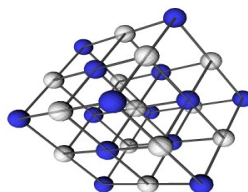


# *SBGN support in BIOCHAM*

## Biochemical Abstract Machine



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INRIA Paris – Rocquencourt, France

**06.10.2010**

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# SBGN support in BIOCHAM



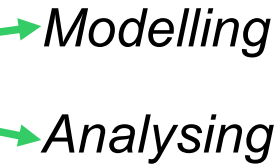
## Outline:


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

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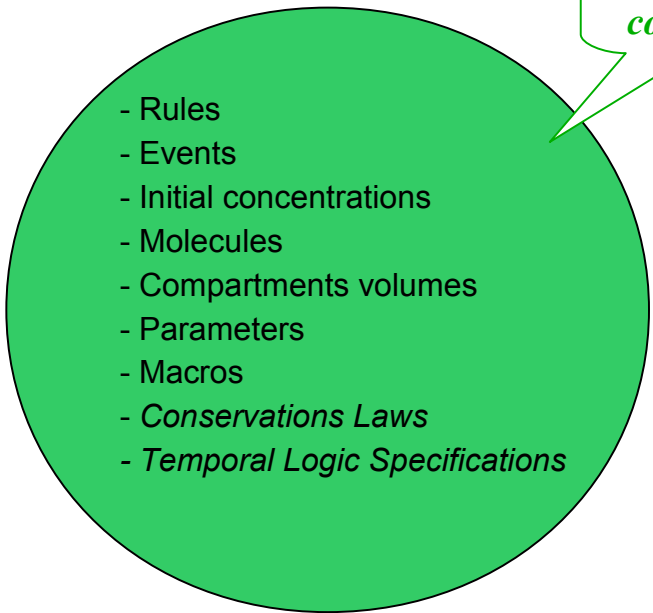
# SBGN support in BIOCHAM

