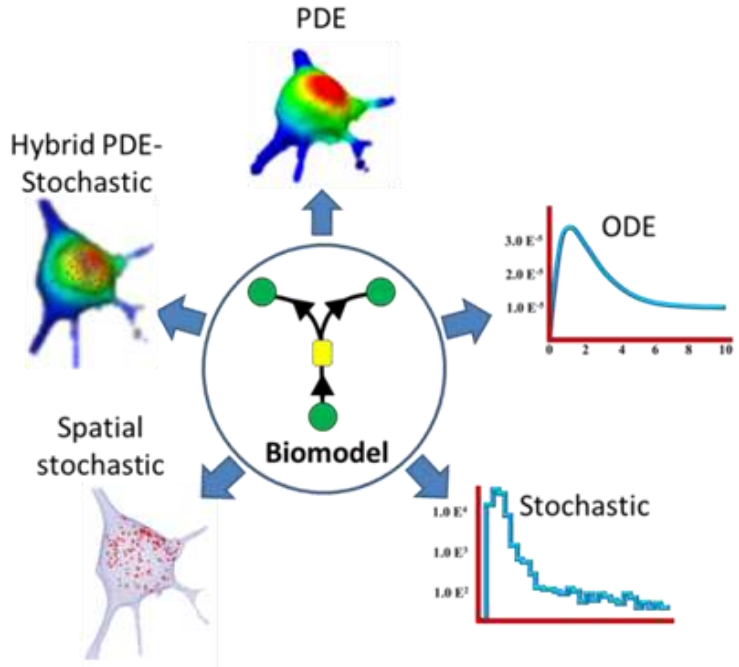
Virtual Cell Tutorials

VCell

modeling environment for mathematical simulation of cellular events.

To run VCell go to:

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)

Contents

VCell Tutorial

PH-GFP binding to PIP2 and IP3

Create a biomodel and 3D spatial (PDE) application to simulate pleckstrin homology domain (PH-GFP) reporter of PIP_2 to IP_3 conversion.

In this tutorial…

- Create a biomodel with reactions involving membrane and volume species.
- Create a compartmental (ODE) application that uses events to include time-dependent triggers.
- Create a spatial deterministic (PDE) application of a model using analytic equations to create a 3D geometry
- Define initial concentrations that are non-uniform in space and create timed events in spatial models using Boolean expressions
- Create output functions for more complex analysis of simulation results, e.g. to sum all fluorescent species in a compartment.

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PIP_2 to IP_3 Conversion

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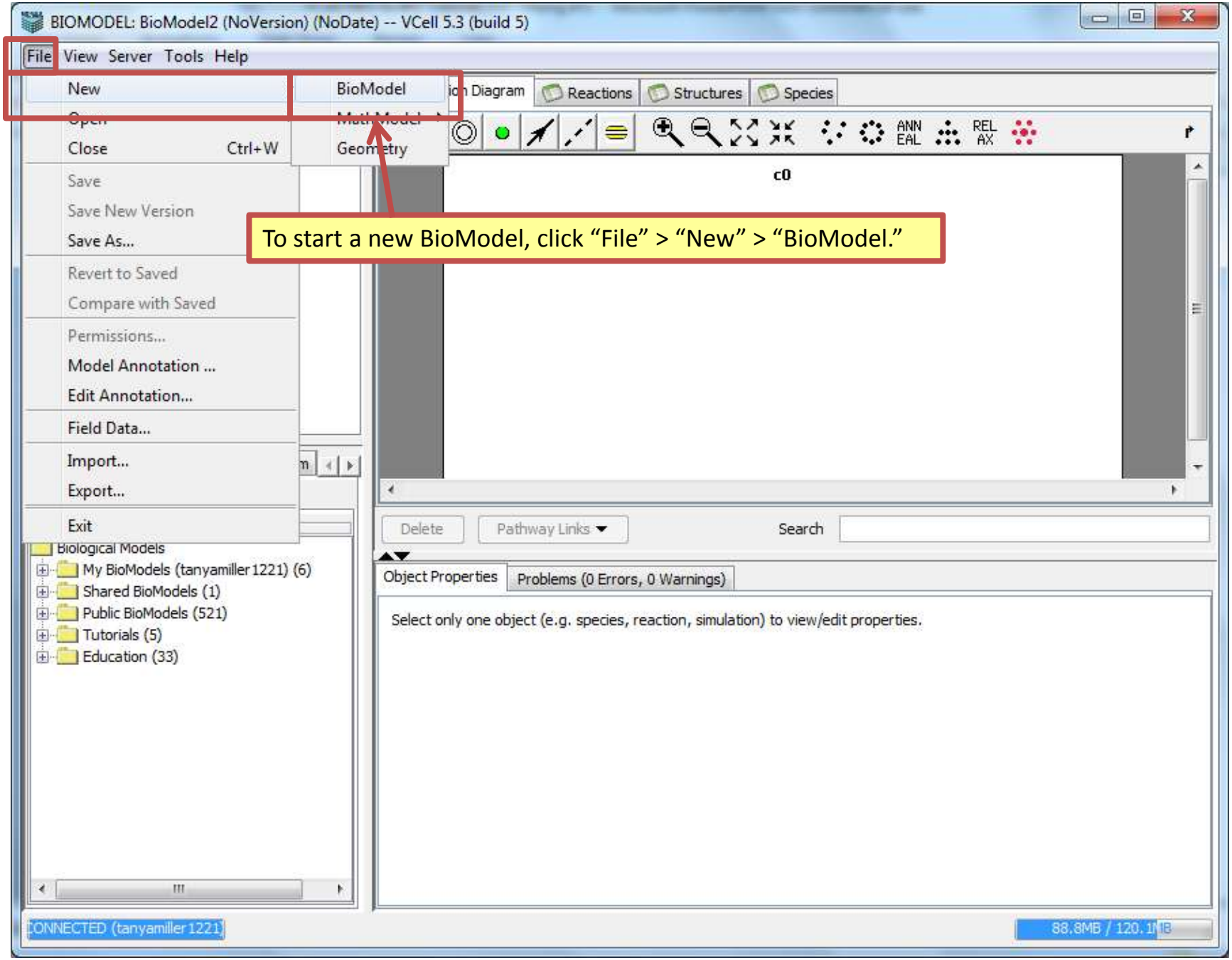

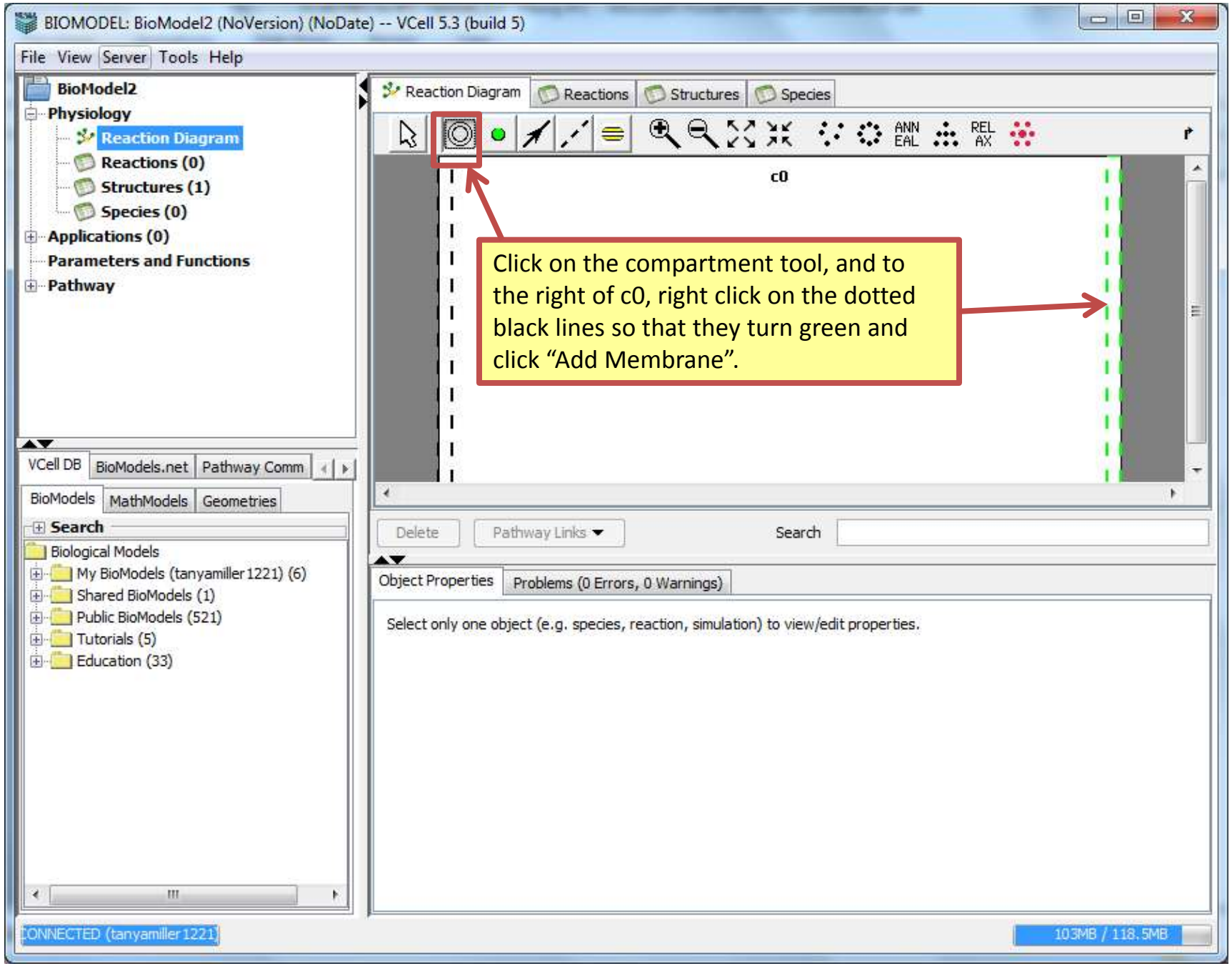
BIOMODEL: BioModel2 (NoVersion) (NoDate) -- VCell 5.3 (build 5)
File View Server Tools Help
BioModel2
Physiology
Reaction Diagram
Reactions (0)
Structures (1)
Species (0)
Applications (0)
Parameters and Functions
Pathway
Reaction Diagram
Reactions
Structures
Species
c0
Click on the compartment tool, and to the right of c0, right click on the dotted black lines so that they turn green and click "Add Membrane".
VCell DB
BioModels.net
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My BioModels (tanyamiller1221) (6)
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Public BioModels (521)
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Education (33)
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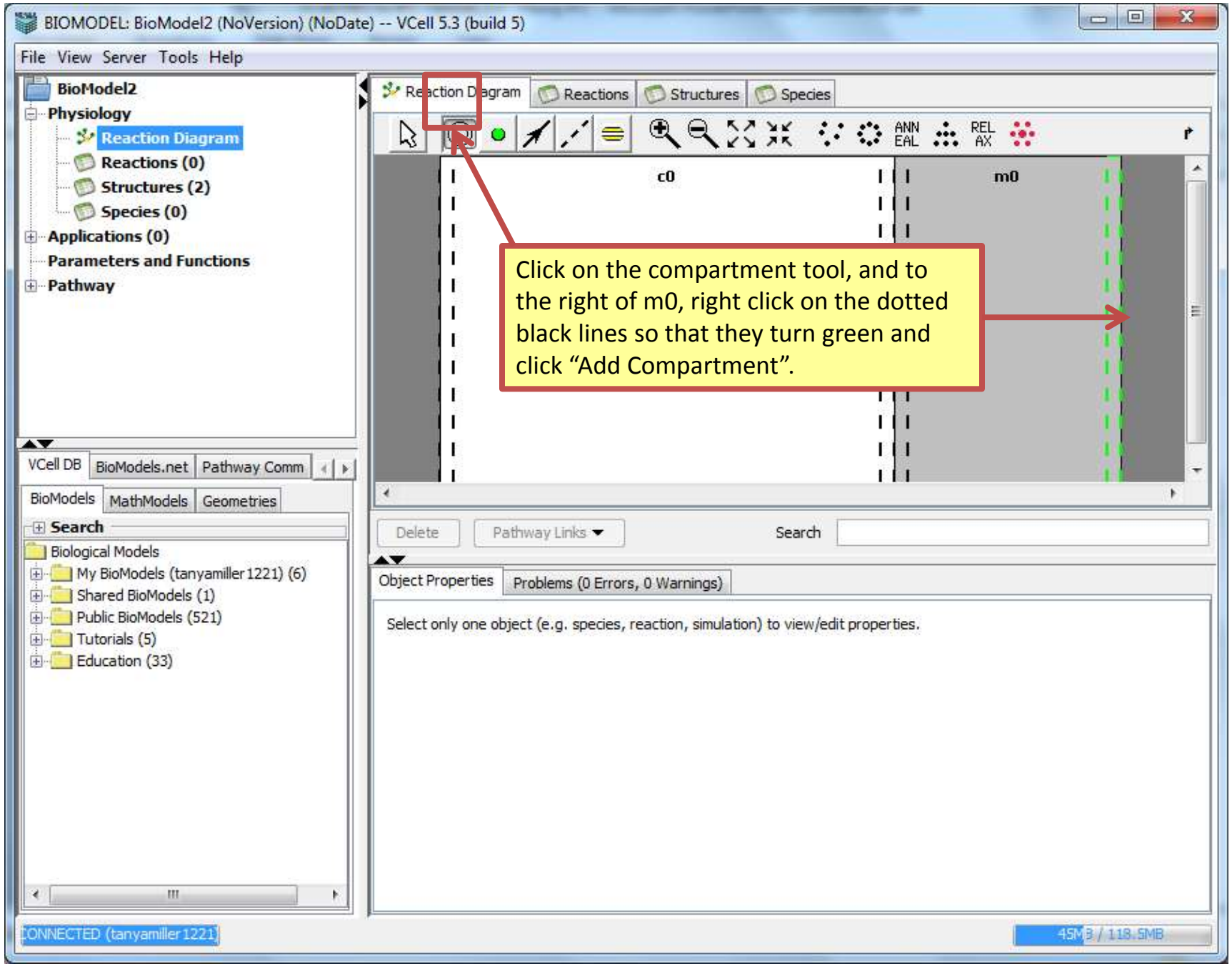
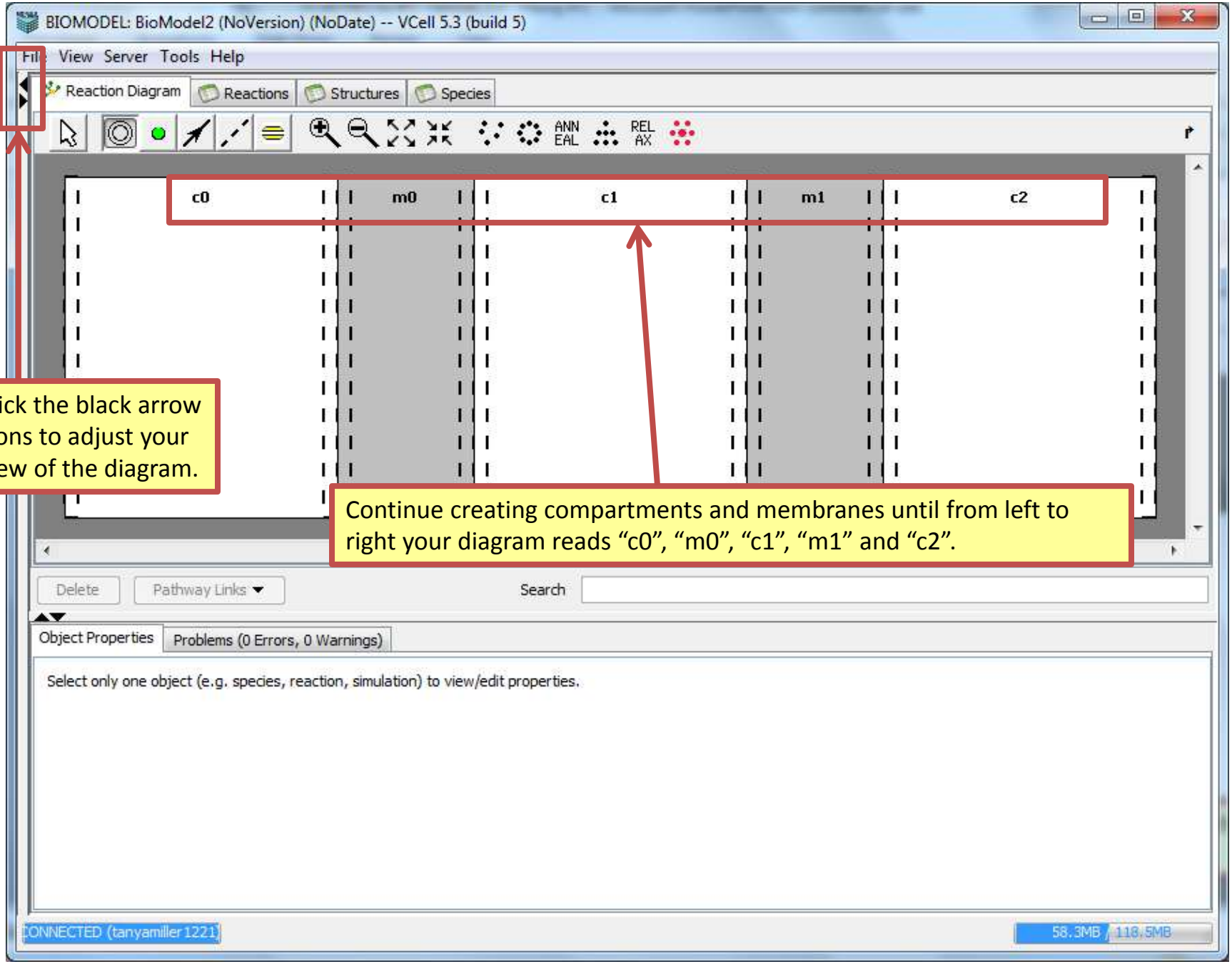
Pathway Links
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (tanyamiller1221)
103MB / 118.5MB

PIP_2 to IP_3 Conversion

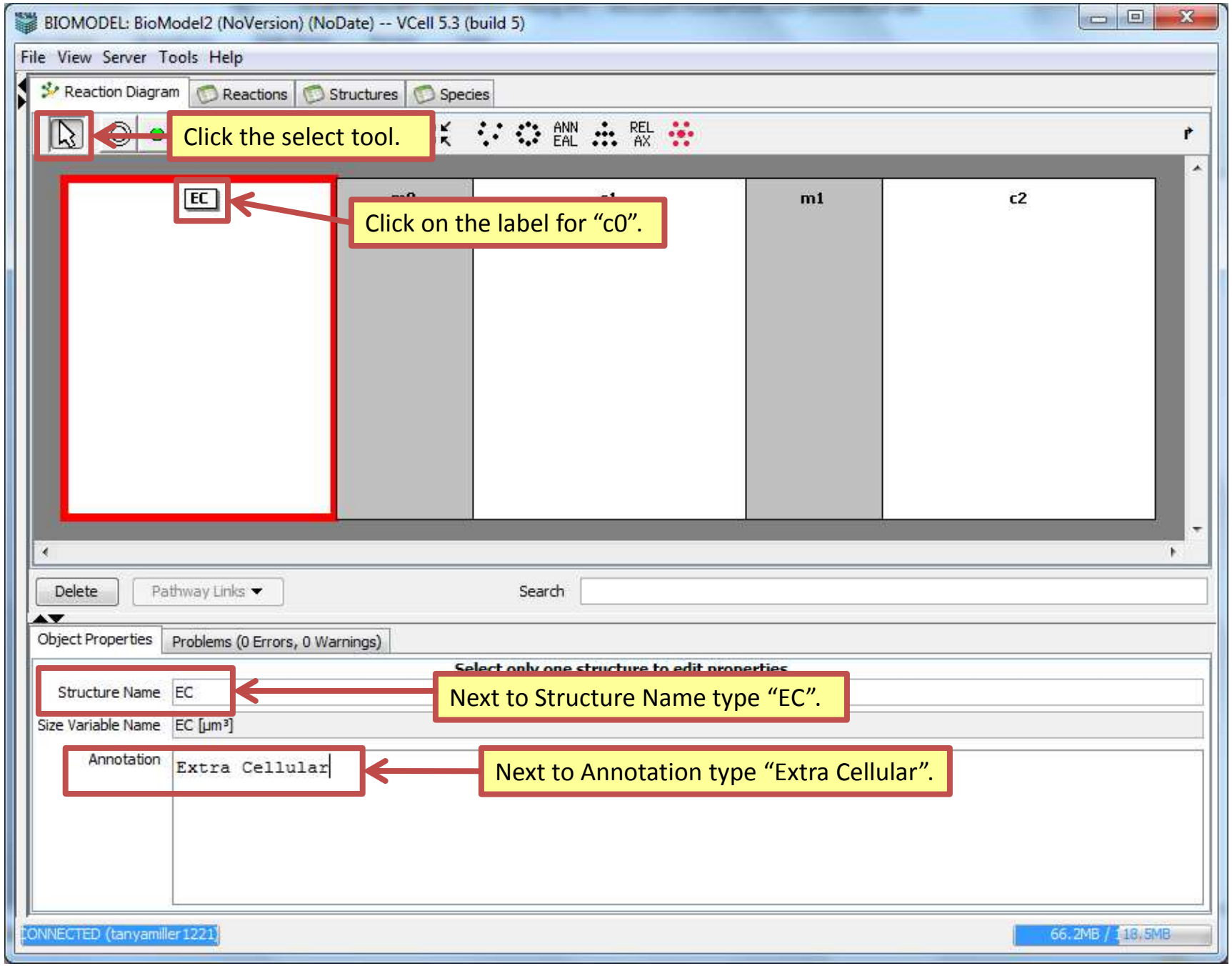
Contents




BIOMODEL: BioModel2 (NoVersion) (NoDate) -- VCell 5.3 (build 5)
File View Server Tools Help
Reaction Diagram
Reactions
Structures
Species
c0
m0
c1
m1
c2
Click the black arrow icons to adjust your view of the diagram.
Continue creating compartments and membranes until from left to right your diagram reads “c0”, “m0”, “c1”, “m1” and “c2”.
Delete
Pathway Links
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (tanyamiller1221)
58.3MB / 118.5MB

