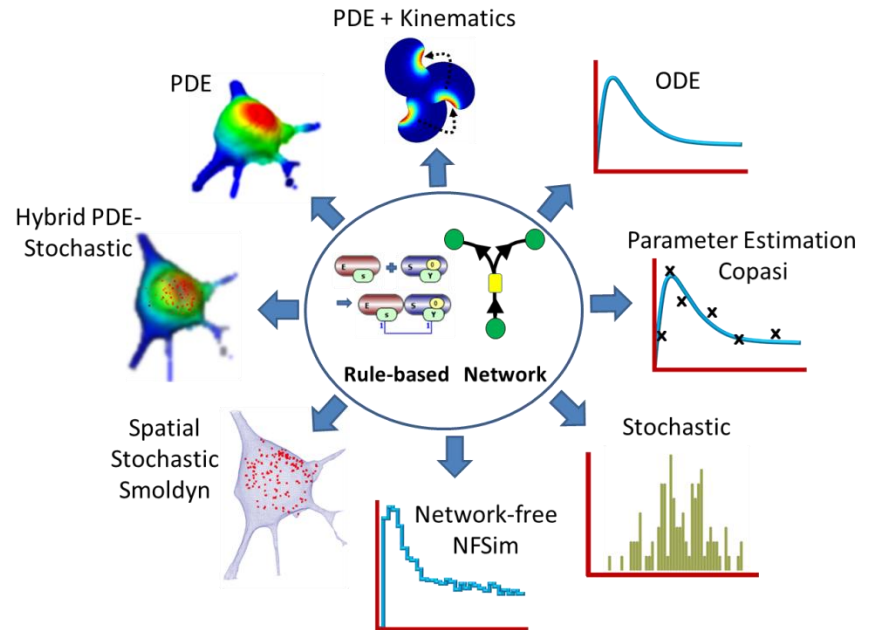


# VCell

modeling environment for  
mathematical simulation of  
cellular events.

To run VCell go to:

[vcell.org](http://vcell.org)



*Virtual Cell is developed by the Center for Cell Analysis and Modeling at the University of Connecticut Health Center. It is funded as a Biomedical Technology Research Resource by the National Institute of General Medical Sciences (NIGMS)*

# 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

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 2018
  - Shared BioModels (0)
  - Public BioModels (514)
  - Tutorials (5)
  - Education (33)
  - Tutorial VCell 6.0 (Rule-based) (7)

Delete | Pathway Links | Search

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

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

**BioModel3**

- 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

EC

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

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BioModels | MathModels | Geometries

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  - My BioModels (astfh234) (3)
  - Shared BioModels (0)
  - Public BioModels (514)
  - Tutorials (5)
  - Education (33)
  - Tutorial VCell 6.0 (Rule-based) (7)

Delete | Pathway Links ▾ | Search

Object Properties | Problems (0 Errors, 0 Warnings)

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

**BioModel3**

- Physiology
  - Reaction Diagram**
  - Reactions (0)
  - Structures (2)
  - Species (0)
  - 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) (3)
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  - Tutorials (5)
  - Education (33)
  - Tutorial VCell 6.0 (Rule-based) (7)

Reaction Diagram Reactions Structures Species Molecules Observables

EC PM

Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

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

**BioModel4**

- Physiology
  - Reaction Diagram
  - 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

**Search**

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

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
- Pathway

Reaction Diagram Reactions Structures Species Molecules Observables

The diagram shows a compartment labeled 'c1' with a vertical membrane structure labeled 'NM' on its left side. A red box highlights the 'NM' label, and a red arrow points from a yellow callout box to it.

Click on the membrane label.

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

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 [um<sup>2</sup>]

**Electrophysiology**

Vo

Pos

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

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



**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.

Delete Pathway Links Search

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".

**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 the species tool.

Cyt	NM	Nuc
		s0 s1 s2
		s3 s4 s5

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

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BioModels | MathModels | Geometries

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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)
- Applications (0)
- Parameters, Functions and Units
- Pathway

Reaction Diagram | Reactions | Structures | Species | Molecules | Observables

Cyt	NM	Nuc
		 s0  <b>s1</b>  s2
		 s3  s4  s5

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

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BioModels | MathModels | Geometries


**Search**

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

Delete | Pathway Links | Search

Object Properties | Problems (0 Errors, 0 Warnings)

Species Name	s1	 Species: <b>s1</b>
Linked Pathway Object(s)		
Annotation		



**BioModel4**

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

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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

The diagram shows three compartments: Cyt, NM, and Nuc. In the Nuc compartment, there are six green circles labeled s0 through s5. A yellow callout box with the text "Click on 's0'." has a red arrow pointing to the green circle labeled 'r' (which is s0).

Delete Pathway Links Search

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".

**BioModel4**

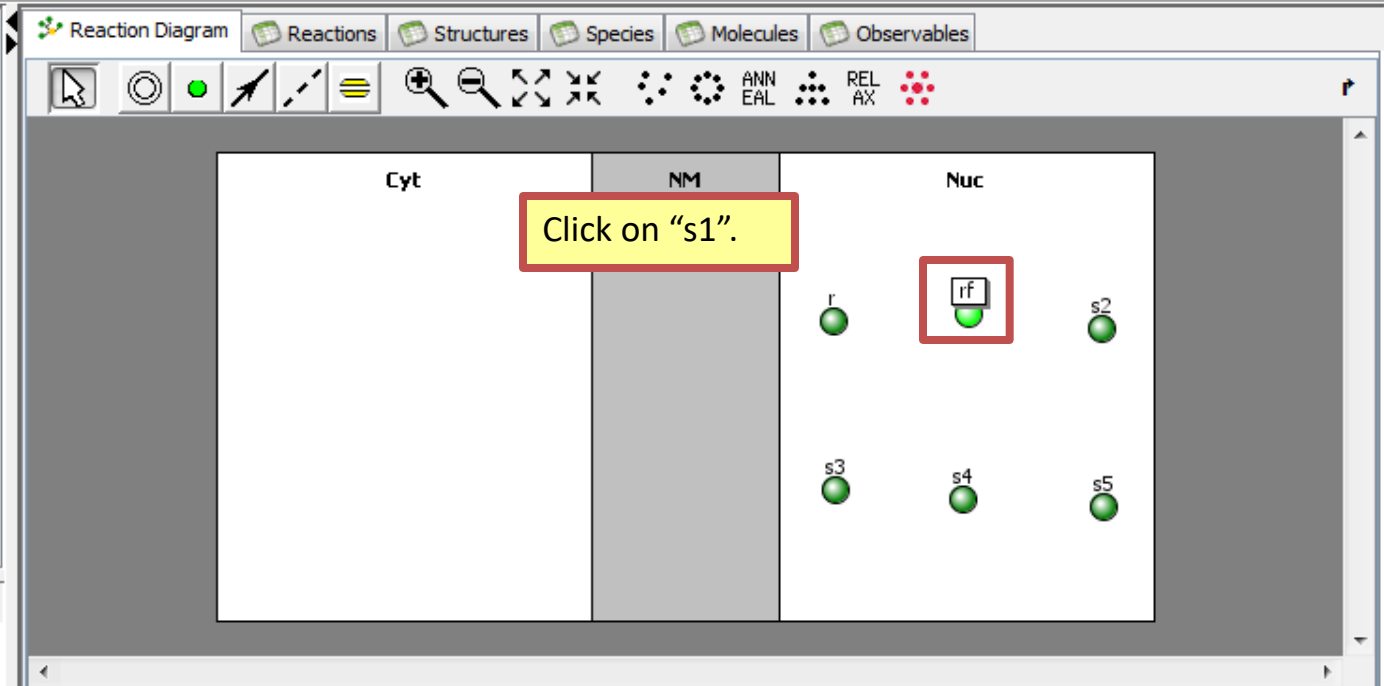
- Physiology
  - Reaction Diagram**
  - Reactions (0)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (0)
- Parameters, Functions and Units
- Pathway

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

**Search**

- Biological Models
  - My BioModels (astfh234) (4)
  - Shared BioModels (0)
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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)

Species Name	rf	Next to Species Name type "rf".
Linked Pathway Object(s)		
Annotation	RAN_FITC	Next to Annotation type "RAN_FITC".

**BioModel4**

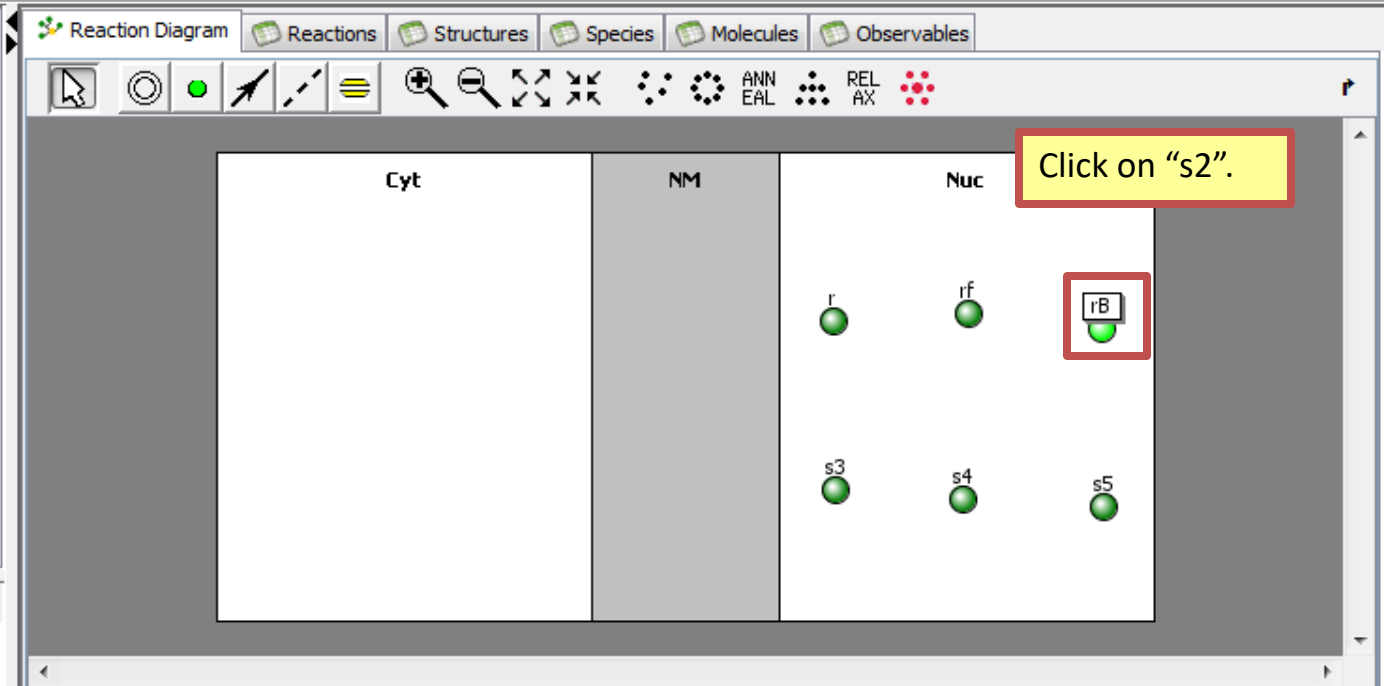
- Physiology
  - Reaction Diagram
  - Reactions (0)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (0)
- Parameters, Functions and Units
- Pathway

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

**Search**

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



Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Species Name  Next to Species Name type "rB".

Linked Pathway Object(s)

Annotation  Next to Annotation type "RAN\_Bound".

The Object Properties panel shows two input fields. The first is labeled 'Species Name' and contains the text 'rB'. A red box highlights this field, with an arrow pointing to a yellow callout box that says 'Next to Species Name type "rB".'. The second field is labeled 'Annotation' and contains the text 'RAN\_Bound'. A red box highlights this field, with an arrow pointing to a yellow callout box that says 'Next to Annotation type "RAN\_Bound".'. Below these fields is a section for 'Linked Pathway Object(s)' which is currently empty, and a small green sphere icon.

**BioModel4**

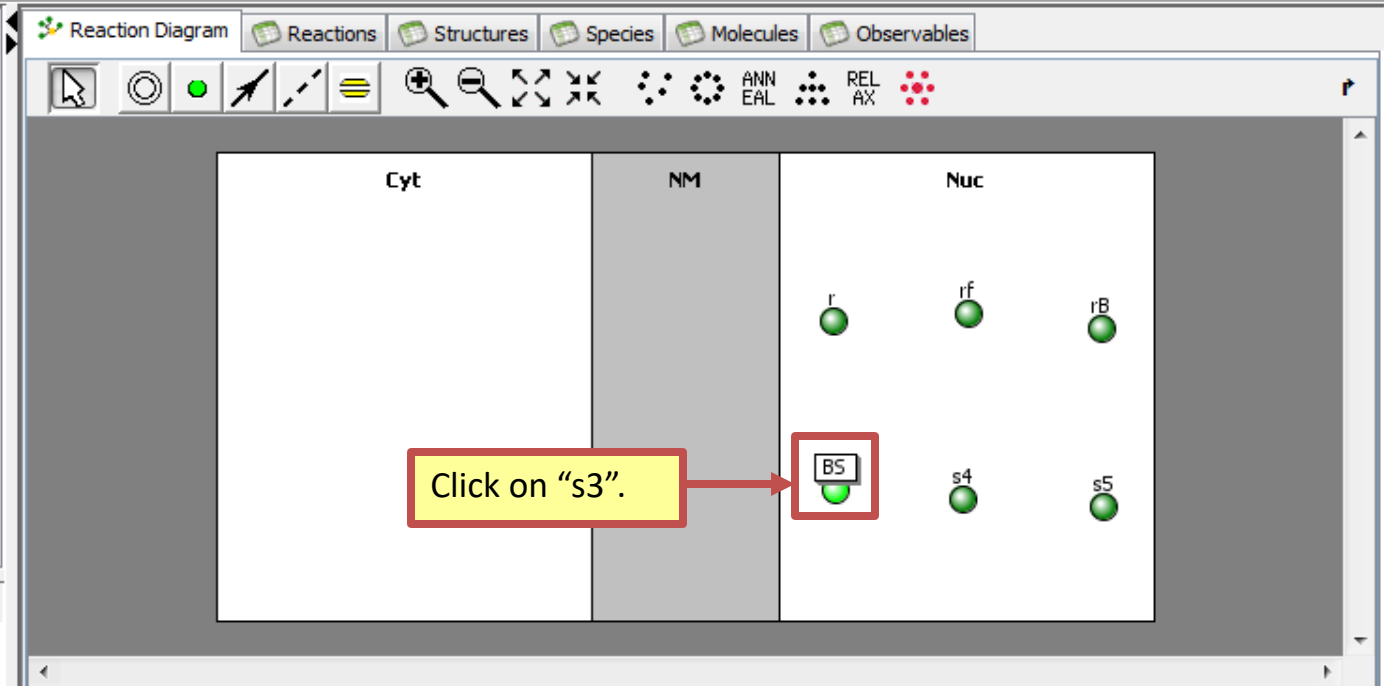
- Physiology
  - Reaction Diagram**
  - Reactions (0)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (0)
- Parameters, Functions and Units
- Pathway

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

**Search**

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



Click on "s3".

Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Species Name BS

Linked Pathway Object(s)

Annotation Binding Sites

Next to Species Name type "BS".

Next to Annotation type "Binding Sites".

**BioModel4**

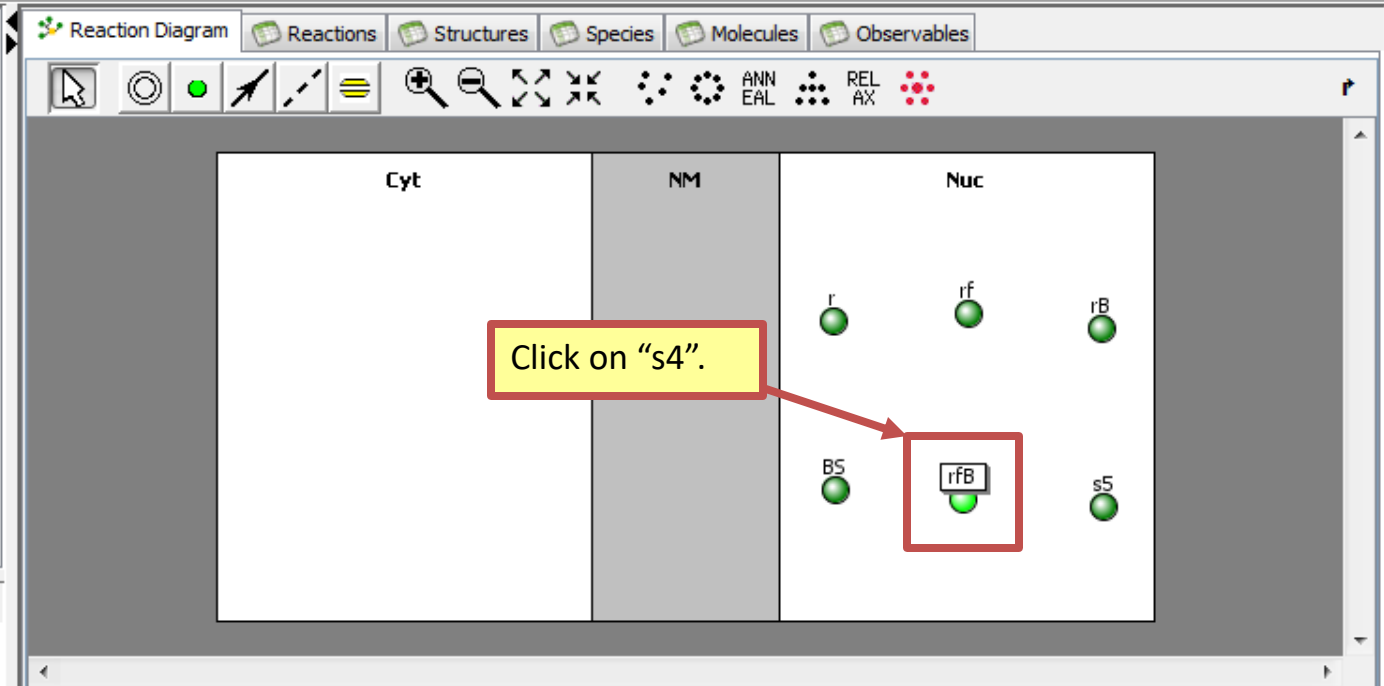
- Physiology
  - Reaction Diagram**
  - Reactions (0)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (0)
- Parameters, Functions and Units
- Pathway

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

**Search**

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



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".