- **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 

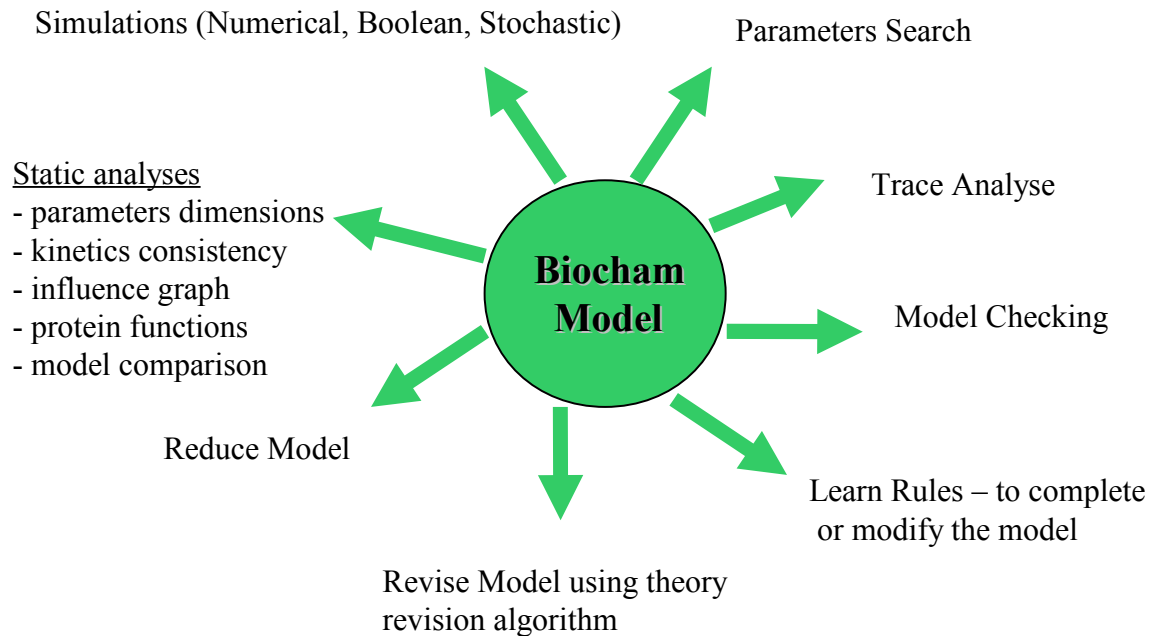


*SBML  
compatible*



# 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:

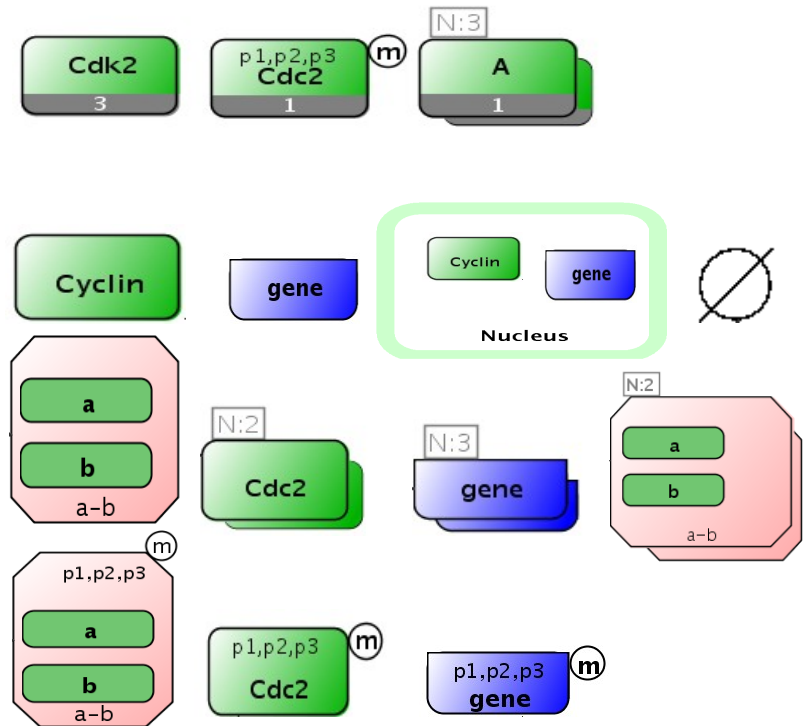
Macromolecule, Nucleic Acid Feature, Multimer, Complex, Source and Sink, Compartment, Unit of Information(cardinality), State Variable(modified), Labeled Clone Marker!!!

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](#) :

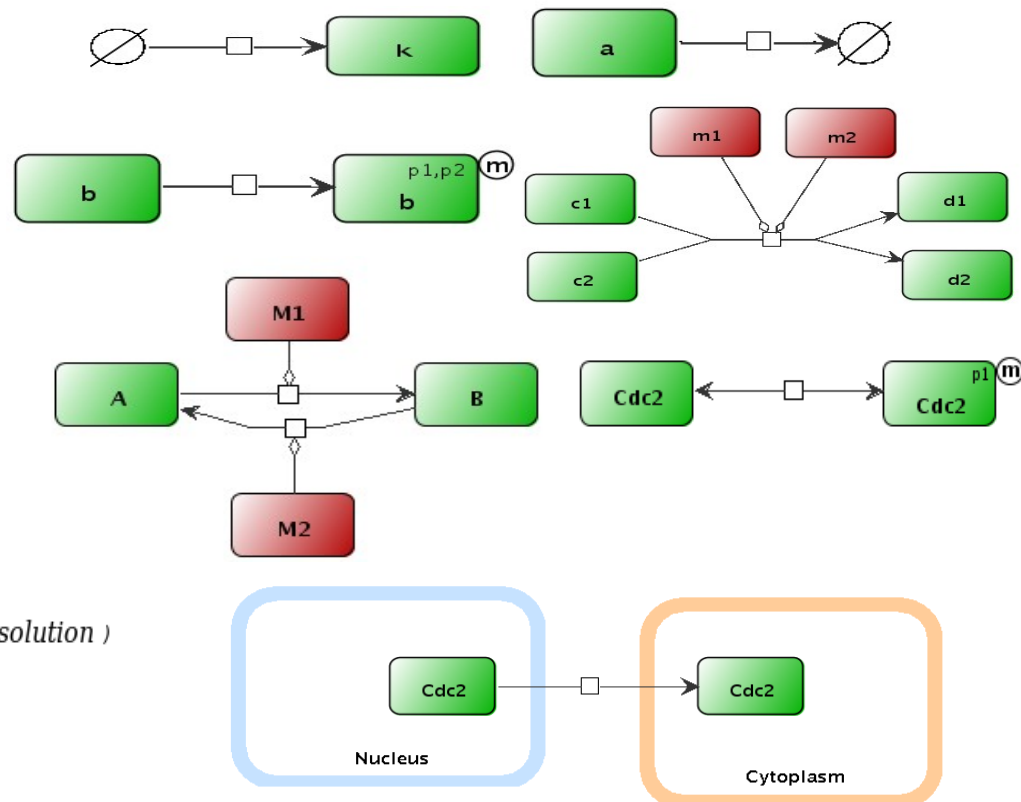
## Process, Association and Dissociation

