

# VCell Tutorial

## FRAP with binding

*Create a simple biomodel and spatial (PDE) application to simulate a photobleaching experiment with both diffusion and binding.*

# In this tutorial...

- Gain a basic introduction to the Virtual Cell interface
- Create a simple biomodel with species and reactions
- Create a compartmental (ODE) application of the model to determine steady state binding conditions.
- Create a spatial deterministic (PDE) application using analytic equations to create a simple geometry
- Define initial concentrations that are non-uniform using Boolean expressions
- Created a timed event in a spatial simulation.
- View and analyze results of a spatial simulation.

**BioModel2**

- Physiology
  - Reaction Diagram**
  - Reactions (0)
  - Structures (1)
  - Species (0)
  - Molecules (0)
  - Observables (0)
- Applications (0)
- Parameters, Functions and Units
- Pathway

Reaction Diagram Reactions Structures Species Molecules Observables

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c0

To re-open a model, click on the folder that the model was saved in and double-click on the model.

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

Search

- Biological Models
  - My BioModels (astfh234) (2)
    - Model 2
    - tutorial 3
    - Private Tue Jun 30 16:47:35 EDT 201
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  - Tutorials (5)
  - Education (33)
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Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings) Database File Info

Spatial Deterministic

- Deterministic
- geom\_20150630\_115646 (3D)

File View Server Tools Help

**BioModel3**

- Physiology
  - Reaction Diagram**
  - Reactions (0)
  - Structures (1)
  - Species (0)
  - Molecules (0)
  - Observables (0)
- Applications (0)
- Parameters, Functions and Units
- Pathway

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

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Reaction Diagram Reactions Structures Species Molecules Observables

Click on the compartment tool, click the dotted black lines so they turn green and click "Add Membrane".

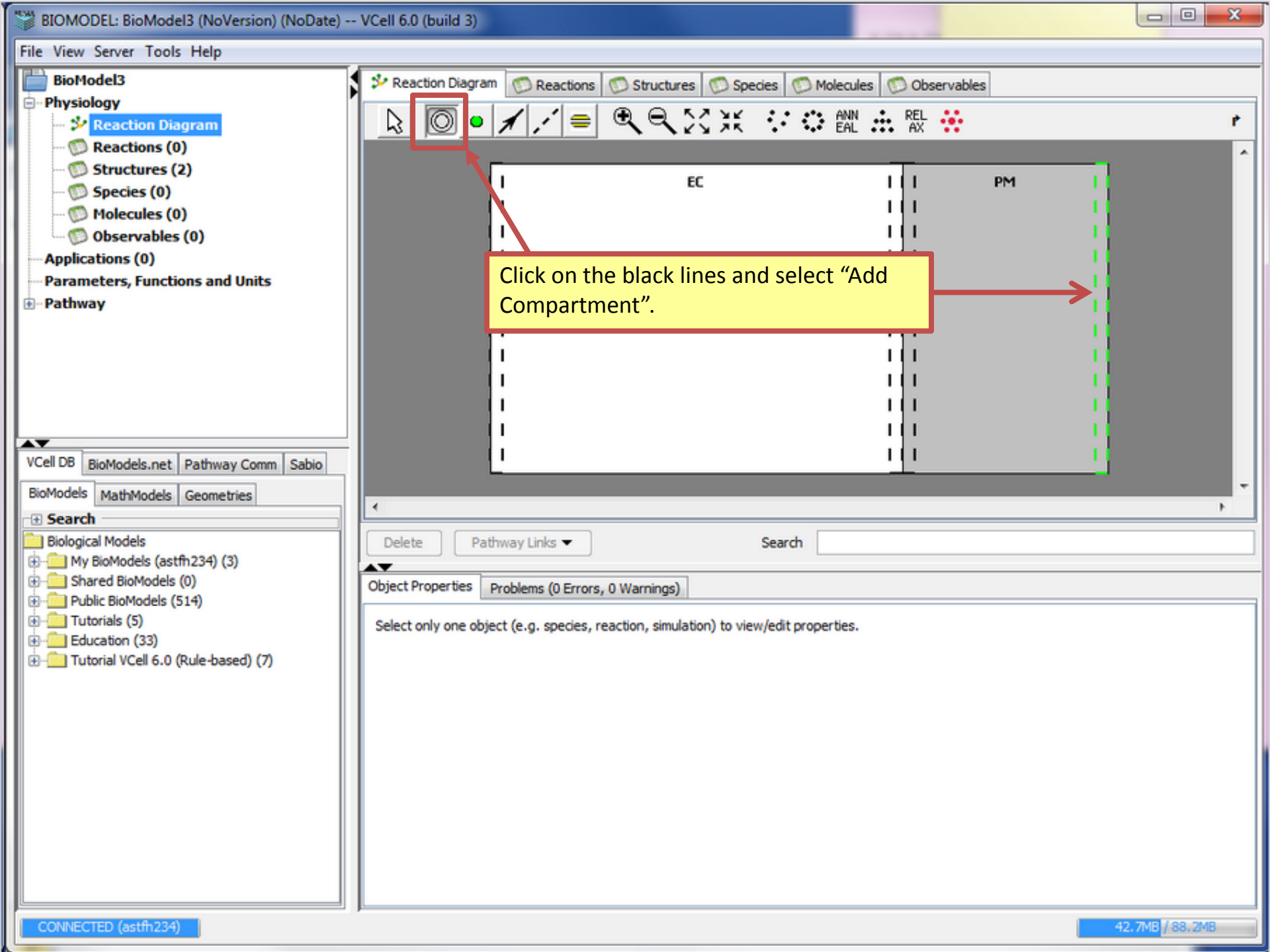
EC

Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Select only one object (e.g. species, reaction, simulation) to view/edit properties.





File View Server Tools Help

**BioModel4**

- Phy
- Reactions (0)
- Structures (3)
- Species (0)
- Molecules (0)
- Observables (0)
- Applications (0)
- Parameters, Functions and Units
- Pathway

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

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Reaction Diagram Reactions Structures Species Molecules Observables

Click the select tool.

Click on the label of the first compartment.

Cyt

Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Select only on

Structure Name Cyt

Size Variable Name Cyt [ $\mu\text{m}^3$ ]

Annotation Cytosol

Next to Structure Name type "Cyt".

Next to Annotation type "Cytosol".

**BioModel4**

- Physiology
  - Reaction Diagram**
  - Reactions (0)
  - Structures (3)
  - Species (0)
  - Molecules (0)
  - Observables (0)
- Applications (0)
- Parameters, Functions and Units
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Reaction Diagram Reactions Structures Species Molecules Observables



Click on the membrane label.

NM

c1

Delete

Pathway Links

Search

Object Properties Problems (0 Errors, 0 Warnings)

Select only one structure to edit properties

Structure Name NM

Size Variable Name NM [μm<sup>2</sup>]

**Electrophysiology**

Next to Structure Name type "NM" (which stands for "Nuclear Membrane").

Negative (outside feature)

**membrane voltage:** "Voltage\_NM" = voltage(inside (+) compartment) - voltage(outside (-) compartment)

**inward currents:** from compartment "outside (-) compartment" into compartment "inside (+) compartment"

*Note: VCell reactions and fluxes specify inward currents (- to +) rather than conventional currents (+ to -).*

Annotation

BIOMODEL: BioModel4 (NoVersion) (NoDate) -- VCell 6.0 (build 3)

File View Server Tools Help

**BioModel4**

**Physiology**

- Reaction Diagram
- Reactions (0)
- Structures (3)
- Species (0)
- Molecules (0)
- Observables (0)
- Applications (0)
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VCell DB BioModels.net Pathway Comm Sabio

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Reaction Diagram Reactions Structures Species Molecules Observables

Click on the label of the second compartment.

Nuc

Object Properties Problems (0 Errors, 0 Warnings)

Select object

Structure Name	Nuc
Size Variable Name	Nuc [ $\mu\text{m}^3$ ]
Annotation	Nucleus

Next to Structure Name type "Nuc".

Next to Annotation type "Nucleus".

CONNECTED (astfh234)

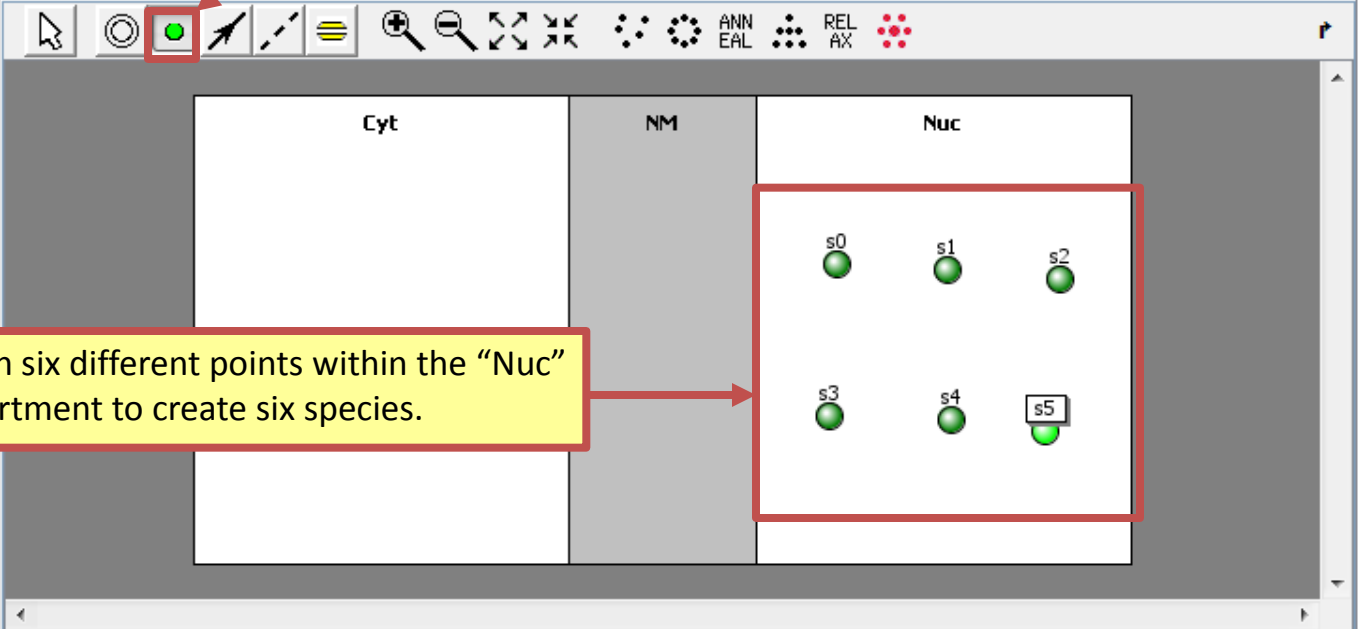
60MB / 112.6MB

Click the species tool.

File View Server Tools Help

**BioModel4**  
**Physiology**  
 Reaction Diagram  
 Reactions (0)  
 Structures (3)  
 Species (6)  
 Molecules (0)  
 Observables (0)  
 Applications (0)  
 Parameters, Functions and Units  
 Pathway

Reaction Diagram Reactions Structures Species Molecules Observables



Click on six different points within the "Nuc" compartment to create six species.

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Delete

Pathway Links

Search

Object Properties

Problems (0 Errors, 0 Warnings)

Species Name s5

Linked Pathway Object(s)

Annotation

Species: s5

**BioModel4**

**Physiology**

- Reaction Diagram**
- Reactions (0)
- Structures (3)
- Species (6)
- Molecules (0)
- Observables (0)
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








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Reaction Diagram Reactions Structures Species Molecules Observables

Cyt NM Nuc

s0 s1 s2

s3 s4 s5

To move a species, click the select tool and click a drag a species to a point.

Delete

Pathway Links ▼

Search

Object Properties

Problems (0 Errors, 0 Warnings)

Species Name	s1
Linked Pathway Object(s)	
Annotation	


Species: **s1**

BIOMODEL: BioModel4 (NoVersion) (NoDate) -- VCell 6.0 (build 3)

File View Server Tools Help

**BioModel4**

- Physiology
  - Reaction Diagram**
  - Reactions (0)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (0)
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Reaction Diagram Reactions Structures Species Molecules Observables

Click on "s0".

Cyt NM Nuc

s1 s2 s3 s4 s5

Object Properties Problems (0 Errors, 0 Warnings)

Species Name

Next to Species Name type "r".

Linked Pathway Object(s)

Annotation

Next to Annotation type "RAN".

CONNECTED (astfh234)

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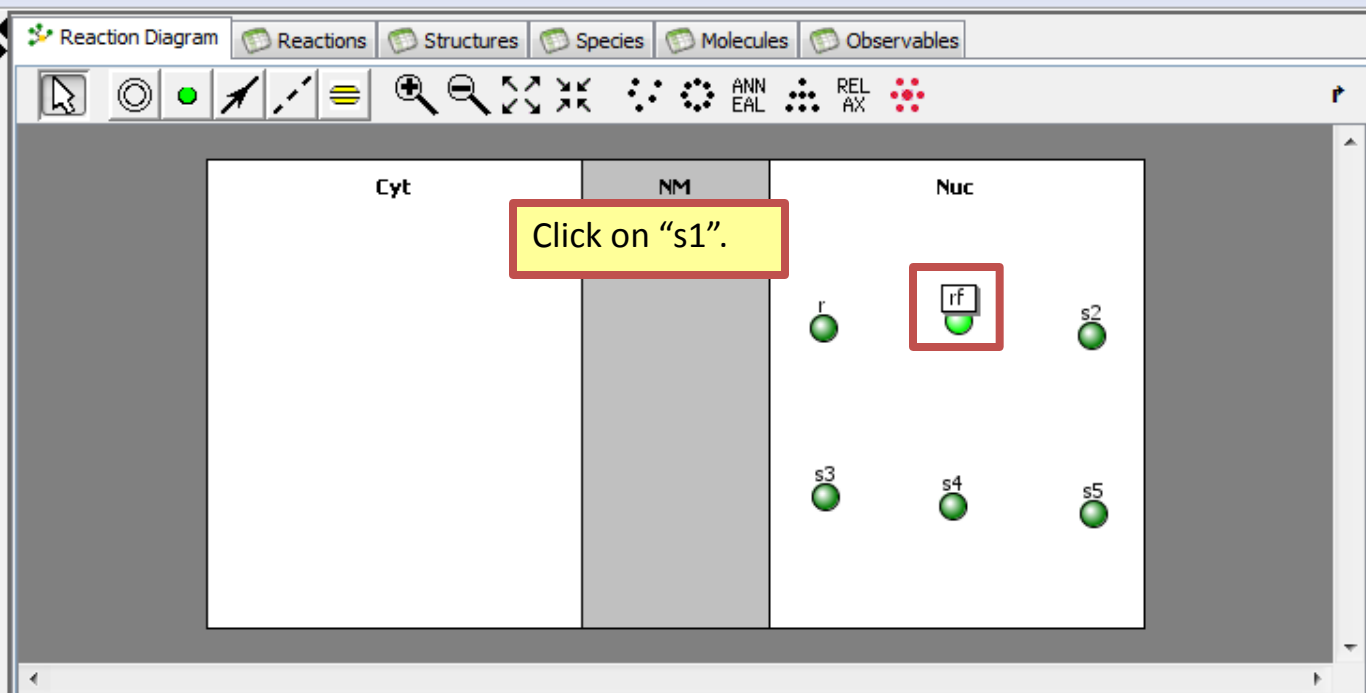
**BioModel4**

- Physiology
  - Reaction Diagram**
  - Reactions (0)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (0)
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Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Species Name rf

Next to Species Name type "rf".

Linked Pathway Object(s)

Annotation RAN\_FITC

Next to Annotation type "RAN\_FITC".



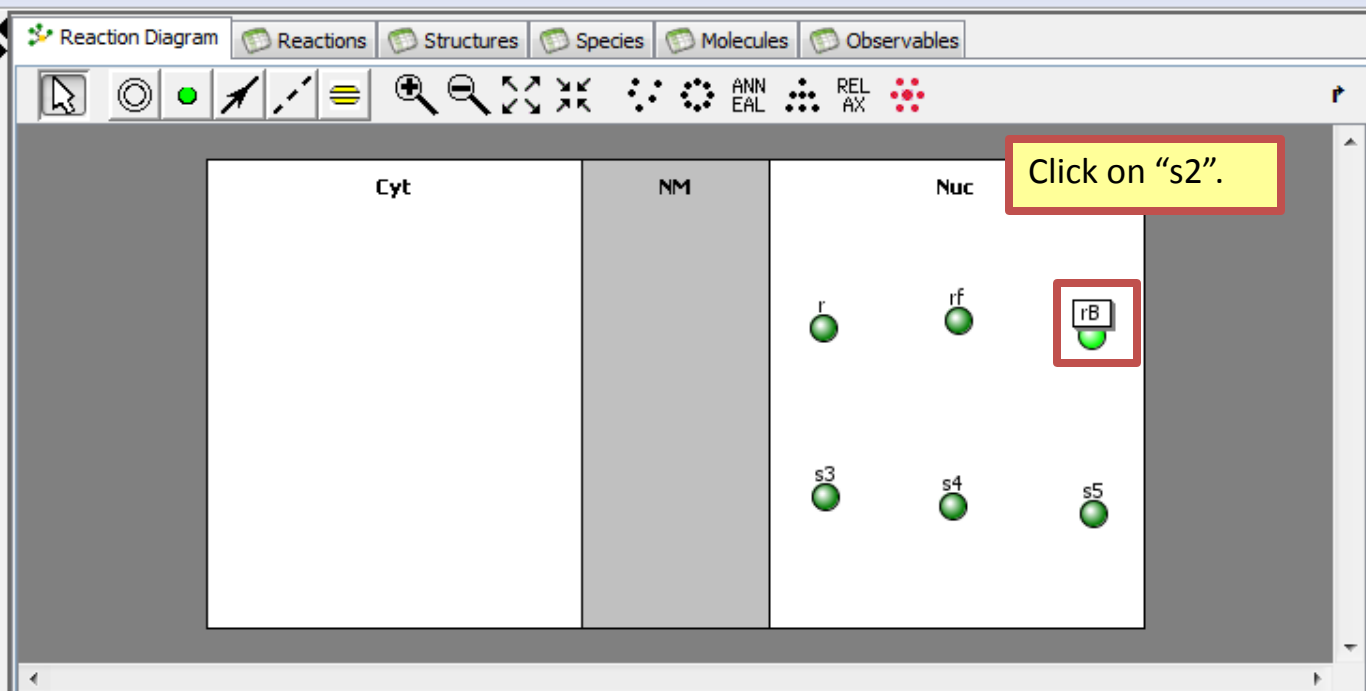
**BioModel4**

- Physiology
  - Reaction Diagram**
  - Reactions (0)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
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Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Species Name	rB
Linked Pathway Object(s)	
Annotation	RAN_Bound

Next to Species Name type "rB".

Next to Annotation type "RAN\_Bound".

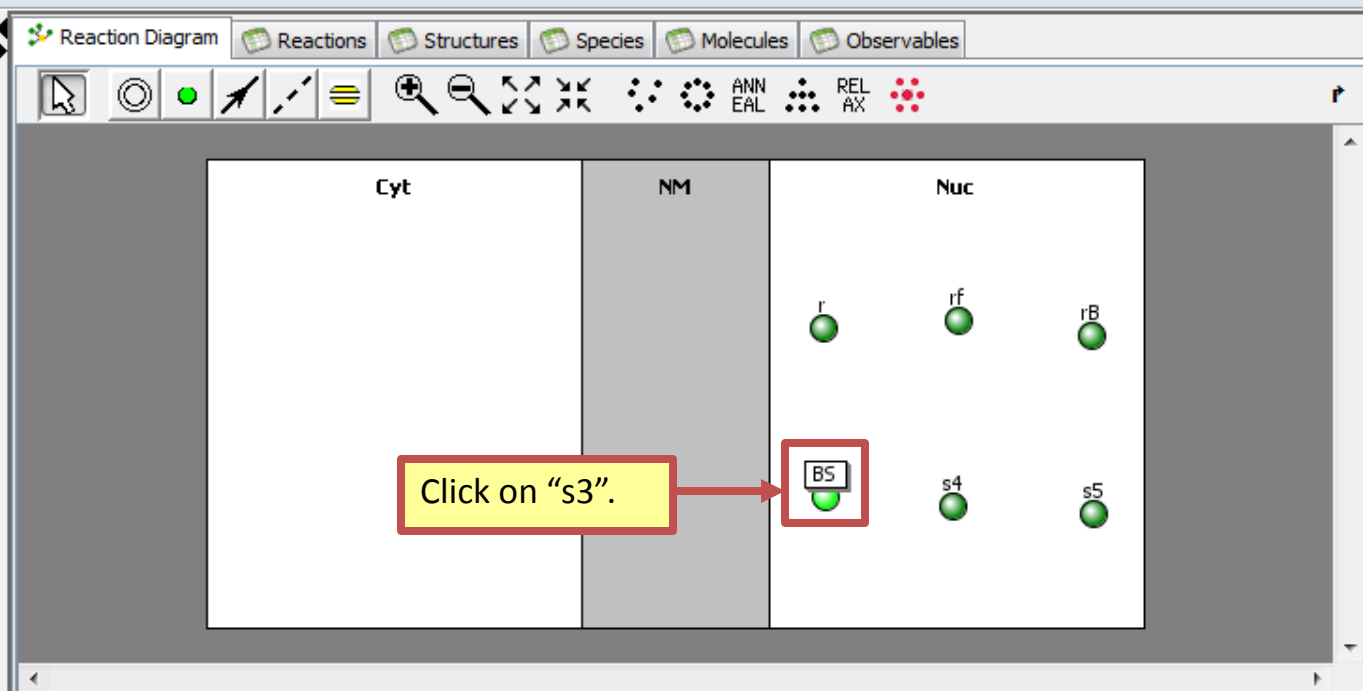
**BioModel4**

- Physiology
  - Reaction Diagram**
  - Reactions (0)
  - Structures (3)
  - Species (6)
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Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Species Name BS

Next to Species Name type "BS".

Linked Pathway Object(s)

Annotation Binding Sites

Next to Annotation type "Binding Sites".

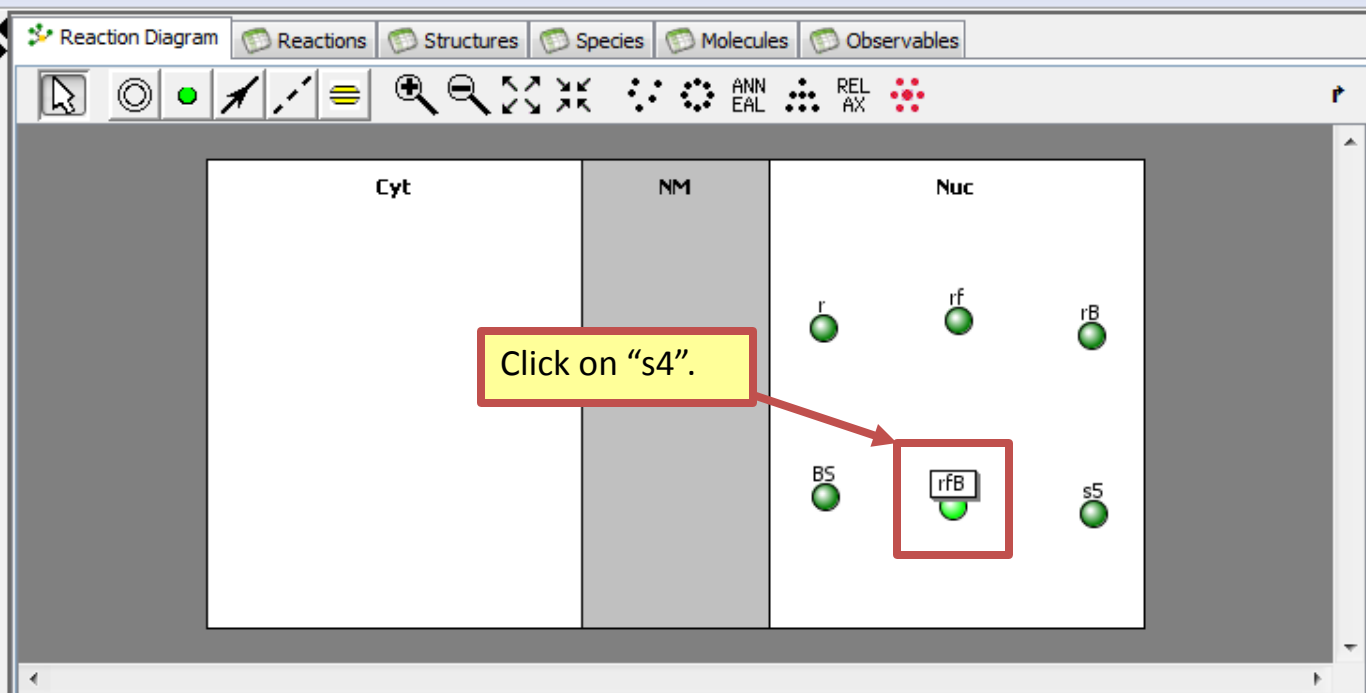
**BioModel4**

- Physiology
  - Reaction Diagram**
  - Reactions (0)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (0)
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Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Species Name rfB

Linked Pathway Object(s)

Annotation RAN\_FITC\_Bound

Next to Species Name type "rfB".

