

# Graphical Exports for BioModels Database

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# Background

- BioModels Database — data resource, targeted at biologists
- Modeling language — different formats
- Graphical diagram — straightforward representation for complex networks

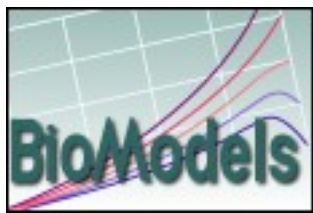




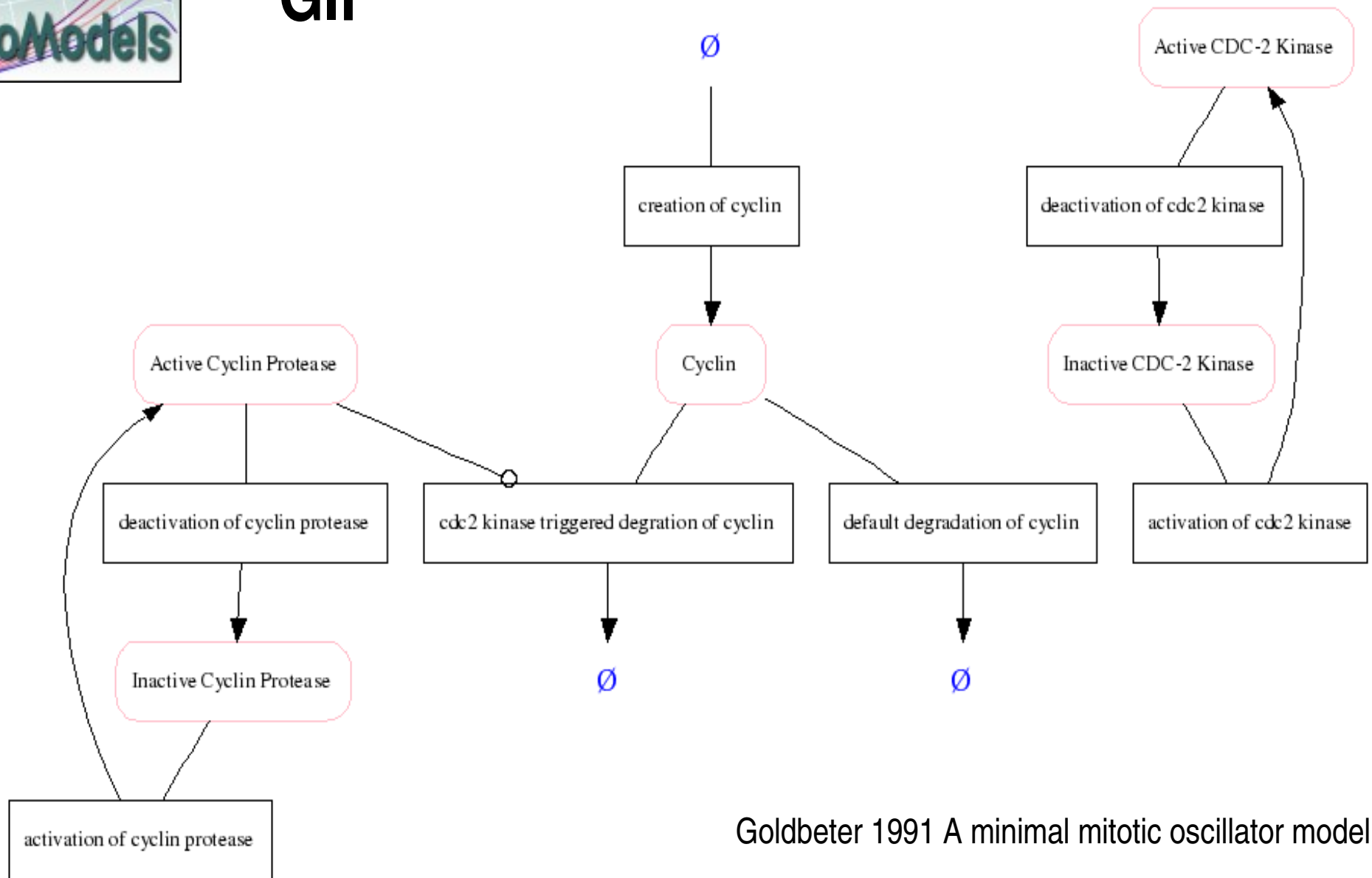
# Graphical formats provided in BioModels database

- GIF
- Scalable vector graphics: SVG
- Dynamic graphics by Java applet.