### 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:

```

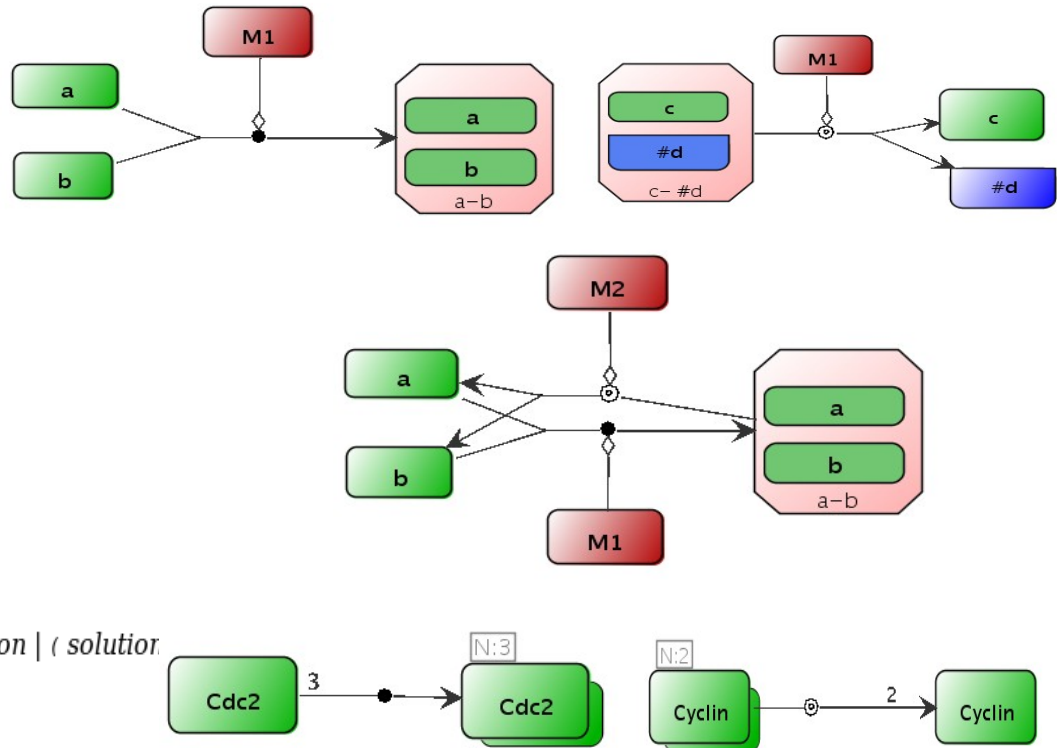
reaction =      kinetics for basic_reaction
                | basic_reaction
                | name : basic_reaction
                | name : kinetics for basic_reaction
    
```

```

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