**BioModel4**

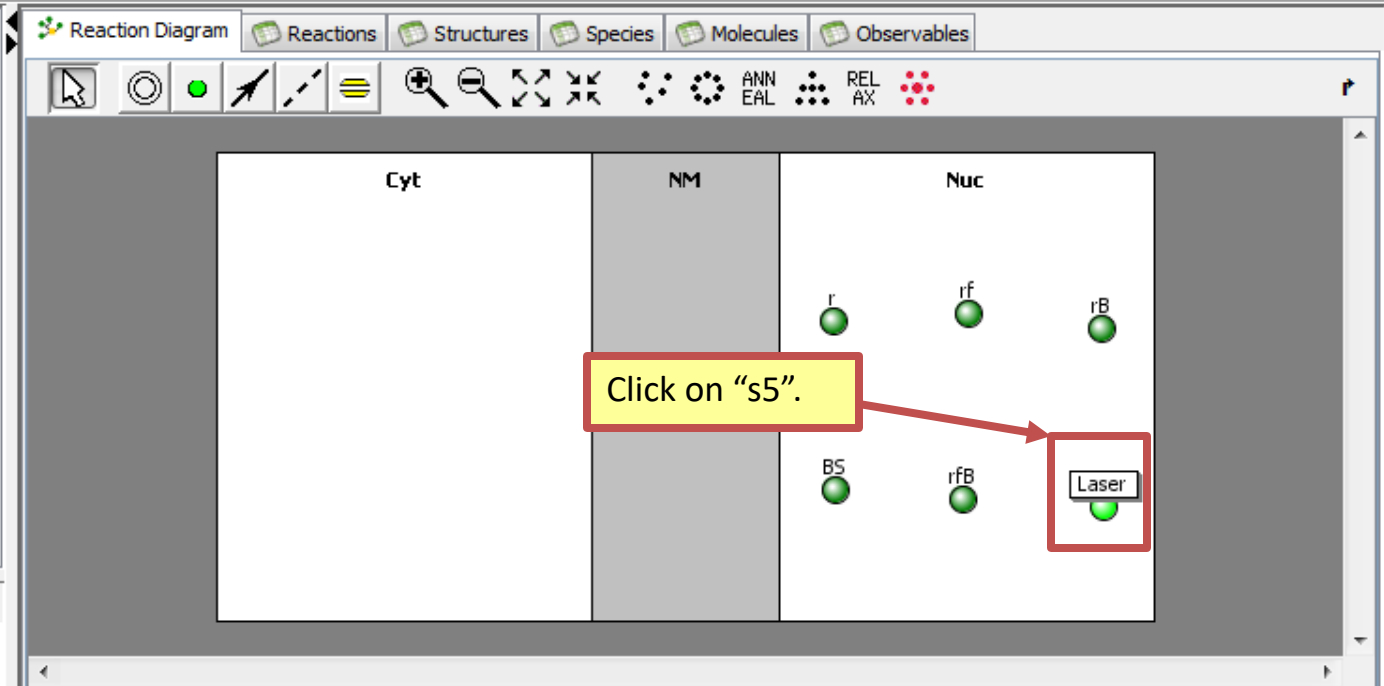
- Physiology
  - Reaction Diagram**
  - Reactions (0)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (0)
- Parameters, Functions and Units
- Pathway

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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)



Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

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

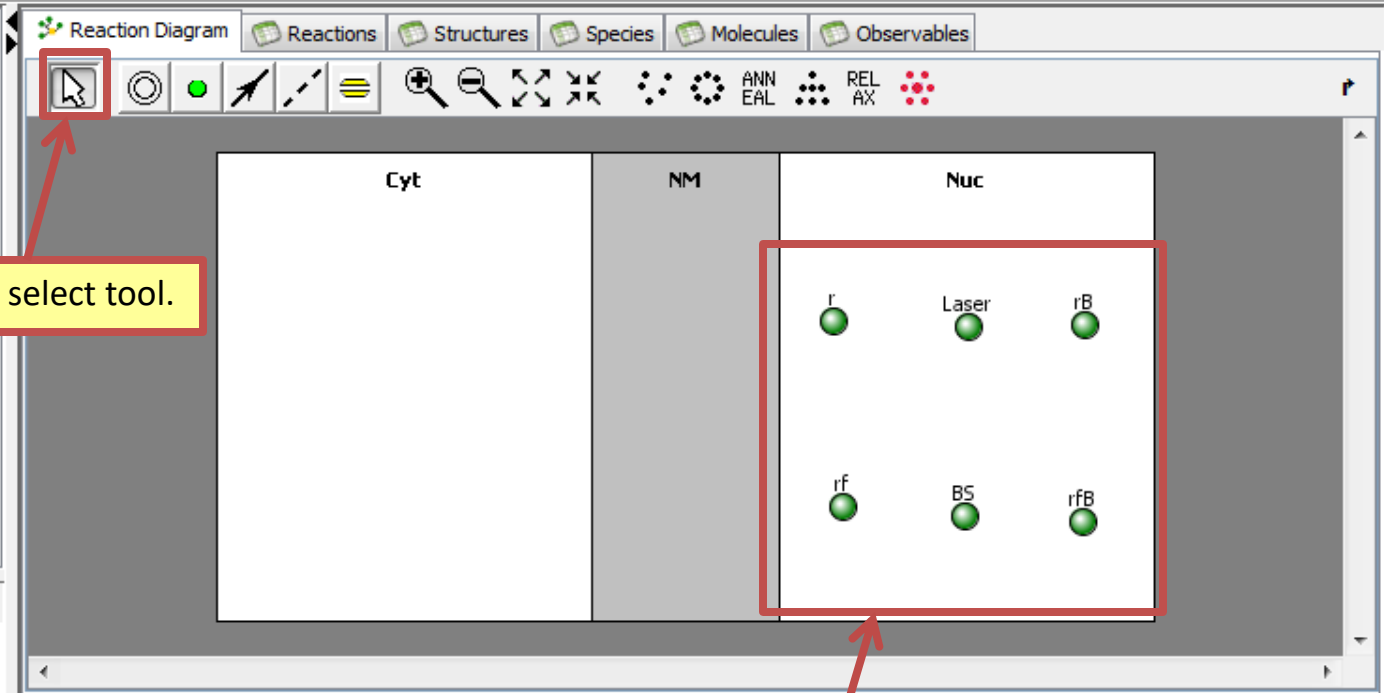
Next to Species Name type "Laser".

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 U...
- Pathway

Click the select tool.



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

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

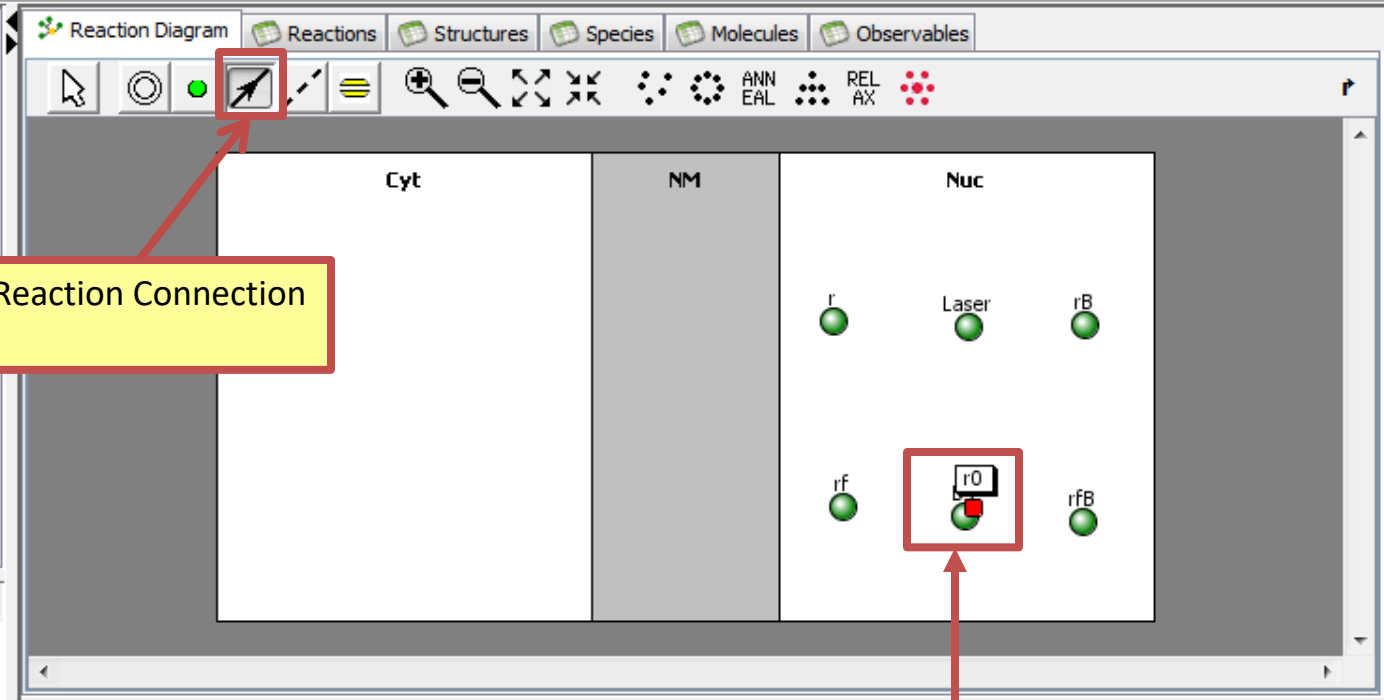
**Search**

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

**BioModel4**

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

Click the Reaction 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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**Search**

- Biological Models
  - My BioModels (astfh234) (4)
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  - Education (33)
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Delete Pathway Links

Object Properties Problems (0 Errors)

Reaction Name: r0

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

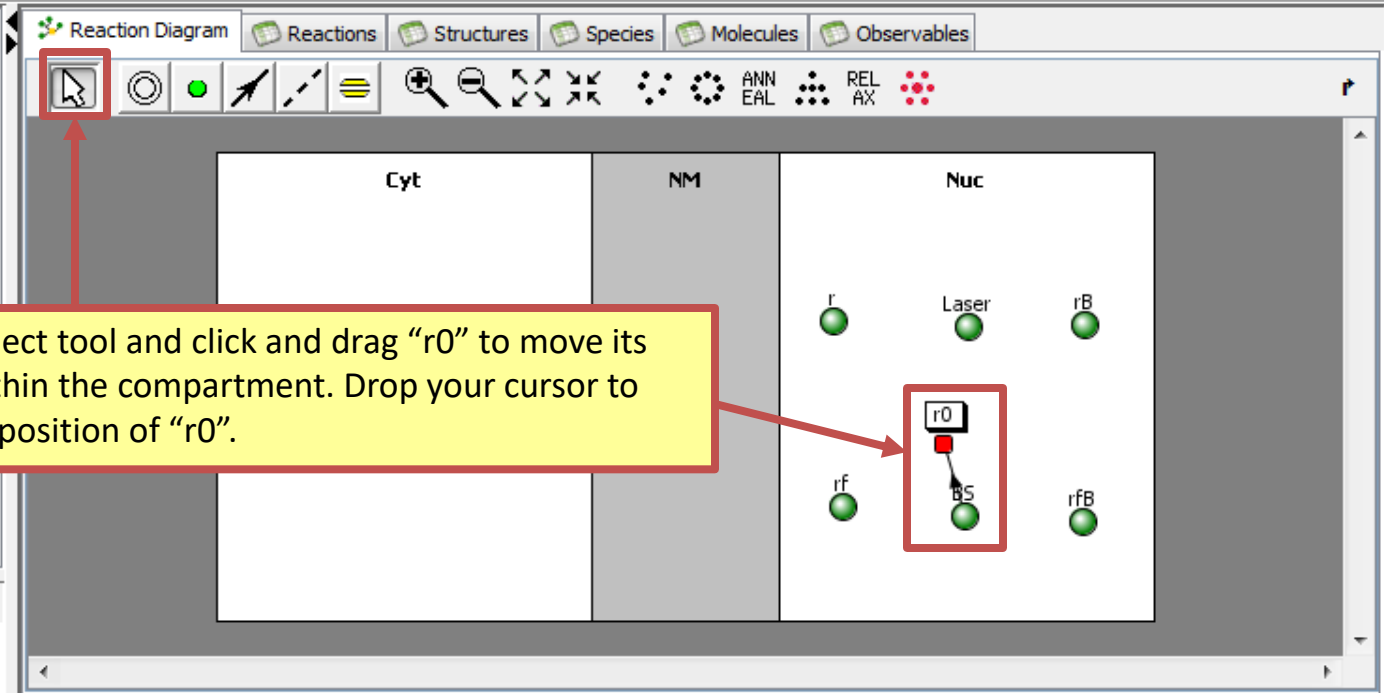
Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$k_f \cdot BS$	$\mu\text{M} \cdot \text{s}^{-1}$
Kf	forward rate constant	<input type="checkbox"/>	0.0	$\text{s}^{-1}$
Kr	reverse rate constant	<input type="checkbox"/>	0.0	$\mu\text{M} \cdot \text{s}^{-1}$
BS	Species Concentration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

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

Annotation and Pathway Links

**BioModel4**

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



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".

VCell DB | BioModels.net | Pathway Comm | Sabio

BioModels | MathModels | Geometries

**Search**

- Biological Models
  - My BioModels (astfh234) (4)
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  - Tutorials (5)
  - Education (33)
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Delete | Pathway Links | Search

Object Properties | Problems (0 Errors, 0 Warnings)

Reaction Name: r0

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

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

Annotation and Pathway Links

**BioModel4**

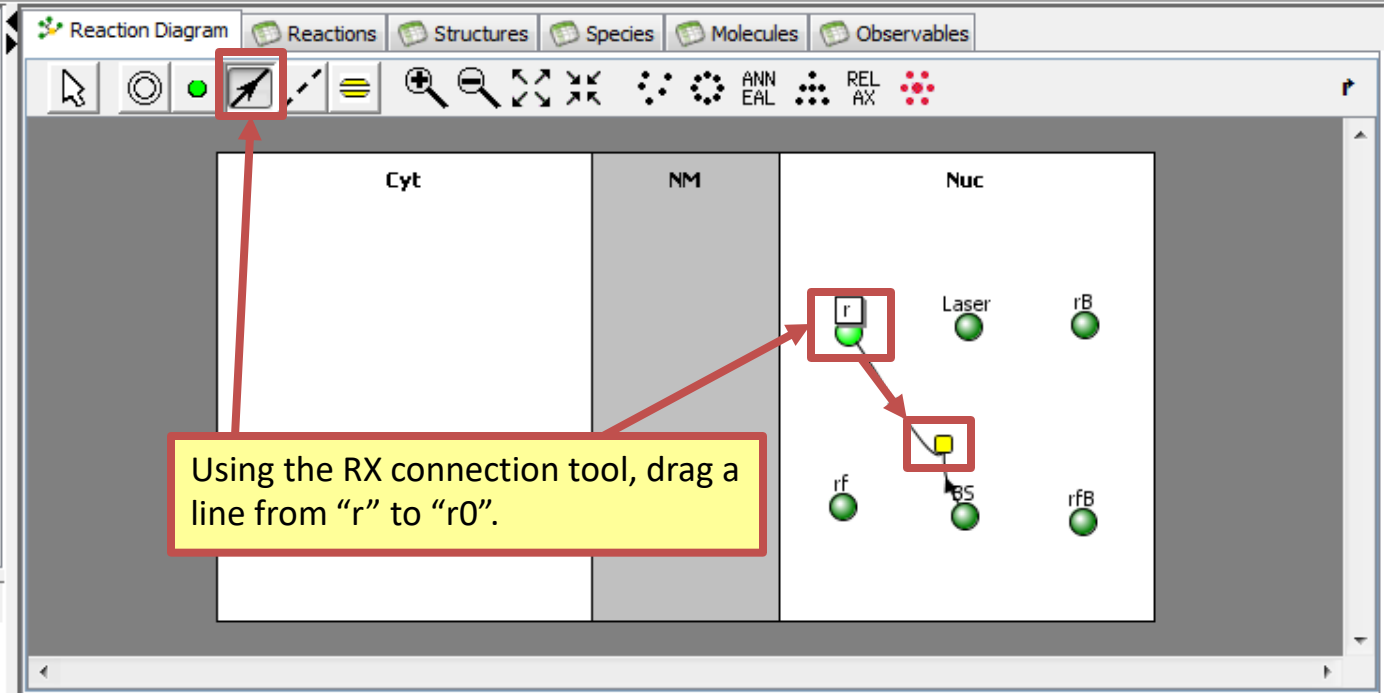
- Physiology
  - Reaction Diagram**
  - Reactions (1)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (0)
- Parameters, Functions and Units
- Pathway

VCell DB BioModels.net Pathway Comm Sabio

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**Search**

- Biological Models
  - My BioModels (astfh234) (4)
  - Shared BioModels (0)
  - Public BioModels (514)
  - Tutorials (5)
  - Education (33)
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Using the RX connection tool, drag a line from "r" to "r0".

Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

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

**BioModel4**

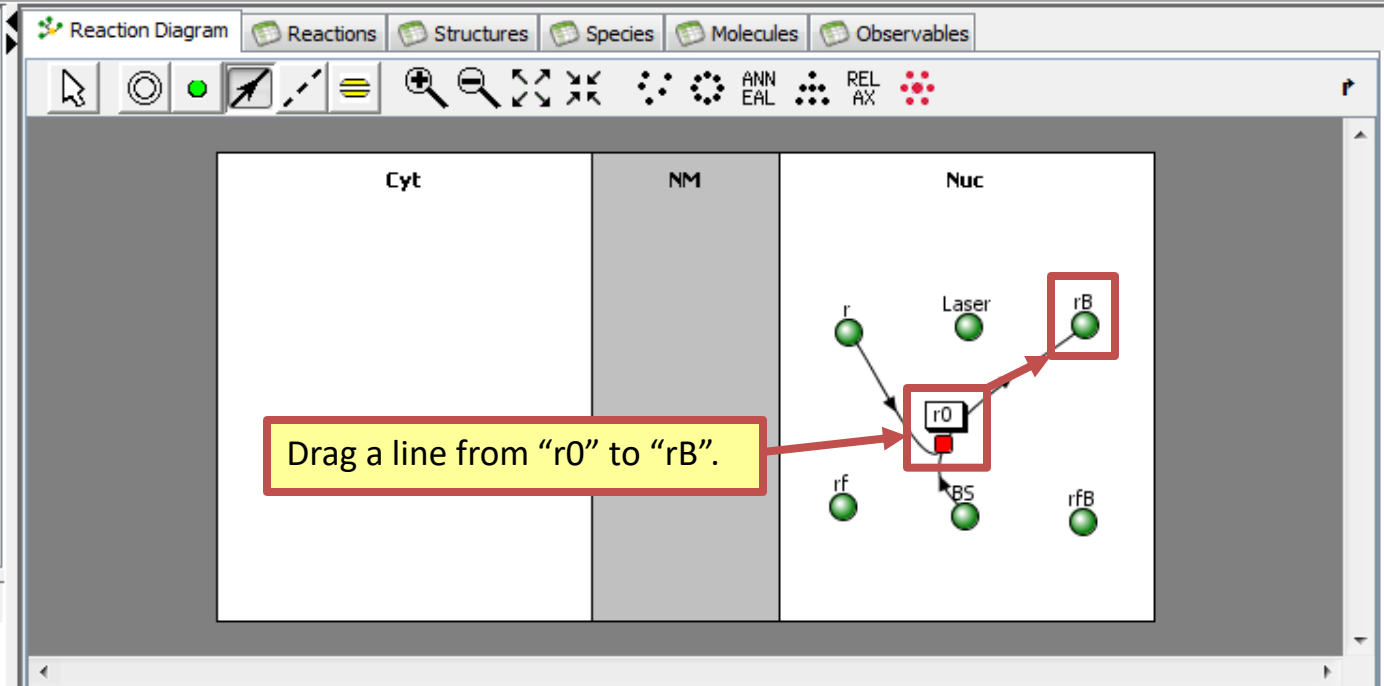
- Physiology
  - Reaction Diagram**
  - Reactions (1)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (0)
- Parameters, Functions and Units
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VCell DB BioModels.net Pathway Comm Sabio

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**Search**

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



Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Reaction Name

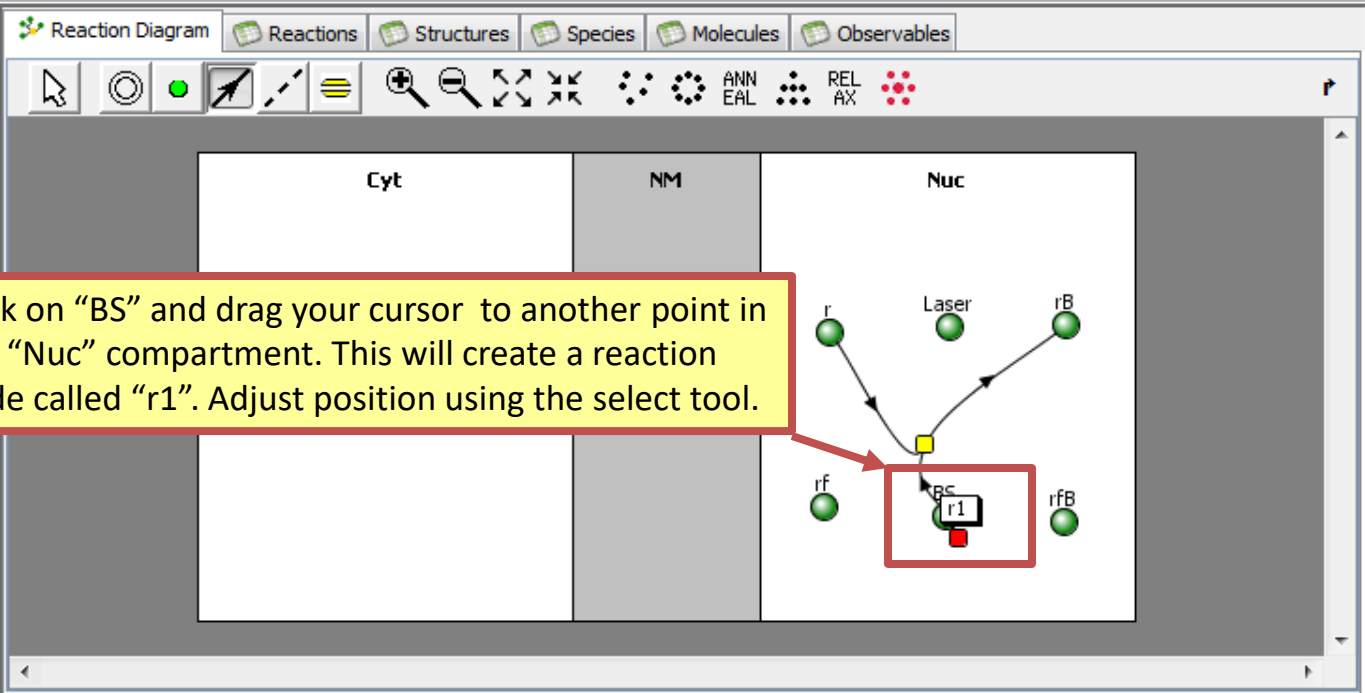
Kinetic Type

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$(K_f \cdot BS \cdot r - K_r \cdot r_B)$	$\mu\text{M} \cdot \text{s}^{-1}$
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)
- Parameters, Functions and Units
- Pathway



Click on "BS" and drag your cursor to another point in the "Nuc" compartment. This will create a reaction node called "r1". Adjust position using the select tool.

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

Kinetic Type

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

Annotation and Pathway Links

**BioModel4**

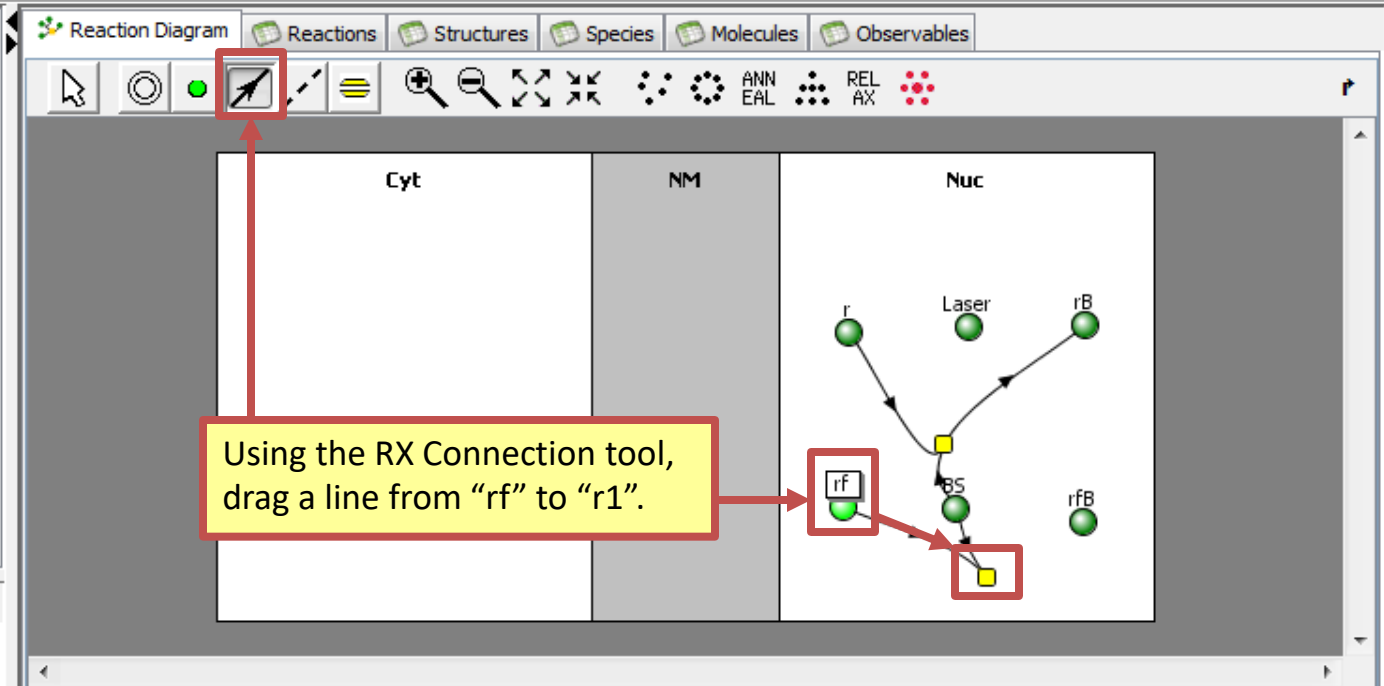
- Physiology
  - Reaction Diagram**
  - Reactions (2)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (0)
- Parameters, Functions and Units
- Pathway

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

**Search**

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



Using the RX Connection tool, drag a line from "rf" to "r1".

Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Species Name	rf
Linked Pathway Object(s)	
Annotation	RAN_FITC

Species: rf



**BioModel4**

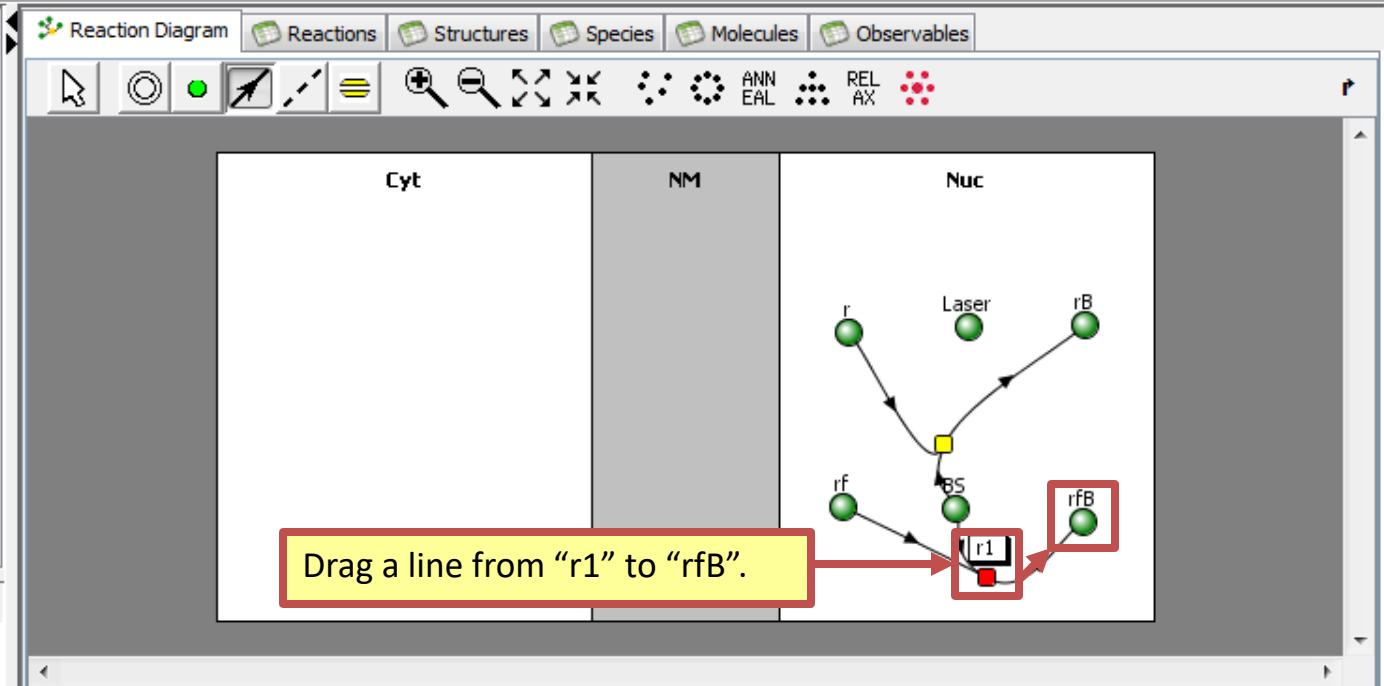
- Physiology
  - Reaction Diagram**
  - Reactions (2)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (0)
- Parameters, Functions and Units
- Pathway

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



Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Reaction Name

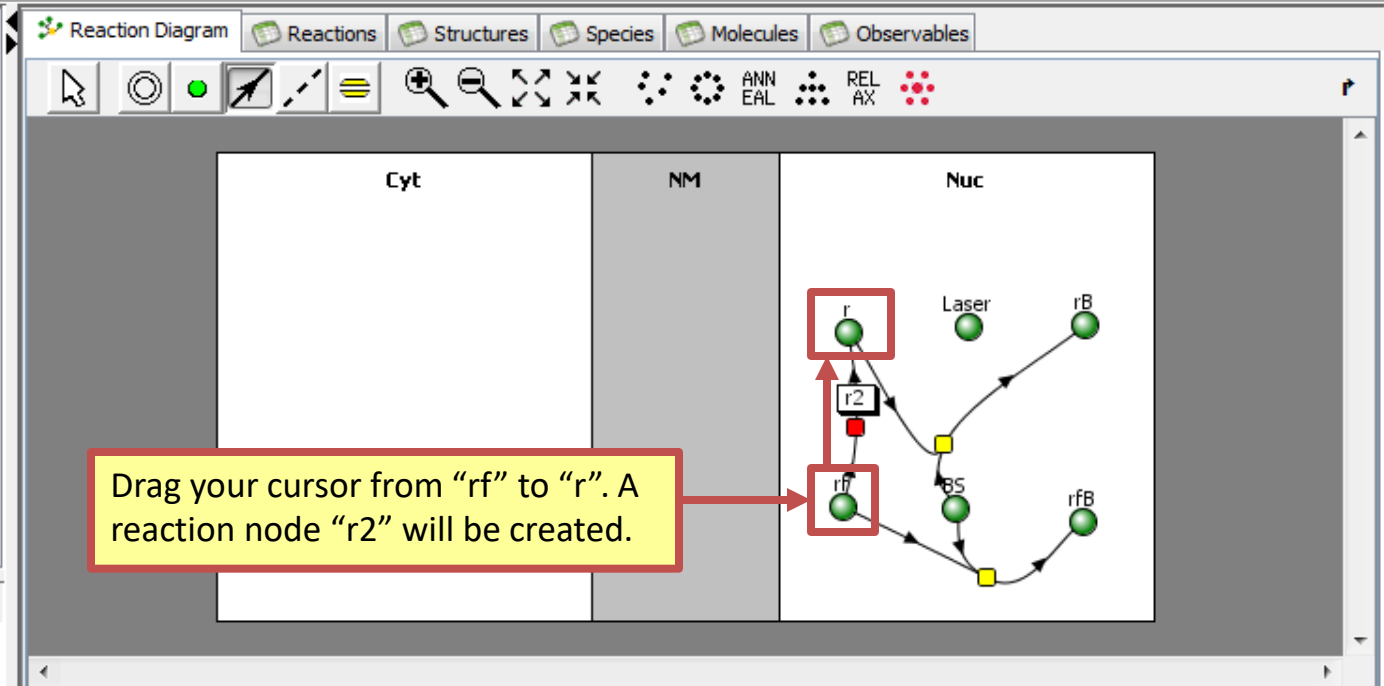
Kinetic Type

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



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

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$(K_f \cdot r_f - K_r \cdot r)$	$\mu\text{M} \cdot \text{s}^{-1}$
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>
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**

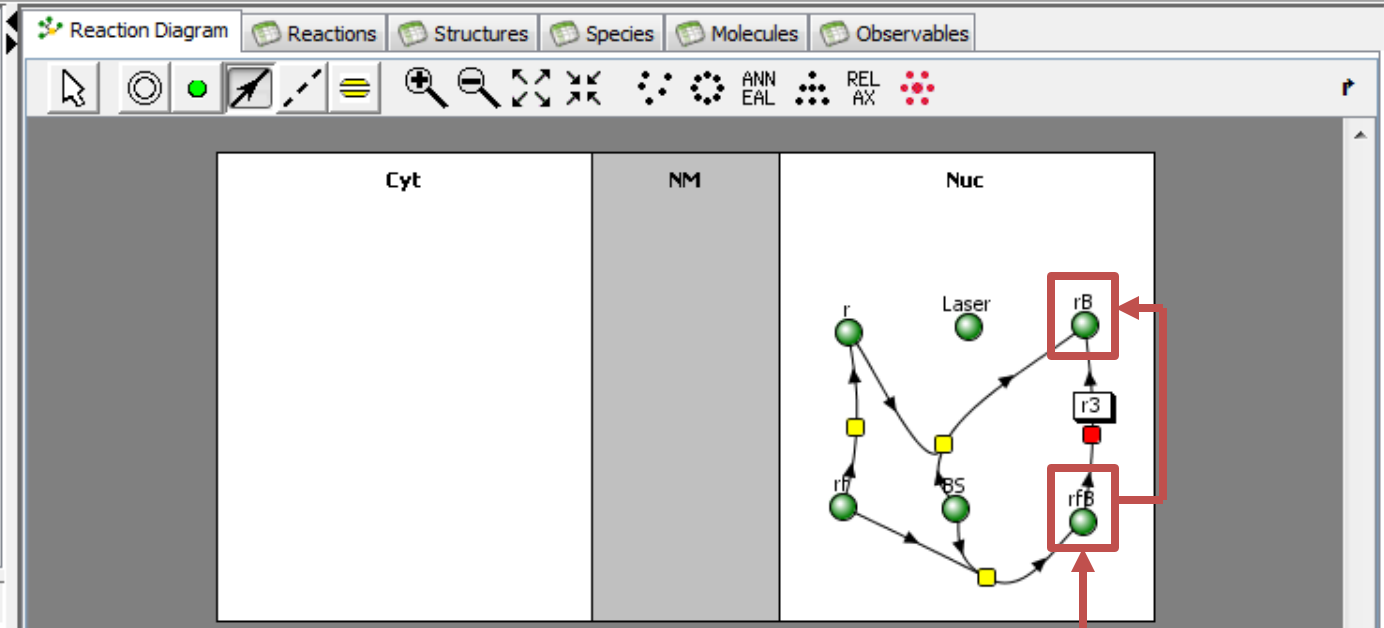
- Physiology
  - Reaction Diagram
  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (0)
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Drag your cursor from "rfB" to "rB". A reaction node "r3" will be created.

