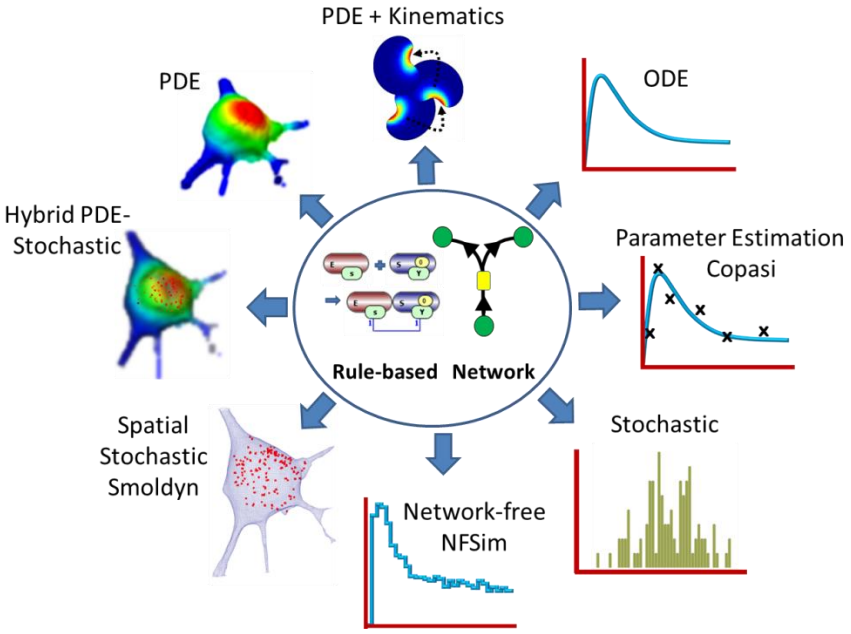
VCell

A modeling environment for the simulation of cellular events, where you can download at 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)

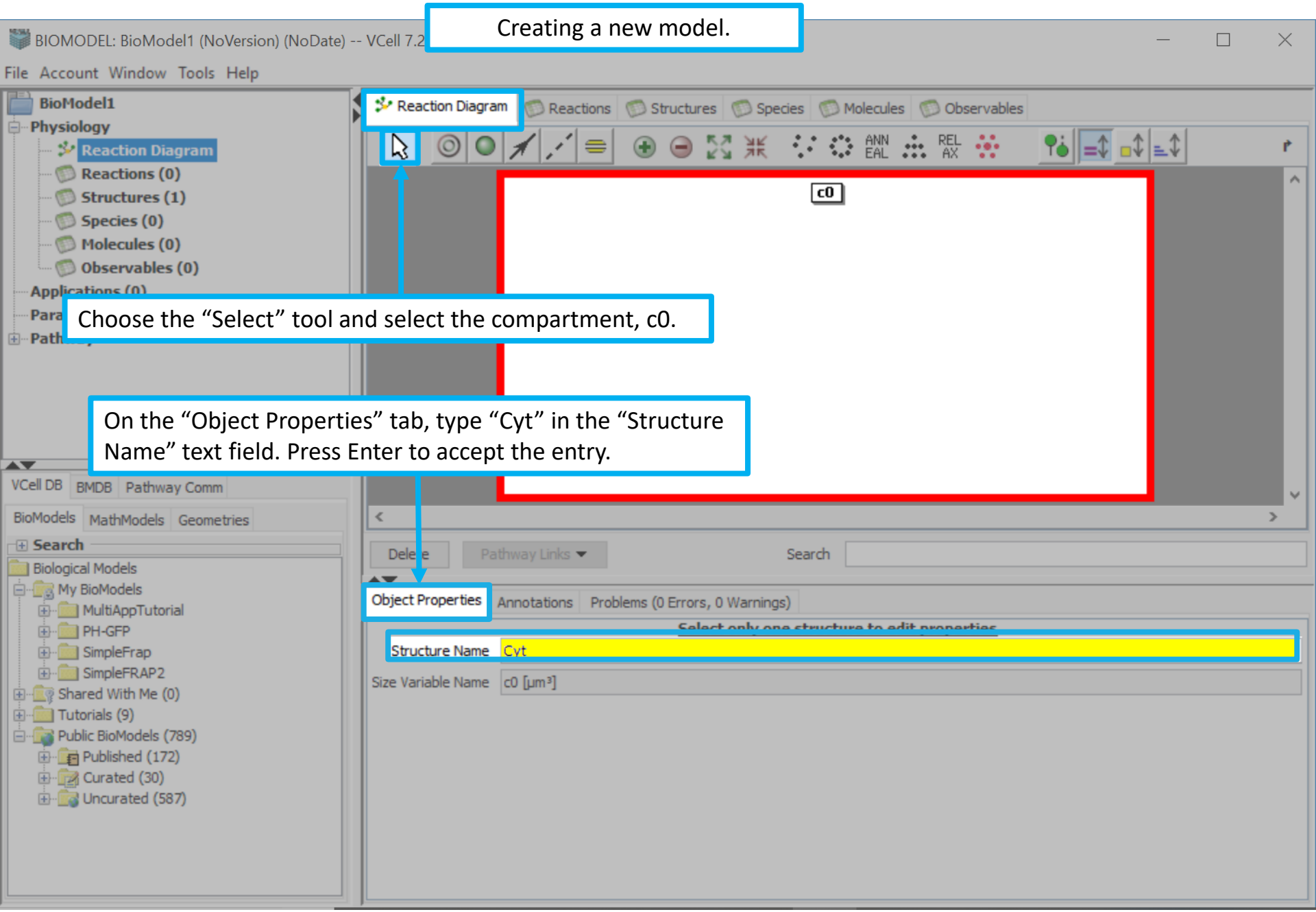
VCell Tutorial

FRAP with binding

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

In this tutorial you will:

- 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
- Create a timed event in a spatial simulation.
- View and analyze results of a spatial simulation.


Creating a new model.
BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 7.2
File Account Window Tools Help
BioModel1
Physiology
Reaction Diagram
Reactions (0)
Structures (1)
Species (0)
Molecules (0)
Observables (0)
Applications (0)
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
c0
Choose the “Select” tool and select the compartment, c0.
On the “Object Properties” tab, type “Cyt” in the “Structure Name” text field. Press Enter to accept the entry.
VCell DB
BMDB
Pathway Comm
BioModels
MathModels
Geometries
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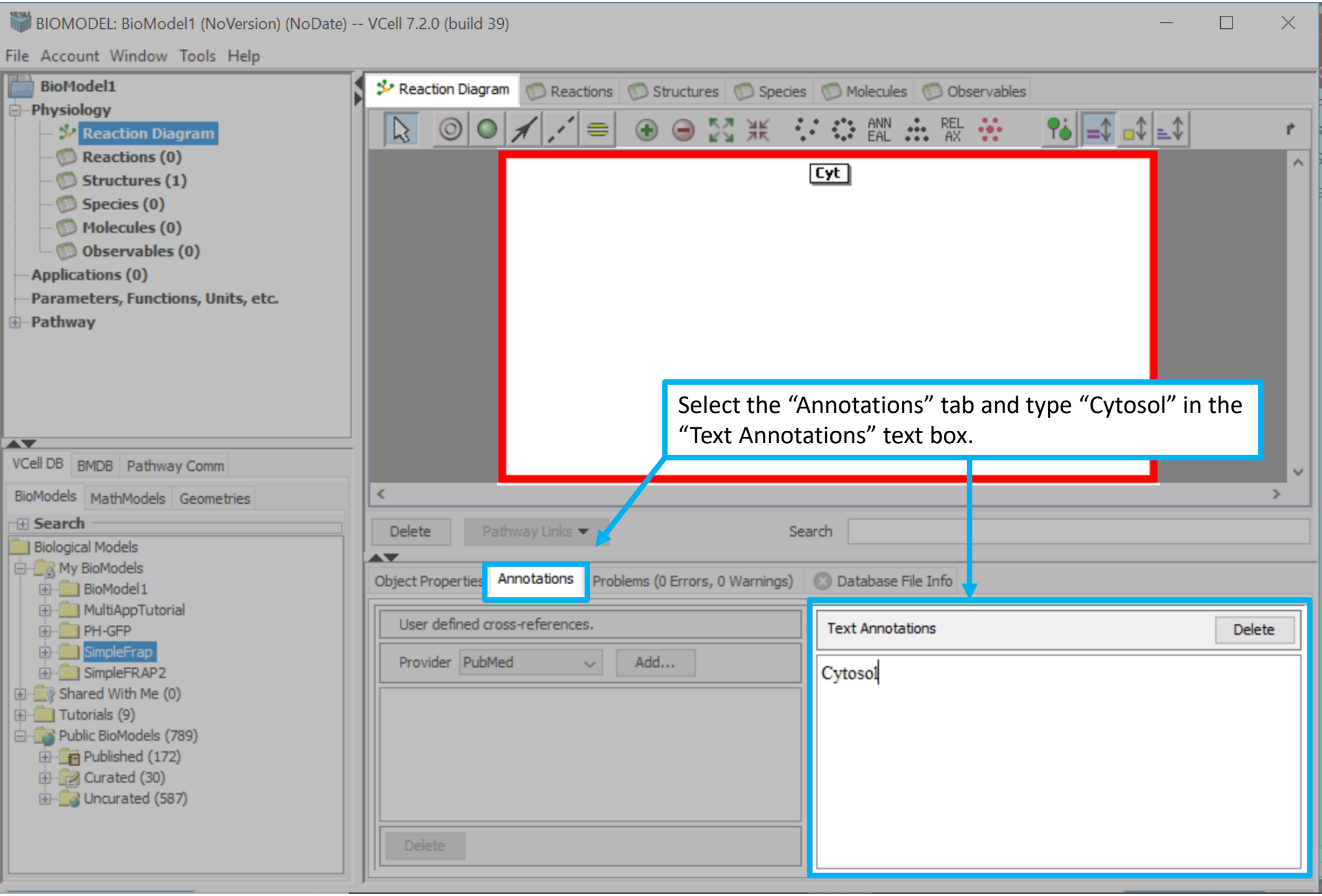
SimpleFrap
SimpleFRAP2
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)
Curated (30)
Uncurated (587)
Delete
Pathway Links
Search
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Structure Name
Cyt
Size Variable Name
c0 [µm³]


BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
BioModel1
Physiology
Reaction Diagram
Reactions (0)
Structures (1)
Species (0)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions, Units, etc.
Pathway
VCell DB BMDB Pathway Comm
BioModels MathModels Geometries
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SimpleFrap
SimpleFRAP2
Shared With Me (0)
Tutorials (9)
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Reaction Diagram
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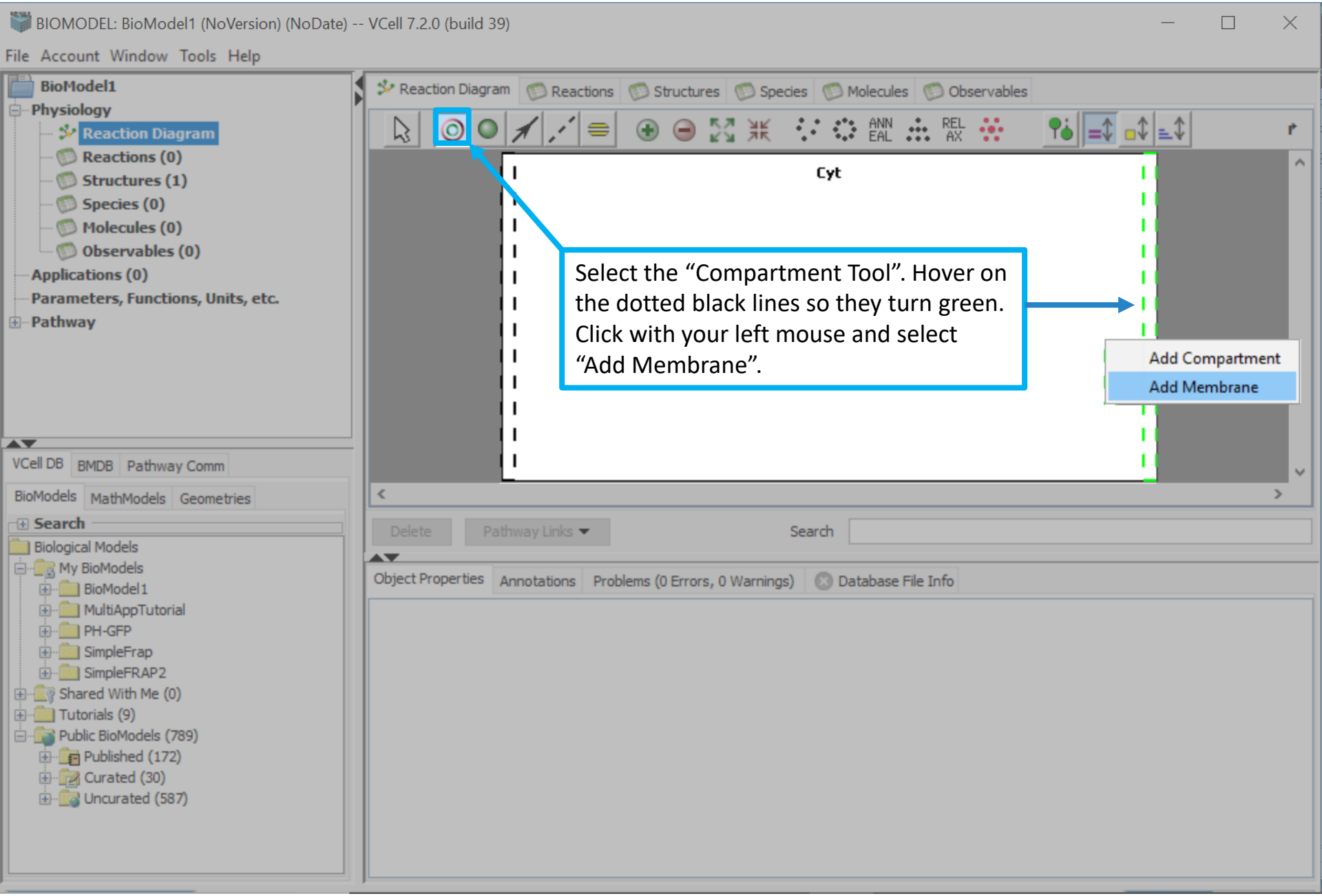
Structures
Species
Molecules
Observables
Cyt
Delete
Pathway Links
Search
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Database File Info
User defined cross-references.
Provider PubMed
Add...
Delete
Text Annotations
Delete
Cytosol
Select the “Annotations” tab and type “Cytosol” in the “Text Annotations” text box.


BIOMODEL: BioModel1 (NoVersion) (NoDate) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
BioModel1
Physiology
Reaction Diagram
Reactions (0)
Structures (1)
Species (0)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions, Units, etc.
Pathway
VCell DB BMDB Pathway Comm
BioModels MathModels Geometries
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Uncurated (587)
Reaction Diagram
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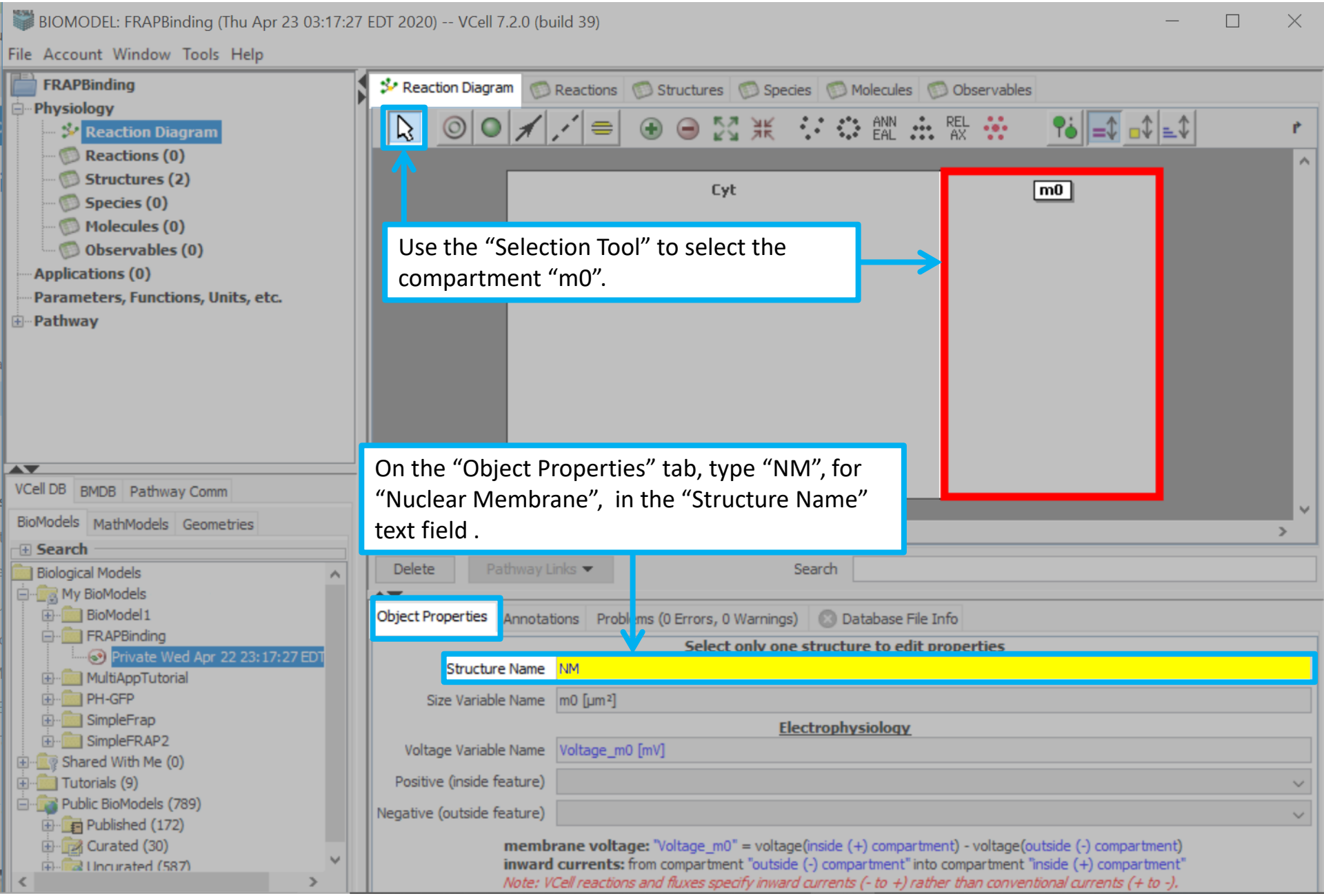
Molecules
Observables
Cyt
Select the "Compartment Tool". Hover on the dotted black lines so they turn green. Click with your left mouse and select "Add Membrane".
Add Compartment
Add Membrane
Delete
Pathway Links
Search
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Database File Info


BIOMODEL: FRAPBinding (Thu Apr 23 03:17:27 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (0)
Structures (2)
Species (0)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions, Units, etc.
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
Cyt
m0
Use the “Selection Tool” to select the compartment “m0”.
On the “Object Properties” tab, type “NM”, for “Nuclear Membrane”, in the “Structure Name” text field .
Delete
Pathway Links
Search
Object Properties
Annotations
Database File Info
Select only one structure to edit properties
Structure Name
NM
Size Variable Name
m0 [µm²]
Electrophysiology
Voltage Variable Name
Voltage_m0 [mV]
Positive (inside feature)
Negative (outside feature)
membrane voltage: "Voltage_m0" = 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 -).
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My BioModels
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FRAPBinding
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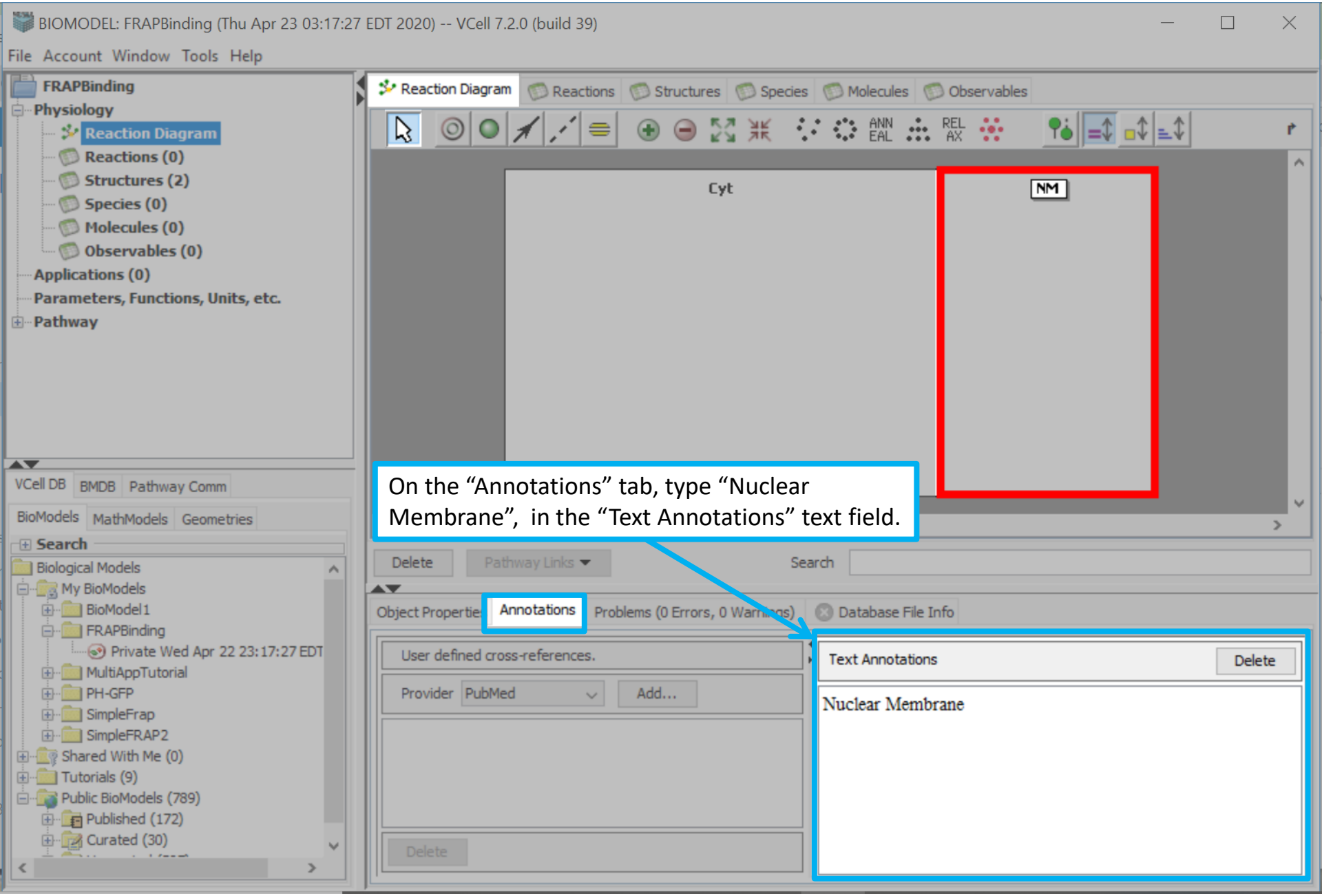
SimpleFrap
SimpleFRAP2
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)
Curated (30)


BIOMODEL: FRAPBinding (Thu Apr 23 03:17:27 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (0)
Structures (2)
Species (0)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions, Units, etc.
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
Cyt
NM
On the “Annotations” tab, type “Nuclear Membrane”, in the “Text Annotations” text field.
Delete
Pathway Links
Search
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Database File Info
User defined cross-references.
Provider PubMed
Add...
Delete
Text Annotations
Delete
Nuclear Membrane
VCell DB
BMDB
Pathway Comm
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Geometries
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SimpleFRAP2
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Tutorials (9)
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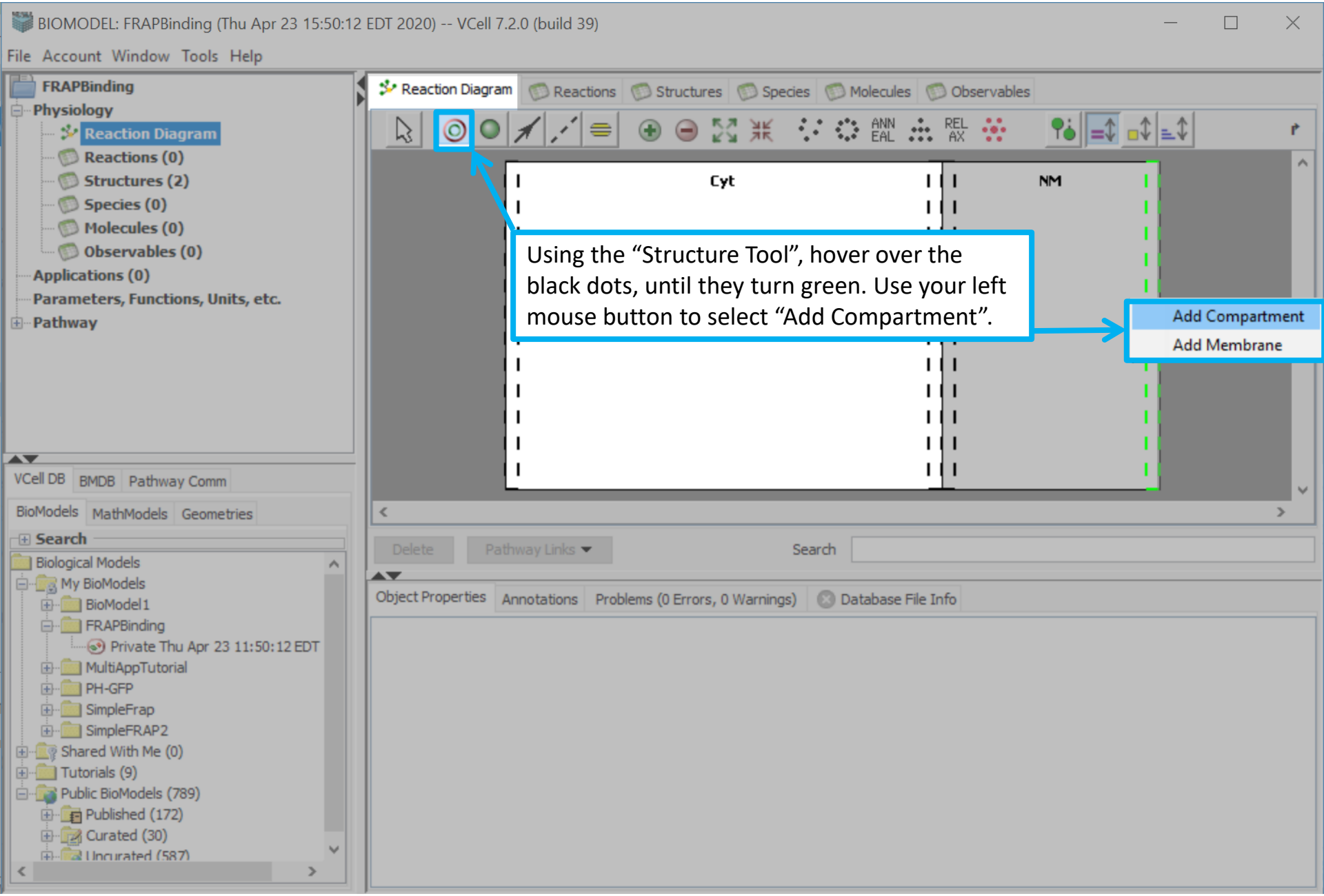
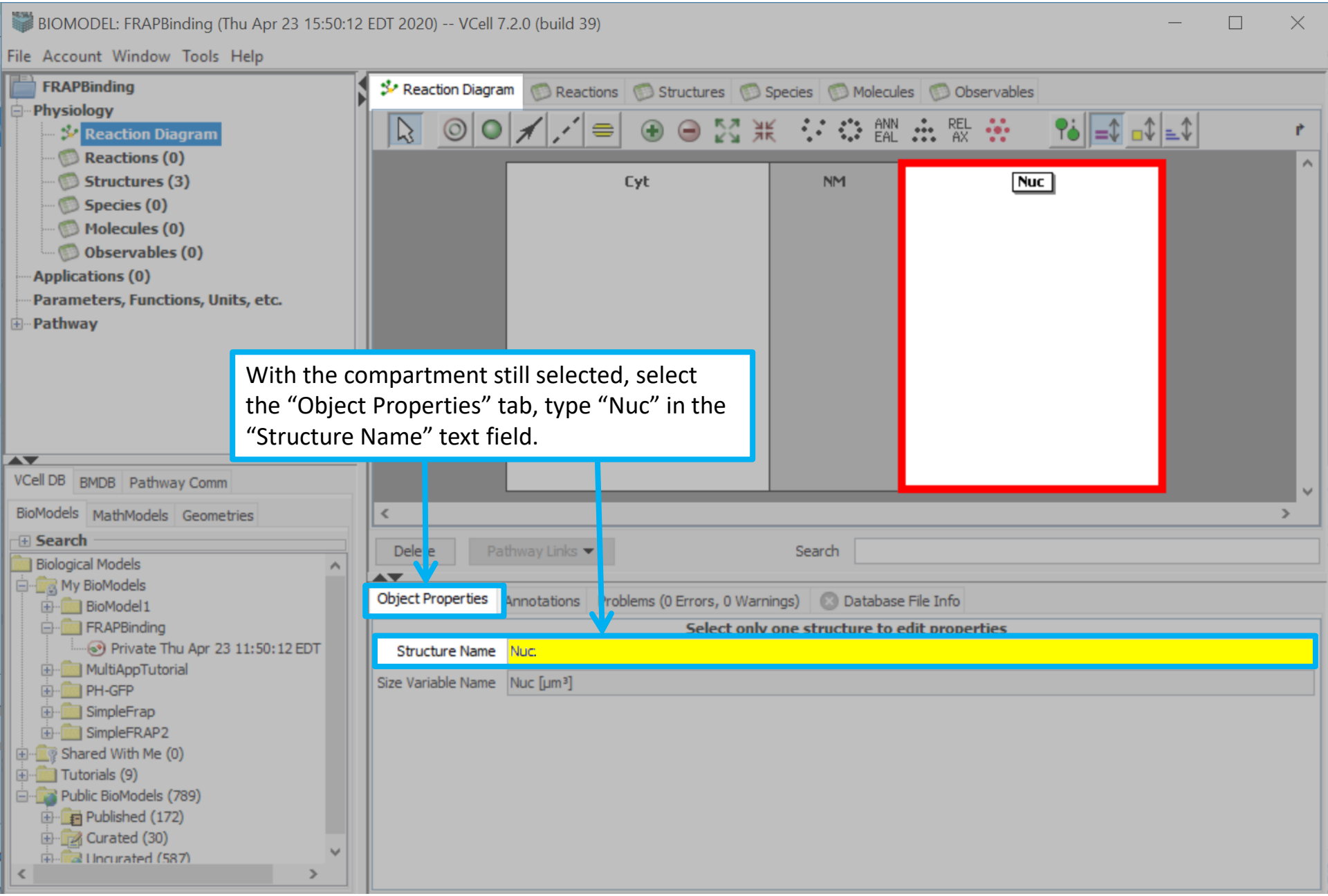
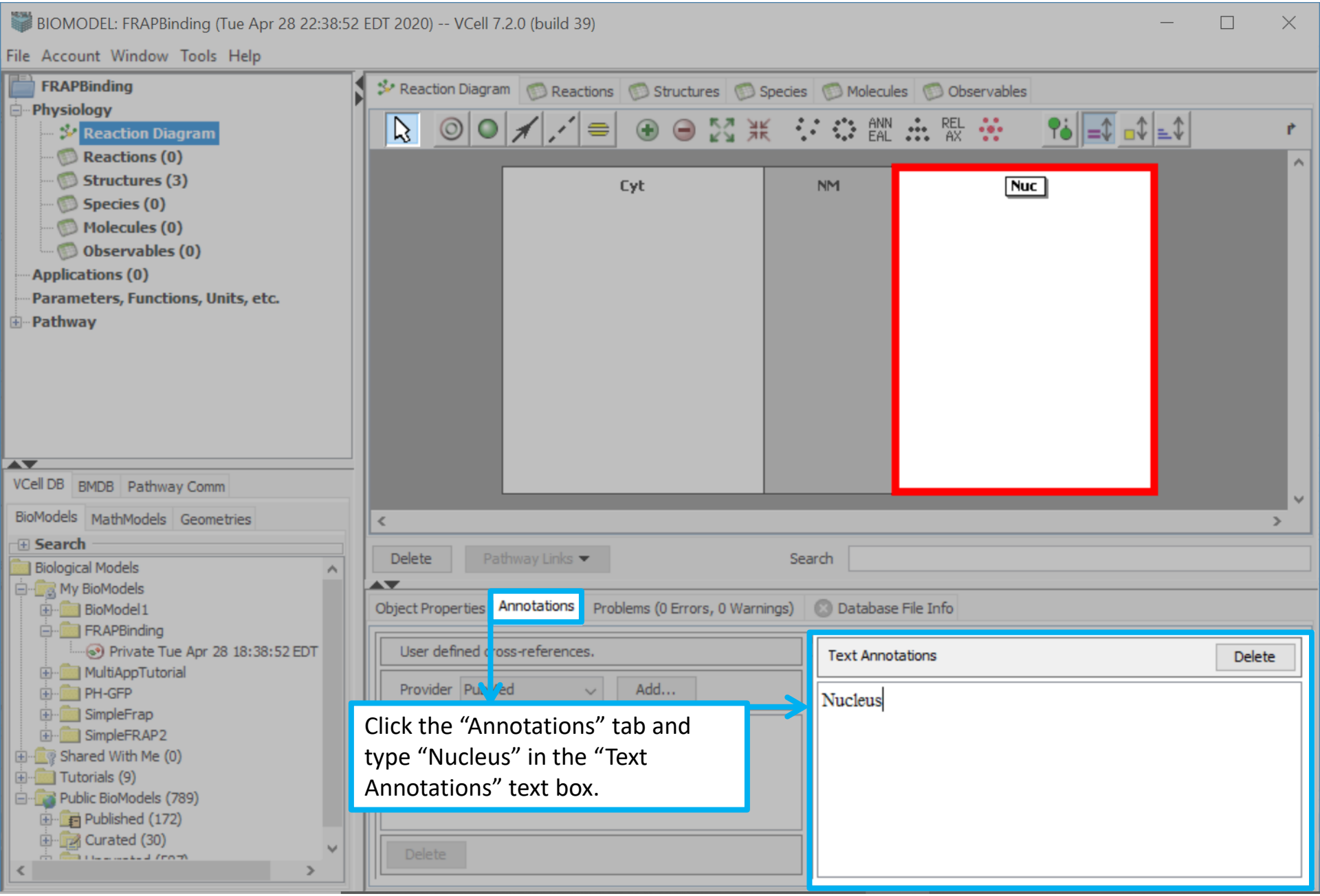
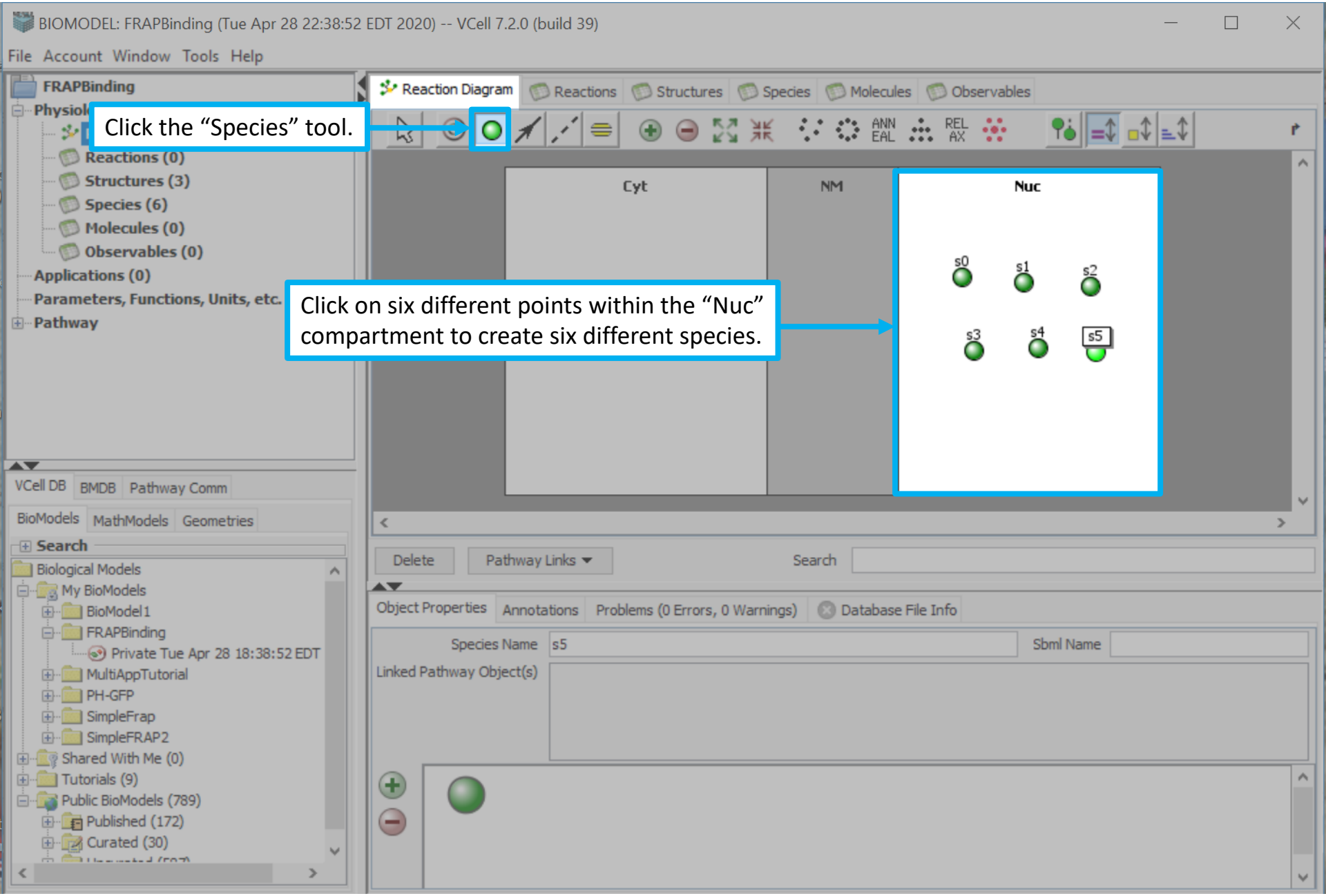
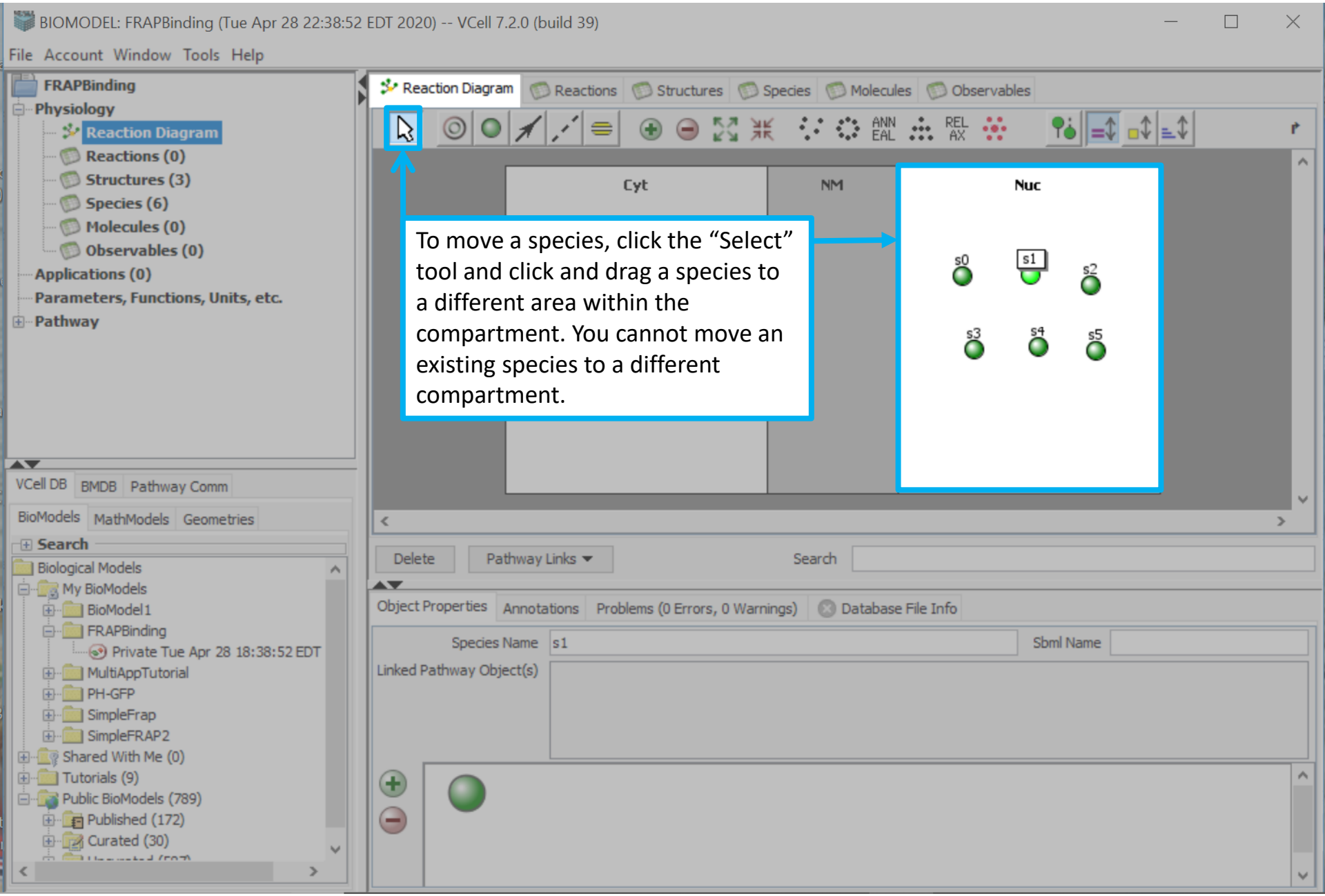
Published (172)
Curated (30)


BIOMODEL: FRAPBinding (Thu Apr 23 15:50:12 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (0)
Structures (2)
Species (0)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions, Units, etc.
Pathway
VCell DB BMDB Pathway Comm
BioModels MathModels Geometries
Search
Biological Models
My BioModels
BioModel1
FRAPBinding
Private Thu Apr 23 11:50:12 EDT
MultiAppTutorial
PH-GFP
SimpleFrap
SimpleFRAP2
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)
Curated (30)
Uncurated (587)
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
Cyt
NM
Using the “Structure Tool”, hover over the black dots, until they turn green. Use your left mouse button to select “Add Compartment”.
Add Compartment
Add Membrane
Delete
Pathway Links
Search
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Database File Info


BIOMODEL: FRAPBinding (Thu Apr 23 15:50:12 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (0)
Structures (3)
Species (0)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions, Units, etc.
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
Cyt
NM
Nuc
With the compartment still selected, select the "Object Properties" tab, type "Nuc" in the "Structure Name" text field.
Delete
Pathway Links
Search
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Database File Info
Select only one structure to edit properties
Structure Name
Nuc
Size Variable Name
Nuc [µm³]
VCell DB
BMDB
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels
BioModel1
FRAPBinding
Private Thu Apr 23 11:50:12 EDT
MultiAppTutorial
PH-GFP
SimpleFrap
SimpleFRAP2
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)
Curated (30)


BIOMODEL: FRAPBinding (Tue Apr 28 22:38:52 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (0)
Structures (3)
Species (0)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions, Units, etc.
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
Cyt
NM
Nuc
Delete
Pathway Links
Search
VCell DB
BMDB
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels
BioModel1
FRAPBinding
Private Tue Apr 28 18:38:52 EDT
MultiAppTutorial
PH-GFP
SimpleFrap
SimpleFRAP2
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)
Curated (30)
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Database File Info
User defined cross-references.
Provider
Add...
Delete
Text Annotations
Delete
Nucleus
Click the “Annotations” tab and type “Nucleus” in the “Text Annotations” text box.