```

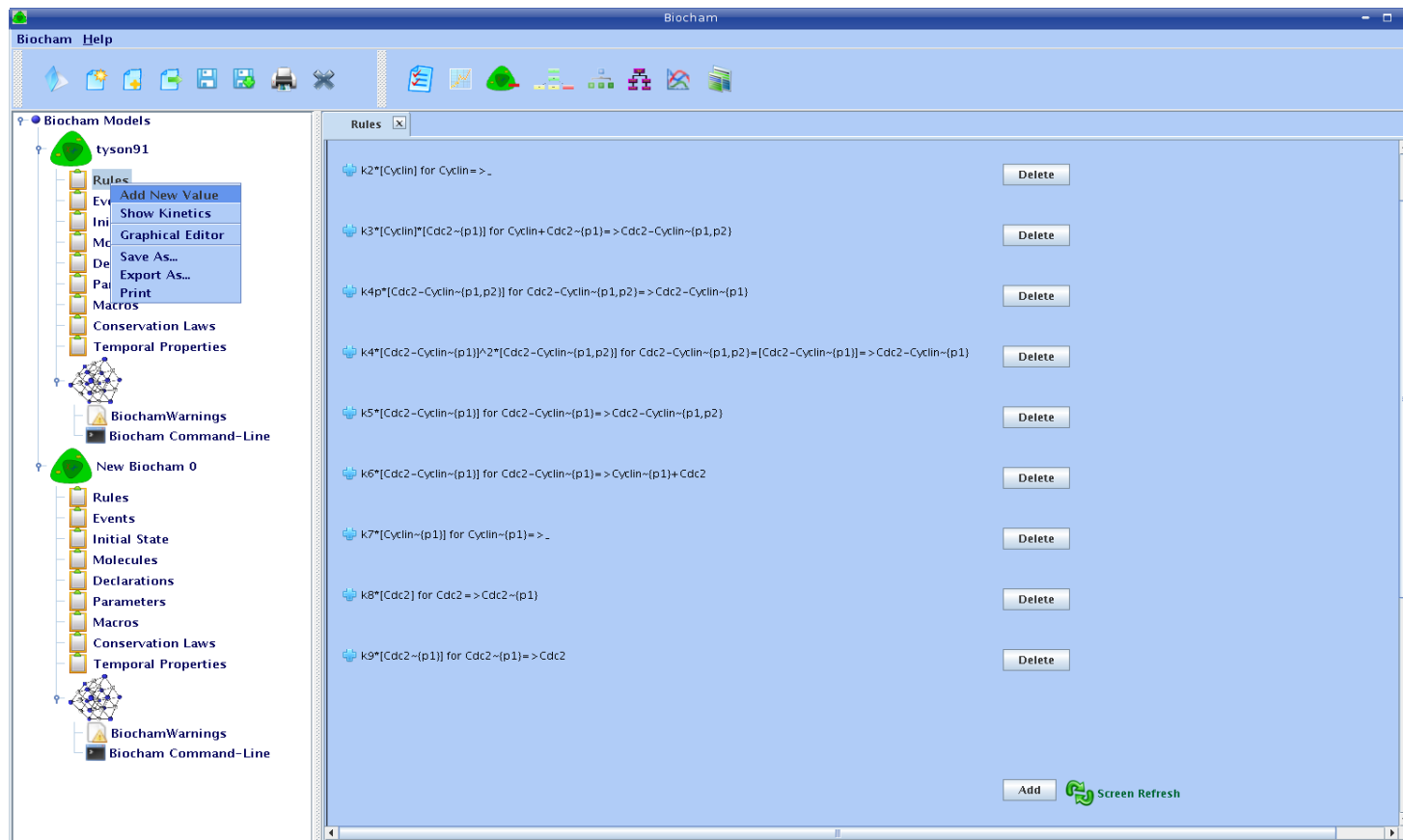
solution =      _ | object | integer*object | solution + solution | ( solution
    
