

Package ‘libsoc’

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Title Read, Create and Write 'PharmML' Standard Output (so) XML Files

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Depends R (>= 2.14.1)

Imports methods

Suggests knitr, rmarkdown, testthat

VignetteBuilder knitr

SystemRequirements libxml2: libxml2-dev (deb), libxml2-devel (rpm)

NeedsCompilation yes

Description

Handle 'PharmML' (Pharmacometrics Markup Language) standard output (SO) XML files. SO files can be created, read, manipulated and written through a data binding from the XML structure to a tree structure of R objects.

URL <https://github.com/rikardn/libsoc>

BugReports <https://github.com/rikardn/libsoc/issues>

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R topics documented:

dv_column	2
dv_column_name	3
idv_column	3
idv_column_name	3
id_column	4

id_column_name	4
libsoc	4
so_Bayesian	5
so_Bayesian_PPE	6
so_DiagnosticIndividualParams	6
so_DiagnosticStructuralModel	7
so_Estimates	7
so_Estimation	8
so_ExternalFile	8
so_IndividualEstimates	9
so_InformationCriteria	9
so_Message	10
so_MissingData	10
so_MLE	11
so_ModelDiagnostic	11
so_OFMeasures	12
so_OptimalDesign	12
so_OptimalDesignBlock	13
so_OtherMethod	13
so_OtherMethod_PPE	14
so_PharmMLRef	14
so_PopulationEstimates	15
so_PrecisionIndividualEstimates	15
so_PrecisionPopulationEstimates	16
so_RandomEffects_IE	16
so_RawResults	17
so_Residuals	17
so_Simulation	18
so_SimulationBlock	18
so_SimulationSubType	19
so_SO	19
so_SOBlock	20
so_SO_read	21
so_TargetToolMessages	21
so_TaskInformation	22
so_ToolSettings	22
Index	23

 dv_column

Get index of the DV column in a data.frame created from an SO object

Description

Function to get the index of the dependent variable from a data.frame created from an SO object

Arguments

table A data.frame extracted from an SO object

dv_column_name *Get the name of the DV column in a data.frame created from an SO object*

Description

Function to get the name of the dependent variable from a data.frame created from an SO object

Arguments

table A data.frame extracted from an SO object

idv_column *Get index of the independent variable column in a data.frame created from an SO object*

Description

Function to get the index of the independent variable from a data.frame created from an SO object

Arguments

table A data.frame extracted from an SO object

idv_column_name *Get the name of the independent variable column in a data.frame created from an SO object*

Description

Function to get the name of the independent variable from a data.frame created from an SO object

Arguments

table A data.frame extracted from an SO object

id_column	<i>Get index of the ID column in a data.frame created from an SO object</i>
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Description

Function to get the index of the ID column from a data.frame created from an SO object

Arguments

table	A data.frame extracted from an SO object
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id_column_name	<i>Get the name of the ID column in a data.frame created from an SO object</i>
----------------	--

Description

Function to get the name of the ID column from a data.frame created from an SO object

Arguments

table	A data.frame extracted from an SO object
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libsoc	<i>A package to handle PharmML standardized output (SO) XML files</i>
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Description

A package to handle PharmML standardized output (SO) XML files. SO files can be created, read, manipulated and written through a data binding from the XML structure to a tree structure of R objects.

Details

Package:	libsoc
Type:	Package
Version:	0.6.2
Date:	2018-01-12
License:	LGPL-3

Depends on libxml2, libiconv and zlib. More information and source code for these libraries can be found on the sites linked below.

libxml2	http://xmlsoft.org
libiconv	https://www.gnu.org/software/libiconv
zlib	http://www.zlib.net

You can view the license for libsoc itself and libiconv with `file.show(system.file("licenses", "COPYING-LIB", package="libsoc"))` and libxml2 with `file.show(system.file("licenses", "COPYING-LIBXML2", package="libsoc"))`

Author(s)

