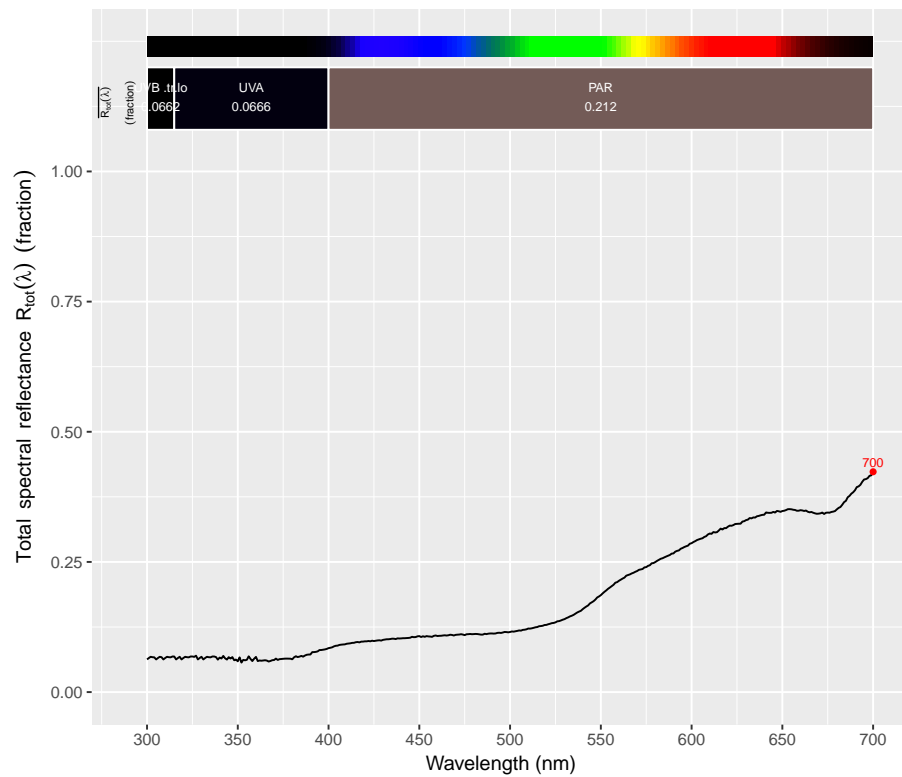
```
fred.spct
```

```
## Object: reflector_spct [401 x 3]
## Wavelength range 300 to 700 nm, step 1 nm
## Label: File: FReDflowerID_157.csv Gazania heterochaeta
## Measured at -28.8751 N, 17.2293 E
##
## # A tibble: 401 x 3
##   flower.id w.length      Rfr
##   <int>     <int>     <dbl>
## 1      157       300 0.0627119
## 2      157       301 0.0654036
## 3      157       302 0.0677941
## # ... with 398 more rows

cat(comment(fred.spct))

## FReD file 'FReDflowerID_157.csv' imported on 2017-03-20 01:10:30 UTC

plot(fred.spct)
```



5.2 ASTER spectral database

The files downloaded from ASTER contain a 25-lines-long header, but at the moment only the first field is decoded, as the whole header copied as a comment.

Name: Dry grass
 Type: Vegetation
 Class: Grasses
 Subclass: Dry grass
 Particle Size: Solid
 Sample No.: drygrass.doc
 Owner: JHU
 Wavelength Range: All
 Origin: The entire spectral range was measured at Johns Hopkins University.

Description: Dry grass. Spectra were assembled from two segments; the bidirectional VNIR and SWIR comprising segment one, and the hemispherical MWIR and TIR comprising segment two. The VNIR/SWIR spectrum was measured in the laboratory at JHU with a GER IRIS Mark IV, using a large piece of sod. The grass was illuminated from directly above and measured at a reflectance angle of 60 degrees to avoid viewing the thatch.
 Measurement: Bidirectional and directional hemispherical reflectance.
 First Column: X
 Second Column: Y
 X Units: Wavelength (micrometers)
 Y Units: Reflectance (percent)
 First X Value: 0.38049
 Last X Value: 14.011
 Number of X Values: 2559
 Additional Information: None.

0.38049 14.249
 0.38299 14.251
 0.38544 14.546
 0.38791 14.694
 ...

```

aster.file <-
  system.file("extdata", "drygrass-spectrum.txt",
             package = "photobiologyInOut", mustWork = TRUE)
aster.spct <- read_ASTER_txt(file = aster.file)
  
```

The label and comment are set from the file header.

```

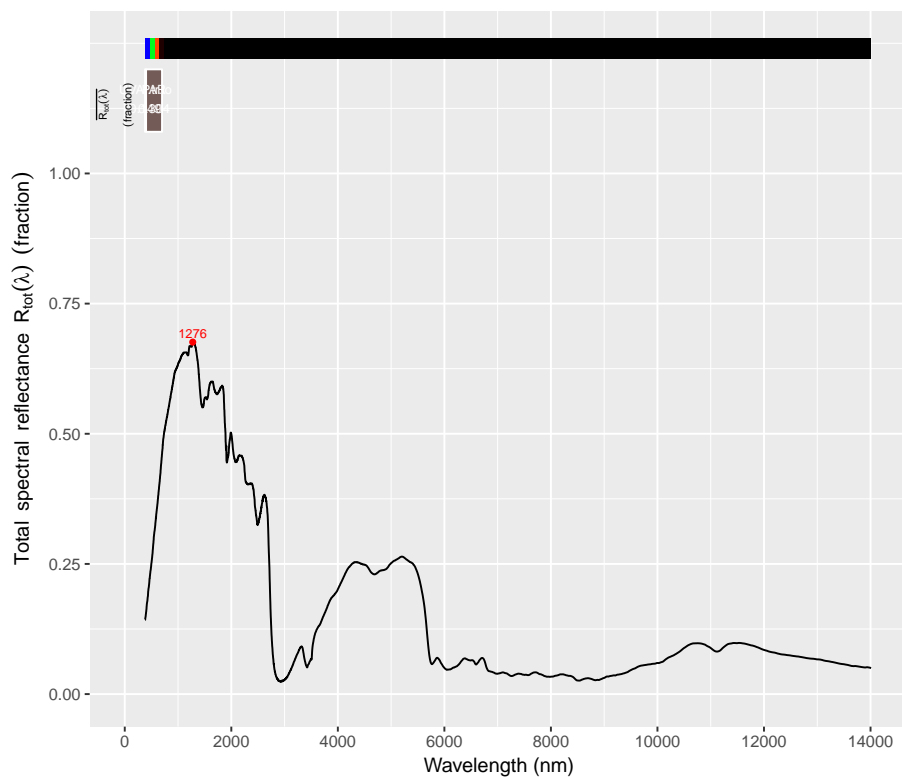
aster.spct

## Object: reflector_spct [2,559 x 2]
## Wavelength range 380.49 to 14011 nm, step 0.8 to 38 nm
## Label: Dry grass
##
##
## # A tibble: 2,559 × 2
##   w.length      Rfr
##   <dbl>    <dbl>
## 1   380.49  0.14249
## 2   382.99  0.14251
## 3   385.44  0.14546
## # ... with 2,556 more rows

cat(comment(aster.spct))
  
