

Package ‘lixoftConnectors’

June 7, 2024

Type Package

Title R connectors for Lixoft Suite (@Lixoft)

Version 2020.1

Date 2019-01-01

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Depends R (>= 3.0.0), RJSONIO

Encoding UTF-8

Collate apiTools.R displayTools.R lixoftEnvironment.R apiManager.R
commons-tools.R commons-data.R commons-projectManagement.R
commons-settings.R commons-scenario.R commons-results.R
mlx-settings.R mlx-scenario.R mlx-populationParameters.R
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mlx-modelBuilding.R pkx-settings.R pkx-scenario.R pkx-results.R
smlx-projectManagement.R smlx-settings.R smlx-definition.R
smlx-scenario.R smlx-results.R

Description This package provides R connectors for Monolix - PKanalix -
Simulx (@Lixoft) to create, edit and run Mlxtran projects from R command prompt.

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RoxygenNote 7.0.2

NeedsCompilation no

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addCategoricalTransformedCovariate

[Monolix] Add categorical transformed covariate

Description

Create a new categorical covariate by transforming an existing one. Transformed covariates cannot be used to produce new covariates. Call [getCovariateInformation](#) to know which covariates can be transformed.

Usage

```
addCategoricalTransformedCovariate(...)
```

Arguments

```
...      A list of comma-separated pairs {transformedCovariateName = { from = (array<(string)>)[ "basicCovariateNames" ], transformed = (array<array<string>)"transformation" } }
```

See Also

[getCovariateInformation](#) [removeCovariate](#)

Examples

```
## Not run:
addCategoricalTransformedCovariate( Country2 = list(reference = "A1",
  from = "Country", transformed = list( A1 = c("A","B"), A2 = c("C")))
)

## End(Not run)
```

```
addContinuousTransformedCovariate
  [Monolix] Add continuous transformed covariate
```

Description

Create a new continuous covariate by transforming an existing one. Transformed covariates cannot be use to produce new covariates. Call [getCovariateInformation](#) to know which covariates can be transformed.

Usage

```
addContinuousTransformedCovariate(...)
```

Arguments

```
...          A list of comma-separated pairs {transformedCovariateName = (string)"transformation" }
```

See Also

[getCovariateInformation](#) [removeCovariate](#)

Examples

```
## Not run:
addContinuousTransformedCovariate( tWt2 = "3*exp(Wt)" )

## End(Not run)
```

```
addGroup          [Simulx] Add simulation group
```

Description

Add a new simulation group.

Usage

```
addGroup(group)
```

Arguments

```
group          (string) Name of the group to add.
```

See Also[getGroups](#)**Examples**

```
## Not run:
  addGroup("group")

## End(Not run)
```

addMixture	<i>[Monolix] Add mixture to the covariate model</i>
------------	---

Description

Add a new latent covariate to the current model giving its name and its modality number.

Usage

```
addMixture(...)
```

Arguments

... A list of comma-separated pairs {latentCovariateName = (int)modalityNumber}

See Also[getCovariateInformation](#) [removeCovariate](#)**Examples**

```
## Not run:
  addMixture(lcat = 2)

## End(Not run)
```

applyFilter	<i>[Monolix - PKanalix] Apply filter</i>
-------------	--

Description

Apply a filter on the current data. Refere to [createFilter](#) for more details about syntax, allowed parameters and examples.

Usage

```
applyFilter(filter, name = "")
```

Arguments

filter (list< list< action = "headerName-comparator-value" > > or "complement") filter definition.

name (string) [optional] created data set name.

See Also

[getAvailableData](#) [createFilter](#) [removeFilter](#)

Examples

```
## Not run:
applyFilter( filter = list(selectLines = "CONC>=5.5", removeLines = "CONC>10"))\cr
applyFilter( filter = list(selectLines = "y1!=2") )\cr
applyFilter( filter = list(selectIds = "SEX==M", selectIds = "WEIGHT<80") )\cr
applyFilter( filter = "complement" )

## End(Not run)
```

computeBins

Compute bins

Description

Compute bins values, middles, and data repartition over bins. Available options are:

"criteria"	(string)	Bins criteria: "equalwidth", "equalsize" or "leastsquare" (default).
"useFixedNb"	(bool)	TRUE to fix the number of bins, FALSE (default) to estimate it.
"fixedNb"	(int)	Fixed number of bins (default: 10).
"estimatedNb"	(pair<int,int>)	Bounds for bins number estimation (default: [5,30]).
"nbBinData"	(pair<int,int>)	Minimum and maximum number of data per bin for bins number estimation (default: [5,30]).

Usage

```
computeBins(data, options = list())
```

Arguments

data (vector<double>) Input data.

options (list) [optional] Computation options.

Value

A list bins values ("values"), middles ("middles") and the actual number of data per bin ("repartition").

Examples

```
## Not run:
computeBins(data = c(1, 1.25, 2.5, 5, 5.5, 5.75, 7.5, 15, 16.5), options = list(nbBinData = c(1,10)))

## End(Not run)
```

computeChartsData *[Monolix - PKanalix - Simulx] Compute the charts data*

Description

Compute and export the charts data of scenario. Notice that it does not impact the current scenario.

Usage

```
computeChartsData(exportVPCSimulations = FALSE, wait = TRUE)
```

Arguments

exportVPCSimulations
 (*bool*) [optional][Monolix] Should VPC simulations be exported if available.
 Equals FALSE by default.

wait (*OBSOLETE*)

Examples

```
## Not run:
computeChartsData()

## End(Not run)
```

computePredictions *[Monolix] Compute predictions from the structural model*

Description

[MlxCore][Prediction]
 Call the monolix prediction function to compute observation models values on observation times for each subject of a set of individuals.

Usage

```
computePredictions(individualParameters, individualIds = NULL)
```

Arguments

individualParameters
 Individual parameter values associated to each one of the individual parameters present in the project, for a set of subjects which must be coherent with the list of individuals ids passed in "individualIds" field (ie, this length of the subject set must be the sum of the subject number of all the individuals selected by the "individualIds" field). This input field accepts a dataframe indexed by individual parameter names (columns) and subject indexes (rows).

individualIds [optional] *vector<int>* Ids of the individuals for which observation models should be computed. By default, all the individuals present in the project are considered.

Value

For each prediction names, a vector giving the computed prediction at observation times for each subject.

See Also

[getIndividualParameterModel](#) [getEstimatedIndividualParameters](#)

Examples

```
## Not run:
ids = c(1,4)
individualValuesForAllIndiv = getEstimatedIndividualParameters()$saem

predictions = computePredictions( individualParameters = individualValuesForAllIndiv[ids,],
                                  individualIds = ids )

predictions
-> $Cc
      [3.8,6.75,...,3.4,5.1,...]
      |   id=1   |   id=4   |
## End(Not run)
```

createAdditionalCovariate

[Monolix - PKanalix] Create additional covariate

Description

Create an additional covariate for stratification purpose. Available column transformations are:

[continuous]	'firstDoseAmount'	(first dose amount)
[continuous]	'doseNumber'	(dose number)
[discrete]	'administrationType'	(administration type)
[discrete]	'administrationSequence'	(administration sequence)
[discrete]	'dosingDesign'	(dose multiplicity)
[continuous]	'observationNumber'	(observation number per individual, for a given observation type)

Usage

```
createAdditionalCovariate(transformation, base = "", name = "")
```

Arguments

transformation *(string)* applied transformation.
 base *(string)* [optional] base data on which the transformation is applied.
 name *(string)* [optional] name of the covariate.

See Also

[deleteAdditionalCovariate](#)

Examples

```
## Not run:
createAdditionalCovariate("firstDoseAmount")\cr
createAdditionalCovariate(transformation = "observationNumberPerIndividual", headerName = "CONC")

## End(Not run)
```

createFilter *[Monolix - PKanalix] Create filter*

Description

Create a new filtered data set by applying a filter on an existing one and/or complementing it.

Usage

```
createFilter(filter, name = "", origin = "")
```

Arguments

filter	(<i>list</i> < <i>list</i> < <i>action</i> = " <i>headerName-comparator-value</i> " > > or "complement") [optional] filter definition./ Existing actions are "selectLines", "selectIds", "removeLines" and "removeIds". First vector level is for set unions, the second one for set intersection. It is possible to give only a list of actions if there is only no high-level union.
name	(<i>string</i>) [optional] created data set name. If not defined, the default name is "currentDataSet_filtered".
origin	(<i>string</i>) [optional] name of the data set to be filtered. The current one is used by default.

Details

The possible actions are line selection (selectLines), line removal (removeLines), Ids selection (selectIds) or removal (removeIds).

The selection is a string containing the header name, a comparison operator and a value
selection = <string> "headerName*-comparator**-value" (ex: "id=='100'", "WEIGHT<70", "SEX!='M'")

Notice that :

- The headerName corresponds to the data set header or one of the header aliases defined in MONOLIX software preferences
- The comparator possibilities are "==" , "!=" for all types of value and "<=", "<", ">=", ">" only for numerical types

Syntax:

* create a simple filter:

```
createFilter( filter = list(act = sel)), e.g. createFilter( filter = list(removeIds = "WEIGHT<50"))
```

=> create a filter with the action act on the selection sel. In this example, we create a filter that removes all subjects with a weight less than 50.

* create a filter with several concurrent conditions, i.e AND condition:

```
createFilter( list(act1 = sel1, act2 = sel2)), e.g. createFilter( filter = list(removeIds = "WEIGHT<50",
removeIds = " AGE<20"))
```

=> create a filter with both the action act1 on sel1 AND the action act2 on sel2. In this example, we create a filter that removes all subjects with a weight less than 50 and an age less than 20. It corresponds to the intersection of the subjects with a weight less than 50 and the subjects with an age less than 20.

* create a filter with several non-concurrent conditions, i.e OR condition:

```
createFilter(filter = list(list(act1 = sel1), list(act2 = sel2)) ), e.g. createFilter( filter = list(list(removeIds
= "WEIGHT<50"),list(removeIds = " AGE<20")))
```

=> create a filter with the action act1 on sel1 OR the action act2 on sel2. In this example, we create a filter that removes all subjects with a weight less than 50 and an age less than 20.

It corresponds to the union of the subjects with a weight less than 50 and the subjects with an age less than 20.

* It is possible to have any combinaison:

```
createFilter(filter = list(list(act1 = sel1), list(act2 = sel2, act3 = sel3)) ) <=> act1,sel1 OR ( act2,sel2
AND act3,sel3 )
```

* It is possible to create the complement of an existing filter:

```
createFilter(filter = "complement")
```

See Also

[applyFilter](#)

Examples

```
## Not run:
```

```
-----
LINE [ int ]
createFilter( filter = list(removeLines = "line>10") ) # keep only the 10th first rows
-----
```

```
ID [ string | int ]
```

If there are only integer identifiers within the data set, ids will be considered as integers. On the contrary, t

```
createFilter( filter = list(selectIds = "id==100") ) # select the subject called '100'
```

```
createFilter( filter = list(list(removeIds = "id!='id_2'")) ) # select all the subjects excepted the one called
```

```
-----
ID INDEX [int]
```

```
createFilter( filter = list(list(removeIds = "idIndex!=2"), list(selectIds = "id<5")) ) # select the 4 first sub
```

```
-----
OCC [ int ]
```

```
createFilter( filter = list(selectIds = "occ1==1", removeIds = "occ2!=3") ) # select the subjects whose first oc
```

```
-----
TIME [ double ]
```

```
createFilter( filter = list(removeIds='TIME>120') ) # remove the subjects who have time over 120
```

```
createFilter( filter = list(selectLines='TIME>120') ) # remove the all the lines where the time is over 120
```

```
-----
OBSERVATION [ double ]
```

```
createFilter( filter = list(selectLines = "CONC>=5.5", removeLines = "CONC>10")) # select the lines where CONC v
```

```
createFilter( filter = list(removeIds = "CONC<0") ) # remove subjects who have negative CONC values
```

```
createFilter( filter = list(removeIds = "E==0") ) # remove subjects for who E equals 0
```

```
-----
```

```

OBSID [ string ]
createFilter( filter = list(removeIds = "y1==1") ) # remove subject who have at least one observation for y1
createFilter( filter = list(selectLines = "y1!=2") ) # select all lines corresponding to observations expected
-----
AMOUNT [ double ]
createFilter( filter = list(selectIds = "AMOUT==10") ) # select subjects who have a dose equals to 10
-----
INFUSION RATE AND INFUSION DURATION [ double ]
createFilter( filter = list(selectIds = "RATE<10") ) # select subjects who have dose with a rate less than 10
-----
COVARIATE [ string (categorical) | double (continuous) ]
createFilter( filter = list(selectIds = "SEX==M", selectIds = "WEIGHT<80") ) # select subjects who are men and w
-----
REGERSOR [ double ]
createFilter( filter = list(selectLines = "REG>10") ) # select the lines where the regressor value is over 10
-----
COMPLEMENT
createFilter(origin = "data_filtered", filter = "complement" )

## End(Not run)

```

```
defineCovariateElement
```

[Simulx] Define covariate element

Description

Define a new covariate element. It can be defined as an external file or as a data.frame. If defined by a data.frame, it can contain only one row.

Usage

```
defineCovariateElement(name, element)
```

Arguments

name	(<i>string</i>) Element name.
element	(<i>string</i> or <i>dataFrame</i>) Element definition from external file path or data frame with covariates as columns.

See Also

[getCovariateElements](#)

Examples

```

## Not run:
defineCovariateElement(name = "name", element = "file/path")
defineCovariateElement(name = "name", element = data.frame(WEIGHT = 70.5, SEX = "M"))

## End(Not run)

```

defineIndividualElement
[Simulx] Define individual element

Description

Define a new individual element. It can be defined as an external file or as a data.frame.

Usage

```
defineIndividualElement(name, element)
```

Arguments

name	(<i>string</i>) Element name.
element	(<i>string</i> or <i>dataFrame</i>) Element definition from external file path or data frame with individual parameters as columns.

See Also

[getIndividualElements](#)

Examples

```
## Not run:  
defineIndividualElement(name = "name", element = "file/path")  
defineIndividualElement(name = "name", element = data.frame(C1 = 1, V = 2.5))  
defineIndividualElement(name = "name", element = data.frame(C1 = c(1, 2), V = c(2.5, 5))  
  
## End(Not run)
```

defineOccasionElement *[Simulx] Define occasion element*

Description

Define a new occasion element. It can be defined as an external file or as a data.frame.

Usage

```
defineOccasionElement(element)
```

Arguments

element	(<i>string</i> or <i>dataFrame</i>) Element definition from external file path or data frame with time and occasion levels as columns.
---------	--

See Also

[getOccasionElements](#)

Examples

```
## Not run:
  defineOccasionElement(element = "file/path")
  defineOccasionElement(element = data.frame(time = c(0, 0.5, 2), occ1 = c(1, 1, 2), occ2 = c(1, 2, 3)))

## End(Not run)
```

defineOutputElement *[Simulx] Define output element*

Description

Define a new output element. It can be defined as an external file or as a data.frame.