Next to Annotation type "RAN\_FITC\_Bound".

File View Server Tools Help

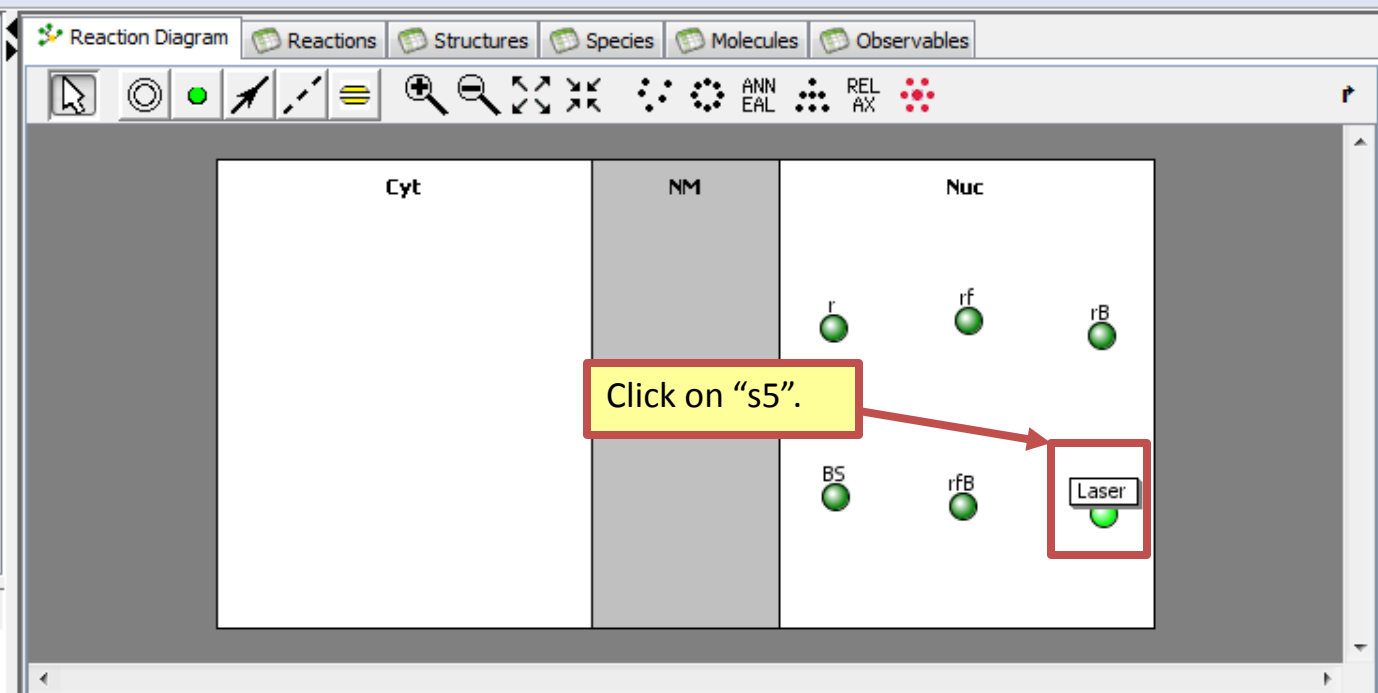
**BioModel4**

- Physiology
  - Reaction Diagram**
  - Reactions (0)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (0)
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Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Species Name	Laser
Linked Pathway Object(s)	
Annotation	Light Source

Next to Species Name type "Laser".

Next to Annotation type "Light Source".

**BioModel4**

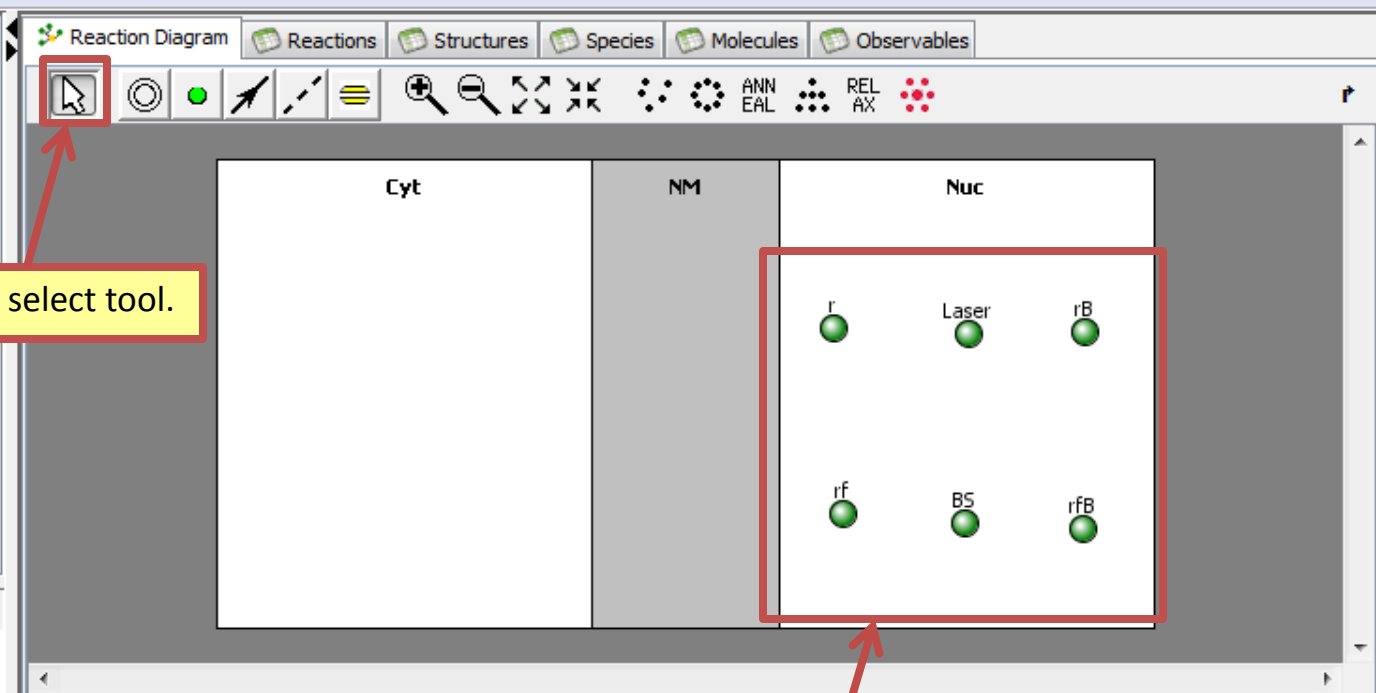
**Physiology**

- Reaction Diagram**
- Reactions (0)
- Structures (3)
- Species (6)
- Molecules (0)
- Observables (0)
- Applications (0)
- Parameters, Functions and Units
- Pathway

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

- Search**
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Click the select tool.

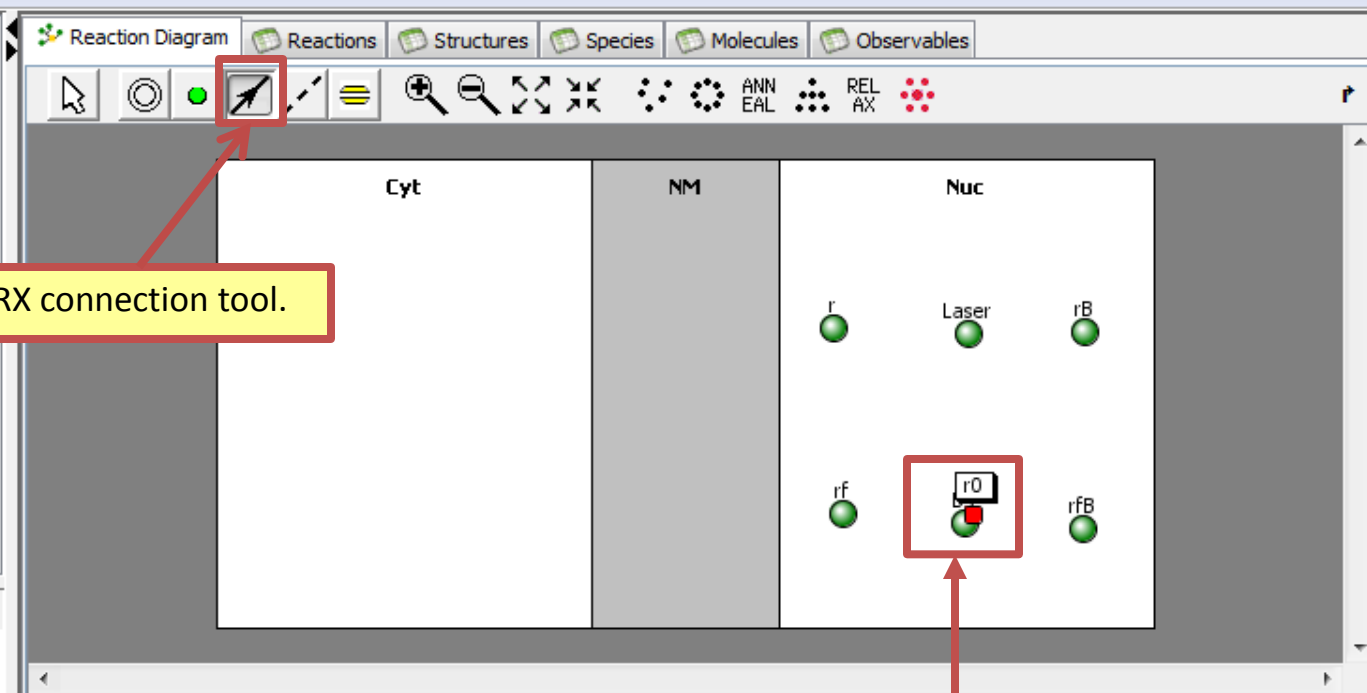
Click and drag the species so that the order is from left to right "r", "Laser", "rB", "rf", "BS", "rfB".

**BioModel4**

**Physiology**

- Reaction Diagram
- Reactions (1)
- Structures (3)
- Species (6)
- Molecules (0)
- Observables (0)
- Applications (0)
- Parameters, Functions and ...
- Pathway

Click the RX connection tool.



Click on "BS" and drag your cursor, which will create a line marked <<REACTANT>>. Drop your cursor anywhere inside the "Nuc" compartment, which will create a reaction node called "r0".

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Delete Pathway Links

Object Properties Problems (0 Errors)

Reaction Name r0

Kinetic Type Mass Action [ $\mu\text{M/s}$ ] (re

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$K_f \cdot BS$	$\mu\text{M.s}^{-1}$
Kf	forward rate constant	<input type="checkbox"/>	0.0	$\text{s}^{-1}$
Kr	reverse rate constant	<input type="checkbox"/>	0.0	$\mu\text{M.s}^{-1}$
BS	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu\text{M}$

Annotation and Pathway Links

**BioModel4**

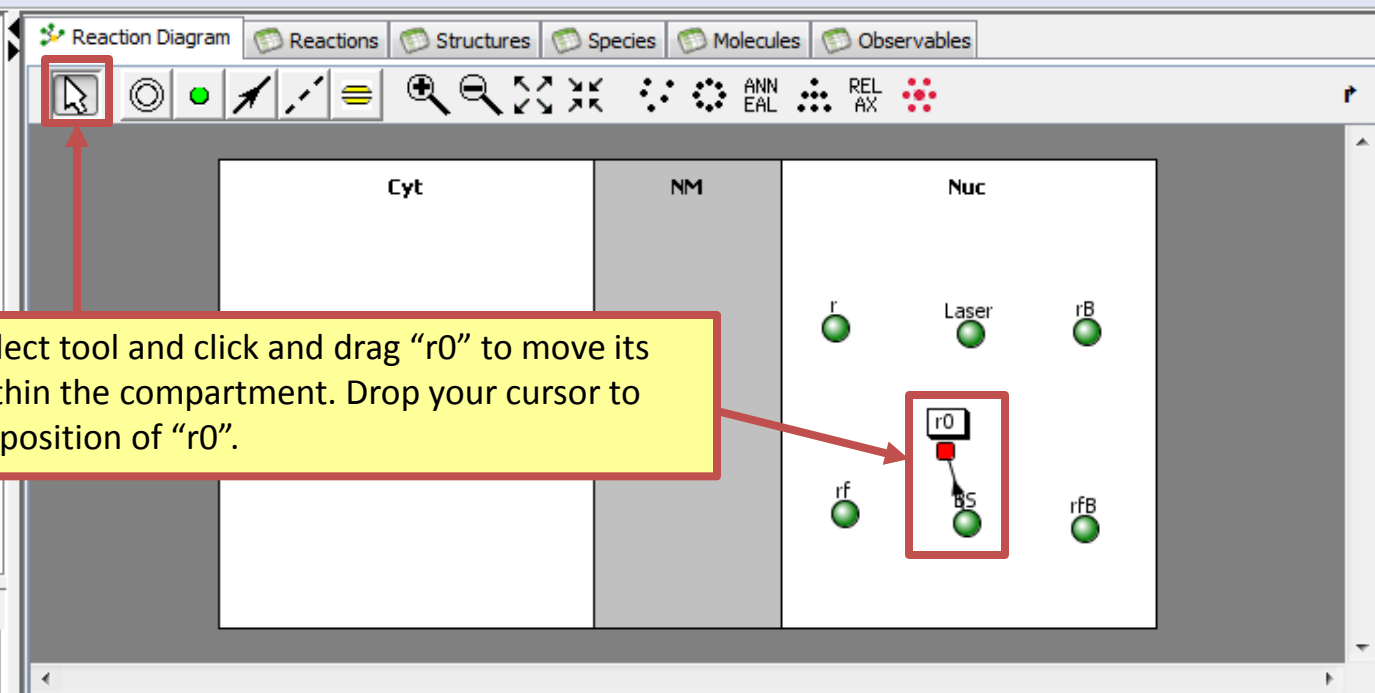
**Physiology**

- Reaction Diagram**
- Reactions (1)
- Structures (3)
- Species (6)
- Molecules (0)
- Observables (0)
- Applications (0)
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VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

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Click the select tool and click and drag "r0" to move its position within the compartment. Drop your cursor to finalize the position of "r0".

Delete

Pathway Links

Search

Object Properties Problems (0 Errors, 0 Warnings)

Reaction Name r0

Kinetic Type Mass Action [ $\mu\text{M/s}$ ] (recommended for stochastic application)

Convert to [ $\text{molecules.s}^{-1}$ ]

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$K_f \cdot BS$	$\mu\text{M.s}^{-1}$
Kf	forward rate constant	<input type="checkbox"/>	0.0	$\text{s}^{-1}$
Kr	reverse rate constant	<input type="checkbox"/>	0.0	$\mu\text{M.s}^{-1}$
BS	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu\text{M}$

Annotation and Pathway Links

**BioModel4**

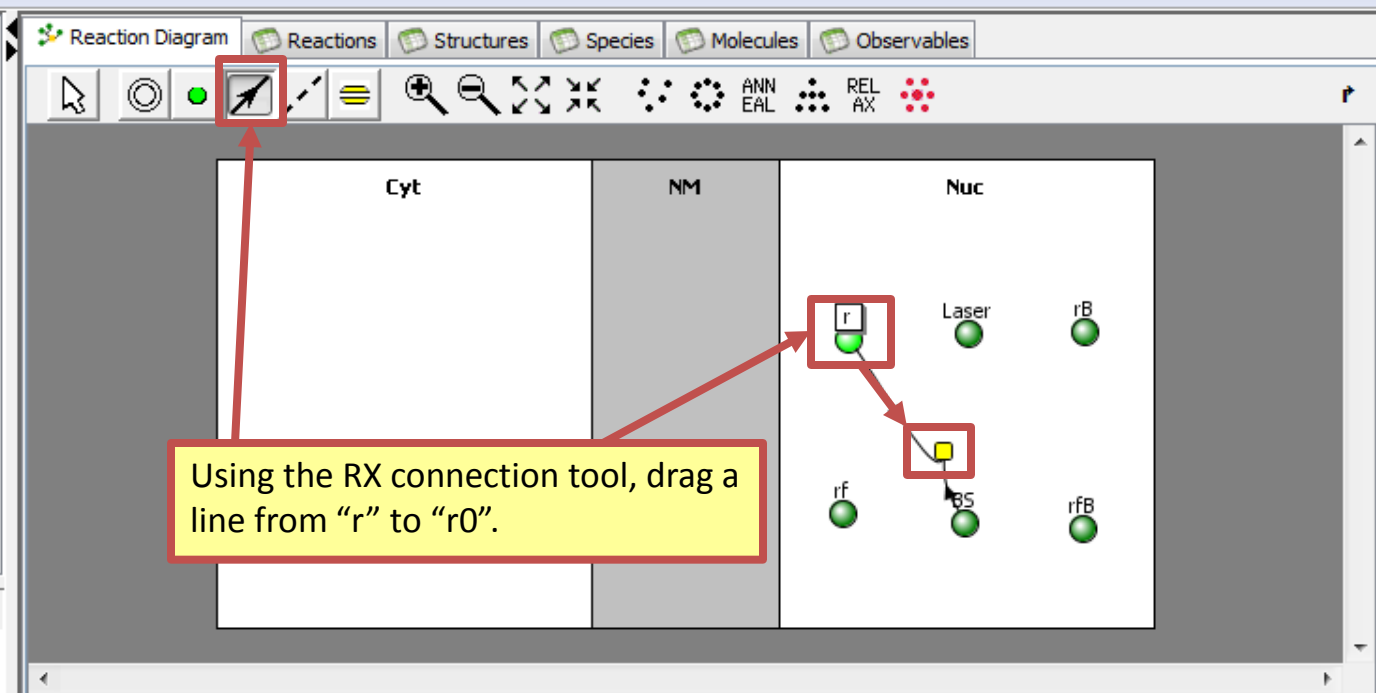
**Physiology**

- Reaction Diagram**
- Reactions (1)
- Structures (3)
- Species (6)
- Molecules (0)
- Observables (0)
- Applications (0)
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    - Education (33)
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Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Species Name	r	Species: r
Linked Pathway Object(s)		
Annotation	RAN	



**BioModel4**

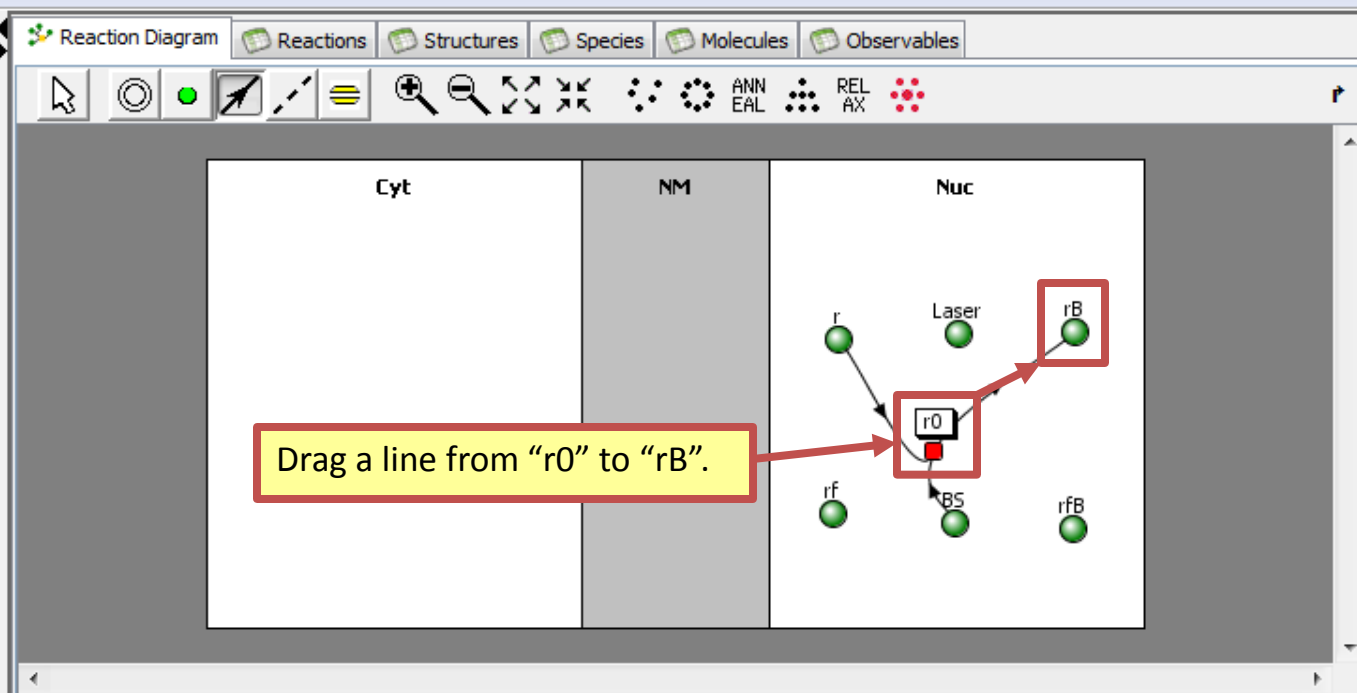
- Physiology
  - Reaction Diagram**
  - Reactions (1)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (0)
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Delete

Pathway Links

Search

Object Properties Problems (0 Errors, 0 Warnings)

Reaction Name r0

Kinetic Type Mass Action [ $\mu\text{M}/\text{s}$ ] (recommended for stochastic application)

Convert to [ $\text{molecules} \cdot \text{s}^{-1}$ ]

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$(K_f \cdot BS \cdot r - K_r \cdot rB)$	$\mu\text{M} \cdot \text{s}^{-1}$
Kf	forward rate constant	<input type="checkbox"/>	0.0	$\text{s}^{-1} \cdot \mu\text{M}^{-1}$
Kr	reverse rate constant	<input type="checkbox"/>	0.0	$\text{s}^{-1}$
BS	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu\text{M}$
r	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu\text{M}$
rB	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu\text{M}$

Annotation and Pathway Links

**BioModel4**

- Physiology
  - Reaction Diagram**
  - Reactions (2)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (0)
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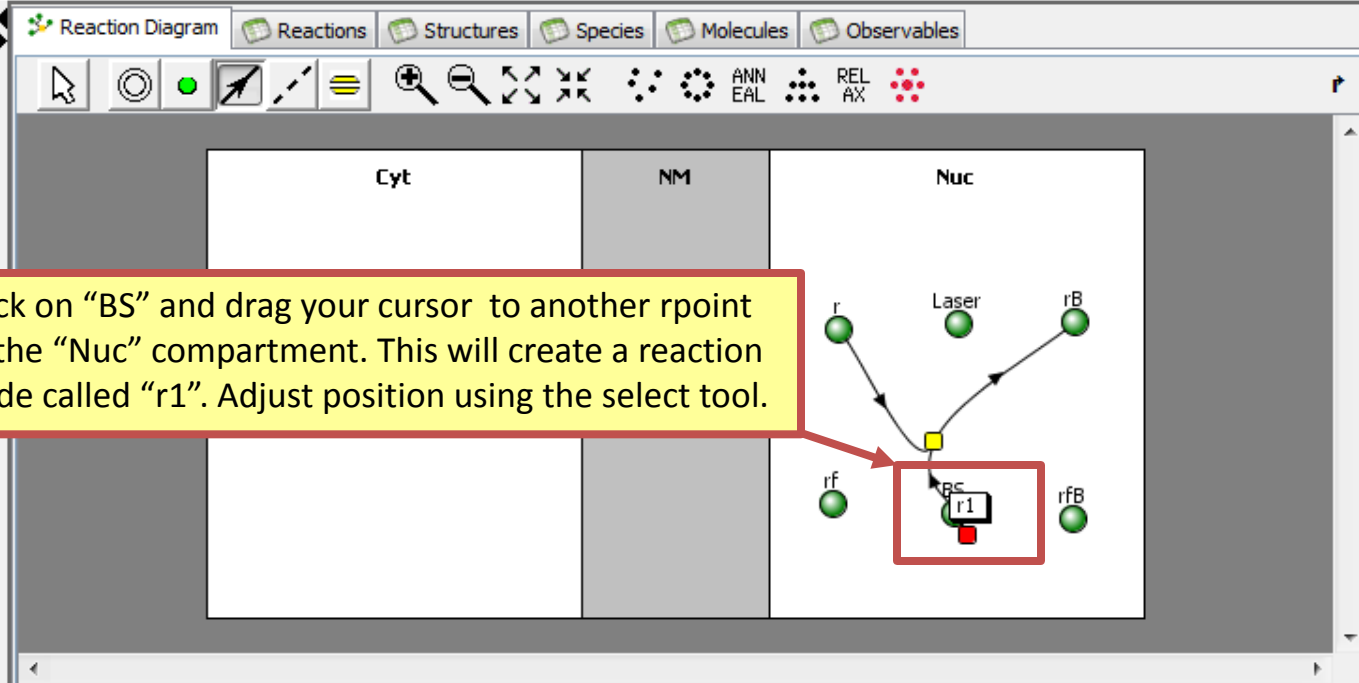
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Click on "BS" and drag your cursor to another rpoint in the "Nuc" compartment. This will create a reaction node called "r1". Adjust position using the select tool.