```

```
## ASTER database file 'drygrass-spectrum.txt' imported on 2017-03-20 01:10:30 UTC
## Name: Dry grass
## Type: Vegetation
## Class: Grasses
## Subclass: Dry grass
## Particle Size: Solid
## Sample No.: drygrass.doc
## Owner: JHU
## Wavelength Range: All
## Origin: The entire spectral range was measured at Johns Hopkins University.
## Description: Dry grass. Spectra were assembled from two segments; the
## bidirectional VNIR and SWIR comprising segment one, and the hemispherical
## MWIR and TIR comprising segment two. The VNIR/SWIR spectrum was
## measured in the laboratory at JHU with a GER IRIS Mark IV, using a large piece
## of sod. The grass was illuminated from directly above and measured at a
## reflectance angle of 60 degrees to avoid viewing the thatch.
## Measurement: Bidirectional and directional hemispherical reflectance.
## First Column: X
## Second Column: Y
## X Units: Wavelength (micrometers)
## Y Units: Reflectance (percent)
## First X Value: 0.38049
## Last X Value: 14.011
## Number of X Values: 2559
## Additional Information: None.
##

plot(aster.spct)
```



6 Other R packages

A general way of exchanging data with other R packages or for use with base R functions is to create a matrix from a collection of spectra, or a collection of spectra from a matrix. However, a matrix is only guaranteed to contain numeric data and a "dim" attribute.

6.1 From R matrix

Spectral data can be stored in a matrix either by row or by column, and the user must supply this information explicitly. We also assume, that wavelengths are not stored as part of the matrix, and so the user needs to supply these values as a separate vector.

We here use artificial data, in this first example with spectra saved by column.

```
x <- matrix(1:100, ncol = 2)
wl <- 501:550 # in nanometres
z <- mat2mspct(x, wl, "filter_spct", "Tpc")
z
```



```
## Object: filter_mspct [1 x 2]
## --- Member: spct_1 ---
## Object: filter_spct [50 x 2]
## Wavelength range 501 to 550 nm, step 1 nm
##
## # A tibble: 50 × 2
##   w.length  Tfr
##   <dbl> <dbl>
## 1     501  0.01
## 2     502  0.02
## 3     503  0.03
## # ... with 47 more rows
## --- Member: spct_2 ---
## Object: filter_spct [50 x 2]
## Wavelength range 501 to 550 nm, step 1 nm
##
## # A tibble: 50 × 2
##   w.length  Tfr
##   <dbl> <dbl>
## 1     501  0.51
## 2     502  0.52
## 3     503  0.53
## # ... with 47 more rows
##
## --- END ---
```

In this second example we supply explicit names for the spectra.

```
z <- mat2mspct(x, wl, "filter_spct", "Tpc", spct.names = c("A", "B"))
z

## Object: filter_mspct [1 x 2]
## --- Member: A ---
## Object: filter_spct [50 x 2]
## Wavelength range 501 to 550 nm, step 1 nm
##
## # A tibble: 50 × 2
##   w.length  Tfr
##   <dbl> <dbl>
## 1     501  0.01
## 2     502  0.02
## 3     503  0.03
## # ... with 47 more rows
## --- Member: B ---
## Object: filter_spct [50 x 2]
## Wavelength range 501 to 550 nm, step 1 nm
##
## # A tibble: 50 × 2
##   w.length  Tfr
##   <dbl> <dbl>
## 1     501  0.51
## 2     502  0.52
## 3     503  0.53
## # ... with 47 more rows
##
## --- END ---
```

There is no change in the call for data stored by row. To demonstrate this, we create a new matrix, with the same data as above, but stored by row, as some other packages do.

```
xrow <- matrix(1:100, nrow = 2, byrow = TRUE)
z1 <- mat2mspct(xrow, wl, "filter_spct", "Tpc")
z1

## Object: filter_mspct [1 x 2]
## --- Member: spct_1 ---
## Object: filter_spct [50 x 2]
## Wavelength range 501 to 550 nm, step 1 nm
##
## # A tibble: 50 × 2
##   w.length Tfr
##   <dbl> <dbl>
## 1     501  0.01
## 2     502  0.02
## 3     503  0.03
## # ... with 47 more rows
## --- Member: spct_2 ---
## Object: filter_spct [50 x 2]
## Wavelength range 501 to 550 nm, step 1 nm
##
## # A tibble: 50 × 2
##   w.length Tfr
##   <dbl> <dbl>
## 1     501  0.51
## 2     502  0.52
## 3     503  0.53
## # ... with 47 more rows
##
## --- END ---
```

There is only one case when an explicit argument for `byrow` is needed: square matrices (same number of spectra as of wavelength values in each spectrum).

