

Package ‘campsismod’

June 17, 2022

Type Package

Title Generic Implementation of a PK/PD Model

Version 0.9.0

Description A generic, easy-to-use and expandable implementation of a pharmacokinetic (PK) / pharmacodynamic (PD) model based on the S4 class system. This package allows the user to read/write a pharmacometric model from/to files and adapt it further on the fly in the R environment. For this purpose, this package provides an intuitive API to add, modify or delete equations, ordinary differential equations (ODE's), model parameters or compartment properties (like infusion duration or rate, bioavailability and initial values). Finally, this package also provides a useful export of the model for use with simulation packages 'RxODE' and 'mrgsolve'. This package is designed and intended to be used with package 'campsis', a PK/PD simulation platform built on top of 'RxODE' and 'mrgsolve'.

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URL <https://github.com/Calvagone/campsismod>,
<https://calvagone.github.io/>

BugReports <https://github.com/Calvagone/campsismod/issues>

Depends R (>= 4.0.0)

Imports assertthat, dplyr, magrittr, methods, plyr, purrr, readr, tibble, utils

Suggests devtools, knitr, pkgdown, rmarkdown, roxygen2, testthat, xfun

VignetteBuilder knitr

Encoding UTF-8

Language en-US

LazyData true

RoxygenNote 7.1.2

Collate 'global.R' 'data.R' 'utilities.R' 'special_operators.R'
 'check.R' 'generic.R' 'generic_element_list.R'
 'generic_element_position.R' 'generic_list.R' 'pattern.R'
 'model_statement.R' 'model_statements.R'
 'model_unknown_statement.R' 'model_comment.R'
 'model_line_break.R' 'model_equation.R' 'model_ode.R'
 'model_if_statement.R' 'compartment.R' 'compartment_property.R'
 'compartment_properties.R' 'compartment_bioavailability.R'
 'compartment_lag_time.R' 'compartment_infusion_duration.R'
 'compartment_infusion_rate.R' 'compartment_initial_condition.R'
 'compartments.R' 'parameter.R' 'parameters.R' 'code_record.R'
 'code_records.R' 'model_parser.R' 'campsis_model.R'
 'rxode_model.R' 'rxode_conversion.R' 'mrgsolve_model.R'
 'mrgsolve_conversion.R'

NeedsCompilation no

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Repository CRAN

Date/Publication 2022-06-17 12:50:02 UTC

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add	<i>Add element to list.</i>
------------	-----------------------------

Description

Add element to list.

Usage

```
add(object, x, ...)

## S4 method for signature 'pmx_list,pmx_element'
add(object, x, pos = NULL)

## S4 method for signature 'pmx_list,pmx_list'
add(object, x)

## S4 method for signature 'pmx_list,list'
add(object, x)

## S4 method for signature 'compartments,compartment_property'
```

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```
add(object, x)

## S4 method for signature 'compartments,compartments'
add(object, x)

## S4 method for signature 'parameters,single_array_parameter'
add(object, x)

## S4 method for signature 'parameters,double_array_parameter'
add(object, x)

## S4 method for signature 'parameters,parameters'
add(object, x)

## S4 method for signature 'code_record,model_statement'
add(object, x, pos = NULL)

## S4 method for signature 'code_record,code_record'
add(object, x)

## S4 method for signature 'code_records,code_records'
add(object, x)

## S4 method for signature 'code_records,model_statement'
add(object, x, pos = NULL)

## S4 method for signature 'campsis_model,compartment_property'
add(object, x)

## S4 method for signature 'campsis_model,parameter'
add(object, x)

## S4 method for signature 'campsis_model,code_record'
add(object, x)

## S4 method for signature 'campsis_model,model_statement'
add(object, x, pos = NULL)

## S4 method for signature 'campsis_model,campsis_model'
add(object, x)
```

Arguments

object	list object
x	element to add
...	extra arguments, unused by this generic list
pos	position where x needs to be added in list

Value

modified list object

as.data.frame *As data frame method.*

Description

As data frame method.

Usage

```
as.data.frame(x, row.names = NULL, optional = FALSE, ...)

## S4 method for signature 'theta,character,logical'
as.data.frame(x, row.names = NULL, optional = FALSE, ...)

## S4 method for signature 'omega,character,logical'
as.data.frame(x, row.names = NULL, optional = FALSE, ...)

## S4 method for signature 'sigma,character,logical'
as.data.frame(x, row.names = NULL, optional = FALSE, ...)
```

Arguments

x	generic object
row.names	row names
optional	optional
...	extra arguments

Value

data frame

assertSingleCharacterString

Assert the given character vector is a single character string.

Description

Assert the given character vector is a single character string.

Usage

```
assertSingleCharacterString(x)
```

Arguments

x	single character string
---	-------------------------

Value

no return value

autoDetectNONMEM	<i>Auto-detect special variables from NONMEM as compartment properties. Bioavailabilities, infusion durations/rates and lag times will be automatically detected.</i>
------------------	---

Description

Auto-detect special variables from NONMEM as compartment properties. Bioavailabilities, infusion durations/rates and lag times will be automatically detected.

Usage

```
autoDetectNONMEM(object, ...)
## S4 method for signature 'campsis_model'
autoDetectNONMEM(object, ...)
```

Arguments

object	object that has NONMEM special variables to be identified
...	extra arguments, unused

Value

updated object

Bioavailability	<i>Create a bioavailability for the specified compartment.</i>
-----------------	--

Description

Create a bioavailability for the specified compartment.

Usage

```
Bioavailability(compartment, rhs = "")
```

Arguments

compartment	compartment index
rhs	right-hand side part of the equation

Value

a bioavailability property

CampsisModel

Create a new CAMPSIS model.

Description

Create a new CAMPSIS model.

Usage

`CampsisModel()`

Value

a CAMPSIS model, empty

campsis_model-class

CAMPSIS model class.

Description

CAMPSIS model class.

Slots

`model` a list of code records
`parameters` model parameters
`compartments` model compartments

CodeRecords	<i>Create a list of code records.</i>
-------------	---------------------------------------

Description

Create a list of code records.

Usage