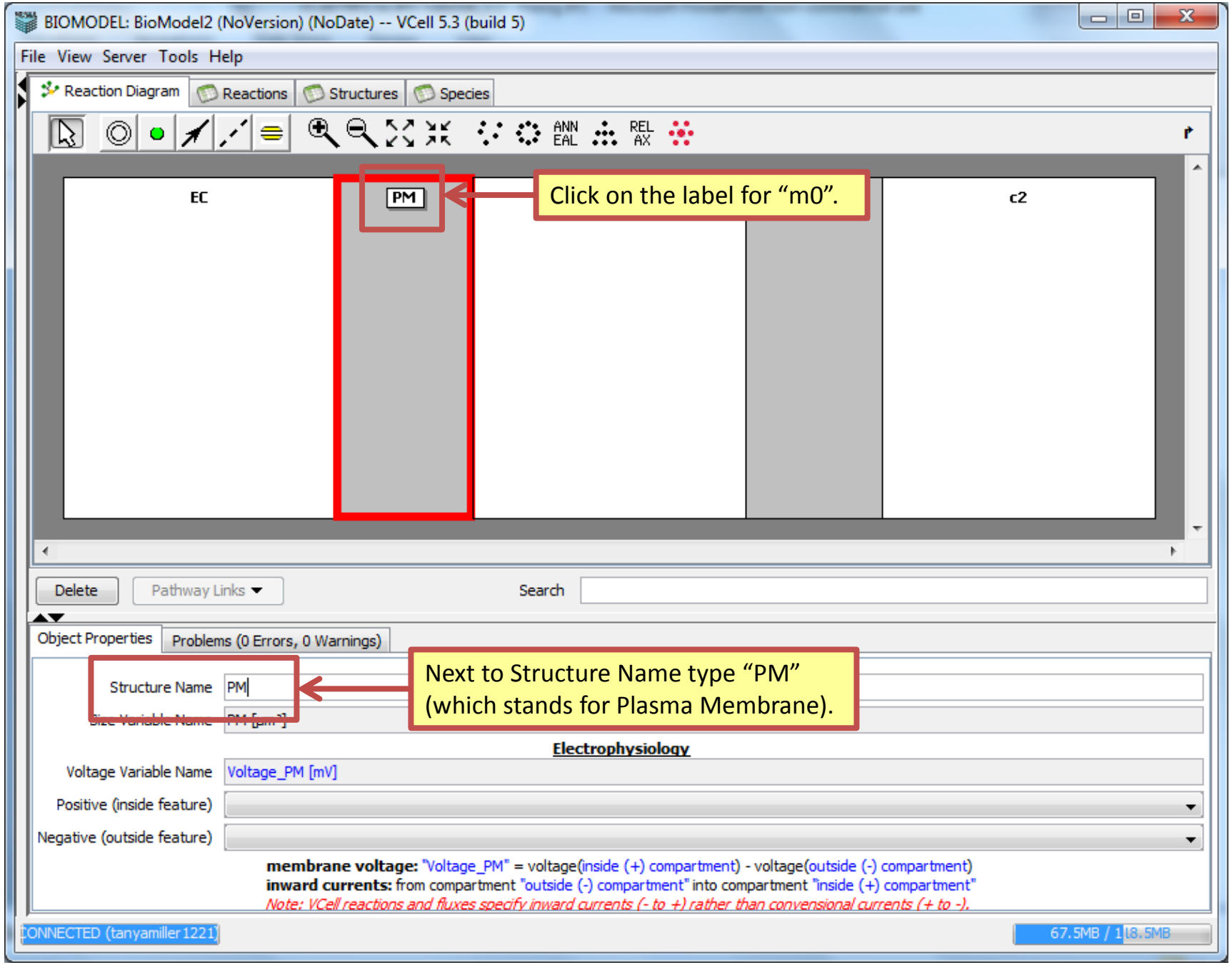
PIP_2 to IP_3 Conversion

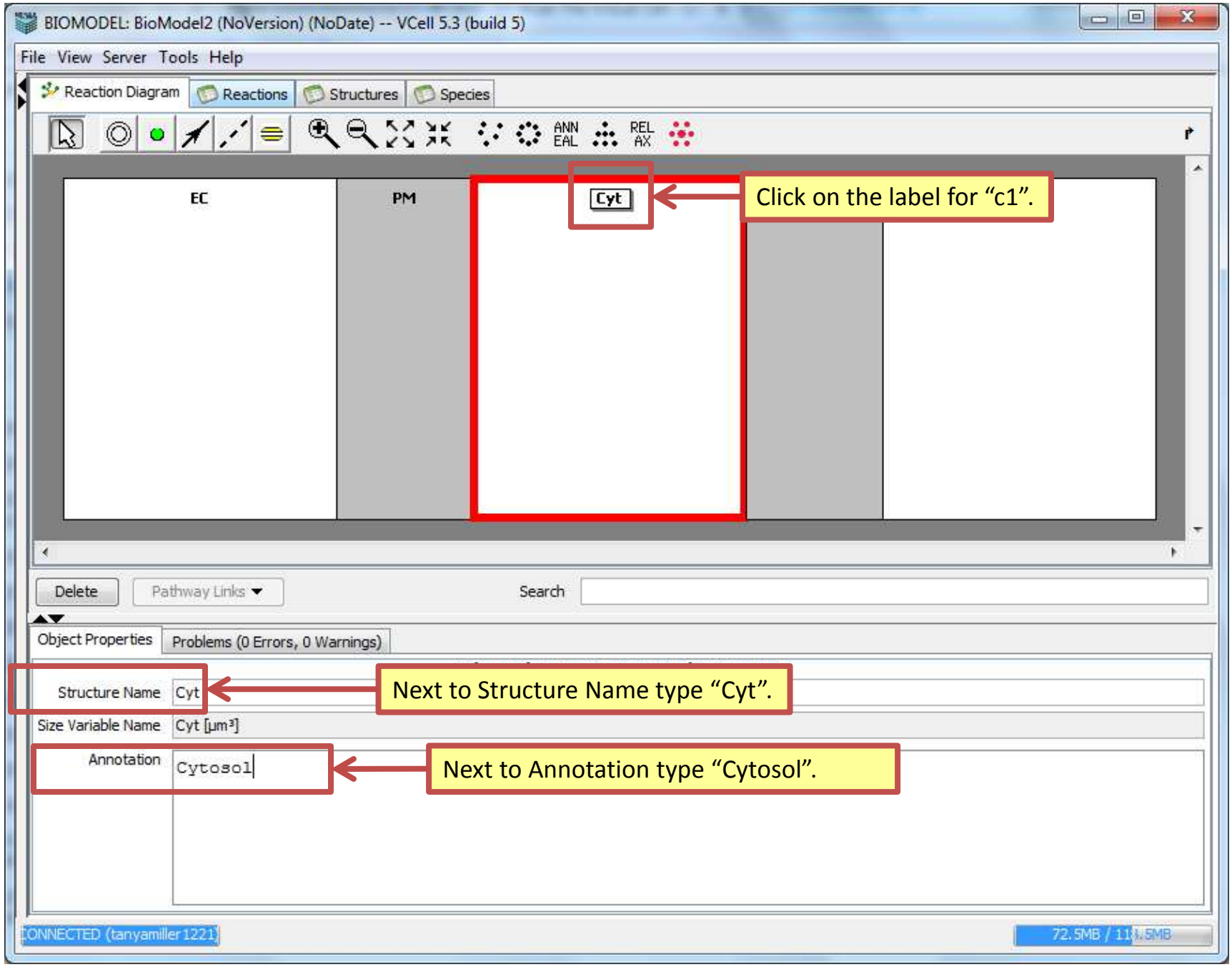
Contents



PIP_2 to IP_3 Conversion

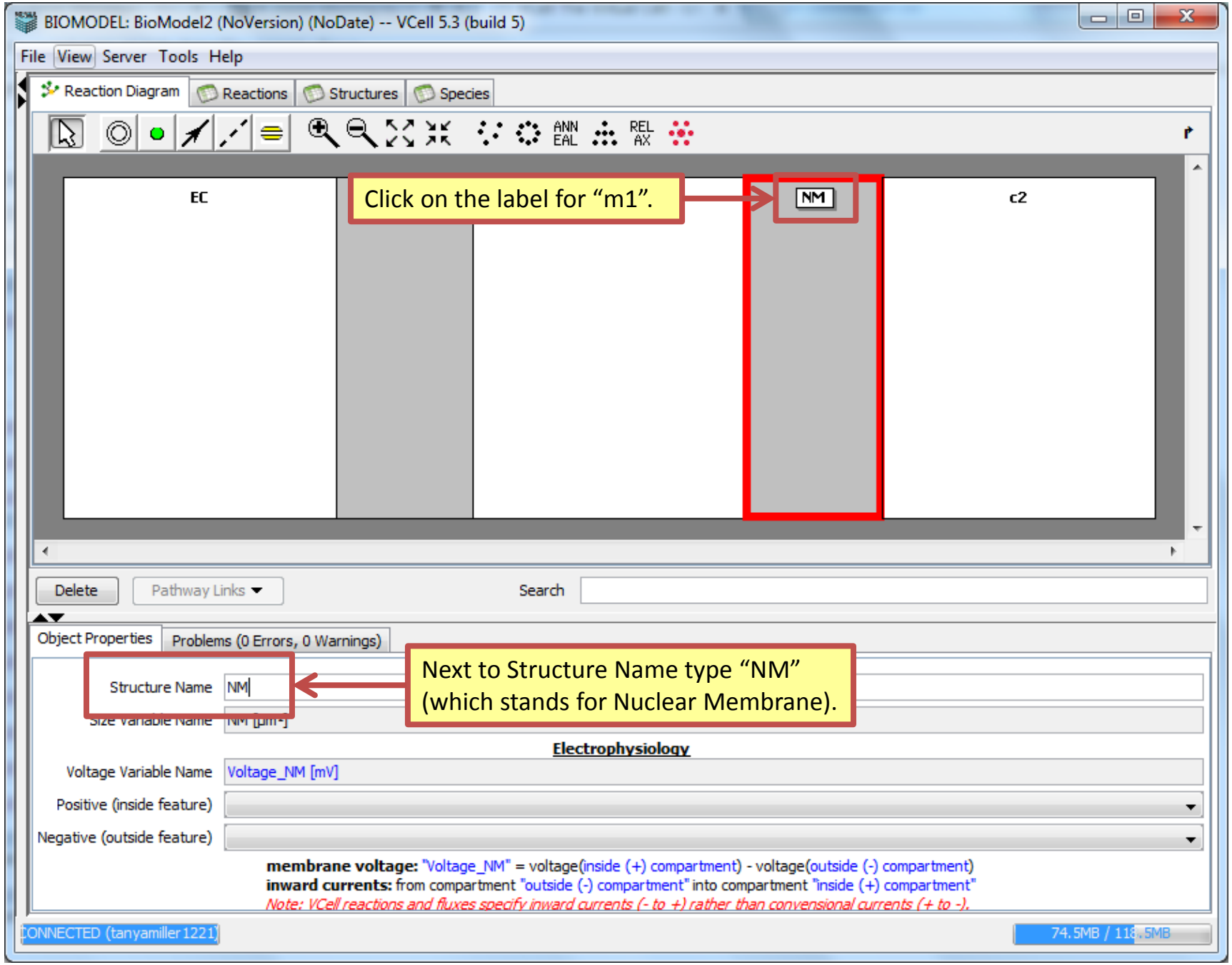
Contents




BIOMODEL: BioModel2 (NoVersion) (NoDate) -- VCell 5.3 (build 5)
File View Server Tools Help
Reaction Diagram
Reactions
Structures
Species
EC
PM
Cyt
Click on the label for “c1”.
Delete
Pathway Links
Search
Object Properties
Problems (0 Errors, 0 Warnings)
Structure Name
Cyt
Next to Structure Name type “Cyt”.
Size Variable Name
Cyt [µm³]
Annotation
Cytosol
Next to Annotation type “Cytosol”.
CONNECTED (tanyamiller1221)
72.5MB / 11

PIP_2 to IP_3 Conversion

Contents



PIP_2 to IP_3 Conversion

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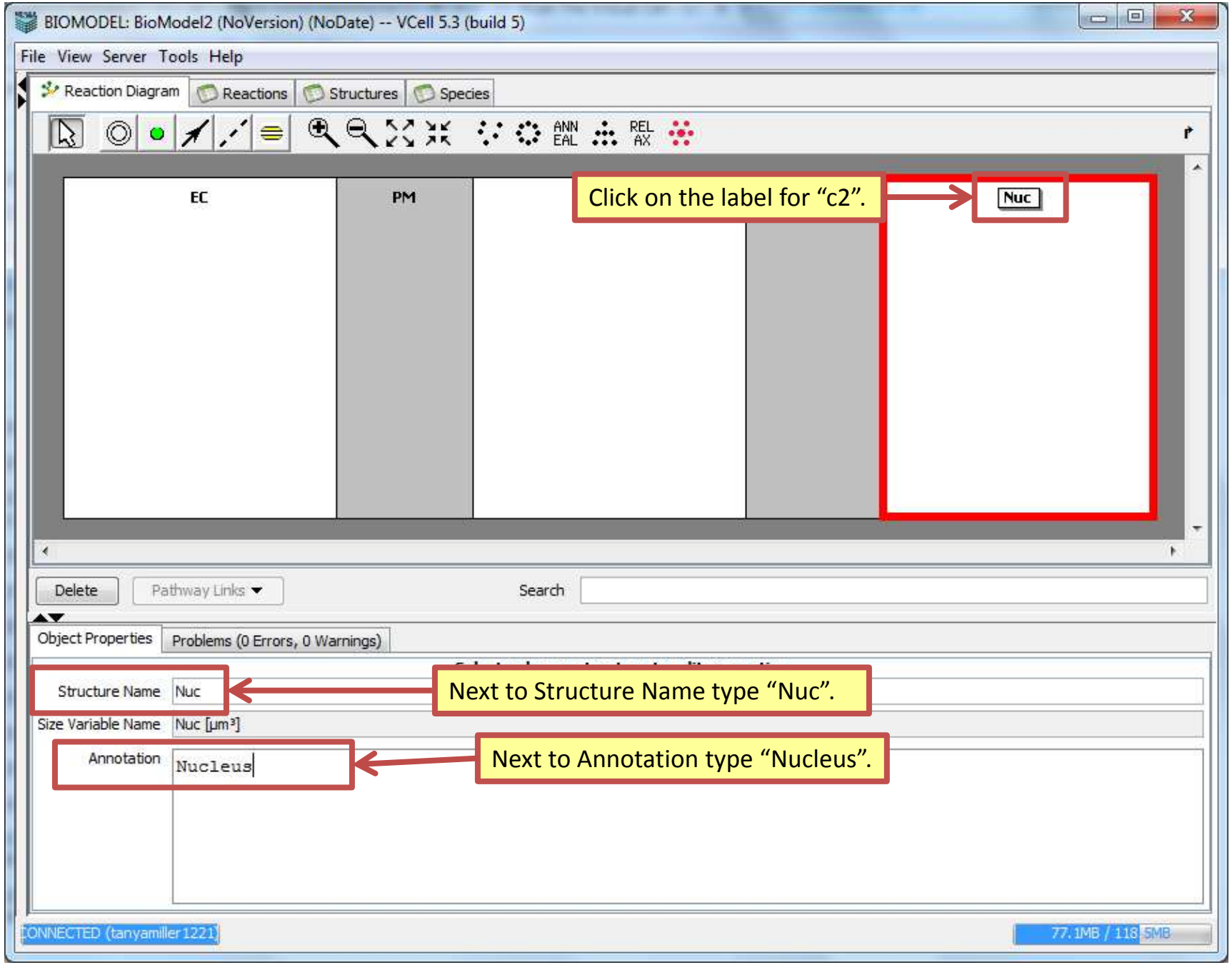

