Package 'OptiCal'

February 16, 2022

Type Package

Title Optimise Calibrants

Version 0.1.0

Description Selecting the optimal oberservations from a calibration series.

License GPL (>= 3)

Encoding UTF-8

LazyData true

Depends R (>= 3.5),
magrittr

Imports purrr,
dplyr

Suggests testthat (>= 3.0.0)

Config/testthat/edition 3

RoxygenNote 7.1.1

Roxygen list(markdown = TRUE)

R topics documented:

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Description

Optimise Calibration Series

Usage

```
optimise(calibration_data, p = 0.6, quad = TRUE)
```

Arguments

`calibration_data`

                   a `data.frame` or `tibble` of calibration data. The data should have two columns named, `area` and `concentration`.

`p`   a numeric value (between 0 and 1) of the minimum percentage of calibration observations to utilise

`quad`   logical; if `TRUE` then quadratic regression is also included alongside linear regression duringf the optimisation

Value

a list of three elements.

- `type`: a character string of the regression type (linear or quadratic)
- `score`: numeric value of the `OptiCal` score
- `data`: a `data.frame` of the optimal set of calibration observations

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