

# Welcome to EasyModel

This tutorial will teach you how to create and simulate your first model using EasyModel.

In each slide you will find general annotations, indicating how you can use the interface to create your model.

To start the tutorial press next (or press skip to use EasyModel).

Information buttons can be found across the application.

Public models. Models can be modified as changes won't be saved.

Create and modify your personal models. Changes will be saved every time the model is validated.



A local SBML model file may be imported to EasyModel.

The screenshot shows the EasyModel application interface. On the left, there is a sidebar with an information icon (i) at the top. Below it, the 'Model Repository' section has two radio buttons: 'Public' and 'Private', with 'Private' selected. Underneath is the 'Import SBML file from disk' section with an 'Import SBML' button. On the right, the main area is titled 'Select Model' and contains a large empty list box. Below this is the 'Model Description' section with another empty text area. At the bottom of the main area are three buttons: 'New Model' (circled in red), 'Delete Model', and 'Load Model'. Red arrows point from text annotations to these elements: from the information icon to the sidebar, from the 'Public' radio button to the 'Public models' text, from the 'Private' radio button to the 'Create and modify your personal models' text, from the 'Import SBML' button to the 'A local SBML model file may be imported' text, from the empty list box to 'List of models (empty)', from the empty description area to 'Selected model description', and from the 'New Model' button to 'Press 'New' to create a new model'.

List of models (empty)

Selected model description

Press 'New' to create a new model















**Name**

BIOMD003 Goldbeter1991 - Min Mit Oscil

**Description**

<div class="dc:title">Goldbeter1991 - Min Mit Os...

**Reactions**

R1		-> C	
R2		C ->	
R3		C -> ; X	
R4		-> M; C; M	
R5		M ->	
R6		-> X; M; X	
R7		X ->	

Add Reaction **Define Rates** Species

Validate

Start by naming your model.

Description is optional, but recommended.

Define reactions using Substrates, Products and Modifiers.

How to write reactions:

$n_1 \cdot S_1 + n_2 \cdot S_2 + \dots \rightarrow m_1 \cdot P_1 + m_2 \cdot P_2 + \dots ; M_1; M_2; \dots$

$n_i, m_i$ : Stoichiometric coefficient.

$S_i, P_i$ : Substrates and Products.

$M_i$ : Modifiers that can activate or inhibit the reaction rate.

Define the rates for each reaction.

When you're done press this

Import predefined rate expressions

Back to Model Editor			
New Rate		Import Rates	
Name	Rate Definition	Edit	Remove
BIOMD003_K1	cell*vi		
BIOMD003_K2	C*cell*kd		
BIOMD003_K3	C*cell*vd*X*(C+Kd)^-1		
BIOMD003_K4	cell*(1+-1*M)*(C*VM1*(C+K...		
BIOMD003_K5	cell*M*V2*(K2+M)^-1		
BIOMD003_K6	cell*(M*VM3)*(1+-1*X)*(K3...		
BIOMD003_K7	cell*V4*X*(K4+X)^-1		

Import Predefined Rates		
<input type="checkbox"/>	Name	Rate Definition
<input type="checkbox"/>	Power Laws	$a X_1^{g1} \dots X_n^{g1n}$
<input type="checkbox"/>	Saturating Cooperative	$v X_1^{g1} \dots X_2^{g1n} / ((KX_1 + X_1)^{g1} \dots (KX_n + X_n)^{g1n})$
<input type="checkbox"/>	Saturating	$v X_1 \dots X_2 / ((KX_1 + X_1) \dots (KX_n + X_n))$
<input type="checkbox"/>	Mass action	$a X_1^n X_1 \dots X_2^n X_n$
<input type="checkbox"/>	Henri-Michaelis menten	$(v * b : XF) / (k + b : XF)$
<input type="checkbox"/>	Hill Cooperativity	$(v * (b : XF^n)) / (k^n + b : XF^n)$
<input type="checkbox"/>	Catalytic activation	$(v * b : XF * b : MF) / ((k + b : XF) * (k_2 + b : MF))$
<input type="checkbox"/>	Competitive inhibition	$(v * b : XF * b : MF) / ((k + b : XF) + (k + b : MF / k_2))$
<input type="checkbox"/>	EZM_KE_1	$k_1 * x_1^{g1} * (x_2)^{g2}$
<div>Ok Cancel</div>		

Edit Rate

Rate Name

BIOMD003\_K1

Rate Definition

cell\*vi

Rate Options

☐ One substrate only

☐ No products

☐ One modifier only

Ok Cancel

**EASY MODEL**

**Name**  
 BIOMD003 Goldbeter1991 - Min Mit Oscil

**Description**  
 <div class="dc:title">Goldbeter1991 - Min Mit Os...

**Reactions**

R1		-> C	
R2		C ->	
R3		C -> ; X	
R4		-> M; C; M	
R5		M ->	
R6		-> X; M; X	
R7		X ->	

Reaction Rate

BIOMD003\_K1

Generic parameter values

Parameter	Numeric	Substrate	Modifier
cell	1		
vi	0.025		

For every reaction in the model select a kinetic rate and set a value for each parameter. Each parameter must have either a numeric value, a reference to a substrate, or a reference to a modifier.

Species

C	0.01	Time dependent
M	0.01	Time dependent
X	0.01	Time dependent

Define the initial values for the species.

Define the type of variable: 'Time dependent' or 'Constant'.