PIP_2 to IP_3 Conversion

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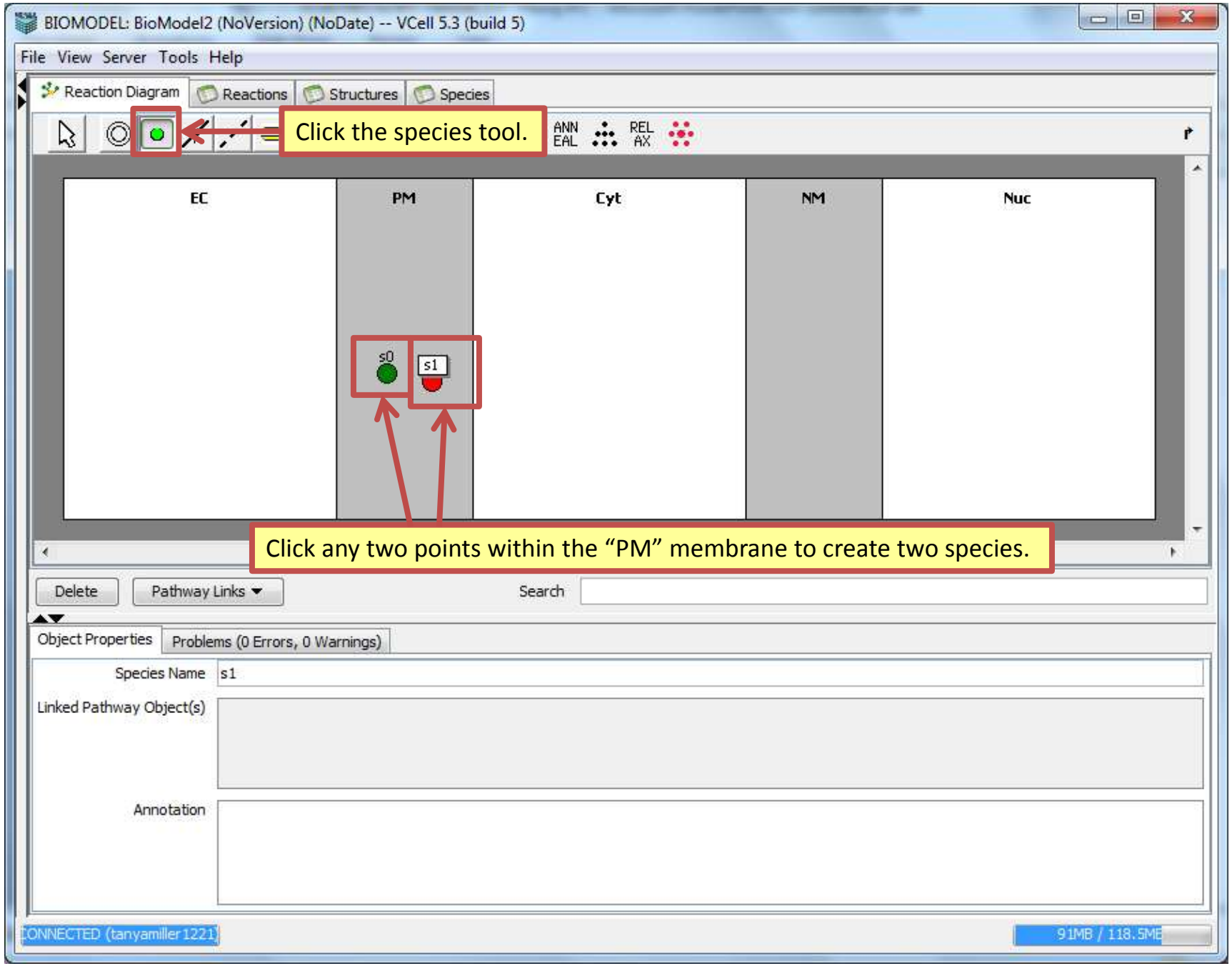
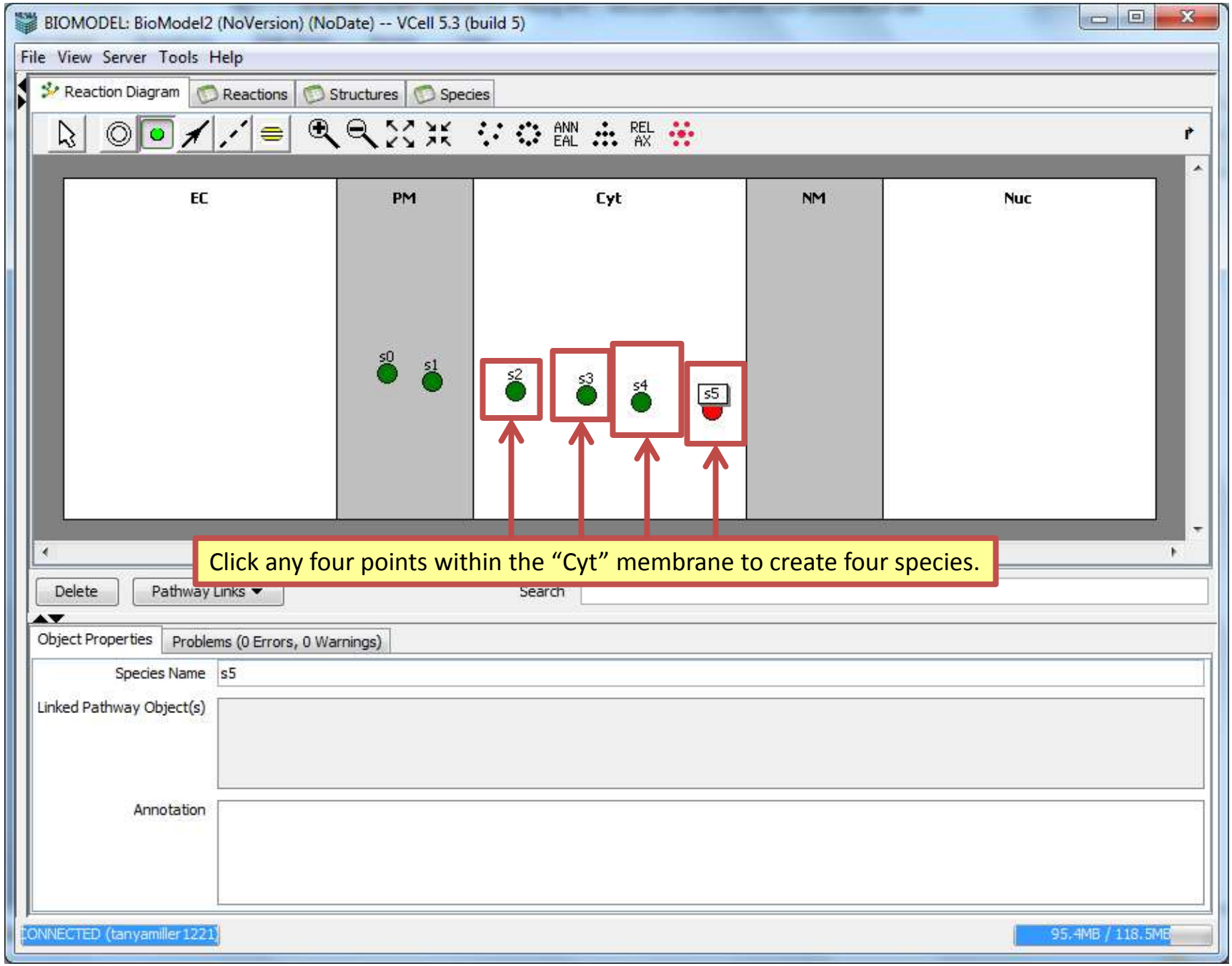
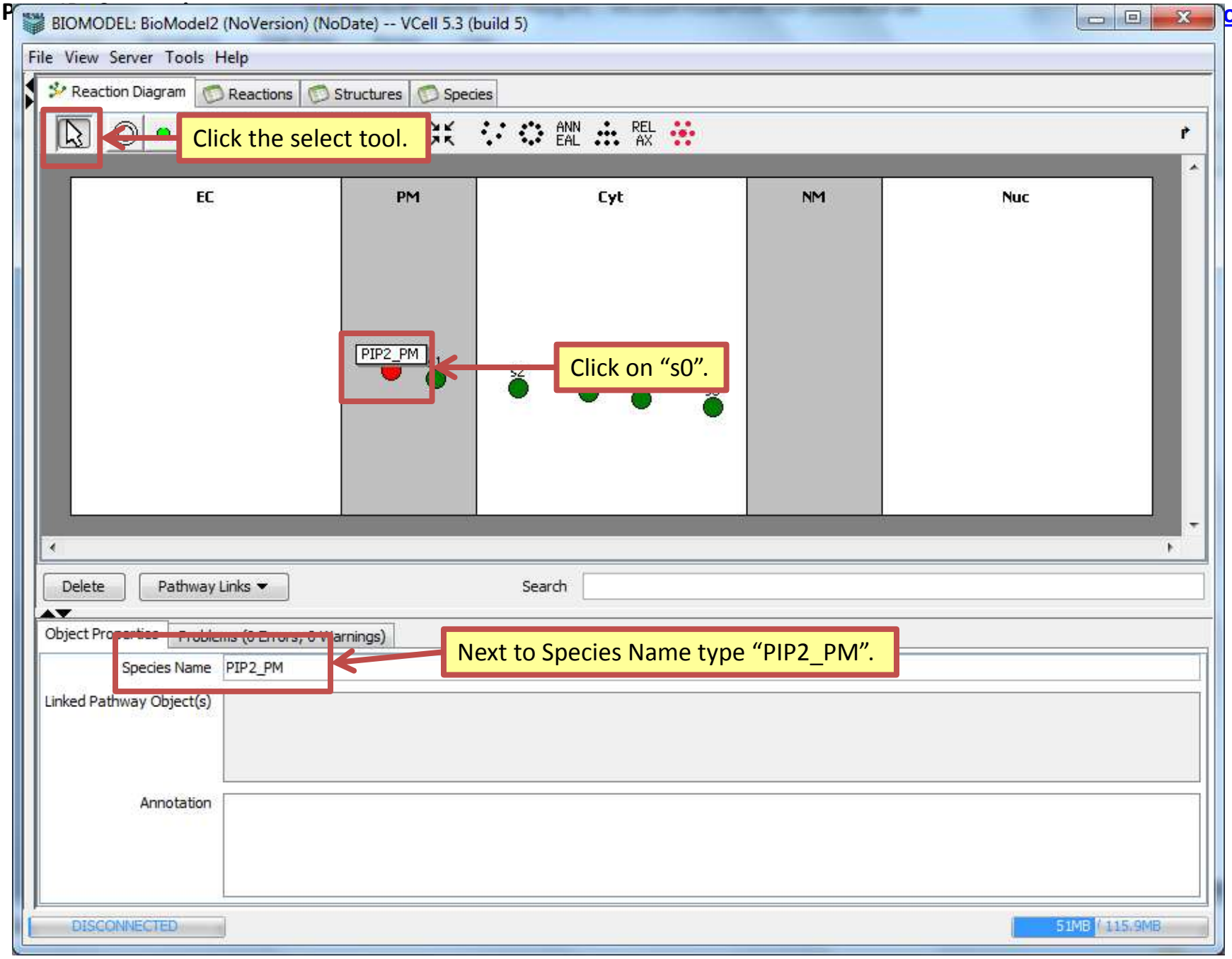
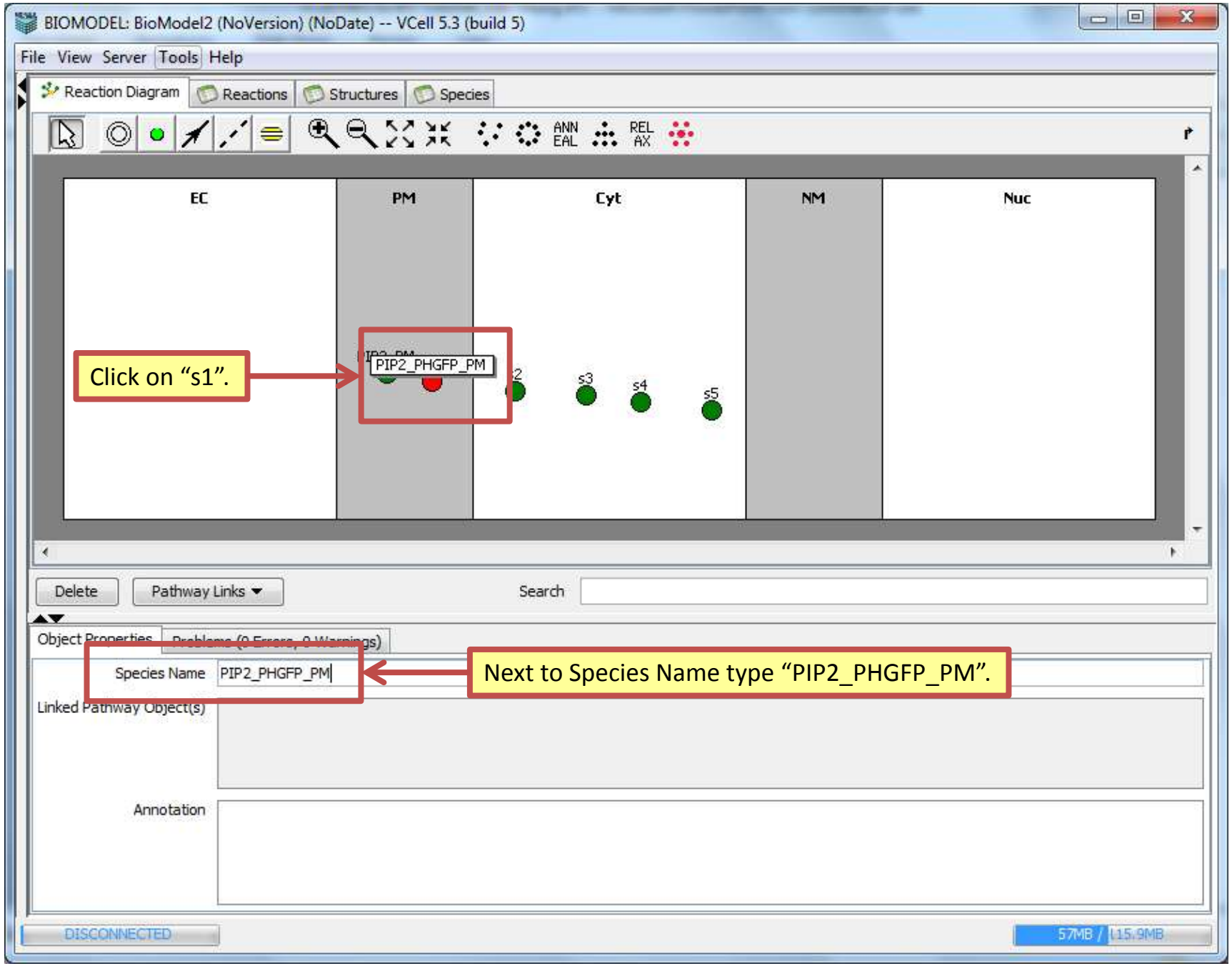


PIP_2 to IP_3 Conversion

Contents




BIOMODEL: BioModel2 (NoVersion) (NoDate) -- VCell 5.3 (build 5)
File View Server Tools Help
Reaction Diagram
Reactions
Structures
Species
Click the select tool.
EC
PM
Cyt
NM
Nuc
PIP2_PM
Click on "s0".
Delete
Pathway Links
Search
Object Properties
Species Name
PIP2_PM
Next to Species Name type "PIP2_PM".
Linked Pathway Object(s)
Annotation
DISCONNECTED
51MB / 115.9MB


BIOMODEL: BioModel2 (NoVersion) (NoDate) -- VCell 5.3 (build 5)
File View Server Tools Help
Reaction Diagram
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PIP2_PHGFP_PM
s3
s4
s5
Click on "s1".
Delete
Pathway Links
Search
Object Properties
Species Name
PIP2_PHGFP_PM
Next to Species Name type "PIP2_PHGFP_PM".
Linked Pathway Object(s)
Annotation
DISCONNECTED
57MB / 115.9MB

PIP_2 to IP_3 Conversion

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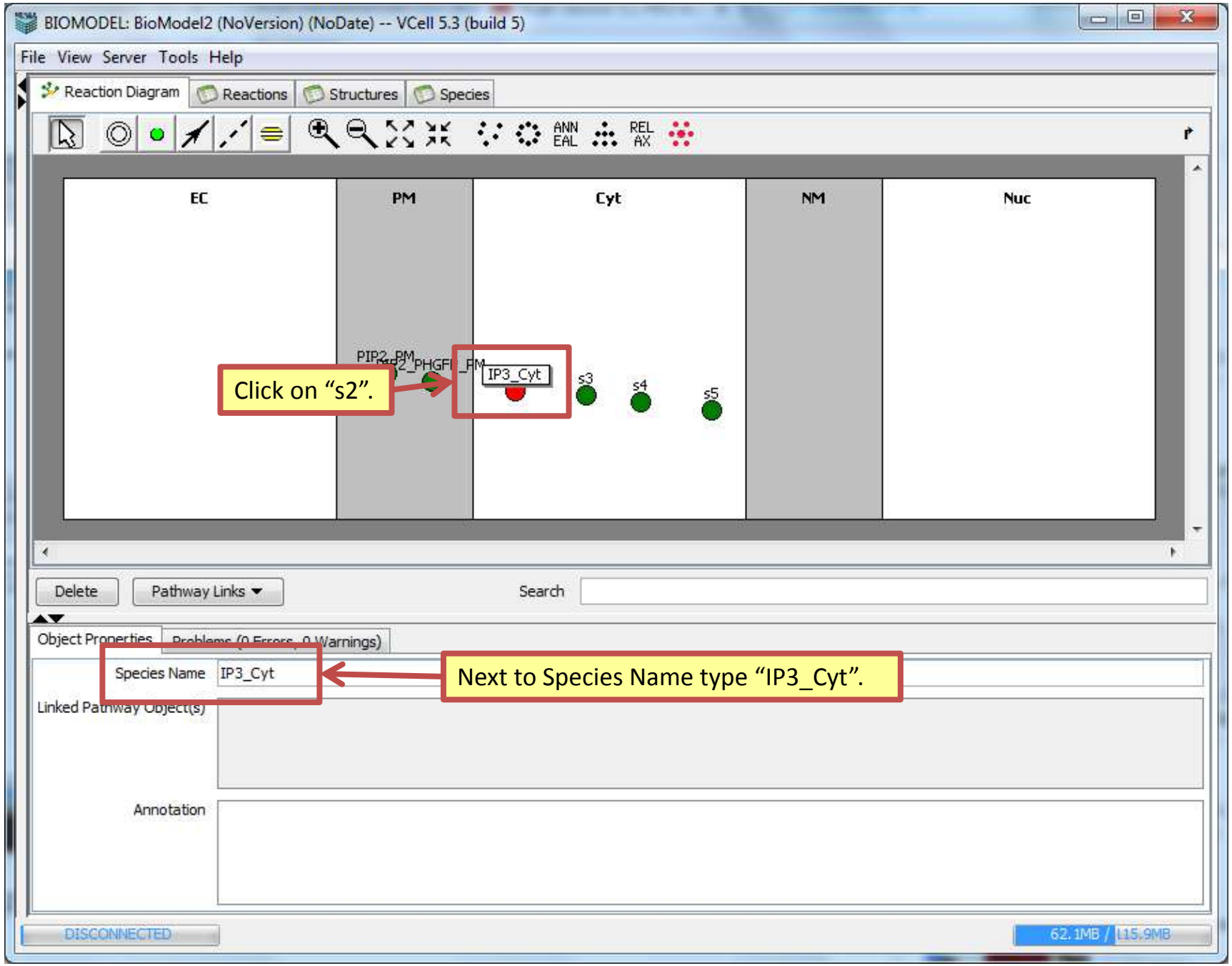

PIP_2 to IP_3 Conversion

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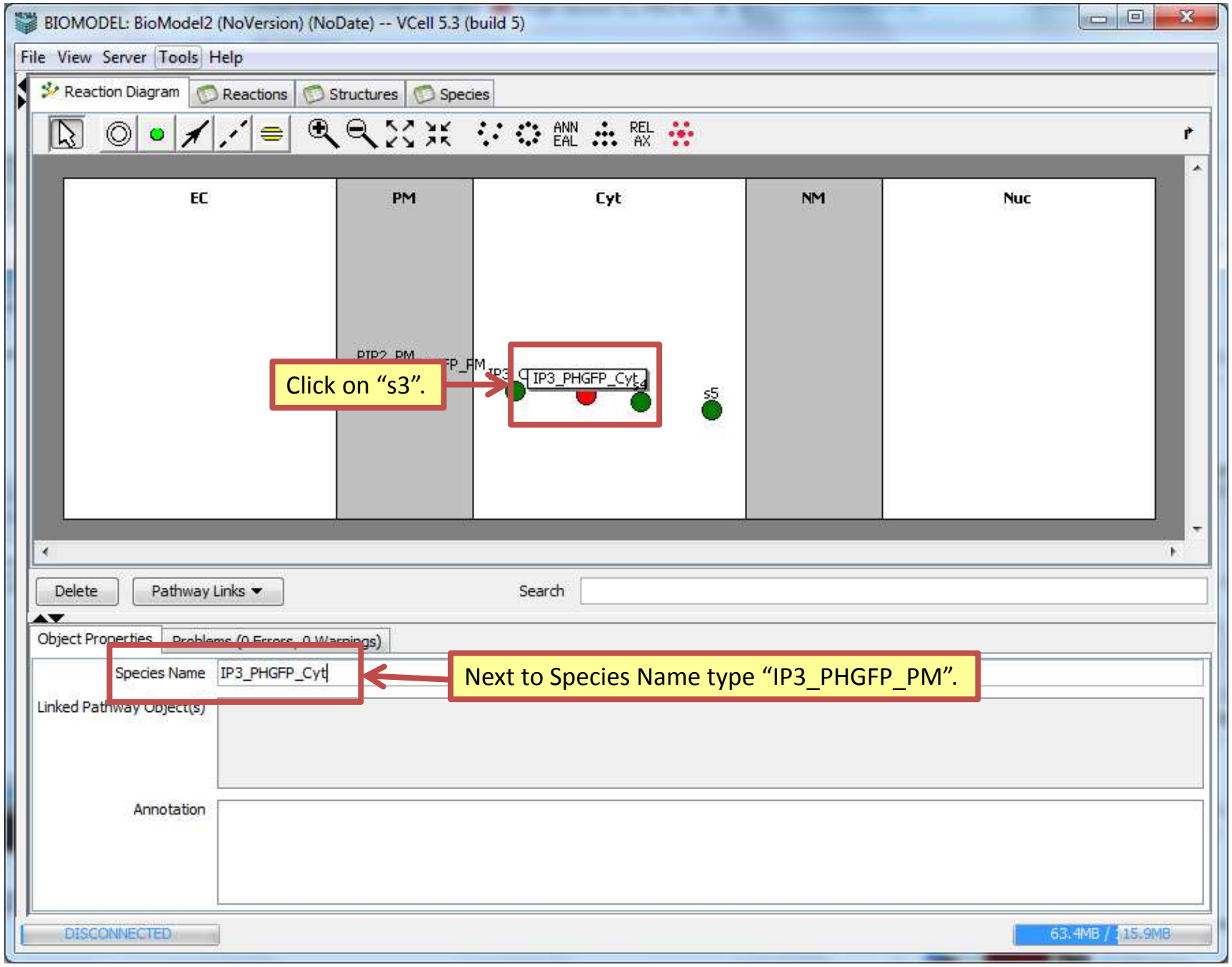

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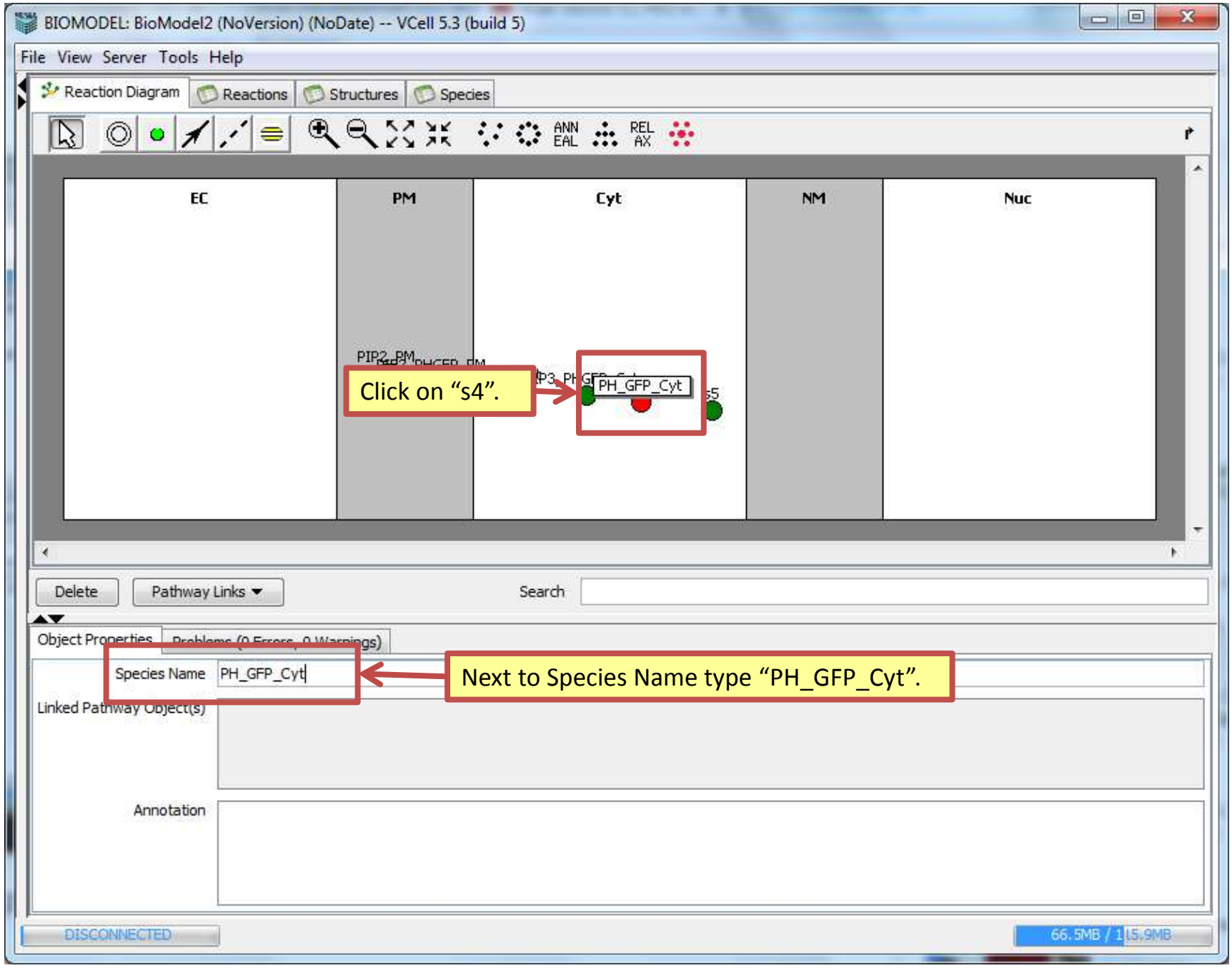