```
CodeRecords()
```

Value

an empty list of code records

code_record-class	<i>Code record class. See this code record as an abstract class. 2 implementations are possible: - properties record (lag, duration, rate & bioavailability properties) - statements record (main, ode & error records)</i>
-------------------	---

Description

Code record class. See this code record as an abstract class. 2 implementations are possible: - properties record (lag, duration, rate & bioavailability properties) - statements record (main, ode & error records)

Slots

```
comment a comment, single character value
statements model statements
```

Comment	<i>Create a new comment.</i>
---------	------------------------------

Description

Create a new comment.

Usage

```
Comment(x)
```

Arguments

x comment, single character string

Value

a comment

comment-class *Comment class. A statement starting with #.*

Description

Comment class. A statement starting with #.

Compartment *Create a compartment.*

Description

Create a compartment.

Usage

`Compartment(index, name = NA)`

Arguments

index compartment index
name compartment name (without prefix)

Value

an empty list of compartments

compartment-class *Compartment class.*

Description

Compartment class.

Slots

name compartment name (without prefix)
index compartment index

Compartments *Create a list of compartments*

Description

Create a list of compartments

Usage

Compartments()

Value

an empty list of compartments

compartments-class *Compartments class.*

Description

Compartments class.

Slots

properties compartment properties of the compartments defined in this class

compartment_bioavailability-class
 Compartment bioavailability class.

Description

Compartment bioavailability class.

compartment_infusion_duration-class
 Compartment infusion duration class.

Description

Compartment infusion duration class.

`compartment_infusion_rate-class`

Compartment infusion rate class.

Description

Compartment infusion rate class.

`compartment_initial_condition-class`

Compartment initial condition class.

Description

Compartment initial condition class.

`compartment_lag_time-class`

Compartment lag time class.

Description

Compartment lag time class.

`compartment_properties-class`

Compartment properties class.

Description

Compartment properties class.

compartment_property-class

Compartment property class.

Description

Compartment property class.

Slots

compartment related compartment index
 rhs right-hand side formula
 comment comment if any, single character string

contains

Check if an element exists in list.

Description

Check if an element exists in list.

Usage

```
contains(object, x)

## S4 method for signature 'pmx_list,pmx_element'
contains(object, x)

## S4 method for signature 'statements_record,model_statement'
contains(object, x)

## S4 method for signature 'campsis_model,pmx_element'
contains(object, x)
```

Arguments

object	list object
x	element to check if exists

Value

logical value, TRUE or FALSE

default	<i>Get default element from list.</i>
---------	---------------------------------------

Description

Get default element from list.

Usage

```
default(object, ...)
```

Arguments

object	list object
...	additional arguments

Value

the default element from list

delete	<i>Delete an element from this list.</i>
--------	--

Description

Delete an element from this list.

Usage

```
delete(object, x)

## S4 method for signature 'pmx_list,pmx_element'
delete(object, x)

## S4 method for signature 'pmx_list,integer'
delete(object, x)

## S4 method for signature 'compartments,compartment_property'
delete(object, x)

## S4 method for signature 'parameters,single_array_parameter'
delete(object, x)

## S4 method for signature 'parameters,double_array_parameter'
delete(object, x)
```

```

## S4 method for signature 'statements_record,model_statement'
delete(object, x)

## S4 method for signature 'statements_record,integer'
delete(object, x)

## S4 method for signature 'code_records,model_statement'
delete(object, x)

## S4 method for signature 'campsis_model,compartment_property'
delete(object, x)

## S4 method for signature 'campsis_model,parameter'
delete(object, x)

## S4 method for signature 'campsis_model,code_record'
delete(object, x)

## S4 method for signature 'campsis_model,model_statement'
delete(object, x)

```

Arguments

object	list object
x	element to delete or element index

Value

the updated list

disable	<i>Disable.</i>
---------	-----------------

Description

Disable.

Usage

```

disable(object, x, ...)

## S4 method for signature 'parameters,character'
disable(object, x, ...)

## S4 method for signature 'campsis_model,character'
disable(object, x, ...)

```

Arguments

object	generic object
x	what needs to be disabled
...	extra arguments needed for disabling

Value

object with some disabled features

double_array_parameter-class

Double-array parameter class. This parameter has 2 indexes. It can thus be used to define correlations between parameters.

Description

Double-array parameter class. This parameter has 2 indexes. It can thus be used to define correlations between parameters.

duration_record-class (Infusion)-duration record class.**Description**

(Infusion)-duration record class.

Equation *Create a new equation.***Description**

Create a new equation.

Usage

```
Equation(lhs, rhs = "", comment = as.character(NA))
```

Arguments

lhs	left-hand side variable corresponding to the assigned variable name
rhs	right-hand side expression corresponding to a formula
comment	comment if any, single character string

Value

an equation

equation-class	<i>Equation class. Any statement in the form A = B.</i>
----------------	---

Description

Equation class. Any statement in the form A = B.

Slots

lhs left-hand side expression
rhs right-hand side expression

ErrorRecord	<i>Create ERROR code record.</i>
-------------	----------------------------------

Description

Create ERROR code record.

Usage

```
ErrorRecord(code = character())
```

Arguments

code code record

Value

an ERROR code record

error_record-class	<i>Error record class.</i>
--------------------	----------------------------

Description

Error record class.

export	<i>Export function.</i>
--------	-------------------------

Description

Export function.

Usage

```
export(object, dest, ...)

