

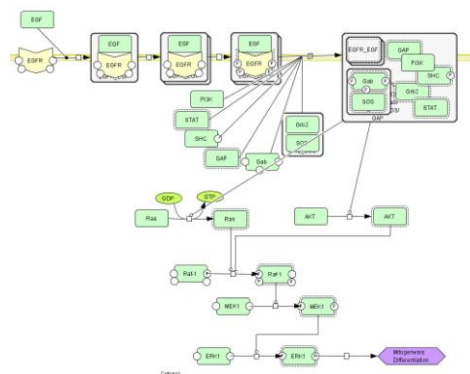
## **How to Use MappingArrayMass plugin**

For CellDesigner 4.1beta plugin

2009/Oct

### **Case A: To map the microarray data to an existing model.**

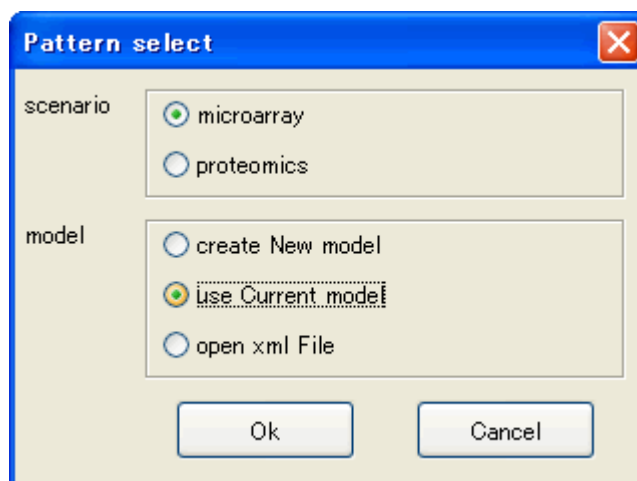
1. Open the sample model "EGF.xml".



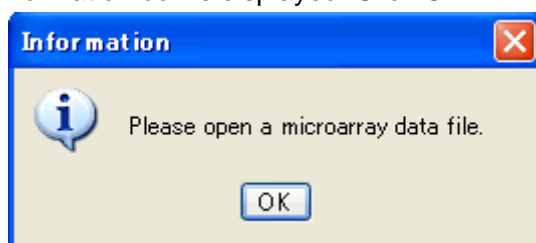
2. Select [Plugin]- [MappingArrayMass] -[Show result].

The [Pattern select] dialog is displayed.

3. Select Scenario:"proteomics", and model: "use Current model".



4. Click OK, then the Information box is displayed. Click OK.



5. Specify the experimental data file, e.g. TestData1.xls.  
Here you can specify the Excel xls. Sheet.  
The [Binding] dialog is displayed.

**Binding**

fileName: C:\Documents and Settings\myukiko\Desktop\TestData1.xls Browse

sheetName: ExptDataSheet

**Set Data**

timeLabel: \* speciesID: \*

keyRow: use dataCol key only speciesName: \*

dataCol: \* mappingKey: ID

dataRow: \* type: GENE

cluster: \*

**Add annotation**

miriamRelation: Reset

dataTypeRow: Clear

dataCols: (can specify multiple columns)

	A	B	C	D	E	F	G	
1	TamRE2						0 min	
2	accession	description	speciesID	name	PubMed	pep_mod	pep_score	pep
3	NP_0010921...	AKT1 substr...	AKT	AKT	18372248	2.0	50.0	1.0
4	NP_0010351...	mitogen-acti...	ERK1	ERK1	19097033	1.0	98.0	1.0

Ok Cancel

6. In the [Binding]. Dialog, you can select the sheet from the Excel file, set Data and add annotation to the model.

Specify the Row/Column number for the items in the following table. You can drag and drop the table numbers.