BIOMODEL: FRAPBinding (Tue Apr 28 22:38:52 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiol
Reactions (0)
Structures (3)
Species (6)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions, Units, etc.
Pathway
Click the “Species” tool.
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
Cyt
NM
Nuc
s0
s1
s2
s3
s4
s5
Click on six different points within the “Nuc” compartment to create six different species.
VCell DB
BMDB
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels
BioModel1
FRAPBinding
Private Tue Apr 28 18:38:52 EDT
MultiAppTutorial
PH-GFP
SimpleFrap
SimpleFRAP2
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)
Curated (30)
Delete
Pathway Links
Search
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Database File Info
Species Name
s5
Sbml Name
Linked Pathway Object(s)


BIOMODEL: FRAPBinding (Tue Apr 28 22:38:52 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (0)
Structures (3)
Species (6)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions, Units, etc.
Pathway
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 and drag a species to a different area within the compartment. You cannot move an existing species to a different compartment.
VCell DB
BMDB
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels
BioModel1
FRAPBinding
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MultiAppTutorial
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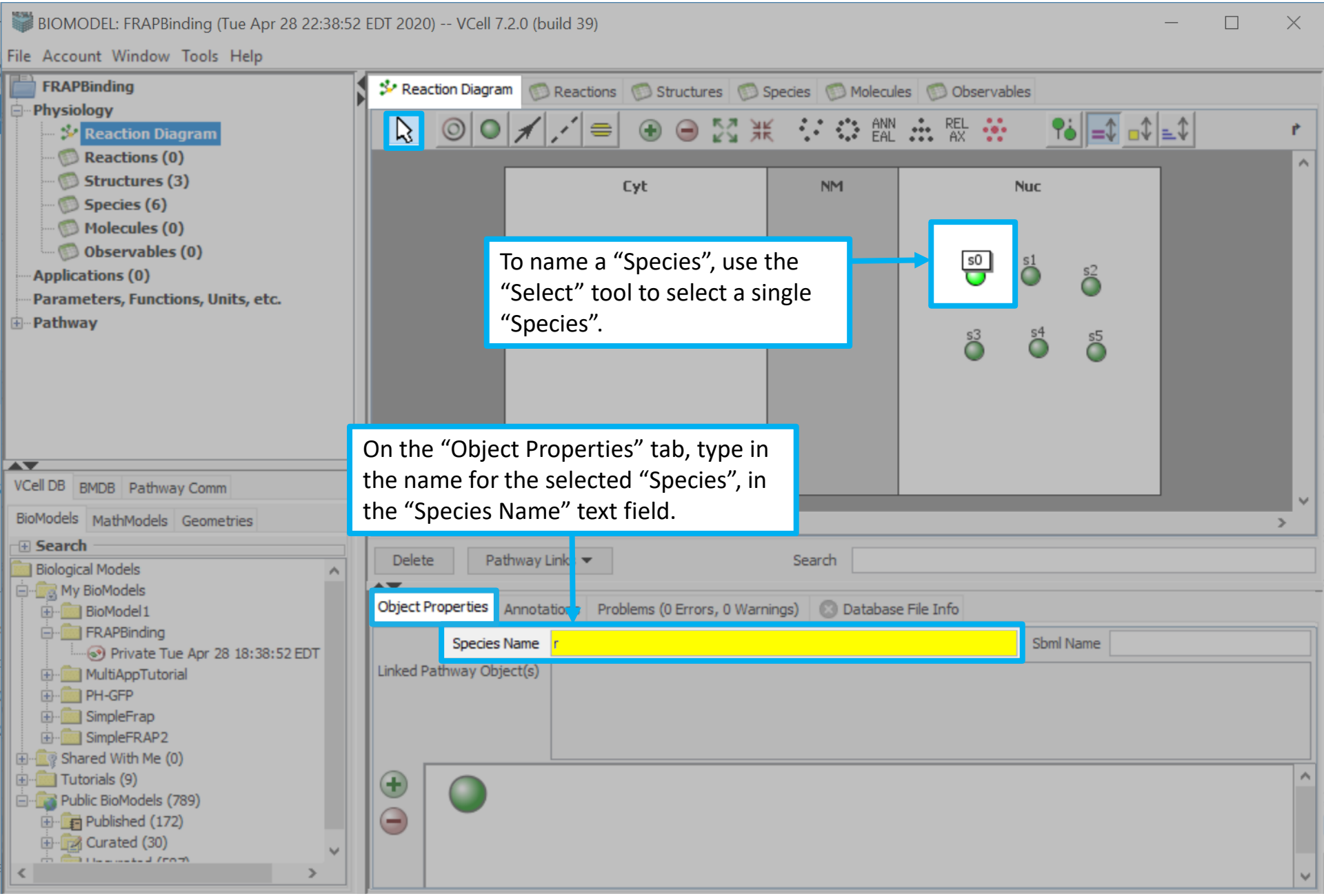
SimpleFrap
SimpleFRAP2
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)
Curated (30)
Delete
Pathway Links
Search
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Database File Info
Species Name
s1
Sbml Name
Linked Pathway Object(s)


BIOMODEL: FRAPBinding (Tue Apr 28 22:38:52 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (0)
Structures (3)
Species (6)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions, Units, etc.
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
Cyt
NM
Nuc
s0
s1
s2
s3
s4
s5
To name a “Species”, use the “Select” tool to select a single “Species”.
On the “Object Properties” tab, type in the name for the selected “Species”, in the “Species Name” text field.
VCell DB
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Pathway Comm
BioModels
MathModels
Geometries
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Biological Models
My BioModels
BioModel1
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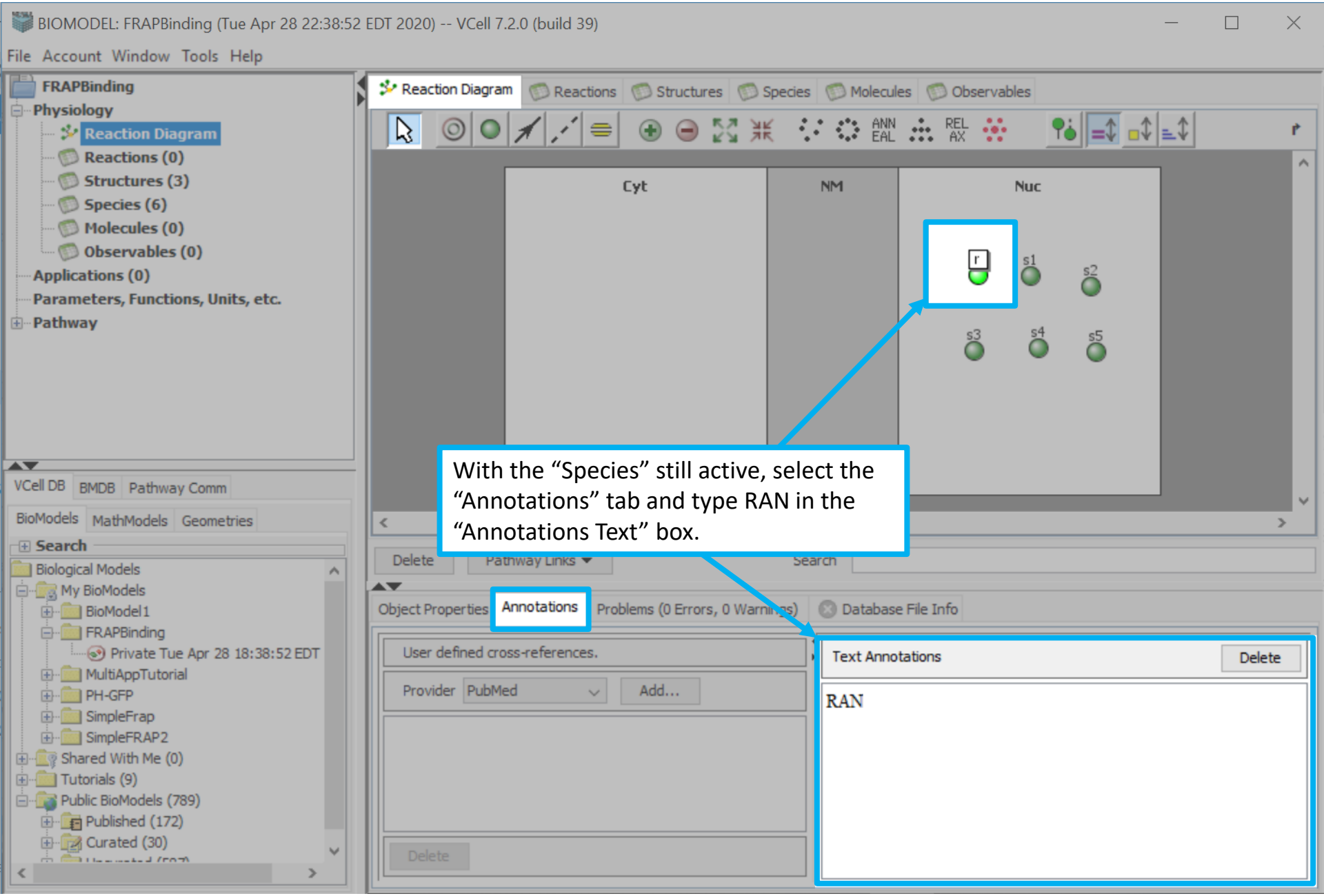
MultiAppTutorial
PH-GFP
SimpleFrap
SimpleFRAP2
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)
Curated (30)
Delete
Pathway Link
Search
Object Properties
Annotation
Problems (0 Errors, 0 Warnings)
Database File Info
Species Name
Sbml Name
Linked Pathway Object(s)


BIOMODEL: FRAPBinding (Tue Apr 28 22:38:52 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (0)
Structures (3)
Species (6)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions, Units, etc.
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
Cyt
NM
Nuc
r
s1
s2
s3
s4
s5
With the “Species” still active, select the “Annotations” tab and type RAN in the “Annotations Text” box.
Delete
Pathway Links
Search
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Database File Info
User defined cross-references.
Provider
PubMed
Add...
Delete
Text Annotations
Delete
RAN
VCell DB
BMDB
Pathway Comm
BioModels
MathModels
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Biological Models
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BioModel1
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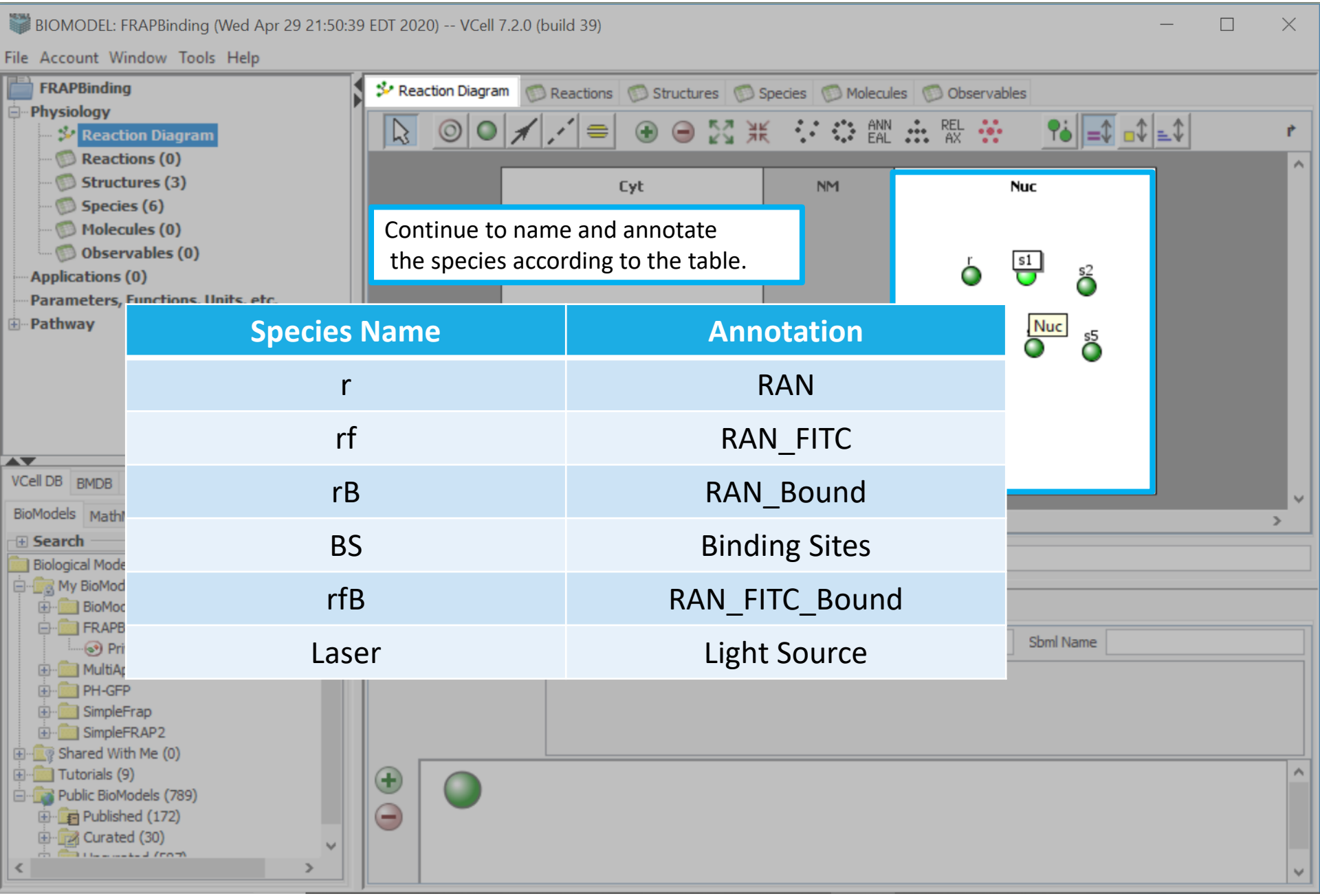
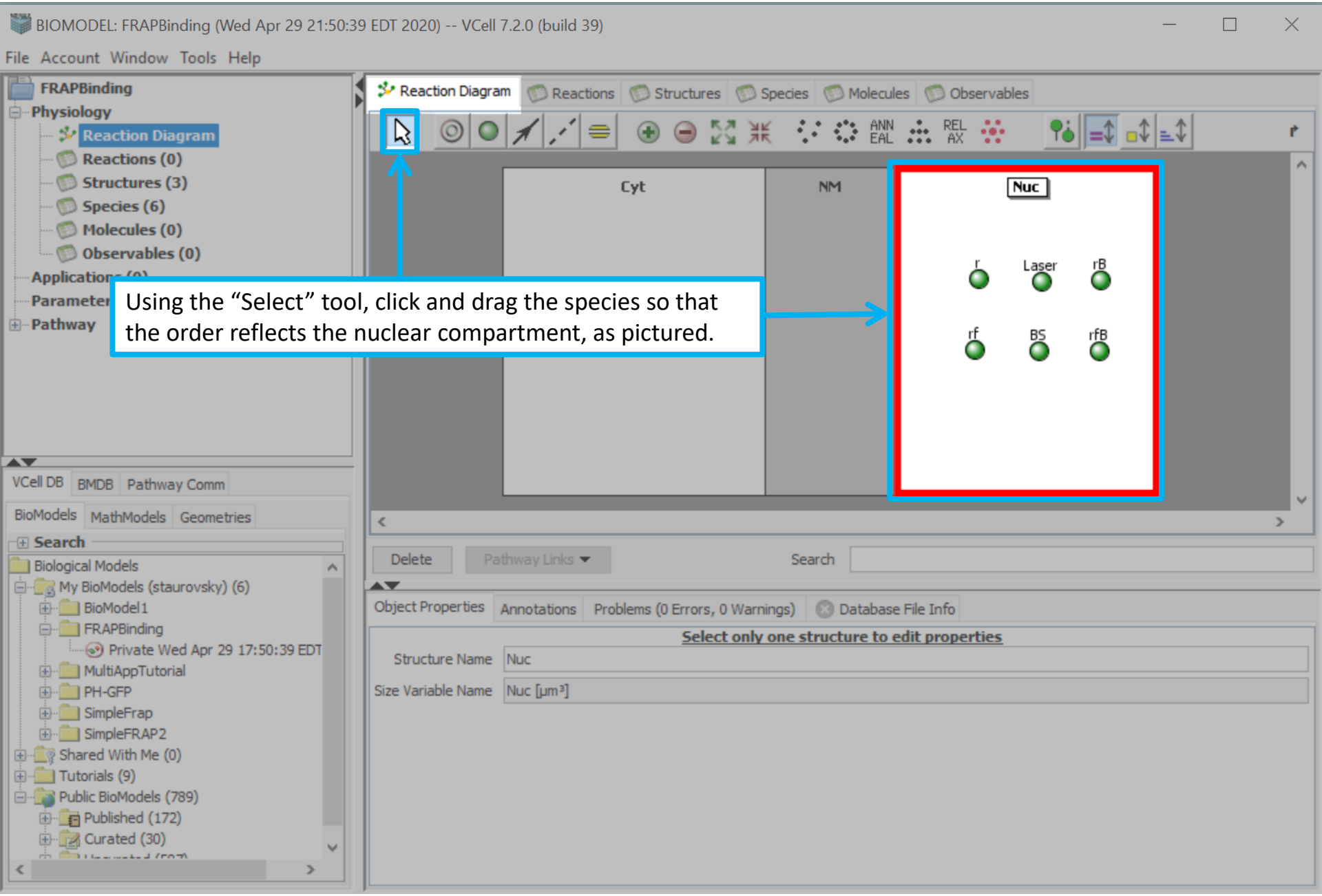
PH-GFP
SimpleFrap
SimpleFRAP2
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)
Curated (30)



Species Name	Annotation
r	RAN
rf	RAN_FITC
rB	RAN_Bound
BS	Binding Sites
rfB	RAN_FITC_Bound
Laser	Light Source


BIOMODEL: FRAPBinding (Wed Apr 29 21:50:39 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (0)
Structures (3)
Species (6)
Molecules (0)
Observables (0)
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
Cyt
NM
Nuc
r
Laser
rB
rf
BS
rfB
Using the “Select” tool, click and drag the species so that the order reflects the nuclear compartment, as pictured.
VCell DB
BMDB
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (staurovsky) (6)
BioModel1
FRAPBinding
Private Wed Apr 29 17:50:39 EDT
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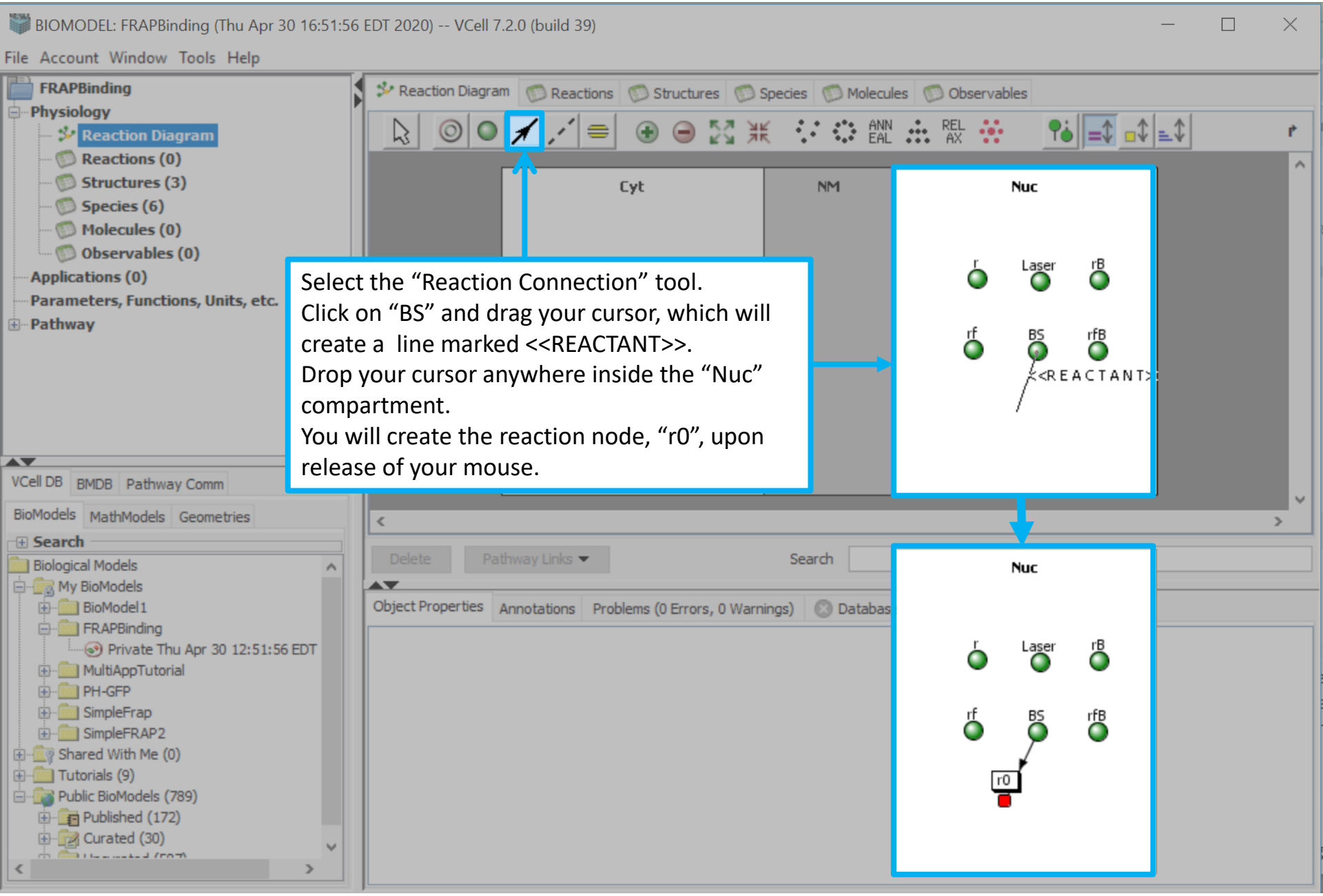
PH-GFP
SimpleFrap
SimpleFRAP2
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)
Curated (30)
Delete
Pathway Links
Search
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Database File Info
Select only one structure to edit properties
Structure Name
Nuc
Size Variable Name
Nuc [µm³]


BIOMODEL: FRAPBinding (Thu Apr 30 16:51:56 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (0)
Structures (3)
Species (6)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions, Units, etc.
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
Cyt
NM
Nuc
r
Laser
rB
rf
BS
rfB
<<REACTANT>>
Select 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.
You will create the reaction node, “r0”, upon release of your mouse.
VCell DB
BMDB
Pathway Comm
BioModels
MathModels
Geometries
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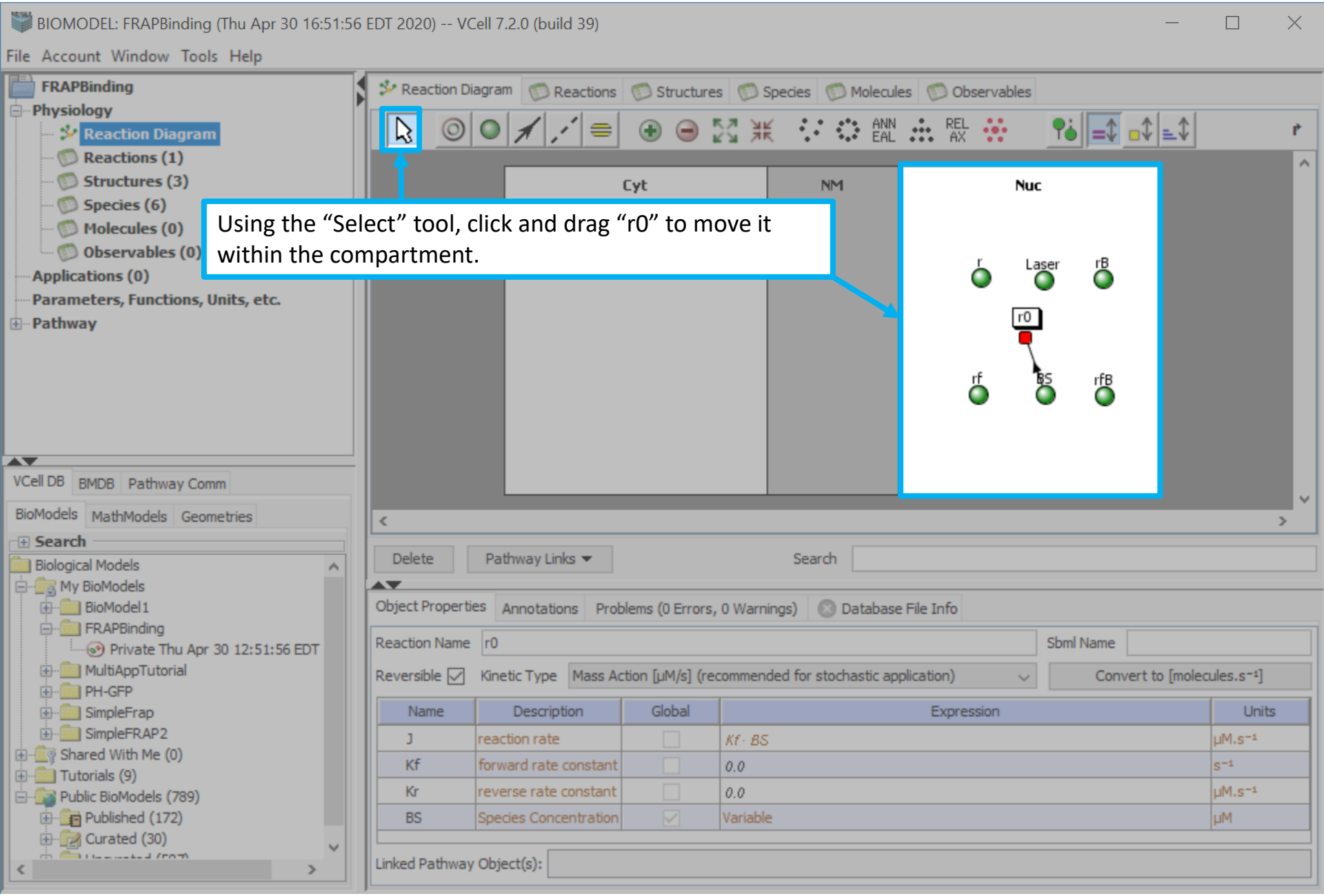
Biological Models
My BioModels
BioModel1
FRAPBinding
Private Thu Apr 30 12:51:56 EDT
MultiAppTutorial
PH-GFP
SimpleFrap
SimpleFRAP2
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)
Curated (30)
Delete
Pathway Links
Search
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
r0


BIOMODEL: FRAPBinding (Thu Apr 30 16:51:56 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (1)
Structures (3)
Species (6)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions, Units, etc.
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
Using the “Select” tool, click and drag “r0” to move it within the compartment.
Cyt
NM
Nuc
r
Laser
rB
r0
rf
BS
rfB
VCell DB
BMDB
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels
BioModel1
FRAPBinding
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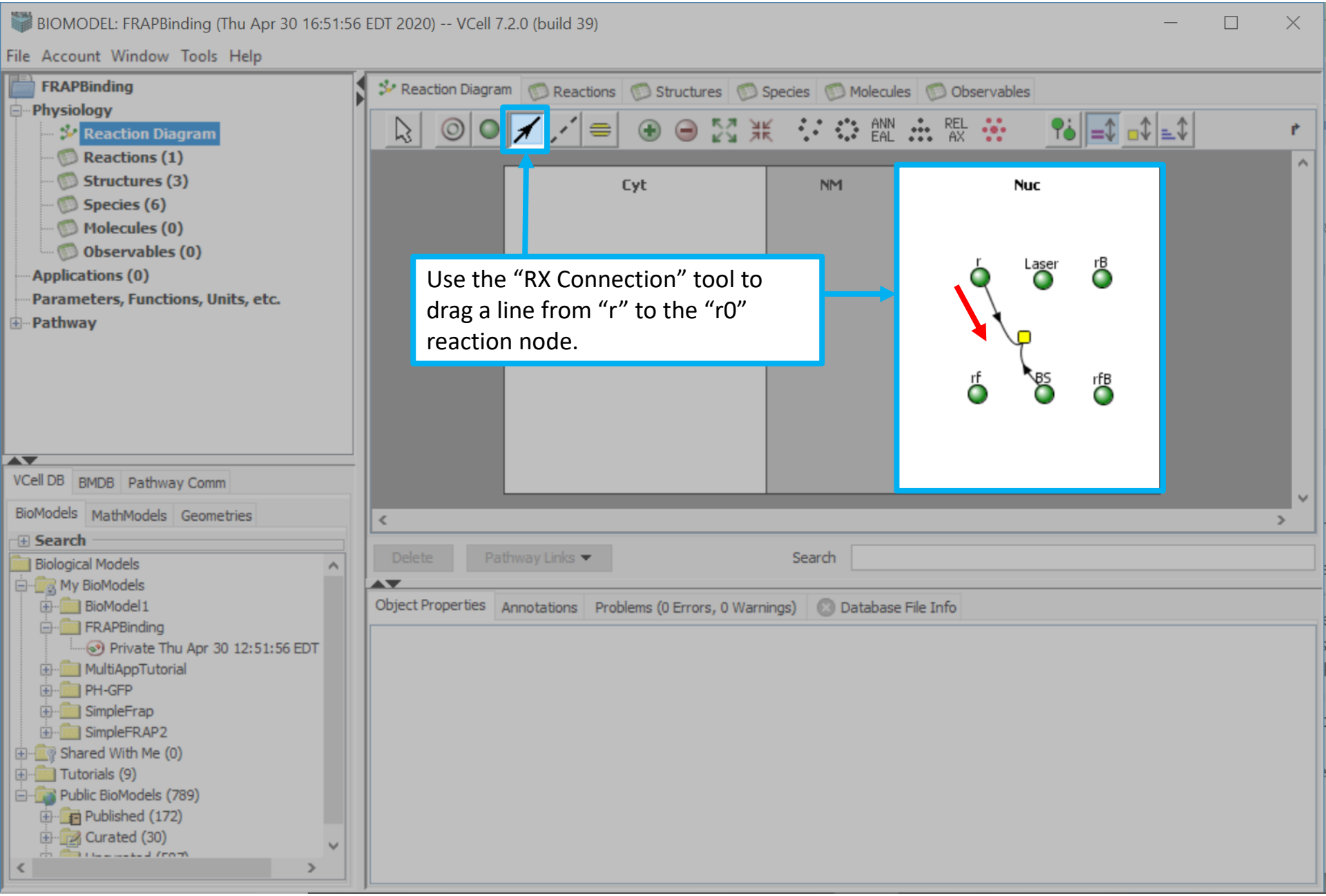
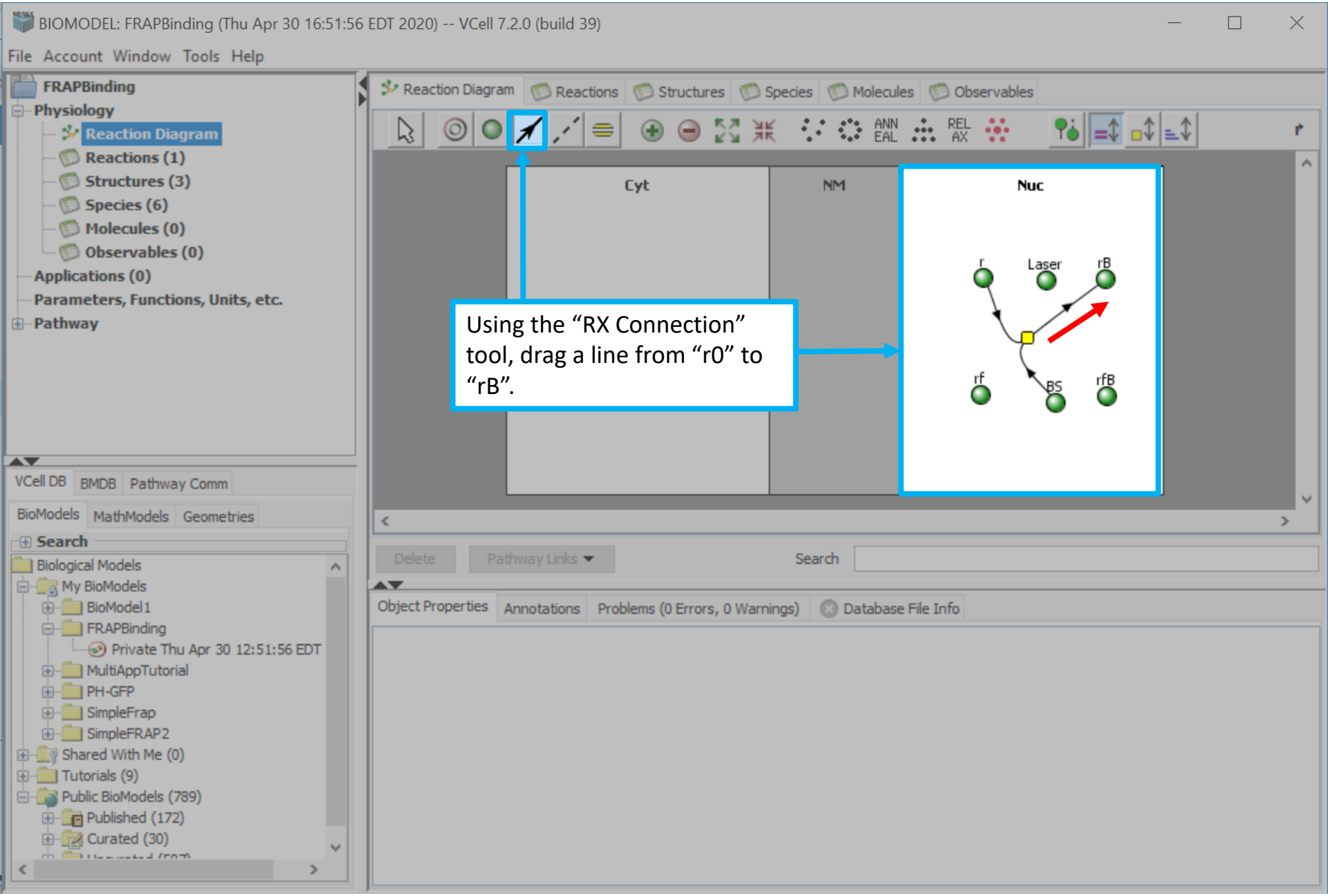
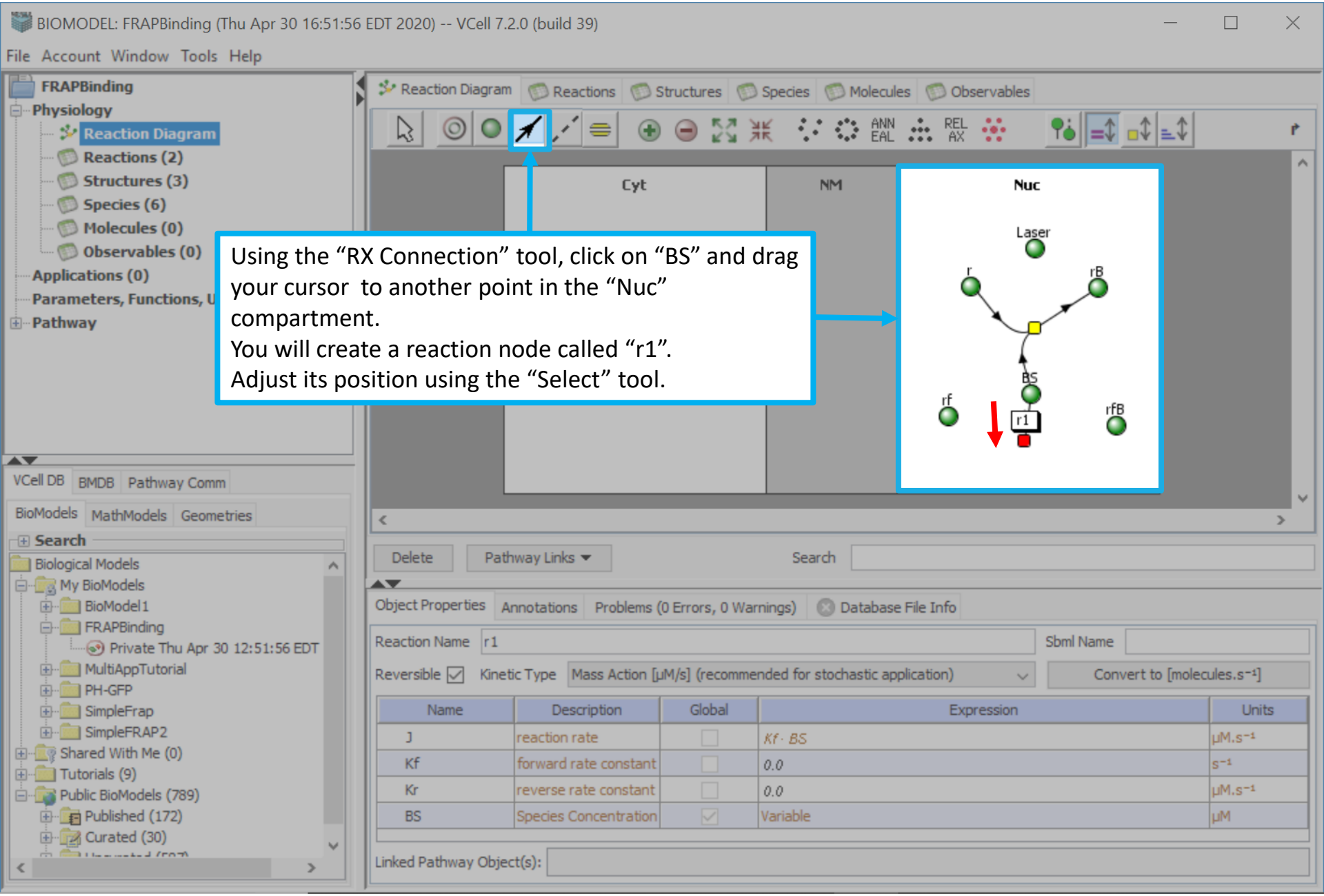
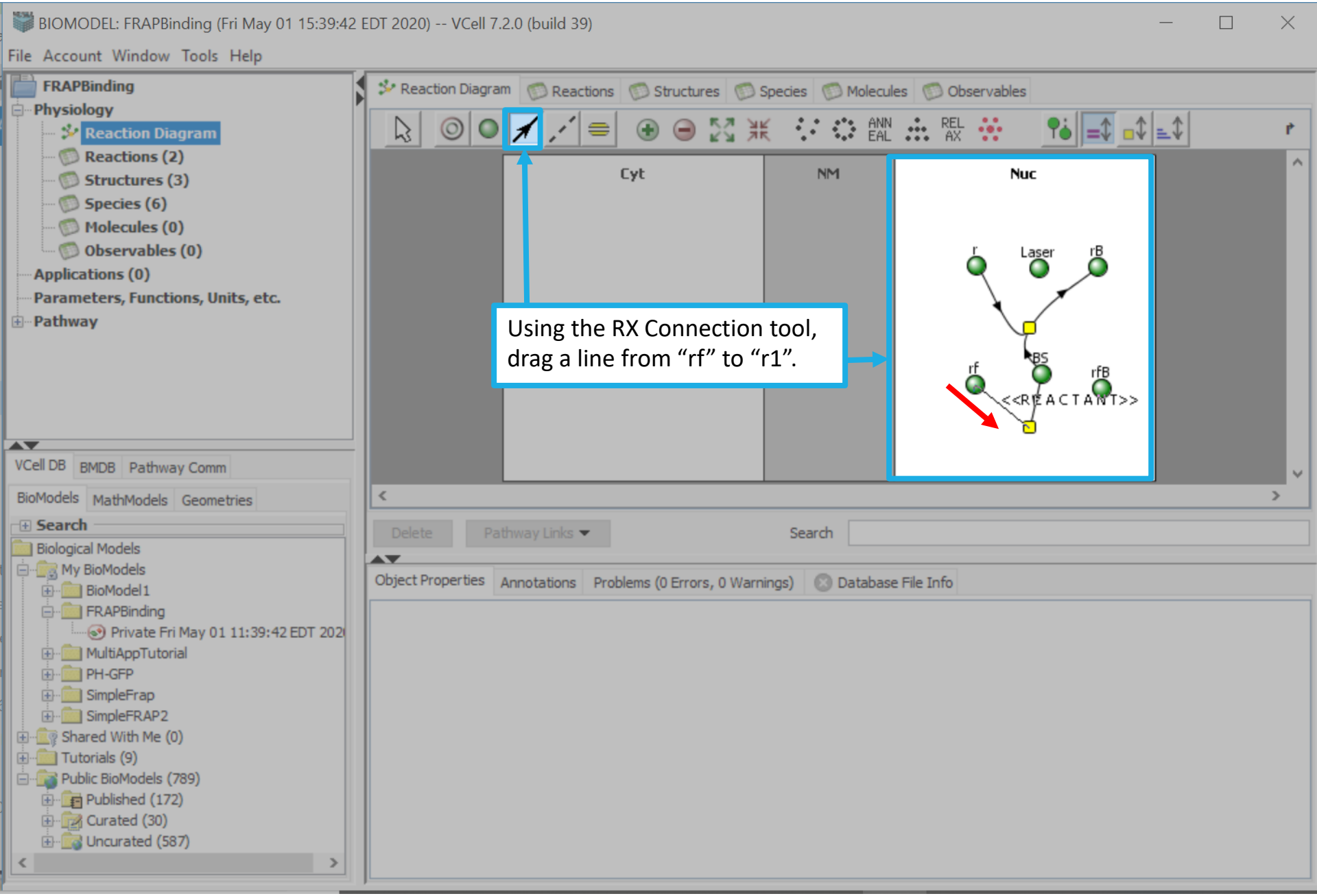
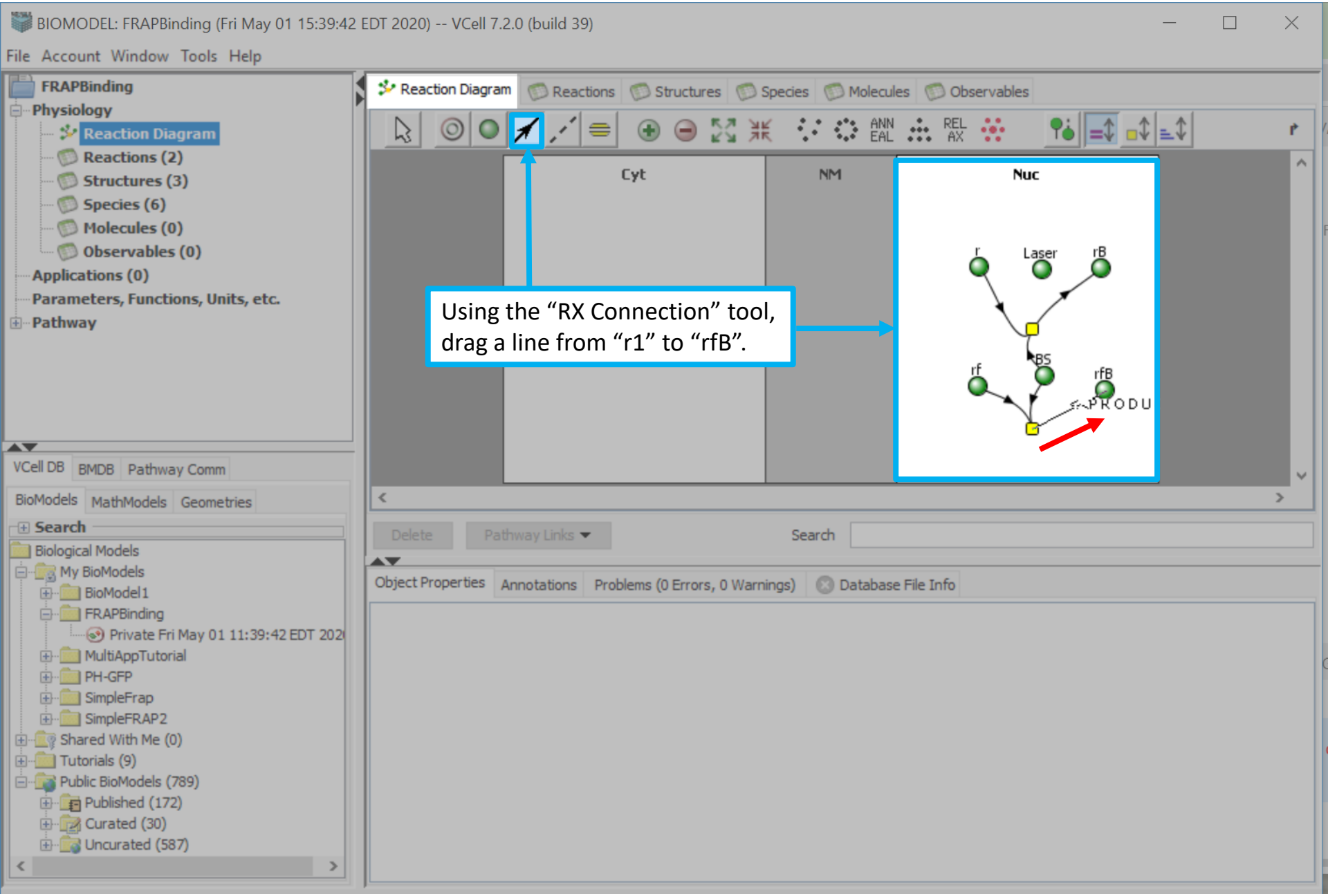
MultiAppTutorial
PH-GFP
SimpleFrap
SimpleFRAP2
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)
Curated (30)
Delete
Pathway Links
Search
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Database File Info
Reaction Name
r0
Sbml Name
Reversible
Kinetic Type
Mass Action [µM/s] (recommended for stochastic application)
Convert to [molecules.s⁻¹]
Name
Description
Global
Expression
Units
J
reaction rate
Kf · BS
µM.s⁻¹
Kf
forward rate constant
0.0
s⁻¹
Kr
reverse rate constant
0.0
µM.s⁻¹
BS
Species Concentration
Variable
µM
Linked Pathway Object(s):