## S4 method for signature 'campsis_model,character'
export(object, dest, outvars = NULL)

## S4 method for signature 'campsis_model,rxode_type'
export(object, dest, ...)

## S4 method for signature 'campsis_model,mrgsolve_type'
export(object, dest, outvars = NULL)
```

Arguments

object	generic object
dest	destination
...	optional arguments
outvars	additional variables to capture

Value

specific object depending on given destination

export_type-class	<i>Export type class.</i>
-------------------	---------------------------

Description

Export type class.

extractLhs*Extract left-hand-side expression.*

Description

Extract left-hand-side expression.

Usage

```
extractLhs(x, split = "=")
```

Arguments

x	character value
split	character where to split

Value

left-hand-side expression, not trimmed

extractRhs*Extract right-hand-side expression.*

Description

Extract right-hand-side expression.

Usage

```
extractRhs(x, split = "=")
```

Arguments

x	character value
split	character where to split

Value

right-hand side expression

extractTextBetweenBrackets

Extract text between brackets.

Description

Extract text between brackets.

Usage

```
extractTextBetweenBrackets(x)
```

Arguments

x	character value
---	-----------------

Value

text between brackets (trimmed)

find

Find an element in list.

Description

Find an element in list.

Usage

```
find(object, x)

## S4 method for signature 'pmx_list,pmx_element'
find(object, x)

## S4 method for signature 'compartments,compartment_property'
find(object, x)

## S4 method for signature 'statements_record,model_statement'
find(object, x)

## S4 method for signature 'code_records,model_statement'
find(object, x)

## S4 method for signature 'campsis_model,compartment'
find(object, x)
```

```
## S4 method for signature 'campsis_model,compartment_property'
find(object, x)

## S4 method for signature 'campsis_model,parameter'
find(object, x)

## S4 method for signature 'campsis_model,code_record'
find(object, x)

## S4 method for signature 'campsis_model,model_statement'
find(object, x)
```

Arguments

object	list object
x	element to find, only key slots need to be filled in

Value

the element from the list that has same name as x, or NULL if no element was found

fixOmega

Fix omega matrix for SAME OMEGA parameters that have NA values due to imperfections in Pharmpy import.

Description

Fix omega matrix for SAME OMEGA parameters that have NA values due to imperfections in Pharmpy import.

Usage

```
fixOmega(object)

## S4 method for signature 'parameters'
fixOmega(object)
```

Arguments

object	generic object
--------	----------------

Value

the parameter that matches

f_record-class *Bioavailability record class.*

Description

Bioavailability record class.

getByIndex *Get element by index.*

Description

Get element by index.

Usage

```
getByIndex(object, x)

## S4 method for signature 'pmx_list,integer'
getByIndex(object, x)

## S4 method for signature 'pmx_list,numeric'
getByIndex(object, x)

## S4 method for signature 'compartment_properties,compartment_property'
getByIndex(object, x)

## S4 method for signature 'parameters,parameter'
getByIndex(object, x)
```

Arguments

object	list object
x	element index

Value

element from the list whose index matches with provided index

`getByName`*Get an element from a list by name. Never return more than 1 element.***Description**

Get an element from a list by name. Never return more than 1 element.

Usage

```
getByName(object, name)

## S4 method for signature 'pmx_list,character'
getByName(object, name)
```

Arguments

<code>object</code>	list object
<code>name</code>	element name to search for

Value

the element that was found or NULL if no element was found with the same name

`getCompartmentIndex`*Get the compartment index for the specified compartment name.***Description**

Get the compartment index for the specified compartment name.

Usage

```
getCompartmentIndex(object, name)

## S4 method for signature 'compartments,character'
getCompartmentIndex(object, name)

## S4 method for signature 'campsis_model,character'
getCompartmentIndex(object, name)
```

Arguments

<code>object</code>	generic object that contains compartments information
<code>name</code>	compartment name

Value

the corresponding compartment index

 getName*Get element name.***Description**

Get element name.

Usage

```
getName(x)

## S4 method for signature 'unknown_statement'
getName(x)

## S4 method for signature 'comment'
getName(x)

## S4 method for signature 'line_break'
getName(x)

## S4 method for signature 'equation'
getName(x)

## S4 method for signature 'ode'
getName(x)

## S4 method for signature 'if_statement'
getName(x)

## S4 method for signature 'compartment'
getName(x)

## S4 method for signature 'compartment_bioavailability'
getName(x)

## S4 method for signature 'compartment_lag_time'
getName(x)

## S4 method for signature 'compartment_infusion_duration'
getName(x)

## S4 method for signature 'compartment_infusion_rate'
getName(x)
```

```

## S4 method for signature 'compartment_initial_condition'
getName(x)

## S4 method for signature 'theta'
getName(x)

## S4 method for signature 'omega'
getName(x)

## S4 method for signature 'sigma'
getName(x)

## S4 method for signature 'main_record'
getName(x)

## S4 method for signature 'ode_record'
getName(x)

## S4 method for signature 'f_record'
getName(x)

## S4 method for signature 'lag_record'
getName(x)

## S4 method for signature 'duration_record'
getName(x)

## S4 method for signature 'rate_record'
getName(x)

## S4 method for signature 'init_record'
getName(x)

## S4 method for signature 'error_record'
getName(x)

```

Arguments

x element to know the name

Value

the name of this element

getNameInModel	<i>Get the name of the given parameter in the CAMPSIS model.</i>
----------------	--

Description

Get the name of the given parameter in the CAMPSIS model.

Usage

```
getNameInModel(x)

## S4 method for signature 'theta'
getNameInModel(x)

## S4 method for signature 'omega'
getNameInModel(x)

## S4 method for signature 'sigma'
getNameInModel(x)
```

Arguments

x element to know the name

Value

the name of this parameter

getNames	<i>Get element names from list.</i>
----------	-------------------------------------

Description

Get element names from list.

Usage

```
getNames(object)

## S4 method for signature 'pmx_list'
getNames(object)
```

Arguments

object list object

Value

character vector with all the element names of this list

<code>getNONMEMName</code>	<i>Get NONMEM name.</i>
----------------------------	-------------------------

Description

Get NONMEM name.

Usage

```
getNONMEMName(object)

## S4 method for signature 'theta'
getNONMEMName(object)

## S4 method for signature 'omega'
getNONMEMName(object)

## S4 method for signature 'sigma'
getNONMEMName(object)
```

Arguments

`object` generic object

Value

the NONMEM name associated with this object

<code>getPrefix</code>	<i>Get prefix.</i>
------------------------	--------------------

Description

Get prefix.

Usage

```
getPrefix(object, ...)