```



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# SBGN support in BIOCHAM

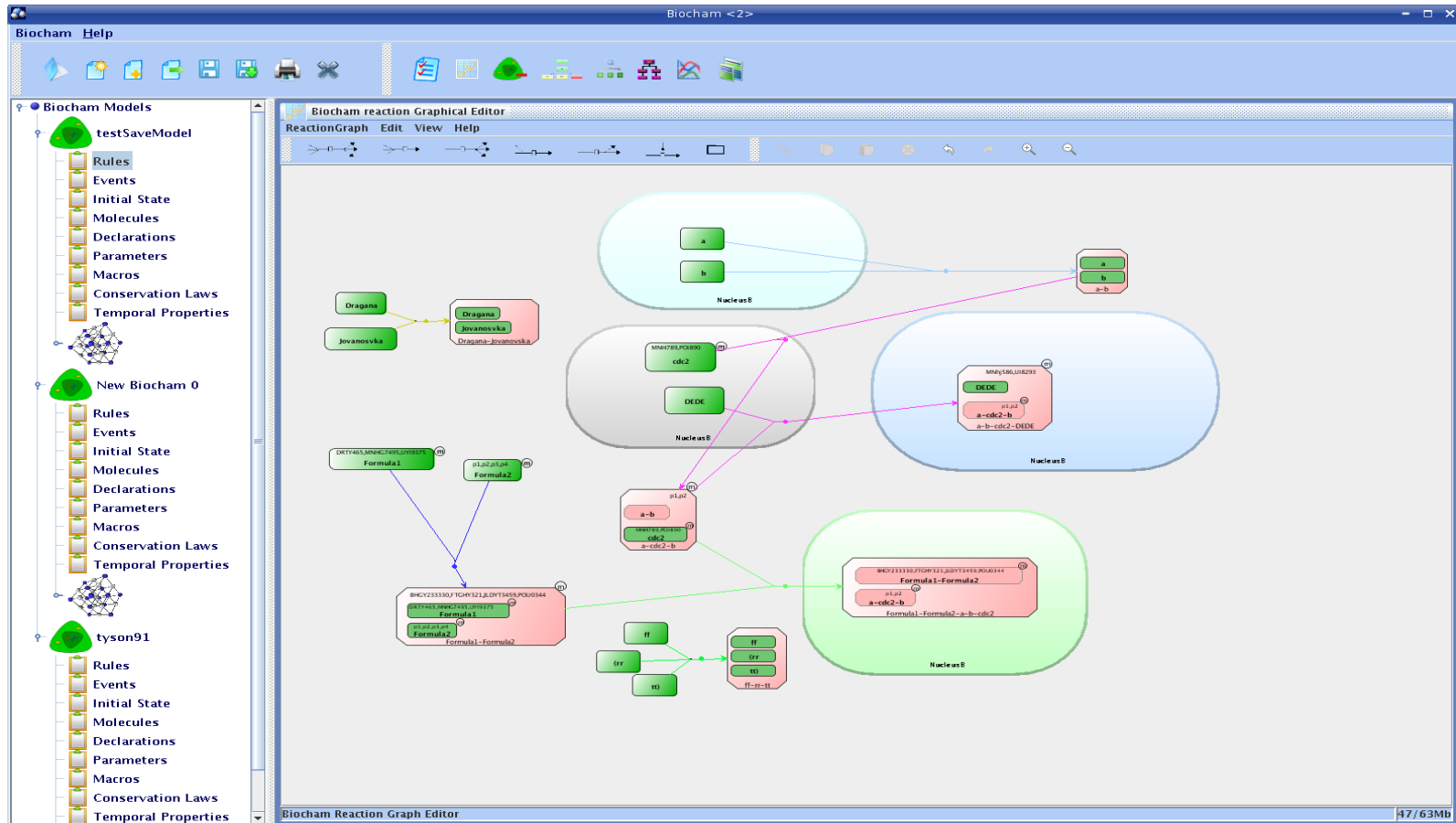
- Biocham Reaction Graph Editor



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# SBGN support in BIOCHAM

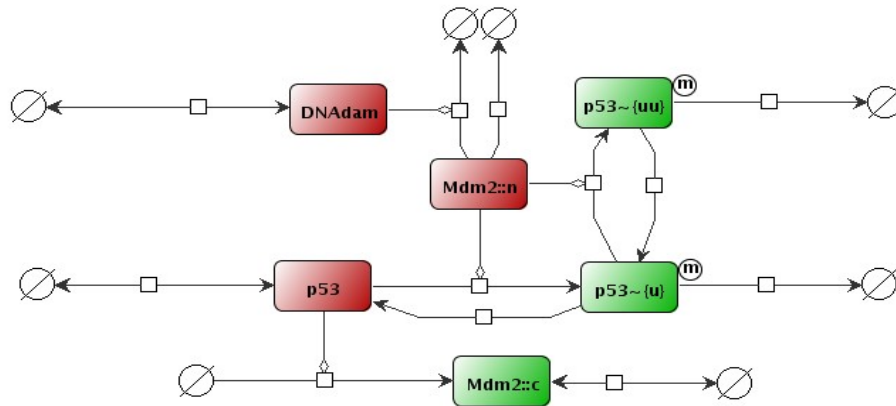
- Biocham Reaction Graph Editor



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# SBGN support in BIOCHAM

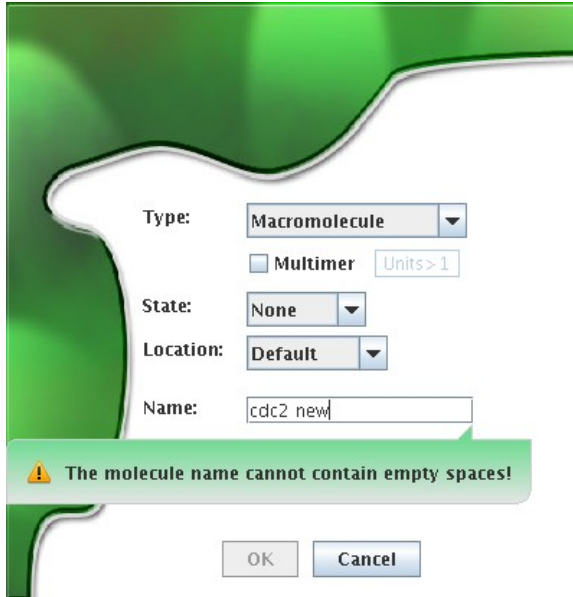
- Biocham Reaction Graph Editor



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# BioCham Reaction Graph Editor

Validation of the syntax and the semantics



The screenshot shows a dialog box for creating a 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)

