

# Welcome to EasyModel

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

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

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



EASY MODEL

Select Model

Model

Simulation

Results

Tools

Model

1. Start by naming your model. Description is optional

BIOMD003 Goldbeter1991 - Min Mit Oscil

Description

Model Options

+ Add Reaction

Species

Reactions

R1

-> C

R2

C ->

R3

C -> ;X

R4

-> M;C;M

R5

M ->

R6

-> X;M;X

R7

X ->

5. Select a rate for each reaction (see next slide)

6. Validate model to advance to the Simulation step

Validate Model

Model editor

How to write reactions using Substrates, Products and Modifiers:

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

$n_i, m_i$ : Stoichiometric coefficient.

$S_i, P_i$ : Substrates and Products.

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

Velocity Rates

4. Create or import rates (see next slide)

+ 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+Kc)^-1...		
BIOMD003_K5	cell*M*V2*(K2+M)^-1		
BIOMD003_K6	cell*(M*VM3)*(1+1*X)*(K3+1*X...		
BIOMD003_K7	cell*V4*X*(K4+X)^-1		

Adjustable Split Bar

Powered by WOLFRAM WEB MATHEMATICA

Rate editor



## Species Settings

Name	Initial Concentration	Variable Type
C	0.01	Time Dependent ▾
M	0.01	Time Dependent ▾
X	0.01	Time Dependent ▾

3. Set initial concentrations and variable types

Ok

Cancel

## Velocity Rates

4. Create or import rates

+ New Rate

Import Rates

## New Rate

## Rate Name

BIOMD003\_K8

## Rate Definition

$$\text{cell} * (1 - M) * (C * VM1 * (C + Kc)^{-1}) * (K1 - M + 1)$$

## Rate Options

- ☐ One substrate only  
☐ No products  
☐ One modifier only

Ok

Cancel

## Import Predefined Rates

<input type="checkbox"/>	Name	Rate Definition
<input checked="" type="checkbox"/>	Power Laws	$a X_1^{g_1} \dots X_n^{g_n}$
<input type="checkbox"/>	Saturating Cooperative	$v X_1^{g_1} \dots X_2^{g_n} / ((KX_1 + X_1)^{g_1} \dots (KX_2 + X_2)^{g_n})$
<input type="checkbox"/>	Saturating	$v X_1 \dots X_2 / ((KX_1 + X_1) \dots (KX_n + X_n))$
<input type="checkbox"/>	Mass action	$a X_1^{n_1} \dots X_2^{n_n}$
<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	$k_1 * x_1 * x_2 / (k_2 + x_2)$

Import

Cancel

## Rate -&gt; Reaction (R3)

BIOMD003\_K3

## Generic parameter values

Parameter	Numeric	Substrate	Modifier
C		C ▾	▾
Kd	0.02		▾
X			X ▾
cell	1		▾
vd	0.25		▾

Ok

Cancel

5. Select a rate for each reaction and set a value for all the rate's parameters. Each parameter must have either a numeric value, a reference to a substrate, or a reference to a modifier.

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

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

**Simulation Type**

- ☒ Deterministic
- ☐ Stochastic

**Plot Settings**

**Run Simulation**

**Dynamic Simulation**

**Dynamic Settings**

Initial time	0
Final time	100
Time step	0.1

☒ Gains  
☒ Sensitivities

**Dynamic Plot Views**

**Parameter Scan**

**Steady State Simulation**

**Steady State Settings**

Threshold	$10^{-30}$
-----------	------------

☒ Stability analysis  
☐ Gains  
☐ Sensitivities

**Parameter Scan**

**Plot Settings**

Font Size:

Image Width (pixels):

☒ Font Bold  
☐ Font Italic

Line Thickness:

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

*"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 displays the EASY MODEL software interface. On the left, the 'Simulation Type' section has 'Deterministic' selected. Below it is a 'Run Simulation' button. The main area is divided into two simulation modes: 'Dynamic Simulation' and 'Steady State Simulation'. Under 'Dynamic Simulation', the 'Dynamic Plot Views' section shows 'View 1' with 'Dependent variables' C, M, and X selected. A red dashed box highlights the 'Deterministic' option and the 'Run Simulation' button. A red arrow points from a text box explaining 'Plot views' to the 'Dependent variables' section. Another red arrow points from a text box explaining 'Parameter scan' to the 'Parameter Scan' section in the 'Steady State Simulation' area.