Delete

Pathway Links

Search

Object Properties Problems (0 Errors, 0 Warnings)

Reaction Name r1

Kinetic Type Mass Action [ $\mu\text{M/s}$ ] (recommended for stochastic application)

Convert to [ $\text{molecules.s}^{-1}$ ]

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$K_f \cdot BS$	$\mu\text{M.s}^{-1}$
Kf	forward rate constant	<input type="checkbox"/>	0.0	$\text{s}^{-1}$
Kr	reverse rate constant	<input type="checkbox"/>	0.0	$\mu\text{M.s}^{-1}$
BS	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu\text{M}$

Annotation and Pathway Links

**BioModel4**

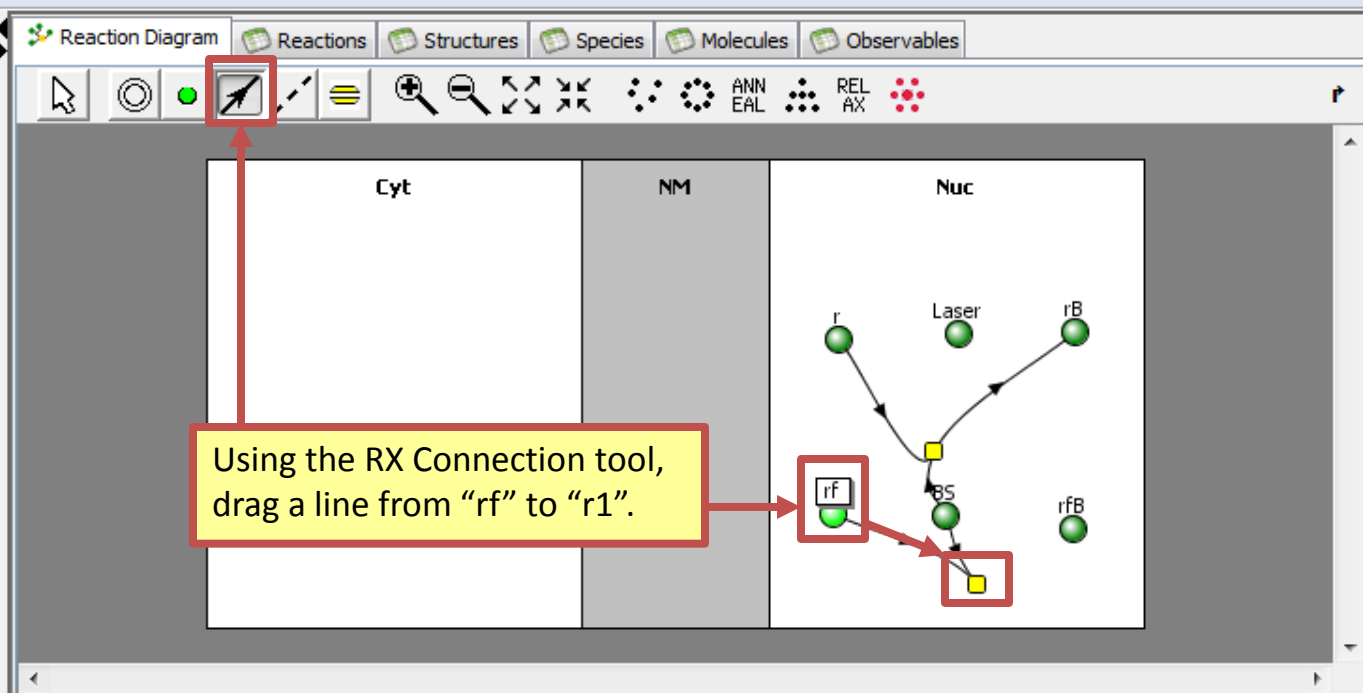
- Physiology
  - Reaction Diagram**
  - Reactions (2)
  - Structures (3)
  - Species (6)
  - Molecules (0)
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Delete

Pathway Links ▼

Search

Object Properties Problems (0 Errors, 0 Warnings)

Species Name	rf
Linked Pathway Object(s)	
Annotation	RAN_FITC



Species: rf

**BioModel4**

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  - Reaction Diagram**
  - Reactions (2)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (0)
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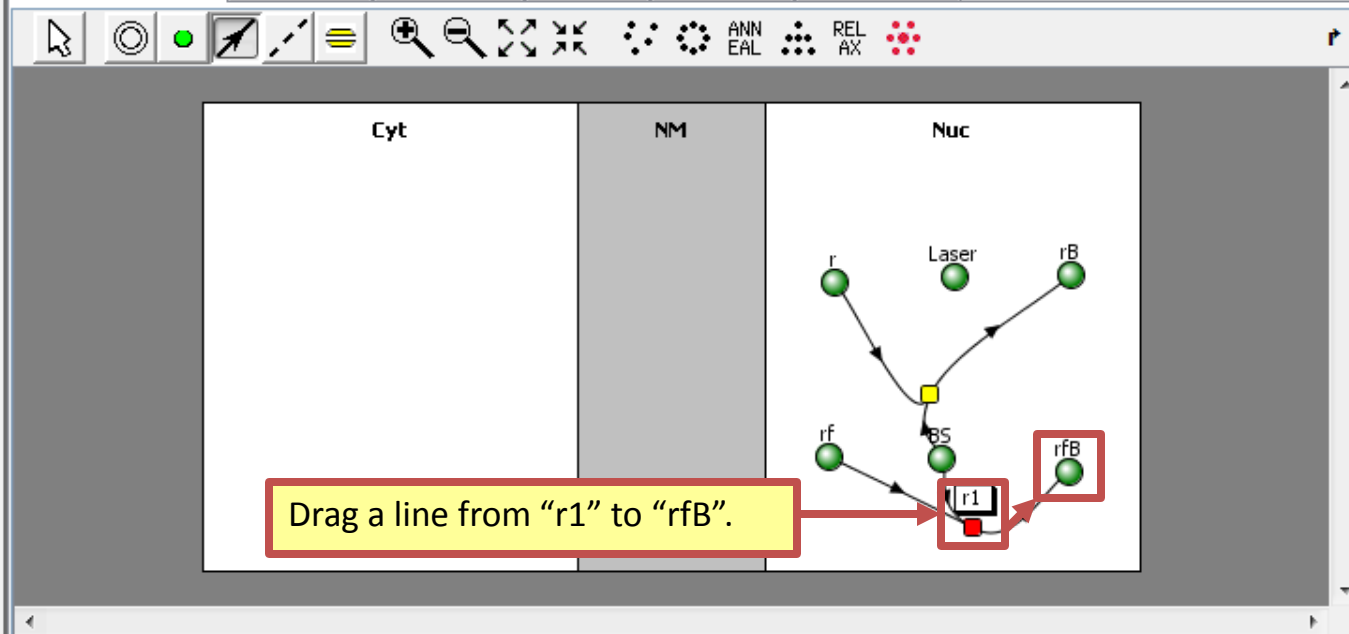
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Reaction Diagram Reactions Structures Species Molecules Observables



Delete

Pathway Links

Search

Object Properties Problems (0 Errors, 0 Warnings)

Reaction Name r1

Kinetic Type Mass Action [ $\mu\text{M}/\text{s}$ ] (recommended for stochastic application)

Convert to [ $\text{molecules} \cdot \text{s}^{-1}$ ]

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$(K_f \cdot BS \cdot rf - K_r \cdot rfb)$	$\mu\text{M} \cdot \text{s}^{-1}$
Kf	forward rate constant	<input type="checkbox"/>	0.0	$\text{s}^{-1} \cdot \mu\text{M}^{-1}$
Kr	reverse rate constant	<input type="checkbox"/>	0.0	$\text{s}^{-1}$
BS	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu\text{M}$
rf	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu\text{M}$
rfb	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu\text{M}$

Annotation and Pathway Links

**BioModel4**

- Physiology
  - Reaction Diagram**
  - Reactions (3)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (0)
- Parameters, Functions and Units
- Pathway

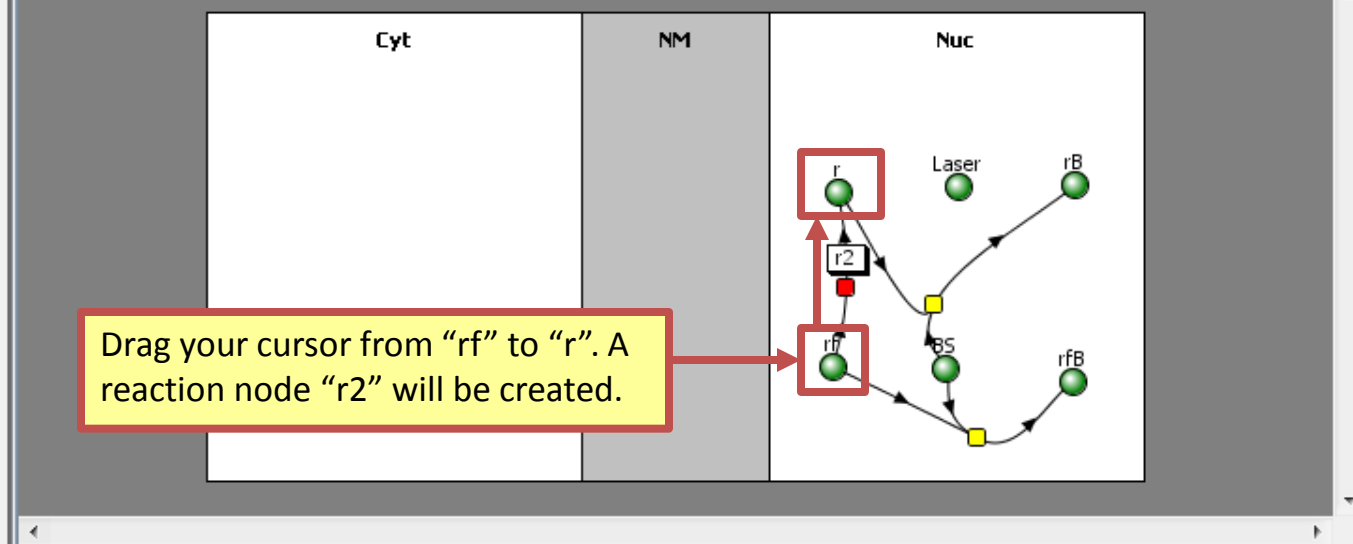
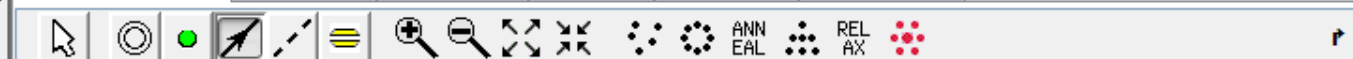
VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

**Search**

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  - Public BioModels (514)
  - Tutorials (5)
  - Education (33)
  - Tutorial VCell 6.0 (Rule-based) (7)

Reaction Diagram Reactions Structures Species Molecules Observables



Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Reaction Name r2

Kinetic Type Mass Action [ $\mu\text{M/s}$ ] (recommended for stochastic application) Convert to [ $\text{molecules.s}^{-1}$ ]

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$(K_f \cdot rf - K_r \cdot r)$	$\mu\text{M.s}^{-1}$
Kf	forward rate constant	<input type="checkbox"/>	0.0	$\text{s}^{-1}$
Kr	reverse rate constant	<input type="checkbox"/>	0.0	$\text{s}^{-1}$
rf	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu\text{M}$
r	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu\text{M}$

Annotation and Pathway Links

**BioModel4**

- Physiology
  - Reaction Diagram**
  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (0)
- Parameters, Functions and Units
- Pathway

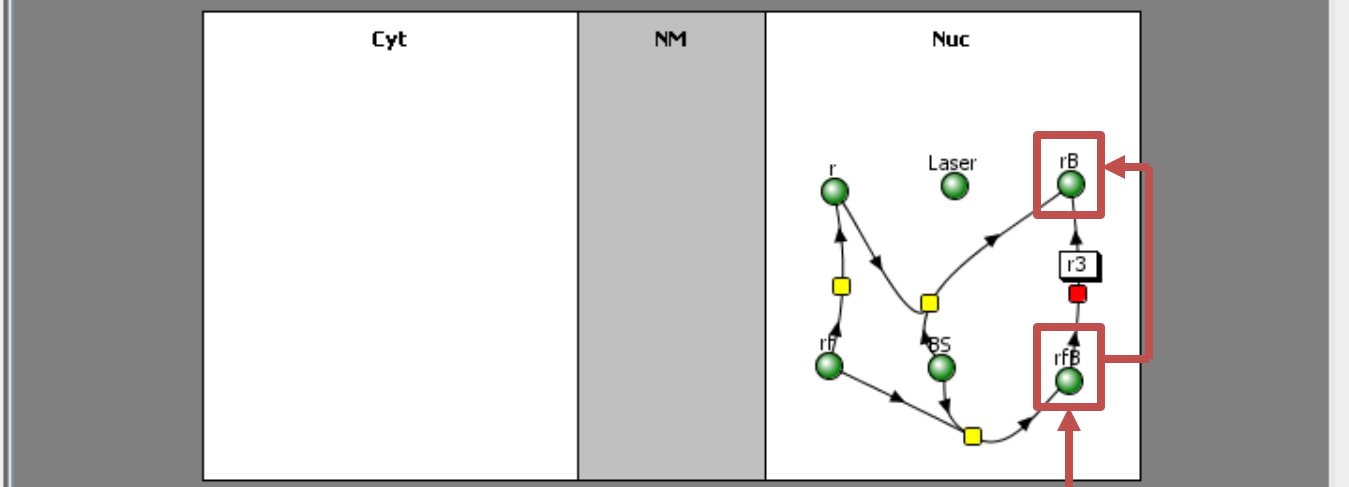
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Biological Models MathModels Geometries

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  - Tutorials (5)
  - Education (33)
  - Tutorial VCell 6.0 (Rule-based) (7)

Reaction Diagram Reactions Structures Species Molecules Observables



Drag your cursor from "rfB" to "rB". A reaction node "r3" will be created.

Delete

Pathway Links

Search

Object Properties Problems (0 Errors, 0 Warnings)

Reaction Name r3

Kinetic Type Mass Action [ $\mu\text{M/s}$ ] (recommended for stochastic application)

Convert to [ $\text{molecules.s}^{-1}$ ]

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$(K_f \cdot rF - K_r \cdot rB)$	$\mu\text{M.s}^{-1}$
Kf	forward rate constant	<input type="checkbox"/>	0.0	$\text{s}^{-1}$
Kr	reverse rate constant	<input type="checkbox"/>	0.0	$\text{s}^{-1}$
rfB	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu\text{M}$
rB	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu\text{M}$

Annotation and Pathway Links

**BioModel4**

**Physiology**

- Reactions (4)
- Structures (3)
- Species (6)
- Molecules (0)
- Observables (0)
- Applications (0)
- Parameters, Functions and Units
- Pathway

Click on the catalyst tool.

Click on "r2" and drag your cursor, which will create a line marked <<CATALYST>>. Drop your cursor on "Laser".

Reaction Diagram Reactions Structures Species Molecules Observables

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

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Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Reaction Name r2

Kinetic Type Mass Action [ $\mu\text{M/s}$ ] (recommended for stochastic application) Convert to [ $\text{molecules.s}^{-1}$ ]

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$(K_f \cdot r_f - K_r \cdot r)$	$\mu\text{M.s}^{-1}$
Kf	forward rate constant	<input type="checkbox"/>	0.0	$\text{s}^{-1}$
Kr	reverse rate constant	<input type="checkbox"/>	0.0	$\text{s}^{-1}$
rf	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu\text{M}$
r	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu\text{M}$

Annotation and Pathway Links

CONNECTED (astfh234) 51.6MB / 112.6MB

File View Server Tools Help

**BioModel4**

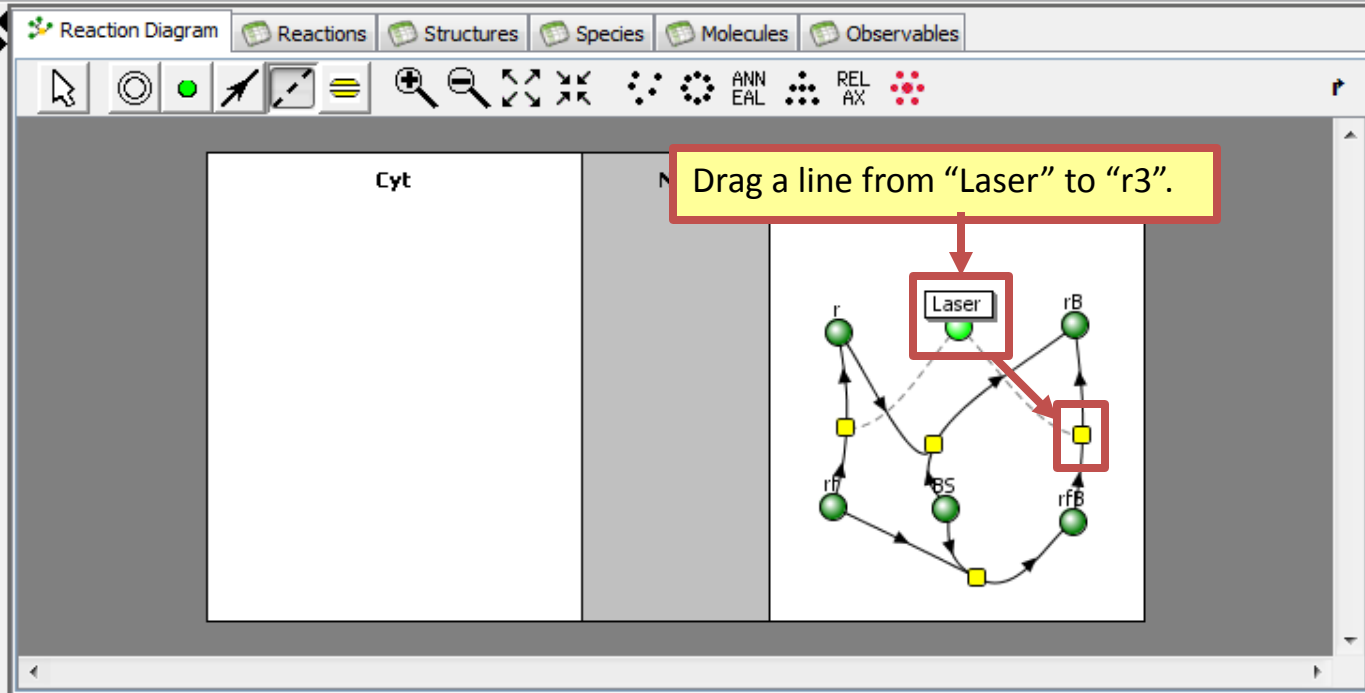
- Physiology
  - Reaction Diagram**
  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (0)
- Parameters, Functions and Units
- Pathway

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

**Search**

- Biological Models
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  - Education (33)
  - Tutorial VCell 6.0 (Rule-based) (7)



Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Species Name	Laser
Linked Pathway Object(s)	
Annotation	Light Source

Species: **Laser**

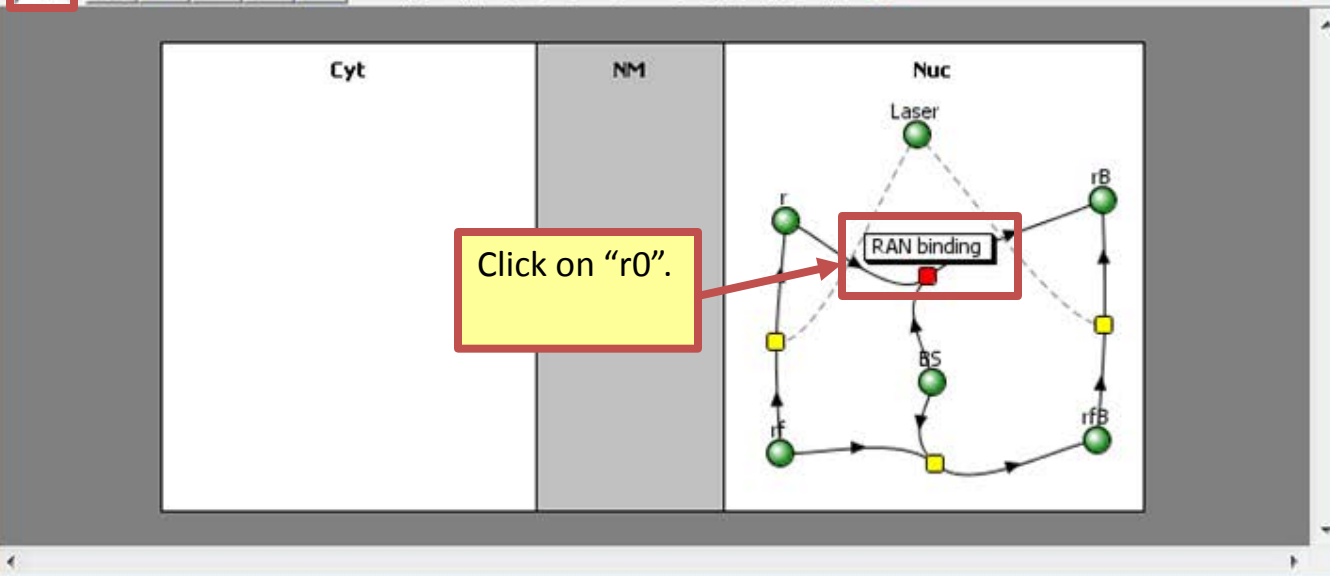


**BioModel4**

- Phys
  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (0)
- Parameters, Functions and Units
- Pathway

Click the select tool.

Reaction Diagram Reactions Structures Species Molecules Observables



Click on "r0".

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BioModels MathModels Geometries

- Search**
- Biological Models
    - My BioModels (astfh234) (4)
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Delete

Pathway Links

Search

Object Properties Problems (0 Errors, 0 Warnings)

Reaction Name RAN binding

Next to Reaction Name type "RAN binding".