Model validation

Validation: OK

Stoichiometric Matrix

	R1	R2	R3	R4	R5	R6	R7
C	1	-1	-1	0	0	0	0
M	0	0	0	1	-1	0	0
X	0	0	0	0	0	1	-1

Regulatory Matrix

	R1	R2	R3	R4	R5	R6	R7
C	0	0	0	1	0	0	0
M	0	0	0	1	0	1	0
X	0	0	1	0	0	1	0

Press 'Validate' to check if model is appropriately defined and ready to be simulated. Model will be saved in your account if you are logged in (a message will be displayed).

The screenshot shows the 'Dynamic Simulation' panel in the EASY MODEL software. At the top is the 'EASY MODEL' logo and an information icon. Below the title bar, there is a section for 'Dynamic Simulation' which includes an 'Enable' checkbox (checked), an 'Initial time' field set to 0, a 'Final time' field set to 60, and a 'Time step' field set to 0.1. There are also checkboxes for 'Gains' and 'Sensitivities', both of which are unchecked. Below this section are tabs for 'Steady State Simulation', 'Plot Settings', and 'Plot Views'. At the bottom of the panel is a 'Run Simulation' button. A red arrow points from the 'Dynamic Simulation' title bar to the explanatory text on the right.

Dynamic simulation: time evolution of the species in the model.

"Gains" option analyses how changes in the independent variables affect the values of the time-dependent variables.


"Sensitivities" option analyses how changes in the parameter values affect the values of the time-dependent variables.

"Stability analysis" calculates if the steady state (homeostasis) is stable (negative real parts for all eigenvalues) or not (non-negative real part for at least one eigenvalue)

The screenshot shows the 'Steady State Simulation' panel in the EASY MODEL software. It features an 'Enable' checkbox (checked), a 'Threshold' field set to  $10^{-30}$ , and checkboxes for 'Stability analysis', 'Gains', and 'Sensitivities', all of which are unchecked. An information icon is located in the top right corner. A red arrow points from the 'Steady State Simulation' title bar to the explanatory text on the right.

Steady state simulation: calculates the steady states (non-trivial equilibriums) of the biological system. These steady states remain constant over the time.

**Plot Settings**

Font Size ☒ Font Bold **Line Thickness** 






 ☐ Font Italic 

Image Width (pixels) 

Plot settings: contains several configuration parameters for the graphical plots that will be performed.


 

Dynamic Simulation

Steady State Simulation

Plot Settings

Plot Views


View 1 × New View 

Dependent variables

☒ C

☒ M

☒ X



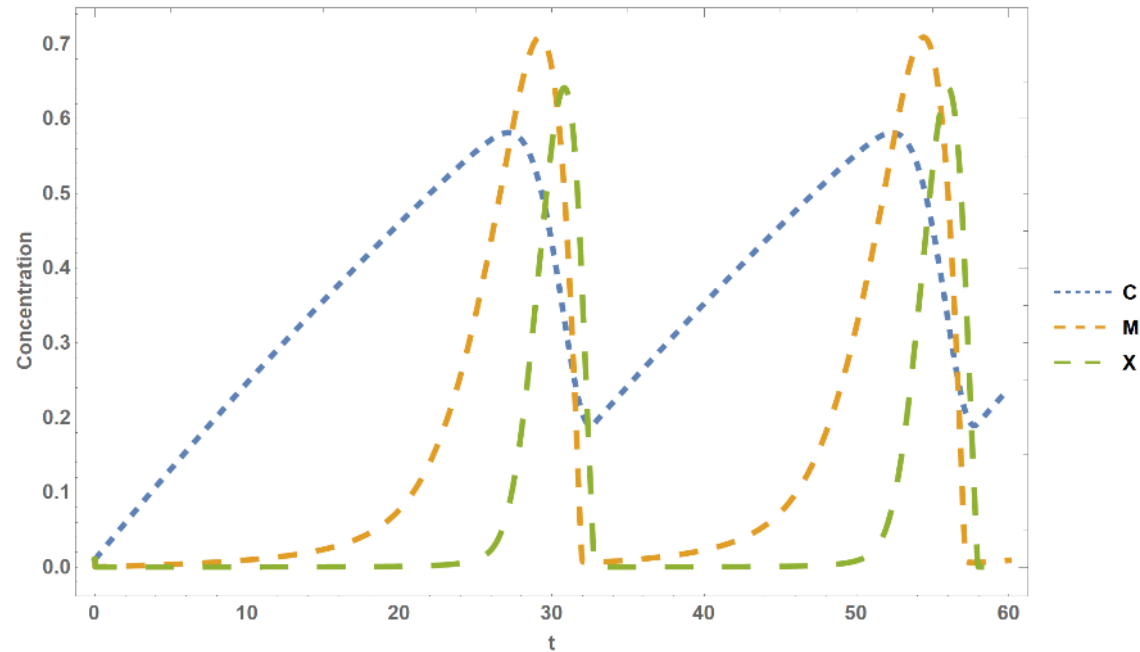
**Run Simulation**

Plot views: you can select which time-dependent species are to be plotted in the simulation graphics. Furthermore, you can define several plot views, each of them with its own selected time-dependent species.

Press 'Run Simulation' to start your simulation

## Results for BIOMD003 Goldbeter1991 - Min Mit Oscil

### Dynamic Simulation



[Download Dynamic Simulation Table](#)

### Generated Files

[Mathematica Notebook](#)

[SBML](#)



The simulation results are displayed in the final step. Clicking the cancel button aborts the simulation.

Left-click images for high-resolution copies.

You can download:

- Images
- Results text files
- Mathematica Notebook of the whole simulation
- SBML file of your model



# You have completed the tutorial!

Press next to start using EasyModel.