Package 'Certara.RsNLME.ModelBuilder'

Title Pharmacometric Model Building Using 'shiny'

Version 3.0.1

Description Develop Nonlinear Mixed Effects (NLME) models for pharmacometrics using a 'shiny' interface. The Pharmacometric Modeling Language (PML) code updates in real time given changes to user inputs. Models can be executed using the 'Certara.RsNLME' package. Additional support to generate the underlying 'Certara.RsNLME' code to recreate the corresponding model in R is provided in the user interface.

Depends R (>= 4.0)

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URL https://certara.github.io/R-RsNLME-model-builder/

Encoding UTF-8

RoxygenNote 7.3.2

Suggests knitr, rmarkdown, testthat (>= 3.0.0)

Imports Certara.RsNLME, shinymeta, shinyAce, bslib (>= 0.7.0), data.table, DT, ggplot2, ggforce, htmltools, htmlwidgets, magrittr, methods, shiny (>= 1.7.0), shinyjs, shinyWidgets, tools, utils, fs

Config/testthat/edition 3

NeedsCompilation no

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Repository CRAN

Date/Publication 2024-12-20 11:00:10 UTC

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create_metamodelBuiltin

Run modelBuilderUI() *and create resulting metamodel*

Description

Used by Pirana to run modelBuilderUI(), saving the resulting metamodel e.g., .mmmdl file given model building operations performed in GUI.

Usage

```
create_metamodelBuiltin(metamodelFile, datafile, author = "")
```

Arguments

metamodelFile	File where the metamodel should be created.
datafile	File with input data.
author	Optional character string to specify the author in the metamodel.

Value

NLME PML model S4 class instance

Examples

```
if (interactive()) {
tmp_data <- tempfile(fileext = ".csv")
write.csv(Certara.RsNLME::pkData, tmp_data, row.names = FALSE)

create_metamodelBuiltin(
  "run1.mmdl",
  tmp_data
  )
}
```

---

create_metamodelTextual

Send metamodel to modelTextualUI() *and run shiny application*

Description

Used by Pirana to send existing metamodel to modelTextualUI() for editing, and after returning, saves it as a metamodel file e.g, .mmdl.

Usage

```
create_metamodelTextual(metamodelFile)
```

Arguments

metamodelFile   Path to existing metmodel file.

Details

If DOSING CYCLE block is presented in the metamodel, it will be transferred to COLDEF block with a warning.

Value

Updated metamodel text.

Examples

```
if (interactive()) {
mmdl_file <- system.file("vignettesdata/OneCpt_IVInfusion.mmdl",
  package = "Certara.RsNLME")

create_metamodelTextual(
  mmdl_file
  )
}
```

---

estimatesUI   *Shiny GUI to examine the model and evaluate estimates for fixed effects.*

Description

Shiny GUI to examine the model and evaluate estimates for fixed effects.

Usage

```
estimatesUI(model, host = NULL)
```

Arguments

model	Model object.
host	Optional host parameter of class hostParams. If NULL, local host will be used.

Value

A model object of class NlmePmlModel

Examples

```
if (interactive()) {
library(Certara.RsNLME)
host <- hostParams(
  parallelMethod = "None",
  hostName = "local",
  numCores = 1
)

model <- pkmodel(
  parameterization = "Clearance",
  absorption = "Intravenous",
  numCompartments = 2,
  data = pkData,
  ID = "Subject",
  A1 = "Amount",
  CObs = "Conc",
  Time = "Act_Time",
  modelName = "pk_model"
)

model <- estimatesUI(model, host)
}
```

---

modelBuilderUI	*Build RsNLME model from Shiny GUI and generate corresponding RsNLME code*

Description

Shiny application to build RsNLME model from Shiny GUI and generate corresponding RsNLME code based on input selections.

Usage

```
modelBuilderUI(
  data,
  modelName = "PKPDmodel",
  workingDir = "",
  baseModel = NULL
)
```

Arguments

data	Input dataset.
modelName	Name of the model; if `missing`, named as 'PKPDmodel.'
workingDir	Working directory to run the model. Current working directory will be used if `workingDir` not specified or does not exist.
baseModel	The model object from where the input dataset and model name are recovered if arguments `data` and `modelName` are not specified.

Value

A model object of class `NlmePmlModel`

Examples

```
if (interactive()) {
model <- modelBuilderUI(data = Certara.RsNLME::pkData, modelName = "PK_Model")
}
```

---

modelTextualUI	*Edit textual RsNLME model from Shiny GUI*

Description

Shiny application to update RsNLME model from Shiny GUI and directly edit PML statements using Ace editor. Syntax and semantic check is performed by TDL executable (if presented). The Shiny application also allows adding input options and column mappings from Shiny GUI.

Usage

```
modelTextualUI(baseModel, initpml, data, modelName = "PKPDmodel")
```

Arguments

baseModel	The model object from where the information is recovered.
initpml	Initial PML model file to be edited. Overrides baseModel@statements, if presented.
data	Input data frame. Overrides baseModel@inputData, if presented.
modelName	Name of the model; if missing, named as 'PKPDmodel'. Overrides baseModel@modelInfo@modelName, if presented.

Value

A model object of class NlmePmlModel

Examples

```
if (interactive()) {
model <- modelBuilderUI(data = Certara.RsNLME::pkData, modelName = "PK_Model")

model <- modelTextualUI(baseModel = model)
}
```

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