PIP_2 to IP_3 Conversion

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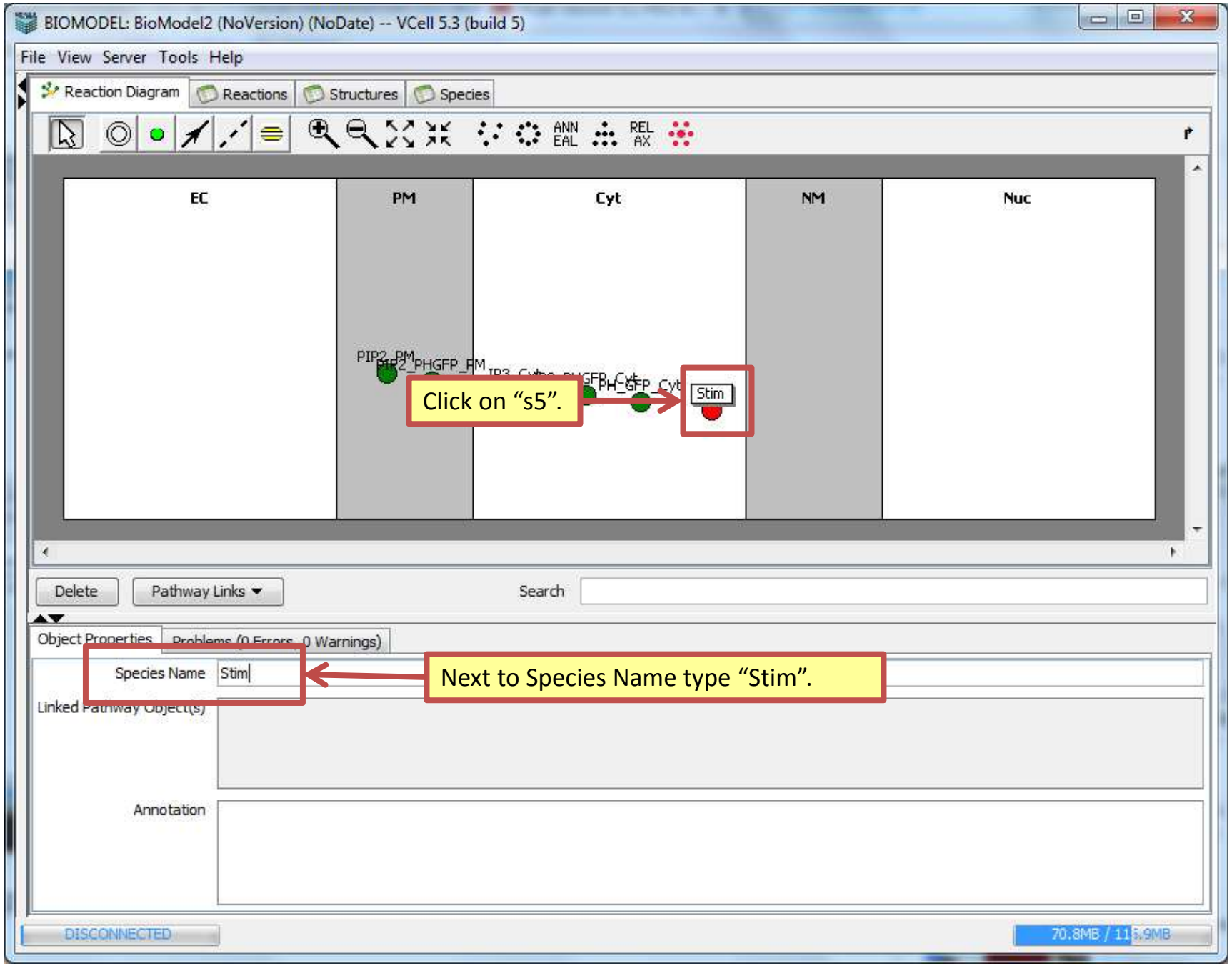

PIP_2 to IP_3 Conversion

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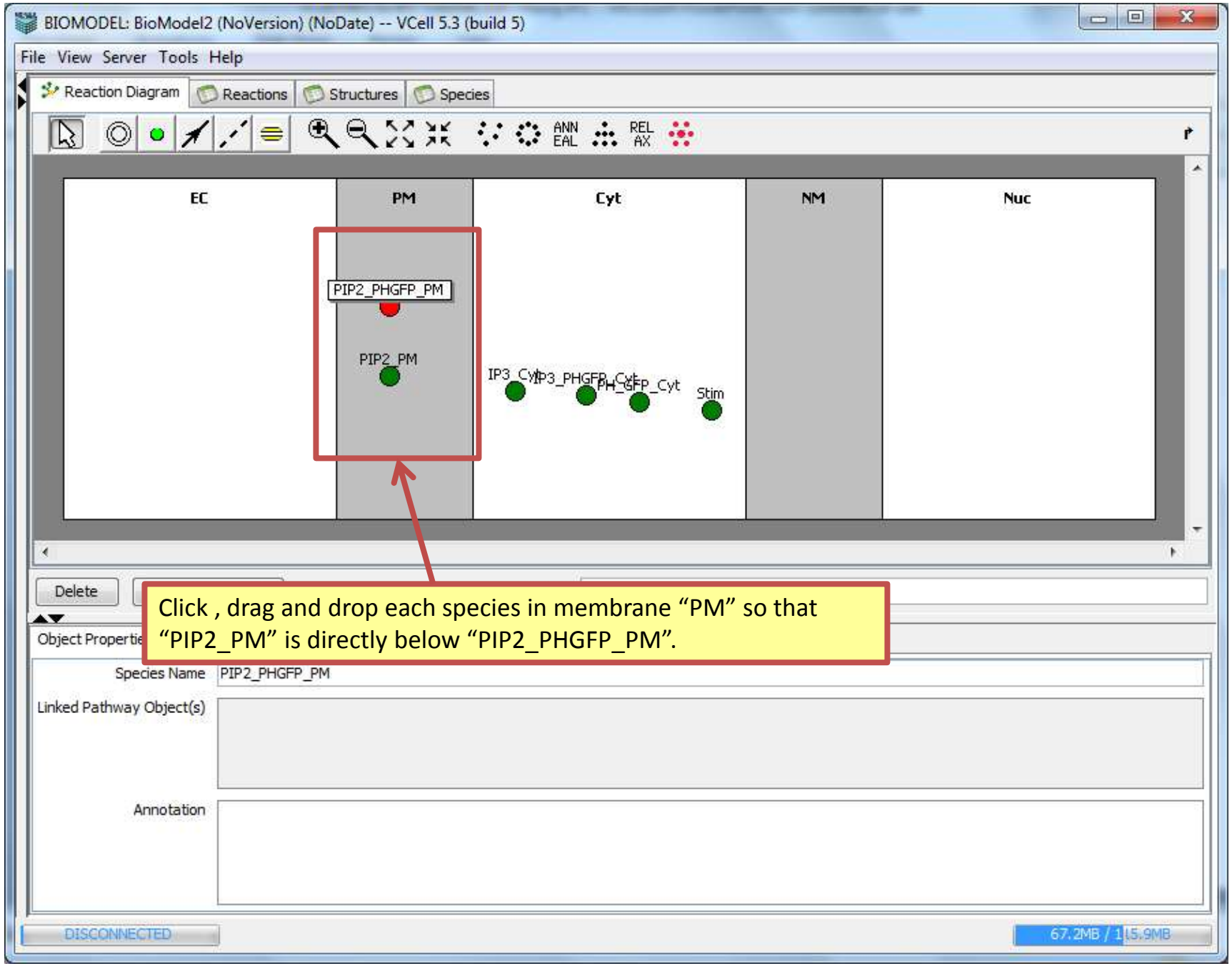

PIP_2 to IP_3 Conversion

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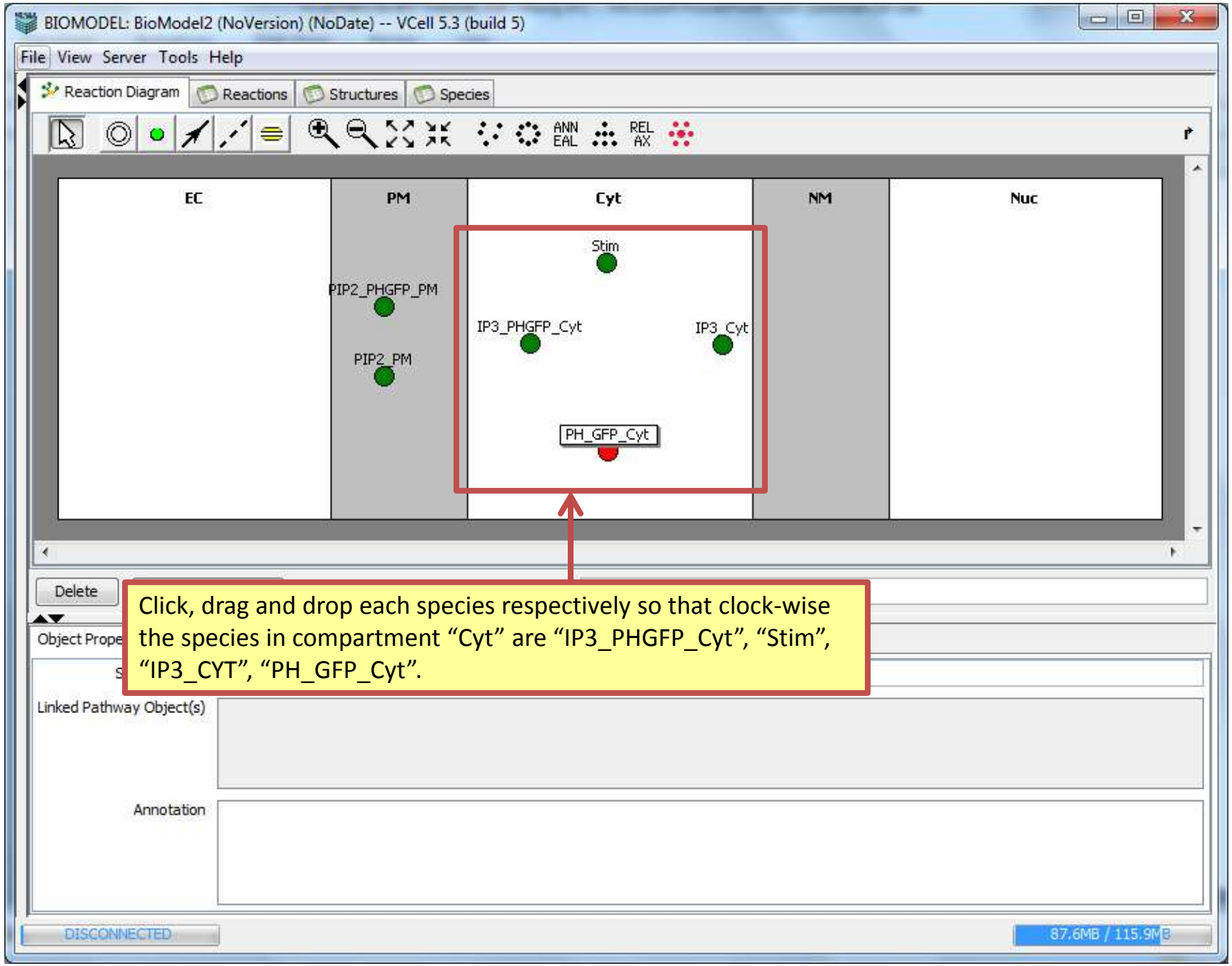

PIP_2 to IP_3 Conversion

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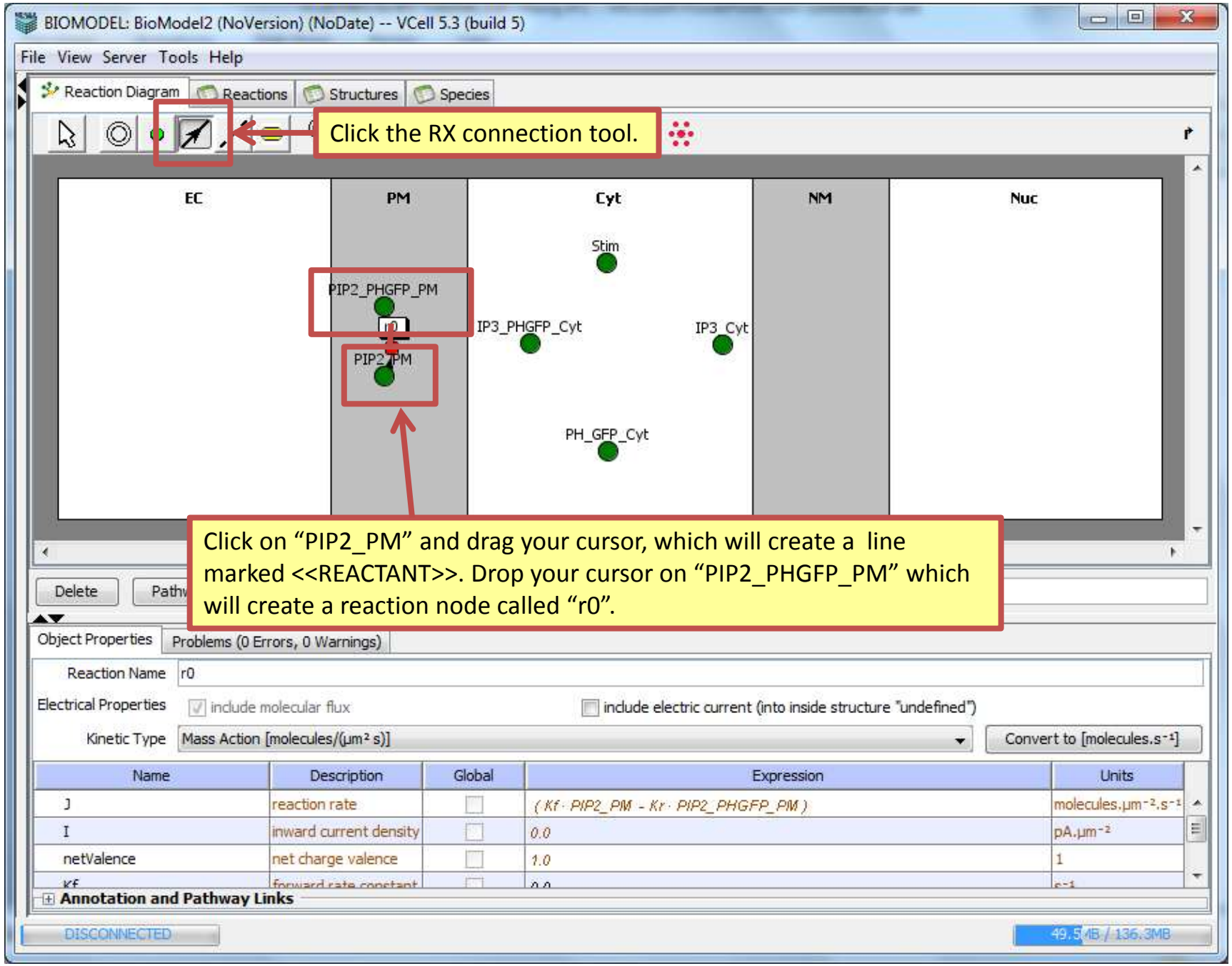

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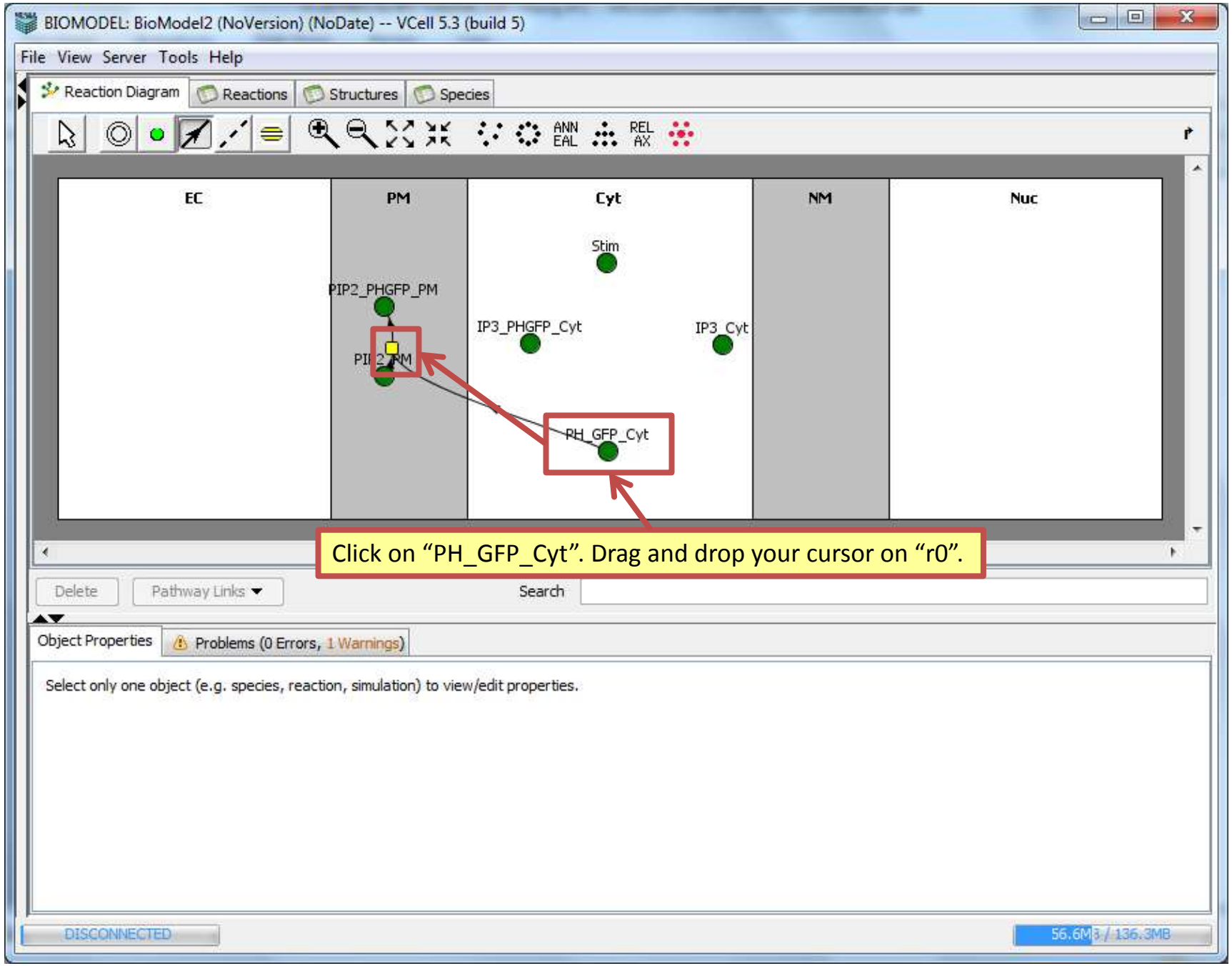