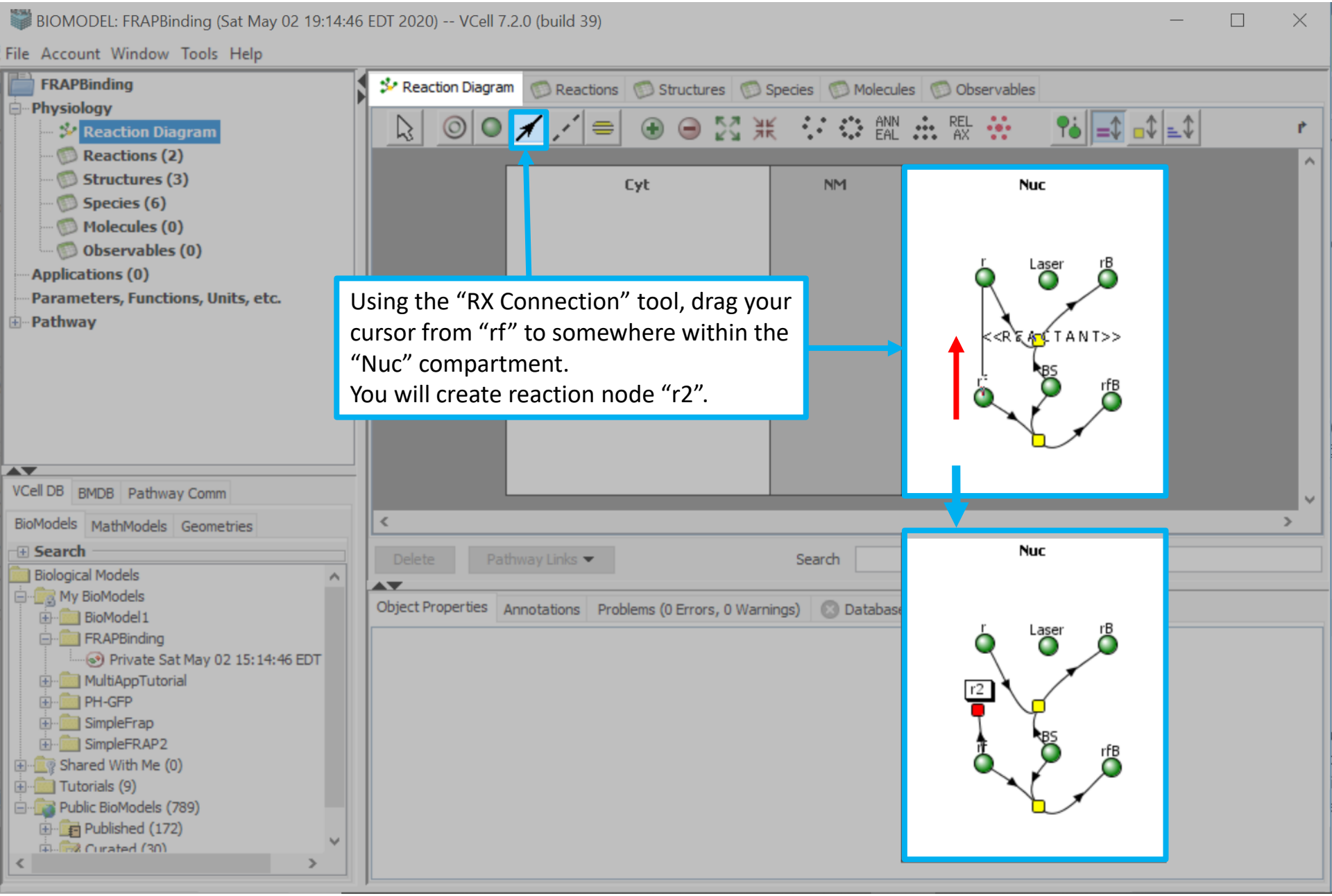

BIOMODEL: FRAPBinding (Thu Apr 30 16:51:56 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (1)
Structures (3)
Species (6)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions, Units, etc.
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
Cyt
NM
Nuc
r
Laser
rB
rf
BS
rfB
Use the “RX Connection” tool to drag a line from “r” to the “r0” reaction node.
VCell DB
BMDB
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels
BioModel1
FRAPBinding
Private Thu Apr 30 12:51:56 EDT
MultiAppTutorial
PH-GFP
SimpleFrap
SimpleFRAP2
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)
Curated (30)
Delete
Pathway Links
Search
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Database File Info

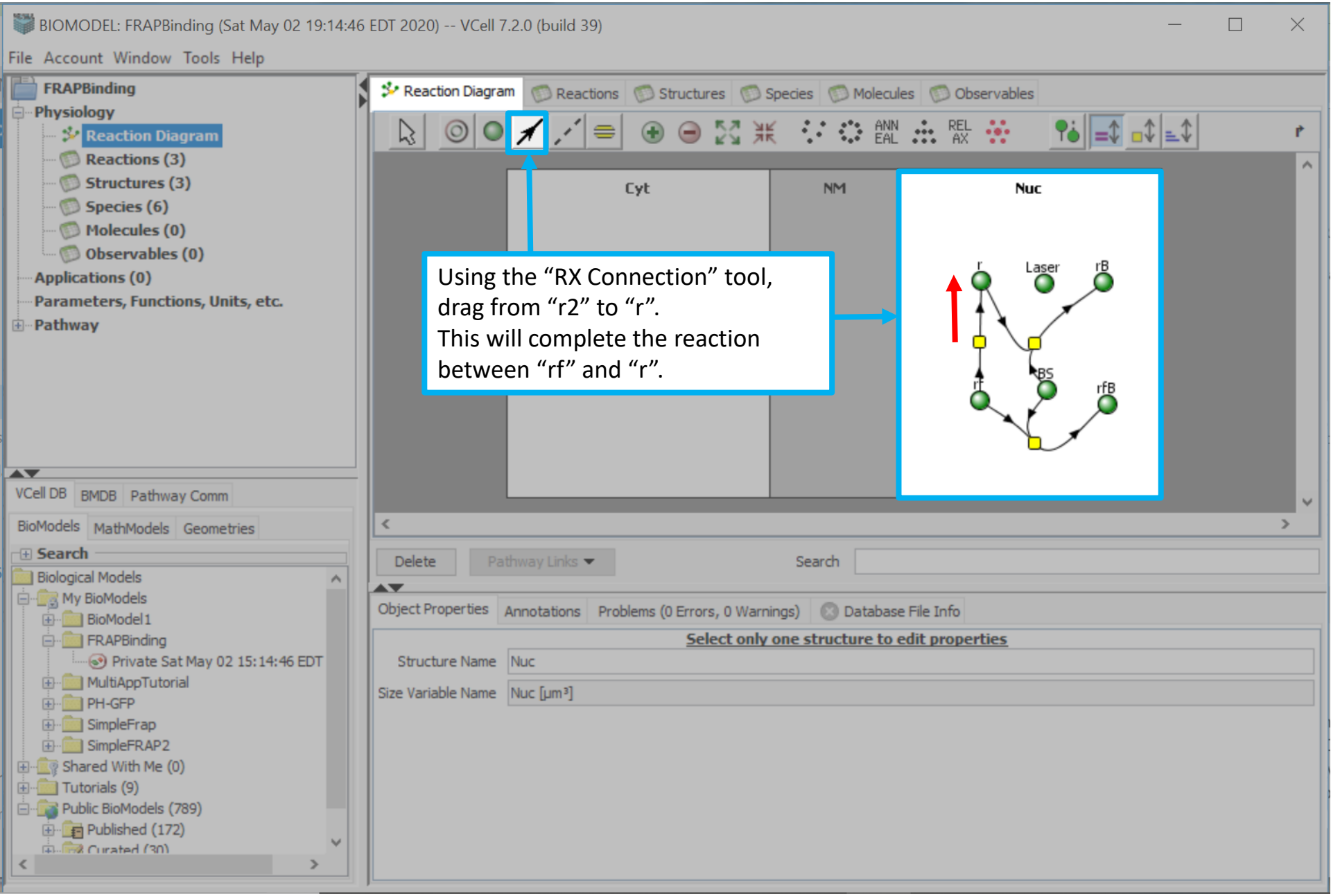

BIOMODEL: FRAPBinding (Thu Apr 30 16:51:56 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (1)
Structures (3)
Species (6)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions, Units, etc.
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
Cyt
NM
Nuc
r
Laser
rB
rf
BS
rfB
Using the “RX Connection” tool, drag a line from “r0” to “rB”.
VCell DB
BMDB
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels
BioModel1
FRAPBinding
Private Thu Apr 30 12:51:56 EDT
MultiAppTutorial
PH-GFP
SimpleFrap
SimpleFRAP2
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)
Curated (30)
Delete
Pathway Links
Search
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Database File Info

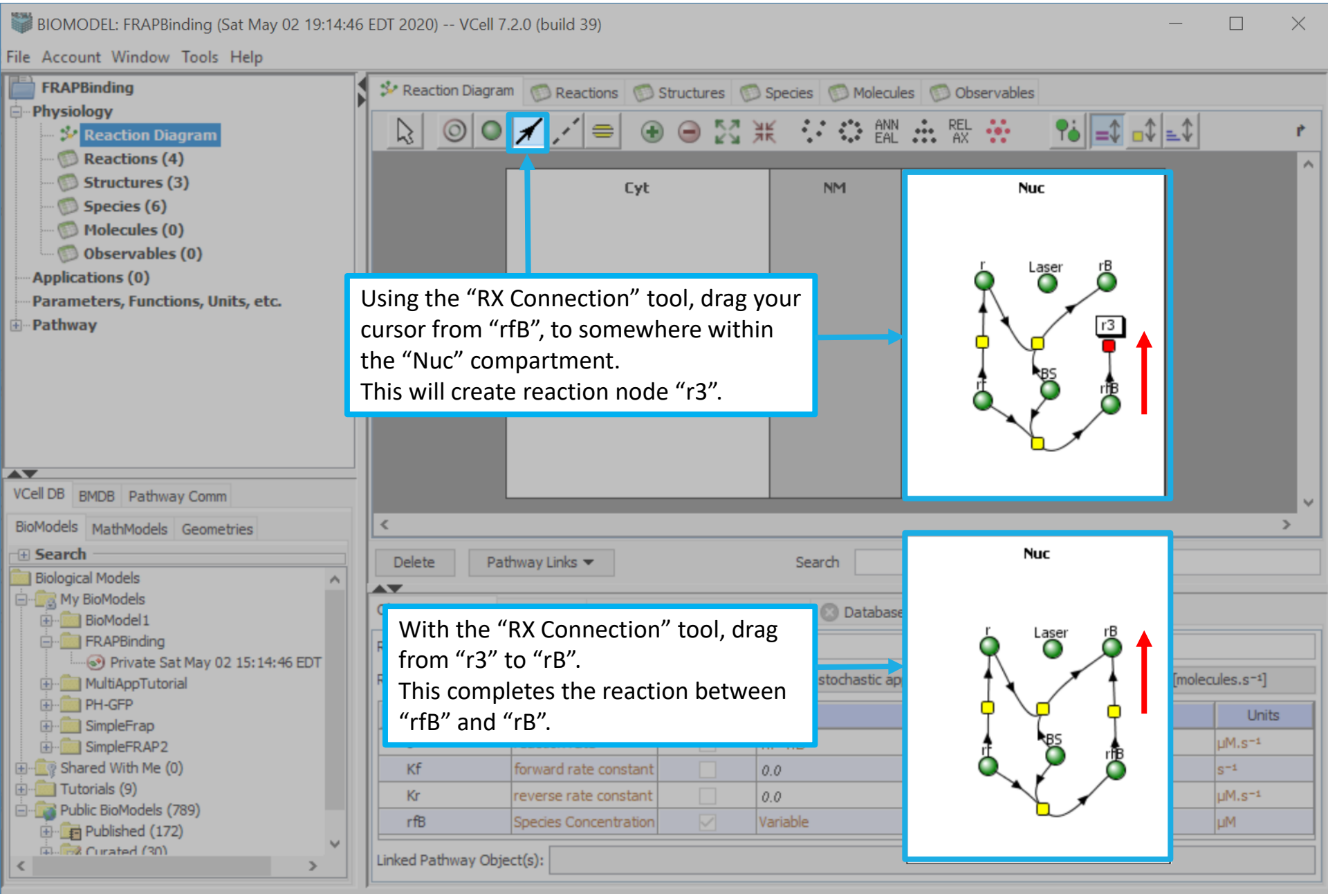

BIOMODEL: FRAPBinding (Thu Apr 30 16:51:56 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (2)
Structures (3)
Species (6)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions, U
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
Cyt
NM
Nuc
Laser
r
rB
BS
rf
r1
rfB
Using the “RX Connection” tool, click on “BS” and drag your cursor to another point in the “Nuc” compartment.
You will create a reaction node called “r1”.
Adjust its position using the “Select” tool.
VCell DB
BMDB
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels
BioModel1
FRAPBinding
Private Thu Apr 30 12:51:56 EDT
MultiAppTutorial
PH-GFP
SimpleFrap
SimpleFRAP2
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)
Curated (30)
Delete
Pathway Links
Search
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Database File Info
Reaction Name
r1
Sbml Name
Reversible
Kinetic Type
Mass Action [µM/s] (recommended for stochastic application)
Convert to [molecules.s⁻¹]
Name
Description
Global
Expression
Units
J
reaction rate
Kf · BS
µM.s⁻¹
Kf
forward rate constant
0.0
s⁻¹
Kr
reverse rate constant
0.0
µM.s⁻¹
BS
Species Concentration
Variable
µM
Linked Pathway Object(s):

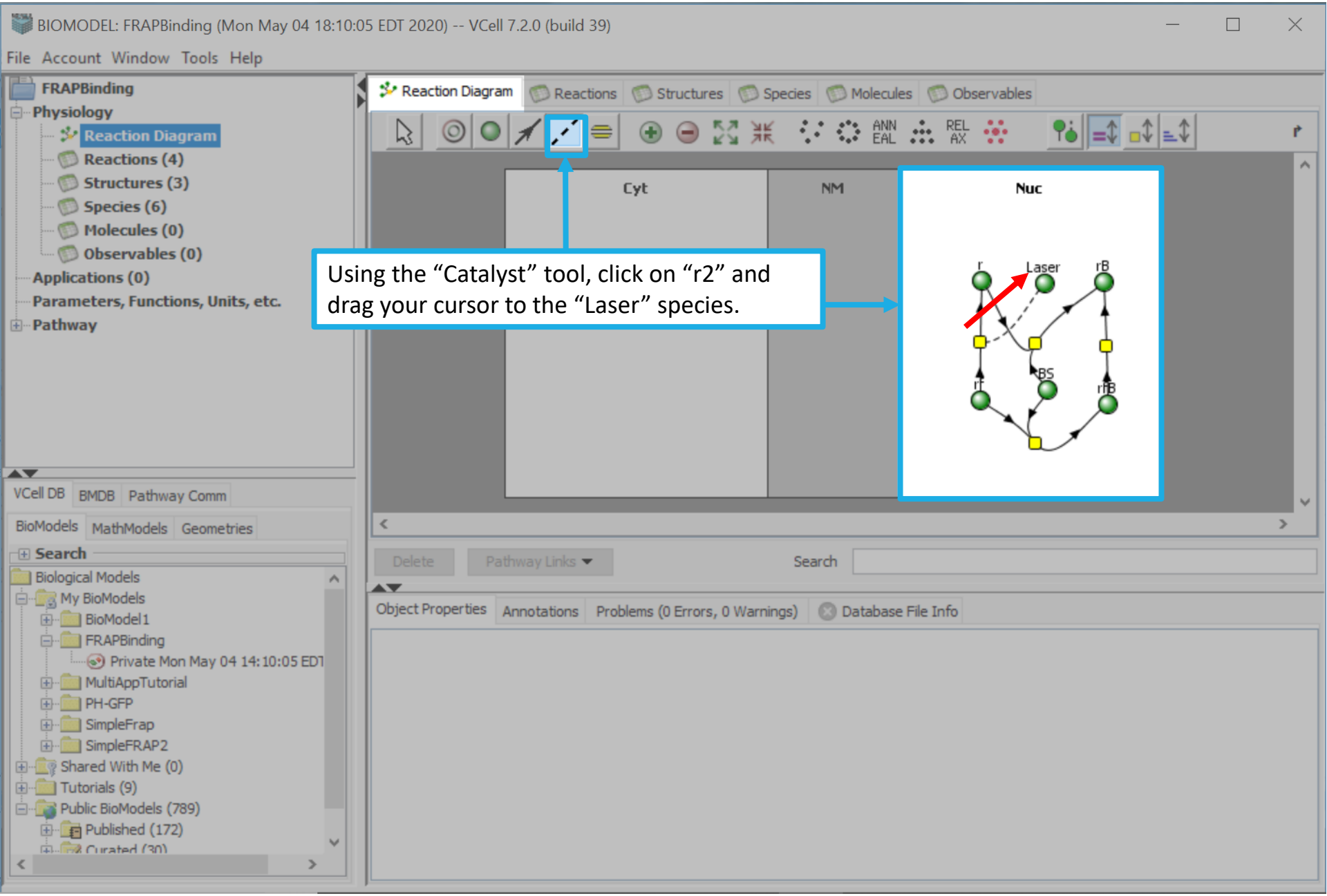

BIOMODEL: FRAPBinding (Fri May 01 15:39:42 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (2)
Structures (3)
Species (6)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions, Units, etc.
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
Cyt
NM
Nuc
r
Laser
rB
BS
rf
rfB
<<REACTANT>>
Using the RX Connection tool, drag a line from “rf” to “r1”.
VCell DB
BMDB
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels
BioModel1
FRAPBinding
Private Fri May 01 11:39:42 EDT 202
MultiAppTutorial
PH-GFP
SimpleFrap
SimpleFRAP2
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)
Curated (30)
Uncurated (587)
Delete
Pathway Links
Search
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Database File Info

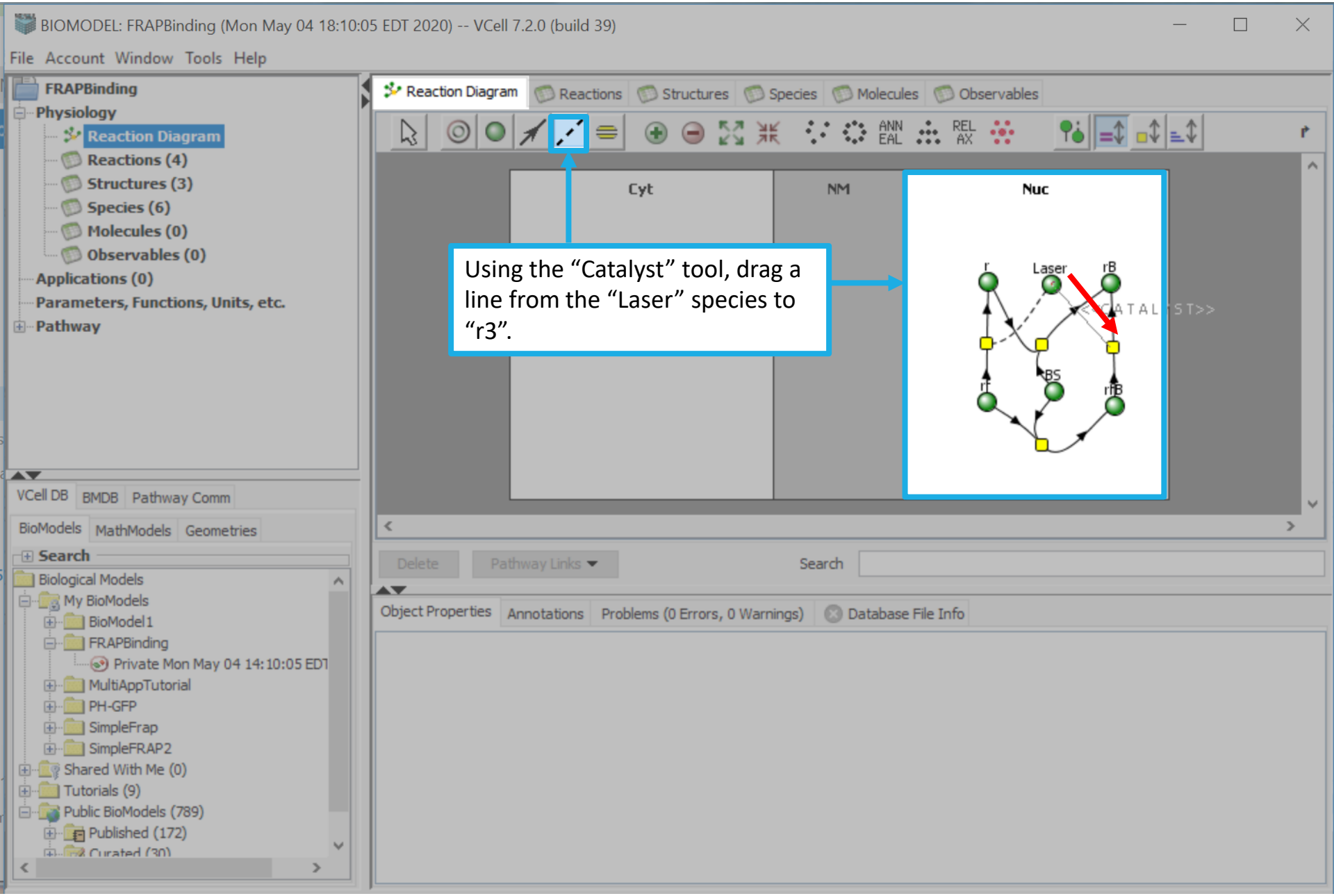

BIOMODEL: FRAPBinding (Fri May 01 15:39:42 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (2)
Structures (3)
Species (6)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions, Units, etc.
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
Cyt
NM
Nuc
r
Laser
rB
BS
rf
rfB
Using the “RX Connection” tool, drag a line from “r1” to “rfB”.
VCell DB
BMDB
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels
BioModel1
FRAPBinding
MultiAppTutorial
PH-GFP
SimpleFrap
SimpleFRAP2
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)
Curated (30)
Uncurated (587)
Delete
Pathway Links
Search
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Database File Info

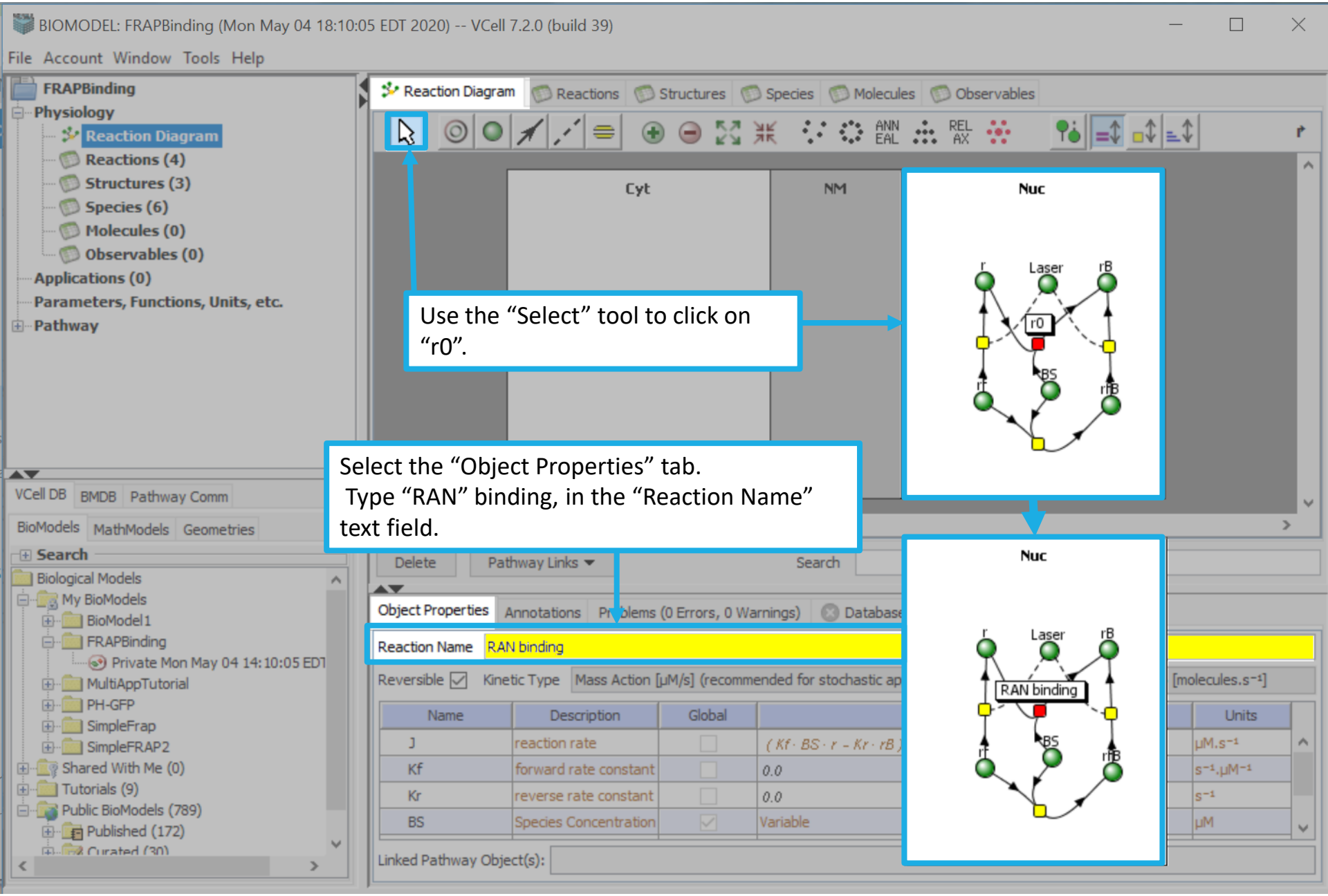

BIOMODEL: FRAPBinding (Sat May 02 19:14:46 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (2)
Structures (3)
Species (6)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions, Units, etc.
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
Cyt
NM
Nuc
Using the “RX Connection” tool, drag your cursor from “rf” to somewhere within the “Nuc” compartment.
You will create reaction node “r2”.
r
Laser
rB
BS
rfB
r2
Delete
Pathway Links
Search
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
VCell DB
BMDB
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels
BioModel1
FRAPBinding
Private Sat May 02 15:14:46 EDT
MultiAppTutorial
PH-GFP
SimpleFrap
SimpleFRAP2
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)

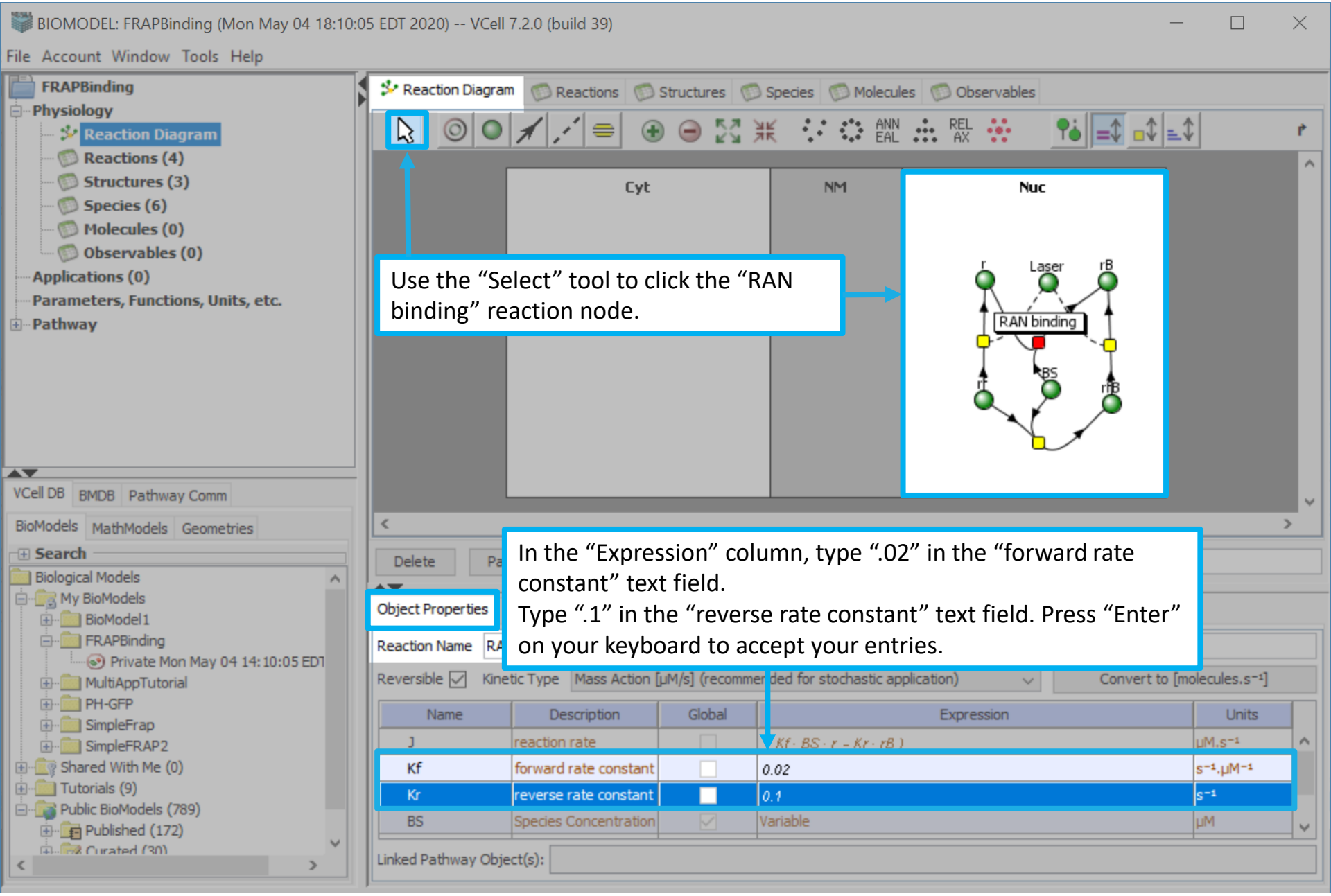

BIOMODEL: FRAPBinding (Sat May 02 19:14:46 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (3)
Structures (3)
Species (6)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions, Units, etc.
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
Cyt
NM
Nuc
r
Laser
rB
BS
rf
rfB
Using the “RX Connection” tool, drag from “r2” to “r”.
This will complete the reaction between “rf” and “r”.
VCell DB
BMDB
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels
BioModel1
FRAPBinding
Private Sat May 02 15:14:46 EDT
MultiAppTutorial
PH-GFP
SimpleFrap
SimpleFRAP2
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)
Delete
Pathway Links
Search
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Database File Info
Select only one structure to edit properties
Structure Name
Nuc
Size Variable Name
Nuc [µm³]

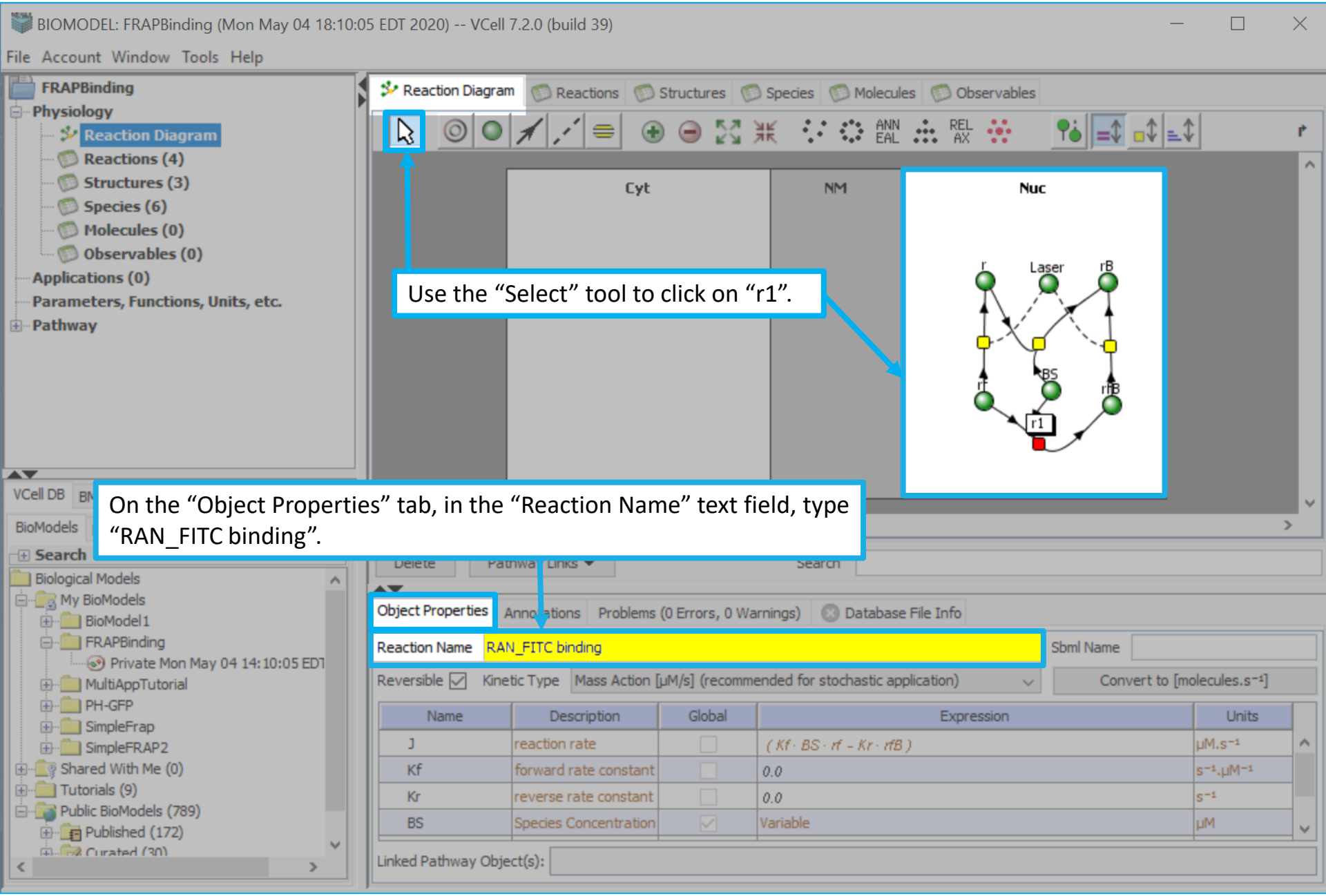

BIOMODEL: FRAPBinding (Sat May 02 19:14:46 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (4)
Structures (3)
Species (6)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions, Units, etc.
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
Cyt
NM
Nuc
r
Laser
rB
r3
BS
rfB
Using the “RX Connection” tool, drag your cursor from “rfB”, to somewhere within the “Nuc” compartment.
This will create reaction node “r3”.
VCell DB
BMDB
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels
BioModel1
FRAPBinding
Private Sat May 02 15:14:46 EDT
MultiAppTutorial
PH-GFP
SimpleFrap
SimpleFRAP2
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)
Delete
Pathway Links
Search
With the “RX Connection” tool, drag from “r3” to “rB”.
This completes the reaction between “rfB” and “rB”.
Kf
forward rate constant
0.0
Kr
reverse rate constant
0.0
rfB
Species Concentration
Variable
Units
μM.s⁻¹
s⁻¹
μM.s⁻¹
μM
[molecules.s⁻¹]
Linked Pathway Object(s):

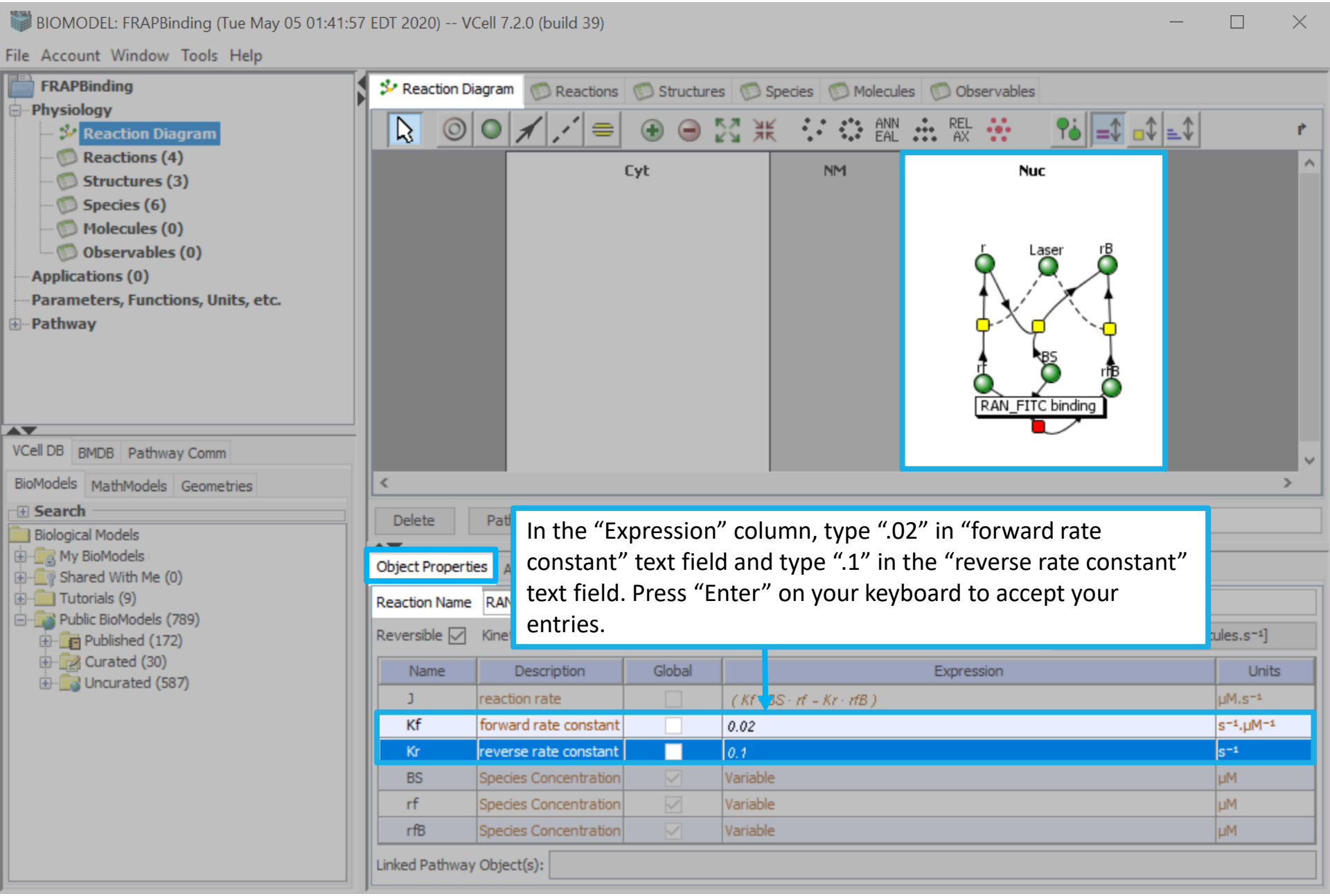

BIOMODEL: FRAPBinding (Mon May 04 18:10:05 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (4)
Structures (3)
Species (6)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions, Units, etc.
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
Cyt
NM
Nuc
r
Laser
rB
BS
rf
rfB
Using the “Catalyst” tool, click on “r2” and drag your cursor to the “Laser” species.
VCell DB
BMDB
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels
BioModel1
FRAPBinding
Private Mon May 04 14:10:05 EDT
MultiAppTutorial
PH-GFP
SimpleFrap
SimpleFRAP2
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)
Delete
Pathway Links
Search
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Database File Info

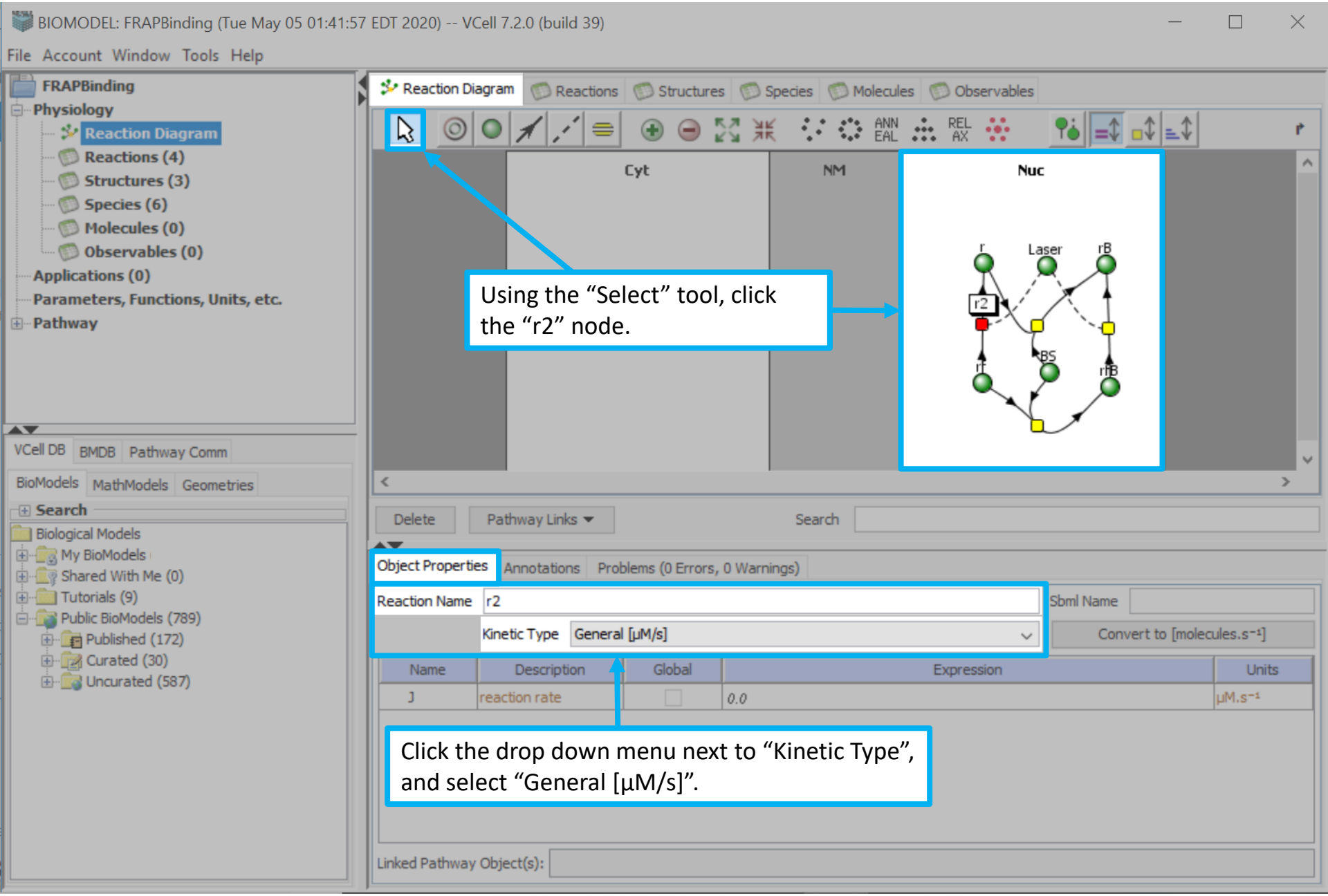

BIOMODEL: FRAPBinding (Mon May 04 18:10:05 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (4)
Structures (3)
Species (6)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions, Units, etc.
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
Cyt
NM
Nuc
Using the “Catalyst” tool, drag a line from the “Laser” species to “r3”.
r
Laser
rB
BS
rf
rfB
Delete
Pathway Links
Search
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Database File Info
VCell DB
BMDB
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels
BioModel1
FRAPBinding
Private Mon May 04 14:10:05 EDT
MultiAppTutorial
PH-GFP
SimpleFrap
SimpleFRAP2
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)