6.2 To R matrix

In this case, the metadata contained in the individual spectral objects is discarded, and only the `"comment"` attribute of the collection of spectra copied to the returned object. The wavelength values are preserved in an attribute named `"w.length"`, but are not included as part of the matrix.

```
z2c.mat <- mspct2mat(z2.mspct, "s.e.irrad")
class(z2c.mat)

## [1] "matrix"

dim(z2c.mat)

## [1] 511 1

head(dimnames(z2c.mat)$spct)
```

```
## [1] "2014_08_21_cum.hel"

head(dimnames(z2c.mat)$w.length)

## [1] "290" "291" "292" "293" "294" "295"

head(attr(z2c.mat, "w.length"))

## [1] 290 291 292 293 294 295
```

Collections of spectra have a `spct.byrow` attribute but it is discarded as it describes dimensions would require spectral data to be stored in a three dimensional array and cannot be mapped to a matrix. The argument `byrow` in the conversion function has the same meaning as in the `matrix` constructor function.

```
z2r.mat <- mspct2mat(z2.mspect, "s.e.irrad", byrow = TRUE)
class(z2r.mat)

## [1] "matrix"

dim(z2r.mat)

## [1] 1 511

head(dimnames(z2r.mat)$spct)

## [1] "2014_08_21_cum.hel"

head(dimnames(z2r.mat)$w.length)

## [1] "290" "291" "292" "293" "294" "295"

head(attr(z2r.mat, "w.length"))

## [1] 290 291 292 293 294 295
```

These functions are not fully automatic, the user needs to provide the name of the variable to extract from each spectrum. If the wavelength values are not consistent among spectra, only those with the same values as the first spectrum in the collection are retained and the remaining ones dropped with a warning.

6.3 To ‘hyperSpec’

Can export to ‘`hyperSpec`’ objects only collections of spectra where all members have identical `w.length` vectors, as objects of class `hyperSpec` store a single vector of wavelengths for the whole collection of spectra.

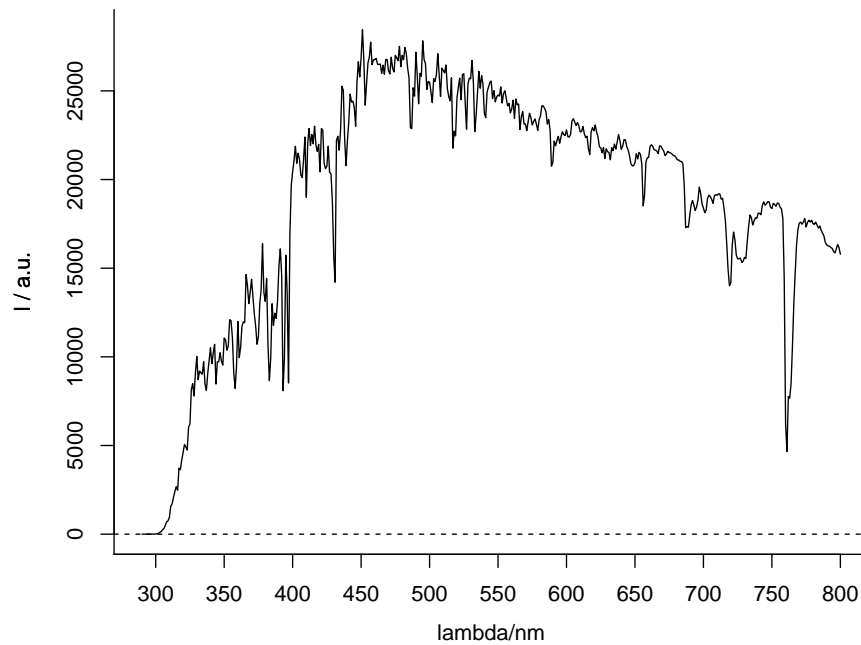
```
z2.hspct <- mspct2hyperSpec(z2.mspect, "s.e.irrad")

## Warning in .local(.Object, ...): Spectra in data are overwritten by argument spc.

class(z2.hspct)
```

```
## [1] "hyperSpec"
## attr(,"package")
## [1] "hyperSpec"

plot(z2.hspct)
```



6.4 From ‘hyperSpec’

Can import only data with wavelength in nanometres. Other quantities and units are not supported by the ‘photobiology’ classes for spectral data. See package ‘hyperSpec’ vignette “laser” for details on the data and the conversion of the original wavelength units into nanometres.

```
class(laser)

## [1] "hyperSpec"
## attr(,"package")
## [1] "hyperSpec"

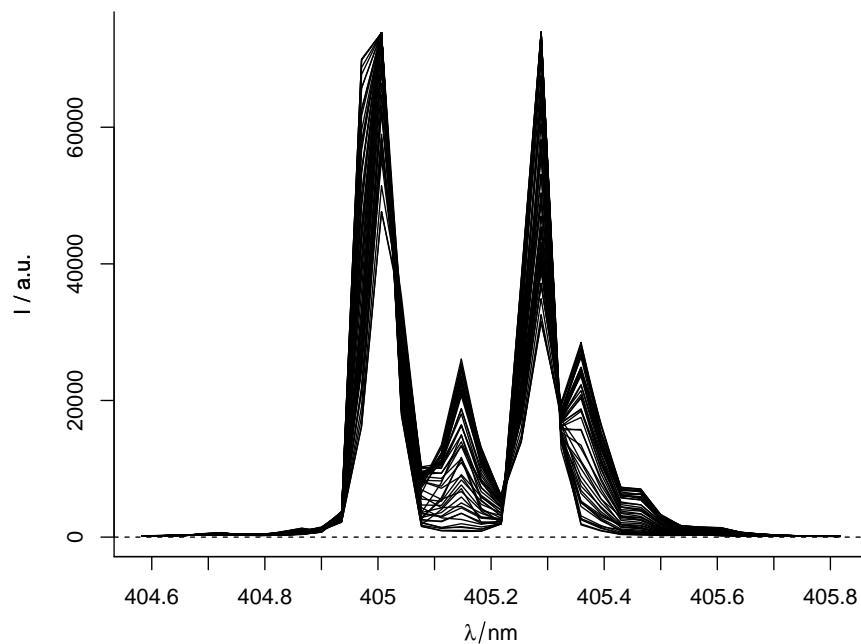
laser

## hyperSpec object
## 84 spectra
```

```
##      2 data columns
##      36 data points / spectrum
## wavelength: lambda/nm [numeric] 404.5828 404.6181 ... 405.8176
## data: (84 rows x 2 columns)
##      1. t: t / s [numeric] 0 2 ... 5722
##      2. spc: I / a.u. [matrix36] 164.650 179.724 ... 112.086

plot(laser)

## Warning in plotspc(x, ...): Number of spectra exceeds spc.nmax. Only the first
50 are plotted.
```



We assume here, that the quantity for the spectral emission of the laser is spectral *energy* irradiance, expressed in $\text{mW m}^{-2} \text{nm}^{-1}$. This is likely to be wrong but for the sake of showing how the conversion takes place is irrelevant. The parameter `multiplier` can be passed a numeric argument to rescale the original data. The default multiplier is 1.