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Examples

```
# Read in parameter estimates
file <- system.file("extdata", "pheno.SO.xml", package="libsoc")
so <- so_SO_read(file)
estimates <- so$SOBlock[[1]]$Estimation$PopulationEstimates$MLE

# For more examples see the examples directory
```

so_Bayesian

so_Bayesian reference class

Description

Reference Class for the SO/SOBlock/Estimation/PopulationEstimates/Bayesian element of a PharmML-SO data structure

Methods

`so_Bayesian$new()` - Create a new empty so_Bayesian object

Fields

`$PosteriorMean` - A data.frame
`$PosteriorMedian` - A data.frame
`$PosteriorMode` - A data.frame

so_Bayesian_PPE *so_Bayesian_PPE reference class*

Description

Reference Class for the SO/SOBlock/Estimation/PrecisionPopulationEstimates/Bayesian element of a PharmML-SO data structure

Methods

so_Bayesian_PPE\$new() - Create a new empty so_Bayesian_PPE object

Fields

\$StandardDeviationPosterior - A data.frame

\$PercentilesCI - A data.frame

so_DiagnosticIndividualParams
so_DiagnosticIndividualParams reference class

Description

Reference Class for the SO/SOBlock/ModelDiagnostic/DiagnosticIndividualParams element of a PharmML-SO data structure

Methods

so_DiagnosticIndividualParams\$new() - Create a new empty so_DiagnosticIndividualParams object

Fields

\$RandomEffects - A data.frame

\$IndivParamsCovariates - A data.frame

\$DistributionIndivParams - A data.frame

so_DiagnosticStructuralModel
so_DiagnosticStructuralModel reference class

Description

Reference Class for the SO/SOBlock/ModelDiagnostic/DiagnosticStructuralModel element of a PharmML-SO data structure

Methods

so_DiagnosticStructuralModel\$new() - Create a new empty so_DiagnosticStructuralModel object

Fields

\$IndivObservationPrediction - A data.frame
\$VPC - A data.frame

so_Estimates *so_Estimates reference class*

Description

Reference Class for the SO/SOBlock/Estimation/IndividualEstimates/Estimates element of a PharmML-SO data structure

Methods

so_Estimates\$new() - Create a new empty so_Estimates object

Fields

\$Mean - A data.frame
\$Median - A data.frame
\$Mode - A data.frame
\$Samples - A data.frame

so_Estimation	<i>so_Estimation reference class</i>
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Description

Reference Class for the SO/SOBlock/Estimation element of a PharmML-SO data structure

Methods

so_Estimation\$new() - Create a new empty so_Estimation object

Fields

\$PopulationEstimates - A [so_PopulationEstimates](#) object
 \$PrecisionPopulationEstimates - A [so_PrecisionPopulationEstimates](#) object
 \$IndividualEstimates - A [so_IndividualEstimates](#) object
 \$PrecisionIndividualEstimates - A [so_PrecisionIndividualEstimates](#) object
 \$Residuals - A [so_Residuals](#) object
 \$Predictions - A data.frame
 \$OFMeasures - A [so_OFMeasures](#) object
 \$TargetToolMessages - A [so_TargetToolMessages](#) object

so_ExternalFile	<i>so_ExternalFile reference class</i>
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Description

Reference Class for the ExternalFile element of a PharmML-SO data structure

Methods

so_ExternalFile\$new() - Create a new empty so_ExternalFile object
 so_ExternalFile\$add_MissingData(object) - Add a MissingData
 so_ExternalFile\$remove_MissingData(object, i) - Remove the MissingData having index i

Fields

\$Description - A character string
 \$path - A character string
 \$format - A character string
 \$delimiter - A character string
 \$MissingData - A list of [so_MissingData](#) objects
 \$oid - A character string attribute

so_IndividualEstimates

so_IndividualEstimates reference class

Description

Reference Class for the SO/SOBlock/Estimation/IndividualEstimates element of a PharmML-SO data structure