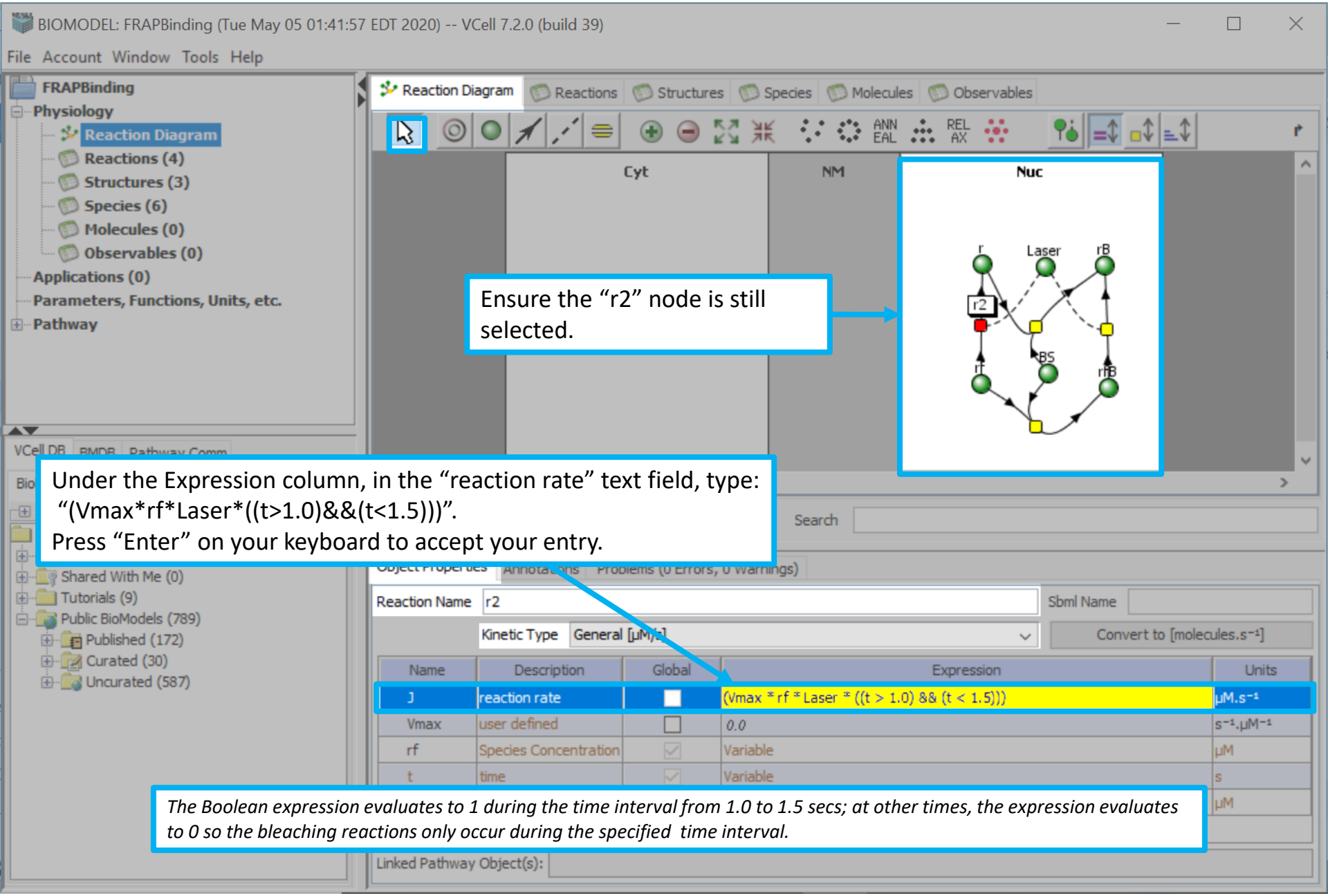

BIOMODEL: FRAPBinding (Mon May 04 18:10:05 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (4)
Structures (3)
Species (6)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions, Units, etc.
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
Cyt
NM
Nuc
r
Laser
rB
r0
BS
rf
rfB
Use the “Select” tool to click on “r0”.
Select the “Object Properties” tab.
Type “RAN” binding, in the “Reaction Name” text field.
Nuc
RAN binding
VCell DB
BMDB
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels
BioModel1
FRAPBinding
Private Mon May 04 14:10:05 EDT
MultiAppTutorial
PH-GFP
SimpleFrap
SimpleFRAP2
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)
Delete
Pathway Links
Search
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Database
Reaction Name
RAN binding
Reversible
Kinetic Type
Mass Action [μM/s] (recommended for stochastic ap
[molecules.s⁻¹]
Name
Description
Global
Units
J
reaction rate
(Kf · BS · r - Kr · rB)
μM.s⁻¹
Kf
forward rate constant
0.0
s⁻¹.μM⁻¹
Kr
reverse rate constant
0.0
s⁻¹
BS
Species Concentration
Variable
μM
Linked Pathway Object(s):

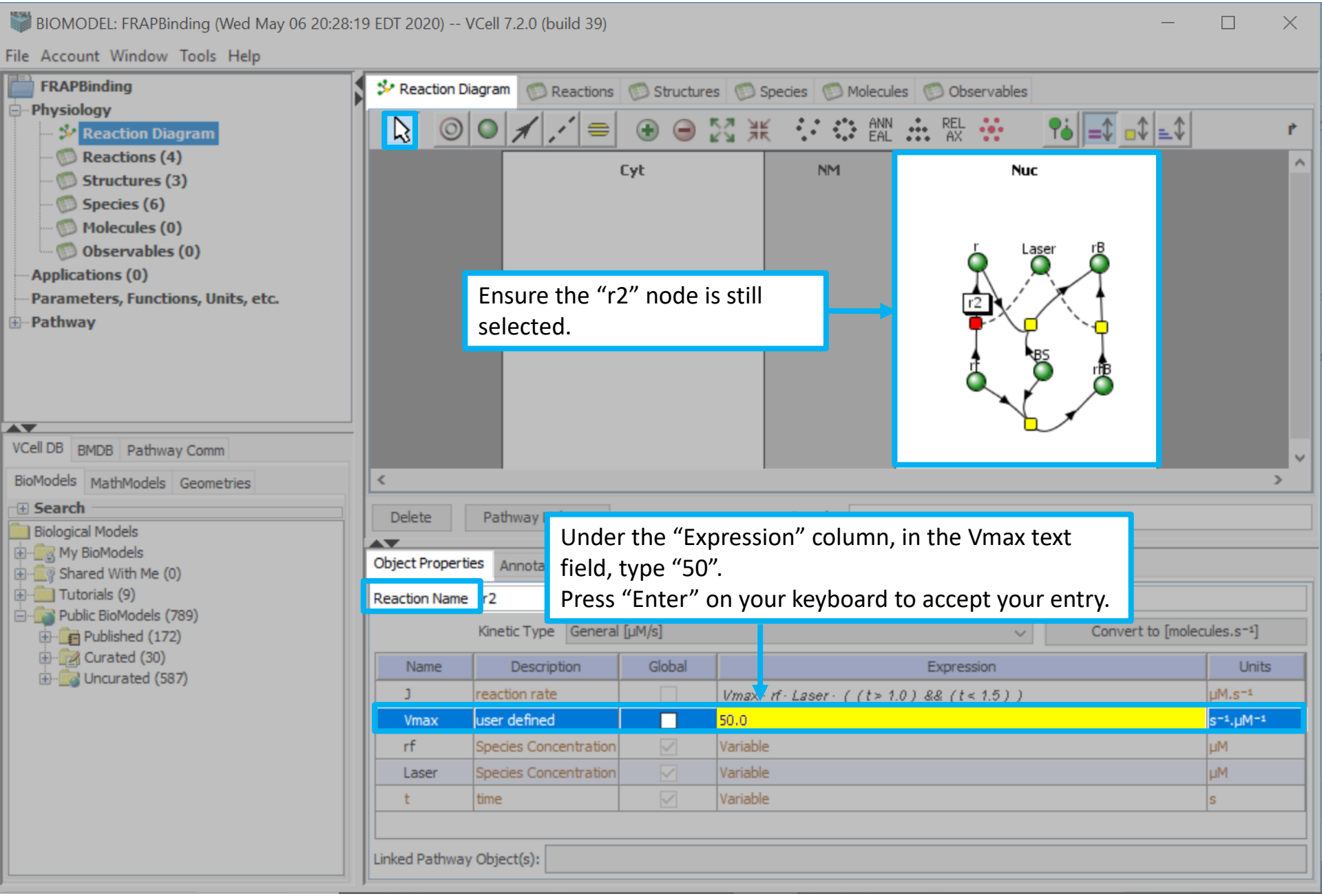

BIOMODEL: FRAPBinding (Mon May 04 18:10:05 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (4)
Structures (3)
Species (6)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions, Units, etc.
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
Cyt
NM
Nuc
r
Laser
rB
RAN binding
BS
rF
rfB
Use the “Select” tool to click the “RAN binding” reaction node.
In the “Expression” column, type “.02” in the “forward rate constant” text field.
Type “.1” in the “reverse rate constant” text field. Press “Enter” on your keyboard to accept your entries.
Object Properties
Reaction Name
Reversible
Kinetic Type
Mass Action [μM/s] (recommended for stochastic application)
Convert to [molecules.s⁻¹]
Name
Description
Global
Expression
Units
J
reaction rate
Kf · BS · r − Kr · rB)
μM.s⁻¹
Kf
forward rate constant
0.02
s⁻¹.μM⁻¹
Kr
reverse rate constant
0.1
s⁻¹
BS
Species Concentration
Variable
μM
Linked Pathway Object(s):
Delete
VCell DB
BMDB
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels
BioModel1
FRAPBinding
Private Mon May 04 14:10:05 EDT
MultiAppTutorial
PH-GFP
SimpleFrap
SimpleFRAP2
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)

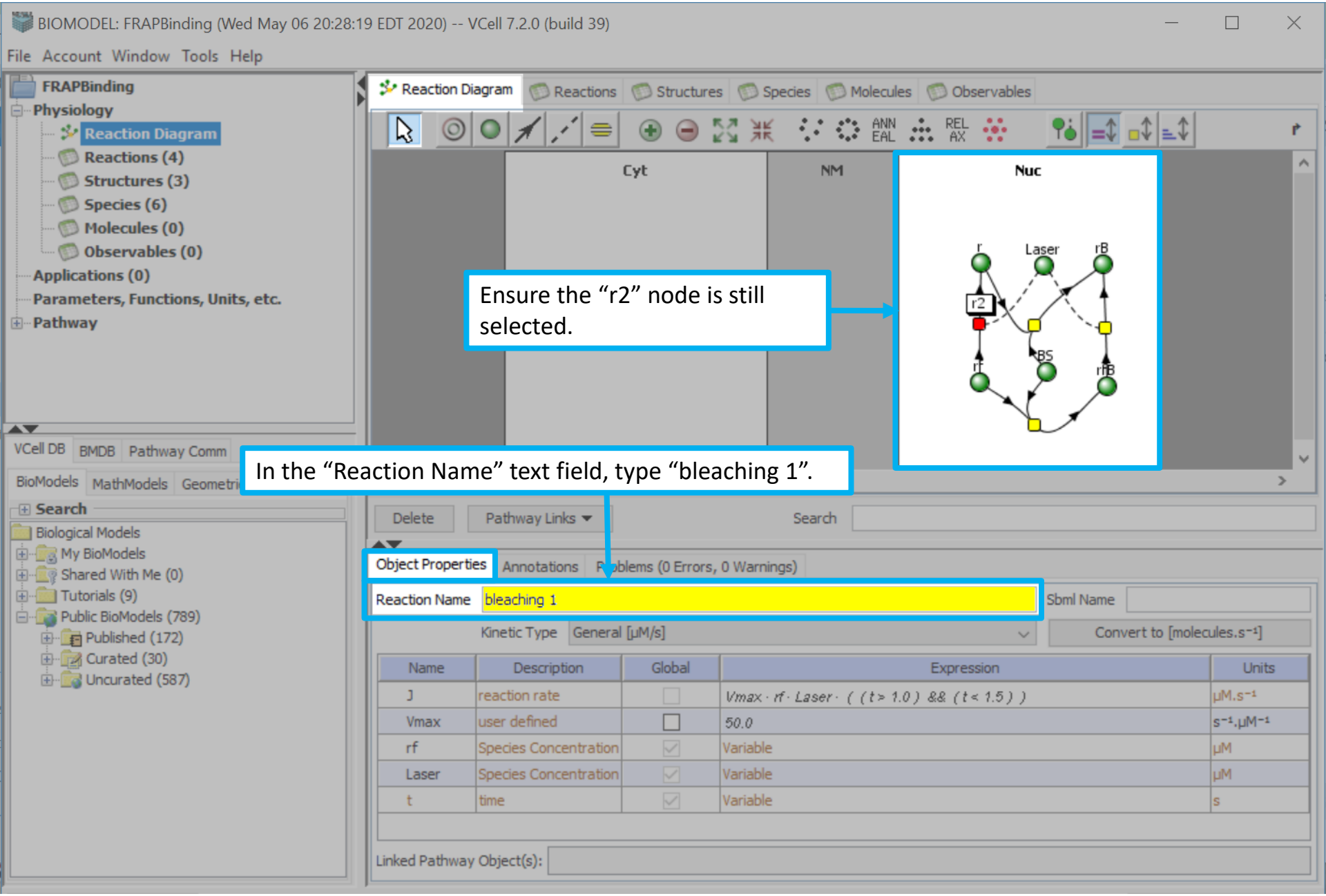

BIOMODEL: FRAPBinding (Mon May 04 18:10:05 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (4)
Structures (3)
Species (6)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions, Units, etc.
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
Cyt
NM
Nuc
r
Laser
rB
BS
rf
rfB
r1
Use the “Select” tool to click on “r1”.
On the “Object Properties” tab, in the “Reaction Name” text field, type “RAN_FITC binding”.
VCell DB
BioModels
Search
Biological Models
My BioModels
BioModel1
FRAPBinding
Private Mon May 04 14:10:05 EDT
MultiAppTutorial
PH-GFP
SimpleFrap
SimpleFRAP2
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)
Delete
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Database File Info
Reaction Name
RAN_FITC binding
Sbml Name
Reversible
Kinetic Type
Mass Action [μM/s] (recommended for stochastic application)
Convert to [molecules.s⁻¹]
Name
Description
Global
Expression
Units
J
reaction rate
(Kf · BS · rf - Kr · rfB)
μM.s⁻¹
Kf
forward rate constant
0.0
s⁻¹.μM⁻¹
Kr
reverse rate constant
0.0
s⁻¹
BS
Species Concentration
Variable
μM
Linked Pathway Object(s):

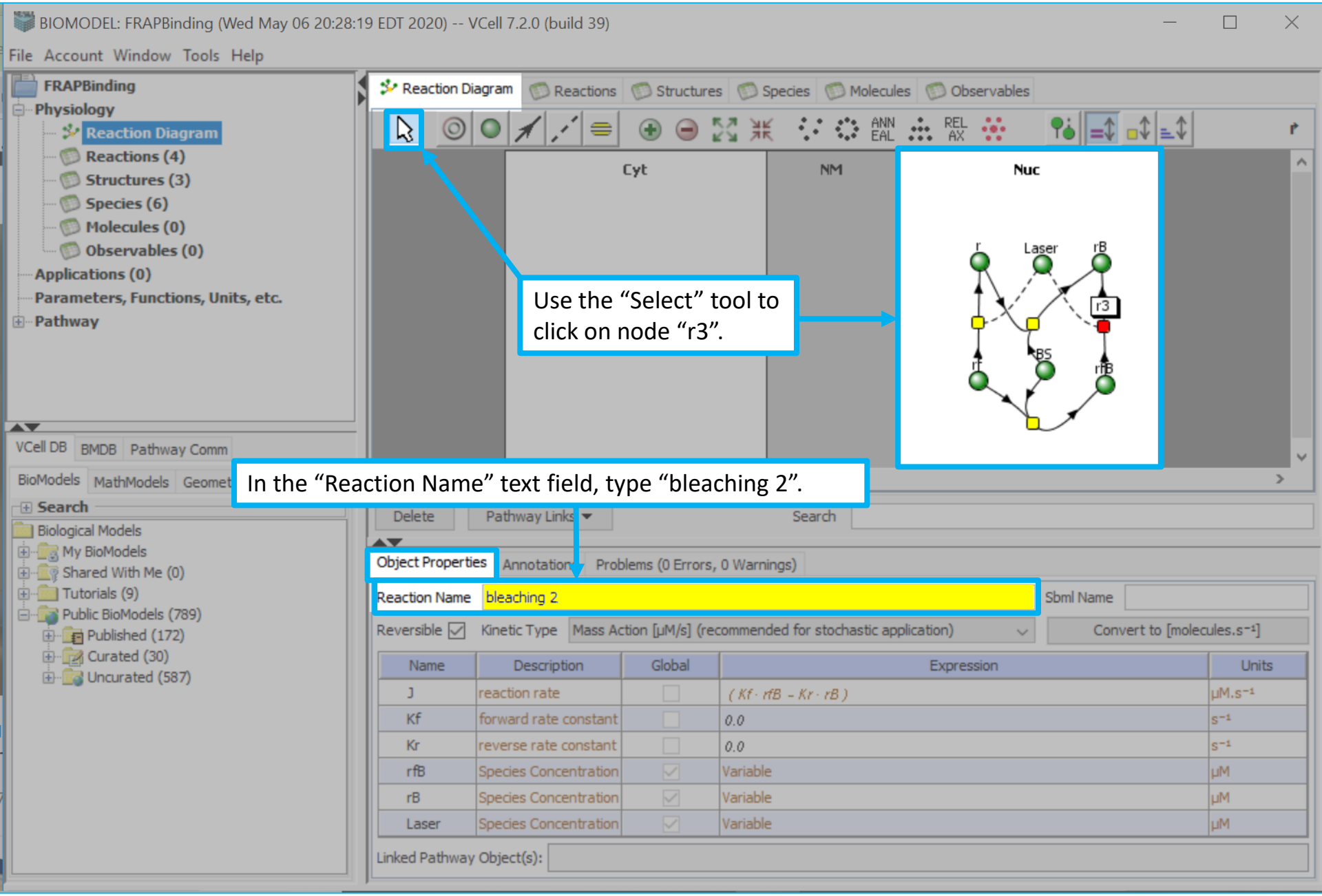

BIOMODEL: FRAPBinding (Tue May 05 01:41:57 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (4)
Structures (3)
Species (6)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions, Units, etc.
Pathway
VCell DB BMDB Pathway Comm
BioModels MathModels Geometries
Search
Biological Models
My BioModels
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)
Curated (30)
Uncurated (587)
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
Cyt
NM
Nuc
r
Laser
rB
BS
rf
rfB
RAN_FITC binding
Delete
Object Properties
Reaction Name
Reversible
In the “Expression” column, type “.02” in “forward rate constant” text field and type “.1” in the “reverse rate constant” text field. Press “Enter” on your keyboard to accept your entries.
Name
Description
Global
Expression
Units
J
reaction rate
(Kf · BS · rf - Kr · rfB)
μM.s⁻¹
Kf
forward rate constant
0.02
s⁻¹.μM⁻¹
Kr
reverse rate constant
0.1
s⁻¹
BS
Species Concentration
Variable
μM
rf
Species Concentration
Variable
μM
rfB
Species Concentration
Variable
μM
Linked Pathway Object(s):

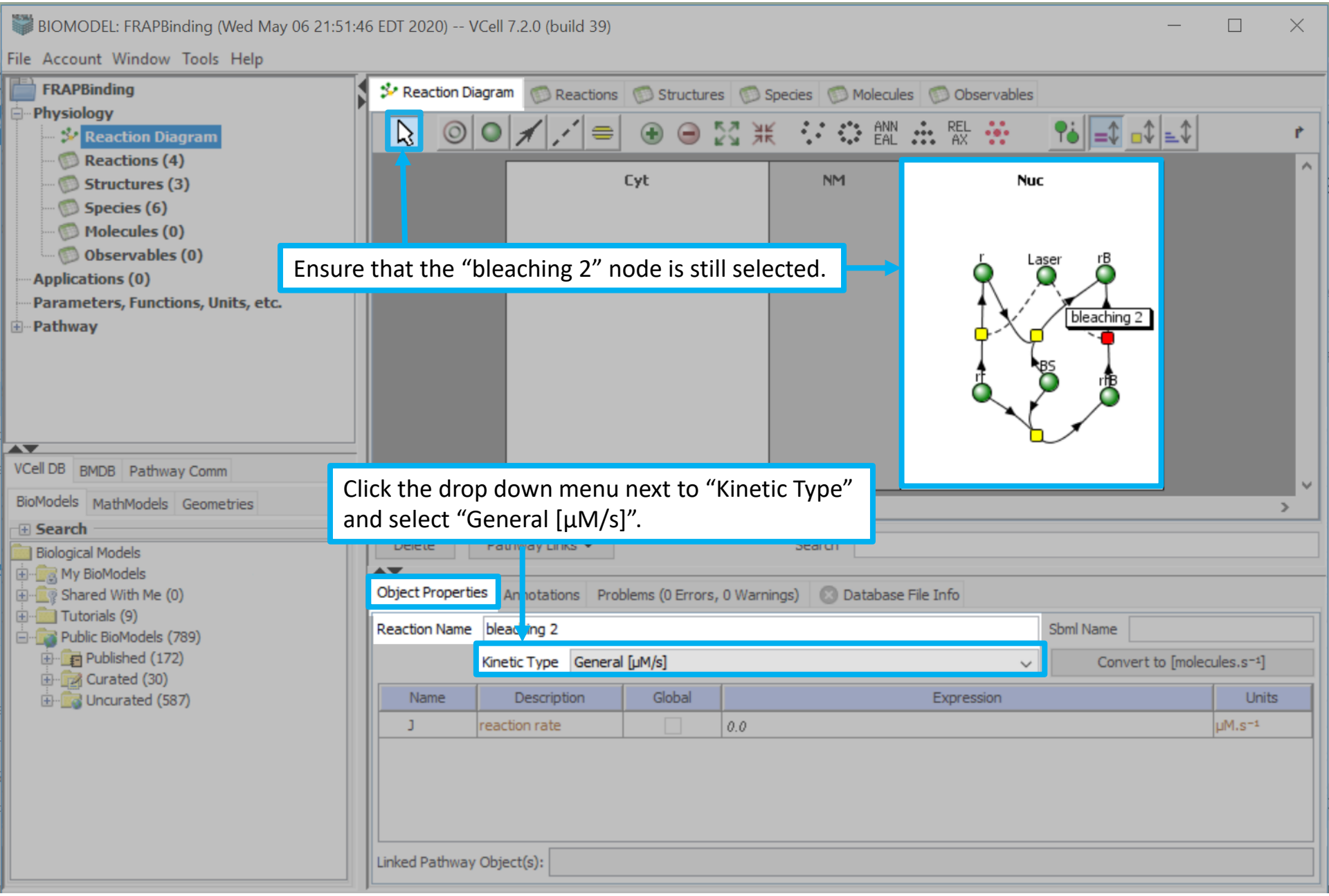

BIOMODEL: FRAPBinding (Tue May 05 01:41:57 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (4)
Structures (3)
Species (6)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions, Units, etc.
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
Cyt
NM
Nuc
r
Laser
rB
r2
BS
rf
rfB
Using the “Select” tool, click the “r2” node.
Delete
Pathway Links
Search
VCell DB
BMDB
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)
Curated (30)
Uncurated (587)
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Reaction Name
r2
Sbml Name
Kinetic Type
General [µM/s]
Convert to [molecules.s⁻¹]
Name
Description
Global
Expression
Units
J
reaction rate
0.0
µM.s⁻¹
Click the drop down menu next to “Kinetic Type”, and select “General [µM/s]”.
Linked Pathway Object(s):

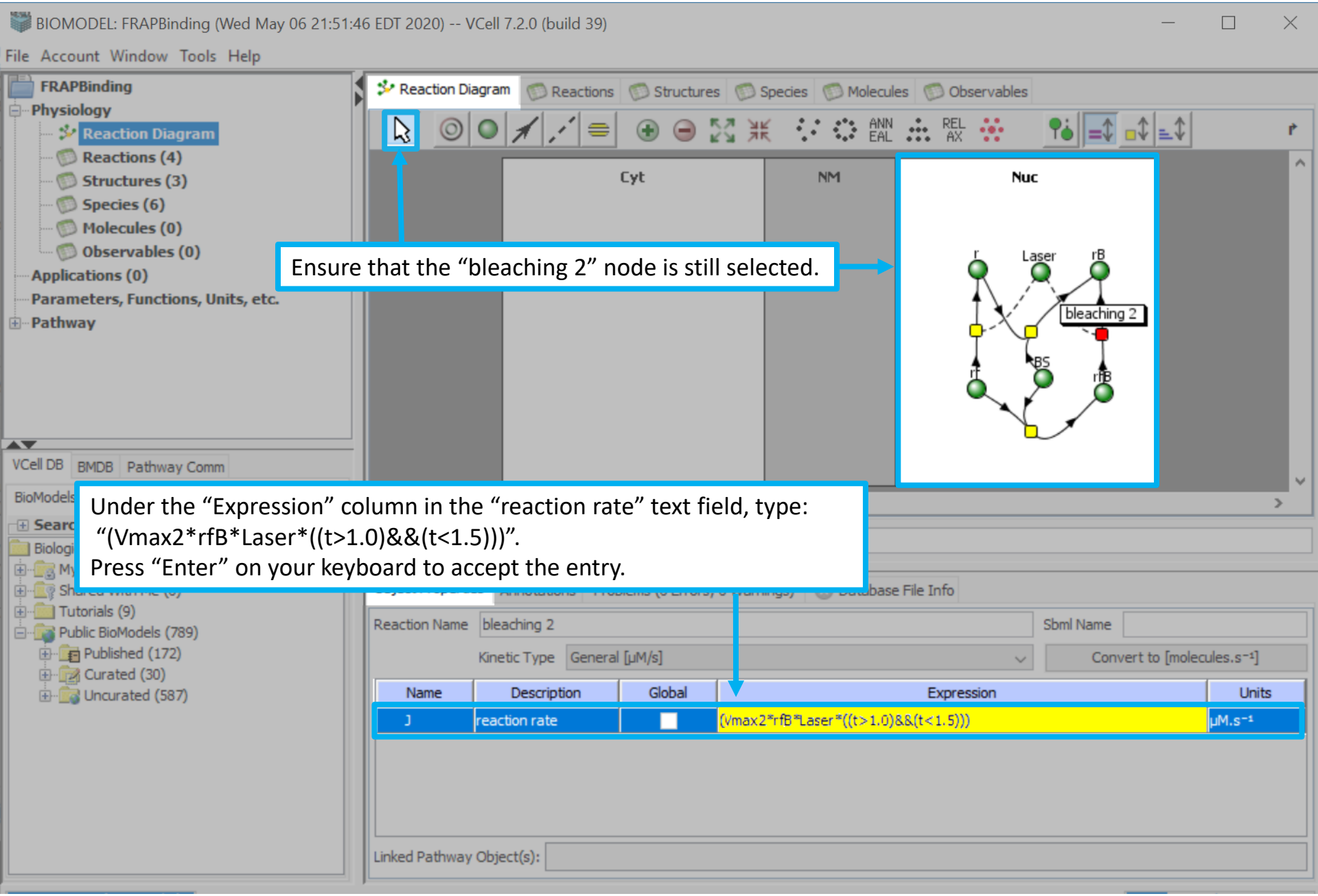

BIOMODEL: FRAPBinding (Tue May 05 01:41:57 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (4)
Structures (3)
Species (6)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions, Units, etc.
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
Cyt
NM
Nuc
r
Laser
rB
r2
BS
rf
rfB
Ensure the “r2” node is still selected.
Under the Expression column, in the “reaction rate” text field, type: “(Vmax*rf*Laser*((t>1.0)&&(t<1.5)))”.
Press “Enter” on your keyboard to accept your entry.
Search
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)
Curated (30)
Uncurated (587)
Reaction Name
r2
Sbml Name
Kinetic Type
General [µM/s]
Convert to [molecules.s⁻¹]
Name
Description
Global
Expression
Units
J
reaction rate
(Vmax * rf * Laser * ((t > 1.0) && (t < 1.5)))
µM.s⁻¹
Vmax
user defined
0.0
s⁻¹.µM⁻¹
rf
Species Concentration
Variable
µM
t
time
Variable
s
µM
Linked Pathway Object(s):
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.

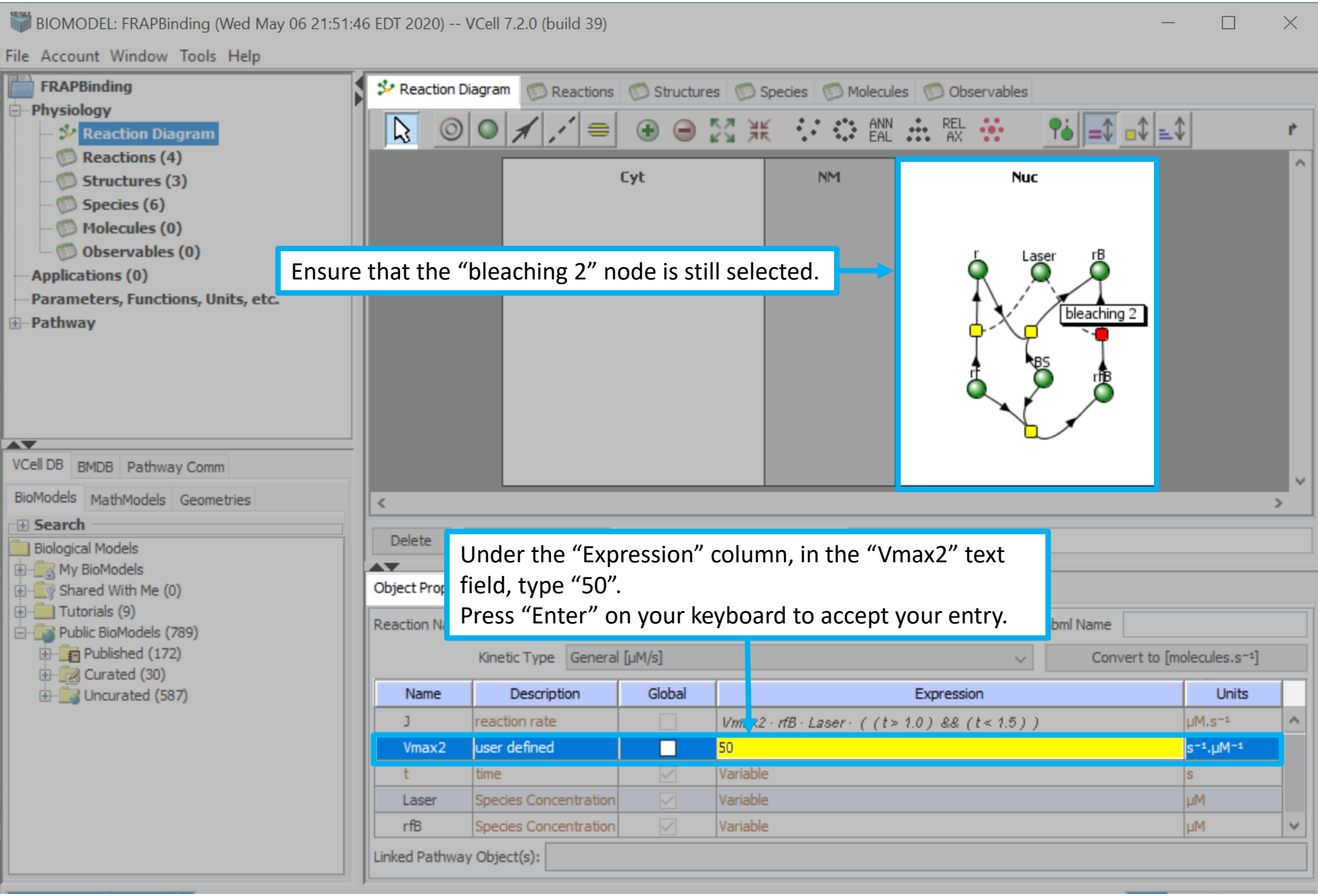

BIOMODEL: FRAPBinding (Wed May 06 20:28:19 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (4)
Structures (3)
Species (6)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions, Units, etc.
Pathway
VCell DB
BMDB
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)
Curated (30)
Uncurated (587)
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
Cyt
NM
Nuc
r
Laser
rB
r2
BS
rf
rfB
Ensure the “r2” node is still selected.
Delete
Object Properties
Reaction Name
r2
Kinetic Type
General [µM/s]
Convert to [molecules.s⁻¹]
Under the “Expression” column, in the Vmax text field, type “50”.
Press “Enter” on your keyboard to accept your entry.
Name
Description
Global
Expression
Units
J
reaction rate
Vmax · rf · Laser · ((t > 1.0) && (t < 1.5))
µM.s⁻¹
Vmax
user defined
50.0
s⁻¹.µM⁻¹
rf
Species Concentration
Variable
µM
Laser
Species Concentration
Variable
µM
t
time
Variable
s
Linked Pathway Object(s):

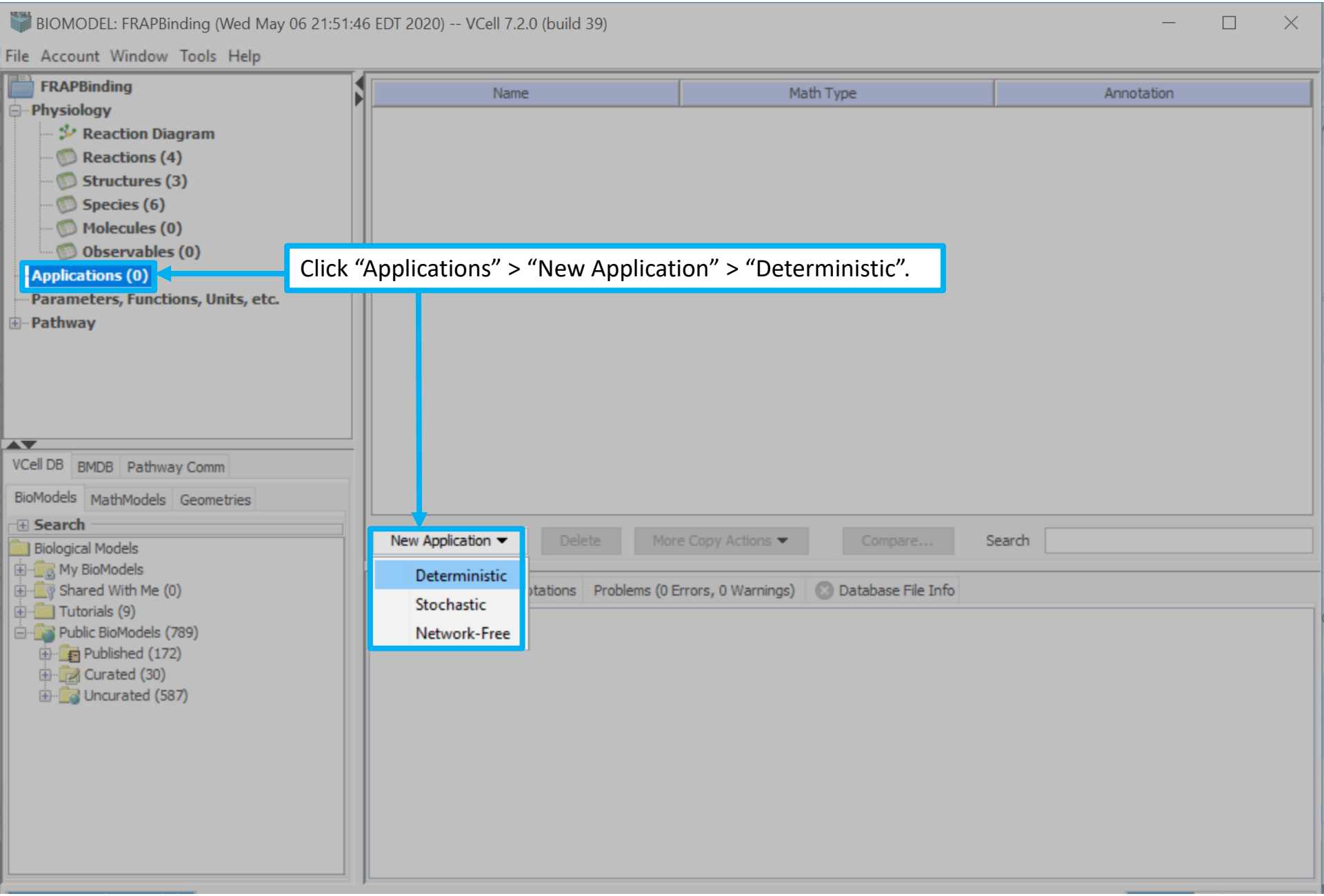

BIOMODEL: FRAPBinding (Wed May 06 20:28:19 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (4)
Structures (3)
Species (6)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions, Units, etc.
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
Cyt
NM
Nuc
r
Laser
rB
r2
BS
rf
rfB
Ensure the "r2" node is still selected.
In the "Reaction Name" text field, type "bleaching 1".
VCell DB
BMDB
Pathway Comm
BioModels
MathModels
Search
Biological Models
My BioModels
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)
Curated (30)
Uncurated (587)
Delete
Pathway Links
Search
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Reaction Name
bleaching 1
Sbml Name
Kinetic Type
General [µM/s]
Convert to [molecules.s⁻¹]
Name
Description
Global
Expression
Units
J
reaction rate
Vmax · rf · Laser · ((t > 1.0) && (t < 1.5))
µM.s⁻¹
Vmax
user defined
50.0
s⁻¹.µM⁻¹
rf
Species Concentration
Variable
µM
Laser
Species Concentration
Variable
µM
t
time
Variable
s
Linked Pathway Object(s):

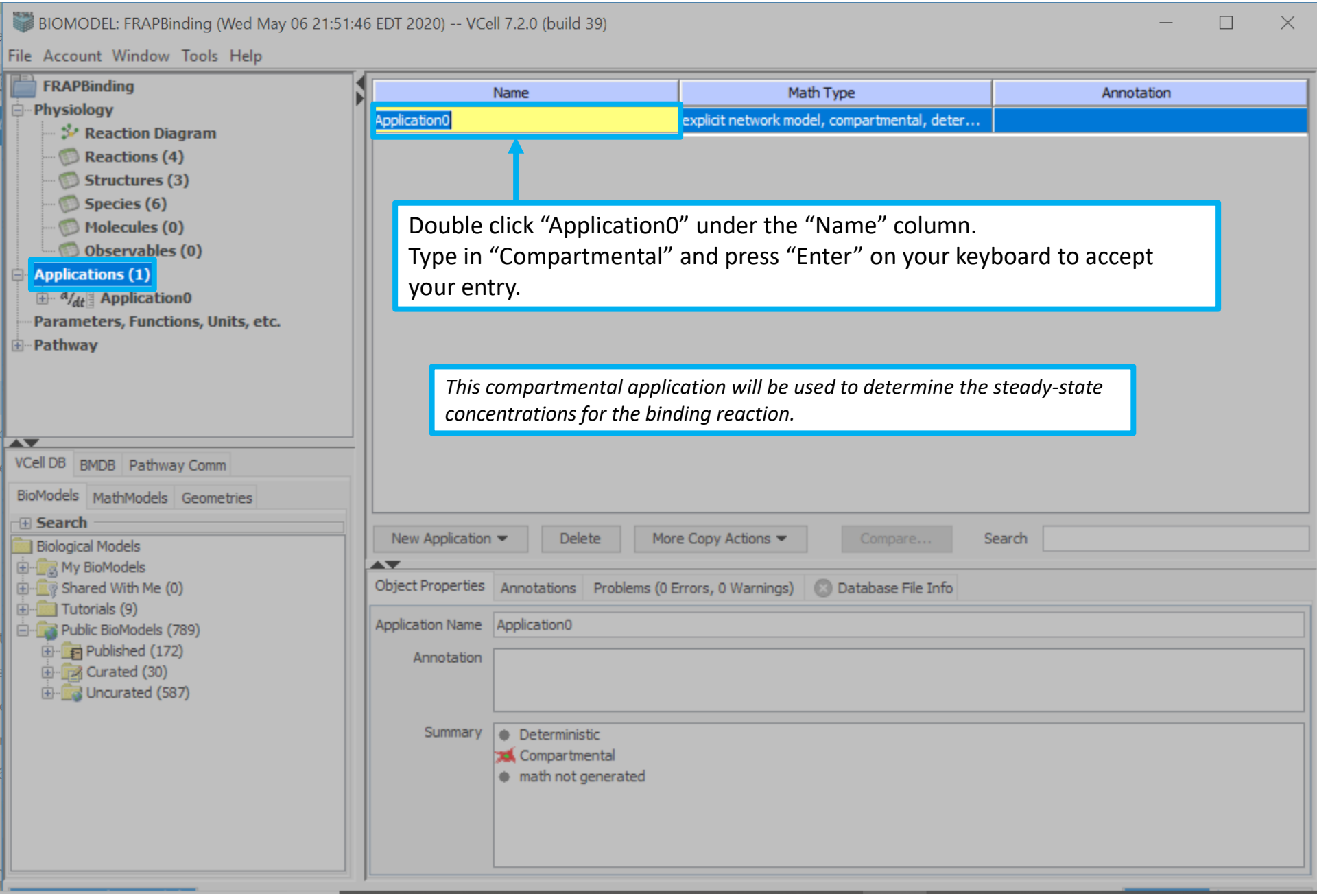

BIOMODEL: FRAPBinding (Wed May 06 20:28:19 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (4)
Structures (3)
Species (6)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions, Units, etc.
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
Cyt
NM
Nuc
r
Laser
rB
r3
BS
rf
rfB
Use the “Select” tool to click on node “r3”.
In the “Reaction Name” text field, type “bleaching 2”.
VCell DB
BMDB
Pathway Comm
BioModels
MathModels
Geomet
Search
Biological Models
My BioModels
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)
Curated (30)
Uncurated (587)
Delete
Pathway Links
Search
Object Properties
Annotation
Problems (0 Errors, 0 Warnings)
Reaction Name
bleaching 2
Sbml Name
Reversible
Kinetic Type
Mass Action [μM/s] (recommended for stochastic application)
Convert to [molecules.s⁻¹]
Name
Description
Global
Expression
Units
J
reaction rate
(Kf · rfB - Kr · rB)
μM.s⁻¹
Kf
forward rate constant
0.0
s⁻¹
Kr
reverse rate constant
0.0
s⁻¹
rfB
Species Concentration
Variable
μM
rB
Species Concentration
Variable
μM
Laser
Species Concentration
Variable
μM
Linked Pathway Object(s):