Usage

```
defineOutputElement(name, element)
```

Arguments

name *(string)* Element name.
 element *(string or dataFrame)* Element definition from external file path or data frame.

See Also

[getOutputElements](#)

Examples

```
## Not run:
  defineOutputElement(name = "name", element = list(data = "file/path", output = "output"))
  defineOutputElement(name = "name", element = list(data = data.frame(time = c(1.25, 2, 5.5)), output = "output"))
  defineOutputElement(name = "name", element = list(data = data.frame(time = c(0, 2, 3, 4, 5), occ1 = c(1, 1, 1, 2, 3)), output = "output"))
  defineOutputElement(name = "name", element = list(data = data.frame(start = 1, interval = 10, final = 100), output = "output"))
  defineOutputElement(name = "name", element = list(data = data.frame(start = c(1, 1, 1, 1), interval = c(10, 5, 10, 5)), output = "output"))

## End(Not run)
```

definePopulationElement

[Simulx] Define population element

Description

Define a new population element. It can be defined as an external file or as a data.frame.

Usage

```
definePopulationElement(name, element)
```

Arguments

name (string) Element name.
 element (string or dataFrame) Element definition from external file path or data frame with population parameters as columns.

See Also

[getPopulationElements](#)

Examples

```
## Not run:
definePopulationElement(name = "name", element = "file/path")
definePopulationElement(name = "name", element = data.frame(CI_pop = 1, V_pop = 2.5))
definePopulationElement(name = "name", element = data.frame(CI_pop = c(1, 3), V_pop = c(2.5, 6)))

## End(Not run)
```

defineRegressorElement

[Simulx] Define regressor element

Description

Define a new regression element. It can be defined as an external file or as a data.frame.

Usage

```
defineRegressorElement(name, element)
```

Arguments

name (string) Element name.
 element (string or dataFrame) Element definition from external file path or data frame with time and regressors as columns.

See Also

[getRegressorElements](#)

Examples

```
## Not run:
defineRegressorElement(name = "name", element = "file/path")
defineRegressorElement(name = "name", element = data.frame(time = c(0, 0.5, 2), reg1 = c(1, 2, 5.25), reg2 = c(1, 2, 5.25)))
defineRegressorElement(name = "name", element = data.frame(time = c(0, 0.5, 2, 5, 6), reg1 = c(1, 2, 5.25, 6, 7)))

## End(Not run)
```


See Also[createAdditionalCovariate](#)**Examples**

```
## Not run:
deleteAdditionalCovariate("firstDoseAmount")\cr
deleteAdditionalCovariate("observationNumberPerIndividual_y1")

## End(Not run)
```

deleteElement	<i>[Simulx] Delete element</i>
---------------	--------------------------------

Description

Delete an element of any type.

Usage

```
deleteElement(name)
```

Arguments

name (*string*) Element name.

Examples

```
## Not run:
deleteElement(name = "name")

## End(Not run)
```

deleteFilter	<i>[Monolix - PKanalix] Delete filter</i>
--------------	---

Description

Delete a data set. Only filtered data set which are not active and whose children are not active either can be deleted.

Usage

```
deleteFilter(name)
```

Arguments

name (*string*) data set name.

See Also[createFilter](#)**Examples**

```
## Not run:
deleteFilter(name = "filter2")

## End(Not run)
```

deleteOccasionElement *[Simulx] Delete occasion element*

Description

Delete the occasion element.

Usage

```
deleteOccasionElement()
```

Examples

```
## Not run:
deleteOccasionElement()

## End(Not run)
```

editFilter *[Monolix - PKanalix] Edit filter*

Description

Edit the definition of an existing filtered data set. Refere to [createFilter](#) for more details about syntax, allowed parameters and examples.

Notice that all the filtered data set which depend on the edited one will be deleted.

Usage

```
editFilter(filter, name = "")
```

Arguments

filter *(list< list< action = "headerName-comparator-value" > >)* filter definition.
name *(string)* [optional] data set name to edit (current one by default)

See Also[createFilter](#)

exportData	<i>[Monolix - PKanalix] Export current data set</i>
------------	---

Description

Export the current data set into a text file.

Usage

```
exportData(dataFile, interpreted = FALSE)
```

Arguments

dataFile (*string*) Path where to export the data file.
interpreted (*boolean*) Should interpreted data be exported. False by default.

Examples

```
## Not run:  
exportData("/path/to/current/data.txt")  
  
## End(Not run)
```

fillInitialParametersByAutoInit	<i>[PKanalix] Automatically estimate initial parameters values.</i>
---------------------------------	---

Description

Run automatic calculation of optimized parameters for CA initial parameters.

Usage

```
fillInitialParametersByAutoInit(parameters)
```

Arguments

parameters (*double*) Initial values to optimized in the same format as initialvalues returned by getCASettings

Examples

```
## Not run:  
getCASettings() -> parameters  
fillInitialParametersByAutoInit(parameters$initialvalues) -> optimizedParameters  
  
## End(Not run)
```

getAddLines	<i>[Simulx] Get lines added to the model</i>
-------------	--

Description

Get the lines that were added to a model.

Usage

```
getAddLines()
```

See Also

[setAddLines](#)

Examples

```
## Not run:  
getAddLines()  
=> "ddt_AUC = Cc"  
  
## End(Not run)
```

getAvailableData	<i>[Monolix - PKanalix] Get data sets descriptions</i>
------------------	--

Description

Get information about the data sets and filters defined in the project.

Usage

```
getAvailableData()
```

Examples

```
## Not run:  
getAvailableData()  
  
## End(Not run)
```

```
getCAIndividualParameters
      [PKanalix] Get CA individual parameters
```

Description

Get the estimated values for each subject of some of the individual CA parameters of the current project.

Usage

```
getCAIndividualParameters(...)
```

Arguments

... (string) Name of the individual parameters whose values must be displayed.

Value

A data frame giving the estimated values of the individual parameters of interest for each subject, and a list of their associated statistics.

Examples

```
## Not run:
indivParams = getCAIndividualParameters() # retrieve all the available individual parameters values.
indivParams = getCAIndividualParameters("ka", "V") # retrieve ka and V values for all individuals.

$parameters->
  id ka  V
  1  0.8 1.2
  .  ...  ...
  N  0.4 2.2

## End(Not run)
```

```
getCASettings      [PKanalix] Get the settings associated to the compartmental analysis
```

Description

Get the settings associated to the compartmental analysis. Associated settings are:

"weightingCA"	(string)	Type of weighting ob
"pool"	(logical)	Fit with individual pa
"initialValues" (list)	list(param = value, ...): value = initial value of individual parameter param.	

"blqMethod" (string)

Method by which the

Usage

```
getCASettings(...)
```

Arguments

... [optional] (string) Name of the settings whose value should be displayed. If no argument is provided, all the settings are returned.

Value

An array which associates each setting name to its current value.

See Also

[setCASettings](#)

Examples

```
## Not run:
getCASettings() # retrieve a list of all the CA methodology settings
getCASettings("weightingca","blqmethod") # retrieve a list containing only the value of the settings whose name
## End(Not run)
```

```
getConditionalDistributionSamplingSettings
```

[Monolix] Get conditional distribution sampling settings

Description

Get the conditional distribution sampling settings. Associated settings are:

"ratio"	(0 < double < 1)	Width of the confidence interval.
"enableMaxIterations"	(bool)	Enable maximum of iterations.
"nbMinIterations"	(int >= 1)	Minimum number of iterations.
"nbMaxIterations"	(int >= 1)	Maximum number of iterations.
"nbSimulatedParameters"	(int >= 1)	Number of replicates.

Usage

```
getConditionalDistributionSamplingSettings(...)
```

Arguments

... [optional] (string) Name of the settings whose value should be displayed. If no argument is provided, all the settings are returned.

Value

An array which associates each setting name to its current value.

See Also

[setConditionalDistributionSamplingSettings](#)

Examples

```
## Not run:
getConditionalDistributionSamplingSettings()
# retrieve all the conditional distribution sampling settings
getConditionalDistributionSamplingSettings("ratio","nbMinIterations")
# retrieve only the ratio and nbMinIterations settings values

## End(Not run)
```

getConditionalModeEstimationSettings

[Monolix] Get conditional mode estimation settings

Description

Get the conditional mode estimation settings. Associated settings are:

"nbOptimizationIterationsMode"	(<i>int</i> ≥ 1)	Maximum number of iterations.
"optimizationToleranceMode"	(<i>double</i> > 0)	Optimization tolerance.

Usage

```
getConditionalModeEstimationSettings(...)
```

Arguments

... [optional] (string) Name of the settings whose value should be displayed. If no argument is provided, all the settings are returned.

Value

An array which associates each setting name to its current value.

See Also

[setConditionalModeEstimationSettings](#)

Examples

```
## Not run:
getConditionalModeEstimationSettings()
# retrieve a list of all the conditional mode estimation settings
getConditionalModeEstimationSettings("nbOptimizationIterationsMode")
# retrieve only the nbOptimizationIterationsMode setting value

## End(Not run)
```

```
getContinuousObservationModel
```

```
[Monolix] Get continuous observation models information
```

Description

Get a summary of the information concerning the continuous observation models in the project. The following informations are provided.

- prediction: (*vector<string>*) name of the associated prediction
- formula: (*vector<string>*) formula applied on the observation
- distribution: (*vector<string>*) distribution of the observation in the Gaussian space. The distribution type can be "normal", "logNormal", or "logitNormal".
- limits: (*vector< pair<double,double> >*) lower and upper limits imposed to the observation. Used only if the distribution is logitNormal. If there is no logitNormal distribution, this field is empty.
- errormodel: (*vector<string>*) type of the associated error model
- autocorrelation: (*vector<bool>*) defines if there is auto correlation

Call [getObservationInformation](#) to get a list of the continuous observations present in the current project.

Usage

```
getContinuousObservationModel()
```

Value

A list associating each continuous observation to its model properties.

See Also

[getObservationInformation](#) [setObservationDistribution](#) [setObservationLimits](#) [setErrorModel](#)
[setAutocorrelation](#)

Examples

```
## Not run:
obsModels = getContinuousObservationModel()
obsModels
-> $prediction
  c(Conc = "Cc")
  $formula
  c(Conc = "Conc = Cc + (a+b*Cc)*e")
  $distribution
  c(Conc = "logitNormal")
  $limits
  list(Conc = c(0,11.5))
  $errormodel
  c(Conc = "combined1")
  $autocorrelation
  c(Conc = TRUE)

## End(Not run)
```

```
getCorrelationOfEstimates
```

[Monolix] Get the inverse of the Fisher Matrix

Description

Get the inverse of the last estimated Fisher matrix computed either by all the Fisher methods used during the last scenario run or by the specific one passed in argument.

WARNING: The Fisher matrix cannot be accessible until the Fisher algorithm has been launched once.

The user can choose to display only the Fisher matrix estimated with a specific method.

Existing Fisher methods :

Fisher by Linearization	"linearization"
Fisher by Stochastic Approximation	"stochasticApproximation"

WARNING: Only the methods which have been used during the last scenario run can provide results.

Usage

```
getCorrelationOfEstimates(method = "")
```

Arguments

method	[optional](string) Fisher method whose results should be displayed. If this field is not specified, the results provided by all the methods used during the last scenario run are displayed.
--------	--

Value

A list whose each field contains the Fisher matrix computed by one of the available Fisher methods used during the ast scenario run. A matrix is defined as a structure containing the following fields :

rownames	list of row names
columnnames	list of column names
rownumber	number of rows
data	vector<...> containing matrix raw values (column major)

Examples

```
## Not run:
getCorrelationOfEstimates("linearization")
-> list( linearization = list(data = c(1,0,0,0,1,-0.06,0,-0.06,1),
                               rownumber = 3,
                               rownames = c("Cl_pop","omega_Cl","a"),
                               columnnames = c("Cl_pop","omega_Cl","a")))

getCorrelationOfEstimates()
-> list(linearization = list(...), stochasticApproximation = list(...))

## End(Not run)
```

getCovariateElements [Simulx] Get covariate elements

Description

Get the list of all available covariate elements for the exploration and simulation.
Each element is a list of

"inputType"	(string)	Type of input definition: can be "manual", "distribution" or "external".
"file"	(string)	Path to the file if the inputType is external. NULL else wise.
"data"	(data.frame)	Values of the element.

Notice that:

- if the project was created from a model file, an covariate element Covariates is created with all values equal 1.
- if the project was created using a Monolix project, – an covariate element mlx_Cov is created with the values corresponding of the covariates values of the project.
- an covariate element mlx_CovDist is created with the values corresponding of the esimation of the distribution of the covariates of the project.

Usage

```
getCovariateElements()
```

See Also

[defineCovariateElement](#)

Examples

```
## Not run:
getCovariateElements()
$mlx_Cov
#'$mlx_Cov$inputType
[1] "external"

$mlx_Cov$file
[1] path/to/file

$mlx_Cov$data
  id WEIGHT
1  1   79.6
2  2   72.4
3  3   70.5
4  4   72.7
5  5   54.6
...

$covMan
$covMan$inputType
[1] "manual"

$covMan$file
NULL

$covMan$data
  id WEIGHT
1 common   75

## End(Not run)
```

getCovariateInformation

[Monolix - PKanalix] Get covariates information

Description

Get the name, the type and the values of the covariates present in the project.

Usage

```
getCovariateInformation()
```

Value

A list containing the following fields :

- name (*vector<string>*): covariate names

- type (*vector<string>*): covariate types. Existing types are "continuous", "continuoustransformed", "categorical", "categoricaltransformed"./ In Monolix mode, "latent" covariates are also allowed.
- [Monolix] modalityNumber (*vector<int>*): number of modalities (for latent covariates only)
- covariate : a data frame giving the values of continuous and categorical covariates for each subject. Latent covariate values exist only if they have been estimated, ie if the covariate is used and if the population parameters have been estimated. Call [getEstimatedIndividualParameters](#) to retrieve them.

Examples

```
## Not run:
info = getCovariateInformation() # Monolix mode with latent covariates
info
-> $name
  c("sex", "wt", "lcat")
-> $type
  c(sex = "categorical", wt = "continuous", lcat = "latent")
-> $modalityNumber
  c(lcat = 2)
-> $covariate
  id  sex  wt
  1   M  66.7
  .   .   .
  N   F  59.0

## End(Not run)
```

getData

[Monolix - PKanalix] Get project data

Description

Get a description of the data used in the current project. Available informations are:

- dataFile (*string*): path to the data file
- header (*array<character>*): vector of header names
- headerTypes (*array<character>*): vector of header types
- observationNames (*vector<string>*): vector of observation names
- observationTypes (*vector<string>*): vector of observation types
- nbSSDoses (*int*): number of doses (if there is a SS column)

Usage

```
getData()
```

Value

A list describing project data.

