



BioUML

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Main new features

- Graphic Notation Editor
- SBGN implementation (prototype)
- Library of predefined kinetic law functions on the base of SBO
- Database references editor
 - use MIRIAM (under construction)
 - gene hub concept
- Microarray plug-in (alpha version)
- BioModels - comparison with other simulators

Graphic notation

formal definition as XML
document

<http://www.biouml.org/sbgn.shtml>

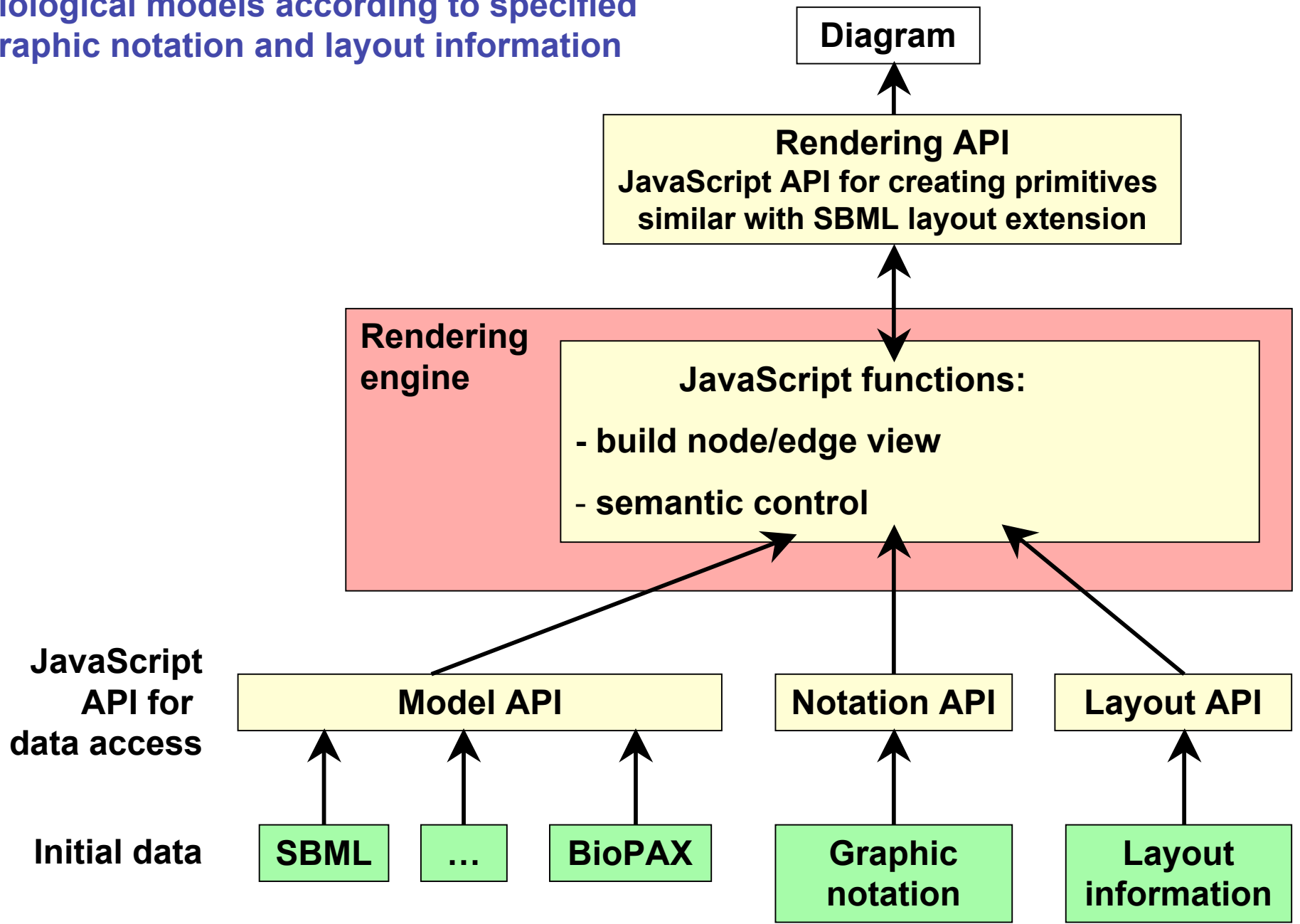
Graphic notation versus graph layout

- allows edit diagram
- allows to create new diagram
- different graphic notations can be applied to the same SBML model
- allows formally define SBGN and use it in SBML models
- allows to reuse graphic notation by many tools

Graphic notation can be defined formally as XML document

- properties – formal definition of properties that can be used as properties of nodes and edges (for example, title, multimer, etc.). Definition of property includes:
 - name
 - type
 - short description
 - controlled vocabulary (optional)
- node types – definition of node includes:
 - name
 - icon
 - properties
 - view function (JavaScript)
 - short description
- edge types – definition of edge includes:
 - name
 - icon
 - properties
 - view function (JavaScript)
 - short description
- semantic controller – defines rules for semantic control of diagram integrity. For this purpose it defines following functions:
 - canAccept (JavaScript)
 - isResizable (JavaScript)
 - move (JavaScript)
- Examples – a set of diagrams that can be used as test cases, legend and examples for the graphic notation. DML - Diagram Markup Language – is used for this purpose.

Basic software architecture for rendering of biological models according to specified graphic notation and layout information



Formal definition of graphic notation as XML document and integration with SBML format

Graphic notation components	Defined as	SBML
Object types	XML	<annotation s>
Object properties	XML	<annotation s>
User defined properties	XML	<annotations >
Rules for visualization	JavaScript	
Rules for semantic control	JavaScript	
Test cases	XML	model, module

Graphic Notation Editor

Graphic notation editor main concepts

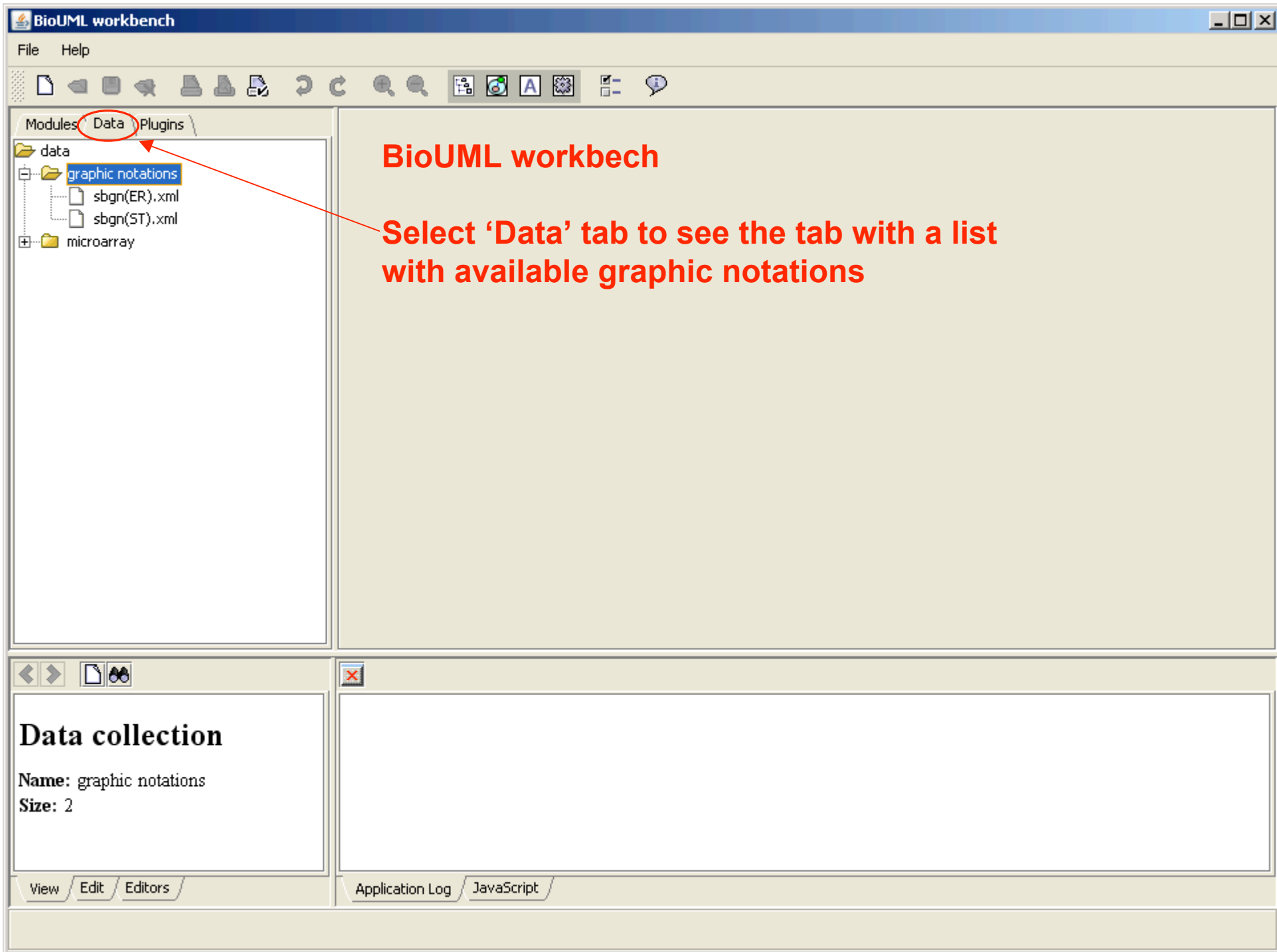
- graphic notation is defined formally as XML document
- graphic notation editor provides user friendly interface for XML document editing
- SBGN graphic notation (prototype) is implemented
- BioUML workbench allows to create and edit diagrams using graphic notation defined as XML document
- May be graphic editor will be useful for SBGN community for:
 - improving SBGN specification
 - for testing SBGN specification by creating different diagrams

