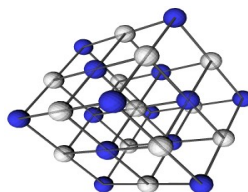


# *SBGN support in BIOCHAM*



## Biochemical Abstract Machine



Dragana JOVANOVSKA  
EPI CONTRAINTES, <http://contraintes.inria.fr>  
INRIA Paris – Rocquencourt, France

**06.10.2010**

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# SBGN support in BIOCHAM



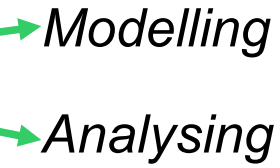
## Outline:

- **BioCham** – *Biochemical Abstract Machine*
- **SBGN** support in *BioCham*
- *Biocham Reaction Graph* **Editor**
- *Conclusion*
- *On-going work*

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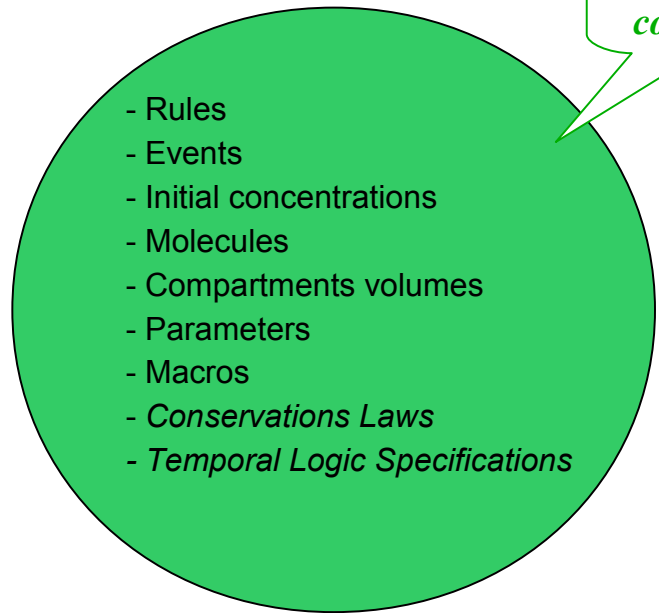
# SBGN support in BIOCHAM

- **BioCham – Biochemical Abstract Machine**
  - <http://contraintes.inria.fr/biocham>
  - different simulators
  - temporal logic based language
  - features for correcting/completing/reducing/relating/coupling models



 **BIOCHAM  
MODEL**

Consists of 

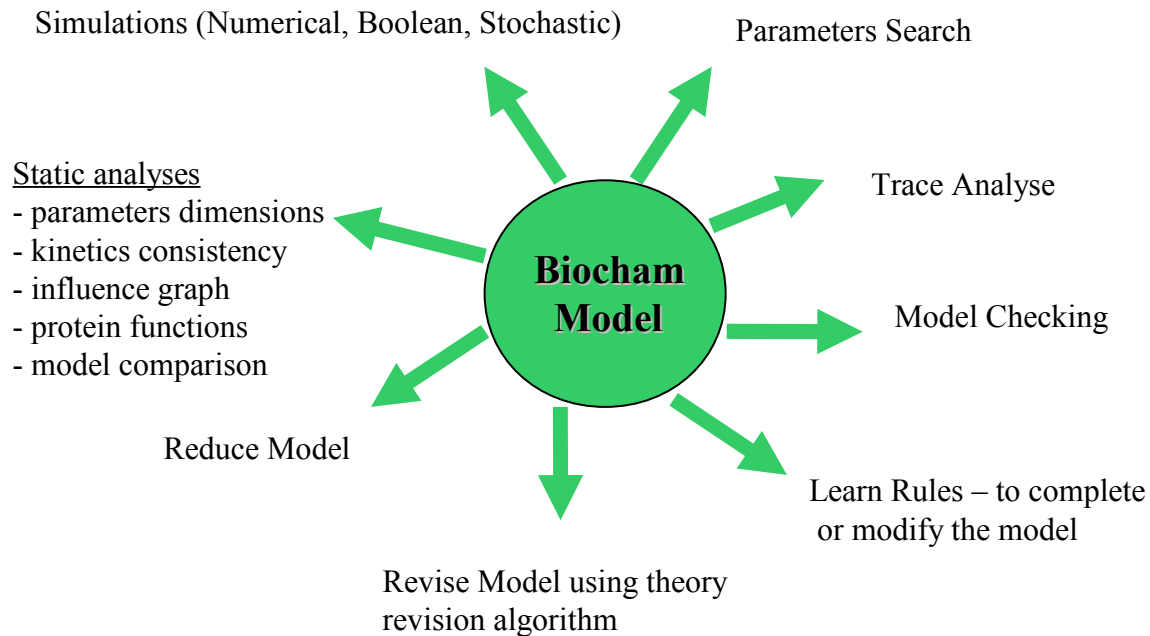


*SBML  
compatible*



# SBGN support in BIOCHAM

- Analysing features in Biocham:



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# SBGN support in BIOCHAM

- SBGN Entity pool nodes, Defined Sets of EPNs and Auxiliary Units:

Macromolecule, Nucleic Acid Feature, Multimer, Complex, Source and Sink, Compartment, Unit of Information(cardinality), State Variable(modified)

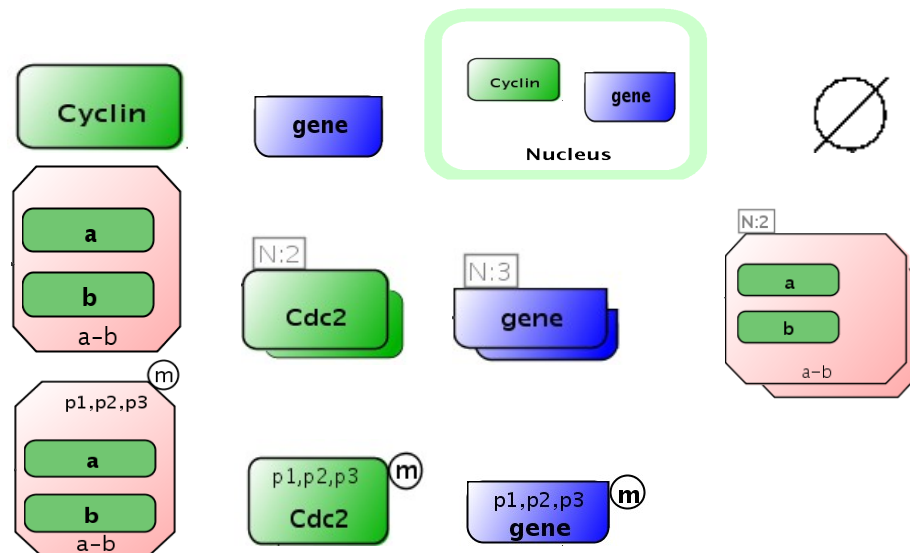
## Biocham objects' grammar:

*object* = *molecule* | *molecule::name* located *molecule*

*molecule* =

*name*  
 | *molecule-molecule*      molecular complex  
 | *molecule~{name,...,name}*   modified molecule  
 | *gene*  
 | ( *molecule* )

*gene* = #*name*



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# SBGN support in BIOCHAM

- SBGN Entity pool nodes, Defined Sets of EPNs and Auxiliary Units:

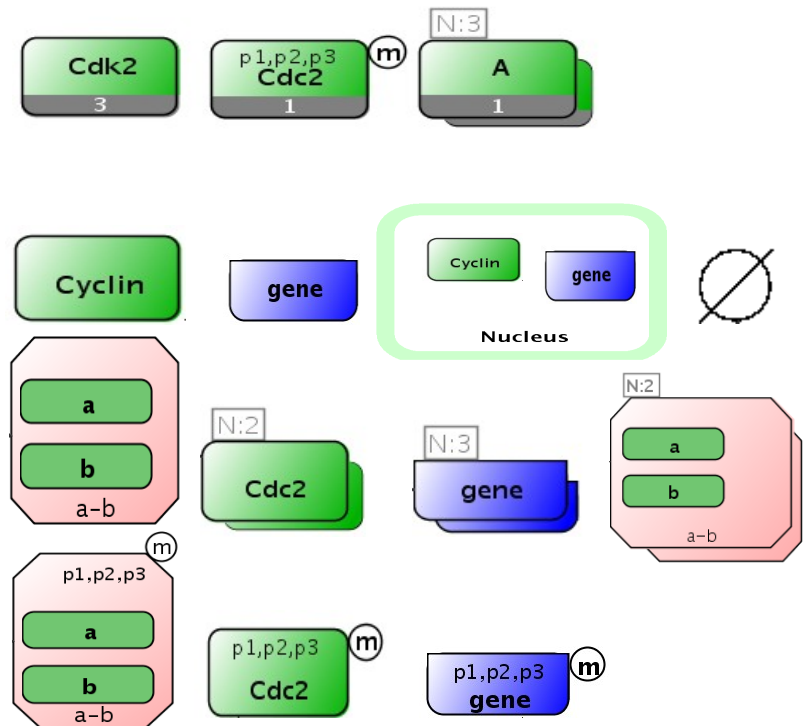
Macromolecule, Nucleic Acid Feature, Multimer, Complex, Source and Sink, Compartment, Unit of Information(cardinality), State Variable(modified), Labeled Clone Marker!!!

Biocham objects' grammar:

*object* = *molecule* | *molecule::name* located *molecule*

*molecule* =  
*name*  
 | *molecule-molecule*      molecular complex  
 | *molecule*-{*name*,...,*name*} modified molecule  
 | *gene*  
 | ( *molecule* )