See Also[setData](#)**Examples**

```
## Not run:
data = getData()
data
-> $dataFile
  "/path/to/data/file.txt"
$header
  c("ID", "TIME", "CONC", "SEX", "OCC")
$headerTypes
  c("ID", "TIME", "OBSERVATION", "CATEGORICAL COVARIATE", "IGNORE")
$observationNames
  c("concentration")
$observationTypes
  c(concentration = "continuous")

## End(Not run)
```

getDataSettings	<i>[PKanalix] Get the data settings associated to the non compartmental analysis</i>
-----------------	--

Description

Get the data settings associated to the non compartmental analysis. Associated settings are:

"urinevolume" (*string*) regressor name used as urine volume.

"datatype" (*list*) list("obsId" = *string*("plasma" or "urine")). The type of data associated with each *obsId*: observ

Usage

```
getDataSettings(...)
```

Arguments

... [optional] (*string*) Name of the settings whose value should be displayed. If no argument is provided, all the settings are returned.

Value

An array which associates each setting name to its current value.

See Also[setNCASettings](#)

Examples

```
## Not run:
getDataSettings() # retrieve a list of all the NCA methodology settings
getDataSettings("urinevolume") # retrieve a list containing only the value of the settings whose name has been p

## End(Not run)
```

```
getEstimatedIndividualParameters
```

```
[Monolix] Get last estimated individual parameter values
```

Description

Get the last estimated values for each subject of some of the individual parameters present within the current project.

WARNING: Estimated individual parameters values cannot be accessible until the individual estimation algorithm has been launched once.

NOTE: The user can choose to display only the individual parameter values estimated with a specific method.

Existing individual estimation methods :

Conditional Mean SAEM	"saem"
Conditional Mean	"conditionalMean"
Conditional Mode	"conditionalMode"

WARNING: Only the methods which have been used during the last scenario run can provide estimation results.

Usage

```
getEstimatedIndividualParameters(..., method = "")
```

Arguments

...	(<i>string</i>) Name of the individual parameters whose values must be displayed. Call getIndividualParameterModel to get a list of the individual parameters present within the current project.
method	[optional](<i>string</i>) Individual parameter estimation method whose results should be displayed. If there are latent covariate used in the model, the estimated modality is displayed too. If this field is not specified, the results provided by all the methods used during the last scenario run are displayed.

Value

A data frame giving, for each wanted method, the last estimated values of the individual parameters of interest for each subject with the corresponding standard deviation values.

See Also

[getEstimatedRandomEffects](#)

Examples

```
## Not run:
indivParams = getEstimatedIndividualParameters()
# retrieve the values of all the available individual parameters for all methods
-> $saem
  id  Cl    V    ka
  1  0.28  7.71  0.29
  .  ...  ...  ...
  N  0.1047.62  1.51

indivParams = getEstimatedIndividualParameters("Cl", "V", method = "conditionalMean")
# retrieve the values of the individual parameters "Cl" and "V"
# estimated by the conditional mode method

## End(Not run)
```

```
getEstimatedLogLikelihood
      [Monolix] Get Log-Likelihood values
```

Description

Get the values computed by using a log-likelihood algorithm during the last scenario run, with or without a method-based filter.

WARNING: The log-likelihood values cannot be accessible until the log-likelihood algorithm has been launched once.

The user can choose to display only the log-likelihood values computed with a specific method.

Existing log-likelihood methods :

Log-likelihood by Linearization	"linearization"
Log-likelihood by Important Sampling	"importanceSampling"

WARNING: Only the methods which have been used during the last scenario run can provide results.

Usage

```
getEstimatedLogLikelihood(method = "")
```

Arguments

method	[optional](string) Log-likelihood method whose results should be displayed. If this field is not specified, the results provided by all the methods used during the last scenario run are retrieved.
--------	--

Value

A list associating the name of each method passed in argument to the corresponding log-likelihood values computed by during the last scenario run.

Examples

```
## Not run:
getEstimatedLogLikelihood()
-> list( linearization = [LL = -170.505, AIC = 350.280, BIC = 365.335] ,
        importanceSampling = [...] )

getEstimatedLogLikelihood("linearization")
-> list( linearization = [LL = -170.505, AIC = 350.280, BIC = 365.335] )

## End(Not run)
```

```
getEstimatedPopulationParameters
```

[Monolix] Get last estimated population parameter value

Description

Get the last estimated value of some of the population parameters present within the current project (fixed effects + individual variances + correlations + latent probabilities + error model parameters).
WARNING: Estimated population parameters values cannot be accessible until the SAEM algorithm has been launched once.

Usage

```
getEstimatedPopulationParameters(...)
```

Arguments

... [optional] (*array<string>*) Names of the population parameters whose value must be displayed. Call [getPopulationParameterInformation](#) to get a list of the population parameters present within the current project. If this field is not specified, the function will retrieve the values of all the available population parameters.

Value

A named vector containing the last estimated value of each one of the population parameters passed in argument.

Examples

```
## Not run:
getEstimatedPopulationParameters("V_pop") -> [V_pop = 0.5]
getEstimatedPopulationParameters("V_pop","Cl_pop") -> [V_pop = 0.5, Cl_pop = 0.25]
getEstimatedPopulationParameters() -> [V_pop = 0.5, Cl_pop = 0.25, ka_pop = 0.05]

## End(Not run)
```

```
getEstimatedRandomEffects
```

[Monolix] Get estimated the random effects

Description

Get the random effects for each subject of some of the individual parameters present within the current project.

WARNING: Estimated random effects cannot be accessible until the individual estimation algorithm has been launched once.

The user can choose to display only the random effects estimated with a specific method.

NOTE: The random effects are defined in the gaussian referential, e.g. if ka is lognormally distributed around ka_pop, $\eta_i = \log(ka_i) - \log(ka_pop)$ Existing individual estimation methods :

Conditional Mean SAEM	"saem"
Conditional Mean	"conditionalMean"
Conditional Mode	"conditionalMode"

WARNING: Only the methods which have been used during the last scenario run can provide estimation results. Please call [getLaunchedTasks](#) to get a list of the methods whose results are available.

Usage

```
getEstimatedRandomEffects(..., method = "")
```

Arguments

...	(<i>string</i>) Name of the individual parameters whose random effects must be displayed. Call getIndividualParameterModel to get a list of the individual parameters present within the current project.
method	[optional](<i>string</i>) Individual parameter estimation method whose results should be displayed. If this field is not specified, the results provided by all the methods used during the last scenario run are displayed.

Value

A data frame giving, for each wanted method, the last estimated eta values of the individual parameters of interest for each subject with the corresponding standard deviation values.

See Also

[getEstimatedIndividualParameters](#)

Examples

```
## Not run:
etaParams = getEstimatedRandomEffects()
# retrieve the values of all the available random effects for all methods
# without the associated standard deviations
-> $saem
```

```

id    Cl    V    ka
1    0.28  7.71  0.29
.    ...   ...   ...
N    0.1047.62  1.51

etaParams = getEstimatedRandomEffects("Cl", "V", method = "conditionalMode")
# retrieve the values of the individual parameters "Cl" and "V"
# estimated by the conditional mean from SAEM algorithm

## End(Not run)

```

```
getEstimatedStandardErrors
```

[Monolix] Get standard errors of population parameters

Description

Get the last estimated standard errors of population parameters computed either by all the Fisher methods used during the last scenario run or by the specific one passed in argument.

WARNING: The standard errors cannot be accessible until the Fisher algorithm has been launched once.

Existing Fisher methods :

Fisher by Linearization	"linearization"
Fisher by Stochastic Approximation	"stochasticApproximation"

WARNING: Only the methods which have been used during the last scenario run can provide results.

Usage

```
getEstimatedStandardErrors(method = "")
```

Arguments

method	[optional](<i>string</i>) Fisher method whose results should be displayed. If this field is not specified, the results provided by all the methods used during the last scenario run are retrieved
--------	--

Value

A list associating each retrieved Fisher algorithm method to the standard errors of population parameters computed during its last run.

Examples

```

## Not run:
getEstimatedStandardErrors() -> list( linearization = [...], stochasticApproximation = [...] )
getEstimatedStandardErrors("linearization") -> list( linearization = [...] )

## End(Not run)

```

```
getFixedEffectsByAutoInit
```

[Monolix] Automatically estimate initial parameters value

Description

Compute optimized values for initial population parameters. The values are returned in the same format as the entry, and can be then used to run the method again.

Usage

```
getFixedEffectsByAutoInit(parameters)
```

Arguments

parameters (*data.frame*), in the same format as the one returned by [getPopulationParameterInformation](#).

Examples

```
## Not run:
getPopulationParameterInformation() -> parameters
getFixedEffectsByAutoInit(parameters) -> optimizedParameters

## End(Not run)
```

```
getGeneralSettings
```

[Monolix] Get project general settings

Description

Get a summary of the common settings for Monolix algorithms. Associated settings are:

"autoChains"	(<i>bool</i>)	Automatically adjusted the number of chains to have at least a minimum number of sub
"nbChains"	(<i>int >0</i>)	Number of chains. <i>Used only if "autoChains" is set to FALSE.</i>
"minIndivForChains"	(<i>int >0</i>)	Minimum number of individuals by chain.

Usage

```
getGeneralSettings(...)
```

Arguments

... [optional] (string) Name of the settings whose value should be displayed. If no argument is provided, all the settings are returned.

Value

An array which associates each setting name to its current value.

See Also[setGeneralSettings](#)**Examples**

```
## Not run:
getGeneralSettings() # retrieve a list of all the general settings

getGeneralSettings("nbChains","autoChains")
# retrieve only the nbChains and autoChains settings values.

## End(Not run)
```

getGlobalObsIdToUse	<i>[PKanalix]</i> Get the global observation id used in both the compartmental and non compartmental analysis
---------------------	---

Description

Get the global observation id used in both the compartmental and non compartmental analysis.

Usage

```
getGlobalObsIdToUse()
```

Value

the observation id used in computations.

See Also[setGlobalObsIdToUse](#)**Examples**

```
## Not run:
getGlobalObsIdToUse() #

## End(Not run)
```

getGroupRemaining	<i>[Simulx] Get simulation group remaining</i>
-------------------	--

Description

Get the values of the remaining elements (coming from the observation model) for a group.

Usage

```
getGroupRemaining(group)
```

Arguments

group (*character*) Group name

See Also

[setGroupRemaining](#)

Examples

```
## Not run:  
  getGroupRemaining( group = "arm1" )  
  
## End(Not run)
```

getGroups	<i>[Simulx] Get simulation groups</i>
-----------	---------------------------------------

Description

Get the structure of each simulation group. Each group is defined as a list of all its elements (population parameters, ...).

Usage

```
getGroups()
```

See Also

[addGroup](#)

Examples

```

## Not run:
getGroups()
[[1]]
[[1]]$name
[1] "simulationGroup1"

[[1]]$covariate
[1] "mlx_Cov"

[[1]]$parameter
[[1]]$parameter$type
[1] "population"

[[1]]$parameter$name
[1] "mlx_Pop"

[[1]]$treatment
[1] "mlx_Adml"

[[1]]$output
[1] "mlx_y1"

[[1]]$size
[1] 12

## End(Not run)

```

getIndividualElements [Simulx] Get individual elements

Description

Get the list of all available individual elements for the exploration and simulation.
Each element is a list of

"inputType"	(string)	Type of input definition: can be "manual" or "external".
"file"	(string)	Path to the file if the inputType is external. NULL else wise.
"data"	(data.frame)	Values of the element.

Notice that:

- if the project was created from a model file, an individual element IndivParameters is created with all values equal 1.
- if the project was created using a Monolix project, – an individual element mlx_IndivInit is created with the values corresponding of the initial population parameters if the population parameters were not estimated.
- an individual element mlx_PopIndiv is created with the values corresponding of the estimated population parameters (without the covariate(s) impact(s)) if the population parameters were estimated.
- an individual element mlx_PopIndivCov is created with the values corresponding of the estimated population parameters (with the covariate(s) impact(s)) if the population parameters were estimated.

- an individual element `mlx_EBEs` is created with the values corresponding of the estimated EBEs if the EBEs were estimated.
- an individual element `mlx_CondMean` is created with the values corresponding of the estimated conditional mean if the conditional distribution task was performed.
- an individual element `mlx_CondDistSample` is created with the values corresponding of the first sample of the conditional ditribution if the conditional distribution task was performed.

Usage

```
getIndividualElements()
```

See Also

[defineIndividualElement](#)

Examples

```
## Not run:
getIndividualElements()
$mlx_PopIndiv
$mlx_PopIndiv$inputType
[1] "manual"

$mlx_PopIndiv$file
NULL

$mlx_PopIndiv$data
  id      C1      V1      Q2      V2      Q3      V3
1 common 2.462069 4.557752 0.1151846 4.355022 1.70242 8.229753

$mlx_EBEs
$mlx_EBEs$inputType
[1] "external"

$mlx_EBEs$file
[1] file/to/path

$mlx_EBEs$data
  id      C1      V1      Q2      V2      Q3      V3
1  1 2.870556 5.801418 2.12758339 5.963084 0.6649303 13.069996
2  2 2.899189 4.443222 0.31646327 5.226719 2.3678264  9.182623
...

## End(Not run)
```

```
getIndividualParameterModel
```

[Monolix] Get individual parameter model

Description

Get a summary of the information concerning the individual parameter model. The available informations are:

- name: (*string*) name of the individual parameter
- distribution: (*string*) distribution of the parameter values. The distribution type can be "normal", "logNormal", or "logitNormal".
- formula: (*string*) formula applied on individual parameters distribution
- variability: a list giving, for each variability level, if individual parameters have variability or not
- covariateModel: a list giving, for each individual parameter, if the related covariates are used or not. If no covariate is used, this field is empty.
- correlationBlocks : a list giving, for each variability level, the blocks of the correlation matrix of the random effects. A block is represented by a vector of individual parameter names. If there is no block, this field is empty.

Usage

```
getIndividualParameterModel()
```

Value

A list of individual parameter model properties.

See Also

[setIndividualParameterDistribution](#) [setIndividualParameterVariability](#) [setCovariateModel](#)

Examples

```
## Not run:
indivModel = getIndividualParameterModel()
indivModel
-> $name
  c("ka","V","Cl")
$distribution
  c(ka = "logNormal", V = "normal", Cl = "logNormal")
$formula
  "\\tlog(ka) = log(ka_pop) + eta_ka\\n\\n
  \\tlog(V) = V_pop + eta_V\\n\\n
  \\tlog(Cl) = log(Cl_pop) + eta_Cl\\n\\n"
$variability
  list( id = c(ka = TRUE, V = FALSE, Cl = TRUE) )
$covariateModel
  list( ka = c(age = TRUE, sex = FALSE, wt = TRUE),
        V = c(age = FALSE, sex = FALSE, wt = FALSE),
        Cl = c(age = FALSE, sex = FALSE, wt = FALSE) )
$correlationBlocks
  list( id = c("ka","V","Tlag") )

## End(Not run)
```

getLastRunStatus *[Monolix - PKanalix] Get last run status*

Description

Return an execution report about the last run with a summary of the error which could have occurred.

