

Package ‘Certara.DarwinReporter’

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Title Data Visualization Utilities for 'pyDarwin' Machine Learning
Pharmacometric Model Development

Version 2.0.1

Description Utilize the 'shiny' interface for visualizing results from a 'pyDarwin' (<<https://certara.github.io/pyDarwin/>>) machine learning pharmacometric model search. It generates Goodness-of-Fit plots and summary tables for selected models, allowing users to customize diagnostic outputs within the interface. The underlying R code for generating plots and tables can be extracted for use outside the interactive session. Model diagnostics can also be incorporated into an R Markdown document and rendered in various output formats.

URL <https://certara.github.io/R-DarwinReporter/>

Depends R (>= 4.1.0)

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Encoding UTF-8

RoxygenNote 7.3.2

Suggests knitr, rmarkdown, data.table, readr, testthat (>= 3.0.0)

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darwinReportUI	<i>Generate and Report Model Diagnostics from NLME or NONMEM runs</i>
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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

```
darwinReportUI(darwin_data, tagged = NULL, settings = NULL, ...)
```

Arguments

darwin_data	Object of class darwin_data. Note, key_models xpose_data must be available.
tagged	List of tagged objects returned from previous tagged <- darwinReportUI() 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()) {
  ddb <- darwin_data("./darwin_search_09") |>
    import_key_models("./darwin_search_09/key_models")

  darwinReportUI(ddb)
}

```

darwin_data	<i>Initialize darwin data structure.</i>
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Description

Initialize darwin data structure.

Usage

```

darwin_data(
  project_dir,
  working_dir = NULL,
  output_dir = NULL,
  key_models_dir = NULL,
  ...
)

```

Arguments

project_dir	Directory containing input files for pyDarwin (e.g., options.json).
working_dir	Directory containing misc results folders generated from a pyDarwin search. This is the default location of the key_models, output, and temp folders.
output_dir	Directory containing output files such as "results.csv" and final control files. Default location is inside working_dir/output.
key_models_dir	Directory of the key_models folder. Default location is inside working_dir/key_models. Note, key models are not imported if argument is NULL, explicitly specify key_models_dir to import files for darwinReportUI .
...	Additional args.

Details

If working_dir and output_dir are sub directories of project_dir, these arguments can be ignored. The key_models_dir is not required to initialize the darwin_data object. If specified, however, key models data will be imported which may take time given the number of key models and size of output tables. See [import_key_models](#).

Value

Object of class darwin_data.

fitness_penalties_vs_iteration

Plot minimum fitness by iteration with penalty composition.

Description

Plot minimum fitness by iteration with penalty composition.

Usage

```
fitness_penalties_vs_iteration(
  darwin_data,
  group_penalties = TRUE,
  scale_ofv = TRUE,
  ...
)
```

Arguments

darwin_data	Object of class darwin_data.
group_penalties	Logical; defaults to TRUE.
scale_ofv	Set to TRUE to rescale OFV axis limit. Used to better observe penalty effects.
...	Additional arguments.

Value

Object of class ggplot.

fitness_vs_iteration *Plot best fitness by iteration.*

Description

Plot best fitness by iteration.

Usage

```
fitness_vs_iteration(darwin_data, ...)
```

Arguments

darwin_data	Object of class darwin_data.
...	Additional arguments.

Value

Object of class ggplot.

get_eps_shk *Get eps shrinkage values xpose_data object*

Description

This function returns eps shrinkage values from xpose_data 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.

get_eta_shk *Get eta shrinkage values from xpose_data object*

Description

This function returns eta shrinkage values from xpose_data 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.

```
import_key_models
```

Imports files from key model output folders

Description

Use to create xpose data object from files in NLME or NONMEM key model output folders.

Usage

```
import_key_models(darwin_data, dir, ...)
```

Arguments

<code>darwin_data</code>	Object of class <code>darwin_data</code> .
<code>dir</code>	File path to key models directory.
<code>...</code>	Additional args.

Value

Object of class `darwin_data`.

Examples

```
if (interactive()) {  
  ddb <- darwin_data(project_dir = "./darwin_search_09") |>  
    import_key_models(dir = "./darwin_search_09/key_models")  
}
```

```
summarise_fitness_by_iteration
```

Summarise fitness by iteration

Description

Summarise minimum, cumulative minimum, and mean fitness values by pyDarwin search iteration/generation.

Usage

```
summarise_fitness_by_iteration(darwin_data)
```

Arguments

<code>darwin_data</code>	Object of class <code>darwin_data</code> .
--------------------------	--

Value

data.frame with columns iteration, min_fitness, mean_fitness, and min_cum_fitness

summarise_fitness_penalties_by_iteration

Summarize minimum fitness and penalty values by iteration

Description

Summarise minimum fitness, ofv, and penalty values used in calculation of overall fitness values by pyDarwin search iteration/generation.

Usage

```
summarise_fitness_penalties_by_iteration(darwin_data, group_penalties = FALSE)
```

Arguments

darwin_data Object of class darwin_data.

group_penalties

Logical. Set to TRUE to group penalties.

Value

data.frame of columns "iteration", "fitness", "ofv" and corresponding penalty columns.

summarise_overall_by_key_models

Summarise overall table by key models

Description

Generate a summary data.frame by key models, which includes columns such as condition number, number of parameters, -2LL, AIC, BIC, fitness, and penalty values.

Usage

```
summarise_overall_by_key_models(darwin_data)
```

Arguments

darwin_data Object of class darwin_data.

Value

data.frame

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() .
...	Additional args

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\(\)](#).

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