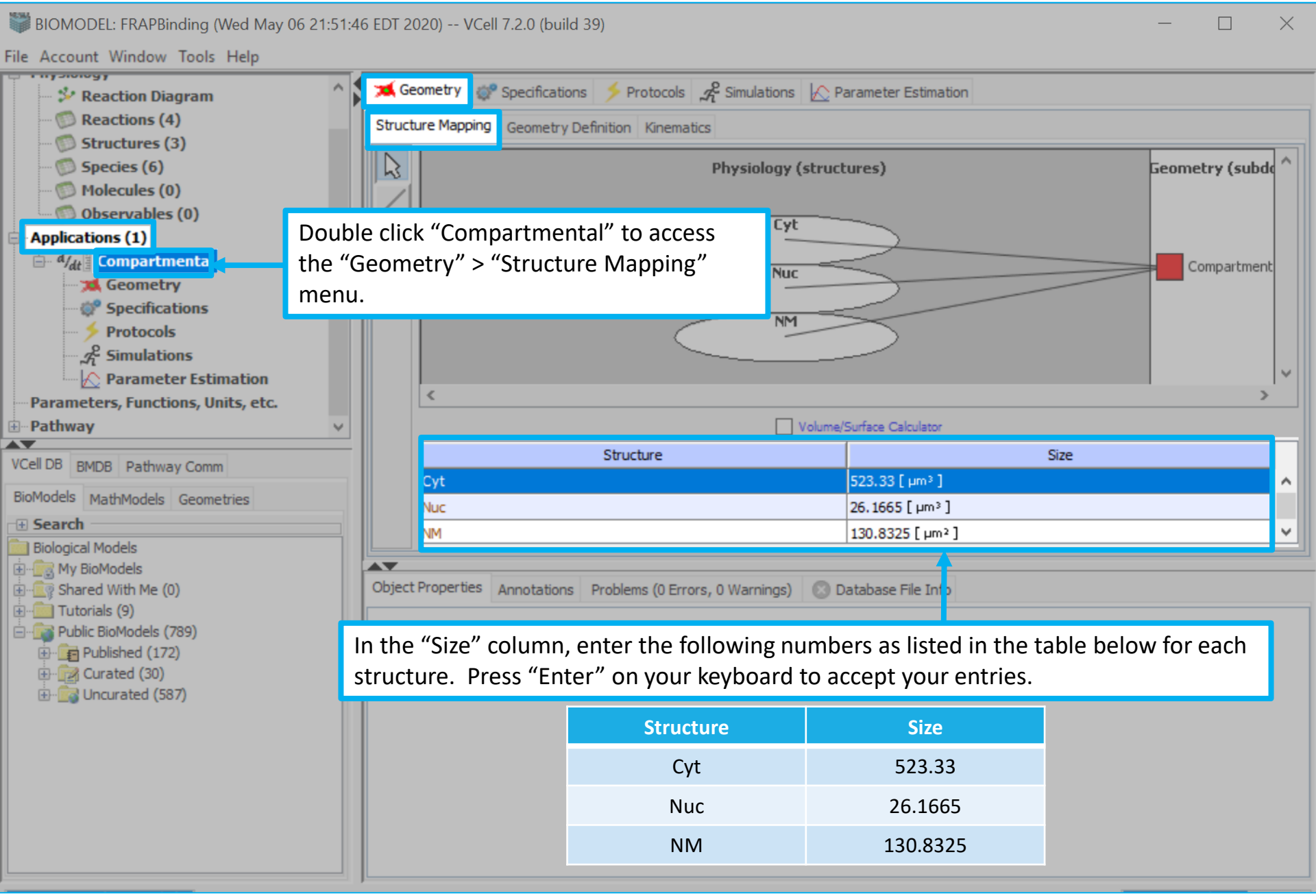

BIOMODEL: FRAPBinding (Wed May 06 21:51:46 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (4)
Structures (3)
Species (6)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions, Units, etc.
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
Cyt
NM
Nuc
r
Laser
rB
bleaching 2
BS
rf
rfB
Ensure that the “bleaching 2” node is still selected.
Click the drop down menu next to “Kinetic Type” and select “General [µM/s]”.
VCell DB
BMDB
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)
Curated (30)
Uncurated (587)
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Database File Info
Reaction Name
bleaching 2
Sbml Name
Kinetic Type
General [µM/s]
Convert to [molecules.s⁻¹]
Name
Description
Global
Expression
Units
J
reaction rate
0.0
µM.s⁻¹
Linked Pathway Object(s):


BIOMODEL: FRAPBinding (Wed May 06 21:51:46 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (4)
Structures (3)
Species (6)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions, Units, etc.
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
Cyt
NM
Nuc
r
Laser
rB
bleaching 2
BS
rf
rfB
Ensure that the “bleaching 2” node is still selected.
Under the “Expression” column in the “reaction rate” text field, type:
“(Vmax2*rfB*Laser*((t>1.0)&&(t<1.5)))”.
Press “Enter” on your keyboard to accept the entry.
VCell DB
BMDB
Pathway Comm
Tutorials (9)
Public BioModels (789)
Published (172)
Curated (30)
Uncurated (587)
Reaction Name
bleaching 2
Sbml Name
Kinetic Type
General [µM/s]
Convert to [molecules.s⁻¹]
Name
Description
Global
Expression
Units
J
reaction rate
(Vmax2*rfB*Laser*((t>1.0)&&(t<1.5)))
µM.s⁻¹
Linked Pathway Object(s):

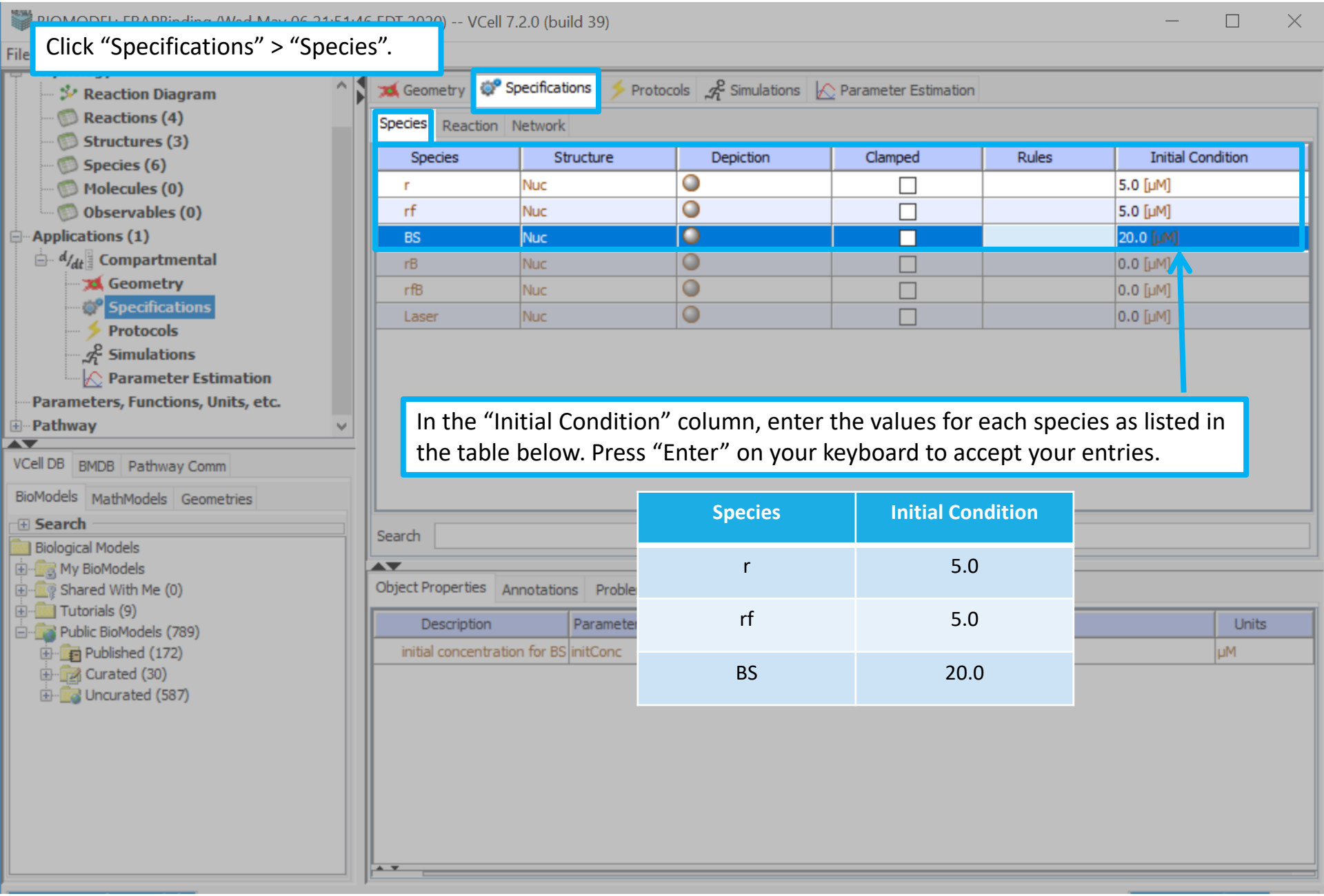

BIOMODEL: FRAPBinding (Wed May 06 21:51:46 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (4)
Structures (3)
Species (6)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions, Units, etc.
Pathway
Reaction Diagram
Reactions
Structures
Species
Molecules
Observables
Cyt
NM
Nuc
r
Laser
rB
bleaching 2
BS
rf
rfB
Ensure that the “bleaching 2” node is still selected.
VCell DB
BMDB
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)
Curated (30)
Uncurated (587)
Delete
Under the “Expression” column, in the “Vmax2” text field, type “50”.
Press “Enter” on your keyboard to accept your entry.
Object Prop
Kinetic Type
General [µM/s]
Convert to [molecules.s⁻¹]
Name
Description
Global
Expression
Units
J
reaction rate
µM.s⁻¹
Vmax2
user defined
50
s⁻¹.µM⁻¹
t
time
Variable
s
Laser
Species Concentration
Variable
µM
rfB
Species Concentration
Variable
µM
Linked Pathway Object(s):


BIOMODEL: FRAPBinding (Wed May 06 21:51:46 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (4)
Structures (3)
Species (6)
Molecules (0)
Observables (0)
Applications (0)
Parameters, Functions, Units, etc.
Pathway
Name
Math Type
Annotation
Click “Applications” > “New Application” > “Deterministic”.
VCell DB
BMDB
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)
Curated (30)
Uncurated (587)
New Application
Deterministic
Stochastic
Network-Free
Delete
More Copy Actions
Compare...
Search
Problems (0 Errors, 0 Warnings)
Database File Info

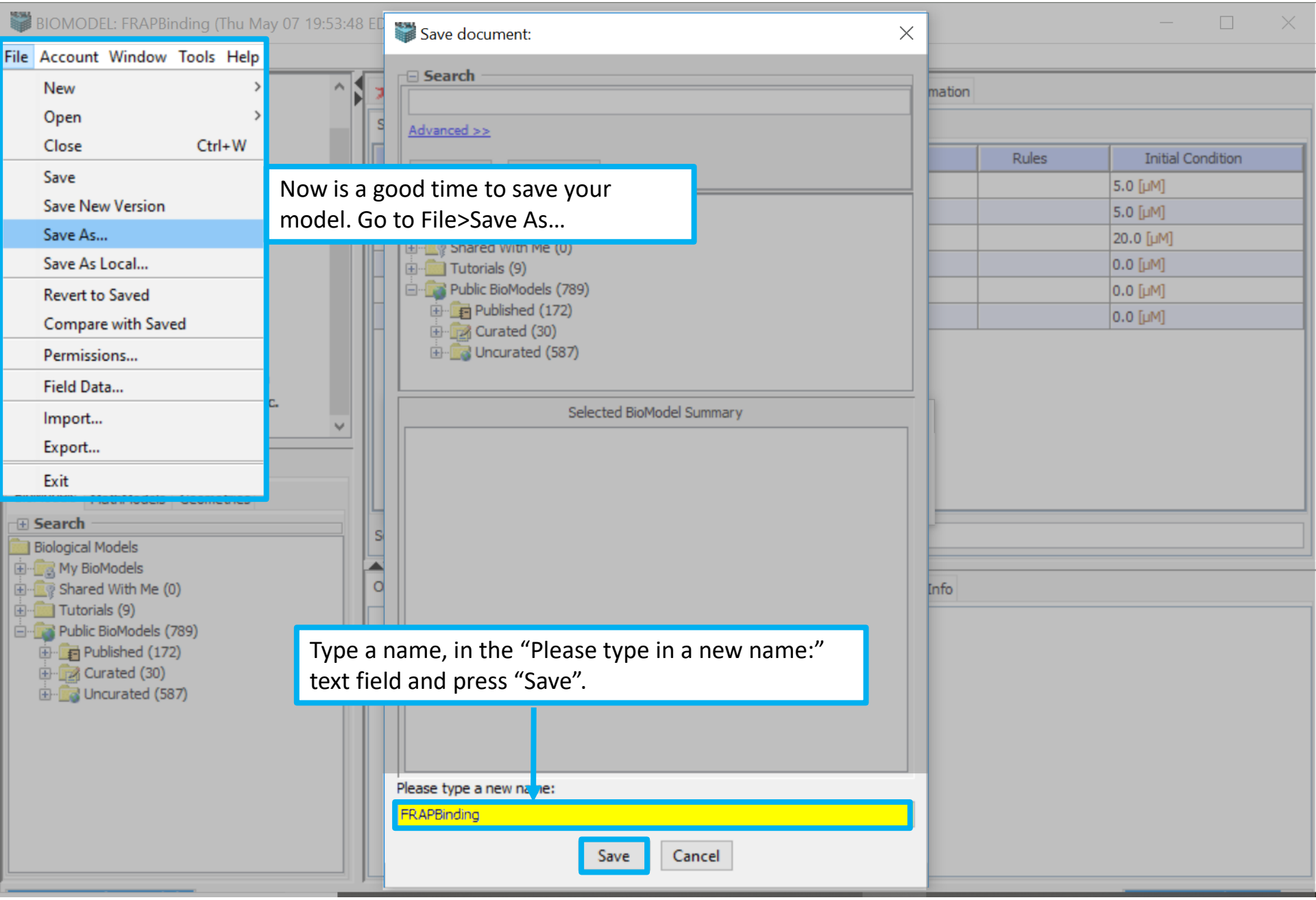

BIOMODEL: FRAPBinding (Wed May 06 21:51:46 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (4)
Structures (3)
Species (6)
Molecules (0)
Observables (0)
Applications (1)
Application0
Parameters, Functions, Units, etc.
Pathway
VCell DB
BMDB
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)
Curated (30)
Uncurated (587)
Name
Math Type
Annotation
Application0
explicit network model, compartmental, deter...
Double click “Application0” under the “Name” column.
Type in “Compartmental” and press “Enter” on your keyboard to accept your entry.
This compartmental application will be used to determine the steady-state concentrations for the binding reaction.
New Application
Delete
More Copy Actions
Compare...
Search
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Database File Info
Application Name
Application0
Annotation
Summary
Deterministic
Compartmental
math not generated

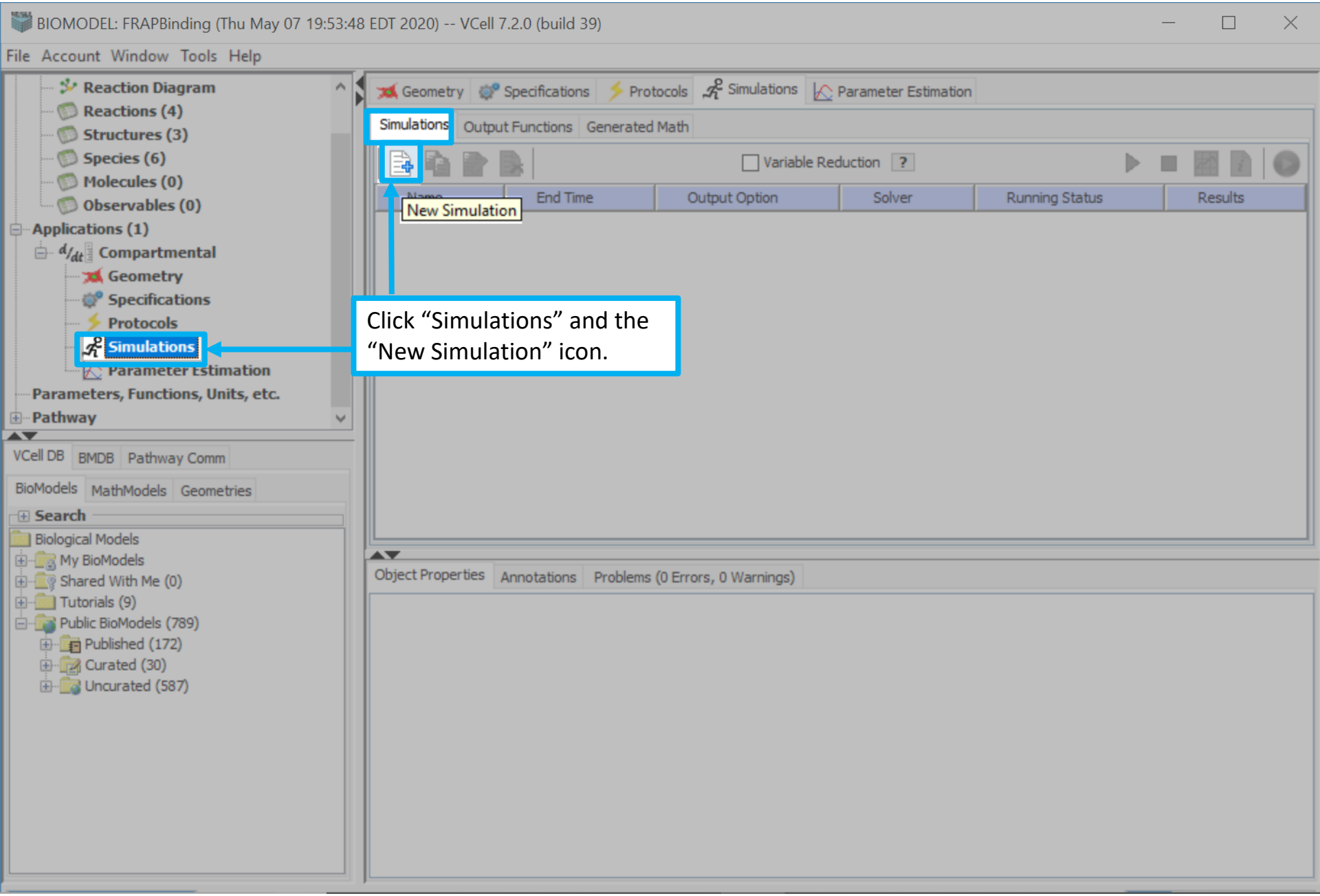


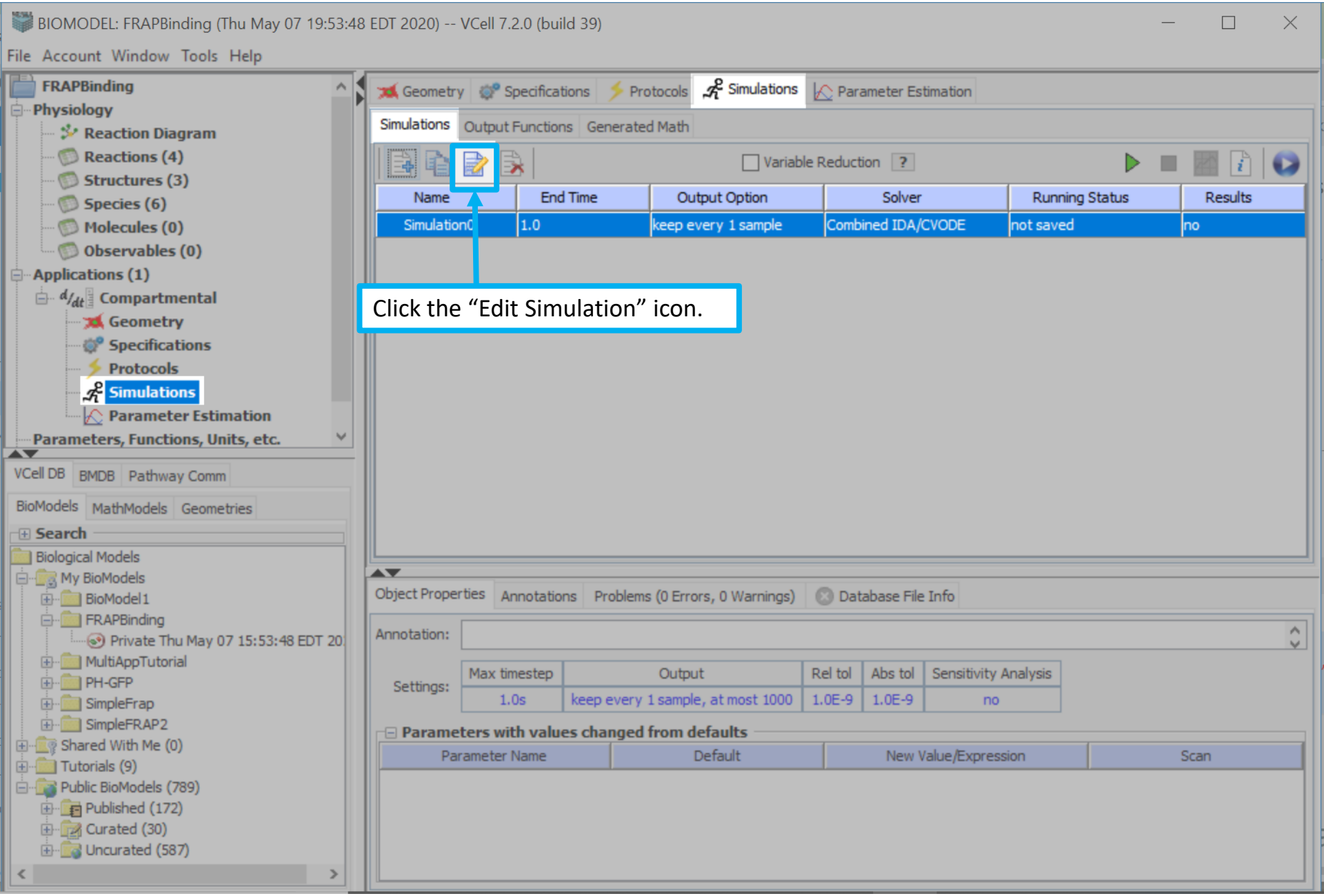
Structure	Size
Cyt	523.33
Nuc	26.1665
NM	130.8325

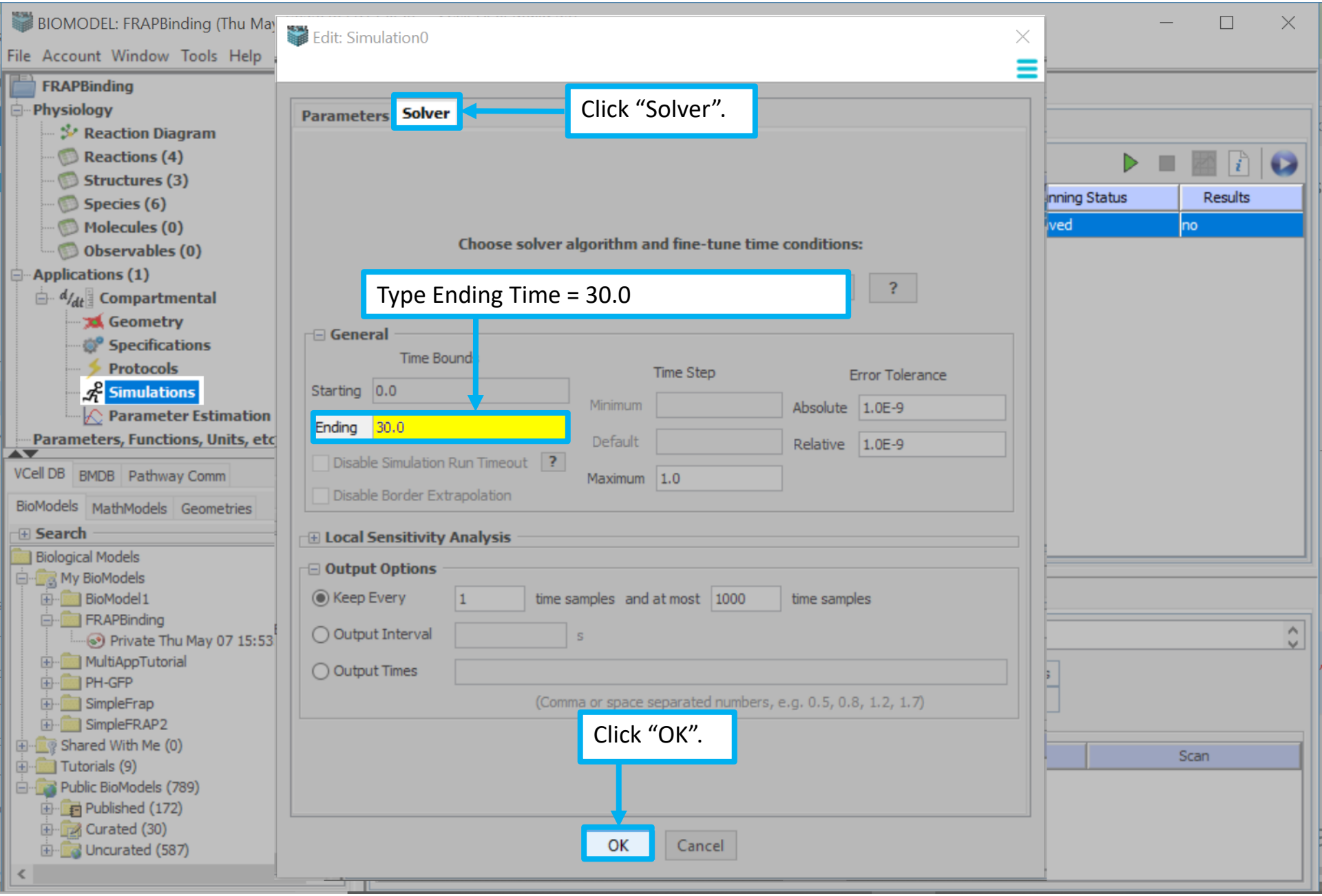


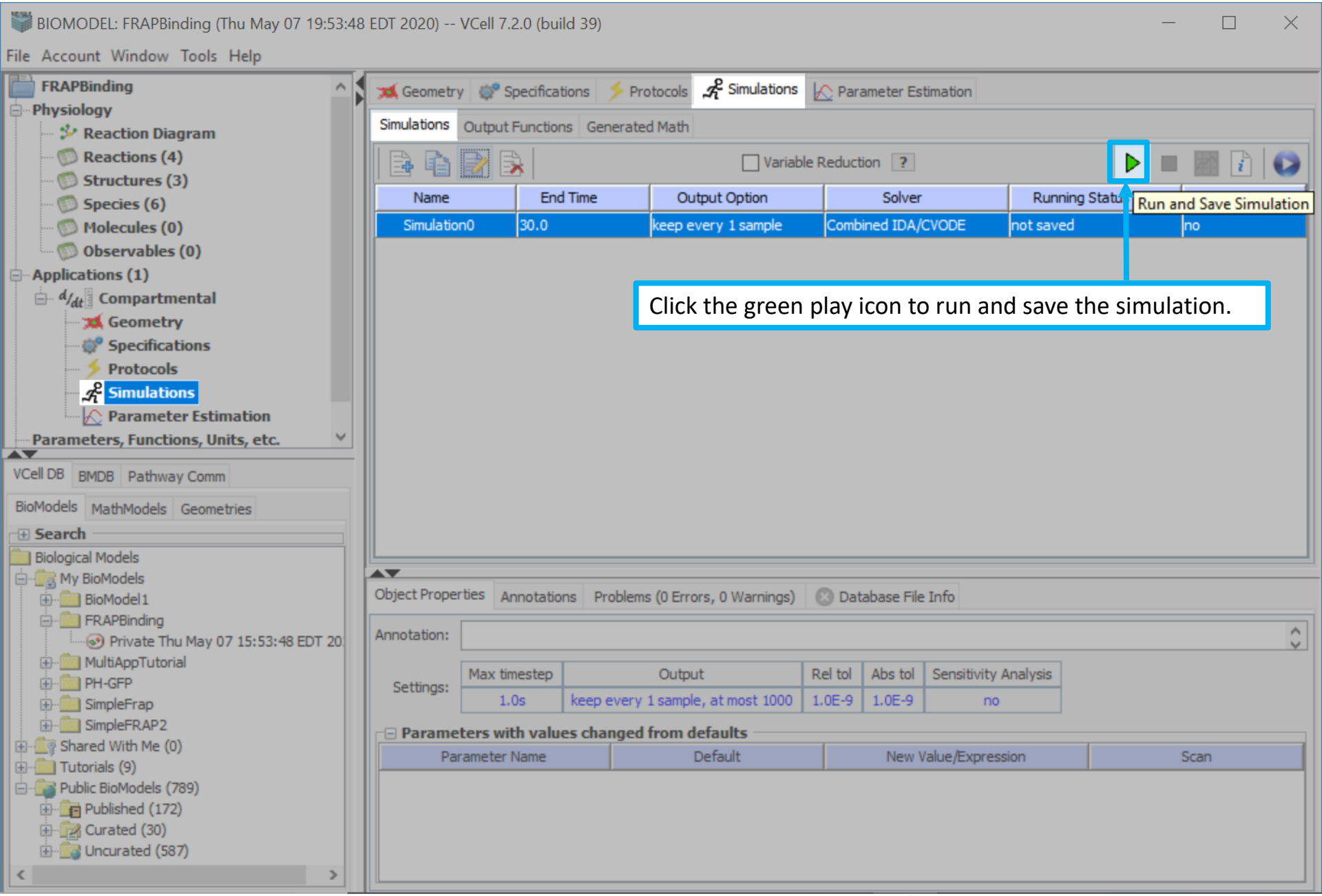
Species	Initial Condition
r	5.0
rf	5.0
BS	20.0


File Account Window Tools Help
New
Open
Close Ctrl+W
Save
Save New Version
Save As...
Save As Local...
Revert to Saved
Compare with Saved
Permissions...
Field Data...
Import...
Export...
Exit
Now is a good time to save your model. Go to File>Save As...
Save document:
Search
Advanced >>
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)
Curated (30)
Uncurated (587)
Selected BioModel Summary
Type a name, in the “Please type in a new name:” text field and press “Save”.
Please type a new name:
FRAPBinding
Save
Cancel
Rules
Initial Condition
5.0 [µM]
5.0 [µM]
20.0 [µM]
0.0 [µM]
0.0 [µM]
0.0 [µM]
Biological Models
My BioModels


BIOMODEL: FRAPBinding (Thu May 07 19:53:48 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
Reaction Diagram
Reactions (4)
Structures (3)
Species (6)
Molecules (0)
Observables (0)
Applications (1)
Compartmental
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Parameters, Functions, Units, etc.
Pathway
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Simulations
Output Functions
Generated Math
Variable Reduction
?
New Simulation
End Time
Output Option
Solver
Running Status
Results
Click “Simulations” and the “New Simulation” icon.
VCell DB
BMDB
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)
Curated (30)
Uncurated (587)
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)


BIOMODEL: FRAPBinding (Thu May 07 19:53:48 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (4)
Structures (3)
Species (6)
Molecules (0)
Observables (0)
Applications (1)
Compartmental
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Parameters, Functions, Units, etc.
VCell DB
BMDB
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels
BioModel1
FRAPBinding
Private Thu May 07 15:53:48 EDT 20
MultiAppTutorial
PH-GFP
SimpleFrap
SimpleFRAP2
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)
Curated (30)
Uncurated (587)
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Simulations
Output Functions
Generated Math
Variable Reduction
?
Name
End Time
Output Option
Solver
Running Status
Results
Simulation0
1.0
keep every 1 sample
Combined IDA/CVODE
not saved
no
Click the “Edit Simulation” icon.
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Database File Info
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


BIOMODEL: FRAPBinding (Thu May
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (4)
Structures (3)
Species (6)
Molecules (0)
Observables (0)
Applications (1)
Compartmental
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Parameters, Functions, Units, etc
VCell DB
BMDB
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels
BioModel1
FRAPBinding
Private Thu May 07 15:53
MultiAppTutorial
PH-GFP
SimpleFrap
SimpleFRAP2
Shared With Me (0)
Tutorials (9)
Public BioModels (789)
Published (172)
Curated (30)
Uncurated (587)
Edit: Simulation0
Parameters
Solver
Click “Solver”.
Choose solver algorithm and fine-tune time conditions:
Type Ending Time = 30.0
?
General
Time Bound
Starting
0.0
Ending
30.0
Disable Simulation Run Timeout
?
Disable Border Extrapolation
Time Step
Minimum
Default
Maximum
1.0
Error Tolerance
Absolute
1.0E-9
Relative
1.0E-9
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
nning Status
Results
ved
no
Scan


BIOMODEL: FRAPBinding (Thu May 07 19:53:48 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (4)
Structures (3)
Species (6)
Molecules (0)
Observables (0)
Applications (1)
Compartmental
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Parameters, Functions, Units, etc.
VCell DB
BMDB
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels
BioModel1
FRAPBinding
Private Thu May 07 15:53:48 EDT 20
MultiAppTutorial
PH-GFP
SimpleFrap
SimpleFRAP2
Shared With Me (0)
Tutorials (9)
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Simulations
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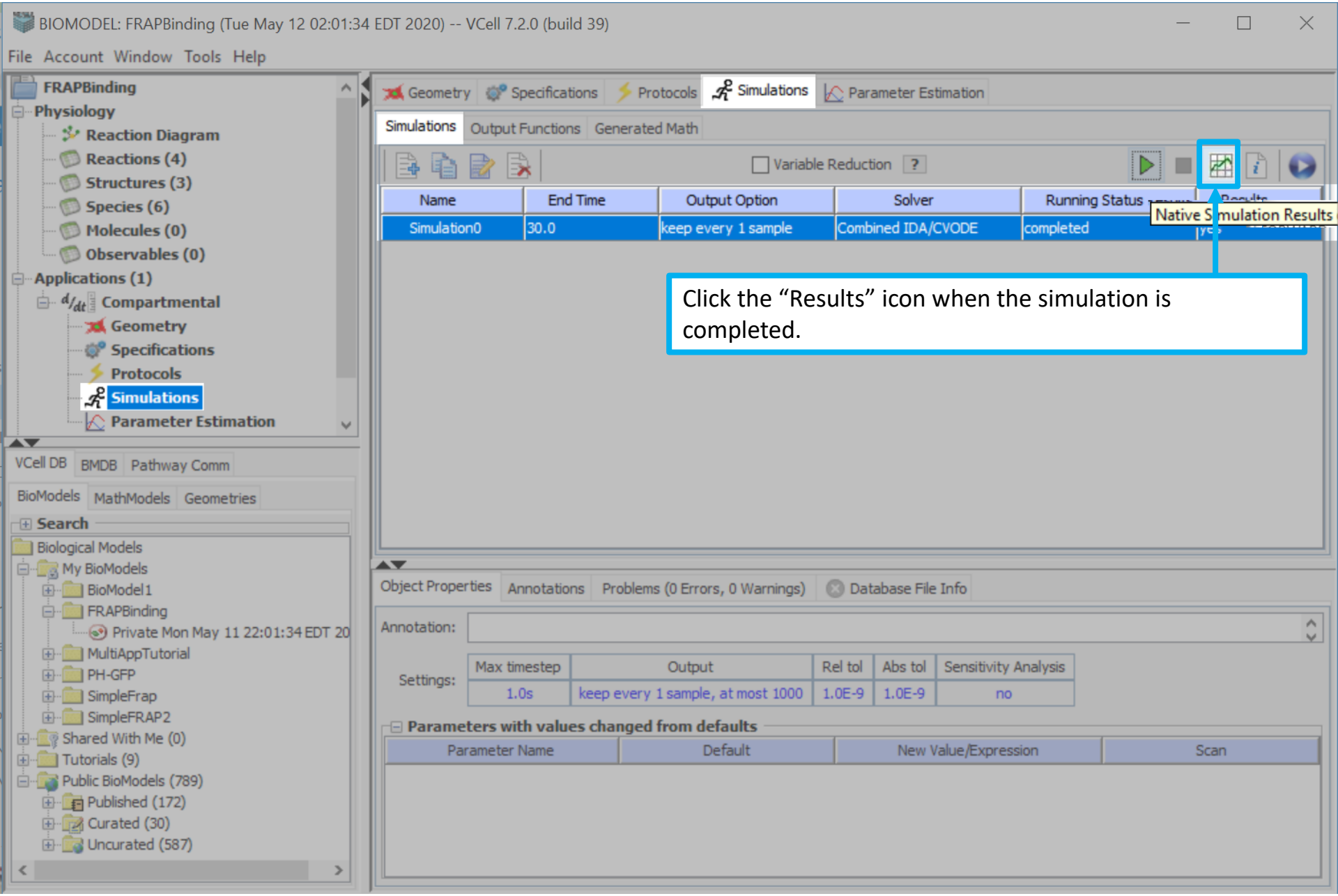
Generated Math
Variable Reduction
?
Run and Save Simulation
Name
End Time
Output Option
Solver
Running Statu
Simulation0
30.0
keep every 1 sample
Combined IDA/CVODE
not saved
no
Click the green play icon to run and save the simulation.
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Database File Info
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


BIOMODEL: FRAPBinding (Tue May 12 02:01:34 EDT 2020) -- VCell 7.2.0 (build 39)
File Account Window Tools Help
FRAPBinding
Physiology
Reaction Diagram
Reactions (4)
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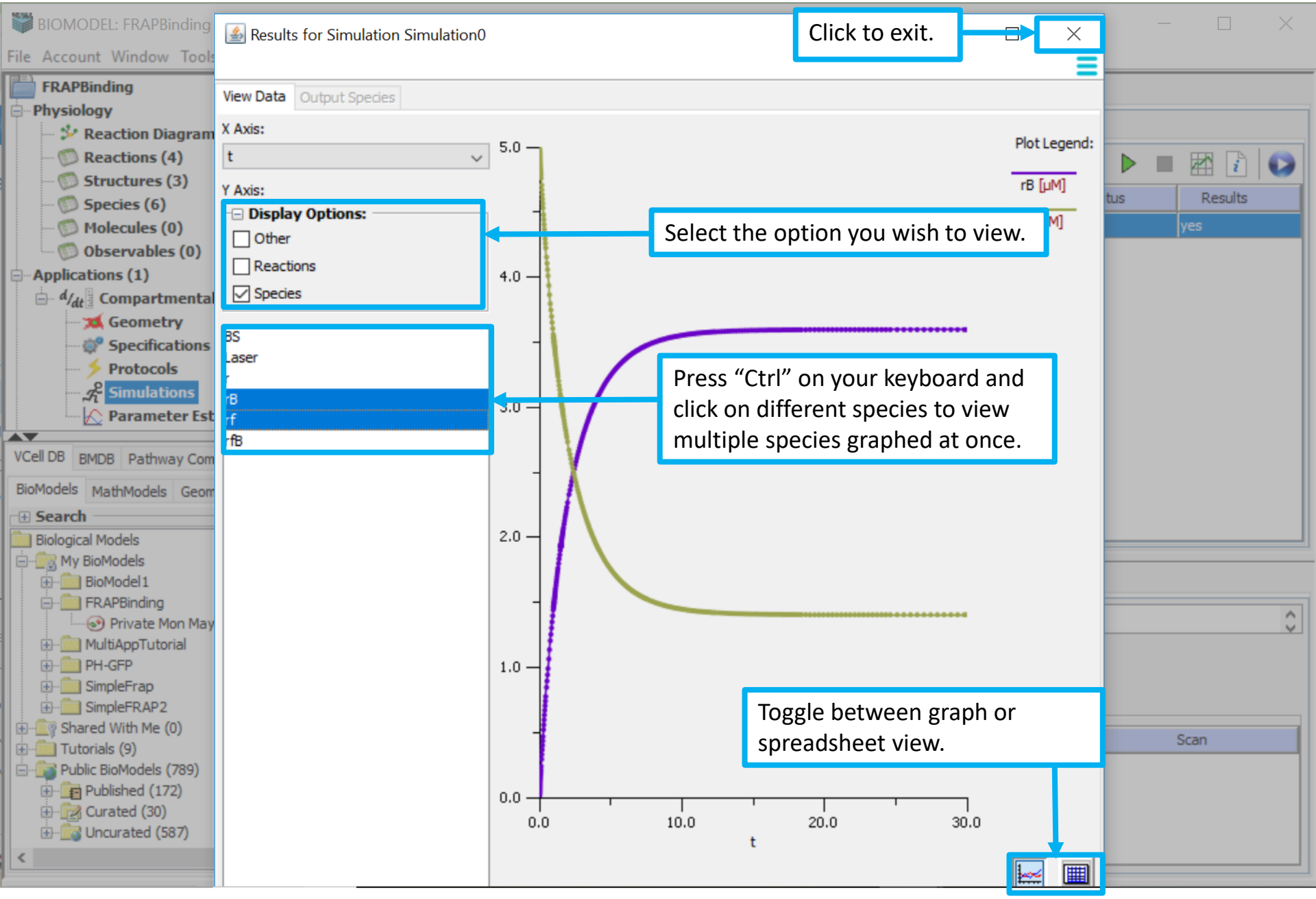
Geometry Specifications Protocols Simulations Parameter Estimation
Simulations Output Functions Generated Math
Variable Reduction ?
Name End Time Output Option Solver Running Status
Simulation0 30.0 keep every 1 sample Combined IDA/CVODE completed
Native Simulation Results
Click the “Results” icon when the simulation is completed.
Object Properties Annotations Problems (0 Errors, 0 Warnings) Database File Info
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


Results for Simulation Simulation0
Click to exit.
View Data
Output Species
X Axis:
t
Y Axis:
Display Options:
Other
Reactions
Species
Plot Legend:
rB [µM]
Select the option you wish to view.
Press “Ctrl” on your keyboard and click on different species to view multiple species graphed at once.
Toggle between graph or spreadsheet view.
5.0
4.0
3.0
2.0
1.0
0.0
0.0
10.0
20.0
30.0
t
FRAPBinding
Physiology
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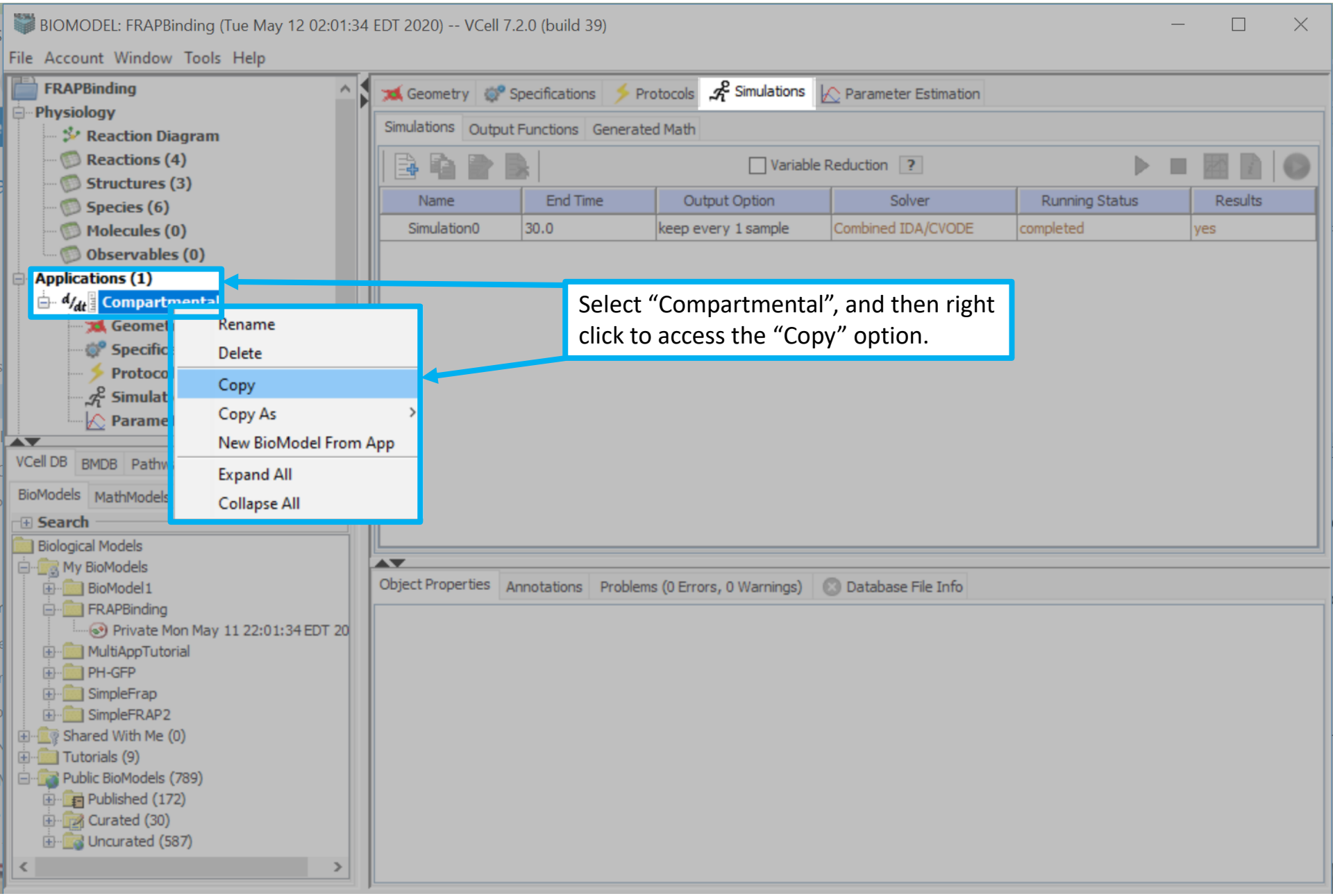
Results
yes
Scan


