

# SBMLeDitor's guide

## Plan

1 - Installing SBMLeditor

2 - How to navigate through SBMLeditor, keyboard shortcuts and right click

3 - How to create an SBML file

## **1- Installing SBMLeditor**

You will find useful information about SBMLeditor installation on the page :  
<http://www.ebi.ac.uk/compneur-srv/SBMLeditor.html>

Here are the information provided on this page :  
In order to run properly SBMLeditor you will need first to install the Java JRE  
you can download from the Java web site :  
<http://java.sun.com/javase/downloads/index.jsp>

After downloading and installing properly the Java JRE, you can download the  
installer on the address cited previously.

SBMLeditor has been successfully tested on Linux, Mac OS X and Windows  
machine.

## **2 – Navigate through SBMLEditor**

SBMLEditor has an really intuitive interface.

Everything can be done by doing right click on the various elements.

We strongly advise users to first try by navigate through the different sub menus displayed by right clicking on the various elements created on the SBMLEditor window and through the tree structure of the SBML file displayed into the main window.

There is also a lot of shortcuts you may want to use.

You can type these shortcuts anywhere in the tree, you will automatically be moved to the right place. If no listOf is present for the element you want to add, it will be added automatically at the same time as your element.

Here is a list of shortcuts to use in the tree :

- Ctrl-I : add a FunctionDefinition
- Ctrl-C : add a Compartment
- Ctrl-S : add a Species
- Ctrl-P : add a Parameter
- Ctrl-T : add a RateRule
- Ctrl-M : add an AssignmentRule
- Ctrl-G : add an AlgebraicRule
- Ctrl-R : add a Reaction
- Ctrl-E : add an Event

Depending on the context you will be able to use those shorcuts :

- ctrl-U : add a UnitDefinition or Unit
- Ctrl-B : add a Product (in a listOfReaction field)
- Ctrl-A : add a Reactant (in a listOfReaction field)
- Ctrl-D : add a Modifier (in a listOfReaction field)
- Ctrl-L : add a local parameter (in a listOfReaction field)
- Ctrl-H : add an EventAssignement (in a listOfEvents field)
- Ctrl-K : add a KineticLaw (in a listOfReaction field) ?

In the main tree you will also be able to use those shortcuts :

- E : edit the selected element
- D : delete the selected element

- Ctrl-N : create a new SBML file
- Ctrl-O : open a SBML file
- Ctrl-V : validate the current model
- Ctrl-F : find/search for a name or id
- Ctrl-W : save the current model to a file

Ctrl-Q : close the window, if it's the last window, close the application  
Ctrl++ : expand all nodes from selected  
Ctrl-- : collapse all nodes from selected

### **3 – How to create an SBML file**

Using SBMLEditor must be really intuitive and users will be using a lot the right click of their mouse (for mac user, the right click can be done by pressing the Ctrl and then click with their mouse).

#### **A – First : Create a new SBML file or import a SBML file**

In order to create a new SBML file, users will have to choose between clicking on the button New on the left side of the button bar or to click on File menu then New.

The id and the name are automatically generated for the model, but you will be able to change the name but not the id.

A structure of an SBML file will be generated. By default, the file will be SBML level 2, version 1, therefore, it is possible to change this to version 1, level 2 by clicking on the File menu and then by choosing the version of the SBML file you want to create.

If you want to import an SBML file, user can click either on the File menu then Open... or they can click on the open file button on the button bar and then choose the file they want to import.

#### **B – Save and validate an SBML file**

Each time you will want to save an SBML file, SBMLEditor will automatically check if the SBML file is compliant with the SBML specifications.

You can also directly check the validity of your SBML file by clicking either on the blue and red button (see fig) or on the File menu and then choosing validate.