Methods

so_IndividualEstimates\$new() - Create a new empty so_IndividualEstimates object

Fields

\$Estimates - A [so_Estimates](#) object
\$RandomEffects - A [so_RandomEffects_IE](#) object
\$EtaShrinkage - A data.frame

so_InformationCriteria

so_InformationCriteria reference class

Description

Reference Class for the SO/SOBlock/Estimation/OFMeasures/InformationCriteria element of a PharmML-SO data structure

Methods

so_InformationCriteria\$new() - Create a new empty so_InformationCriteria object

Fields

\$AIC - A numeric
\$BIC - A numeric
\$DIC - A numeric

so_Message	<i>so_Message reference class</i>
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Description

Reference Class for the SO/SOBlock/TaskInformation/Message element of a PharmML-SO data structure

Methods

so_Message\$new() - Create a new empty so_Message object

Fields

\$Toolname - A character string
\$Name - A character string
\$Content - A character string
\$Severity - An integer
\$type - A character string attribute

so_MissingData	<i>so_MissingData reference class</i>
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Description

Reference Class for the MissingData element of a PharmML-SO data structure

Methods

so_MissingData\$new() - Create a new empty so_MissingData object

Fields

\$dataCode - A character string attribute
\$missingDataType - A character string attribute

so_MLE	<i>so_MLE reference class</i>
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Description

Reference Class for the SO/SOBlock/Estimation/PrecisionPopulationEstimates/MLE element of a PharmML-SO data structure

Methods

so_MLE\$new() - Create a new empty so_MLE object

Fields

\$FIM - A matrix
\$CovarianceMatrix - A matrix
\$CorrelationMatrix - A matrix
\$StandardError - A data.frame
\$RelativeStandardError - A data.frame
\$AsymptoticCI - A data.frame
\$ConditionNumber - A numeric

so_ModelDiagnostic	<i>so_ModelDiagnostic reference class</i>
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Description

Reference Class for the SO/SOBlock/ModelDiagnostic element of a PharmML-SO data structure

Methods

so_ModelDiagnostic\$new() - Create a new empty so_ModelDiagnostic object

Fields

\$DiagnosticStructuralModel - A [so_DiagnosticStructuralModel](#) object
\$DiagnosticIndividualParams - A [so_DiagnosticIndividualParams](#) object

so_OFMeasures	<i>so_OFMeasures reference class</i>
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Description

Reference Class for the SO/SOBlock/Estimation/OFMeasures element of a PharmML-SO data structure

Methods

so_OFMeasures\$new() - Create a new empty so_OFMeasures object

Fields

\$Likelihood - A numeric
 \$LogLikelihood - A numeric
 \$Deviance - A numeric
 \$ToolObjFunction - A numeric
 \$IndividualContribToLL - A data.frame
 \$InformationCriteria - A [so_InformationCriteria](#) object

so_OptimalDesign	<i>so_OptimalDesign reference class</i>
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Description

Reference Class for the SO/SOBlock/OptimalDesign element of a PharmML-SO data structure

Methods

so_OptimalDesign\$new() - Create a new empty so_OptimalDesign object
 so_OptimalDesign\$add_OptimalDesignBlock(object) - Add a OptimalDesignBlock
 so_OptimalDesign\$remove_OptimalDesignBlock(object, i) - Remove the OptimalDesignBlock having index i

Fields

\$OptimalDesignBlock - A list of [so_OptimalDesignBlock](#) objects
 \$type - A character string attribute

so_OptimalDesignBlock *so_OptimalDesignBlock reference class*

Description

Reference Class for the SO/SOBlock/OptimalDesign/OptimalDesignBlock element of a PharmML-SO data structure

Methods

so_OptimalDesignBlock\$new() - Create a new empty so_OptimalDesignBlock object

Fields

\$FIM - A matrix
\$CovarianceMatrix - A matrix
\$ParameterPrecision - A data.frame
\$Criteria - A data.frame
\$Tests - A data.frame
\$SimulatedData - A [so_ExternalFile](#) object
\$Design - A [so_ExternalFile](#) object
\$blockNumber - An integer attribute

so_OtherMethod *so_OtherMethod reference class*

Description

Reference Class for the SO/SOBlock/Estimation/PopulationEstimates/OtherMethod element of a PharmML-SO data structure

