Package: rbioacc (via r-universe)

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Title Inference and Prediction of Toxicokinetic Models

Version 1.3.1

Description Provides bioaccumulation factors from a toxicokinetic model fitted to accumulation-depuration data. It is designed to fulfil the requirements of regulators when examining applications for market authorization of active substances.

URL https://gitlab.in2p3.fr/mosaic-software/rbioacc

BugReports https://gitlab.in2p3.fr/mosaic-software/rbioacc/-/issues

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`rbioacc-package` *The 'rbioacc' package.*

Description

A DESCRIPTION OF THE PACKAGE

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References

Stan Development Team (NA). RStan: the R interface to Stan. R package version NA. https://mc-stan.org

See Also

Useful links:

- https://gitlab.in2p3.fr/mosaic-software/rbioacc
- Report bugs at https://gitlab.in2p3.fr/mosaic-software/rbioacc/-/issues

.fonte *A simple implementation of to pivot_longer of tidyr*

Description

A simple implementation of to pivot_longer of tidyr

Usage

```
.fonte(df, names_to, values_to)
```

Arguments

df	A data frame to pivot.
names_to	A string specifying the name of the column to create from the data stored in the column names of df.
values_to	A string specifying the name of the column to create from the data stored in cell values.

Value

The data frame with a "lengthens" shape: more rows, less columns

.index_col_exposure *Return column matching "expw", "exps", "expf", "exppw" of a data.frame*

Description

Return column matching "expw", "exps", "expf", "exppw" of a data.frame

Usage

```
.index_col_exposure(data_frame)
```

Arguments

data_frame	a dataframe

Value

A vector of numeric

.index_col_metabolite *Return column matching "concX" of a* data.frame *where X is metabolite*

Description

Return column matching "concX" of a data.frame where X is metabolite

Usage

```
.index_col_metabolite(data_frame)
```

Arguments

data_frame	a dataframe

Value

A vector of numeric

.is_equal_rmInf *Check if two vectors* x *and* y *are equal after remove* Inf

Description

Check if two vectors x and y are equal after remove Inf

Usage

```
.is_equal_rmInf(x, y)
```

Arguments

x	A vector
y	A vector

Value

A logical value

bioacc_metric *Biaccumulation metrics*

Description

Biaccumulation metrics

Usage

```
bioacc_metric(fit, ...)

## S3 method for class 'fitTK'
bioacc_metric(fit, type = "k", route = "all", ...)
```

Arguments

fit	An stanFit object
...	Further arguments to be passed to generic methods
type	A string with the type of metric: k for the kinetics BioConcentration Factor, ss for the steady state BioConcentration Factor.
route	Provide exposure route: all

Value

a data frame

Chiro_Creuzot *Data on Chironomus with several exposure routes.*

Description

Data on Chironomus with several exposure routes.

Usage

```
data(Chiro_Creuzot)
```

Format

A dataframe with 24 observations on the following four variables:

time A vector of class numeric with the time points in days.

expw A vector of class numeric with the exposure in water.

expw A vector of class numeric with the exposure in pore water.

`replicate` A vector of class `integer` for replicate identification.

`conc` A vector of class `numeric` with concentration in organism.

`concm1` A vector of class `numeric` with metabolite concentration in organism.

`concm2` A vector of class `numeric` with metabolite concentration in organism.

`Chironomus_benzoapyrene` *Data on Chironomus exposed to benzoapyrene*

Description

Data on Chironomus exposed to benzoapyrene

Usage

```
data(Chironomus_benzoapyrene)
```

`corrMatrix` *Correlations between parameters: colored matrix*

Description

Correlations between parameters: colored matrix

Usage

```
corrMatrix(fit)
```

Arguments

`fit`	An object of class `fitTK`

Value

A heatmap of class `ggplot`.

corrPlot *Correlations between parameters: pairs plot*

Description

Correlations between parameters: pairs plot

Usage

```
corrPlot(fit, plots = c("all", "deterministic", "stochastic"))
```

Arguments

fit	An object of class fitTK
plots	A string selecting the parameters. Defaults is "all" and select all parameters. Determinstc parameters can be selected by setting "deterministic" and stochastic parameter with "stochastic"

Value

A pairsplot of class ggmatrix containing planes of parameter pairs (lower triangle), marginal posterior distribution of each parameter (diagonal) and Pearson correlation coefficients (upper triangle)

df_ppc *PPC data.frame*

Description

This is the generic ppc S3 method for plots of the predicted values along with 95\ versus the observed values for fitTK objects.