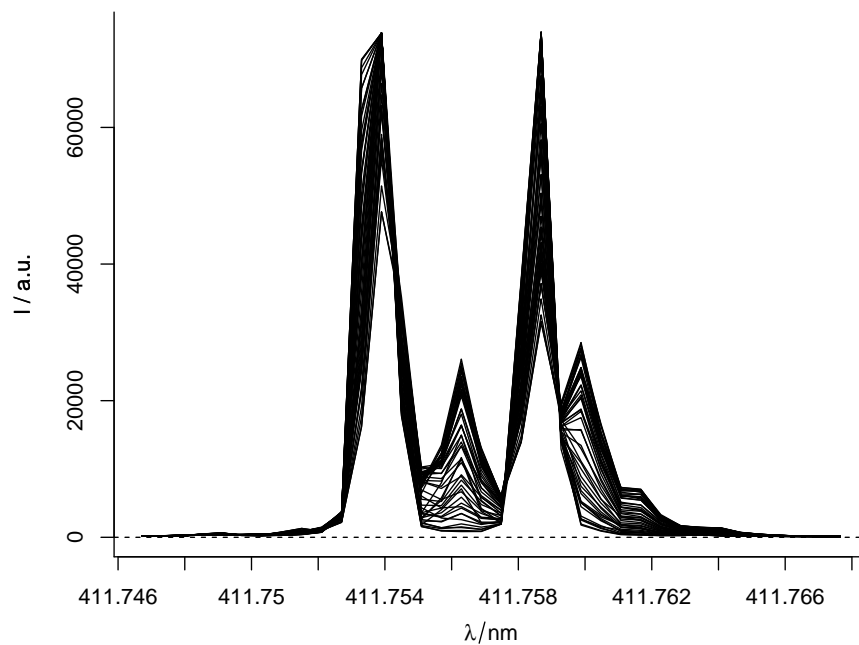
```
wl(laser) <- list (
  wl = 1e7 / (1/405e-7 - wl (laser)),
  label = expression (lambda / nm)
)
laser
## hyperSpec object
```

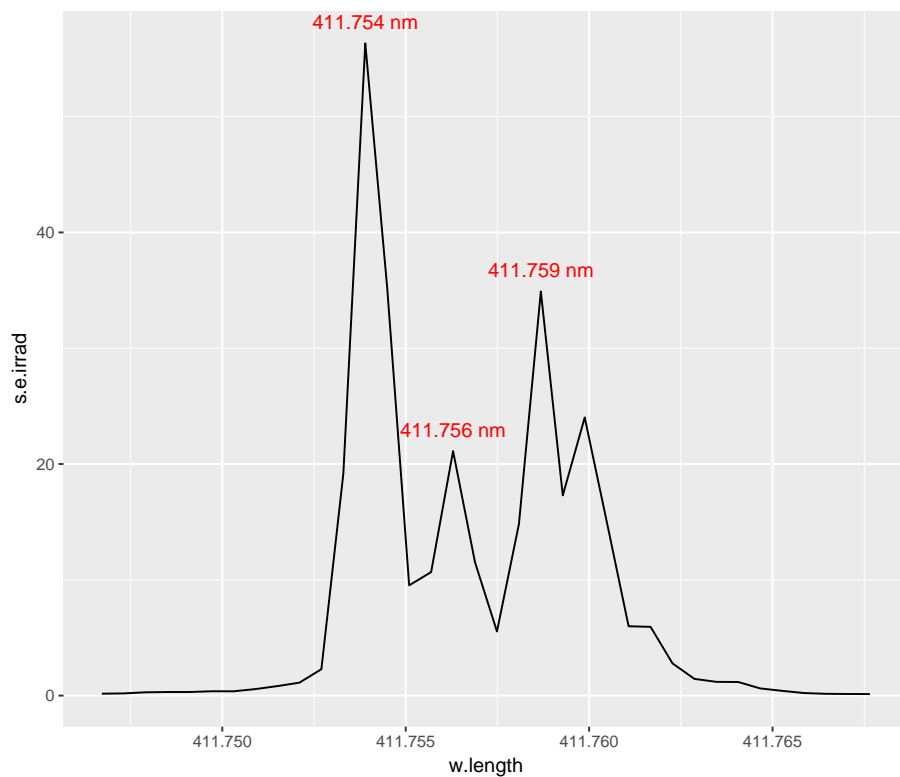
```
##      84 spectra
##      2 data columns
##      36 data points / spectrum
## wavelength: lambda/nm [numeric] 411.7467 411.7473 ... 411.7677
## data: (84 rows x 2 columns)
##      1. t: t / s [numeric] 0 2 ... 5722
##      2. spc: I / a.u. [matrix36] 164.650 179.724 ... 112.086

plot(laser)

## Warning in plotspc(x, ...): Number of spectra exceeds spc.nmax. Only the first
## 50 are plotted.

laser.mspct <-
  hyperSpec2mspct(laser, "source_spect", "s.e.irrad", multiplier = 1e-3)
ggplot(laser.mspct[[1]]) +
  geom_line() +
  stat_peaks(geom = "text", vjust = -1, label.fmt = "%.6g nm", color = "red")
```





6.5 From ‘colorSpec’

```
fluorescent.mspct <- colorSpec2mspct(Fs.5nm)
print(fluorescent.mspct, n = 3, n.members = 3)

## Object: source_mspct [12 x 1]
## --- Member: F1 ---
## Object: source_spct [81 x 2]
## Wavelength range 380 to 780 nm, step 5 nm
## Time unit is
##
## # A tibble: 81 x 2
##   w.length s.e.irrad
##   <dbl>     <dbl>
## 1     380       1.87
## 2     385       2.36
## 3     390       2.94
## # ... with 78 more rows
## --- Member: F2 ---
## Object: source_spct [81 x 2]
## Wavelength range 380 to 780 nm, step 5 nm
## Time unit is
##
## # A tibble: 81 x 2
```

```
##   w.length s.e.irrad
##   <dbl>     <dbl>
## 1     380     1.18
## 2     385     1.48
## 3     390     1.84
## # ... with 78 more rows
## --- Member: F3 ---
## Object: source_spct [81 x 2]
## Wavelength range 380 to 780 nm, step 5 nm
## Time unit 1s
##
## # A tibble: 81 × 2
##   w.length s.e.irrad
##   <dbl>     <dbl>
## 1     380     0.82
## 2     385     1.02
## 3     390     1.26
## # ... with 78 more rows
## .....
## 9 other member spectra not shown
##
## --- END ---
```

