Package ‘Certara.ModelResults’

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Title Generate Diagnostics for Pharmacometric Models Using 'shiny'

Version 3.0.1

Description Utilize the 'shiny' interface to generate Goodness of Fit (GOF) plots and tables for Non-Linear Mixed Effects (NLME / NONMEM) pharmacometric models. From the interface, users can customize model diagnostics and generate the underlying R code to reproduce the diagnostic plots and tables outside of the 'shiny' session. Model diagnostics can be included in a 'rmarkdown' document and rendered to desired output format.

Depends R (>= 4.0)

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URL `https://certara.github.io/R-model-results/`

Encoding UTF-8

LazyData true

RoxygenNote 7.3.2

Suggests knitr, rmarkdown, testthat (>= 3.0.0), Certara.RsNLME

Imports colourpicker, shinyAce, shinymeta, Certara.Xpose.NLME, xpose, dplyr, flextable, shinyjqui, grDevices, ggplot2, plotly, magrittr, scales, shiny (>= 1.7.0), shinyjs, shinyWidgets, shinyTree (>= 0.3.1), sortable, tidyr, rlang, bslib (>= 0.7.0)

Config/testthat/edition 3

NeedsCompilation no

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`get_eps_shk` *Get eps skrinkage values xpdb*

Description

This function returns eps shrinkage values from xpdb object as a `data.frame`.

Usage

```
get_eps_shk(xpdb)
```

Arguments

`xpdb`	Object of class `xpose_data`.

Value

Returns an object of class `data.frame`.

Examples

```
get_eps_shk(xpdb_NLME$TwCpt_IVBolus_FOCE_ELS)
```

`get_eta_shk` *Get eta skrinkage values xpdb*

Description

This function returns eta shrinkage values from xpdb object as a `data.frame`.

Usage

```
get_eta_shk(xpdb)
```

Arguments

`xpdb`	Object of class `xpose_data`.

Value

Returns an object of class `data.frame`.

Examples

```
get_eta_shk(xpdb_NLME$TwCpt_IVBolus_FOCE_ELS)
```

`resultsUI` *Generate and Report Model Diagnostics from NLME or NONMEM runs*

Description

Shiny application to generate, customize, and report diagnostic plots and tables from NLME or NONMEM output files. Create an Rmarkdown file of tagged model diagnostics and render into submission ready report.

Usage

```
resultsUI(model, xpdb = NULL, tagged = NULL, settings = NULL, ...)
```

Arguments

`model`	A single object, vector, or list of objects of class `NlmePmlModel`.
`xpdb`	A single object or list of objects of class `xpose_data`.
`tagged`	List of tagged objects returned from previous `tagged <- resultsUI()` session.
`settings`	List of settings (e.g., settings.Rds) returned from previous Shiny session.
`...`	Additional arguments for Pirana integration.

Value

If `interactive()`, returns a list of tagged diagnostics from the Shiny application, otherwise returns `TRUE`.

Examples

```
if (interactive()) {


# RsNLME
library(Certara.RsNLME)
library(Certara.ModelResults)

model1 <- pkmodel(numCompartments = 1,
                 data = pkData,
                 ID = "Subject",
                 Time = "Act_Time",
                 A1 = "Amount",
                 CObs = "Conc",
                 modelName = "OneCpt_IVBolus_FOCE-ELS")

baseFitJob1 <- fitmodel(model1)


model2 <- pkmodel(numCompartments = 2,
                 data = pkData,
                 ID = "Subject",
                 Time = "Act_Time",
                 A1 = "Amount",
                 CObs = "Conc",
                 modelName = "TwCpt_IVBolus_FOCE-ELS")

baseFitJob2 <- fitmodel(model2)

# Run Model Results
resultsUI(model = c(model1, model2))


# NONMEM via xpose

library(Certara.ModelResults)
library(xpose)

xpdb <- xpose_data(
  runno = "1",
  prefix = "run",
  ext = ".lst",
  dir = "./NONMEM/Hands_onB/")

resultsUI(xpdb = xpdb)

# Multiple models

xpdb_multiple <- list(
 run1 = xpose_data(file = "run1.lst"),
 run2 = xpose_data(file = "run2.lst"),
 run3 = xpose_data(file = "run3.lst"),
 run4 = xpose_data(file = "run4.lst")
)
}
```

`theme_certara` *A ggplot2 theme for Certara.*

Description

A ggplot2 theme for Certara.

Usage

```
theme_certara(
  base_size = 11,
  base_family = "",
  base_line_size = base_size/22,
  base_rect_size = base_size/22,
  grid = c("none", "horizontal", "both")
)
```

Arguments

`base_size` base font size, given in pts.

`base_family` base font family

`base_line_size` base size for line elements

`base_rect_size` base size for rect elements

`grid` Which grid lines should appear? Horizontal only, both horizontal and vertical, or none (default). `continuous_scale()`.

Details

There are 3 variants of the theme: no grid `theme_certara()`, full grid `theme_certara(grid = "both")`, and horizontal grid lines only `theme_certara(grid = "horizontal")`.

Value

An object of class `theme()`.

write_code — *Write code to R script from tagged diagnostics*

Description

Use this function to write code to R script from diagnostics tagged in Certara's Model Results Shiny Application.

Usage

```
write_code(tagged, file)
```

Arguments

`tagged`	List of tagged objects from returned from `resultsUI()`.
`file`	Character specifying path of output file. If missing, it will be saved as `code.R` in working directory.

Value

Returns `NULL` after writing to `file`.

Examples

```
if (interactive()) {
tagged_diagnostics <- resultsUI(xpdb = xpdb_NLME)

write_code(tagged_diagnostics, "tagged_results.R")

}
```

xpdb_NLME — *List of xpose data objects from RsNLME example tutorials*

Description

The following object contains a list of 2 `xpose_data` objects generated in the RsNLME example script `TwoCptIVBolus_FitBaseModel_CovariateSearch_VPC_BootStrapping.R`.

Usage

```
xpdb_NLME
```

Format

List of 2 `xpose_data` objects constructed from NLME model output.

Details

- xpdb_NLME$`TwCpt_IVBolus_FOCE-ELS` is an xpose_data object created from the base model in RsNLME example script. The model can be used as a reference to compare model diagnostics in final model.
- xpdb_NLME$`TwCpt_IVBolus_SelectedCovariateModel_FOCE-ELS` is an xpose_data object created from the final model in the RsNLME example script. The final model includes selected covariate BodyWeight added from the results of stepwise covariate search.

Source

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xpdb_NONMEM *List of xpose data objects from NONMEM model output*

Description

The following object contains of list of 2 xpose_data objects:

Usage

```
xpdb_NONMEM
```

Format

List of 2 xpose_data objects constructed from NONMEM model output.

Details

- xpdb_NONMEM$ex_pk is an xpose_data object from xpose::xpdb_ex_pk. The model contains multiple covariates and can be used to explore covariate model diagnostics.
- xpdb_NONMEM$mult_obs is an xpose_data object created from NONMEM model with multiple observed variables. Users will see that appropriate model diagnostic plots are automatically facetted by DVID in the Shiny GUI.

Source

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