Usage

```
df_ppc(fit, ...)

## S3 method for class 'fitTK'
df_ppc(fit, ...)

ppc(fit, ...)

## S3 method for class 'fitTK'
ppc(fit, ...)
```

Arguments

`fit`	And object returned by fitTK
`...`	Additional arguments

Details

The black points show the observed number of survivors (pooled replicates, on X-axis) against the corresponding predicted number (Y-axis). Predictions come along with 95\ intervals, which are depicted in green when they contain the observed value and in red otherwise. Samples with equal observed value are shifted on the X-axis. For that reason, the bisecting line (y = x), is represented by steps when observed values are low. That way we ensure green intervals do intersect the bisecting line.

Value

A data frame with median and 95\

a plot of class `ggplot`

`df_PriorPost` *Data frame of Posterior over Prior*

Description

Data frame of Posterior over Prior

Data frame of Posterior over Prior

Usage

```
df_PriorPost(fit, ...)

## S3 method for class 'fitTK'
df_PriorPost(fit, select = "all", ...)
```

Arguments

`fit`	An object of class `fitTK` returned by the function `fitTK()`.
`...`	Additional arguments
`select`	A string selecting the parameters. Defaults is `"all"` and select all parameters.Determinstc parameters can be selected by setting `"deterministic"` and stochastic parameter with `"stochastic"`

Value

An object of class `data.frame`

equations *Equations of the mathematical model used for the fit*

Description

Equations of the mathematical model used for the fit

Usage

```
equations(fit, object)
```

Arguments

fit	An object of class fitTK
object	The data.frame used as the base as the fit object

Value

A vector of strings each containing an equation

exposure_names *Retrieve exposure routes names from object*

Description

Retrieve exposure routes names from object

Usage

```
exposure_names(object)
```

Arguments

object	a data frame.

Value

A vector of string

Exposure_Sialis_lutaria *Data on Sialis lutaria exposure time series*

Description

Data on Sialis lutaria exposure time series

Usage

```
data(Exposure_Sialis_lutaria)
```

fitTK *Posterior predictive check*

Description

Posterior predictive check

Bayesian inference of TK model with Stan

Bayesian inference of TK model with variable exposure profile (BETA version)

Usage

```
fitTK(stanTKdata, ...)

## S3 method for class 'stanTKdataCST'
fitTK(stanTKdata, ...)

## S3 method for class 'stanTKdataVAR'
fitTK(stanTKdata, ...)
```

Arguments

stanTKdata	List of Data require for computing
...	Arguments passed to rstan::sampling (e.g. iter, chains).

Value

An object of class fitTK containing two object: stanTKdata the data set used for inference and stanfit returned by rstan::sampling

Gammarus_azoxistrobine_1d_Rosch2017

Data on Gammarus exposed to azoxistrobine

Description

Data on Gammarus exposed to azoxistrobine

Usage

```
data(Gammarus_azoxistrobine_1d_Rosch2017)
```

Internal_Sialis_lutaria

Data on Sialis lutaria internal time series

Description

Data on Sialis lutaria internal time series

Usage

```
data(Internal_Sialis_lutaria)
```

Male_Gammarus_Merged

Male Gammarus fossarum *exposed to Hg spiked water. Three exposure concentrations were tested in triplicates. The duration of the accumulation phase is 4 days for 0.0000708021 and 0.000283208* $\mu g.mL\hat{}-1$ *exposure concentrations, and 7 days for 0.000141604* $\mu g.mL\hat{}-1$ *exposure concentration.*

Description

Male Gammarus fossarum exposed to Hg spiked water. Three exposure concentrations were tested in triplicates. The duration of the accumulation phase is 4 days for 0.0000708021 and 0.000283208 $\mu g.mL^{-1}$ exposure concentrations, and 7 days for 0.000141604 $\mu g.mL^{-1}$ exposure concentration.

Usage

```
data(Male_Gammarus_Merged)
```

Format

A dataframe with 72 observations on the following four variables:

`time` A vector of class `numeric` with the time points in days.

`expw` A vector of class `numeric` with Hg exposure in water in $\mu g.mL^{-1}$.

`replicate` A vector of class `integer` for replicate identification.

`conc` A vector of class `numeric` with Hg concentration in organism in $\mu g.mL^{-1}$.

References

Ciccia, T. (2019). Accumulation et devenir du mercure chez l'espèce sentinelle Gammarus fossarum : de l'expérimentation au développement d'un modèle toxicocinétique multi-compartiments. Rapport de stage de Master 2, INRAE.

`Male_Gammarus_seanine_growth`

Male `Gammarus pulex` *exposed to seanine spiked water. A single exposure concentration was tested. The duration of the accumulation phase is 1.417 days. Three metabolites were quantified. The growth of organism was included.*

Description

Male `Gammarus pulex` exposed to seanine spiked water. A single exposure concentration was tested. The duration of the accumulation phase is 1.417 days. Three metabolites were quantified. The growth of organism was included.