## S4 method for signature 'compartment_bioavailability'
getPrefix(object, ...)

## S4 method for signature 'compartment_lag_time'
getPrefix(object, ...)

## S4 method for signature 'compartment_infusion_duration'
getPrefix(object, ...)

## S4 method for signature 'compartment_infusion_rate'
getPrefix(object, ...)

## S4 method for signature 'compartment_initial_condition'
getPrefix(object, ...)
```

Arguments

object	generic object
...	e.g. dest='mrgsolve'

Value

the prefix of this object

getRecordDelimiter *Get record delimiter.*

Description

Get record delimiter.

Usage

```
getRecordDelimiter(line)
```

Arguments

line	any line, single character value
------	----------------------------------

Value

the record delimiter between brackets

getRecordName

*Get record name.***Description**

Get record name.

Usage

```
getRecordName(object)

## S4 method for signature 'compartment_bioavailability'
getRecordName(object)

## S4 method for signature 'compartment_lag_time'
getRecordName(object)

## S4 method for signature 'compartment_infusion_duration'
getRecordName(object)

## S4 method for signature 'compartment_infusion_rate'
getRecordName(object)

## S4 method for signature 'compartment_initial_condition'
getRecordName(object)
```

Arguments

object	generic object
--------	----------------

Value

the name of the record

getUncertainty

*Get uncertainty on the parameters.***Description**

Get uncertainty on the parameters.

Usage

```
getUncertainty(object, ...)

## S4 method for signature 'parameter'
getUncertainty(object, varcov, ...)

## S4 method for signature 'parameters'
getUncertainty(object, ...)

## S4 method for signature 'campsis_model'
getUncertainty(object, ...)
```

Arguments

object	generic object
...	extra arguments
varcov	variance covariance matrix

Value

data frame with standard error (se) and relative standard error (rse)

getVarCov	<i>Get variance-covariance matrix.</i>
-----------	--

Description

Get variance-covariance matrix.

Usage

```
getVarCov(object)

## S4 method for signature 'parameters'
getVarCov(object)

## S4 method for signature 'campsis_model'
getVarCov(object)
```

Arguments

object	generic object
--------	----------------

Value

a variance-covariance matrix (data frame) or NULL if no matrix present

hasComment*Check if string contains CAMPSIS-style comments.***Description**

Check if string contains CAMPSIS-style comments.

Usage

```
hasComment(x)
```

Arguments

x	character vector
---	------------------

Value

logical value

IfStatement*Create a new IF-statement.***Description**

Create a new IF-statement.

Usage

```
IfStatement(condition, equation, comment = as.character(NA))
```

Arguments

condition	condition, single character string
equation	equation if condition is met
comment	comment if any, single character string

Value

an IF-statement

if_statement-class *If-statement class. Any statement in the form if (condition) A = B.*

Description

If-statement class. Any statement in the form if (condition) A = B.

Slots

condition IF statement condition
equation any equation or ODE

indexOf *Get the index of an element in list.*

Description

Get the index of an element in list.

Usage

```
indexOf(object, x)  
  
## S4 method for signature 'pmx_list,pmx_element'  
indexOf(object, x)
```

Arguments

object	list object
x	element to know the index

Value

index of this element

InfusionDuration *Create an infusion duration.*

Description

Create an infusion duration.

Usage

```
InfusionDuration(compartment, rhs = "")
```

Arguments

compartment	compartment index
rhs	right-hand side part of the equation

Value

an infusion duration property

InfusionRate *Create an infusion rate.*

Description

Create an infusion rate.

Usage

```
InfusionRate(compartment, rhs = "")
```

Arguments

compartment	compartment index
rhs	right-hand side part of the equation

Value

an infusion rate property

InitialCondition	<i>Create an initial condition.</i>
------------------	-------------------------------------

Description

Create an initial condition.

Usage

```
InitialCondition(compartment, rhs = "")
```

Arguments

compartment	compartment index
rhs	right-hand side part of the equation

Value

an initial condition property

init_record-class	<i>Init record class.</i>
-------------------	---------------------------

Description

Init record class.

isComment	<i>Check if string is a CAMPSIS comment (i.e. not an equation).</i>
-----------	---

Description

Check if string is a CAMPSIS comment (i.e. not an equation).

Usage

```
isComment(x)
```

Arguments

x	character vector
---	------------------

Value

logical value

isDiag	<i>Is diagonal.</i>
--------	---------------------

Description

Is diagonal.

Usage

```
isDiag(object)

## S4 method for signature 'double_array_parameter'
isDiag(object)
```

Arguments

object generic object

Value

logical value

isEmptyLine	<i>Check if string is an empty line.</i>
-------------	--

Description

Check if string is an empty line.

Usage

```
isEmptyLine(x)
```

Arguments

x character vector

Value

logical value

isEquation	<i>Say if line in record is an equation not.</i>
------------	--

Description

Say if line in record is an equation not.

Usage

`isEquation(x)`

Arguments

x character value

Value

logical value

isIfStatement	<i>Say if line in record is an IF-statement.</i>
---------------	--

Description

Say if line in record is an IF-statement.

Usage

`isIfStatement(x)`

Arguments

x character value

Value

logical value

isODE *Say if line(s) in record is/are ODE or not.*

Description

Say if line(s) in record is/are ODE or not.

Usage

`isODE(x)`

Arguments

`x` character vector

Value

logical vector

isRecordDelimiter *Is record delimiter: A record delimiter is any line starting with [...].*

Description

Is record delimiter. A record delimiter is any line starting with [...].

Usage

`isRecordDelimiter(line)`

Arguments

`line` any line, single character value

Value

a logical value

isStrictRecordDelimiter

Is strict record delimiter. A strict record delimiter is any line starting with [...] and followed by nothing but spaces or a possible comment.

Description

Is strict record delimiter. A strict record delimiter is any line starting with [...] and followed by nothing but spaces or a possible comment.

Usage