# GIF

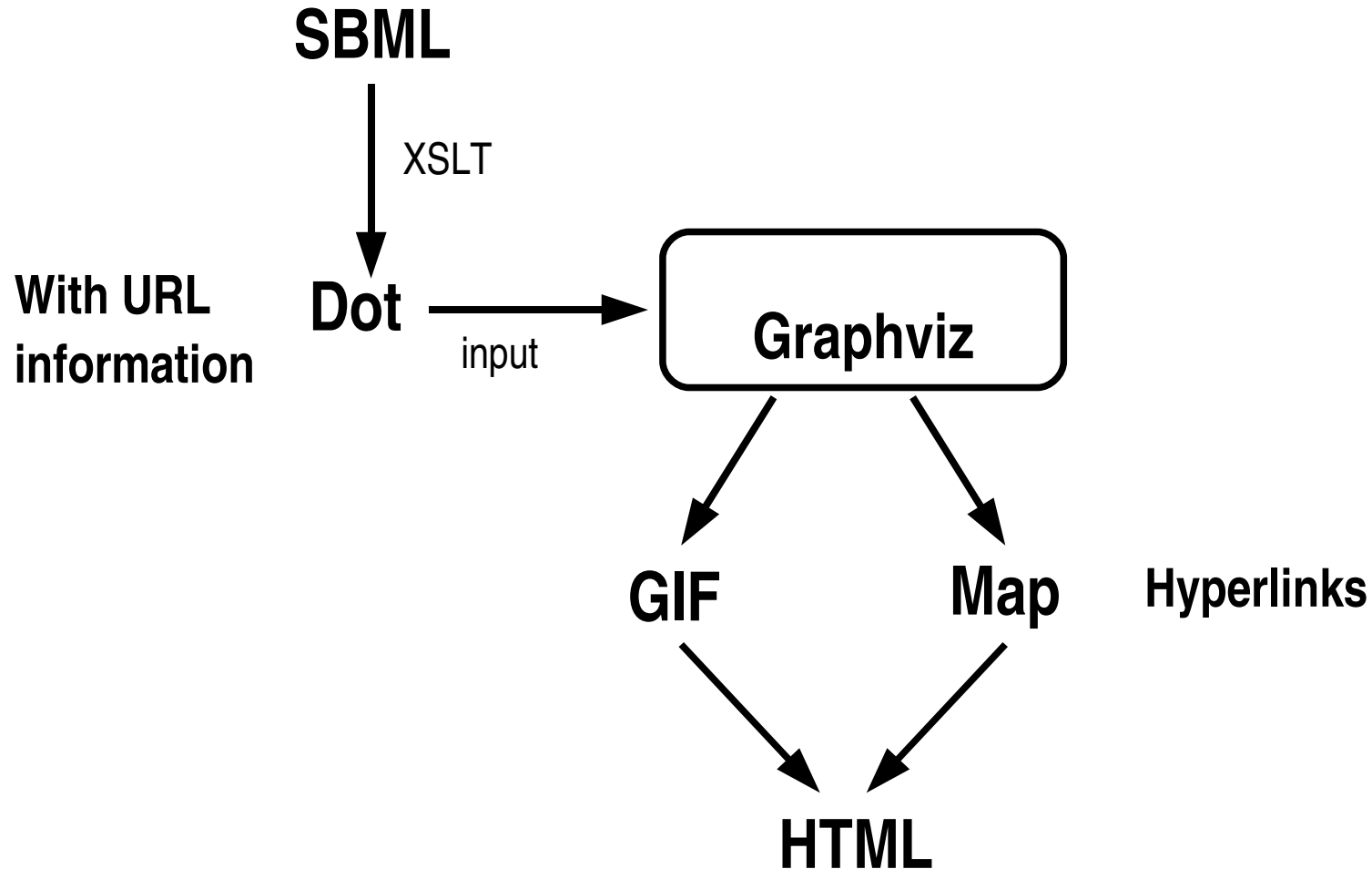


Goldbeter 1991 A minimal mitotic oscillator model.





# Implementation





# Features and Problems

- GIF — easy to view and download models
- Hyperlinks — convenient to search and curate models.
- Problems:
  - Complexity of big models
  - Raster Graphics, not scalable

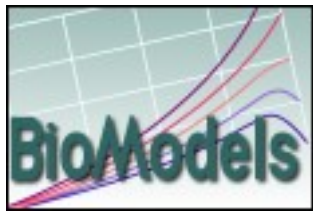




# Scalable Vector Graphics (SVG)

- Vector Graphics — Scalable
- W3C recommendation
- An application of XML
- Combining with JavaScript — Interactive graphics
- Growing interest in SVG





# Scalable vector graphics (SVG)

- Basic Structure

```
<?xml version="1.0" encoding="UTF-8"?>
```

```
<!DOCTYPE svg PUBLIC "-//W3C//DTD SVG 1.0//EN"
```

```
"http://www.w3.org/TR/2001/REC-SVG-20010904/DTD/svg10.dtd">
```

```
<svg width="200" height="200" viewBox="1 1 20 20"
```

```
xmlns:xlink="http://www.w3.org/1999/xlink">
```

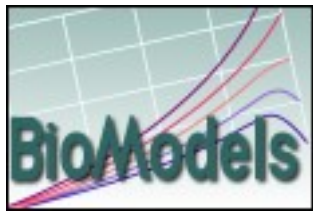
```
  <script xlink:href="JavaScriptFile_forSVG.js" type="text/ecmascript"/>
```

```
  .....
```

```
</svg>
```