Usage

```
data(Male_Gammarus_seanine_growth)
```

Format

A dataframe with 22 observations on the following four variables:

`time` A vector of class `numeric` with the time points in days.

`expw` A vector of class `numeric` with seanine exposure in water in $\mu g.mL^{-1}$.

`replicate` A vector of class `integer` for replicate identification.

`conc` A vector of class `numeric` with concentration in organism.

`concm1` A vector of class `numeric` with metabolite concentration in organism.

`concm2` A vector of class `numeric` with metabolite concentration in organism.

`concm3` A vector of class `numeric` with metabolite concentration in organism.

`growth` A vector of class `numeric` with growth of the organism.

References

Ashauer, R. et al. (2012). Significance of xenobiotic metabolism for bioaccumulation kinetics of organic chemicals in Gammarus pulex. Environmental Science Technology, 46: 3498-3508.

`Male_Gammarus_Single` *Bio-accumulation data set for* Gammarus fossarum *exposed to Hg spiked water.*

Description

Male *Gammarus fossarum* exposed to Hg spiked water. A single exposure concentration was tested. The duration of the accumulation phase is 4 days.

Usage

```
data(Male_Gammarus_Single)
```

Format

A dataframe with 23 observations on the following four variables:

`time` A vector of class `numeric` with the time points in days.

`expw` A vector of class `numeric` with Hg exposure in water in $\mu g.mL^{-1}$.

`replicate` A vector of class `integer` for replicate identification.

`conc` A vector of class `numeric` with Hg concentration in organism in $\mu g.mL^{-1}$.

References

Ciccia, T. (2019). Accumulation et devenir du mercure chez l'espèce sentinelle Gammarus fossarum : de l'expérimentation au développement d'un modèle toxicocinétique multi-compartiments. Rapport de stage de Master 2, INRAE.

`mcmcTraces` *Traces of MCMC iterations*

Description

Traces of MCMC iterations

Usage

```
mcmcTraces(fit, plots = "all")
```

Arguments

fit	An object of class fitTK
plots	A string selecting the parameters. Defaults is "all" and select all parameters. Determinstc parameters can be selected by setting "deterministic" and stochastic parameter with "stochastic"

Value

A traceplot of class ggplot.

---

modelData *Create a list giving data and parameters to use in the model inference.*

Description

Create a list giving data and parameters to use in the model inference.

Usage

```
modelData(object, ...)

## S3 method for class 'data.frame'
modelData(object, time_accumulation, elimination_rate = NA, ...)
```

Arguments

object	An object of class data.frame
...	Further arguments to be passed to generic methods
time_accumulation	A scalar givin accumulation time
elimination_rate	A scalar for the elimination rate. Default is NA. To remove elimination rate, set elimination_rate = 0.

Value

A list with data and parameters require for model inference.

`modelData_ode` *Create a list giving data and parameters to use in the model inference.*

Description

Create a list giving data and parameters to use in the model inference.

Usage

```
modelData_ode(
  df_exposure,
  df_internal,
  y0 = 1,
  t0 = -0.001,
  unifMax = 10,
  time_accumulation = NULL,
  minK = -5,
  maxK = 5,
  ...
)

modelData_ode(
  df_exposure,
  df_internal,
  y0 = 1,
  t0 = -0.001,
  unifMax = 10,
  time_accumulation = NULL,
  minK = -5,
  maxK = 5,
  ...
)
```

Arguments

`df_exposure`	Dataframe of exposure with 2 column (`time` and `value`)
`df_internal`	Dataframe of internal concentration with 2 column (`time` and `value`)
`y0`	Initial concentration
`t0`	initial time point
`unifMax`	Hyperparameter value
`time_accumulation`	Time of accumulation
`minK`	Hyperparameter value
`maxK`	Hyperparameter value
`...`	Additional arguments

Value

A `list` with data and parameters require for model inference.

`Oncorhynchus_two` *Data on Oncorhynchus exposition*

Description

Data on Oncorhynchus exposition

Usage

```
data(Oncorhynchus_two)
```

`plot.bioaccMetric` *Plot function for object of class* `bioaccMetric`

Description

Plot function for object of class `bioaccMetric`

Usage

```
## S3 method for class 'bioaccMetric'
plot(x, ...)
```

Arguments

`x`	a data frame
`...`	Additional arguments

Value

A plot of class `ggplot`

plot.fitTK *Plotting method for* fitTK *objects*

Description

This is the generic plot S3 method for the fitTK. It plots the fit obtained for each variable in the original dataset.

Usage

```
## S3 method for class 'fitTK'
plot(x, time_interp = NULL, ...)
```

Arguments

x	And object returned by fitTK
time_interp	A vector with additional time point to interpolate. Time point of the original data set are conserved.
...	Additional arguments

Value

a plot of class ggplot

plot.predictTK *Plotting method for* predictTK *objects*

Description

This is the generic plot S3 method for the predictTK.

