Package ‘xpose.nlmixr’

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Type Package

Title Graphical Diagnostics for Pharmacometric Models: Extension to 'nlmixr'

Version 0.3.0

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Description Extension to 'xpose' to support 'nlmixr'. Provides functions to import 'nlmixr' fit data into an 'xpose' data object, allowing the use of 'xpose' for 'nlmixr' model diagnostics.

License GPL (>= 2)

Encoding UTF-8

LazyData true

Depends R (>= 3.2), xpose (>= 0.4.2)

Imports ggplot2 (>= 2.2.1), nlmixr (>= 1.1.0-0), dplyr (>= 0.7.4), tibble (>= 2.0.0), stringr (>= 1.2.0), tidyr (>= 0.7.2), magrittr (>= 1.5), methods (>= 3.4.1), vpc (>= 1.0.2), nlme, crayon, rlang

RoxygenNote 7.1.2

NeedsCompilation no

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### nlmixr_vpc_theme

**Default VPC theme for 'xpose.nlmixr'**

**Description**

Default VPC theme for 'xpose.nlmixr'.

**Usage**

```r
nlmixr_vpc_theme
```

**Format**

An object of class `vpc_theme` of length 23.

**Value**

A list with 'vpc' theme specifiers.

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### summarise_nlmixr_model

**Data summary function**

**Description**

Convert 'nlmixr' model output into an 'xpose' database

**Usage**

```r
summarise_nlmixr_model(obj, model, software, rounding, runname)
```
theme_xp_nlmixr

Arguments

- **obj**: nlmixr fit object to be evaluated
- **model**: Model. Can be blank
- **software**: Software that generated the model fit
- **rounding**: Number of figures to round estimates to
- **runname**: Name of the model object being converted

Value

A summary data object used by xpose_data_nlmixr.

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theme_xp_nlmixr

*Default* *nlmixr* theme for *xpose*

Description

Default *nlmixr* theme for *xpose*.

Usage

theme_xp_nlmixr()

Value

A list with *xpose* theme specifiers.

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theo_sd_fit

*Single-dose theophylline PK data fit*

Description

Single-dose theophylline PK data fit using the first-order conditional estimation method with interaction (FOCEI) in *nlmixr*, a modified tibble.

Usage

data("theo_sd_fit")
Format

A **tibble** with 132 observations and 22 variables, and an additional 13 properties.

- **ID** Individual identifier, a factor
- **TIME** Time in hours, a numeric vector
- **DV** Theophylline concentration, a numeric vector
- **EVID** Event identifier, a numeric vector
- **PRED** Population predictions, a numeric vector
- **RES** Residuals, a numeric vector
- **WRES** Weighted residuals, a numeric vector
- **IPRED** Individual predictions, a numeric vector
- **IRES** Individual residuals, a numeric vector
- **IWRES** Individual weighted residuals, a numeric vector
- **CPRED** Conditional predictions, a numeric vector
- **CRES** Conditional residuals, a numeric vector
- **CWRES** Conditional weighted residuals, a numeric vector
- **eta.ka** Interindividual variability in $ka$, a numeric vector
- **eta.cl** Interindividual variability in $CL/F$, a numeric vector
- **eta.v** Interindividual variability in $V/F$, a numeric vector
- **ka** Absorption rate in $/h$, a numeric vector
- **cl** Apparent clearance in $L/h$, a numeric vector
- **v** Apparent volume of distribution in $L$, a numeric vector
- **cp** Theophylline concentration, a numeric vector
- **depot** Amount of theophylline in the depot compartment, a numeric vector
- **center** Amount of theophylline in the central compartment, a numeric vector
- **omega** Omega matrix
- **omegaR** Omega Correlation matrix
- **shrink** Shrinkage table, includes skewness, kurtosis, and eta p-values
- **parFixed** Fixed Effect Parameter Table
- **theta** Fixed Parameter Estimates
- **eta** Individual Parameter Estimates
- **seed** Seed (if applicable)
- **coefficients** Fixed and random coefficients
- **meta** Model meta information environment
- **modelName** Model name (from R function)
- **dataName** Name of R data input
- **simInfo** RxODE list for simulation
- **sigma** List of sigma components and their values
Details

This dataset is an nlmixr fit object for demonstrating the use of xpose.nlmixr.

Source

NONMEM/nlme.

Examples

data(theo_sd_fit)
str(theo_sd_fit)

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**xpose_data_nlmixr** Import nlmixr output into xpose

Description

Convert 'nlmixr' model output into an 'xpose' database.

Usage

```r
xpose_data_nlmixr(
  obj = NULL,
  pred = NULL,
  wres = NULL,
  gg_theme = theme_readable(),
  xp_theme = theme_xp_default(),
  quiet,
  skip = NULL,
  ...
)
```

Arguments

- **obj** nlmixr fit object to be evaluated.
- **pred** Name of the population prediction variable to use for plotting. If unspecified, it will choose either "NPDE", "CWRES", and "RES" (in that order) if the column exists in the data.
- **wres** Name of the weighted residual variable to use for plotting. If unspecified, it will choose either "NPDE", "CWRES", and "RES" (in that order) if the column exists in the data.
- **gg_theme** A ggplot2 theme object.
- **xp_theme** An xpose theme or vector of modifications to the xpose theme (eg. `c(point_color = 'red', line_linetype = 'dashed')`).
- **quiet** Logical, if FALSE messages are printed to the console.
- **skip** Character vector be used to skip the import/generation of: 'data', 'files', 'summary' or any combination of the three.
- **...** Additional arguments to be passed to the `read_delim` functions.
Value

An \texttt{xpose_data} object suitable for use in 'xpose'.

Examples

\texttt{xpdb <- xpose_data_nlmixr(obj = theo_sd_fit)}
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