Usage

```
getLastRunStatus()
```

Value

A structure containing

1. a boolean which equals TRUE if the last run has successfully completed,
2. a summary of the errors which could have occurred.

Examples

```
## Not run:  
lastRunInfo = getLastRunStatus()  
lastRunInfo$status  
-> TRUE  
lastRunInfo$report  
-> ""  
  
## End(Not run)
```

getLaunchedTasks *[Monolix] Get tasks with results*

Description

Get a list of the tasks which have results to provide. A task is the association of:

- an algorithm (string)
- a vector of methods (string) relative to this algorithm for the standardErrorEstimation and the loglikelihoodEstimation, TRUE or FALSE for the other one.

Usage

```
getLaunchedTasks()
```

Value

The list of tasks with results, indexed by algorithm names.

Examples

```
## Not run:
tasks = getLaunchedTasks()
tasks
-> $populationParameterEstimation = TRUE
   $conditionalModeEstimation = TRUE
   $standardErrorEstimation = "linearization"

## End(Not run)
```

```
getLixoftConnectorsState
```

Get lixoftConnectors API current state

Description

Retrieve information about the Lixoft software the lixoftConnectors are currently interfacing with.

Usage

```
getLixoftConnectorsState(quietly = FALSE)
```

Arguments

`quietly` *boolean* If TRUE, no warning is raised when lixoftConnectors package is not initialized. Equals FALSE by default.

Value

A structure containing:

- `path`: path to Lixoft installation directory
- `software`: software name
- `version`: Lixoft softwares suite version

```
getLixoftEnvInfo
```

Get information about LixoftEnvironment object

Description

Get information about LixoftEnvironment object

Usage

```
getLixoftEnvInfo()
```

```
getLogLikelihoodEstimationSettings
      [Monolix] Get LogLikelihood algorithm settings
```

Description

Get the loglikelihood estimation settings. Associated settings are:

"nbFixedIterations"	(<i>int</i> >0)	Monte Carlo size for the loglikelihood evaluation.
"samplingMethod"	(<i>string</i>)	Should the loglikelihood estimation use a given number of freedom d
"nbFreedomDegrees"	(<i>int</i> >0)	Degree of freedom of the Student t-distribution. <i>Used only if "samplin</i>
"freedomDegreesSampling"	(<i>vector</i> < <i>int</i> (>0)>)	Sequence of freedom degrees to be tested. <i>Used only if "samplingMet</i>

Usage

```
getLogLikelihoodEstimationSettings(...)
```

Arguments

... [optional] (*string*) Name of the settings whose value should be displayed. If no argument is provided, all the settings are returned.

Value

An array which associates each setting name to its current value.

See Also

[setLogLikelihoodEstimationSettings](#)

Examples

```
## Not run:
getLogLikelihoodEstimationSettings() # retrieve a list of all the loglikelihood estimation settings
getLogLikelihoodEstimationSettings("nbFixedIterations","samplingMethod")
# retrieve only nbFixedIterations and samplingMethod settings values

## End(Not run)
```

```
getMCMCSettings      [Monolix] Get MCMC algorithm settings
```

Description

Get the MCMC algorithm settings of the current project. Associated settings are:

"strategy"	(<i>vector</i> < <i>int</i> >[3])	Number of calls for each one of the three MCMC kernels.
"acceptanceRatio"	(<i>double</i>)	Target acceptance ratio.

Usage

```
getMCMCSettings(...)
```

Arguments

```
... [optional] (string) Names of the settings whose value should be displayed. If no
argument is provided, all the settings are returned.
```

Value

An array which associates each setting name to its current value.

See Also

[setMCMCSettings](#)

Examples

```
## Not run:
getMCMCSettings() # retrieve a list of all the MCMC settings
getMCMCSettings("strategy") # retrieve only the strategy setting

## End(Not run)
```

```
getModelBuildingResults
```

[Monolix] Get the results of the model building

Description

Get the results (detailed models) of the model building.

Usage

```
getModelBuildingResults()
```

Value

The results of model building All the detailed tried models are returned

- LL: result of $-2 \times \text{Log-Likelihood}$
- BICc: modified BIC.
- individualModels: (*data.frame*) individual model for each individual parameter. The columns are the covariates and the elements of the data.frame notes if a covariate is used or not for the current parameter.

COSSAC send 2 additional fields:

- tested: (*vector<string>*) first element is the individual parameter and the second one is the covariate. This combination notes if the covariate is tested or not with respect to the previous model.

- `bestModel` (*boolean*) best model amongst all the tried models according to the chosen criterion.

SAMBA send the error model and covariance model information if there are exist

- `errorModels`: chosen type for each error model
- `covarianceModels`: chosen correlations between individual parameters

See Also

[runModelBuilding](#)

Examples

```
## Not run:
getModelBuildingResults()

## End(Not run)
```

```
getModelBuildingSettings
```

[Monolix] Get model building settings

Description

Get the settings that will be used during the run of model building.

Usage

```
getModelBuildingSettings()
```

Value

The list of settings

- `covariates`: (*list<string>*) covariate names
- `parameters`: (*list<string>*) parameters names
- `strategy`: (*string*) strategy to search best model ([`COSSAC`], `samba`, `scm`)
- `criterion`: (*string*) criterion to search best model ([`BIC`], `LRT`)
- `relationships`: (*data.frame<parameters, covariates, locked>*) Use to lock relationships between parameters and covariates. By default, all the combinations are possible. This parameter forces the use or not of some combinations. See example where *ka* must have *SEX* and *V* must not have *WEIGHT*
- `threshold$lrt`: threshold used by criterion `LRT` to continue or not to improve the model (first element is for forward and the second one is for the backward method)
- `threshold$correlation`: threshold used by `COSSAC` to choose what combinations (parameter-covariate) must be tried as next candidate model (first element is for forward and the second one is for the backward method)
- `useLin`: (*boolean*) computes linearization ([`TRUE`]) or the Importance Sampling (`FALSE`)
- `useSAMBABeforeCossac`: (*boolean*) gives the possibility to launch one `SAMBA` iteration before the `COSSAC` strategy (`TRUE`, [`FALSE`])

See Also[runModelBuilding](#)**Examples**

```
## Not run:
set = getModelBuildingSettings()
set$relationships[1,] = c("ka", "SEX", TRUE)
set$relationships[2,] = c("V", "WEIGHT", FALSE)

-> set$relationships
  parameters covariates locked
1         ka         SEX  TRUE
2          V        WEIGHT FALSE

runModelBuilding(settings = set)

## End(Not run)
```

`getNbReplicates`*[Simulx] Get number of replicates*

Description

Get the number of replicates.

Usage

```
getNbReplicates()
```

See Also[setNbReplicates](#)**Examples**

```
## Not run:
getNbReplicates()

## End(Not run)
```

```
getNCAIndividualParameters  
    [PKanalix] Get NCA individual parameters
```

Description

Get the estimated values for each subject of some of the individual NCA parameters of the current project.

Usage

```
getNCAIndividualParameters(...)
```

Arguments

```
...          (string) Name of the individual parameters whose values must be displayed.
```

Value

A data frame giving the estimated values of the individual parameters of interest for each subject, and a list of their associated statistics.

Examples

```
## Not run:  
indivParams = getNCAIndividualParameters()  
# retrieve the values of all the available parameters.  
  
indivParams = getNCAIndividualParameters("Tmax","Clast")  
# retrieve only the values of Tmax and Clast for all individuals.  
  
$parameters->  
  id Tmax Clast  
  1  0.8  1.2  
  .  ...  ...  
  N  0.4  2.2  
  
## End(Not run)
```

```
getNCASettings          [PKanalix] Get the settings associated to the non compartmental analysis
```

Description

Get the settings associated to the non compartmental analysis. Associated settings are:

"administrationType"	(<i>list</i>)	list(key = "admId", value = <i>string</i> ("intravenous" or "extravascular")). <i>admId</i>
"integralMethod"	(<i>string</i>)	Method for AUC and AUMC calculation and interpolation.
"partialAucTime"	(<i>list</i>)	The first element of the list is a boolean describing if this setting is used. The
"blqMethodBeforeTmax"	(<i>string</i>)	Method by which the BLQ data before Tmax should be replaced.
"blqMethodAfterTmax"	(<i>string</i>)	Method by which the BLQ data after Tmax should be replaced.
"ajdr2AcceptanceCriteria"	(<i>list</i>)	The first element of the list is a boolean describing if this setting is used. Th
"extrapAucAcceptanceCriteria"	(<i>list</i>)	The first element of the list is a boolean describing if this setting is used. Th
"spanAcceptanceCriteria"	(<i>list</i>)	The first element of the list is a boolean describing if this setting is used. Th
"lambdaRule"	(<i>string</i>)	Main rule for the lambda_Z estimation.
"timeInterval"	(<i>vector</i>)	Time interval for the lambda_Z estimation when " <i>lambdaRule</i> " = "interval"
"timeValuesPerId"	(<i>list</i>)	list("idName" = idTimes,...): <i>idTimes</i> Observation times to use for the calcul
"nbPoints"	(<i>integer</i>)	Number of points for the lambda_Z estimation when " <i>lambdaRule</i> " = "point
"maxNbOfPoints"	(<i>list</i>)	The first element of the list is a boolean describing if this setting is used. Th
"startTimeNotBefore"	(<i>list</i>)	The first element of the list is a boolean describing if this setting is used. Th
"weightingNCA"	(<i>string</i>)	Weighting method used for the regression that estimates lambda_Z.
"computedNCAParameters"	(<i>vector</i>)	All the parameters to compute during the analysis."

Usage

```
getNCASettings(...)
```

Arguments

... [optional] (*string*) Name of the settings whose value should be displayed. If no argument is provided, all the settings are returned.

Value

An array which associates each setting name to its current value.

See Also

[setNCASettings](#)

Examples

```
## Not run:
getNCASettings() # retrieve a list of all the NCA methodology settings
getNCASettings("lambdaRule","integralMethod") # retrieve a list containing only the value of the settings whose

## End(Not run)
```

```
getObservationInformation
      [Monolix - PKanalix] Get observations information
```

Description

Get the name, the type and the values of the observations present in the project.

Usage

```
getObservationInformation()
```

Value

A list containing the name of the observations and their values (id, time and observationName (and occasion if present in the data set)).

In Monolix mode, the observation type and the mapping with data set names is also retrieved.

In PKanalix mode, the observation type and the mapping are not provided as there is only one used output and this one is necessarily continuous..

Examples

```
## Not run:
info = getObservationInformation()
info
-> $name
  c("concentration")
-> $type # [Monolix]
  c(concentration = "continuous")
-> $mapping # [Monolix]
  c(concentration = "CONC")
-> $concentration
  id  time concentration
  1   0.5      0.0
  .   .       .
  N   9.0     10.8

## End(Not run)
```

getOccasionElements *[Simulx] Get occasion elements*

Description

Get the list of the occasion element for the simulation. It is a list of

"id"	(string)	Ids of the occasions
"names"	(string)	Name of the occasions.
"times"	(data.frame)	Times of the occasions.
"occasions"	(data.frame)	Values of the element.

Usage

```
getOccasionElements()
```

See Also

[defineOccasionElement](#)

getOutputElements *[Simulx] Get output elements*

Description

Get the list of all available output elements for the exploration and simulation.
Each element is a list of

"output"	(string)	Output name.
"inputType"	(string)	Type of input definition: can be "manual" or "external".
"file"	(string)	Path to the file if the inputType is external. NULL else wise.
"data"	(data.frame)	Values of the element.

Importantly, all the variables in the model file can be used as an output. The user is not constrained to the ones defined in the OUTPUT: section. Notice that:

- if the project was created from a model file, an output element is created for each output of the section OUTPUT: with regular grid from 0 to 100 by 1.
- if the project was created using a Monolix project, with for exemple CC as a prediction and y as measurement – an individual element mlx_y1 is created as an external file with the values corresponding of the output values for each id of the project.
- an individual element mlx_Cc is created with a regular grid starting from the first time measurement of the project to the final time measurement of the project.

Usage

```
getOutputElements()
```

See Also[defineOutputElement](#)**Examples**

```
## Not run:
$output
[1] "y1"

$inputType
[1] "manual"

$file
NULL

$data
      id time
1  common  0
2  common  1
3  common  2
...

## End(Not run)
```

getPopulationElements *[Simulx] Get population elements*

Description

Get the list of all available population elements for the simulation.
Each element is a list of

"inputType"	(<i>string</i>)	Type of input definition: can be "manual" or "external".
"file"	(<i>string</i>)	Path to the file if the inputType is external. NULL else wise.
"data"	(<i>data.frame</i>)	Values of the element.

Notice that:

- if the project was created from a model file, a population element PopParameters is created with all values equal 1.
- if the project was created using a Monolix project, – a population element mlx_Pop is created with the values corresponding of the Monolix estimated population parameters.
- a population element mlx_PopInit is created with the values corresponding of the Monolix initial population parameters if the parameters were not estimated.

Usage

```
getPopulationElements()
```

See Also[definePopulationElement](#)

Examples

```
## Not run:
getPopulationElements()
$mLx_Pop
$mLx_Pop$inputType
[1] "manual"

$mLx_Pop$file
NULL

$mLx_Pop$data
  id C1_pop V1_pop Q2_pop V2_pop Q3_pop V3_pop omega_C1 omega_Q2 omega_Q3 omega_V1 omega_V2 omega
1 common 2.462069 4.557752 0.1151846 4.355022 1.70242 8.229753 0.2272315 0.92641 0.5745623 0.4080015 0.8127517

## End(Not run)
```

```
getPopulationParameterEstimationSettings
```

[Monolix] Get population parameter estimation settings

Description

Get the population parameter estimation settings. Associated settings are:

"nbBurningIterations"	(int >=0)	Number of iterations in the burn-in phase.
"nbExploratoryIterations"	(int >=0)	If "exploratoryAutoStop" is set to FALSE, it is the number of iterations.
"exploratoryAutoStop"	(bool)	Should the exploratory step automatically stop.
"exploratoryInterval"	(int >0)	Minimum number of iteration in the exploratory phase. <i>Used only if "exploratoryAutoStop" is FALSE.</i>
"exploratoryAlpha"	(0<= double <=1)	Convergence memory in the exploratory phase. <i>Used only if "exploratoryAutoStop" is FALSE.</i>
"nbSmoothingIterations"	(int >=0)	If "smoothingAutoStop" is set to FALSE, it is the number of iterations.
"smoothingAutoStop"	(bool)	Should the smoothing step automatically stop.
"smoothingInterval"	(int >0)	Minimum number of iteration in the smoothing phase. <i>Used only if "smoothingAutoStop" is FALSE.</i>
"smoothingAlpha"	(0.5< double <=1)	Convergence memory in the smoothing phase. <i>Used only if "smoothingAutoStop" is FALSE.</i>
"smoothingRatio"	(0< double <1)	Width of the confidence interval. <i>Used only if "smoothingAutoStop" is FALSE.</i>
"simulatedAnnealing"	(bool)	Should annealing be simulated.
"tauOmega"	(double >0)	Proportional rate on variance. <i>Used only if "simulatedAnnealing" is TRUE.</i>
"tauErrorModel"	(double >0)	Proportional rate on error model. <i>Used only if "simulatedAnnealing" is TRUE.</i>
"variability"	(string)	Estimation method for parameters without variability: "firstStage" "common"
"nbOptimizationIterations"	(int >=1)	Number of optimization iterations.
"optimizationTolerance"	(double >0)	Tolerance for optimization.