# Scalable vector graphics (SVG)

- Grouping and Reference

**<def>**

**<g id="xxxx">.....</g>**

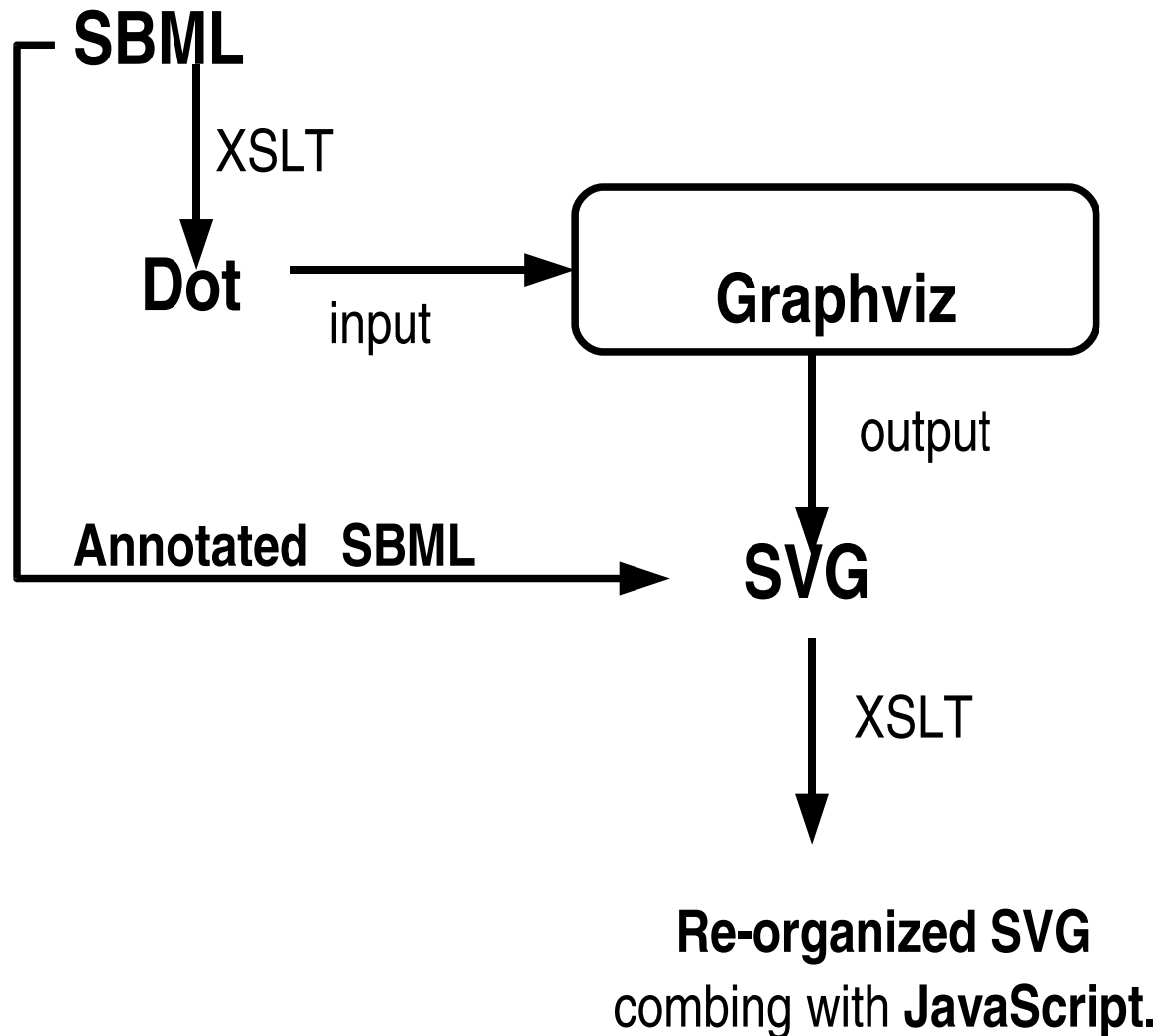
**<symbol id="xxxx">.....</symbol>**

**</def>**

**<use xlink:href="local/external object id"/>**

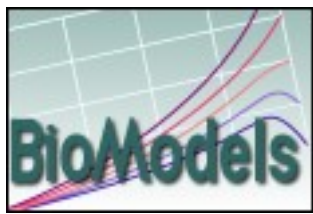


# Implementation



- Re-render SVG:
  - Grouping reactions
  - Changing ID
  - Adding URL link



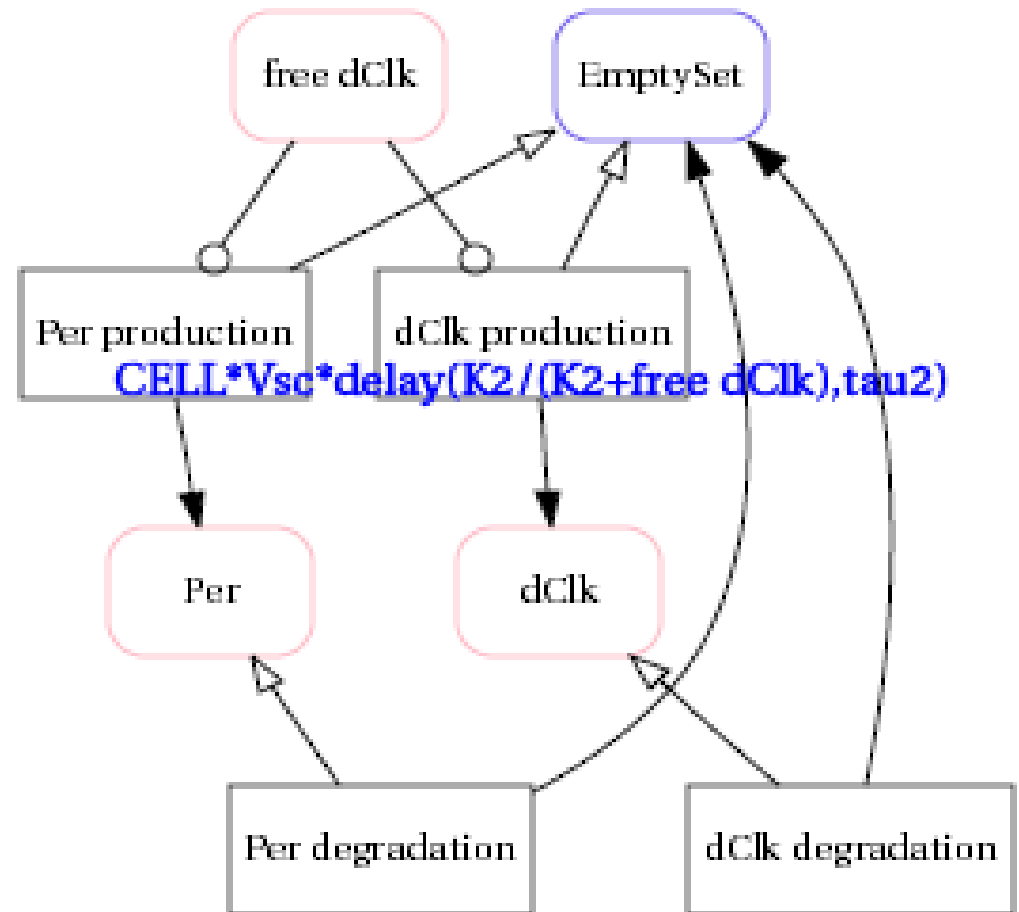
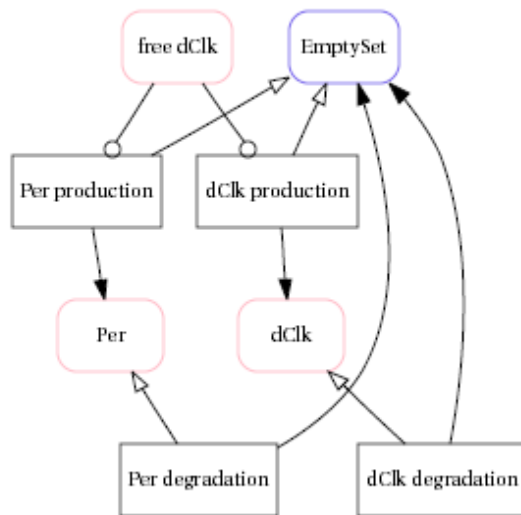


