

# Package: nlmixr2lib (via r-universe)

July 18, 2024

**Type** Package

**Version** 0.2.0.9000

**Title** A Model Library for 'nlmixr2'

**Description** A model library for 'nlmixr2'. The models include (and plan to include) pharmacokinetic, pharmacodynamic, and disease models used in pharmacometrics. Where applicable, references for each model are included in the meta-data for each individual model. The package also includes model composition and modification functions to make model updates easier.

**Depends** R (>= 4.0)

**Imports** checkmate, cli, methods, nlmixr2est, rxode2 (>= 2.0.12)

**License** GPL (>= 2)

**LazyData** true

**RoxygenNote** 7.3.2

**VignetteBuilder** knitr

**URL** <https://github.com/nlmixr2/nlmixr2lib>,  
<https://nlmixr2.github.io/nlmixr2lib/>

**Encoding** UTF-8

**Language** en-US

**Suggests** covr, knitr, rmarkdown, testthat (>= 3.0.0)

**Config/testthat/edition** 3

**Repository** <https://nlmixr2.r-universe.dev>

**RemoteUrl** <https://github.com/nlmixr2/nlmixr2lib>

**RemoteRef** HEAD

**RemoteSha** cd58212f1a828981afed3bb881e9cb0a7e35a2f2

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addComp	<i>To add additional compartments to the model</i>
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### Description

To add additional compartments to the model

### Usage

```
addComp(
  model,
  numPeripheral,
  central = "central",
  depot = "depot",
  peripheralComp = "peripheral",
  vp = "vp",
  vc = "vc",
  q = "q"
)
```

### Arguments

model	The model as a function
numPeripheral	number of peripheral compartments to be added to the model
central	a character vector representing the central compartment
depot	a character vector representing the depot compartment
peripheralComp	A character vector representing the prefix of peripheral compartments

vp	parameter representing the peripheral volume of the first (central) compartment and the prefix of the other compartments
vc	parameter representing the central volume of the first (central) compartment and the prefix of the other compartment's volume
q	inter-compartmental clearance parameter or prefix (depending on the model)

**Value**

A rxode2 model function with an additional compartment added

**Examples**

```
readModelDb("PK_1cmt_des") |>
  addComp(1)
```

---

addDepot	<i>To convert from infusion/intravenous administration to first-order oral absorption</i>
----------	---

---

**Description**

To convert from infusion/intravenous administration to first-order oral absorption

**Usage**

```
addDepot(
  model,
  central = "central",
  depot = "depot",
  absRate = "ka",
  lag = paste0("lag", depot),
  lagIni = NA,
  fdepotIni = NA,
  absRateIni = 1
)
```

**Arguments**

model	The model as a function (or something convertible to an rxUi object)
central	central compartment name
depot	depot compartment name
absRate	absorption rate parameter name
lag	lag parameter name
lagIni	Initial value for the lag time ('NA' to omit)
fdepotIni	Initial value for the depot bioavailability ('NA' to omit)
absRateIni	Initial value for the first order rate

**Value**

a model with the depot added

**Examples**

```
# most of the examples in the model library already have a depot.  
# for this example we will remove the depot and then add it back  
readModelDb("PK_1cmt_des") |>  
  removeDepot() |>  
  addDepot()
```

---

addDirToModelDb	<i>Add a directory to the modeldb</i>
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**Description**

Add a directory to the modeldb

**Usage**

```
addDirToModelDb(dir, modeldb = data.frame())
```

```
addFileToModelDb(dir, file, modeldb)
```

**Arguments**

dir	Directory name containing model files
modeldb	The starting modeldb data.frame
file	The file name (without the directory name)

**Value**

The updated modeldb data.frame  
the model database

**Functions**

- addFileToModelDb(): Add a file to the modeldb

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addEta	<i>Add random effects to a model</i>
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**Description**

Add random effects to a model

**Usage**

```
addEta(model, eta)
```

**Arguments**

model	The model as a function
eta	vector with the parameters to add random effects (sometimes referred to as inter-individual variability, IIV) on

**Value**

The model with eta added to the requested parameters

**Examples**

```
library(rxode2)
readModelDb("PK_1cmt") |> addEta("ka")
```

---

addResErr	<i>Add residual error to a model</i>
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**Description**

Add residual error to a model

**Usage**

```
addResErr(model, reserr)
```

**Arguments**

model	The model as a function
reserr	The type or types of residual error (currently "addSd", "propSd", and "lnormSd" are accepted)

**Details**

For reserr, the parameter will be named with the dependent variable from the model as a prefix. For example, if the dependent variable in the model is Cc, the parameter name for propSd will become CcpropSd.