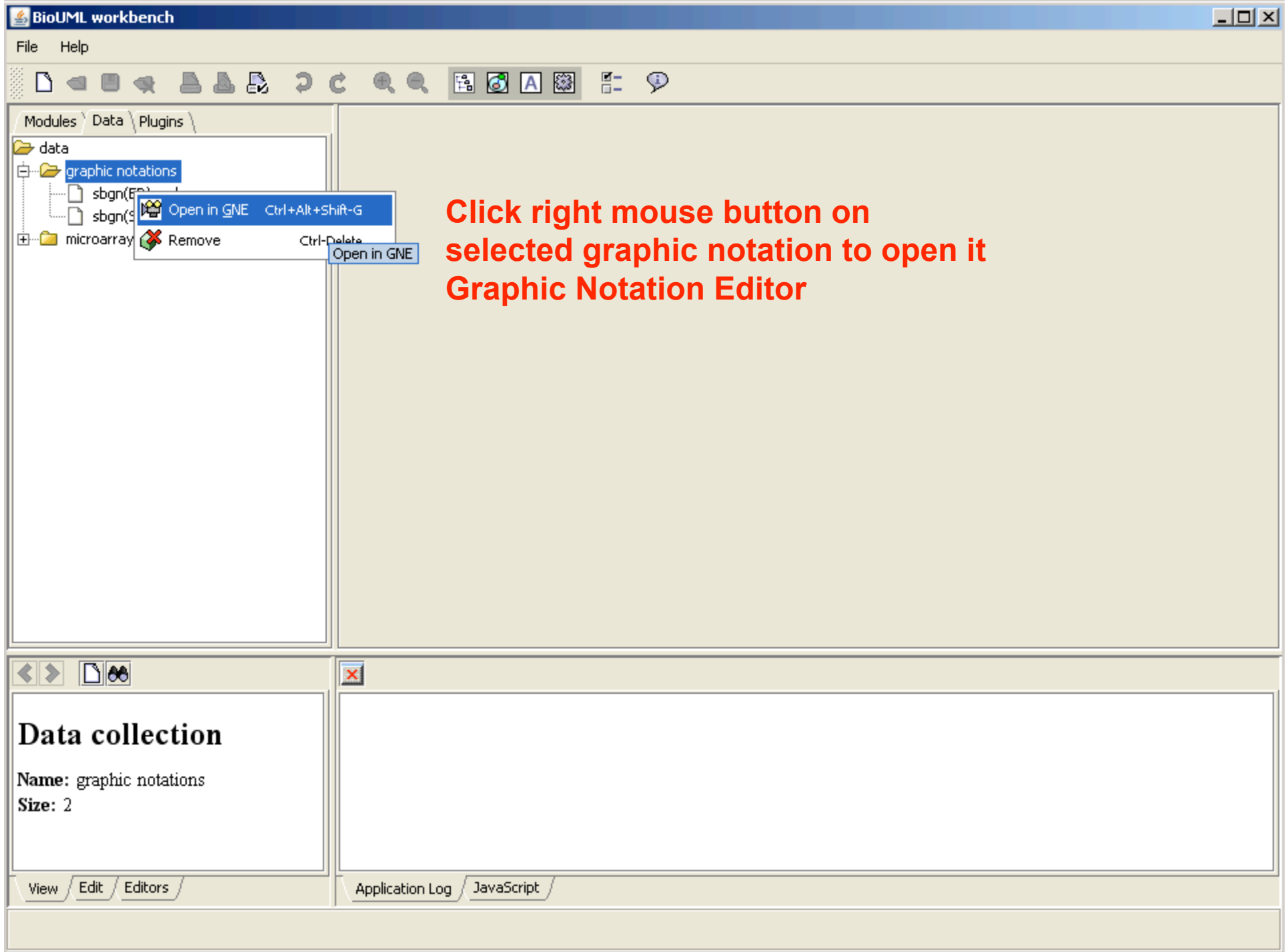
Details:

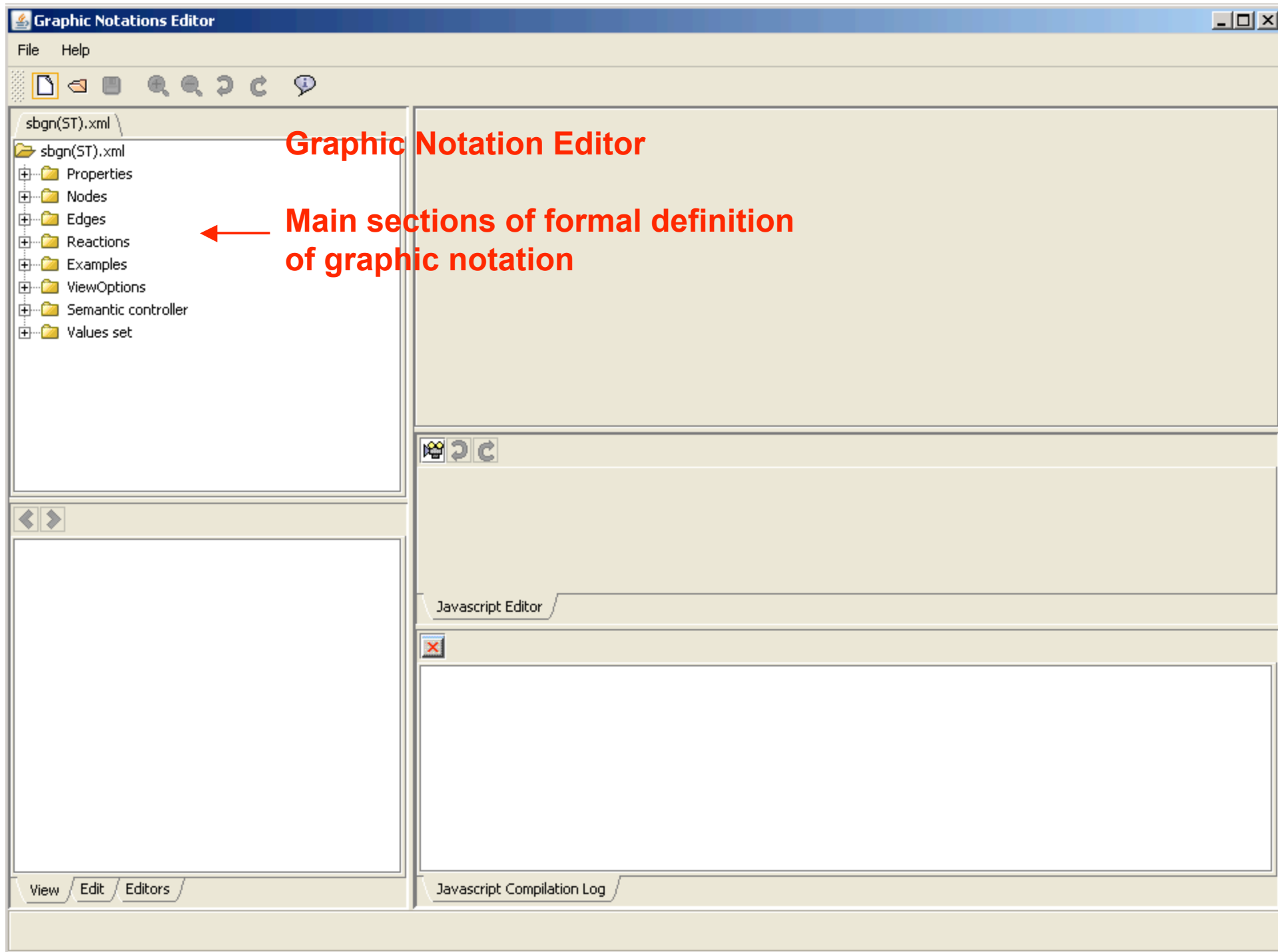
<http://www.biouml.org/sbgn.shtml>

Graphic Notation Editor

user interface







Graphic Notations Editor

File Help

sbgn(ST).xml \

- sbgn(ST).xml
 - Properties
 - multimer**
 - text
 - value
 - Nodes
 - Edges
 - Reactions
 - Examples
 - ViewOptions
 - Semantic controller
 - Values set