Methods

so_OtherMethod\$new() - Create a new empty so_OtherMethod object

Fields

\$Mean - A data.frame
\$Median - A data.frame
\$method - A character string attribute

so_OtherMethod_PPE *so_OtherMethod_PPE reference class*

Description

Reference Class for the SO/SOBlock/Estimation/PrecisionPopulationEstimates/OtherMethod element of a PharmML-SO data structure

Methods

so_OtherMethod_PPE\$new() - Create a new empty so_OtherMethod_PPE object

Fields

\$CovarianceMatrix - A matrix
\$CorrelationMatrix - A matrix
\$StandardDeviation - A data.frame
\$StandardError - A data.frame
\$AsymptoticCI - A data.frame
\$PercentilesCI - A data.frame

so_PharmMLRef *so_PharmMLRef reference class*

Description

Reference Class for the SO/PharmMLRef element of a PharmML-SO data structure

Methods

so_PharmMLRef\$new() - Create a new empty so_PharmMLRef object

Fields

\$Description - A character string
\$name - A character string attribute
\$id - A character string attribute

so_PopulationEstimates

so_PopulationEstimates reference class

Description

Reference Class for the SO/SOBlock/Estimation/PopulationEstimates element of a PharmML-SO data structure

Methods

so_PopulationEstimates\$new() - Create a new empty so_PopulationEstimates object

Fields

\$MLE - A data.frame

\$Bayesian - A [so_Bayesian](#) object

\$OtherMethod - A [so_OtherMethod](#) object

so_PrecisionIndividualEstimates

so_PrecisionIndividualEstimates reference class

Description

Reference Class for the SO/SOBlock/Estimation/PrecisionIndividualEstimates element of a PharmML-SO data structure

Methods

so_PrecisionIndividualEstimates\$new() - Create a new empty so_PrecisionIndividualEstimates object

Fields

\$StandardDeviation - A data.frame

\$PercentilesCI - A data.frame

so_PrecisionPopulationEstimates

so_PrecisionPopulationEstimates reference class

Description

Reference Class for the SO/SOBlock/Estimation/PrecisionPopulationEstimates element of a PharmML-SO data structure

Methods

so_PrecisionPopulationEstimates\$new() - Create a new empty so_PrecisionPopulationEstimates object

Fields

\$MLE - A [so_MLE](#) object

\$Bayesian - A [so_Bayesian_PPE](#) object

\$OtherMethod - A [so_OtherMethod_PPE](#) object

so_RandomEffects_IE *so_RandomEffects_IE reference class*

Description

Reference Class for the SO/SOBlock/Estimation/IndividualEstimates/RandomEffects element of a PharmML-SO data structure

Methods

so_RandomEffects_IE\$new() - Create a new empty so_RandomEffects_IE object

Fields

\$EffectMean - A data.frame

\$EffectMedian - A data.frame

\$EffectMode - A data.frame

\$Samples - A data.frame

so_RawResults *so_RawResults reference class*

Description

Reference Class for the SO/SOBlock/RawResults element of a PharmML-SO data structure

Methods

so_RawResults\$new() - Create a new empty so_RawResults object
so_RawResults\$add_DataFile(object) - Add a DataFile
so_RawResults\$remove_DataFile(object, i) - Remove the DataFile having index i
so_RawResults\$add_GraphicsFile(object) - Add a GraphicsFile
so_RawResults\$remove_GraphicsFile(object, i) - Remove the GraphicsFile having index i

Fields

\$DataFile - A list of data.frames
\$GraphicsFile - A list of [so_ExternalFile](#) objects

so_Residuals *so_Residuals reference class*

Description

Reference Class for the SO/SOBlock/Estimation/Residuals element of a PharmML-SO data structure