**Value**

The model with residual error modified

**Examples**

```
library(rxode2)
readModelDb("PK_1cmt") |> addResErr("addSd")
readModelDb("PK_1cmt") |> addResErr("lnormSd")
readModelDb("PK_1cmt") |> addResErr(c("addSd", "propSd"))
```

---

addTransit

*To add transit compartments to the model*

---

**Description**

To add transit compartments to the model

**Usage**

```
addTransit(
  model,
  transit,
  central = "central",
  depot = "depot",
  transitComp = "transit",
  ktr = "ktr"
)
```

**Arguments**

model	The model as a function
transit	the number of transit compartments to be added
central	a character vector representing the central compartment
depot	a character vector representing the depot compartment
transitComp	the transit compartment prefix
ktr	the parameter name for the transit compartment rate

**Value**

a model with transit compartment added

**Examples**

```
readModelDb("PK_1cmt_des") |>
  addTransit(3)
```

---

`convertMM`*Convert models from linear elimination to MM elimination*

---

**Description**

Convert models from linear elimination to MM elimination

**Usage**

```
convertMM(  
  ui,  
  central = "central",  
  elimination = "kel",  
  vm = "vm",  
  km = "km",  
  vc = "vc"  
)
```

**Arguments**

<code>ui</code>	model to convert
<code>central</code>	the central compartment where the elimination is present
<code>elimination</code>	variable for the elimination constant in the model
<code>vm</code>	variable name for Vmax in the model
<code>km</code>	variable name for Km in the model
<code>vc</code>	variable name for Vc in the model

**Value**

new model changing linear elimination to MM elimination

**Author(s)**

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**Examples**

```
readModelDb("PK_1cmt_des") |> convertMM()

readModelDb("PK_2cmt_des") |> convertMM()

readModelDb("PK_3cmt_des") |> convertMM()

readModelDb("PK_3cmt_des") |> removeDepot() |> convertMM()
```

---

 modeldb

*Model library for nlmixr2*


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**Description**

This is a data frame of the available models in nlmixr2lib, it is generated with the package. Custom modeldb may be used.

**Usage**

```
modeldb
```

**Format**

A data frame with 17 rows and 9 columns

**name** Model name that can be used to extract the model from the model library

**description** Model description in free form text; in model itself

**parameters** A comma separated string listing either the parameter in the model defined by population/individual effects or a population effect parameter

**DV** The definition of the dependent variable(s)

**linCmt** Logical flag indicating if solved models are used (TRUE) or not (FALSE)

**algebraic** Logical flag indicating if the model is purely algebraic: TRUE no linCmt() and no ODEs; FALSE otherwise

**dosing** A comma separated string of identified dosing compartments

**depends** A comma separated string of objects the model depends on

**filename** Filename of the model. By default these are installed in the model library and read on demand



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modellib	<i>Get the model from the model library</i>
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**Description**

This function gets a model from the available model library

**Usage**

```
modellib(name = NULL, eta = NULL, reserr = NULL)
```

**Arguments**

name	character with the name of the model to load (if NULL, lists all available base models)
eta	vector with the parameters to add random effects (sometimes referred to as inter-individual variability, IIV) on
reserr	The type or types of residual error (currently "addSd", "propSd", and "lnormSd" are accepted)

**Details**

This is a very first draft just to look at the proof of concept

**Value**

The function returns a function the model code (or NULL if the model = NULL)

**Examples**

```
modellib(name = "PK_1cmt")  
modellib(name = "PK_1cmt", eta = c("ka", "vc"), reserr = "addSd")  
modellib(name = "PK_1cmt", reserr = "addSd")
```

---

readModelDb	<i>Read a model from the nlmixr2 model database</i>
-------------	---