List of specific properties that are used by graphic notation

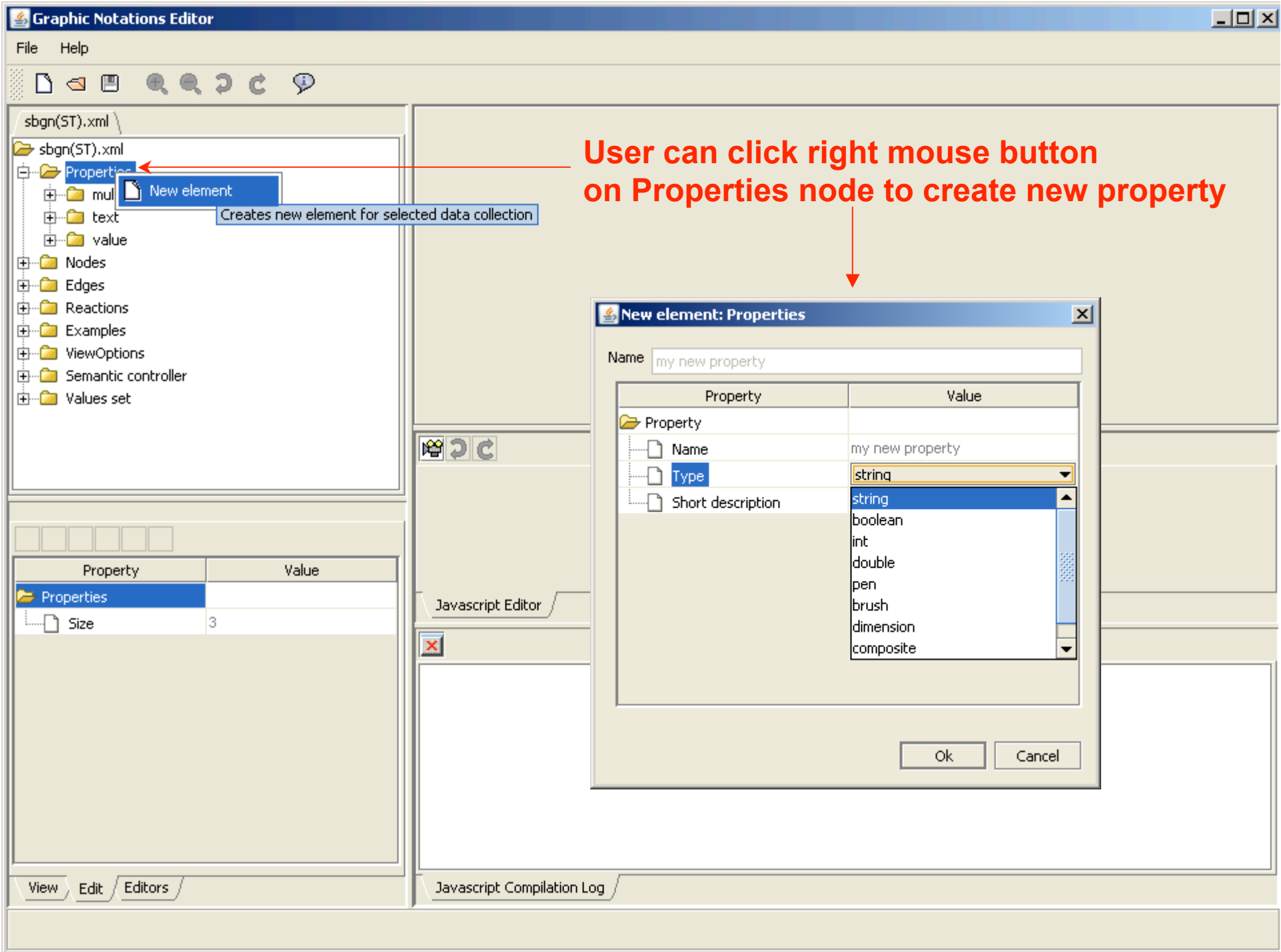
Properties editor

Property	Value
Property	
Name	multimer
Type	int
Short description	multimer

Javascript Editor

Javascript Compilation Log

View Edit Editors



Graphic Notations Editor

File Help

sbgn(ST).xml \

- sbgn(ST).xml
 - Properties
 - multimer
 - text
 - value
 - Nodes ← **Nodes – contains list of all node types used by graphic notation**
 - source-sink
 - tag
 - unspecified entity
 - simple chemical
 - multimer
 - macromolecule
 - complex
 - compartment
 - unit of information
 - variable
 - and
 - or
 - xor
 - not
 - transition

```
function f(container, node, options, g)
{
    var d, pen, brush;
    d = new Dimension(50,50);
    brush = new Brush(new Color(1.0, 0.9, 1.0));
    pen = options.getDefaultPen();
    var multimer = node.getValue("multimer", 0);
    if(multimer>1)
    {
        var ellipse = new EllipseView(pen, brush, 5, 5, d.width, d.height);
    }
}
```

Property	Value
Properties	
Name	simple chemical
Property count	1
Icon	<input type="radio"/> Select...

View Edit Editors

Javascript Editor

Javascript Compilation Log

Graphic Notations Editor

File Help

sbgn(ST).xml \

- sbgn(ST).xml
 - Properties
 - multimer
 - text
 - value
 - Nodes
 - source-sink
 - tag
 - unspecified entity
 - simple chemical
 - multimer
 - macromolecule
 - complex
 - compartment
 - unit of information
 - variable
 - and
 - or
 - xor
 - not
 - transition

For each node type user can define:

- name
- properties
- icon
- view function (JavaScript)

```
function f(container, node, options, g)
{
    var d, pen, brush;
    d = new Dimension(50,50);
    brush = new Brush(new Color(1.0, 0.9, 1.0));
    pen = options.getDefaultPen();
    var multimer = node.getValue("multimer", 0);
    if(multimer>1)
    {
        var ellipse = new EllipseView(pen, brush, 5, 5, d.width, d.height);
    }
}
```

Property	Value
Properties	
Name	simple chemical
Property count	1
Icon	<input type="radio"/> Select...

Javascript Editor

Javascript Compilation Log

Graphic Notations Editor

File Help

sbgn(ST).xml \

- sbgn(ST).xml
 - Properties
 - multimer
 - text
 - value
 - Nodes
 - source-sink
 - tag
 - unspecified entity
 - simple chemical
 - multimer
 - macromolecule
 - complex
 - compartment
 - unit of information
 - variable
 - and
 - or
 - xor
 - not
 - transition

By clicking right mouse button on "Nodes" user can create new node type

New element: Nodes

Name: my new node type

Property	Value
Properties	
Name	my new node type
Icon	Select...

is compartment

Ok Cancel

```
function f
(  

  var d,  

  d = new  

  brush =  

  pen = c  

  var mul  

  if(mult  

  (  

  var  

  d.height);
```

Javascript Editor

Javascript Compilation Log

View Edit Editors

Graphic Notations Editor

File Help

sbgn(ST).xml \

- sbgn(ST).xml
 - Properties
 - multimer
 - text
 - value
 - Nodes
 - Edges
 - consumption
 - production
 - modulation
 - stimulation
 - catalysis
 - inhibition
 - Reactions
 - Examples
 - ViewOptions
 - Semantic controller
 - Values set

By the same way user can define edge type:

- name
- properties
- icon
- view function (JavaScript)

```
function f(container, edge, inPoint, outPoint, options, g)
{
    var pen, brush;
    brush = new Brush(new Color(0.0, 0.0, 0.0));
    pen = options.getDefaultPen();
    var arrow = new ArrowView(pen, brush, inPoint.x, inPoint.y, outPoint.x, outPoint.y, 0);
    container.add(arrow);
    return false;
}
```

Property	Value
Properties	
Name	consumption
Property count	0
Icon	— <input type="button" value="Select..."/>

View Edit Editors

Javascript Editor

Javascript Compilation Log

Graphic Notations Editor

File Help

sbgn(ST).xml \

- sbgn(ST).xml
 - Properties
 - Nodes
 - Edges
 - Reactions
 - Examples
 - complex
 - modulation
 - test
 - simple
 - transition
 - transition2
 - test4
 - test2
 - test3
 - ViewOptions
 - Semantic controller
 - Values set

sbgn(ST).xml : complex \

“Examples” node contains a set of diagrams that demonstrates usage of graphic notation.

```
function f(container, node, options, g)
{
  var d, pen, brush;
}
```

Property	Value
Compartment	
Title	label1
Comment	
ShapeColor	<input type="text" value="white"/>
Size	
Attributes	

View Edit Editors

Javascript Editor

Javascript Compilation Log

Graphic Notations Editor

File Help

sbgn(ST).xml \

- sbgn(ST).xml
 - Properties
 - Nodes
 - Edges
 - Reactions
 - Examples
 - complex
 - modulation
 - test
 - simple
 - transition
 - transition2
 - test4
 - test2
 - test3
 - ViewOptions
 - Semantic controller
 - Values set

sbgn(ST).xml : complex \

User can create and edit such diagram.

Property	Value
Compartment	
Title	label1
Comment	
ShapeColor	<input type="text" value="white"/>
Size	
Attributes	

```
function f(container, node, options, g)
{
  var d, pen, brush;
```

Javascript Editor

Javascript Compilation Log

Graphic Notations Editor

File Help

sbgn(ST).xml \

- sbgn(ST).xml
 - Properties
 - Nodes
 - Edges
 - Reactions
 - Examples
 - complex
 - modulation
 - test
 - simple
 - transition
 - transition2
 - test4
 - test2
 - test3
 - ViewOptions
 - Semantic controller
 - Values set

When user selects some element on the diagram he can edit:

- object properties
- JavaScript that builds a view for selected diagram element

sbgn(ST).xml : complex \

```
function f(container, node, options, g)
{
    var d, pen, brush;
    d = new Dimension(50,50);
    brush = new Brush(new Color(1.0, 0.9, 1.0));
    pen = options.getDefaultPen();
    var multimer = node.getValue("multimer", 0);
    f(multimer);
}
```

Property	Value
Node	
Title	label4
Comment	
Size	
Attributes	

View Edit Editors

Javascript Editor

Javascript Compilation Log

Graphic Notations Editor

File Help

sbgn(ST).xml \

- sbgn(ST).xml
 - Properties
 - Nodes
 - Edges
 - Reactions
 - Examples
 - ViewOptions
 - Semantic controller
 - Can accept
 - Is resizable
 - Move
 - Values set

“Semantic controller” node contains list of JavaScript functions that provide semantic constraints and semantic integrity of the diagram.

Property	Value
Data Collection	
Size	0

```
function f(container, de)
{
    var deType = de.getValue('kernel', '').getType();
    if(deType == "unspecified entity" || deType == "xor" || deType == "or" || deType == '
    || deType == "transition" || deType == "uncertain process" || deType == "omitted pro
    {
        var type = container.getValue('kernel', '').getType();
        if(type == "xor" || deType == "or" || deType == "omitted process" || deType == "uncertain process" || deType == "transition" || deType == "unspecified entity")
        {
            return false;
        }
    }
    return true;
}
```