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

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$(K_f \cdot r_fB - K_r \cdot r_B)$	$\mu\text{M.s}^{-1}$
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	$\mu\text{M}$

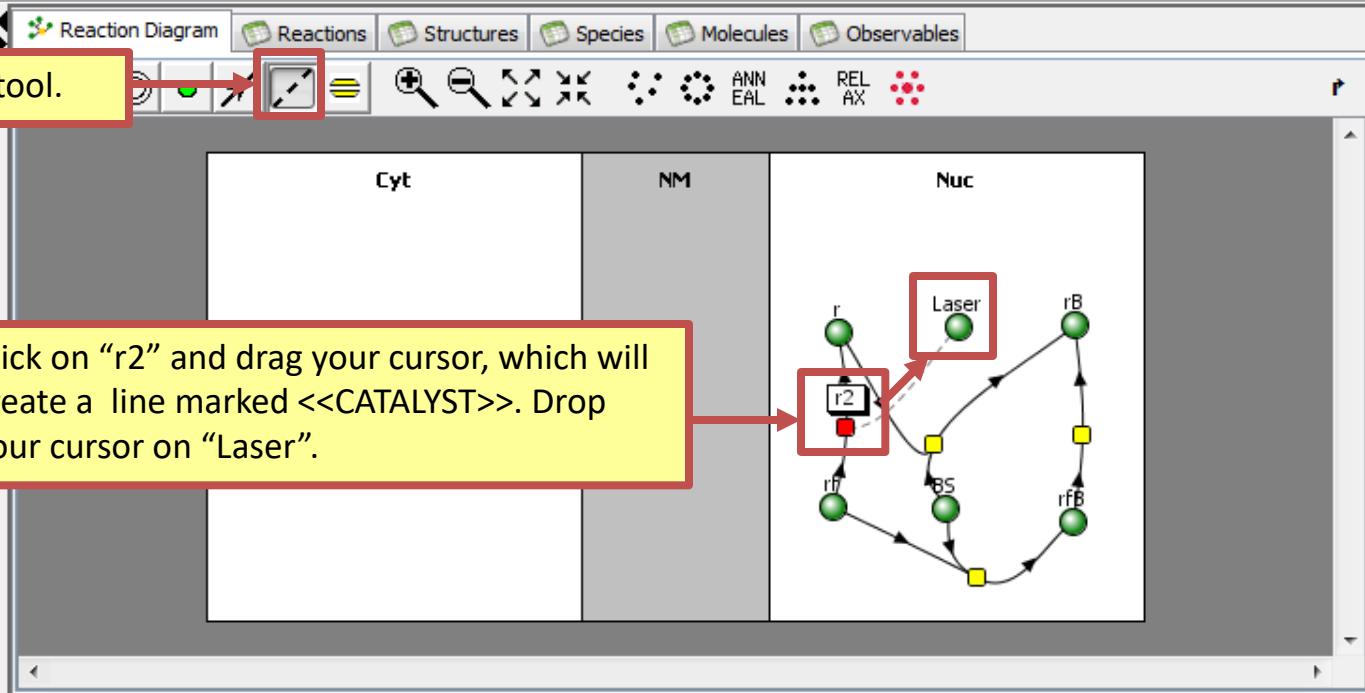
Annotation and Pathway Links

**BioModel4**

- Physiology
  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
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Click on the catalyst tool.

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



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

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$(K_f \cdot r_f - K_r \cdot r)$	$\mu\text{M.s}^{-1}$
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>
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**

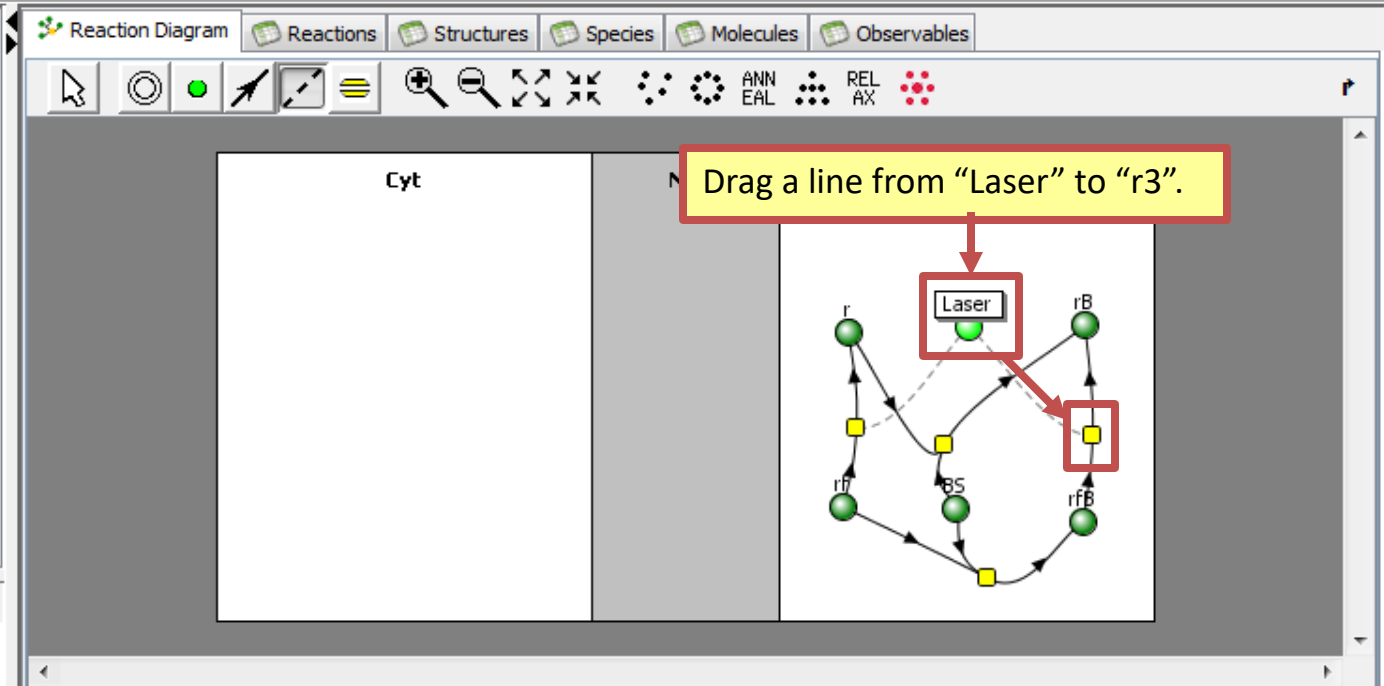
- Physiology
  - Reaction Diagram**
  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
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Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

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

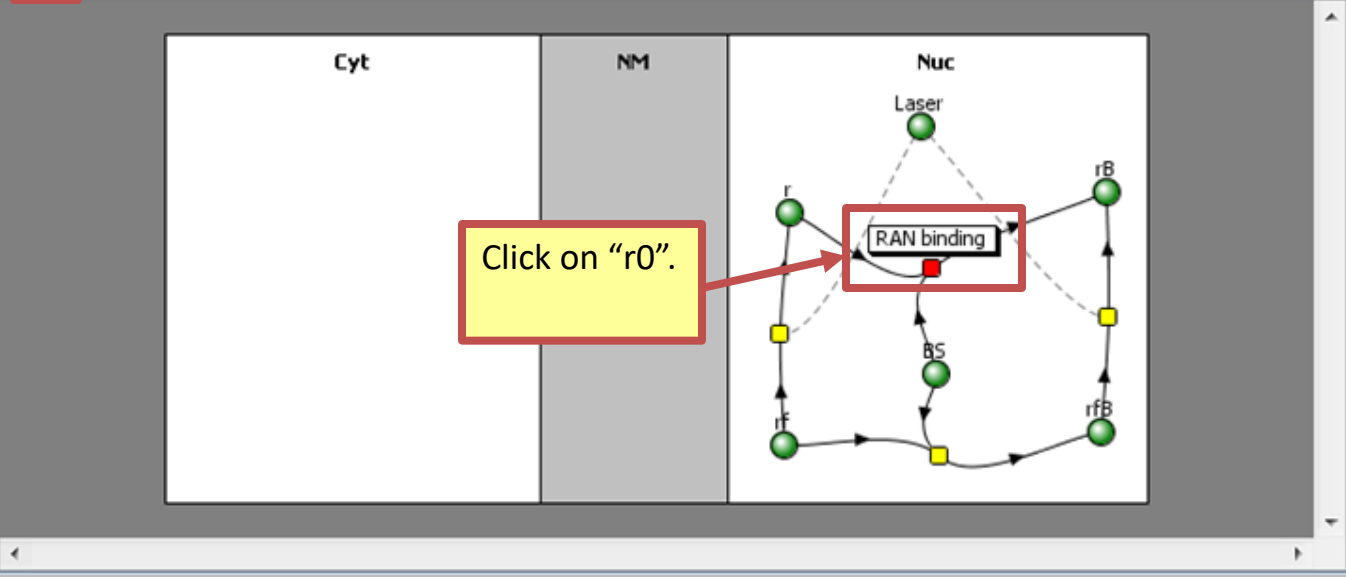
**BioModel4**

- Phys
- Reactions (4)
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- Molecules (0)
- Observables (0)
- Applications (0)
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Click the select tool.

Reaction Diagram Reactions Structures Species Molecules Observables

Toolbar icons: select, pan, zoom, etc.



Click on "r0".

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Biological Models

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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 [μM/s] (recommended for stochastic application) Convert to [molecules.s<sup>-1</sup>]

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

Annotation and Pathway Links

**BioModel4**

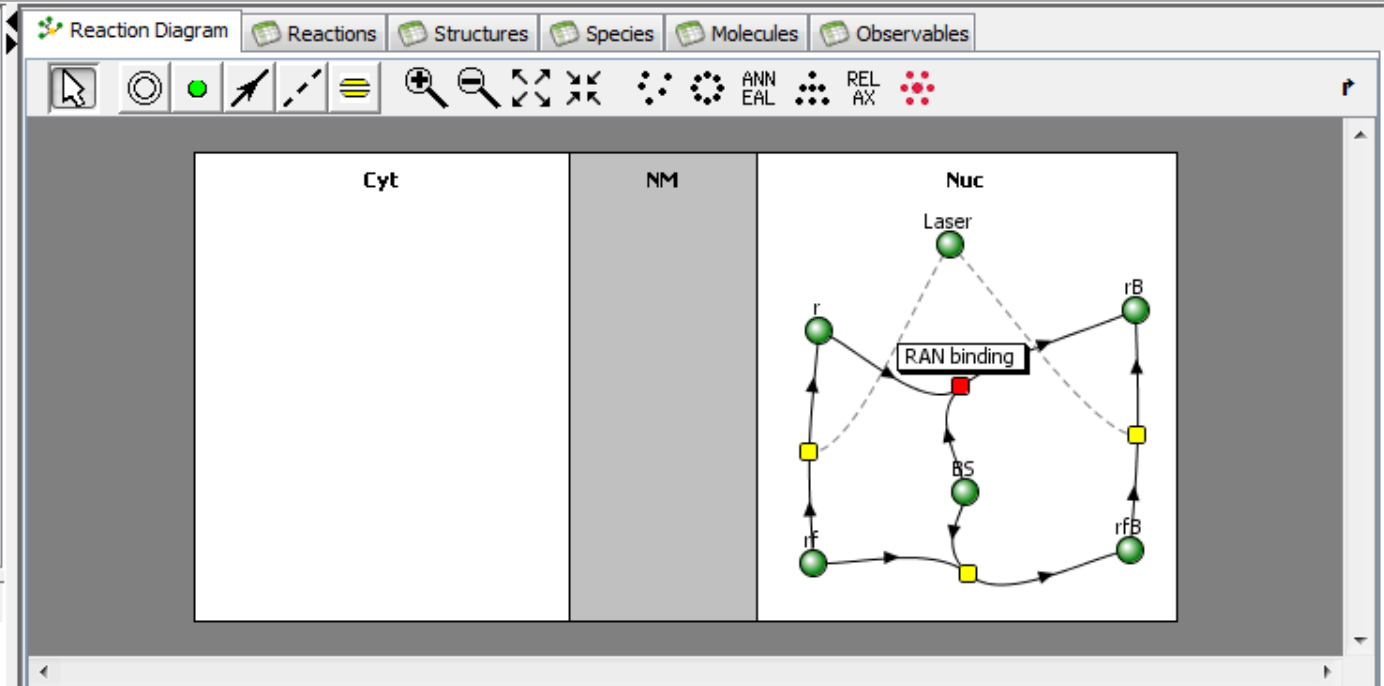
- Physiology
  - Reaction Diagram
  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (0)
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Delete Pathway Links Search

Object

Reaction

Kind

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

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

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**

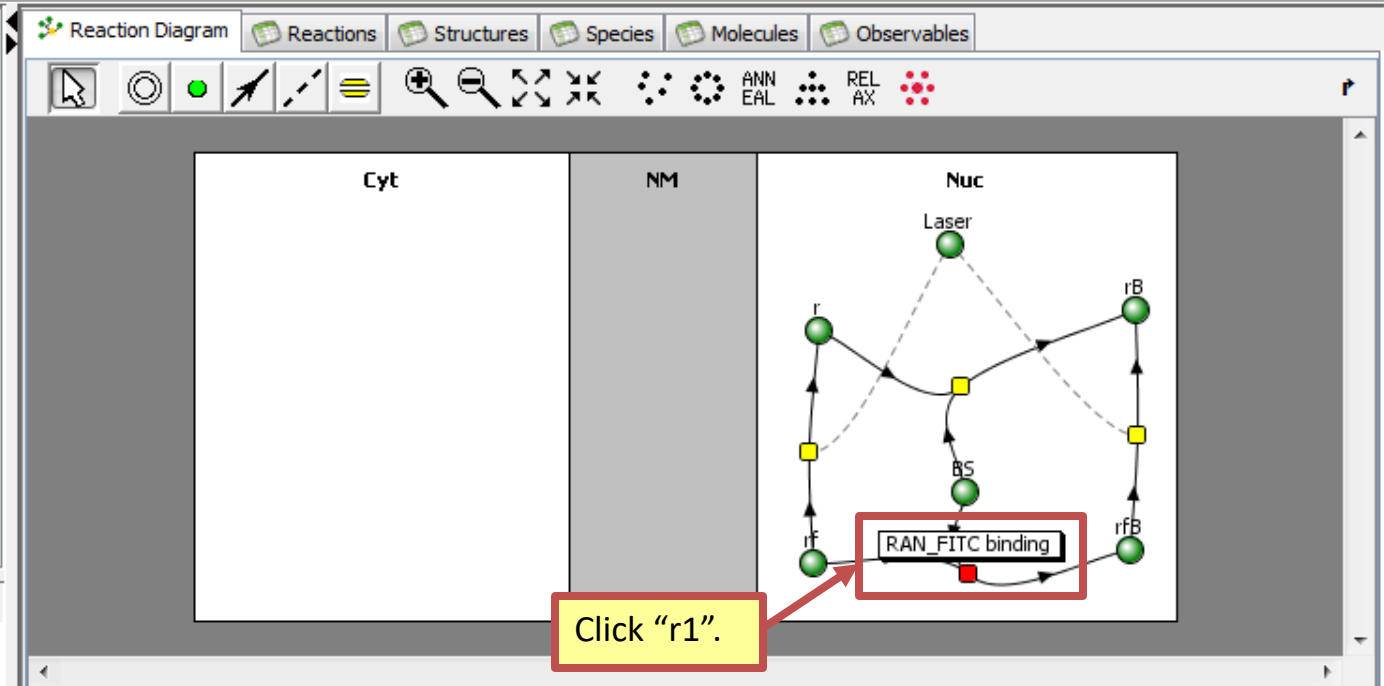
- Physiology
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  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
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Click "r1".

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

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

Name	Description	Global	Expression	Units
<i>rFB</i>				$\mu\text{M} \cdot \text{s}^{-1}$
<i>rFB</i>				$\text{s}^{-1} \cdot \mu\text{M}^{-1}$
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	$\mu\text{M}$

Annotation and Pathway Links



**BioModel4**

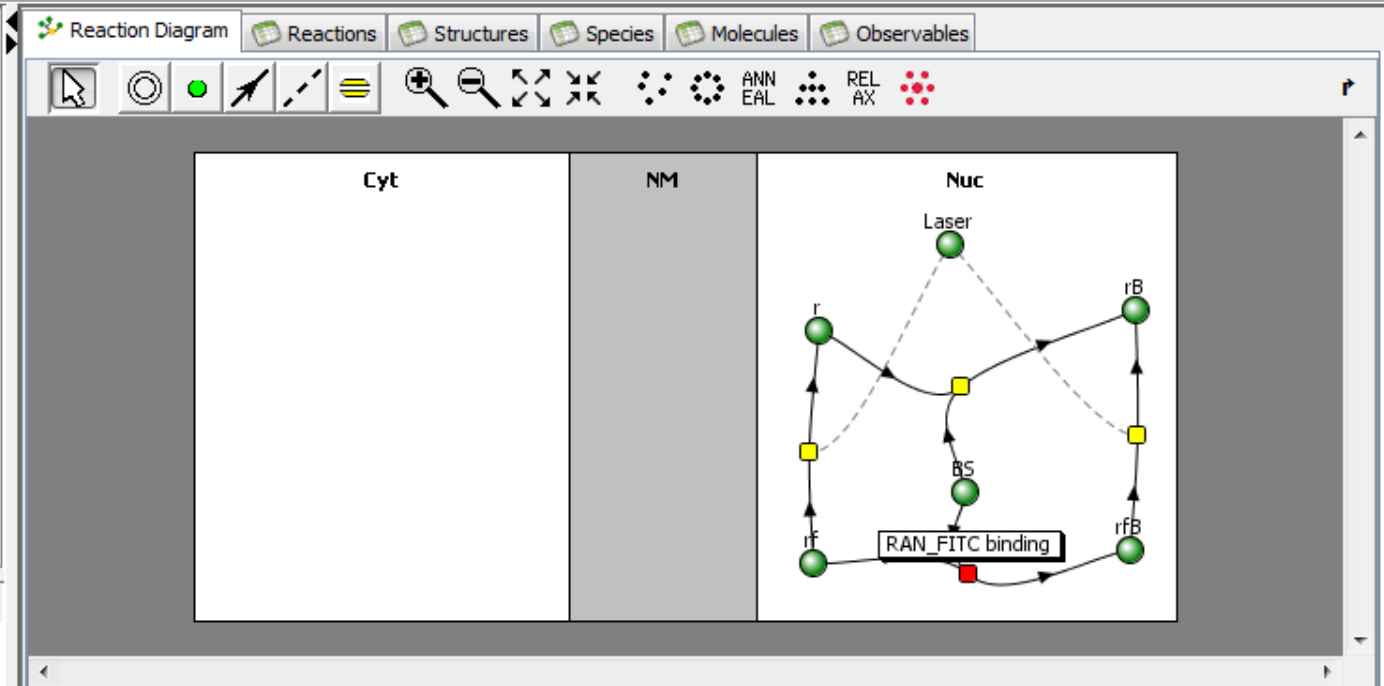
- Physiology
  - Reaction Diagram**
  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (0)
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Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