# Result

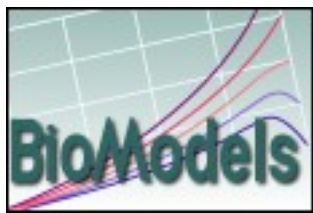
## — High lighten Rate Law

Search For Species  
Search For Reaction

Search For Species  
Search For Reaction



Smolen 2002, A Drosophila circadian oscillator model



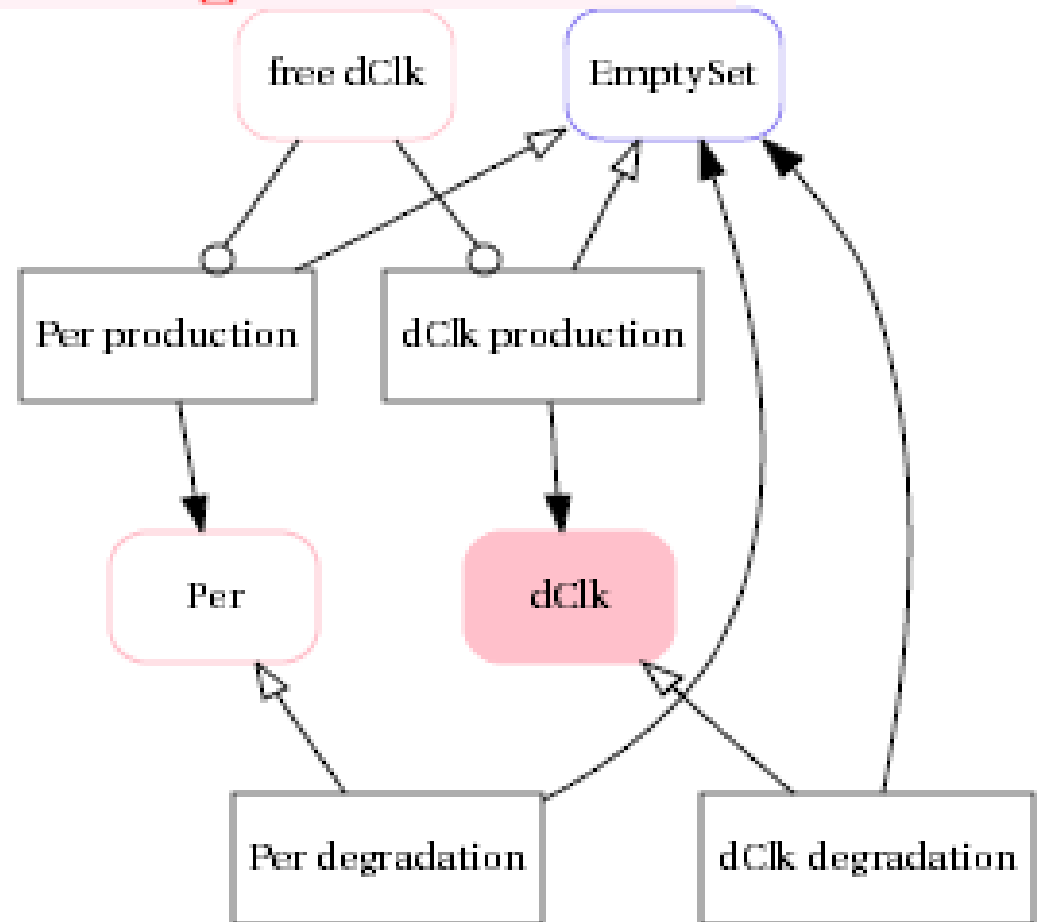
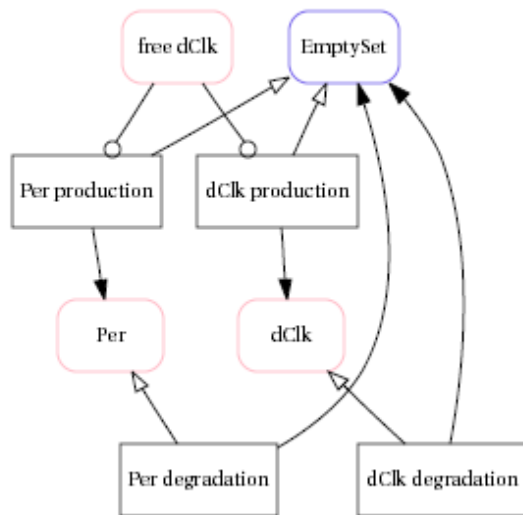
# Result

## — Selecte species

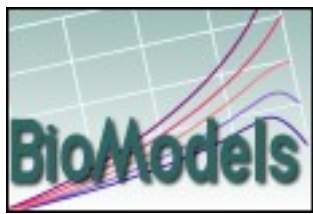
Search For Species

|           |     |      |
|-----------|-----|------|
| EmptySet  | Per | dClk |
| free dClk | ✗   |      |