BIOMODEL: FRAPBinding (Tue May 12 02:01:34 EDT 2020) -- VCell 7.2.0 (build 39)
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FRAPBinding
Physiology
Reaction Diagram
Reactions (4)
Structures (3)
Species (6)
Molecules (0)
Observables (0)
Applications (1)
Compartmental
Rename
Delete
Copy
Copy As
New BioModel From App
Expand All
Collapse All
Select “Compartmental”, and then right click to access the “Copy” option.
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Simulations
Output Functions
Generated Math
Variable Reduction
Name
End Time
Output Option
Solver
Running Status
Results
Simulation0
30.0
keep every 1 sample
Combined IDA/CVODE
completed
yes
VCell DB
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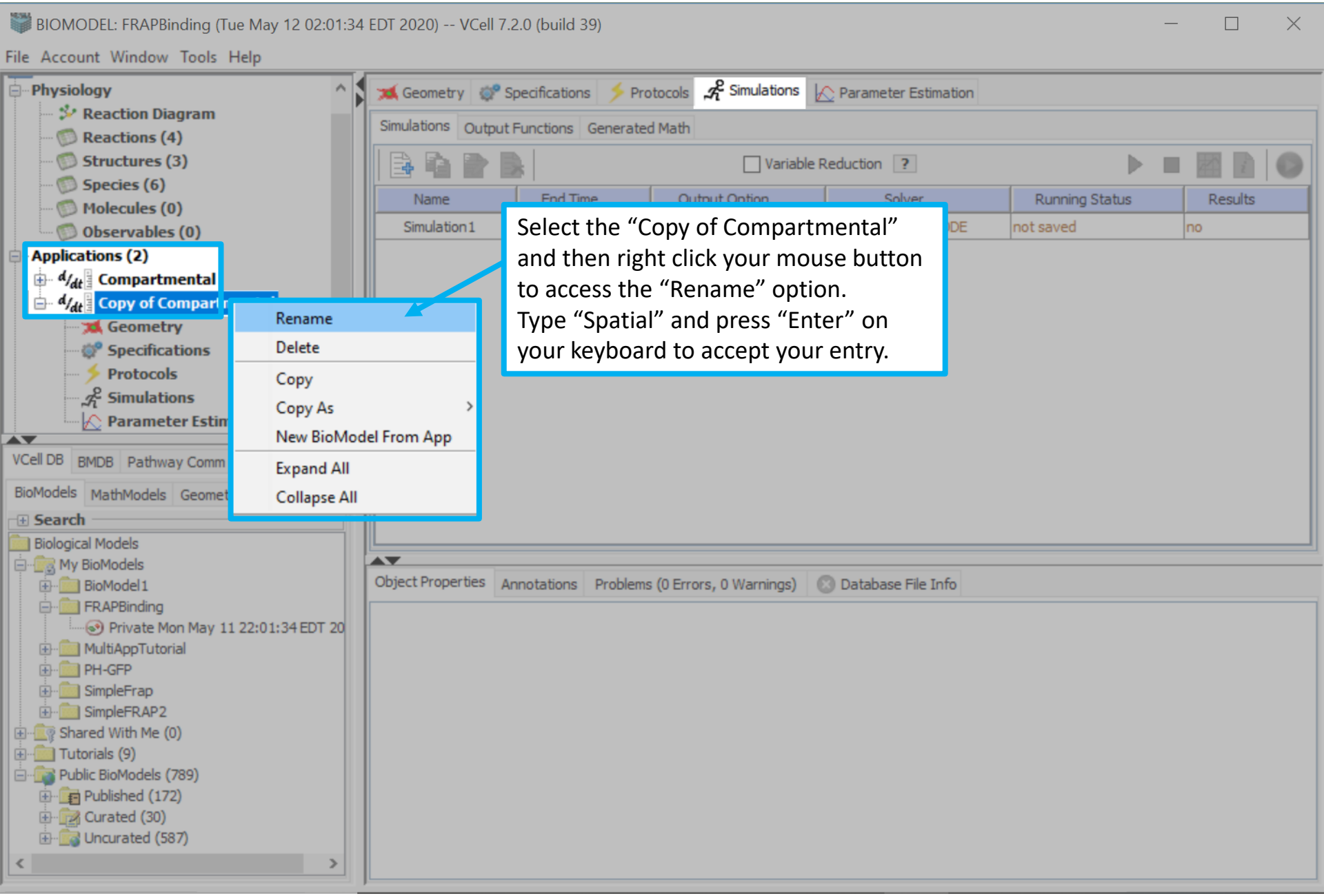
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Database File Info


BIOMODEL: FRAPBinding (Tue May 12 02:01:34 EDT 2020) -- VCell 7.2.0 (build 39)
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Molecules (0)
Observables (0)
Applications (2)
Compartmental
Copy of Compart
Geometry
Specifications
Protocols
Simulations
Parameter Estim
Rename
Delete
Copy
Copy As
New BioModel From App
Expand All
Collapse All
Select the “Copy of Compartmental” and then right click your mouse button to access the “Rename” option.
Type “Spatial” and press “Enter” on your keyboard to accept your entry.
Geometry
Specifications
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Simulations
Output Functions
Generated Math
Variable Reduction
Name
End Time
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Simulation1
not saved
no
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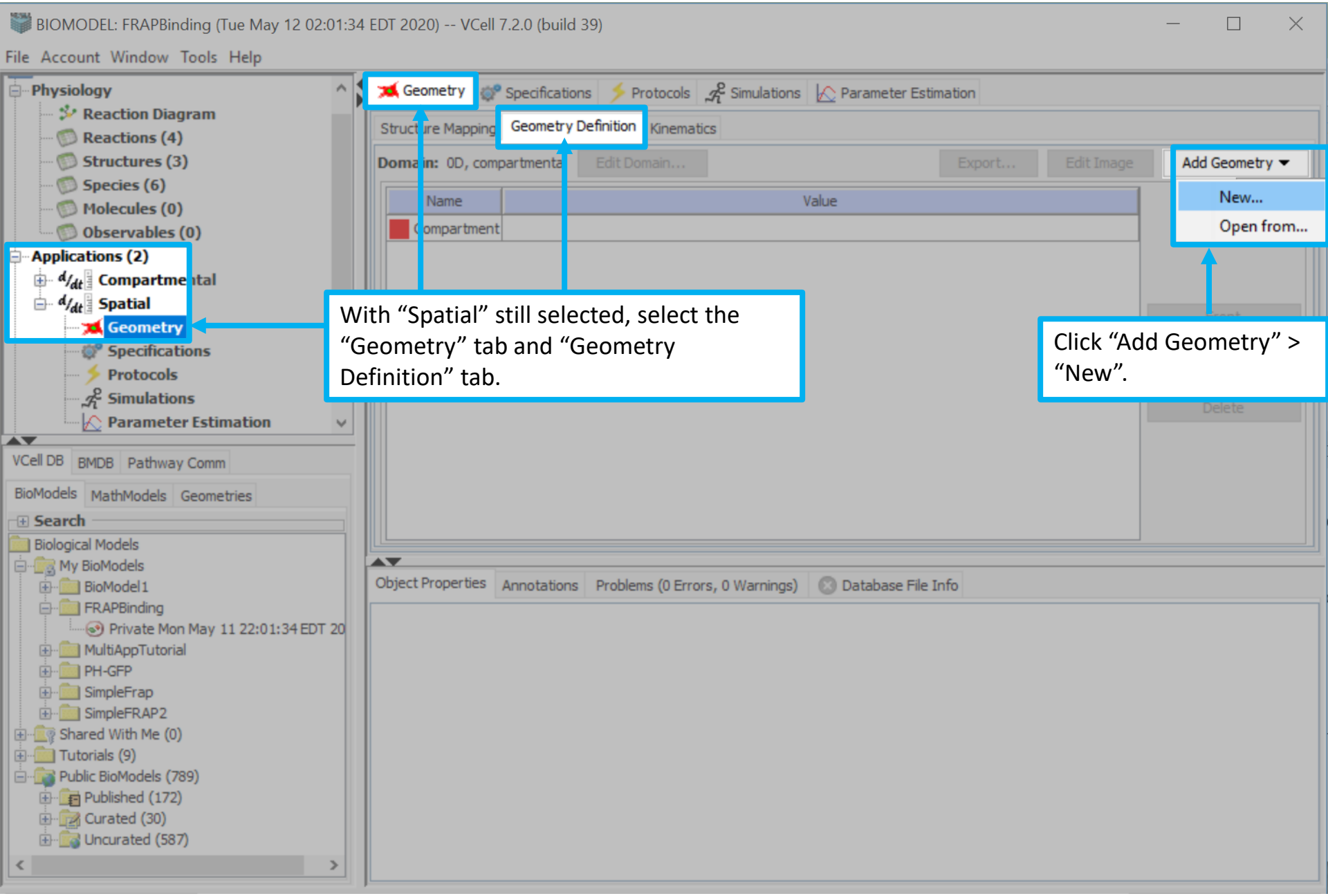
Database File Info


BIOMODEL: FRAPBinding (Tue May 12 02:01:34 EDT 2020) -- VCell 7.2.0 (build 39)
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Parameter Estimation
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Structure Mapping
Geometry Definition
Kinematics
Domain: 0D, compartmenta
Edit Domain...
Export...
Edit Image
Add Geometry
New...
Open from...
Name
Value
Compartment
Delete
With “Spatial” still selected, select the “Geometry” tab and “Geometry Definition” tab.
Click “Add Geometry” > “New”.
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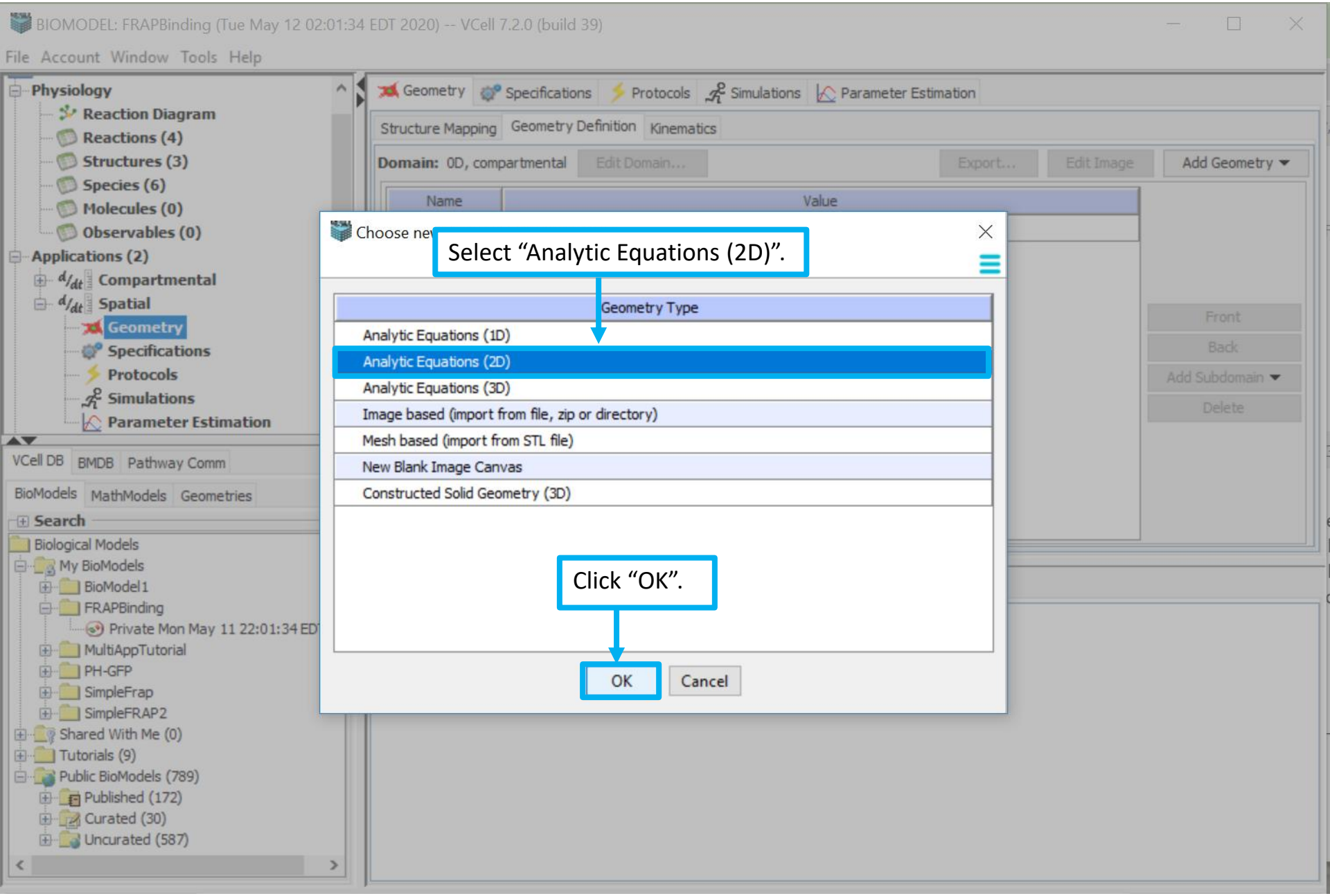
Problems (0 Errors, 0 Warnings)
Database File Info


BIOMODEL: FRAPBinding (Tue May 12 02:01:34 EDT 2020) -- VCell 7.2.0 (build 39)
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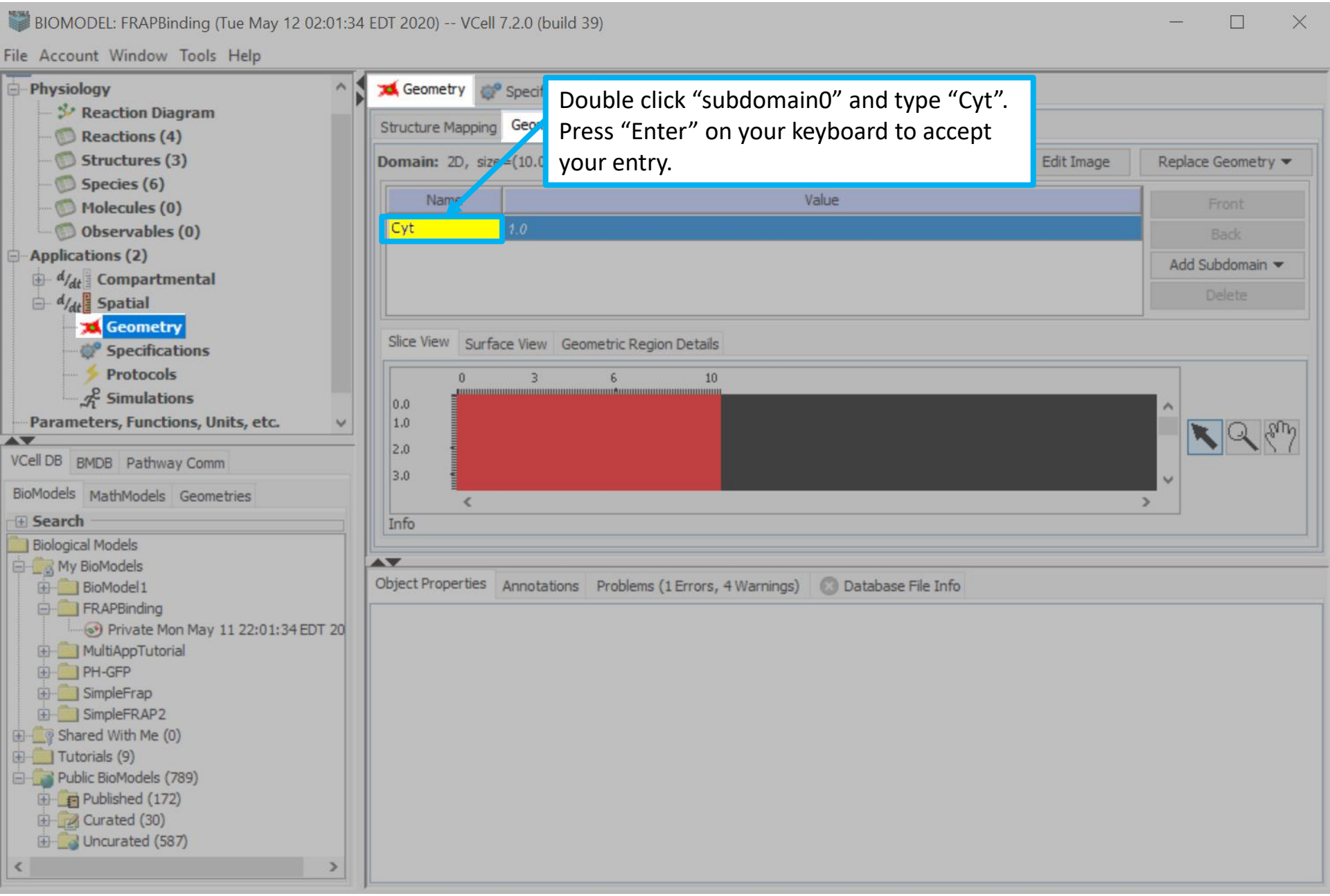
Structure Mapping
Geometry Definition
Kinematics
Domain: 0D, compartmental
Edit Domain...
Export...
Edit Image
Add Geometry
Name
Value
Front
Back
Add Subdomain
Delete
Choose ne
Select “Analytic Equations (2D)”.
Geometry Type
Analytic Equations (1D)
Analytic Equations (2D)
Analytic Equations (3D)
Image based (import from file, zip or directory)
Mesh based (import from STL file)
New Blank Image Canvas
Constructed Solid Geometry (3D)
Click “OK”.
OK
Cancel


BIOMODEL: FRAPBinding (Tue May 12 02:01:34 EDT 2020) -- VCell 7.2.0 (build 39)
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Observables (0)
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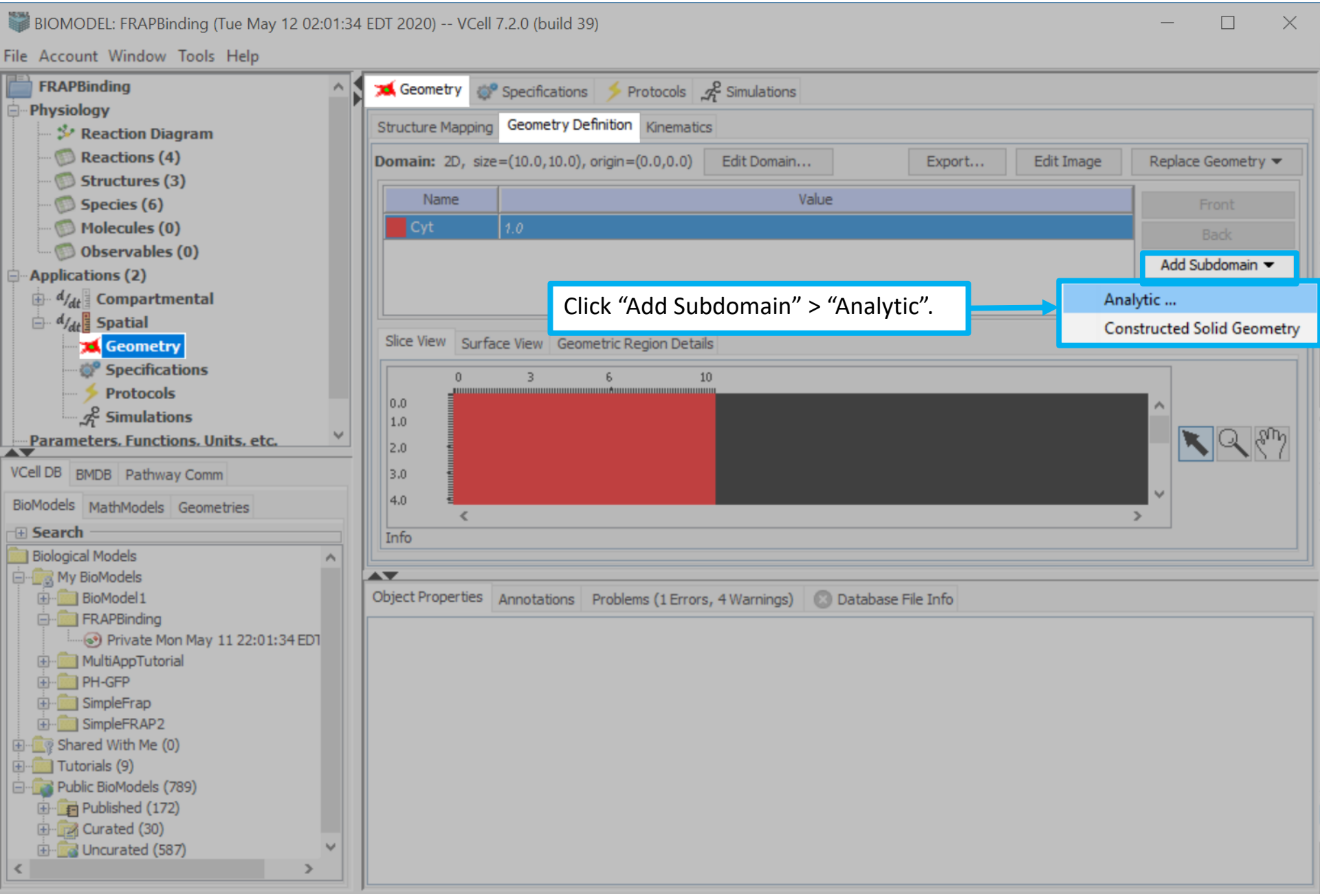
Geometry
Structure Mapping
Domain: 2D, size=(10.0
Edit Image
Replace Geometry
Name
Value
Cyt
1.0
Front
Back
Add Subdomain
Delete
Slice View
Surface View
Geometric Region Details
0
3
6
10
0.0
1.0
2.0
3.0
Info
Object Properties
Annotations
Problems (1 Errors, 4 Warnings)
Database File Info
Double click “subdomain0” and type “Cyt”. Press “Enter” on your keyboard to accept your entry.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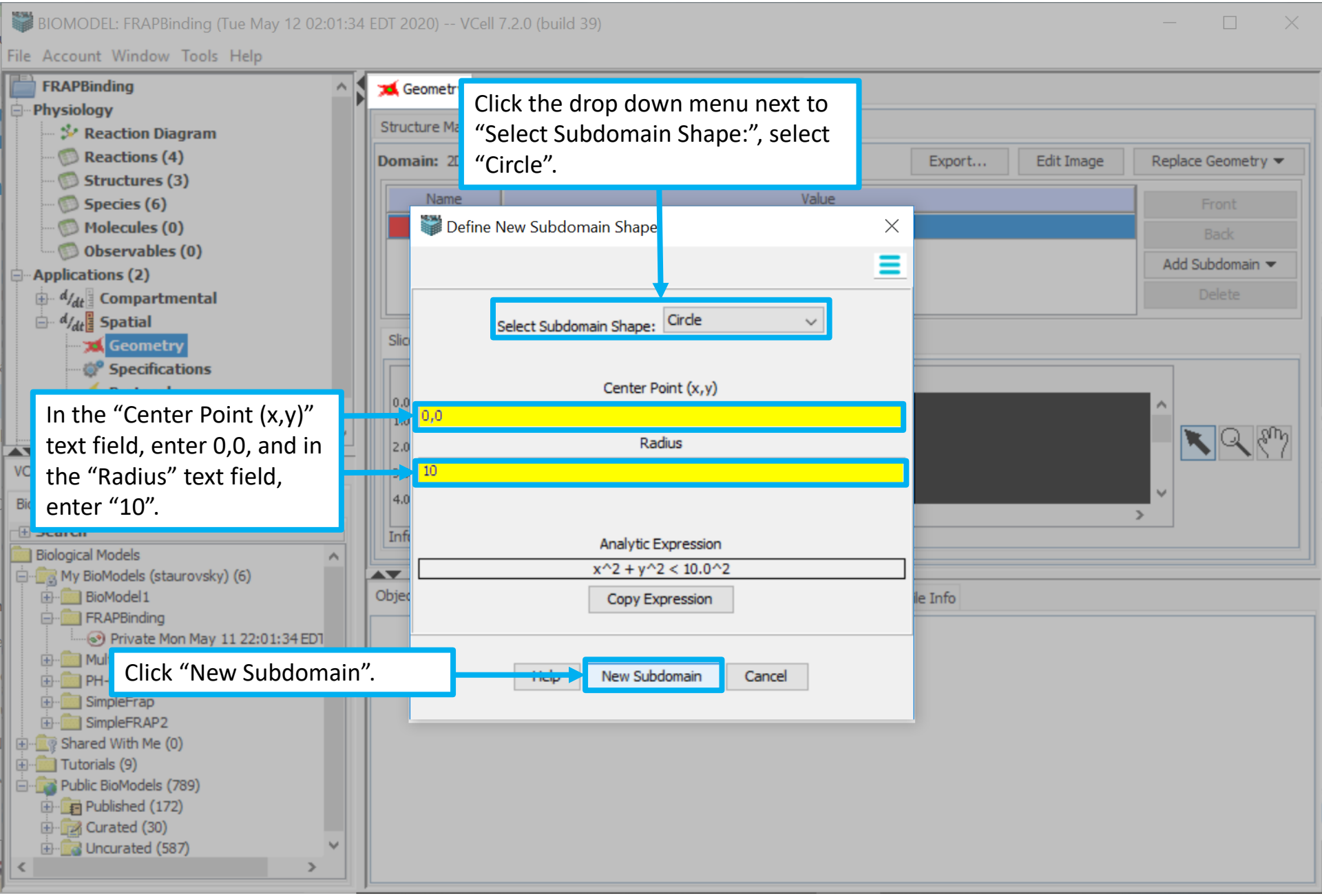
Structure Mapping
Geometry Definition
Kinematics
Domain: 2D, size=(10.0,10.0), origin=(0.0,0.0)
Edit Domain...
Export...
Edit Image
Replace Geometry
Name
Value
Cyt
1.0
Front
Back
Add Subdomain
Click “Add Subdomain” > “Analytic”.
Analytic ...
Constructed Solid Geometry
Slice View
Surface View
Geometric Region Details
0
3
6
10
0.0
1.0
2.0
3.0
4.0
Info
Object Properties
Annotations
Problems (1 Errors, 4 Warnings)
Database File Info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Observables (0)
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Biological Models
My BioModels (staurovsky) (6)
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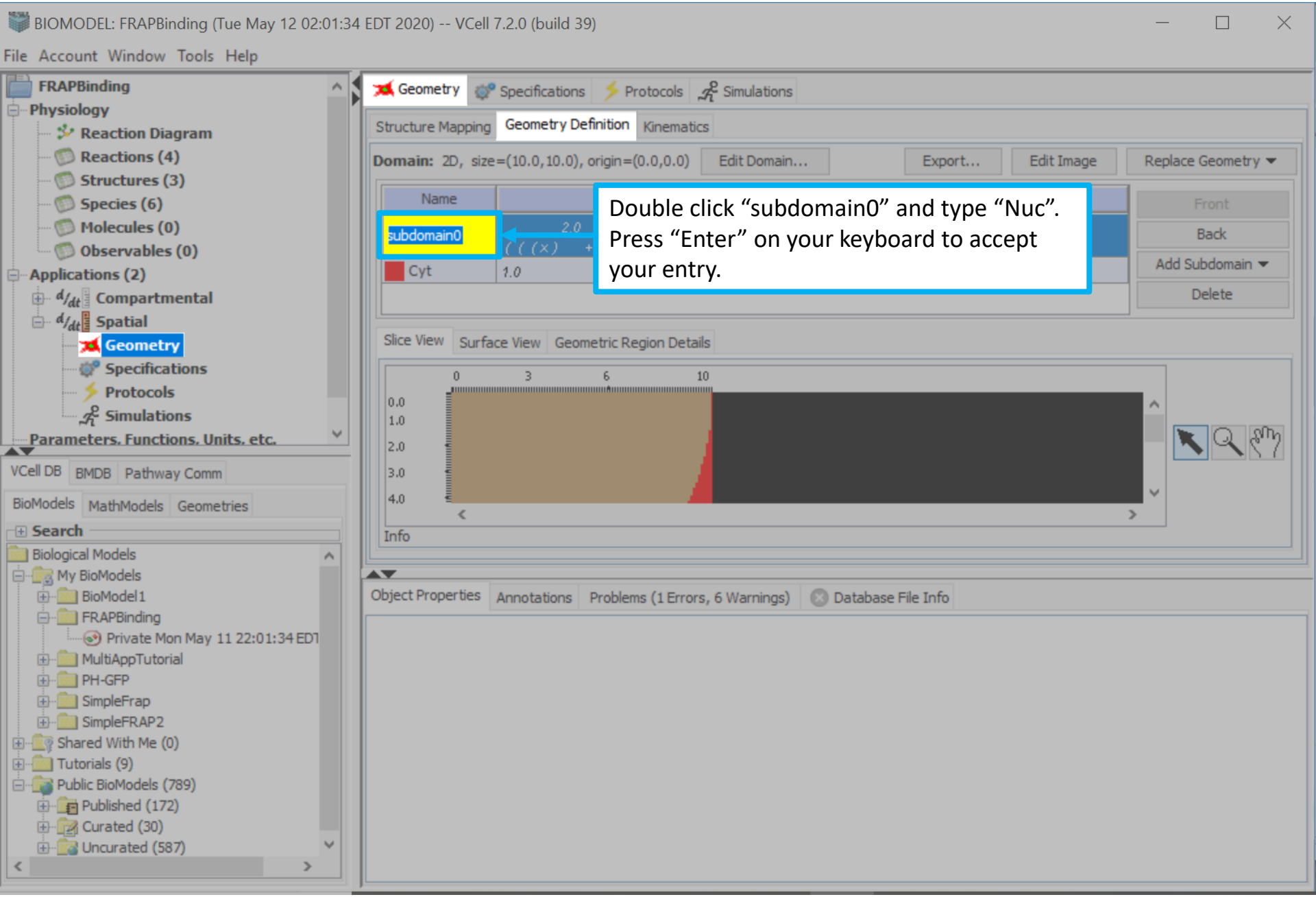
Geometry
Structure Ma
Domain: 2D
Export...
Edit Image
Replace Geometry
Name
Value
Front
Back
Add Subdomain
Delete
Define New Subdomain Shape
Select Subdomain Shape:
Circle
Center Point (x,y)
0,0
Radius
10
Analytic Expression
x^2 + y^2 < 10.0^2
Copy Expression
Help
New Subdomain
Cancel
Click the drop down menu next to "Select Subdomain Shape:", select "Circle".
In the "Center Point (x,y)" text field, enter 0,0, and in the "Radius" text field, enter "10".
Click "New Subdomain".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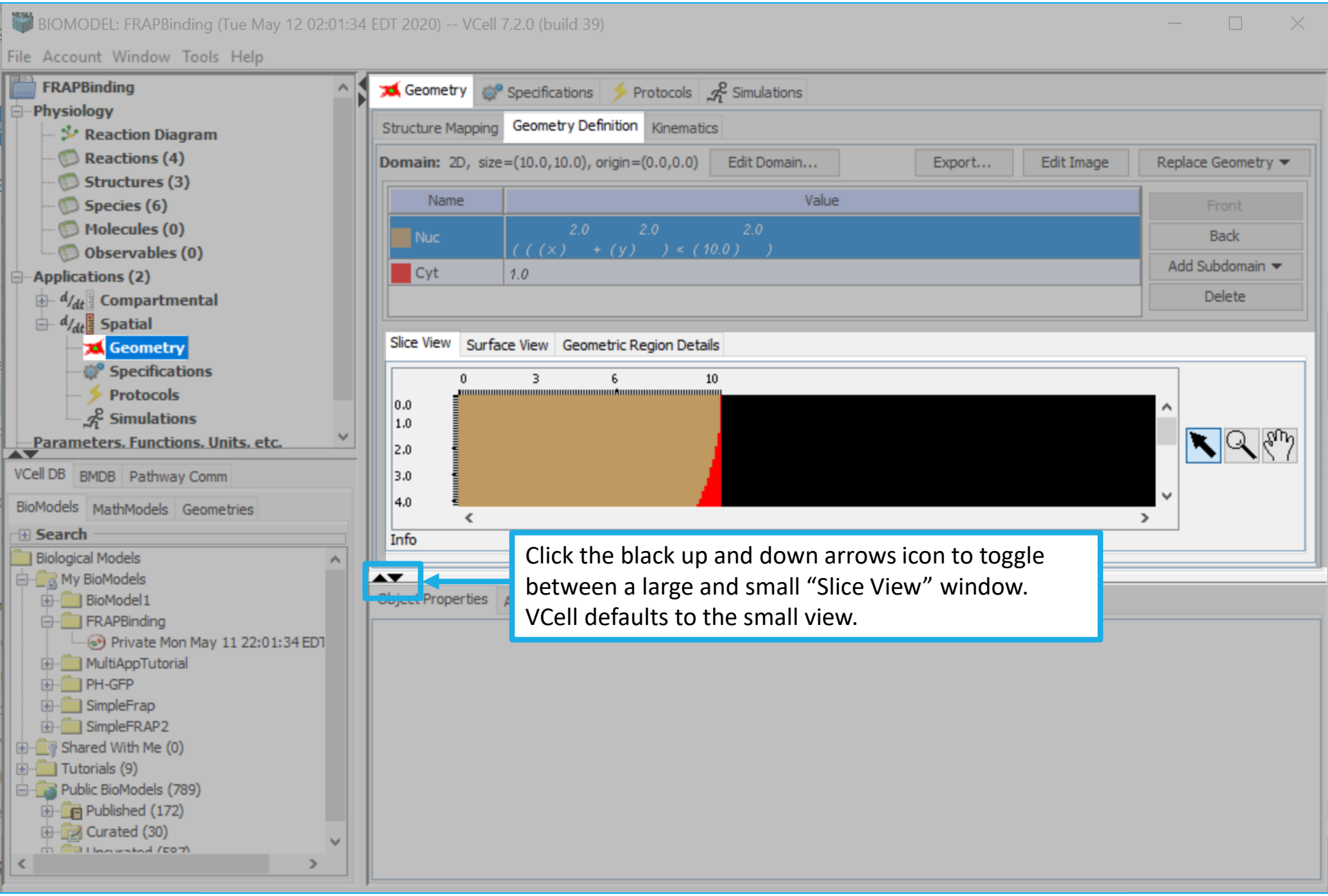
Kinematics
Domain: 2D, size=(10.0,10.0), origin=(0.0,0.0)
Edit Domain...
Export...
Edit Image
Replace Geometry
Name
subdomain0
2.0
Cyt
1.0
Front
Back
Add Subdomain
Delete
Slice View
Surface View
Geometric Region Details
0
3
6
10
0.0
1.0
2.0
3.0
4.0
Info
Object Properties
Annotations
Problems (1 Errors, 6 Warnings)
Database File Info
Double click “subdomain0” and type “Nuc”. Press “Enter” on your keyboard to accept your entry.


BIOMODEL: FRAPBinding (Tue May 12 02:01:34 EDT 2020) -- VCell 7.2.0 (build 39)
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FRAPBinding
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Species (6)
Molecules (0)
Observables (0)
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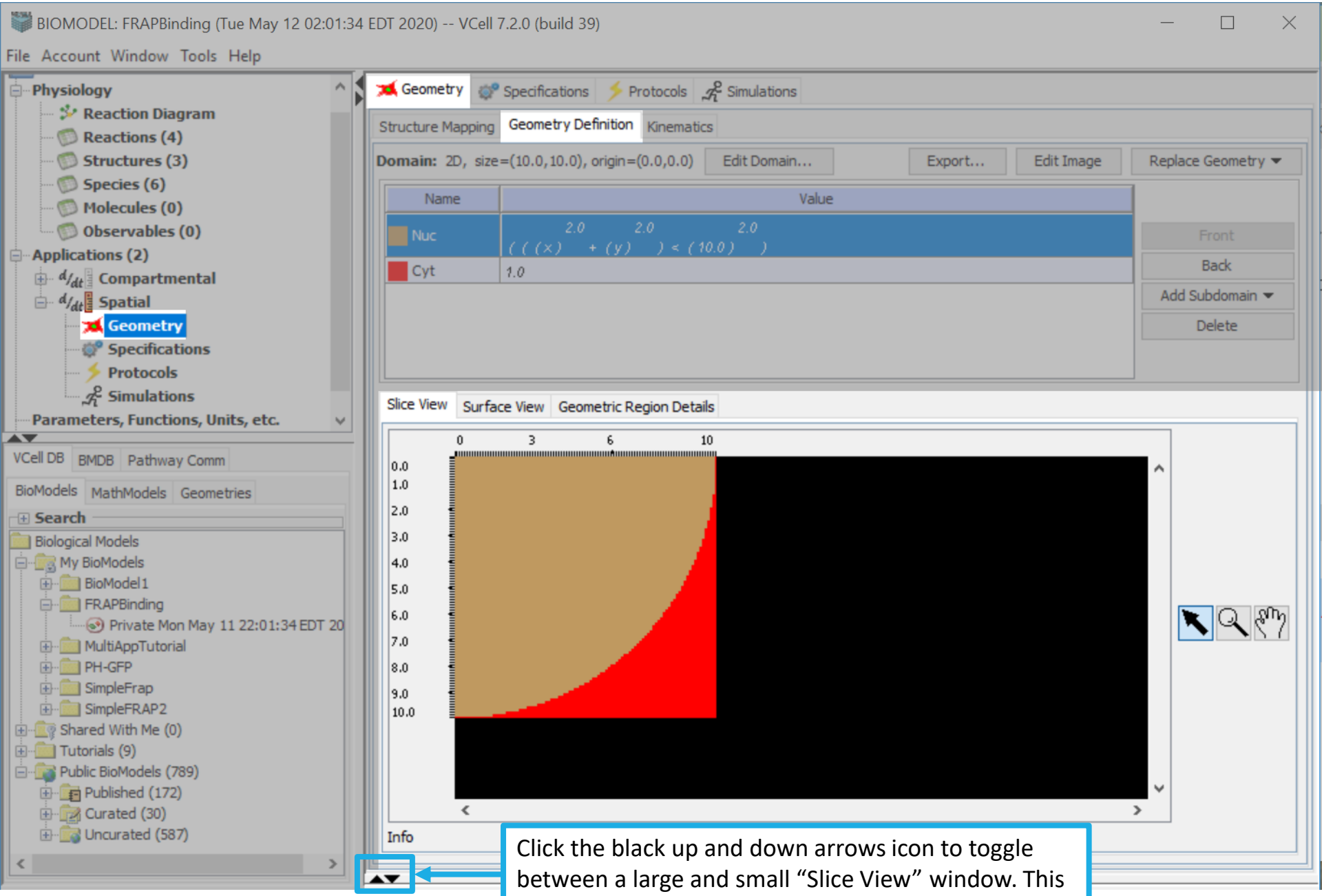
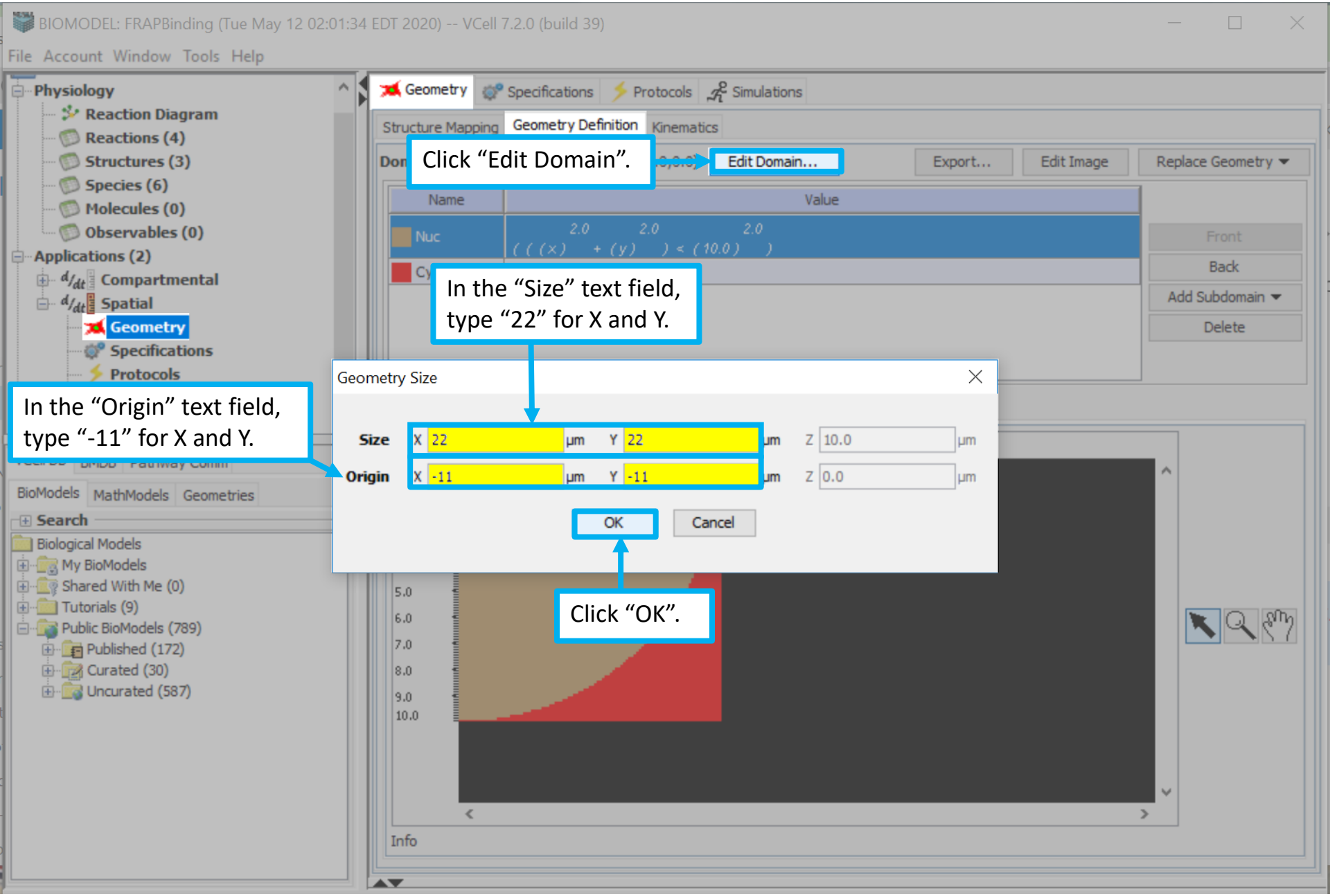
Specifications
Protocols
Simulations
Structure Mapping
Geometry Definition
Kinematics
Domain: 2D, size=(10.0,10.0), origin=(0.0,0.0)
Edit Domain...
Export...
Edit Image
Replace Geometry
Name
Value
Nuc
2.0 2.0 2.0
(((x) + (y)) < (10.0))
Cyt
1.0
Front
Back
Add Subdomain
Delete
Slice View
Surface View
Geometric Region Details
0
3
6
10
0.0
1.0
2.0
3.0
4.0
Info
Object Properties
Click the black up and down arrows icon to toggle between a large and small “Slice View” window. VCell defaults to the small view.



Click the black up and down arrows icon to toggle between a large and small “Slice View” window. This is the large view.


