

Package: SmartPK (via r-universe)

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Type Package

Title Automated Noncompartmental Pharmacokinetic Analysis

Version 0.1.0

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Description Provides functions for automated noncompartmental pharmacokinetic (NCA) analysis using concentration-time data. The package estimates pharmacokinetic parameters including area under the concentration-time curve (AUC), area under the first moment curve (AUMC), maximum concentration (Cmax), time to maximum concentration (Tmax), terminal elimination rate constant (Kel), elimination half-life, clearance, volume of distribution, and mean residence time (MRT). It supports automatic terminal phase selection, bootstrap confidence intervals, and publication-ready concentration-time profiles. Methods are based on Gibaldi and Perrier (1982, ISBN:9780824710422).

License GPL-3

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Imports ggplot2, rlang

Suggests knitr, rmarkdown, testthat (>= 3.0.0)

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Description

Provides functions for automated noncompartmental pharmacokinetic (NCA) analysis using concentration-time data. The package estimates pharmacokinetic parameters including area under the concentration-time curve (AUC), area under the first moment curve (AUMC), maximum concentration (Cmax), time to maximum concentration (Tmax), terminal elimination rate constant (Kel), elimination half-life, clearance, volume of distribution, and mean residence time (MRT). It supports automatic terminal phase selection, bootstrap confidence intervals, and publication-ready concentration-time profiles.

Usage

```
SmartPK(
  data,
  dose,
  time_col = "Time",
  conc_col = "Concentration",
  route = c("iv", "extravascular"),
  min_terminal_points = 3,
  max_terminal_points = 6,
  lambda_method = c("auto", "lastn", "manual"),
  terminal_idx = NULL,
  n_boot = 0,
  conf_level = 0.95,
  plot = TRUE,
  log_plot = TRUE,
  return_plot = TRUE
)
```

Arguments

<code>data</code>	A data frame containing concentration-time observations.
<code>dose</code>	A single positive numeric dose value.
<code>time_col</code>	Name of the time column in data. Default is "Time".
<code>conc_col</code>	Name of the concentration column in data. Default is "Concentration".
<code>route</code>	Route of administration. Must be "iv" or "extravascular".
<code>min_terminal_points</code>	Minimum number of points used to estimate the terminal phase.

<code>max_terminal_points</code>	Maximum number of points used to estimate the terminal phase.
<code>lambda_method</code>	Method for terminal slope estimation: "auto", "lastn", or "manual".
<code>terminal_idx</code>	Integer indices of terminal points when <code>lambda_method</code> is "lastn" or "manual".
<code>n_boot</code>	Number of bootstrap resamples used to estimate confidence intervals. Set to 0 to skip bootstrapping.
<code>conf_level</code>	Confidence level for bootstrap intervals. Default is 0.95.
<code>plot</code>	Logical; whether to generate a concentration-time plot.
<code>log_plot</code>	Logical; whether the plot should use a log10 y-axis.
<code>return_plot</code>	Logical; whether to include the plot in the returned object.

Details

The function computes observed AUC and AUMC using the trapezoidal rule, then extrapolates to infinity using the terminal elimination rate constant estimated from a log-linear regression of the terminal phase. The terminal phase may be selected automatically, manually, or using the last `n` points depending on the value of `lambda_method`.

Value

A list with the following components:

- `summary`: A data frame of estimated PK parameters.
- `terminal_fit`: A list containing the terminal points used, fit statistics, and the estimated K_{el} .
- `plot`: A ggplot object showing the concentration-time profile, if `plot = TRUE`.

References

Gibaldi, M. and Perrier, D. (1982). *Pharmacokinetics*. 2nd Edition. Marcel Dekker, New York. ISBN: 9780824710422.

Examples

```
df <- data.frame(  
  Time = c(0, 1, 2, 4, 6, 8),  
  Concentration = c(0, 12, 9, 5, 2, 0.8)  
)  
  
SmartPK(df, dose = 100)
```

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