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"/>	$K_f \cdot BS \cdot rf - K_r \cdot rfB$	$\mu\text{M} \cdot \text{s}^{-1}$
Kf	forward rate constant	<input type="checkbox"/>	0.02	$\text{s}^{-1} \cdot \mu\text{M}^{-1}$
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	$\mu\text{M}$
				$\mu\text{M}$

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

**BioModel4**

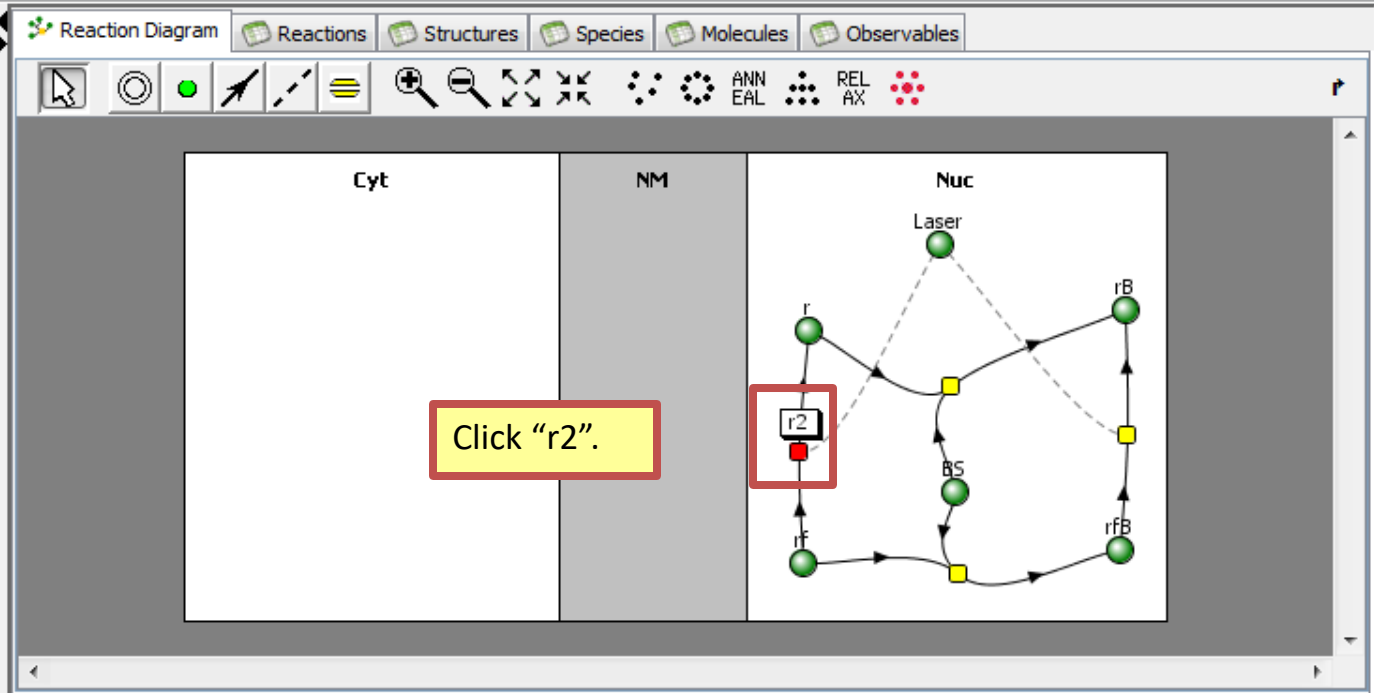
- Physiology
  - Reaction Diagram**
  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (0)
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Delete Pathway Links Search

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"/>	0.0	μM.s <sup>-1</sup>

Click the drop down menu next to Kinetic Type. Select "General [μM/s]".

Annotation and Pathway Links

**BioModel4**

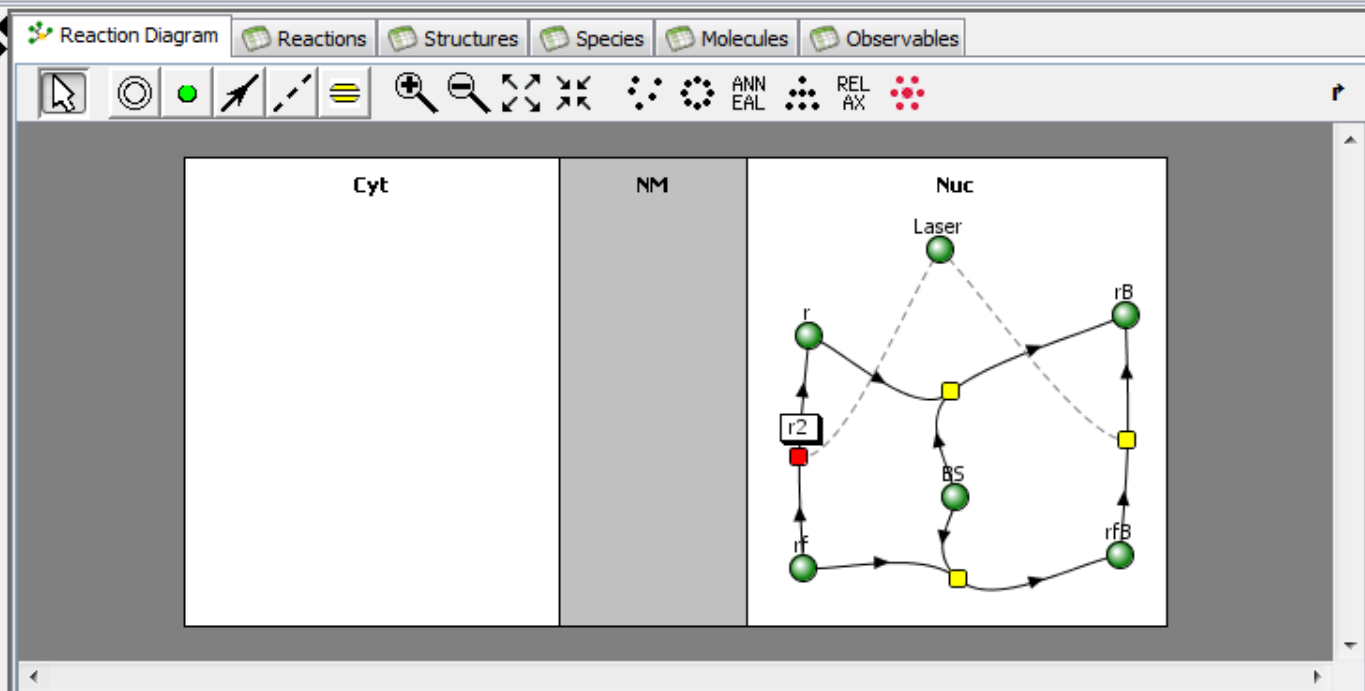
- Physiology
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  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (0)
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Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Reaction Name: r2  
 Kinetic Type: General [μM/s] Convert to [molecules.s<sup>-1</sup>]

Name	Description	Global	Expression	Units
r2	reaction rate	<input type="checkbox"/>	$(V_{max} * r_f * Laser * ((t > 1.0) \&\& (t < 1.5)))$	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.

**BioModel4**

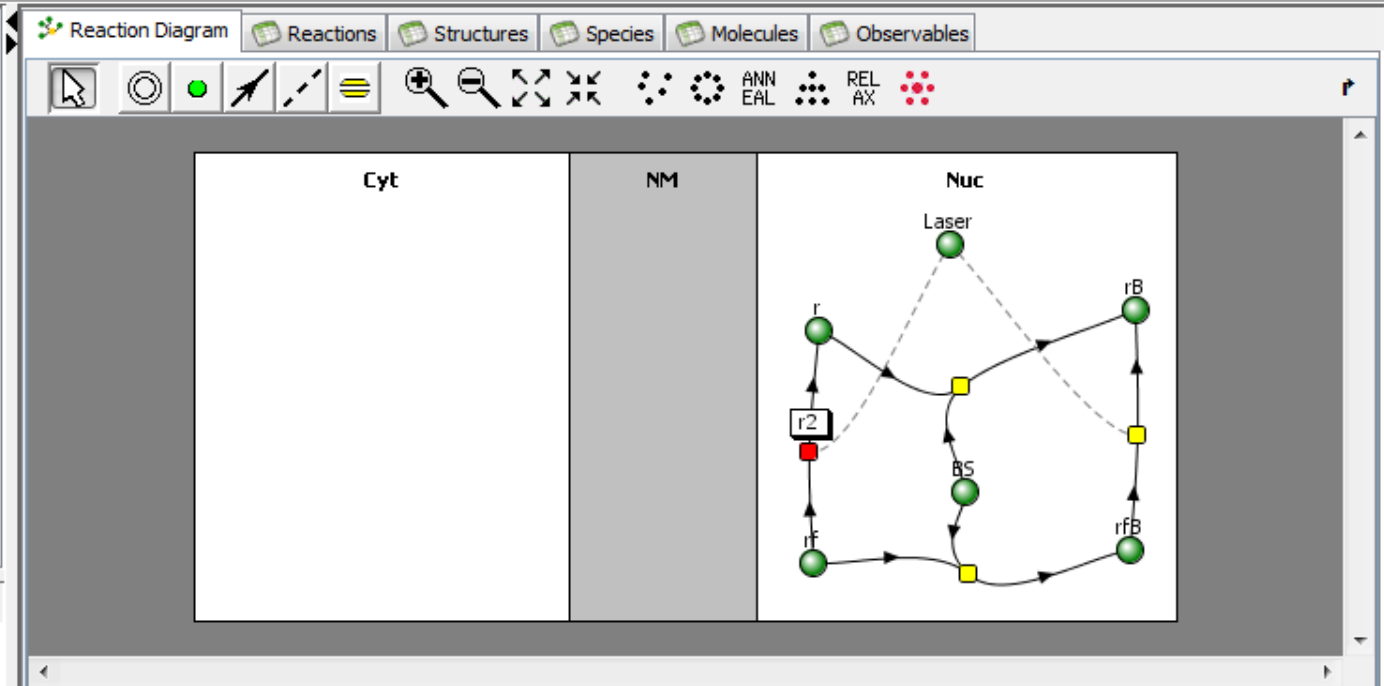
- Physiology
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  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
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Delete Pathway Links Search

Object Properties Problem

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

Reaction Name: r2  
 Kinetic Type: General [ ] Convert to [molecules.s<sup>-1</sup>]

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

Annotation and Pathway Links

**BioModel4**

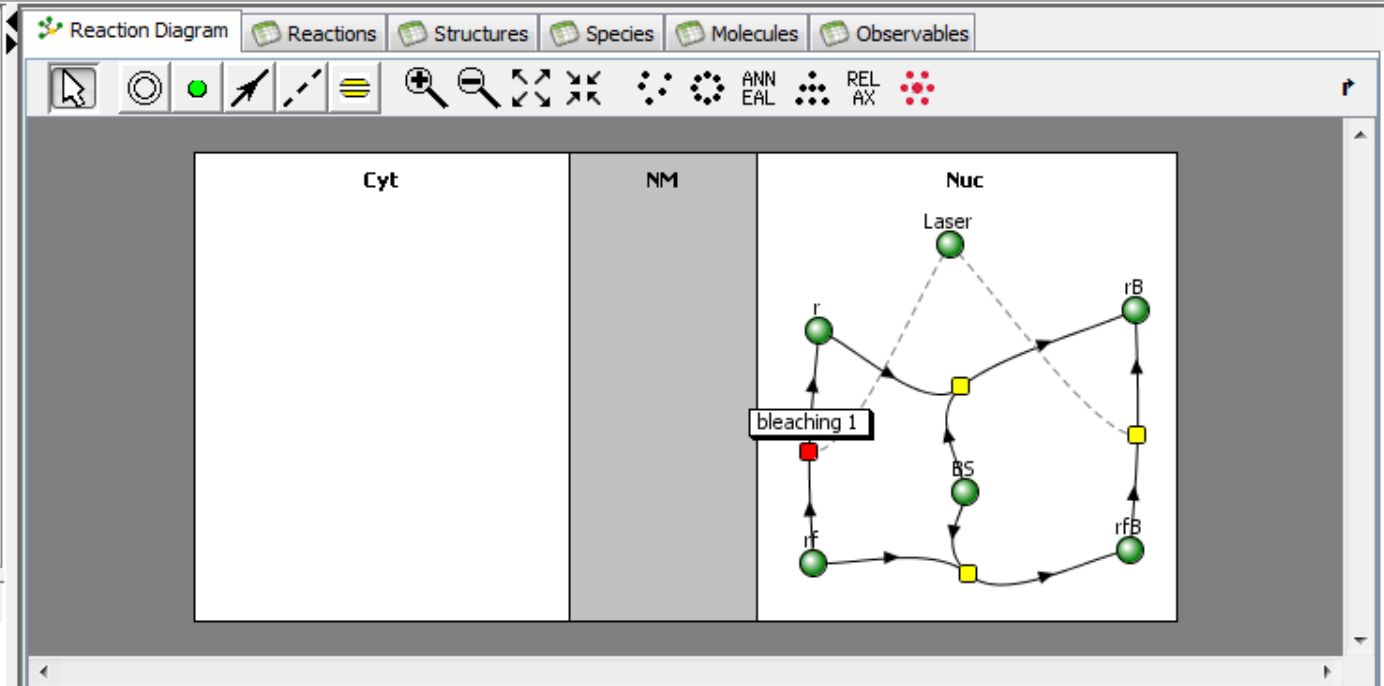
- Physiology
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  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
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Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Reaction Name  Next to Reaction Name type "bleaching 1".

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

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

Annotation and Pathway Links

**BioModel4**

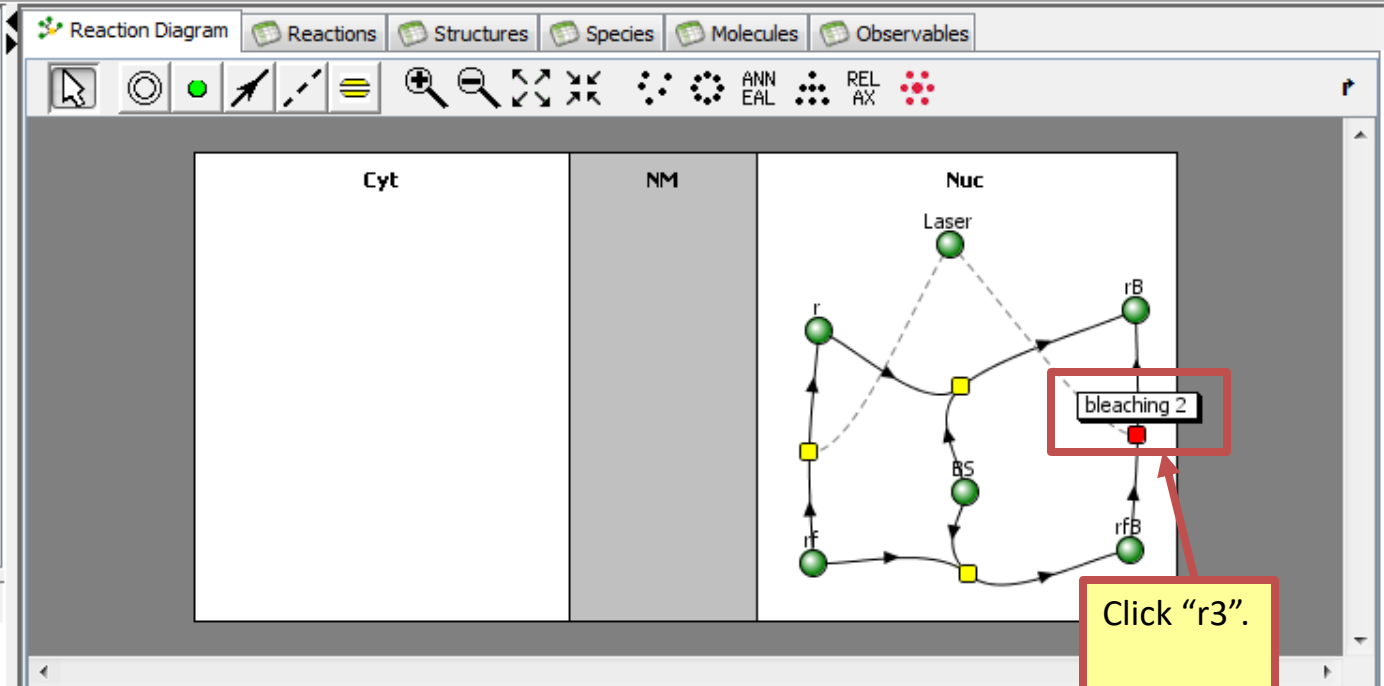
- Physiology
  - Reaction Diagram**
  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (0)
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BioModels MathModels Geometries

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  - Tutorials (5)
  - Education (33)
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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 [μM/s] (recommended for stochastic application) Convert to [molecules.s<sup>-1</sup>]

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$(K_f \cdot r_{fB} - K_r \cdot r_B)$	$\mu\text{M} \cdot \text{s}^{-1}$
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>
r <sub>fB</sub>	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM
r <sub>B</sub>	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM

Annotation and Pathway Links

**BioModel4**

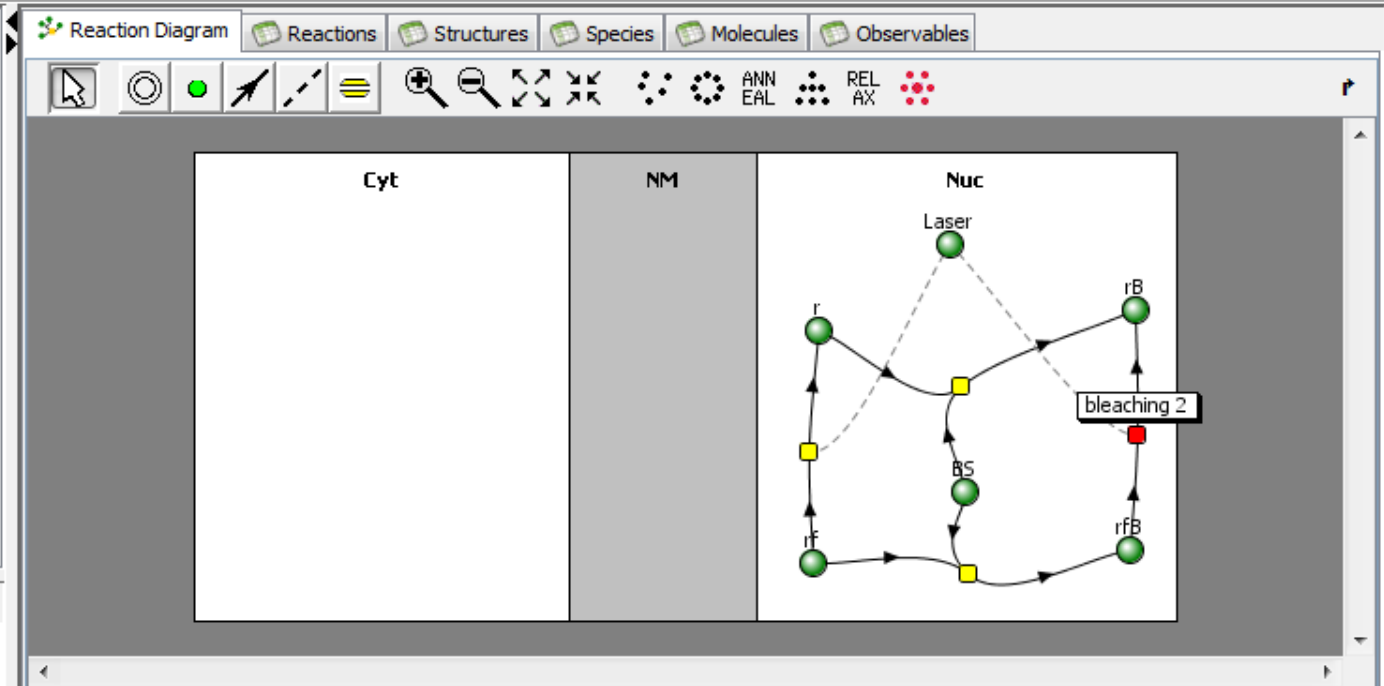
- Physiology
  - Reaction Diagram**
  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (0)
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Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Reaction Name bleaching 2