BIOMODEL: FRAPBinding (Tue May 12 02:01:34 EDT 2020) -- VCell 7.2.0 (build 39)
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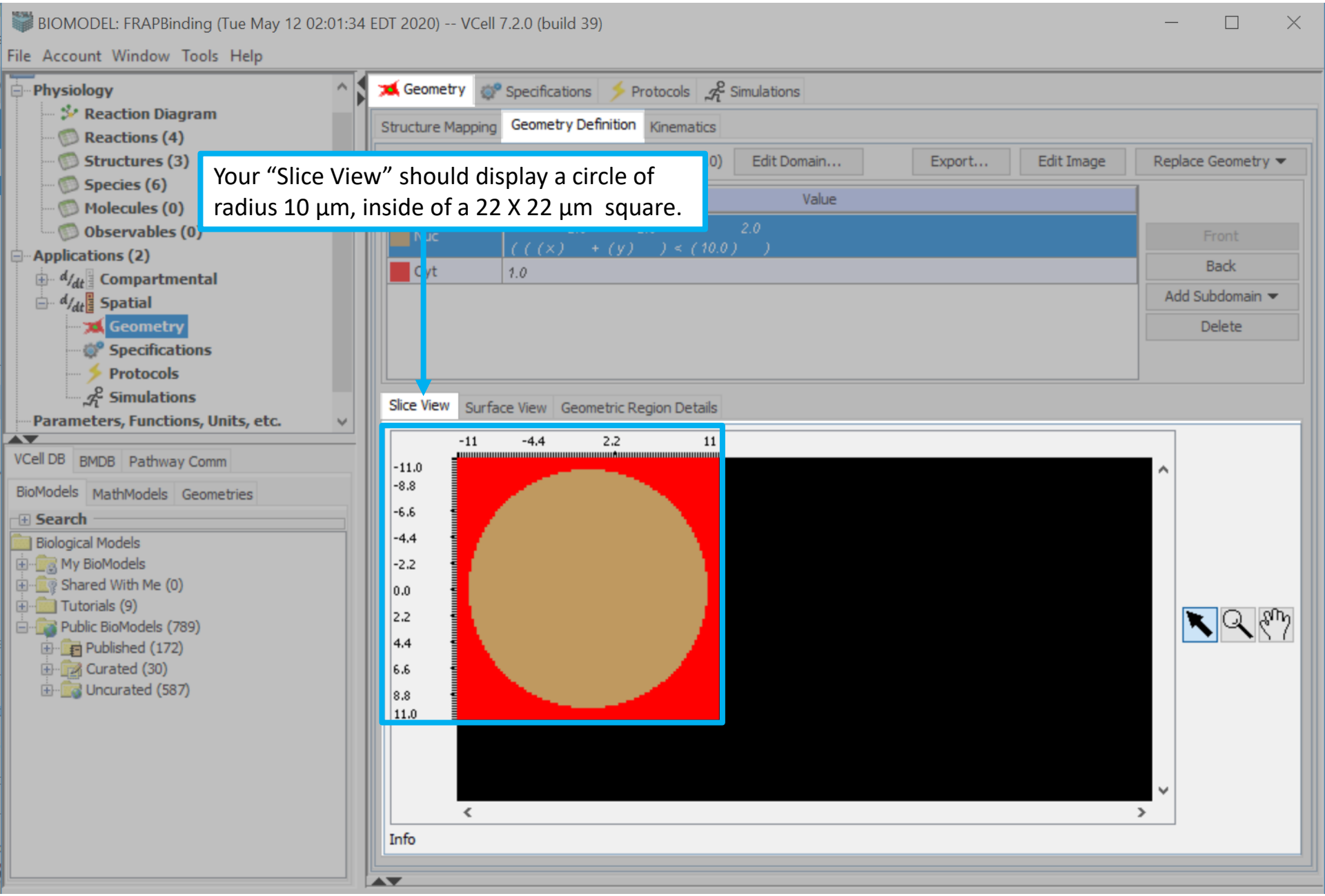
Geometry Specifications Protocols Simulations
Structure Mapping Geometry Definition Kinematics
Edit Domain...
Export... Edit Image Replace Geometry
Name Value
Nuc
Front
Back
Add Subdomain
Delete
Click “Edit Domain”.
In the “Size” text field, type “22” for X and Y.
In the “Origin” text field, type “-11” for X and Y.
Geometry Size
Size X 22 µm Y 22 µm Z 10.0 µm
Origin X -11 µm Y -11 µm Z 0.0 µm
OK
Cancel
Click “OK”.
Info


BIOMODEL: FRAPBinding (Tue May 12 02:01:34 EDT 2020) -- VCell 7.2.0 (build 39)
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Applications (2)
Compartmental
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Parameters, Functions, Units, etc.
Your "Slice View" should display a circle of radius 10 µm, inside of a 22 X 22 µm square.
Geometry
Specifications
Protocols
Simulations
Structure Mapping
Geometry Definition
Kinematics
Edit Domain...
Export...
Edit Image
Replace Geometry
Value
2.0
(((x) + (y)) < (10.0))
1.0
Front
Back
Add Subdomain
Delete
Slice View
Surface View
Geometric Region Details
-11
-4.4
2.2
11
-11.0
-8.8
-6.6
-4.4
-2.2
0.0
2.2
4.4
6.6
8.8
11.0
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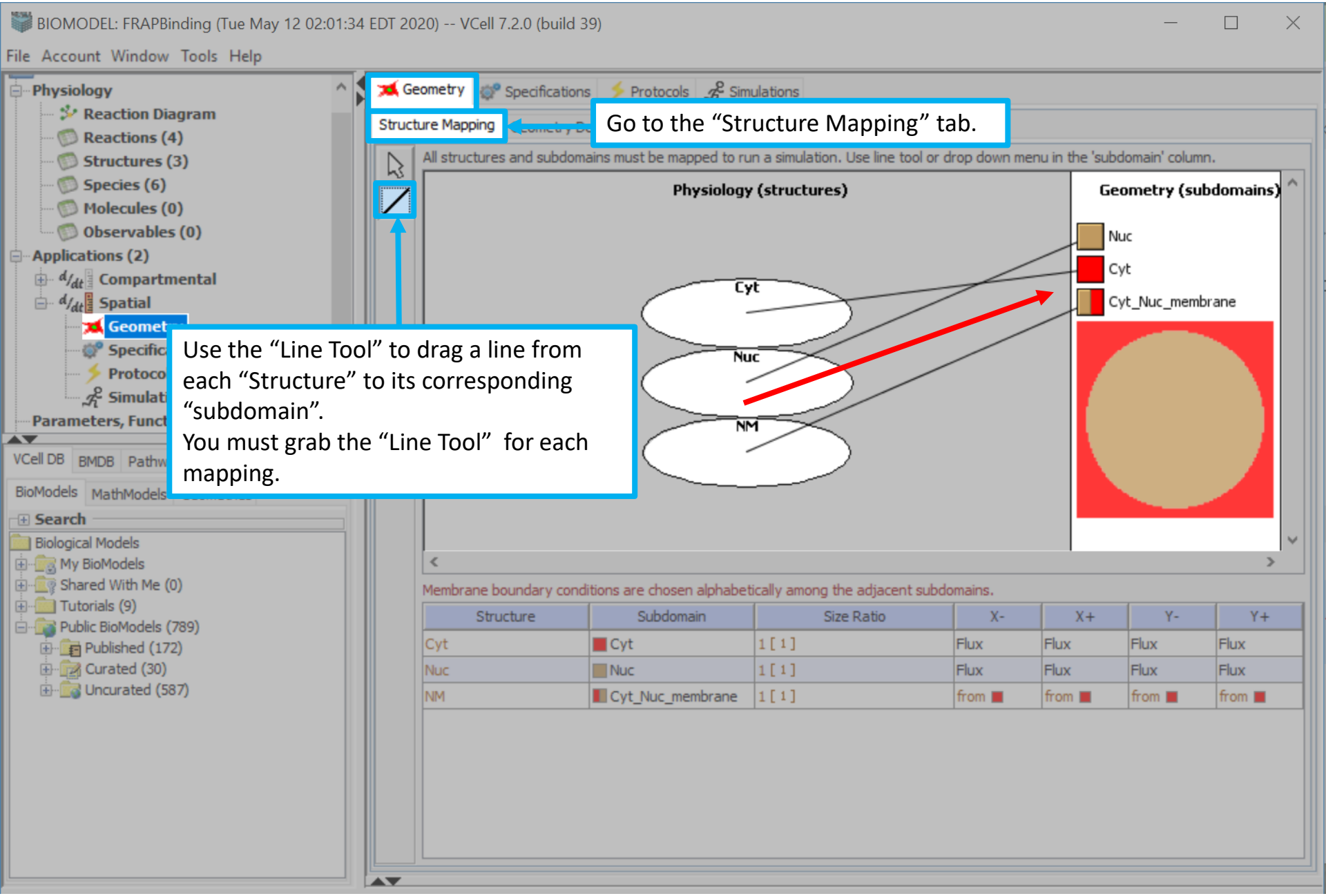
BIOMODEL: FRAPBinding (Tue May 12 02:01:34 EDT 2020) -- VCell 7.2.0 (build 39)
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Observables (0)
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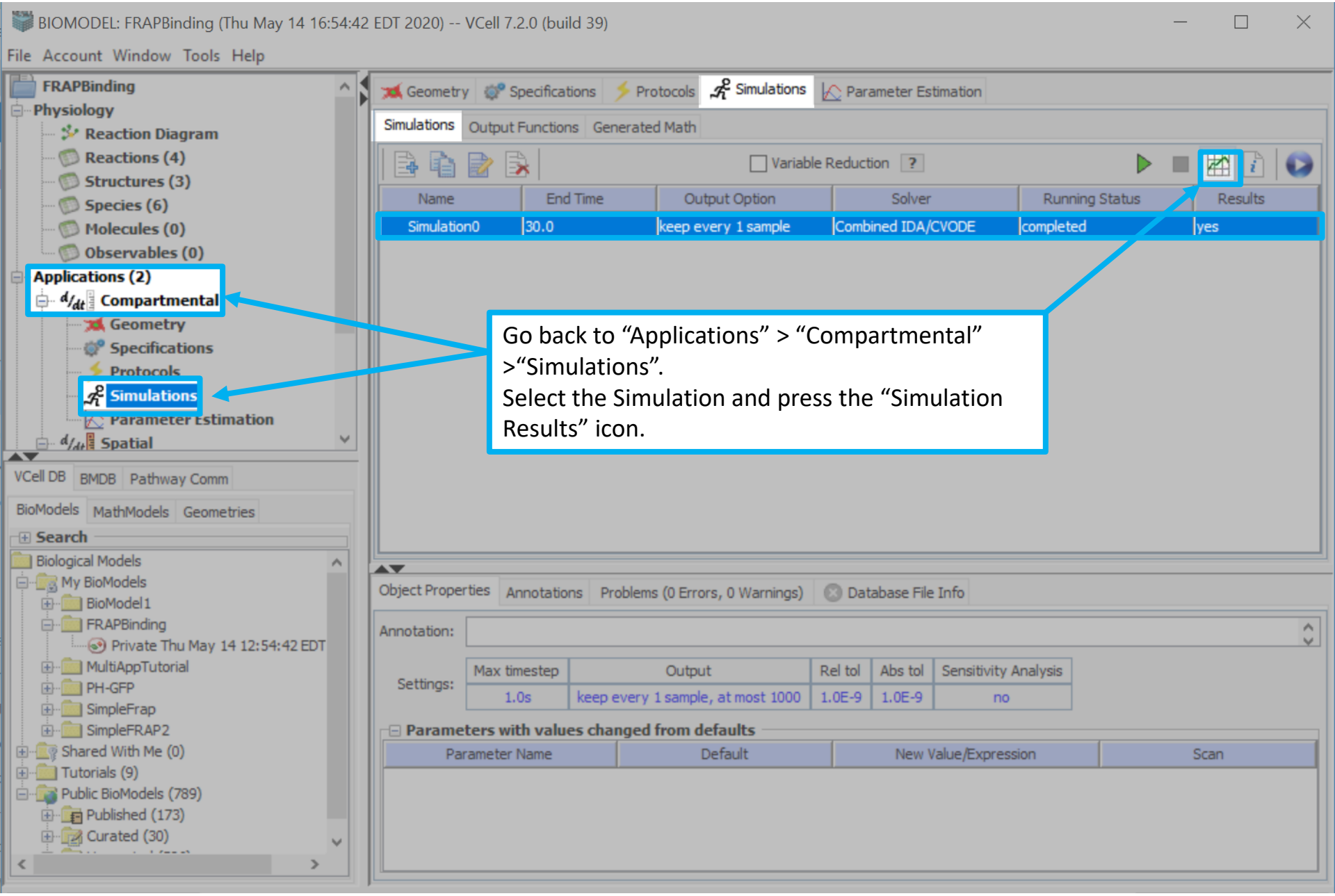
Structure Mapping
Go to the “Structure Mapping” tab.
All structures and subdomains must be mapped to run a simulation. Use line tool or drop down menu in the 'subdomain' column.
Physiology (structures)
Geometry (subdomains)
Cyt
Nuc
NM
Nuc
Cyt
Cyt_Nuc_membrane
Use the “Line Tool” to drag a line from each “Structure” to its corresponding “subdomain”.
You must grab the “Line Tool” for each mapping.
Membrane boundary conditions are chosen alphabetically among the adjacent subdomains.
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]
from
from
from
from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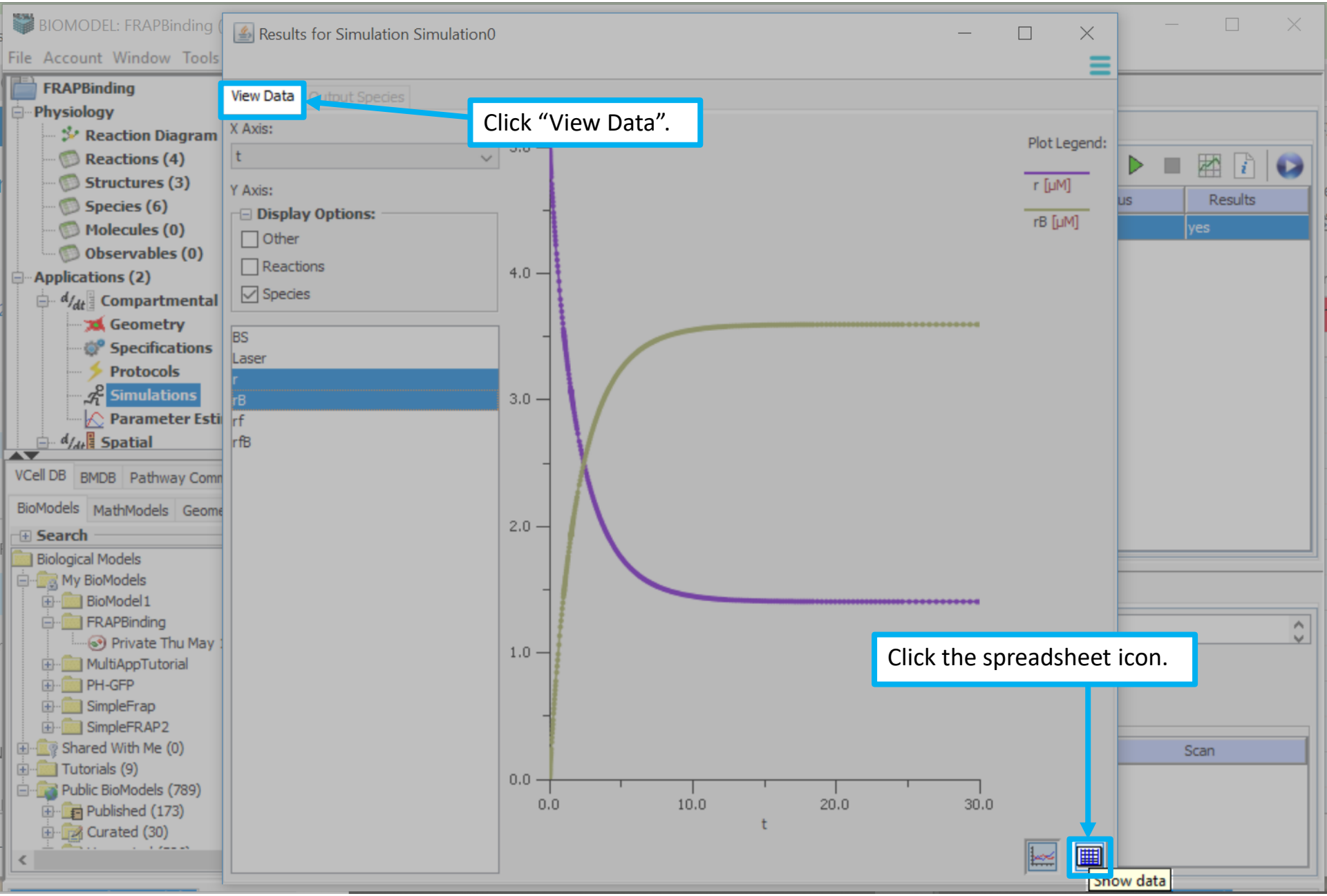
Generated Math
Variable Reduction
?
Name
End Time
Output Option
Solver
Running Status
Results
Simulation0
30.0
keep every 1 sample
Combined IDA/CVODE
completed
yes
Go back to “Applications” > “Compartmental” >“Simulations”.
Select the Simulation and press the “Simulation Results” icon.
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Database File Info
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


Results for Simulation Simulation0
View Data
Click “View Data”.
X Axis:
t
Y Axis:
Display Options:
Other
Reactions
Species
BS
Laser
r
rB
rf
rfB
Plot Legend:
r [µM]
rB [µM]
4.0
3.0
2.0
1.0
0.0
0.0
10.0
20.0
30.0
t
Click the spreadsheet icon.
Show data
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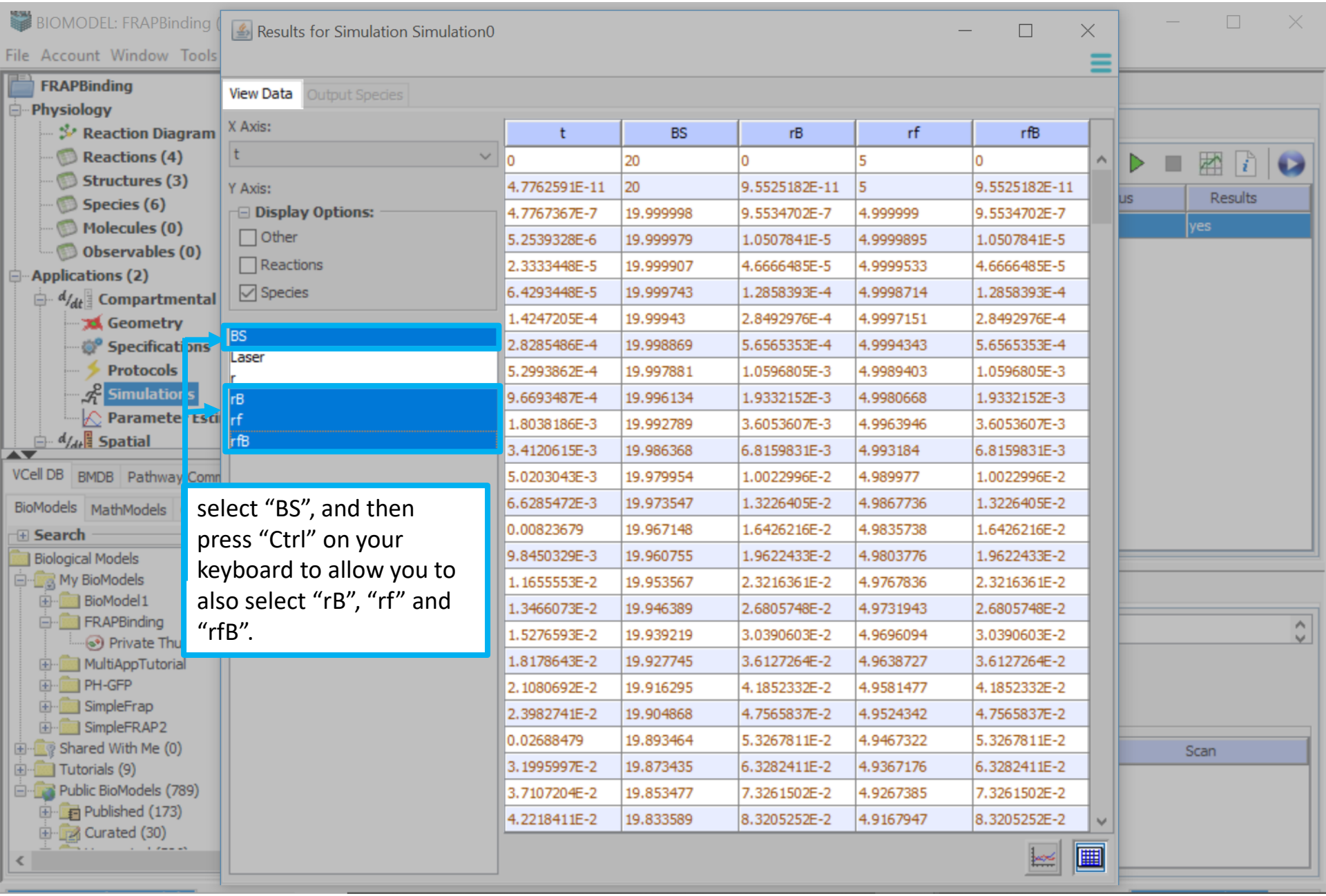
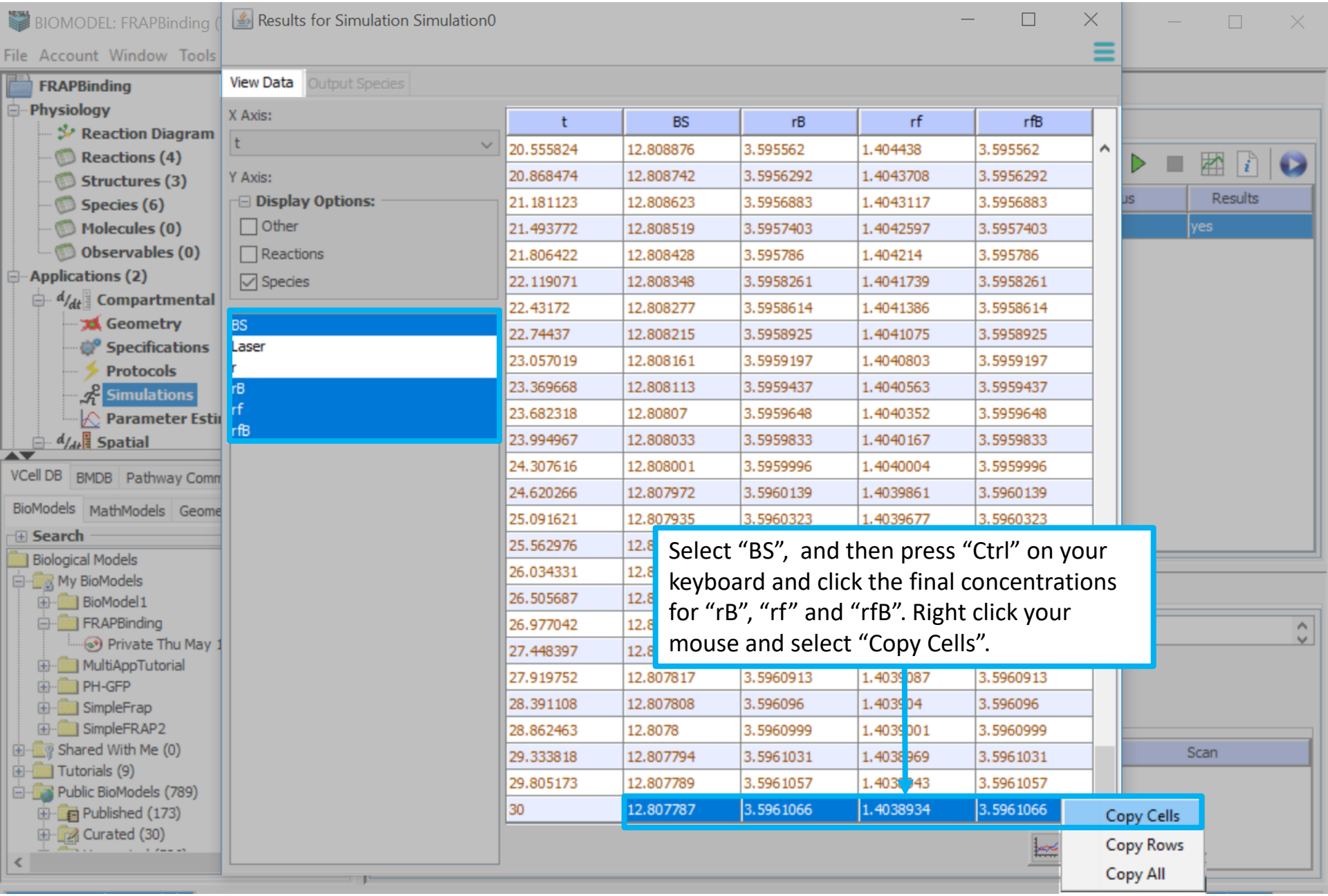
Spatial
Results
yes
Scan



t	BS	rB	rf	rfB
0	20	0	5	0
4.7762591E-11	20	9.5525182E-11	5	9.5525182E-11
4.7767367E-7	19.999998	9.5534702E-7	4.999999	9.5534702E-7
5.2539328E-6	19.999979	1.0507841E-5	4.9999895	1.0507841E-5
2.3333448E-5	19.999907	4.6666485E-5	4.9999533	4.6666485E-5
6.4293448E-5	19.999743	1.2858393E-4	4.9998714	1.2858393E-4
1.4247205E-4	19.99943	2.8492976E-4	4.9997151	2.8492976E-4
2.8285486E-4	19.998869	5.6565353E-4	4.9994343	5.6565353E-4
5.2993862E-4	19.997881	1.0596805E-3	4.9989403	1.0596805E-3
9.6693487E-4	19.996134	1.9332152E-3	4.9980668	1.9332152E-3
1.8038186E-3	19.992789	3.6053607E-3	4.9963946	3.6053607E-3
3.4120615E-3	19.986368	6.8159831E-3	4.993184	6.8159831E-3
5.0203043E-3	19.979954	1.0022996E-2	4.989977	1.0022996E-2
6.6285472E-3	19.973547	1.3226405E-2	4.9867736	1.3226405E-2
0.00823679	19.967148	1.6426216E-2	4.9835738	1.6426216E-2
9.8450329E-3	19.960755	1.9622433E-2	4.9803776	1.9622433E-2
1.1655553E-2	19.953567	2.3216361E-2	4.9767836	2.3216361E-2
1.3466073E-2	19.946389	2.6805748E-2	4.9731943	2.6805748E-2
1.5276593E-2	19.939219	3.0390603E-2	4.9696094	3.0390603E-2
1.8178643E-2	19.927745	3.6127264E-2	4.9638727	3.6127264E-2
2.1080692E-2	19.916295	4.1852332E-2	4.9581477	4.1852332E-2
2.3982741E-2	19.904868	4.7565837E-2	4.9524342	4.7565837E-2
0.02688479	19.893464	5.3267811E-2	4.9467322	5.3267811E-2
3.1995997E-2	19.873435	6.3282411E-2	4.9367176	6.3282411E-2
3.7107204E-2	19.853477	7.3261502E-2	4.9267385	7.3261502E-2
4.2218411E-2	19.833589	8.3205252E-2	4.9167947	8.3205252E-2


BIOMODEL: FRAPBinding
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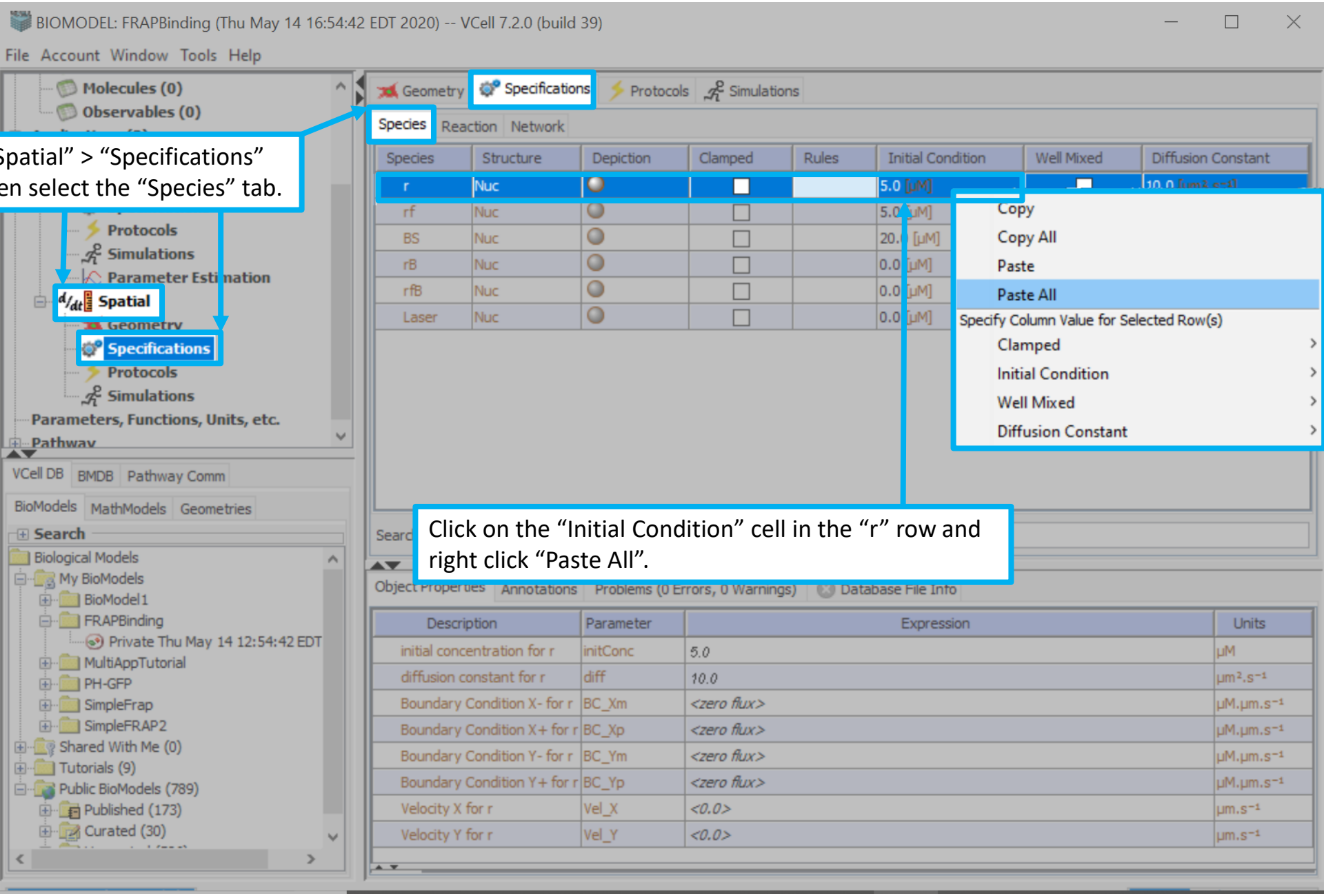
Output Species
X Axis:
t
Y Axis:
Display Options:
Other
Reactions
Species
BS
Laser
r
rB
rf
rfB
t
BS
rB
rf
rfB
20.555824 12.808876 3.595562 1.404438 3.595562
20.868474 12.808742 3.5956292 1.4043708 3.5956292
21.181123 12.808623 3.5956883 1.4043117 3.5956883
21.493772 12.808519 3.5957403 1.4042597 3.5957403
21.806422 12.808428 3.595786 1.404214 3.595786
22.119071 12.808348 3.5958261 1.4041739 3.5958261
22.43172 12.808277 3.5958614 1.4041386 3.5958614
22.74437 12.808215 3.5958925 1.4041075 3.5958925
23.057019 12.808161 3.5959197 1.4040803 3.5959197
23.369668 12.808113 3.5959437 1.4040563 3.5959437
23.682318 12.80807 3.5959648 1.4040352 3.5959648
23.994967 12.808033 3.5959833 1.4040167 3.5959833
24.307616 12.808001 3.5959996 1.4040004 3.5959996
24.620266 12.807972 3.5960139 1.4039861 3.5960139
25.091621 12.807935 3.5960323 1.4039677 3.5960323
25.562976
26.034331
26.505687
26.977042
27.448397
27.919752 12.807817 3.5960913 1.4039087 3.5960913
28.391108 12.807808 3.596096 1.4039 3.596096
28.862463 12.8078 3.5960999 1.4039 3.5960999
29.333818 12.807794 3.5961031 1.4038 3.5961031
29.805173 12.807789 3.5961057 1.4038 3.5961057
30 12.807787 3.5961066 1.4038934 3.5961066
Select “BS”, and then press “Ctrl” on your keyboard and click the final concentrations for “rB”, “rf” and “rfB”. Right click your mouse and select “Copy Cells”.
Copy Cells
Copy Rows
Copy All
Results
yes
Scan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Molecules (0)
Observables (0)
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Pathway
Spatial" > "Specifications"
en select the "Species" tab.
Geometry
Specifications
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Reaction
Network
Species
Structure
Depiction
Clamped
Rules
Initial Condition
Well Mixed
Diffusion Constant
r
Nuc
5.0 [µM]
rf
Nuc
5.0 [µM]
BS
Nuc
20. [µM]
rB
Nuc
0.0 [µM]
rfB
Nuc
0.0 [µM]
Laser
Nuc
0.0 [µM]
Copy
Copy All
Paste
Paste All
Specify Column Value for Selected Row(s)
Clamped
Initial Condition
Well Mixed
Diffusion Constant
Click on the "Initial Condition" cell in the "r" row and right click "Paste All".
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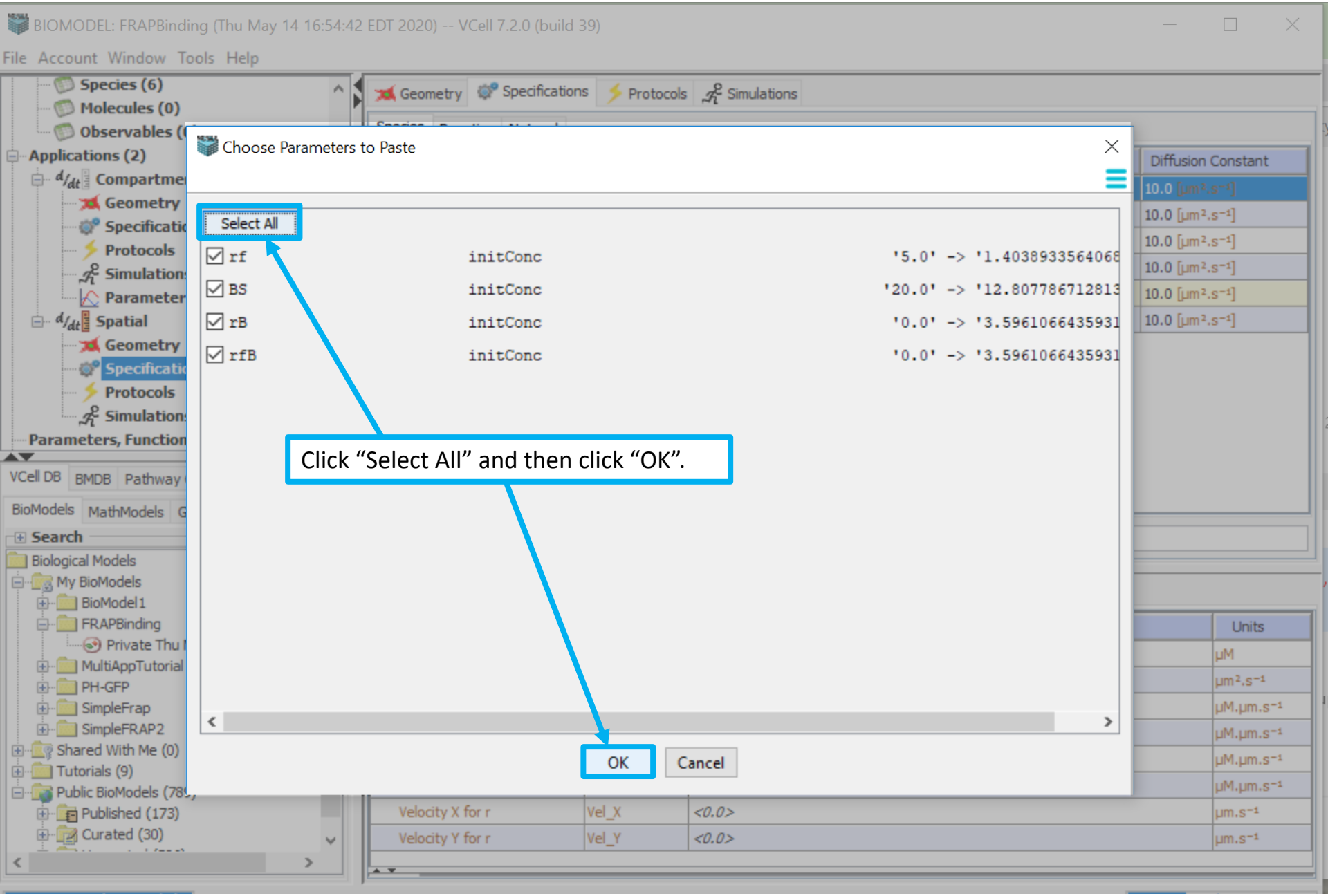
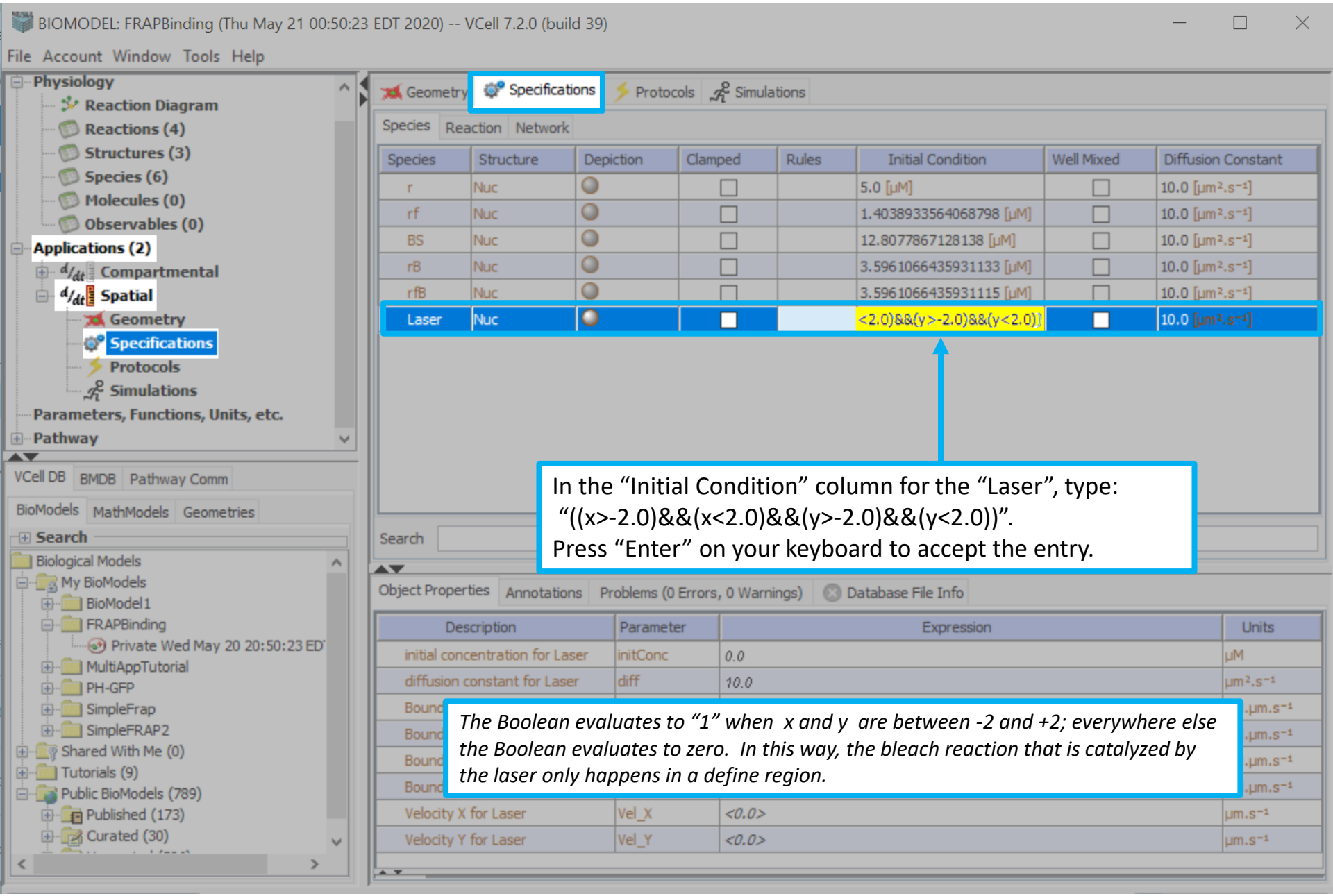
Problems (0 Errors, 0 Warnings)
Database File Info
Description
Parameter
Expression
Units
initial concentration for r
initConc
5.0
µM
diffusion constant for r
diff
10.0
µm².s⁻¹
Boundary Condition X- for r
BC_Xm
<zero flux>
µM.µm.s⁻¹
Boundary Condition X+ for r
BC_Xp
<zero flux>
µM.µm.s⁻¹
Boundary Condition Y- for r
BC_Ym
<zero flux>
µM.µm.s⁻¹
Boundary Condition Y+ for r
BC_Yp
<zero flux>
µM.µm.s⁻¹
Velocity X for r
Vel_X
<0.0>
µm.s⁻¹
Velocity Y for r
Vel_Y
<0.0>
µm.s⁻¹


Choose Parameters to Paste
Select All
rf initConc '5.0' -> '1.4038933564068
BS initConc '20.0' -> '12.807786712813
rB initConc '0.0' -> '3.5961066435931
rfB initConc '0.0' -> '3.5961066435931
Click “Select All” and then click “OK”.
OK
Cancel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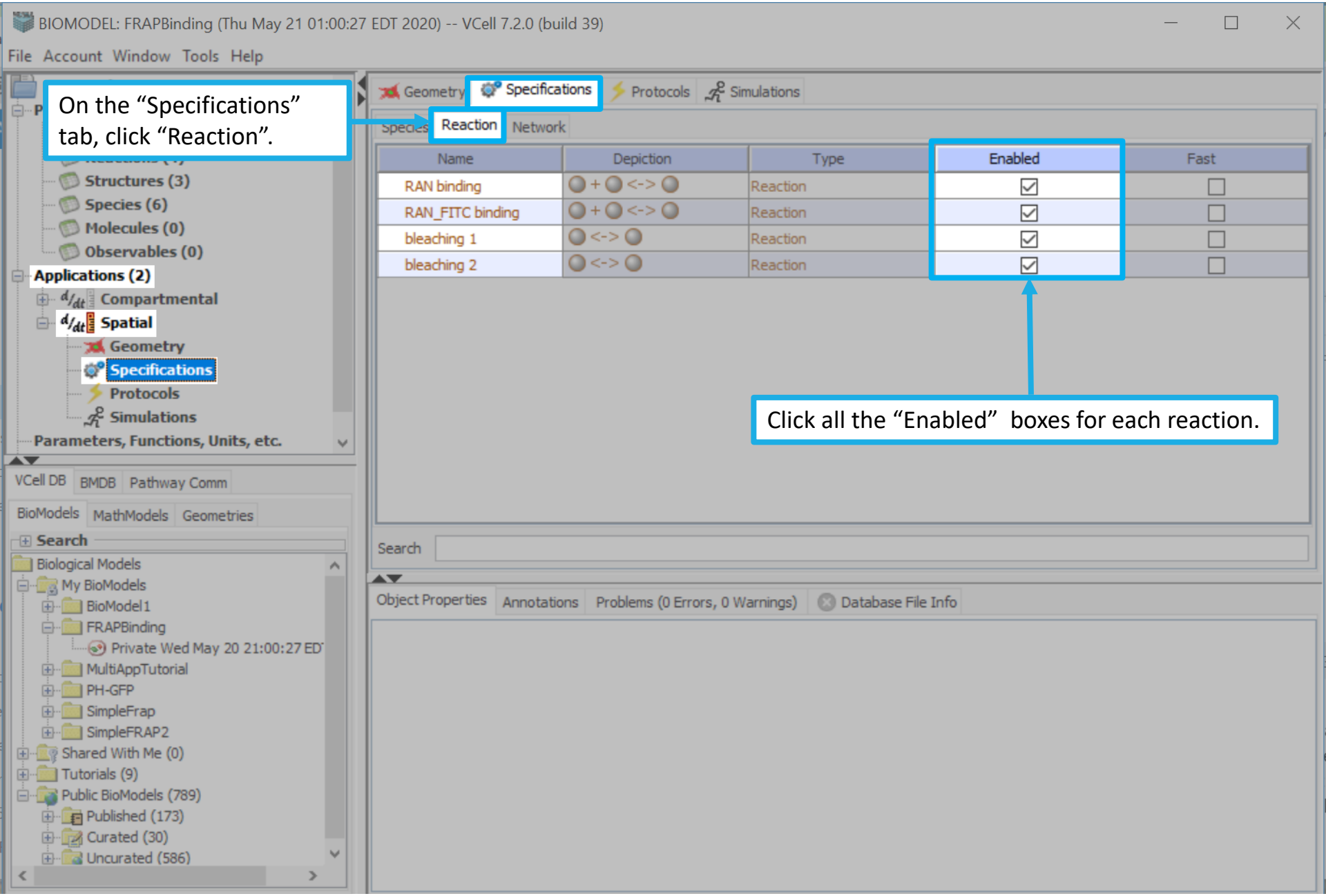
Clamped
Rules
Initial Condition
Well Mixed
Diffusion Constant
r
Nuc
5.0 [µM]
10.0 [µm².s⁻¹]
rf
Nuc
1.4038933564068798 [µM]
10.0 [µm².s⁻¹]
BS
Nuc
12.8077867128138 [µM]
10.0 [µm².s⁻¹]
rB
Nuc
3.5961066435931133 [µM]
10.0 [µm².s⁻¹]
rfB
Nuc
3.5961066435931115 [µM]
10.0 [µm².s⁻¹]
Laser
Nuc
<2.0)&&(y>-2.0)&&(y<2.0))
10.0 [µm².s⁻¹]
Search
In the “Initial Condition” column for the “Laser”, type:
“((x>-2.0)&&(x<2.0)&&(y>-2.0)&&(y<2.0))”.
Press “Enter” on your keyboard to accept the entry.
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Database File Info
Description
Parameter
Expression
Units
initial concentration for Laser
initConc
0.0
µM
diffusion constant for Laser
diff
10.0
µm².s⁻¹
Velocity X for Laser
Vel_X
<0.0>
µm.s⁻¹
Velocity Y for Laser
Vel_Y
<0.0>
µm.s⁻¹
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 the laser only happens in a define region.