```
isStrictRecordDelimiter(line)
```

Arguments

line	any line, single character value
------	----------------------------------

Value

a logical value

LagTime

Create a lag time for the specified compartment.

Description

Create a lag time for the specified compartment.

Usage

```
LagTime(compartment, rhs = "")
```

Arguments

compartment	compartment index
rhs	right-hand side part of the equation

Value

a lag time property

lag_record-class *Lag record class.*

Description

Lag record class.

length,pmx_list-method
Return the length of this list.

Description

Return the length of this list.

Usage

```
## S4 method for signature 'pmx_list'  
length(x)  
  
## S4 method for signature 'statements_record'  
length(x)
```

Arguments

x list object

Value

the length of this list, integer value

LineBreak *Create a new line break.*

Description

Create a new line break.

Usage

LineBreak()

Value

a line break

`line_break-class` *Line-break class. A linebreak in the model.*

Description

Line-break class. A linebreak in the model.

`MainRecord` *Create MAIN code record.*

Description

Create MAIN code record.

Usage

```
MainRecord(code = character())
```

Arguments

`code` code record

`main_record-class` *Main record class.*

Description

Main record class.

maxIndex

Max index.

Description

Max index.

Usage

```
maxIndex(object)

## S4 method for signature 'parameters'
maxIndex(object)
```

Arguments

object generic object

Value

max index

minIndex

Min index.

Description

Min index.

Usage

```
minIndex(object)

## S4 method for signature 'parameters'
minIndex(object)
```

Arguments

object generic object

Value

min index

ModelStatements	<i>Create an empty list of model statements.</i>
-----------------	--

Description

Create an empty list of model statements.

Usage

```
ModelStatements()
```

Value

a model statements object

model_library	<i>CAMPSIS model library.</i>
---------------	-------------------------------

Description

A list containing pharmacokinetic (PK) and pharmacodynamic (PD) model templates.

Usage

```
model_library
```

Format

A list with all the models:

advan1_trans1 1-compartment PK model (K,V)
advan1_trans2 1-compartment PK model (CL,V)
advan2_trans1 1-compartment PK model with absorption compartment (KA,K,V)
advan2_trans2 1-compartment PK model with absorption compartment (KA,CL,V)
advan3_trans1 2-compartment PK model (K,V,K12,K21)
advan3_trans3 2-compartment PK model (CL,V,Q,VSS)
advan3_trans4 2-compartment PK model (CL,V1,V2,Q)
advan4_trans1 2-compartment PK model with absorption compartment (KA,K,V,K12,K21)
advan4_trans3 2-compartment PK model with absorption compartment (KA,CL,V,Q,VSS)
advan4_trans4 2-compartment PK model with absorption compartment (KA,CL,V1,V2,Q)
advan11_trans4 3-compartment PK model (CL,V1,V2,V3,Q2,Q3)
advan12_trans4 3-compartment PK model with absorption compartment (KA,CL,V1,V2,V3,Q2,Q3)

direct_effect_model direct effect PD model (EMAX,EC50,GAMMA,E0)
effect_cmt_model effect compartment PD model (KE0)
irm_kin_inhibition indirect response PD model - inhibition of KIN (IC50,KIN,KOUT)
irm_kin_stimulation indirect response PD model - stimulation of KIN (EMAX,EC50,KIN,KOUT)
irm_kout_inhibition indirect response PD model - inhibition of KOUT (IC50,KIN,KOUT)
irm_kout_stimulation indirect response PD model - stimulation of KOUT (EMAX,EC50,KIN,KOUT)
transit_cmt_model transit compartment PD model (BASE,POWER,MTT,SLOPE,KTR)
filgrastim_pkpd_krzyzanski PK/PD model of filgrastim (Krzyszanski et al., see URL below)
my_model1 Example of 2-compartment PK model with variance-covariance matrix

Source

<https://www.iconplc.com/innovation/nonmem/>
<http://repository.ddmore.eu/model/DDMODEL00000077/>
<https://calvagone.github.io/campsis.doc/>

model_statement-class *Model statement class. Any statement in a code record.*

Description

Model statement class. Any statement in a code record.

Slots

comment a comment associated to this model statement

model_statements-class

Model statements class. A list of statements.

Description

Model statements class. A list of statements.

model_suite	<i>CAMPSIS model suite.</i>
-------------	-----------------------------

Description

A library of models of all kinds, ready to be simulated in Campsis. These model templates are sorted into the following categories: pharmacokinetic (PK), pharmacodynamic (PD), target-mediated drug disposition (TMDD), NONMEM, literature and other (custom models).

Usage

```
model_suite
```

Format

A list with all the models:

pk extensive list of pharmacokinetic (PK) model templates

pd list of pharmacodynamic (PD) model templates, to be plugged into any pharmacokinetic (PK) model

tmdd extensive list of target-mediated drug disposition (TMDD) model templates

nonmem list of model templates translated from standard NONMEM control streams

literature a couple of models coming from the literature

other a couple of custom models

Source

<https://calvagone.github.io/campsis.doc/>

<https://www.iconplc.com/innovation/nonmem/>

<http://repository.ddmore.eu/model/DDMODEL00000077/>

mrgsolveBlock	<i>Convert code record for mrgsolve.</i>
---------------	--

Description

Convert code record for mrgsolve.

Usage