Usage

```
getPopulationParameterEstimationSettings(...)
```

Arguments

... [optional] (string) Name of the settings whose value should be displayed. If no argument is provided, all the settings are returned.

Value

An array which associates each setting name to its current value.

See Also

[setPopulationParameterEstimationSettings](#)

Examples

```
## Not run:
getPopulationParameterEstimationSettings()
# retrieve a list of all the population parameter estimation settings

getPopulationParameterEstimationSettings("nbBurningIterations", "smoothingInterval")
# retrieve only the nbBurningIterations and smoothingInterval settings values

## End(Not run)
```

getPopulationParameterInformation

[Monolix] Get population parameters information

Description

Get the name, the initial value, the estimation method and, if relevant, MAP parameters value of the population parameters present in the project. It is available for fixed effects, random effects, error model parameters, and latent covariates probabilities.

Usage

```
getPopulationParameterInformation()
```

Value

A data frame giving, for each population parameter, the corresponding :

- `initialValue` : (*double*) initial value
- `method` : (*string*) estimation method
- `priorValue` : (*double*) [MAP] typical value
- `priorSD` : (*double*) [MAP] standard deviation

See Also

[setPopulationParameterInformation](#)

Examples

```
## Not run:
info = getPopulationParameterInformation()
info
  name      initialValue  method  typicalValue  stdDeviation
ka_pop      1.0         MLE      NA             NA
V_pop      10.0         MAP     10.0          0.5
omega_ka    1.0         FIXED   NA             NA

## End(Not run)
```

getPreferences *[Monolix - PKanalix - Simulx] Get project preferences*

Description

Get a summary of the project preferences. Preferences are:

"relativepath"	<i>(bool)</i>	Use relative path for save/load operations.
"threads"	<i>(int >0)</i>	Number of threads.
"timestamping"	<i>(bool)</i>	Create an archive containing result files after each run.
"delimiter"	<i>(string)</i>	Character use as delimiter in exported result files.
"exportchartsData"	<i>(bool)</i>	Should graphics data be exported.
"exportsimulationfiles"	<i>(bool)</i>	[Simulx] Should simulation results files be exported.
"headeraliases"	<i>(list("header" = vector<string>))</i>	For each header, the list of the recognized aliases.
"ncaparameters"	<i>(vector<string>)</i>	[PKanalix] Defaultly computed NCA parameters.

Usage

```
getPreferences(...)
```

Arguments

... [optional] (string) Name of the preference whose value should be displayed. If no argument is provided, all the preferences are returned.

Value

An array which associates each preference name to its current value.

Examples

```
## Not run:
getPreferences() # retrieve a list of all the general settings

getPreferences("imageFormat","exportCharts")
# retrieve only the imageFormat and exportCharts settings values

## End(Not run)
```

getProjectSettings *[Monolix - Pkanalix - Simulx] Get project settings*

Description

Get a summary of the project settings. Associated settings for Monolix projects are:

"directory"	<i>(string)</i>	Path to the folder where simulation results will be saved. It sh
"exportResults"	<i>(bool)</i>	Should results be exported.
"seed"	<i>(0 < int < 2147483647)</i>	Seed used by random generators.
"grid"	<i>(int)</i>	Number of points for the continuous simulation grid.
"nbSimulations"	<i>(int)</i>	Number of simulations.
"dataAndModelNextToProject"	<i>(bool)</i>	Should data and model files be saved next to project.

Associated settings for Pkanalix projects are:

"directory"	<i>(string)</i>	Path to the folder where simulation results will be saved. It should be a writable director
"dataNextToProject"	<i>(bool)</i>	Should data files be saved next to project.

Associated settings for Simulx projects are:

"directory"	<i>(string)</i>	Path to the folder where simulation results will be saved. It should be
"seed"	<i>(0 < int < 2147483647)</i>	Seed used by random generators.
"userfilesnexttoproject"	<i>(bool)</i>	Should user files be saved next to project.

Usage

```
getProjectSettings(...)
```

Arguments

... [optional] (string) Name of the settings whose value should be displayed. If no argument is provided, all the settings are returned.

Value

An array which associates each setting name to its current value.

See Also

[getProjectSettings](#)

Examples

```
## Not run:
getProjectSettings() # retrieve a list of all the project settings

getProjectSettings("directory","seed")
# retrieve only the directopry and the seed settings values

## End(Not run)
```

getRegressorElements *[Simulx] Get regressor elements*

Description

Get the list of all available regressor elements for the exploration and simulation.
Each element is a list of

"inputType"	(<i>string</i>)	Type of input definition: can be "manual" or "external".
"file"	(<i>string</i>)	Path to the file if the inputType is external. NULL else wise.
"data"	(<i>data.frame</i>)	Values of the element.

Usage

```
getRegressorElements()
```

See Also

[defineRegressorElement](#)

Examples

```
## Not run:
$inputType
[1] "manual"

$file
NULL

$data
      id time
1  common  0
2  common  1
3  common  2
...

## End(Not run)
```

getSAEMIterations *[Monolix] Get SAEM algorithm iterations*

Description

Retrieve the successive values of some of the population parameters present within the current project (fixed effects + individual variances + correlations + latent probabilities + error model parameters) during the previous run of the SAEM algorithm.

WARNING: Convergence history of population parameters values cannot be accessible until the SAEM algorithm has been launched once.

Usage

```
getSAEMiterations(...)
```

Arguments

... [optional] (*array<string>*) Names of the population parameters whose convergence history must be displayed. Call [getPopulationParameterInformation](#) to get a list of the population parameters present within the current project. If this field is not specified, the function will retrieve the values of all the available population parameters.

Value

A list containing a pair composed by the number of exploratory and smoothing iterations and a data frame which associates each wanted population parameter to its successive values over SAEM algorithm iterations.

Examples

```
## Not run:
report = getSAEMiterations()
report
-> $iterationNumbers
  c(50,25)
$estimates
  V    C1
0.25  0
  0.3  0.5
  .    .
0.35  0.25

## End(Not run)
```

```
getSameIndividualsAmongGroups
```

[Simulx] Get same individuals among groups

Description

Get the informations if the same individuals are simulated among all groups.

Usage

```
getSameIndividualsAmongGroups()
```

See Also

[setSameIndividualsAmongGroups](#)

Examples

```
## Not run:
  getSameIndividualsAmongGroups()

## End(Not run)
```

getSamplingMethod *[Simulx] Get sampling method*

Description

Define which sampling methods is used for the simulation. The possibilities are to keep the order, sample with replacement and sample without replacement.

Usage

```
getSamplingMethod()
```

See Also

[setSamplingMethod](#)

Examples

```
## Not run:
  getSamplingMethod()

## End(Not run)
```

getScenario *[Monolix] Get current scenario*

Description

Get the list of tasks that will be run at the next call to [runScenario](#), the associated method (linearization true or false), and the associated list of plots. The list of tasks consist of the following tasks: `populationParameterEstimation`, `conditionalDistributionSampling`, `conditionalModeEstimation`, `standardErrorEstimation`, `logLikelihoodEstimation`, and plots.

Usage

```
getScenario()
```

Value

The list of tasks that corresponds to the current scenario, indexed by algorithm names.

See Also

[setScenario](#)

Examples

```
## Not run:
scenario = getScenario()
scenario
-> $tasks
  populationParameterEstimation conditionalDistributionSampling conditionalModeEstimation standardErrorEsti
  TRUE TRUE TRUE FALSE FALSE FALSE
  $linearization = T
  $plotList = "outputplot", "vpc"

## End(Not run)
```

```
getSharedIds [Simulx] Get simulation groups sharedIds
```

Description

Get the elements for the shared group.

Usage

```
getSharedIds()
```

See Also

[setSharedIds](#)

Examples

```
## Not run:
getSharedIds()

## End(Not run)
```

```
getSimulatedIndividualParameters
[Monolix] Get simulated individual parameters
```

Description

Get the simulated values for each replicate of each subject of some of the individual parameters present within the current project.

WARNING: Simulated individual parameters values cannot be accessible until the individual estimation with conditional mean algorithm has been launched once.

Usage

```
getSimulatedIndividualParameters(...)
```

Arguments

... (string) Name of the individual parameters whose values must be displayed. Call [getIndividualParameterModel](#) to get a list of the individual parameters present within the current project.

Value

A list giving the last simulated values of the individual parameters of interest for each replicate of each subject.

See Also

[getSimulatedRandomEffects](#)

Examples

```
## Not run:
simParams = getSimulatedIndividualParameters()
# retrieve the values of all the available individual parameters

simParams
  rep  id  Cl  V  ka
  1   1  0.022 0.37 1.79
  1   2  0.033 0.42 -0.92
  .   .   ...   ...   ...
  2   1  0.021 0.33 1.47
  .   .   ...   ...   ...

## End(Not run)
```

```
getSimulatedRandomEffects
```

[Monolix] Get simulated random effects

Description

Get the simulated values for each replicate of each subject of some of the individual random effects present within the current project.

WARNING: Simulated individual random effects values cannot be accessible until the individual estimation algorithm with conditional mean has been launched once.

Usage

```
getSimulatedRandomEffects(...)
```

Arguments

... (string) Name of the individual parameters whose values must be displayed. Call [getIndividualParameterModel](#) to get a list of the individual parameters present within the current project.

Value

A list giving the last simulated values of the individual random effects of interest for each replicate of each subject.

See Also

[getIndividualParameterModel](#)

Examples

```
## Not run:
simEtas = getSimulatedRandomEffects()
# retrieve the values of all the available individual random effects

simEtas
  rep  id  Cl   V   ka
  ---  ---  ---  ---  ---
1     1   0.022 0.37 1.79
1     2   0.033 0.42 -0.92
.     .   ...   ...   ...
2     1   0.021 0.33 1.47
.     .   ...   ...   ...

## End(Not run)
```

getSimulationResults *[Simulx] Get simulation results*

Description

Get the results of the simulation.

The output is a list of two elements: res and IndividualParameters.

A first element called res is provided. It corresponds to the list of the output(s) of the simulation. There is a data frame for each output with the columns id, time, outputName, and group (corresponding to the group name if there are several groups).

A second element called IndividualParameters is provided. It corresponds to the list of data.frame. Each data.frame of the list corresponds to the individual parameters for each group.

Usage

```
getSimulationResults()
```

See Also

[runSimulation](#)

Examples

```
## Not run:
getSimulationResults()

## End(Not run)
```

```
getStandardErrorEstimationSettings
    [Monolix] Get standard error estimation settings
```

Description

Get the standard error estimation settings. Associated settings are:

```
"minIterations" (int >=1) Minimum number of iterations.
"maxIterations" (int >=1) Maximum number of iterations.
```

Usage

```
getStandardErrorEstimationSettings(...)
```

Arguments

```
... [optional] (string) Name of the settings whose value should be displayed. If no
argument is provided, all the settings are returned.
```

Value

An array which associates each setting name to its current value.

See Also

[setStandardErrorEstimationSettings](#)

Examples

```
## Not run:
getStandardErrorEstimationSettings()
# retrieve a list of all the standard error estimation settings

getStandardErrorEstimationSettings("minIterations","maxIterations")
# retrieve only minIterations and maxIterations settings values

## End(Not run)
```

```
getStructuralModel    [Monolix - PKanalix - Simulx] Get structural model file
```

Description

Get the model file for the structural model used in the current project. For Simulx, this function will return the structural model only if the project was imported from Monolix, and NULL otherwise.

Usage

```
getStructuralModel()
```

Value

A string corresponding to the path to the structural model file.

See Also

[setStructuralModel](#)

Examples

```
## Not run:  
getStructuralModel() => "/path/to/model/inclusion/modelFile.txt"  
  
## End(Not run)
```

getTests

[Monolix] Get statistical tests results

Description

Get the results of performed statistical tests.

Existing tests: Wald, Individual parameters normality, individual parameters marginal distribution, random effects normality, random effects correlation, individual parameters vs covariates correlation, random effects vs covariates correlation, residual normality and residual symmetry.

WARNING: Only the tests performed during the last scenario run can provide results.

Usage

```
getTests()
```

Value

A list associating the name of the test to the corresponding results values computed during the last scenario run.

Examples

```
## Not run:  
getTests()  
-> list( wald = [...] ,  
        individualParametersNormality = [...] ,  
        ... )  
  
## End(Not run)
```

getTreatmentElements *[Simulx] Get treatment elements*

Description

Get the list of all available treatments elements for the exploration and simulation.
Each element is a list of

"inputType"	(<i>string</i>)	Type of input definition: can be "manual" or "external".
"file"	(<i>string</i>)	Path to the file if the inputType is external. NULL else wise.
"data"	(<i>data.frame</i>)	Values of the element.

Notice that:

- if the project was created from a model file, no treatment is added.
- if the project was created using a Monolix project, for each administration type of the project, – an individual element `mlx_adm` is created as an external file with the values corresponding of the treatment values for each id of the project.

Usage

```
getTreatmentElements()
```

See Also

[defineTreatmentElement](#)

Examples

```
## Not run:
$mlx_Adm1
$mlx_Adm1$inputType
[1] "external"

$mlx_Adm1$file
[1] path/to/file

$mlx_Adm1$data
  id time amount washout
1  1   0   320  FALSE
2  2   0   320  FALS
...

## End(Not run)
```

getVariabilityLevels *[Monolix] Get variability levels*

Description

Get a summary of the variability levels (inter-individual and/or intra-individual variability) present in the current project.

Usage

```
getVariabilityLevels()
```

Value

A collection of the variability levels present in the currently loaded project.

Examples

```
## Not run:  
getVariabilityLevels()  
  
## End(Not run)
```

importMonolixProject *[Simulx] Import project from Monolix*

Description

Import all the elements coming from a Monolix project. It imports - the model file, - the population parameters (if estimated, else wise an element is created with all values at 1), - the individual parameters (if estimated, else wise an element is created with all values at 1), - the outputs as an external element, - the treatments (if any) as an external element, - the regressors (if any) as an external element, - the occasion structure (if any) as an external element.

Usage

```
importMonolixProject(projectFile)
```

Arguments

projectFile *(string)* Path to the project file. Can be absolute or relative to the current working directory.

Details

WARNING: R is sensitive between '\` and `/`, only `/` can be used.

