Package 'chromr'

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Type Package

Title Read and Plot FPLC Chromatograms

Version 0.1.0

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Description For reading files from BioRad QuadTec machines and making plots of the charomatograms.

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URL https://github.com/BradyAJohnston/chromr

BugReports https://github.com/BradyAJohnston/chromr/issues

Imports dplyr, ggplot2, glue, janitor, lifecycle, magrittr, purrr, readr, rlang, scales, stringr, tibble, tidyr

Suggests covr, testthat (>= 3.0.0)

Config/testthat/edition 3

Encoding UTF-8

RoxygenNote 7.2.1

R topics documented:

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chrom_add_volume   *Add Volume Column From Time Units*

Description

Adds a column with calculated volums from the time column given a particular flow rate. Currently only constant flow rates are supported.

Usage

```
chrom_add_volume(.data, flow_rate = 0.5, time = "second")
```

Arguments

.data	Data frame or tibble with a column called 'time'.
flow_rate	Flow rate in ml/min.
time	Time unit when exported.

Value

a [tibble][tibble::tibble-package]

Examples

```
fl <- system.file(
  "extdata",
  "sec_no_volume.txt",
  package = "chromr"
)
# read just the data
dat <- fl |>
  chrom_read_quadtech()
dat
# add a volume given a constant flow rate
dat |>
  chrom_add_volume(0.3)
```

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chrom_find_data_start_line
                    Find the Line Where Data Begins

Description

Finds the line where the tabular data begins. This is then used to start the reading of the data with 'readr::read_csv()' and end the reading of the metadata.

Usage

```
chrom_find_data_start_line(file, n_lines = 50)
```

Arguments

file	File path to the file to read.
n_lines	Number of lines to search for the start of the data.

Value

Single integer of the start of the data.

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chrom_get_meta_quadtech

Reads Metadata from QuadTech Chromatogram

Description

Reads Metadata from QuadTech Chromatogram

Usage

```
chrom_get_meta_quadtech(file, start_line)
```

Arguments

file	Path to the chromatogram file.
start_line	Start of the data and thus end of the metadata. Determined with 'chromr::chrom_find_data_start_line(

Value

a [tibble][tibble::tibble-package]

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chrom_interp_volume   *Interpolate Volume from Time*

Description

Interpolates the volume column values, based on the time column values.

Usage

```
chrom_interp_volume(.data, time, volume)
```

Arguments

.data	Data frame with a volume column to be interpolated.
time	Name of the time column to use for interpolation.
volume	Name of the volumn column to interpolate along the time.

Details

Some FPLC systems don't report accurate volume data, but do report accurate timing data. This function takes the time and volume data and interpolates the otherwise constant volume data in accordance with the time points.

Value

a [tibble][tibble::tibble-package]

Examples

```
fl <- system.file(
  "extdata",
  "sec.txt",
  package = "chromr"
)

dat <- fl |>
  chrom_read_quadtech(interp_volume = FALSE)

dat

dat |>
  chrom_interp_volume(time, volume)
```

---

chrom_plot   *Plot a Chromatogram*

Description

Plot a Chromatogram

Usage

```
chrom_plot(data, channels = NULL, xlim = NULL, ylim = NULL)
```

Arguments

data	Data frame that contains columns for wavelength ('wl'), volume ('volume') and absorbance ('abs').
channels	Character vector of wavelengths to plot (e.g. c("280","260")). If none supplied, all wavelengths plotted.
xlim	Limits for the x axis.
ylim	Limits for the y axis.

Value

a 'ggplot2::ggplot()' plot.

Examples

```
fl <- system.file(
  "extdata",
  "sec_no_volume.txt",
  package = "chromr"
)

fl |>
  chrom_read_quadtech() |>
  chrom_add_volume(0.3) |>
  chrom_plot(xlim = c(0, 3), ylim = c(NA, 0.01))
```

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chrom_read_ngc   *Read .csv Chromatogram from the BioRad NGC*

Description

Read .csv Chromatogram from the BioRad NGC

Usage

```
chrom_read_ngc(file, skip = 1)
```

Arguments

file   File path to the '.csv' file.

skip   Number of lines to skip before begin reading. Usually 1 line.

Value

a [tibble][tibble::tibble-package]

Examples

```
fl <- system.file(
  "extdata",
  "ngc_sec.csv",
  package = "chromr"
)

dat <- chrom_read_ngc(fl)
dat
```

chrom_read_quadtech   *Read BioRad QuadTech Chromatogram Files*

Description

Read BioRad QuadTech Chromatogram Files

Usage

```
chrom_read_quadtech(file, interp_volume = TRUE)
```

Arguments

file   Exported '.TXT' chromatogram file from the BioRad QuadTech.

interp_volume   Logical. If TRUE, interpolates the values in the volume column based on the
                values in the time column.

Value

a [tibble][tibble::tibble-package]

Examples

```
fl <- system.file("extdata",
                  "sec.txt",
                  package = "chromr")
# just read
fl |>
  chrom_read_quadtech()

# read without interpolating volume
fl |>
  chrom_read_quadtech(interp_volume = FALSE)
# read then plot
fl |>
  chrom_read_quadtech() |>
  chrom_plot()
```