```
mrgsolveBlock(record, init = NULL, capture = FALSE)
```

Arguments

record	code record
init	name of mrgsolve block
capture	'capture' instead of 'double'

Value

translated record for mrgsolve

`mrgsolveCapture` *Get the CAPTURE block for mrgsolve.*

Description

Get the CAPTURE block for mrgsolve.

Usage

`mrgsolveCapture(outvars, model)`

Arguments

outvars	outvars in method simulate
model	CAMPSIS model

Value

CAPTURE block or character(0) if no variable in outvars

`mrgsolveCompartm` *Get the compartment block for mrgsolve.*

Description

Get the compartment block for mrgsolve.

Usage

`mrgsolveCompartm(model)`

Arguments

model	CAMPSIS model
-------	---------------

Value

character vector, each value is a line

mrgsolveMain

Get the MAIN block for mrgsolve.

Description

Get the MAIN block for mrgsolve.

Usage

```
mrgsolveMain(model)
```

Arguments

model CAMPSIS model

Value

MAIN block

mrgsolveMatrix

Get the OMEGA/SIGMA matrix for mrgsolve.

Description

Get the OMEGA/SIGMA matrix for mrgsolve.

Usage

```
mrgsolveMatrix(model, type = "omega")
```

Arguments

model CAMPSIS model

type either omega or sigma

Value

named matrix or character(0) if matrix is empty

`mrgsolveOde`

Get the ODE block for mrgsolve.

Description

Get the ODE block for mrgsolve.

Usage

```
mrgsolveOde(model)
```

Arguments

model CAMPSIS model

Value

ODE block

`mrgsolveParam`

Get the parameters block for mrgsolve.

Description

Get the parameters block for mrgsolve.

Usage

```
mrgsolveParam(model)
```

Arguments

model CAMPSIS model

Value

character vector, 1 parameter per line. First one is header [PARAM].

mrgsolveTable *Get the TABLE block for mrgsolve.*

Description

Get the TABLE block for mrgsolve.

Usage

```
mrgsolveTable(model)
```

Arguments

model CAMPSIS model

Value

TABLE block if at least one line in error record, character(0) otherwise

mrgsolve_type-class *Mrgsolve export type class.*

Description

Mrgsolve export type class.

Ode *Create a new ordinary differential equation (ODE).*

Description

Create a new ordinary differential equation (ODE).

Usage

```
Ode(lhs, rhs = "", comment = as.character(NA))
```

Arguments

lhs left-hand side variable corresponding to derivative name, must start with 'A_'

rhs right-hand side expression corresponding to derivative value

comment comment if any, single character string

Value

an ODE

ode-class

ODE class. Any statement in the form d/dt(A_CMT) = B.

Description

ODE class. Any statement in the form $d/dt(A_CMT) = B$.

OdeRecord

Create ODE code record.

Description

Create ODE code record.

Usage

```
OdeRecord(code = character())
```

Arguments

code code record

Value

an ODE code record

ode_record-class

ODE record class.

Description

ODE record class.

Omega

Create an OMEGA parameter.

Description

Create an OMEGA parameter.

Usage

```
Omega(  
  name = NA,  
  index = NA,  
  index2 = NA,  
  value = NA,  
  fix = FALSE,  
  type = NULL,  
  same = NA  
)
```

Arguments

name	parameter name, e.g. CL (prefix OMEGA will be added automatically)
index	parameter index
index2	second parameter index
value	parameter value
fix	parameter was fixed in estimation, logical value
type	variance type: 'var', 'sd', 'covar', 'cor', 'cv' or 'cv%'
same	NA by default, FALSE for first OMEGA followed by 'SAME' OMEGA's, TRUE for 'SAME' OMEGA's

Value

an OMEGA parameter

omega-class

Omega parameter class.

Description

Omega parameter class.

Slots

same logical value, tell if this omega is the same as the previous one

parameter-class*Parameter class. Any parameter in a pharmacometric model.***Description**

Parameter class. Any parameter in a pharmacometric model.

Slots

- `name` parameter name, optional (although recommended)
- `index` parameter index, integer
- `value` parameter value (e.g. the estimated value from a modelling tool)
- `fix` logical value, say if parameter was fixed in the modelling phase

Parameters*Create a list of parameters.***Description**

Create a list of parameters.

Usage

```
Parameters()
```

Value

an empty list of parameters

parameters-class*Parameters class.***Description**

Parameters class.

Slots

- `varcov` associated variance-covariance matrix

parseIfStatement *Parse IF-statement. Assumption: isIfStatement method already called and returned TRUE.*

Description

Parse IF-statement. Assumption: isIfStatement method already called and returned TRUE.

Usage

```
parseIfStatement(line, comment = as.character(NA))
```

Arguments

line	IF-statement as single character string value, comment omitted
comment	any comment, NA by default

Value

an IF statement object

parseStatements *Parse statements code and return CAMPSIS statements.*

Description

Parse statements code and return CAMPSIS statements.

Usage

```
parseStatements(code)
```

Arguments

code	character vector containing all statements (text form)
------	--

Value

a list of CAMPSIS statements

Pattern	<i>Create a pattern.</i>
---------	--------------------------

Description

Create a pattern.

Usage

`Pattern(x)`

Arguments

x	regular expression
---	--------------------

Value

a pattern

pattern-class	<i>Pattern class.</i>
---------------	-----------------------

Description

Pattern class.

pmx_element-class	<i>PMX element class.</i>
-------------------	---------------------------

Description

PMX element class.

pmx_list-class	<i>PMX list class.</i>
----------------	------------------------

Description

PMX list class.

Slots

list effective list which will contain the elements
type type of the elements this list may contain

pmx_position-class *PMX position class.*

Description

PMX position class.

pmx_position_by_element-class
 PMX position by element class.

Description

PMX position by element class.

pmx_position_by_index-class
 PMX position by index class.

Description

PMX position by index class.

Position *Element position in list.*

Description

Element position in list.

Usage

`Position(x, after = TRUE)`

Arguments

- | | |
|-------|--|
| x | either an integer position (useful to add an element in a code record at a specified position) or an model element (element can be a model statement or a code record) |
| after | element to be added will be added after x (if after is TRUE) or before x (if after is FALSE) |

Value

a position object

processExtraArg	<i>Process extra arguments.</i>
-----------------	---------------------------------

Description

Process extra arguments.

Usage