PIP_2 to IP_3 Conversion

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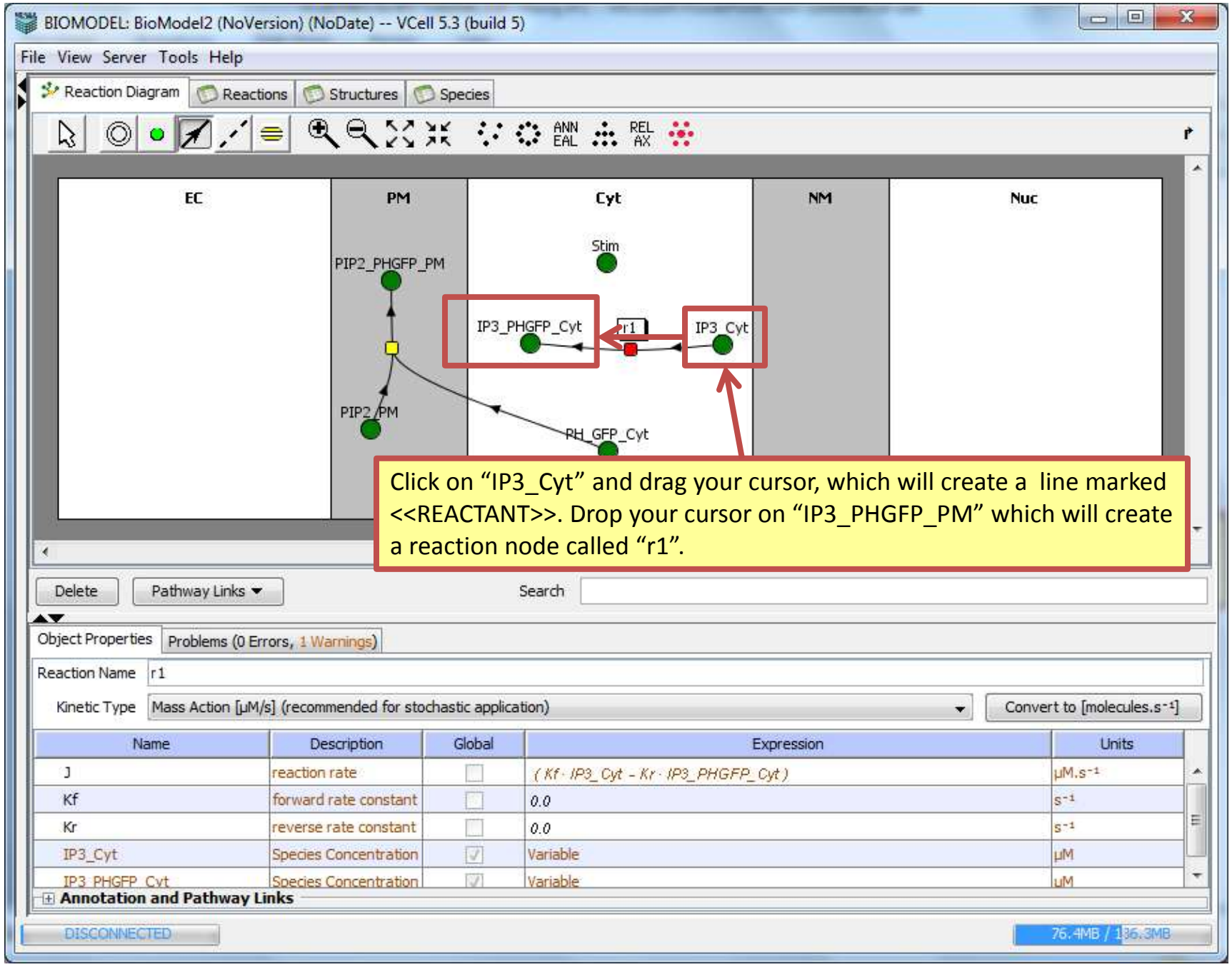

PIP_2 to IP_3 Conversion

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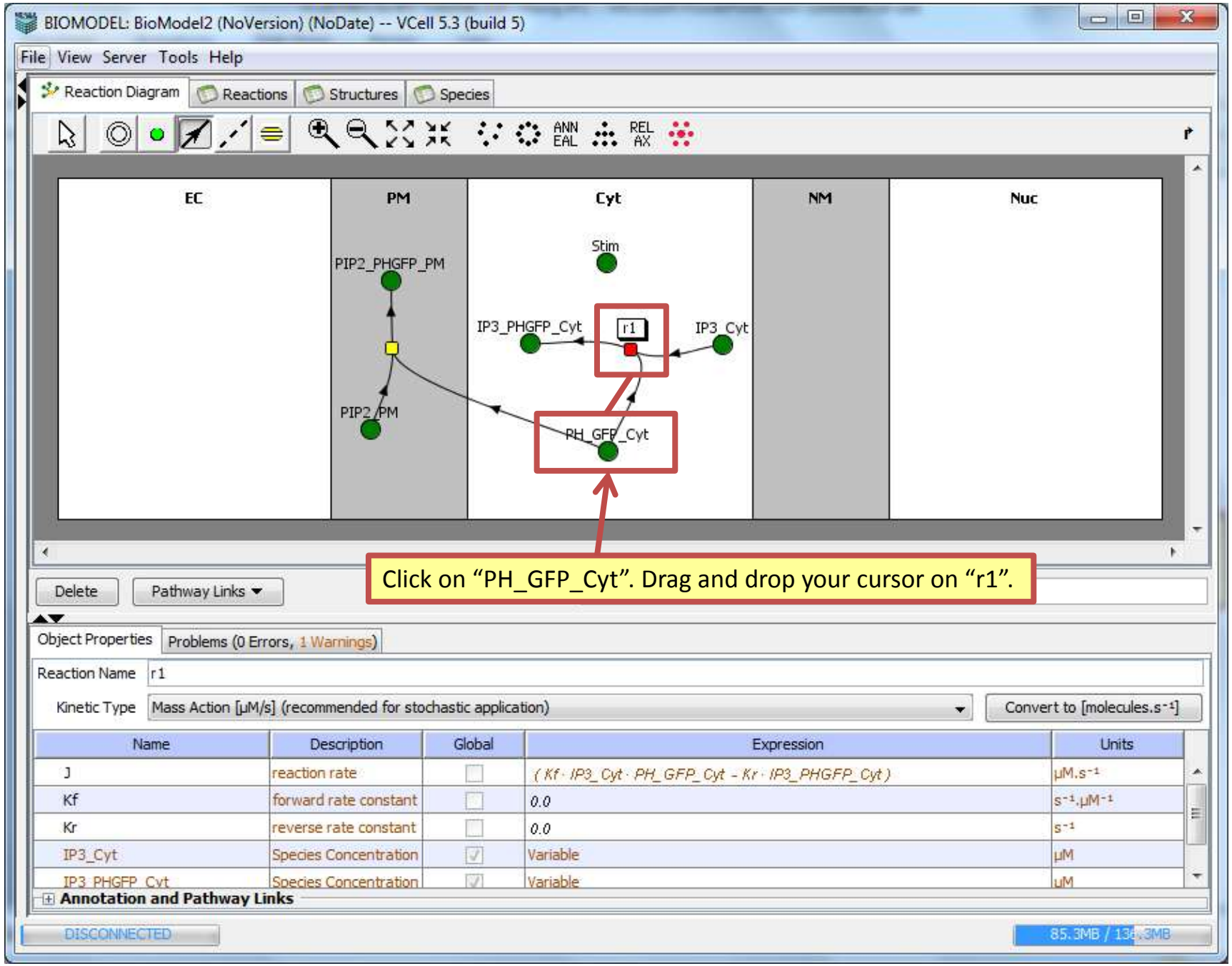
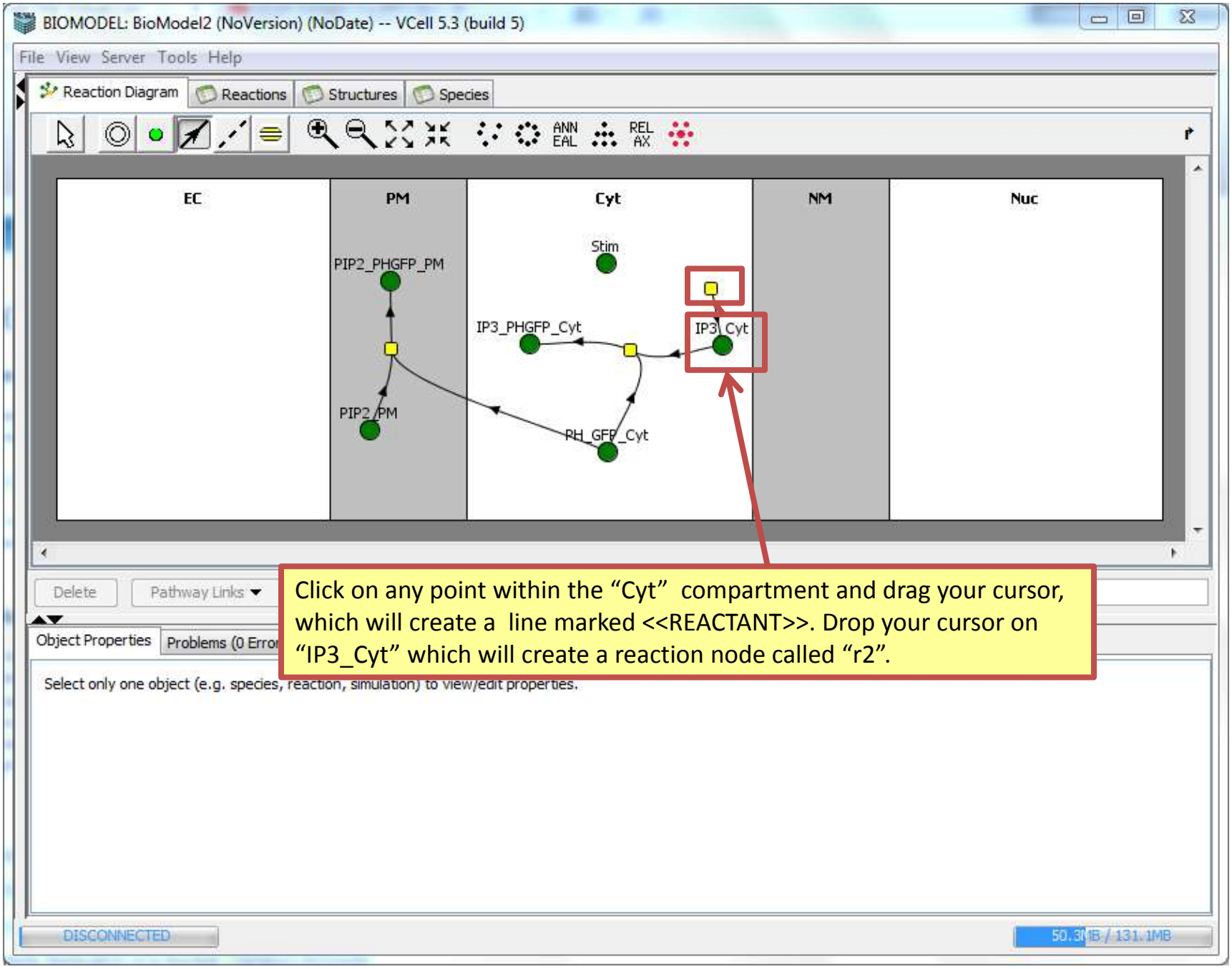


PIP_2 to IP_3 Conversion

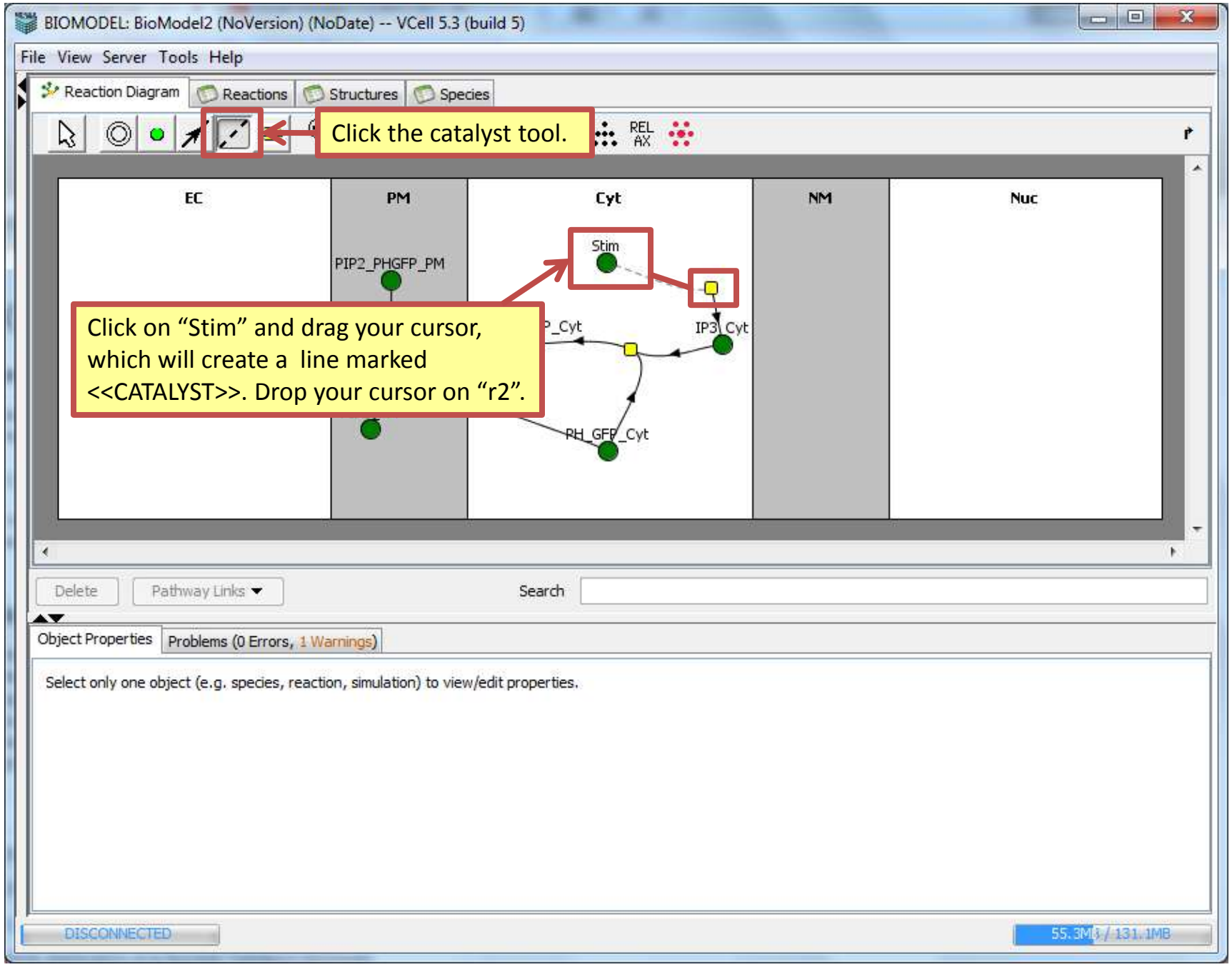
Contents



Click on any point within the "Cyt" compartment and drag your cursor, which will create a line marked <<REACTANT>>. Drop your cursor on "IP3_Cyt" which will create a reaction node called "r2".