**Binding**

fileName: C:\Documents and Settings\myukiko\Desktop\TestData1.xls Browse

sheetName: ExptDataSheet

**Set Data**

timeLabel: 1 \*  
 keyRow: 2 \*  
☒ use dataCol key only  
 dataCol: G \*  
 dataRow: 3 \*

speciesID: C \*  
 speciesName: D  
 mappingKey: ID  
 type: PROTEIN  
 cluster:

**Add annotation**

miriamRelation: Reset  
 dataTypeRow:  
 dataCols: (can specify multiple columns) Clear

	A	B	C	D	E	F	G	
1	TamRE2						0 min	
2	accession	description	speciesID	name	PubMed	pep_mod	pep_score	pep
3	NP_0010921...	AKT1 substr...	AKT	AKT	18372248	2.0	50.0	1.0
4	NP_0010351...	mitogen-acti...	ERK1	ERK1	19097033	1.0	98.0	1.0

Ok Cancel

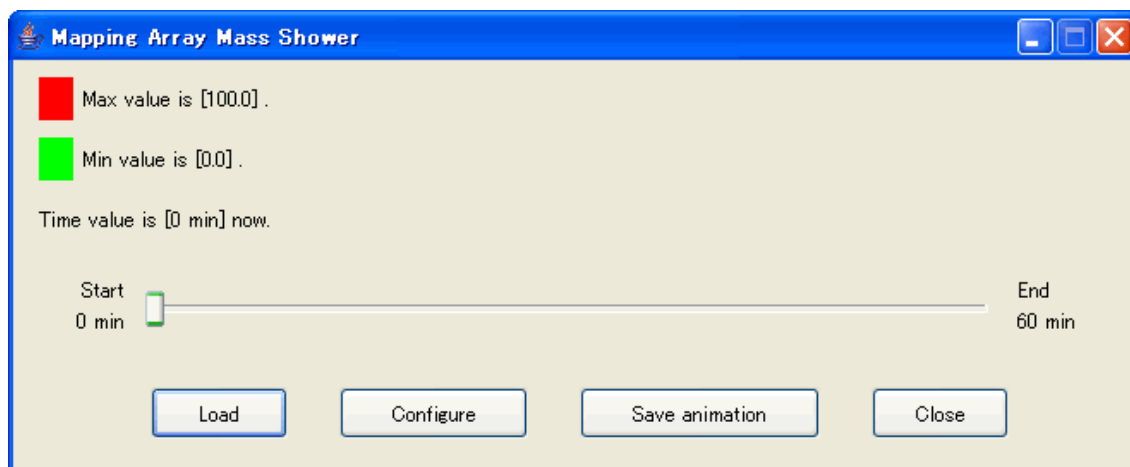
timeLabel	Select the header row which contains the time points.
keyRow	Select the header row of the data. If you check "same key", the values are selected and mapped according to the same header key name. (e.g. "pep_score") If there is no check at "same key" option, all the column data will be used.
dataRow	Select the first row of the data.
dataCol	Select the data column for mapping. Select the first time point data column only. For other time points, data from the column with the same header name (e.g. pep_score) will be used.
speciesID	Specify the column where speciesIDs are listed.

speciesName	Specify the column where speciesNames are listed.
mappingKey	Specify the key type for data mapping.
type	When you create a new model, the type specified here will be used to generate new species.
cluster	When you create a new model, the clusters specified here will be generated as Compartments and all the Species newly generated will be stored inside the specified Compartments.