#### **C – Adding parts to the SBML file**

When a file is created you can, by doing a right click on *model*, choose every part you want to create in your SBML file. See Figure 1 for details :

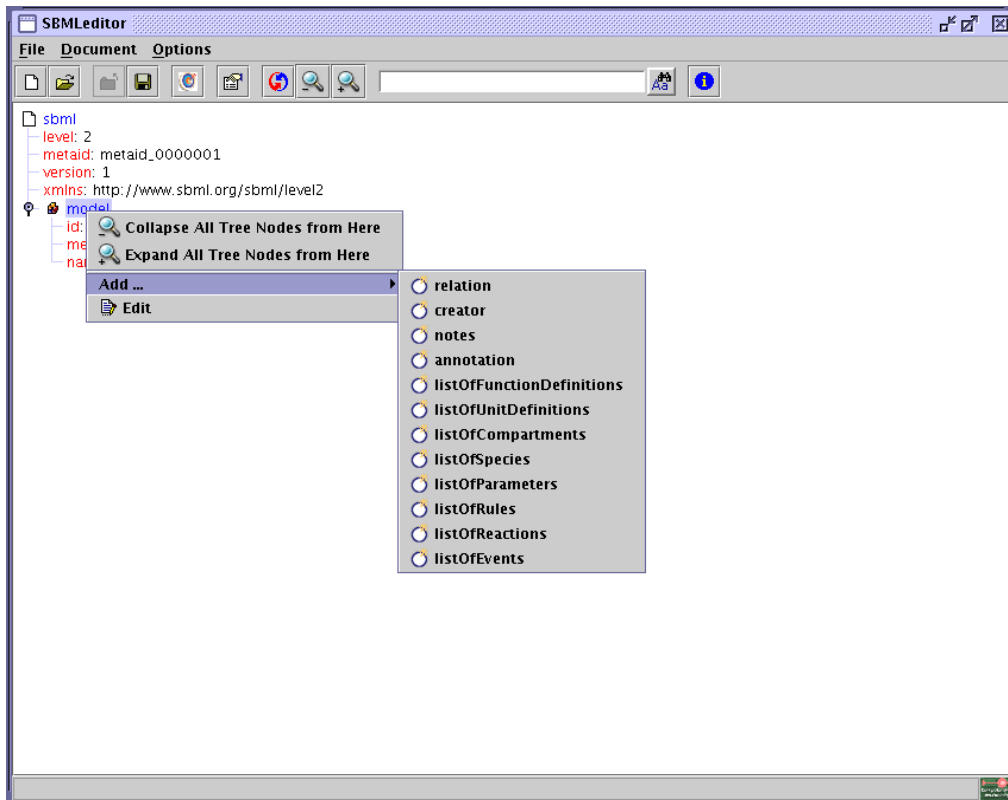


Figure 1: Mouse Menu on the model element

Every time you will want to add an element you will have to create first the list of corresponding to the part you want to create and then to right click on the list of and choose "Add New ". See Figure 2 for example :