Examples

```
## Not run:
importfrommonolix("/path/to/project/file.mlxtran") for Linux platform
importfrommonolix("C:/Users/path/to/project/file.mlxtran") for Windows platform

## End(Not run)
```

```
initializeLixoftConnectors
```

Initialize lixoftConnectors API

Description

Initialize lixoftConnectors API for a given software

Usage

```
initializeLixoftConnectors(software = "monolix", path = "", force = FALSE)
```

Arguments

software	<i>(character)</i> [optional] Name of the software to be loaded. By default, "monolix" software is used.
path	<i>(character)</i> [optional] Path to installation directory of the Lixoft suite. If lixoft-Connectors library is not already loaded and no path is given, the directory written in the lixoft.ini file is used for initialization.
force	<i>(bool)</i> [optional] Should software switch security be overpassed or not. Equals FALSE by default.

Value

A boolean equaling TRUE if the initialization has been successful and FALSE if not.

Examples

```
## Not run:
initializeLixoftConnectors(software = "monolix", path = "/path/to/lixoftRuntime/")

## End(Not run)
```

lixoftDisplay	<i>Display Lixoft API Structures</i>
---------------	--------------------------------------

Description

[Tools][Display]

Display the structures retrieved by the LixoftConnectors library in a user-friendly way.

Usage

```
lixoftDisplay(structure)
```

Arguments

structure *[miscellaneous]* The data structure to be displayed.

Examples

```
## Not run:
settings = getProjectSettings()
lixoftDisplay(settings)

## End(Not run)
```

loadProject	<i>[Monolix - PKanalix - Simulx] Load project from file</i>
-------------	---

Description

Load a project by parsing the Mlxtran-formated file whose path has been given as an input. The extensions are .mlxtran for Monolix, .pkx for PKanalix, and .smlx for Simulx. **WARNING:** R is sensitive between '\ ' and ' / ', only ' / ' can be used.

Usage

```
loadProject(projectFile)
```

Arguments

projectFile *(character)* Path to the project file. Can be absolute or relative to the current working directory.

See Also

[saveProject](#)

Examples

```
## Not run:
loadProject("/path/to/project/file.mlxtran") for Linux platform
loadProject("C:/Users/path/to/project/file.mlxtran") for Windows platform

## End(Not run)
```

newProject

[Monolix - PKanalix - Simulx] Create new project

Description

Create a new empty project providing model and data specification. The data specification is:

- Monolix, PKanalix**
- `dataFile` (*string*): path to the data file
 - `headerTypes` (*array<character>*): vector of headers
 - `observationTypes` [optional] (*list*): a list, indexed by observation name, giving the type of each observation present in the data file. If omitted, all the observations will be considered as "continuous"
 - `nbSSDoses` (*int*): number of steady-state doses (if there is a SS column)
 - `mapping` [optional] (*list*): a list giving the observation name associated to each y-type present in the data file (this field is mandatory when there is a column tagged with the "obsid" headerType)

Please refer to [setData](#) documentation for a comprehensive description of the "data" argument structure.

- Monolix only**
- `projectFile` (*string*): path to the datxplore or pkanalix project file defining the data

Usage

```
newProject(modelFile = NULL, data = NULL)
```

Arguments

- | | |
|------------------------|--|
| <code>modelFile</code> | (<i>character</i>) Path to the model file. Can be absolute or relative to the current working directory. To use a model from the libraries, you can set <code>modelFile = "lib:modelName.txt"</code> , e.g. <code>modelFile = "lib:oral1_1cpt_kaVCl.txt"</code> |
| <code>data</code> | (<i>list</i>) Structure describing the data. In case of PKanalix, data is mandatory and <code>modelFile</code> is optional (used only for the CA part and must be from the library). In case of Monolix, data and <code>modelFile</code> are mandatory. It can be replaced by a <code>projectFile</code> corresponding to a Datxplore or PKanalix project file. In case of Simulx, <code>modelFile</code> is mandatory and <code>data = NULL</code> . It can be replaced by a <code>projectFile</code> corresponding to a Monolix project. In that case, the Monolix project will be imported into Simulx. |

See Also

[newProject](#) [saveProject](#)

Examples

```
## Not run:
newProject(data = list(dataFile = "/path/to/data/file.txt",
                      headerTypes = c("IGNORE", "OBSERVATION"),
                      observationTypes = "continuous"),
           modelFile = "/path/to/model/file.txt")
```

```
newProject(data = list(dataFile = "/path/to/data/file.txt",
                      headerTypes = c("IGNORE", "OBSERVATION", "OBSID"),
                      observationTypes = list(concentration = "continuous", effect = "discrete"),
                      mapping = list("1" = "concentration", "2" = "effect")),
          modelFile = "/path/to/model/file.txt")
```

[Monolix only]

```
newProject(data = list(projectFile = "/path/to/project/file.datxplre"),
          modelFile = "/path/to/model/file.txt")
```

[Simulx only]

```
newProject(modelFile = "/path/to/model/file.txt")
new project from an import of a structural model

newProject(modelFile = "/path/to/monolix/project/file.mlxtran")
new project from an import of a monolix model
```

```
## End(Not run)
```

removeCovariate	<i>[Monolix] Remove covariate</i>
-----------------	-----------------------------------

Description

Remove some of the transformed covariates (discrete and continuous) and/or latent covariates. Call [getCovariateInformation](#) to know which covariates can be removed.

Usage

```
removeCovariate(...)
```

Arguments

... A list of covariate names.

See Also

[getCovariateInformation](#) [addContinuousTransformedCovariate](#) [addCategoricalTransformedCovariate](#)
[addMixture](#)

Examples

```
## Not run:
removeCovariate("tWt", "lcat1")

## End(Not run)
```

removeFilter *[Monolix - PKanalix] Remove filter*

Description

Remove the last filter applied on the current data set.

Usage

```
removeFilter()
```

See Also

[applyFilter](#) [selectData](#)

Examples

```
## Not run:  
removeFilter()  
  
## End(Not run)
```

removeGroup *[Simulx] Remove simulation group*

Description

Remove a simulation group.

Usage

```
removeGroup(group)
```

Arguments

group (*string*) Name of the group to remove.

See Also

[getGroups](#), [addGroup](#)

Examples

```
## Not run:  
removeGroup("group")  
  
## End(Not run)
```

removeGroupElement *[Simulx] Remove element from simulation group*

Description

Remove an element of the simulation.

Usage

```
removeGroupElement(group, element)
```

Arguments

group (*character*) Group name
element (*character*) Element to remove

Examples

```
## Not run:  
removeGroupElement(group = "group", element = "element")  
  
## End(Not run)
```

renameAdditionalCovariate
 [Monolix - PKanalix] Rename additional covariate

Description

Rename an existing additional covariate.

Usage

```
renameAdditionalCovariate(oldName, newName)
```

Arguments

oldName (*string*) current name of the covariate to rename
newName (*string*) new name.

See Also

[createAdditionalCovariate](#)

Examples

```
## Not run:  
renameAdditionalCovariate(oldName = "observationNumberPerIndividual_y1", newName = "nbObsForY1")  
  
## End(Not run)
```

renameData *[Monolix - PKanalix] Rename data set*

Description

Rename a data set. Only filtered data sets can be renamed.

Usage

```
renameData(oldName, newName)
```

Arguments

oldName (string) previous data set name.
newName (string) new data set name.

See Also

[getAvailableData](#)

Examples

```
## Not run:  
renameData(oldName = "data1", newName = "data2")  
  
## End(Not run)
```

renameFilter *[Monolix - PKanalix] Rename filter*

Description

Rename an existing filtered data set.

Usage

```
renameFilter(newName, oldName = "")
```

Arguments

newName (string) new name.
oldName (string) [optional] current name of the data set to rename (current one by default)

See Also

[createFilter](#) [editFilter](#)

Examples

```
## Not run:
renameFilter("newFilter")\cr
renameFilter(oldName = "filter", newName = "newFilter")

## End(Not run)
```

renameGroup	<i>[Simulx] Rename simulation group</i>
-------------	---

Description

Rename a simulation group.

Usage

```
renameGroup(currentGroupName, newGroupName)
```

Arguments

currentGroupName *(string)* Name of the current group name.
newGroupName *(string)* Name of the new group name.

See Also

[getGroups](#)

Examples

```
## Not run:
renameGroup("currentGroupName", "newGroupName")

## End(Not run)
```

runCAEstimation	<i>[PKanalix] Estimate the individual parameters using compartmental analysis.</i>
-----------------	--

Description

Estimate the CA parameters for each individual of the project.

Usage

```
runCAEstimation(wait = TRUE)
```

Arguments

wait *(OBSOLETE)*

Examples

```
## Not run:
runCAEstimation()

## End(Not run)
```

```
runConditionalDistributionSampling
      [Monolix] Sampling from the conditional distribution
```

Description

Estimate the individual parameters using conditional distribution sampling algorithm. The associated method keyword is "conditionalMean".

Usage

```
runConditionalDistributionSampling(wait = TRUE)
```

Arguments

```
wait          (OBSOLETE)
```

Examples

```
## Not run:
runConditionalDistributionSampling()

## End(Not run)
```

```
runConditionalModeEstimation
      [Monolix] Estimation of the conditional modes (EBEs)
```

Description

Estimate the individual parameters using the conditional mode estimation algorithm (EBEs). The associated method keyword is "conditionalMode".

Usage

```
runConditionalModeEstimation(wait = TRUE)
```

Arguments

```
wait          (OBSOLETE)
```

Examples

```
## Not run:
runConditionalModeEstimation()

## End(Not run)
```

```
runEstimation          [PKanalix] Run both non compartmental and compartmental analysis.
```

Description

Run the NCA analysis and the CA analysis if the structural model for the CA calculation is defined.

Usage

```
runEstimation(wait = TRUE)
```

Arguments

```
wait          (OBSOLETE)
```

Examples

```
## Not run:
runEstimation()

## End(Not run)
```

```
runLogLikelihoodEstimation
          [Monolix] Log-Likelihood estimation
```

Description

Run the log-Likelihood estimation algorithm. By default, this task is not processed in the background of the R session. Existing methods:

<i>Method</i>	<i>Identifier</i>
Log-Likelihood estimation by linearization	linearization = T
Log-Likelihood estimation by Importance Sampling (default)	linearization = F

The Log-likelihood outputs(-2LL, AIC, BIC) are available using [getEstimatedLogLikelihood](#) function

Usage

```
runLogLikelihoodEstimation(linearization = FALSE, wait = TRUE)
```

Arguments

```
linearization  option (boolean)[optional] method to be used. When no method is given, the
               importance sampling is used by default.
wait          (OBSOLETE)
```

Examples

```
## Not run:
runLogLikelihoodEstimation(linearization = T)

## End(Not run)
```

```
runModelBuilding      [Monolix] Run model building
```

Description

Run model building. To change the initialization before a run, use [getModelBuildingSettings](#) to receive all the settings. See example.

Usage

```
runModelBuilding(wait = TRUE, ...)
```

Arguments

```
wait      (OBSOLETE)
...       (list<settings>) Settings to initialize the model buildign algorithm. See getModelBuildingSettings
```

See Also

[getModelBuildingSettings](#) [getModelBuildingResults](#)

Examples

```
## Not run:
runModelBuilding()
set = getModelBuildingSettings()
runModelBuilding(settings = set)

## End(Not run)
```

```
runNCAEstimation      [PKanalix] Estimate the individual parameters using non compart-  
mental analysis.
```

Description

Estimate the NCA parameters for each individual of the project.

Usage

```
runNCAEstimation(wait = TRUE)
```

Arguments

```
wait      (OBSOLETE)
```

Examples

```
## Not run:  
runNCAEstimation()  
  
## End(Not run)
```

```
runPopulationParameterEstimation  
      [Monolix] Population parameter estimation
```

Description

Estimate the population parameters with the SAEM method. The associated method keyword is "saem". The initial values of the population parameters can be accessed by calling [getPopulationParameterInformation](#) and customized with [setPopulationParameterInformation](#). The estimated population parameters are available using [getEstimatedPopulationParameters](#) function.

Usage

```
runPopulationParameterEstimation(wait = TRUE)
```

Arguments

```
wait          (OBSOLETE)
```

Examples

```
## Not run:  
runPopulationParameterEstimation()  
  
## End(Not run)
```

```
runScenario          [Monolix] Run current scenario
```

Description

Run the current scenario.

Usage

```
runScenario(wait = TRUE)
```

Arguments

```
wait          (OBSOLETE)
```

See Also

[setScenario](#) [getScenario](#)

Examples

```
## Not run:
runScenario()

## End(Not run)
```

```
runSimulation          [Simulx] Run simulation
```

Description

Run the simulation task.

Usage

```
runSimulation(wait = TRUE)
```

Arguments

```
wait          (OBSOLETE)
```

See Also

[getSimulationResults](#)

```
runStandardErrorEstimation
          [Monolix] Standard error estimation
```

Description

Estimate the Fisher Information Matrix and the standard errors of the population parameters. By default, this task is not processed in the background of the R session. Existing methods:

<i>Method</i>	<i>Identifier</i>
Estimate the FIM by Stochastic Approximation	linearization = F (default)
Estimate the FIM by Linearization	linearization = T

The Fisher Information Matrix is available using [getCorrelationOfEstimates](#) function, while the standard errors are available using [getEstimatedStandardErrors](#) function.

Usage

```
runStandardErrorEstimation(linearization = FALSE, wait = TRUE)
```

Arguments

```
linearization  option (boolean)[optional] method to be used. When no method is given, the
                stochastic approximation is used by default.
wait          (OBSOLETE)
```

Examples

```
## Not run:
runStandardErrorEstimation(linearization = T)

## End(Not run)
```

saveProject	<i>[Monolix - PKanalix - Simulx] Save current project</i>
-------------	---

Description

Save the current project as an Mlxtran-formated file.
The extensions are .mlxtran for Monolix, .pkx for PKanalix, and .smlx for Simulx.
WARNING: R is sensitive between '\ ' and ' / ', only ' / ' can be used.

Usage

```
saveProject(projectFile = "")
```

Arguments

projectFile [optional](*character*) Path where to save a copy of the current mlxtran model.
Can be absolute or relative to the current working directory. If no path is given,
the file used to build the current configuration is updated.

See Also

[newProject](#) [loadProject](#)

Examples

```
## Not run:
[Pkanalix only]
saveProject("/path/to/project/file.pqx") # save a copy of the model
[Monolix only]
saveProject("/path/to/project/file.mlxtran") # save a copy of the model
[Simulx only]
saveProject("/path/to/project/file.smlx") # save a copy of the model
[Monolix - PKanalix - Simulx]
saveProject() # update current model

## End(Not run)
```

selectData	<i>[Monolix - PKanalix] Select data set</i>
------------	---

Description

Choose the new current data set within the previously defined ones.

Usage

```
selectData(name)
```

Arguments

name (*string*) data set name.