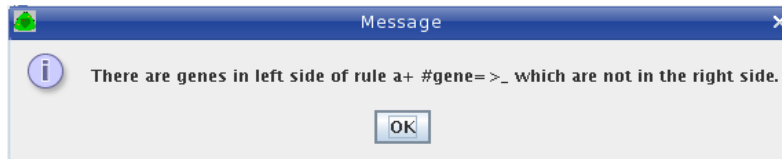
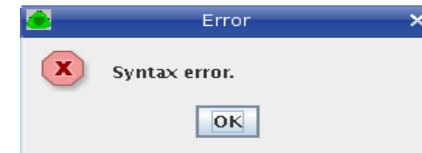
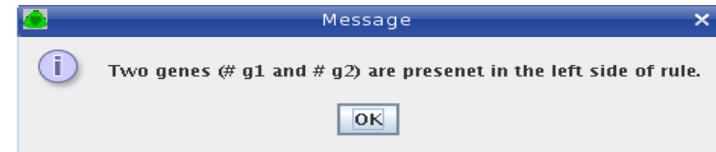
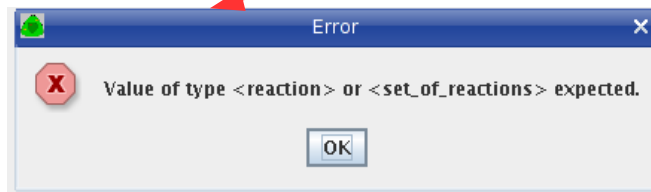
A green error message box is displayed at the bottom of the dialog, containing a warning icon and the text: "The molecule name cannot contain empty spaces!". Below the error message are "OK" and "Cancel" buttons.

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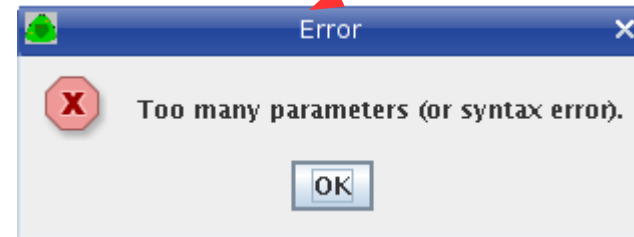
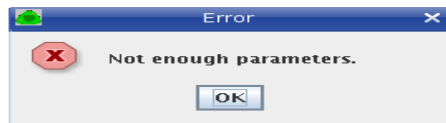