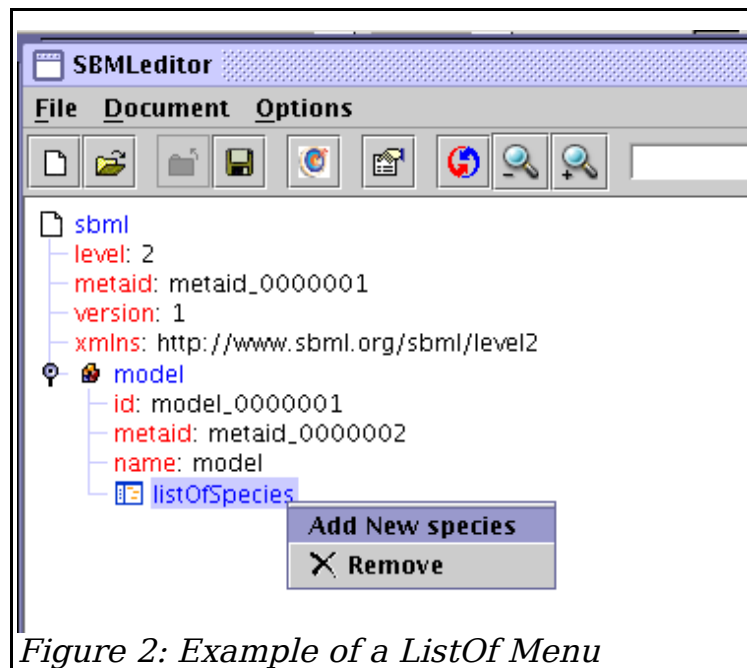
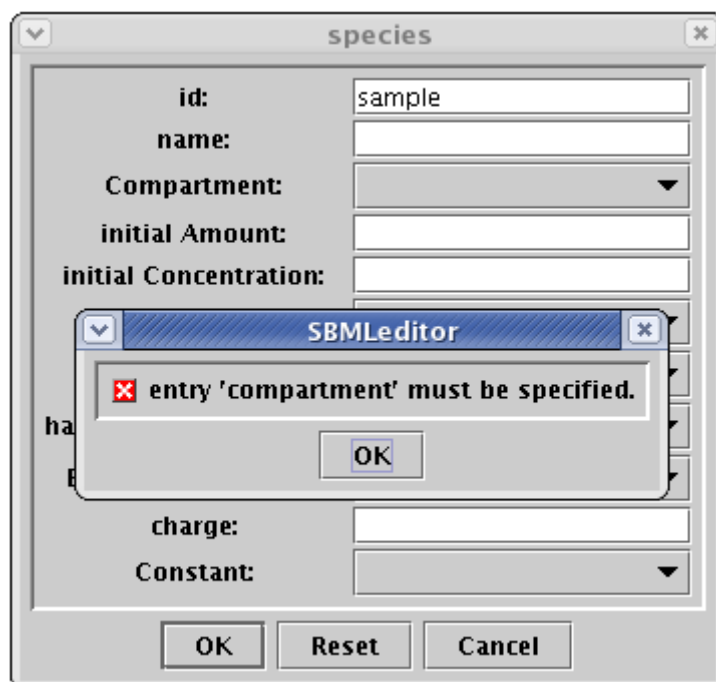


Figure 2: Example of a ListOf Menu

For everything you will create you will be asked to give an id and all the information required for the type of SBML element you have added. The id

must be chosen carefully because it will not be possible to change it afterwards with SBMLeditor, you may be able to change it directly in the SBML file with a text editor but users must be aware that it could create problem of id conflict in the model. In addition, the id must begin with a letter or an underscore and can't have symbol others that letter, number or underscore.

If in SBMLeditor you are not giving all the information required or if you are doing a mistake, SBMLeditor will tell you what is the mistake and eventually how to correct it (see figure 3).



*Figure 3 – SBMLeditor detects the error and provides an help in order to correct it*

For further information about the SBML specifications we strongly recommend to look to the SBML website : <http://www.sbml.org/> and search in the documentation section for the latest specifications.

## **D – Details for each Element**

### **1) Creation of Annotations, Notes, Contributors, Creators**

SBMLeditor provides a way to add useful informations to the SBML file for further use of the file by other people not used to the model described by the file.

So, by right clicking on “sbml” in the main window and then clicking on Add...

you can choose to add Contributors, Notes, Annotations (see fig 4).

Contributor fields are : Family Name, Given Name, email, and Organization name.

For Notes and Annotations, a new window is provided with the tags which will be inserted into the XML. Therefore, the user need to write between those tags in order to avoid to have an error message because SBMLEditor check the integrity of the SBML file and does not authorize error in it

By right clicking on “model” in addition of those previously cited, the user will be able to add a Creator field which has the same fields as Contributor.

Then, for every field, the user will be able to create annotations or notes.

## **2) Creation of a relation field**

By right clicking on model, as previously explained, the user will be able to create every fields allowed by SBML lib.

So, it is possible to create an Relation field (see fig 5) where the user is able to define the Qualifier (see [http://sbml.org/wiki/Biomodels\\_Qualifiers](http://sbml.org/wiki/Biomodels_Qualifiers) for details) and the URIs (see [http://sbml.org/wiki/MIRIAM\\_URI\\_Set](http://sbml.org/wiki/MIRIAM_URI_Set) for details). When the user clicks on one URIs among the selection, SBMLEditor automatically fill in the URI field and the user therefore has to enter a proper ID compliant with the URI. For example, if the user clicks on Gene Ontology, the ID will be automatically filled by the tern “GO:” and if you put your mouse on the ID field, an contextual help will be provided to help user to enter the correct form of the ID (see fig 6).