*gene* = #*name*



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# SBGN support in BIOCHAM

- **SBGN support in BioCham: [SBGN Process Nodes](#) :**

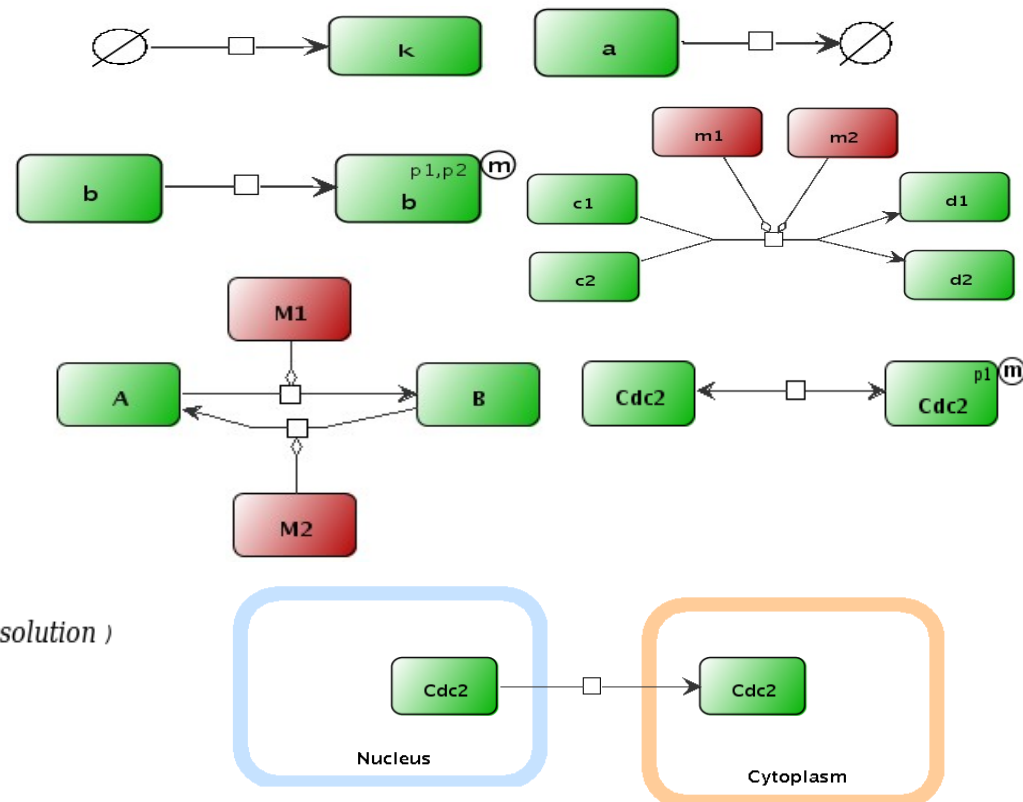
## Process, Association and Dissociation

### Biocham reactions' grammar:

*reaction* =        *kinetics for basic\_reaction*  
                       | *basic\_reaction*  
                       | *name : basic\_reaction*  
                       | *name : kinetics for basic\_reaction*

*basic\_reaction* = *solution => solution.*  
                       | *solution =[{object}]=> solution.*  
                       | *solution =[{solution => solution}]=> solution.*  
                       | *solution <=> solution.*  
                       | *solution <=[object]=> solution.*

*solution* =        \_ | *object* | *integer\*object* | *solution + solution* | ( *solution* )



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# SBGN support in BIOCHAM

• SBGN support in BioCham: SBGN Process Nodes and Arcs :

Process, Association and Dissociation; Consumption, Production and Modulation

Biocham reactions' grammar:

```

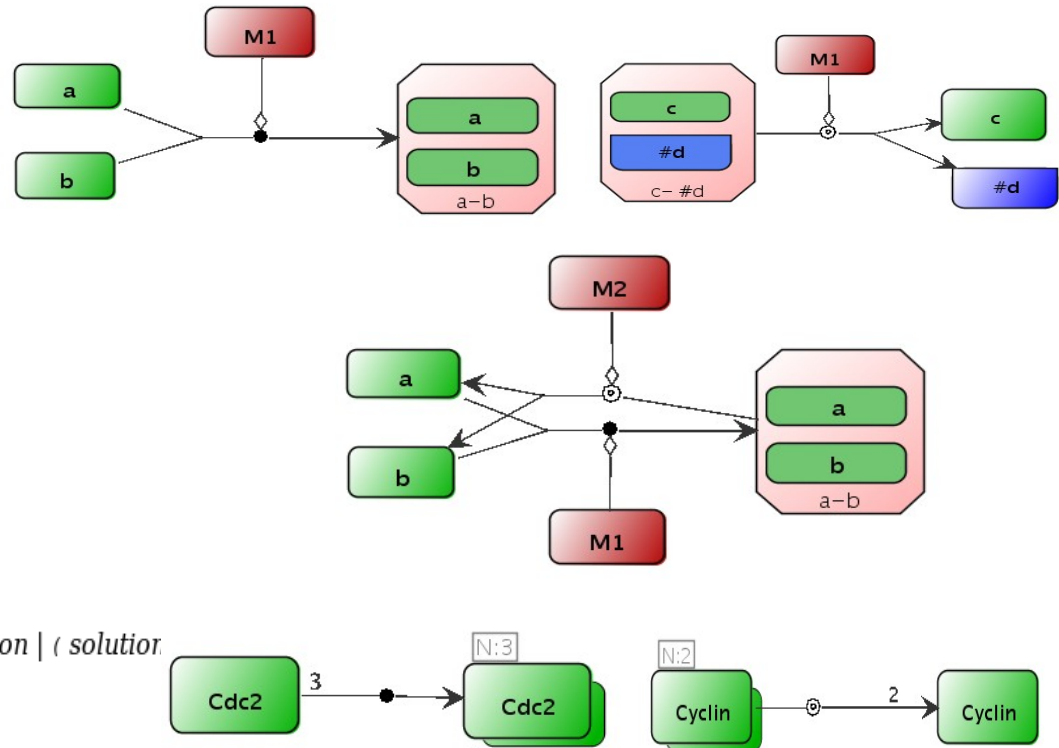
reaction =      kinetics for basic_reaction
               | basic_reaction
               | name : basic_reaction
               | name : kinetics for basic_reaction
    
```

```

basic_reaction = solution => solution.
                | solution =[object]=> solution.
                | solution =[solution => solution]=> solution.
                | solution <=> solution.
                | solution <=[object]=> solution.
    
```

```

solution =     _ | object | integer*object | solution + solution | ( solution.
    
```