```
processExtraArg(args, name, default = NULL, mandatory = FALSE)
```

Arguments

args	arguments list
name	argument name to retrieve
default	default value if argument is not present
mandatory	mandatory argument, logical value

Value

requested argument value

properties_record-class	<i>Properties record class.</i>
-------------------------	---------------------------------

Description

Properties record class.

rate_record-class	<i>(Infusion)-rate record class.</i>
-------------------	--------------------------------------

Description

(Infusion)-rate record class.

read

Generic read method to read data from a file or a folder.

Description

Generic read method to read data from a file or a folder.

Usage

```
read(file, ...)
```

Arguments

file	path to the file or folder to be read
...	extra arguments

Value

the object representation of the data contained in the file

read.allparameters

Read all parameters files at once.

Description

Read all parameters files at once.

Usage

```
read.allparameters(folder)
```

Arguments

folder	path to folder or path to zipped project
--------	--

Value

parameters object

`read.campsis` *Read a CAMPSIS model.*

Description

Read a CAMPSIS model.

Usage

```
read.campsis(file)
```

Arguments

`file` path to folder

Value

a CAMPSIS model

`read.model` *Read model file.*

Description

Read model file.

Usage

```
read.model(file)
```

Arguments

`file` path to records

Value

records object

read.parameters *Read parameters file.*

Description

Read parameters file.

Usage

```
read.parameters(file, type)
```

Arguments

file	path to CSV file
type	parameter type: 'theta', 'omega' or 'sigma'

Value

parameters sub list

read.varcov *Read variance-covariance file.*

Description

Read variance-covariance file.

Usage

```
read.varcov(file)
```

Arguments

file	path to CSV file
------	------------------

Value

variance-covariance matrix

replace

Replace element by another in list.

Description

Replace element by another in list.

Usage

```
replace(object, x)

## S4 method for signature 'pmx_list,pmx_element'
replace(object, x)

## S4 method for signature 'pmx_list,pmx_list'
replace(object, x)

## S4 method for signature 'pmx_list,list'
replace(object, x)

## S4 method for signature 'compartments,compartment_property'
replace(object, x)

## S4 method for signature 'parameters,single_array_parameter'
replace(object, x)

## S4 method for signature 'parameters,double_array_parameter'
replace(object, x)

## S4 method for signature 'statements_record,model_statement'
replace(object, x)

## S4 method for signature 'code_records,model_statement'
replace(object, x)

## S4 method for signature 'campsis_model,compartment'
replace(object, x)

## S4 method for signature 'campsis_model,compartment_property'
replace(object, x)

## S4 method for signature 'campsis_model,parameter'
replace(object, x)

## S4 method for signature 'campsis_model,code_record'
replace(object, x)
```

```
## S4 method for signature 'campsis_model,model_statement'  
replaceAll(object, x)
```

Arguments

object	list object
x	element to replace

Value

list object or an error if the element does not exist in the list

replaceAll	<i>Replace all occurrences in object.</i>
------------	---

Description

Replace all occurrences in object.

Usage

```
replaceAll(object, pattern, replacement, ...)  
  
## S4 method for signature 'character,variable_pattern,character'  
replaceAll(object, pattern, replacement, ...)  
  
## S4 method for signature 'character,pattern,character'  
replaceAll(object, pattern, replacement, ...)  
  
## S4 method for signature 'model_statement,pattern,character'  
replaceAll(object, pattern, replacement, ...)  
  
## S4 method for signature 'equation,pattern,character'  
replaceAll(object, pattern, replacement, ...)  
  
## S4 method for signature 'if_statement,pattern,character'  
replaceAll(object, pattern, replacement, ...)  
  
## S4 method for signature 'code_record,pattern,character'  
replaceAll(object, pattern, replacement, ...)  
  
## S4 method for signature 'code_records,pattern,character'  
replaceAll(object, pattern, replacement, ...)  
  
## S4 method for signature 'campsis_model,pattern,character'  
replaceAll(object, pattern, replacement, ...)  
  
## S4 method for signature 'campsis_model,character,character'  
replaceAll(object, pattern, replacement, ...)
```

Arguments

object	generic object (e.g. model, code_record(s), etc.)
pattern	pattern to be replaced
replacement	replacement string
...	extra arguments

Value

the same object with all occurrences replaced

<i>rxodeCode</i>	<i>Get code for RxODE.</i>
------------------	----------------------------

Description

Get code for RxODE.

Usage

```
rxodeCode(model)
```

Arguments

model	CAMPSIS model
-------	---------------

Value

corresponding model code for RxODE

<i>rxodeMatrix</i>	<i>Get the OMEGA/SIGMA matrix for RxODE.</i>
--------------------	--

Description

Get the OMEGA/SIGMA matrix for RxODE.

Usage

```
rxodeMatrix(model, type = "omega")
```

Arguments

model	CAMPSIS model
type	either omega or sigma

Value

omega/sigma named matrix

rxodeParams *Get the parameters vector for RxODE.*

Description

Get the parameters vector for RxODE.

Usage

```
rxodeParams(model)
```

Arguments

model CAMPSIS model

Value

named vector with THETA values

rxode_type-class *RxODE export type class.*

Description

RxODE export type class.

select *Get a subset of an object.*

Description

Get a subset of an object.

Usage

```
select(object, ...)