## **3) Creation of an Function Definition**

The first thing to do is to create an listOfFunctionDefinitions by right clicking on “model”. After it is created, right click on listOfFunctionDefinitions and choose “Add New functionDefinition”, a new window will be displayed (see figure 7), where you will be able to rename the id, give a name (if you want) and edit the MathML. If you've written your MathML formula directly between the tags you can choose to untick the “Open mathML editor”.

### **a) MathML editor**

If you have problem with the MathML syntax, you can avoid to write anything into the mathML field, let the “Open mathML editor” ticked and click on Ok. You will be then invited to write directly the formula into the mathML editor (see figure 8).

In this window you can write directly using infix notation which is more natural, the MathML editor will translate the formula in a MathML format.

In addition, MathML editor window displays a lot of options. As in any other editor, you can cut, paste, undo, redo (all available from the button bar or the Edit menu). You can also Save in order to write the MathML formula into your

SBML file (you can do it either by clicking on the floppy disk in the button bar or in the File menu). After you saved you will have to Exit in order to get back to the main SBMLeditor window.

In the File menu you also can Export in image format (png, jpg), text format (txt) or in Windows Meta format (wmf) and choose where you want to save the file.

It is possible to export under mathML format (mml) by choosing either Presentation Markup or Content Markup.

If you want to use power in your formula or fraction you will have either to write the formula in its mathematical form (e.g :  $2/3$ ) or you may choose the Layout button under the button bar (or in the Insert menu), you will therefore choose what to put in power or which part to divide by another part.

If you have problem with having a clear view of the different levels you can choose in the View menu to Highlights the Levels.

As you cannot write your formula in more than one line you may experience problem with having a general view of your entire formula, especially if it is a long one. In the View menu you will be able to Zoom Out or Zoom in. If you choose Zoom normal, the view will go back to the default one.

In the Help menu you can have a look to all the shortcuts you can use into the Equation editor by clicking on Readme (see fig 9).

#### **4) Creation of a list of unit definitions**

To create a list of unit definition you need to right click on “model” and then choose Add... and finally listOfUnitDefinitions (see fig10 ?)

A new field listOfUnitDefinitions will appear, you then have to right click on this field and click on Add New UnitDefinition. A new window will be displayed and you will be able to change the id which is automatically generated and give a name (this is optional). Pay attention to the id you choose because once you've clicked on Ok, you won't be allowed to change the id.

When your list of units is created you have to click right on the field “list of Units” and then choose “Add New unit”. In the new window, you will have to choose what is the unit kind between the 33 values possible. It is the only field you have to fill (if you don't, SBMLeditor will display an error and ask you to choose a unit kind). You can after this choose what to enter in the different optional fields (Exponent, Scale, Multiplier).

#### **5) Creation of a list of Compartments**

To create a list of unit definition you need to right click on “model” and then choose Add... and finally listOfCompartments (see fig11 ?).

A new field ListOfCompartments will appear, you then have to right click on this field and click on Add New Compartment.

In the new window, there is no required field except the id which is automatically pre-filled. You can choose to modify everything you need between the fields id, name, size, spatialDimensions, unit, outside, constant (see fig 12).

From the new compartment you create you can add a relation as described on part C, 1. But you will not be able to choose the URI which is Gene ontology.

Please notice that the list of URIs are following the definitions of the SBML site (<http://www.biomodels.net/miriam/>). If you want to add your own URI, you can use the "Submit New" form on the web site.

## **6) Creation of a list of Species**

To create a list of Species you need to right click on "model" and then choose Add... and finally listOfSpecies (see fig12 ?).

A new field ListOfSpecies will appear, you then have to right click on this field and click on Add New species.