Javascript Editor

Javascript Compilation Log

View Edit Editors

Graphic Notations Editor

File Help

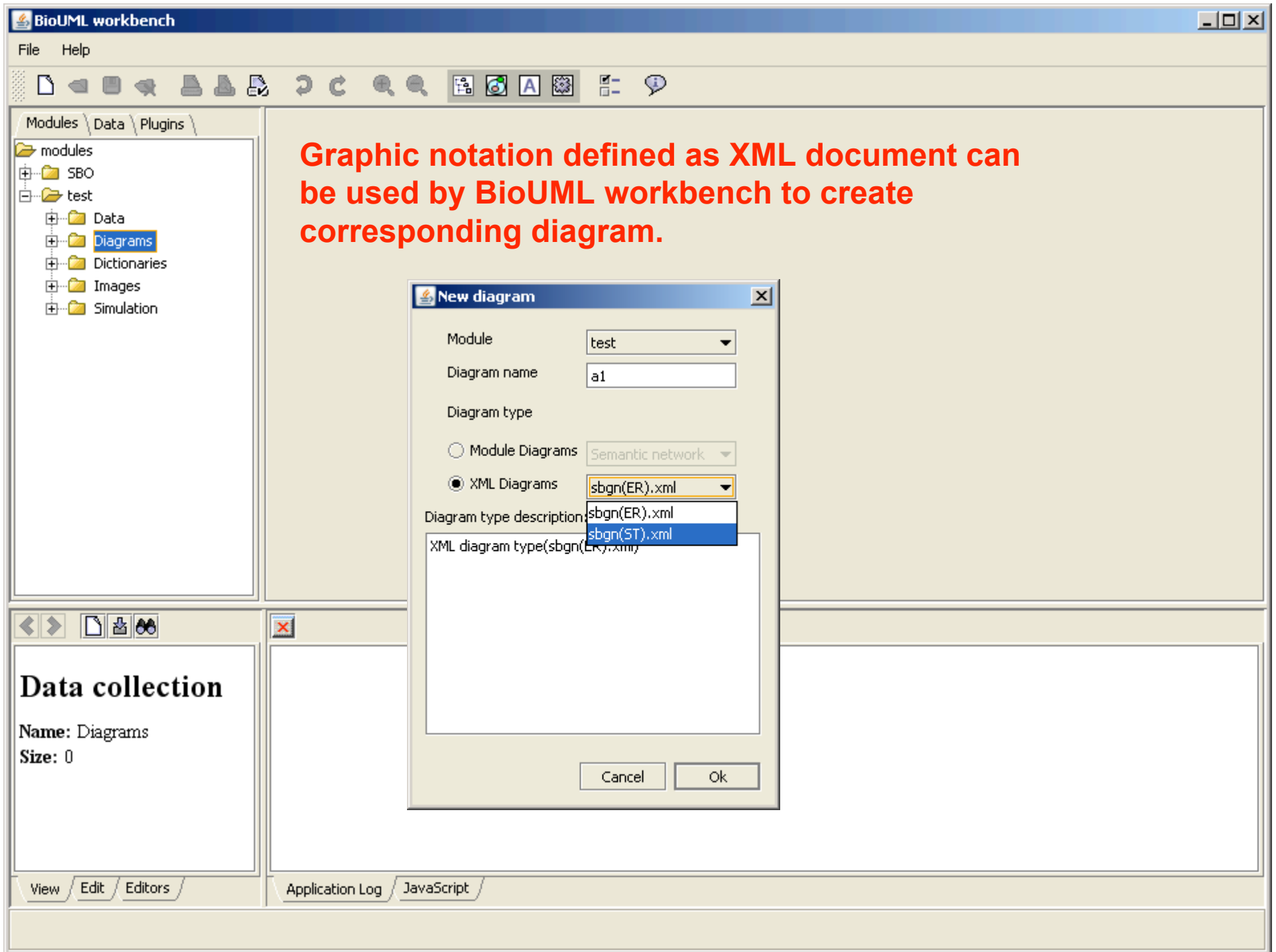
sbgn(ST).xml sbgn(ER).xml

- sbgn(ER).xml
 - Properties
 - Nodes
 - Edges
 - Reactions
 - Examples
 - ViewOptions
 - Semantic controller
 - Values set

“Value set” node contains list of controlled vocabularies for property values (not completed yet).

Property	Value
Values set	
Size	0

```
function f(container, de)
{
    var deType = de.getValue('kernel', '').getType();
    if(deType == "unspecified entity" || deType == "xor" || deType == "or" || deType == '
    || deType == "transition" || deType == "uncertain process" || deType == "omitted pro
    {
        var type = container.getValue('kernel', '').getType();
        </pre>
```



BioUML workbench

File Help

Modules | Data | Plugins

test : a1

modules

- SBO
- test
 - Data
 - Diagrams
 - a1
 - a
 - a(2)
 - b
 - catalysis_0: \$macromolecule
 - consumption_0: \$a to \$"a(2)
 - macromolecule
 - production_0: \$"a(2)" to \$b
 - Dictionaries
 - Images
 - Simulation

Diagram

Diagram description: A reaction diagram showing a macromolecule (p453) catalyzing the conversion of species 'a' to species 'b'. The macromolecule is represented by a green rounded rectangle labeled 'p453' and 'macromolecule'. Species 'a' and 'b' are represented by pink circles. A reaction arrow points from 'a' to 'b', with a small white circle containing a question mark above it. A vertical line connects the macromolecule to this question mark.

Property	Value
Diagram	
Title	a1
Diagram type	XmlDiagramType
Layouter	"...forceDirectedLayout..."
Comment	
Data	

Normal
Html
Preview

Description | References | Application Log | Clipboard | Layouter pane | JavaScript | Search linked

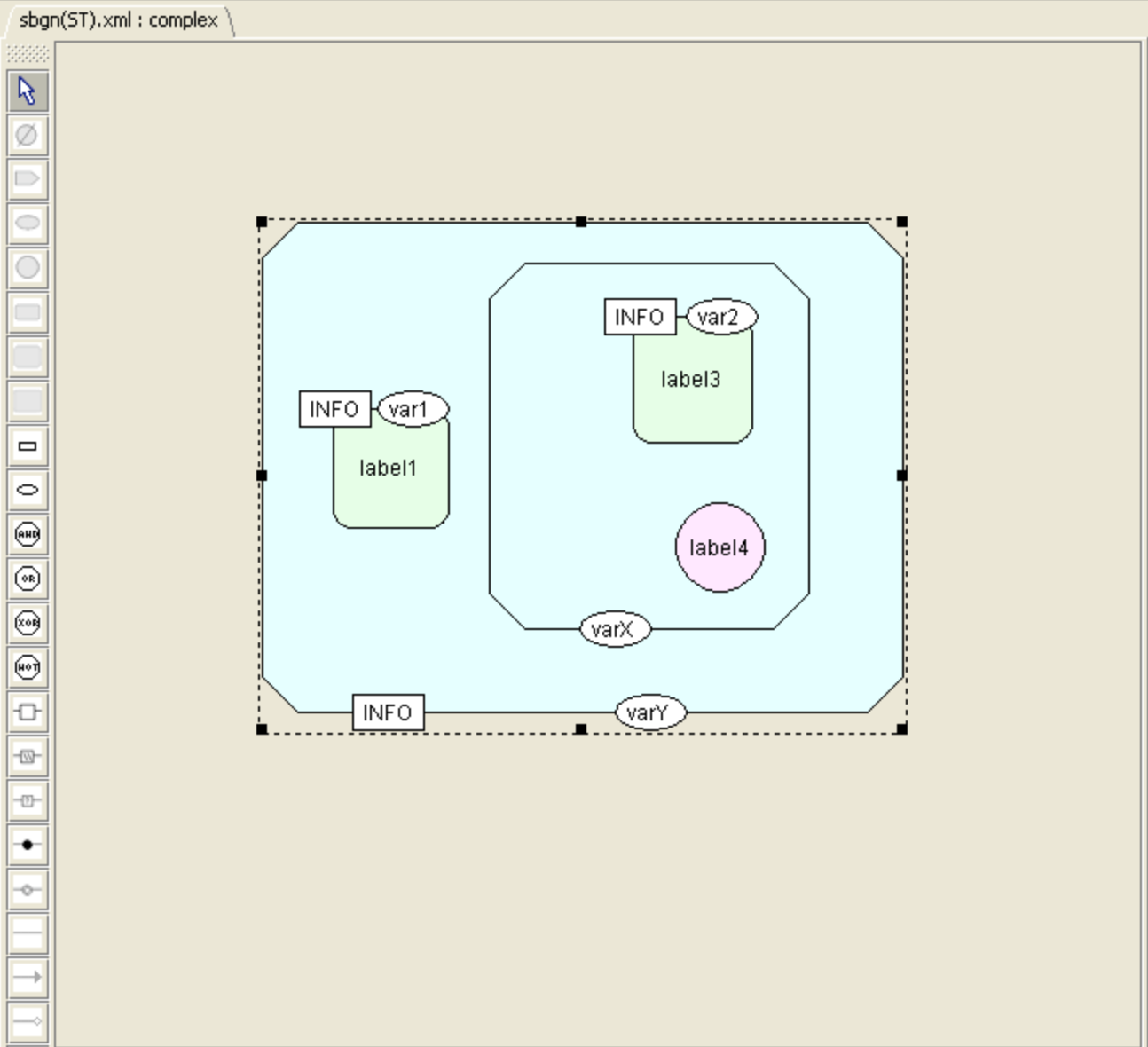
Graphic Notation Editor

SBGN examples
created in BioUML



sbgn(ST).xml \ sbgn(ER).xml \

- sbgn(ST).xml
 - Properties
 - Nodes
 - Edges
 - Reactions
 - Examples
 - complex
 - modulation
 - test
 - simple
 - transition
 - transition2
 - test4
 - test2
 - test3
 - ViewOptions
 - Semantic controller
 - Values set



Property	Value
Compartment	
Title	dscsdacsd
Comment	
ShapeColor	<input type="text" value="white"/>
Size	
Attributes	

Graphic Notations Editor

File Help

sbgn(ST).xml \ sbgn(ER).xml \

- sbgn(ST).xml
 - Properties
 - Nodes
 - Edges
 - Reactions
 - Examples
 - complex
 - modulation
 - test
 - simple
 - transition
 - transition2
 - test4
 - test2
 - test3
 - ViewOptions
 - Semantic controller
 - Values set

sbgn(ST).xml : complex \ sbgn(ST).xml : modulation \

```

graph TD
  nicotine((nicotine)) --- diamond{ }
  diamond --> nAChr[nAChr]
  diamond --> nAChr2[nAChr2]
  style nicotine fill:#f9f,stroke:#333,stroke-width:1px
  style diamond fill:#fff,stroke:#333,stroke-width:1px
  style nAChr fill:#9ff,stroke:#333,stroke-width:1px
  style nAChr2 fill:#9ff,stroke:#333,stroke-width:1px
  
```

Property	Value
Diagram	
Title	modulation
Diagram type	XmlDiagramType
Layouter	"...forceDirectedLayout..."
Comment	
Data	

View Edit Editors

Graphic Notations Editor

File Help

sbgn(ST).xml \

- sbgn(ST).xml
 - Properties
 - Nodes
 - Edges
 - Reactions
 - Examples
 - complex
 - modulation
 - test
 - cdscdc
 - fdvfdvdf
 - sdcascsac
 - test1
 - test2
 - vfdvdf
 - simple
 - transition
 - transition2
 - test4
 - test2
 - test3

sbgn(ST).xml : test

Diagram Properties:

Property	Value
Diagram	
Title	test
Diagram type	XmlDiagramType
Layouter	"...forceDirectedLayout..."
Comment	
Data	

