# Package 'ruminate'

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Title A Pharmacometrics Data Transformation and Analysis Tool

Version 0.3.1

**Description** Exploration of pharmacometrics data involves both general tools (transformation and plotting) and specific techniques (non-compartmental analysis). This kind of exploration is generally accomplished by utilizing different packages. The purpose of 'ruminate' is to create a 'shiny' interface to make these tools more broadly available while creating reproducible results.

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BugReports https://github.com/john-harrold/ruminate/issues

URL https://ruminate.ubiquity.tools/

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**Depends** R (>= 4.2.0)

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# Description

Used to convert nonstandard dose route values (i.e. "IV") to standard values ("intravascular").

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#### Usage

```
apply_route_map(route_map = list(), route_col = NULL, DS = NULL)
```

# Arguments

route\_map List with names corresponding to the route replacement and a vector of regular expressions to match.

route\_col Column name with the route data.

DS Dataframe containing the dataset.

#### Value

Dataset with the route mapping applied.

#### **Examples**

CTS\_add\_covariate

Add Covariate to Elemetnt

## **Description**

Takes the ui elements in the module state and processes the covariate elements for addition.

## Usage

```
CTS_add_covariate(state, element)
```

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## **Arguments**

```
state CTS state from CTS_fetch_state()
element Element list from CTS_fetch_current_element()
```

#### **Details**

This depends on the following UI values in the state

```
state[["CTS"]][["ui"]][["covariate_value"]]state[["CTS"]][["ui"]][["covariate_type_selected"]]state[["CTS"]][["ui"]][["selected_covariate"]]
```

#### Value

Element with the results of adding the covariate. The cares list element can be used to determine the exit status of the function.

- COV\_IS\_GOOD If TRUE if the covariate was good and added, and FALSE if there were any
  issues
- msgs Vector of messages.

```
# For more information see the Clinical Trial Simulation vignette:
# https://ruminate.ubiquity.tools/articles/clinical_trial_simulation.html
# None of this will work if rxode2 isn't installed:
library(formods)
if( Sys.getenv("ruminate_rxfamily_found") == "TRUE"){
# This will populate the session variable with the model building (MB) module
sess_res = MB_test_mksession()
session = sess_res[["session"]]
id
      = "CTS"
id\_ASM = "ASM"
id\_MB = "MB"
input = list()
# Configuration files
FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml")
MOD_yaml_file = system.file(package = "ruminate", "templates", "CTS.yaml")
state = CTS_fetch_state(id
                                        = id,
                        id_ASM
                                       = id_ASM,
                        id_MB
                                       = id_MB,
                        input
                                       = input,
                        session
                                       = session,
                        FM_yaml_file = FM_yaml_file,
                        MOD_yaml_file = MOD_yaml_file,
```

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= NULL)

react\_state

```
# Fetch a list of the current element
current_ele = CTS_fetch_current_element(state)
# You can modify the element
current_ele[["element_name"]] = "A more descriptive name"
# Defining the source model
state[["CTS"]][["ui"]][["source_model"]] = "MB_obj_1_rx"
current_ele = CTS_change_source_model(state, current_ele)
# Single visit
current_ele[["ui"]][["visit_times"]]
                                                    = "0"
current_ele[["ui"]][["cts_config_nsteps"]]
                                                    = "5"
# Creating a dosing rule
state[["CTS"]][["ui"]][["rule_condition"]]
                                                  = "time == 0"
                                                    = "dose"
state[["CTS"]][["ui"]][["rule_type"]]
state[["CTS"]][["ui"]][["action_dosing_state"]]
                                                   = "central"
                                                 = "c(1)"
state[["CTS"]][["ui"]][["action_dosing_values"]]
                                                    = "c(0)"
state[["CTS"]][["ui"]][["action_dosing_times"]]
state[["CTS"]][["ui"]][["action_dosing_durations"]] = "c(0)"
                                                    = "Single_Dose"
state[["CTS"]][["ui"]][["rule_name"]]
# Adding the rule:
current_ele = CTS_add_rule(state, current_ele)
# Appending the plotting details as well
                                          = "1"
current_ele[["ui"]][["fpage"]]
current_ele[["ui"]][["dvcols"]]
                                          = "Cc"
# Reducing the number of subjects and steps to speed things up on CRAN
current_ele[["ui"]][["nsub"]]
                                          = "2"
current_ele[["ui"]][["cts_config_nsteps"]] = "5"
# Putting the element back in the state forcing code generation
state = CTS_set_current_element(
 state = state,
 element = current_ele)
# Now we pull out the current element, and simulate it
current_ele = CTS_fetch_current_element(state)
#current_ele = CTS_simulate_element(state, current_ele)
# Next we plot the element
current_ele = CTS_plot_element(state, current_ele)
# Now we save those results back into the state:
state = CTS_set_current_element(
 state = state,
 element = current_ele)
```

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```
# This will extract the code for the current module
code = CTS_fetch_code(state)
code
# This will update the checksum of the module state
state = CTS_update_checksum(state)
# Access the datasets generated from simulations
ds = CTS_fetch_ds(state)
# CTS_add_covariate
                                                       = "70, .1"
state[["CTS"]][["ui"]][["covariate_value"]]
state[["CTS"]][["ui"]][["covariate_type_selected"]]
                                                       = "cont_lognormal"
state[["CTS"]][["ui"]][["selected_covariate"]]
                                                       = "WT"
current_ele = CTS_add_covariate(state, current_ele)
# Creates a new empty element
state = CTS_new_element(state)
# Delete the current element
state = CTS_del_current_element(state)
```

CTS\_add\_rule

Add Rule to Element

#### **Description**

Takes the ui elements in the state and element and attempts to add a rule.

## Usage

```
CTS_add_rule(state, element)
```

## **Arguments**

state CTS state from CTS\_fetch\_state()

#### **Details**

This depends on the following UI values in the state and element

```
• state[["CTS"]][["ui"]][["rule_name"]]
```

- state[["CTS"]][["ui"]][["rule\_condition"]]
- state[["CTS"]][["ui"]][["rule\_type"]]

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```
- For rule type "dose"
    * state[["CTS"]][["ui"]][["action_dosing_state"]]
    * state[["CTS"]][["ui"]][["action_dosing_values"]]
    * state[["CTS"]][["ui"]][["action_dosing_times"]]
    * state[["CTS"]][["ui"]][["action_dosing_durations"]]
- For rule type "set state"
    * state[["CTS"]][["ui"]][["action_set_state_state"]]
    * state[["CTS"]][["ui"]][["action_set_state_values"]]
- For rule type "manual code"
    * state[["CTS"]][["ui"]][["action_manual_code"]]
```

#### Value

Element with the results of adding the rule. The rares list element can be used to determine the exit status of the function.

- RULE\_IS\_GOOD If true it indicates that the pieces of the rule from the UI check out.
- RULE\_UPDATED If RULE\_IS\_GOOD and RULE\_UPDATED is true then a previous rule definition was overwritten. If RULE\_IS\_GOOD is TRUE and RULE\_UPDATED is FALSE then a new rule was added.
- notify\_text Text for notify message
- notify\_id Notification ID
- notify\_type Notification type
- msgs Vector of messages.

```
# For more information see the Clinical Trial Simulation vignette:
# https://ruminate.ubiquity.tools/articles/clinical_trial_simulation.html
# None of this will work if rxode2 isn't installed:
library(formods)
if( Sys.getenv("ruminate_rxfamily_found") == "TRUE"){
# This will populate the session variable with the model building (MB) module
sess_res = MB_test_mksession()
session = sess_res[["session"]]
      = "CTS"
id
id\_ASM = "ASM"
id_MB = "MB"
input = list()
# Configuration files
FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml")
MOD_yaml_file = system.file(package = "ruminate", "templates", "CTS.yaml")
state = CTS_fetch_state(id
                                        = id,
```

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```
id_ASM
                                       = id_ASM,
                       id_MB
                                       = id_MB,
                       input
                                      = input,
                                      = session,
                       session
                       FM_yaml_file = FM_yaml_file,
                       MOD_yaml_file = MOD_yaml_file,
                       react_state = NULL)
# Fetch a list of the current element
current_ele = CTS_fetch_current_element(state)
# You can modify the element
current_ele[["element_name"]] = "A more descriptive name"
# Defining the source model
state[["CTS"]][["ui"]][["source_model"]] = "MB_obj_1_rx"
current_ele = CTS_change_source_model(state, current_ele)
# Single visit
                                                    = "0"
current_ele[["ui"]][["visit_times"]]
                                                    = "5"
current_ele[["ui"]][["cts_config_nsteps"]]
# Creating a dosing rule
                                                  = "time == 0"
state[["CTS"]][["ui"]][["rule_condition"]]
                                                    = "dose"
state[["CTS"]][["ui"]][["rule_type"]]
state[["CTS"]][["ui"]][["action_dosing_state"]]
                                                    = "central"
state[["CTS"]][["ui"]][["action_dosing_values"]]
                                                   = "c(1)"
state[["CTS"]][["ui"]][["action_dosing_times"]]
                                                   = "c(0)"
state[["CTS"]][["ui"]][["action_dosing_durations"]] = "c(0)"
state[["CTS"]][["ui"]][["rule_name"]]
                                                    = "Single_Dose"
# Adding the rule:
current_ele = CTS_add_rule(state, current_ele)
# Appending the plotting details as well
                                          = "1"
current_ele[["ui"]][["fpage"]]
                                          = "Cc"
current_ele[["ui"]][["dvcols"]]
# Reducing the number of subjects and steps to speed things up on CRAN
current_ele[["ui"]][["nsub"]]
                                        = "2"
current_ele[["ui"]][["cts_config_nsteps"]] = "5"
# Putting the element back in the state forcing code generation
state = CTS_set_current_element(
 state = state,
 element = current_ele)
# Now we pull out the current element, and simulate it
current_ele = CTS_fetch_current_element(state)
#current_ele = CTS_simulate_element(state, current_ele)
# Next we plot the element
```

CTS\_append\_report

```
current_ele = CTS_plot_element(state, current_ele)
# Now we save those results back into the state:
state = CTS_set_current_element(
 state = state,
 element = current_ele)
# This will extract the code for the current module
code = CTS_fetch_code(state)
code
# This will update the checksum of the module state
state = CTS_update_checksum(state)
# Access the datasets generated from simulations
ds = CTS_fetch_ds(state)
# CTS_add_covariate
                                                       = "70, .1"
state[["CTS"]][["ui"]][["covariate_value"]]
state[["CTS"]][["ui"]][["covariate_type_selected"]] = "cont_lognormal"
state[["CTS"]][["ui"]][["selected_covariate"]]
                                                       = "WT"
current_ele = CTS_add_covariate(state, current_ele)
# Creates a new empty element
state = CTS_new_element(state)
# Delete the current element
state = CTS_del_current_element(state)
}
```

CTS\_append\_report

Append Report Elements

## **Description**

Appends report elements to a formods report.

#### Usage

```
CTS_append_report(state, rpt, rpttype, gen_code_only = FALSE)
```

## Arguments

cTS state from CTS\_fetch\_state()

Report with the current content of the report which will be appended to in this function. For details on the structure see the documentation for onbrand::template\_details()

rpttype Type of report to generate (supported "xlsx", "pptx", "docx").

gen\_code\_only Boolean value indicating that only code should be generated (FALSE).

## Value

list containing the following elements

- isgood: Return status of the function.
- hasrptele: Boolean indicator if the module has any reportable elements.
- code: Code to generate reporting elements.
- msgs: Messages to be passed back to the user.
- rpt: Report with any additions passed back to the user.

#### See Also

```
formods::FM_generate_report() and onbrand::template_details()
```

```
CTS_change_source_model
```

Change the Source Model

# Description

Takes the ui elements in the state and element and processes any changes to the source model and updates the element accordingly.

# Usage

```
CTS_change_source_model(state, element)
```

## **Arguments**

state CTS state from CTS\_fetch\_state()

#### **Details**

This depends on the following UI values in the state.

```
• state[["CTS"]][["ui"]][["source_model"]]
```

#### Value

Element with the necessary changes to the source model.

```
# For more information see the Clinical Trial Simulation vignette:
# https://ruminate.ubiquity.tools/articles/clinical_trial_simulation.html
# None of this will work if rxode2 isn't installed:
library(formods)
if( Sys.getenv("ruminate_rxfamily_found") == "TRUE"){
# This will populate the session variable with the model building (MB) module
sess_res = MB_test_mksession()
session = sess_res[["session"]]
      = "CTS"
id
id\_ASM = "ASM"
id\_MB = "MB"
input = list()
# Configuration files
FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml")
MOD_yaml_file = system.file(package = "ruminate", "templates", "CTS.yaml")
state = CTS_fetch_state(id
                                      = id,
                       id_ASM
                                     = id_ASM,
                       id_MB
                                     = id_MB,
                       input
                                     = input,
                       session
                                     = session,
                       FM_yaml_file = FM_yaml_file,
                       MOD_yaml_file = MOD_yaml_file,
                       react_state
                                     = NULL)
# Fetch a list of the current element
current_ele = CTS_fetch_current_element(state)
# You can modify the element
current_ele[["element_name"]] = "A more descriptive name"
# Defining the source model
state[["CTS"]][["ui"]][["source_model"]] = "MB_obj_1_rx"
current_ele = CTS_change_source_model(state, current_ele)
# Single visit
                                                  = "0"
current_ele[["ui"]][["visit_times"]]
                                                  = "5"
current_ele[["ui"]][["cts_config_nsteps"]]
# Creating a dosing rule
                                                 = "time == 0"
state[["CTS"]][["ui"]][["rule_condition"]]
state[["CTS"]][["ui"]][["rule_type"]]
                                                   = "dose"
                                                  = "central"
state[["CTS"]][["ui"]][["action_dosing_state"]]
state[["CTS"]][["ui"]][["action_dosing_values"]] = "c(1)"
                                                  = "c(0)"
state[["CTS"]][["ui"]][["action_dosing_times"]]
state[["CTS"]][["ui"]][["action_dosing_durations"]] = "c(0)"
```

```
state[["CTS"]][["ui"]][["rule_name"]]
                                                  = "Single_Dose"
# Adding the rule:
current_ele = CTS_add_rule(state, current_ele)
# Appending the plotting details as well
                                          = "1"
current_ele[["ui"]][["fpage"]]
                                          = "Cc"
current_ele[["ui"]][["dvcols"]]
# Reducing the number of subjects and steps to speed things up on CRAN
                              = "2"
current_ele[["ui"]][["nsub"]]
current_ele[["ui"]][["cts_config_nsteps"]] = "5"
# Putting the element back in the state forcing code generation
state = CTS_set_current_element(
 state = state,
 element = current_ele)
# Now we pull out the current element, and simulate it
current_ele = CTS_fetch_current_element(state)
#current_ele = CTS_simulate_element(state, current_ele)
# Next we plot the element
current_ele = CTS_plot_element(state, current_ele)
# Now we save those results back into the state:
state = CTS_set_current_element(
 state = state,
 element = current_ele)
# This will extract the code for the current module
code = CTS_fetch_code(state)
# This will update the checksum of the module state
state = CTS_update_checksum(state)
# Access the datasets generated from simulations
ds = CTS_fetch_ds(state)
# CTS_add_covariate
state[["CTS"]][["ui"]][["covariate_value"]]
                                                      = "70, .1"
state[["CTS"]][["ui"]][["covariate_type_selected"]]
                                                     = "cont_lognormal"
                                                      = "WT"
state[["CTS"]][["ui"]][["selected_covariate"]]
current_ele = CTS_add_covariate(state, current_ele)
# Creates a new empty element
state = CTS_new_element(state)
# Delete the current element
state = CTS_del_current_element(state)
```

```
CTS_del_current_element
```

Deletes Current cohort

## **Description**

Takes a CTS state and deletes the current cohort. If that is the last element, then a new default will be added.

## Usage

```
CTS_del_current_element(state)
```

#### **Arguments**

state CTS state from CTS\_fetch\_state()

#### Value

CTS state object with the current cohort deleted.

```
# For more information see the Clinical Trial Simulation vignette:
# https://ruminate.ubiquity.tools/articles/clinical_trial_simulation.html
# None of this will work if rxode2 isn't installed:
library(formods)
if( Sys.getenv("ruminate_rxfamily_found") == "TRUE"){
# This will populate the session variable with the model building (MB) module
sess_res = MB_test_mksession()
session = sess_res[["session"]]
      = "CTS"
id
id\_ASM = "ASM"
id\_MB = "MB"
input = list()
# Configuration files
FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml")
MOD_yaml_file = system.file(package = "ruminate", "templates", "CTS.yaml")
state = CTS_fetch_state(id
                                        = id,
                        id_ASM
                                        = id_ASM,
                        id_MB
                                       = id_MB,
                        input
                                       = input,
                        session
                                        = session,
```

```
FM_yaml_file
                                      = FM_yaml_file,
                       MOD_yaml_file = MOD_yaml_file,
                       react_state
                                      = NULL)
# Fetch a list of the current element
current_ele = CTS_fetch_current_element(state)
# You can modify the element
current_ele[["element_name"]] = "A more descriptive name"
# Defining the source model
state[["CTS"]][["ui"]][["source_model"]] = "MB_obj_1_rx"
current_ele = CTS_change_source_model(state, current_ele)
# Single visit
                                                    = "0"
current_ele[["ui"]][["visit_times"]]
                                                    = "5"
current_ele[["ui"]][["cts_config_nsteps"]]
# Creating a dosing rule
state[["CTS"]][["ui"]][["rule_condition"]]
                                                  = "time == 0"
                                                   = "dose"
state[["CTS"]][["ui"]][["rule_type"]]
state[["CTS"]][["ui"]][["action_dosing_state"]]
                                                  = "central"
state[["CTS"]][["ui"]][["action_dosing_values"]] = "c(1)"
state[["CTS"]][["ui"]][["action_dosing_times"]]
                                                  = "c(0)"
state[["CTS"]][["ui"]][["action_dosing_durations"]] = "c(0)"
state[["CTS"]][["ui"]][["rule_name"]]
                                                    = "Single_Dose"
# Adding the rule:
current_ele = CTS_add_rule(state, current_ele)
# Appending the plotting details as well
                                          = "1"
current_ele[["ui"]][["fpage"]]
current_ele[["ui"]][["dvcols"]]
                                          = "Cc"
# Reducing the number of subjects and steps to speed things up on CRAN
                                         = "2"
current_ele[["ui"]][["nsub"]]
current_ele[["ui"]][["cts_config_nsteps"]] = "5"
# Putting the element back in the state forcing code generation
state = CTS_set_current_element(
 state = state,
 element = current_ele)
# Now we pull out the current element, and simulate it
current_ele = CTS_fetch_current_element(state)
#current_ele = CTS_simulate_element(state, current_ele)
# Next we plot the element
current_ele = CTS_plot_element(state, current_ele)
# Now we save those results back into the state:
state = CTS_set_current_element(
```

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```
state = state,
 element = current_ele)
# This will extract the code for the current module
code = CTS_fetch_code(state)
code
# This will update the checksum of the module state
state = CTS_update_checksum(state)
# Access the datasets generated from simulations
ds = CTS_fetch_ds(state)
# CTS_add_covariate
state[["CTS"]][["ui"]][["covariate_value"]]
                                                       = "70, .1"
                                                      = "cont_lognormal"
state[["CTS"]][["ui"]][["covariate_type_selected"]]
                                                       = "WT"
state[["CTS"]][["ui"]][["selected_covariate"]]
current_ele = CTS_add_covariate(state, current_ele)
# Creates a new empty element
state = CTS_new_element(state)
# Delete the current element
state = CTS_del_current_element(state)
```

CTS\_fetch\_code

Fetch Module Code

## **Description**

Fetches the code to generate results seen in the app

## Usage

```
CTS_fetch_code(state)
```

## Arguments

state

CTS state from CTS\_fetch\_state()

# Value

Character object vector with the lines of code

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```
# For more information see the Clinical Trial Simulation vignette:
# https://ruminate.ubiquity.tools/articles/clinical_trial_simulation.html
# None of this will work if rxode2 isn't installed:
library(formods)
if( Sys.getenv("ruminate_rxfamily_found") == "TRUE"){
# This will populate the session variable with the model building (MB) module
sess_res = MB_test_mksession()
session = sess_res[["session"]]
      = "CTS"
id
id\_ASM = "ASM"
id\_MB = "MB"
input = list()
# Configuration files
FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml")
MOD_yaml_file = system.file(package = "ruminate", "templates", "CTS.yaml")
state = CTS_fetch_state(id
                                      = id,
                       id_ASM
                                     = id_ASM,
                       id_MB
                                     = id_MB,
                       input
                                     = input,
                       session
                                     = session,
                       FM_yaml_file = FM_yaml_file,
                       MOD_yaml_file = MOD_yaml_file,
                       react_state
                                     = NULL)
# Fetch a list of the current element
current_ele = CTS_fetch_current_element(state)
# You can modify the element
current_ele[["element_name"]] = "A more descriptive name"
# Defining the source model
state[["CTS"]][["ui"]][["source_model"]] = "MB_obj_1_rx"
current_ele = CTS_change_source_model(state, current_ele)
# Single visit
                                                  = "0"
current_ele[["ui"]][["visit_times"]]
                                                  = "5"
current_ele[["ui"]][["cts_config_nsteps"]]
# Creating a dosing rule
                                                 = "time == 0"
state[["CTS"]][["ui"]][["rule_condition"]]
state[["CTS"]][["ui"]][["rule_type"]]
                                                   = "dose"
                                                  = "central"
state[["CTS"]][["ui"]][["action_dosing_state"]]
state[["CTS"]][["ui"]][["action_dosing_values"]] = "c(1)"
                                                  = "c(0)"
state[["CTS"]][["ui"]][["action_dosing_times"]]
state[["CTS"]][["ui"]][["action_dosing_durations"]] = "c(0)"
```

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```
state[["CTS"]][["ui"]][["rule_name"]]
                                                   = "Single_Dose"
# Adding the rule:
current_ele = CTS_add_rule(state, current_ele)
# Appending the plotting details as well
                                          = "1"
current_ele[["ui"]][["fpage"]]
current_ele[["ui"]][["dvcols"]]
                                          = "Cc"
# Reducing the number of subjects and steps to speed things up on CRAN
                               = "2"
current_ele[["ui"]][["nsub"]]
current_ele[["ui"]][["cts_config_nsteps"]] = "5"
# Putting the element back in the state forcing code generation
state = CTS_set_current_element(
 state = state,
 element = current_ele)
# Now we pull out the current element, and simulate it
current_ele = CTS_fetch_current_element(state)
#current_ele = CTS_simulate_element(state, current_ele)
# Next we plot the element
current_ele = CTS_plot_element(state, current_ele)
# Now we save those results back into the state:
state = CTS_set_current_element(
 state = state,
 element = current_ele)
# This will extract the code for the current module
code = CTS_fetch_code(state)
# This will update the checksum of the module state
state = CTS_update_checksum(state)
# Access the datasets generated from simulations
ds = CTS_fetch_ds(state)
# CTS_add_covariate
state[["CTS"]][["ui"]][["covariate_value"]]
                                                      = "70, .1"
state[["CTS"]][["ui"]][["covariate_type_selected"]]
                                                      = "cont_lognormal"
                                                      = "WT"
state[["CTS"]][["ui"]][["selected_covariate"]]
current_ele = CTS_add_covariate(state, current_ele)
# Creates a new empty element
state = CTS_new_element(state)
# Delete the current element
state = CTS_del_current_element(state)
```

```
CTS_fetch_current_element
```

Fetches Current cohort

## **Description**

Takes a CTS state and returns the current active cohort

#### Usage

```
CTS_fetch_current_element(state)
```

#### **Arguments**

state

CTS state from CTS\_fetch\_state()