Search For Species  
Search For Reaction



Smolen 2002, A Drosophila circadian oscillator model

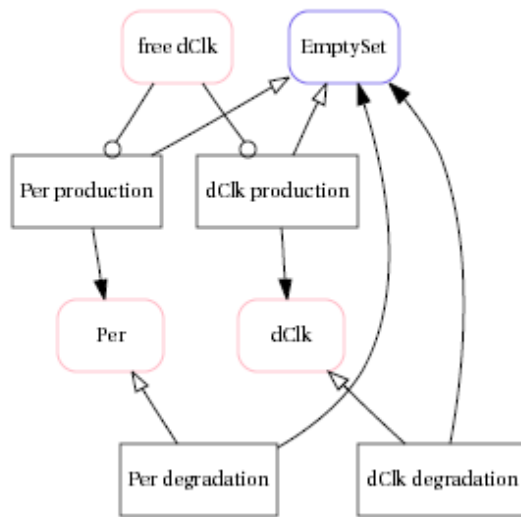


# Result

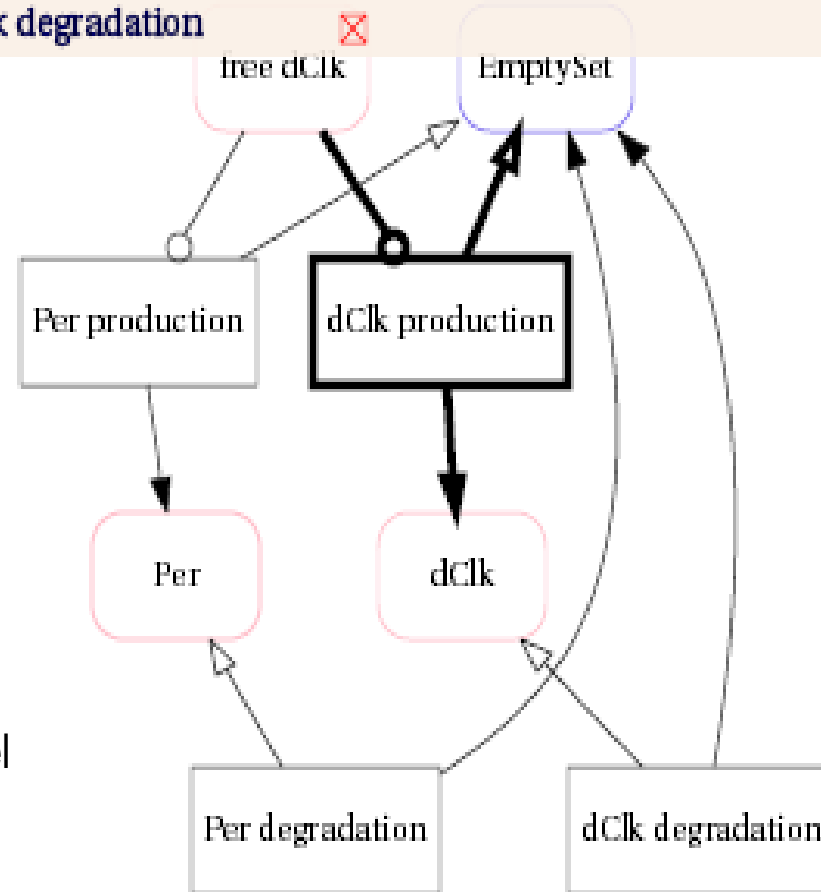
## — Select reaction

Search For Species  
Search For Reaction

Search For Species  
Search For Reaction



Per production      dClk production      Per degradation  
dClk degradation      free dClk      EmptySet



Smolen 2002, A Drosophila circadian oscillator model



# Problems

- SVG supporting
- Impossible unlimited zoom-in
- Static constructions with a fixed geometry

