

Package ‘lightr’

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Title Read Spectrometric Data and Metadata

Version 0.1

Description Parse various reflectance/transmittance/absorbance spectra file formats to extract spectral data and metadata, as described in Gruson, White & Maia (2019) <doi:10.21105/joss.01857>.

This package has been peer-reviewed by rOpenSci (v. 0.1).

Depends R (>= 3.5.0)

Imports pbmcapply, xml2 (>= 1.0.0)

Suggests knitr, pavo, rmarkdown, spelling, testthat (>= 2.0.0)

URL <https://docs.ropensci.org/lightr>,
<https://github.com/ropensci/lightr>

BugReports <https://github.com/ropensci/lightr/issues>

License GPL (>= 2)

Encoding UTF-8

LazyData true

RoxygenNote 7.0.0

Language en-GB

VignetteBuilder knitr

NeedsCompilation no

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lr_convert_tocsv	<i>Convert spectral data files to csv files</i>
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Description

Convert spectral data files to csv files

Usage

```
lr_convert_tocsv(
  where = NULL,
  ext = "txt",
  decimal = ".",
  sep = NULL,
  subdir = FALSE,
  cores = getOption("mc.cores", 2L),
  ignore.case = TRUE,
  overwrite = FALSE
)
```

Arguments

where	Folder in which files are located (defaults to current working directory).
ext	File extension to be searched for, without the "." (defaults to txt).
decimal	Character to be used to identify decimal plates (defaults to .).
sep	Column delimiting characters to be considered in addition to the default (which are: tab, space, and ";")
subdir	Should subdirectories within the where folder be included in the search? (defaults to FALSE).
cores	Number of cores to be used. If greater than 1, import will use parallel processing (not available in Windows).
ignore.case	Should the extension search be case insensitive? (defaults to TRUE)
overwrite	logical. Should the function overwrite existing files with the same name? (defaults to FALSE).

Value

Convert input files to csv and invisibly return the list of created file paths

Warning

This step loses all metadata associated to the spectra. This metadata is critical to ensure reproducibility. We recommended you use `lr_get_metadata()` to extract this information from your raw data.

lr_get_metadata	<i>Extract metadata from spectra files</i>
-----------------	--

Description

Finds and imports metadata from spectra files in a given location.

Usage

```
lr_get_metadata(
  where = getwd(),
  ext = "ProcSpec",
  sep = NULL,
  subdir = FALSE,
  subdir.names = FALSE,
  cores = getOption("mc.cores", 2L),
  ignore.case = TRUE
)
```

Arguments

where	Folder in which files are located (defaults to current working directory).
ext	File extension to be searched for, without the "." (defaults to txt).
sep	Column delimiting characters to be considered in addition to the default (which are: tab, space, and ";")
subdir	Should subdirectories within the where folder be included in the search? (defaults to FALSE).
subdir.names	Should subdirectory path be included in the name of the spectra? (defaults to FALSE).
cores	Number of cores to be used. If greater than 1, import will use parallel processing (not available in Windows).
ignore.case	Should the extension search be case insensitive? (defaults to TRUE)

Value

A data.frame containing one file per row and the following columns:

- name: File name (without the extension)
- user: Name of the spectrometer operator
- date: Timestamp of the recording
- spec_model: Model of the spectrometer
- spec_ID: Unique ID of the spectrometer
- white_inttime: Integration time of the white reference (in ms)
- dark_inttime: Integration time of the dark reference (in ms)
- sample_inttime: Integration time of the sample (in ms)
- white_avgs: Number of averaged measurements for the white reference
- dark_avgs: Number of averaged measurements for the dark reference
- sample_avgs: Number of averaged measurements for the sample
- white_boxcar: Boxcar width for the white reference
- dark_boxcar: Boxcar width for the dark reference
- sample_boxcar: Boxcar width for the sample reference

Warning

white_inttime, dark_inttime and sample_inttime should be equal. The normalised data may be inaccurate otherwise.

References

White TE, Dalrymple RL, Noble DWA, O'Hanlon JC, Zurek DB, Umbers KDL. Reproducible research in the study of biological coloration. *Animal Behaviour*. 2015 Aug 1;106:51-7 (doi: [10.1016/j.anbehav.2015.05.007](https://doi.org/10.1016/j.anbehav.2015.05.007)).

Examples

```
lr_get_metadata(system.file("testdata", "procspec_files",  
                           package = "lightr"),  
               ext = "ProcSpec")
```

lr_get_spec

*Extract spectral data from spectra files***Description**

Finds and imports reflectance/transmittance/absorbance data from spectra files in a given location.