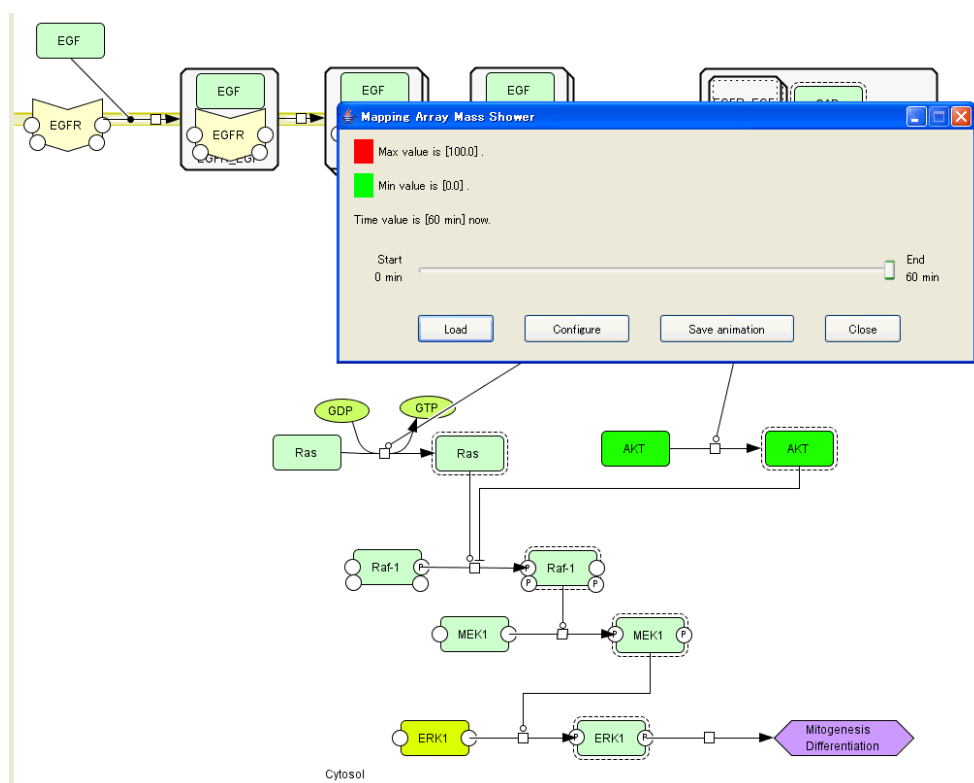
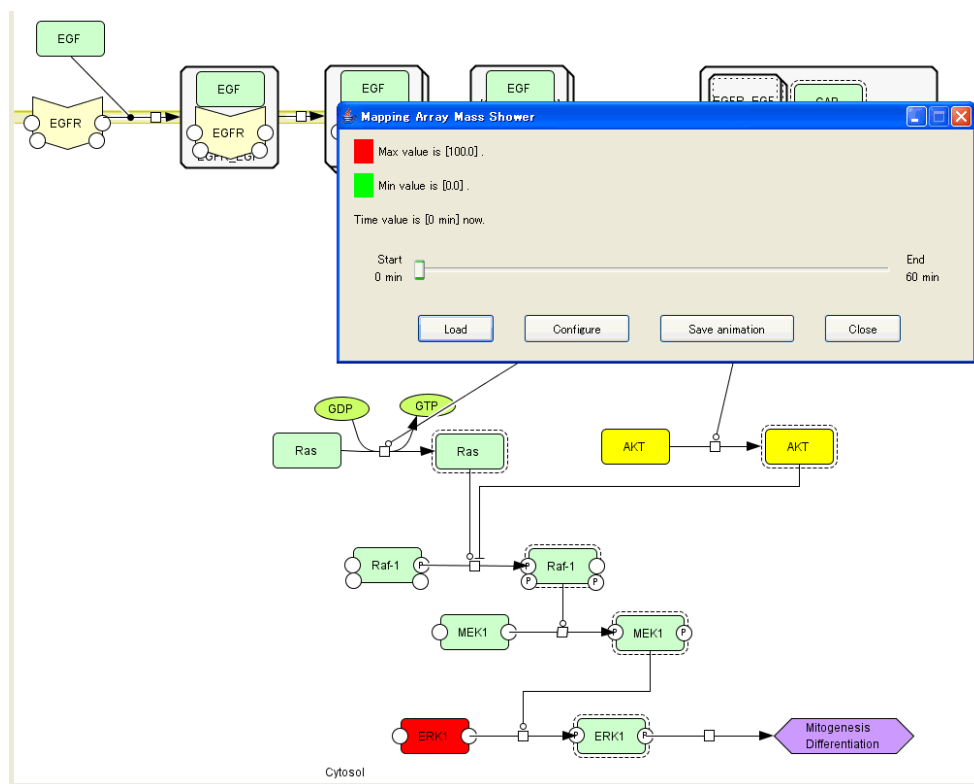
miriamRelation	Specify miriamRelation
dataTypeRow	Specify the header row
dataTypeRow	In the text area: Specify the columns where MIRIAM data is stored. MIRIAM information will be associated with the relevant Species. You can specify multiple columns with comma delimiters. If the header names are same as MIRIAM resource names, the header names will become the resource names, and IDs specified in the data field columns become IDs of the MIRIAM data for the Species.