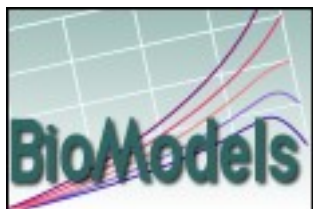




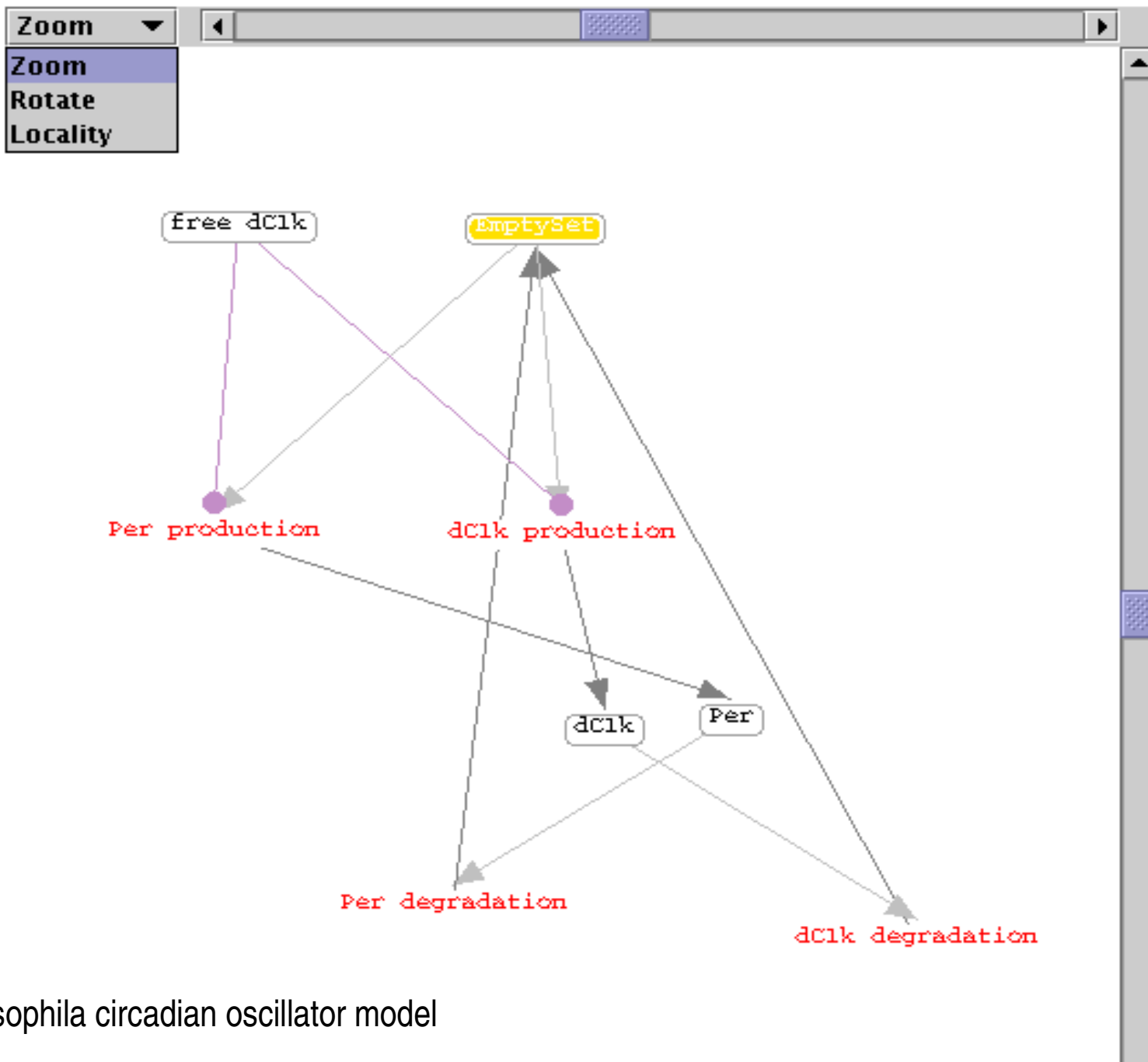
# Dynamic Graph by Java Applet

- Based on TouchGraph software (<http://www.touchgraph.com/>)  
NanoXML parser (<http://nanoxml.sourceforge.net>)
- Easy to load and view
- Crossing platform
- Dynamically control the model display

