

# Package ‘rbioacc’

September 26, 2025

**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>

**License** MIT + file LICENSE

**Encoding** UTF-8

**LazyData** true

**RoxygenNote** 7.3.2

**Biarch** true

**Depends** R (>= 3.5.0)

**Imports** ggplot2, methods, Rcpp, rstan (>= 2.26.0), rstantools (>= 2.1.1), ggmcmc, GGally, loo, stringr, stats, zoo

**LinkingTo** BH (>= 1.66.0), Rcpp, RcppEigen (>= 0.3.3.3.0), RcppParallel (>= 5.0.1), rstan (>= 2.26.0), StanHeaders (>= 2.26.0)

**SystemRequirements** GNU make

**Config/testthat/edition** 3

**Suggests** knitr, rmarkdown, testthat

**VignetteBuilder** knitr

**NeedsCompilation** yes

**Author** Virgile Baudrot [aut, cre],  
Sandrine Charles [aut],  
Ophélie Gestin [ctb],  
Miléna Kaag [aut],  
Christelle Lopes [ctb],  
Gauthier Multari [ctb],  
Alain Pavé [ctb],

Aude Ratier [aut],  
Aur lie Siberchicot [aut]

**Maintainer** Virgile Baudrot <virgile.baudrot@qonfluens.com>

**Repository** CRAN

**Date/Publication** 2025-09-26 09:40:02 UTC

## Contents

|                                               |    |
|-----------------------------------------------|----|
| rbioacc-package . . . . .                     | 3  |
| .fonte . . . . .                              | 4  |
| .index_col_exposure . . . . .                 | 4  |
| .index_col_metabolite . . . . .               | 5  |
| .is_equal_rmInf . . . . .                     | 5  |
| bioacc_metric . . . . .                       | 6  |
| Chironomus_benzoapyrene . . . . .             | 6  |
| Chiro_Creuzot . . . . .                       | 7  |
| corrMatrix . . . . .                          | 7  |
| corrPlot . . . . .                            | 8  |
| df_ppc . . . . .                              | 8  |
| df_PriorPost . . . . .                        | 9  |
| equations . . . . .                           | 10 |
| exposure_names . . . . .                      | 10 |
| Exposure_Sialis_lutaria . . . . .             | 11 |
| fitTK . . . . .                               | 11 |
| Gammarus_azoxistrobine_1d_Rosch2017 . . . . . | 12 |
| Internal_Sialis_lutaria . . . . .             | 12 |
| Male_Gammarus_Merged . . . . .                | 12 |
| Male_Gammarus_seanine_growth . . . . .        | 13 |
| Male_Gammarus_Single . . . . .                | 14 |
| mcmcTraces . . . . .                          | 14 |
| modelData . . . . .                           | 15 |
| modelData_ode . . . . .                       | 16 |
| Oncorhynchus_two . . . . .                    | 17 |
| plot.bioaccMetric . . . . .                   | 17 |
| plot.fitTK . . . . .                          | 18 |
| plot.predictTK . . . . .                      | 18 |
| plot_exposure . . . . .                       | 19 |
| plot_PriorPost . . . . .                      | 19 |
| predict.fitTK . . . . .                       | 20 |
| psrf . . . . .                                | 21 |
| quantile_table . . . . .                      | 22 |
| replace_ . . . . .                            | 22 |
| rmMessWarn . . . . .                          | 23 |
| t95 . . . . .                                 | 23 |
| waic . . . . .                                | 24 |

**Index**

**25**

---

|                 |                               |
|-----------------|-------------------------------|
| rbioacc-package | <i>The 'rbioacc' package.</i> |
|-----------------|-------------------------------|

---

## Description

A DESCRIPTION OF THE PACKAGE

## Author(s)

**Maintainer:** Virgile Baudrot <virgile.baudrot@qonfluens.com>

Authors:

- Sandrine Charles
- Miléna Kaag
- Aude Ratier
- Aurélie Siberchicot

Other contributors:

- Ophélie Gestin [contributor]
- Christelle Lopes [contributor]
- Gauthier Multari [contributor]
- Alain Pavé [contributor]

## 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 | <i>A simple implementation of to_pivot_longer of tidyr</i> |
|--------|------------------------------------------------------------|

---

**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 | <i>Return column matching "expw", "exps", "expf", "exppw" of a data.frame</i> |
|---------------------|-------------------------------------------------------------------------------|

---

**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 | <i>Biaccumulation metrics</i> |
|---------------|-------------------------------|

---

**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

---

|                         |                                                   |
|-------------------------|---------------------------------------------------|
| Chironomus_benzoapyrene | <i>Data on Chironomus exposed to benzoapyrene</i> |
|-------------------------|---------------------------------------------------|

---

**Description**

Data on Chironomus exposed to benzoapyrene

**Usage**

```
data(Chironomus_benzoapyrene)
```

---

|               |                                                         |
|---------------|---------------------------------------------------------|
| Chiro_Creuzot | <i>Data on Chironomus with several exposure routes.</i> |
|---------------|---------------------------------------------------------|

---

**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.

---

|            |                                                        |
|------------|--------------------------------------------------------|
| corrMatrix | <i>Correlations between parameters: colored matrix</i> |
|------------|--------------------------------------------------------|

---

**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 <code>fitTK</code>                                                                                                                                                          |
| plots | 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 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 | <i>Data frame of Posterior over Prior</i> |
|--------------|-------------------------------------------|