# BioCham Reaction Graph Editor

## 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 under "Biocham Models" with a "New Biocham 0" model selected. The tree view includes folders for "Rules", "Events", "Initial State", "Molecules", "Declarations", "Parameters", "Macros", "Conservation Laws", and "Temporal Properties". Below these is a "BiochamWarnings" folder and a "Biocham Command-Line" folder. The main area displays the "BiochamWarnings and Errors" panel, which contains the following messages:

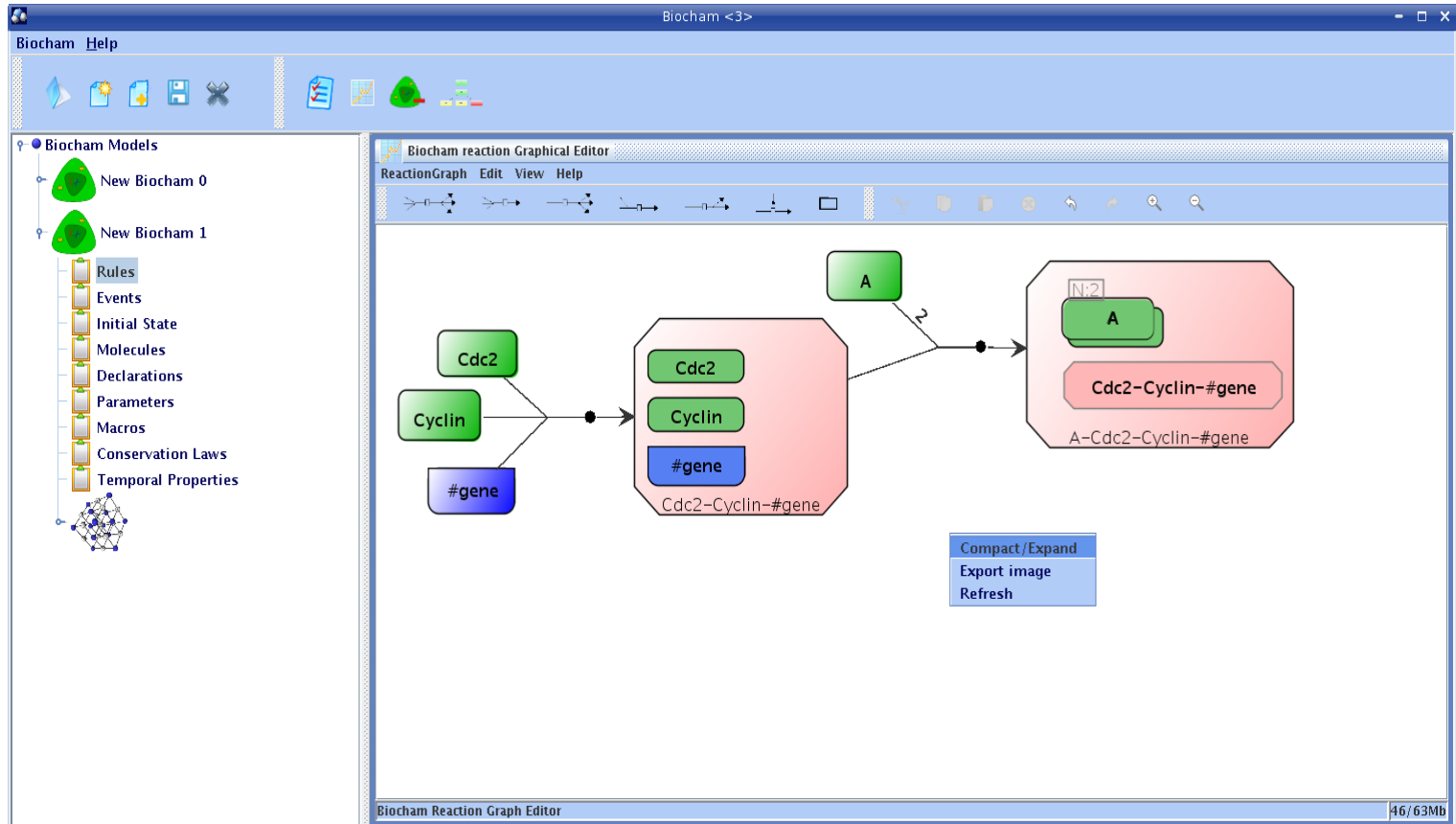
- Error:** Value of type <reaction> or <set\_of\_reactions> expected.
- Warning:** There are genes in left side of rule  $a + \#gene = \_$  which are not in the right side.
