Package: PKPDindex (via r-universe)

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Title Optimal PK/PD Index Finder

Version 0.2.1

Description Fits Emax models to pharmacokinetic/pharmacodynamic (PK/PD) data, estimate key parameters, and visualise model fits for multiple PK/PD indices. Methods are described in Macdougall J (2006) <doi:10.1007/0-387-33706-7_9>, Spiess AN, Neumeyer N (2010) <doi:10.1186/1471-2210-10-6>, and Burnham KP, Anderson DR (2004) <doi:10.1177/0049124104268644>.

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Contents

PKPDindex *PKPDindex: Optimal PK/PD Index Finder*

Description

This function fits various Emax models to a given dataset, allowing for flexibility in model selection, initial parameter estimates, and plotting options.

Usage

```
PKPDindex(
  dataset,
  x_columns = NULL,
  y_column = "response",
  E0_fix,
  Emax_fix,
  EI50_init = NULL,
  maxiter = 500,
  tol = 1e-05,
  minFactor = 1e-07,
  select_mod = NULL,
  plot_results = FALSE,
  srow = FALSE,
  xlim = NULL,
  ylim = NULL,
  point_color = NULL,
  line_color = NULL,
  x_label = NULL,
  y_label = NULL,
  plot_title = NULL,
  log_scale_x = NULL,
  title_cex = 1.2,
  label_cex = 1,
  axis_cex = 1,
  detail_cex = 1
)
```

Arguments

`dataset`	A data frame containing the independent (x) and dependent (y) variables.
`x_columns`	A character vector specifying the x-axis variables (PK/PD indices). If NULL (default), the function attempts to detect appropriate columns from the dataset, specifically `"auc_mic"`, `"cmax_mic"`, and `"t_mic"`. If these are not found, the user must specify the names manually.

- `"auc_mic"`: area under the concentration-time curve divided by the MIC.
- `"cmax_mic"`: peak drug concentration divided by the MIC.

- "t_mic": time above MIC (duration the drug concentration exceeds MIC). Users should calculate these indices based on their PK data before using this function.

y_column	A character string specifying the response variable. Default name is "response".The response should be the log10-transformed change in CFU/ml (Delta log10 CFU/ml). Users can either provide a column with pre-calculated log10 CFU/ml changes, or provide raw CFU/ml counts at the initial (CFU_init) and 24-hour timepoint (CFU_24) , and the function will automatically calculate the log10 change in CFU/ml (Delta log10 CFU/ml).
E0_fix	Fixed E0 (baseline effect) value.
Emax_fix	Fixed Emax (maximum effect) value.
EI50_init	Optional numeric vector specifying initial EI50 values for each x_column. Defaults to NULL, and values are estimated automatically.
maxiter	Maximum number of iterations - Specifies the maximum number of iterations allowed for the nonlinear least squares (NLS) fitting process. Higher values may help convergence for complex models. Default maxiter = 500.
tol	Tolerance level - Defines the tolerance for convergence in the NLS algorithm. Lower values indicate stricter convergence criteria. Default tol = 1e-5.
minFactor	Minimum step factor - Determines the smallest step size used in parameter updates during the NLS fitting process, controlling the precision of optimisation. Default minFactor = 1e-7.
select_mod	Optional named list specifying preferred models for each x_column.
plot_results	Logical; if TRUE, the function generates model fit plots.
srow	Single row plotting - Logical (TRUE or FALSE). If TRUE, plots all best model fits in a single row for visual comparison.
xlim	A numeric vector of length 2 specifying x-axis limits.
ylim	A numeric vector of length 2 specifying y-axis limits.
point_color	Optional character string specifying the point colour in plots.
line_color	Optional character string specifying the line colour in plots.
x_label	Optional named list specifying custom x-axis labels.
y_label	Optional character string specifying a custom y-axis label.
plot_title	Optional character string specifying a custom plot title.
log_scale_x	Optional named list specifying whether to apply log10 scaling to x-axis for each x_column.
title_cex	Size of the plot title text. Default title_cex = 1.2.
label_cex	Size of the axis title. Default label_cex = 1.0.
axis_cex	Size of the axis labels. Default axis_cex = 1.0.
detail_cex	Size of the model detail text on the plot. Default detail_cex = 1.0.

Details

The function fits different variations of the Emax model to describe the relationship between PK/PD indices and response. The available models (m1 to m8) are defined as follows:

- **m1**: Fixed E0 and Emax, no Hill coefficient.
- **m2**: Fixed E0 and Emax, with Hill coefficient (gam).
- **m3**: Fixed E0, estimated Emax, no Hill coefficient.
- **m4**: Fixed E0, estimated Emax, with Hill coefficient.
- **m5**: Estimated E0, fixed Emax, no Hill coefficient.
- **m6**: Estimated E0, fixed Emax, with Hill coefficient.
- **m7**: Estimated E0 and Emax, no Hill coefficient.
- **m8**: Fully estimated model (E0, Emax, EI50, and gam).

Users can select specific models using the `select_mod` argument.

Value

A list containing:

- **All_Model_Results**: A data frame with results from all fitted models.
- **Best_Models**: A data frame with the best model (lowest AIC) for each PK/PD index.
- **Plots**: A list of recorded plots (if `plot_results = TRUE`).

Examples

```
# Basic usage with default settings
 output <- PKPDindex(
  dataset = PKPDindex_data,
  E0_fix = 1.5,
  Emax_fix = 4.8
)
# Custom x and y columns and initial data
 output <- PKPDindex(
  dataset = PKPDindex_data,
  E0_fix = 1.5,
  Emax_fix = 4.8,
  x_columns = c("auc_mic","cmax_mic","t_mic"),
  y_column = "response",
  EI50_init = c(1,1,1)
)

# Generate and custom plots
 output <- PKPDindex(
  dataset = PKPDindex_data,
  E0_fix = 1.5,
  Emax_fix = 4.8,
  plot_results = TRUE,
  srow=TRUE,
  xlim = c(0, 50),
```

```
  ylim = c(-2, 10),
  point_color = "green",
  line_color = "purple",
  select_mod = list(auc_mic = "m5", t_mic = "m1"),
  x_label = list(auc_mic = "AUC/MIC", cmax_mic = "Cmax/MIC", t_mic = "Time>MIC"),
  y_label = "Log10 Change in CFU",
  plot_title = "Model Fitting Results",
  log_scale_x = list(auc_mic = TRUE, cmax_mic = TRUE,t_mic=FALSE),
  title_cex = 2,
  label_cex = 1.5,
  axis_cex = 1.4,
  detail_cex = 1.3
)

#' # To view the best models:
output$Best_Models

# To view all model results:
output$All_Model_Results

# To access a specific plot:
output$Plots[["cmax_mic"]]
```

`PKPDindex_data` *PKPDindex_data*

Description

Example dataset for Emax model fitting.

Usage

```
PKPDindex_data
```

Format

A data frame with 20 rows and 4 columns:

auc_mic Area under the concentration-time curve (numeric)

cmax_mic Maximum concentration of the drug (numeric)

t_mic Time above minimum inhibitory concentration (numeric)

response Observed drug response (numeric; Delta log10 CFU/ml)

Details

This dataset contains information about drug concentrations (AUC/MIC, Cmax/MIC, and Time above MIC) and their corresponding response values, used for modelling the drug's effect based on the Emax model.

Source

Generated for package example purposes.

Examples

```
data(PKPDindex_data)
```

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