Methods

so_Residuals\$new() - Create a new empty so_Residuals object

Fields

\$ResidualTable - A data.frame
\$EpsShrinkage - A data.frame

so_Simulation	<i>so_Simulation reference class</i>
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Description

Reference Class for the SO/SOBlock/Simulation element of a PharmML-SO data structure

Methods

so_Simulation\$new() - Create a new empty so_Simulation object
 so_Simulation\$add_SimulationBlock(object) - Add a SimulationBlock
 so_Simulation\$remove_SimulationBlock(object, i) - Remove the SimulationBlock having index i

Fields

\$SimulationBlock - A list of [so_SimulationBlock](#) objects

so_SimulationBlock	<i>so_SimulationBlock reference class</i>
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Description

Reference Class for the SO/SOBlock/Simulation/SimulationBlock element of a PharmML-SO data structure

Methods

so_SimulationBlock\$new() - Create a new empty so_SimulationBlock object
 so_SimulationBlock\$add_SimulatedProfiles(object) - Add a SimulatedProfiles
 so_SimulationBlock\$remove_SimulatedProfiles(object, i) - Remove the SimulatedProfiles having index i
 so_SimulationBlock\$add_IndivParameters(object) - Add a IndivParameters
 so_SimulationBlock\$remove_IndivParameters(object, i) - Remove the IndivParameters having index i
 so_SimulationBlock\$add_RandomEffects(object) - Add a RandomEffects
 so_SimulationBlock\$remove_RandomEffects(object, i) - Remove the RandomEffects having index i
 so_SimulationBlock\$add_Covariates(object) - Add a Covariates
 so_SimulationBlock\$remove_Covariates(object, i) - Remove the Covariates having index i
 so_SimulationBlock\$add_Regressors(object) - Add a Regressors
 so_SimulationBlock\$remove_Regressors(object, i) - Remove the Regressors having index i
 so_SimulationBlock\$add_PopulationParameters(object) - Add a PopulationParameters
 so_SimulationBlock\$remove_PopulationParameters(object, i) - Remove the PopulationParameters

having index i

so_SimulationBlock\$add_Dosing(object) - Add a Dosing

so_SimulationBlock\$remove_Dosing(object, i) - Remove the Dosing having index i

Fields

\$SimulatedProfiles - A list of [so_SimulationSubType](#) objects

\$IndivParameters - A list of [so_SimulationSubType](#) objects

\$RandomEffects - A list of [so_SimulationSubType](#) objects

\$Covariates - A list of [so_SimulationSubType](#) objects

\$Regressors - A list of [so_SimulationSubType](#) objects

\$PopulationParameters - A list of [so_SimulationSubType](#) objects

\$Dosing - A list of [so_SimulationSubType](#) objects

\$RawResultsFile - A [so_ExternalFile](#) object

\$replicate - An integer attribute

so_SimulationSubType	<i>so_SimulationSubType reference class</i>
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Description

Reference Class for the SimulationSubType element of a PharmML-SO data structure

Methods

so_SimulationSubType\$new() - Create a new empty so_SimulationSubType object

Fields

\$name - A character string attribute

\$extFileNo - An integer attribute

so_SO	<i>so_SO reference class</i>
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Description

Reference Class for the SO element of a PharmML-SO data structure

Methods

so_SO\$new() - Create a new empty so_SO object
 so_SO\$write(filename, pretty=TRUE) - Write an SO to file. Set pretty to FALSE to not get pretty printed xml
 so_SO\$add_SOBlock(object) - Add a SOBlock
 so_SO\$remove_SOBlock(object, i) - Remove the SOBlock having index i
 so_SO\$all_population_estimates() - Get a data.frame with the population estimates from all SOBlocks
 so_SO\$all_standard_errors() - Get a data.frame with the standard errors from all SOBlocks
 so_SO\$variability_type(parameter_names) - Given an array of parameter names return an array with the variability type of the parameters
 Types are: structParameter, parameterVariability and residualError
 so_SO\$correlation_parameters(parameter_names) - Given an array of parameter names return an array of whether each parameter is a correlation or not
 so_SO\$random_variable_from_variability_parameter(parameter_names) - Given an array of parameter names return an array of names of the corresponding random variable