Usage

```
lr_get_spec(
  where = getwd(),
  ext = "txt",
  lim = c(300, 700),
  decimal = ".",
  sep = NULL,
  subdir = FALSE,
  subdir.names = FALSE,
  cores = getOption("mc.cores", 2L),
  ignore.case = TRUE
)
```

Arguments

where	Folder in which files are located (defaults to current working directory).
ext	File extension to be searched for, without the "." (defaults to txt).
lim	A vector with two numbers determining the wavelength limits to be considered (defaults to c(300, 700)).
decimal	Character to be used to identify decimal plates (defaults to .).
sep	Column delimiting characters to be considered in addition to the default (which are: tab, space, and ";")
subdir	Should subdirectories within the where folder be included in the search? (defaults to FALSE).
subdir.names	Should subdirectory path be included in the name of the spectra? (defaults to FALSE).
cores	Number of cores to be used. If greater than 1, import will use parallel processing (not available in Windows).
ignore.case	Should the extension search be case insensitive? (defaults to TRUE)

Value

A data.frame, containing the wavelengths in the first column and individual imported spectral files in the subsequent columns. Reflectance values are interpolated to the nearest wavelength integer.

Examples

```
lr_get_spec(system.file("testdata", package = "lightr"), ext = "jdx")
```

lr_parse_generic	<i>Generic function to parse spectra files that don't have a specific parser</i>
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Description

Generic function to parse spectra files that don't have a specific parser

Usage

```
lr_parse_generic(filename, decimal = ".", sep = NULL)
```

Arguments

filename	Path of the file to parse
decimal	Character to be used to identify decimal plates (defaults to .).
sep	Column delimiting characters to be considered in addition to the default (which are: tab, space, and ";")

Value

A list of two elements:

- a dataframe with columns "wl", "dark", "white", "scope" and "processed", in that order
- a list with metadata including

Examples

```
lr_parse_generic(system.file("testdata", "spec.csv", package = "lightr"),  
                 sep = ",")  
lr_parse_generic(system.file("testdata", "CRAIC_export.txt",  
                             package = "lightr"))
```

lr_parse_jaz	<i>Parse OceanOptics converted file</i>
--------------	---

Description

Parse OceanOptics converted file. <https://oceanoptics.com/>

Usage

```
lr_parse_jaz(filename)
```

```
lr_parse_jazirrad(filename)
```

Arguments

filename Path of the file to parse

Value

A list of two elements:

- a dataframe with columns "wl", "dark", "white", "scope" and "processed", in that order
- a list with metadata including

Examples

```
lr_parse_jaz(system.file("testdata", "jazspec.jaz", package = "lightr"))
lr_parse_jazirrad(system.file("testdata", "irrad.JazIrrad",
                             package = "lightr"))
```

lr_parse_jdx	<i>Parse OceanOptics JCAMP-DX (.jdx) file</i>
--------------	---

Description

Parse OceanOptics JCAMP-DX (.jdx) file. <https://oceanoptics.com/>

Usage

```
lr_parse_jdx(filename)
```

Arguments

filename Path of the file to parse

Value

A list of two elements:

- a dataframe with columns "wl", "dark", "white", "scope" and "processed", in that order
- a list with metadata including

References

McDonald RS, Wilks PA. JCAMP-DX: A Standard Form for Exchange of Infrared Spectra in Computer Readable Form. Applied Spectroscopy. 1988;42(1):151-62.

Examples

```
lr_parse_jdx(system.file("testdata", "OceanOptics.jdx", package = "lightr"))
```

lr_parse_procspec *Parse OceanOptics ProcSpec file*

Description

Parse OceanOptics ProcSpec file. <https://oceanoptics.com/>

Usage

```
lr_parse_procspec(filename)
```

Arguments

filename Path of the file to parse

Value

A list of two elements:

- a dataframe with columns "wl", "dark", "white", "scope" and "processed", in that order
- a list with metadata including

References

<https://oceanoptics.com/faq/extract-data-procspec-file-without-spectrasuite/>

Examples

```
lr_parse_procspec(system.file("testdata", "procspec_files",  
                             "OceanOptics_Linux.ProcSpec",  
                             package = "lightr"))
```

lr_parse_trm *Parse Avantes binary file*

Description

Parse Avantes binary file. <https://www.avantes.com/products/spectrometers>

Usage

```
lr_parse_trm(filename)
```

```
lr_parse_abs(filename)
```

```
lr_parse_roh(filename)
```


Arguments

filename Path of the file to parse

Value

A list of two elements:

- a dataframe with columns "wl", "dark", "white", "scope" and "processed", in that order
- a list with metadata including

Examples

```
lr_parse_trm(system.file("testdata", "avantes_trans.TRM",
                        package = "lightr"))
lr_parse_roh(system.file("testdata", "avantes_reflect.ROH",
                        package = "lightr"))
```

lr_parse_ttt *Parse Avantes converted file*

Description

Parse Avantes converted file. <https://www.avantes.com/products/spectrometers>

Usage

```
lr_parse_ttt(filename)
```

```
lr_parse_trt(filename)
```

Arguments

filename Path of the file to parse

Value

A list of two elements:

- a dataframe with columns "wl", "dark", "white", "scope" and "processed", in that order
- a list with metadata including

Examples

```
lr_parse_ttt(system.file("testdata", "avantes_export.ttt",
                        package = "lightr"))
lr_parse_trt(system.file("testdata", "avantes_export2.trt",
                        package = "lightr"))
```

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