In the new window (see fig 13), you can choose the id, the name, Compartment (beware that if you didn't previously create an compartment you will not be allowed to create species), initial Amount, initial Concentrations, substanceUnits, spatialSizeUnits, OnlySubstanceUnits, Boundary Conditions, charge, constant (by default the charge is positive, you will have to specify the negative charge, e.g : -2).

According to SBML specifications, the fields hasOnlySubstanceUnits, boundaryCondition, constant, have default value "false". It is not specified into the window and you can either "confirm" the value false or change the value to "true".

## **7) Creation of a list of Parameters**

To create a list of Parameters you need to right click on "model" and then choose Add... and finally listOfParameters (see fig14 ?).

A new field ListOfParameters will appear, you then have to right click on this field and click on Add New parameter.

In the new window, you will be able to choose the id, name, value, unit, constant. Except for the id which is automatically generated and that you have to specify, none of the fields are required. Please pay attention to the fact that the constant field has two choices true and false and by default, as defined on the SBML specifications, the value is true.

SBML allows two kind of parameters, the one you create from the list of Parameters will be global.

But you will be also allowed to create a local parameter which will be assigned to a specific reaction (this can be done from the MathML editor, for ruther explanation please see the section 9 – a) MathML editor).

## **8) Creation of a list of Rules**

To create a list of Rules you need to right click on “model” and then choose Add... and finally listOfRules (see fig15 ?).

A new field ListOfRules will appear, you then have to right click on this field and by selection “Add new...” you will have to choose between 3 different rules (see fig 16).

### **a) Algebraic Rules**

A new window will be displayed in which you will be able to enter the formula directly in MathML format or you can choose to open the MathML editor by clicking on OK without deticking the field “Open mathML editor”. Behaviour of MathML editor will be described in the d) part of this section.

### **b) Assignment rules**

In this window where you will be invited to enter the formula directly in mathML format, you will also have the possibility to choose your Tag type and you will have to choose the variable, otherwise SBMLEditor will not allow you to continue.

Then if you want to use the MathML editor, click on OK without deticking the Open MathML editor field. Behaviour of MathML editor will be described in the d) part of this section.

### **c) Rate Rule**

In this window where you will be invited to enter the formula directly in mathML format, you will also have the possibility to choose your Tag type and you will have to choose the variable, otherwise SBMLEditor will not allow you to continue.

Then if you want to use the MathML editor, click on OK without deticking the Open MathML editor field. Behaviour of MathML editor will be described in the d) part of this section.

### **d) MathML editor**

In this window you can write either directly in mathML or in a mathematical way, the MathML editor will translate the formula in a MathML format. But you also can use the both ways in the same formula.

In addition, MathML editor window displays a lot of options. As in any other editor, you can cut, paste, undo, redo (all available from the button bar or the

Edit menu). You can also Save in order to write the MathML formula into your SBML file (you can do it either by clicking on the floppy disk in the button bar or in the File menu). After you saved you will have to Exit in order to get back to the main SBMLeditor window.

In the File menu you also can Export in image format (png, jpg), text format (txt) or in Windows Meta format (wmf) and choose where you want to save the file.

It is possible to export under mathML format (mml) by choosing either Presentation Markup or Content Markup.

If you want to use power in your formula or fraction you will have either to write the formula in its mathematical form (e.g :  $2/3$ ) or you may choose the Layout button under the button bar (or in the Insert menu), you will therefore choose what to put in power or which part to divide by another part.

If you have problem with having a clear view of the different levels you can choose in the View menu to Highlights the Levels.

As you cannot write your formula in more than one line you may experience problem with having a general view of your entire formula, especially if it is a long one. In the View menu you will be able to Zoom Out or Zoom in. If you choose Zoom normal, the view will go back to the default one.

In the Help menu you can have a look to all the shortcuts you can use into the Equation editor by clicking on Readme (see fig 9).

At the bottom at the window you have three different menus.

Starting from the left, the first menu allows you to choose if you want to add into you rule a functionDefinition, a compartement, a specie, a parameter.