## S4 method for signature 'data.frame'
select(object, ...)

## S4 method for signature 'compartment_properties'
select(object, ...)

## S4 method for signature 'parameters'
select(object, ...)
```

Arguments

object	generic object
...	arguments to select

Value

subset of an object

Sigma	<i>Create a SIGMA parameter.</i>
-------	----------------------------------

Description

Create a SIGMA parameter.

Usage

```
Sigma(name = NA, index = NA, index2 = NA, value = NA, fix = FALSE, type = NULL)
```

Arguments

name	parameter name, e.g. CL (prefix SIGMA will be added automatically)
index	parameter index
index2	second parameter index
value	parameter value
fix	parameter was fixed in estimation, logical value
type	variance type: 'var', 'sd', 'covar', 'cv' or 'cv%'

Value

a SIGMA parameter

sigma-class	<i>Sigma parameter class.</i>
-------------	-------------------------------

Description

Sigma parameter class.

single_array_parameter-class

Single-array parameter class. This parameter has a single index value.

Description

Single-array parameter class. This parameter has a single index value.

sort

Sort the specified list.

Description

Sort the specified list.

Usage

```
sort(x, decreasing = FALSE, ...)

## S4 method for signature 'compartment_properties'
sort(x, decreasing = FALSE, ...)

## S4 method for signature 'compartments'
sort(x, decreasing = FALSE, ...)

## S4 method for signature 'parameters'
sort(x, decreasing = FALSE, ...)

## S4 method for signature 'code_records'
sort(x, decreasing = FALSE, ...)

## S4 method for signature 'campsis_model'
sort(x, decreasing = FALSE, ...)
```

Arguments

x	list object
decreasing	increasing or decreasing order
...	extra arguments

Value

same list but ordered

standardise	<i>Standardise.</i>
-------------	---------------------

Description

Standardise.

Usage

```
standardise(object, ...)

## S4 method for signature 'theta'
standardise(object, ...)

## S4 method for signature 'double_array_parameter'
standardise(object, parameters = NULL, ...)

## S4 method for signature 'parameters'
standardise(object, ...)
```

Arguments

object	generic object
...	extra arguments needed for standardisation
parameters	the list of parameters, to be provided only if parameter type is 'cor'

Value

standardised object

statements_record-class	<i>Statements record class.</i>
-------------------------	---------------------------------

Description

Statements record class.

Theta	<i>Create a THETA parameter.</i>
-------	----------------------------------

Description

Create a THETA parameter.

Usage

```
Theta(name = NA, index = NA, value = NA, fix = FALSE)
```

Arguments

name	parameter name, e.g. CL (prefix THETA will be added automatically)
index	parameter index
value	parameter value
fix	parameter was fixed in estimation, logical value

Value

a THETA parameter

theta-class	<i>Theta parameter class.</i>
-------------	-------------------------------

Description

Theta parameter class.

toString	<i>ToString generic method.</i>
----------	---------------------------------

Description

ToString generic method.

Usage

```
toString(object, ...)

## S4 method for signature 'unknown_statement'
toString(object, ...)

## S4 method for signature 'comment'
toString(object, ...)

## S4 method for signature 'line_break'
toString(object, ...)

## S4 method for signature 'equation'
toString(object, ...)

## S4 method for signature 'ode'
toString(object, ...)

## S4 method for signature 'if_statement'
toString(object, ...)

## S4 method for signature 'compartment'
toString(object, ...)

## S4 method for signature 'compartment_property'
toString(object, ...)

## S4 method for signature 'compartment_initial_condition'
toString(object, ...)

## S4 method for signature 'mrgsolve_model'
toString(object, ...)
```

Arguments

object	generic object
...	extra arguments needed for <code>toString</code> conversion

Value

character value/vector

trim

Trim character vector. Remove all leading and trailing spaces.

Description

Trim character vector. Remove all leading and trailing spaces.

Usage

```
trim(x)
```

Arguments

x character vector

Value

character vector without leading and trailing spaces

UnknownStatement

Create a new ordinary differential equation (ODE).

Description

Create a new ordinary differential equation (ODE).

Usage

```
UnknownStatement(line, comment = as.character(NA))
```

Arguments

line line which was not recognised
comment comment if any, single character string

Value

an unknown statement

unknown_statement-class

Unknown statement class. Any statement not recognized by campsismod.

Description

Unknown statement class. Any statement not recognized by campsismod.

updateCompartments	<i>Update compartments list from the persisted records. Exported especially for package pmxtran. However, this method should not be called.</i>
--------------------	---

Description

Update compartments list from the persisted records. Exported especially for package pmxtran. However, this method should not be called.

Usage

```
updateCompartments(model)
```

Arguments

model	CAMPSIS model
-------	---------------

Value

an updated CAMPSIS model, with an updated compartments list

VariablePattern	<i>Create a variable pattern.</i>
-----------------	-----------------------------------

Description

Create a variable pattern.

Usage

```
VariablePattern(x)
```

Arguments

x	variable name
---	---------------

Value

a variable pattern

variable_pattern-class

Variable pattern class.

Description

Variable pattern class.

write

Write generic object to files.

Description

Write generic object to files.

Usage

```
write(object, file, ...)

## S4 method for signature 'parameters,character'
write(object, file, ...)

## S4 method for signature 'code_records,character'
write(object, file, ...)

## S4 method for signature 'campsis_model,character'
write(object, file, ...)
```

Arguments

object	generic object
file	path of the output file or directory
...	extra arguments

Value

logical value, TRUE for success, FALSE for failure

`writeParameters`

Write subset of parameters (theta, omega or sigma).

Description

Write subset of parameters (theta, omega or sigma).

Usage

```
writeParameters(object, file, ...)
```

Arguments

object	subset of parameters
file	filename
...	extra arguments, like defaultDf for empty parameters list

Value

TRUE if success

`writeVarcov`

Write variance-covariance matrix.

Description

Write variance-covariance matrix.

Usage

```
writeVarcov(object, file)
```

Arguments

object	matrix
file	filename

Value

TRUE if success

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