Kinetic Type Mass Action [ $\mu\text{M}/\text{s}$ ] (recommended for stochastic application)

Convert to [ $\text{molecules}\cdot\text{s}^{-1}$ ]

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$(K_f \cdot BS \cdot r - K_r \cdot rB)$	$\mu\text{M}\cdot\text{s}^{-1}$
Kf	forward rate constant	<input type="checkbox"/>	0.0	$\text{s}^{-1}\cdot\mu\text{M}^{-1}$
Kr	reverse rate constant	<input type="checkbox"/>	0.0	$\text{s}^{-1}$
BS	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu\text{M}$
r	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu\text{M}$
rB	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu\text{M}$

Annotation and Pathway Links

**BioModel4**

**Physiology**

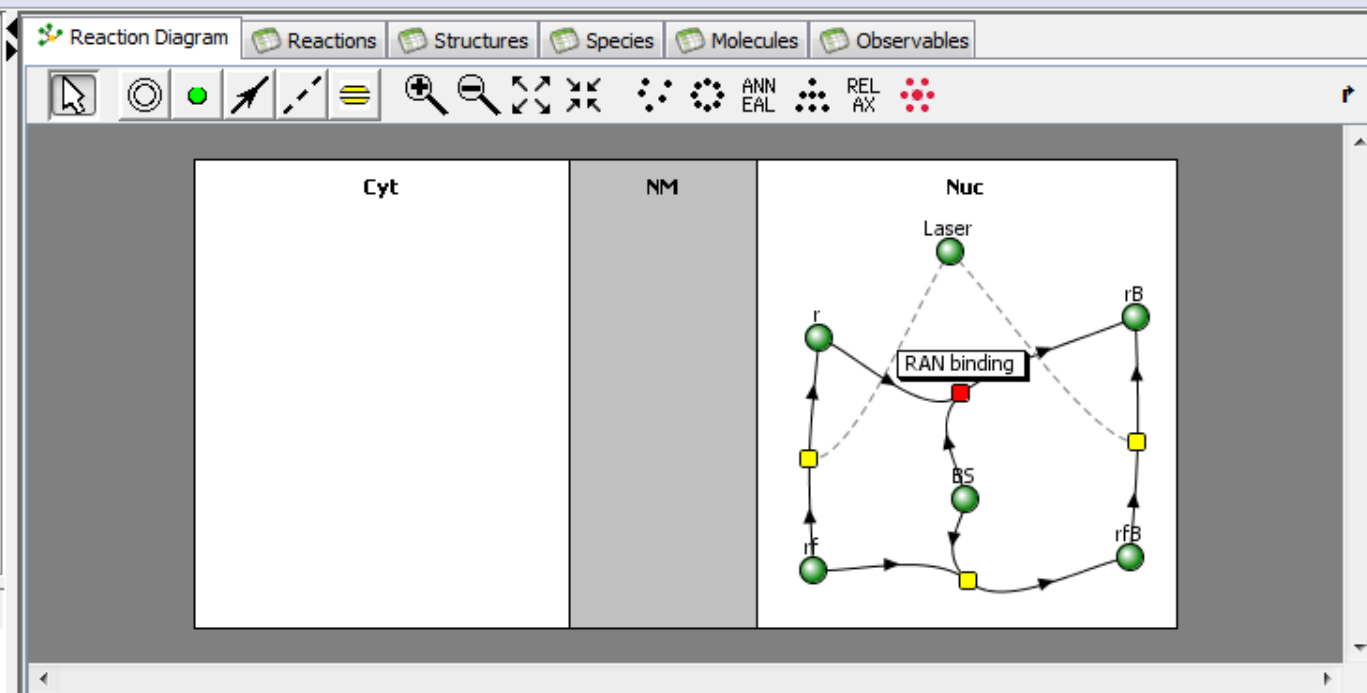
- Reaction Diagram
- Reactions (4)
- Structures (3)
- Species (6)
- Molecules (0)
- Observables (0)
- Applications (0)
- Parameters, Functions and Units
- Pathway

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

+ Search

- Biological Models
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  - Tutorial VCell 6.0 (Rule-based) (7)



Delete

Pathway Links

Search

Object

React

Kin

Convert to [molecules.s<sup>-1</sup>]

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$K_f \cdot BS \cdot r - K_r \cdot rB$	$\mu M \cdot s^{-1}$
Kf	forward rate constant	<input type="checkbox"/>	0.02	$s^{-1} \cdot \mu M^{-1}$
Kr	reverse rate constant	<input checked="" type="checkbox"/>	.1	$s^{-1}$
BS	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu M$
r	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu M$
rB				$\mu M$

+ Ar

In the forward rate constant row, type ".02" under the Expression column. Press "Enter" on your keyboard to finalize.

In the reverse rate constant row, type ".1" under the Expression column. Press "Enter" on your keyboard to finalize.

**BioModel4**

**Physiology**

- Reaction Diagram
- Reactions (4)
- Structures (3)
- Species (6)
- Molecules (0)
- Observables (0)
- Applications (0)
- Parameters, Functions and Units
- Pathway

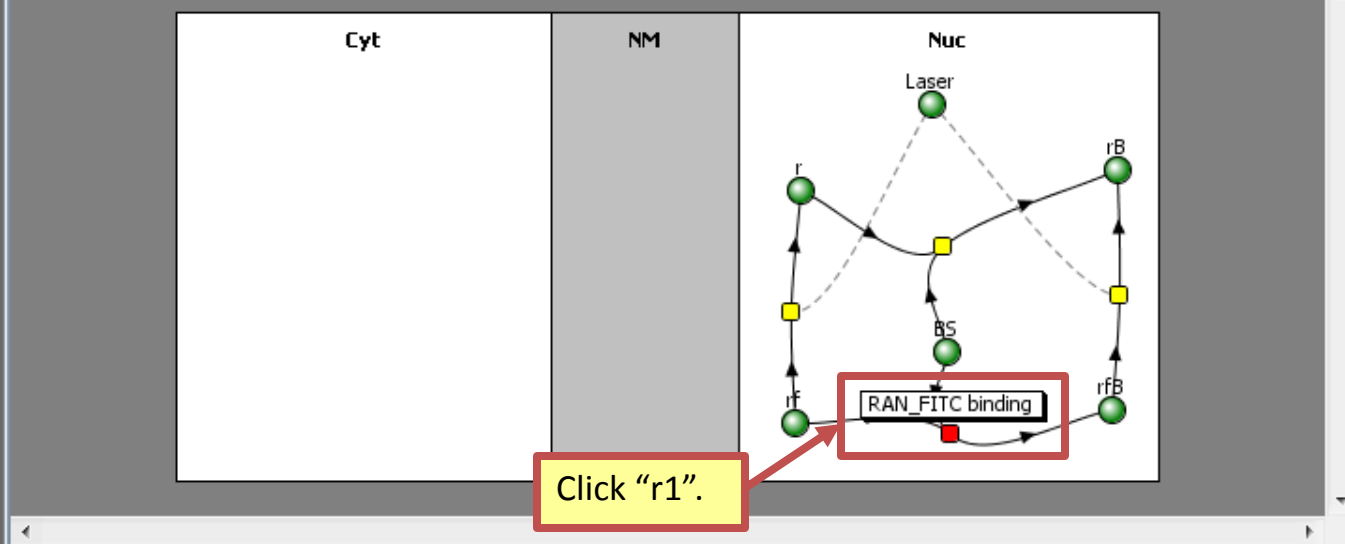
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BioModels MathModels Geometries

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Reaction Diagram Reactions Structures Species Molecules Observables



Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Reaction Name RAN\_FITC binding

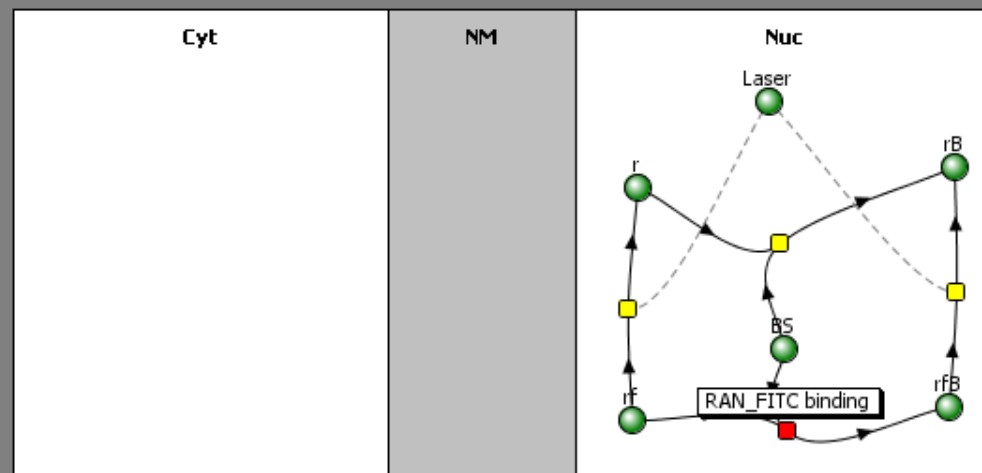
Kinetic Type Mass Action [ $\mu\text{M}/\text{s}$ ] (recommended for stochastic application)

Convert to [ $\text{molecules} \cdot \text{s}^{-1}$ ]

Name	Description	Global	Expression	Units
Kr	reverse rate constant	<input type="checkbox"/>	0.1	$\text{s}^{-1}$
BS	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu\text{M}$
rf	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu\text{M}$
rfB	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu\text{M}$

Next to Reaction Name, type "RAN\_FITC binding".

Annotation and Pathway Links



Pathway Links ▼

Search

Object Properties Problems (0 Errors, 0 Warnings)

In the forward rate constant row, type “.02” under the Expression column. Press “Enter” on your keyboard to finalize.

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$K_f \cdot BS \cdot rf - K_r \cdot rfB$	$\mu M \cdot s^{-1}$
Kf	forward rate constant	<input type="checkbox"/>	0.02	$s^{-1} \cdot \mu M^{-1}$
Kr	reverse rate constant	<input type="checkbox"/>	0.1	$s^{-1}$
BS	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu M$
rf	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu M$
				$\mu M$

In the reverse rate constant row, type “.1” under the Expression column. Press “Enter” on your keyboard to finalize.

**BioModel4**

**Physiology**

- Reaction Diagram
- Reactions (4)
- Structures (3)
- Species (6)
- Molecules (0)
- Observables (0)
- Applications (0)
- Parameters, Functions and Units
- Pathway

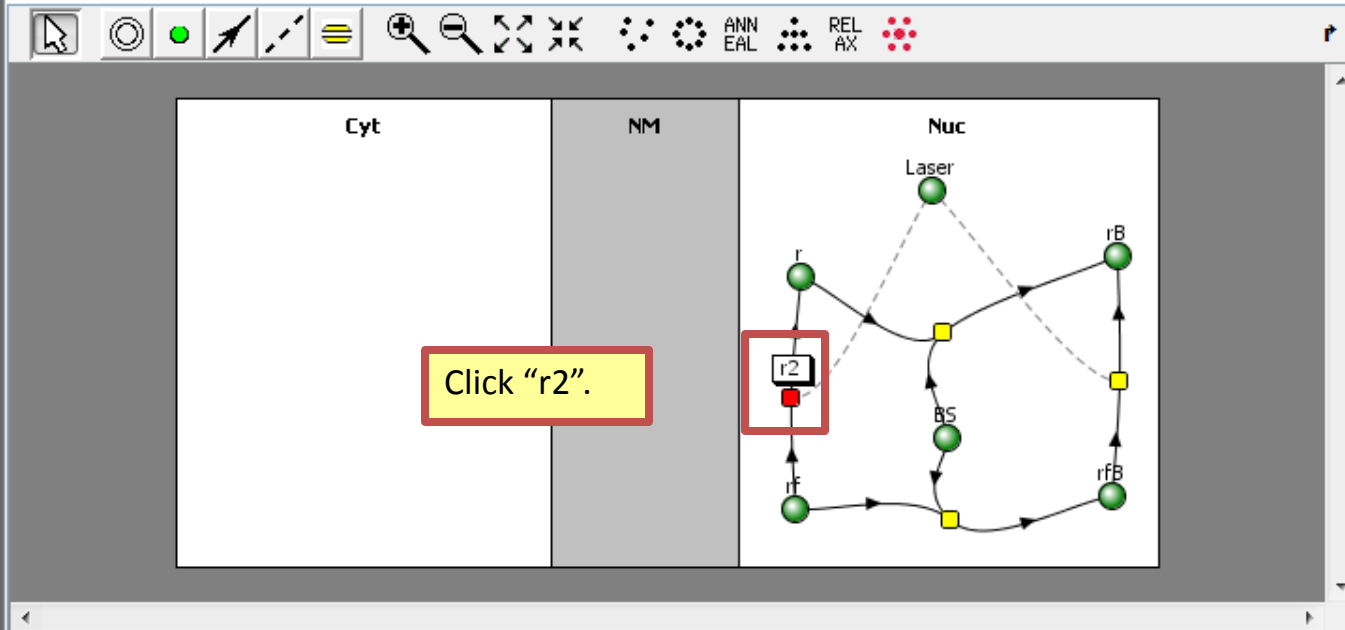
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BioModels MathModels Geometries

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Reaction Diagram Reactions Structures Species Molecules Observables



Click "r2".

Delete

Pathway Links

Search

Object Properties Problems (0 Errors, 0 Warnings)

Reaction Name r2

Kinetic Type General [ $\mu\text{M/s}$ ]

Convert to [ $\text{molecules.s}^{-1}$ ]

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	0.0	$\mu\text{M.s}^{-1}$

Click the drop down menu next to Kinetic Type.  
Click "General [ $\mu\text{M/s}$ ]".

Annotation and Pathway Links

BIOMODEL: BioModel4 (NoVersion) (NoDate) -- VCell 6.0 (build 3)

File View Server Tools Help

**BioModel4**

**Physiology**

- Reaction Diagram
- Reactions (4)
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**Reaction Diagram** Reactions Structures Species Molecules Observables

Diagram showing a reaction network across three compartments: Cyt, NM, and Nuc. The network includes species like Laser, r, rB, rf, rfB, and BS, connected by reactions r, r2, rB, rf, rfB, and BS. A yellow box highlights reaction r2.

**Object Properties** Problems (0 Errors, 0 Warnings)

Reaction Name: r2

Kinetic Type: General [μM/s]

Convert to [molecules.s<sup>-1</sup>]

Name	Description	Global	Expression	Units
j	reaction rate	<input type="checkbox"/>	$(Vmax * rf * Laser * ((t > 1.0) \&\& (t < 1.5)))$	μM.s <sup>-1</sup>

In the reaction rate row, type “(Vmax\*rf\*Laser\*((t>1.0)&&(t<1.5)))” under the Expression column. Press “Enter” on your keyboard to finalize. The Boolean expression evaluates to 1 during the time interval from 1.0 to 1.5 secs; at other times, the expression evaluates to 0 so the bleaching reactions only occur during the specified time interval.

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File View Server Tools Help

**BioModel4**

**Physiology**

- Reaction Diagram
- Reactions (4)
- Structures (3)
- Species (6)
- Molecules (0)
- Observables (0)
- Applications (0)
- Parameters, Functions and Units
- Pathway

VCell DB BioModels.net Pathway Comm Sabio

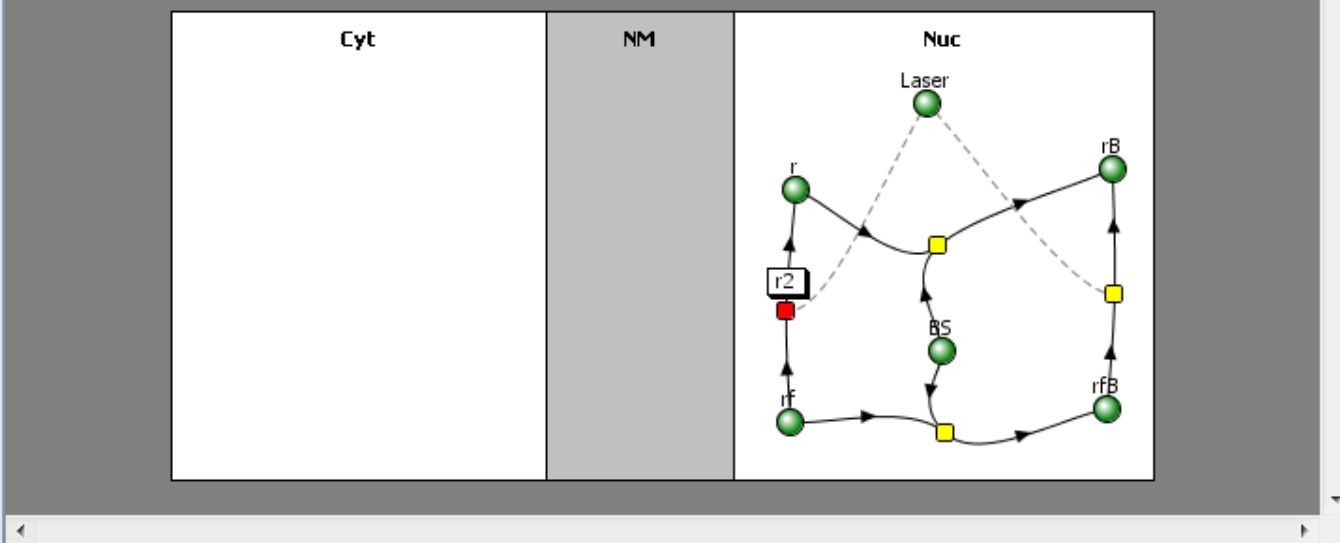
BioModels MathModels Geometries

+ Search

Biological Models

- My BioModels (astfh234) (4)
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- Tutorial VCell 6.0 (Rule-based) (7)

Reaction Diagram Reactions Structures Species Molecules Observables



Delete Pathway Links Search

Object Properties Problem

Reaction Name r2

Kinetic Type General

In the Vmax row, type "50" under the Expression column. Press "Enter" on your keyboard to finalize.

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$v_{max} \cdot r_f \cdot Laser \cdot ((t > 1.0) \&\& (t < 1.5))$	$\mu M \cdot s^{-1}$
Vmax	user defined	<input type="checkbox"/>	50	$s^{-1} \cdot \mu M^{-1}$
rf	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu M$
Laser	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu M$
t	time	<input checked="" type="checkbox"/>	Variable	s

+ Annotation and Pathway Links

File View Server Tools Help

**BioModel4**

- Physiology
  - Reaction Diagram**
  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (0)
- Parameters, Functions and Units
- Pathway

VCell DB BioModels.net Pathway Comm Sabio

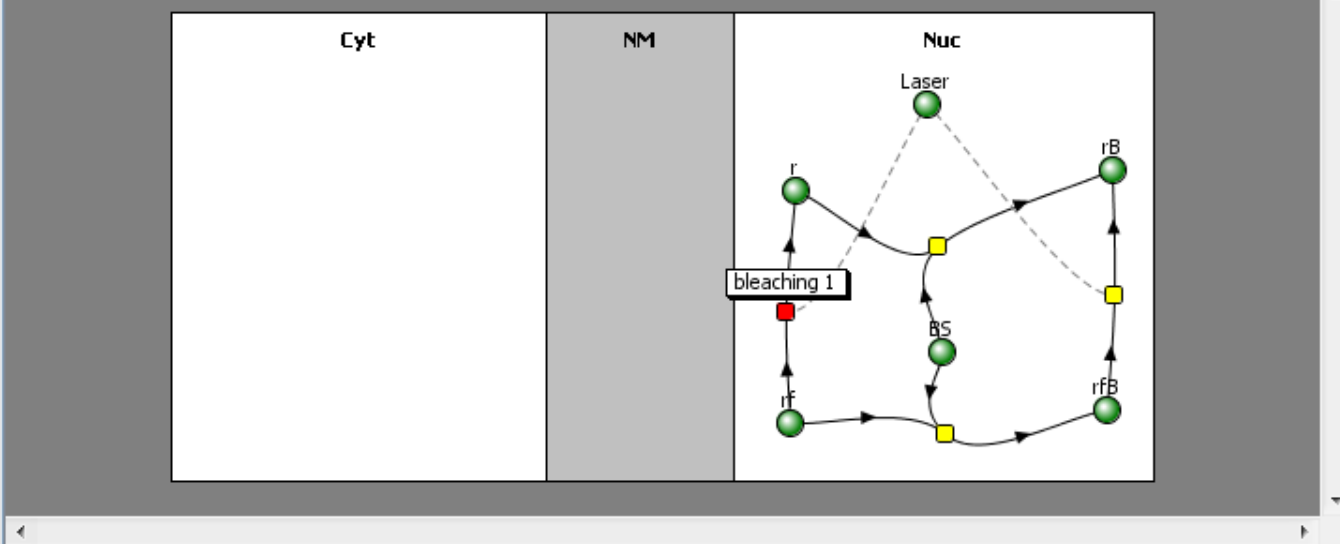
BioModels MathModels Geometries

+ Search

Biological Models

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Reaction Diagram Reactions Structures Species Molecules Observables



Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Reaction Name bleaching 1

Next to Reaction Name type "bleaching 1".

Kinetic Type General [μM/s]

Convert to [molecules.s<sup>-1</sup>]

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$V_{max} \cdot rf \cdot Laser \cdot ((t > 1.0) \&\& (t < 1.5))$	μM.s <sup>-1</sup>
Vmax	user defined	<input type="checkbox"/>	50.0	s <sup>-1</sup> .μM <sup>-1</sup>
rf	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM
Laser	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM
t	time	<input checked="" type="checkbox"/>	Variable	s

+ Annotation and Pathway Links



**BioModel4**

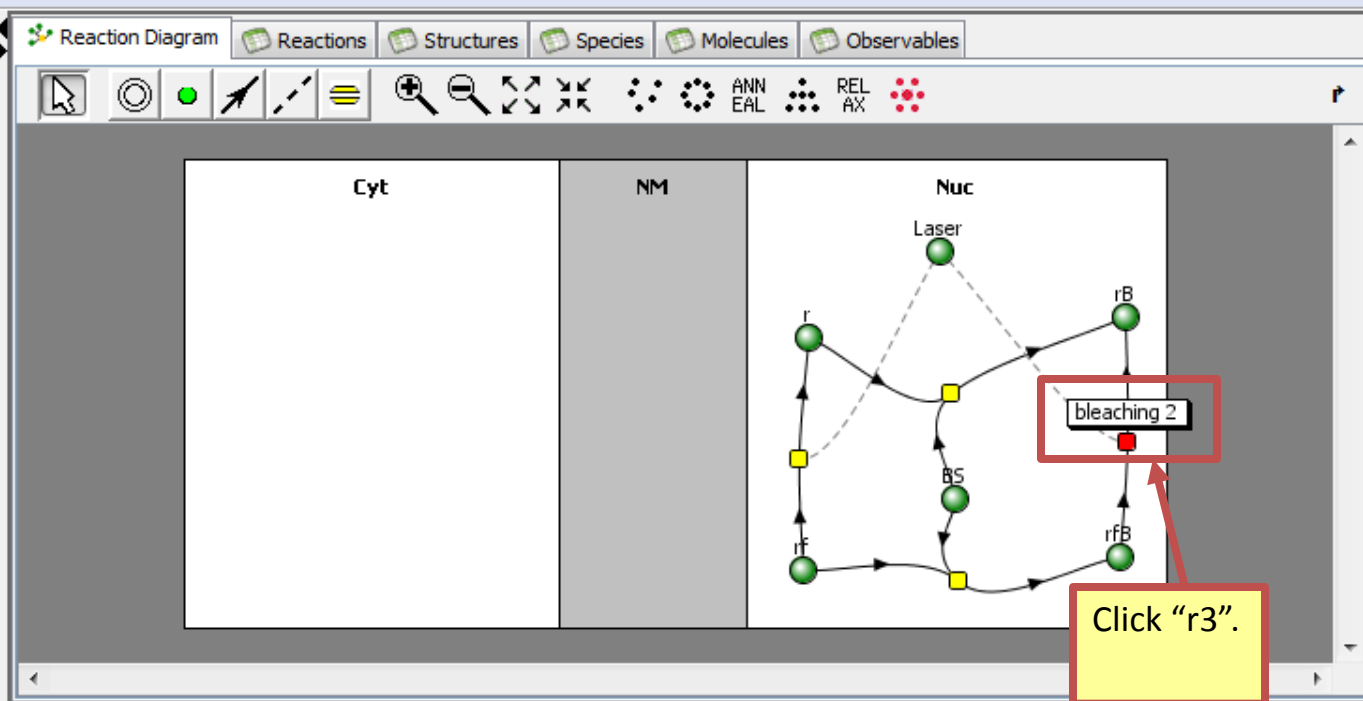
- Physiology
  - Reaction Diagram**
  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (0)
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VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

+ Search

- Biological Models
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  - Tutorials (5)
  - Education (33)
  - Tutorial VCell 6.0 (Rule-based) (7)



Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Reaction Name **bleaching 2** Next to Reaction Name type "bleaching 2".

Kinetic Type Mass Action [ $\mu\text{M/s}$ ] (recommended for stochastic application) Convert to [molecules.s<sup>-1</sup>]

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$(K_f \cdot r_F - K_r \cdot r_B)$	$\mu\text{M.s}^{-1}$
Kf	forward rate constant	<input type="checkbox"/>	0.0	s <sup>-1</sup>
Kr	reverse rate constant	<input type="checkbox"/>	0.0	s <sup>-1</sup>
rFB	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu\text{M}$
rB	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu\text{M}$

+ Annotation and Pathway Links

BIOMODEL: BioModel4 (NoVersion) (NoDate) -- VCell 6.0 (build 3)

File View Server Tools Help

**BioModel4**

**Physiology**

- Reaction Diagram
- Reactions (4)
- Structures (3)
- Species (6)
- Molecules (0)
- Observables (0)
- Applications (0)
- Parameters, Functions and Units
- Pathway

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

**Search**

- Biological Models
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  - Tutorial VCell 6.0 (Rule-based) (7)

**Reaction Diagram** Reactions Structures Species Molecules Observables

Cyt NM Nuc

Laser

rB

bleaching 2

r

rf

BS

rfB

Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Reaction Name bleaching 2

Kinetic Type General [ $\mu\text{M/s}$ ] Convert to [ $\text{molecules.s}^{-1}$ ]

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	0.0	$\mu\text{M.s}^{-1}$

Click the drop down menu next to Kinetic Type. Click "General [ $\mu\text{M/s}$ "].