**Simulation Type**

- ☒ Deterministic
- ☐ Stochastic

**Plot Settings**

**Run Simulation**

**Dynamic Simulation**

**Dynamic Settings**

**Dynamic Plot Views**

View 1 × New View

**Dependent variables**

- ☒ C
- ☒ M
- ☒ X

**Parameter Scan**

**Steady State Simulation**

**Steady State Settings**

**Parameter Scan**

Select Parameters

Select Independent Variables

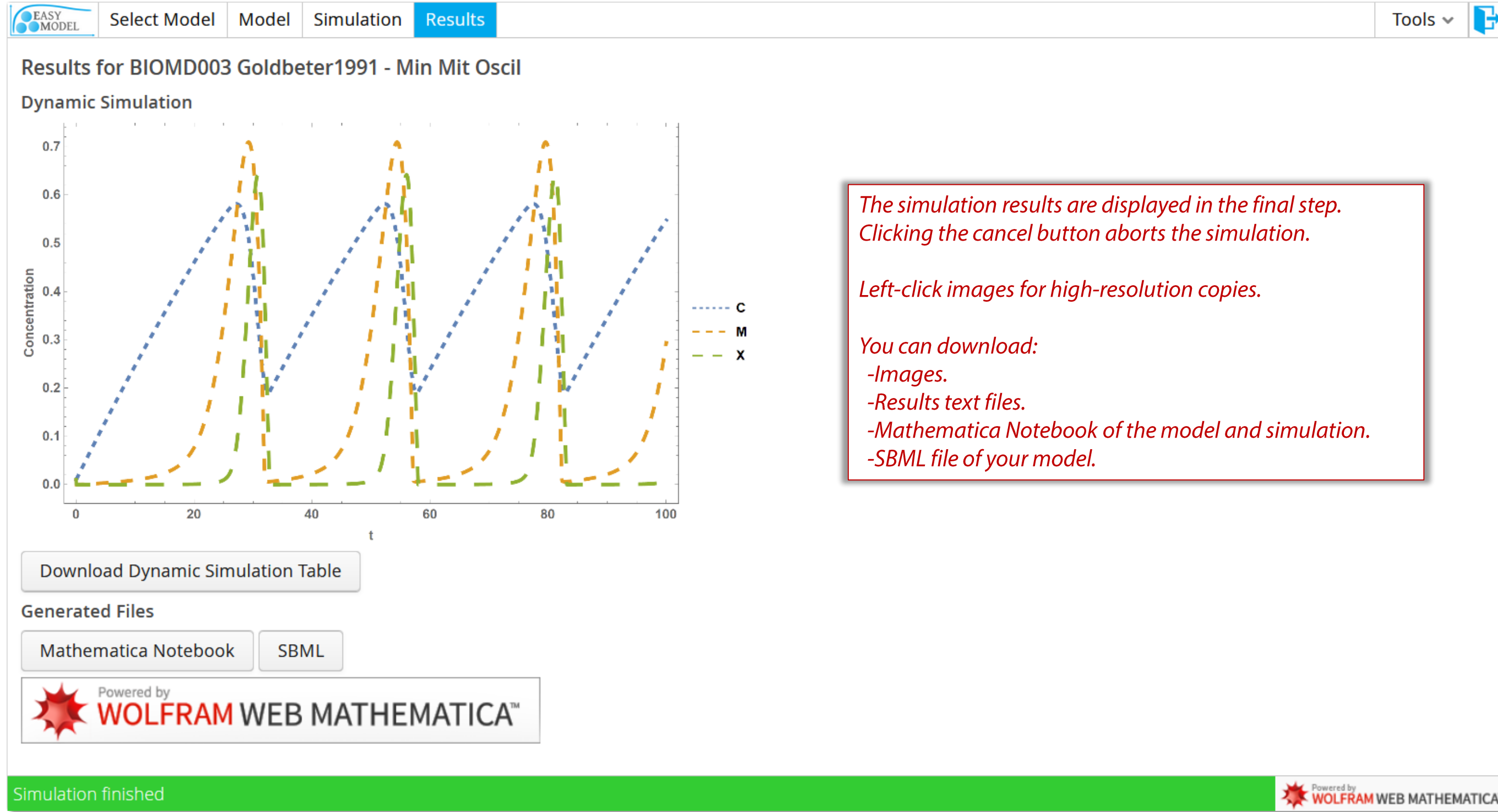
Reset Selection

*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.*

*Parameter scan: perform the simulation for several values of the rate parameters or independent variables. Select a numerical range and the number of range intervals for the parameter you want to scan to observe how the system evolves with the values variation. Each parameter scan is simulated separated from the others.*









# You have completed the tutorial!

Press next to start using EasyModel.