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

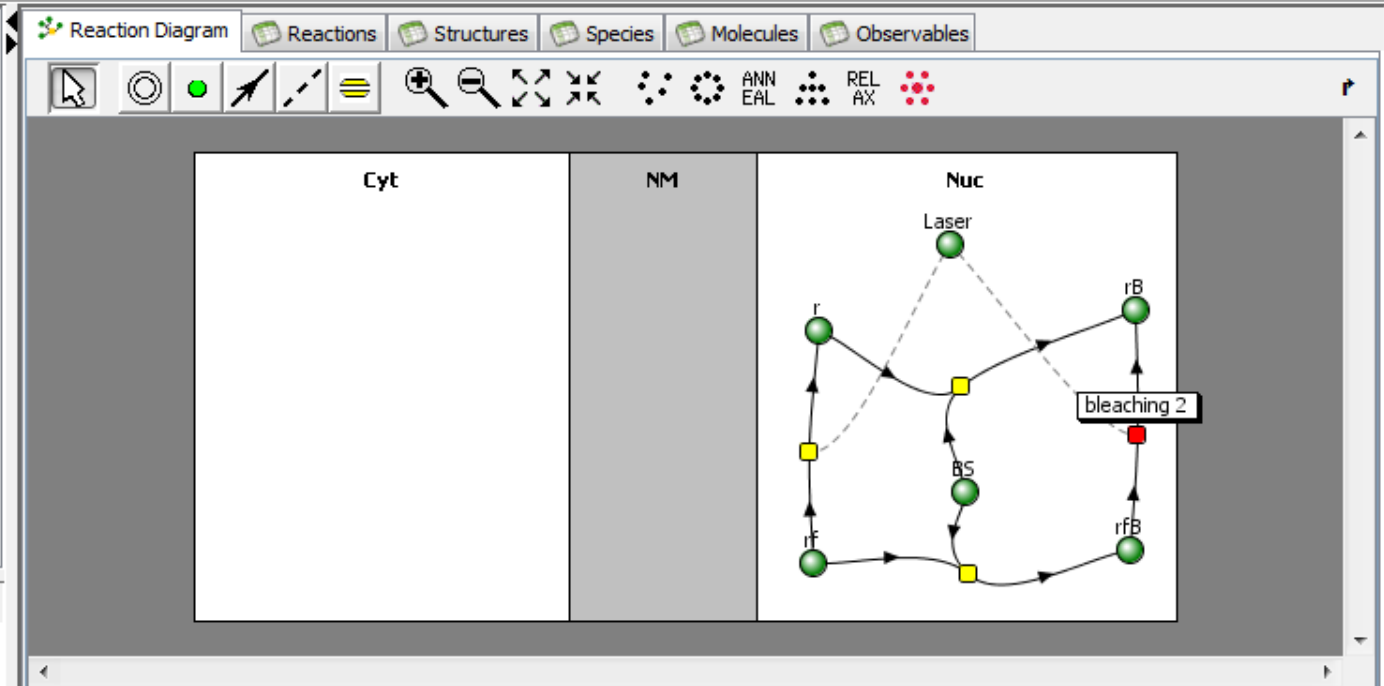
Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	0.0	$\mu\text{M}\cdot\text{s}^{-1}$

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

Annotation and Pathway Links

**BioModel4**

- Physiology
  - Reaction Diagram**
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Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings)

Reaction Name: bleaching 2  
 Kinetic Type: General [μM/s] Convert to [molecules.s<sup>-1</sup>]

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$(Vmax2 * rFB * Laser * ((t > 1.0) \& \& (t < 1.5)))$	μM.s <sup>-1</sup>

In the reaction rate row, type “(Vmax2\*rFB\*Laser\*((t>1.0)&&(t<1.5)))” under the Expression column. Press “Enter” on your keyboard to finalize.

Annotation and Pathway Links



**BioModel4**

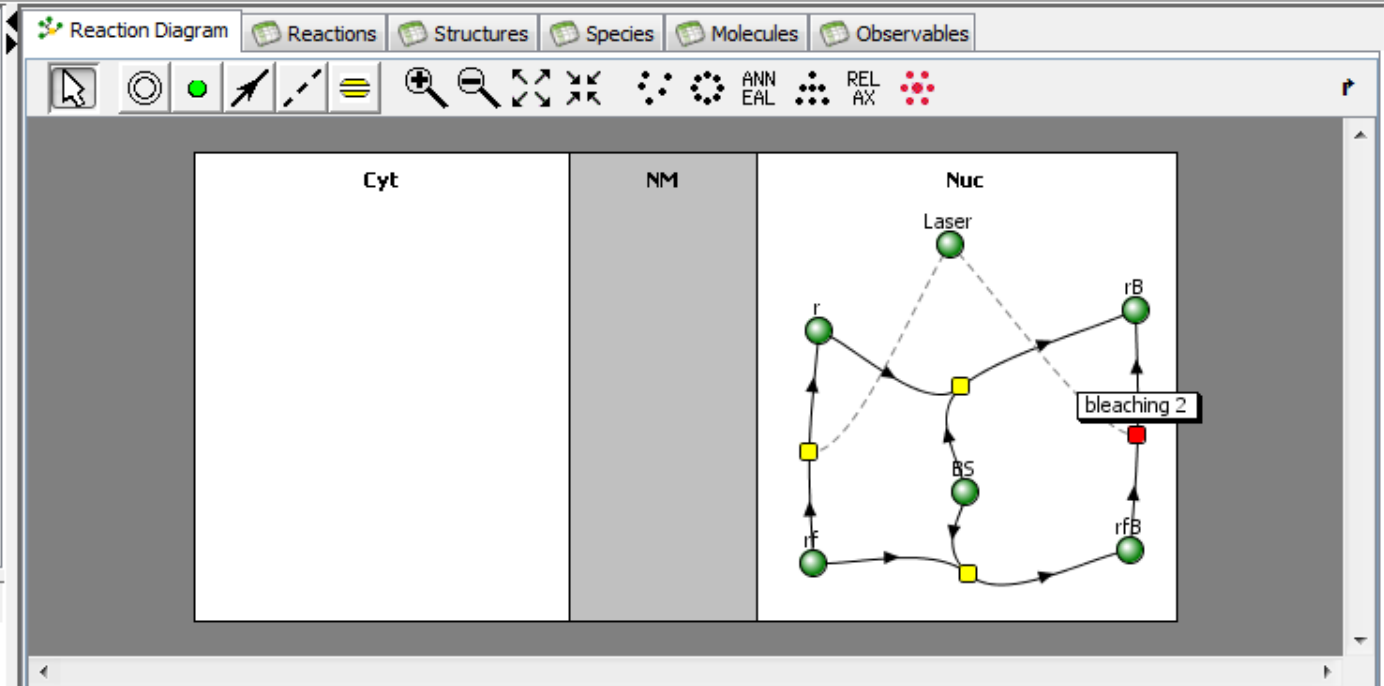
- Physiology
  - Reaction Diagram
  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (0)
- Parameters, Functions and Units
- Pathway

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

**Search**

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



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"/>	$V_{max2} \cdot rFB \cdot Laser \cdot ((t > 1.0) \ \&\& \ (t < 1.5))$	$\mu\text{M} \cdot \text{s}^{-1}$
Vmax2	user defined	<input type="checkbox"/>	50	$\text{s}^{-1} \cdot \mu\text{M}^{-1}$
rFB	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu\text{M}$
Laser	Species Concentration	<input checked="" type="checkbox"/>	Variable	$\mu\text{M}$
t	time	<input checked="" type="checkbox"/>	Variable	s

Annotation and Pathway Links

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

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

Click "Applications" > "New Application" > "Deterministic".

Name	Math Type	Annotation

VCell DB | BMDB | Pathway Comm | Sabio

BioModels | MathModels | Geometries

**Search**

- Biological Models
  - My BioModels (Zkhan) (5)
    - BioModel2
    - delete
    - FRAP-Binding
      - Private Tue Jun 26 11:53:48 EDT 2018
    - PHGFP Tutorial
    - PHGFP Tutorial 7.0
  - Shared BioModels (0)
  - Public BioModels (639)
  - Tutorials (8)
  - Education (33)

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

**BioModel4**

- Physiology
  - Reaction Diagram
  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (1)
  - 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**

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  - My BioModels (astfh234) (4)
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  - 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

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

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

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.

**BioModel4**

- Physiology
  - Reaction Diagram
  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (1)
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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	$\mu\text{M}$

File Server Window Tools Help

- BioModel4
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    - Reaction Diagram
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**Search**

Advanced >>

Search Show All

- Biological Models
  - My BioModels (astfh234) (4)
    - FRAPTutorial
    - BioModel4
    - Model2
    - tutorial 3
  - Shared BioModels (0)
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Selected BioModel Summary

Please type a new name:  
FRAPBindingTutorial

Save Cancel

Now is a good time to save your model.

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

ation

Initial Condition	
	5.0
	5.0
	0.0
	20.0

ion Units

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

**FRAPBindingTutorial**

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Geometry Specifications Protocols Simulations Parameter Estimation

Simulations Output Functions Generated Math

+

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.

**FRAPBindingTutorial**

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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.

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

**Search**

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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
----------------	---------	----------------------	------



**FRAP-Binding**

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Edit: Simulation0

**Parameters Solver** ← Click "Solver".

Choose solver algorithm and fine-tune time conditions:

Type Ending Time = 30.0

**General**

Time Bounds		Time Step		Error Tolerance	
Starting	0.0	Minimum		Absolute	1.0E-9
Ending	30.0	Default		Relative	1.0E-9
		Maximum	1.0		

**Local Sensitivity Analysis**

**Output Options**

- Keep Every 1 time samples and at most 1000 time samples
- Output Interval [ ] s
- Output Times [ ]

(Comma or space separated numbers, e.g. 0.5, 0.8, 1.2, 1.7)

Click "OK".

OK Cancel

Running Status Results

Running Status	Results
Running	yes

Scan

File Server Window Tools Help

**FRAPBindingTutorial**

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Geometry Specifications Protocols Simulations Parameter Estimation

Simulations Output Functions Generated Math

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

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

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 Server Window Tools Help

**FRAPBindingTutorial**

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Geometry Specifications Protocols Simulations Parameter Estimation

Simulations Output Functions Generated Math

Results icon (highlighted with a red box and arrow)

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
----------------	---------	----------------------	------

**Tutorial\_FRAPbinding**

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- Applications (2)
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  - Spatial

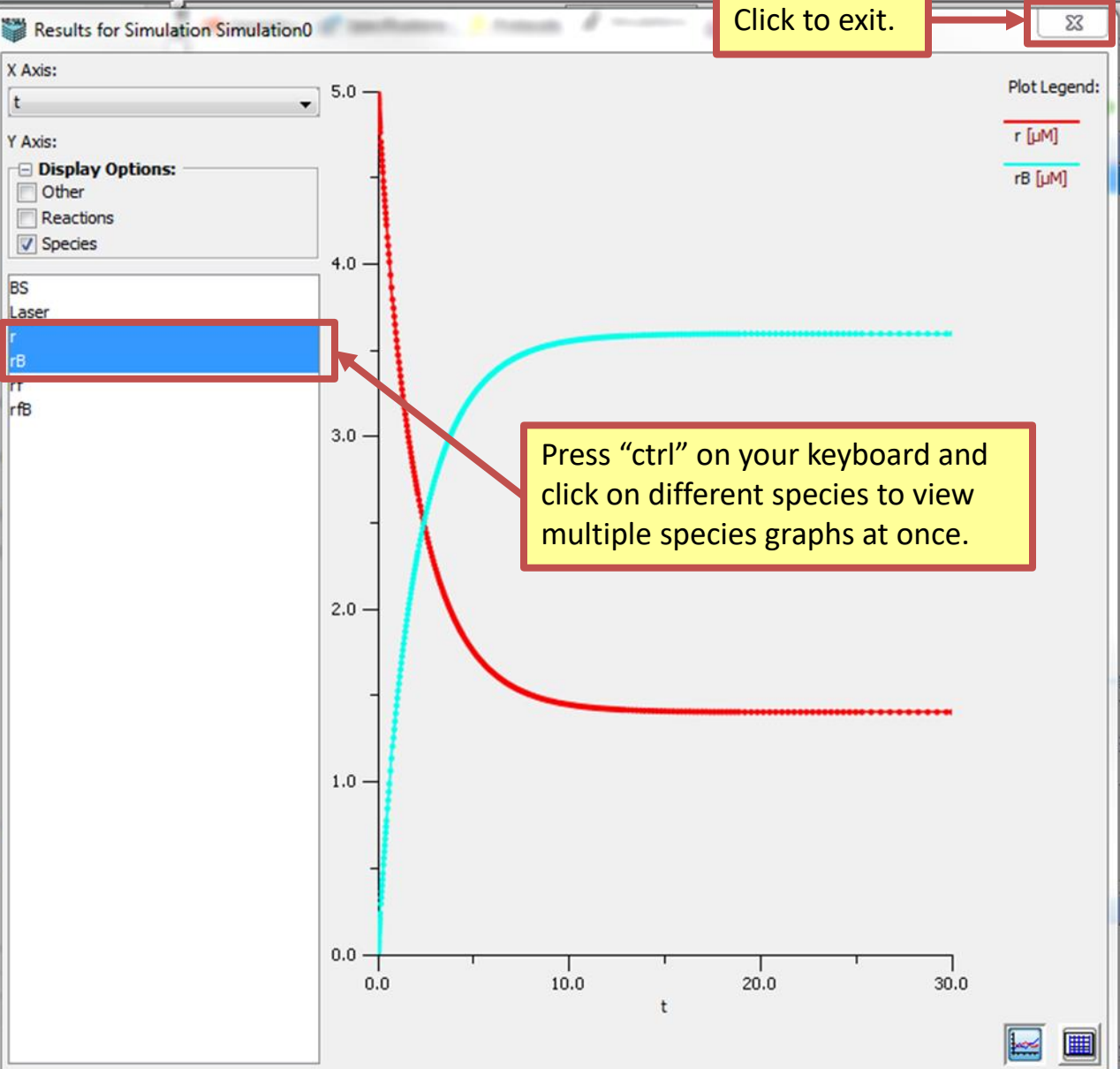
Parameters, Functions and

VCell DB BioModels.net Pathway

BioModels MathModels Geom

**Search**

- test
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- vFRAPtest1\_APCcell
- vFRAPtest1\_APCcell
- vFRAPtest1\_APCcell
- VICE FRAP 3-09 VICE



Click to exit.

r  
rB

Press "ctrl" on your keyboard and click on different species to view multiple species graphs at once.

Results
yes

Scan

**FRAPBindingTutorial**

- Physiology
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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**

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Object Properties Problems (0 Errors, 0 Warnings)

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

**FRAPBindingTutorial**

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Geometry Specifications Protocols Simulations Parameter Estimation

Simulations Output Functions Generated Math

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

Right click "Copy of Compartmental". Click "Rename". Type "Spatial". Press "Enter" on your keyboard to finalize.

Object Properties Problems (0 Errors, 0 Warnings)

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

**FRAP-Binding**

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Geometry Specifications Protocols Simulations Parameter Estimation

Structure Mapping Geometry Definition Kinematics

Domain: 0D, compartmental Edit Domain... Export... Edit Image Add Geometry ▾

Name	Value
Compartment	

Front  
Back  
Add Subdomain ▾  
Delete

Double click "Spatial" and click "Geometry" > "Geometry Definition".

Click "Add Geometry" > "New".

VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

+ Search

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

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

**FRAP-Binding**

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Parameters, Functions and Units

VCell DB | BMDB | Pathway Comm | Sabio

BioModels | MathModels | Geometries

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Geometry Specifications Protocols Simulations Parameter Estimation

Structure Mapping Geometry Definition Kinematics

Domain: OD, compartmental Edit Domain... Export... Edit Image Add Geometry ▾

Name	Value
Compartment	

Front

Back

Add Subdomain ▾

Delete

Choose

Click "Analytic Equations (2D)".

Geometry Type
Analytic Equations (1D)
<b>Analytic Equations (2D)</b>
Analytic Equations (3D)
Image based (import from file, zip or directory)
Mesh based (import from STL file)
New Blank Image Canvas
Constructed Solid Geometry (3D)
Import from Fiji/Imagej
Import from Blender

Click "OK".

OK Cancel



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Geometry Specifications Protocols Simulations

Structure Mapping Geometry De

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

Name	Value
Cyt	

Replace Geometry ▾

Front

Back

Add Subdomain ▾

Delete

Slice View Surface View Geometric Region Details

Info

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

Object Properties Problems (0 Errors, 4 Warnings)

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

**FRAP-Binding**

- Physiology
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BioModels | MathModels | Geometries

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Geometry | Specifications | Protocols | Simulations

Structure Mapping | Geometry Definition | Kinematics

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" > "Analytic".

Front | Back | Add Subdomain ▾ | Delete

Slice View | Surface View | Geometric Region Details

Info

Object Properties | Problems (0 Errors, 4 Warnings) | Database File Info

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

**FRAP-Binding**

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Geometry Specifications Protocols Simulations

Structure Mapping Geometry Definition Kinematics

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

Front Back Add Subdomain ▾ Delete

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

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

Help New Subdomain Cancel

Under "Radius" type "10".