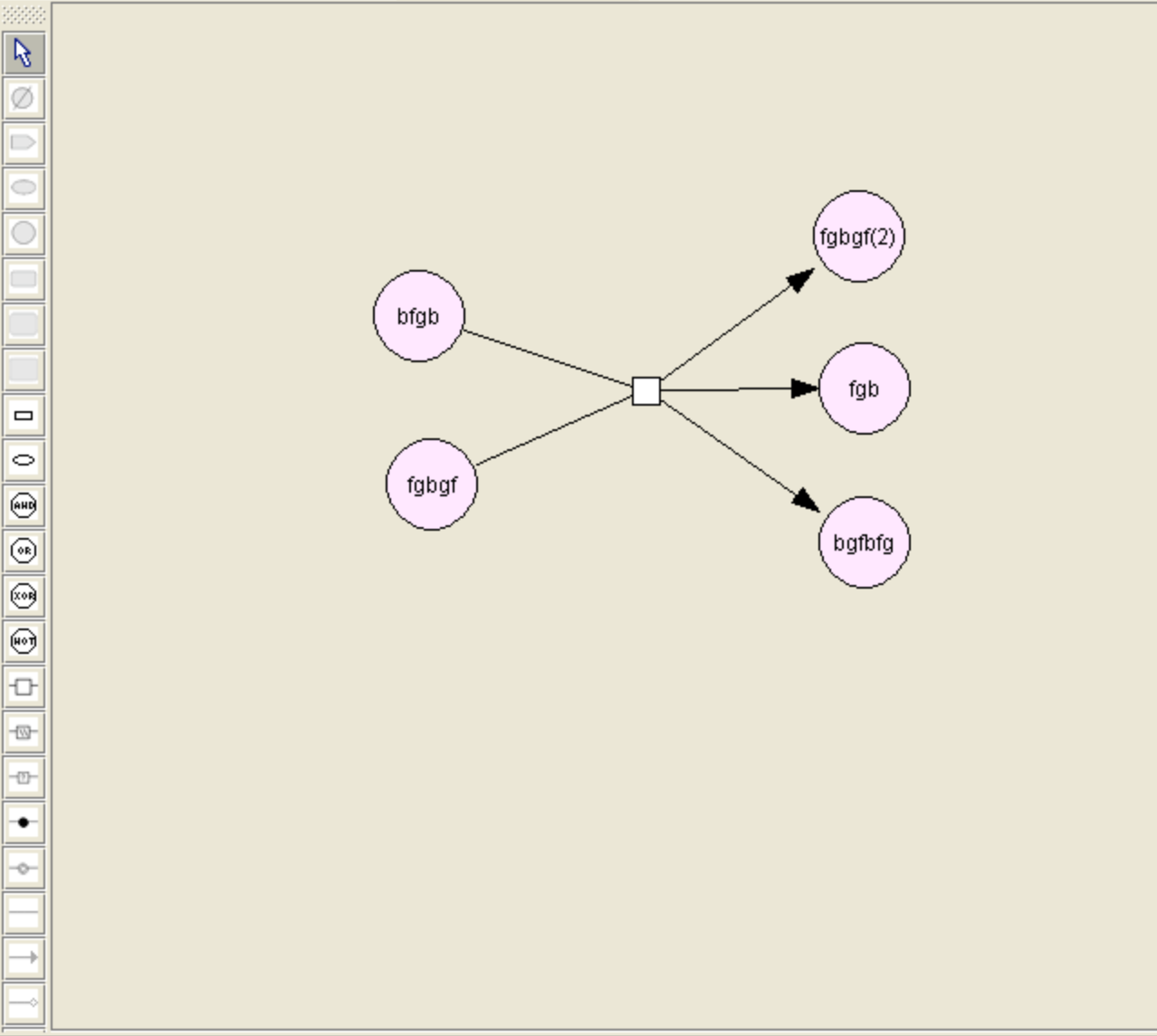
View Edit Editors



sbgn(ST).xml \

- sbgn(ST).xml
 - Properties
 - Nodes
 - Edges
 - Reactions
 - Examples
 - complex
 - modulation
 - test
 - simple
 - transition
 - bfgb
 - bgfbfg
 - consumption_0: \$bfgb to \$klnhkjb
 - consumption_0: \$fgbgf to \$klnhkjb
 - fgb
 - fgbgf
 - fgbgf(2)
 - klnhkjb
 - production_0: \$klnhkjb to \$"fgbgf(2)"
 - production_0: \$klnhkjb to \$bgfbfg

sbgn(ST).xml : test | sbgn(ST).xml : simple | sbgn(ST).xml : transition

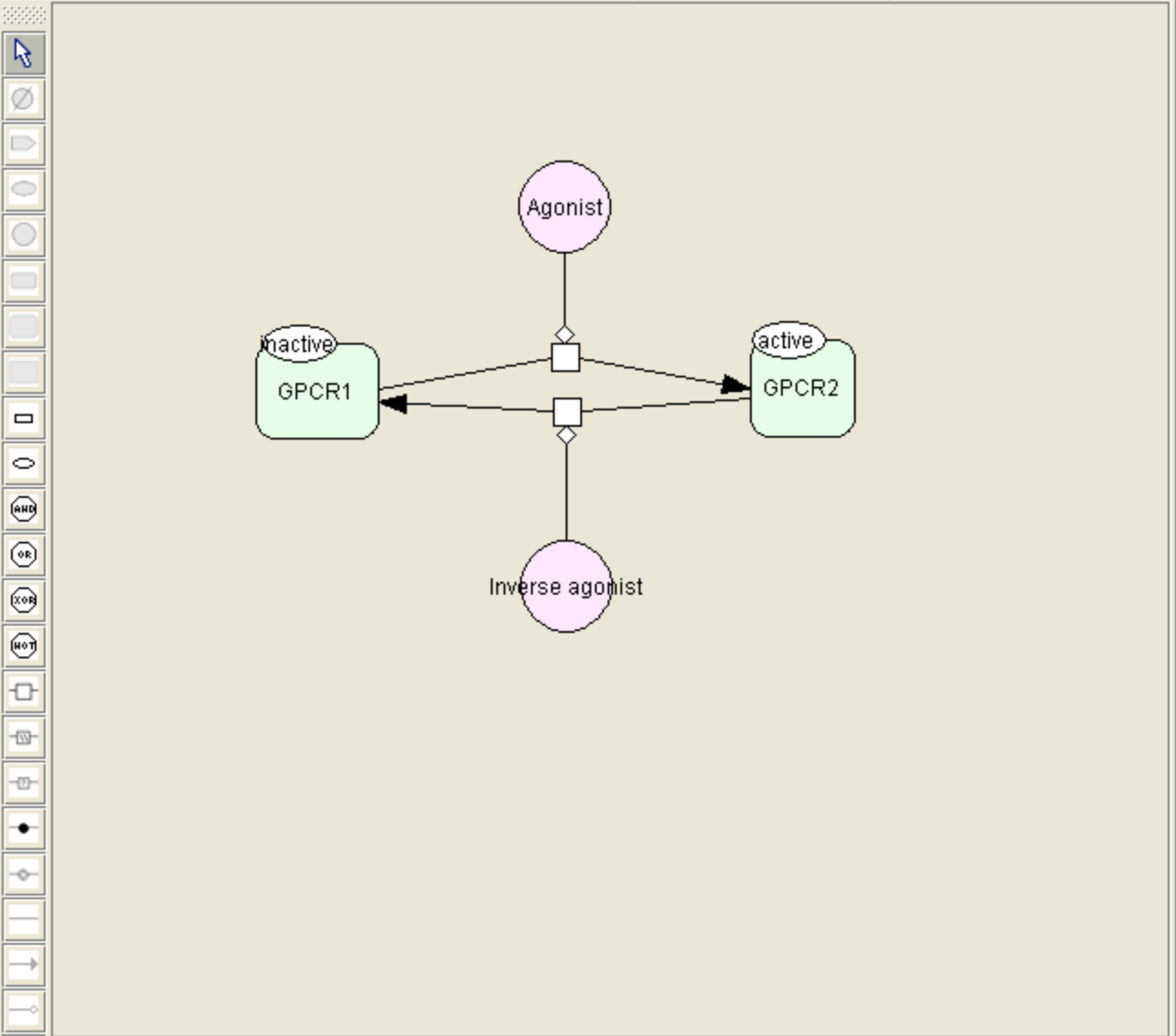


Property	Value
Diagram	
Title	transition
Diagram type	XmlDiagramType
Layouter	"...forceDirectedLayout..."
Comment	
Data	



sbgn(ST).xml \

- sbgn(ST).xml
 - Properties
 - Nodes
 - Edges
 - Reactions
 - Examples
 - complex
 - modulation
 - test
 - simple
 - transition
 - transition2
 - Agonist
 - GPCR1
 - GPCR2
 - Inverse agonist
 - consumption_0: \$GPCR1 to \$kjbk
 - consumption_0: \$GPCR2 to \$hjbkjh
 - hjbkjh
 - kjbk



Property	Value
Diagram	
Title	transition2
Diagram type	XmlDiagramType
Layouter	"...forceDirectedLayout..."
Comment	
Data	

Graphic Notations Editor

File Help

sbgn(ST).xml

- sbgn(ST).xml
 - Properties
 - Nodes
 - Edges
 - Reactions
 - Examples
 - complex
 - modulation
 - test
 - simple
 - transition
 - transition2
 - test4
 - test2
 - catalysis_0: \$"fdvf(2)" to \$knljkb
 - consumption_0: \$csdcd to \$csdsds
 - consumption_0: \$fdvfv to \$knljkb
 - consumption_0: \$fdvfv to \$klnljk
 - consumption_0: \$vdfvdf to \$ferfer
 - consumption_0: \$vfdvdfv to \$vljkdf
 - csdcd

sbgn(ST).xml : test2

sbgn(ST).xml : test | sbgn(ST).xml : simple | sbgn(ST).xml : transition | sbgn(ST).xml : transition2 | sbgn(ST).xml : test4

Diagram

Property	Value
Title	test2
Diagram type	XmlDiagramType
Layouter	"...forceDirectedLayout..."
Comment	
Data	