#### Value

List containing the details of the active data view. The structure of this list is the same as the structure of state\$CTS\$elements in the output of CTS\_fetch\_state().

```
# For more information see the Clinical Trial Simulation vignette:
# https://ruminate.ubiquity.tools/articles/clinical_trial_simulation.html
# None of this will work if rxode2 isn't installed:
library(formods)
if( Sys.getenv("ruminate_rxfamily_found") == "TRUE"){
# This will populate the session variable with the model building (MB) module
sess_res = MB_test_mksession()
session = sess_res[["session"]]
      = "CTS"
id
id\_ASM = "ASM"
id\_MB = "MB"
input = list()
# Configuration files
FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml")
MOD_yaml_file = system.file(package = "ruminate", "templates", "CTS.yaml")
state = CTS_fetch_state(id
                                        = id,
                        id_ASM
                                        = id_ASM,
                        id_MB
                                       = id_MB,
                        input
                                       = input,
                        session
                                        = session,
```

```
FM_yaml_file
                                      = FM_yaml_file,
                       MOD_yaml_file = MOD_yaml_file,
                       react_state
                                      = NULL)
# Fetch a list of the current element
current_ele = CTS_fetch_current_element(state)
# You can modify the element
current_ele[["element_name"]] = "A more descriptive name"
# Defining the source model
state[["CTS"]][["ui"]][["source_model"]] = "MB_obj_1_rx"
current_ele = CTS_change_source_model(state, current_ele)
# Single visit
                                                    = "0"
current_ele[["ui"]][["visit_times"]]
                                                    = "5"
current_ele[["ui"]][["cts_config_nsteps"]]
# Creating a dosing rule
state[["CTS"]][["ui"]][["rule_condition"]]
                                                  = "time == 0"
                                                  = "dose"
state[["CTS"]][["ui"]][["rule_type"]]
state[["CTS"]][["ui"]][["action_dosing_state"]]
                                                  = "central"
state[["CTS"]][["ui"]][["action_dosing_values"]] = "c(1)"
state[["CTS"]][["ui"]][["action_dosing_times"]]
                                                  = "c(0)"
state[["CTS"]][["ui"]][["action_dosing_durations"]] = "c(0)"
state[["CTS"]][["ui"]][["rule_name"]]
                                                    = "Single_Dose"
# Adding the rule:
current_ele = CTS_add_rule(state, current_ele)
# Appending the plotting details as well
                                          = "1"
current_ele[["ui"]][["fpage"]]
current_ele[["ui"]][["dvcols"]]
                                          = "Cc"
# Reducing the number of subjects and steps to speed things up on CRAN
                                         = "2"
current_ele[["ui"]][["nsub"]]
current_ele[["ui"]][["cts_config_nsteps"]] = "5"
# Putting the element back in the state forcing code generation
state = CTS_set_current_element(
 state = state,
 element = current_ele)
# Now we pull out the current element, and simulate it
current_ele = CTS_fetch_current_element(state)
#current_ele = CTS_simulate_element(state, current_ele)
# Next we plot the element
current_ele = CTS_plot_element(state, current_ele)
# Now we save those results back into the state:
state = CTS_set_current_element(
```

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```
state
        = state,
 element = current_ele)
# This will extract the code for the current module
code = CTS_fetch_code(state)
code
# This will update the checksum of the module state
state = CTS_update_checksum(state)
# Access the datasets generated from simulations
ds = CTS_fetch_ds(state)
# CTS_add_covariate
state[["CTS"]][["ui"]][["covariate_value"]]
                                                       = "70, .1"
                                                       = "cont_lognormal"
state[["CTS"]][["ui"]][["covariate_type_selected"]]
                                                       = "WT"
state[["CTS"]][["ui"]][["selected_covariate"]]
current_ele = CTS_add_covariate(state, current_ele)
# Creates a new empty element
state = CTS_new_element(state)
# Delete the current element
state = CTS_del_current_element(state)
```

CTS\_fetch\_ds

Fetch Clinical Trial Simulator Module Datasets

## **Description**

Fetches the datasets produced by the module. For each cohort this will be the simulation timecourse and the event table

#### Usage

```
CTS_fetch_ds(state)
```

## **Arguments**

state

CTS state from CTS\_fetch\_state()

#### Value

Character object vector with the lines of code

list containing the following elements

• isgood: Return status of the function.

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- hasds: Boolean indicator if the module has any datasets
- msgs: Messages to be passed back to the user.
- ds: List with datasets. Each list element has the name of the R-object for that dataset. Each element has the following structure:
  - label: Text label for the dataset
  - MOD\_TYPE: Short name for the type of module.
  - id: module ID
  - DS: Dataframe containing the actual dataset.
  - DSMETA: Metadata describing DS
  - code: Complete code to build dataset.
  - checksum: Module checksum.
  - DSchecksum: Dataset checksum.

```
# For more information see the Clinical Trial Simulation vignette:
# https://ruminate.ubiquity.tools/articles/clinical_trial_simulation.html
# None of this will work if rxode2 isn't installed:
library(formods)
if( Sys.getenv("ruminate_rxfamily_found") == "TRUE"){
# This will populate the session variable with the model building (MB) module
sess_res = MB_test_mksession()
session = sess_res[["session"]]
      = "CTS"
id_ASM = "ASM"
id_MB = "MB"
input = list()
# Configuration files
FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml")
MOD_yaml_file = system.file(package = "ruminate", "templates", "CTS.yaml")
state = CTS_fetch_state(id
                                     = id,
                                  = id_ASM,
                       id_ASM
                       id_MB
                                     = id_MB,
                                     = input,
                       input
                       session
                                    = session,
                       FM_yaml_file = FM_yaml_file,
                       MOD_yaml_file = MOD_yaml_file,
                       react_state
                                     = NULL)
# Fetch a list of the current element
current_ele = CTS_fetch_current_element(state)
# You can modify the element
current_ele[["element_name"]] = "A more descriptive name"
```

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```
# Defining the source model
state[["CTS"]][["ui"]][["source_model"]] = "MB_obj_1_rx"
current_ele = CTS_change_source_model(state, current_ele)
# Single visit
                                                    = "0"
current_ele[["ui"]][["visit_times"]]
current_ele[["ui"]][["cts_config_nsteps"]]
                                                    = "5"
# Creating a dosing rule
                                                  = "time == 0"
state[["CTS"]][["ui"]][["rule_condition"]]
                                                    = "dose"
state[["CTS"]][["ui"]][["rule_type"]]
                                                 = "central"
state[["CTS"]][["ui"]][["action_dosing_state"]]
                                                = "c(1)"
= "c(0)"
state[["CTS"]][["ui"]][["action_dosing_values"]]
state[["CTS"]][["ui"]][["action_dosing_times"]]
state[["CTS"]][["ui"]][["action_dosing_durations"]] = "c(0)"
state[["CTS"]][["ui"]][["rule_name"]]
                                                    = "Single_Dose"
# Adding the rule:
current_ele = CTS_add_rule(state, current_ele)
# Appending the plotting details as well
                                          = "1"
current_ele[["ui"]][["fpage"]]
                                          = "Cc"
current_ele[["ui"]][["dvcols"]]
# Reducing the number of subjects and steps to speed things up on CRAN
current_ele[["ui"]][["nsub"]]
                               = "2"
current_ele[["ui"]][["cts_config_nsteps"]] = "5"
# Putting the element back in the state forcing code generation
state = CTS_set_current_element(
 state = state,
 element = current_ele)
# Now we pull out the current element, and simulate it
current_ele = CTS_fetch_current_element(state)
#current_ele = CTS_simulate_element(state, current_ele)
# Next we plot the element
current_ele = CTS_plot_element(state, current_ele)
# Now we save those results back into the state:
state = CTS_set_current_element(
 state = state,
 element = current_ele)
# This will extract the code for the current module
code = CTS_fetch_code(state)
code
# This will update the checksum of the module state
state = CTS_update_checksum(state)
```

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CTS\_fetch\_sc\_meta

Fetches Simulation Parameter Meta Information

## **Description**

This provides meta information about simulatino options. This includes option names, text descriptions, ui\_names used, etc.

# Usage

```
CTS_fetch_sc_meta(
   MOD_yaml_file = system.file(package = "ruminate", "templates", "CTS.yaml")
)
```

#### **Arguments**

MOD\_yaml\_file Module configuration file with MC as main section.

## Value

List with the following elements:

- config List from the YAML->MC->sim\_config.
- summary: Dataframe with elements of config in tabular format.
- ui\_config Vector of all the ui\_ids for configuration options.

```
CTS_fetch_sc_meta()
```

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CTS_fetch_sta	эt	e
---------------	----	---

Fetch Clinical Trial Simulator State

#### **Description**

Merges default app options with the changes made in the UI

## Usage

```
CTS_fetch_state(
  id,
  id_ASM,
  id_MB,
  input,
  session,
  FM_yaml_file,
  MOD_yaml_file,
  react_state
)
```

## **Arguments**

id	Shiny module ID
id_ASM	ID string for the app state management module used to save and load app states
id_MB	An ID string that corresponds with the ID used to call the MB modules
input	Shiny input variable
session	Shiny session variable
FM_yaml_file	App configuration file with FM as main section.
MOD_yaml_file	Module configuration file with MC as main section.
react_state	Variable passed to server to allow reaction outside of module (NULL)

## Value

list containing the current state of the app including default values from the yaml file as well as any changes made by the user. The list has the following structure:

- yaml: Full contents of the supplied yaml file.
- MC: Module components of the yaml file.
- CTS:
  - isgood: Boolean object indicating if the file was successfully loaded.
  - checksum: This is an MD5 sum of the contents element and can be used to detect changes in the state.
- MOD\_TYPE: Character data containing the type of module "CTS"
- id: Character data containing the module id module in the session variable.
- FM\_yaml\_file: App configuration file with FM as main section.
- MOD\_yaml\_file: Module configuration file with MC as main section.

### **Examples**

```
# Within shiny both session and input variables will exist,
# this creates examples here for testing purposes:
sess_res = MB_test_mksession()
session = sess_res$session
input = sess_res$input
# Configuration files
FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml")
MOD_yaml_file = system.file(package = "ruminate", "templates", "CTS.yaml")
# Creating an empty state object
state = CTS_fetch_state(id
                                       = "CTS",
                       id_ASM
                                      = "ASM",
                       id MB
                                      = "MB",
                                      = input,
                       input
                       session
                                      = session,
                       FM_yaml_file = FM_yaml_file,
                       MOD_yaml_file = MOD_yaml_file,
                       react_state
                                       = NULL)
```

CTS\_init\_element\_model

Initializes Cohort When Model Changes

# Description

When a source model changes this will update information about that model like the default dvcols and selection information about the dvcols

#### Usage

```
CTS_init_element_model(state, element)
```

## **Arguments**

state CTS state from CTS\_fetch\_state()
element Element list from CTS\_fetch\_current\_element()

#### Value

CTS state object with the current cohort ui elements initialized based on the current model selected

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CTS\_init\_state

Initialize CTS Module State

### **Description**

Creates a list of the initialized module state

#### Usage

```
CTS_init_state(FM_yaml_file, MOD_yaml_file, id, id_MB, session)
```

## Arguments

FM\_yaml\_file App configuration file with FM as main section

MOD\_yaml\_file Module configuration file with MC as main section

id ID string for the module

id\_MB An ID string that corresponds with the ID used to call the MB modules

session Shiny session variable

## Value

list containing an empty CTS state

```
# Within shiny both session and input variables will exist,
# this creates examples here for testing purposes:
sess_res = MB_test_mksession()
session = sess_res$session
input = sess_res$input
state = CTS_init_state(
  FM_yaml_file = system.file(package = "formods",
                               "templates",
                               "formods.yaml"),
  MOD_yaml_file = system.file(package = "ruminate",
                               "templates",
                               "CTS.yaml"),
                  = "CTS",
  id
  id_MB
                  = "MB",
                  = session)
  session
state
```

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CTS\_mk\_preload

Make List of Current CTS State

# Description

Reads in the app state from yaml files.

## Usage

```
CTS_mk_preload(state)
```

## **Arguments**

state

CTS state object

#### Value

list with the following elements

- isgood: Boolean indicating the exit status of the function.
- msgs: Messages to be passed back to the user.
- yaml\_list: Lists with preload components.

# **Examples**

```
sess_res = CTS_test_mksession()
state = sess_res$state
res = CTS_mk_preload(state)
```

CTS\_new\_element

New Clinical Trial Simulation Cohort

# Description

Appends a new empty cohort to the CTS state object and makes this new cohort the active cohort.

# Usage

```
CTS_new_element(state)
```

## **Arguments**

state

CTS state from CTS\_fetch\_state()

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#### Value

CTS state object containing a new cohort and that cohort is set as the current active cohort. See the help for CTS\_fetch\_state() for ===ELEMENT== format.

```
# For more information see the Clinical Trial Simulation vignette:
# https://ruminate.ubiquity.tools/articles/clinical_trial_simulation.html
# None of this will work if rxode2 isn't installed:
library(formods)
if( Sys.getenv("ruminate_rxfamily_found") == "TRUE"){
# This will populate the session variable with the model building (MB) module
sess_res = MB_test_mksession()
session = sess_res[["session"]]
     = "CTS"
id
id_ASM = "ASM"
id\_MB = "MB"
input = list()
# Configuration files
FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml")
MOD_yaml_file = system.file(package = "ruminate", "templates", "CTS.yaml")
state = CTS_fetch_state(id
                                    = id,
                      id_ASM
                                   = id_ASM,
                                    = id_MB,
                      id_MB
                                    = input,
                      input
                      session = session,
                      FM_yaml_file = FM_yaml_file,
                      MOD_yaml_file = MOD_yaml_file,
                      react_state = NULL)
# Fetch a list of the current element
current_ele = CTS_fetch_current_element(state)
# You can modify the element
current_ele[["element_name"]] = "A more descriptive name"
# Defining the source model
state[["CTS"]][["ui"]][["source_model"]] = "MB_obj_1_rx"
current_ele = CTS_change_source_model(state, current_ele)
# Single visit
current_ele[["ui"]][["visit_times"]]
                                                 = "0"
current_ele[["ui"]][["cts_config_nsteps"]]
                                                 = "5"
# Creating a dosing rule
```

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```
state[["CTS"]][["ui"]][["rule_type"]]
                                                     = "dose"
                                                     = "central"
state[["CTS"]][["ui"]][["action_dosing_state"]]
state[["CTS"]][["ui"]][["action_dosing_values"]]
                                                 = "c(1)"
state[["CTS"]][["ui"]][["action_dosing_times"]]
                                                    = "c(0)"
state[["CTS"]][["ui"]][["action_dosing_durations"]] = "c(0)"
state[["CTS"]][["ui"]][["rule_name"]]
                                                     = "Single_Dose"
# Adding the rule:
current_ele = CTS_add_rule(state, current_ele)
# Appending the plotting details as well
                                           = "1"
current_ele[["ui"]][["fpage"]]
                                           = "Cc"
current_ele[["ui"]][["dvcols"]]
# Reducing the number of subjects and steps to speed things up on CRAN
current_ele[["ui"]][["nsub"]]
                                         = "2"
current_ele[["ui"]][["cts_config_nsteps"]] = "5"
# Putting the element back in the state forcing code generation
state = CTS_set_current_element(
 state = state,
 element = current_ele)
# Now we pull out the current element, and simulate it
current_ele = CTS_fetch_current_element(state)
#current_ele = CTS_simulate_element(state, current_ele)
# Next we plot the element
current_ele = CTS_plot_element(state, current_ele)
# Now we save those results back into the state:
state = CTS_set_current_element(
 state = state,
 element = current_ele)
# This will extract the code for the current module
code = CTS_fetch_code(state)
code
# This will update the checksum of the module state
state = CTS_update_checksum(state)
# Access the datasets generated from simulations
ds = CTS_fetch_ds(state)
# CTS_add_covariate
state[["CTS"]][["ui"]][["covariate_value"]]
                                                      = "70, .1"
state[["CTS"]][["ui"]][["covariate_type_selected"]]
                                                      = "cont_lognormal"
state[["CTS"]][["ui"]][["selected_covariate"]]
                                                       = "WT"
current_ele = CTS_add_covariate(state, current_ele)
# Creates a new empty element
```

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```
state = CTS_new_element(state)

# Delete the current element
state = CTS_del_current_element(state)
}
```

CTS\_plot\_element

Plots the Specified Element

## **Description**

Takes a CTS state and element and simulates the current set of rules.

#### Usage

```
CTS_plot_element(state, element)
```

## **Arguments**

state CTS state from CTS\_fetch\_state()

#### Value

Simulation element with plot results stored in the '"plotres" element.

- isgood Boolean value indicating the state of the figure generation code.
- msgs Any messages to be passed to the user.
- capture Captured figure generation output from plot\_sr\_tc()

```
# For more information see the Clinical Trial Simulation vignette:
# https://ruminate.ubiquity.tools/articles/clinical_trial_simulation.html
# None of this will work if rxode2 isn't installed:
library(formods)
if( Sys.getenv("ruminate_rxfamily_found") == "TRUE"){
# This will populate the session variable with the model building (MB) module sess_res = MB_test_mksession() session = sess_res[["session"]]
id = "CTS"
id_ASM = "ASM"
id_MB = "MB"
input = list()
```

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```
# Configuration files
FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml")
MOD_yaml_file = system.file(package = "ruminate", "templates", "CTS.yaml")
state = CTS_fetch_state(id
                                      = id,
                       id_ASM
                                     = id_ASM,
                       id_MB
                                     = id_MB,
                                     = input,
                       input
                                   = session,
                       session
                       FM_yaml_file = FM_yaml_file,
                       MOD_yaml_file = MOD_yaml_file,
                       react_state = NULL)
# Fetch a list of the current element
current_ele = CTS_fetch_current_element(state)
# You can modify the element
current_ele[["element_name"]] = "A more descriptive name"
# Defining the source model
state[["CTS"]][["ui"]][["source_model"]] = "MB_obj_1_rx"
current_ele = CTS_change_source_model(state, current_ele)
# Single visit
                                                   = "0"
current_ele[["ui"]][["visit_times"]]
                                                   = "5"
current_ele[["ui"]][["cts_config_nsteps"]]
# Creating a dosing rule
state[["CTS"]][["ui"]][["rule_condition"]]
                                                   = "time == 0"
                                                  = "dose"
state[["CTS"]][["ui"]][["rule_type"]]
state[["CTS"]][["ui"]][["action_dosing_state"]]
                                                 = "central"
state[["CTS"]][["ui"]][["action_dosing_values"]] = "c(1)"
                                                = "c(0)"
state[["CTS"]][["ui"]][["action_dosing_times"]]
state[["CTS"]][["ui"]][["action_dosing_durations"]] = "c(0)"
state[["CTS"]][["ui"]][["rule_name"]]
                                                   = "Single_Dose"
# Adding the rule:
current_ele = CTS_add_rule(state, current_ele)
# Appending the plotting details as well
current_ele[["ui"]][["fpage"]]
                                          = "1"
current_ele[["ui"]][["dvcols"]]
                                          = "Cc"
# Reducing the number of subjects and steps to speed things up on CRAN
                                         = "2"
current_ele[["ui"]][["nsub"]]
current_ele[["ui"]][["cts_config_nsteps"]] = "5"
# Putting the element back in the state forcing code generation
state = CTS_set_current_element(
 state = state,
 element = current_ele)
```

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```
# Now we pull out the current element, and simulate it
current_ele = CTS_fetch_current_element(state)
#current_ele = CTS_simulate_element(state, current_ele)
# Next we plot the element
current_ele = CTS_plot_element(state, current_ele)
# Now we save those results back into the state:
state = CTS_set_current_element(
 state = state,
 element = current_ele)
# This will extract the code for the current module
code = CTS_fetch_code(state)
code
# This will update the checksum of the module state
state = CTS_update_checksum(state)
# Access the datasets generated from simulations
ds = CTS_fetch_ds(state)
# CTS_add_covariate
state[["CTS"]][["ui"]][["covariate_value"]]
                                                       = "70, .1"
                                                       = "cont_lognormal"
state[["CTS"]][["ui"]][["covariate_type_selected"]]
state[["CTS"]][["ui"]][["selected_covariate"]]
                                                       = "WT"
current_ele = CTS_add_covariate(state, current_ele)
# Creates a new empty element
state = CTS_new_element(state)
# Delete the current element
state = CTS_del_current_element(state)
```

CTS\_preload

Preload Data for CTS Module

# Description

Populates the supplied session variable with information from list of sources.

# Usage

```
CTS_preload(
   session,
   src_list,
   yaml_res,
```

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```
mod_ID = NULL,
  react_state = list(),
  quickload = FALSE
)
```

### Arguments

session Shiny session variable (in app) or a list (outside of app)
src\_list List of preload data (all read together with module IDs at the top level)
yaml\_res List data from module yaml config
mod\_ID Module ID of the module being loaded.
react\_state Reactive shiny object (in app) or a list (outside of app) used to trigger reactions.
quickload Logical TRUE to load reduced analysis FALSE to load the full analysis

## Value

list with the following elements

- isgood: Boolean indicating the exit status of the function.
- msgs: Messages to be passed back to the user.
- session: Session object
- input: The value of the shiny input at the end of the session initialization.
- state: App state.
- react\_state: The react\_state components.

CTS\_Server

Clinical Trial Simulator State Server

## Description

Server function for the Clinical Trial Simulator Shiny Module

### Usage

```
CTS_Server(
  id,
  id_ASM = "ASM",
  id_MB = "MB",
  FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml"),
  MOD_yaml_file = system.file(package = "ruminate", "templates", "CTS.yaml"),
  deployed = FALSE,
  react_state = NULL
)
```

### **Arguments**

An ID string that corresponds with the ID used to call the modules UI elements
ID string for the app state managment module used to save and load app states
An ID string that corresponds with the ID used to call the MB modules
App configuration file with FM as main section.

 ${\tt MOD\_yaml\_file} \quad Module \ configuration \ file \ with \ MC \ as \ main \ section.$ 

deployed Boolean variable indicating whether the app is deployed or not.

react\_state Variable passed to server to allow reaction outside of module (NULL)

#### Value

**UD** Server object

```
CTS_set_current_element
```

Sets the Value for the Current cohort

#### **Description**

Takes a CTS state and returns the current active cohort

#### Usage

```
CTS_set_current_element(state, element)
```

## Arguments

state CTS state from CTS\_fetch\_state()

#### Value

CTS state object with the current cohort set using the supplied value.