Annotation and Pathway Links

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BIOMODEL: BioModel4 (NoVersion) (NoDate) -- VCell 6.0 (build 3)

File View Server Tools Help

**BioModel4**

**Physiology**

- Reaction Diagram
- Reactions (4)
- Structures (3)
- Species (6)
- Molecules (0)
- Observables (0)
- Applications (0)
- Parameters, Functions and Units
- Pathway

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

**Search**

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  - My BioModels (astfh234) (4)
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  - Public BioModels (514)
  - Tutorials (5)
  - Education (33)
  - Tutorial VCell 6.0 (Rule-based) (7)

**Reaction Diagram**

Reactions Structures Species Molecules Observables

Cyt NM Nuc

Laser

r

rB

bleaching 2

BS

rf

rfB

Delete Pathway Links Search

**Object Properties** Problems (0 Errors, 0 Warnings)

Reaction Name bleaching 2

Kinetic Type General  $\mu\text{M/s}$  Convert to  $[\text{molecules.s}^{-1}]$

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$(V_{\text{max}2} * r_{\text{fB}} * \text{Laser} * ((t > 1.0) \& \& (t < 1.5)))$	$\mu\text{M.s}^{-1}$

**Annotation and Pathway Links**

CONNECTED (astfh234) 66.2MB / 1.2.6MB

In the reaction rate row, type “ $(V_{\text{max}2} * r_{\text{fB}} * \text{Laser} * ((t > 1.0) \& \& (t < 1.5)))$ ” under the Expression column. Press “Enter” on your keyboard to finalize.

File View Server Tools Help

# BioModel4

## Physiology

### Reaction Diagram

#### Reactions (4)

#### Structures (3)

#### Species (6)

#### Molecules (0)

#### Observables (0)

## Applications (0)

## Parameters, Functions and Units

## Pathway

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

## Search

### Biological Models

My BioModels (astfh234) (4)

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## Reaction Diagram

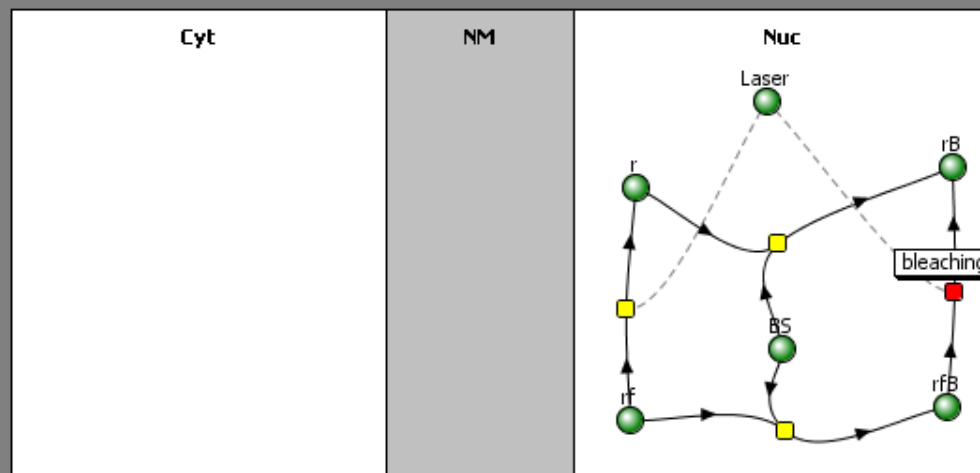
## Reactions

## Structures

## Species

## Molecules

## Observables



Delete

Pathway Links

Search

## Object Properties

Reaction Name

bleach

Kinetic Type

General

Convert to [molecules.s<sup>-1</sup>]

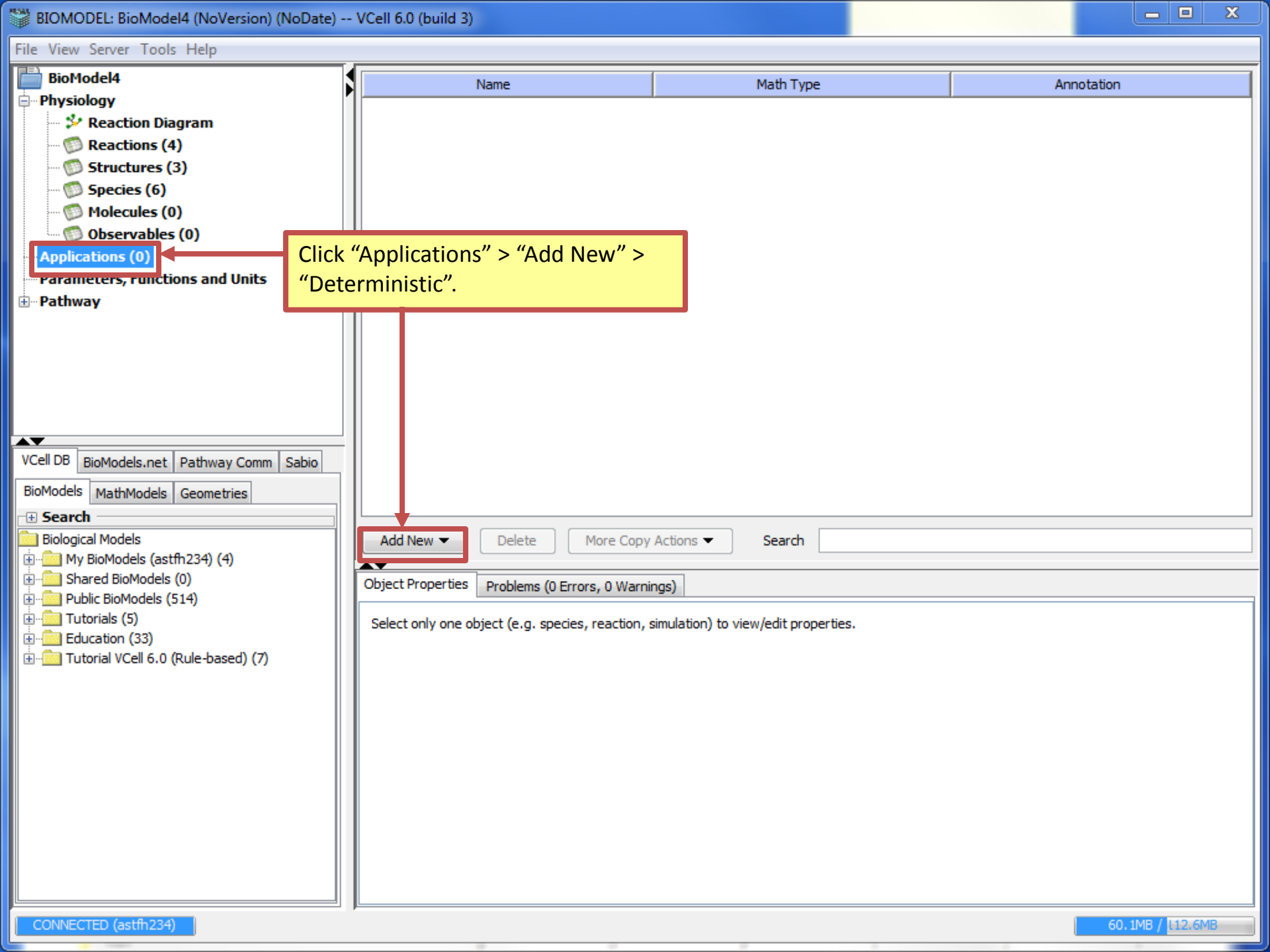
Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$V_{max2} \cdot rfB \cdot Laser \cdot ((t > 1.0) \&\& (t < 1.5))$	$\mu M \cdot s^{-1}$
Vmax2	user defined	<input checked="" type="checkbox"/>	50	$s^{-1} \cdot \mu M^{-1}$
rfB	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu M$
Laser	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu M$
t	time	<input checked="" type="checkbox"/>	Variable	s

## Annotation and Pathway Links

CONNECTED (astfh234)

75.4MB / 112.6MB

In the Vmax row, type "50" under the Expression column. Press "Enter" on your keyboard to finalize.



Click "Applications" > "Add New" > "Deterministic".

Buttons: Add New, Delete, More Copy Actions, Search

Object Properties Problems (0 Errors, 0 Warnings)

Select only one object (e.g. species, reaction, simulation) to view/edit properties.

File View Server Tools Help

**BioModel4**

- Physiology**
  - Reaction Diagram
  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (1)**
  - $d/dt$  Application0
- Parameters, Functions and Units
- Pathway

Name	Math Type	Annotation
Compartmental	compartmental deterministic	

Double click "Application0" under the Name column. Type in "Compartmental". Press "Enter" on your keyboard to finalize. This compartmental application will be used to determine the steady-state concentrations for the binding reaction.

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

+ Search

- Biological Models
  - My BioModels (astfh234) (4)
  - Shared BioModels (0)
  - Public BioModels (514)
  - Tutorials (5)
  - Education (33)
  - Tutorial VCell 6.0 (Rule-based) (7)

Add New ▼

Delete

More Copy Actions ▼

Search

Object Properties Problems (0 Errors, 0 Warnings)

Application Name Application0

Annotation

Summary

- Deterministic
- ✖ Compartmental
- math not generated

BIOMODEL: BioModel4 (NoVersion) (NoDate) -- VCell 6.0 (build 3)

File View Server Tools Help

BioModel4

Physiology

- Reaction Diagram
- Reactions (4)
- Structures (3)
- Species (6)
- Molecules (0)
- Observables (0)

Applications (1)

- Compartmental
- Geometry
- Specifications
- Protocols
- Simulations
- Parameter Estimation

Parameters, Functions and Units

Pathway

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

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Geometry Specifications Protocols Simulations Parameter Estimation

Structure Mapping Geometry Definition

Physiology (structures)

Cyt

Geometry (subd

Compartment

Volume and Surface Calculator >>

Structure	Size
Cyt	523.33 [ $\mu\text{m}^3$ ]
NM	130.8325 [ $\mu\text{m}^2$ ]
Nuc	26.1665

Object Properties Problems (0 Errors, 0 Warnings)

Select only one object (e.g. species, reaction, simulation) to view/edit properties.

Double click "Compartmental" and click "Geometry" > "Structure Mapping".

In the Size column for "Cyt", "NM" and "Nuc", type in "523.33", "130.8325" and "26.1665" respectively. Press "Enter" on your keyboard to finalize.

CONNECTED (astfh234)

60.8MB / 112.6MB

**BioModel4**

**Physiology**

- Reaction Diagram
- Reactions (4)
- Structures (3)
- Species (6)
- Molecules (0)
- Observables (0)

**Applications (1)**

- Compartmental
- Geometry
- Specifications**
- Protocols
- Simulations
- Parameter Estimation

**Parameters, Functions and Units**

**Pathway**

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

+ Search

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Geometry Specifications Protocols Simulations Parameter Estimation

Species

Reaction Network

Click "Specifications" > "Species".

Species	Structure	Clamped	Initial Condition
r	Nuc	<input type="checkbox"/>	5.0
rf	Nuc	<input type="checkbox"/>	5.0
rB	Nuc	<input type="checkbox"/>	0.0
BS	Nuc	<input type="checkbox"/>	20
rFB	Nuc	<input type="checkbox"/>	0.0
Laser	Nuc	<input type="checkbox"/>	0.0

In the Initial Condition column for "r", "rf" and "BS", type in "5", "5" and "20" respectively. Press "Enter" on your keyboard to finalize.

Search

Object Properties Problems (0 Errors, 0 Warnings)

Description	Parameter	Expression	Units
initial concentration for BS	initConc	0.0	$\mu\text{M}$



To save your model, click "File" > "Save As".

	Structure	Clamped	Initial Condition
		<input type="checkbox"/>	5.0
rf	Nuc	<input type="checkbox"/>	5.0
rB	Nuc	<input type="checkbox"/>	0.0
BS	Nuc	<input type="checkbox"/>	20
rfB	Nuc	<input type="checkbox"/>	0.0
Laser	Nuc	<input type="checkbox"/>	0.0

Description	Parameter	Expression	Units
initial concentration for BS	initConc	0.0	$\mu\text{M}$

File View Server Tools Help

**BioModel4**

- Physiology
  - Reaction Diagram
  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (1)
  - Compartmental
  - Geometry
  - Specifications**
  - Protocols
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  - Parameter Estimation
- Parameters, Functions and Units
- Pathway

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

**Search**

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  - Tutorials (5)
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  - Tutorial VCell 6.0 (Rule-based) (7)

CONNECTED (astfh234)

Save document:

Search

[Advanced >>](#)

Search Show All

- Biological Models
  - My BioModels (astfh234) (4)**
    - FRAPTutorial
    - BioModel4
    - Model2
    - tutorial 3
  - Shared BioModels (0)
  - Public BioModels (514)
  - Tutorials (5)

Selected BioModel Summary

Please type a new name:

FRAPBindingTutorial

Save Cancel

Click on a folder to select the location for your model to be saved.

Type in a name under "Please type in a new name:" and click "Save".

Initial Condition

	5.0
	5.0
	0.0
	20.0

Units

	$\mu\text{M}$
--	---------------

79MB / 112.6MB

File View Server Tools Help

**FRAPBindingTutorial**

- Physiology**
  - Reaction Diagram
  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (1)**
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  - Geometry
  - Specifications
  - Protocols
  - Simulations**
  - Parameter Estimation
- Parameters, Functions and Units**

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

+ Search

- Biological Models
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Geometry Specifications Protocols Simulations Parameter Estimation

Simulations Output Functions Generated Math

Simulations

Name	End Time	Output Option	Solver	Running Status	Results
------	----------	---------------	--------	----------------	---------

Click "Simulations" and the new simulation icon.

Object Properties Problems (0 Errors, 0 Warnings)

Select only one object (e.g. species, reaction, simulation) to view/edit properties.

File View Server Tools Help

**FRAPBindingTutorial**

- Physiology**
  - Reaction Diagram
  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (1)**
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  - Protocols
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  - Parameter Estimation
- Parameters, Functions and Units**

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

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  - Education (33)
  - Tutorial VCell 6.0 (Rule-based) (7)

Geometry Specifications Protocols Simulations Parameter Estimation

Simulations Output Functions Generated Math

Name	End Time	Output Option	Solver	Running Status	Results
Simulation	1.0	keep every 1 sample	Combined IDA/CVODE	not saved	no

Click the edit simulation icon.

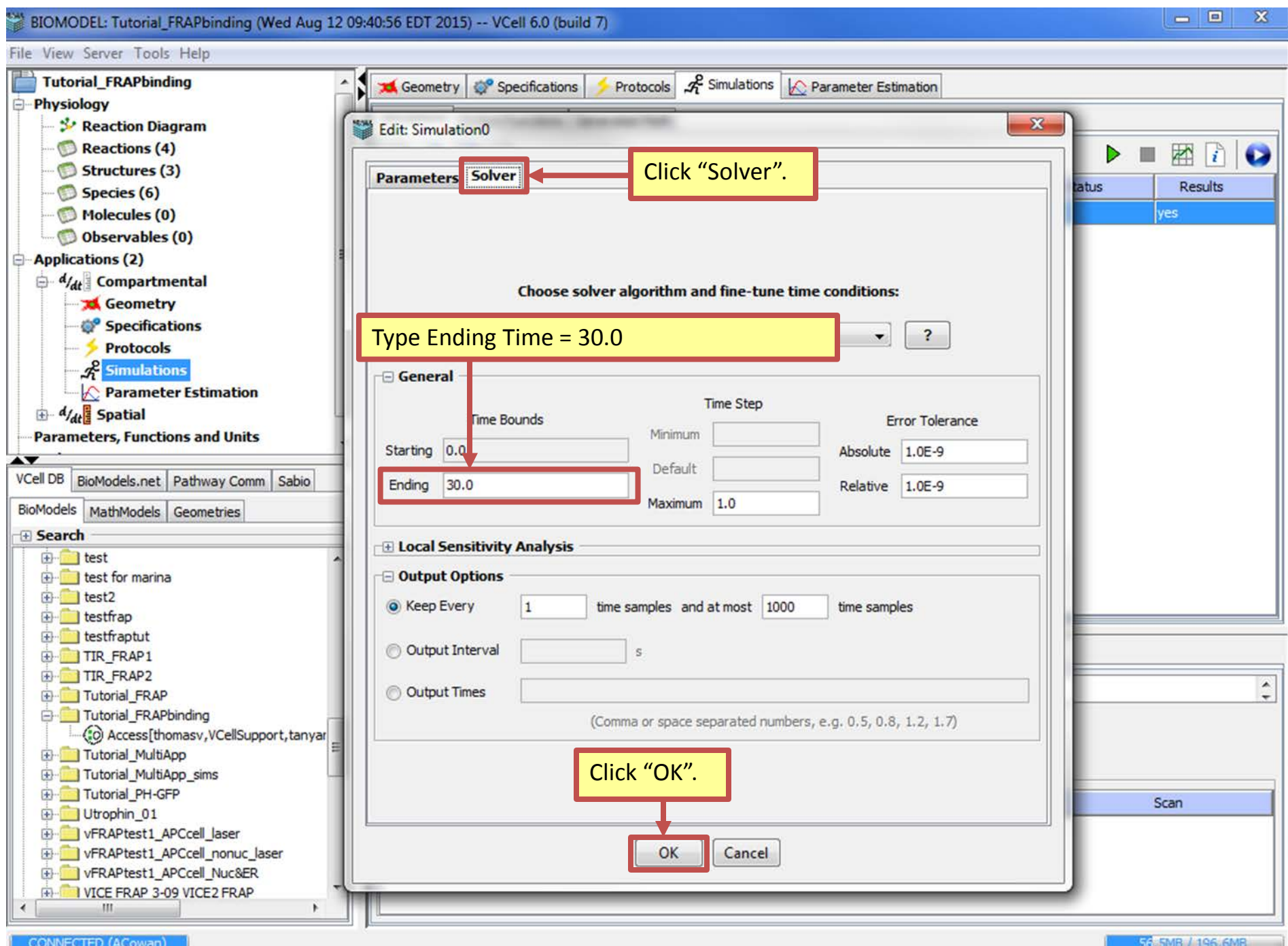
Object Properties Problems (0 Errors, 0 Warnings)

Annotation:

Settings:	max timestep	output	rel tol	abs tol	Sensitivity Analysis
	1.0s	keep every 1 sample, at most 1000	1.0E-9	1.0E-9	no

Parameters with values changed from defaults

Parameter Name	Default	New Value/Expression	Scan



File View Server Tools Help

**FRAPBindingTutorial**

- Physiology**
  - Reaction Diagram
  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (1)**
  - $d/dt$  Compartmental
  - Geometry
  - Specifications
  - Protocols
  - Simulations**
  - Parameter Estimation
- Parameters, Functions and Units**

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

+ Search

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  - Public BioModels (514)
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  - Tutorial VCell 6.0 (Rule-based) (7)

Geometry
 Specifications
 Protocols
 **Simulations**
 Parameter Estimation

Simulations
 Output Functions
 Generated Math

Name	End Time	Output Option	Solver	Running Status	Results
Simulation0	1.0	keep every 1 sample	Runge-Kutta-Fehlberg	not saved	no

Click the green play icon to run and save the simulation.

Object Properties Problems (0 Errors, 0 Warnings)

Annotation:

Settings:	max timestep	output	rel tol	abs tol	Sensitivity Analysis
	0.1s	keep every 1 sample, at most 1000	1.0E-9	1.0E-9	no

☐ Parameters with values changed from defaults

Parameter Name	Default	New Value/Expression	Scan

**FRAPBindingTutorial**

- Physiology
  - Reaction Diagram
  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (1)
  - Compartmental
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  - Simulations**
  - Parameter Estimation
- Parameters, Functions and Units

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

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  - Tutorial VCell 6.0 (Rule-based) (7)

Geometry
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 Protocols
 **Simulations**
 Parameter Estimation

Simulations
 Output Functions
 Generated Math

Name	End Time	Output Option	Solver	Running Status	Results
Simulation0	1.0	keep every 1 sample	Runge-Kutta-Fehlberg	completed	yes

Click the results icon when the simulation is completed.

Object Properties Problems (0 Errors, 0 Warnings)

Annotation:

Settings:	max timestep	output	rel tol	abs tol	Sensitivity Analysis
	0.1s	keep every 1 sample, at most 1000	1.0E-9	1.0E-9	no

Parameters with values changed from defaults

Parameter Name	Default	New Value/Expression	Scan



File View Server Tools Help

**Tutorial\_FRAPbinding**

- Physiology
  - Reaction Diagram
  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (2)
  - $d/dt$  Compartmental
    - Geometry
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    - Protocols
    - Simulations**
    - Parameter Estimation
  - $d/dt$  Spatial
- Parameters, Functions and...

VCell DB BioModels.net Pathway

BioModels MathModels Geometry

**Search**

- test
- test for marina
- test2
- testfrap
- testfraptut
- TIR\_FRAP1
- TIR\_FRAP2
- Tutorial\_FRAP
- Tutorial\_FRAPbinding
- Access[thomasv,
- Tutorial\_MultiApp
- Tutorial\_MultiApp\_sim
- Tutorial\_PH-GFP
- Utrophin\_01
- vFRAPtest1\_APCcell
- vFRAPtest1\_APCcell
- vFRAPtest1\_APCcell
- VICE FRAP 3-09 VICE

Results for Simulation Simulation0

X Axis:

t

Y Axis:

Display Options:

☐ Other  
☐ Reactions  
☒ Species

BS

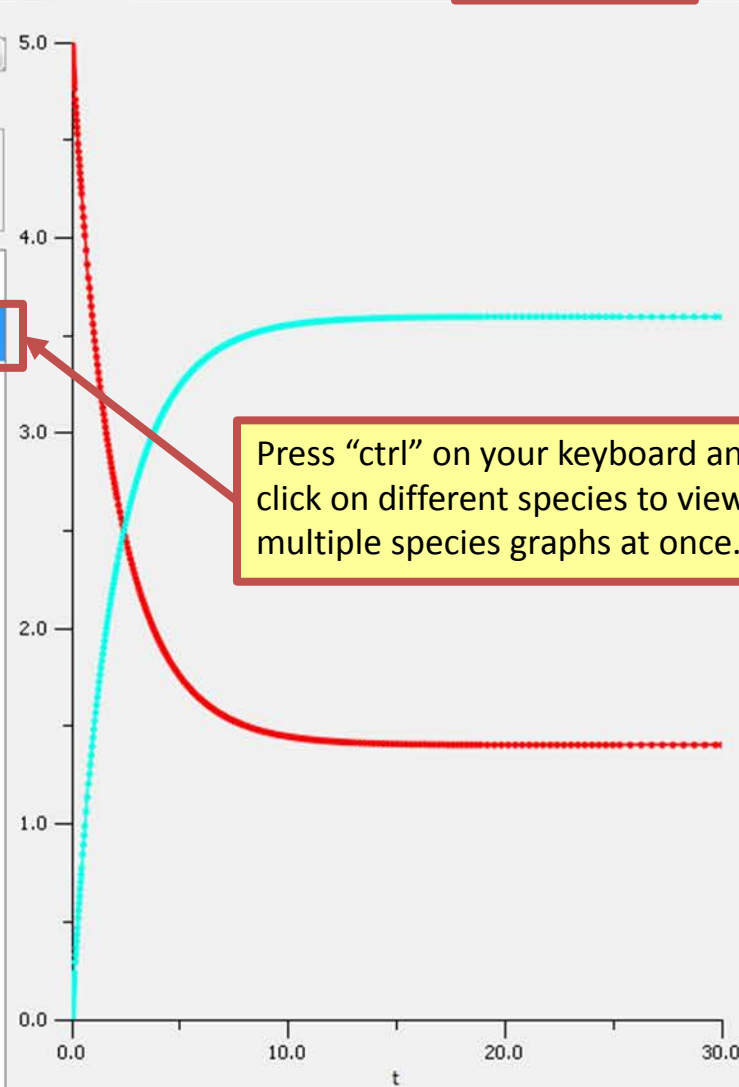
Laser

r

rB

r1

rFB



Click to exit.