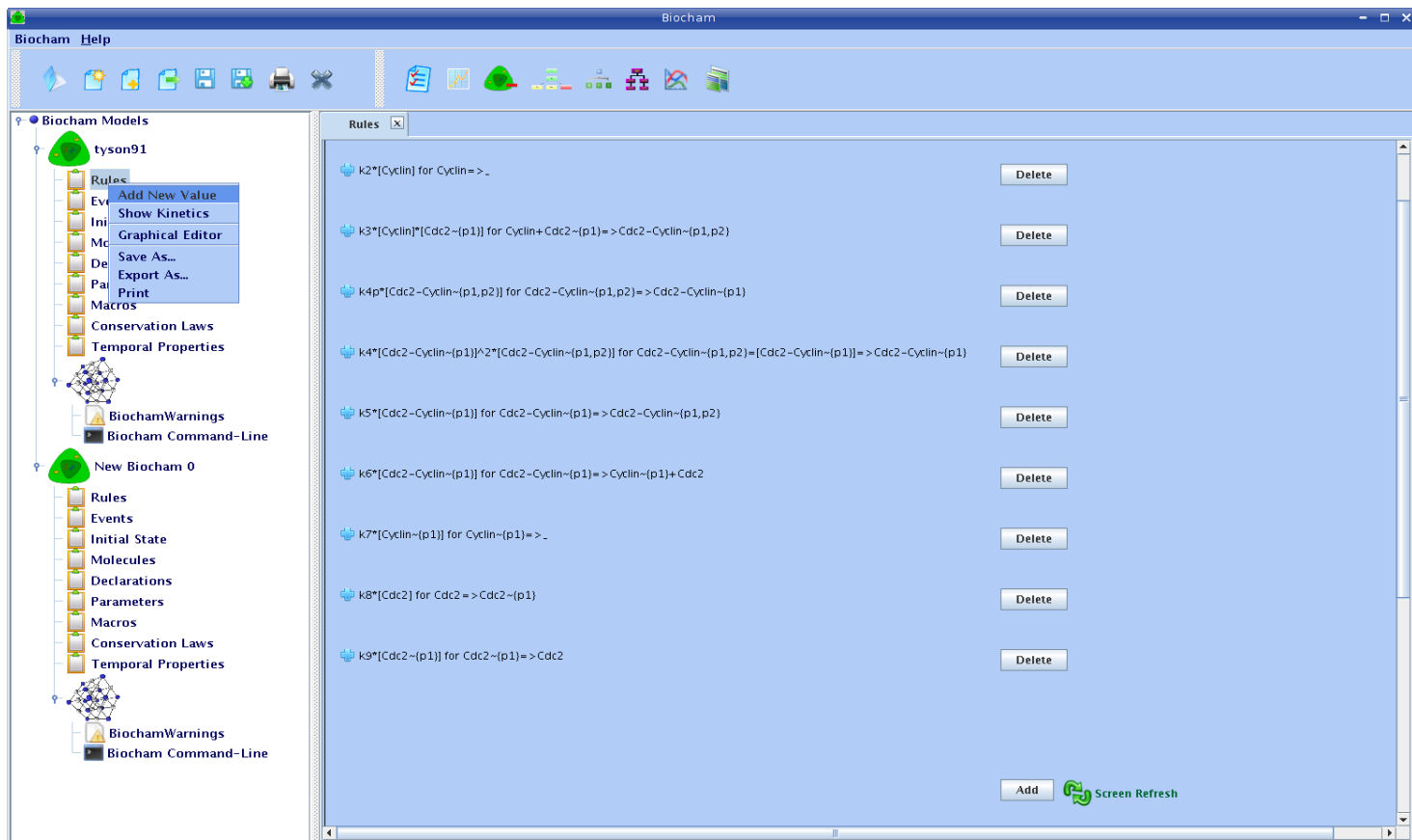


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# SBGN support in BIOCHAM

- Biocham Reaction Graph Editor



The screenshot shows the Biocham Reaction Graph Editor interface. The window title is "Biocham". The left sidebar displays a tree view of "Biocham Models" with "tyson91" selected. A context menu is open over "tyson91", listing options: "Add New Value", "Show Kinetics", "Graphical Editor", "Save As...", "Export As...", "Print", "Conservation Laws", and "Temporal Properties". The main area is titled "Rules" and contains a list of reaction rules with "Delete" buttons next to each:

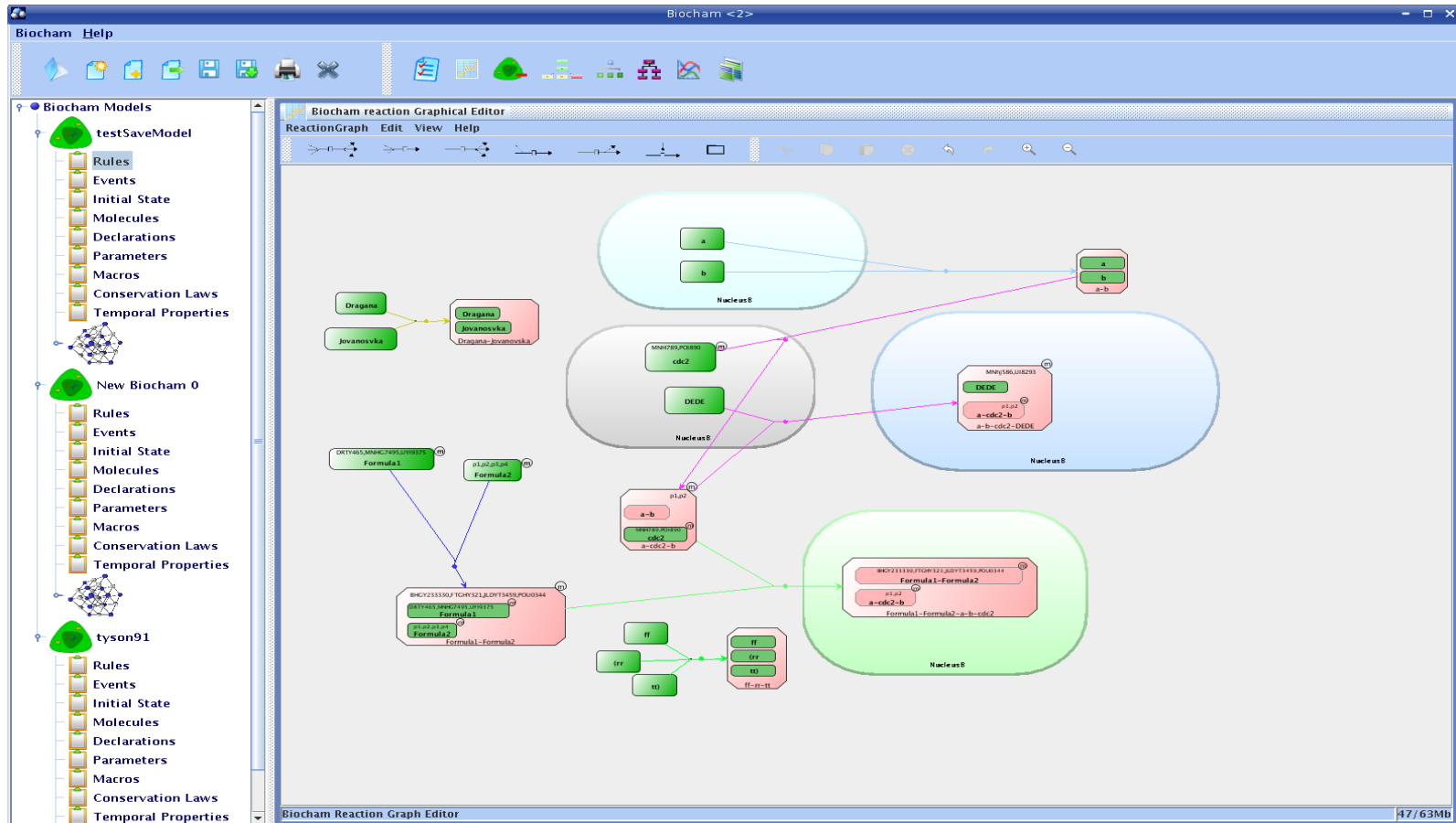
- $k2$ \*[Cyclin] for Cyclin=>..
- $k3$ \*[Cyclin]\*[Cdc2~(p1)] for Cyclin+Cdc2~(p1)=>Cdc2~Cyclin~(p1,p2)
- $k4p$ \*[Cdc2~Cyclin~(p1,p2)] for Cdc2~Cyclin~(p1,p2)=>Cdc2~Cyclin~(p1)
- $k4$ \*[Cdc2~Cyclin~(p1)]^2\*[Cdc2~Cyclin~(p1,p2)] for Cdc2~Cyclin~(p1,p2)=[Cdc2~Cyclin~(p1)]=>Cdc2~Cyclin~(p1)
- $k5$ \*[Cdc2~Cyclin~(p1)] for Cdc2~Cyclin~(p1)=>Cdc2~Cyclin~(p1,p2)
- $k6$ \*[Cdc2~Cyclin~(p1)] for Cdc2~Cyclin~(p1)=>Cyclin~(p1)+Cdc2
- $k7$ \*[Cyclin~(p1)] for Cyclin~(p1)=>..
- $k8$ \*[Cdc2] for Cdc2=>Cdc2~(p1)
- $k9$ \*[Cdc2~(p1)] for Cdc2~(p1)=>Cdc2

At the bottom right, there are "Add" and "Screen Refresh" buttons.