```
# For more information see the Clinical Trial Simulation vignette:
# https://ruminate.ubiquity.tools/articles/clinical_trial_simulation.html
# None of this will work if rxode2 isn't installed:
library(formods)
if( Sys.getenv("ruminate_rxfamily_found") == "TRUE"){
# This will populate the session variable with the model building (MB) module sess_res = MB_test_mksession()
session = sess_res[["session"]]
```

```
id = "CTS"
id_ASM = "ASM"
id\_MB = "MB"
input = list()
# Configuration files
FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml")
MOD_yaml_file = system.file(package = "ruminate", "templates", "CTS.yaml")
state = CTS_fetch_state(id
                                      = id,
                       id_ASM
                                    = id_ASM,
                                     = id_MB,
                       id_MB
                       MOD_yaml_file = MOD_yaml_file,
                       react_state = NULL)
# Fetch a list of the current element
current_ele = CTS_fetch_current_element(state)
# You can modify the element
current_ele[["element_name"]] = "A more descriptive name"
# Defining the source model
state[["CTS"]][["ui"]][["source_model"]] = "MB_obj_1_rx"
current_ele = CTS_change_source_model(state, current_ele)
# Single visit
                                                   = "0"
current_ele[["ui"]][["visit_times"]]
                                                   = "5"
current_ele[["ui"]][["cts_config_nsteps"]]
# Creating a dosing rule
                                                = "time == 0"
= "dose"
state[["CTS"]][["ui"]][["rule_condition"]]
state[["CTS"]][["ui"]][["rule_type"]]
state[["CTS"]][["ui"]][["action_dosing_state"]] = "central"
state[["CTS"]][["ui"]][["action_dosing_values"]] = "c(1)"
state[["CTS"]][["ui"]][["action_dosing_times"]] = "c(0)"
state[["CTS"]][["ui"]][["action_dosing_durations"]] = "c(0)"
state[["CTS"]][["ui"]][["rule_name"]]
                                                   = "Single_Dose"
# Adding the rule:
current_ele = CTS_add_rule(state, current_ele)
# Appending the plotting details as well
                                         = "1"
current_ele[["ui"]][["fpage"]]
current_ele[["ui"]][["dvcols"]]
                                         = "Cc"
# Reducing the number of subjects and steps to speed things up on CRAN
current_ele[["ui"]][["cts_config_nsteps"]] = "5"
```

```
# Putting the element back in the state forcing code generation
state = CTS_set_current_element(
 state = state,
 element = current_ele)
# Now we pull out the current element, and simulate it
current_ele = CTS_fetch_current_element(state)
#current_ele = CTS_simulate_element(state, current_ele)
# Next we plot the element
current_ele = CTS_plot_element(state, current_ele)
# Now we save those results back into the state:
state = CTS_set_current_element(
 state = state,
 element = current_ele)
# This will extract the code for the current module
code = CTS_fetch_code(state)
code
# This will update the checksum of the module state
state = CTS_update_checksum(state)
# Access the datasets generated from simulations
ds = CTS_fetch_ds(state)
# CTS_add_covariate
                                                       = "70, .1"
state[["CTS"]][["ui"]][["covariate_value"]]
state[["CTS"]][["ui"]][["covariate_type_selected"]]
                                                      = "cont_lognormal"
                                                       = "WT"
state[["CTS"]][["ui"]][["selected_covariate"]]
current_ele = CTS_add_covariate(state, current_ele)
# Creates a new empty element
state = CTS_new_element(state)
# Delete the current element
state = CTS_del_current_element(state)
}
```

### **Description**

Takes a CTS state and element and simulates the current set of rules.

#### Usage

```
CTS_simulate_element(state, element)
```

### **Arguments**

state CTS state from CTS\_fetch\_state()
element Element list from CTS\_fetch\_current\_element()

#### Value

Simulation element with simulation results stored in the "simres" element.

```
# For more information see the Clinical Trial Simulation vignette:
# https://ruminate.ubiquity.tools/articles/clinical_trial_simulation.html
# None of this will work if rxode2 isn't installed:
library(formods)
if( Sys.getenv("ruminate_rxfamily_found") == "TRUE"){
# This will populate the session variable with the model building (MB) module
sess_res = MB_test_mksession()
session = sess_res[["session"]]
       = "CTS"
id
id\_ASM = "ASM"
id\_MB = "MB"
input = list()
# Configuration files
FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml")
MOD_yaml_file = system.file(package = "ruminate", "templates", "CTS.yaml")
state = CTS_fetch_state(id
                                         = id,
                                      = id_ASM,
                         id_ASM
                         id_MB
                                         = id_MB,
                         input
                                         = input,
                         session
                                        = session,
                         FM_yaml_file = FM_yaml_file,
                         MOD_yaml_file = MOD_yaml_file,
                         react_state
                                          = NULL)
# Fetch a list of the current element
current_ele = CTS_fetch_current_element(state)
# You can modify the element
current_ele[["element_name"]] = "A more descriptive name"
# Defining the source model
```

```
state[["CTS"]][["ui"]][["source_model"]] = "MB_obj_1_rx"
current_ele = CTS_change_source_model(state, current_ele)
# Single visit
                                                      = "0"
current_ele[["ui"]][["visit_times"]]
                                                      = "5"
current_ele[["ui"]][["cts_config_nsteps"]]
# Creating a dosing rule
                                                   = "time == 0"
state[["CTS"]][["ui"]][["rule_condition"]]
                                                    = "dose"
state[["CTS"]][["ui"]][["rule_type"]]
state[["CTS"]][["ui"]][["action_dosing_state"]] = "central"
state[["CTS"]][["ui"]][["action_dosing_values"]] = "c(1)"
state[["CTS"]][["ui"]][["action_dosing_times"]] = "c(0)"
state[["CTS"]][["ui"]][["action_dosing_durations"]] = "c(0)"
                                                      = "Single_Dose"
state[["CTS"]][["ui"]][["rule_name"]]
# Adding the rule:
current_ele = CTS_add_rule(state, current_ele)
# Appending the plotting details as well
                                           = "1"
current_ele[["ui"]][["fpage"]]
                                           = "Cc"
current_ele[["ui"]][["dvcols"]]
# Reducing the number of subjects and steps to speed things up on CRAN
                               = "2"
current_ele[["ui"]][["nsub"]]
current_ele[["ui"]][["cts_config_nsteps"]] = "5"
# Putting the element back in the state forcing code generation
state = CTS_set_current_element(
 state = state,
 element = current_ele)
# Now we pull out the current element, and simulate it
current_ele = CTS_fetch_current_element(state)
#current_ele = CTS_simulate_element(state, current_ele)
# Next we plot the element
current_ele = CTS_plot_element(state, current_ele)
# Now we save those results back into the state:
state = CTS_set_current_element(
 state = state,
 element = current_ele)
# This will extract the code for the current module
code = CTS_fetch_code(state)
code
# This will update the checksum of the module state
state = CTS_update_checksum(state)
```

# Access the datasets generated from simulations

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CTS\_sim\_isgood

Checks Simulation in Element for Goodness

# **Description**

Takes the supplied element and determines if the underlying simulation is in a good state or not.

## Usage

```
CTS_sim_isgood(state, element)
```

## **Arguments**

state CTS state from CTS\_fetch\_state()

#### Value

List with the following elements:

- isgood: Boolean object indicating if the file was successfully loaded.
- msgs: Text description of failure.

CTS\_test\_mksession 41

CTS\_test\_mksession

Populate Session Data for Module Testing

### **Description**

Populates the supplied session variable for testing.

# Usage

```
CTS_test_mksession(session = list(), full = FALSE)
```

### **Arguments**

session Shiny session variable (in app) or a list (outside of app)

full Boolean indicating if the full test session should be created (TRUE) or a minimal

test session should be created (FALSE, default)

### Value

The CTS portion of the all\_sess\_res returned from FM\_app\_preload

#### See Also

```
FM_app_preload
```

### **Examples**

```
session = shiny::MockShinySession$new()
sess_res = CTS_test_mksession(session=session)
```

CTS\_update\_checksum

Updates CTS Module Checksum

## **Description**

Takes a CTS state and updates the checksum used to trigger downstream updates

### Usage

```
CTS_update_checksum(state)
```

### **Arguments**

state

CTS state from CTS\_fetch\_state()

#### Value

CTS state object with the checksum updated

```
# For more information see the Clinical Trial Simulation vignette:
# https://ruminate.ubiquity.tools/articles/clinical_trial_simulation.html
# None of this will work if rxode2 isn't installed:
library(formods)
if( Sys.getenv("ruminate_rxfamily_found") == "TRUE"){
# This will populate the session variable with the model building (MB) module
sess_res = MB_test_mksession()
session = sess_res[["session"]]
id = "CTS"
id\_ASM = "ASM"
id_MB = "MB"
input = list()
# Configuration files
FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml")
MOD_yaml_file = system.file(package = "ruminate", "templates", "CTS.yaml")
state = CTS_fetch_state(id
                                     = id,
                       id_ASM
                                     = id_ASM,
                       id_MB
                                     = id_MB,
                                     = input,
                       input
                                 = session,
                       session
                       FM_yaml_file = FM_yaml_file,
                       MOD_yaml_file = MOD_yaml_file,
                       react_state = NULL)
# Fetch a list of the current element
current_ele = CTS_fetch_current_element(state)
# You can modify the element
current_ele[["element_name"]] = "A more descriptive name"
# Defining the source model
state[["CTS"]][["ui"]][["source_model"]] = "MB_obj_1_rx"
current_ele = CTS_change_source_model(state, current_ele)
# Single visit
                                                   = "0"
current_ele[["ui"]][["visit_times"]]
current_ele[["ui"]][["cts_config_nsteps"]]
                                                   = "5"
# Creating a dosing rule
                                                = "time == 0"
state[["CTS"]][["ui"]][["rule_condition"]]
                                                   = "dose"
state[["CTS"]][["ui"]][["rule_type"]]
```

```
state[["CTS"]][["ui"]][["action_dosing_state"]]
                                                    = "central"
state[["CTS"]][["ui"]][["action_dosing_values"]] = "c(1)"
state[["CTS"]][["ui"]][["action_dosing_times"]]
                                                   = "c(0)"
state[["CTS"]][["ui"]][["action_dosing_durations"]] = "c(0)"
state[["CTS"]][["ui"]][["rule_name"]]
                                                    = "Single_Dose"
# Adding the rule:
current_ele = CTS_add_rule(state, current_ele)
# Appending the plotting details as well
                                          = "1"
current_ele[["ui"]][["fpage"]]
                                          = "Cc"
current_ele[["ui"]][["dvcols"]]
# Reducing the number of subjects and steps to speed things up on CRAN
current_ele[["ui"]][["nsub"]]
                                        = "2"
current_ele[["ui"]][["cts_config_nsteps"]] = "5"
# Putting the element back in the state forcing code generation
state = CTS_set_current_element(
 state = state,
 element = current_ele)
# Now we pull out the current element, and simulate it
current_ele = CTS_fetch_current_element(state)
#current_ele = CTS_simulate_element(state, current_ele)
# Next we plot the element
current_ele = CTS_plot_element(state, current_ele)
# Now we save those results back into the state:
state = CTS_set_current_element(
 state = state,
 element = current_ele)
# This will extract the code for the current module
code = CTS_fetch_code(state)
code
# This will update the checksum of the module state
state = CTS_update_checksum(state)
# Access the datasets generated from simulations
ds = CTS_fetch_ds(state)
# CTS_add_covariate
state[["CTS"]][["ui"]][["covariate_value"]]
                                                      = "70, .1"
state[["CTS"]][["ui"]][["covariate_type_selected"]]
                                                    = "cont_lognormal"
state[["CTS"]][["ui"]][["selected_covariate"]]
                                                      = "WT"
current_ele = CTS_add_covariate(state, current_ele)
# Creates a new empty element
state = CTS_new_element(state)
```

dose\_records\_builder

```
# Delete the current element
state = CTS_del_current_element(state)
}
```

dose\_records\_builder Builds Dose Records Dataframe

# Description

Takes information about columns in dataset and constructs the dosing records.

# Usage

```
dose_records_builder(
  NCA_DS = NULL,
  dose_from = NULL,
  col_id = NULL,
  col_time = NULL,
  col_ntime = NULL,
  col_route = NULL,
  col_dose = NULL,
  col_dycle = NULL,
  col_dur = NULL,
  col_evid = NULL,
  col_evid = NULL,
  col_analyte = NULL,
  col_group = NULL
)
```

## **Arguments**

NCA_DS	Dataset containing dosing records.
dose_from	Method of dose extraction either "cols" or "rows".
col_id	Name of column with subject ID.
col_time	Name of column with time since first dose.
col_ntime	Name of column with time since the last dose (required with ${\tt dose\_from="cols"}).$
col_route	Name of column with route information.
col_dose	Name of column with last dose given.
col_cycle	Name of column with dose cycle (required with dose_from="cols").
col_dur	Name of column with dose duration.
col_evid	Name of column with event ID (required with dose_from="rows").
col_analyte	Name of column with analyte (optional).
col_group	Names of columns with grouping information (optionl).

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#### Value

list containing the following elements

- isgood: Return status of the function.
- msgs: Messages to be passed back to the user.
- dose\_rec:

```
if(system.file(package="readxl") !=""){
library(dplyr)
library(readxl)
library(stringr)
# Example data file:
data_file = system.file(package="formods","test_data","TEST_DATA.xlsx")
# Dataset formatted to extract dosing from columns
DS_cols = readxl::read_excel(path=data_file, sheet="DATA")
                                                                 |>
dplyr::filter(EVID == 0)
                                                        |>
 dplyr::filter(DOSE %in% c(3))
                                                        |>
dplyr::filter(str_detect(string=Cohort, "^MD"))
                                                        |>
 dplyr::filter(CMT == "C_ng_ml")
drb_res = dose_records_builder(
NCA_DS = DS_cols,
dose_from = "cols",
col_id = "ID",
col_time = "TIME_DY",
col_ntime = "NTIME_DY",
col_route = "ROUTE",
col_cycle = "DOSE_NUM",
col_dose = "DOSE",
 col_group = "Cohort")
utils::head(drb_res$dose_rec)
# Dataset formatted to extract dosing from rows (records)
DS_rows = readxl::read_excel(path=data_file, sheet="DATA")
                                                                 |>
dplyr::filter(DOSE %in% c(3))
                                                                |>
 dplyr::filter(str_detect(string=Cohort, "^MD"))
                                                                |>
dplyr::filter(CMT %in% c("Ac", "C_ng_ml"))
drb_res = dose_records_builder(
NCA_DS = DS_rows,
dose_from = "rows",
col_id = "ID",
col_time = "TIME_DY",
col_ntime = "NTIME_DY",
col_route = "ROUTE",
col_dose = "AMT",
col_evid = "EVID",
```

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```
col_group = "Cohort")
utils::head(drb_res$dose_rec)
}
```

fetch\_rxinfo

Fetches Information from an rxode2 Object

### **Description**

This will provide information like parameter names, covriates, etc from an rxode2 object.

## Usage

```
fetch_rxinfo(object)
```

### **Arguments**

object

rxode2 model object An ID string that corresponds with the ID used to call the modules UI elements

#### Value

List with the following elements.

- isgood: Boolean variable indicating if the model is good.
- msgs: Any messages from parsing the model.
- elements: List with names of simulation elements:
  - covariates: Names of the covariates in the system.
  - parameters: Names of the parameters (subject level) in the system.
  - iiv: Names of the iiv parameters in the system.
  - states: Names of the states/compartments in the system.
- txt\_info: Summary information in text format.
- list\_info: Summary information in list format used with onbrand reporting.
- ht\_info: Summary information in HTML formot.

```
library(formods)
library(ggplot2)

# For more information see the Clinical Trial Simulation vignette:
# https://ruminate.ubiquity.tools/articles/clinical_trial_simulation.html

# None of this will work if rxode2 isn't installed:
if(is_installed("rxode2")){
library(rxode2)
```

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```
set.seed(8675309)
rxSetSeed(8675309)
my_model = function ()
  description <- "One compartment PK model with linear clearance using differential equations"
    ini({
        lka <- 0.45
        label("Absorption rate (Ka)")
        lcl <- 1
        label("Clearance (CL)")
        lvc <- 3.45
        label("Central volume of distribution (V)")
        propSd <- c(0, 0.5)
        label("Proportional residual error (fraction)")
        etalcl ~ 0.1
    })
    model({
        ka <- exp(lka)</pre>
        cl <- exp(lcl + etalcl)</pre>
        vc <- exp(lvc)</pre>
        kel <- cl/vc
        d/dt(depot) <- -ka * depot
        d/dt(central) <- ka * depot - kel * central</pre>
        Cc <- central/vc</pre>
        Cc ~ prop(propSd)
    })
}
# This creates an rxode2 object
object = rxode(my_model)
# If you want details about the parameters, states, etc
# in the model you can use this:
rxdetails = fetch_rxinfo(object)
rxdetails$elements
# Next we will create subjects. To do that we need to
# specify information about covariates:
nsub = 2
covs = list(
  WT
             = list(type
                            = "continuous",
                    sampling = "log-normal",
                    values = c(70, .15))
)
subs = mk_subjects(object = object,
                   nsub = nsub,
                   covs = covs)
head(subs$subjects)
```

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```
rules = list(
 dose = list(
   condition = "TRUE",
   action = list(
     type = "dose",
     state = "central",
     values = "c(1)",
     times = "c(0)",
     durations = "c(0)")
   )
)
\# We evaulate the rules for dosing at time 0
eval_times = 0
# Stop 2 months after the last dose
output\_times = seq(0, 56, 1)
# This runs the rule-based simulations
simres =
 simulate_rules(
             = object,
   object
               = subs[["subjects"]],
   subjects
   eval_times = eval_times,
   output_times = output_times,
   rules
                = rules)
# First subject data:
sub_1 = simres$simall[simres$simall$id == 1, ]
# First subjects events
evall = as.data.frame(simres$evall)
ev_sub_1 = evall[evall$id ==1, ]
# All of the simulation data
simall = simres$simall
simall$id = as.factor(simall$id)
# Timecourse
psim =
 plot_sr_tc(
   sro = simres,
   dvcols = "Cc")
psim$fig
# Events
pev =
 plot_sr_ev(
   sro = simres,
   ylog = FALSE)
pev$fig
```

fetch\_rxtc 49

fetch	rvtc
16000	1 X L.C.

Extracts Timecourse and Merges Covariates

## **Description**

Takes the output of rxSolve() and merges in any missing covariates that are present in params but not in sim

## Usage

```
fetch_rxtc(rx_details, sim)
```

## **Arguments**

rx\_details Output of fetch\_rxinfo()
sim output of rxSolve()

## Value

Dataframe of the simulated time course.

MR	append	report
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Append Report Elements

### **Description**

Appends report elements to a formods report.

## Usage

```
MB_append_report(state, rpt, rpttype, gen_code_only = FALSE)
```

# Arguments

state	MB state	from MB_	_fetch_	state()
-------	----------	----------	---------	---------

rpt Report with the current content of the report which will be appended to in this

function. For details on the structure see the documentation for formods::FM\_generate\_report()

rpttype Type of report to generate (supported "xlsx", "pptx", "docx").

gen\_code\_only Boolean value indicating that only code should be generated (FALSE).

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## Value

list containing the following elements

- isgood: Return status of the function.
- hasrptele: Boolean indicator if the module has any reportable elements.
- code: Code to generate reporting elements.
- msgs: Messages to be passed back to the user.
- rpt: Report with any additions passed back to the user.

#### See Also

```
formods::FM_generate_report()
```

MB\_build\_code

Build Code to Generate Model

## **Description**

Takes the function definition from an rxode object, a function object name and an rxode object name and creates the code to build those objects.

## Usage

```
MB_build_code(
    state,
    session,
    fcn_def,
    time_scale,
    fcn_obj_name,
    rx_obj_name,
    ts_obj_name
)
```

# Arguments

state	MB state from MB_fetch_state()
session	Shiny session variable
fcn_def	Character string containing the function definition for the model
time_scale	$Short name for the model timescale (see names of state $MC\$ formatting $time\_scales $choices).$
fcn_obj_name	Object name of the function to create.
rx_obj_name	Object name of the rxode2 object to create.
ts_obj_name	Object name of the tiemscale object to create.

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### Value

List with the following elements

- model\_code Block of code to create the model in the context of a larger script.
- model\_code\_sa Same as the model\_code element but meant to stand alone.

```
#library(ruminate)
# This will get the full session:
library(formods)
if( Sys.getenv("ruminate_rxfamily_found") == "TRUE"){
 sess_res = MB_test_mksession()
 # This is just for CRAN
 #sess_res = MB_test_mksession(session=list())
 session = sess_res$session
 input = sess_res$input
 # Configuration files
 FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml")
MOD_yaml_file = system.file(package = "ruminate", "templates", "MB.yaml")
 # Creating an empty state object
 state = MB_fetch_state(id
                                           = "MB",
                                         = input,
                          input
                          session
                                         = session,
                          FM_yaml_file = FM_yaml_file,
                          MOD_yaml_file = MOD_yaml_file,
                                           = NULL)
                          react_state
 # This will provide a list of the available models
 models = MB_fetch_catalog(state)
 # This is a summary of the tables in the model:
 models$summary
 # This will test the models in the catalog, set as_cran
 # to FALSE to test all the models.
 mtres = MB_test_catalog(state, as_cran=TRUE)
 mtres$isgood
 # Creates a new empty element
 state = MB_new_element(state)
 # Delete the current element
 state = MB_del_current_element(state)
 # Fetch a list of the current element
 element = MB_fetch_current_element(state)
 # This will attach a model to it:
 # Pulling the first model from the catalog
```

```
fcn_def = models[["summary"]][1, ][["Model"]]
fcn_obj = models[["summary"]][1, ][["Object"]]
mdl_type = models[["summary"]][1, ][["Type"]]
fcn_desc = models[["summary"]][1, ][["Description"]]
# This will build the rxode2 object from the model
mk_rx_res = mk_rx_obj(
  type = mdl_type,
 model = list(fcn_def = fcn_def,
               fcn_obj = fcn_obj))
# This will attach the model to the current element
element = MB_update_model(
             = state,
  state
  session
             = session,
  current_ele = element,
             = mk_rx_res[["capture"]][["rx_obj"]],
  rx_obj
             = fcn_desc,
  note
  reset
             = TRUE)
# You can now place element back in the state
state = MB_set_current_element(state, element)
# This will fetch the current component
component = MB_fetch_component(state, element)
fares = MB_fetch_appends(state, element)
# You can use the component to build the code to generate the model:
gen_code =
 MB_build_code(state
                            = state, session = session,
              fcn_def
                           = component[["fcn_def"]],
              time_scale = element[["ui"]][["time_scale"]],
              fcn_obj_name = "my_fcn_obj",
              rx_obj_name
                            = "my_obj_name",
                            = "my_ts_name")
              ts_obj_name
# Model code to be included in a larger script
message(paste0(gen_code$model_code, collapse="\n"))
# Stand-alone model code
message(paste0(gen_code$model_code_sa, collapse="\n"))
# This will fetch the code to regenerate all of the components of this module
message(MB_fetch_code(state))
```

MB\_del\_current\_element

}

Deletes Current model

### **Description**

Takes a MB state and deletes the current model. If that is the last element, then a new default will be added.

# Usage

```
MB_del_current_element(state)
```

### **Arguments**

```
state MB state from MB_fetch_state()
```

#### Value

MB state object with the current model deleted.

```
#library(ruminate)
# This will get the full session:
library(formods)
if( Sys.getenv("ruminate_rxfamily_found") == "TRUE"){
 sess_res = MB_test_mksession()
 \ensuremath{\text{\#}} This is just for CRAN
 #sess_res = MB_test_mksession(session=list())
 session = sess_res$session
 input = sess_res$input
 # Configuration files
 FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml")
 MOD_yaml_file = system.file(package = "ruminate", "templates", "MB.yaml")
 # Creating an empty state object
                                         = "MB",
 state = MB_fetch_state(id
                                        = input,
                         input
                         session
                                        = session,
                         FM_yaml_file = FM_yaml_file,
                         MOD_yaml_file = MOD_yaml_file,
                                         = NULL)
                         react_state
 # This will provide a list of the available models
 models = MB_fetch_catalog(state)
 # This is a summary of the tables in the model:
 models$summary
 # This will test the models in the catalog, set as_cran
 # to FALSE to test all the models.
 mtres = MB_test_catalog(state, as_cran=TRUE)
 mtres$isgood
 # Creates a new empty element
```

```
state = MB_new_element(state)
# Delete the current element
state = MB_del_current_element(state)
# Fetch a list of the current element
element = MB_fetch_current_element(state)
# This will attach a model to it:
# Pulling the first model from the catalog
fcn_def = models[["summary"]][1, ][["Model"]]
fcn_obj = models[["summary"]][1, ][["Object"]]
mdl_type = models[["summary"]][1, ][["Type"]]
fcn_desc = models[["summary"]][1, ][["Description"]]
# This will build the rxode2 object from the model
mk_rx_res = mk_rx_obj(
  type = mdl_type,
  model = list(fcn_def = fcn_def,
               fcn_obj = fcn_obj))
# This will attach the model to the current element
element = MB_update_model(
             = state,
  state
             = session,
  session
  current_ele = element,
             = mk_rx_res[["capture"]][["rx_obj"]],
  rx_obj
  note
             = fcn_desc,
  reset
             = TRUE)
# You can now place element back in the state
state = MB_set_current_element(state, element)
# This will fetch the current component
component = MB_fetch_component(state, element)
fares = MB_fetch_appends(state, element)
# You can use the component to build the code to generate the model:
gen_code =
 MB_build_code(state
                            = state, session = session,
              fcn_def
                            = component[["fcn_def"]],
              time_scale
                            = element[["ui"]][["time_scale"]],
              fcn_obj_name = "my_fcn_obj",
              rx_obj_name = "my_obj_name",
              ts_obj_name
                            = "my_ts_name")
# Model code to be included in a larger script
message(paste0(gen_code$model_code, collapse="\n"))
# Stand-alone model code
message(paste0(gen_code$model_code_sa, collapse="\n"))
```

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```
# This will fetch the code to regenerate all of the components of this module
message(MB_fetch_code(state))
}
```

MB\_fetch\_appends

Fetches List of Available Models

# **Description**

Creates a catalog of the models available in the system file.

#### Usage

```
MB_fetch_appends(state, current_ele)
```

### **Arguments**

```
state MB state from MB_fetch_state()
current_ele MB model element from MB_fetch_current_element()
```

#### Value

List with the following attributes:

- isgood: Boolean variable indicating success or failure.
- msgs: Messages to be passed back to the user.
- hasappends: Boolean variable indicating if appendable models were found.
- select\_plain: Flat list with the models (ungrouped).
- choicesOpt List with the subtext filled out.