⌵

Results

yes

Scan

CONNECTED (ACowan)

80.8M / 192.4MB



File View Server Tools Help

**FRAPBindingTutorial**

- Physiology
  - Reaction Diagram
  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (1)
  - Compartmental**
- Parameters, Functions and Units
- Pathway

Geometry Specifications Protocols Simulations Parameter Estimation

Simulations Output Functions Generated Math

Name	End Time	Output Option	Solver	Running Status	Results
Simulation0	1.0	keep every 1 sample	Runge-Kutta-Fehlberg	completed	yes

Right click "Compartmental". Click "Copy".

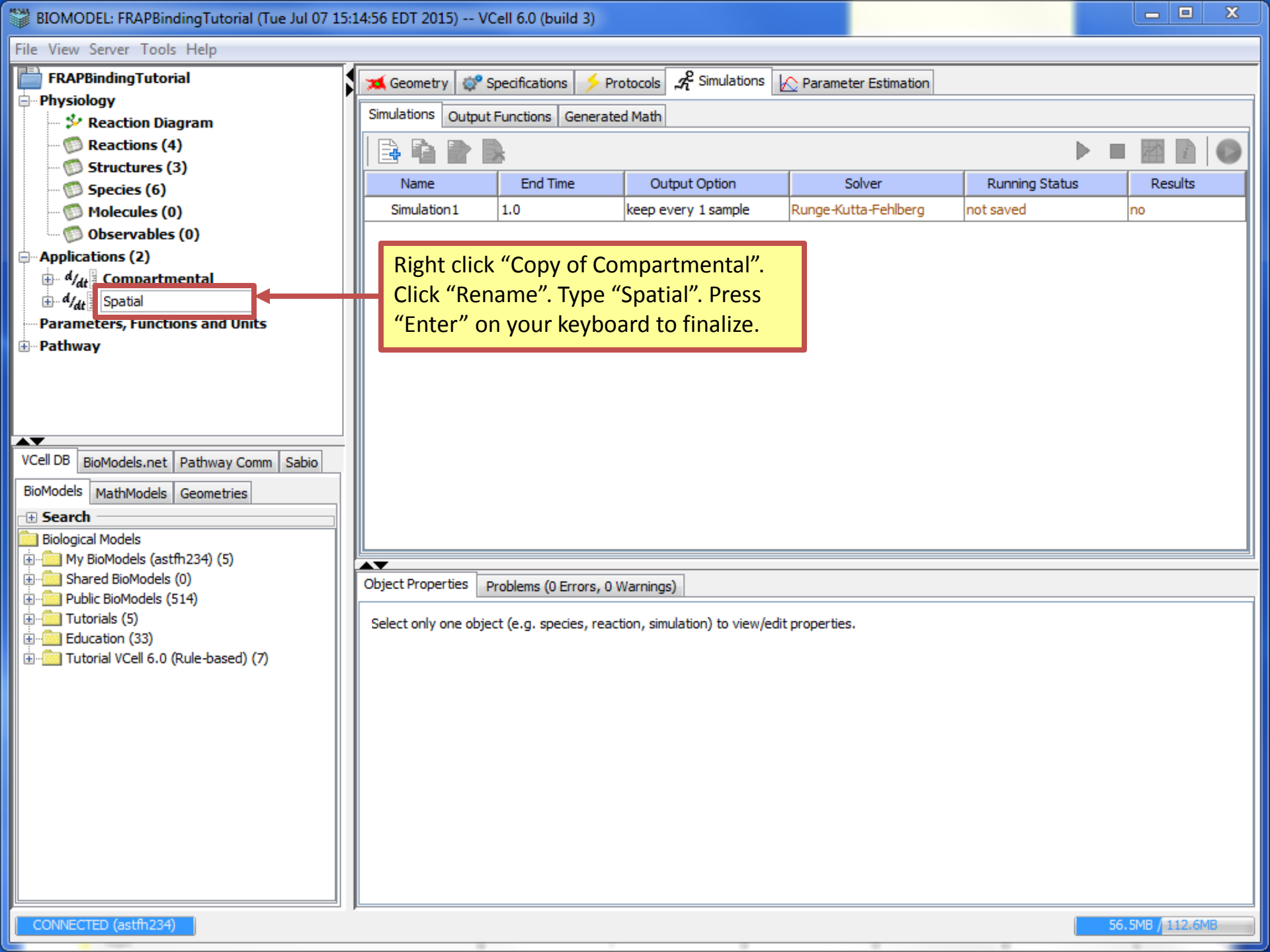
VCell DB BioModels.net Pathway Comm Sabio

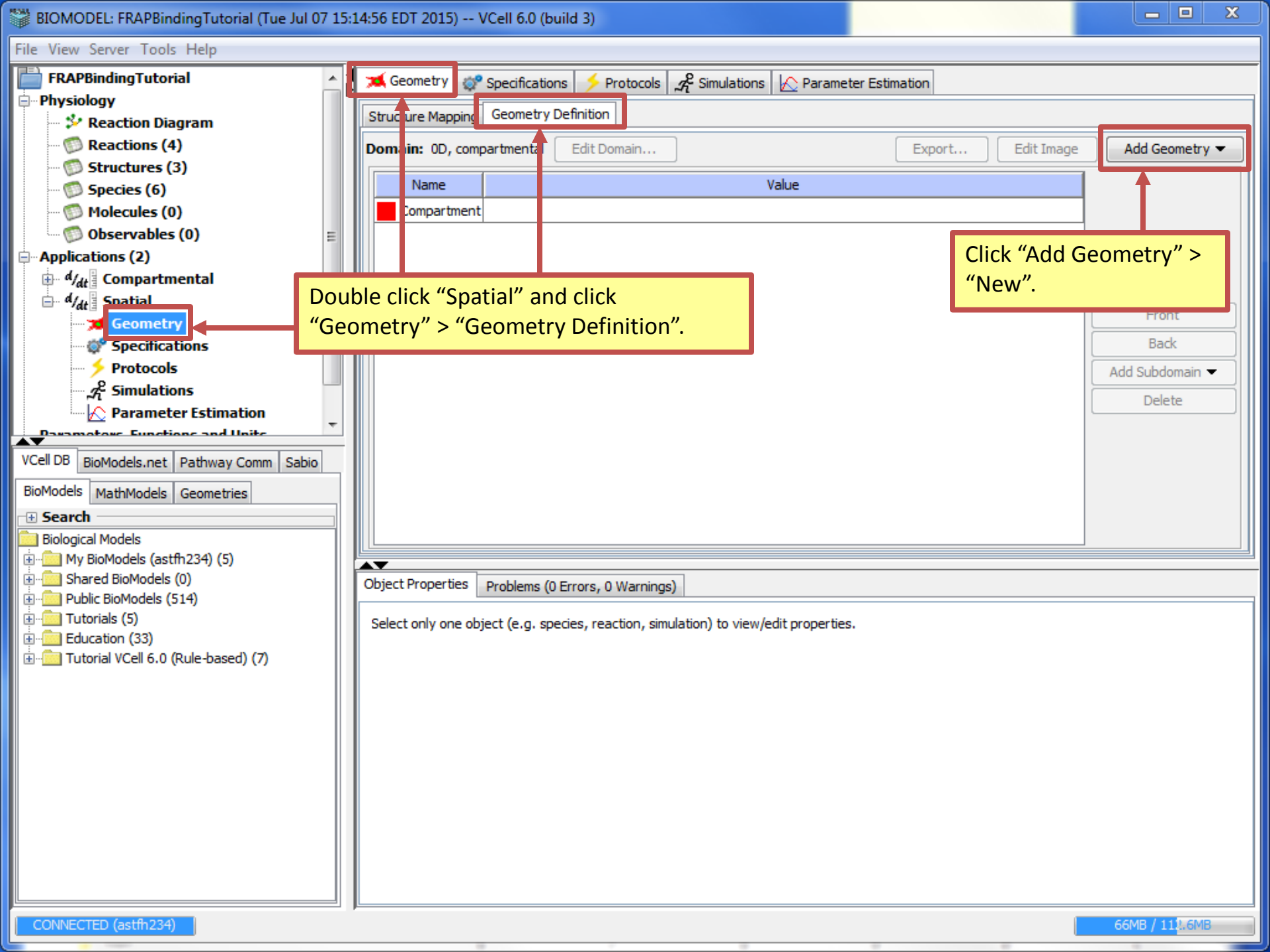
BioModels MathModels Geometries

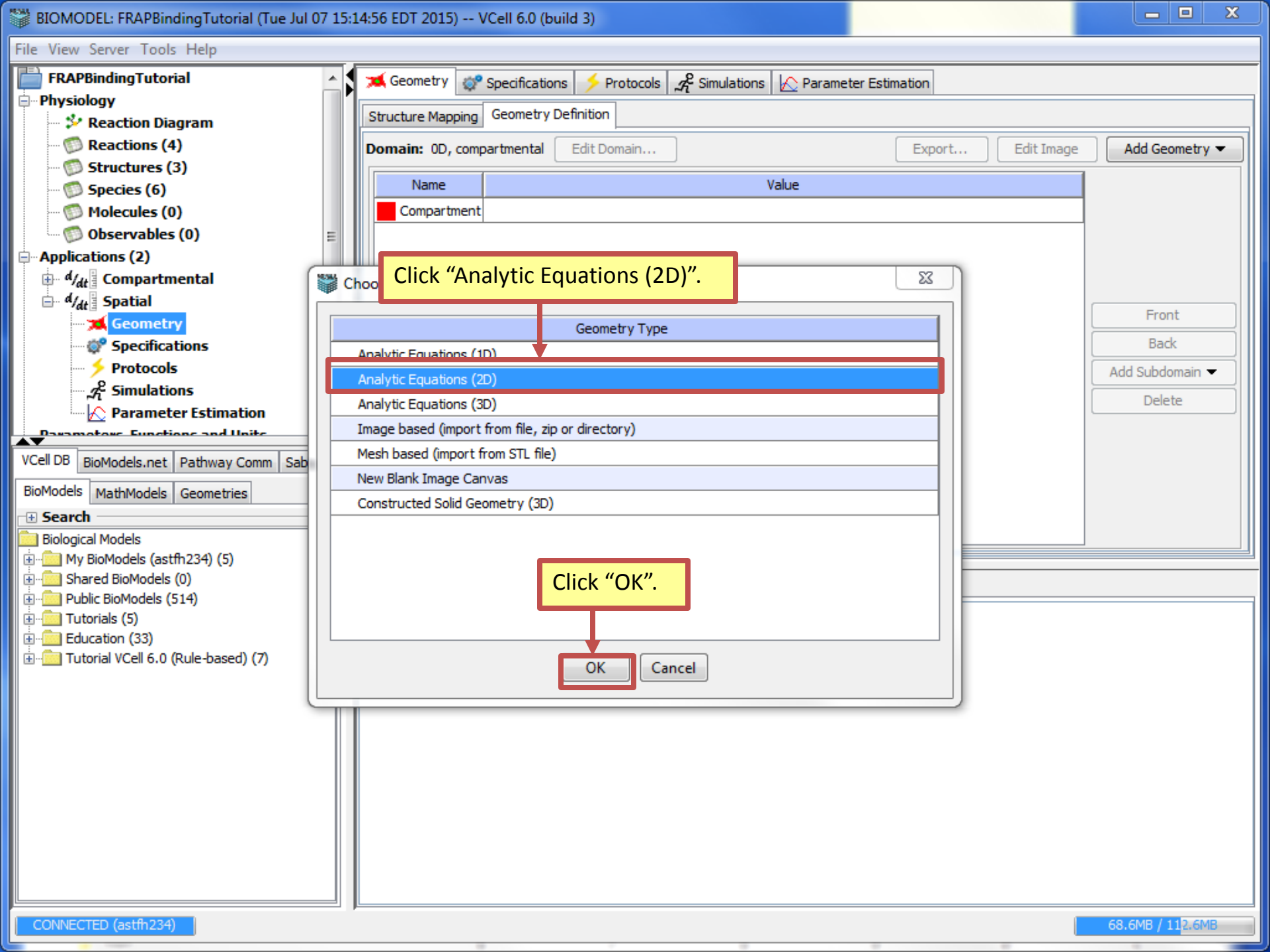
- Search**
- Biological Models
    - My BioModels (astfh234) (5)
    - Shared BioModels (0)
    - Public BioModels (514)
    - Tutorials (5)
    - Education (33)
    - Tutorial VCell 6.0 (Rule-based) (7)

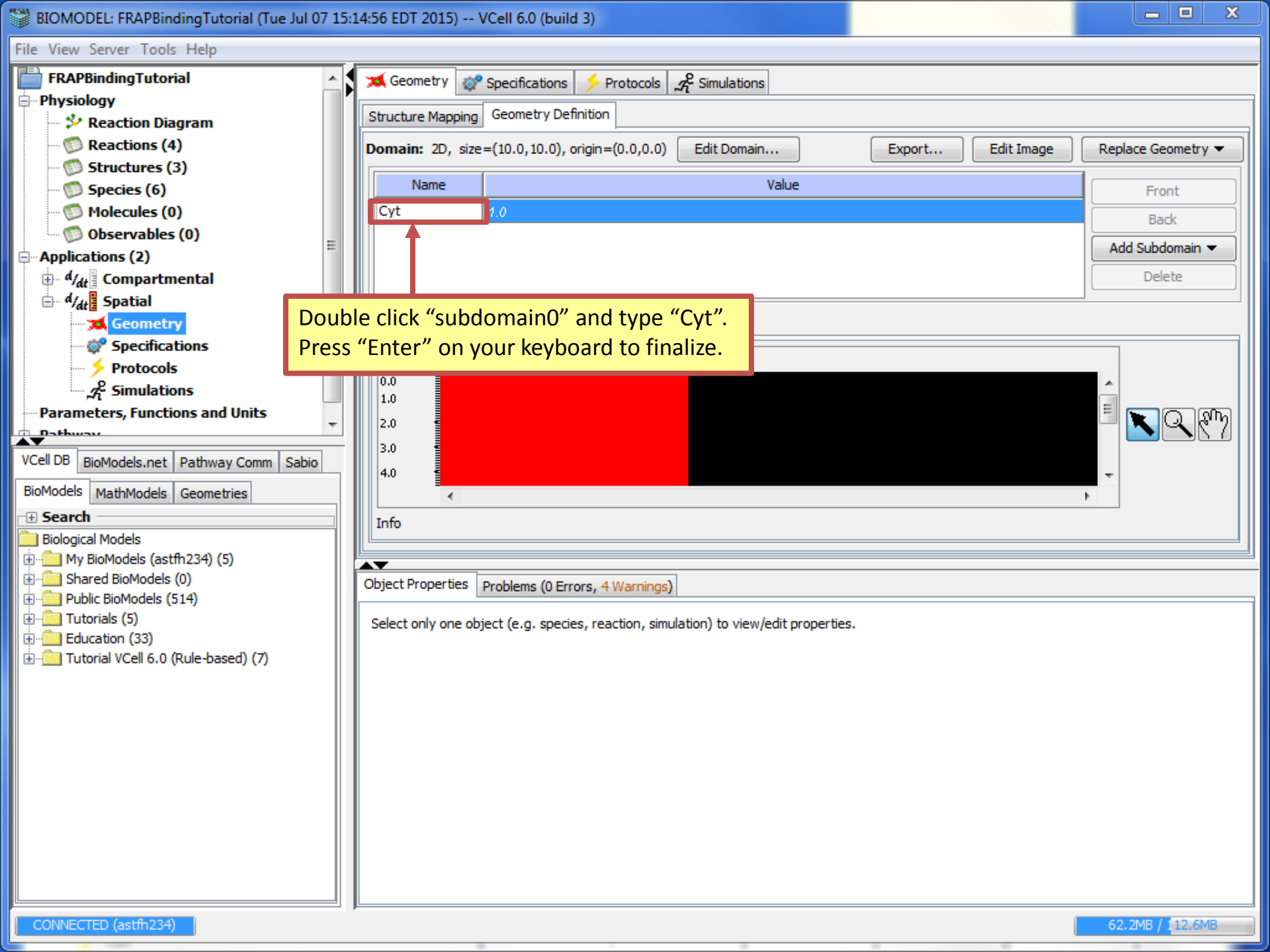
Object Properties Problems (0 Errors, 0 Warnings)

Select only one object (e.g. species, reaction, simulation) to view/edit properties.









File View Server Tools Help

**FRAPBindingTutorial**

- Physiology
  - Reaction Diagram
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VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

+ Search

- Biological Models
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  - Tutorial VCell 6.0 (Rule-based) (7)

Geometry Specifications Protocols Simulations

Structure Mapping Geometry Definition

Domain: 2D, size=(10.0,10.0), origin=(0.0,0.0)

Edit Domain...

Export...

Edit Image

Replace Geometry ▾

Name	Value
Cyt	1.0

Click "Add Subdomain" &gt; "Analytic".

Front

Back

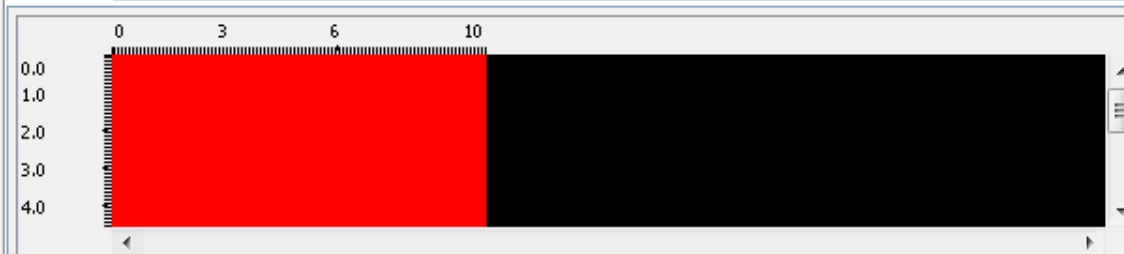
Add Subdomain ▾

Delete

Slice View

Surface View

Geometric Region Details



Info

Object Properties

Problems (0 Errors, 4 Warnings)

Select only one object (e.g. species, reaction, simulation) to view/edit properties.

File View Server Tools Help

**FRAPBindingTutorial**

**Physiology**

- Reaction Diagram
- Reactions (4)
- Structures (3)
- Species (6)
- Molecules (0)
- Observables (0)

**Applications (2)**

- Compartmental
- Spatial
- Geometry**
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**Parameters, Functions and Units**

VCell DB

BioModels MathModels Geometries

**Search**

- Biological Models
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- Tutorial

Geometry Specifications Protocols Simulations

Structure Mapping Geometry Definition

Domain: 2D, size=(10.0,10.0), origin=(0.0,0.0) Edit Domain... Export... Edit Image Replace Geometry ▾

Front Back Add Subdomain ▾ Delete

**Define New Subdomain Shape**

Select Subdomain Shape: Circle ▾

Center Point (x,y)  
0,0

Radius  
10

Analytic Expression  
 $x^2 + y^2 < 10.0^2$   
Copy Expression

Add New Subdomain Cancel

Click the drop down menu next to "Select Subdomain Shape:".  
Click "Circle".

Under "Radius" type "10".

Click "Add New Subdomain".

File View Server Tools Help

**FRAPBindingTutorial**

- Physiology
  - Reaction Diagram
  - Reactions (4)
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  - Observables (0)
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Geometry Specifications Protocols Simulations

Structure Mapping Geometry Definition

Domain: 2D, size=(10.0,10.0), origin=(0.0,0.0) Edit Domain... Export... Edit Image Replace Geometry ▾

Name	Value
Nuc	$\sqrt{(x)^2 + (y)^2} < (10.0)$
Cyt	1.0

Front Back Add Subdomain ▾ Delete

0.0 1.0 2.0 3.0 4.0

Info

Object Properties Problems (0 Errors, 6 Warnings)

Select only one object (e.g. species, reaction, simulation) to view/edit properties.

Double click "subdomain0" and type "Nuc". Press "Enter" on your keyboard to finalize.



File View Server Tools Help

**FRAPBindingTutorial**

- Physiology
  - Reaction Diagram
  - Reactions (4)
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  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (2)
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VCell DB BioModels.net Pathway Comm Sabio

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- Search**
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Geometry
Specifications
Protocols
Simulations

Structure Mapping Geometry Definition

Domain: 2D, size=(10.0,10.0), origin=(0.0,0.0)

Edit Domain...

Export...

Edit Image

Replace Geometry ▾

Name	Value
Nuc	$((x) + (y)) < (10.0)$
Cyt	1.0

Front

Back

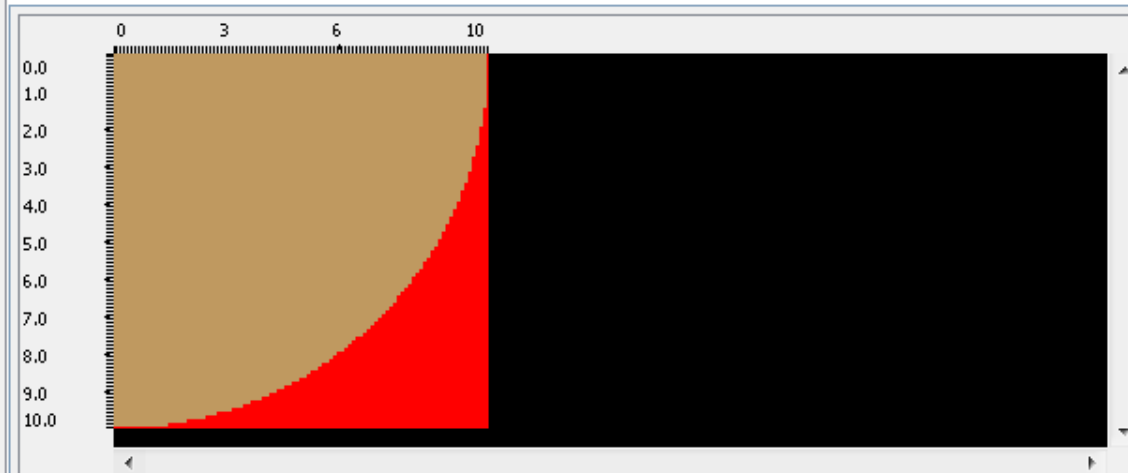
Add Subdomain ▾

Delete

Slice View

Surface View

Geometric Region Details



Info



Click the black down arrow icon to adjust the Slice View window.

Object Properties

Select only one object (e.g. species, reaction, simulation) to view/edit properties.

**FRAPBindingTutorial**

- Physiology
  - Reaction Diagram
  - Reactions (4)
  - Structures (3)
  - Species (6)
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  - Observables (0)
- Applications (2)
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VCell DB BioModels.net Pathway Comm Sabio

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Geometry Specifications Protocols Simulations

Structure Mapping Geometry Definition

Domain: 2D, size=(10.0,10.0), origin=(0.0,0.0)

Edit Domain...

Export...

Edit Image

Replace Geometry ▾

Name	Value
Nuc	$((x) + (y))$
Cyt	1.0

Click "Edit Domain".