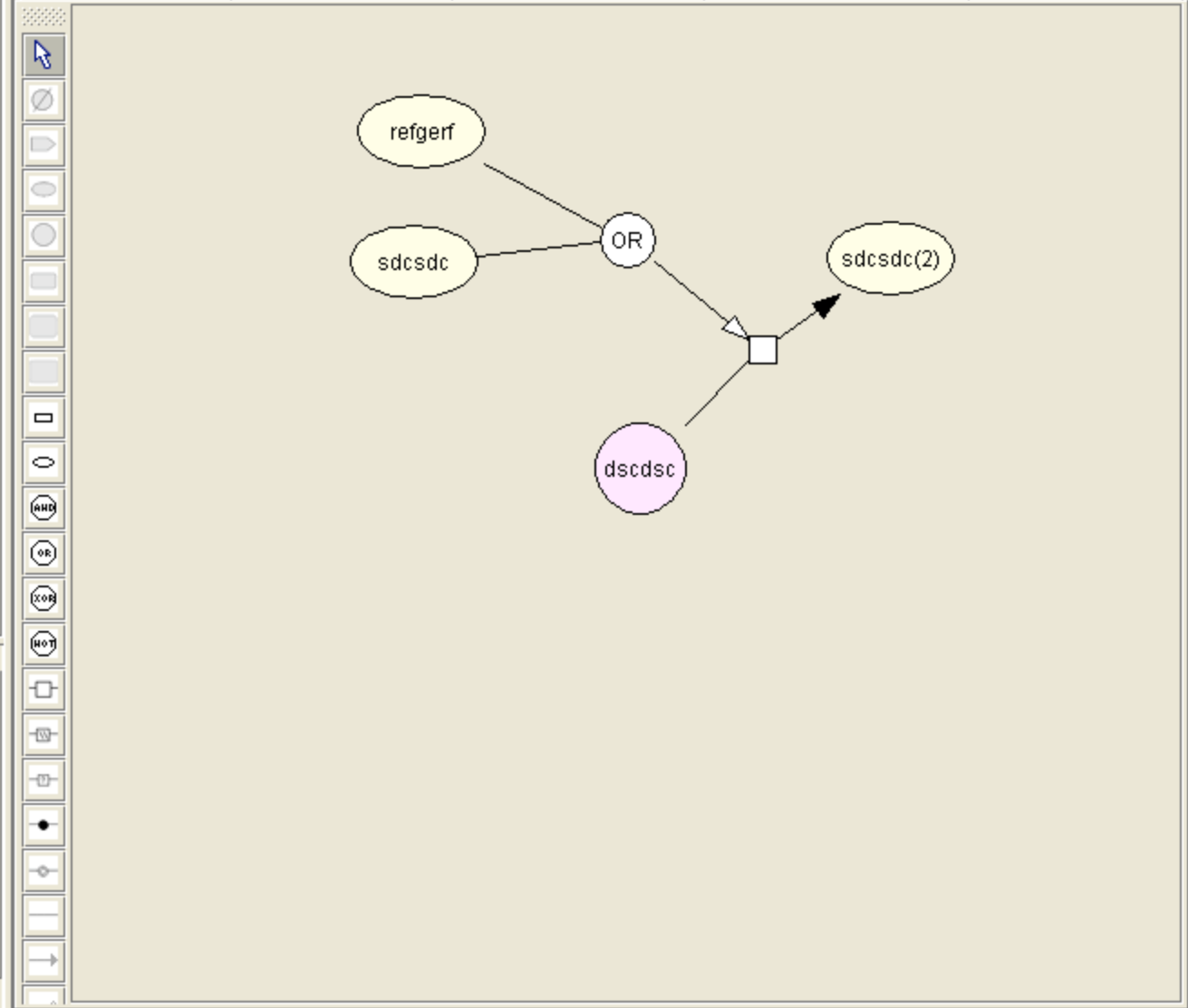
View Edit Editors



sbgn(ST).xml \

- sbgn(ST).xml
 - Properties
 - Nodes
 - Edges
 - Reactions
 - Examples
 - complex
 - modulation
 - test
 - simple
 - transition
 - transition2
 - test4
 - test2
 - test3
 - consumption_0: \$dscdsc to \$ojnkj
 - consumption_0: \$refgerf to \$"lm,n"
 - consumption_0: \$dscdsc to \$"lm,n"
 - dscdsc
 - lm,n
 - ojnkj

sbgn(ST).xml : test2 sbgn(ST).xml : test3
sbgn(ST).xml : test sbgn(ST).xml : simple sbgn(ST).xml : transition sbgn(ST).xml : transition2 sbgn(ST).xml : test4



Property	Value
Diagram	
Title	test3
Diagram type	XmlDiagramType
Layouter	"...forceDirectedLayout..."
Comment	
Data	

Library of predefined kinetic law
functions on the base of SBO
(Systems Biology Ontology)

The screenshot displays the BioUML workbench interface. The top menu bar includes 'File' and 'Help'. Below it is a toolbar with various icons for file operations and editing. The main workspace is divided into two panes. The left pane, titled 'Modules | Data | Plugins', shows a tree view of the 'modules' directory. Under 'modules', there is a folder 'SBO', which contains a sub-folder 'Data'. The 'Data' folder is expanded to show 'instances', 'relations', and 'terms'. The 'terms' folder is further expanded to show a list of SBO terms, with 'SBO:0000000' selected. The right pane is currently empty. Below the main workspace, there is a toolbar with icons for navigation and editing. The bottom section of the interface is divided into two panes. The left pane, titled 'Concept', displays the details for the selected term 'SBO:0000000'. The details include: ID: SBO:0000000, TY: concept, TI: Systems Biology Ontology, NM: Systems Biology Ontology, and DE: Set of relational controlled vocabularies intended to increase the semantic content of quantitative efforts in. The right pane is empty. At the bottom of the interface, there is a toolbar with buttons for 'View', 'Edit', and 'Editors'. Below this, there is a row of buttons for 'Description', 'References', 'Application Log', 'Clipboard', 'Layouter pane', 'JavaScript', and 'Search linked'.

Distribution of BioUML workbench includes SBO as a module.

List of SBO terms and selected term description.

Concept

ID: SBO:0000000
TY: concept
TI: Systems Biology Ontology
NM: Systems Biology Ontology
DE: Set of relational controlled vocabularies intended to increase the semantic content of quantitative efforts in

View Edit Editors

Description References Application Log Clipboard Layouter pane JavaScript Search linked

BioUML workbench

File Help

Modules | Data | Plugins

test : simulation

modules

- SBO
- test
 - Data
 - Diagrams
 - a1
 - simulation
- Dictionaries
- Images
- Simulation

enzyme 0.0

a 0.0 $\xrightarrow{\text{SBS000001} \rightarrow \text{SBS000002}}$ b 0.0

Let us create reaction: a ----> b

Property	Value
Node	
Title	SBS000001 -> SBS000002
Comment	
Size	50.0 50.0
Data	
Identifier	RCT000001
Name	SBS000001 -> SBS000002

Normal
Html
Preview

Description References Math editor Filter Application Log Clipboard Layouter pane Parameters
Variables JAVA MATLAB JavaScript Search linked

New reaction

Add/remove reaction component:

Component: Role:

Variable name: Click element on the diagram to select it as reaction component

Reaction components:

	Identifier	Name	Role	Stoichio...	Modifier...	Partisip...	Title	Comme...	Attributes
0	SBS000001	SBS000001	reactant	1		direct	SBS000001		
1	SBS000002	SBS000002	product	1		direct	SBS000002		

Reaction dialog

Reaction rate:

List of possible reaction rates will be automatically selected from SBO templates.

Simple \ SBO template

first order forward, first order reverse, reversible mass action kinetics, continuous scheme

first order forward, first order reverse, reversible mass action kinetics, continuous scheme

first order forward, second order reverse with one product, reversible mass action kinetics, continuous scheme

first order forward, third order reverse with one product, reversible mass action kinetics, continuous scheme

second order forward with one reactant, first order reverse, reversible mass action kinetics, continuous scheme

second order forward with one reactant, second order reverse with one product, reversible mass action kinetics, continuous scheme

second order forward with one reactant, third order reverse with one product, reversible mass action kinetics, continuous scheme

third order forward with one reactant, first order reverse, reversible mass action kinetics, continuous scheme

third order forward with one reactant, second order reverse with one product, reversible mass action kinetics, continuous scheme

reactant act proportion

al to the quantity of one reactant. The rate of the reverse process is proportional to the quantity of one product. It is to be used in a reaction modelled using a continuous framework.

New reaction

Add/remove reaction component:

Component: Role:

Variable name: Click element on the diagram to select it as reaction component

Reaction components:

	Identifier	Name	Role	Stoichio...	Modifier...	Partisip...	Title	Comme...	Attributes
0	SBS000001	SBS000001	reactant	1		direct	SBS000001		
1	SBS000002	SBS000002	product	1		direct	SBS000002		

Reaction rate:

Simple \ SBO template \

first order forward, first order reverse, reversible mass action kinetics, continuous scheme

Name	Value	Comment
kf	kf	forward unimolecular rate constant, continuous case
kr	kr	reverse unimolecular rate constant, continuous case
R	\$SBS000001	reactant
P	\$SBS000002	product

Reaction scheme where the products are created from the reactants and the change of a product quantity is proportional to the product of reactant activities. The reaction scheme does include a reverse process that creates the reactants from the products. The rate of the forward process is proportional to the quantity of one reactant. The rate of the reverse process is proportional to the quantity of one product. It is to be used in a reaction modelled using a continuous framework.

When user have selected reaction rate from the list, then variables for reactant, product and modifier will be set up automatically in reaction template.

Description of parameters from SBO.

Description of reaction rate from SBO.

New reaction

Add/remove reaction component:

Component: SBS000002 Role: product Add Remove

Variable name: \$SBS000002 Click element on the diagram to select it as reaction component

Reaction components:

Table with 10 columns: Identifier, Name, Role, Stoichio..., Modifier..., Partisip..., Title, Comme..., Attributes. It lists two reaction components: SBS000001 (reactant) and SBS000002 (product).

After pressing "Apply" button corresponding reaction rate will be generated on the base of selected SBO template.

Reaction rate:

Chemical equation: kf*\$SBS000001 - kr*\$SBS000002

Simple SBO template

first order forward, first order reverse, reversible mass action kinetics, continuous scheme Apply

Table with 3 columns: Name, Value, Comment. It lists parameters kf, kr, R, and P with their respective values and descriptions.