BIOMODEL: FRAPBinding (Thu May 21 01:00:27 EDT 2020) -- VCell 7.2.0 (build 39)
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On the “Specifications” tab, click “Reaction”.
Structures (3)
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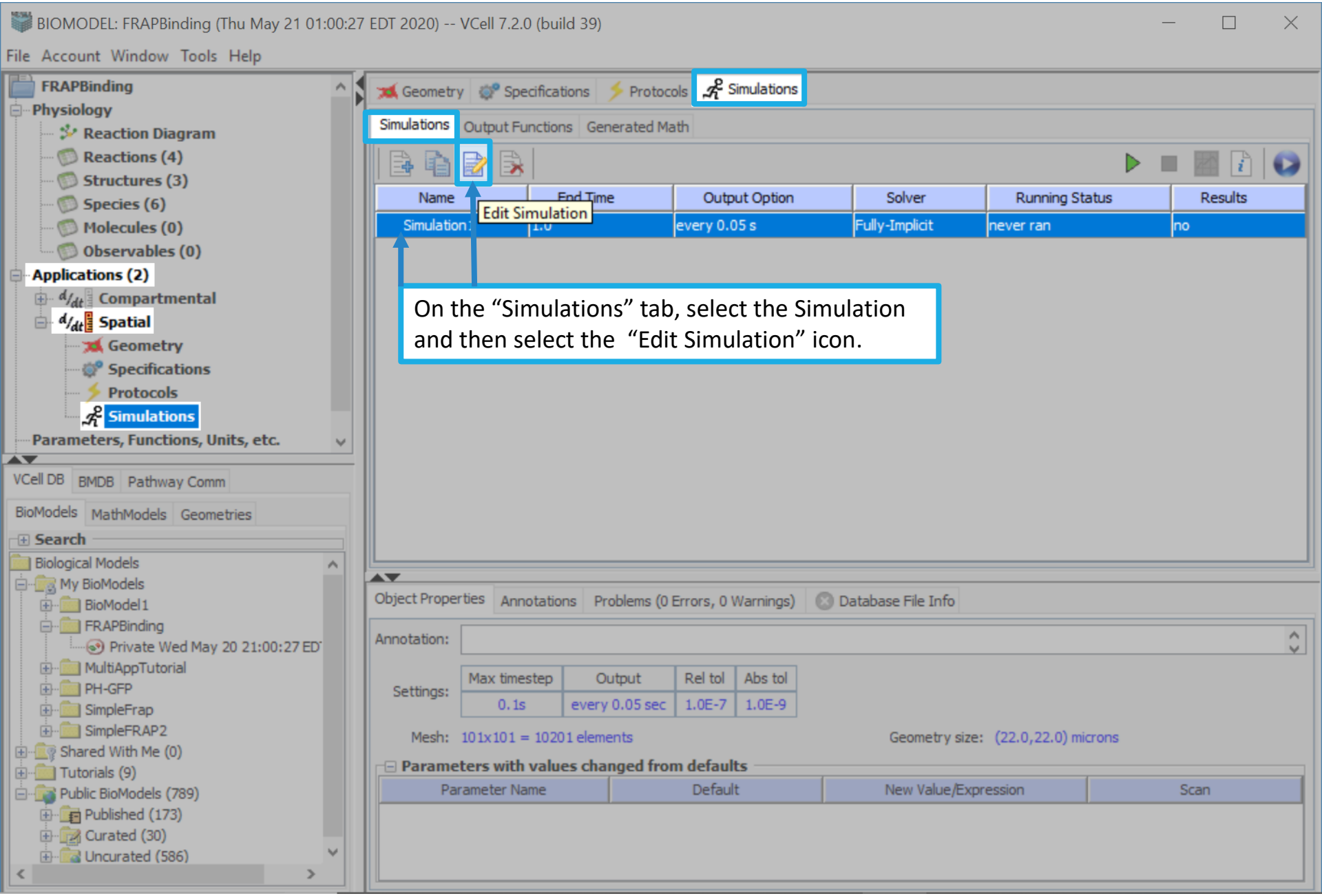
Reaction
Network
Name
Depiction
Type
Enabled
Fast
RAN binding
RAN_FITC binding
bleaching 1
bleaching 2
Reaction
Search
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Database File Info
Click all the “Enabled” boxes for each reaction.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Simulations
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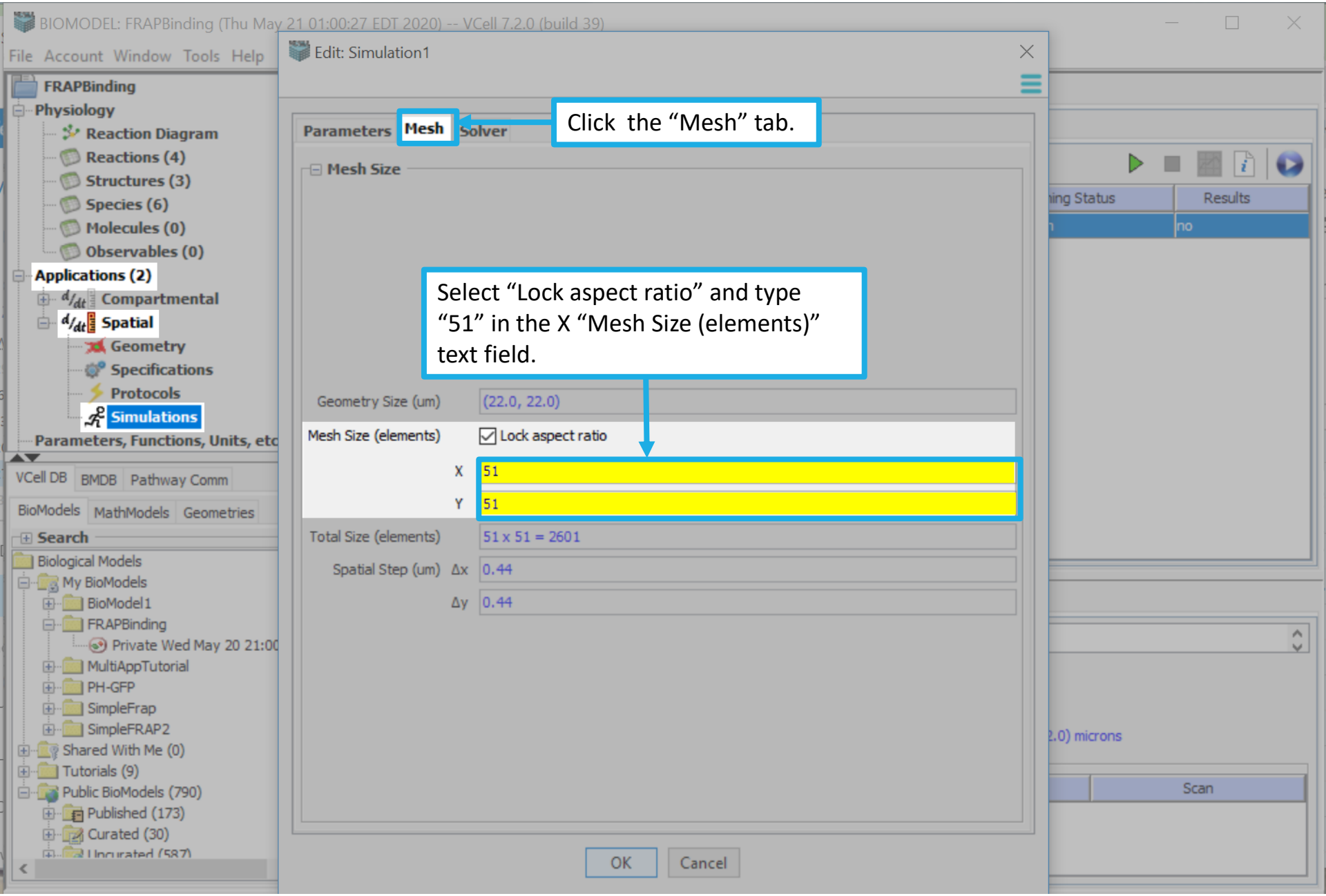
Generated Math
Edit Simulation
Name
End Time
Output Option
Solver
Running Status
Results
Simulation 1
1.0
every 0.05 s
Fully-Implicit
never ran
no
On the “Simulations” tab, select the Simulation and then select the “Edit Simulation” icon.
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Database File Info
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
Parameter Name
Default
New Value/Expression
Scan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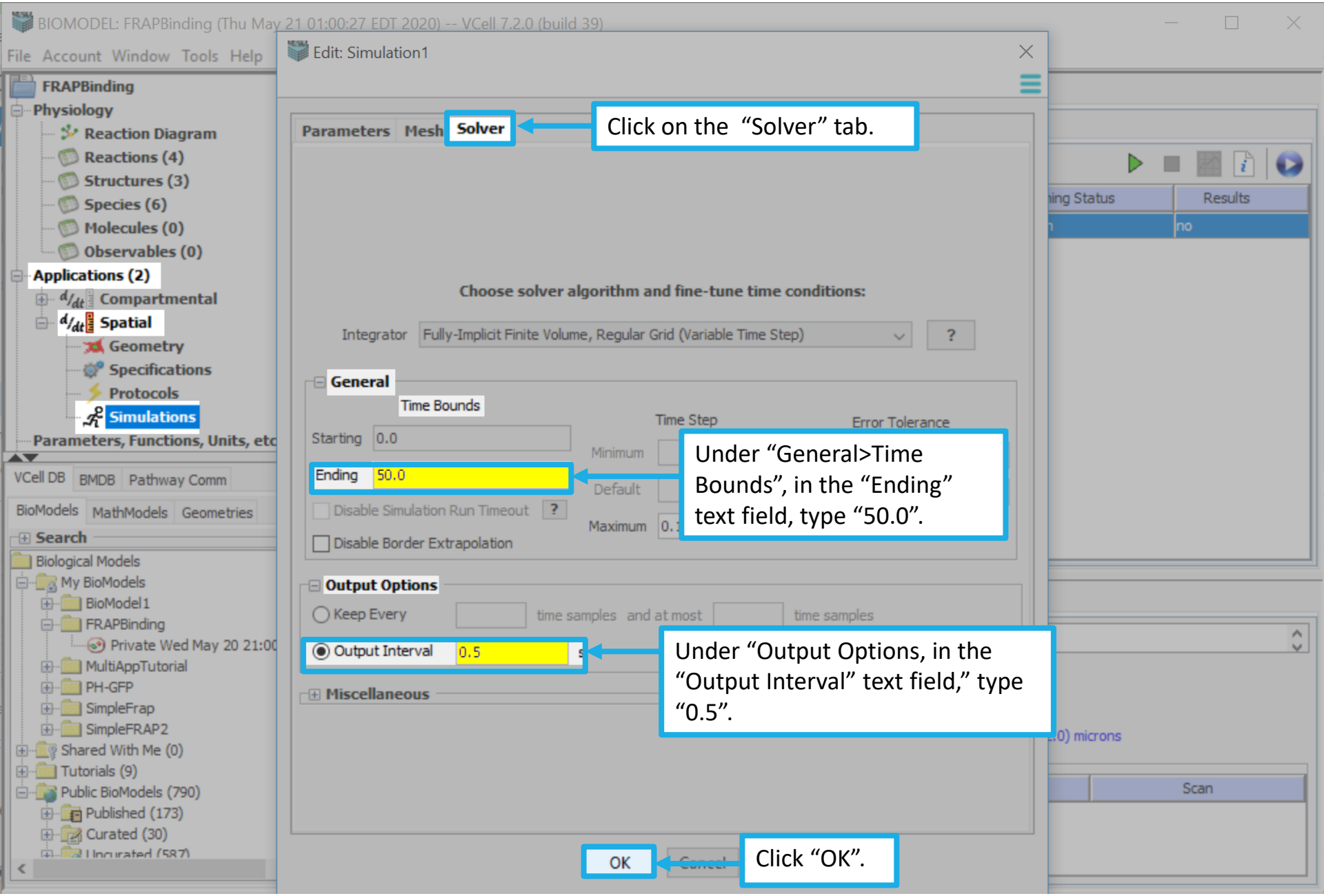
Uncurated (587)
Edit: Simulation1
Parameters
Mesh
Solver
Click the “Mesh” tab.
Mesh Size
Select “Lock aspect ratio” and type “51” in the X “Mesh Size (elements)” text field.
Geometry Size (um)
(22.0, 22.0)
Mesh Size (elements)
Lock aspect ratio
X
51
Y
51
Total Size (elements)
51 x 51 = 2601
Spatial Step (um) Δx
0.44
Δy
0.44
OK
Cancel
ing Status
Results
no
2.0) microns
Scan


Edit: Simulation1
Parameters
Mesh
Solver
Click on the "Solver" tab.
Choose solver algorithm and fine-tune time conditions:
Integrator
Fully-Implicit Finite Volume, Regular Grid (Variable Time Step)
General
Time Bounds
Starting
0.0
Ending
50.0
Under "General>Time Bounds", in the "Ending" text field, type "50.0".
Time Step
Error Tolerance
Minimum
Default
Maximum
Disable Simulation Run Timeout
Disable Border Extrapolation
Output Options
Keep Every
time samples
and at most
time samples
Output Interval
0.5
Under "Output Options, in the "Output Interval" text field," type "0.5".
Miscellaneous
OK
Click "OK".
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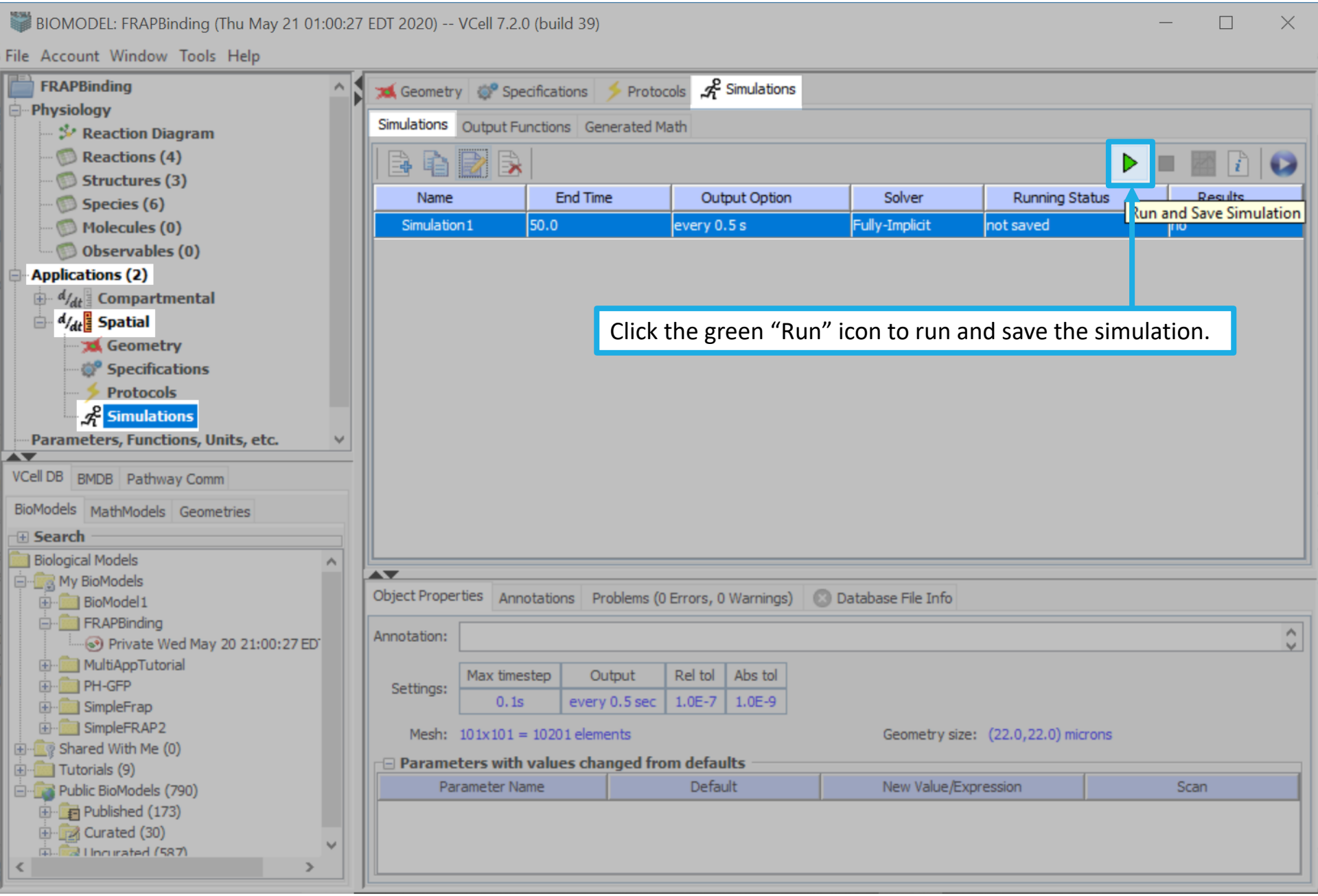
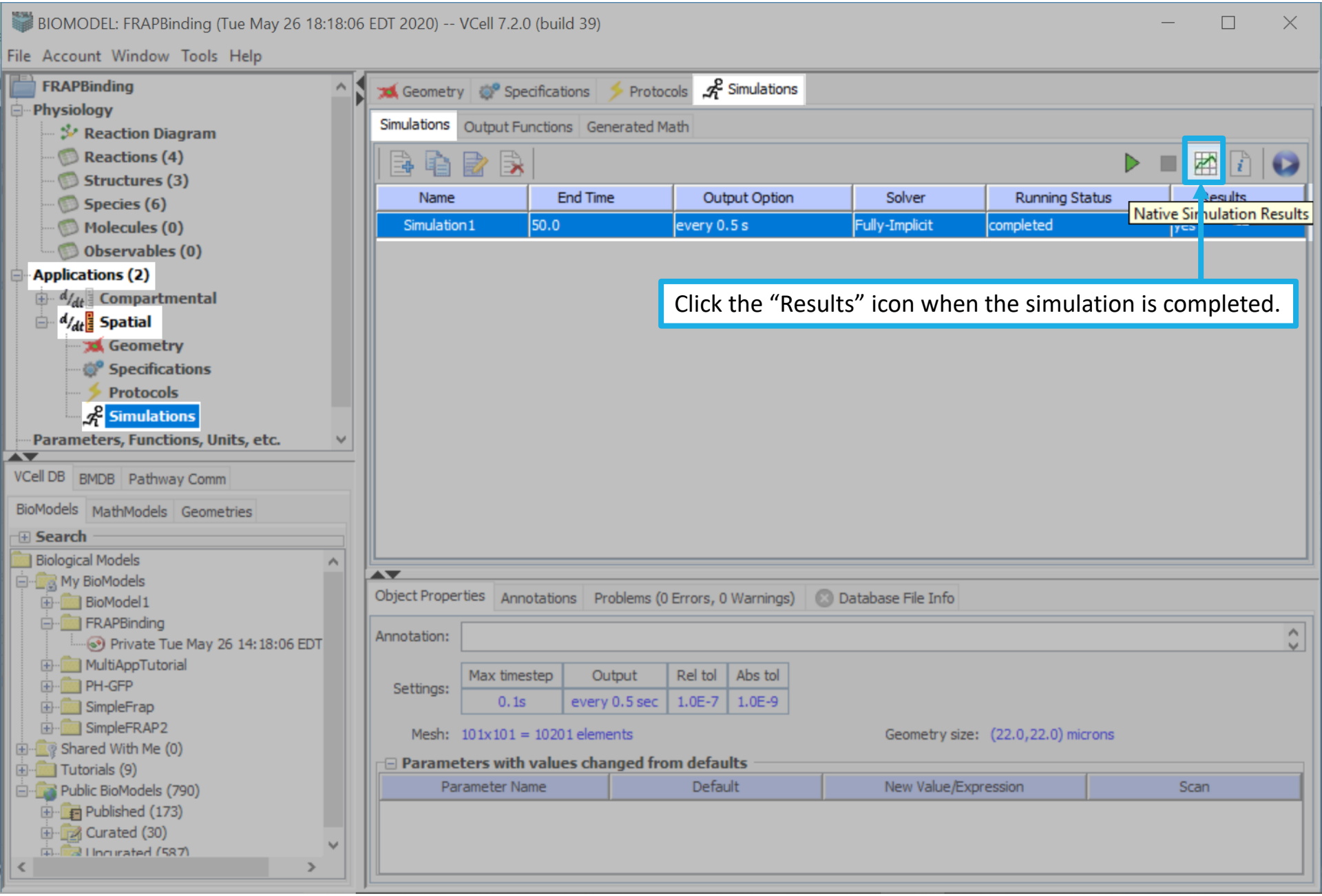
Results
no
Scan



Click the green “Run” icon to run and save the simulation.


BIOMODEL: FRAPBinding (Tue May 26 18:18:06 EDT 2020) -- VCell 7.2.0 (build 39)
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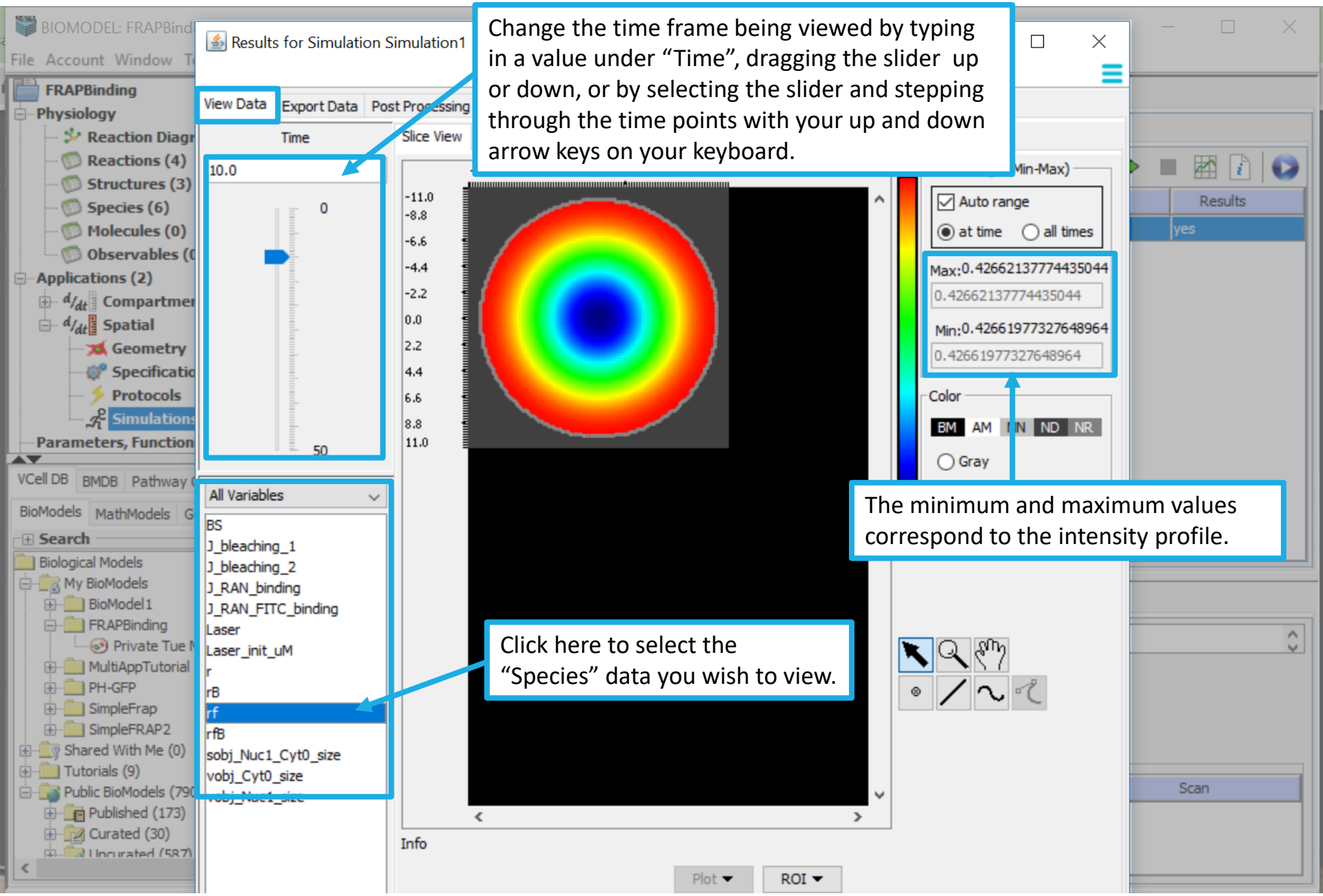
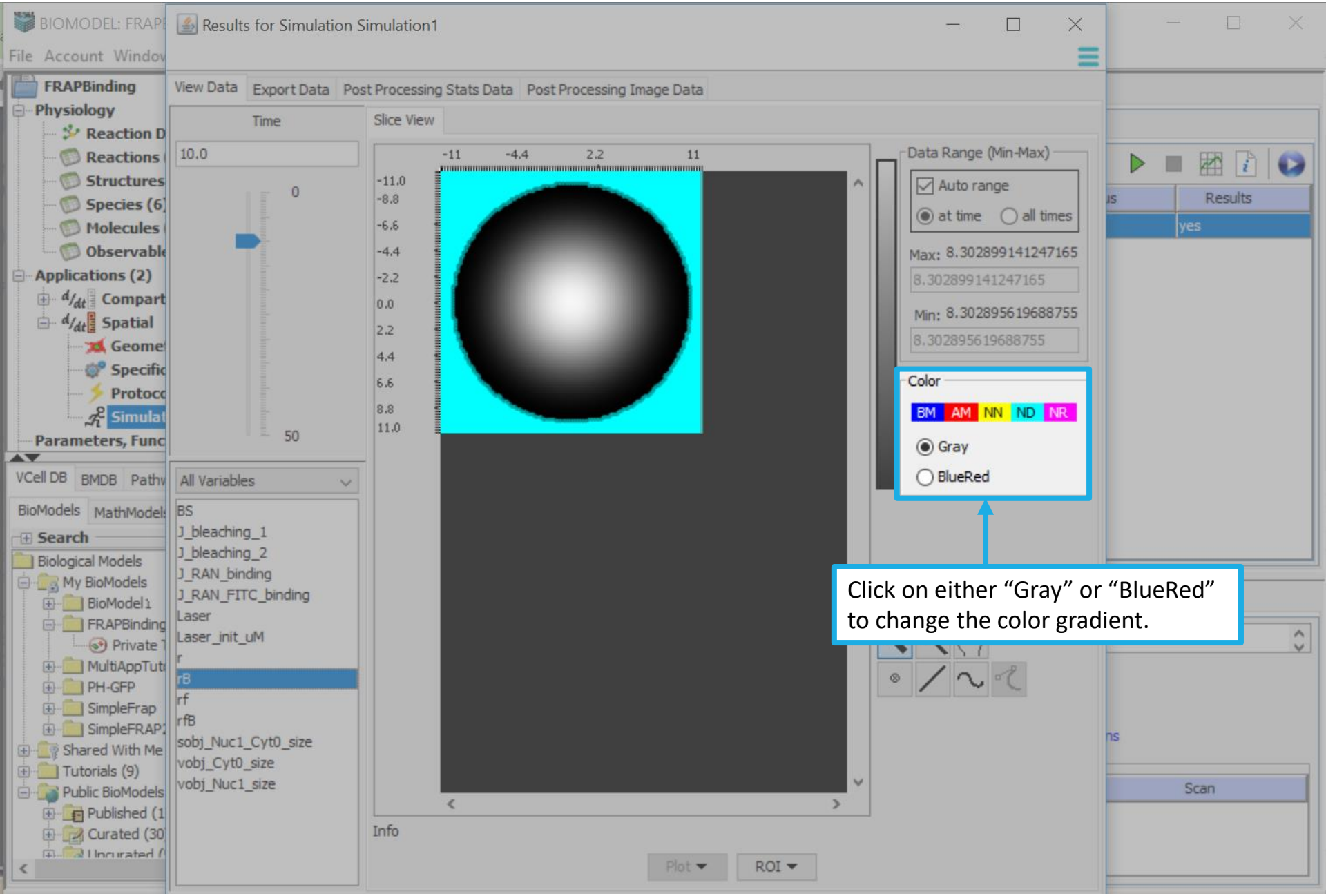
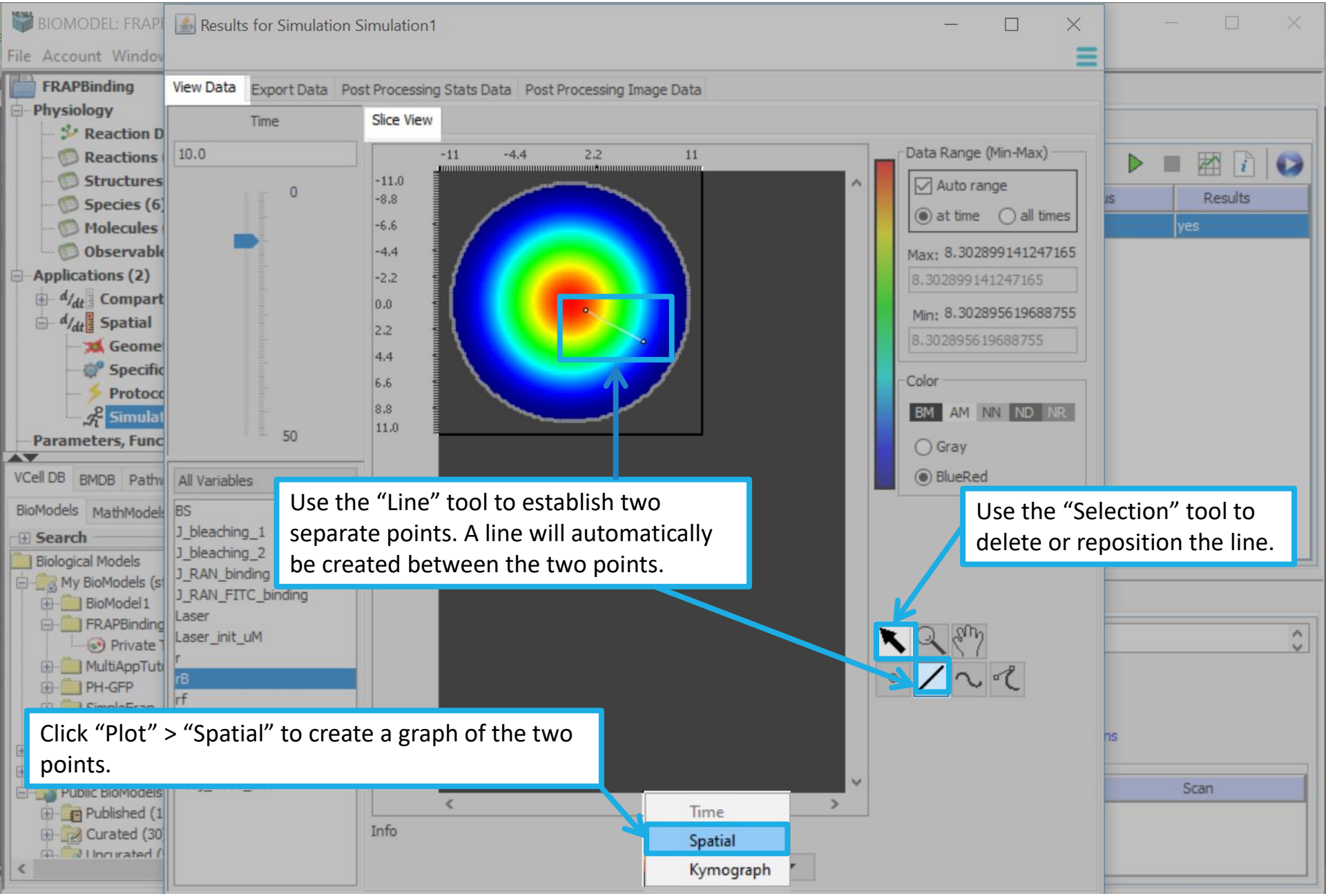
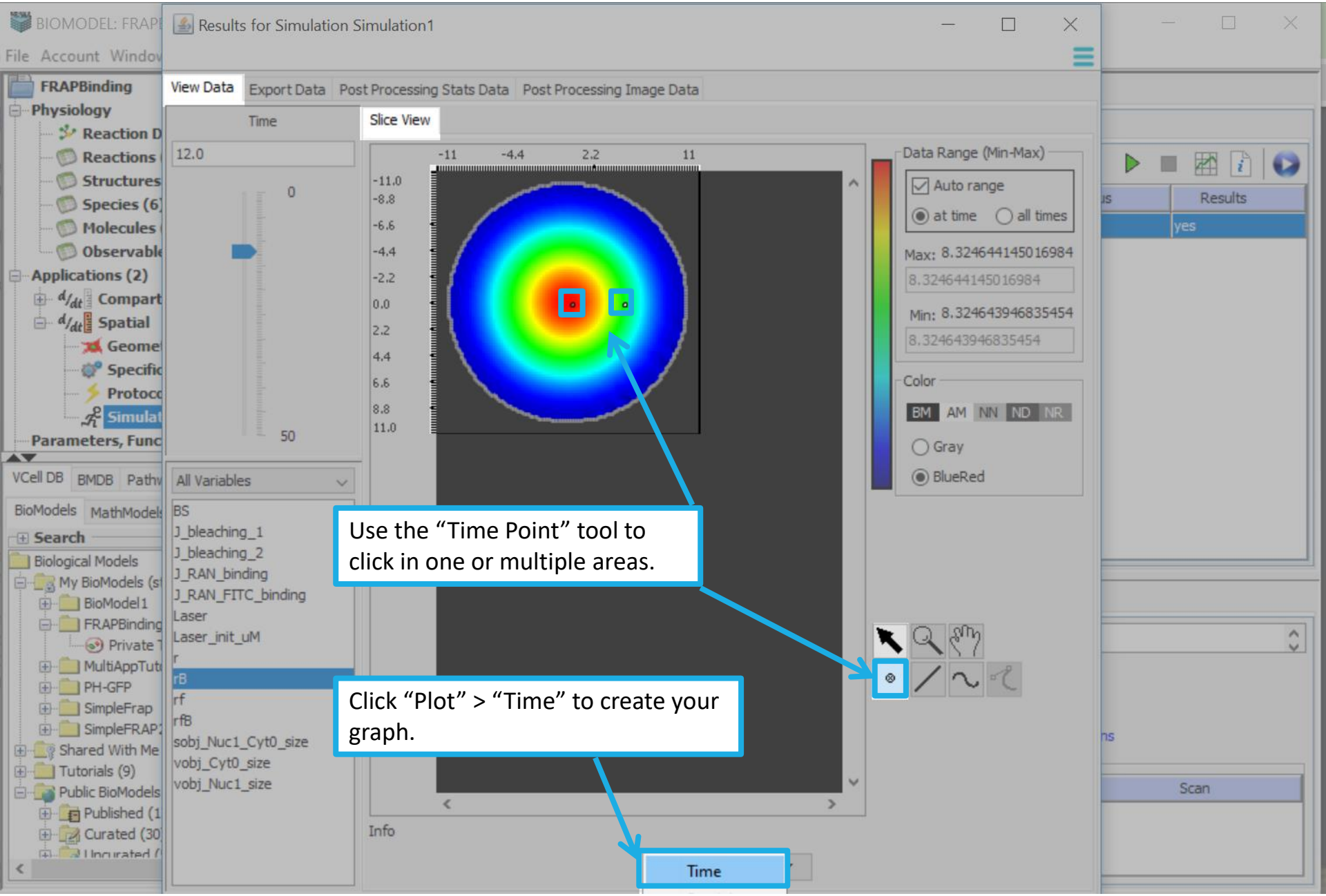
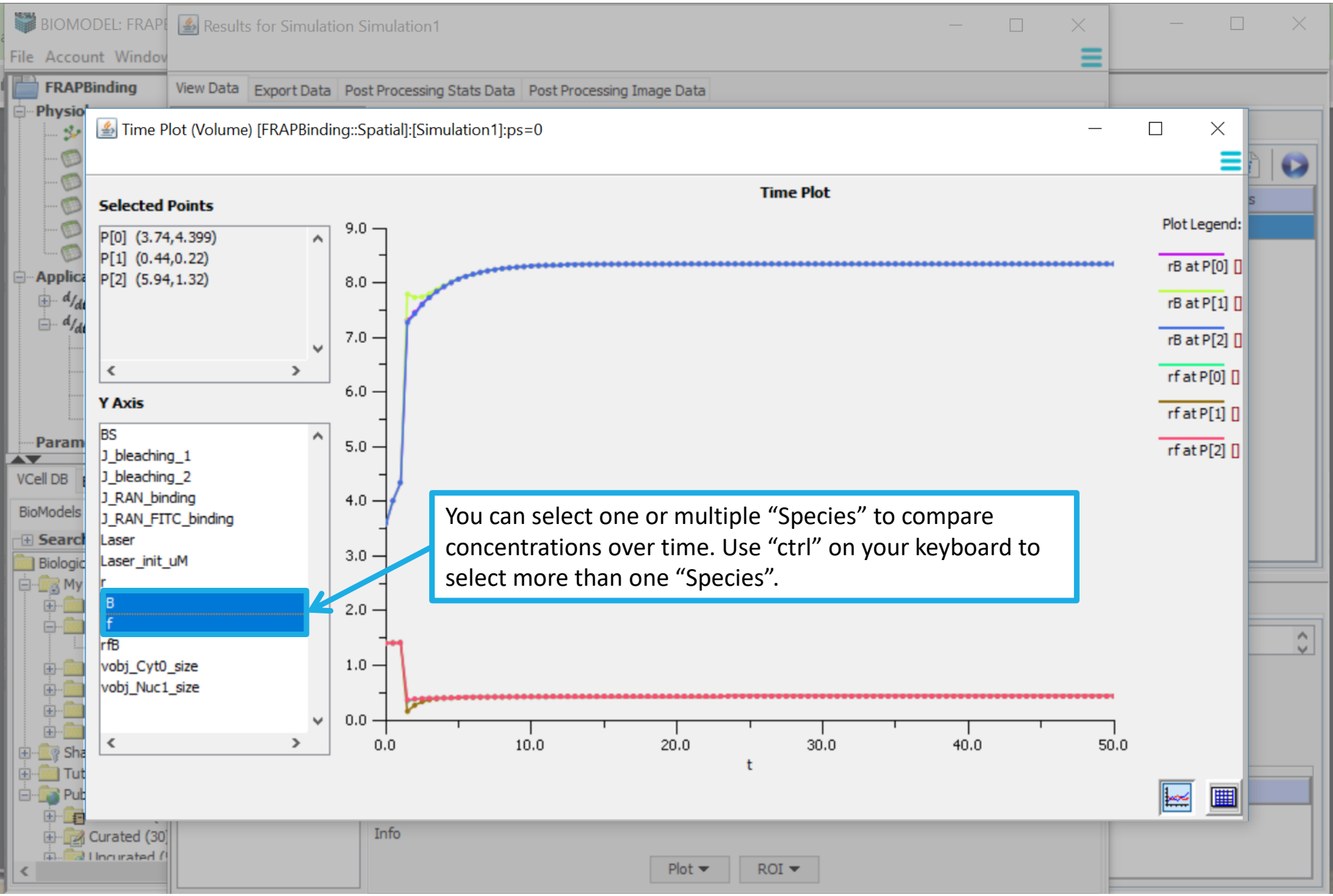
Simulations
Output Functions
Generated Math
Name
End Time
Output Option
Solver
Running Status
Simulation1
50.0
every 0.5 s
Fully-Implicit
completed
Native Simulation Results
Click the “Results” icon when the simulation is completed.
Object Properties
Annotations
Problems (0 Errors, 0 Warnings)
Database File Info
Annotation:
Settings:
Max timestep
Output
Rel tol
Abs tol
0.1s
every 0.5 sec
1.0E-7
1.0E-9
Mesh: 101x101 = 10201 elements
Geometry size: (22.0,22.0) microns
Parameters with values changed from defaults
Parameter Name
Default
New Value/Expression
Scan


Change the time frame being viewed by typing in a value under “Time”, dragging the slider up or down, or by selecting the slider and stepping through the time points with your up and down arrow keys on your keyboard.
The minimum and maximum values correspond to the intensity profile.
Click here to select the “Species” data you wish to view.
Results for Simulation Simulation1
View Data
Export Data
Post Processing
Time
10.0
0
50
Slice View
All Variables
BS
J_bleaching_1
J_bleaching_2
J_RAN_binding
J_RAN_FITC_binding
Laser
Laser_init_uM
r
rB
rf
rfB
sobj_Nuc1_Cyt0_size
vobj_Cyt0_size
Auto range
at time
all times
Max:0.42662137774435044
Min:0.42661977327648964
Color
BM
AM
ND
NR
Gray
Info
Plot
ROI


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: 8.302899141247165
Min: 8.302895619688755
Color
BM
AM
NN
ND
NR
Gray
BlueRed
All Variables
BS
J_bleaching_1
J_bleaching_2
J_RAN_binding
J_RAN_FITC_binding
Laser
Laser_init_uM
r
rB
rf
rfB
sobj_Nuc1_Cyt0_size
vobj_Cyt0_size
vobj_Nuc1_size
Info
Plot
ROI
Click on either “Gray” or “BlueRed” to change the color gradient.


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: 8.302899141247165
Min: 8.302895619688755
Color
BM
AM
NN
ND
NR
Gray
BlueRed
All Variables
Use the “Line” tool to establish two separate points. A line will automatically be created between the two points.
Use the “Selection” tool to delete or reposition the line.
Click “Plot” > “Spatial” to create a graph of the two points.
Time
Spatial
Kymograph
Info


Results for Simulation Simulation1
View Data
Export Data
Post Processing Stats Data
Post Processing Image Data
Time
12.0
Slice View
Data Range (Min-Max)
Auto range
at time
all times
Max: 8.324644145016984
Min: 8.324643946835454
Color
BM
AM
NN
ND
NR
Gray
BlueRed
All Variables
BS
J_bleaching_1
J_bleaching_2
J_RAN_binding
J_RAN_FITC_binding
Laser
Laser_init_uM
rB
rf
rfB
sobj_Nuc1_Cyt0_size
vobj_Cyt0_size
vobj_Nuc1_size
Info
Time
Use the “Time Point” tool to click in one or multiple areas.
Click “Plot” > “Time” to create your graph.


Time Plot (Volume) [FRAPBinding::Spatial]:[Simulation1]:ps=0
Selected Points
P[0] (3.74,4.399)
P[1] (0.44,0.22)
P[2] (5.94,1.32)
Y Axis
BS
J_bleaching_1
J_bleaching_2
J_RAN_binding
J_RAN_FITC_binding
Laser
Laser_init_uM
B
f
rfB
vobj_Cyt0_size
vobj_Nuc1_size
Time Plot
Plot Legend:
rB at P[0]
rB at P[1]
rB at P[2]
rf at P[0]
rf at P[1]
rf at P[2]
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
0.0
10.0
20.0
30.0
40.0
50.0
t
You can select one or multiple “Species” to compare concentrations over time. Use “ctrl” on your keyboard to select more than one “Species”.

Acknowledgements

The following students worked on this tutorial:

Tanya Miller (2015) – Pomperaug High School
Nathan Schaumburger (2017) – Hall High School
Arundeep Singh (2018) – Sport and Medical Sciences Academy
Zaiba Khan (2018) – East Windsor High School

Their work was supported by the Department of Health Career Opportunity Programs; the Aetna Foundation, Connecticut Collegiate Awareness and Preparation Program, Office of Higher Education; Connecticut State Legislative Fund; The Hartford; William and Alice Mortensen Foundation; John and Valerie Rowe Health Professions Scholars Program; the University of Connecticut Foundation; the Friends of the Department of Health Career Opportunity Programs and UConn Health.