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# SBGN support in BIOCHAM

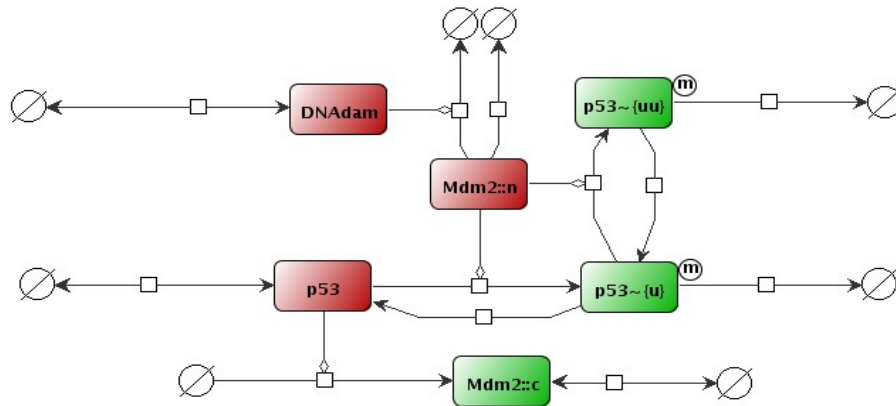
- Biocham Reaction Graph Editor



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# SBGN support in BIOCHAM

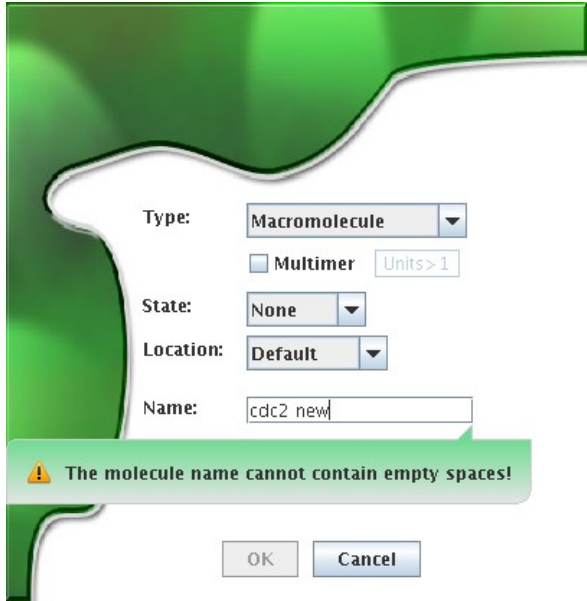
- Biocham Reaction Graph Editor



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# BioCham Reaction Graph Editor

Validation of the syntax and the semantics



The screenshot shows a dialog box for creating a new molecule. The fields are as follows:

- Type: Macromolecule (dropdown)
- Multimer:  (checkbox) Units > 1 (text input)
- State: None (dropdown)
- Location: Default (dropdown)
- Name: cdc2 new (text input)

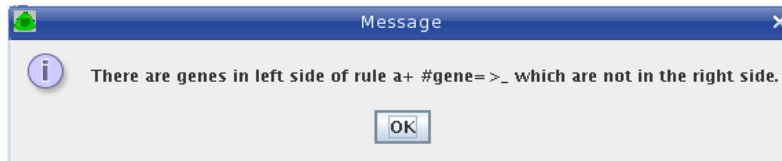
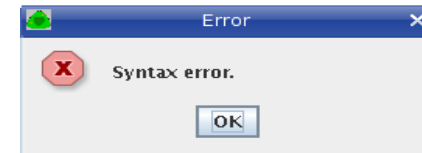
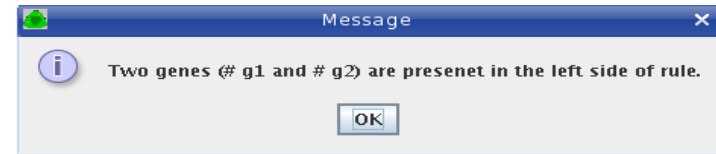
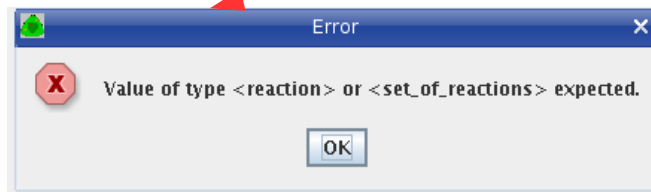
A green error message box is displayed at the bottom of the dialog, containing a warning icon and the text: "The molecule name cannot contain empty spaces!". Below the error message are "OK" and "Cancel" buttons.