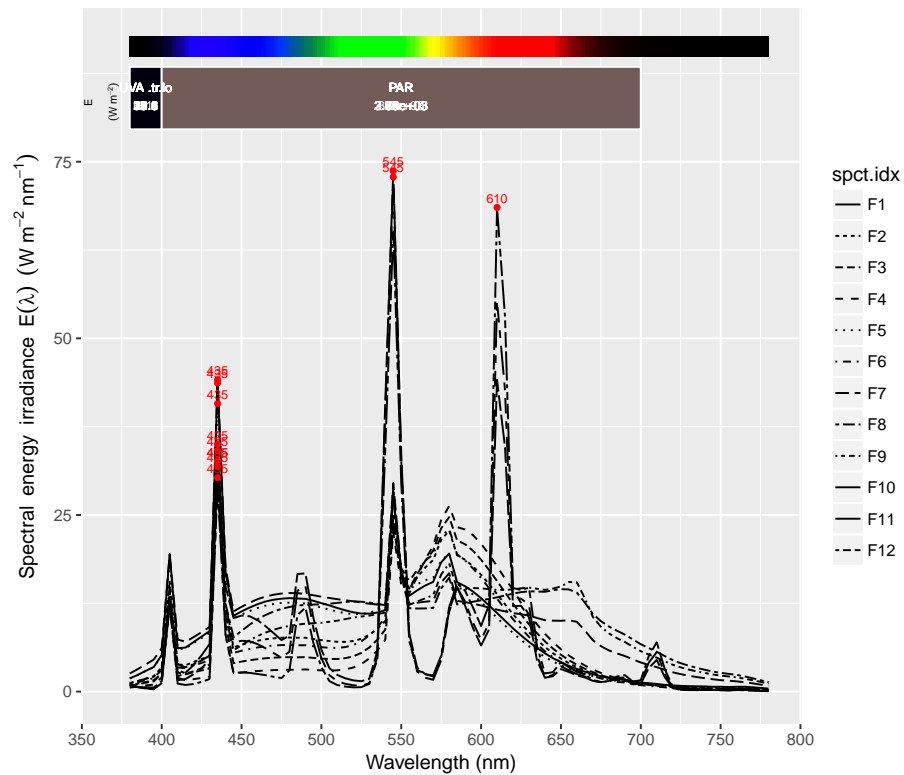
```
colorSpec2mspct(Hoya)

## Object: filter_mspct [4 x 1]
## --- Member: R-60 ---
## Object: filter_spct [46 x 2]
## Wavelength range 300 to 750 nm, step 10 nm
##
## # A tibble: 46 × 2
##   w.length Tfr
##   <dbl> <dbl>
## 1     300     0
## 2     310     0
## 3     320     0
## # ... with 43 more rows
## --- Member: G-533 ---
## Object: filter_spct [46 x 2]
## Wavelength range 300 to 750 nm, step 10 nm
##
## # A tibble: 46 × 2
##   w.length Tfr
##   <dbl> <dbl>
## 1     300     0
## 2     310     0
## 3     320     0
## # ... with 43 more rows
## --- Member: B-440 ---
## Object: filter_spct [46 x 2]
## Wavelength range 300 to 750 nm, step 10 nm
##
## # A tibble: 46 × 2
##   w.length Tfr
##   <dbl> <dbl>
## 1     300     0
```



```
## 2      310      0
## 3      320      0
## # ... with 43 more rows
## --- Member: LB-120 ---
## Object: filter_spct [46 x 2]
## Wavelength range 300 to 750 nm, step 10 nm
##
## # A tibble: 46 x 2
##   w.length    Tfr
##   <dbl>    <dbl>
## 1      300 0.00003
## 2      310 0.00580
## 3      320 0.08100
## # ... with 43 more rows
##
## --- END ---
```

```
fluorescent.spct <- colorSpec2spct(Fs.5nm)
plot(fluorescent.spct) + aes(linetype = spct.idx)
```

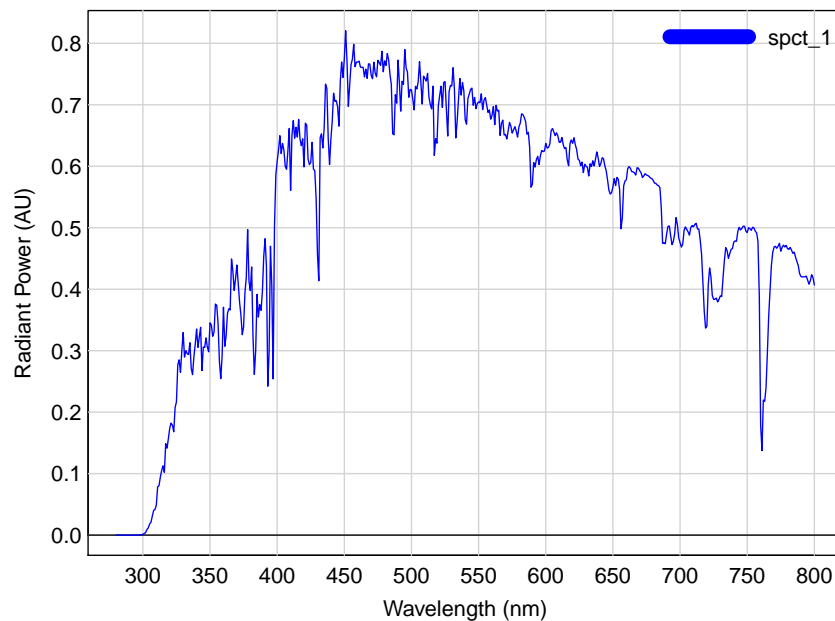


```
colorSpec2chroma_spct(xyz1931.5nm)
## Object: chroma_spct [81 x 4]
```

```
## Wavelength range 380 to 780 nm, step 5 nm
##
## # A tibble: 81 × 4
##   x     y     z w.length
## * <dbl> <dbl> <dbl>   <dbl>
## 1 0.0014 0e+00 0.0065     380
## 2 0.0022 1e-04 0.0105     385
## 3 0.0042 1e-04 0.0201     390
## # ... with 78 more rows
```