- Warning:** Two genes ( $\# g1$  and  $\# g2$ ) are present in the left side of rule.
- Warning:** There are genes in left side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

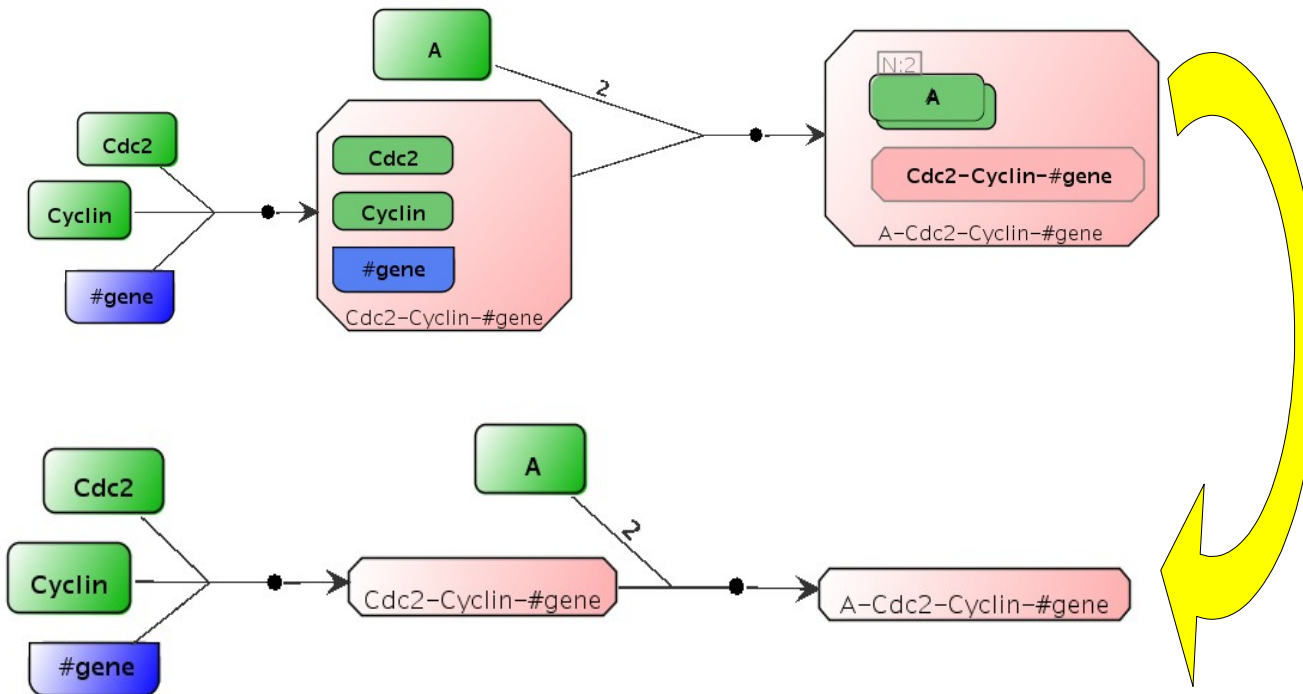


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# CONCLUSION

## 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!!!!***

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

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# Thank You!!!!

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

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

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Dragana Jovanovska (INRIA engineer)



# BIOCHAM