```
#library(ruminate)
# This will get the full session:
library(formods)
if( Sys.getenv("ruminate_rxfamily_found") == "TRUE"){
    sess_res = MB_test_mksession()
    # This is just for CRAN
    #sess_res = MB_test_mksession(session=list())
    session = sess_res$session
    input = sess_res$input

# Configuration files
FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml")
MOD_yaml_file = system.file(package = "ruminate", "templates", "MB.yaml")
# Creating an empty state object
```

```
state = MB_fetch_state(id
                                      = "MB",
                       input
                                      = input,
                       session
                                     = session,
                       FM_yaml_file = FM_yaml_file,
                       MOD_yaml_file = MOD_yaml_file,
                       react_state
                                      = NULL)
# This will provide a list of the available models
models = MB_fetch_catalog(state)
# This is a summary of the tables in the model:
models$summary
# This will test the models in the catalog, set as_cran
# to FALSE to test all the models.
mtres = MB_test_catalog(state, as_cran=TRUE)
mtres$isgood
# Creates a new empty element
state = MB_new_element(state)
# Delete the current element
state = MB_del_current_element(state)
# Fetch a list of the current element
element = MB_fetch_current_element(state)
# This will attach a model to it:
# Pulling the first model from the catalog
fcn_def = models[["summary"]][1, ][["Model"]]
fcn_obj = models[["summary"]][1, ][["Object"]]
mdl_type = models[["summary"]][1, ][["Type"]]
fcn_desc = models[["summary"]][1, ][["Description"]]
# This will build the rxode2 object from the model
mk_rx_res = mk_rx_obj(
  type = mdl_type,
 model = list(fcn_def = fcn_def,
               fcn_obj = fcn_obj))
# This will attach the model to the current element
element = MB_update_model(
  state
             = state,
  session
             = session,
  current_ele = element,
            = mk_rx_res[["capture"]][["rx_obj"]],
             = fcn_desc,
  note
             = TRUE)
  reset
\mbox{\#} You can now place element back in the state
state = MB_set_current_element(state, element)
# This will fetch the current component
```

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```
component = MB_fetch_component(state, element)
 fares = MB_fetch_appends(state, element)
 # You can use the component to build the code to generate the model:
 gen_code =
   MB_build_code(state
                             = state, session = session,
                            = component[["fcn_def"]],
               fcn_def
               time_scale = element[["ui"]][["time_scale"]],
               fcn_obj_name = "my_fcn_obj",
               rx_obj_name = "my_obj_name"
                             = "my_ts_name")
               ts_obj_name
 # Model code to be included in a larger script
 message(paste0(gen_code$model_code, collapse="\n"))
 # Stand-alone model code
 message(paste0(gen_code$model_code_sa, collapse="\n"))
 # This will fetch the code to regenerate all of the components of this module
 message(MB_fetch_code(state))
}
```

MB\_fetch\_catalog

Fetches List of Available Models

### **Description**

Creates a catalog of the models available in the system file.

#### Usage

```
MB_fetch_catalog(state)
```

## **Arguments**

state MB state from MB\_fetch\_state()

### Value

List with the following attributes:

- summary: Dataframe with a summary of the models in the catlog
- sources: Same information a that found in the summary table but in list form.
- select\_group: List with the models grouped by source.
- select\_plain: Flat list with the models (ungrouped).
- select\_subtext: Subtext for pulldown menus.

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- msgs: Messages to be passed back to the user.
- hasmdl: Boolean value indicating if any models were found.
- isgood: Boolean variable indicating success or failure.

```
#library(ruminate)
# This will get the full session:
library(formods)
if( Sys.getenv("ruminate_rxfamily_found") == "TRUE"){
 sess_res = MB_test_mksession()
 # This is just for CRAN
 #sess_res = MB_test_mksession(session=list())
 session = sess_res$session
 input = sess_res$input
 # Configuration files
 FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml")
 MOD_yaml_file = system.file(package = "ruminate", "templates", "MB.yaml")
 # Creating an empty state object
 state = MB_fetch_state(id
                                        = "MB",
                                      = input,
                        input
                        session
                                      = session,
                        FM_yaml_file = FM_yaml_file,
                        MOD_yaml_file = MOD_yaml_file,
                        react_state = NULL)
 # This will provide a list of the available models
 models = MB_fetch_catalog(state)
 # This is a summary of the tables in the model:
 models$summary
 # This will test the models in the catalog, set as_cran
 # to FALSE to test all the models.
 mtres = MB_test_catalog(state, as_cran=TRUE)
 mtres$isgood
 # Creates a new empty element
 state = MB_new_element(state)
 # Delete the current element
 state = MB_del_current_element(state)
 # Fetch a list of the current element
 element = MB_fetch_current_element(state)
 # This will attach a model to it:
 # Pulling the first model from the catalog
 fcn_def = models[["summary"]][1, ][["Model"]]
 fcn_obj = models[["summary"]][1, ][["Object"]]
```

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```
mdl_type = models[["summary"]][1, ][["Type"]]
fcn_desc = models[["summary"]][1, ][["Description"]]
# This will build the rxode2 object from the model
mk_rx_res = mk_rx_obj(
  type = mdl_type,
 model = list(fcn_def = fcn_def,
               fcn_obj = fcn_obj))
# This will attach the model to the current element
element = MB_update_model(
             = state,
  state
  session
             = session,
  current_ele = element,
             = mk_rx_res[["capture"]][["rx_obj"]],
  rx_obj
             = fcn_desc,
  note
  reset
             = TRUE)
# You can now place element back in the state
state = MB_set_current_element(state, element)
# This will fetch the current component
component = MB_fetch_component(state, element)
fares = MB_fetch_appends(state, element)
# You can use the component to build the code to generate the model:
gen_code =
 MB_build_code(state
                           = state, session = session,
              fcn_def
                           = component[["fcn_def"]],
              time_scale = element[["ui"]][["time_scale"]],
              fcn_obj_name = "my_fcn_obj",
              rx_obj_name = "my_obj_name",
              ts_obj_name
                            = "my_ts_name")
# Model code to be included in a larger script
message(paste0(gen_code$model_code, collapse="\n"))
# Stand-alone model code
message(paste0(gen_code$model_code_sa, collapse="\n"))
# This will fetch the code to regenerate all of the components of this module
message(MB_fetch_code(state))
```

MB\_fetch\_code

Fetch Module Code

### **Description**

}

Fetches the code to generate results seen in the app

MB\_fetch\_code

### Usage

```
MB_fetch_code(state)
```

### **Arguments**

state MB state from MB\_fetch\_state()

#### Value

Character object vector with the lines of code

```
#library(ruminate)
# This will get the full session:
library(formods)
if( Sys.getenv("ruminate_rxfamily_found") == "TRUE"){
 sess_res = MB_test_mksession()
 # This is just for CRAN
 #sess_res = MB_test_mksession(session=list())
 session = sess_res$session
 input = sess_res$input
 # Configuration files
 FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml")
 MOD_yaml_file = system.file(package = "ruminate", "templates", "MB.yaml")
 # Creating an empty state object
 state = MB_fetch_state(id
                                      = "MB",
                        input
                                      = input,
                        session = session,
                        FM_yaml_file = FM_yaml_file,
                        MOD_yaml_file = MOD_yaml_file,
                        react_state
                                        = NULL)
 # This will provide a list of the available models
 models = MB_fetch_catalog(state)
 # This is a summary of the tables in the model:
 models$summary
 # This will test the models in the catalog, set as_cran
 # to FALSE to test all the models.
 mtres = MB_test_catalog(state, as_cran=TRUE)
 mtres$isgood
 # Creates a new empty element
 state = MB_new_element(state)
 # Delete the current element
 state = MB_del_current_element(state)
```

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```
# Fetch a list of the current element
element = MB_fetch_current_element(state)
# This will attach a model to it:
# Pulling the first model from the catalog
fcn_def = models[["summary"]][1, ][["Model"]]
fcn_obj = models[["summary"]][1, ][["Object"]]
mdl_type = models[["summary"]][1, ][["Type"]]
fcn_desc = models[["summary"]][1, ][["Description"]]
# This will build the rxode2 object from the model
mk_rx_res = mk_rx_obj(
  type = mdl_type,
  model = list(fcn_def = fcn_def,
               fcn_obj = fcn_obj))
# This will attach the model to the current element
element = MB_update_model(
  state
             = state,
  session
             = session,
  current_ele = element,
             = mk_rx_res[["capture"]][["rx_obj"]],
  rx_obj
             = fcn_desc,
 note
             = TRUE)
  reset
# You can now place element back in the state
state = MB_set_current_element(state, element)
# This will fetch the current component
component = MB_fetch_component(state, element)
fares = MB_fetch_appends(state, element)
# You can use the component to build the code to generate the model:
gen_code =
  MB_build_code(state
                            = state, session = session,
              fcn_def
                            = component[["fcn_def"]],
              time_scale = element[["ui"]][["time_scale"]],
              fcn_obj_name = "my_fcn_obj",
                             = "my_obj_name"
              rx_obj_name
              ts_obj_name
                             = "my_ts_name")
# Model code to be included in a larger script
message(paste0(gen_code$model_code, collapse="\n"))
# Stand-alone model code
message(paste0(gen_code$model_code_sa, collapse="\n"))
# This will fetch the code to regenerate all of the components of this module
message(MB_fetch_code(state))
```

}

MB\_fetch\_component Fetch Selected Current Model Component

### **Description**

Fetches the selected component of the provided model.

## Usage

```
MB_fetch_component(state, current_ele, component_id = NULL)
```

## **Arguments**

```
state MB state from MB_fetch_state()

current_ele MB model element from MB_fetch_current_element()

component_id The numeric component id to select (default NULL) will return the selected ID.
```

#### Value

list with the current component with the following attributes

- isgood: Boolean object indicating success.
- rx\_obj: rxode2 object for the model.
- ts\_obj: timescale object for the model.
- fcn\_def: Just the model function definition.
- note: Note field from the components\_table
- model\_code: Code to generate model.
- model code sa: Stand-alone code to generate model with
- msgs: Messages to be passed back to the user.

```
#library(ruminate)
# This will get the full session:
library(formods)
if( Sys.getenv("ruminate_rxfamily_found") == "TRUE"){
    sess_res = MB_test_mksession()
    # This is just for CRAN
    #sess_res = MB_test_mksession(session=list())
    session = sess_res$session
    input = sess_res$input

# Configuration files
FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml")
MOD_yaml_file = system.file(package = "ruminate", "templates", "MB.yaml")
```

```
# Creating an empty state object
state = MB_fetch_state(id
                                      = "MB",
                                      = input,
                      input
                       session
                                      = session,
                       FM_yaml_file = FM_yaml_file,
                      MOD_yaml_file = MOD_yaml_file,
                       react_state
                                      = NULL)
# This will provide a list of the available models
models = MB_fetch_catalog(state)
# This is a summary of the tables in the model:
models$summary
# This will test the models in the catalog, set as_cran
# to FALSE to test all the models.
mtres = MB_test_catalog(state, as_cran=TRUE)
mtres$isgood
# Creates a new empty element
state = MB_new_element(state)
# Delete the current element
state = MB_del_current_element(state)
# Fetch a list of the current element
element = MB_fetch_current_element(state)
# This will attach a model to it:
# Pulling the first model from the catalog
fcn_def = models[["summary"]][1, ][["Model"]]
fcn_obj = models[["summary"]][1, ][["Object"]]
mdl_type = models[["summary"]][1, ][["Type"]]
fcn_desc = models[["summary"]][1, ][["Description"]]
# This will build the rxode2 object from the model
mk_rx_res = mk_rx_obj(
  type = mdl_type,
 model = list(fcn_def = fcn_def,
               fcn_obj = fcn_obj))
# This will attach the model to the current element
element = MB_update_model(
  state
             = state,
  session
             = session,
  current_ele = element,
            = mk_rx_res[["capture"]][["rx_obj"]],
  rx_obj
  note
             = fcn_desc,
  reset
             = TRUE)
# You can now place element back in the state
state = MB_set_current_element(state, element)
```

```
# This will fetch the current component
 component = MB_fetch_component(state, element)
 fares = MB_fetch_appends(state, element)
 # You can use the component to build the code to generate the model:
 gen_code =
   MB_build_code(state
                              = state, session = session,
               fcn_def
                              = component[["fcn_def"]],
                              = element[["ui"]][["time_scale"]],
                time_scale
               fcn_obj_name = "my_fcn_obj",
                              = "my_obj_name",
                rx_obj_name
                ts_obj_name
                              = "my_ts_name")
 # Model code to be included in a larger script
 message(paste0(gen_code$model_code, collapse="\n"))
 # Stand-alone model code
 message(paste0(gen_code$model_code_sa, collapse="\n"))
 # This will fetch the code to regenerate all of the components of this module
 message(MB_fetch_code(state))
}
```

MB\_fetch\_current\_element

Fetches Current model

## **Description**

Takes a MB state and returns the current active model object.

### Usage

```
MB_fetch_current_element(state)
```

#### **Arguments**

state MB state from MB\_fetch\_state()

#### Value

List containing the details of the active data view. The structure of this list is the same as the structure of state\$MB\$elements in the output of MB\_fetch\_state().

```
#library(ruminate)
# This will get the full session:
library(formods)
if( Sys.getenv("ruminate_rxfamily_found") == "TRUE"){
 sess_res = MB_test_mksession()
 # This is just for CRAN
 #sess_res = MB_test_mksession(session=list())
 session = sess_res$session
 input = sess_res$input
 # Configuration files
 FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml")
 MOD_yaml_file = system.file(package = "ruminate", "templates", "MB.yaml")
 # Creating an empty state object
                                       = "MB",
 state = MB_fetch_state(id
                                      = input,
                        input
                        session
                                      = session,
                        FM_yaml_file = FM_yaml_file,
                        MOD_yaml_file = MOD_yaml_file,
                        react_state
                                        = NULL)
 # This will provide a list of the available models
 models = MB_fetch_catalog(state)
 # This is a summary of the tables in the model:
 models$summary
 # This will test the models in the catalog, set as_cran
 # to FALSE to test all the models.
 mtres = MB_test_catalog(state, as_cran=TRUE)
 mtres$isgood
 # Creates a new empty element
 state = MB_new_element(state)
 # Delete the current element
 state = MB_del_current_element(state)
 # Fetch a list of the current element
 element = MB_fetch_current_element(state)
 # This will attach a model to it:
 # Pulling the first model from the catalog
 fcn_def = models[["summary"]][1, ][["Model"]]
 fcn_obj = models[["summary"]][1, ][["Object"]]
 mdl_type = models[["summary"]][1, ][["Type"]]
 fcn_desc = models[["summary"]][1, ][["Description"]]
 # This will build the rxode2 object from the model
 mk_rx_res = mk_rx_obj(
```

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```
type = mdl_type,
  model = list(fcn_def = fcn_def,
               fcn_obj = fcn_obj))
# This will attach the model to the current element
element = MB_update_model(
  state
             = state,
           = session,
  session
 current_ele = element,
             = mk_rx_res[["capture"]][["rx_obj"]],
  rx_obj
             = fcn_desc,
 note
             = TRUE)
  reset
# You can now place element back in the state
state = MB_set_current_element(state, element)
# This will fetch the current component
component = MB_fetch_component(state, element)
fares = MB_fetch_appends(state, element)
# You can use the component to build the code to generate the model:
gen_code =
                            = state, session = session,
 MB_build_code(state
                            = component[["fcn_def"]],
              fcn_def
              time_scale
                            = element[["ui"]][["time_scale"]],
              fcn_obj_name = "my_fcn_obj",
              rx_obj_name
                           = "my_obj_name",
              ts_obj_name
                           = "my_ts_name")
# Model code to be included in a larger script
message(paste0(gen_code$model_code, collapse="\n"))
# Stand-alone model code
message(paste0(gen_code$model_code_sa, collapse="\n"))
# This will fetch the code to regenerate all of the components of this module
message(MB_fetch_code(state))
```

MB\_fetch\_mdl

Fetch Model Builder Module Models

### **Description**

}

Fetches the models contained in the module.

### Usage

```
MB_fetch_mdl(state)
```

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## **Arguments**

state MB state from MB\_fetch\_state()

### Value

list containing the following elements

- isgood: Return status of the function.
- hasmdl: Boolean indicator if the module has any models
- msgs: Messages to be passed back to the user.
- mdl: List with models. Each list element has the name of the R-object for that dataset. Each element has the following structure:
  - label: Text label for the model (e.g. one-compartment model).
  - MOD\_TYPE: Type of module.
  - id: Module ID.
  - rx\_obj: The rxode2 object.
  - rx\_obj\_name: The rxode2 object name that holds the model.
  - ts\_obj List with elements system and details
  - ts\_obj\_name: The object name that holds the model time scale information.
  - fcn\_def: Text to define the model
  - MDLMETA: Notes about the model.
  - code: Code to generate the model.
  - checksum: Module checksum.
  - MDLchecksum: Model checksum.

## **Examples**

```
# We need a module state:
sess_res = MB_test_mksession()
state = sess_res$state

mdls = MB_fetch_mdl(state)
names(mdls)
```

MB\_fetch\_state

Fetch Model Builder State

### Description

Merges default app options with the changes made in the UI

MB\_fetch\_state

### Usage

```
MB_fetch_state(
   id,
   id_ASM,
   input,
   session,
   FM_yaml_file,
   MOD_yaml_file,
   react_state
)
```

# Arguments

id	Shiny module ID
id_ASM	ID string for the app state management module used to save and load app states
input	Shiny input variable
session	Shiny session variable
FM_yaml_file	App configuration file with FM as main section.
MOD_yaml_file	Module configuration file with MC as main section.
react_state	Variable passed to server to allow reaction outside of module (NULL)

#### Value

list containing the current state of the app including default values from the yaml file as well as any changes made by the user. The list has the following structure:

- yaml: Full contents of the supplied yaml file.
- MC: Module components of the yaml file.
- MB:
  - isgood: Boolean object indicating if the file was successfully loaded.
  - checksum: This is an MD5 sum of the contents element and can be used to detect changes in the state.
- MOD\_TYPE: Character data containing the type of module "MB"
- id: Character data containing the module id module in the session variable.
- FM\_yaml\_file: App configuration file with FM as main section.
- MOD\_yaml\_file: Module configuration file with MC as main section.

```
# Within shiny both session and input variables will exist,
# this creates examples here for testing purposes:
sess_res = MB_test_mksession()
session = sess_res$session
input = sess_res$input
```

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```
# Configuration files
FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml")
MOD_yaml_file = system.file(package = "ruminate", "templates", "MB.yaml")
# Creating an empty state object
state = MB_fetch_state(id
                                      = "MB",
                                     = "ASM",
                      id_ASM
                      input
                                     = input,
                      session
                                     = session,
                      FM_yaml_file = FM_yaml_file,
                      MOD_yaml_file = MOD_yaml_file,
                                      = NULL)
                      react_state
```

MB\_init\_state

Initialize MB Module State

### **Description**

Creates a list of the initialized module state

### Usage

```
MB_init_state(FM_yaml_file, MOD_yaml_file, id, session)
```

## Arguments

FM\_yaml\_file App configuration file with FM as main section.

MOD\_yaml\_file Module configuration file with MC as main section.

id ID string for the module.

session Shiny session variable

#### Value

list containing an empty MB state

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```
"MB.yam1"),
id = "MB",
session = session)
state
```

MB\_mk\_preload

Make List of Current MB State

# Description

Reads in the app state from yaml files.

# Usage

```
MB_mk_preload(state)
```

## **Arguments**

state

MB state object

## Value

list with the following elements

- isgood: Boolean indicating the exit status of the function.
- msgs: Messages to be passed back to the user.
- yaml\_list: Lists with preload components.

## **Examples**

```
sess_res = MB_test_mksession()
state = sess_res$state
res = MB_mk_preload(state)
```

MB\_new\_element

New Model Building Model

## **Description**

Appends a new empty model to the MB state object and makes this new model the active model.

# Usage

```
MB_new_element(state)
```

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## **Arguments**

state MB state from MB\_fetch\_state()

#### Value

MB state object containing a new model and that model is set as the current active model. See the help for MB\_fetch\_state() for model format.

```
#library(ruminate)
# This will get the full session:
library(formods)
if( Sys.getenv("ruminate_rxfamily_found") == "TRUE"){
 sess_res = MB_test_mksession()
 # This is just for CRAN
 #sess_res = MB_test_mksession(session=list())
 session = sess_res$session
 input = sess_res$input
 # Configuration files
 FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml")
 MOD_yaml_file = system.file(package = "ruminate", "templates", "MB.yaml")
 # Creating an empty state object
                                        = "MB",
 state = MB_fetch_state(id
                        input
                                       = input,
                                      = session,
                        session
                        FM_yaml_file = FM_yaml_file,
                        MOD_yaml_file = MOD_yaml_file,
                        react_state
                                        = NULL)
 # This will provide a list of the available models
 models = MB_fetch_catalog(state)
 # This is a summary of the tables in the model:
 models$summary
 # This will test the models in the catalog, set as_cran
 # to FALSE to test all the models.
 mtres = MB_test_catalog(state, as_cran=TRUE)
 mtres$isgood
 # Creates a new empty element
 state = MB_new_element(state)
 # Delete the current element
 state = MB_del_current_element(state)
 # Fetch a list of the current element
 element = MB_fetch_current_element(state)
```

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```
# This will attach a model to it:
# Pulling the first model from the catalog
fcn_def = models[["summary"]][1, ][["Model"]]
fcn_obj = models[["summary"]][1, ][["Object"]]
mdl_type = models[["summary"]][1, ][["Type"]]
fcn_desc = models[["summary"]][1, ][["Description"]]
# This will build the rxode2 object from the model
mk_rx_res = mk_rx_obj(
  type = mdl_type,
  model = list(fcn_def = fcn_def,
               fcn_obj = fcn_obj))
# This will attach the model to the current element
element = MB_update_model(
  state
             = state,
  session
             = session,
  current_ele = element,
             = mk_rx_res[["capture"]][["rx_obj"]],
  note
              = fcn_desc,
              = TRUE)
  reset
# You can now place element back in the state
state = MB_set_current_element(state, element)
# This will fetch the current component
component = MB_fetch_component(state, element)
fares = MB_fetch_appends(state, element)
# You can use the component to build the code to generate the model:
gen_code =
 MB_build_code(state
                            = state, session = session,
                            = component[["fcn_def"]],
              fcn_def
                            = element[["ui"]][["time_scale"]],
              time_scale
              fcn_obj_name = "my_fcn_obj",
                             = "my_obj_name"
              rx_obj_name
                            = "my_ts_name")
              ts_obj_name
# Model code to be included in a larger script
message(paste0(gen_code$model_code, collapse="\n"))
# Stand-alone model code
message(paste0(gen_code$model_code_sa, collapse="\n"))
# This will fetch the code to regenerate all of the components of this module
message(MB_fetch_code(state))
```

}

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# **Description**

Populates the supplied session variable with information from list of sources.