Usage

```
## S3 method for class 'predictTK'
plot(x, ...)

## S3 method for class 'predictTKstan'
plot(x, add_data = FALSE, ...)
```

Arguments

x	An object of class predictTK returned by predict
...	Additional arguments
add_data	logical TRUE or FALSE to add the orignal data of the fit object x

Value

A plot of class ggplot

`plot_exposure` *Plot exposure profile*

Description

Plot exposure profile

Usage

```
plot_exposure(object)
```

Arguments

`object`	a data frame with exposure column

Value

a plot of class ggplot

`plot_PriorPost` *Plot Posterior over Prior*

Description

Plot Posterior over Prior

Plot Posterior over Prior

Usage

```
plot_PriorPost(x, ...)

## S3 method for class 'fitTK'
plot_PriorPost(x, select = "all", ...)

## S3 method for class 'df_PP'
plot_PriorPost(x, select = "all", ...)
```

Arguments

`x`	A data.frame of class `df_PP` returned by the function `df_PriorPost()`.
`...`	addition arguments
`select`	A string selecting the parameters. Defaults is `"all"` and select all parameters. Deterministic parameters can be selected by setting `"deterministic"` and stochastic parameter with `"stochastic"`.

Value

A plot of class ggplot.

A plot of class ggplot.

---

predict.fitTK *Prediction function using* fitTK *object*

Description

Use when parameter are manually given by the user.

Usage

```
## S3 method for class 'fitTK'
predict(object, data, mcmc_size = NULL, fixed_init = TRUE, ...)

predict_stan(
  object,
  data,
  mcmc_size = NULL,
  fixed_init = TRUE,
  time_interp = NULL,
  iter = 1000,
  ...
)

predict_manual(
  param,
  data,
  time_accumulation = NULL,
  C0 = 0,
  G0 = NA,
  gmax = NA
)
```

Arguments

object	An object of stanfit
data	A data set with one column time and 1 to 4 exposure
mcmc_size	Size of mcmc chain if needed to be reduced
fixed_init	If TRUE fix the initial conditions of internal concentration. columns with name in expw, exps, expf and exppw
...	Additional arguments
time_interp	A vector with additional time point to interpolate. Time point of the original data set are conserved.

iter	Number of time steps
param	A dataframe with name of parameters kee, keg, ku1, ku2, ..., km1, km2, ... and kem1, kem2, ..., sigmaConc, sigmaCmet (if metabolites) and sigmaGrowth (if growth). The parameter kee is mandatory.
time_accumulation	the time of accumulation.
C0	Gives the initial conditions of internal concentration.
G0	initial condition of G0 (require if keg is provided)
gmax	gmax (require if keg is provided) columns with name in expw, exps, expf and exppw

Value

An object of class predictTK

An object of class predictTK

---

psrf *Potential Scale Reduction Factors (PSRF) of the parameters*

Description

Potential Scale Reduction Factors (PSRF) of the parameters

Usage

```
psrf(fit)
```

Arguments

fit	An object of class fitTK

Value

An object of class data.frame with two columns: PSRF and parameter

a data frame with Potential Scale Reduction Factors

quantile_table *Quantiles of parameters*

Description

Quantiles of parameters

Usage

```
quantile_table(fit, probs = c(0.025, 0.5, 0.975))
```

Arguments

fit	An object of class fitTK
probs	Scalar or Vector of quantiles. Default is 0.025, 0.5 and 0.975 giving median and 95% credible interval

Value

A data frame with quantiles

replace_ *Replace element of a vector*

Description

Replace element of a vector

Usage

```
replace_(x, from, to)
```

Arguments

x	a vector
from	a vector of elements to replace
to	a vector with replacing elements

Value

a vector

Examples

```
replace_(1:10,c(2,4,5,8), c(0,0,0,0))
replace_(c(1,2,2,3,2),c(3,2), c(4,5))
```

rmMessWarn *remove message and warning*

Description

Remove message and warning which is usefull when running a model and removing all outputs messages and warnings#'

Usage

```
rmMessWarn(...)
```

Arguments

...	any function, but a fit function.

t95 *Return the time at 95% depuration of the parent component*

Description

Return the time at 95% depuration of the parent component

Usage

```
t95(fit)
```

Arguments

fit	An object of class `fitTK`

Value

a numeric object

`waic` *Widely Applicable Information Criterion (WAIC)*

Description

Compute WAIC using the `waic()` method of the loo package.

Usage

```
waic(fit)
```

Arguments

`fit`	An object of class `fitTK`

Value

A numeric containing the WAIC

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