Click "Add New Subdomain".

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Geometry Specification

Structure Mapping Geometry

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

Name	Value
Nuc	2.0 2.0 2.0 $((x)^2 + (y)^2) < (10.0)^2$
Cyt	1.0

Replace Geometry

Front

Back

Add Subdomain

Delete

Slice View Surface View Geometric Region Details

Info

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

Object Properties Problems (0 Errors, 6 Warnings)

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

**FRAP-Binding**

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Geometry Specifications Protocols Simulations

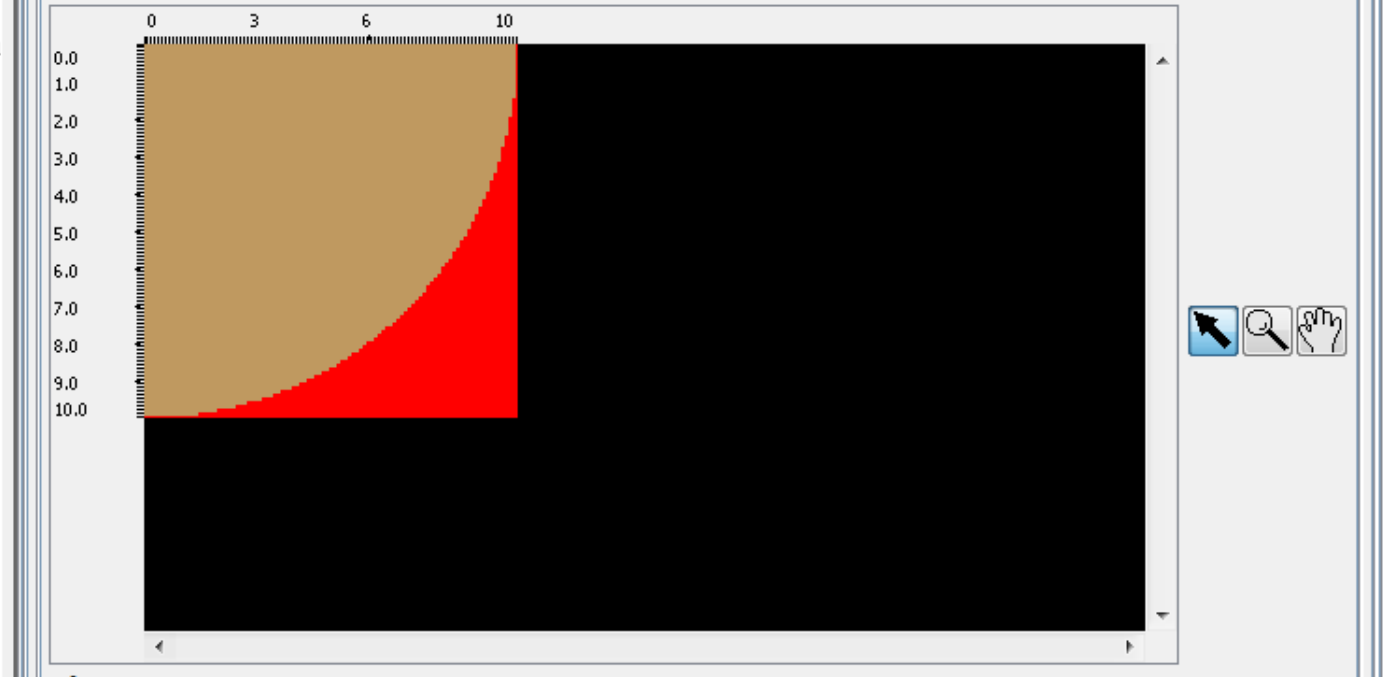
Structure Mapping Geometry Definition Kinematics

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

Name	Value
subdomain0	$((x)^2 + (y)^2) < (10.0)^2$
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.

**FRAP-Binding**

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Geometry Specifications Protocols Simulations

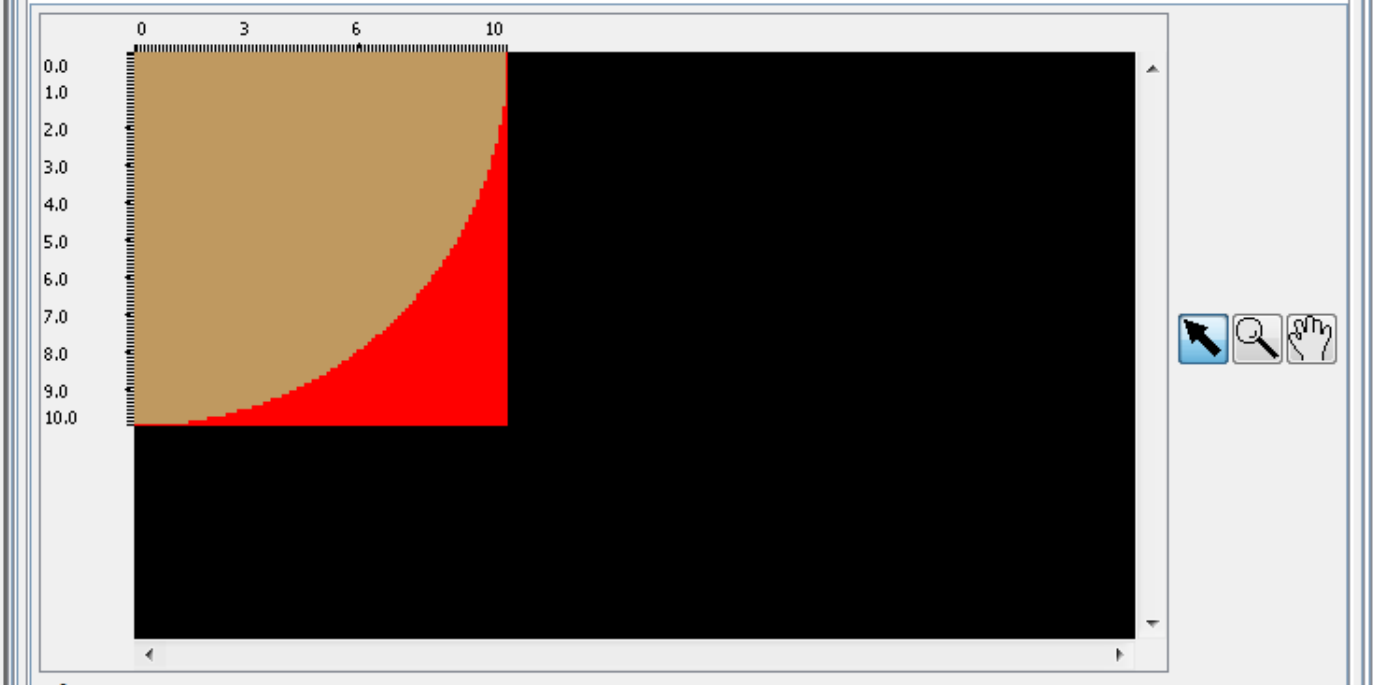
Structure Mapping Geometry Definition Kinematics

Domain: **Click "Edit Domain".** Edit Domain... Export... Edit Image Replace Geometry ▾

Name	Value
subdomain0	$\left( \left( \frac{x}{2.0} \right)^2 + \left( \frac{y}{2.0} \right)^2 \right) < (10.0)$
Cyt	1.0

Front  
Back  
Add Subdomain ▾  
Delete

Slice View Surface View Geometric Region Details



**FRAP-Binding**

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

VCell DB BMDB Pathway Comm Sabio

BioModels MathModels Geometries

**Search**

- Biological Models
  - My BioModels (Zkhan) (5)
  - Shared BioModels (0)
  - Public BioModels (639)
  - Tutorials (8)
  - Education (33)

Geometry Specifications Protocols Simulations

Structure Mapping Geometry Definition Kinematics

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

Name	Value
subdomain0	$((x)^2 + (y)^2) < (10.0)^2$
Cyt	1.0

Front Back Add Subdomain Delete

Next to "Size", type "22" for X and Y.

Geometry Size

Size X 22 μm Y 22 μm Z 10.0

Origin X -11 μm Y -11 μm Z 0

OK Cancel

Next to "Origin", type "-11" for X and Y.

Click "OK".

Info

**FRAPBindingTutorial**

- Physiology
  - Reaction Diagram
  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (2)
  - Compartmental
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    - Geometry**
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    - Protocols
    - Simulations
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VCeLL DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

**Search**

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

Geometry Specifications Protocols Simulations

Structure

**Domain:**

Name	Value
Nuc	2.0 2.0 2.0 $((x) + (y) < (10.0))$
Cyt	1.0

Front Back Add Subdomain Delete

Slice View Surface View Geometric Region Details

Info

Your "Slice View" should now be a circle of radius 10 μm inside of an 22 X 22 μm square.

Object Properties Problems (0 Errors, 6 Warnings)

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



Geometry Specifications Protocols Simulations

**FRAPBindingTutorial**

- Physiology
  - Reaction Diagram
  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (2)
  - Compartmental
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  - Geometry**
  - Specifications
  - Protocols
  - Simulation
- Parameters, Functions

Structure Mapping
Go to Structure Mapping

Physiology (structures)

Cyt

Nuc

NM

Geometry (subdomains)

- Nuc
- Cyt
- Cyt\_Nuc\_membrane

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

Use the line tool to drag a line from the structures to their corresponding subdomains

Object Properties Problems (0 Errors, 0 Warnings)

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

**FRAPBindingTutorial**

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

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

Go back to the "Compartmental" Applications (Double click "Compartmental" ), then select "Simulations" > results icon.

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

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

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
----------------	---------	----------------------	------

**FRAP-Binding**

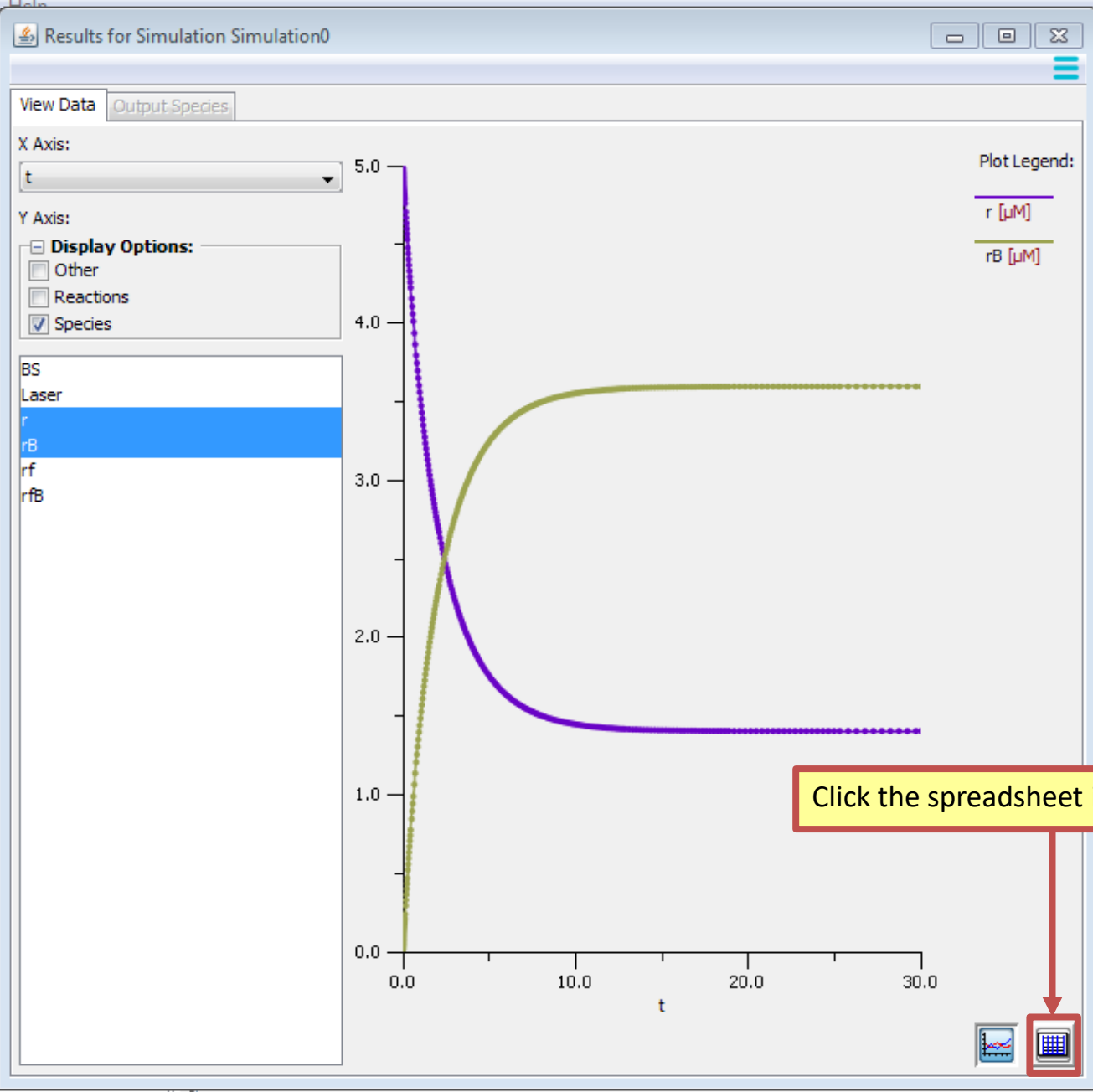
- Physiology
  - Reaction Diagram
  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (2)
  - Compartment
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VCell DB BMDB Pathway Co

BioModels MathModels Ge

**Search**

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Click the spreadsheet icon.

us	Results
	yes

Scan

**FRAP-Binding**

- Physiology
  - Reaction Diagram
  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables (0)
- Applications (2)
  - Compartment
  - Spatial
- Geometry
- Specification
- Protocols
- Simulations
- Parameters, Functions

Results for Simulation Simulation0

View Data Output Species

X Axis: t

Y Axis:  Display Options:  Other  Reactions  Species

t	BS	rB	rf	rfB
0	20	0	5	0
4.7762591E-11	20	9.5525535E-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
0.01346038	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	5.3265665E-2	4.9467343	5.3265665E-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".

Results

Results
yes

Scan

**FRAP-Binding**

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

VCell DB BMDB Pathway Co

BioModels MathModels Ge

**Search**

- Biological Models
  - My BioModels (Zkhan)
  - Shared BioModels (0)
  - Public BioModels (639)
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  - Education (33)

Results for Simulation Simulation0

View Data Output Species

X Axis: t

Y Axis:
 

- Display Options:
  - Other
  - Reactions
  - Species

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
21.112715	12.808648	3.595676	1.404324	3.595676
21.434518	12.808538	3.595731	1.404269	3.595731
21.756321	12.808442	3.595779	1.404221	3.595779
22.078124	12.808358	3.5958212	1.4041788	3.5958212
22.399927	12.808284	3.595858	1.404142	3.595858
22.72173	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
25.296155	12.807922	3.5960399	1.4039622	3.5960399
25.617958	12.807902	3.5960508	1.4039542	3.5960508
25.939761	12.807884	3.5960607	1.4039481	3.5960607
26.261564	12.807867	3.5960697	1.4039437	3.5960697
26.583367	12.807852	3.5960778	1.4039408	3.5960778
26.90517	12.807838	3.596085	1.4039393	3.596085
27.226973	12.807825	3.5960913	1.4039391	3.5960913
27.548776	12.807813	3.5960966	1.4039401	3.5960966
27.870579	12.807802	3.5960989	1.4039421	3.5960989
28.192382	12.807792	3.5960999	1.4039451	3.5960999
28.514185	12.807783	3.5961004	1.4039491	3.5961004
28.835988	12.807775	3.5961004	1.4039541	3.5961004
29.157791	12.807768	3.5961001	1.4039591	3.5961001
29.479594	12.807762	3.5961001	1.4039641	3.5961001
29.801397	12.807757	3.5961001	1.4039691	3.5961001
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".

Results

yes
-----

Scan

- 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

Geometry Specifications Protocols Simulations

Species Reaction Network

Species	Structure	Clamped	Initial Condition	Well Mixed	Diffusion Constant
laser	Nuc	<input type="checkbox"/>	0.0	<input type="checkbox"/>	10.0
B	Nuc	<input type="checkbox"/>	0.0	<input type="checkbox"/>	10.0
fb	Nuc	<input type="checkbox"/>	0.0	<input type="checkbox"/>	10.0
	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".

VCCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

Search

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

Object Properties Problems (0 Errors, 0 Warnings)

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

Applications (2)

- Compartmental
  - Geometry
  - Specifications
  - Protocols
  - Simulations
- Spatial
  - Geometry
  - Specifications
  - Protocols
  - Simulations

Species Reactions

Species	Structure	Clamped	Initial Condition	Well Mixed	Diffusion Constant
rf_nucleus			'5.0'	->	'1.40389335666'
rB_nucleus			'0.0'	->	'3.59610664333'
BS_nucleus			'20.0'	->	'12.8077867133'
rfB_nucleus			'0.0'	->	'3.59610664333'

Choose Parameters to Paste

Select All

- rf\_nucleus
- rB\_nucleus
- BS\_nucleus
- rfB\_nucleus

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

OK Cancel

Velocity Y for r\_nucleus | Vel\_Y | <0.0>

Applications (2)

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

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. The Boolean evaluates to "1" when x and y are between -2 and +2; everywhere else the Boolean evaluates to zero. In this way, the bleach reaction that is catalyzed by laser only happens in a define region.

Description		Units
initial concentration for Laser_nucleus	initConc	$((x > -2.0) \ \&\& \ (x < 2.0) \ \&\& \ (y > -2.0) \ \&\& \ (y < 2.0))$ $\mu\text{M}$
diffusion constant for Laser_nucleus	diff	0.0 $\mu\text{m}^2 \cdot \text{s}^{-1}$



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
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  - 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 Server Window Tools Help

Species (0)  
Molecules (0)  
Observables (0)  
Applications (2)  
 - d/dt Compartmental
 

- Geometry
- Specifications
- Protocols
- Simulations
- Parameter Estimation

 - d/dt Spatial
 

- Geometry
- Specifications
- Protocols
- Simulations

 Parameters, Functions and Units  
Pathway

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

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Geometry Specifications Protocols **Simulations**

Simulations Output Functions Generated Math

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

Click "Simulations" > edit simulation icon.