See Also

[getAvailableData](#)

Examples

```
## Not run:  
selectData(name = "filter1")  
  
## End(Not run)
```

setAddLines	<i>[Simulx] Add lines to the model</i>
-------------	--

Description

Lines that can be added to the model file. The goal is to complete/add new element in the model without rewriting it from scratch.

Notice that all the variable defined in the add lines will be available as an output.

Usage

```
setAddLines(lines)
```

Arguments

lines (*string*) Additional lines to define.

See Also

[getAddLines](#)

Examples

```
## Not run:
  setAddLines("ddt_AUC = Cc")
  setAddLines(c("if t>24", "ddt_AUC = Cc", "end"))

## End(Not run)
```

setAutocorrelation *[Monolix] Set auto-correlation*

Description

Add or remove auto-correlation from the error model used on some of the observation models. Call [getObservationInformation](#) to get a list of the observation models present in the current project.

Usage

```
setAutocorrelation(...)
```

Arguments

... Sequence of comma-separated pairs $\{(string)"observationModel", (boolean)hasAutoCorrelation\}$.

See Also

[getContinuousObservationModel](#)

Examples

```
## Not run:
  setAutocorrelation(Conc = TRUE)
  setAutocorrelation(Conc = TRUE, Effect = FALSE)

## End(Not run)
```

setCASettings *[PKanalix] Get the settings associated to the compartmental analysis*

Description

Set the settings associated to the compartmental analysis. Associated settings names are:

"weightingCA"	(string)	Type of weighting ob
"pool"	(logical)	If TRUE, fit with ind
"initialValues" (list)	list(param = value, ...): value = initial value of individual parameter param.	
"blqMethod"	(string)	Method by which the

Usage

```
setCASettings(...)
```

Arguments

```
...           A collection of comma-separated pairs {settingName = settingValue}.
```

See Also

[getCASettings](#)

Examples

```
## Not run:
setCASettings(weightingCA = "uniform", blqMethod = "zero") # set the settings whose name has been passed in argu
setCASettings(initialValues = list(CL=0.4, V=.5, ka=0.04) # set the paramters CL, V, and ka to .4, .5 and .04 res

## End(Not run)
```

```
setConditionalDistributionSamplingSettings
```

[Monolix] Set conditional distribution sampling settings

Description

Set the value of one or several of the conditional distribution sampling settings. Associated settings are:

"ratio"	(0 < double < 1)	Width of the confidence interval.
"nbMinIterations"	(int >= 1)	Minimum number of iterations.
"nbSimulatedParameters"	(int >= 1)	Number of replicates.

Usage

```
setConditionalDistributionSamplingSettings(...)
```

Arguments

```
...           A collection of comma-separated pairs {settingName = settingValue}.
```

See Also

[getConditionalDistributionSamplingSettings](#)

Examples

```
## Not run:
setConditionalDistributionSamplingSettings(ratio = 0.05, nbMinIterations = 50)

## End(Not run)
```

```
setConditionalModeEstimationSettings
    [Monolix] Set conditional mode estimation settings
```

Description

Set the value of one or several of the conditional mode estimation settings. Associated settings are:

"nbOptimizationIterationsMode"	(<i>int</i> >=1)	Maximum number of iterations.
"optimizationToleranceMode"	(<i>double</i> >0)	Optimization tolerance.

Usage

```
setConditionalModeEstimationSettings(...)
```

Arguments

... A collection of comma-separated pairs {settingName = settingValue}.

See Also

[getConditionalModeEstimationSettings](#)

Examples

```
## Not run:
setConditionalModeEstimationSettings(nbOptimizationIterationsMode = 20,
                                     optimizationToleranceMode = 0.1)

## End(Not run)
```

```
setCorrelationBlocks   [Monolix] Set correlation block structure
```

Description

Define the correlation block structure associated to some of the variability levels of the current project. Call [getVariabilityLevels](#) to get a list of the variability levels and [getIndividualParameterModel](#) to get a list of the available individual parameters within the current project.

Usage

```
setCorrelationBlocks(...)
```

Arguments

... A list of comma-separated pairs {variabilityLevel = vector<(array<string>)parameterNames> }.

See Also

[getVariabilityLevels](#) [getIndividualParameterModel](#)

Examples

```
## Not run:
setCorrelationBlocks(id = list( c("ka", "V", "Tlag") ), iov1 = list( c("ka", "Cl"), c("Tlag", "V") ) )

## End(Not run)
```

setCovariateModel *[Monolix] Set covariate model*

Description

Set which are the covariates influencing individual parameters present in the project. Call [getIndividualParameterModel](#) to get a list of the individual parameters present within the current project. and [getCovariateInformation](#) to know which are the available covariates for a given level of variability and a given individual parameter.

Usage

```
setCovariateModel(...)
```

Arguments

... A list of comma-separated pairs { parameterName = { covariateName = (*bool*)isInfluent, ... } }

See Also

[getCovariateInformation](#)

Examples

```
## Not run:
setCovariateModel( ka = c( Wt = FALSE, tWt = TRUE, lcat2 = TRUE),
                  Cl = c( SEX = TRUE )
                  )

## End(Not run)
```

setData	[Monolix - PKanalix] Set project data
---------	---------------------------------------

Description

Set project data giving a data file and specifying headers and observations types.

Usage

```
setData(dataFile, headerTypes, observationTypes, nbSSDoses = NULL)
```

Arguments

dataFile	(<i>character</i>): Path to the data file. Can be absolute or relative to the current working directory.
headerTypes	(<i>array<character></i>): A collection of header types. The possible header types are: "ignore", "id", "time", "observation", "amount", "contcov", "catcov", "occ", "evid", "mdv", "obsid", "cens", "limit", "regressor", "admid", "rate", "tinf", "ss", "ii", "addl", "date". Notice that these are not the types displayed in the interface, these one are short-cuts.
observationTypes	[optional] (<i>list</i>): A list giving the type of each observation present in the data file. If there is only one y-type, the corresponding observation name can be omitted. The possible observation types are "continuous", "discrete", and "event".
nbSSDoses	[optional] (<i>int</i>): Number of doses (if there is a SS column).

See Also

[getData](#)

Examples

```
## Not run:
setData(dataFile = "/path/to/data/file.txt",
        headerTypes = c("IGNORE", "OBSERVATION"), observationTypes = "continuous")
setData(dataFile = "/path/to/data/file.txt",
        headerTypes = c("IGNORE", "OBSERVATION", "YTYPE"),
        observationTypes = list(Concentration = "continuous", Level = "discrete"))

## End(Not run)
```

setDataSettings	<i>[PKanalix]</i> Set the value of one or several of the data settings associated to the non compartmental analysis
-----------------	---

Description

Set the value of one or several of the data settings associated to the non compartmental analysis. Associated settings names are:

"urinevolume" (*string*) regressor name used as urine volume.

"datatype" (*list*) list("obsId" = *string*("plasma" or "urine")). The type of data associated with each *obsId*. Default

Usage

```
setDataSettings(...)
```

Arguments

... A collection of comma-separated pairs {settingName = settingValue}.

See Also

[getDataSettings](#)

Examples

```
## Not run:
setDataSettings("datatype" = list("Y" = "plasma")) # set the settings whose name has been passed in argument

## End(Not run)
```

setErrorModel	<i>[Monolix]</i> Set error model
---------------	----------------------------------

Description

Set the error model type to be used with some of the observation models. Call [getObservationInformation](#) to get a list of the observation models present in the current project.

Usage

```
setErrorModel(...)
```

Arguments

... A list of comma-separated pairs {observationModel = (*string*)errorModelType}.

Details

Available error model types are :

"constant"	obs = pred + a*err
"proportional"	obs = pred + (b*pred)*err
"combined1"	obs = pred + (b*pred^c + a)*err
"combined2"	obs = pred + sqrt(a^2 + (b^2)*pred^(2c))*err

Error model parameters will be initialized to 1 by default. Call [setPopulationParameterInformation](#) to modify their initial value.

The value of the exponent parameter is fixed by default when using the "combined1" and "combined2" models.

Use [setPopulationParameterInformation](#) to enable its estimation.

See Also

[getContinuousObservationModel](#) [setPopulationParameterInformation](#)

Examples

```
## Not run:
setErrorModel(Conc = "constant", Effect = "combined1")

## End(Not run)
```

setGeneralSettings *[Monolix] Set common settings for algorithms*

Description

Set the value of one or several of the common settings for Monolix algorithms. Associated settings are:

"autoChains"	<i>(bool)</i>	Automatically adjusted the number of chains to have at least a minimum number of sub
"nbChains"	<i>(int >0)</i>	Number of chains to be used if "autoChains" is set to FALSE.
"minIndivForChains"	<i>(int >0)</i>	Minimum number of individuals by chain.

Usage

```
setGeneralSettings(...)
```

Arguments

... A collection of comma-separated pairs {settingName = settingValue}.

See Also

[getGeneralSettings](#)

Examples

```
## Not run:
setGeneralSettings(autoChains = FALSE, nbchains = 10)

## End(Not run)
```

setGlobalObsIdToUse *[PKanalix] Set the global observation id used in both the compartmental and non compartmental analysis*

Description

Get the global observation id used in both the compartmental and non compartmental analysis.

Usage

```
setGlobalObsIdToUse(...)
```

Arguments

... ("id" *string*) the observation id from data section to use for computations.

See Also

[getGlobalObsIdToUse](#)

Examples

```
## Not run:
setGlobalObsIdToUse("id") #

## End(Not run)
```

setGroupElement *[Simulx] Set elements to simulation group*

Description

Set the new element of a specific group.

Usage

```
setGroupElement(group, elements)
```

Arguments

group (*character*) Group name
elements (*character*) Vector of new elements that are already defined

See Also[getGroups](#)**Examples**

```
## Not run:
  setGroupElement(group = "group", newElement = c("element1", "element2"))

## End(Not run)
```

setGroupRemaining	<i>[Simulx] Set simulation group remaining</i>
-------------------	--

Description

Set the values of the remaining elements (coming from the observation model) for a group.

Usage

```
setGroupRemaining(group, remaining)
```

Arguments

group	(<i>character</i>) Group name
remaining	(<i>vector</i>) list of the remaining variables

See Also[getGroupRemaining](#)**Examples**

```
## Not run:
  setGroupRemaining(group="arm1", remaining = list(a = 12, b = 3))

## End(Not run)
```

setGroupSize	<i>[Simulx] Set simulation group size</i>
--------------	---

Description

Define the size of a simulation group.

Usage

```
setGroupSize(group, size)
```

Arguments

group (*string*) Name of the group where the size will be changed.
 size (*int*) Size of the new group.

See Also

[getGroups](#)

Examples

```
## Not run:
  setGroupSize("group", 10)

## End(Not run)
```

setIndividualLogitLimits

[Monolix] Set individual parameter distribution limits

Description

Set the minimum and the maximum values between the individual parameter can be used. Used only if the distribution of the parameter is "logitNormal", else wise it will not be taken into account

Usage

```
setIndividualLogitLimits(...)
```

Arguments

... A list of comma-separated pairs {individualParameter = [(double)min,(double)max]
 }

See Also

[getIndividualParameterModel](#)

Examples

```
## Not run:
  setIndividualLogitLimits( V = c(0, 1), ka = c(-1, 2) )

## End(Not run)
```

```
setIndividualParameterDistribution
```

[Monolix] Set individual parameter distribution

Description

Set the distribution of the estimated parameters. Available distributions are "normal", "logNormal" and "logitNormal".

Call [getIndividualParameterModel](#) to get a list of the available individual parameters within the current project.

Usage

```
setIndividualParameterDistribution(...)
```

Arguments

... A list of comma-separated pairs {parameterName = (*string*)"distribution"}.

See Also

[getIndividualParameterModel](#)

Examples

```
## Not run:
setIndividualParameterDistribution(V = "logNormal")
setIndividualParameterDistribution(CI = "normal", V = "logNormal")

## End(Not run)
```

```
setIndividualParameterModel
```

[Monolix] Set individual parameter model

Description

Set the information concerning the individual parameter model. The editable informations are:

- **distribution**: (*string*) distribution of the parameter values. The distribution type can be "normal", "logNormal", or "logitNormal".
- **limits**: a list giving the distribution limits for each parameter following a "logitNormal" distribution
- **variability**: a list giving, for each variability level, if individual parameters have variability or not
- **covariateModel**: a list giving, for each individual parameter, if the related covariates are used or not.
- **correlationBlocks** : a list giving, for each variability level, the blocks of the correlation matrix of the random effects. A block is represented by a vector of individual parameter names.

Usage

```
setIndividualParameterModel(...)
```

Arguments

```
...          A list of comma-separated pairs {[info] = [value]}.
```

```
setIndividualParameterVariability
```

```
[Monolix] Individual variability management
```

Description

Add or remove inter-individual and/or intra-individual variability from some of the individual parameters present in the project.

Call [getIndividualParameterModel](#) to get a list of the available parameters within the current project.

Usage

```
setIndividualParameterVariability(...)
```

Arguments

```
...          A list of comma-separated pairs {variabilityLevel = {individualParameterName  
= (bool)hasVariability} }.
```

See Also

[getIndividualParameterModel](#)

Examples

```
## Not run:  
setIndividualParameterVariability(ka = TRUE, V = FALSE)  
setIndividualParameterVariability(id = list(ka = TRUE), iov1 = list(ka = FALSE))  
  
## End(Not run)
```

```
setInitialEstimatesToLastEstimates
```

[Monolix] Initialize population parameters with the last estimated ones

Description

Set the initial value of all the population parameters present within the current project to the ones previously estimated. These the values will be used in the population parameter estimation algorithm during the next scenario run.

WARNING: If there is any set after a run, it will not be possible to set the initial values as the structure of the project has changed since last results.

Usage

```
setInitialEstimatesToLastEstimates(fixedEffectsOnly = FALSE)
```

Arguments

```
fixedEffectsOnly
```

(bool) If this boolean is set to TRUE, only the fixed effects are initialized to their last estimated values. Otherwise, individual variances and error model parameters are re-initialized too. Equals FALSE by default.

See Also

[getEstimatedPopulationParameters](#) [getPopulationParameterInformation](#)

Examples

```
## Not run:
setInitialEstimatesToLastEstimates() # fixedEffectsOnly = FALSE by default
setInitialEstimatesToLastEstimates(TRUE)

## End(Not run)
```

```
setLogLikelihoodEstimationSettings
```

[Monolix] Set loglikelihood estimation settings

Description

Set the value of the loglikelihood estimation settings. Associated settings are:

"nbFixedIterations"	<i>(int >0)</i>	Monte Carlo size for the loglikelihood evaluation.
"samplingMethod"	<i>(string)</i>	Should the loglikelihood estimation use a given number of freedom d
"nbFreedomDegrees"	<i>(int >0)</i>	Degree of freedom of the Student t-distribution. <i>Used only if "samplin</i>
"freedomDegreesSampling"	<i>(vector<int(>0)>)</i>	Sequence of freedom degrees to be tested. <i>Used only if "samplingMet</i>

Usage

```
setLogLikelihoodEstimationSettings(...)
```

Arguments

```
...           A collection of comma-separated pairs {settingName = settingValue}.
```

See Also

[getLogLikelihoodEstimationSettings](#)

Examples

```
## Not run:
setLogLikelihoodEstimationSettings(nbFixedIterations = 20000)

## End(Not run)
```

setMCMCSettings *[Monolix] Set settings associated to the MCMC algorithm*

Description

Set the value of one or several of the MCMC algorithm specific settings of the current project. Associated settings are:

"strategy"	(<i>vector<int>[3]</i>)	Number of calls for each one of the three MCMC kernels.
"acceptanceRatio"	(<i>double</i>)	Target acceptance ratio.