6.6 To ‘colorSpec’

```
sun.cspect <- spct2colorSpec(sun.spct)
plot(sun.cspect, col = "blue")
```



```
spct2colorSpec(yellow_gel.spct)

##
## colorSpec object. The organization is 'vector'. Object size is 11488 bytes.
## the object describes 1 transparent materials, and the quantity is 'transmittance'.
## Wavelength range: 190 to 800 nm. Step size is 1 nm.
##
```

```
## 1 spectra
## 611 data points / spectrum
##
##   Material   Min    Max LambdaMax Integral
## 1   spct_1 1e-05 0.9025    768.5 260.3194

chroma_spct2colorSpec(beesxyzCMF.spct)

##
## colorSpec object. The organization is 'matrix'. Object size is 4128 bytes.
## the object describes a responder to light with 3 output channels, and the quantity is 'power->neural'.
## Wavelength range: 300 to 700 nm. Step size is 5 nm.
##
## 3 spectra
## 81 data points / spectrum
##
##   Channel   Min Max LambdaMax E.response
## 1       x 0.000  1    340    68.965
## 2       y 0.000  1    435   103.850
## 3       z 0.006  1    560   135.620
```

6.7 From ‘pavo’

In this example we convert an `rspec` object from package ‘pavo’ into a collection of spectra and then we plot it with `ggplot` methods from package ‘ggspectra’ (an extension to ‘ggplot2’). The data are the spectral reflectance of the plumage from seven different individual birds of the same species, measured in three different body parts.

```
data(sicalis)
class(sicalis)

## [1] "rspec"      "data.frame"

names(sicalis)

## [1] "w1"      "ind1.C" "ind1.T" "ind1.B" "ind2.C"
## [6] "ind2.T" "ind2.B" "ind3.C" "ind3.T" "ind3.B"
## [11] "ind4.C" "ind4.T" "ind4.B" "ind5.C" "ind5.T"
## [16] "ind5.B" "ind6.C" "ind6.T" "ind6.B" "ind7.C"
## [21] "ind7.T" "ind7.B"
```

We convert the data into a collection of spectra, and calculate summaries for three spectra.

```
sicalis.mspect <- rspec2mspect(sicalis, "reflector_spct", "Rpc")
summary(sicalis.mspect[[1]])

## Summary of object: reflector_spct [401 x 2]
## Wavelength range 300 to 700 nm, step 1 nm
##
##   w.length      Rfr
```

```
## Min. :300 Min. :0.001798
## 1st Qu.:400 1st Qu.:0.008288
## Median :500 Median :0.031709
## Mean :500 Mean :0.052848
## 3rd Qu.:600 3rd Qu.:0.098775
## Max. :700 Max. :0.114807

summary(sicalis.mspct[[2]])

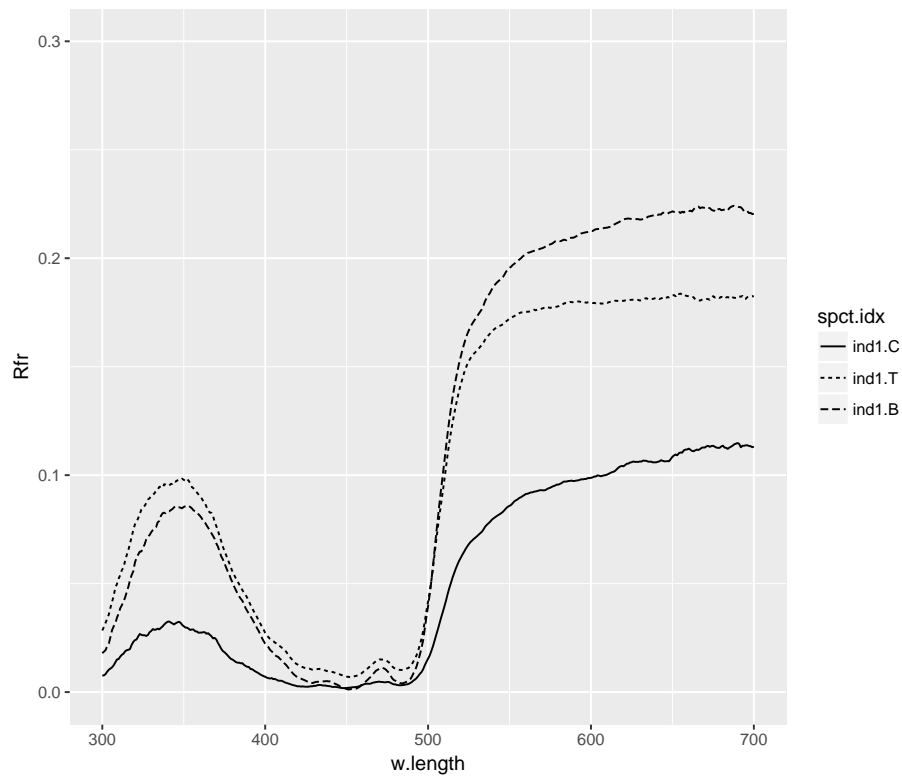
## Summary of object: reflector_spct [401 x 2]
## Wavelength range 300 to 700 nm, step 1 nm
##
##      w.length      Rfr
## Min. :300 Min. :0.006783
## 1st Qu.:400 1st Qu.:0.030112
## Median :500 Median :0.096994
## Mean :500 Mean :0.105449
## 3rd Qu.:600 3rd Qu.:0.179691
## Max. :700 Max. :0.183823

summary(sicalis.mspct[[3]])

## Summary of object: reflector_spct [401 x 2]
## Wavelength range 300 to 700 nm, step 1 nm
##
##      w.length      Rfr
## Min. :300 Min. :0.001191
## 1st Qu.:400 1st Qu.:0.022293
## Median :500 Median :0.085235
## Mean :500 Mean :0.116253
## 3rd Qu.:600 3rd Qu.:0.212554
## Max. :700 Max. :0.224162
```

We convert the subset of the collection corresponding to the first individual into a single spectra object for plotting with `ggplot`.

```
ggplot(rbindspct(sicalis.mspct[1:3])) +
  aes(linetype = spct.idx) +
  ylim(0,0.3) +
  geom_line()
```