Error

**Application geometry does not match Simulation geometry**  
Update Math before editing

OK

Click "OK" to acknowledge the error.  
The error arises in this tutorial because the math for the original compartmental application will be different from the spatial geometry. In the next slide we will refresh the math to fix the error.

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
----------------	---------	----------------------	------

The screenshot shows the VCell software interface. On the left is a tree view with categories like Species, Molecules, Observables, Applications (2), Parameters, and Pathway. The main area has tabs for Geometry, Specifications, Protocols, and Simulations. Under the Simulations tab, there are sub-tabs for Simulations, Output Functions, and Generated Math. The 'Generated Math' tab is selected and highlighted with a red box. Below it, there are radio buttons for 'Math Equations' (selected) and 'Math Description Language'. A 'Refresh Math' button is highlighted with a red box. Below the buttons is a tree view for 'math description' containing folders for constants, functions, volume domains, and membrane domains.

To fix the error message, click "Generated Math" > "Refresh Math".

The screenshot shows an error dialog box with a yellow warning icon. The text inside reads: "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))". An 'OK' button is highlighted with a red box.

Click "OK".

- 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

Geometry Specifications Protocols **Simulations**

Simulations Output Functions Generated Math

Icons: Add, Edit, Delete, Run, Stop, Help, Refresh

Name	End Time	Output Option	Solver	Running Status	Results
Simulation 1	1.0	every 0.05 sec	Fully-Implicit	not saved	no

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

VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

Search

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

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 Server Window Tools Help

- Species (0)
- Molecules (0)
- Observables (0)
- Applications (2)
  - Compartmental
    - Geometry
    - Specifications
    - Protocols
    - Simulations
    - Parameter Estimation
  - Spatial
    - Geometry
    - Specifications
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VCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

Search

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  - Tutorials (5)
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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

Total Size (elements) 51 x 51 = 2601

Spatial Step (um)  $\Delta x$  0.44

$\Delta y$  0.44

OK Cancel

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

Mesh: 101x101 = 10201 elements Geometry size: (22.0,22.0) microns

Parameters with values changed from defaults

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

VCCell DB BioModels.net Pathway Comm Sabio

BioModels MathModels Geometries

Search

Biological Models

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

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 Maximum 0.1

Ending 50.0 Default

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".

Results

Results	no
---------	----

Mesh: 101x101 = 10201 elements Geometry size: (22.0,22.0) microns

Parameters with values changed from defaults

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

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.

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)

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

**TRAP binding to cellular**

- 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



**FRAP-Binding**

- Physiology
  - Reaction Diagram
  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables
- Applications (2)
  - $d/dt$  Compartmental
  - $d/dt$  Spatial
    - Geometry
    - Specifications
    - Protocols
    - Simulation
- Parameters, Functions
- Pathways
  - VCell DB
  - BMDB
  - Pathway
- BioModels
  - MathModels
  - Search
    - Biological Models
      - My BioModels (Zkhan)
      - Shared BioModels (6)
      - Public BioModels (6)
      - Tutorials (8)
      - Education (33)

Results for Simulation Simulation1

View Data | Export Data | Post Processing

Time: 10.0

Slice View

0

47

All Variables

- BS
- J\_bleaching\_1
- J\_bleaching\_2
- J\_RAN\_binding
- J\_RAN\_FITC
- Laser
- Laser\_init\_uM
- r
- rB
- rF**
- rFB
- sobj\_Nuc1\_Cyt0\_size
- vobj\_Cyt0\_size
- vobj\_Nuc1\_size

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

Data Range (Min-Max)

Auto range

at time  all times

Max: 0.48158401927638794

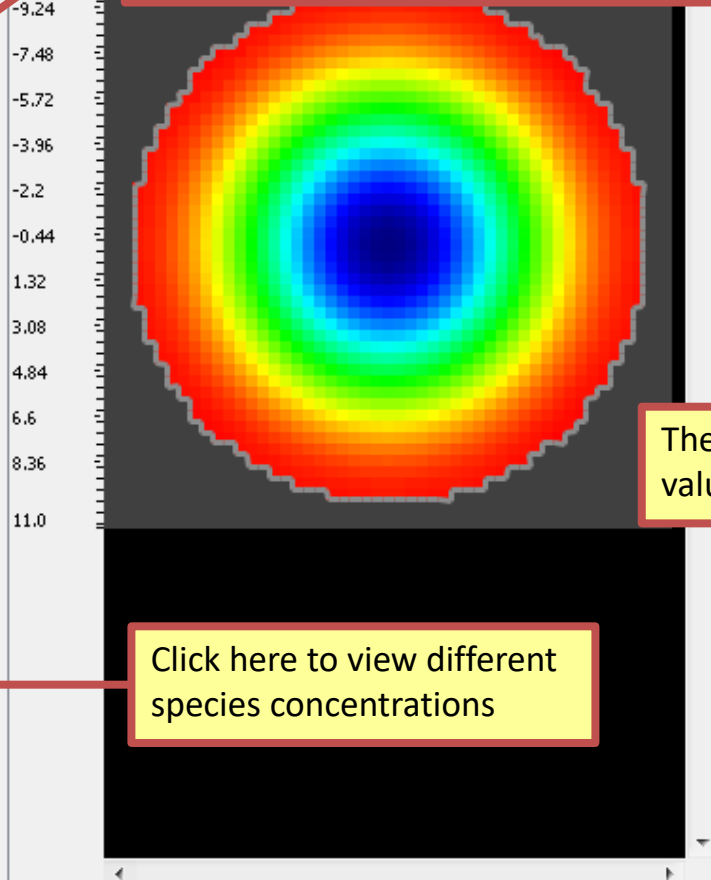
0.48158401927638794

Min: 0.481582402688458

0.481582402688458

The minimum and maximum values correspond to the colors

Click here to view different species concentrations



Navigation icons: arrow, magnifying glass, hand, pan, zoom, and other plot controls.

Plot | ROI

Results

yes

Scan

**FRAP-Binding**

- Physiology
  - Reaction Diagram
  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables
- Applications (2)
  - $d/dt$  Compartment
  - $d/dt$  Spatial
    - Geometry
    - Specification
    - Protocols
    - Simulation
- Parameters, Functions
- Pathway

VCell DB BMDB Pathway

BioModels MathModels

**Search**

- Biological Models
  - My BioModels (Zkhan)
  - Shared BioModels
  - Public BioModels (6)
  - Tutorials (8)
  - Education (33)

All Variables

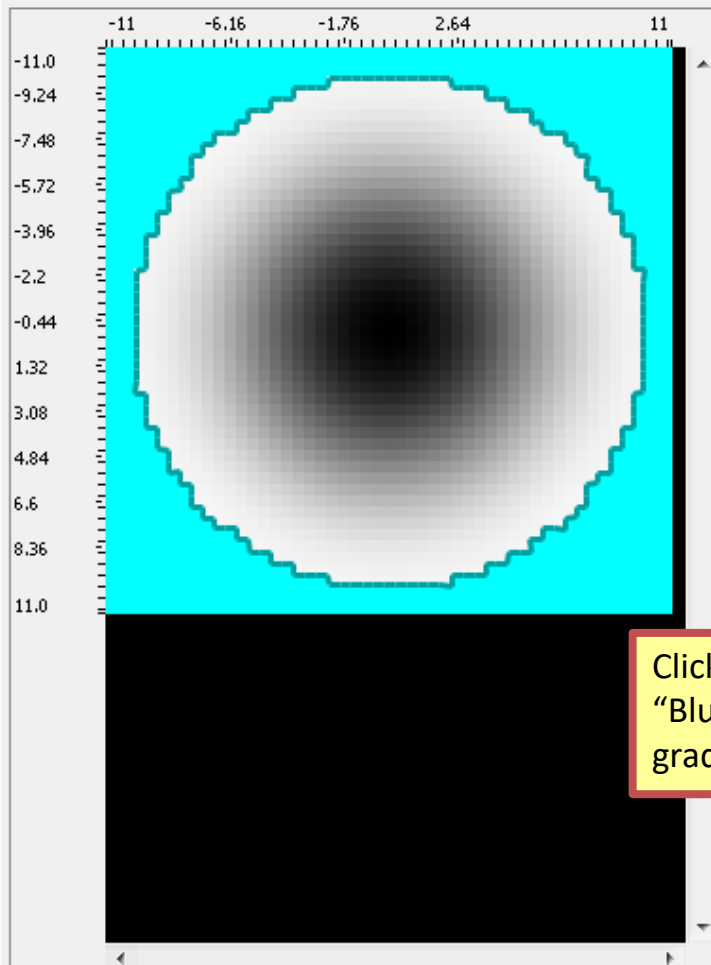
- BS
- J\_bleaching\_1
- J\_bleaching\_2
- J\_RAN\_binding
- J\_RAN\_FITC
- Laser
- Laser\_init\_uM
- r
- rB
- r**
- rB
- sobj\_Nuc1\_Cyt0\_size
- vobj\_Cyt0\_size
- vobj\_Nuc1\_size

Results for Simulation Simulation1

View Data Export Data Post Processing Stats Data Post Processing Image Data

Time: 10.0

Slice View



Data Range (Min-Max)

Auto range

at time  all times

Max: 0.48158401927638794

0.48158401927638794

Min: 0.481582402688458

0.481582402688458

Color

BM AM NN ND NR

Gray

BlueRed

Plot ROI

Click on either "Gray" or "BlueRed" to change the color gradient.

Results

yes

Scan

**FRAP-Binding**

- Physiology
  - Reaction Diagram
  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables
- Applications (2)
  - $d/dt$  Compartment
  - $d/dt$  Spatial
    - Geometry
    - Specification
    - Protocols
    - Simulation
- Parameters, Functions
- Pathway
  - VCell DB
  - BMDB
  - Pathway
- BioModels
  - MathModels
  - Search
    - Biological Models
      - My BioModels (Zkhan)
      - Shared BioModels (6)
      - Public BioModels (6)
      - Tutorials (8)
      - Education (33)

Results for Simulation Simulation1

View Data | Export Data | Post Processing Stats Data | Post Processing Image Data

Time: 10.0

Slice View

Data Range (Min-Max)

- Auto range
- at time  all times
- Max: 0.48158401927638794
- 0.48158401927638794
- Min: 0.481582402688458
- 0.481582402688458

Color

- BM  AM  NN  ND  NR
- Gray
- BlueRed

All Variable

- BS
- J\_bleaching
- J\_bleaching
- J\_RAN\_bin
- J\_RAN\_FIT
- Laser
- Laser\_init\_uM
- r
- rB
- rf
- rfB
- sobj\_Nuc1\_Cyt0\_size
- vobj\_Cyt0\_size
- vobj\_Nuc1\_size

Info

Plot | ROI

Click on a point within the data and click on another point. A line will form and connect the two points.

Click on the line tool.

Click "Plot" > "Spatial" to create a graph of the two points.

**FRAP-Binding**

- Physiology
  - Reaction Diagram
  - Reactions (4)
  - Structures (3)
  - Species (6)
  - Molecules (0)
  - Observables
- Applications (2)
  - Compartment
  - Spatial
  - Geometry
  - Specification
  - Protocols
  - Simulation
- Parameters, Functions
- Pathway

VCell DB | BMDB | Pathway

BioModels | MathModels

**Search**

- Biological Models
  - My BioModels (Zkhan)
  - Shared BioModels (6)
  - Public BioModels (6)
  - Tutorials (8)
  - Education (33)

All Variables

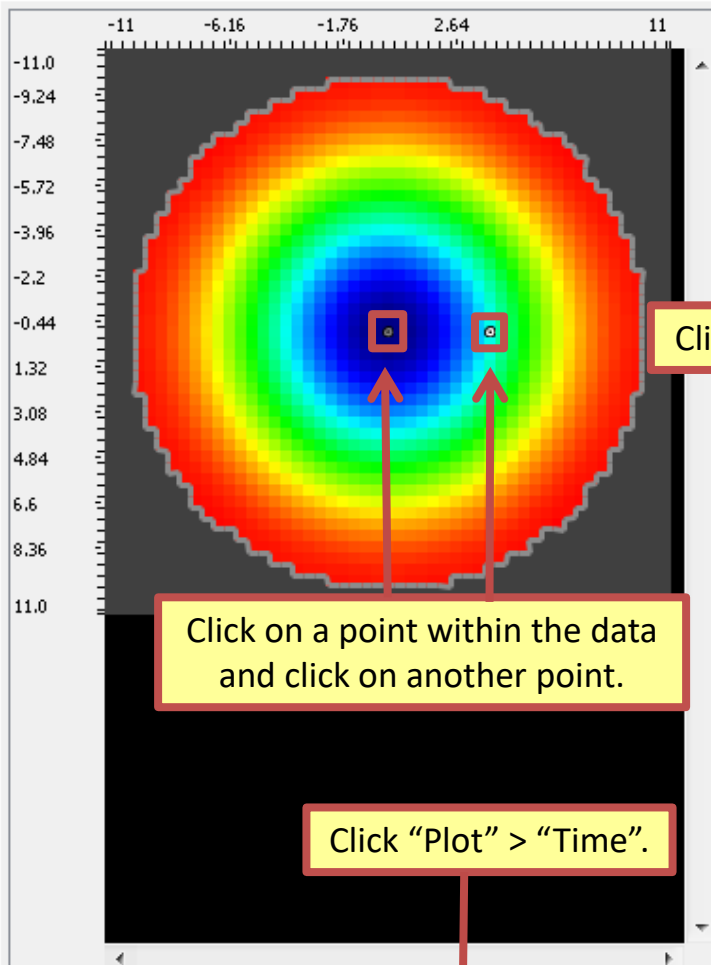
- BS
- J\_bleaching\_1
- J\_bleaching\_2
- J\_RAN\_binding
- J\_RAN\_FITC
- Laser
- Laser\_init\_uM
- r
- rB
- r**
- rFB
- sobj\_Nuc1\_Cyt0\_size
- vobj\_Cyt0\_size
- vobj\_Nuc1\_size

Results for Simulation Simulation1

View Data | Export Data | Post Processing Stats Data | Post Processing Image Data

Time: 10.0

Slice View



Data Range (Min-Max)

- Auto range
- at time  all times
- Max: 0.48158401927638794
- 0.48158401927638794
- Min: 0.481582402688458
- 0.481582402688458

BM AM NN ND NR

- Gray
- BlueRed

Click the dot tool.

Click on a point within the data and click on another point.

Click "Plot" > "Time".

Plot ROI

Results

yes

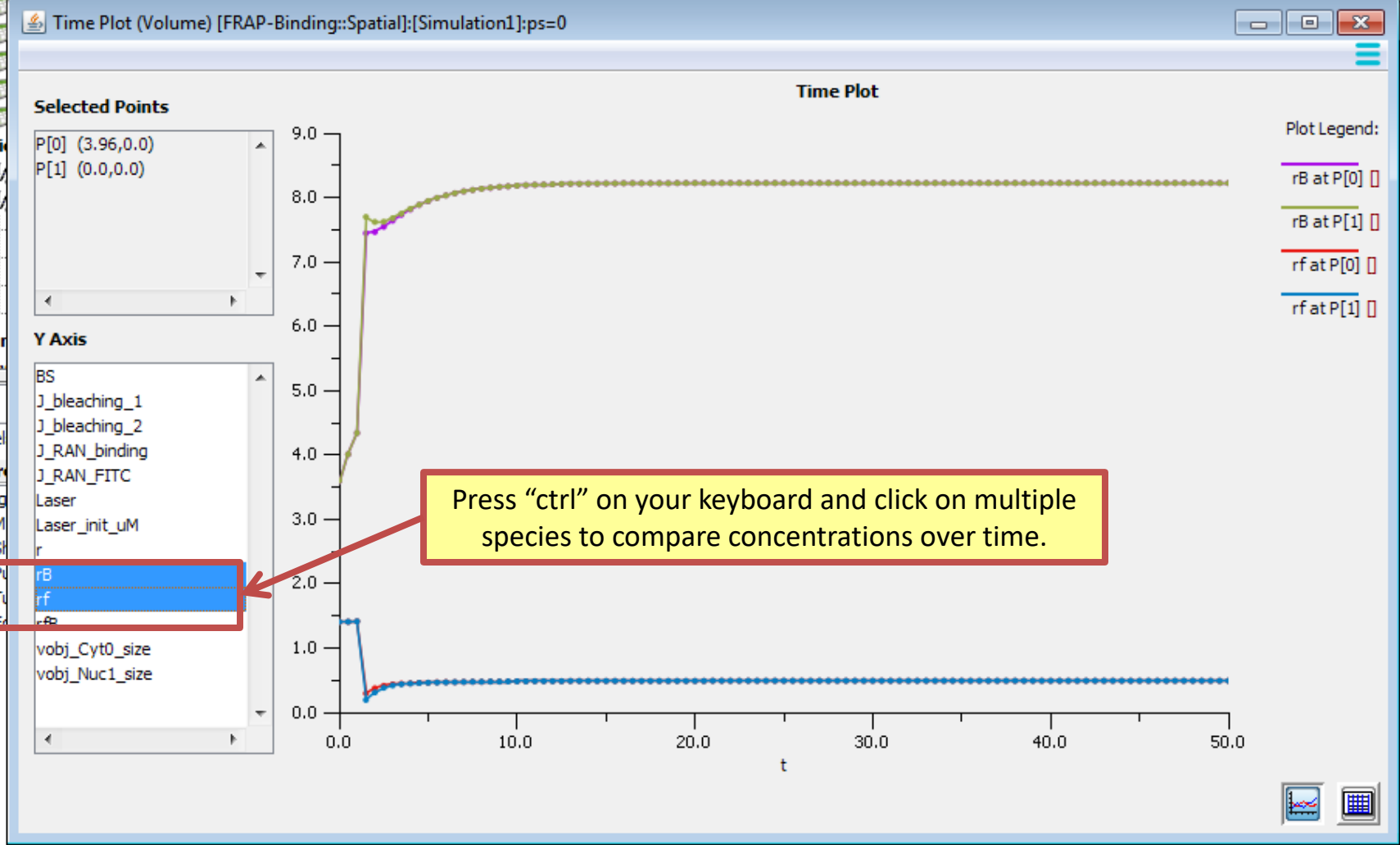
Scan

FRAP-Binding

- Physiology
- Reaction Diagram
- Applic
- Param
- Path
- VCell DB
- BioModel
- Search
- Biolog
- M
- St
- P
- T
- E

Results for Simulation Simulation1

View Data | Export Data | Post Processing Stats Data | Post Processing Image Data



Press "ctrl" on your keyboard and click on multiple species to compare concentrations over time.

# Acknowledgements

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Tanya Miller (2015) – Pomperaug High School

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Zaiba Khan (2018) – East Windsor High School

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