---

**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. Deterministic 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**

|                     |                                                                |
|---------------------|----------------------------------------------------------------|
| <code>fit</code>    | An object of class <code>fitTK</code>                          |
| <code>object</code> | The <code>data.frame</code> 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**

|                     |               |
|---------------------|---------------|
| <code>object</code> | 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  $\mu\text{g.mL}^{-1}$  exposure concentrations, and 7 days for 0.000141604  $\mu\text{g.mL}^{-1}$  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  $\mu\text{g.mL}^{-1}$  exposure concentrations, and 7 days for 0.000141604  $\mu\text{g.mL}^{-1}$  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 | <i>Bio-accumulation data set for Gammarus fossarum exposed to Hg spiked water.</i> |
|----------------------|------------------------------------------------------------------------------------|

---

## 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 | <i>Traces of MCMC iterations</i> |
|------------|----------------------------------|

---

## 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. Deterministic parameters can be selected by setting "deterministic" and stochastic parameter with "stochastic" |

**Value**

A traceplot of class ggplot.

---

|           |                                                                                |
|-----------|--------------------------------------------------------------------------------|
| modelData | <i>Create a list giving data and parameters to use in the model inference.</i> |
|-----------|--------------------------------------------------------------------------------|

---

**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 | <i>Data on Oncorhynchus exposition</i> |
|------------------|----------------------------------------|

---

**Description**

Data on Oncorhynchus exposition

**Usage**

data(Oncorhynchus\_two)

---

|                   |                                                       |
|-------------------|-------------------------------------------------------|
| plot.bioaccMetric | <i>Plot function for object of class bioaccMetric</i> |
|-------------------|-------------------------------------------------------|

---

**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 | <i>Plotting method for fitTK objects</i> |
|------------|------------------------------------------|

---

**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 | <i>Plotting method for predictTK objects</i> |
|----------------|----------------------------------------------|

---

**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 original data of the fit object x |

**Value**

A plot of class ggplot

---

|               |                              |
|---------------|------------------------------|
| plot_exposure | <i>Plot exposure profile</i> |
|---------------|------------------------------|

---

**Description**

Plot exposure profile

**Usage**

```
plot_exposure(object)
```

**Arguments**

object                    a data frame with exposure column

**Value**

a plot of class ggplot

---

|                |                                  |
|----------------|----------------------------------|
| plot_PriorPost | <i>Plot Posterior over Prior</i> |
|----------------|----------------------------------|

---

**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 | <i>Prediction function using fitTK object</i> |
|---------------|-----------------------------------------------|

---

**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.        |

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

**Value**

An object of class `predictTK`

An object of class `predictTK`

---

|                   |                                                                   |
|-------------------|-------------------------------------------------------------------|
| <code>psrf</code> | <i>Potential Scale Reduction Factors (PSRF) of the parameters</i> |
|-------------------|-------------------------------------------------------------------|

---

**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 | <i>Quantiles of parameters</i> |
|----------------|--------------------------------|

---

**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_ | <i>Replace element of a vector</i> |
|----------|------------------------------------|

---

**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 | <i>remove message and warning</i> |
|------------|-----------------------------------|

---

**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 | <i>Return the time at 95% depuration of the parent component</i> |
|-----|------------------------------------------------------------------|

---

**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



# Index

## \* dataset

Chiro\_Creuzot, [7](#)  
Chironomus\_benzoapyrene, [6](#)  
Exposure\_Sialis\_lutaria, [11](#)  
Gammarus\_azoxistrobine\_1d\_Rosch2017, [12](#)  
Internal\_Sialis\_lutaria, [12](#)  
Male\_Gammarus\_Merged, [12](#)  
Male\_Gammarus\_seanine\_growth, [13](#)  
Male\_Gammarus\_Single, [14](#)  
Oncorhynchus\_two, [17](#)  
.fonte, [4](#)  
.index\_col\_exposure, [4](#)  
.index\_col\_metabolite, [5](#)  
.is\_equal\_rmInf, [5](#)  
  
bioacc\_metric, [6](#)  
  
Chiro\_Creuzot, [7](#)  
Chironomus\_benzoapyrene, [6](#)  
corrMatrix, [7](#)  
corrPlot, [8](#)  
  
df\_ppc, [8](#)  
df\_PriorPost, [9](#)  
  
equations, [10](#)  
exposure\_names, [10](#)  
Exposure\_Sialis\_lutaria, [11](#)  
  
fitTK, [11](#)  
  
Gammarus\_azoxistrobine\_1d\_Rosch2017, [12](#)  
  
Internal\_Sialis\_lutaria, [12](#)  
  
Male\_Gammarus\_Merged, [12](#)  
Male\_Gammarus\_seanine\_growth, [13](#)  
Male\_Gammarus\_Single, [14](#)  
mcmcTraces, [14](#)  
  
modelData, [15](#)  
modelData\_ode, [16](#)  
  
Oncorhynchus\_two, [17](#)  
  
plot.bioaccMetric, [17](#)  
plot.fitTK, [18](#)  
plot.predictTK, [18](#)  
plot.predictTKstan (plot.predictTK), [18](#)  
plot\_exposure, [19](#)  
plot\_PriorPost, [19](#)  
ppc (df\_ppc), [8](#)  
predict.fitTK, [20](#)  
predict\_manual (predict.fitTK), [20](#)  
predict\_stan (predict.fitTK), [20](#)  
psrf, [21](#)  
  
quantile\_table, [22](#)  
  
rbioacc (rbioacc-package), [3](#)  
rbioacc-package, [3](#)  
replace\_, [22](#)  
rmMessWarn, [23](#)  
  
t95, [23](#)  
  
waic, [24](#)