7. After specifying necessary data, press OK.

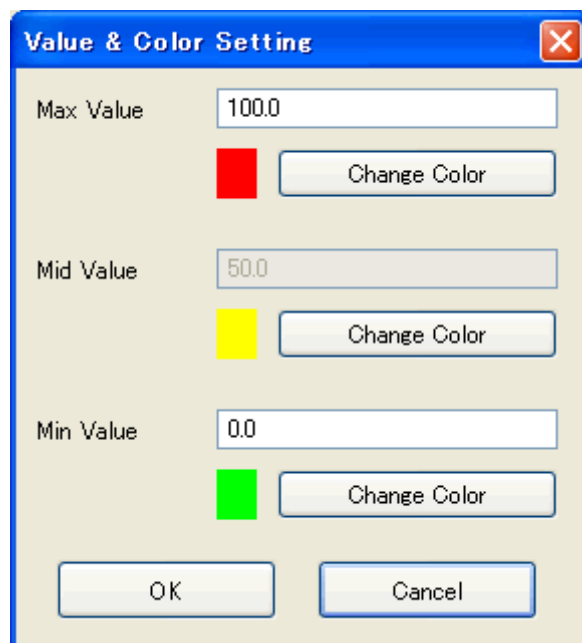
The [Mapping Array Mass Shower] dialog is displayed.



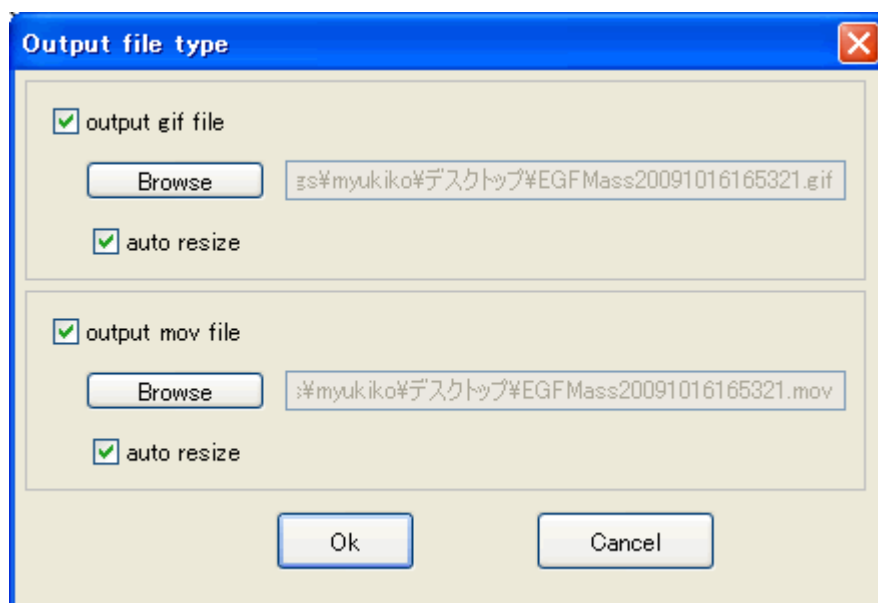
7. When you slide the Time value slide bar, you can see the color changed over the species in the model.



8. To change the colors and the values, click [Configure] button.

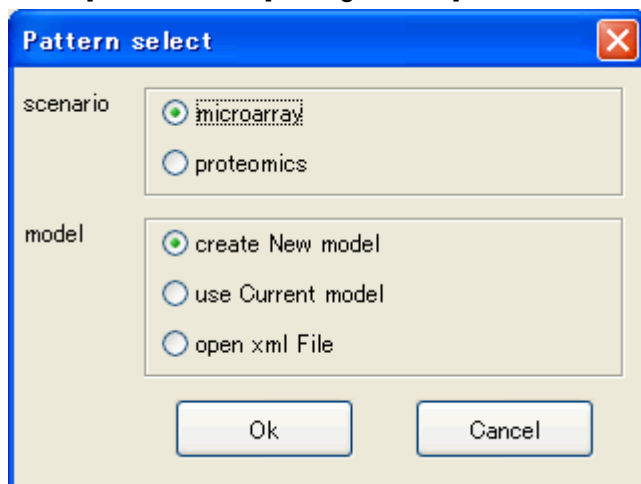


9. To save the images as animation, click the [Save animation] button.  
Specify the output file and storage, then you can store the image data.



**Case B: Create a new model out from the experimental data.**

1. In the [Pattern select] dialog, select [create New model] option.



2. Select the data file; specify the data set same as the Case A procedure. Just change the [type] of the [Set Data] to “GENE”, instead of “PROTEIN”.
3. New model is created according to the experimental data. (as below).  
\*Please note there is no reaction connected between the nodes.