Usage

```
setMCMCSettings(...)
```

Arguments

```
...           A collection of comma-separated pairs {settingName = settingValue}.
```

See Also

[getMCMCSettings](#)

Examples

```
## Not run:
setMCMCSettings(strategy = c(2,1,2))

## End(Not run)
```

setNbReplicates	<i>[Simulx] Set number of replicates</i>
-----------------	--

Description

Define the number of replicates of the simulation.

Usage

```
setNbReplicates(nb)
```

Arguments

nb (int) Number of replicates.

See Also

[getNbReplicates](#)

Examples

```
## Not run:
  setNbReplicates( nb = 1 )

## End(Not run)
```

setNCASettings	<i>[PKanalix] Set the value of one or several of the settings associated to the non compartmental analysis</i>
----------------	--

Description

Set the value of one or several of the settings associated to the non compartmental analysis. Associated settings are:

"administrationType"	(list)	list(key = "admId", value = string("intravenous" or "extravascular")). <i>admId</i>
"integralMethod"	(string)	Method for AUC and AUMC calculation and interpolation.
"partialAucTime"	(list)	The first element of the list is a boolean describing if this setting is used. The
"blqMethodBeforeTmax"	(string)	Method by which the BLQ data before Tmax should be replaced. Possible r
"blqMethodAfterTmax"	(string)	Method by which the BLQ data after Tmax should be replaced. Possible me
"ajdr2AcceptanceCriteria"	(list)	The first element of the list is a boolean describing if this setting is used. Th
"extrapAucAcceptanceCriteria"	(list)	The first element of the list is a boolean describing if this setting is used. Th
"spanAcceptanceCriteria"	(list)	The first element of the list is a boolean describing if this setting is used. Th

"lambdaRule"	(string)	Main rule for the lambda_Z estimation. Possible rules are "R2", "interval", "
"timeInterval"	(vector)	Time interval for the lambda_Z estimation when "lambdaRule" = "interval", "
"timeValuesPerId"	(list)	list("idName" = idTimes,...): idTimes Observation times to use for the calcul
"nbPoints"	(integer)	Number of points for the lambda_Z estimation when "lambdaRule" = "point
"maxNbOfPoints"	(list)	The first element of the list is a boolean describing if this setting is used. Th
"startTimeNotBefore"	(list)	The first element of the list is a boolean describing if this setting is used. Th
"weightingNca"	(string)	Weighting method used for the regression that estimates lambda_Z. Possible
"computedNCAParameters"	(vector)	All the parameters to compute during the analysis."

Usage

```
setNCASettings(...)
```

Arguments

... A collection of comma-separated pairs {settingName = settingValue}.

See Also

[getNCASettings](#)

Examples

```
## Not run:
setNCASettings(integralMethod = "LinLogTrapLinLogInterp", weightingnca = "uniform") # set the settings whose n
setNCASettings(administrationType = list("1"="extravasculard")) # set the administration id "1" to extravascula
setNCASettings(startTimeNotBefore = list(TRUE, 15)) # set the estimation of the lambda_z with points with time o
setNCASettings(timeValuesPerId = list('1'=c(4, 6, 8, 30), '4'=c(8, 12, 18, 24, 30))) # set the points to use for
setNCASettings(timeValuesPerId = NULL) # set the points to use for the lambda_z to the default rule

## End(Not run)
```

setObservationDistribution

[Monolix] Set observation model distribution

Description

Set the distribution in the Gaussian space of some of the observation models. Available distribution types are "normal", "logNormal", or "logitNormal". Call [getObservationInformation](#) to get a list of the available observation models within the current project.

Usage

```
setObservationDistribution(...)
```

Arguments

```
...          A list of comma-separated pairs { observationModel = (string)"distribution"}.
```

See Also

[getContinuousObservationModel](#)

Examples

```
## Not run:
setObservationDistribution(Conc = "normal")
setObservationDistribution(Conc = "normal", Effect = "logNormal")

## End(Not run)
```

setObservationLimits *[Monolix] Set observation model distribution limits*

Description

Set the minimum and the maximum values between which some of the observations can be found. Used only if the distribution of the error model is "logitNormal", else wise it will not be taken into account

Usage

```
setObservationLimits(...)
```

Arguments

```
...          A list of comma-separated pairs { observationModel = [(double)min,(double)max]
}

```

See Also

[getContinuousObservationModel](#) [getObservationInformation](#)

Examples

```
## Not run:
setObservationLimits( Conc = c(-Inf,Inf), Effect = c(0,Inf) )

## End(Not run)
```

 setPopulationParameterEstimationSettings

[Monolix] Set population parameter estimation settings

Description

Set the value of one or several of the population parameter estimation settings. Associated settings are:

"nbBurningIterations"	(int >=0)	Number of iterations in the burn-in phase.
"nbExploratoryIterations"	(int >=0)	If "exploratoryAutoStop" is set to FALSE, it is the number of iterations.
"exploratoryAutoStop"	(bool)	Should the exploratory step automatically stop.
"exploratoryInterval"	(int >0)	Minimum number of iteration in the exploratory phase. <i>Used only if "exploratoryAutoStop" is FALSE.</i>
"exploratoryAlpha"	(0<= double <=1)	Convergence memory in the exploratory phase. <i>Used only if "exploratoryAutoStop" is FALSE.</i>
"nbSmoothingIterations"	(int >=0)	If "smoothingAutoStop" is set to FALSE, it is the number of iterations.
"smoothingAutoStop"	(bool)	Should the smoothing step automatically stop.
"smoothingInterval"	(int >0)	Minimum number of iteration in the smoothing phase. <i>Used only if "smoothingAutoStop" is FALSE.</i>
"smoothingAlpha"	(0.5< double <=1)	Convergence memory in the smoothing phase. <i>Used only if "smoothingAutoStop" is FALSE.</i>
"smoothingRatio"	(0< double <1)	Width of the confidence interval. <i>Used only if "smoothingAutoStop" is FALSE.</i>
"simulatedAnnealing"	(bool)	Should annealing be simulated.
"tauOmega"	(double >0)	Proportional rate on variance. <i>Used only if "simulatedAnnealing" is TRUE.</i>
"tauErrorModel"	(double >0)	Proportional rate on error model. <i>Used only if "simulatedAnnealing" is TRUE.</i>
"variability"	(string)	Estimation method for parameters without variability: "firstStage" "c".
"nbOptimizationIterations"	(int >=1)	Number of optimization iterations.
"optimizationTolerance"	(double >0)	Tolerance for optimization.

Usage

```
setPopulationParameterEstimationSettings(...)
```

Arguments

... A collection of comma-separated pairs {settingName = SettingValue}.

See Also

[getPopulationParameterEstimationSettings](#)

Examples

```
## Not run:
setPopulationParameterEstimationSettings(exploratoryAutoStop = TRUE, tauOmega = 0.95)

## End(Not run)
```

`setPopulationParameterInformation`*[Monolix] Population parameters initialization and estimation method*

Description

Set the initial value, the estimation method and, if relevant, the MAP parameters of one or several of the population parameters present within the current project (fixed effects + individual variances + error model parameters). Available methods are:

- "FIXED": Fixed
- "MLE": Maximum Likelihood Estimation
- "MAP": Maximum A Posteriori

Call [getPopulationParameterInformation](#) to get a list of the initializable population parameters present within the current project.

Usage

```
setPopulationParameterInformation(...)
```

Arguments

... A list of comma-separated pairs {paramName = list(initialValue = (*double*), method = (*string*)"method"}. In case of "MAP" method, the user can specify the associated typical value and standard deviation values by using an additional list elements {paramName = list(priorValue = (*double*)1, priorSD = (*double*)2)}. By default, the prior value corresponds to the the population parameter and the prior standard deviation is set to 1.

See Also

[getPopulationParameterInformation](#)

Examples

```
## Not run:
setPopulationParameterInformation(Cl_pop = list(initialValue = 0.5, method = "FIXED"),
                                V_pop = list(intialValue = 1),
                                ka_pop = list(method = "MAP", priorValue = 1, priorSD = 0.1))

## End(Not run)
```

setPreferences *[Monolix - PKanalix - Simulx] Set preferences*

Description

Set the value of one or several of the project preferences. Preferences are:

"relativepath"	(<i>bool</i>)	Use relative path for save/load operations.
"threads"	(<i>int >0</i>)	Number of threads.
"timestamping"	(<i>bool</i>)	Create an archive containing result files after each run.
"delimiter"	(<i>string</i>)	Character use as delimiter in exported result files.
"exportchartsData"	(<i>bool</i>)	Should graphics data be exported.
"exportsimulationfiles"	(<i>bool</i>)	[Simulx] Should simulation results files be exported.
"headeraliases"	(<i>list("header" = vector<string>)</i>)	For each header, the list of the recognized aliases.
"ncaparameters"	(<i>vector<string></i>)	[PKanalix] Defaultly computed NCA parameters.

Usage

```
setPreferences(...)
```

Arguments

... A collection of comma-separated pairs {preferenceName = settingValue}.

See Also

[getPreferences](#)

Examples

```
## Not run:
setPreferences(exportCharts = FALSE, delimiter = ",")

## End(Not run)
```

setProjectSettings *[Monolix - PKanalix - Simulx] Set project settings*

Description

Set the value of one or several of the settings of the project. Associated settings for Monolix projects are:

"directory"	(<i>string</i>)	Path to the folder where simulation results will be saved. It sh
"exportResults"	(<i>bool</i>)	Should results be exported.
"seed"	(<i>0 < int < 2147483647</i>)	Seed used by random generators.
"grid"	(<i>int</i>)	Number of points for the continuous simulation grid.
"nbSimulations"	(<i>int</i>)	Number of simulations.
"dataAndModelNextToProject"	(<i>bool</i>)	Should data and model files be saved next to project.

Associated settings for Pkanalix projects are:

"directory"	(string)	Path to the folder where simulation results will be saved. It should be a writable directory.
"dataNextToProject"	(bool)	Should data files be saved next to project.

Associated settings for Simulx projects are:

"directory"	(string)	Path to the folder where simulation results will be saved. It should be a writable directory.
"seed"	(0 < int < 2147483647)	Seed used by random generators.
"userfilesnexttoproject"	(bool)	Should user files be saved next to project.

Usage

```
setProjectSettings(...)
```

Arguments

... A collection of comma-separated pairs {settingName = settingValue}.

See Also

[getProjectSettings](#)

Examples

```
## Not run:
setProjectSettings(directory = "/path/to/export/directory", seed = 12345)

## End(Not run)
```

```
setSameIndividualsAmongGroups
  [Simulx] Set same individuals among groups
```

Description

Define if the same individuals will be simulated among all groups.

Usage

```
setSameIndividualsAmongGroups(value)
```

Arguments

value (boolean) Boolean to define if the same individuals will be the same for all groups.

See Also

[getSameIndividualsAmongGroups](#)

Examples

```
## Not run:
  setSameIndividualsAmongGroups( value = TRUE )

## End(Not run)
```

setSamplingMethod *[Simulx] Set sampling method*

Description

Define which sampling methods will be used for the simulation. The possibilities are to keep the order, sample with replacement and sample without replacement.

Usage

```
setSamplingMethod(method)
```

Arguments

method (*character*) keepOrder, withReplacement, withoutReplacement

See Also

[getSamplingMethod](#)

Examples

```
## Not run:
  setSamplingMethod( method = "" )

## End(Not run)
```

setScenario *[Monolix] Set scenario*

Description

Clear the current scenario and build a new one from a given list of tasks, the linearization option and the list of plots. A task is the association of:

- a task
- a boolean

NOTE: by default the boolean is false, thus, the user can only state what will run during the scenario.
 NOTE: Within a MONOLIX scenario, the order according which the different algorithms are run is fixed:

Algorithm	Algorithm Keyword
Population Parameter Estimation	"populationParameterEstimation"
Conditional Mode Estimation (EBEs)	"conditionalModeEstimation"
Sampling from the Conditional Distribution	"conditionalDistributionSampling"
Standard Error and Fisher Information Matrix Estimation	"standardErrorEstimation"
LogLikelihood Estimation	"logLikelihoodEstimation"
Plots	"plots"

Usage

```
setScenario(...)
```

Arguments

... A list of tasks as previously defined.

See Also

[getScenario](#)

Examples

```
## Not run:

scenario = getScenario()
scenario$tasks = c(populationParameterEstimation = T, conditionalModeEstimation = T, conditionalDistributionS
setScenario(scenario)

## End(Not run)
```

setSharedIds *[Simulx] Set simulation groups sharedIds*

Description

Set the elements for the shared group.

Usage

```
setSharedIds(sharedIds)
```

Arguments

sharedIds (*vector<string>*) List of element types. The available types are: covariate, output, treatment, regressor, population, individual

See Also

[getSharedIds](#)

Examples

```
## Not run:
  setSharedIds( sharedIds = c("output", "treatment") )

## End(Not run)
```

```
setStandardErrorEstimationSettings
  [Monolix] Set standard error estimation settings
```

Description

Set the value of one or several of the standard error estimation settings. Associated settings are:

```
"minIterations"  (int >=1)  Minimum number of iterations.
"maxIterations"  (int >=1)  Maximum number of iterations.
```

Usage

```
setStandardErrorEstimationSettings(...)
```

Arguments

```
...           A collection of comma-separated pairs {settingName = settingValue}.
```

See Also

[getStandardErrorEstimationSettings](#)

Examples

```
## Not run:
  setStandardErrorEstimationSettings(minIterations = 20, maxIterations = 250)

## End(Not run)
```

```
setStructuralModel  [Monolix - PKanalix] Set structural model file
```

Description

Set the structural model.

NOTE: In case of PKanalix, the user can only use a structural model from the library for the CA analysis. Thus, the structural model should be written 'lib:modelFromLibrary.txt'.

Usage

```
setStructuralModel(modelFile)
```


Arguments

modelFile (*character*) Path to the model file. Can be absolute or relative to the current working directory.

See Also

[getStructuralModel](#)

Examples

```
## Not run:  
setStructuralModel("/path/to/model/file.txt") # for Monolix  
setStructuralModel("'lib:oral1_2cpt_kaClV1QV2.txt'") # for PKanalix or Monolix  
  
## End(Not run)
```

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