## Usage

```
MB_preload(
   session,
   src_list,
   yaml_res,
   mod_ID = NULL,
   react_state = list(),
   quickload = FALSE
)
```

# Arguments

session	Shiny session variable (in app) or a list (outside of app)
src_list	List of preload data (all read together with module IDs at the top level)
yaml_res	List data from module yaml config
mod_ID	Module ID of the module being loaded.
react_state	Reactive shiny object (in app) or a list (outside of app) used to trigger reactions.
quickload	Logical TRUE to load reduced analysis FALSE to load the full analysis

## Value

list with the following elements

- isgood: Boolean indicating the exit status of the function.
- msgs: Messages to be passed back to the user.
- session: Session object
- input: The value of the shiny input at the end of the session initialization.
- state: App state.
- react\_state: The react\_state components.

MB_Server	Model Builder State Server	

# Description

Server function for the Model Builder Shiny Module

### **Usage**

```
MB_Server(
   id,
   id_ASM = "ASM",
   FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml"),
   MOD_yaml_file = system.file(package = "ruminate", "templates", "MB.yaml"),
   deployed = FALSE,
   react_state = NULL
)
```

### **Arguments**

An ID string that corresponds with the ID used to call the modules UI elements id\_ASM ID string for the app state managment module used to save and load app states FM\_yaml\_file App configuration file with FM as main section.

MOD\_yaml\_file Module configuration file with MC as main section.

deployed Boolean variable indicating whether the app is deployed or not.

react\_state Variable passed to server to allow reaction outside of module (NULL)

#### Value

MB Server object

```
MB_set_current_element
```

Sets the Value for the Current model

## **Description**

Takes a MB state and returns the current active model

### Usage

```
MB_set_current_element(state, element)
```

## **Arguments**

state MB state from MB\_fetch\_state()

#### Value

MB state object with the current model set using the supplied value.

```
#library(ruminate)
# This will get the full session:
library(formods)
if( Sys.getenv("ruminate_rxfamily_found") == "TRUE"){
 sess_res = MB_test_mksession()
 # This is just for CRAN
 #sess_res = MB_test_mksession(session=list())
 session = sess_res$session
 input = sess_res$input
 # Configuration files
 FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml")
 MOD_yaml_file = system.file(package = "ruminate", "templates", "MB.yaml")
 # Creating an empty state object
                                       = "MB",
 state = MB_fetch_state(id
                                      = input,
                        input
                        session
                                      = session,
                        FM_yaml_file = FM_yaml_file,
                        MOD_yaml_file = MOD_yaml_file,
                        react_state
                                        = NULL)
 # This will provide a list of the available models
 models = MB_fetch_catalog(state)
 # This is a summary of the tables in the model:
 models$summary
 # This will test the models in the catalog, set as_cran
 # to FALSE to test all the models.
 mtres = MB_test_catalog(state, as_cran=TRUE)
 mtres$isgood
 # Creates a new empty element
 state = MB_new_element(state)
 # Delete the current element
 state = MB_del_current_element(state)
 # Fetch a list of the current element
 element = MB_fetch_current_element(state)
 # This will attach a model to it:
 # Pulling the first model from the catalog
 fcn_def = models[["summary"]][1, ][["Model"]]
 fcn_obj = models[["summary"]][1, ][["Object"]]
 mdl_type = models[["summary"]][1, ][["Type"]]
 fcn_desc = models[["summary"]][1, ][["Description"]]
 # This will build the rxode2 object from the model
 mk_rx_res = mk_rx_obj(
```

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```
type = mdl_type,
  model = list(fcn_def = fcn_def,
               fcn_obj = fcn_obj))
# This will attach the model to the current element
element = MB_update_model(
  state
             = state,
           = session,
  session
 current_ele = element,
             = mk_rx_res[["capture"]][["rx_obj"]],
  rx_obj
             = fcn_desc,
 note
             = TRUE)
  reset
# You can now place element back in the state
state = MB_set_current_element(state, element)
# This will fetch the current component
component = MB_fetch_component(state, element)
fares = MB_fetch_appends(state, element)
# You can use the component to build the code to generate the model:
gen_code =
                            = state, session = session,
 MB_build_code(state
                            = component[["fcn_def"]],
              fcn_def
              time_scale
                            = element[["ui"]][["time_scale"]],
              fcn_obj_name = "my_fcn_obj",
              rx_obj_name
                           = "my_obj_name",
              ts_obj_name
                           = "my_ts_name")
# Model code to be included in a larger script
message(paste0(gen_code$model_code, collapse="\n"))
# Stand-alone model code
message(paste0(gen_code$model_code_sa, collapse="\n"))
# This will fetch the code to regenerate all of the components of this module
message(MB_fetch_code(state))
```

MB\_test\_catalog

Tests the Model Catalog

## **Description**

}

Reads in models in the catalog and attempts to build them.

### Usage

```
MB_test_catalog(state, as_cran = FALSE, verbose = TRUE)
```

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## **Arguments**

state	MB state from MB_fetch_state()
as_cran	Boolean to indicate if you're running this on CRAN
verbose	Boolean to indicate if messages should be displayed.

#### Value

List with the following attributes:

- isgood: Boolean variable indicating if all the models in the catalog passed the test.
- msgs: Messages indicating if the test was successful or not.

```
#library(ruminate)
# This will get the full session:
library(formods)
if( Sys.getenv("ruminate_rxfamily_found") == "TRUE"){
 sess_res = MB_test_mksession()
 # This is just for CRAN
 #sess_res = MB_test_mksession(session=list())
 session = sess_res$session
 input = sess_res$input
 # Configuration files
 FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml")
 MOD_yaml_file = system.file(package = "ruminate", "templates", "MB.yaml")
 # Creating an empty state object
                                      = "MB",
 state = MB_fetch_state(id
                                      = input,
                        input
                                = session,
                        session
                        FM_yaml_file = FM_yaml_file,
                        MOD_yaml_file = MOD_yaml_file,
                        react_state
                                     = NULL)
 # This will provide a list of the available models
 models = MB_fetch_catalog(state)
 # This is a summary of the tables in the model:
 models$summary
 # This will test the models in the catalog, set as_cran
 # to FALSE to test all the models.
 mtres = MB_test_catalog(state, as_cran=TRUE)
 mtres$isgood
 # Creates a new empty element
 state = MB_new_element(state)
 # Delete the current element
```

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```
state = MB_del_current_element(state)
# Fetch a list of the current element
element = MB_fetch_current_element(state)
# This will attach a model to it:
# Pulling the first model from the catalog
fcn_def = models[["summary"]][1, ][["Model"]]
fcn_obj = models[["summary"]][1, ][["Object"]]
mdl_type = models[["summary"]][1, ][["Type"]]
fcn_desc = models[["summary"]][1, ][["Description"]]
# This will build the rxode2 object from the model
mk_rx_res = mk_rx_obj(
  type = mdl_type,
  model = list(fcn_def = fcn_def,
               fcn_obj = fcn_obj))
# This will attach the model to the current element
element = MB_update_model(
  state
             = state,
             = session,
  session
 current_ele = element,
             = mk_rx_res[["capture"]][["rx_obj"]],
  rx_obj
             = fcn_desc,
 note
  reset
             = TRUE)
# You can now place element back in the state
state = MB_set_current_element(state, element)
# This will fetch the current component
component = MB_fetch_component(state, element)
fares = MB_fetch_appends(state, element)
# You can use the component to build the code to generate the model:
gen_code =
 MB_build_code(state
                           = state, session = session,
              fcn_def
                            = component[["fcn_def"]],
              time_scale
                            = element[["ui"]][["time_scale"]],
              fcn_obj_name = "my_fcn_obj",
              rx_obj_name = "my_obj_name",
              ts_obj_name = "my_ts_name")
# Model code to be included in a larger script
message(paste0(gen_code$model_code, collapse="\n"))
# Stand-alone model code
message(paste0(gen\_code\$model\_code\_sa, collapse="\n"))
# This will fetch the code to regenerate all of the components of this module
message(MB_fetch_code(state))
```

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}

MB\_test\_mksession

Populate Session Data for Module Testing

# Description

Populates the supplied session variable for testing.

# Usage

```
MB_test_mksession(session = list())
```

# Arguments

session

Shiny session variable (in app) or a list (outside of app)

#### Value

The MB portion of the all\_sess\_res returned from FM\_app\_preload

### See Also

```
FM_app_preload
```

# **Examples**

```
session = shiny::MockShinySession$new()
sess_res = MB_test_mksession(session=session)
```

MB\_update\_checksum

Update MB Module Checksum

## **Description**

Takes a MB state and updates the checksum used to trigger downstream updates

# Usage

```
MB_update_checksum(state)
```

# **Arguments**

state

MB state from MB\_fetch\_state()

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### Value

MB state object with the checksum updated

# Examples

```
# Within shiny both session and input variables will exist,
# this creates examples here for testing purposes:
sess_res = MB_test_mksession()
session = sess_res$session
input = sess_res$input

# We also need a state variable
state = sess_res$state
state = MB_update_checksum(state)
```

MB\_update\_model

Updates Current Element with rxode2 Model

### **Description**

Takes an rxode2 object and updates the model components of the current element.

# Usage

```
MB_update_model(state, session, current_ele, rx_obj, note, reset = FALSE)
```

## **Arguments**

state MB state from MB\_fetch\_state()

session Shiny session variable

rx\_obj rxode2 model from rxode2::rxode2()

note text indicating what this update does (e.g. "added parameter")

reset boolean indicating that the element needs to be reset (i.e. if you change the base

model) default: FALSE.

### Value

current\_element with model attached

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```
#library(ruminate)
# This will get the full session:
library(formods)
if( Sys.getenv("ruminate_rxfamily_found") == "TRUE"){
 sess_res = MB_test_mksession()
 # This is just for CRAN
 #sess_res = MB_test_mksession(session=list())
 session = sess_res$session
 input = sess_res$input
 # Configuration files
 FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml")
 MOD_yaml_file = system.file(package = "ruminate", "templates", "MB.yaml")
 # Creating an empty state object
                                       = "MB",
 state = MB_fetch_state(id
                                      = input,
                        input
                        session
                                      = session,
                        FM_yaml_file = FM_yaml_file,
                        MOD_yaml_file = MOD_yaml_file,
                        react_state
                                        = NULL)
 # This will provide a list of the available models
 models = MB_fetch_catalog(state)
 # This is a summary of the tables in the model:
 models$summary
 # This will test the models in the catalog, set as_cran
 # to FALSE to test all the models.
 mtres = MB_test_catalog(state, as_cran=TRUE)
 mtres$isgood
 # Creates a new empty element
 state = MB_new_element(state)
 # Delete the current element
 state = MB_del_current_element(state)
 # Fetch a list of the current element
 element = MB_fetch_current_element(state)
 # This will attach a model to it:
 # Pulling the first model from the catalog
 fcn_def = models[["summary"]][1, ][["Model"]]
 fcn_obj = models[["summary"]][1, ][["Object"]]
 mdl_type = models[["summary"]][1, ][["Type"]]
 fcn_desc = models[["summary"]][1, ][["Description"]]
 # This will build the rxode2 object from the model
 mk_rx_res = mk_rx_obj(
```

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```
type = mdl_type,
  model = list(fcn_def = fcn_def,
               fcn_obj = fcn_obj))
# This will attach the model to the current element
element = MB_update_model(
  state
             = state,
           = session,
  session
  current_ele = element,
            = mk_rx_res[["capture"]][["rx_obj"]],
  rx_obj
             = fcn_desc,
 note
             = TRUE)
  reset
# You can now place element back in the state
state = MB_set_current_element(state, element)
# This will fetch the current component
component = MB_fetch_component(state, element)
fares = MB_fetch_appends(state, element)
# You can use the component to build the code to generate the model:
gen_code =
 MB_build_code(state
                            = state, session = session,
                            = component[["fcn_def"]],
              fcn_def
              time_scale
                            = element[["ui"]][["time_scale"]],
              fcn_obj_name = "my_fcn_obj",
              rx_obj_name = "my_obj_name",
              ts_obj_name
                           = "my_ts_name")
# Model code to be included in a larger script
message(paste0(gen_code$model_code, collapse="\n"))
# Stand-alone model code
message(paste0(gen_code$model_code_sa, collapse="\n"))
# This will fetch the code to regenerate all of the components of this module
message(MB_fetch_code(state))
```

mk\_figure\_ind\_obs

Creates Figures of Individual Observations from PKNCA Result

### **Description**

}

Takes the output of PKNCA and creates ggplot figures faceted by subject id highlighting of certain NCA aspects (e.g. points used for half-life)

mk\_figure\_ind\_obs 83

## Usage

```
mk_figure_ind_obs(
   nca_res,
   OBS_LAB = "Concentration ===CONCUNITS===",
   TIME_LAB = "Time ===TIMEUNITS===",
   OBS_STRING = "Observation",
   BLQ_STRING = "BLQ",
   NA_STRING = "Missing",
   log_scale = TRUE,
   scales = "fixed",
   nfrows = 4,
   nfcols = 3
)
```

## **Arguments**

nca_res	Output of PKNCA.
OBS_LAB	Label of the observation axis with optional ===CONCUNITS=== placeholder for units.
TIME_LAB	Label of the time axis with optional ===TIMEUNITS=== placeholder for units.
OBS_STRING	Label for observation data.
BLQ_STRING	Label for BLQ data.
NA_STRING	Label for missing data.
log_scale	Boolean variable to control y-scale (TRUE: Log 10, FALSE: linear).
scales	String to determine the scales used when faceting. Can be either "fixed", "free", "free_x", or "free_y".
nfrows	Number of facet rows per page.
nfcols	Number of facet cols per page.

#### Value

List containing the element figures which is a list of figure pages ("Figure 1", "Figure 2", etc.). Each of these is a also a list containing two elements:

- gg: A ggplot object for that page.
- notes: Placeholder for future notes, but NULL now.

```
# We need a state variable to be define
sess_res = NCA_test_mksession()

state = sess_res$state

# Pulls out the active analysis
current_ana = NCA_fetch_current_ana(state)
```

 $mk_rx_obj$ 

```
# This is the raw PKNCA output
pknca_res = NCA_fetch_ana_pknca(state, current_ana)
# Building the figure
mk_res = mk_figure_ind_obs(nca_res = pknca_res)
mk_res$figures$Figure_1$gg
```

mk\_rx\_obj

Makes an rxode2 Object

### **Description**

Creates an rxode2 object from a model (either rxode2 function or a NONMEM file)

### Usage

```
mk_rx_obj(type, model)
```

## **Arguments**

type

Type of supplied model can be "rxode2", "NONMEM"

mode1

List containing the relevant information about the model. This will depend on the model types.

- rxode2: The supplied model is in the rxode2 format.
  - fcn\_def: Character string containing function definition.
  - fcn\_obj: Name of the function object created in fcn\_def.
- NONMEM: The supplied model is in NONMEM format (either a control
  - model\_file: Character string containing the NONMEM model file.

### Value

Results of FM\_tc() when running the model. This will include a field isgood which is a boolean variable indicating success or failure. See the documentation for FM\_tc() for the format returned when evaluation results in a failure and how to address those. When successful the capture field will contain the following:

- fcn\_obj: The function name.
- rx\_obj: The built rxode2 object.

```
label("Absorption rate (Ka)")
           lcl <- 1
           label("Clearance (CL)")
           lvc <- 3.45
           label("Central volume of distribution (V)")
           propSd <- c(0, 0.5)
           label("Proportional residual error (fraction)")
       })
       model({
           ka <- exp(lka)
           cl <- exp(lcl)</pre>
           vc <- exp(lvc)
           cp <- linCmt()</pre>
           cp ~ prop(propSd)
       })
   }'
fcn_obj = "my_func"
model = list(fcn_def = fcn_def,
             fcn_obj = fcn_obj)
rx_res = mk_rx_obj("rxode2", model)
# function object
rx_res[["capture"]][["fcn_obj"]]
# rxode2 object
rx_res[["capture"]][["rx_obj"]]
```

mk\_subjects

Fetches Information from an rxode2 Object

# Description

This will provide information like parameter names, covriates, etc from an rxode2 object.

### Usage

```
mk_subjects(object, nsub = 10, covs = NULL)
```

# Arguments

object	rxode2 model object An ID string that corresponds with the ID used to call the modules UI elements.
nsub	Number of subjects to generate. If set to 1 it will return the typical values (IIV set to zero).
covs	List describing how covariates should be generated.

#### **Details**

See below.

The underlying simulations are run using rxode2, and as such we need an rxode2 system object. From that we can either simulate subjects or load them from a file. Next we need to define a set of rules. These will be a set of conditions and actions. At each evaluation time point the conditions are evaluated. When a condition is met the actions associated with that condition are executed. For example, if during a visit (an evaluation time point) the trough PK is below a certain level (condition) we may want to increase the dosing regimen for the next dosing cycle (action).

#### **Creating subjects:**

Subjects are expected in a data frame with the following column headers:

- · id Individual subject id
- Names of parameters and iiv as specified in the ini section of the rxode2 function specification
- Names of covariates used in the model.

mk\_subjects() — Creates subjects for simulation by sampling based on between-subject variability and generating covariate information based on user specifications.

#### Covariates:

The covs input is a list with the following structure:

- type: Can be either "fixed", "discrete", or "continuous".
- sampling: This field is only needed for a "continuous" covariate ' type and can be either "random", "normal" or "log-normal".
- values: This field depends on the type and optional sampling above.
  - fixed: A single value.
  - discrete: A vector of possible discrete elements.
  - continuous, random: Two values the first is the lower bound and the second is the upper bound.
  - continuous, normal: Two values the first is the mean and the second is the variance.
  - continuous, log-normal: Two values the first is the mean and the second is the variance.

This examples shows the SEX\_ID randomly sampled from the values specified, SUBTYPE\_ID fixed at a value, and WT sampled from a log-normal distribution.

```
covs = list(
                              = "discrete",
  SEX_ID
             = list(type
                    values
                             = c(0,1)),
                              = "fixed",
  SUBTYPE_ID = list(type
                    values
                             = c(0)),
  WT
             = list(type
                             = "continuous",
                    sampling = "log-normal",
                    values
                             = c(70, .15))
)
```

#### **Rule-based simulations:**

simulate\_rules() — This will run simulations based on the rule definitions below.

### Rules:

Rules are a named list where the list name can be a short descriptive label used to remember what the rule does. These names will be returned as columns in the simulated data frame.

• condition: Character string that evaluates to either TRUE or FALSE. When true the action portion will be triggered. For a list of objects available see the Rule-evaluation environment below.

- fail\_flag: Flag set in the rule\_id column when the condition is not met (set to "false" if not specified).
- true\_flag: Flag set in the rule\_id column when the condition is met (set to "true" if not specified).
- action: This is what the rule will trigger can be any of the following:
  - type: This defines the action type and can be either "dose", "set state", or "manual".

Based on the type the action field will expect different elements.

#### Dosing:

- action
  - type: "dose"
  - values: Character string that evaluates as a numeric vector dosing amounts (e.g. "c(3, 3, 3, 3)")
  - times: Character string that evaluates as a numeric vector of times (e.g. "c(0, 14, 28, 42)")
  - durations: Character string that evaluates as a numeric vector of durations (e.g. "c(0, 0, 0, 0)", zero for bolus dosing)

#### Changing a state value:

- action
  - type: "set state"
  - state: Character string with the name of the state to set ("Ac")
  - value: Character string that evaluates as a numeric value for state (e.g. "Ac/2" would set the state to half the value of Ac at the evaluation point)

Manual modification of the simulation:

- action
  - type: "manual"
  - code: Character string of code to evaluate.

#### Rule-evaluation environment:

Beyond simple simulations it will be necessary to execute actions based on the current or previous state of the system. For this reason, when a condition or elements of the action (e.g., the values, times and durations of a dose action type) are being evaluated, the following objects will be available at each evaluation point:

- outputs: The value of each model output.
- states: The value of each named state or compartment.
- covariates: The value of each named covariate.
- subject-level parameters: The value of each named parameter.
- rule value: The last value the rule evaluated as.
- id: Current subject id.
- time: Current evaluation time.
- SI\_SUB\_HISTORY: A data frame of the simulation history of the current subject up to the current evaluation point.
- SI\_subjects: The subjects data frame.

- SI\_eval\_times: Vector of the evaluation times.
- SI\_interval\_ev: The events table in it's current state for the given simulation interval.
- SI\_ev\_history: This is the history of the event table containing all the events leading up to the current interval.
- SI\_ud\_history: This is a free form object the user can define or alter within the "man-ual" action type (ud-user defined, history).

The following functions will be available::

• SI\_fpd: This function will fetch the previous dose (fpd) for the given id and state. For example for the current id and the state Ac you would do the following:

```
SI_fpd(id=id, state="Ac")
```

#### Time scales:

You can include columns in your output for different time scales if you wish. You need to create a list in the format below. One element should be system with a short name for the system time scale. The next should be details which is a list containing short names for each time scale you want to include. Each of these is a list with a verbose name for the time scale (verb) and a numerical conversion indicating how that time scale relates to the others. Here we define weeks and days on the basis of seconds.

#### Value

List with the following elements.

- isgood: Return status of the function.
- msgs: Error or warning messages if any issues were encountered.
- subjects: Data frame of parameters and covariates for the subjects generated.
- iCov: Data frame of the covariates.
- params: Data frame of the parameters.

### See Also

```
vignette("clinical_trial_simulation", package = "ruminate")
```

```
library(formods)
library(ggplot2)

# For more information see the Clinical Trial Simulation vignette:
# https://ruminate.ubiquity.tools/articles/clinical_trial_simulation.html

# None of this will work if rxode2 isn't installed:
if(is_installed("rxode2")){
library(rxode2)
```

```
set.seed(8675309)
rxSetSeed(8675309)
my_model = function ()
  description <- "One compartment PK model with linear clearance using differential equations"
    ini({
        lka <- 0.45
        label("Absorption rate (Ka)")
        lcl <- 1
        label("Clearance (CL)")
        lvc <- 3.45
        label("Central volume of distribution (V)")
        propSd <- c(0, 0.5)
        label("Proportional residual error (fraction)")
        etalcl ~ 0.1
    })
    model({
        ka <- exp(lka)</pre>
        cl <- exp(lcl + etalcl)</pre>
        vc <- exp(lvc)</pre>
        kel <- cl/vc
        d/dt(depot) <- -ka * depot
        d/dt(central) <- ka * depot - kel * central</pre>
        Cc <- central/vc</pre>
        Cc ~ prop(propSd)
    })
}
# This creates an rxode2 object
object = rxode(my_model)
# If you want details about the parameters, states, etc
# in the model you can use this:
rxdetails = fetch_rxinfo(object)
rxdetails$elements
# Next we will create subjects. To do that we need to
# specify information about covariates:
nsub = 2
covs = list(
  WT
             = list(type
                            = "continuous",
                    sampling = "log-normal",
                    values = c(70, .15))
)
subs = mk_subjects(object = object,
                   nsub = nsub,
                   covs = covs)
head(subs$subjects)
```

```
rules = list(
 dose = list(
   condition = "TRUE",
   action = list(
     type = "dose",
     state = "central",
     values = "c(1)",
     times = "c(0)",
     durations = "c(0)")
   )
)
\# We evaulate the rules for dosing at time 0
eval_times = 0
# Stop 2 months after the last dose
output\_times = seq(0, 56, 1)
# This runs the rule-based simulations
simres =
 simulate_rules(
             = object,
   object
               = subs[["subjects"]],
   subjects
   eval_times = eval_times,
   output_times = output_times,
   rules
                = rules)
# First subject data:
sub_1 = simres$simall[simres$simall$id == 1, ]
# First subjects events
evall = as.data.frame(simres$evall)
ev_sub_1 = evall[evall$id ==1, ]
# All of the simulation data
simall = simres$simall
simall$id = as.factor(simall$id)
# Timecourse
psim =
 plot_sr_tc(
   sro = simres,
   dvcols = "Cc")
psim$fig
# Events
pev =
 plot_sr_ev(
   sro = simres,
   ylog = FALSE)
pev$fig
}
```

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 ${\tt mk\_table\_ind\_obs}$ 

Creates Tables of Individual Observations from PKNCA Result

# Description

Takes the output of PKNCA and creates a tabular view of the individual observation data. This can be spread out of over several tables (pages) if necessary.