Reaction scheme where the products are created from the reactants and the change of a product quantity is proportional to the product of reactant activities. The reaction scheme does include a reverse process that creates the reactants from the products. The rate of the forward process is proportional to the quantity of one reactant. The rate of the reverse process is proportional to the quantity of one product. It is to be used in a reaction modelled using a continuous framework.

Cancel Ok

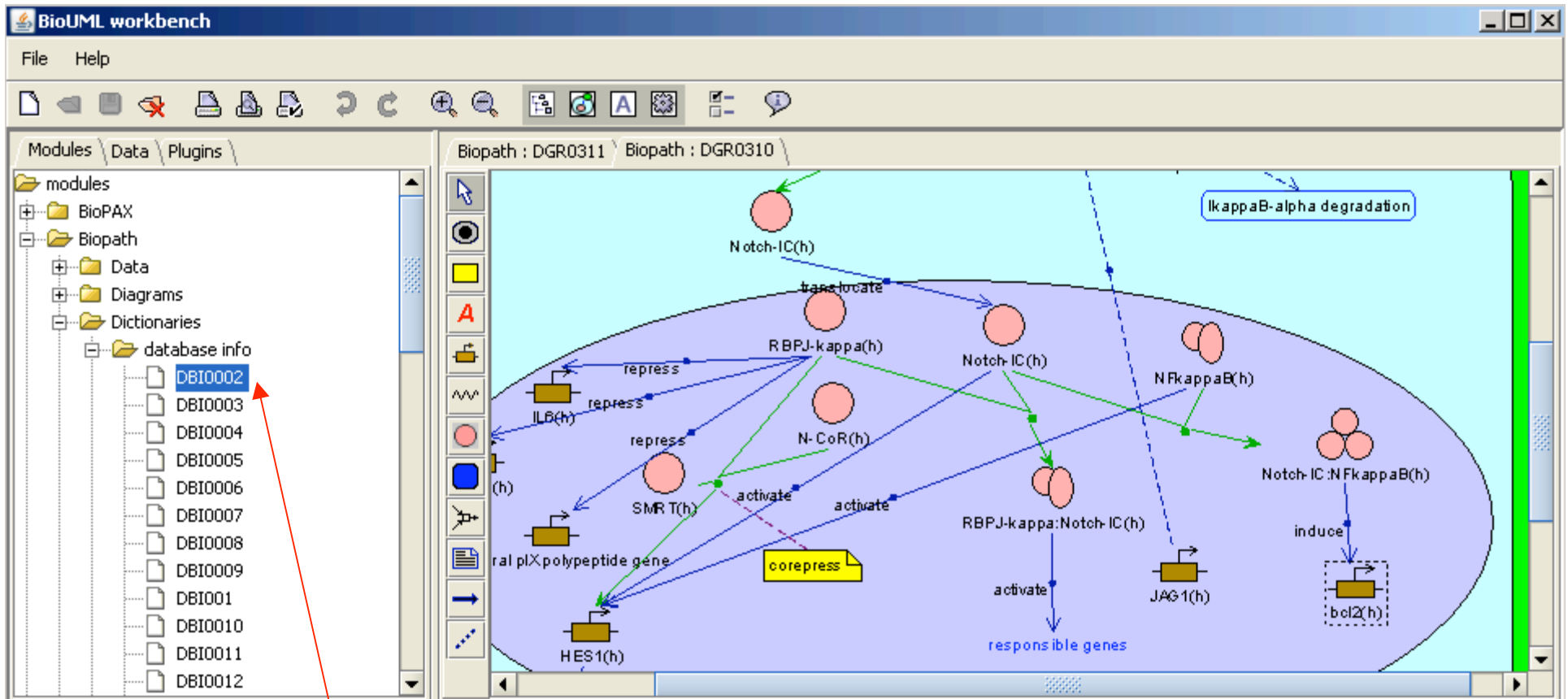
Database references editor

Database references editor

main concepts

- BioUML has DatabaseInfo type for description external database (quite similar with MIRIAM)
- Diagram element has Data object that contains references to databases (again, quite similar with MIRIAM)
- Database reference editor provides user interface for
 - database references creating/editing
 - open corresponding links in browser
 - finding related database links using gene hub. For example, user may specify some reference to Ensembl database. Using Ensembl gene hub all database references from Ensembl for the specified gene will be found and shown automatically.

By this way it is quite convenient to find and copy database references for the selected diagram element from different databases.



DatabaseInfo type:
 - list of external databases
 - description of external database

Database info

ID: DBI0002
TI: EMBL
DE: A comprehensive database of DNA and RNA sequences collected from the scientific literature, patent applications, and directly submitted from researchers and sequencing groups.
QID: [http://srs.ebi.ac.uk/srs6bin/cgi-bin/wgetz?-e+\[embl-id:\\$id\\$](http://srs.ebi.ac.uk/srs6bin/cgi-bin/wgetz?-e+[embl-id:id)
QAC: [http://srs.ebi.ac.uk/srs6bin/cgi-bin/wgetz?-e+\[embl-acc:\\$ac\\$](http://srs.ebi.ac.uk/srs6bin/cgi-bin/wgetz?-e+[embl-acc:ac)
CC:

Current DB references for DC/title

Database	ID	AC	Relation	Comment
TRANSFAC	G003555	null		null
OMIM	151430			
HGNC	990			
UniGene	150749			
Entrez Gene	596			

Description References Microarray Text search Filter Application Log Clipboard
 Layouter pane JavaScript Search linked

BioUML workbench

File Help

Modules | Data | Plugins

modules

- BioPAX
- Biopath
 - Data
 - Diagrams
 - Dictionaries
 - database info
 - DBI0002
 - DBI0003
 - DBI0004
 - DBI0005
 - DBI0006
 - DBI0007
 - DBI0008
 - DBI0009
 - DBI0010
 - DBI0011
 - DBI0012

Biopath : DGR0311 Biopath : DGR0310

Database info

ID: DBI0002
 TI: EMBL
 DE: A comprehensive database of DNA and RNA sequences collected from the scientific literature, patent applications, and directly submitted from researchers and sequencing groups.
 QID: [http://srs.ebi.ac.uk/srs6bin/cgi-bin/wgetz?-e+\[embl-id:\\$id\\$](http://srs.ebi.ac.uk/srs6bin/cgi-bin/wgetz?-e+[embl-id:id)
 QAC: [http://srs.ebi.ac.uk/srs6bin/cgi-bin/wgetz?-e+\[embl-acc:\\$ac\\$](http://srs.ebi.ac.uk/srs6bin/cgi-bin/wgetz?-e+[embl-acc:ac)
 CC:

View Edit Editors

List of database references for selected diagram element

Current DB references for DC/title

Database	ID	AC	Relation	Comment
TRANSFAC	G003555	null		null
OMIM	151430			
HGNC	990			
UniGene	150749			
Entrez Gene	596			

Description References Microarray Text search Filter Application Log Clipboard
 Layouter pane JavaScript Search linked

Database references editor

Database References Editor [X]

Gene hub

New database reference:

Database: ID: AC:

Relation: Comment:

Gene hub search options:

Gene hub:

Organism:

Database:

Current DB references for gene/title:

Database	ID	AC	Relation	Comment
TRANSFAC	G003555	null		null
OMIM	151430			
HGNC	990			
UniGene	150749			
Entrez G...	596			

Gene hub references:

Database	ID	AC	Relation	Comment
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Database references editor

current work

- Complete correspondence to MIRIAM standard
 - list of databases
 - controlled vocabularies
- MIRIAM file is included into BioUML distribution by default
- Gene hub is essential part for binding pathway elements with experimental data (microarray, proteom data, metabolome data).
- Gene hub (we are preparing separate document about it)

Microarray plug-in (alpha version)

Microarray plug-in

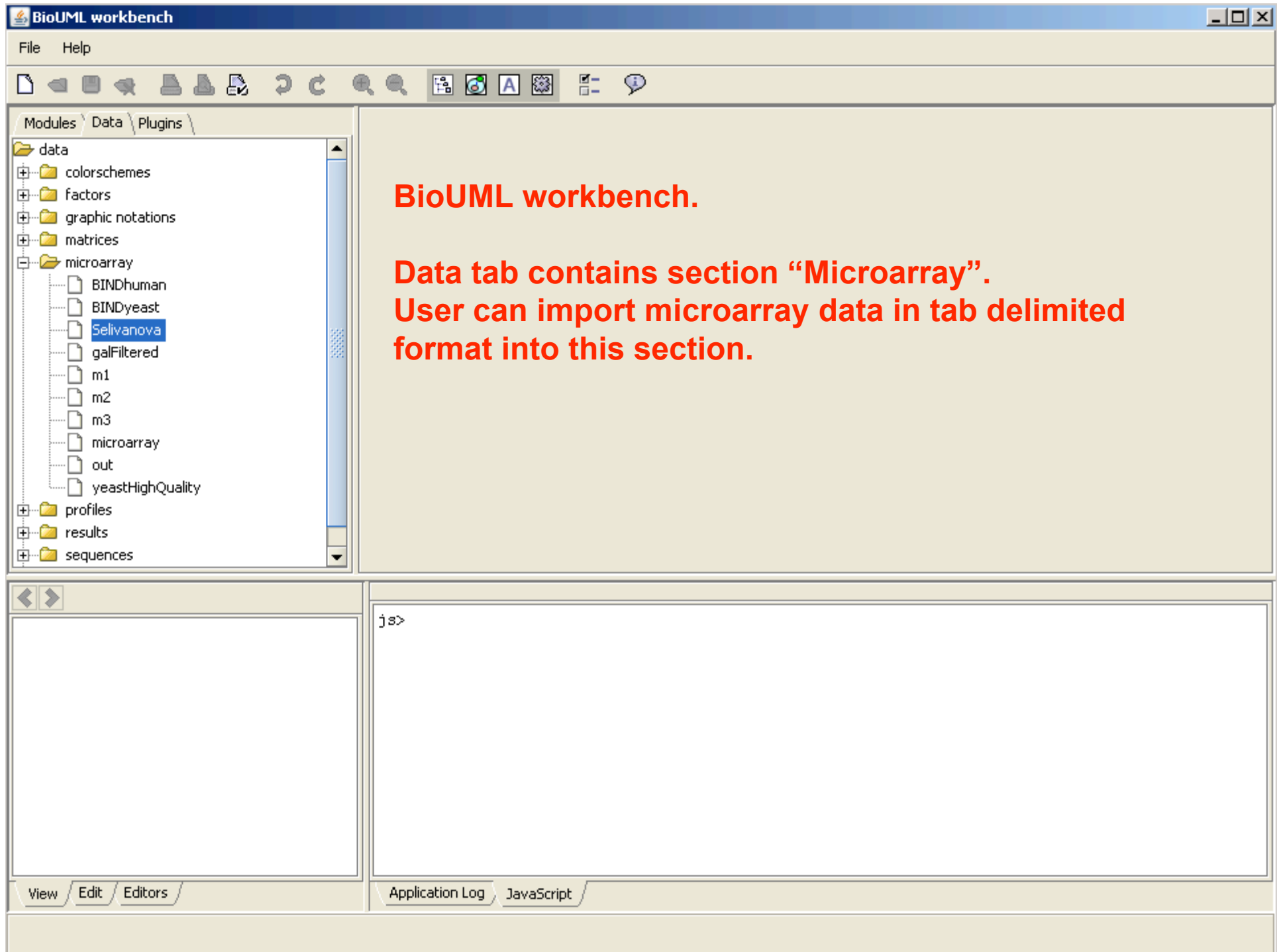
- Import microarray data in tab delimited format (the same as Cytoscape)
- Show data as a table
- Binding with diagram nodes by ID
- Coloring diagrams