Front

Back

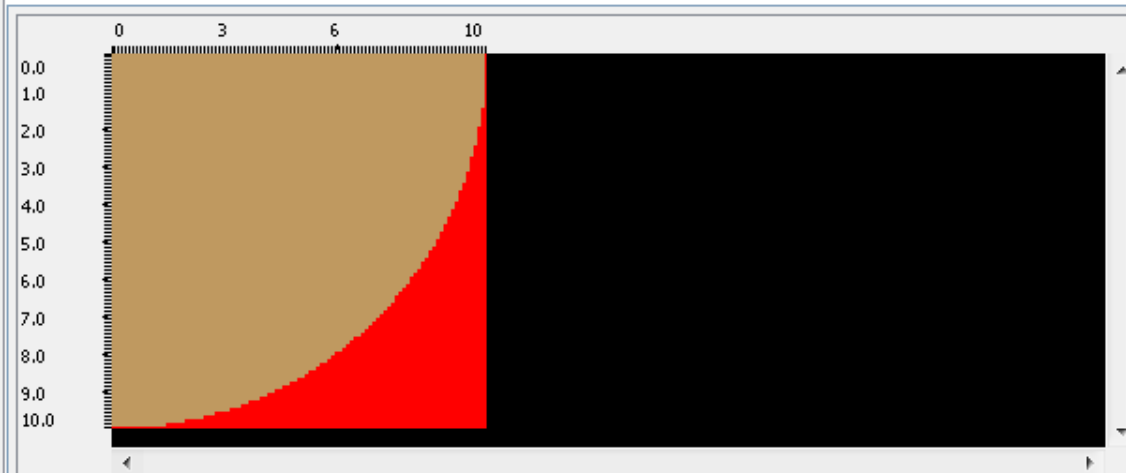
Add Subdomain ▾

Delete

Slice View

Surface View

Geometric Region Details

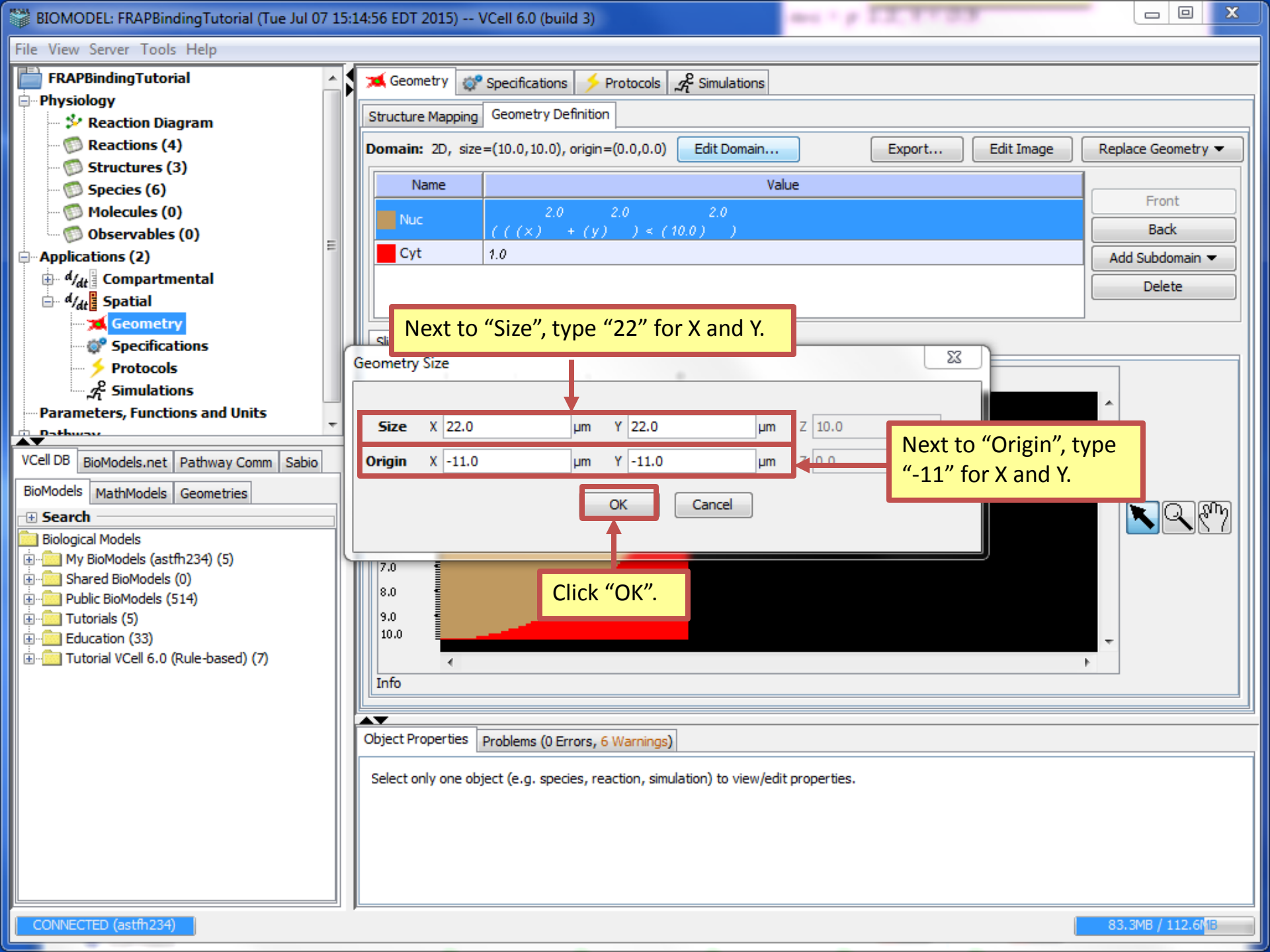


Info

Object Properties

Problems (0 Errors, 6 Warnings)

Select only one object (e.g. species, reaction, simulation) to view/edit properties.



Geometry

Specifications

Protocols

Simulations

Structure Mapping

Geometry Definition



**Domain:** 2D, size=(22.0,22.0), origin=(-11.0,-11.0)
 

Edit Domain...

Export...

Edit Image

Replace Geometry ▼

Name	Value
 Nuc	$\left( \left( \frac{x}{2.0} + \frac{y}{2.0} \right) < \left( \frac{10.0}{2.0} \right) \right)$
 Cyt	1.0

Front

Back

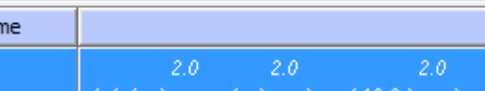
Add Subdomain ▼

Delete

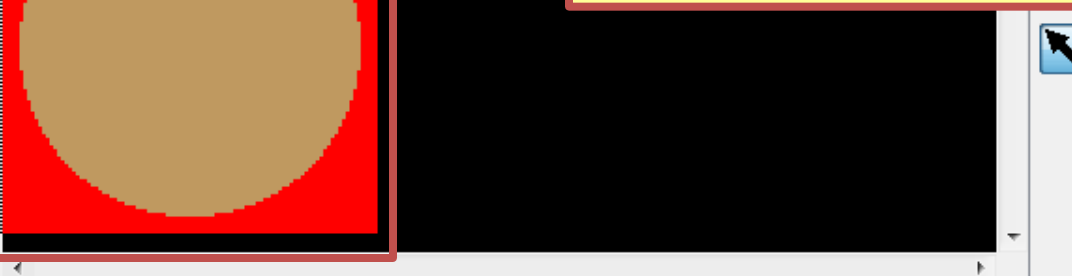
Slice View

Surface View

Geometric Region Details



Your "Slice View" should now be a



your Slice view should now be a circle inside of a square.

Info

Object Properties Problems (0 Errors, 6 Warnings)

Select only one object (e.g. species, reaction, simulation) to view/edit properties.

Go to Structure Mapping

Structure Mapping Geometry Definition

All structures and subdomains must be mapped to run a simulation.  
Use line tool or drop down menu in the 'subdomain' column.

**Physiology (structures)**

Cyt

Nuc

NM

**Geometry (subdomains)**

Nuc

Cyt

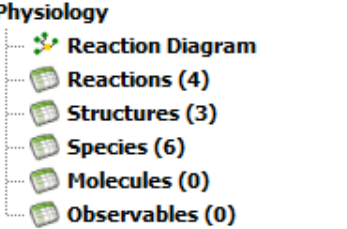
Cyt\_Nuc\_membrane

Tool to drag a line from the their corresponding

Structure	Subdomain	Size Ratio	X-	X+	Y-	Y+
Cyt	Cyt	1 [ 1 ]	Flux	Flux	Flux	Flux
Nuc	Nuc	1 [ 1 ]	Flux	Flux	Flux	Flux
NM	Cyt_Nuc_membrane	1 [ 1 ]	Flux	Flux	Flux	Flux

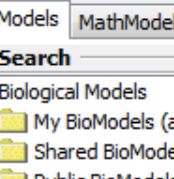
Object Properties Problems (0 Errors, 0 Warnings)

Select only one object (e.g. species, reaction, simulation) to view/edit properties.



The screenshot shows the COPASI Project Explorer. The 'Applications' folder is expanded, revealing a list of application types. Two red boxes are drawn around 'Compartmental' and 'Simulations'. Red arrows point from the right edge of the image towards these two items. The 'Simulations' item is highlighted with a blue background.

- FRAPBindingTutorial
  - Physiology
    - Reaction Diagram
    - Reactions (4)
    - Structures (3)
    - Species (6)
    - Molecules (0)
    - Observables (0)
  - Applications (2)
    - $d/dt$  Compartmental
    - Geometry
    - Specifications
    - Protocols
    - Simulations
    - Parameter Estimation
  - $d/dt$  Spatial



The screenshot shows the VCell DB application window. At the top, there are tabs for 'VCell DB', 'BioModels.net', 'Pathway Comm', and 'Sabio'. Below these, there are sub-tabs for 'BioModels', 'MathModels', and 'Geometries'. A 'Search' bar is located below the sub-tabs. The main content area displays a hierarchical tree of biological models under the 'Biological Models' category. The tree structure is as follows:

- Biological Models
  - My BioModels (astfh234) (5)
  - Shared BioModels (0)
  - Public BioModels (514)
  - Tutorials (5)
    - Education (33)
    - Tutorial VCell 6.0 (Rule-based) (7)

Double click "Compartmental" > " Simulations" > results icon.

Object Properties Problems (0 Errors, 0 Warnings)

Annotation:

Settings:

max timestep	output	rel tol	abs tol	Sensitivity Analysis
0.1s	keep every 1 sample, at most 1000	1.0E-9	1.0E-9	no

☐ Parameters with values changed from defaults

Parameter Name	Default	New Value/Expression	Scan
----------------	---------	----------------------	------

File View Server Tools

Tutorial\_FRAPbinding

Physiology

Reaction Diagram

Reactions (4)

Structures (3)

Species (6)

Applications (2)

Compartment

Geometry

Specifications

Protocols

Simulation

Parameters

Spatial

Parameters and Functions

VCell DB

BioModels.net

BioModels

MathModels

Search

Biological Models

My BioModels (tanyamiller)

Shared BioModels (0)

ACowan : Tutorial

Access[VCell]

ACowan : Tutorial

astfh234 : new

astfh234 : Run

Public BioModels (52)

Tutorials (5)

Education (33)

Results for Simulation Simulation0

X Axis:

t

Y Axis:

Display Options:

Reactions

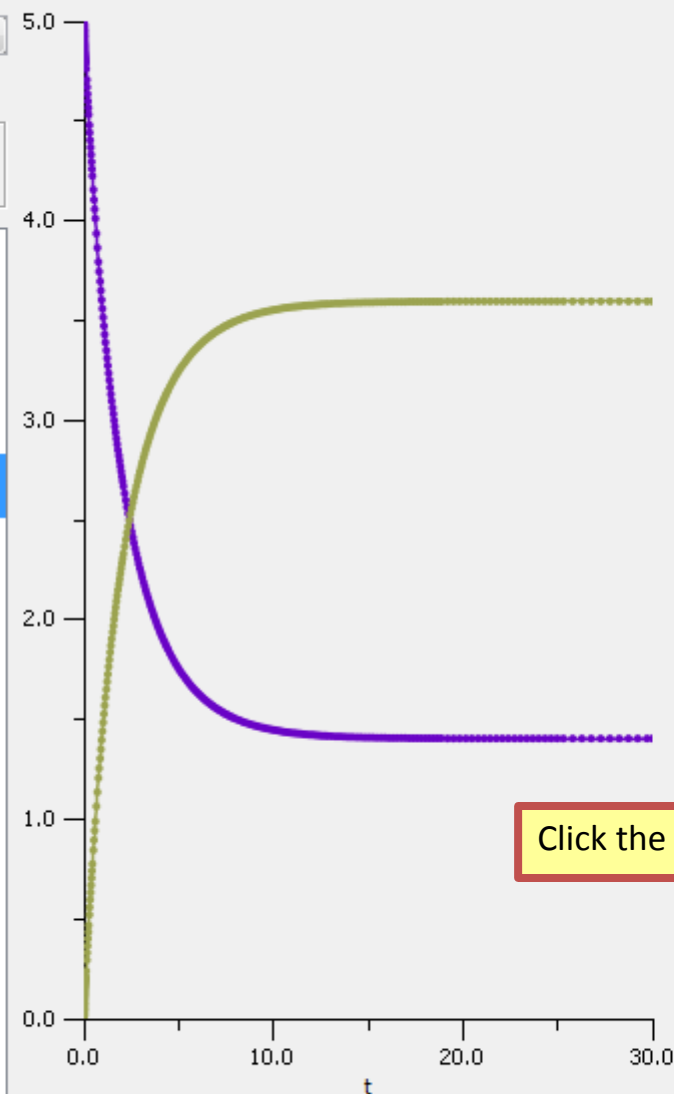
Species

t  
BS\_nucleus  
J\_bleaching1  
J\_bleaching2  
J\_RAN\_binding  
J\_RAN\_FITC\_binding  
Laser\_nucleus  
r\_nucleus  
rB\_nucleus  
rf\_nucleus  
rB\_nucleus

Plot Legend:

r\_nucleus

rB\_nucleus



Click the spreadsheet icon.



Finest Level Mesh:

View Level Mesh:

Scan



File View Server Tools

**Tutorial\_FRAPbinding**

- Physiology
  - Reaction Diagram
  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (2)
  - Compartment
  - Geometry
  - Specification
  - Protocols
  - Simulation
  - Parameter

Results for Simulation Simulation0

X Axis: t

Y Axis: ☐ Other ☐ Reactions ☒ Species

t	BS	rB	rf	rfB
0	20	0	5	0
4.7762591E-11	20	9.5525358E-11	5	9.5525182E-11
4.7767367E-7	19.999998	9.5534703E-7	4.999999	9.5534702E-7
5.2539328E-6	19.999979	1.0507841E-5	4.9999895	1.0507841E-5
2.3320245E-5	19.999907	4.6640077E-5	4.9999534	4.6640077E-5
6.4240719E-5	19.999743	1.2847847E-4	4.9998715	1.2847847E-4
1.4233739E-4	19.999431	2.8466048E-4	4.9997153	2.8466048E-4
2.8256877E-4	19.99887	5.6508148E-4	4.9994349	5.6508148E-4
5.2938242E-4	19.997883	1.0585685E-3	4.9989414	1.0585685E-3
9.6589107E-4	19.996138	1.9311290E-3	4.9980689	1.9311290E-3
1.8017288E-3	19.992798	3.6011863E-3	4.9963988	3.6011863E-3
3.4098637E-3	19.986377	6.8115980E-3	4.9931884	6.8115980E-3
5.0179986E-3	19.979963	1.0018401E-2	4.9899816	1.0018401E-2
6.6261336E-3	19.973557	0.0132216	4.9867784	0.0132216
8.2342685E-3	19.967158	1.6421201E-2	4.9835788	1.6421201E-2
9.8424034E-3	19.960766	0.01961721	4.9803828	0.01961721
1.1651391E-2	19.953584	2.3208105E-2	4.9767919	2.3208105E-2
1.3460379E-2	19.946411	2.6794467E-2	4.9732055	2.6794467E-2
1.5269368E-2	19.939247	3.0376305E-2	4.9696237	3.0376305E-2
0.01817295	19.927768	3.6116023E-2	4.963884	3.6116023E-2
2.1076532E-2	19.916312	4.1844135E-2	4.9581559	4.1844135E-2
2.3980115E-2	19.904879	4.7560672E-2	4.9524393	4.7560672E-2
2.6883697E-2	19.893469	5.3265666E-2	4.9467343	5.3265666E-2
3.1991248E-2	19.873454	6.3273121E-2	4.9367269	6.3273121E-2
3.7098798E-2	19.85351	7.3245119E-2	4.9267549	7.3245119E-2
4.2206348E-2	19.833636	8.3181825E-2	4.9168182	8.3181825E-2
5.1753439E-2	19.796677	0.10166156	4.8983384	0.10166156

Press "Ctrl" on your keyboard and select "BS", "rB", "rf" and "rfB".



File View Server Tools

Results for Simulation Simulation0

Tutorial\_FRAPbinding

Physiology

Reaction Diagram

Reactions (4)

Structures (3)

Species (6)

Molecules (0)

Observables (0)

Applications (2)

d/dt Compartment

Geometry

Specification

Protocols

Simulations

Parameter

d/dt Spatial

Cell DB BioModels.net

BioModels MathModels

Search

- test
- test for marina
- test2
- testfrap
- testfraptut
- TIR\_FRAP1
- TIR\_FRAP2
- Tutorial\_FRAP
- Tutorial\_FRAPbinding
- Access[thom]
- Tutorial\_MultiApp
- Tutorial\_MultiApp
- Tutorial\_PH-GFP
- Utrophin\_01
- vFRAPtest1\_APC

X Axis:

t

Y Axis:

Display Options:

- ☐ Other
- ☐ Reactions
- ☒ Species

BS

Laser

r

rB

rf

rfB

t	BS	rB	rf	rfB
20.147306	12.80908	3.59546	1.40454	3.59546
20.469109	12.808917	3.5955417	1.4044583	3.5955417
20.790912	12.808773	3.5956133	1.4043867	3.5956133
21.112716	12.808648	3.595676	1.404324	3.595676
21.434519	12.808538	3.595731	1.404269	3.595731
21.756322	12.808442	3.595779	1.404221	3.595779
22.078125	12.808358	3.5958212	1.4041788	3.5958212
22.399928	12.808284	3.595858	1.404142	3.595858
22.721731	12.808219	3.5958903	1.4041097	3.5958903
23.043534	12.808163	3.5959186	1.4040814	3.5959186
23.365337	12.808113	3.5959434	1.4040566	3.5959434
23.68714	12.80807	3.5959651	1.4040349	3.5959651
24.008943	12.808032	3.5959841	1.4040159	3.5959841
24.330746	12.807999	3.5960007	1.4039993	3.5960007
24.652549	12.807969	3.5960153	1.4039847	3.5960153
24.974352	12.807944	3.596028	1.403972	3.596028
25.296156	12.807922	3.5960392	1.4039608	3.5960392
25.787234				
26.278313				
26.769391				
27.26047				
27.751549	12.807821	3.5960894	1.4039106	3.5960894
28.242627	12.807811	3.5960946	1.4039054	3.5960946
28.733706	12.807802	3.5960989	1.4039011	3.5960989
29.224785	12.807795	3.5961024	1.4038976	3.5961024
29.715863	12.80779	3.5961052	1.4038948	3.5961052
30	12.807787	3.5961066	1.4038934	3.5961066

Press "Ctrl" on your keyboard and click the final concentrations for "BS", "rB", "rf" and "rfB". Right click and click "Copy".

Species (0)  
Molecules (0)  
Observables (0)  
Applications (2)  
Compartmental  
Geometry  
Specifications  
Protocols  
Simulations  
Parameter Estimation  
Spatial  
Geometry  
Specifications  
Protocols  
Simulations  
Parameters, Functions and Units  
Pathway

Species	Reaction	Network				
Species	Structure	Clamped	Initial Condition	Well Mixed	Diffusion Constant	
laser	Nuc	<input type="checkbox"/>	0.0	<input type="checkbox"/>	10.0	
rB	Nuc	<input type="checkbox"/>	0.0	<input type="checkbox"/>	10.0	
rfB	Nuc	<input type="checkbox"/>	0.0	<input type="checkbox"/>	10.0	
r	Nuc	<input type="checkbox"/>	5.0	<input type="checkbox"/>	10.0	
		<input type="checkbox"/>	5.0	<input type="checkbox"/>	10.0	
		<input type="checkbox"/>	20.0	<input type="checkbox"/>	10.0	

Click "Spatial" > "Specifications" > "Species".

Click on the cell in the "r" row and Initial Condition column. Right click "Paste All".

Search

Biological Models

- My BioModels (astfh234) (5)
- Shared BioModels (0)
- Public BioModels (514)
- Tutorials (5)
- Education (33)
- Tutorial VCell 6.0 (Rule-based) (7)

Description	Parameter	Expression	Units
initial concentration for r for r	initConc	5.0	$\mu\text{M}$
diffusion constant for r for r	diff	10.0	$\mu\text{m}^2.\text{s}^{-1}$
Boundary Condition X- for r for r	BC_Xm	<zero flux>	$\mu\text{M}.\mu\text{m}.\text{s}^{-1}$
Boundary Condition X+ for r for r	BC_Xp	<zero flux>	$\mu\text{M}.\mu\text{m}.\text{s}^{-1}$
Boundary Condition Y- for r for r	BC_Ym	<zero flux>	$\mu\text{M}.\mu\text{m}.\text{s}^{-1}$

File View Server Tools Help

Applications (2)

Compartmental

Geometry

Specifications

Protocols

Simulations

Space

Species

Reactions

Species

Structure

Clamped

Initial Condition

Well Mixed

Diffusion Constant

Parameter

Pathway

VCell DB

BioModels

Search

Biological Mo

My BioM

Shared B

ACo

ACo

astl

astl

Public Bio

Tutorials

Education

Velocity Y for r\_nucleus

Vel\_Y

<0.0>

CONNECTED (tanyamiller1221)

50.1MB / 130.5MB

Units

$\mu\text{M}$

$\mu\text{m}^2.\text{s}^{-1}$

$\mu\text{M}$

$\mu\text{M}$

$\mu\text{M}$

$\mu\text{M}$

$\mu\text{m}.\text{s}^{-1}$

$\mu\text{m}.\text{s}^{-1}$

OK

Cancel

Select All

rf\_nucleus

initConc

'5.0' -> '1.40389335666'

rB\_nucleus

initConc

'0.0' -> '3.59610664333'

BS\_nucleus

initConc

'20.0' -> '12.8077867133'

rfB\_nucleus

initConc

'0.0' -> '3.59610664333'

Click "Select All" and then click "OK".

BIOMODEL: Tutorial\_FRAPbinding (Thu Jul 23 16:23:09 EDT 2015) -- VCell 5.3 (build 9)

FileViewServerToolsHelp

Applications (2)

Compartmental

Geometry

Specifications

Protocols

Simulations

Parameter Estimation

Spatial

Geometry

Specifications

Protocols

Simulations

Parameters and Functions

Pathway

VCell DBBioModels.netPath...

BioModelsMathModelsGeometries

Search

Biological Models

My BioModels (tanyamiller1221) (7)

Shared BioModels (4)

ACowan : Tutorial\_FRAPbind

Access[VCellSupport,thom

ACowan : Tutorial\_MultiApp\_

astfh234 : new stuff

astfh234 : Rule Based

Public BioModels (521)

Tutorials (5)

Education (33)

GeometrySpecificationsProtocolsSimulations

SpeciesReactions

Species	Structure	Clamped	Initial Condition	Well Mixed	Diffusion Constant
r_nucleus	nucleus	<input type="checkbox"/>	5.0	<input type="checkbox"/>	10.0
rf_nucleus	nucleus	<input type="checkbox"/>	1.4038933566697134	<input type="checkbox"/>	10.0
rB_nucleus	nucleus	<input type="checkbox"/>	3.5961066433302924	<input type="checkbox"/>	0.0
BS_nucleus	nucleus	<input type="checkbox"/>	12.807786713339414	<input type="checkbox"/>	0.0
rfB_nucleus	nucleus	<input type="checkbox"/>	3.596106643330292	<input type="checkbox"/>	0.0
Laser_nud...	nucleus	<input type="checkbox"/>	x > - 2.0 && (x < 2.0) && (y > - 2.0) && (y < 2.0))	<input type="checkbox"/>	0.0

In the "Laser" row and "Initial Condition" column, type  
"((x>-2.0)&&(x<2.0)&&(y>-2.0)&&(y<2.0))". Press "Enter"  
on your keyboard to finalize.

Search

Object PropertiesProblems (0 Errors, 0 Warnings)Database File Info

Description	Parameter	Expression	Units
initial concentration for Laser_nucleus	initConc	(( x > - 2.0 ) && ( x < 2.0 ) && ( y > - 2.0 ) && ( y < 2.0 ) )	μM
diffusion constant for Laser_nucleus	diff	0.0	μm <sup>2</sup> .s <sup>-1</sup>

CONNECTED (tanyamiller1221)78.4MB / 130.5MB

File View Server Tools Help

Species (0)  
Molecules (0)  
Obs

Application

- Compartmental
  - Geometry
  - Specifications
  - Protocols
  - Simulations
  - Parameter Estimation
- Spatial
  - Geometry
  - Specifications
  - Protocols
  - Simulations
- Parameters, Functions and Units
- Pathway

Click "Reactions".

Geometry Specifications Protocols Simulations

Species Reaction Network

Name	Type	Enabled	Fast
RAN binding	Reaction	<input checked="" type="checkbox"/>	<input type="checkbox"/>
RAN_FITC binding	Reaction	<input checked="" type="checkbox"/>	<input type="checkbox"/>
bleaching 1	Reaction	<input checked="" type="checkbox"/>	<input type="checkbox"/>
bleaching 2	Reaction	<input checked="" type="checkbox"/>	<input type="checkbox"/>

Click on all boxes in the Enabled column so that they are checked off if they are not already.

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

+ Search

- Biological Models
  - My BioModels (astfh234) (5)
  - Shared BioModels (0)
  - Public BioModels (514)
  - Tutorials (5)
  - Education (33)
  - Tutorial VCell 6.0 (Rule-based) (7)

Search

Object Properties Problems (0 Errors, 0 Warnings)

Select only one object (e.g. species, reaction, simulation) to view/edit properties.