Fields

\$Description - A character string
 \$PharmMLRef - A [so_PharmMLRef](#) object
 \$SOBlock - A list of [so_SOBlock](#) objects
 \$id - A character string attribute
 \$metadataFile - A character string attribute

 so_SOBlock

so_SOBlock reference class

Description

Reference Class for the SO/SOBlock element of a PharmML-SO data structure

Methods

so_SOBlock\$new() - Create a new empty so_SOBlock object

Fields

\$ToolSettings - A [so_ToolSettings](#) object
 \$RawResults - A [so_RawResults](#) object
 \$TaskInformation - A [so_TaskInformation](#) object
 \$Estimation - A [so_Estimation](#) object
 \$Simulation - A [so_Simulation](#) object
 \$ModelDiagnostic - A [so_ModelDiagnostic](#) object
 \$OptimalDesign - A [so_OptimalDesign](#) object

\$blkId - A character string attribute

so_SO_read *Read an SO file*

Description

Function to read an SO file from disk into a Reference Class tree structure

so_TargetToolMessages *so_TargetToolMessages reference class*

Description

Reference Class for the SO/SOBlock/Estimation/TargetToolMessages element of a PharmML-SO data structure

Methods

so_TargetToolMessages\$new() - Create a new empty so_TargetToolMessages object

Fields

\$Termination - A character string
\$Warnings - A character string
\$Errors - A character string
\$ElapsedTime - A numeric
\$OutputFilePath - A [so_ExternalFile](#) object
\$ChainsNumber - A numeric
\$IterationNumber - A numeric

so_TaskInformation *so_TaskInformation reference class*

Description

Reference Class for the SO/SOBlock/TaskInformation element of a PharmML-SO data structure

Methods

so_TaskInformation\$new() - Create a new empty so_TaskInformation object
so_TaskInformation\$add_Message(object) - Add a Message
so_TaskInformation\$remove_Message(object, i) - Remove the Message having index i
so_TaskInformation\$add_OutputFilePath(object) - Add a OutputFilePath
so_TaskInformation\$remove_OutputFilePath(object, i) - Remove the OutputFilePath having index i

Fields

\$Message - A list of [so_Message](#) objects
\$OutputFilePath - A list of [so_ExternalFile](#) objects
\$RunTime - A numeric
\$NumberChains - An integer
\$NumberIterations - An integer

so_ToolSettings *so_ToolSettings reference class*

Description

Reference Class for the SO/SOBlock/ToolSettings element of a PharmML-SO data structure

Methods

so_ToolSettings\$new() - Create a new empty so_ToolSettings object
so_ToolSettings\$add_File(object) - Add a File
so_ToolSettings\$remove_File(object, i) - Remove the File having index i