Here we extract the “crown” data from all individuals and plot these spectra in a single plot.

```
print(sicalis.mspct[c(TRUE, FALSE, FALSE)])

## Object: reflector_mspct [7 x 1]
## --- Member: ind1.C ---
## Object: reflector_spct [401 x 2]
## Wavelength range 300 to 700 nm, step 1 nm
##
## # A tibble: 401 x 2
##   w.length      Rfr
##   <dbl>      <dbl>
## 1     300 0.007594984
## 2     301 0.007727841
## 3     302 0.008288000
## # ... with 398 more rows
## --- Member: ind2.C ---
## Object: reflector_spct [401 x 2]
## Wavelength range 300 to 700 nm, step 1 nm
##
## # A tibble: 401 x 2
##   w.length      Rfr
##   <dbl>      <dbl>
## 1     300 0.002971167
## 2     301 0.002326722
```

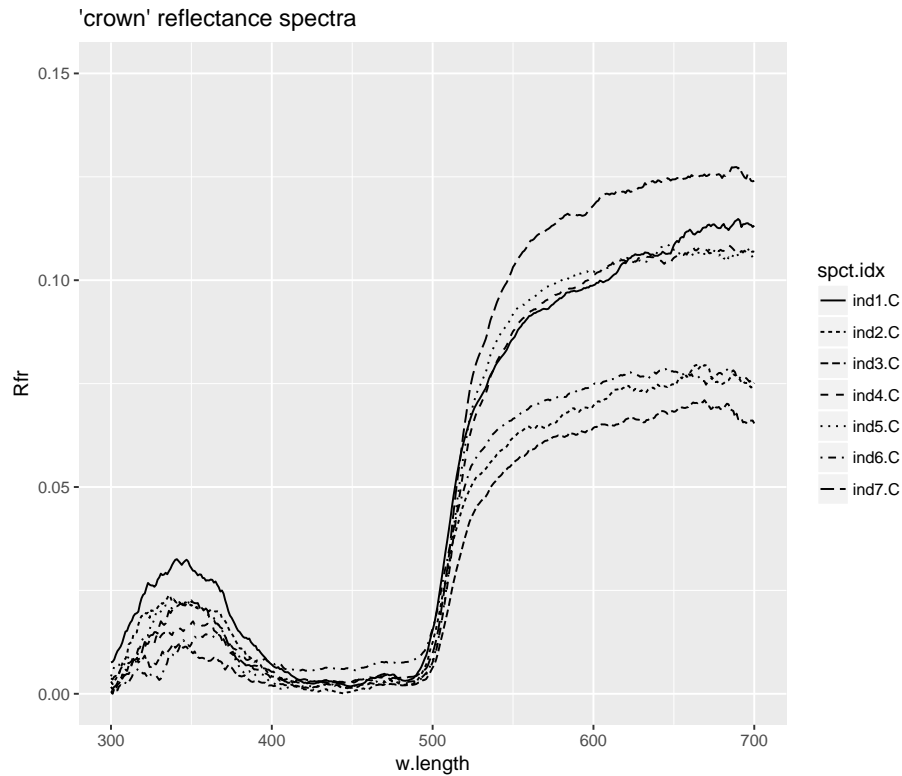
```

## 3      302 0.003227833
## # ... with 398 more rows
## --- Member: ind3.C ---
## Object: reflector_spct [401 x 2]
## Wavelength range 300 to 700 nm, step 1 nm
##
## # A tibble: 401 × 2
##   w.length      Rfr
##   <dbl>      <dbl>
## 1      300 0.0005947619
## 2      301 0.0000000000
## 3      302 0.0011853968
## # ... with 398 more rows
## --- Member: ind4.C ---
## Object: reflector_spct [401 x 2]
## Wavelength range 300 to 700 nm, step 1 nm
##
## # A tibble: 401 × 2
##   w.length      Rfr
##   <dbl>      <dbl>
## 1      300 0.003750159
## 2      301 0.003465714
## 3      302 0.004133333
## # ... with 398 more rows
## --- Member: ind5.C ---
## Object: reflector_spct [401 x 2]
## Wavelength range 300 to 700 nm, step 1 nm
##
## # A tibble: 401 × 2
##   w.length      Rfr
##   <dbl>      <dbl>
## 1      300 0.004225349
## 2      301 0.005361222
## 3      302 0.006554556
## # ... with 398 more rows
## --- Member: ind6.C ---
## Object: reflector_spct [401 x 2]
## Wavelength range 300 to 700 nm, step 1 nm
##
## # A tibble: 401 × 2
##   w.length      Rfr
##   <dbl>      <dbl>
## 1      300 0.0006326984
## 2      301 0.0006136508
## 3      302 0.0001934921
## # ... with 398 more rows
## --- Member: ind7.C ---
## Object: reflector_spct [401 x 2]
## Wavelength range 300 to 700 nm, step 1 nm
##
## # A tibble: 401 × 2
##   w.length      Rfr
##   <dbl>      <dbl>
## 1      300 0.001680730
## 2      301 0.001043270
## 3      302 0.001702476
## # ... with 398 more rows