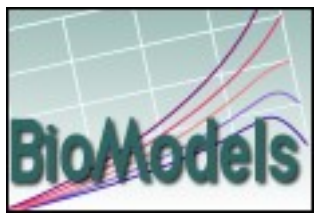




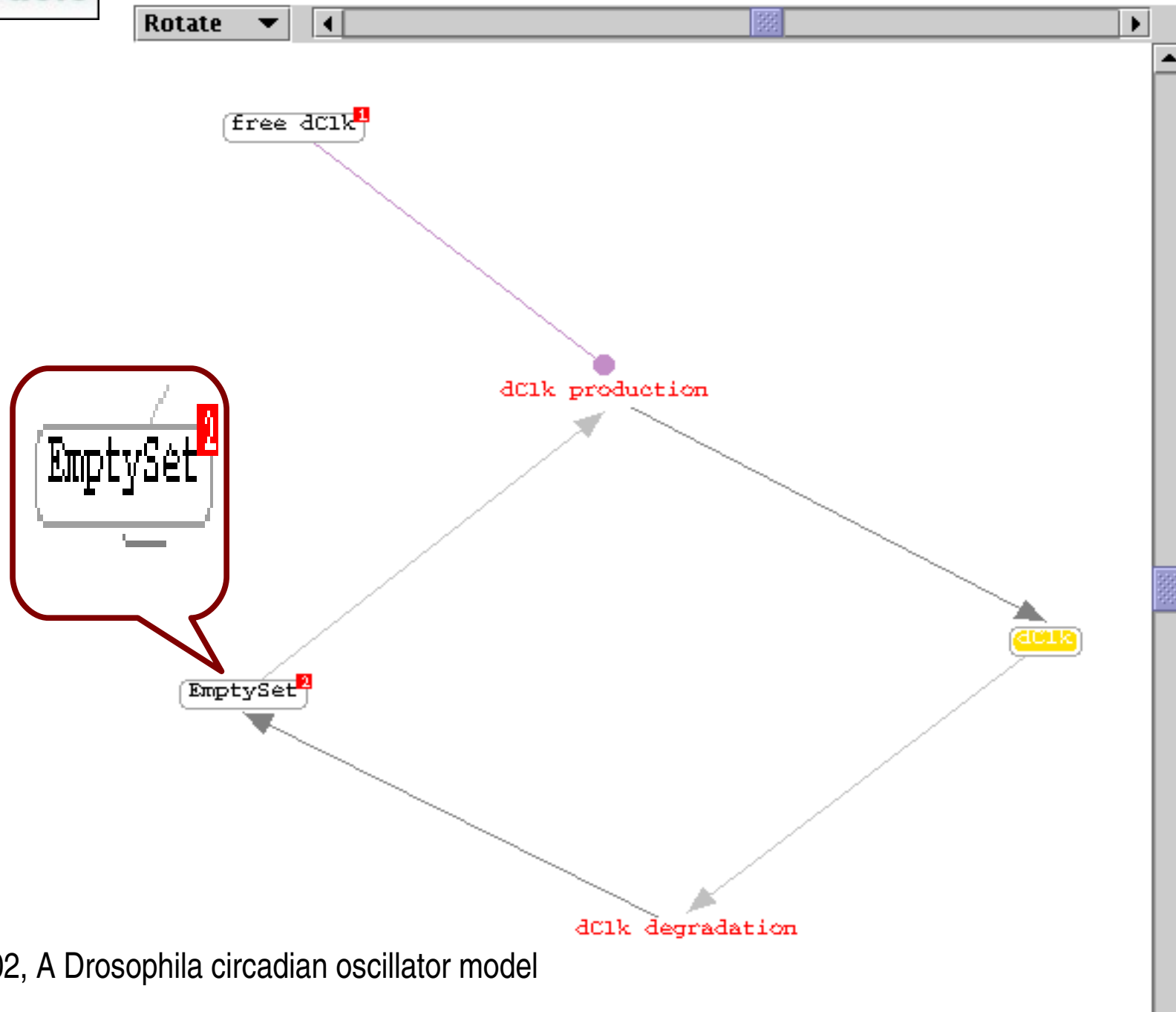
# Dynamic Graph by Java Applet







# Dynamic Graph by Java Applet





# Disadvantages

- The applet requires the Java plug-in, which isn't available by default on all web browsers.
- If untrusted, it has severely limited access to the user's system.