Once you have chosen the category you want, the middle menu will display all the elements contained into your category.

If you realized that you forgot to create an element you can still click on the right button named "Add New..." and choose to create a new compartment, species or parameter.

A window corresponding to the element you want to create is displayed and you can create it.

For further informations about those elements you can create, please refer to the corresponding parts.

## **9) Creation of a listOfReactions**

To create a list of Reactions you need to right click on "model" and then choose Add... and finally listOfReactions (see fig17 ?).

A new field ListOfReactions will appear , you then have to right click on this field and by selection "Add new...".

In the window displayed you will be able to change the id, the name and the reversible and fast fields. Please note that the default value of the optional field Reversible is true, according to SBML specifications.

Once you have filled all the field you want, you will be able to choose if you want to create the kinetic law or not.

If you don't want to create the kinetic law you will have to detick the "Open mathML editor" field.

If you want to right the kinetic law with the help of the mathML editor, just click on OK.

#### a) MathML editor

In this window you can write either directly in mathML or in a mathematical way, the MathML editor will translate the formula in a MathML format. But you also can use the both ways in the same formula.

In addition, MathML editor window displays a lot of options. As in any other editor, you can cut, paste, undo, redo (all available from the button bar or the Edit menu). You can also Save in order to write the MathML formula into your SBML file (you can do it either by clicking on the floppy disk in the button bar or in the File menu). After you saved you will have to Exit in order to get back to the main SBMLeditor window.

In the File menu you also can Export in image format (png, jpg), text format (txt) or in Windows Meta format (wmf) and choose where you want to save the file.

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If you want to use power in your formula or fraction you will have either to write the formula in its mathematical form (e.g :  $2/3$ ) or you may choose the Layout button under the button bar (or in the Insert menu), you will therefore choose what to put in power or which part to divide by another part.

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In the Help menu you can have a look to all the shortcuts you can use into the Equation editor by clicking on Readme (see fig 9).

At the bottom at the window you have three different menus.

Starting from the left, the first menu allows you to choose if you want to add into you rule a functionDefinition, a compartement, a specie, a parameter, a local parameter.

Once you have chosen the category you want, the middle menu will display all the elements contained into your category.

If you realized that you forgot to create an element you can still click on the right button named "Add New..." and choose to create a new compartment, species or parameter.

A window corresponding to the element you want to create is displayed and you can create it.

For further informations about those elements you can create, please refer to the corresponding parts.

#### b) Additional parts to the reaction

Once you've created and defined the kinetic law. You may have to create Reactants, Products or Modifiers.

This can be done by right clicking on reaction then choosing either listOfReactants, listOfProducts or listOfProducts.

You will have then to right click of the list you've created and choose "Add a new speciesReference". A new window will appear

In this window you will have to choose the specie you want to add with the species menu (on top). Then you will be able to choose the stoichiometry.

You can directly write in the huge StoichiometryMath white space the mathML equation.

If you want to have the help of the MathML editor don't forget to tick the Open MathML editor box on bottom left.

For further explanations about the MathML editor please refer to the previous section.

### **10) Creation of a list of Events**

To create a list of Events you need to right click on "model" and then choose Add... and finally listOfEvents (see fig17 ?).

A new field ListOfEvents will appear , you then have to right click on this field and by selection "Add new Event".

In the window displayed you will be able to change the id, name and timeUnits.

Once you've written what you want and clicked on OK a new window named "Define a trigger" will appear. It's basically a mathML editor window (for more explanations about this editor please see the section 9-a) MathML editor).

Once you've written your trigger, validate it by clicking on OK.

In the trigger sub-tree you will have a creation of a List of Event Assignments.

By right clicking on List of Event Assignments and then choosing "Add New eventAssignment" you will make appearing a new window.

In this window, you will be asked to choose the Tag types and variable from the two top menu.

Then in the great blank MathML screen you will be able to write directly the formula you want in a mathML format or you can click on OK and let ticked the Open mathML editor box.

By doing this you will have the possibility to write directly the formula into the Equation editor window.

More explanations about this window in the 9 - a section.