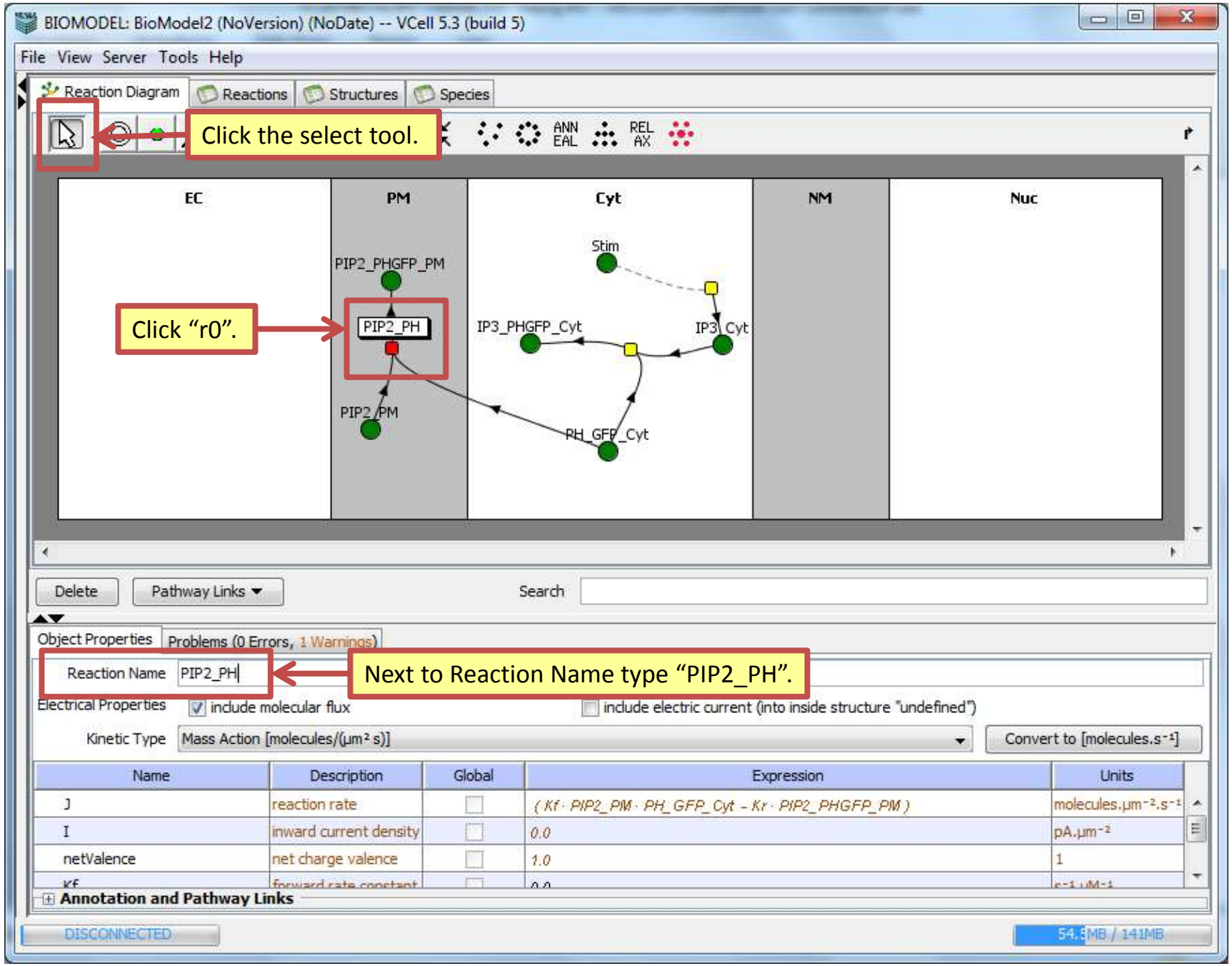
PIP_2 to IP_3 Conversion

Contents



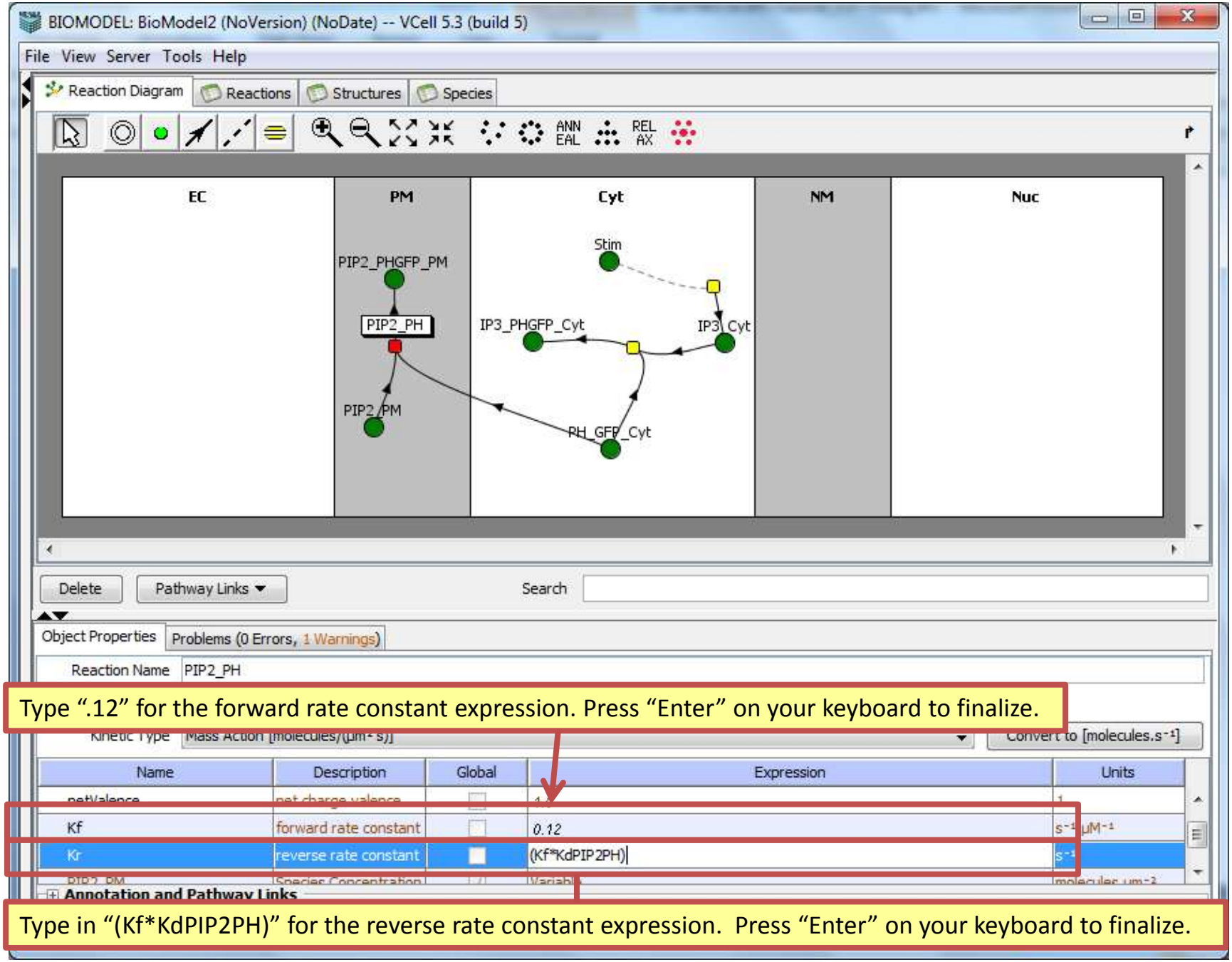
PIP_2 to IP_3 Conversion

Contents



PIP_2 to IP_3 Conversion

Contents

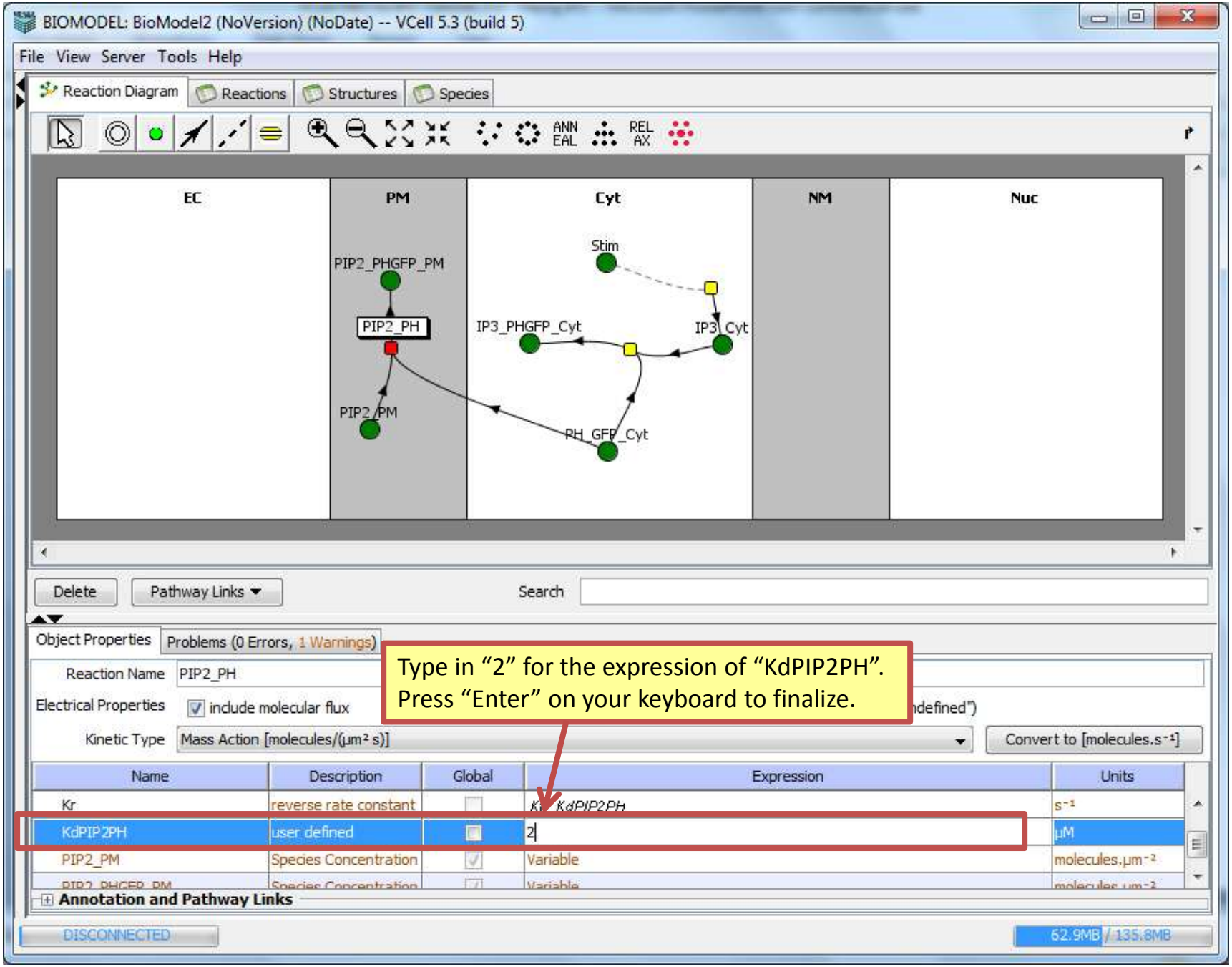


Type ".12" for the forward rate constant expression. Press "Enter" on your keyboard to finalize.

Type in "(Kf*KdPIP2PH)" for the reverse rate constant expression. Press "Enter" on your keyboard to finalize.

PIP_2 to IP_3 Conversion

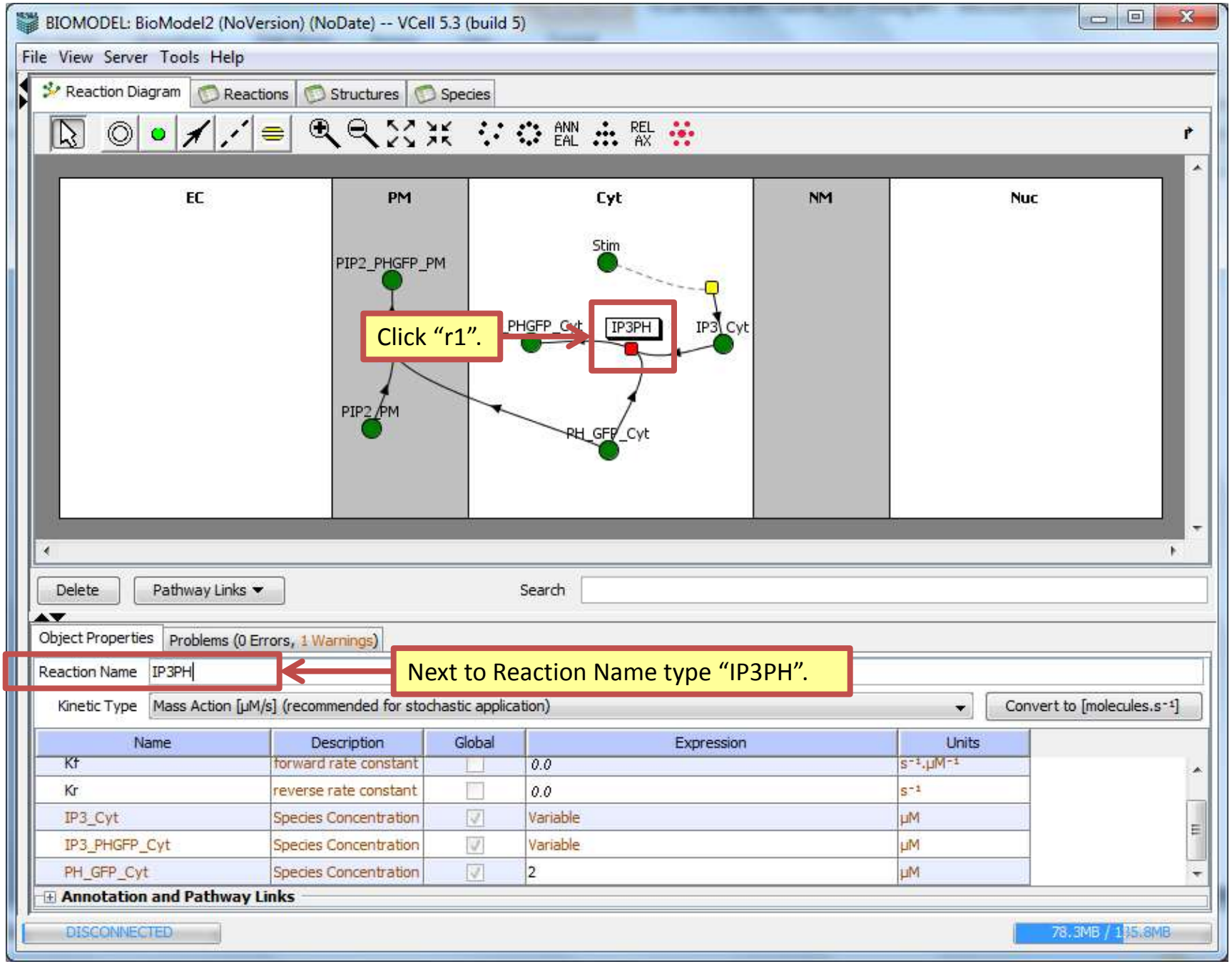
Contents



Type in “2” for the expression of “KdPIP2PH”.
Press “Enter” on your keyboard to finalize.

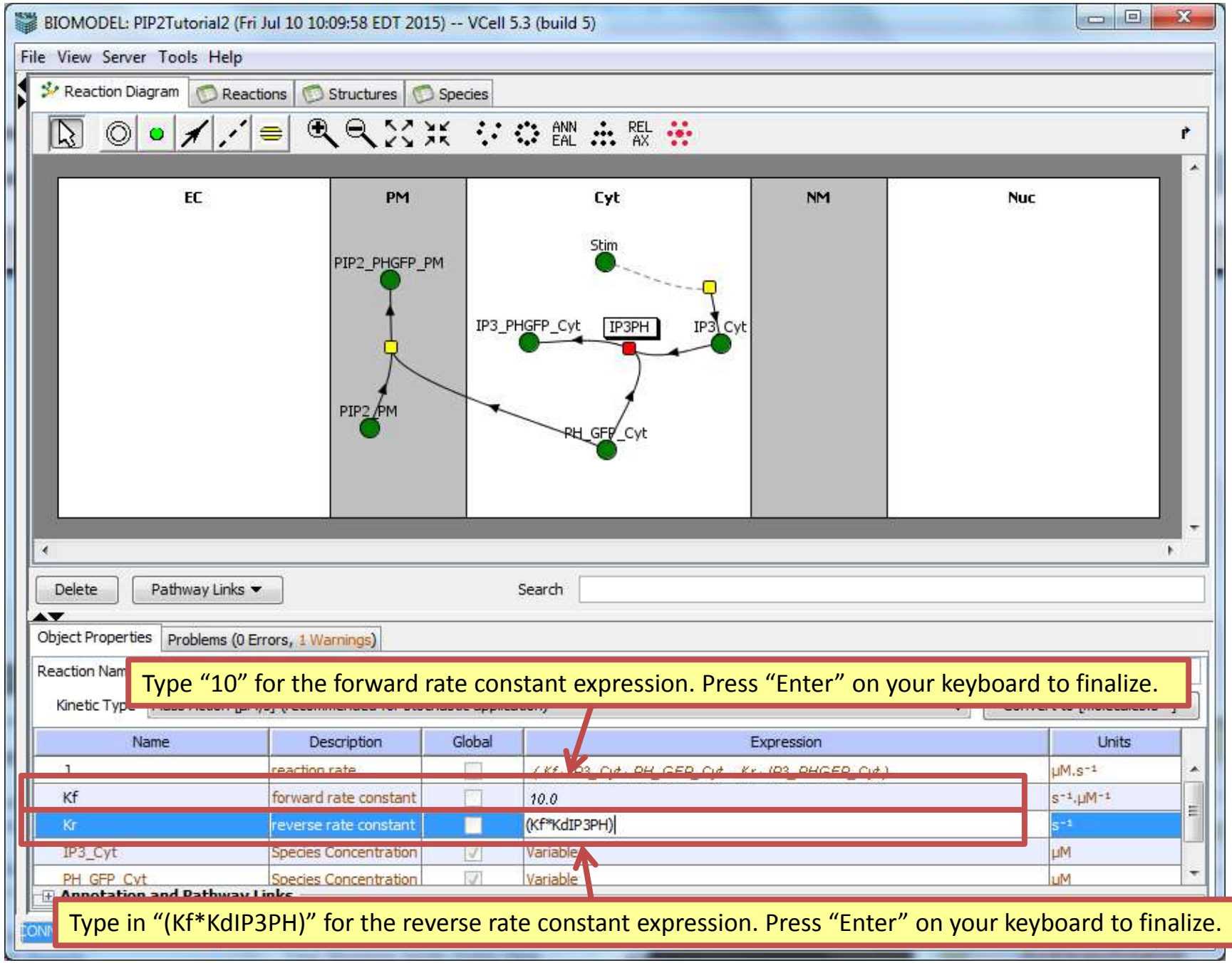
PIP_2 to IP_3 Conversion

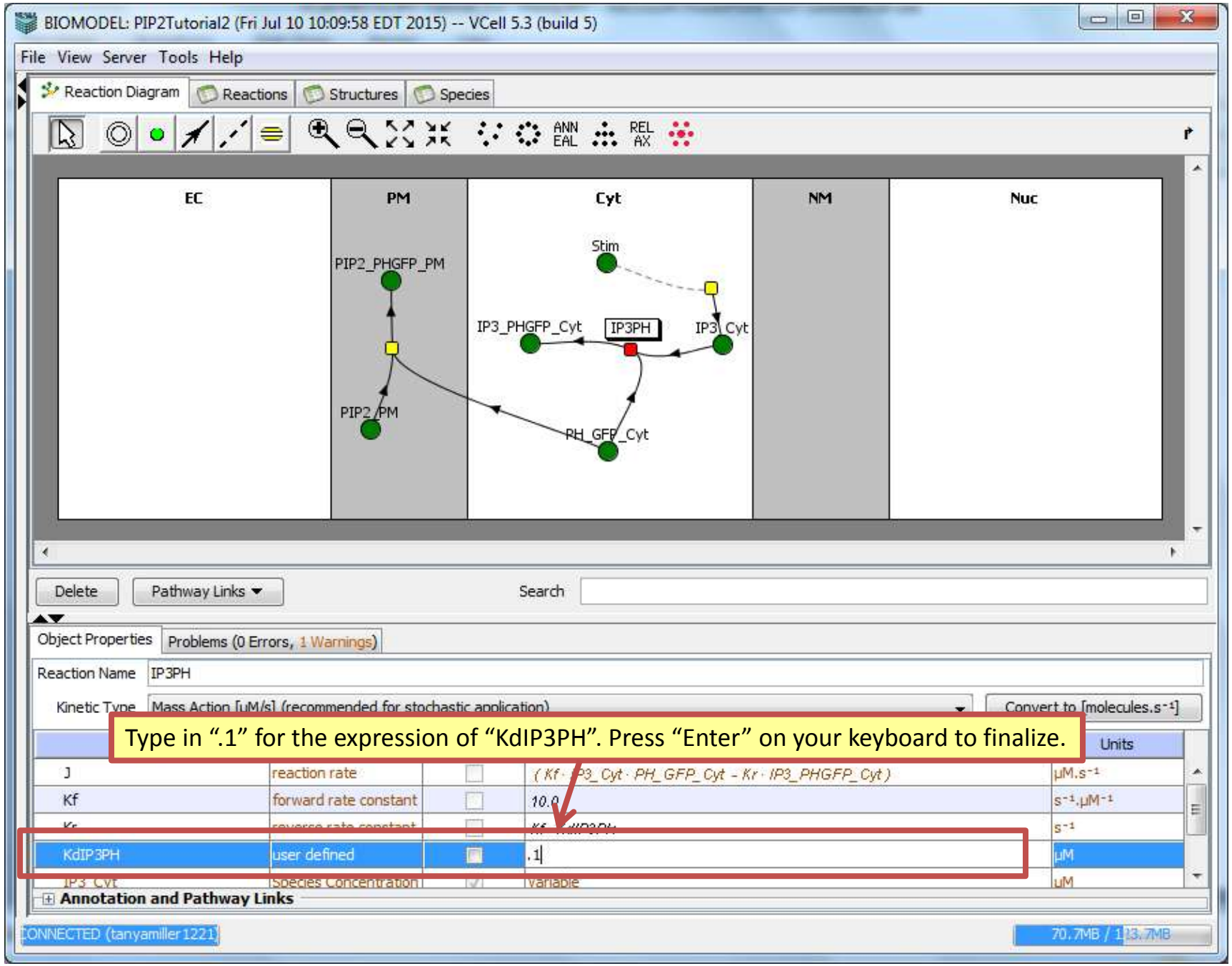
Contents



PIP_2 to IP_3 Conversion

Contents




BIOMODEL: PIP2Tutorial2 (Fri Jul 10 10:09:58 EDT 2015) -- VCell 5.3 (build 5)
File View Server Tools Help
Reaction Diagram
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Species
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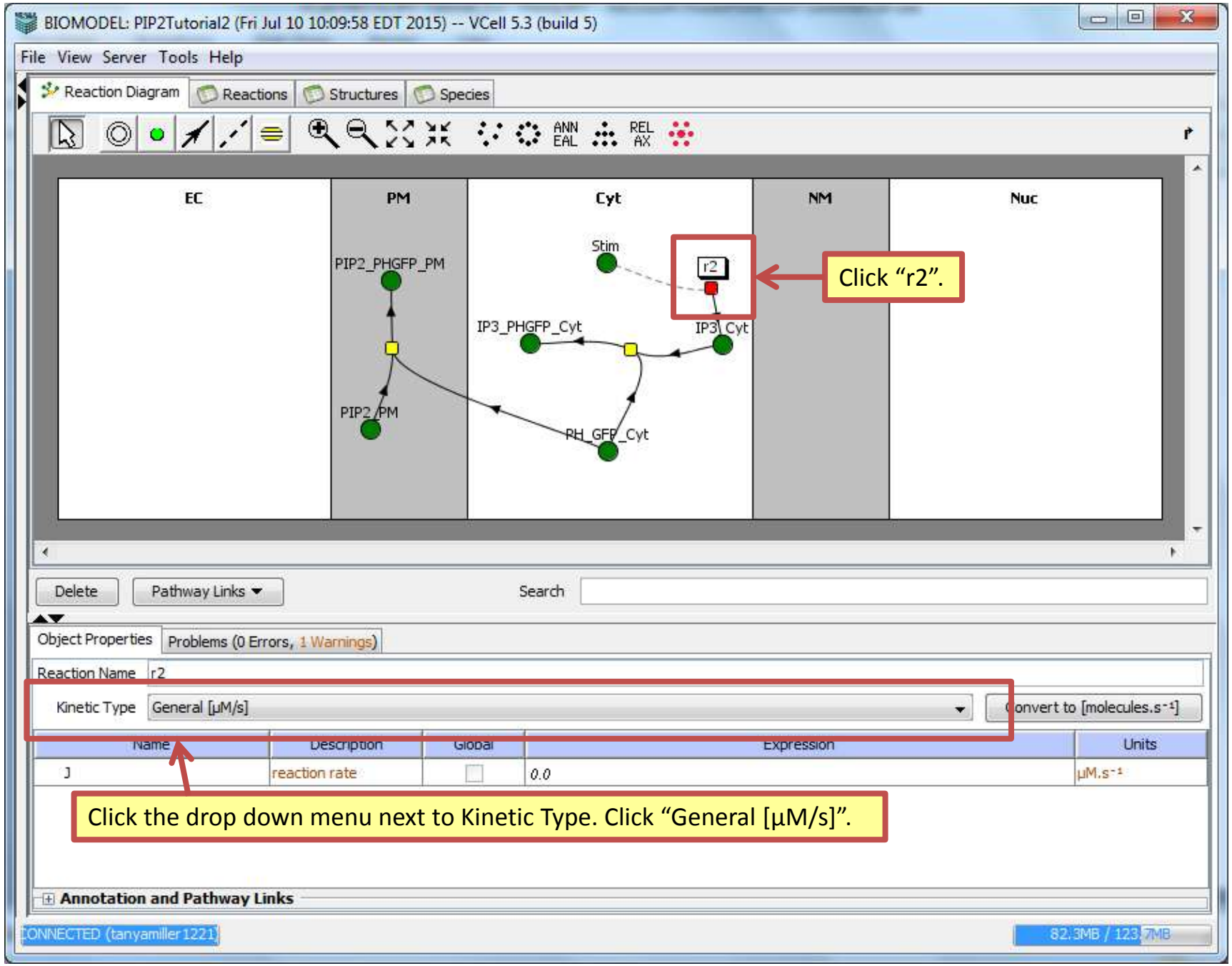
Nuc
Stim
PIP2_PHGFP_PM
IP3_PHGFP_Cyt
IP3PH
IP3_Cyt
PIP2_PM
PH_GFP_Cyt
Delete
Pathway Links
Search
Object Properties
Problems (0 Errors, 1 Warnings)
Reaction Name
IP3PH
Kinetic Type
Mass Action [uM/s] (recommended for stochastic application)
Convert to [molecules.s-1]
Type in ".1" for the expression of "KdIP3PH". Press "Enter" on your keyboard to finalize.
Units
J
reaction rate
(Kf · IP3_Cyt · PH_GFP_Cyt - Kr · IP3_PHGFP_Cyt)
µM.s-1
Kf
forward rate constant
10.0
s-1.µM-1
s-1
KdIP3PH
user defined
.1
µM
Species Concentration
Variable
uM
Annotation and Pathway Links
CONNECTED (tanyamiller1221)
70.7MB / 1