Fields

\$File - A list of [so_ExternalFile](#) objects

Index

- *Topic **dv_column_name**
 - dv_column_name, 3
- *Topic **dv_column**
 - dv_column, 2
- *Topic **id_column_name**
 - id_column_name, 4
- *Topic **id_column**
 - id_column, 4
- *Topic **idv_column_name**
 - idv_column_name, 3
- *Topic **idv_column**
 - idv_column, 3
- *Topic **package**
 - libsoc, 4
- *Topic **so_Bayesian_PPE**
 - so_Bayesian_PPE, 6
- *Topic **so_Bayesian**
 - so_Bayesian, 5
- *Topic **so_DiagnosticIndividualParams**
 - so_DiagnosticIndividualParams, 6
- *Topic **so_DiagnosticStructuralModel**
 - so_DiagnosticStructuralModel, 7
- *Topic **so_Estimates**
 - so_Estimates, 7
- *Topic **so_Estimation**
 - so_Estimation, 8
- *Topic **so_ExternalFile**
 - so_ExternalFile, 8
- *Topic **so_IndividualEstimates**
 - so_IndividualEstimates, 9
- *Topic **so_InformationCriteria**
 - so_InformationCriteria, 9
- *Topic **so_MLE**
 - so_MLE, 11
- *Topic **so_Message**
 - so_Message, 10
- *Topic **so_MissingData**
 - so_MissingData, 10
- *Topic **so_ModelDiagnostic**
 - so_ModelDiagnostic, 11
- *Topic **so_OFMeasures**
 - so_OFMeasures, 12
- *Topic **so_OptimalDesignBlock**
 - so_OptimalDesignBlock, 13
- *Topic **so_OptimalDesign**
 - so_OptimalDesign, 12
- *Topic **so_OtherMethod_PPE**
 - so_OtherMethod_PPE, 14
- *Topic **so_OtherMethod**
 - so_OtherMethod, 13
- *Topic **so_PharmMLRef**
 - so_PharmMLRef, 14
- *Topic **so_PopulationEstimates**
 - so_PopulationEstimates, 15
- *Topic **so_PrecisionIndividualEstimates**
 - so_PrecisionIndividualEstimates, 15
- *Topic **so_PrecisionPopulationEstimates**
 - so_PrecisionPopulationEstimates, 16
- *Topic **so_RandomEffects_IE**
 - so_RandomEffects_IE, 16
- *Topic **so_RawResults**
 - so_RawResults, 17
- *Topic **so_Residuals**
 - so_Residuals, 17
- *Topic **so_SOBlock**
 - so_SOBlock, 20
- *Topic **so_SO_read**
 - so_SO_read, 21
- *Topic **so_SO**
 - so_SO, 19
- *Topic **so_SimulationBlock**
 - so_SimulationBlock, 18
- *Topic **so_SimulationSubType**

- so_SimulationSubType, 19
- *Topic **so_Simulation**
 - so_Simulation, 18
- *Topic **so_TargetToolMessages**
 - so_TargetToolMessages, 21
- *Topic **so_TaskInformation**
 - so_TaskInformation, 22
- *Topic **so_ToolSettings**
 - so_ToolSettings, 22

- dv_column, 2
- dv_column_name, 3

- id_column, 4
- id_column_name, 4
- idv_column, 3
- idv_column_name, 3

- libsoc, 4
- libsoc-package (libsoc), 4

- so_Bayesian, 5, 15
- so_Bayesian_PPE, 6, 16
- so_DiagnosticIndividualParams, 6, 11
- so_DiagnosticStructuralModel, 7, 11
- so_Estimates, 7, 9
- so_Estimation, 8, 20
- so_ExternalFile, 8, 13, 17, 19, 21, 22
- so_IndividualEstimates, 8, 9
- so_InformationCriteria, 9, 12
- so_Message, 10, 22
- so_MissingData, 8, 10
- so_MLE, 11, 16
- so_ModelDiagnostic, 11, 20
- so_OFMeasures, 8, 12
- so_OptimalDesign, 12, 20
- so_OptimalDesignBlock, 12, 13
- so_OtherMethod, 13, 15
- so_OtherMethod_PPE, 14, 16
- so_PharmMLRef, 14, 20
- so_PopulationEstimates, 8, 15
- so_PrecisionIndividualEstimates, 8, 15
- so_PrecisionPopulationEstimates, 8, 16
- so_RandomEffects_IE, 9, 16
- so_RawResults, 17, 20
- so_Residuals, 8, 17
- so_Simulation, 18, 20
- so_SimulationBlock, 18, 18
- so_SimulationSubType, 19, 19
- so_S0, 19
- so_S0_read, 21
- so_S0Block, 20, 20
- so_TargetToolMessages, 8, 21
- so_TaskInformation, 20, 22
- so_ToolSettings, 20, 22