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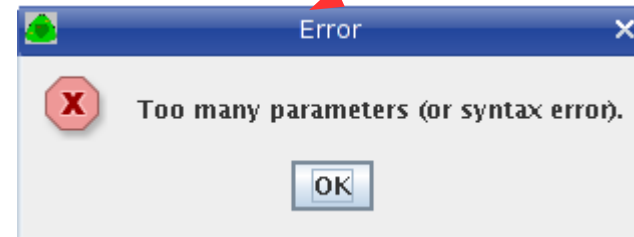
# BioCham Reaction Graph Editor

## Validation of the syntax and the semantics

*Wrong kinetics*



*Wrong molecules name*



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# BioCham Reaction Graph Editor

## Validation of the syntax and the semantics

The screenshot shows the BioCham Reaction Graph Editor interface. The window title is "Biocham <3>". The menu bar includes "Biocham" and "Help". The toolbar contains icons for file operations (open, save, close) and editing (undo, redo, delete). The left sidebar shows a tree view of "Biocham Models" with a sub-tree for "New Biocham 0" containing: Rules, Events, Initial State, Molecules, Declarations, Parameters, Macros, Conservation Laws, and Temporal Properties. Below this is a network diagram icon and a "BiochamWarnings" icon. The right pane, titled "BiochamWarnings and Errors", displays the following messages:

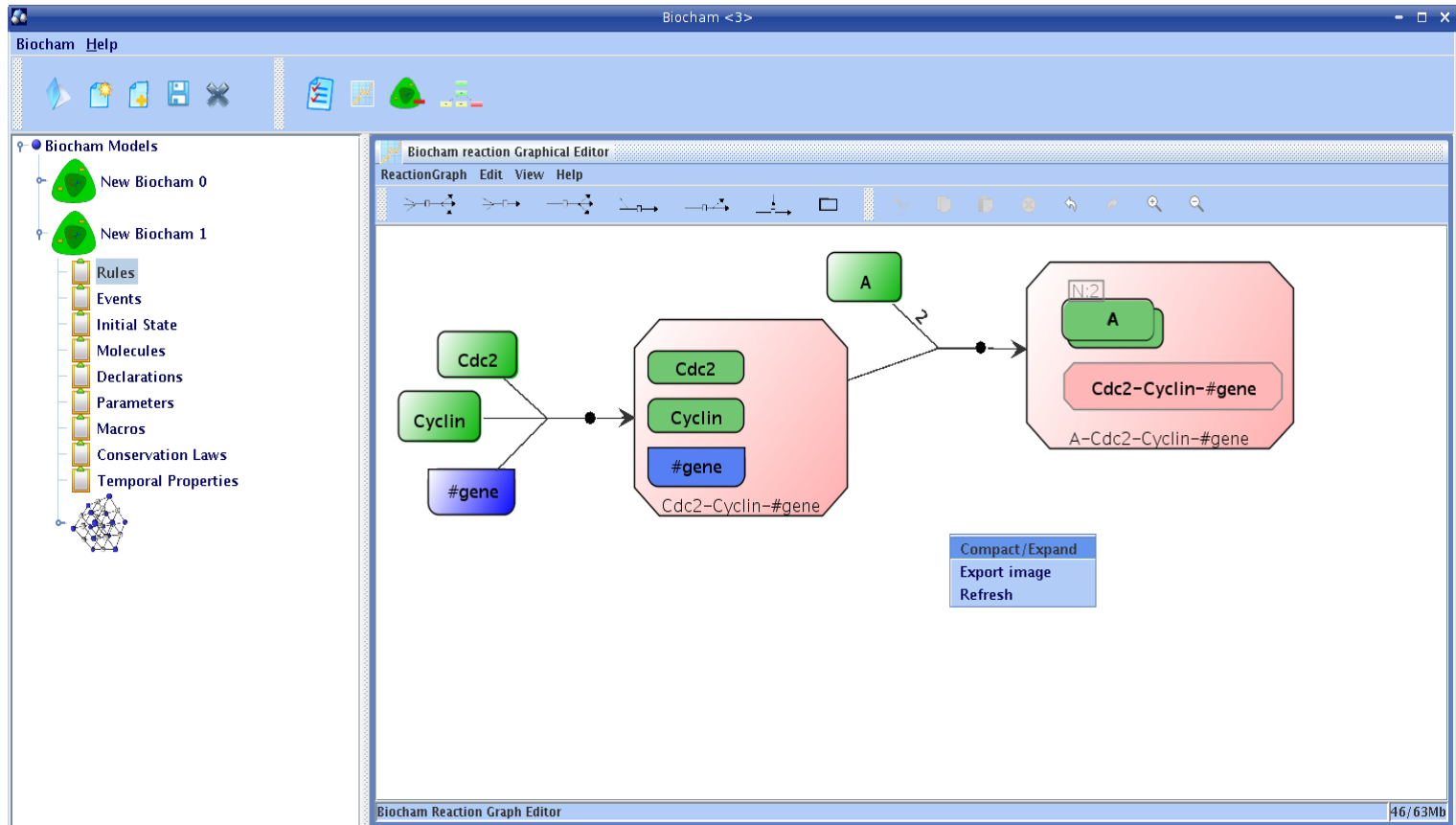
- Error:** Value of type <reaction> or <set\_of\_reactions> expected.
- Warning:** There are genes in left side of rule  $a + \#gene = \_$  which are not in the right side.
- Warning:** Two genes ( $\# g1$  and  $\# g2$ ) are present in the left side of rule.
- Warning:** There are genes in left side of rule  $\#g1 + \#g2 = \> \#g1 - \#g2$  which are not in the right side.
- Error:** Value of type <reaction> or <set\_of\_reactions> expected.
- Error:** Too many parameters (or syntax error).
- Error:** Not enough parameters.
- Error:** Syntax error.