BIOMODEL: PIP2Tutorial2 (Fri Jul 10 10:09:58 EDT 2015) -- VCell 5.3 (build 5)
File View Server Tools Help
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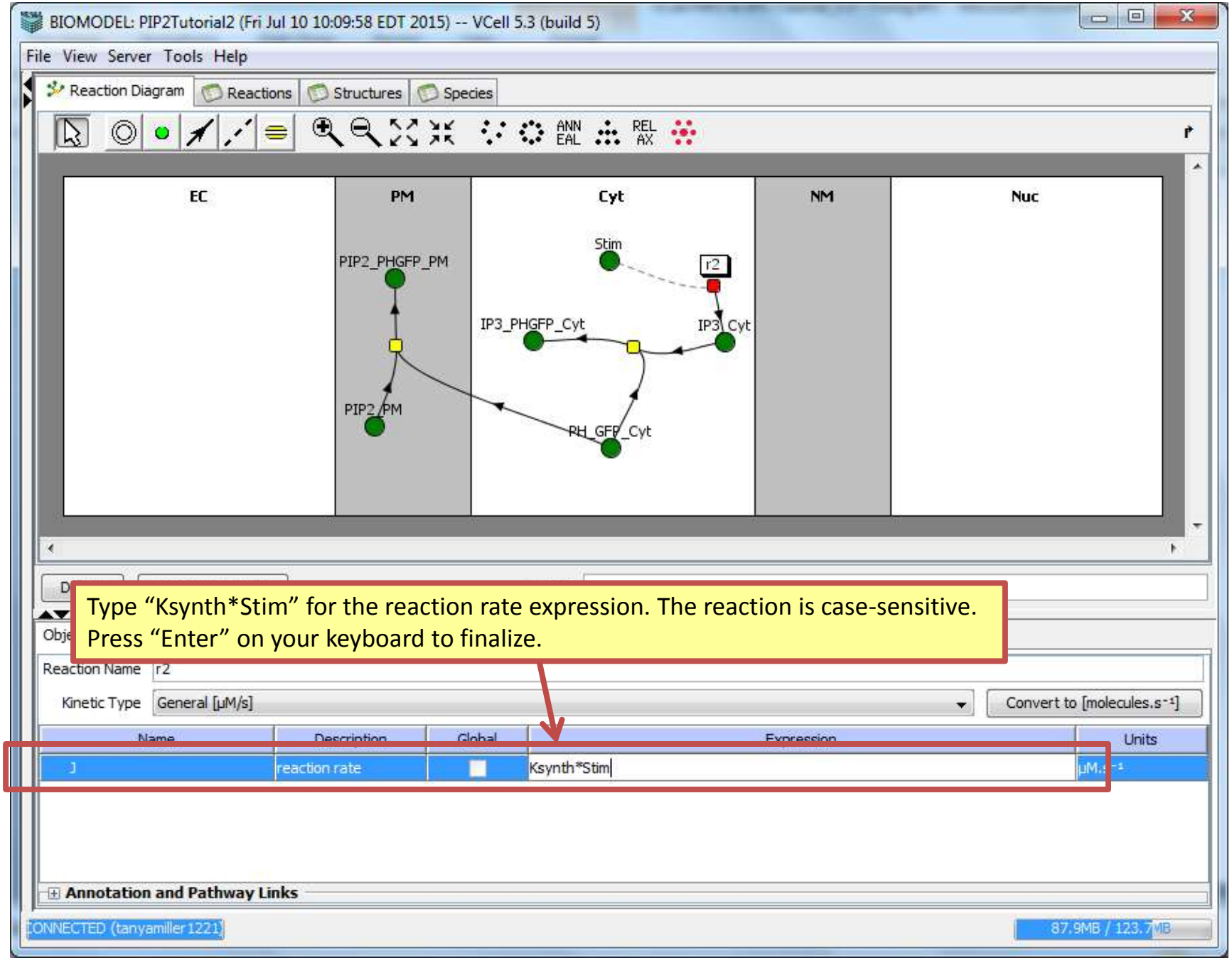
Nuc
Stim
r2
PIP2_PHGFP_PM
IP3_PHGFP_Cyt
IP3_Cyt
PIP2_PM
PH_GFP_Cyt
Click "r2".
Delete
Pathway Links
Search
Object Properties
Problems (0 Errors, 1 Warnings)
Reaction Name
r2
Kinetic Type
General [µM/s]
Convert to [molecules.s⁻¹]
Name
Description
Global
Expression
Units
J
reaction rate
0.0
µM.s⁻¹
Click the drop down menu next to Kinetic Type. Click "General [µM/s]".
Annotation and Pathway Links
CONNECTED (tanyamiller1221)
82.3MB / 123.7MB


BIOMODEL: PIP2Tutorial2 (Fri Jul 10 10:09:58 EDT 2015) -- VCell 5.3 (build 5)
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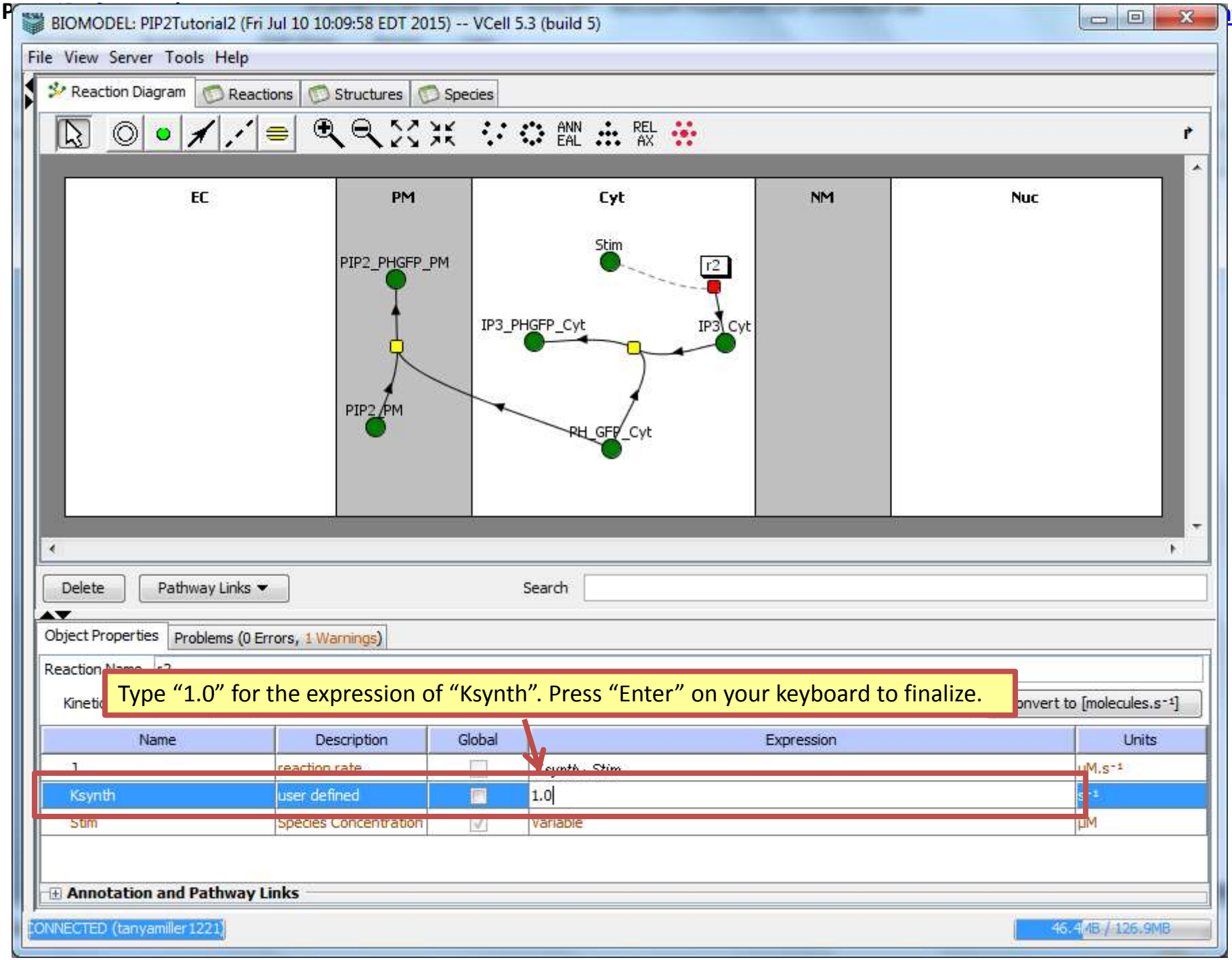
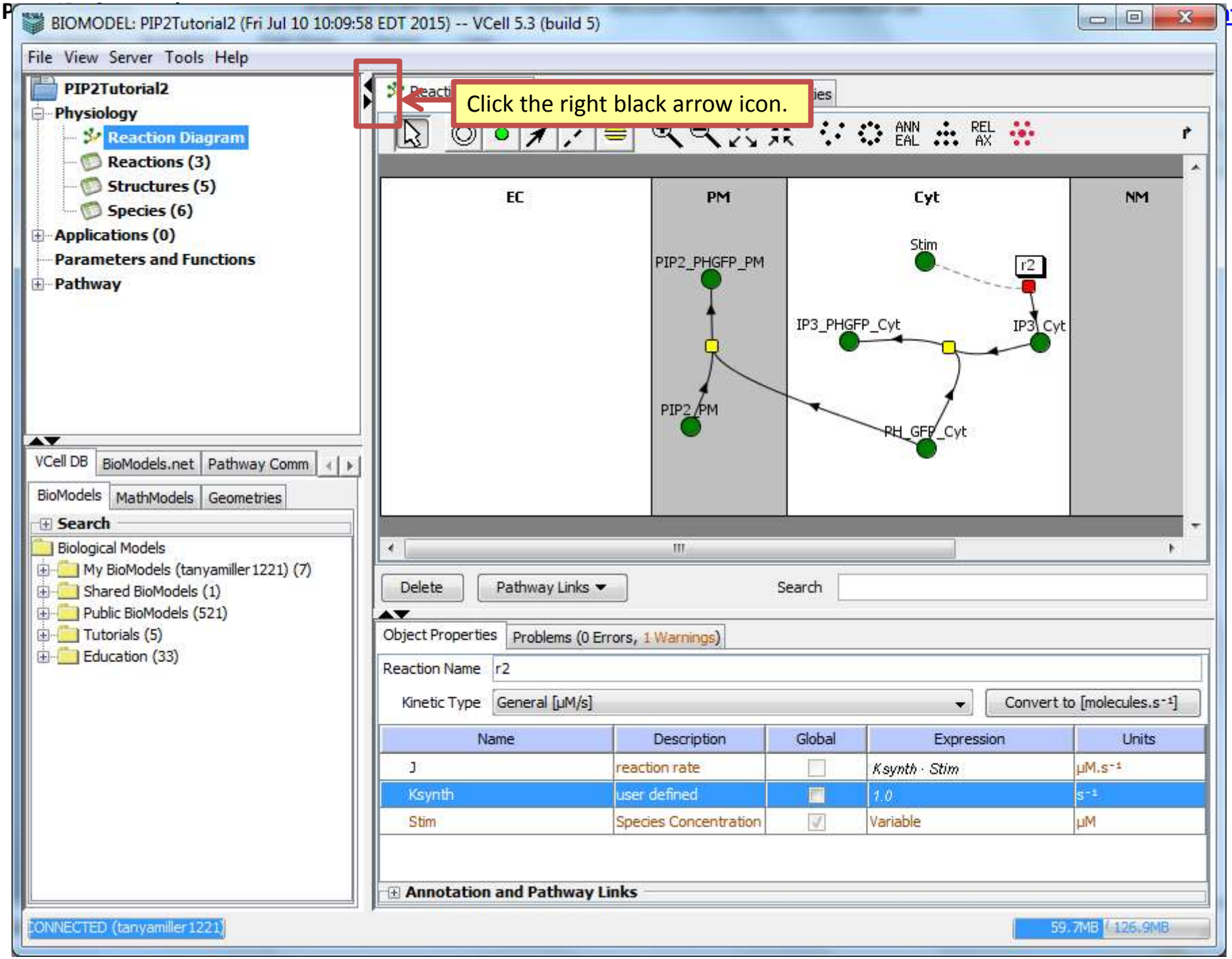
Cyt
NM
Nuc
Stim
r2
PIP2_PHGFP_PM
IP3_PHGFP_Cyt
IP3_Cyt
PIP2_PM
PH_GFP_Cyt
Type "Ksynth*Stim" for the reaction rate expression. The reaction is case-sensitive.
Press "Enter" on your keyboard to finalize.
Reaction Name
r2
Kinetic Type
General [µM/s]
Convert to [molecules.s⁻¹]
Name
Description
Global
Expression
Units
J
reaction rate
Ksynth*Stim
Annotation and Pathway Links
CONNECTED (tanyamiller1221)
87.9MB / 123.7MB



Type “1.0” for the expression of “Ksynth”. Press “Enter” on your keyboard to finalize.


BIOMODEL: PIP2Tutorial2 (Fri Jul 10 10:09:58 EDT 2015) -- VCell 5.3 (build 5)
File View Server Tools Help
PIP2Tutorial2
Physiology
Reaction Diagram
Reactions (3)
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Species (6)
Applications (0)
Parameters and Functions
Pathway
Click the right black arrow icon.
EC
PM
Cyt
NM
PIP2_PHGFP_PM
Stim
r2
IP3_PHGFP_Cyt
IP3_Cyt
PIP2_PM
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Public BioModels (521)
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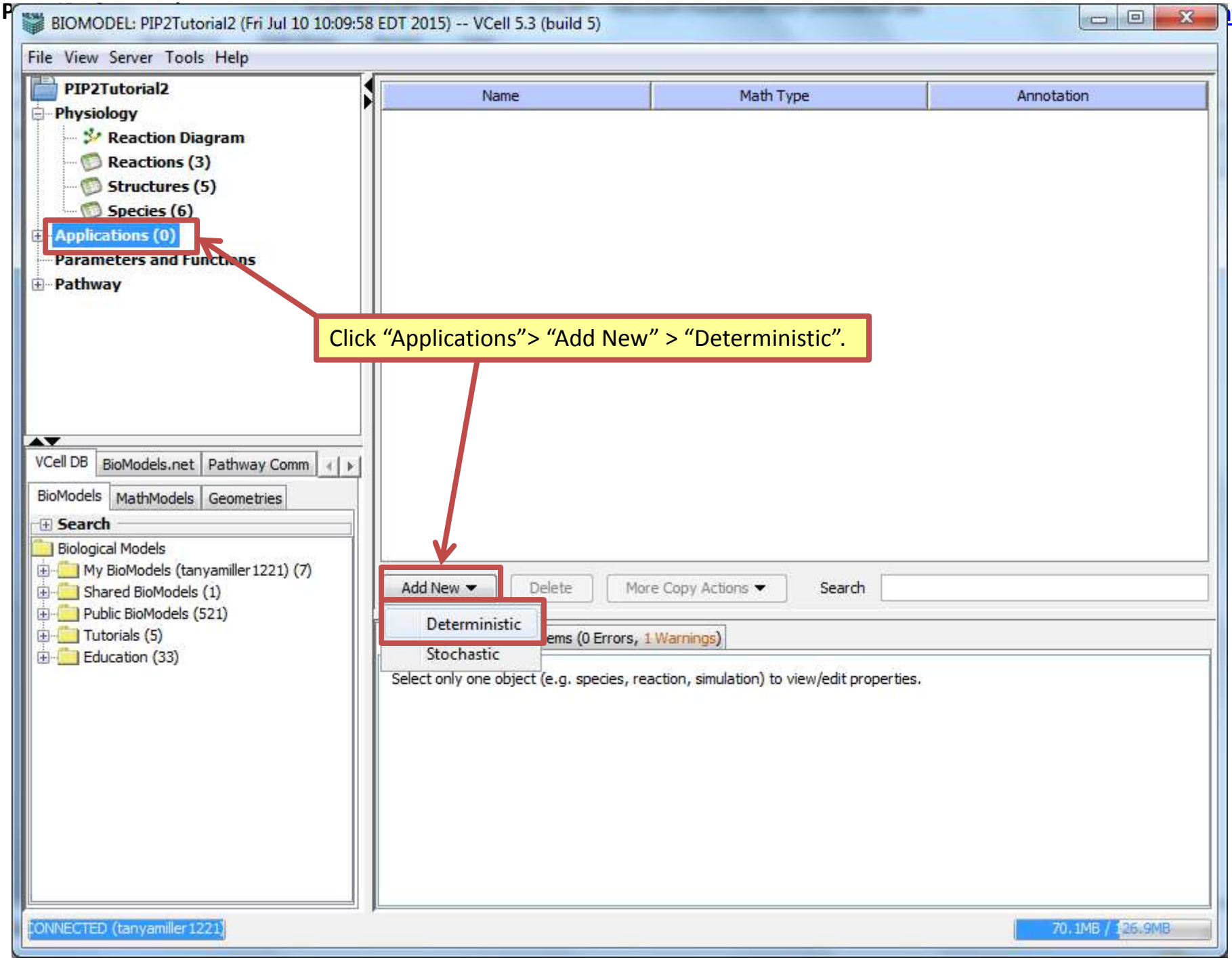
Education (33)
Delete
Pathway Links
Search
Object Properties
Problems (0 Errors, 1 Warnings)
Reaction Name
r2
Kinetic Type
General [µM/s]
Convert to [molecules.s-1]
Name
Description
Global
Expression
Units
J
reaction rate
Ksynth · Stim
µM.s-1
Ksynth
user defined
1.0
s-1
Stim
Species Concentration
Variable
µM
Annotation and Pathway Links
CONNECTED (tanyamiller1221)
59.7MB
126.9MB