# Require for second generation graphs

- Current graphs — basic network display, but poor biochemical semantics
- Requirements for meaningful graphs :
  - Standard visual notation — **SBGN**
  - Well annotated models — **BioModels Database**
- Second generation graphs — Parsing annotation, connecting to SBGN





# SBGN

([www.sbgn.org](http://www.sbgn.org))

- Aim : to provide organized information in a concise graphical manner with sufficient detail for simulation.
- The two languages of SBGN:
  - State Transition diagram
  - Entity Relation diagram
- Nodes defined in SBGN:
  - state/entity nodes (SENs)
  - transition/relationships nodes (TRNs)





# Two possible directions

- SBML – BioPAX – SBGN
  - Parsing annotation
  - MIRIAM web services
- SBML – SBO – SBGN
  - sboTerm** attribute included in most SBML (L2V2) classes



• **State / Entity nodes**

*macromolecule*  
SBO:0000245



*simple chemical*  
SBO:0000247



*unknown entity*  
SBO:0000285



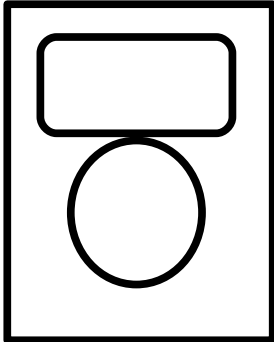
*empty set*  
SBO:0000291




*multimer*  
SBO:0000286



*complex*  
SBO:0000253



state variable  
SBO:0000214 - 221  
0000212  
0000233  
0000224



unit of information  
no SBL term



additional  
information  
for species

SBML: *species*

***SBO and SBGN connections***

could also be judged by  
**bqmodel:relation element**

• Transition / relationship nodes

*yield*  
no SBO item



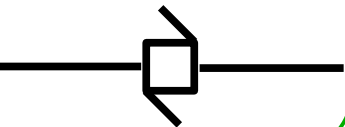
*reset*  
no SBO item



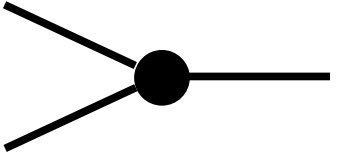
*irreversible*  
no SBO item



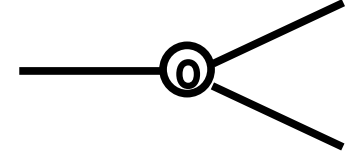
*reversible*  
no SBO item



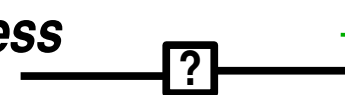
*association*  
SBO:0000177



*dissociation*  
SBO:0000180



*omitted process*  
no SBO item



*uncertain process*  
no SBO item



can be judged  
from reaction

SBML : reaction

need more  
information

*modulation*  
SBO:0000168



*stimulation*  
SBO:0000170



*trigger*  
SBO:0000171

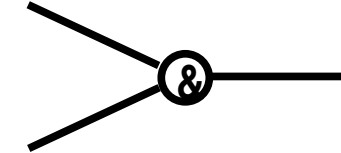


*inhibition*  
SBO:000169

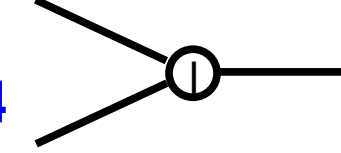


SBML:modifier

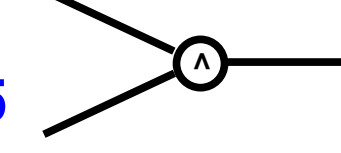
*and*  
SBO:0000173



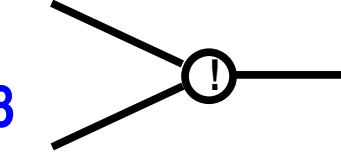
*or*  
SBO:0000174

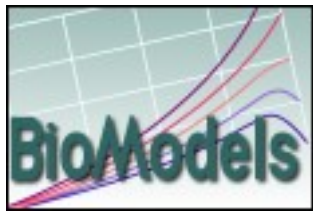


*xor*  
SBO:0000175



*not*  
SBO:0000238



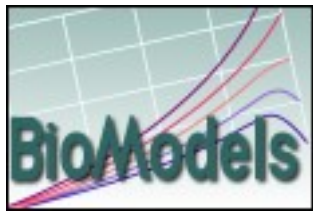


# Difficulties

- Connection between SBML and SBGN
- Lack of efficient free rendering algorithm
- Complexity of big models







Your suggestions and discussion will be most appreciated.