Current work:

- Powerful user interface for coloring diagrams
- Support of other formats for microarray data and results of analyses
- Sophisticated binding algorithm using different database references and ID (gene hub)

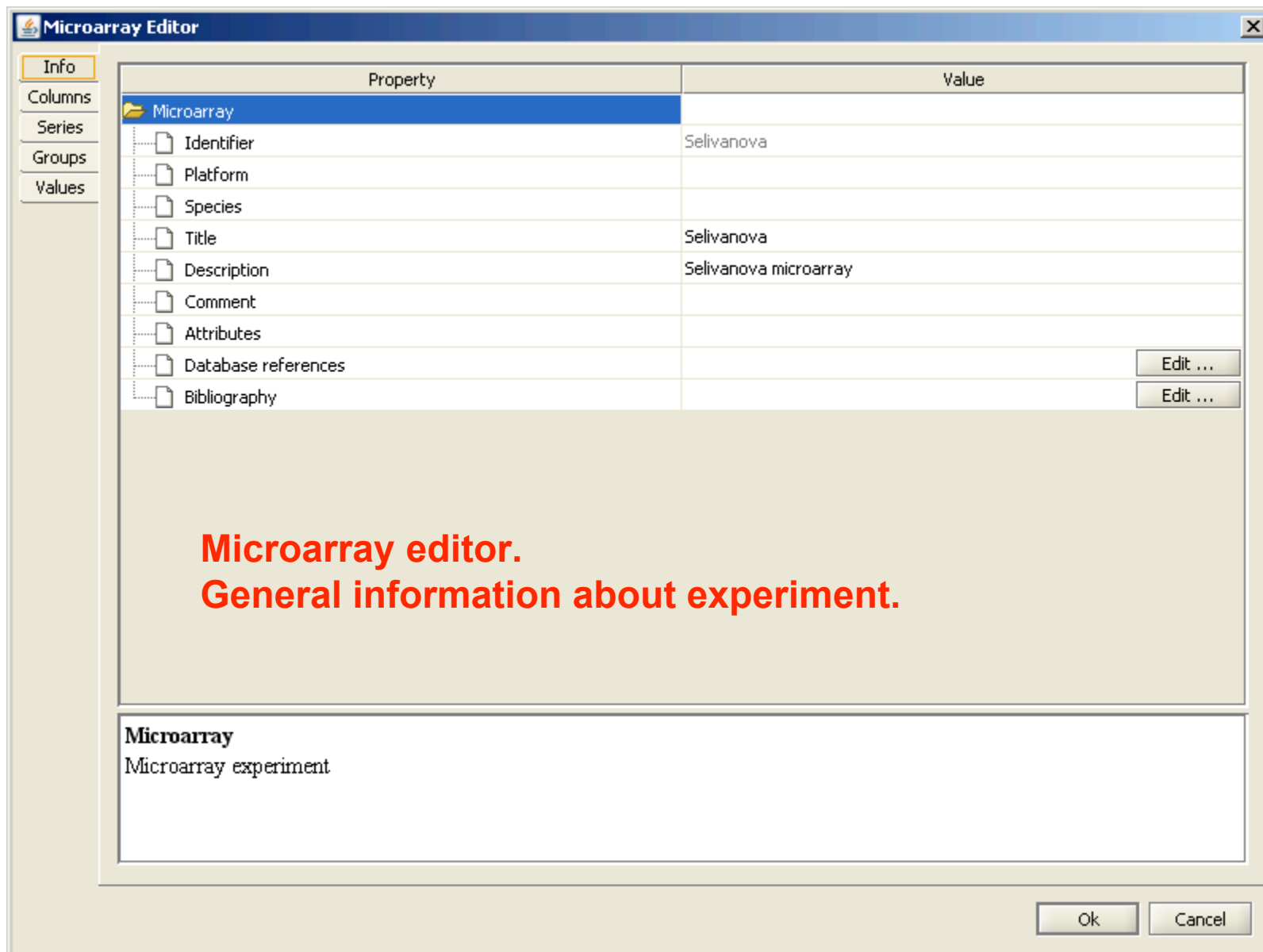
Further work:

- Server module that will provide access to ArrayExpress data



BioUML workbench.

**Data tab contains section "Microarray".
User can import microarray data in tab delimited
format into this section.**



Microarray editor provides possibility to filter probe sets:

- by column values
- selecting only those probesets that can be linked to the specified diagram

The screenshot shows the 'Microarray Editor' window. On the left is a sidebar with tabs: Info, Columns, Series, Groups, and Values (selected). The main area is divided into two panels: 'Filter by column' and 'Filter by diagram'. The 'Filter by column' panel has a 'Column:' dropdown set to 'id', a text input for 'Values (separated by comma):', and an 'Apply' button. The 'Filter by diagram' panel has dropdowns for 'Module:' (Biopath), 'Diagram:' (316_new), and 'GeneHub:' (Ensembl), along with an 'Apply' button. Below these panels is a table with 6 columns and 20 rows of data. At the bottom, there are tabs for 'Values' and 'Columns', and buttons for 'Add experiment', 'Remove experiment', 'Ok', and 'Cancel'.

id	null.untr<->...	null.untr<->...	null.12h<->...	wt.untr<->...	null.12h<->...
204995_at	-0.598978	0.870959	-4.034031	-3.813265	1.459187
215195_at	2.070853	2.124593	3.405656	3.591895	-0.936971
209693_at	1.736705	-2.192375	1.615612	3.875506	-3.292119
213716_s_at	-0.694441	-3.000195	-1.864673	0.371655	-2.410478
203765_at	-0.950785	-8.399035	-7.220017	1.840271	-8.304233
207859_s_at	0.774395	3.050078	0.90309	-0.908897	1.515161
219944_at	-1.23509	2.109801	3.373582	1.233055	2.510442
218764_at	0.425519	-0.459243	4.593501	4.869904	0.367648
201746_at	-4.042248	-11.038752	-11.772484	-1.944731	-10.948575
220761_s_at	0.532354	-6.869036	1.229193	6.383228	-7.361719
211475_s_at	-0.305626	-0.84818	-3.721242	-3.00117	-0.820027
219073_s_at	1.694772	-2.11339	2.858096	4.36393	-2.811219
220334_at	0.564119	-3.094801	1.988387	4.624332	-3.706741
213016_at	1.500005	-0.459243	3.18261	5.461951	-1.092072
201141_at	-1.915486	-3.416209	0.699773	2.952151	-2.645406
207709_at	-1.538003	-4.385207	-1.365542	0.467387	-1.981945
221000_at	0.268270	1.780867	2.405456	4.202620	1.401206

BiOPLM Workbench

File Help

Modules Data Plugins

data

- classifications
- colorschemes
- factors
- graphic notations
- matrices
- microarray
 - galExpData
 - m1
 - m2
 - m3
- profiles
- results
- sequences
- test

Biopath (local) : DGR0003a

Microarray: m2

Experiment	
v1	<input checked="" type="checkbox"/>
v2	<input checked="" type="checkbox"/>
v3	<input checked="" type="checkbox"/>

**Coloring diagram according to microarray data.
Each bar corresponds to one value from
corresponding microarray series.**

View Edit Editors

Description Microarray Application Log Clipboard Layouter pane JavaScript Search linked

BioModels –
comparison BioUML simulation
results with other simulators

http://www.biouml.org/_biomodels/

Simulators comparison criteria

Passed – CSV file was generated by simulator

interval criteria

no difference - $0.999 * \min < x < 1.001 * \max$ or
 $x < \text{ZERO}$ and $\max < \text{ZERO}$

small difference – $0.5 * \min < x < 1.5 * \max$

significant difference - otherwise

median criteria

no difference - $0.999 * \text{median} < x < 1.001 * \text{median}$ or
 $x < \text{ZERO}$ and $\text{median} < \text{ZERO}$

small difference – $0.5 * \text{median} < x < 1.5 * \text{median}$

significant difference – otherwise

x – variable value provided by compared simulator

min, max, median – calculated from values provided by other simulators with which the specified simulator is being compared.

Implementation note: if result file was not generated by BioUML, then other simulators can be compared one to each other.

Summary of results

Simulator	passed	no difference		small difference		significant difference	
SBWOdeSolver	149	122	102	12	16	5	21
BioUML	140	120	100	3	10	17	30
MathSBML	138	103	94	10	8	15	26
roadRunner	138	96	88	1	16	31	24
Copasi	127	85	86	3	7	29	24
JSim	93	70	63	0	2	13	18
Jarnac	79	58	55	0	2	11	12
Oscill8 Core	44	25	24	2	1	7	9
CVODE	17	4	4	2	1	1	2

Availability

BioUML workbench (including source code) is freely available at <http://www.biouml.org>

Supplementary materials:

<http://www.biouml.org/sbgn.shtml>

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