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# CONCLUSION

## Proposal for SBGN

### ★ Nested complexes

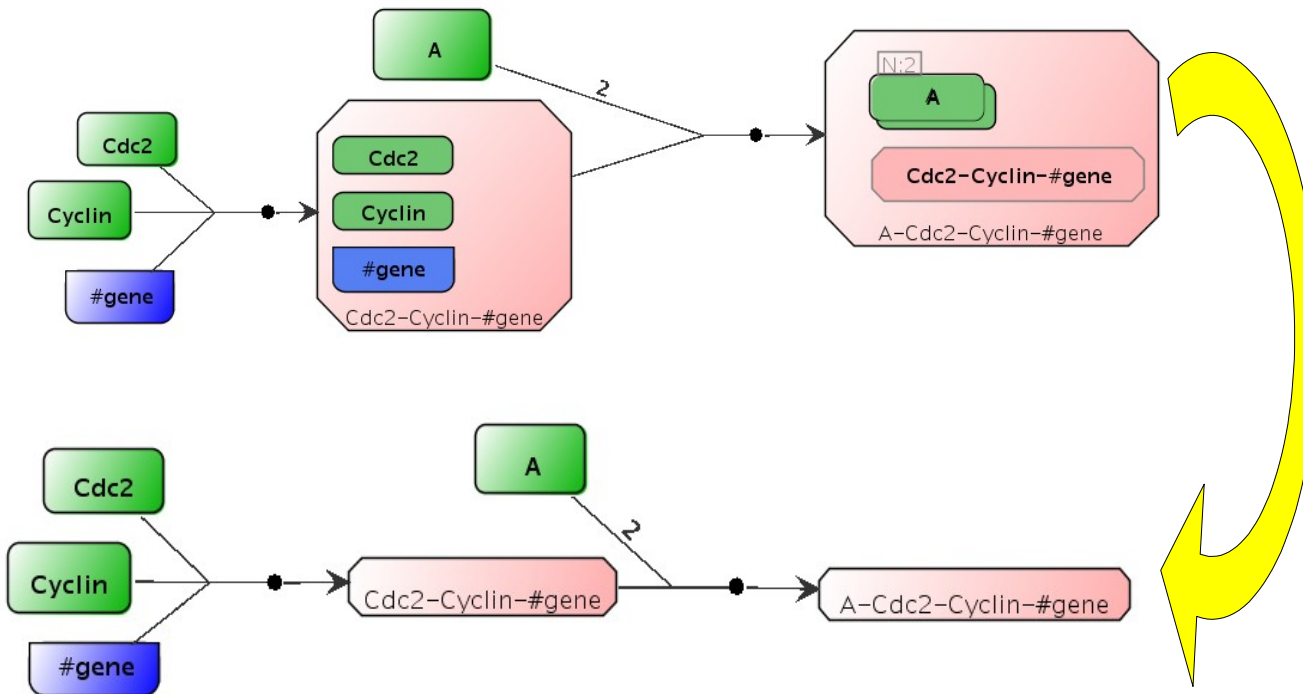


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# CONCLUSION

## Proposal for SBGN

### ★ Nested complexes



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# CONCLUSION

- ◆ *Biocham is based on a formal language for modelling biochemical systems*
- ◆ *Static analyses in the Graphical User Interface*
- ◆ *SBGN Graphical Editor - The best of the both worlds (formal and graphical)*

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# ***On-going work***

- ◆ *Better automatic Layout*
- ◆ *Layout saving format and reuse of layout*
- ◆ *Generalization of graphical operations to edit model reductions [Gay Soliman Fages bioinformatics 2010]*

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# ***SBGN support in BIOCHAM***

***Thank You!!!!***

***biocham@inria.fr***

***http://contraintes.inria.fr/BIOCHAM/***

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# Thank You!!!!

## Members of Constraints:

[François Fages](#) (INRIA senior research scientist, team leader)

[Grégory Batt](#) (INRIA research scientist)

[Pierre Deransart](#) (INRIA senior research scientist)

[Sylvain Soliman](#) (INRIA research scientist, vice-leader)

[Nicolas Beldiceanu](#) (associate, professor EMIN Nantes)

Denis Thieffry (associate, professor ENS Ulm)

Elisabetta De Maria (INRIA post-doctorate engineer)

Sylvain Pradalier (INRIA post-doctorate fellow)

Xavier Duportet (PhD student, INRIA)

Steven Gay (PhD student, INRIA)

[Domitille Heitzler](#) (PhD student, ASC INRA Tours)

[Julien Martin](#) (PhD student, INRIA)

[Thierry Martinez](#) (PhD student, INRIA)

Faten Nabli (PhD student, INRIA)

[Aurélien Rizk](#) (PhD student, INRIA)

Jannis Ullendorff (PhD student, INRIA)

Dragana Jovanovska (INRIA engineer)



# BIOCHAM