# Usage

```
mk_table_ind_obs(
  nca_res,
  obnd = NULL,
  not_sampled = "NS",
  blq = "BLQ",
  digits = 3,
  text_format = "text",
  max_height = 7,
  max_width = 6.5,
  max_row = NULL,
  max_col = 9,
  notes_detect = NULL,
  rows_by = "time"
)
```

## **Arguments**

nca_res	Output of PKNCA.
obnd	onbrand reporting object.
not_sampled	Character string to use for missing data when pivoting.
blq	Character string to use to indicate data below the level of quantification (value of 0 in the dataset).
digits	Number of significant figures to report (set to NULL to disable rounding)
text_format	Either "md" for markdown or "text" (default) for plain text.
max_height	Maximum height of the final table in inches (A value of NULL will use 100 inches).
max_width	Maximum width of the final table in inches (A value of NULL will use 100 inches).
max_row	Maximum number of rows to have on a page. Spillover will hang over the side of the page
max_col	Maximum number of columns to have on a page. Spillover will be wrapped to multiple pages.

rows\_by

Can be either "time" or "id". If it is "time", there will be a column for time and separate column for each subject ID. If rows\_by is set to "id" there will be a column for ID and a column for each individual time.

#### Value

List containing the following elements

- isgood: Boolean indicating the exit status of the function.
- one\_table: Dataframe of the entire table with the first lines containing the header.
- one\_body: Dataframe of the entire table (data only).
- one\_header: Dataframe of the entire header (row and body, no data).
- tables: Named list of tables. Each list element is of the output
- msgs: Vector of text messages describing any errors that were found. format from build\_span.

## **Examples**

```
# We need a state variable to be define
sess_res = NCA_test_mksession()

state = sess_res$state

# Pulls out the active analysis
current_ana = NCA_fetch_current_ana(state)

# This is the raw PKNCA output
pknca_res = NCA_fetch_ana_pknca(state, current_ana)

# Building the figure
mk_res = mk_table_ind_obs(nca_res = pknca_res)
mk_res$tables[["Table 1"]]$ft
```

mk\_table\_nca\_params

Create Tabular Output from PKNCA Results

### Description

Create paginated tables from PKNCA to use in reports and Shiny apps.

# Usage

```
mk_table_nca_params(
  nca_res,
  type = "individual",
  grouping = "interval",
  not_calc = "NC",
```

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```
obnd = NULL,
nps = NULL,
mult_str = "*",
infinity = "inf",
digits = NULL,
text_format = "text",
notes_detect = NULL,
max_height = 7,
max_width = 6.5,
max_row = NULL,
max_col = NULL
```

# Arguments

nca_res	Output of PKNCA.
type	Type of table to generate. Can be either "individual" or "summary"].
grouping	How to group columns in tables. Can be either "interval" or "parameter"].
not_calc	Text string to replace NA values with to indicated values were not calculated.
obnd	onbrand reporting object.
nps	NCA parameter summary table with the following columns.
	• parameter: PKNCA Paramter name.
	• text: Name used in text output.
	md: Name used markdown output.
	• latex: Name used in latex output.
	• description: Verbose textual description of the parameter.
mult_str	Text string to replace * values in units.
infinity	Text string to replace infinity in time intervals in column headers.
digits	Number of significant figures to report (set to NULL to disable rounding)
text_format	Either "md" for markdown or "text" (default) for plain text.
notes_detect	Vector of strings to detect in output tables (example c("NC", "BLQ")).
max_height	Maximum height of the final table in inches (A value of NULL will use 100 inches).
max_width	Maximum width of the final table in inches (A value of NULL will use 100 inches).
max_row	Maximum number of rows to have on a page. Spillover will hang over the side of the page
max_col	Maximum number of columns to have on a page. Spillover will be wrapped to multiple pages.

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#### Value

list containing the following elements

- raw\_nca: Raw PKNCA output.
- isgood: Boolean indicating the exit status of the function.
- one\_table: Dataframe of the entire table with the first lines containing the header.
- one\_body: Dataframe of the entire table (data only).
- one\_header: Dataframe of the entire header (row and body, no data).
- tables: Named list of tables. Each list element is of the output
- msgs: Vector of text messages describing any errors that were found. format from build\_span.

# **Examples**

```
# We need a state variable to be define
sess_res = NCA_test_mksession()

state = sess_res$state

# Pulls out the active analysis
current_ana = NCA_fetch_current_ana(state)

# This is the raw PKNCA output
pknca_res = NCA_fetch_ana_pknca(state, current_ana)

# Parameter reporting details from the ruminate configuration
nps = state[["NCA"]][["nca_parameters"]][["summary"]]

# Building the figure
mk_res = mk_table_nca_params(nca_res = pknca_res, nps=nps, digits=3)
mk_res$tables[["Table 1"]]$ft
```

NCA\_add\_int

Adds Analysis Interval to Current Analysis

# **Description**

Takes the start time, stop time, and NCA parameters and adds them to the intervals table of the current analysis

#### Usage

```
NCA_add_int(state, interval_start, interval_stop, nca_parameters)
```

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## **Arguments**

```
state NCA state from NCA_fetch_state()
interval_start Interval start time (numeric).
interval_stop Interval stop time (numeric).
nca_parameters list of NCA parameters in the interval
```

#### Value

State with interval added to the current analysis.

NCA_append_report	Append Report Elements	

## **Description**

Takes an NCA state object and appends any reportable elements for the specified report type. On NCA analyses that are in a "good" state will be reported. Those not in a good state will be ignored.

#### **Usage**

```
NCA_append_report(state, rpt, rpttype, gen_code_only = FALSE)
```

## **Arguments**

state	NCA state from NCA_fetch_state()
rpt	Report with the current content of the report which will be appended to in this function. For details on the structure see the documentation for formods::FM_generate_report()
rpttype	Type of report to generate (supported "xlsx", "pptx", "docx").
gen_code_only	Boolean value indicating that only code should be generated (FALSE).

### Value

list containing the following elements

- isgood: Return status of the function.
- hasrptele: Boolean indicator if the module has any reportable elements.
- code: Code to create report elements.
- msgs: Messages to be passed back to the user.
- rpt: Report with any additions passed back to the user.

### See Also

```
formods::FM_generate_report()
```

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### **Examples**

```
# We need a state object to use below
sess_res = NCA_test_mksession()
state = sess_res$state
# here we need an empty report object for tabular data
rpt = list(summary = list(), sheets=list())
# Now we append the report indicating we want
# Excel output:
rpt_res = NCA_append_report(state,
               = rpt,
  rpt
  rpttype = "xlsx",
  gen_code_only = TRUE)
# Shows if report elements are present
rpt_res$hasrptele
# Code chunk to generate report element
cat(paste(rpt_res$code, collapse="\n"))
```

nca\_builder

Builds NCA Code from ui Elements

# **Description**

Takes the current analysis in the state object and creates the code to run the analysis

### Usage

```
nca_builder(state)
```

### **Arguments**

state

NCA state from NCA\_fetch\_state()

### Value

NCA state with the NCA for the current analysis built.

```
# We need a module variables to be defined
sess_res = NCA_test_mksession()
state = sess_res$state
state = nca_builder(state)
```

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NCA\_fetch\_ana\_ds

Fetch Analysis Dataset

### **Description**

Fetches the dataset used for the specified analysis

## Usage

```
NCA_fetch_ana_ds(state, current_ana)
```

### **Arguments**

```
state NCA state from NCA_fetch_state()
current_ana Current value in the analysis
```

#### Value

Dataset from the ds field of FM\_fetch\_ds()

```
library(ruminate)
# Module IDs
      = "NCA"
id_UD = "UD"
id_DW = "DW"
id_ASM = "ASM"
# We need session and input variables to be define
sess_res = NCA_test_mksession()
# Extracting the session and input variables
         = sess_res$session
session
input
            = sess_res$input
react_state = list()
# We also need configuration files
FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml")
MOD_yaml_file = system.file(package = "ruminate", "templates", "NCA.yaml")
# Getting the current module state
state = NCA_fetch_state(id
                                     = id,
                      input
                                     = input,
                      session
                                     = session,
                      FM_yaml_file
                                     = FM_yaml_file,
                      MOD_yaml_file = MOD_yaml_file,
                      id_ASM
                                     = id_ASM,
                      id_UD
                                     = id_UD,
                      id_DW
                                     = id_DW,
```

```
react_state
                                       = react_state)
# Pulls out the active analysis
current_ana = NCA_fetch_current_ana(state)
# This will get the dataset associated with this analysis
ds = NCA_fetch_ana_ds(state, current_ana)
# After making changes you can update those in the state
state = NCA_set_current_ana(state, current_ana)
# You can use this to check the current analysis
current_ana = NCA_process_current_ana(state)
# This will pull out the code for the module
fc_res = NCA_fetch_code(state)
# This will use patterns defined for the site to detect
# columns. In this example we are detecting the id column:
id_col = NCA_find_col(
  patterns = state[["MC"]][["detect_col"]][["id"]],
  dscols = names(ds$DS))
# This creates a new analysis
state = NCA_new_ana(state)
```

NCA\_fetch\_ana\_pknca

Fetch PKNCA Results Object

# **Description**

Fetches the PKNCA output for a specified analysis

# Usage

```
NCA_fetch_ana_pknca(state, current_ana)
```

# **Arguments**

state NCA state from NCA\_fetch\_state()

current\_ana Current value in the analysis

### Value

Dataset from the ds field of FM\_fetch\_ds()

```
library(ruminate)
# Module IDs
id = "NCA"
id_UD = "UD"
id_DW = "DW"
id\_ASM = "ASM"
# We need session and input variables to be define
sess_res = NCA_test_mksession()
# Extracting the session and input variables
session = sess_res$session
input
            = sess_res$input
react_state = list()
# We also need configuration files
FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml")
MOD_yaml_file = system.file(package = "ruminate", "templates", "NCA.yaml")
# Getting the current module state
state = NCA_fetch_state(id
                                     = id,
                                    = input,
                      input
                      session
                                     = session,
                      FM_yaml_file = FM_yaml_file,
                      MOD_yaml_file = MOD_yaml_file,
                      id_ASM
                                     = id_ASM,
                      id_UD
                                    = id_UD,
                      id_DW
                                    = id_DW,
                      react_state = react_state)
# Pulls out the active analysis
current_ana = NCA_fetch_current_ana(state)
# This will get the dataset associated with this analysis
ds = NCA_fetch_ana_ds(state, current_ana)
# After making changes you can update those in the state
state = NCA_set_current_ana(state, current_ana)
# You can use this to check the current analysis
current_ana = NCA_process_current_ana(state)
# This will pull out the code for the module
fc_res = NCA_fetch_code(state)
# This will use patterns defined for the site to detect
# columns. In this example we are detecting the id column:
id_col = NCA_find_col(
 patterns = state[["MC"]][["detect_col"]][["id"]],
 dscols = names(ds$DS))
# This creates a new analysis
```

NCA\_fetch\_code

```
state = NCA_new_ana(state)
```

NCA\_fetch\_code

Fetch Module Code

## **Description**

Fetches the code to generate results seen in the app

### Usage

```
NCA_fetch_code(state)
```

# **Arguments**

state

NCA state from NCA\_fetch\_state()

### Value

Character object vector with the lines of code

```
library(ruminate)
# Module IDs
     = "NCA"
id UD = "UD"
id_DW = "DW"
id_ASM = "ASM"
# We need session and input variables to be define
sess_res = NCA_test_mksession()
# Extracting the session and input variables
        = sess_res$session
session
           = sess_res$input
input
react_state = list()
# We also need configuration files
FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml")
MOD_yaml_file = system.file(package = "ruminate", "templates", "NCA.yaml")
# Getting the current module state
state = NCA_fetch_state(id
                                     = id,
                      input
                                    = input,
                      session
                                    = session,
                      FM_yaml_file = FM_yaml_file,
                      MOD_yaml_file = MOD_yaml_file,
                      id_ASM = id_ASM,
                      id_UD
                                   = id_UD,
                      id_DW
                                    = id_DW,
```

```
react_state
                                      = react_state)
# Pulls out the active analysis
current_ana = NCA_fetch_current_ana(state)
# This will get the dataset associated with this analysis
ds = NCA_fetch_ana_ds(state, current_ana)
# After making changes you can update those in the state
state = NCA_set_current_ana(state, current_ana)
# You can use this to check the current analysis
current_ana = NCA_process_current_ana(state)
# This will pull out the code for the module
fc_res = NCA_fetch_code(state)
# This will use patterns defined for the site to detect
# columns. In this example we are detecting the id column:
id_col = NCA_find_col(
 patterns = state[["MC"]][["detect_col"]][["id"]],
 dscols = names(ds$DS))
# This creates a new analysis
state = NCA_new_ana(state)
```

NCA\_fetch\_current\_ana Fetches Current Analysis

# **Description**

Takes an NCA state and returns the current active analysis

### Usage

```
NCA_fetch_current_ana(state)
```

#### **Arguments**

state

NCA state from NCA\_fetch\_state()

#### Value

List containing the details of the current analysis. The structure of this list is the same as the structure of state\$NCA\$anas in the output of NCA\_fetch\_state().

```
library(ruminate)
# Module IDs
id = "NCA"
id_UD = "UD"
id_DW = "DW"
id\_ASM = "ASM"
# We need session and input variables to be define
sess_res = NCA_test_mksession()
# Extracting the session and input variables
session = sess_res$session
input
            = sess_res$input
react_state = list()
# We also need configuration files
FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml")
MOD_yaml_file = system.file(package = "ruminate", "templates", "NCA.yaml")
# Getting the current module state
state = NCA_fetch_state(id
                                     = id,
                                    = input,
                      input
                      session
                                    = session,
                      FM_yaml_file = FM_yaml_file,
                      MOD_yaml_file = MOD_yaml_file,
                      id_ASM
                                    = id_ASM,
                      id_UD
                                    = id_UD,
                      id_DW
                                    = id_DW,
                      react_state = react_state)
# Pulls out the active analysis
current_ana = NCA_fetch_current_ana(state)
# This will get the dataset associated with this analysis
ds = NCA_fetch_ana_ds(state, current_ana)
# After making changes you can update those in the state
state = NCA_set_current_ana(state, current_ana)
# You can use this to check the current analysis
current_ana = NCA_process_current_ana(state)
# This will pull out the code for the module
fc_res = NCA_fetch_code(state)
# This will use patterns defined for the site to detect
# columns. In this example we are detecting the id column:
id_col = NCA_find_col(
 patterns = state[["MC"]][["detect_col"]][["id"]],
 dscols = names(ds$DS))
# This creates a new analysis
```

```
state = NCA_new_ana(state)
```

NCA\_fetch\_current\_obj Fetches the Current Analysis Object

## **Description**

Takes the current state and object type and returns the currently selected object. For example if you have specified figure, it will look at the output figure selected and the figure number of that figure and return the ggplot object for that. by subject id highlighting of certain NCA aspects (e.g. points used for half-life)

### Usage

```
NCA_fetch_current_obj(state, obj_type)
```

### **Arguments**

```
state NCA state from NCA_fetch_state()
obj_type Type of object to return (either "table" or "figure").
```

#### Value

List with a format that depends on the obj\_type. For figures:

- ggplot: ggplot object of the figure.
- isgood: Return status of the function.
- msgs: Messages to be passed back to the user.

#### For tables:

- df: Dataframe of the current table.
- ft: Flextable object of the current table.
- notes: Any table notes to be included.
- isgood: Return status of the function.
- msgs: Messages to be passed back to the user.

```
# We need a state object to use below
sess_res = NCA_test_mksession()
state = sess_res$state

# Current active table:
res = NCA_fetch_current_obj(state, "table")
res$ft

# Current active figure:
res = NCA_fetch_current_obj(state, "figure")
res$ggplot
```

NCA\_fetch\_ds

NCA\_fetch\_data\_format Fetches Details About Data Requirements

## **Description**

Use this to get information about data formats.

# Usage

```
NCA_fetch_data_format(
   MOD_yaml_file = system.file(package = "ruminate", "templates", "NCA.yaml")
)
```

# Arguments

### Value

List with details about the data formats

# **Examples**

```
NCA_fetch_data_format()
```

NCA\_fetch\_ds

Fetch Module Datasets

# **Description**

Fetches the datasets contained in the module

## Usage

```
NCA_fetch_ds(state)
```

## **Arguments**

state

NCA state from NCA\_fetch\_state()

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### Value

list containing the following elements

- isgood: Return status of the function.
- hasds: Boolean indicator if the module has any datasets
- msgs: Messages to be passed back to the user.
- ds: List with datasets. Each list element has the name of the R-object for that dataset. Each element has the following structure:
  - label: Text label for the dataset
  - MOD\_TYPE: Short name for the type of module.
  - id: module ID
  - DS: Dataframe containing the actual dataset.
  - DSMETA: Metadata describing DS
  - code: Complete code to build dataset.
  - checksum: Module checksum.
  - DSchecksum: Dataset checksum.

# **Examples**

```
# We need a state object to use below
sess_res = NCA_test_mksession()
state = sess_res$state

myDs = NCA_fetch_ds(state)
```

NCA\_fetch\_np\_meta

Fetches NCA Parameter Meta Information

## **Description**

This provides meta information about NCA parameters. This includes parameter names, text descriptions, formatting (md and LaTeX).

### Usage

```
NCA_fetch_np_meta(
   MOD_yaml_file = system.file(package = "ruminate", "templates", "NCA.yaml")
)
```

# **Arguments**

MOD\_yaml\_file Module configuration file with MC as main section.

## Value

List with the following elements:

- choices: List parameter choices grouped by values specified in the module configuration file.
- summary: Data frame with meta data about the NCA parameters with the following columns:
  - parameter: Name of parameter in PKNCA.
  - text: Name of parameter in plain text.
  - md: Parameter name formatted in Markdown.
  - latex: Parameter name formatted using LaTeX.
  - description: Verbose description in plain text for the parameter.

# **Examples**

```
NCA_fetch_np_meta()
```

NCA\_fetch\_PKNCA\_meta Fetches PKNCA Metadata

# Description

Compiles Metadata from PKNCA

## Usage

```
NCA_fetch_PKNCA_meta()
```

#### Value

Dataframe containing PKCNA metadata for NCA parameters.

```
PKNCA_meta = NCA_fetch_PKNCA_meta()
utils::head(PKNCA_meta)
```

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# Description

Merges default app options with the changes made in the UI

# Usage

```
NCA_fetch_state(
  id,
  input,
  session,
  FM_yaml_file,
  MOD_yaml_file,
  id_ASM,
  id_UD,
  id_DW,
  react_state
)
```

## **Arguments**

id	Shiny module ID
input	Shiny input variable
session	Shiny session variable
FM_yaml_file	App configuration file with FM as main section.
MOD_yaml_file	Module configuration file with MC as main section.
id_ASM	ID string for the app state management module used to save and load app states
id_UD	ID string for the upload data module used to save and load app states
id_DW	ID string for the data wrangling module used to save and load app states
react_state	Variable passed to server to allow reaction outside of module (NULL)

## Value

list containing the current state of the app including default values from the yaml file as well as any changes made by the user. The list has the following structure:

- yaml: Full contents of the supplied yaml file.
- MC: Module components of the yaml file.
- NCA:
  - ana\_cntr: Analysis counter.
  - anas: List of analyses: Each analysis has the following structure:

NCA\_fetch\_state

\* ana\_dsview: Dataset view/ID (name from DSV) selected as a data source for this analysis.

- \* ana\_scenario: Analysis scenario selected in the UI
- \* checksum: checksum of the analysis (used to detect changes in the analysis).
- code: Code to generate analysis from start to finish or error messages if code generation/analysis failed.
- \* code\_components: List containing the different components from code
- \* col\_conc: Column from ana\_dsview containing the concentration data.
- \* col\_dose: Column from ana\_dsview containing the dose amount.
- \* col\_dur: Column from ana\_dsview containing the infusion duration or N/A if unused.
- \* col\_group: Columns from ana\_dsview containing other grouping variables.
- \* col\_id: Column from ana\_dsview containing the subject IDs.
- \* col\_ntime: Column from ana\_dsview containing the nominal time values
- \* col\_route: Column from ana\_dsview containing the dosing route.
- \* col\_time: Column from ana\_dsview containing the time values.
- \* id: Character id (ana\_idx).
- \* idx: Numeric id (1).
- \* include\_units: Boolean variable indicating in units should included in the analysis.
- \* interval\_range: Vector with the first element representing he beginning of the interval and the second element containing the end of the interval.
- \* intervals: List of the intervals to include.
- \* isgood: Current status of the analysis.
- \* key: Analysis key acts as a title/caption (user editable)
- \* msgs: Messages generated when checking configuration and analysis options.
- \* nca config: List of NCA configuration options for this analysis.
- \* nca\_object\_name: Prefix for NCA objects associated with this analyis.
- \* nca parameters: NCA parameters selected for calculation in the UI.
- \* notes: Analysis notes (user editable)
- \* objs: List of names and values for objects created with generated code.
- \* sampling: Sampling method either "sparse" or "serial"
- \* units amt: Amount units.
- \* units\_conc: Concentration units.
- \* units\_dose: Dosing units.
- \* units\_time: Time units.
- current\_ana: Currently selected analysis (list name element from anas).
- DSV: Available data source views (see FM\_fetch\_ds)
- checksum: This is an MD5 sum of the module (checksum of the analysis checksums).
- nca\_config: List of PKNCA configuration options for this analysis.
- nca\_parameters: List with two elements
  - \* choices: List consisting of "Common Parameters" and "Other" (used for grouping in the UI). Each of these is a list of text parameter names with a value of the PKNCA parameter name.
  - \* summary: Summary table with the following columns:

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- · parameter: PKNCA Paramter name.
- · text: Name used in text output.
- · md: Name used markdown output.
- · latex: Name used in latex output.
- · description: Verbose textual description of the parameter.
- ui: Current value of form elements in the UI.
- ui\_ana\_map: Map between UI element names and analysis in the object you get from NCA\_fetch\_current\_ana
- ui\_ids: Vector of UI elements for the module.
- ui\_hold: List of hold elements to disable updates before a full ui referesh is complete.
- MOD\_TYPE: Character data containing the type of module "NCA"
- id: Character data containing the module id module in the session variable.
- FM\_yaml\_file: App configuration file with FM as main section.
- MOD\_yaml\_file: Module configuration file with MC as main section.

