

# Package ‘libsoc’

February 3, 2022

**Version** 0.7.3

**Date** 2022-02-03

**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>

**License** LGPL-3

**Copyright** 2015-2022 Rikard Nordgren

**Repository** CRAN

**Date/Publication** 2022-02-03 15:40:02 UTC

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 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>
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---

**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	<a href="http://xmlsoft.org">http://xmlsoft.org</a>
libiconv	<a href="https://www.gnu.org/software/libiconv">https://www.gnu.org/software/libiconv</a>
zlib	<a href="http://www.zlib.net">http://www.zlib.net</a>

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*

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### 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

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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

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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

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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    *so\_SimulationSubType reference class*

---

### 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                            *so\_SO reference class*

---

### 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

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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

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