File View Server Tools Help

Species (0)  
Molecules (0)  
Observables (0)  
Applications (2)  
  Compartmental  
    Geometry  
    Specifications  
    Protocols  
    Simulations  
    Parameter Estimation  
  Spatial  
    Geometry  
    Specifications  
    Protocols  
    Simulations  
Parameters, Functions and Units  
Pathway

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

+ Search  
Biological Models  
  My BioModels (astfh234) (5)  
  Shared BioModels (0)  
  Public BioModels (514)  
  Tutorials (5)  
  Education (33)  
  Tutorial VCell 6.0 (Rule-based) (7)

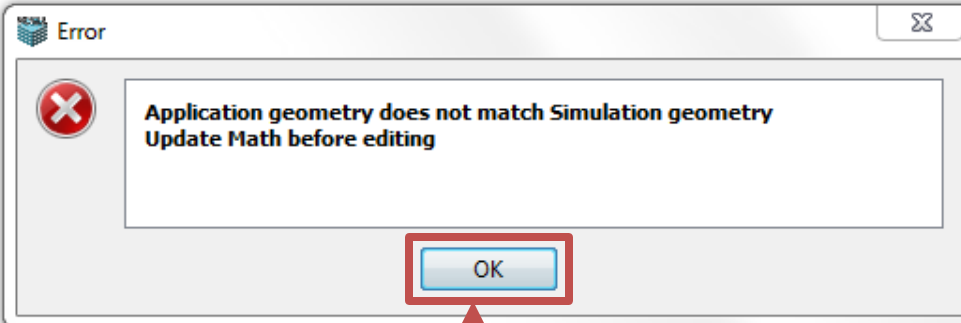
Geometry Specifications Protocols Simulations

Simulations Output Functions Generated Math



Click "Simulations" > edit simulation icon.

Name	End Time	Output Option	Solver	Running Status	Results
Simulation	1.0	keep every 1 sample	Runge-Kutta-Fehlberg	not saved	no



If an error message appears, click "OK".

Object Properties Problems (0 Errors, 0 Warnings)

Annotation:

Settings:	max timestep	output	rel tol	abs tol	Sensitivity Analysis
	0.1s	keep every 1 sample, at most 1000	1.0E-9	1.0E-9	no

Parameters with values changed from defaults

Parameter Name	Default	New Value/Expression	Scan
----------------	---------	----------------------	------

File View Server Tools Help

Species (0)  
Molecules (0)  
Observables (0)  
Applications (2)  
Compartmental  
Geometry  
Specifications  
Protocols  
Simulations  
Parameter Estimation  
Spatial  
Geometry  
Specifications  
Parameters  
Pathway

Geometry Specifications Protocols Simulations

Simulations Output Functions **Generated Math**

Choose View: ☒ Math Equations ☐ Math Description Language **Refresh Math** Create Math Model

math description  
+ constants  
+ functions  
+ volume domains  
+ membrane domains

**Issues encountered during Math Generation:**  
Units warning : expected=[uM], observed=[1] for exp = ((x > - 5.0) && (x < 5.0) && (y > - 5.0) && (y < 5.0))

**OK**

Click "OK".

Object Properties Problems (0 Errors, 0 Warnings)

Select only one object (e.g. species, reaction, simulation) to view/edit properties.

CONNECTED (astfh234) 63.9MB / 122.1MB

File View Server Tools Help

Species (0)  
Molecules (0)  
Observables (0)  
Applications (2)  
Compartmental  
Geometry  
Specifications  
Protocols  
Simulations  
Parameter Estimation  
Spatial  
Geometry  
Specifications  
Protocols  
Simulations  
Parameters, Functions and Units  
Pathway

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

+ Search  
Biological Models  
My BioModels (astfh234) (5)  
Shared BioModels (0)  
Public BioModels (514)  
Tutorials (5)  
Education (33)  
Tutorial VCell 6.0 (Rule-based) (7)

Geometry Specifications Protocols Simulations

Simulations Output Functions Generated Math



Name	End Time	Output Option	Solver	Running Status	Results
Simulation1	1.0	every 0.05 sec	Fully-Implicit	not saved	no

Go back to simulations, select Simulation1 and click the edit simulation icon.

Object Properties Problems (0 Errors, 0 Warnings)

Annotation:

Settings:

max timestep	output	rel tol	abs tol
0.1s	every 0.05 sec	1.0E-7	1.0E-9

Mesh: 101x101 = 10201 elements

Geometry size: (22.0,22.0) microns

Parameters with values changed from defaults



File View Server Tools Help

Species (0)  
Molecules (0)  
Observables (0)  
Applications (2)  
Compartmental  
Geometry  
Specifications  
Protocols  
Simulations  
Parameter Estimation  
Spatial  
Geometry  
Specifications  
Protocols  
Simulations  
Parameters, Functions and Units  
Pathway

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

Search

Biological Models  
My BioModels (astfh234) (5)  
Shared BioModels (0)  
Public BioModels (514)  
Tutorials (5)  
Education (33)  
Tutorial VCell 6.0 (Rule-based) (7)

Edit: Simulation1

Parameters Mesh Solver

Click "Mesh".

Mesh Size

Geometry Size (um) (22.0, 22.0)

Mesh Size (elements) ☒ Lock aspect ratio

X

51

Y

51

Click "Lock aspect ratio" if it is not checked off already. Type in "51" next to Mesh Size for X.

Total Size (elements) 51 x 51 = 2601

Spatial Step (um) Δx

0.44

Δy

0.44

OK

Cancel

Mesh: 101x101 = 10201 elements

Geometry size: (22.0,22.0) microns

Parameters with values changed from defaults

CONNECTED (astfh234)

65.4MB / 122.1MB

Edit: Simulation1

Parameters Mesh **Solver**

Click "Solver".

Choose solver algorithm and fine-tune time conditions:

Integrator Fully-Implicit Finite Volume, Regular Grid (Variable Time Step)

General

Time Bounds Time Step Error Tolerance  
Starting 0.0 Minimum Default Maximum 0.1  
Ending 50.0

Type "50.0" next to Ending, under Time Bounds.

Local Sensitivity Analysis

Output Options

Keep Every time samples and at most time samples  
Output Interval 0.5 secs

Type "0.5" next to Output Interval.

Miscellaneous

OK

Cancel

Click "OK".

Mesh: 101x101 = 10201 elements

Geometry size: (22.0,22.0) microns

Parameters with values changed from defaults

File View Server Tools Help

Species (0)  
Molecules (0)  
Observables (0)  
Applications (2)  
  Compartmental  
    Geometry  
    Specifications  
    Protocols  
    Simulations  
    Parameter Estimation  
  Spatial  
    Geometry  
    Specifications  
    Protocols  
    Simulations  
Parameters, Functions and Units  
Pathway

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

+ Search  
Biological Models  
  My BioModels (astfh234) (5)  
  Shared BioModels (0)  
  Public BioModels (514)  
  Tutorials (5)  
  Education (33)  
  Tutorial VCell 6.0 (Rule-based) (7)

Geometry Specifications Protocols Simulations

Simulations Output Functions Generated Math

Name	End Time	Output Option	Solver	Running Status	Results
Simulation 1	50.0	every 0.5 sec	Fully-Implicit	not saved	no

Click the green play icon to run and save the simulation.

Object Properties Problems (0 Errors, 0 Warnings)

Annotation:

Settings:

max timestep	output	rel tol	abs tol
0.1s	every 0.5 sec	1.0E-7	1.0E-9

Mesh: 51x51 = 2601 elements

Geometry size: (22.0,22.0) microns

Parameters with values changed from defaults

File View Server Tools Help

### FRAPBindingTutorial

- Physiology
  - Reaction Diagram
  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (2)
  - Compartmental
  - Spatial
  - Geometry
  - Specifications
  - Protocols
  - Simulations
- Parameters, Functions and Units
- Pathway

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

#### Search

- Biological Models
  - My BioModels (astfh234) (5)
  - Shared BioModels (0)
  - Public BioModels (514)
  - Tutorials (5)
  - Education (33)
  - Tutorial VCell 6.0 (Rule-based) (7)

Geometry Specifications Protocols Simulations

Simulations Output Functions Generated Math

Name	End Time	Output Option	Solver	Running Status	Results
Simulation 1	50.0	every 0.5 sec	Fully-Implicit	completed	yes

Click the results icon when the simulation is completed.

Object Properties Problems (0 Errors, 0 Warnings)

Annotation:

Settings:

max timestep	output	rel tol	abs tol
0.1s	every 0.5 sec	1.0E-7	1.0E-9

Mesh: 51x51 = 2601 elements

Geometry size: (22.0,22.0) microns

Parameters with values changed from defaults

CONNECTED (astfh234)

90.8MB / 122.1MB

simulation results for FRAP binding

View Data Export Data Post Processing

Time

39.5

0

50

Slice View

-11.0

-9.24

-7.48

-5.72

-3.96

-2.2

-0.44

1.32

3.08

4.84

6.6

8.36

11.0

All Variables

BS  
J\_bleaching1  
J\_bleaching2  
J\_RAN\_binding  
J\_RAN\_FITC\_binding  
Laser  
Laser\_init\_uM  
r  
rB  
rf  
rfB

To change the time frame being viewed, type in a value under "Time" or hold down and drag the slider under "Time".

Click here to view different species concentrations

Data Range (Min-Max)

☒ Auto (current time)

Max: 1.2892572668295028

1.2892572668295028

Min: 1.284306269805525

1.284306269805525

Color

BM

AM

NN

ND

NR

☐ Gray

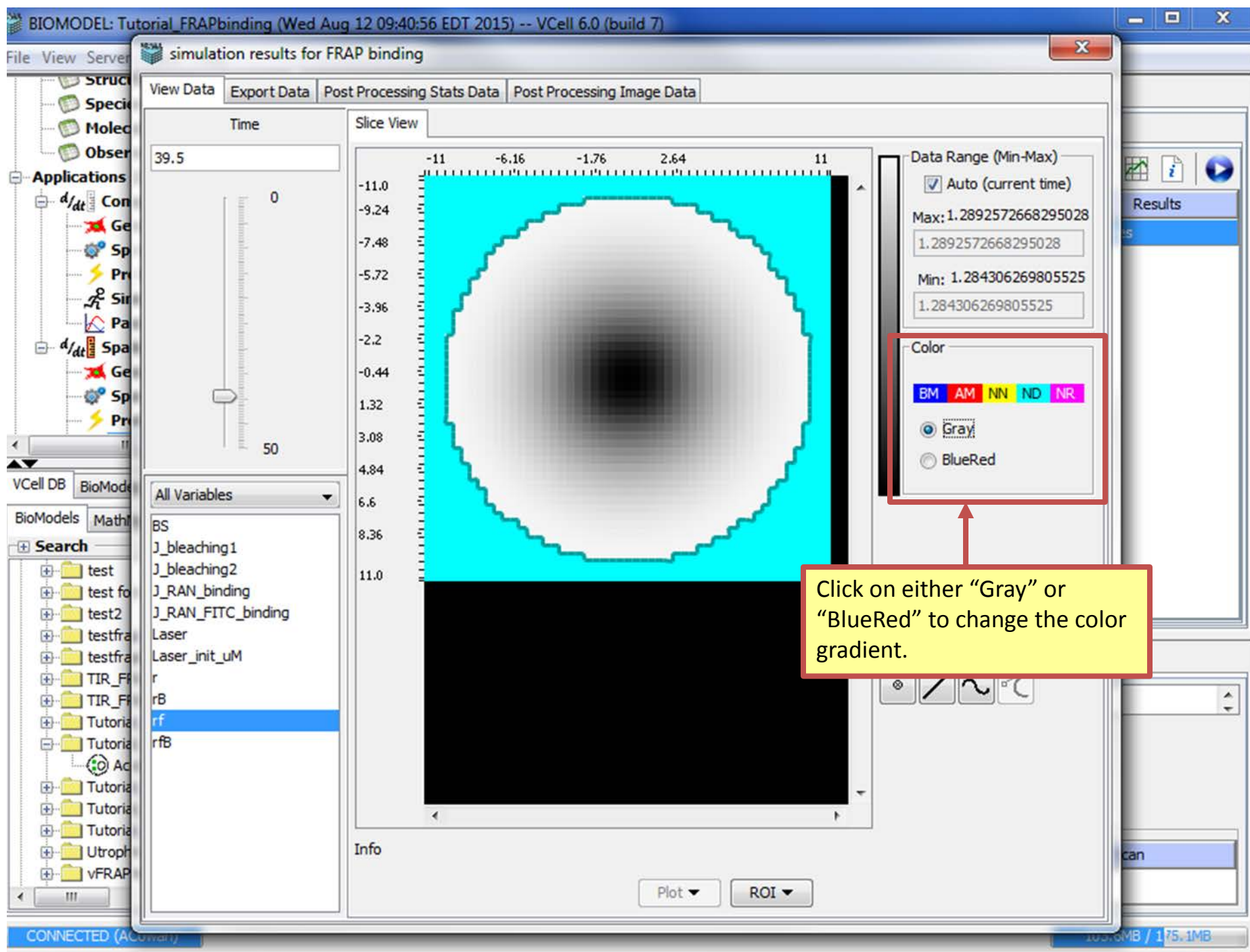
The minimum and maximum values correspond to the colors

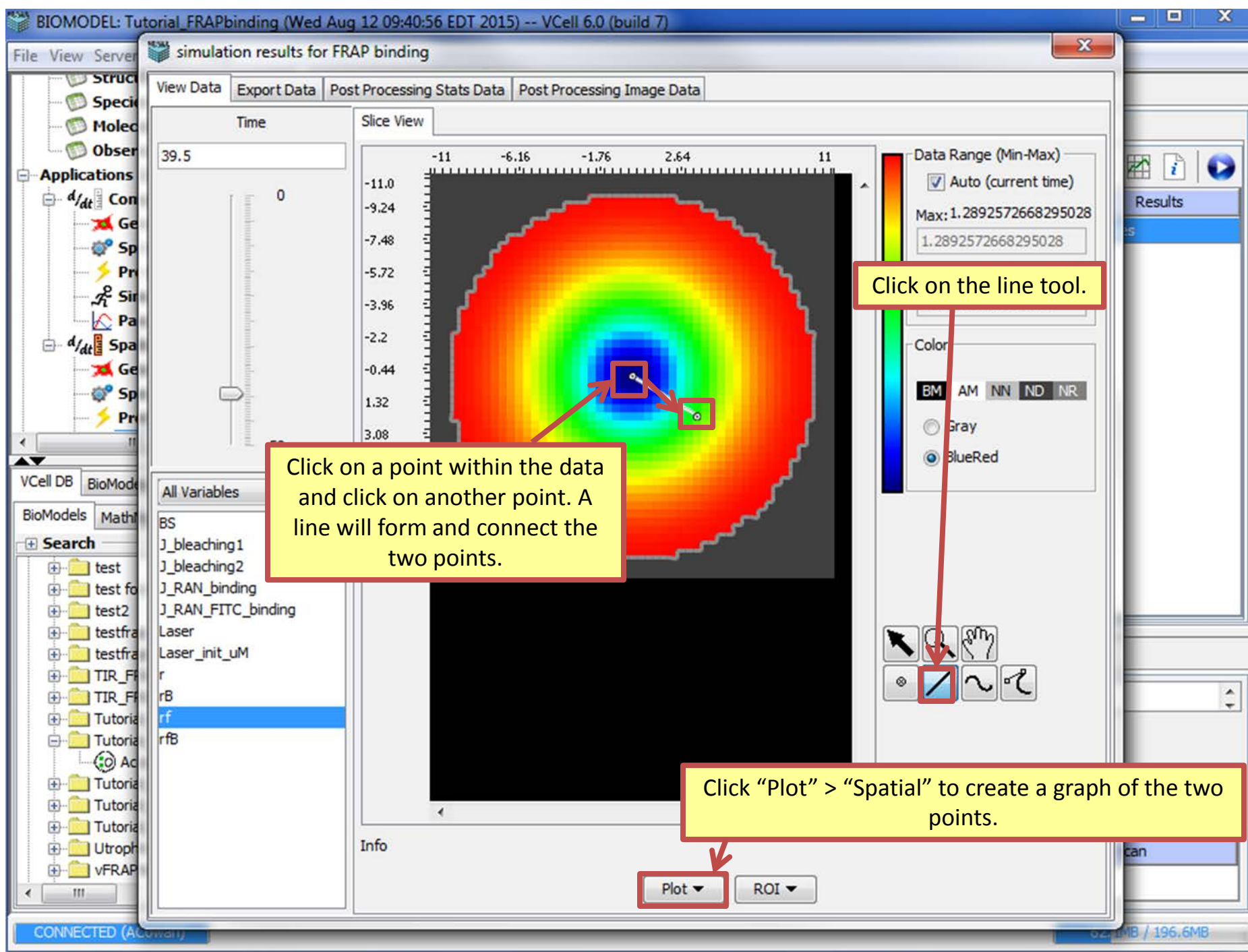


Plot

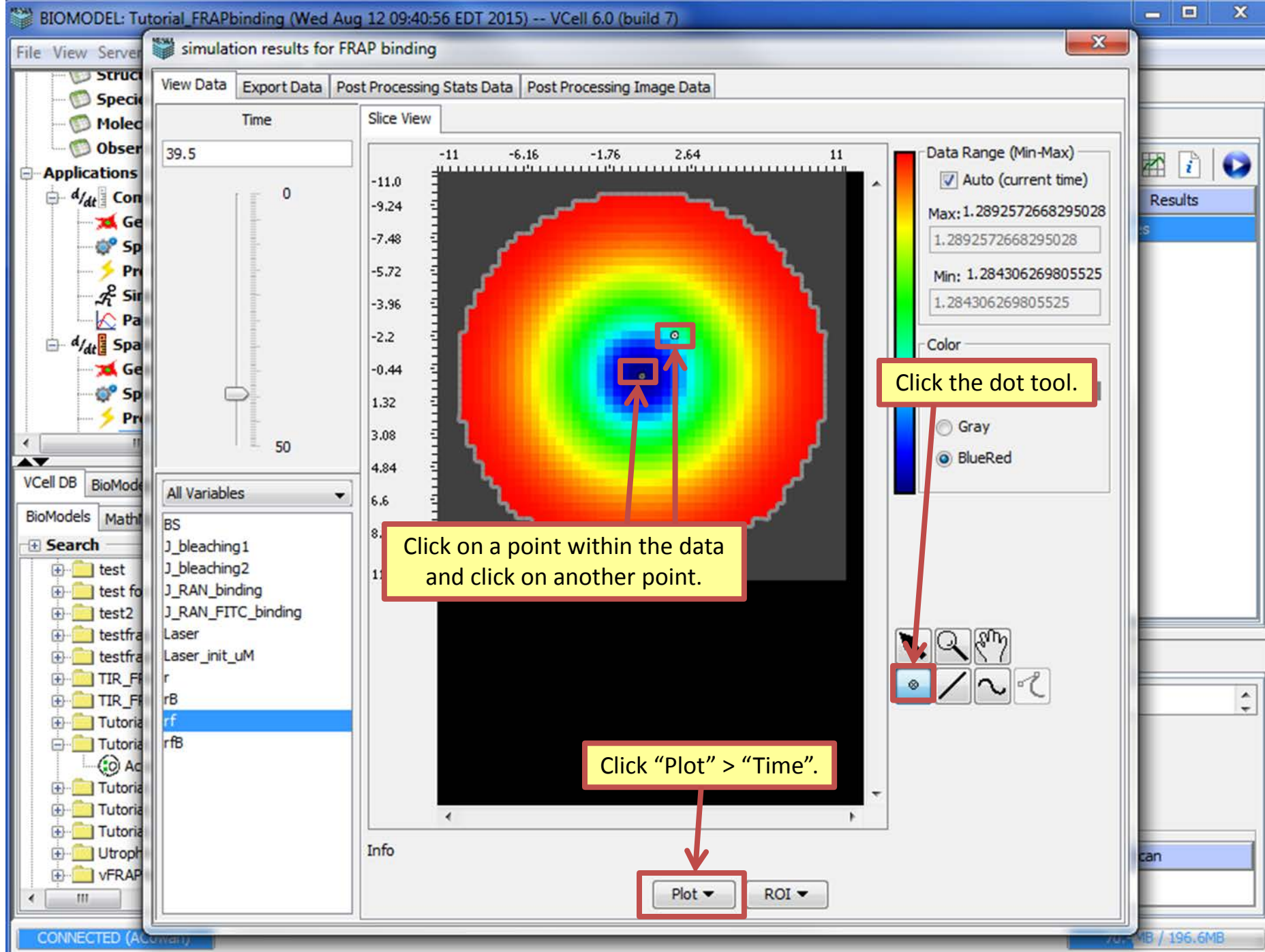
ROI

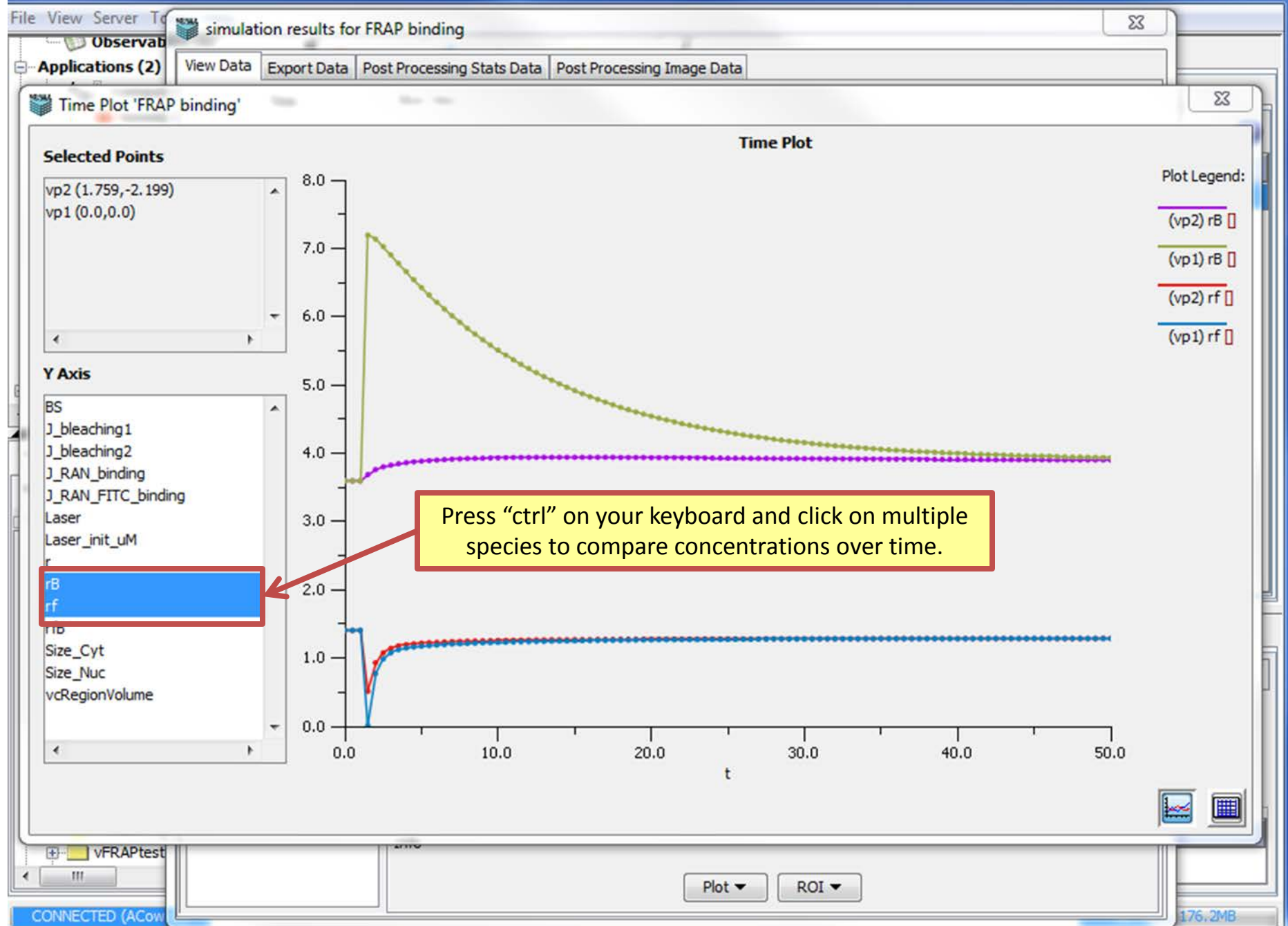












Next: VCell PIP2  
to IP3 Tutorial