```
library(ruminate)
# Module IDs
id = "NCA"
id_UD = "UD"
id_DW = "DW"
id\_ASM = "ASM"
# We need session and input variables to be define
sess_res = NCA_test_mksession()
# Extracting the session and input variables
session = sess_res$session
          = sess_res$input
input
react_state = list()
# We also need configuration files
FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml")
MOD_yaml_file = system.file(package = "ruminate", "templates", "NCA.yaml")
# Getting the current module state
state = NCA_fetch_state(id
                                    = id,
                                   = input,
                      input
                      input = input,
session = session,
                      FM_yaml_file = FM_yaml_file,
                      MOD_yaml_file = MOD_yaml_file,
                                    = id_ASM,
                      id_ASM
                                    = id_UD,
                      id_UD
                             - ___
= id_DW,
                      id_DW
                      react_state = react_state)
# Pulls out the active analysis
current_ana = NCA_fetch_current_ana(state)
```

NCA\_find\_col

```
# This will get the dataset associated with this analysis
ds = NCA_fetch_ana_ds(state, current_ana)

# After making changes you can update those in the state
state = NCA_set_current_ana(state, current_ana)

# You can use this to check the current analysis
current_ana = NCA_process_current_ana(state)

# This will pull out the code for the module
fc_res = NCA_fetch_code(state)

# This will use patterns defined for the site to detect
# columns. In this example we are detecting the id column:
id_col = NCA_find_col(
    patterns = state[["MC"]][["detect_col"]][["id"]],
    dscols = names(ds$DS))

# This creates a new analysis
state = NCA_new_ana(state)
```

NCA\_find\_col

Determines Default Column Name

#### **Description**

Based on the current analysis, value from the UI, an optional list of patterns to search, and column names from a dataset this function tries to find a default value for a column in the analysis (e.g. subject id, dose, concentration, etc).

Generally the following is done:

- If curr\_ui has a non-NULL, non-"" value it is compared to dscols. If it is found there that value is returned.
- If not then the patterns are considered. If the patterns from the YAML file are not NULL they are compared sequentially to the columns names. The first match found is returned.
- If nothing is found then the first value of dscols is returned.

#### Usage

```
NCA_find_col(
  curr_ana = NULL,
  curr_ui = NULL,
  patterns = NULL,
  dscols,
  null_ok = FALSE
)
```

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# **Arguments**

curr_ana	Current value in the analysis
curr_ui	Current value in UI
patterns	List of regular expression patterns to consider.
dscols	Columns from the dataset.
null_ok	Logical value indicating if a null result (nothing found) is OK (default: FALSE)

#### Value

Name of column found based on the rules above.

```
library(ruminate)
# Module IDs
id = "NCA"
id_UD = "UD"
id_DW = "DW"
id_ASM = "ASM"
# We need session and input variables to be define
sess_res = NCA_test_mksession()
# Extracting the session and input variables
session = sess_res$session
          = sess_res$input
react_state = list()
# We also need configuration files
FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml")
MOD_yaml_file = system.file(package = "ruminate", "templates", "NCA.yaml")
# Getting the current module state
state = NCA_fetch_state(id
                                    = id,
                     session = input,
                                   = session,
                      FM_yaml_file = FM_yaml_file,
                      MOD_yaml_file = MOD_yaml_file,
                      id_ASM
                                  = id_ASM,
                      id_UD
                                   = id_UD,
                      id_DW
                                   = id_DW,
                      react_state = react_state)
# Pulls out the active analysis
current_ana = NCA_fetch_current_ana(state)
# This will get the dataset associated with this analysis
ds = NCA_fetch_ana_ds(state, current_ana)
# After making changes you can update those in the state
state = NCA_set_current_ana(state, current_ana)
```

NCA\_init\_state

```
# You can use this to check the current analysis
current_ana = NCA_process_current_ana(state)

# This will pull out the code for the module
fc_res = NCA_fetch_code(state)

# This will use patterns defined for the site to detect
# columns. In this example we are detecting the id column:
id_col = NCA_find_col(
  patterns = state[["MC"]][["detect_col"]][["id"]],
  dscols = names(ds$DS))

# This creates a new analysis
state = NCA_new_ana(state)
```

NCA\_init\_state

Initialize NCA Module State

## **Description**

Creates a list of the initialized module state

# Usage

```
NCA_init_state(FM_yaml_file, MOD_yaml_file, id, id_UD, id_DW, session)
```

# Arguments

FM_yaml_file	App configuration file with FM as main section.
MOD_yaml_file	Module configuration file with MC as main section.
id	ID string for the module.
id_UD	ID string for the upload data module used to handle uploads or the name of the list element in react_state where the data set is stored.
id_DW	ID string for the data wrangling module to process any uploaded data
session	Shiny session variable (in app) or a list (outside of app)

# Value

list containing an empty NCA state

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NCA\_load\_scenario

Loads Pre-Defined Scenario

# Description

Loads a pre-defined analysis scneario from the NCA YAML config file.

## Usage

```
NCA_load_scenario(state, ana_scenario)
```

#### **Arguments**

state NCA state from NCA\_fetch\_state()

ana\_scenario Short name of the analysis scenario to load from the config file.

#### Value

NCA state object with the scenario loaded and relevant notifications set.

NCA\_mkactive\_ana

Fetch PKNCA Results Object

# Description

Fetches the PKNCA output for a specified analysis

## Usage

```
NCA_mkactive_ana(state, ana_id)
```

## **Arguments**

state NCA state from NCA\_fetch\_state()

ana\_id Analysis ID to make active.

#### Value

State with the analysis ID made active. JMH add to example script below

114 NCA\_mkactive\_ana

```
library(ruminate)
# Module IDs
id = "NCA"
id_UD = "UD"
id_DW = "DW"
id\_ASM = "ASM"
# We need session and input variables to be define
sess_res = NCA_test_mksession()
# Extracting the session and input variables
session = sess_res$session
input
            = sess_res$input
react_state = list()
# We also need configuration files
FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml")
MOD_yaml_file = system.file(package = "ruminate", "templates", "NCA.yaml")
# Getting the current module state
state = NCA_fetch_state(id
                                     = id,
                                   = input,
                      input
                      session
                                    = session,
                      FM_yaml_file = FM_yaml_file,
                      MOD_yaml_file = MOD_yaml_file,
                      id_ASM
                                    = id_ASM,
                      id_UD
                                    = id_UD,
                      id_DW
                                    = id_DW,
                      react_state = react_state)
# Pulls out the active analysis
current_ana = NCA_fetch_current_ana(state)
# This will get the dataset associated with this analysis
ds = NCA_fetch_ana_ds(state, current_ana)
# After making changes you can update those in the state
state = NCA_set_current_ana(state, current_ana)
# You can use this to check the current analysis
current_ana = NCA_process_current_ana(state)
# This will pull out the code for the module
fc_res = NCA_fetch_code(state)
# This will use patterns defined for the site to detect
# columns. In this example we are detecting the id column:
id_col = NCA_find_col(
 patterns = state[["MC"]][["detect_col"]][["id"]],
 dscols = names(ds$DS))
# This creates a new analysis
```

NCA\_mk\_preload 115

```
state = NCA_new_ana(state)
```

NCA\_mk\_preload

Make List of Current NCA State

# Description

Reads in the app state from yaml files.

#### Usage

```
NCA_mk_preload(state)
```

## **Arguments**

state

NCA state object

#### Value

list with the following elements

- isgood: Boolean indicating the exit status of the function.
- msgs: Messages to be passed back to the user.
- yaml\_list: Lists with preload components.

# Examples

```
sess_res = NCA_test_mksession()
state = sess_res$state
res = NCA_mk_preload(state)
```

NCA\_new\_ana

Initialize New Analysis

# Description

Creates a new NCA analysis in an NCA module

#### Usage

```
NCA_new_ana(state)
```

# **Arguments**

state

NCA state from NCA\_fetch\_state()

NCA\_new\_ana

#### Value

NCA state object containing a new empty analysis and that analysis is set as the current active analysis

```
library(ruminate)
# Module IDs
id = "NCA"
id_UD = "UD"
id DW = "DW"
id\_ASM = "ASM"
# We need session and input variables to be define
sess_res = NCA_test_mksession()
# Extracting the session and input variables
         = sess_res$session
session
          = sess_res$input
input
react_state = list()
# We also need configuration files
FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml")
MOD_yaml_file = system.file(package = "ruminate", "templates", "NCA.yaml")
# Getting the current module state
state = NCA_fetch_state(id
                                     = id,
                      input
                                   = input,
                                   = session,
                      session
                      FM_yaml_file = FM_yaml_file,
                      MOD_yaml_file = MOD_yaml_file,
                      id_ASM
                                    = id_ASM,
                                    = id_UD,
                      id_UD
                      id_DW
                                    = id_DW,
                      react_state = react_state)
# Pulls out the active analysis
current_ana = NCA_fetch_current_ana(state)
# This will get the dataset associated with this analysis
ds = NCA_fetch_ana_ds(state, current_ana)
# After making changes you can update those in the state
state = NCA_set_current_ana(state, current_ana)
# You can use this to check the current analysis
current_ana = NCA_process_current_ana(state)
# This will pull out the code for the module
fc_res = NCA_fetch_code(state)
# This will use patterns defined for the site to detect
# columns. In this example we are detecting the id column:
```

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```
id_col = NCA_find_col(
  patterns = state[["MC"]][["detect_col"]][["id"]],
  dscols = names(ds$DS))

# This creates a new analysis
state = NCA_new_ana(state)
```

NCA\_preload

Preload Data for NCA Module

# Description

Populates the supplied session variable with information from list of sources.

# Usage

```
NCA_preload(
    session,
    src_list,
    yaml_res,
    mod_ID = NULL,
    react_state = list(),
    quickload = FALSE
)
```

## **Arguments**

session	Shiny session variable (in app) or a list (outside of app)
src_list	List of preload data (all read together with module IDs at the top level)
yaml_res	List data from module yaml config
mod_ID	Module ID of the module being loaded.
react_state	Reactive shiny object (in app) or a list (outside of app) used to trigger reactions.
quickload	Logical TRUE to load reduced analysis FALSE to load the full analysis

# Value

list with the following elements

- isgood: Boolean indicating the exit status of the function.
- msgs: Messages to be passed back to the user.
- session: Session object
- input: The value of the shiny input at the end of the session initialization.
- state: App state.
- react\_state: The react\_state components.

```
NCA_process_current_ana
```

Processes Current Analysis to be Run

#### **Description**

Takes the current analysis and checks different aspects to for any issues to make sure it's good to go.

## Usage

```
NCA_process_current_ana(state)
```

#### **Arguments**

```
state NCA state from NCA_fetch_state()
```

#### Value

Current analysis list with isgood and msgs set

```
library(ruminate)
# Module IDs
      = "NCA"
id UD = "UD"
id_DW = "DW"
id_ASM = "ASM"
# We need session and input variables to be define
sess_res = NCA_test_mksession()
# Extracting the session and input variables
         = sess_res$session
session
input
            = sess_res$input
react_state = list()
# We also need configuration files
FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml")
MOD_yaml_file = system.file(package = "ruminate", "templates", "NCA.yaml")
# Getting the current module state
state = NCA_fetch_state(id
                                     = id,
                      input
                                     = input,
                      session
                                     = session,
                      FM_yaml_file
                                     = FM_yaml_file,
                      MOD_yaml_file = MOD_yaml_file,
                      id_ASM
                                     = id_ASM,
                      id_UD
                                     = id_UD,
                      id_DW
                                     = id_DW,
```

```
react_state
                                       = react_state)
# Pulls out the active analysis
current_ana = NCA_fetch_current_ana(state)
# This will get the dataset associated with this analysis
ds = NCA_fetch_ana_ds(state, current_ana)
# After making changes you can update those in the state
state = NCA_set_current_ana(state, current_ana)
# You can use this to check the current analysis
current_ana = NCA_process_current_ana(state)
# This will pull out the code for the module
fc_res = NCA_fetch_code(state)
# This will use patterns defined for the site to detect
# columns. In this example we are detecting the id column:
id_col = NCA_find_col(
 patterns = state[["MC"]][["detect_col"]][["id"]],
 dscols = names(ds$DS))
# This creates a new analysis
state = NCA_new_ana(state)
```

NCA\_Server

Fetch Non-Compartmental Analysis State

#### Description

Merges default app options with the changes made in the UI

## Usage

```
NCA_Server(
  id,
FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml"),
  MOD_yaml_file = system.file(package = "ruminate", "templates", "NCA.yaml"),
  id_ASM = "ASM",
  id_UD = "UD",
  id_DW = "DW",
  deployed = FALSE,
  react_state = NULL
)
```

# **Arguments** id

An ID string that corresponds with the ID used to call the modules UI elements

FM_yaml_file	App configuration file with FM as main section.
MOD_yaml_file	Module configuration file with MC as main section.
id_ASM	ID string for the app state management module used to save and load app states
id_UD	ID string for the upload data module used to save and load app states
id_DW	ID string for the data wrangling module used to save and load app states
deployed	Boolean variable indicating whether the app is deployed or not.
react_state	Variable passed to server to allow reaction outside of module (NULL)

#### Value

list containing the current state of the app including default values from the yaml file as well as any changes made by the user. The list has the following structure:

- yaml: Full contents of the supplied yaml file.
- MC: Module components of the yaml file.
- NCA:
  - isgood: Boolean object indicating if the file was successfully loaded.
  - checksum: This is an MD5 sum of the contents element and can be used to detect changes in the state.
- MOD\_TYPE: Character data containing the type of module "NCA"
- id: Character data containing the module id module in the session variable.
- FM\_yaml\_file: App configuration file with FM as main section.
- MOD\_yaml\_file: Module configuration file with MC as main section.

```
if(interactive()){
 # original file: inst/templates/ruminate.R
 library(formods)
library(ruminate)
 # These are suggested packages
 library(shinydashboard)
 #library(ggpubr)
  #library(plotly)
  #library(shinybusy)
 library(prompter)
  #library(utils)
  tags$style("@import url(https://use.fontawesome.com/releases/v6.4.0/css/all.css);")
  # You can copy these locally and customize them for your own needs. Simply
  # change the assignment to the local copy you've modified.
formods.yaml = system.file(package="formods", "templates",

ASM.yaml = system.file(package="formods", "templates",

UD.yaml = system.file(package="formods", "templates",

DW yaml = system.file(package="formods", "templates",

"templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", "templates", 
                                                                                                                                                                                                                                                                        "formods.yaml")
                                                                                                                                                                                                                                                                       "ASM.yaml")
                                                                                                                                                                                                                                                                      "UD.yaml")
                                                          = system.file(package="formods", "templates", "DW.yaml")
 DW.yaml
```

```
FG.yaml
              = system.file(package="formods", "templates",
                                                              "FG.yaml")
NCA.yaml
              = system.file(package="ruminate", "templates",
                                                              "NCA.yaml")
# Name of file to indicate we need to load testing data
ftmptest = file.path(tempdir(), "ruminate.test")
# Making sure that the deployed object is created
if(!exists("deployed")){
  deployed = FALSE
# If the DEPLOYED file marker existrs we set deployed to TRUE
if(file.exists("DEPLOYED")){
  deployed = TRUE
}
# # Making sure that the run_dev object is created
# if(file.exists(file.path(tempdir(), "RUMINTE_DEVELOPMENT"))){
# run_dev = TRUE
# }else{
   run_dev = FALSE
# }
# If the SETUP.R file exists we source it
if(file.exists("SETUP.R")){
  source("SETUP.R")
}
CSS <- "
.wrapfig {
  float: right;
  shape-margin: 20px;
  margin-right: 20px;
  margin-bottom: 20px;
#https://fontawesome.com/icons?from=io
logo_url =
  "https://raw.githubusercontent.com/john-harrold/ruminate/main/man/figures/logo.png"
data_url =
  "https://github.com/john-harrold/formods/raw/master/inst/test_data/TEST_DATA.xlsx"
run_url =
  "https://runruminate.ubiquity.tools/"
use_url =
  "https://useruminate.ubiquity.tools/"
main_url =
  "https://ruminate.ubiquity.tools/"
issue_url =
```

```
"https://github.com/john-harrold/ruminate/issues"
intro_text = tags$p(
"Ruminate is a shiny module for pharmacometric data processing,
visualization, and analysis. It consists of separate shiny modules that
provide interfaces into common R packages and provides the underlying code.
This is done to facilitate usage of those packages and to provide reproducible
analyses.",
tags$li( "To find out more visit ",
        tags$a("ruminate.ubiquity.tools", href=main_url),""),
tags$li( "To give it a try you can download a test dataset ",
        tags$a("here", href=data_url),""),
tags$li( "Go to ",
        tags$a("useruminate.ubiquity.tools", href=use_url)," for a video
        demonstrating how to use ruminate"),
tags$li( "If you run into any problems, have questions, or want a feature please
       visit the ",
       tags$a("issues", href=issue_url)," page")
)
ui <- shinydashboard::dashboardPage(</pre>
 skin="black",
 shinydashboard::dashboardHeader(title="ruminate"),
 shinydashboard::dashboardSidebar(
     shinydashboard::sidebarMenu(
       shinydashboard::menuItem("Load/Save",
                                tabName="loadsave",
                                icon=icon("arrow-down-up-across-line")) ,
    shinydashboard::menuItem("Transform Data", tabName="wrangle", icon=icon("shuffle")),
    shinydashboard::menuItem("Visualize", tabName="plot", icon=icon("chart-line")),
     shinydashboard::menuItem("NCA",
                                            tabName="nca",
                                                               icon=icon("chart-area")),
    shinydashboard::menuItem("App Info", tabName="sysinfo", icon=icon("book-medical"))
 ),
  shinydashboard::dashboardBody(
 tags$head(
    tags$style(HTML(CSS))
    shinydashboard::tabItems(
       shinydashboard::tabItem(tabName="nca",
               shinydashboard::box(title="Non-Compartmental Analysis", width=12,
               fluidRow( prompter::use_prompt(),
               column(width=12,
               htmlOutput(NS("NCA", "NCA_ui_compact")))))
       shinydashboard::tabItem(tabName="loadsave",
               shinydashboard::box(title=NULL, width=12,
               shinydashboard::tabBox(
                 width = 12,
                 title = NULL,
                 shiny::tabPanel(id="load_data",
                          title=tagList(shiny::icon("file-arrow-up"),
```

"Load Data"),

```
fluidRow(
              column(width=6,
                div(style="display:inline-block;width:100%",
                htmlOutput(NS("UD", "ui_ud_load_data"))),
                htmlOutput(NS("UD", "ui_ud_clean")),
                htmlOutput(NS("UD", "ui_ud_select_sheets")),
                htmlOutput(NS("UD", "ui_ud_workflows")),
                htmlOutput(NS("UD", "ui_ud_text_load_result"))),
              column(width=6,
                  tags$p(
                      tags$img(
                      class = "wrapfig",
                      src = logo_url,
                      width = 150,
                      alt = "formods logo" ),
                  intro_text
                  ))
            ),
          fluidRow(
            column(width=12,
                   div(style="display:inline-block;vertical-align:top",
                             htmlOutput(NS("UD", "ui_ud_data_preview")))
                   ))
          ),
          shiny::tabPanel(id="save_state",
                   title=tagList(shiny::icon("arrow-down-up-across-line"),
                                  "Save or Load Analysis"),
          fluidRow(
            column(width=5,
                   div(style="display:inline-block;vertical-align:top",
            htmlOutput(NS("ASM", "ui_asm_compact"))
            ))
            )
          )
  #
shinydashboard::tabItem(tabName="wrangle",
    shinydashboard::box(title="Transform and Create Views of Your Data", width=12,
        fluidRow(
        column(width=12,
        htmlOutput(NS("DW", "DW_ui_compact")))))
        ),
shinydashboard::tabItem(tabName="plot",
        shinydashboard::box(title="Visualize Data", width=12,
        htmlOutput(NS("FG", "FG_ui_compact")))),
shinydashboard::tabItem(tabName="sysinfo",
        box(title="System Details", width=12,
        shinydashboard::tabBox(
          width = 12,
          title = NULL,
          shiny::tabPanel(id="sys_packages",
```

```
title=tagList(shiny::icon("box-open"),
                                         "Installed Packages"),
                 htmlOutput(NS("ASM", "ui_asm_sys_packages"))
                 shiny::tabPanel(id="sys_modules",
                          title=tagList(shiny::icon("cubes"),
                                         "Loaded Modules"),
                 htmlOutput(NS("ASM", "ui_asm_sys_modules"))
                 ),
                 shiny::tabPanel(id="sys_log",
                          title=tagList(shiny::icon("clipboard-list"),
                                         "Log"),
                 verbatimTextOutput(NS("ASM", "ui_asm_sys_log"))
                 shiny::tabPanel(id="sys_options",
                          title=tagList(shiny::icon("sliders"),
                                         "R Options"),
                 htmlOutput(NS("ASM", "ui_asm_sys_options"))
         #
                 )
               ))
     )
   )
# Main app server
server <- function(input, output, session) {</pre>
 # Empty reactive object to track and react to
 # changes in the module state outside of the module
 react_FM = reactiveValues()
 # Module IDs and the order they are needed for code generation
 mod_ids = c("UD", "DW", "FG", "NCA", "MB")
 # If the ftmptest file is present we load test data
 if(file.exists(ftmptest)){
                                                 "preload", "ASM_preload.yaml"),
   sources = c(system.file(package="formods",
                                                 "preload", "UD_preload.yaml"),
                system.file(package="formods",
                                                 "preload", "FG_preload.yaml"),
"preload", "DW_preload.yaml"),
                system.file(package="formods",
                system.file(package="formods",
                system.file(package="ruminate", "preload", "NCA_preload.yaml"))
   res = FM_app_preload(session=session, sources=sources)
 # Otherwise we look for a preload file and load that if it exists
 } else if(file.exists("preload.yaml")){
  shinybusy::show_modal_spinner(text="Preloading analysis, be patient", session=session)
   res = FM_app_preload(session=session, sources="preload.yaml")
   shinybusy::remove_modal_spinner(session = session)
 }
 # Module servers
 formods::ASM_Server( id="ASM",
```

NCA\_set\_current\_ana 125

```
deployed
                                  = deployed,
                     react_state = react_FM,
                     FM_yaml_file = formods.yaml,
                     MOD_yaml_file = ASM.yaml,
                     mod_ids
                               = mod_ids)
 formods::UD_Server(
                    id ="UD", id_ASM = "ASM",
                     deployed
                                = deployed,
                     react_state = react_FM,
                     MOD_yaml_file = UD.yaml,
                     FM_yaml_file = formods.yaml)
                                  id\_ASM = "ASM",
 formods::DW_Server(
                     id="DW",
                     id_UD = "UD",
                     deployed
                                    = deployed,
                     react_state
                                    = react_FM,
                     MOD_yaml_file = DW.yaml,
                     FM_yaml_file = formods.yaml)
 formods::FG_Server( id="FG",
                               id\_ASM = "ASM",
                     id_UD = "UD", id_DW = "DW",
                     react_state
                     deployed
                                   = deployed,
                                    = react_FM,
                     MOD_yaml_file = FG.yaml,
                     FM_yaml_file = formods.yaml)
                         ="NCA", id_ASM = "ASM",
 ruminate::NCA_Server(id
                     id_UD = "UD", id_DW = "DW",
                     deployed
                                    = deployed,
                     react_state
                                   = react_FM,
                     MOD_yaml_file = NCA.yaml,
                     FM_yaml_file
                                     = formods.yaml)
}
shinyApp(ui, server)
```

#### **Description**

Takes an NCA state and an analysis list and sets that figure list as the value for the active figure

# Usage

```
NCA_set_current_ana(state, ana)
```

#### **Arguments**

```
state NCA state from NCA_fetch_state()
ana Analysis list from NCA_fetch_current_ana
```

#### Value

State with the current analysis updated

```
library(ruminate)
# Module IDs
id = "NCA"
id UD = "UD"
id_DW = "DW"
id_ASM = "ASM"
# We need session and input variables to be define
sess_res = NCA_test_mksession()
# Extracting the session and input variables
session = sess res$session
          = sess_res$input
input
react_state = list()
# We also need configuration files
FM_yaml_file = system.file(package = "formods", "templates", "formods.yaml")
MOD_yaml_file = system.file(package = "ruminate", "templates", "NCA.yaml")
# Getting the current module state
state = NCA_fetch_state(id = id,
                      input = input,
session = session,
                      input
                      FM_yaml_file = FM_yaml_file,
                      MOD_yaml_file = MOD_yaml_file,
                      id_ASM
                                    = id_ASM,
                                    = id_UD,
                      id_UD
                      id DW
                                    = id_DW,
                      react_state = react_state)
# Pulls out the active analysis
current_ana = NCA_fetch_current_ana(state)
# This will get the dataset associated with this analysis
ds = NCA_fetch_ana_ds(state, current_ana)
# After making changes you can update those in the state
state = NCA_set_current_ana(state, current_ana)
# You can use this to check the current analysis
current_ana = NCA_process_current_ana(state)
# This will pull out the code for the module
fc_res = NCA_fetch_code(state)
# This will use patterns defined for the site to detect
# columns. In this example we are detecting the id column:
id_col = NCA_find_col(
```

NCA\_test\_mksession 127

```
patterns = state[["MC"]][["detect_col"]][["id"]],
dscols = names(ds$DS))

# This creates a new analysis
state = NCA_new_ana(state)
```

 $NCA\_test\_mksession$ 

Populate Session Data for Module Testing

# **Description**

Populates the supplied session variable for testing.