---

**Description**

Read a model from the nlmixr2 model database

**Usage**

```
readModelDb(name)
```

**Arguments**

name                    The name of the model (must be one of modeldb\$name)

**Value**

The model as a function

**Examples**

```
readModelDb("PK_1cmt")
```

---

removeComp	<i>To remove peripheral compartments from the model</i>
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---

**Description**

To remove peripheral compartments from the model

**Usage**

```
removeComp(
  model,
  peripheral,
  central = "central",
  depot = "depot",
  peripheralComp = "peripheral",
  vp = "vp",
  vc = "vc",
  q = "q"
)
```

**Arguments**

model	The model as a function
peripheral	The number of peripheral compartments to remove
central	a character vector representing the central compartment
depot	a character vector representing the depot compartment
peripheralComp	A character vector representing the prefix of peripheral compartments
vp	parameter representing the peripheral volume of the first (central) compartment and the prefix of the other compartments
vc	parameter representing the central volume of the first (central) compartment and the prefix of the other compartment's volume
q	inter-compartmental clearance parameter or prefix (depending on the model)

**Value**

rxode2 model function/ui with a compartment removed

**Examples**

```
library(rxode2)
readModelDb("PK_2cmt_des") |> removeComp(1)
```

---

removeDepot	<i>To convert from first order oral absorption to IV/Intravenous</i>
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---

**Description**

To convert from first order oral absorption to IV/Intravenous

**Usage**

```
removeDepot(model, central = "central", depot = "depot")
```

**Arguments**

model	The model as a function
central	This is a character vector that represents the central compartment in the model
depot	This is a character vector that represents the depot in the model

**Value**

Returns a model with the depot from a first order absorption model removed

**Examples**

```
readModelDb("PK_1cmt_des") |>
  removeDepot()
```

---

removeTransit	<i>To remove transit compartments from the model</i>
---------------	--

---

### Description

To remove transit compartments from the model

### Usage

```
removeTransit(  
  model,  
  transit,  
  central = "central",  
  depot = "depot",  
  transitComp = "transit",  
  ktr = "ktr"  
)
```

### Arguments

model	The model as a function
transit	The number of transit compartments to remove
central	a character vector representing the central compartment
depot	a character vector representing the depot compartment
transitComp	the transit compartment prefix
ktr	the parameter name for the transit compartment rate

### Value

rxode2 model with transit compartment removed

### Examples

```
# In this example the transit is added and then a few are removed  
  
readModelDb("PK_1cmt_des") |>  
  addTransit(4) |>  
  removeTransit(3)
```

---

searchReplace	<i>Search within a model to replace part of the model</i>
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---

**Description**

Search within a model to replace part of the model

**Usage**

```
searchReplace(object, find, replace)
```

```
searchReplaceHelper(object, find, replace)
```

**Arguments**

object            function specifying the nlmixr2 model

find, replace    Character scalars of parts of the model to replace

**Value**

object with find replaced with replace

**Functions**

- `searchReplaceHelper()`: A helper function for `searchReplace` (not intended for users to use directly)

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updateOncologyXenograftSimeoni2004	
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*Update an oncology xenograft model based on Simeoni 2004*

---

**Description**

Update an oncology xenograft model based on Simeoni 2004

**Usage**

```
updateOncologyXenograftSimeoni2004(
  object,
  ncmt,
  damagedCmtName = "damagedCells",
  drugEffectName = "drugEffectCyclingCells",
  undamagedCmtName = "cyclingCells",
  tumorVolName = "tumorVol",
  transitRateName = "damageTransit"
)
```

**Arguments**

`object` Fitted object or function specifying the model.  
`ncmt` The desired number of damaged cell compartments  
`damagedCmtName, undamagedCmtName, tumorVolName`  
character string names for the compartments for damaged cells, undamaged cells, and the calculated tumor volume (the sum of undamaged and damaged cells)  
`drugEffectName, transitRateName`  
character string names of the drug effect and transit rate (as used in the model block)

**Value**

An updated model with the new number of compartments

**Examples**

```
library(rxode2)
readModelDb("oncology_xenograft_simeoni_2004") %>%
  updateOncologyXenograftSimeoni2004(ncmt = 5)
```

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