```

```
##
## --- END ---

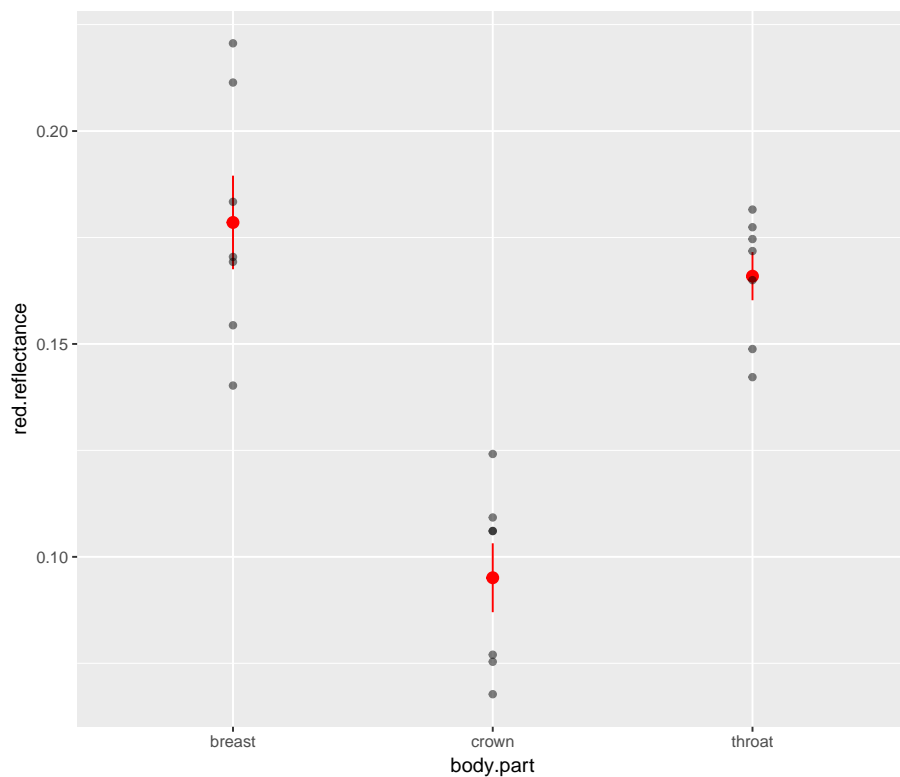
ggplot(rbindspct(sicalis.mspct[c(TRUE, FALSE, FALSE)])) +
  aes(linetype = spct.idx) +
  ylim(0,0.15) +
  geom_line() +
  ggtitle("'crown' reflectance spectra")
```



We calculate the mean reflectance in wavebands corresponding to ISO colors obtaining a data frame. We then add to this returned data frame a factor indicating the body parts.

```
refl.by.band <- reflectance(sicalis.mspct, w.band = list(Red(), Green(), Blue(), UVA()))
refl.by.band$body.part <- c("crown", "throat", "breast")
```

```
refl.red <- reflectance(sicalis.mspct, w.band = Red())
names(refl.red)[2] <- "red.reflectance"
refl.red$body.part <- c("crown", "throat", "breast")
ggplot(refl.red, aes(x = body.part, y = red.reflectance)) +
  stat_summary(fun.data = "mean_se", color = "red") +
  geom_point(alpha = 0.5)
```



7 Dealing with odd and bad data

7.1 Using locales

Most functions in this package have a parameter `locale`, that accepts `readr::locale` objects as arguments. At the moment only the time zone and decimal mark are respected. This allows files using comma for decimal marker be easily imported, or the dates and times **in the input file** be interpreted in a given time zone. Setting the correct time zone is very important to avoid errors. Time coordinates are always stored in the created objects using universal time coordinates ("UTC").

```
jaz.irrad.comma.file <-
  system.file("extdata", "spectrum-comma.JazIrrad",
              package = "photobiologyInOut", mustWork = TRUE)
my.locale <- locale(decimal_mark = ",", tz = "EET")
jaz00.spct <- read_oo_jazirrad(file = jaz.irrad.comma.file,
                              locale = my.locale)

## Parsed with column specification:
## cols(
##   W = col_double(),
```



```
## D = col_double(),
## S = col_double(),
## P = col_double()
## )
```

```
jaz00.spct

## Object: source_spct [2,048 x 2]
## Wavelength range 188.82523 to 1033.1483 nm, step 0.357056 to 0.459625 nm
## Label: File: spectrum-comma.JazIrrad
## Measured on 2015-02-03 07:44:41 UTC
## Time unit 1s
##
## # A tibble: 2,048 × 2
##   w.length s.e.irrad
##   <dbl>     <dbl>
## 1 188.8252         0
## 2 189.2849         0
## 3 189.7444         0
## # ... with 2,045 more rows
```

7.2 Overriding default metadata

We revisit now the Jaz irradiance data to show how the metadata can be changed by the user if needed (e.g. clock settings at the time of data acquisition were wrong).

A variable with the user supplied date and time data, or the date read from the header (the text itself) not the file date as the file date may not reflect the creation date and time.

```
jaz.s.irrad.file <-
  system.file("extdata", "spectrum.JazIrrad",
             package = "photobiologyInOut", mustWork = TRUE)
```

```
jaz01.spct <- read_oo_jazirrad(file = jaz.s.irrad.file,
                             date = NULL)
```

```
## Parsed with column specification:
## cols(
##   W = col_double(),
##   D = col_double(),
##   S = col_double(),
##   P = col_double()
## )
```

```
getWhenMeasured(jaz01.spct)
```

```
## [1] "2015-02-03 09:44:41 UTC"
```

```
jaz02.spct <- read_oo_jazirrad(file = jaz.s.irrad.file,
                             date = ymd_hms("2015-11-15 12:00:00"))

## Parsed with column specification:
## cols(
##   W = col_double(),
##   D = col_double(),
##   S = col_double(),
##   P = col_double()
## )

getWhenMeasured(jaz02.spct)

## [1] "2015-11-15 12:00:00 UTC"
```

```
jaz03.spct <- read_oo_jazirrad(file = jaz.s.irrad.file,
                             date = now())

## Parsed with column specification:
## cols(
##   W = col_double(),
##   D = col_double(),
##   S = col_double(),
##   P = col_double()
## )

getWhenMeasured(jaz03.spct)

## [1] "2017-03-20 01:10:38 UTC"
```

7.3 Adding additional metadata

When can add a geocode, either directly by giving latitude and longitude coordinates or by generating it from a Google maps search using function `ggmap::geocode()` as shown here.

```
jaz04.spct <- read_oo_jazirrad(file = jaz.s.irrad.file,
                             geocode = geocode("Vikki, 00790 Helsinki, Finland",
                                                source = "google"))

jaz04.spct

## Object: source_spct [2,048 x 2]
## Wavelength range 188.82523 to 1033.1483 nm, step 0.357056 to 0.459625 nm
## Label: File: spectrum.JazIrrad
## Measured on 2015-02-03 09:44:41 UTC
## Measured at 60.2251453 N, 25.0200552 E
## Time unit 1s
##
## # A tibble: 2,048 × 2
##   w.length s.e.irrad
##   <dbl>     <dbl>
## 1 188.8252     0
## 2 189.2849     0
```

```
## 3 189.7444      0
## # ... with 2,045 more rows

getWhereMeasured(jaz04.spct)

##      lon      lat
## 1 25.02006 60.22515
```