# Usage

```
NCA_test_mksession(session = list(), full = FALSE)
```

## **Arguments**

session Shiny session variable (in app) or a list (outside of app)

full Boolean indicating if the full test session should be created

# Value

The NCA portion of the all\_sess\_res returned from FM\_app\_preload

# See Also

```
FM_app_preload
```

```
session = shiny::MockShinySession$new()
sess_res = NCA_test_mksession(session=session)
```

plot\_sr\_ev

plot\_sr\_ev

Plots Timecourse of Rules Simulations

## **Description**

Plots the timecourse of `simulate\_rules()` output.

## Usage

```
plot_sr_ev(
    sro = NULL,
    fpage = 1,
    fcol = "id",
    xcol = "time",
    error_msgs = NULL,
    ylog = TRUE,
    ylab_str = "Amount",
    xlab_str = "Time",
    post_proc = "fig = fig + ggplot2::theme_light()",
    evplot = c(1, 4),
    fncol = 4,
    fnrow = 2
)
```

#### **Arguments**

Output of 'simulate_rules()'.
If facets are selected and multiple pages are generated then this indicates the page to return.
Name of column to facet by or NULL to disable faceting ("id").
Name of column to take x-data from ("time").
Named list with error messages to overwrite (NULL
Boolean to enable log10 scaling of the y-axis (TRUE
Label for the y-axis ("Output"
Label for the x-axis ("Output"
Character object with post processing post-processing code for the figure object named fig internall ("fig = fig + theme_light()")
Evids to plot can be 1 or 4
Number of columns in faceted output.
Number of rows in faceted output.

# **Details**

For a detailed examples see vignette ("clinical\_trial\_simulation", package = "ruminate").

plot\_sr\_ev 129

#### Value

List with the followin1g elements:

- isgood: Return status of the function.
- msgs: Error or warning messages if any issues were encountered.
- npages: Total number of pages using the current configuration.
- error\_msgs: List of error messages used.
- dsp: Intermediate dataset generated from sro to plot in ggplot.
- fig: Figure generated.

```
library(formods)
library(ggplot2)
# For more information see the Clinical Trial Simulation vignette:
# https://ruminate.ubiquity.tools/articles/clinical_trial_simulation.html
# None of this will work if rxode2 isn't installed:
if(is_installed("rxode2")){
library(rxode2)
set.seed(8675309)
rxSetSeed(8675309)
my_model = function ()
  description <- "One compartment PK model with linear clearance using differential equations"
    ini({
        lka <- 0.45
        label("Absorption rate (Ka)")
        lcl <- 1
        label("Clearance (CL)")
        lvc <- 3.45
        label("Central volume of distribution (V)")
        propSd <- c(0, 0.5)
        label("Proportional residual error (fraction)")
        etalcl ~ 0.1
    })
    model({
        ka <- exp(lka)</pre>
        cl <- exp(lcl + etalcl)</pre>
        vc <- exp(lvc)
        kel <- cl/vc
        d/dt(depot) <- -ka * depot</pre>
        d/dt(central) <- ka * depot - kel * central</pre>
        Cc <- central/vc</pre>
        Cc ~ prop(propSd)
    })
}
```

plot\_sr\_ev

```
# This creates an rxode2 object
object = rxode(my_model)
# If you want details about the parameters, states, etc
# in the model you can use this:
rxdetails = fetch_rxinfo(object)
rxdetails$elements
# Next we will create subjects. To do that we need to
# specify information about covariates:
nsub = 2
covs = list(
 WT
            = list(type = "continuous",
                   sampling = "log-normal",
                   values = c(70, .15))
)
subs = mk_subjects(object = object,
                  nsub = nsub,
                  covs = covs)
head(subs$subjects)
rules = list(
 dose = list(
   condition = "TRUE",
   action = list(
     type = "dose",
     state = "central",
     values = "c(1)",
            = "c(0)",
     times
     durations = "c(0)")
   )
)
\# We evaulate the rules for dosing at time 0
eval_times = 0
# Stop 2 months after the last dose
output\_times = seq(0, 56, 1)
# This runs the rule-based simulations
simres =
 simulate_rules(
    object = object,
    subjects
               = subs[["subjects"]],
    eval_times = eval_times,
   output_times = output_times,
                 = rules)
   rules
# First subject data:
sub_1 = simres$simall[simres$simall$id == 1, ]
```

```
# First subjects events
evall = as.data.frame(simres$evall)
ev_sub_1 = evall[evall$id ==1, ]
# All of the simulation data
simall = simres$simall
simall$id = as.factor(simall$id)
# Timecourse
psim =
 plot_sr_tc(
   sro = simres,
   dvcols = "Cc")
psim$fig
# Events
pev =
 plot_sr_ev(
   sro = simres,
   ylog = FALSE)
pev$fig
}
```

plot\_sr\_tc

Plots Timecourse of Rules Simulations

# **Description**

Plots the timecourse of `simulate\_rules()` output.

# Usage

```
plot_sr_tc(
    sro = NULL,
    dvcols = NULL,
    fpage = 1,
    fcol = "id",
    xcol = "time",
    error_msgs = NULL,
    ylog = TRUE,
    ylab_str = "Output",
    xlab_str = "Time",
    post_proc = "fig = fig + ggplot2::theme_light()",
    fncol = 4,
    fnrow = 2
)
```

# Arguments

sro	Output of 'simulate_rules()'.
dvcols	Character vector of dependent variables.
fpage	If facets are selected and multiple pages are generated then this indicates the page to return.
fcol	Name of column to facet by or NULL to disable faceting ("id").
xcol	Name of column to take x-data from ("time").
error_msgs	Named list with error messages to overwrite (NULL
ylog	Boolean to enable log10 scaling of the y-axis (TRUE
ylab_str	Label for the y-axis ("Output"
xlab_str	Label for the x-axis ("Output"
post_proc	Character object with post processing post-processing code for the figure object named fig internall ("fig = fig + theme_light()")
fncol	Number of columns in faceted output.
fnrow	Number of rows in faceted output.

#### **Details**

For a detailed examples see vignette("clinical\_trial\_simulation", package = "ruminate").

#### Value

List with the followin1g elements:

- isgood: Return status of the function.
- msgs: Error or warning messages if any issues were encountered.
- npages: Total number of pages using the current configuration.
- error\_msgs: List of error messages used.
- dsp: Intermediate dataset generated from sro to plot in ggplot.
- fig: Figure generated.

```
library(formods)
library(ggplot2)

# For more information see the Clinical Trial Simulation vignette:
# https://ruminate.ubiquity.tools/articles/clinical_trial_simulation.html

# None of this will work if rxode2 isn't installed:
if(is_installed("rxode2")){
library(rxode2)
set.seed(8675309)
rxSetSeed(8675309)
```

```
my_model = function ()
  description <- "One compartment PK model with linear clearance using differential equations"
        lka <- 0.45
        label("Absorption rate (Ka)")
        lcl <- 1
        label("Clearance (CL)")
        lvc <- 3.45
        label("Central volume of distribution (V)")
        propSd <- c(0, 0.5)
        label("Proportional residual error (fraction)")
        etalcl ~ 0.1
    })
    model({
        ka <- exp(lka)</pre>
        cl <- exp(lcl + etalcl)</pre>
        vc <- exp(lvc)</pre>
        kel <- cl/vc
        d/dt(depot) <- -ka * depot</pre>
        d/dt(central) <- ka * depot - kel * central</pre>
        Cc <- central/vc</pre>
        Cc ~ prop(propSd)
    })
}
# This creates an rxode2 object
object = rxode(my_model)
# If you want details about the parameters, states, etc
# in the model you can use this:
rxdetails = fetch_rxinfo(object)
rxdetails$elements
# Next we will create subjects. To do that we need to
# specify information about covariates:
nsub = 2
covs = list(
  WT
             = list(type
                             = "continuous",
                     sampling = "log-normal",
                     values = c(70, .15))
)
subs = mk_subjects(object = object,
                   nsub = nsub,
                    covs = covs)
head(subs$subjects)
rules = list(
  dose = list(
    condition = "TRUE",
```

```
action = list(
     type = "dose",
     state = "central",
     values = "c(1)",
     times = "c(0)",
     durations = "c(0)")
   )
)
\# We evaulate the rules for dosing at time 0
eval_times = 0
# Stop 2 months after the last dose
output\_times = seq(0, 56, 1)
# This runs the rule-based simulations
simres =
 simulate_rules(
   object = object,
    subjects
               = subs[["subjects"]],
   eval_times = eval_times,
   output_times = output_times,
   rules
                = rules)
# First subject data:
sub_1 = simres$simall[simres$simall$id == 1, ]
# First subjects events
evall = as.data.frame(simres$evall)
ev_sub_1 = evall[evall$id ==1, ]
# All of the simulation data
simall = simres$simall
simall$id = as.factor(simall$id)
# Timecourse
psim =
 plot_sr_tc(
   sro = simres,
   dvcols = "Cc")
psim$fig
# Events
pev =
 plot_sr_ev(
   sro = simres,
   ylog = FALSE)
pev$fig
}
```

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ruminate	ruminate: Shiny app and module to facilitate pharamacometrics analysis
----------	--

## **Description**

This is done by creating a Shiny interface to different tools for data transformation (dplyr and tidyr), plotting (ggplot2), and noncompartmental analysis (PKNCA). These results can be reported in Excel, Word or PowerPoint. The state of the app can be saved and loaded at a later date. When saved, a script is generated to reproduce the different actions in the Shiny interface.

Runs the pharmacometrics ruminate app.

#### Usage

```
ruminate(
  host = "127.0.0.1",
  port = 3838,
  server_opts = list(shiny.maxRequestSize = 30 * 1024^2),
  devmode = FALSE,
  mksession = FALSE
)
```

#### **Arguments**

host Hostname of the server ("127.0.0.1")

port Port number for the app (3838)

server\_opts List of options (names) and their vlues (value) e.g. list(shiny.maxRequestSize = 30 \* 1024^2).

devmode Boolean value, when TRUE will run ruminate with development modules.

mksession Boolean value, when TRUE will load test session data for app testing.

#### Value

Nothing is returned, this function just runs the built-in ruminate app.

# Author(s)

```
Maintainer: John Harrold < john.m.harrold@gmail.com> (ORCID)
```

#### See Also

```
https://ruminate.ubiquity.tools/
```

run\_nca\_components

## **Examples**

```
if (interactive()) {
ruminate()
}
```

ruminate\_check

Checks ruminate Dependencies

# Description

Looks at the suggested dependencies and checks to make sure they are installed.

# Usage

```
ruminate_check(verbose = TRUE)
```

## **Arguments**

verbose

Logical indicating if messages should be displayed

#### Value

List with the following elements:

- all\_found: Boolean indicating if all packages were found
- found\_pkgs: Character vector of found packages
- missing\_pkgs: Character vector of missing packages

## **Examples**

```
fcres =ruminate_check()
```

run\_nca\_components

Runs NCA for the Current Analysis

## **Description**

Takes the current state and runs the current analysis in that state.

# Usage

```
run_nca_components(
   state,
   components = c("nca", "fg_ind_obs", "tb_ind_obs", "tb_ind_params"),
   verbose = TRUE
)
```

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#### Arguments

state NCA state from NCA\_fetch\_state()

components List of components to run. By default it will run all of the following. If you just

need to regenerate a figure based on the current nca results you can just specify

that component. These are the valid

verbose Logical to enable or disable messaging components:

• nca: Run NCA analysis

• fg\_ind\_obs: Build the figure(s) with the individual observations.

• tb\_ind\_obs: Build the table(s) with the individual observations.

• tb\_ind\_params: Build the table(s) with the individual parameters.

#### Value

List with the following components:

- isgood: Return status of the function.
- · msgs: Error messages if any issues were encountered.
- nca\_res: PKNCA results if run was successful.

#### **Examples**

```
# We need a state object to use below
sess_res = NCA_test_mksession()
state = sess_res$state
state = run_nca_components(state, components="tb_ind_params")
```

rx2other

Converts an rxode2 Object Into Specified Model Format

#### **Description**

If you have an rxode2 or nlmixr2 model object you can use this function to translate that object into other formats. See output\_type below for the allowed formats.

In order to do this you need at least one between-subject variability term and one endpoint. If these are missing then dummy values will be added. The dummy values for between-subject variability are IIV will be POP\_RUMINATE, TV\_RUMINATE, and ETA.RUMINATE. The dummy terms for endpoints are OUT\_RUMINATE and add.OUT\_RUMINATE.

# Usage

```
rx2other(
  object,
  out_type = "nonmem",
  dataset = NULL,
  export_name = "my_model",
  export_path = tempfile(pattern = "dir")
)
```

rx2other

#### **Arguments**

object	rxode2 model object
out_type	Output type (either "nonmem", "monolix")
dataset	Optional dataset
export_name	Basename for models used
export_path	Location to place output files (default tempdir())

#### **Details**

Known issues: If you have specified bioavailability in the model, it will fail on the Monolix conversion.

#### Value

List with the following elements:

- isgood: Return status of the function.
- msgs: Error or warning messages if any issues were encountered.
- files: If successful this will contain a list with an entry for each file generated to support the requested format. the current file format. For example if "nonmem" was selected this will include elements for "ctl" and "csv". Each of these are lists with the following format:
  - fn: Exported file name
  - fn\_full: Exported file name with the full path.
  - contents: Contents of the file.

```
library(ruminate)
if( Sys.getenv("ruminate_rxfamily_found") == "TRUE"){
# First create an rxode2 model:
library(rxode2)
one.compartment <- function() {</pre>
   rxode2::ini({
     tka <- log(1.57); label("Ka")
     tcl <- log(2.72); label("Cl")
     tv <- log(31.5); label("V")
     eta.ka ~ 0.6
     eta.cl ~ 0.3
     eta.v ~ 0.1
     add.sd <- 0.7
   })
   # and a model block with the error specification and model specification
   rxode2::model({
     ka <- exp(tka + eta.ka)
     cl <- exp(tcl + eta.cl)</pre>
     v <- exp(tv + eta.v)
     d/dt(depot) <- -ka * depot</pre>
     d/dt(center) <- ka * depot - cl / v * center</pre>
```

```
cp <- center / v
   cp ~ add(add.sd)
  })
}
nmout = rx2other(one.compartment, out_type="nonmem")
}</pre>
```

simulate\_rules

Rule-Based simulates

# Description

Simulate an rxode2 model based on rules evaluated at specified time-points. For example if you want to titrate dosing based on individual plasma levels you could create a rule that changes dosing at specified time points based on the last observation of the user.

## Usage

```
simulate_rules(
  object,
  subjects,
  eval_times,
  output_times,
  time_scales = NULL,
  rules,
  rx_options = list(),
  preamble = "",
  pbm = "Evaluation times",
  smooth_sampling = TRUE
)
```

## **Arguments**

object	rxode2 model object An ID string that corresponds with the ID used to call the modules UI elements
subjects	Dataframe of subject level information.
eval_times	Vector of simulation times to evaulate the rules (units are time units of the system).
output_times	Specific output times to include. Other times will be included as well to ensure proper evaluation of the rules.
time_scales	Optional list with timescale information to include in the output.
rules	List of rules, see below for a description of the format.
rx_options	List of options to pass through to rxSolve().

Preamble Character string of user-defined code to execute in rule-evaluation environment (e.g. you can put user-defined functions here).

pbm Progress bar message, set to NULL to disable.

smooth\_sampling

Boolean when TRUE will insert sampling just before dosing to make sampling smooth.

#### Details

For a detailed examples see vignette("clinical\_trial\_simulation", package = "ruminate")

The underlying simulations are run using rxode2, and as such we need an rxode2 system object. From that we can either simulate subjects or load them from a file. Next we need to define a set of rules. These will be a set of conditions and actions. At each evaluation time point the conditions are evaluated. When a condition is met the actions associated with that condition are executed. For example, if during a visit (an evaluation time point) the trough PK is below a certain level (condition) we may want to increase the dosing regimen for the next dosing cycle (action).

#### **Creating subjects:**

Subjects are expected in a data frame with the following column headers:

- · id Individual subject id
- Names of parameters and iiv as specified in the ini section of the rxode2 function specification
- Names of covariates used in the model.

mk\_subjects() — Creates subjects for simulation by sampling based on between-subject variability and generating covariate information based on user specifications.

#### Covariates:

The covs input is a list with the following structure:

- type: Can be either "fixed", "discrete", or "continuous".
- sampling: This field is only needed for a "continuous" covariate ' type and can be either "random", "normal" or "log-normal".
- values: This field depends on the type and optional sampling above.
  - fixed: A single value.
  - discrete: A vector of possible discrete elements.
  - continuous, random: Two values the first is the lower bound and the second is the upper bound.
  - continuous, normal: Two values the first is the mean and the second is the variance.
  - continuous, log-normal: Two values the first is the mean and the second is the variance.

This examples shows the SEX\_ID randomly sampled from the values specified, SUBTYPE\_ID fixed at a value, and WT sampled from a log-normal distribution.

```
sampling = "log-normal",
values = c(70, .15))
)
```

#### **Rule-based simulations:**

simulate\_rules() — This will run simulations based on the rule definitions below.

#### Rules:

Rules are a named list where the list name can be a short descriptive label used to remember what the rule does. These names will be returned as columns in the simulated data frame.

- condition: Character string that evaluates to either TRUE or FALSE. When true the action portion will be triggered. For a list of objects available see the Rule-evaluation environment below.
- fail\_flag: Flag set in the rule\_id column when the condition is not met (set to "false" if not specified).
- true\_flag: Flag set in the rule\_id column when the condition is met (set to "true" if not specified).
- action: This is what the rule will trigger can be any of the following:
  - type: This defines the action type and can be either "dose", "set state", or "manual".

Based on the type the action field will expect different elements.

# Dosing:

- action
  - type: "dose"
  - values: Character string that evaluates as a numeric vector dosing amounts (e.g. "c(3, 3, 3, 3)")
  - times: Character string that evaluates as a numeric vector of times (e.g. "c(0, 14, 28, 42)")
  - durations: Character string that evaluates as a numeric vector of durations (e.g. "c(0, 0, 0, 0)", zero for bolus dosing)

#### Changing a state value:

- action
  - type: "set state"
  - state: Character string with the name of the state to set ("Ac")
  - value: Character string that evaluates as a numeric value for state (e.g. "Ac/2" would set the state to half the value of Ac at the evaluation point)

#### Manual modification of the simulation:

- action
  - type: "manual"
  - code: Character string of code to evaluate.

#### Rule-evaluation environment:

Beyond simple simulations it will be necessary to execute actions based on the current or previous state of the system. For this reason, when a condition or elements of the action (e.g., the values, times and durations of a dose action type) are being evaluated, the following objects will be available at each evaluation point:

- outputs: The value of each model output.
- states: The value of each named state or compartment.

- covariates: The value of each named covariate.
- subject-level parameters: The value of each named parameter.
- rule value: The last value the rule evaluated as.
- id: Current subject id.
- time: Current evaluation time.
- SI\_SUB\_HISTORY: A data frame of the simulation history of the current subject up to the current evaluation point.
- SI\_subjects: The subjects data frame.
- SI\_eval\_times: Vector of the evaluation times.
- SI\_interval\_ev: The events table in it's current state for the given simulation interval.
- SI\_ev\_history: This is the history of the event table containing all the events leading up to the current interval.
- SI\_ud\_history: This is a free form object the user can define or alter within the "man-ual" action type (ud-user defined, history).

The following functions will be available::

• SI\_fpd: This function will fetch the previous dose (fpd) for the given id and state. For example for the current id and the state Ac you would do the following:

```
SI_fpd(id=id, state="Ac")
```

#### Time scales:

You can include columns in your output for different time scales if you wish. You need to create a list in the format below. One element should be system with a short name for the system time scale. The next should be details which is a list containing short names for each time scale you want to include. Each of these is a list with a verbose name for the time scale (verb) and a numerical conversion indicating how that time scale relates to the others. Here we define weeks and days on the basis of seconds.

#### Value

List with the following elements:

- isgood: Return status of the function.
- msgs: Error or warning messages if any issues were encountered.
- · simall: Simulation results.
- ev\_history: The event table for the entire simulation history.
- eval\_times: Evaluation time points at the system time scale
- eval\_times\_df: Data frame of the evaluation time points with a column for the system time scale and then columns for named time scales.

```
library(formods)
library(ggplot2)
# For more information see the Clinical Trial Simulation vignette:
# https://ruminate.ubiquity.tools/articles/clinical_trial_simulation.html
# None of this will work if rxode2 isn't installed:
if(is_installed("rxode2")){
library(rxode2)
set.seed(8675309)
rxSetSeed(8675309)
my_model = function ()
  description <- "One compartment PK model with linear clearance using differential equations"
    ini({
        lka <- 0.45
        label("Absorption rate (Ka)")
        lcl <- 1
        label("Clearance (CL)")
        lvc <- 3.45
        label("Central volume of distribution (V)")
        propSd <- c(0, 0.5)
        label("Proportional residual error (fraction)")
        etalcl ~ 0.1
    })
    model({
        ka <- exp(lka)</pre>
        cl <- exp(lcl + etalcl)</pre>
        vc <- exp(lvc)
        kel <- cl/vc
        d/dt(depot) <- -ka * depot</pre>
        d/dt(central) <- ka * depot - kel * central</pre>
        Cc <- central/vc</pre>
        Cc ~ prop(propSd)
    })
}
# This creates an rxode2 object
object = rxode(my_model)
# If you want details about the parameters, states, etc
# in the model you can use this:
rxdetails = fetch_rxinfo(object)
rxdetails$elements
# Next we will create subjects. To do that we need to
# specify information about covariates:
nsub = 2
covs = list(
```

```
= list(type = "continuous",
                   sampling = "log-normal",
                   values = c(70, .15))
)
subs = mk_subjects(object = object,
                  nsub = nsub,
                  covs = covs)
head(subs$subjects)
rules = list(
 dose = list(
   condition = "TRUE",
   action = list(
     type = "dose",
     state = "central",
     values = "c(1)",
     times = "c(0)",
     durations = "c(0)")
)
\mbox{\#} We evaulate the rules for dosing at time 0
eval_times = 0
# Stop 2 months after the last dose
output\_times = seq(0, 56, 1)
# This runs the rule-based simulations
simres =
 simulate_rules(
   object
               = object,
   subjects
               = subs[["subjects"]],
   eval_times = eval_times,
   output_times = output_times,
   rules
                 = rules)
# First subject data:
sub_1 = simres$simall[simres$simall$id == 1, ]
# First subjects events
evall = as.data.frame(simres$evall)
ev_sub_1 = evall[evall$id ==1, ]
# All of the simulation data
simall = simres$simall
simall$id = as.factor(simall$id)
# Timecourse
psim =
 plot_sr_tc(
   sro = simres,
```

```
dvcols = "Cc")
psim$fig

# Events
pev =
   plot_sr_ev(
       sro = simres,
       ylog = FALSE)
pev$fig
}
```

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