BIOMODEL: PIP2Tutorial2 (Fri Jul 10 10:09:58 EDT 2015) -- VCell 5.3 (build 5)
File View Server Tools Help
PIP2Tutorial2
Physiology
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Name
Math Type
Annotation
Click “Applications”> “Add New” > “Deterministic”.
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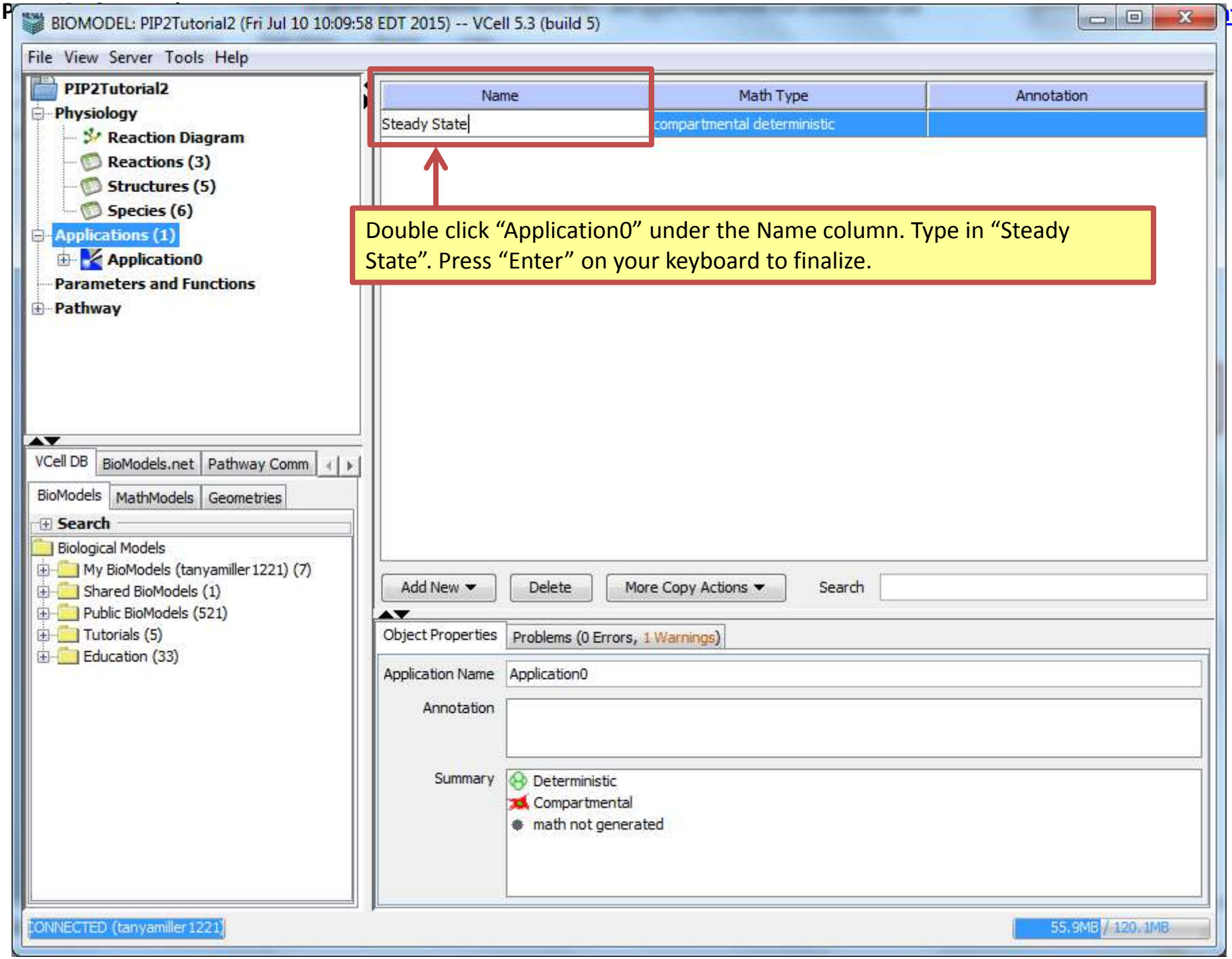
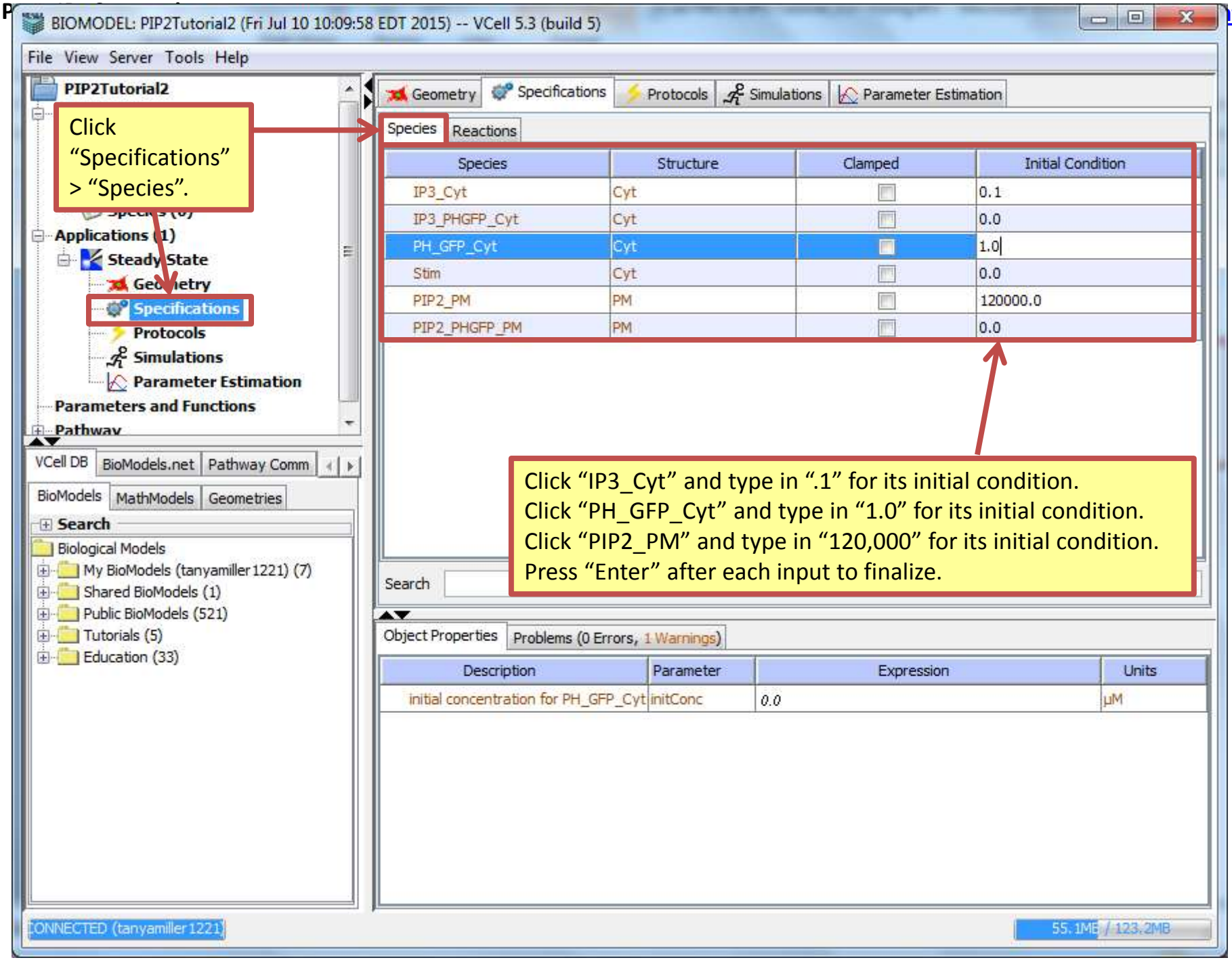
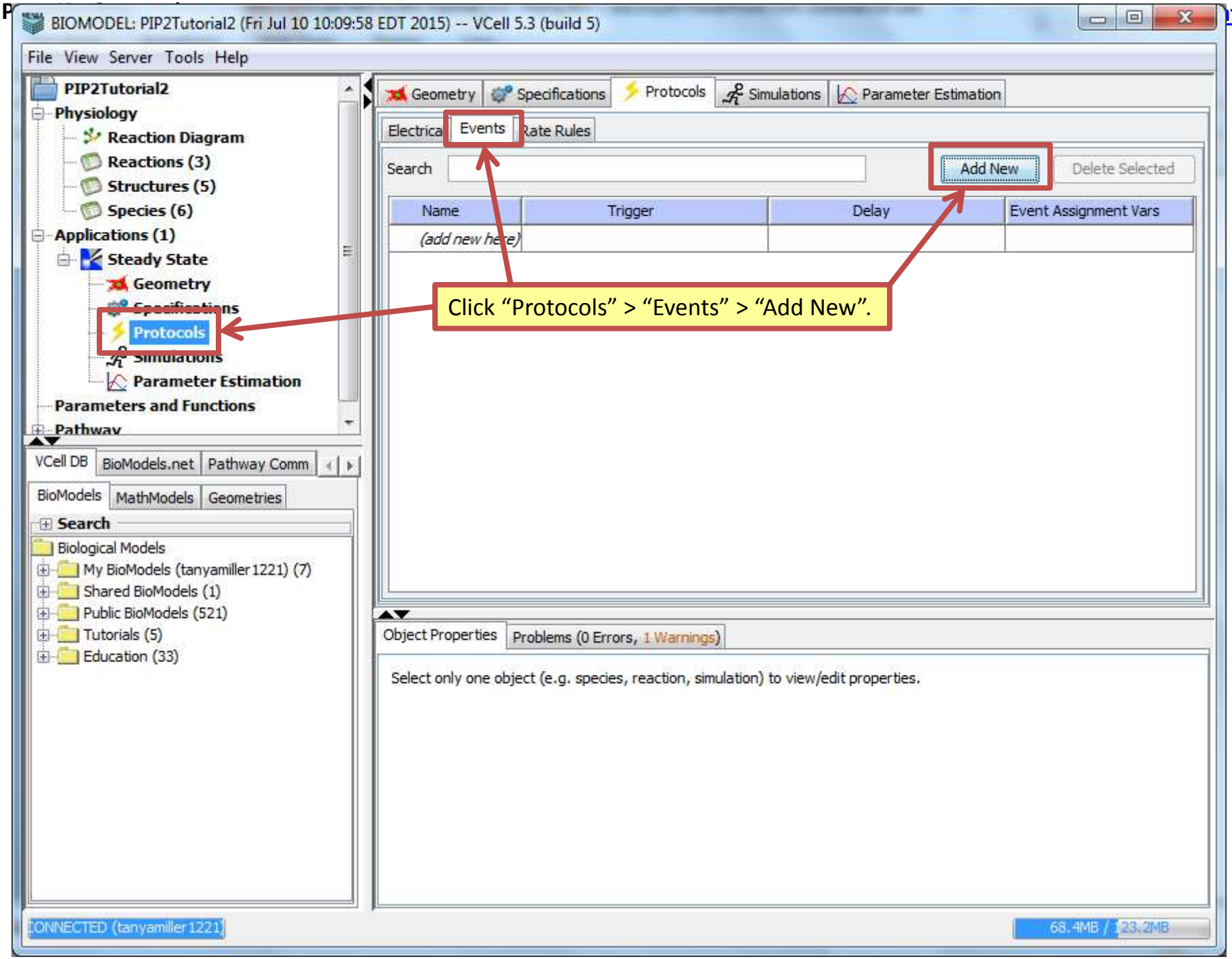
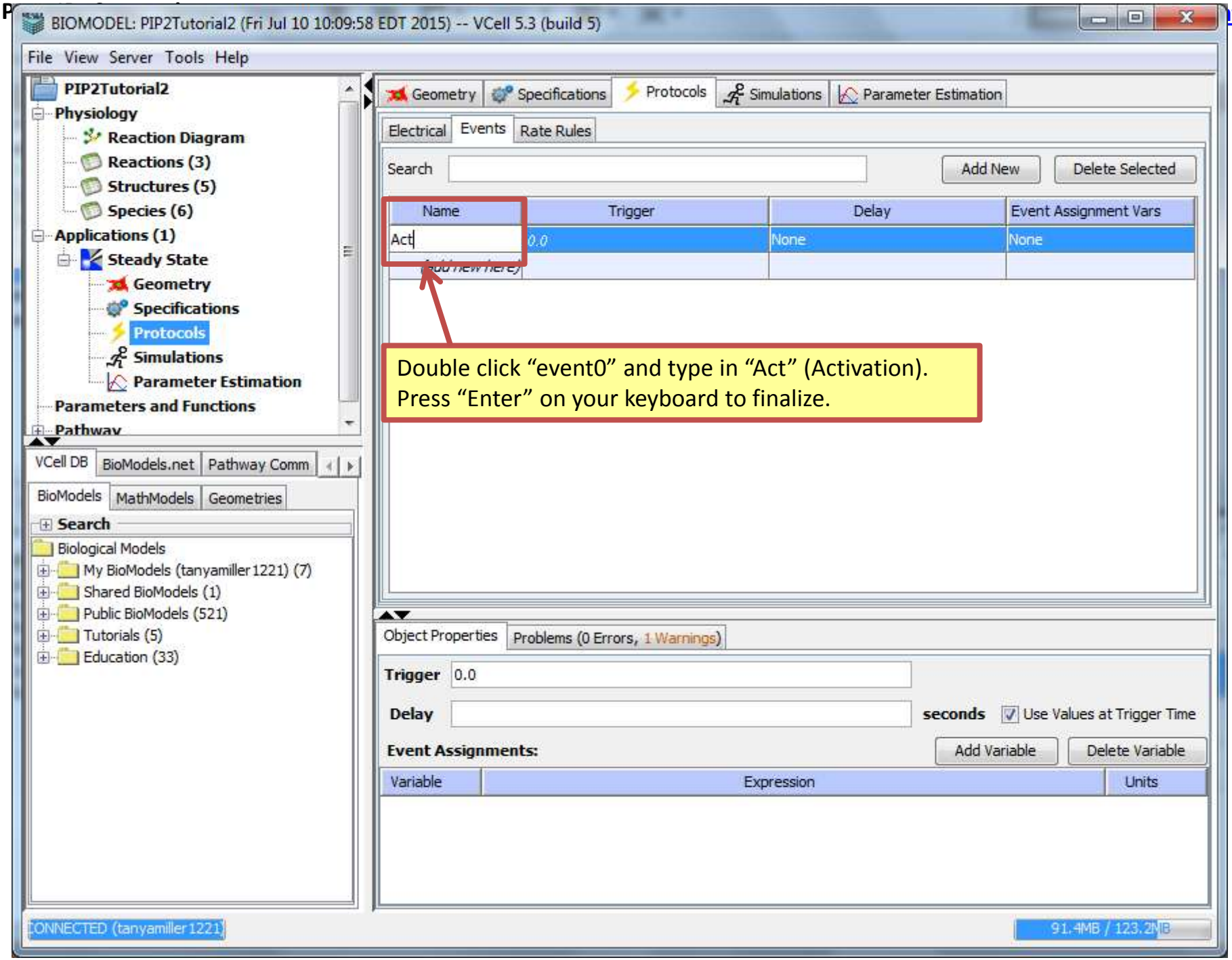
Public BioModels (521)
Tutorials (5)
Education (33)
Add New
Delete
More Copy Actions
Search
Deterministic
Stochastic
ems (0 Errors, 1 Warnings)
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (tanyamiller1221)
70.1MB / 126.9MB


BIOMODEL: PIP2Tutorial2 (Fri Jul 10 10:09:58 EDT 2015) -- VCell 5.3 (build 5)
File View Server Tools Help
PIP2Tutorial2
Physiology
Reaction Diagram
Reactions (3)
Structures (5)
Species (6)
Applications (1)
Application0
Parameters and Functions
Pathway
Name
Math Type
Annotation
Steady State
compartmental deterministic
Double click “Application0” under the Name column. Type in “Steady State”. Press “Enter” on your keyboard to finalize.
VCell DB
BioModels.net
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (tanyamiller1221) (7)
Shared BioModels (1)
Public BioModels (521)
Tutorials (5)
Education (33)
Add New
Delete
More Copy Actions
Search
Object Properties
Problems (0 Errors, 1 Warnings)
Application Name
Application0
Annotation
Summary
Deterministic
Compartmental
math not generated
CONNECTED (tanyamiller1221)
55.9MB / 120.1MB


BIOMODEL: PIP2Tutorial2 (Fri Jul 10 10:09:58 EDT 2015) -- VCell 5.3 (build 5)
File View Server Tools Help
PIP2Tutorial2
Applications (1)
Steady State
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Parameters and Functions
Pathway
Click "Specifications" > "Species".
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Species
Reactions
Species
Structure
Clamped
Initial Condition
IP3_Cyt
Cyt
0.1
IP3_PHGFP_Cyt
Cyt
0.0
PH_GFP_Cyt
Cyt
1.0
Stim
Cyt
0.0
PIP2_PM
PM
120000.0
PIP2_PHGFP_PM
PM
0.0
Click "IP3_Cyt" and type in ".1" for its initial condition.
Click "PH_GFP_Cyt" and type in "1.0" for its initial condition.
Click "PIP2_PM" and type in "120,000" for its initial condition.
Press "Enter" after each input to finalize.
Search
VCell DB
BioModels.net
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (tanyamiller1221) (7)
Shared BioModels (1)
Public BioModels (521)
Tutorials (5)
Education (33)
Object Properties
Problems (0 Errors, 1 Warnings)
Description
Parameter
Expression
Units
initial concentration for PH_GFP_Cyt
initConc
0.0
µM
CONNECTED (tanyamiller1221)
55.1MB / 123.2MB


BIOMODEL: PIP2Tutorial2 (Fri Jul 10 10:09:58 EDT 2015) -- VCell 5.3 (build 5)
File View Server Tools Help
PIP2Tutorial2
Physiology
Reaction Diagram
Reactions (3)
Structures (5)
Species (6)
Applications (1)
Steady State
Geometry
Protocols
Parameter Estimation
Parameters and Functions
Pathway
VCell DB
BioModels.net
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (tanyamiller1221) (7)
Shared BioModels (1)
Public BioModels (521)
Tutorials (5)
Education (33)
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Electrica
Events
Rate Rules
Search
Add New
Delete Selected
Name
Trigger
Delay
Event Assignment Vars
(add new here)
Click “Protocols” > “Events” > “Add New”.
Object Properties
Problems (0 Errors, 1 Warnings)
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (tanyamiller1221)
68.4MB / 123.2MB


BIOMODEL: PIP2Tutorial2 (Fri Jul 10 10:09:58 EDT 2015) -- VCell 5.3 (build 5)
File View Server Tools Help
PIP2Tutorial2
Physiology
Reaction Diagram
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Applications (1)
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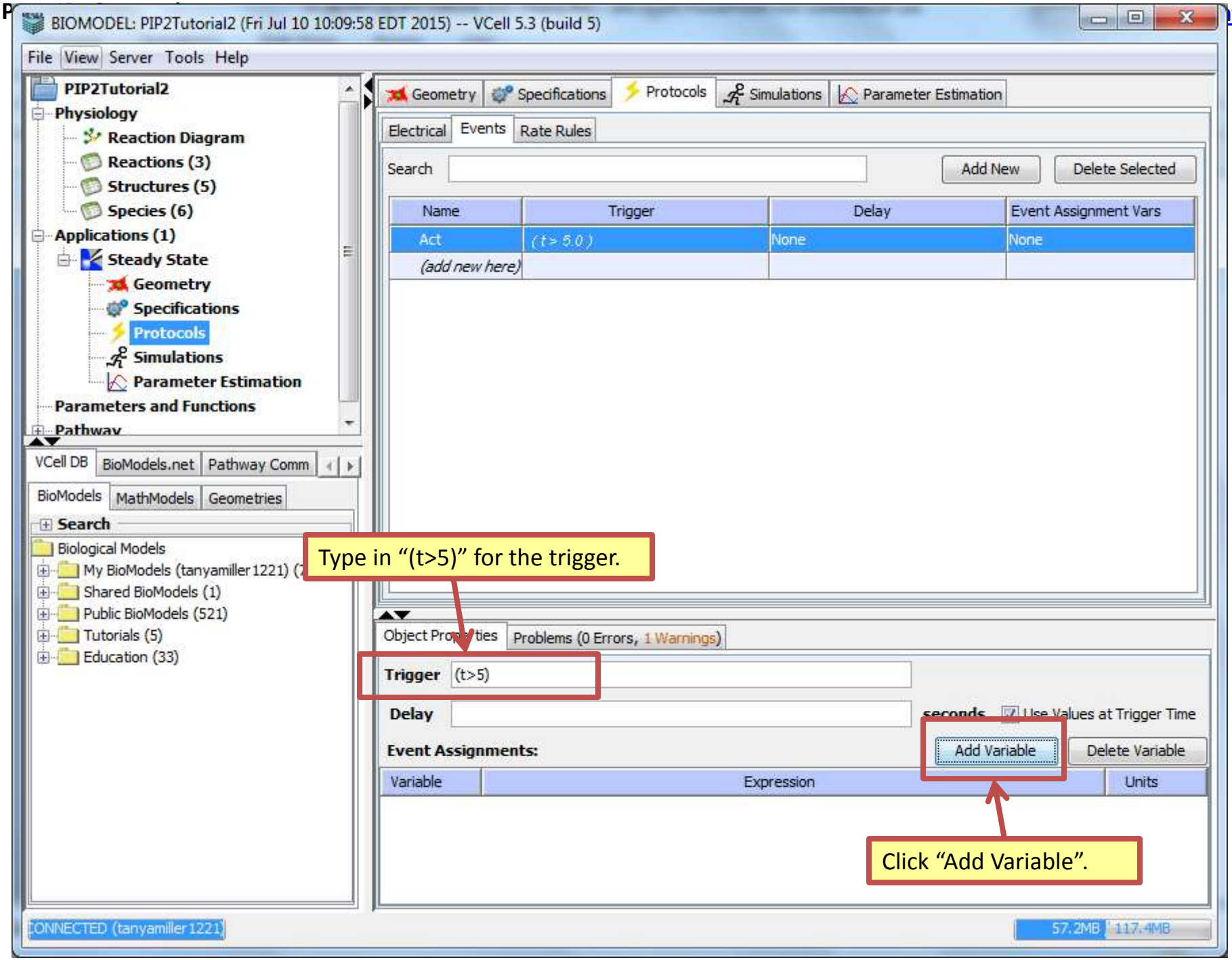
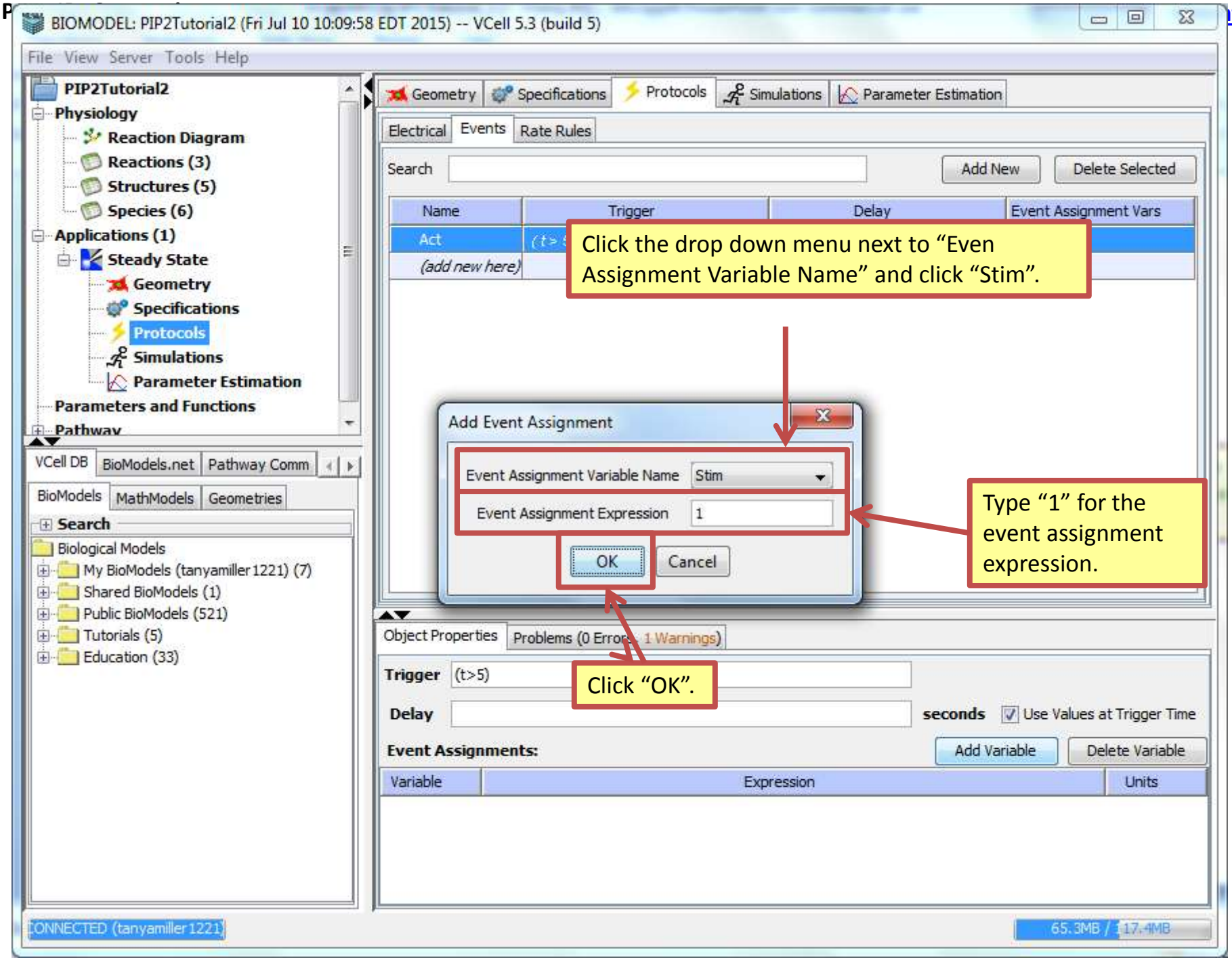
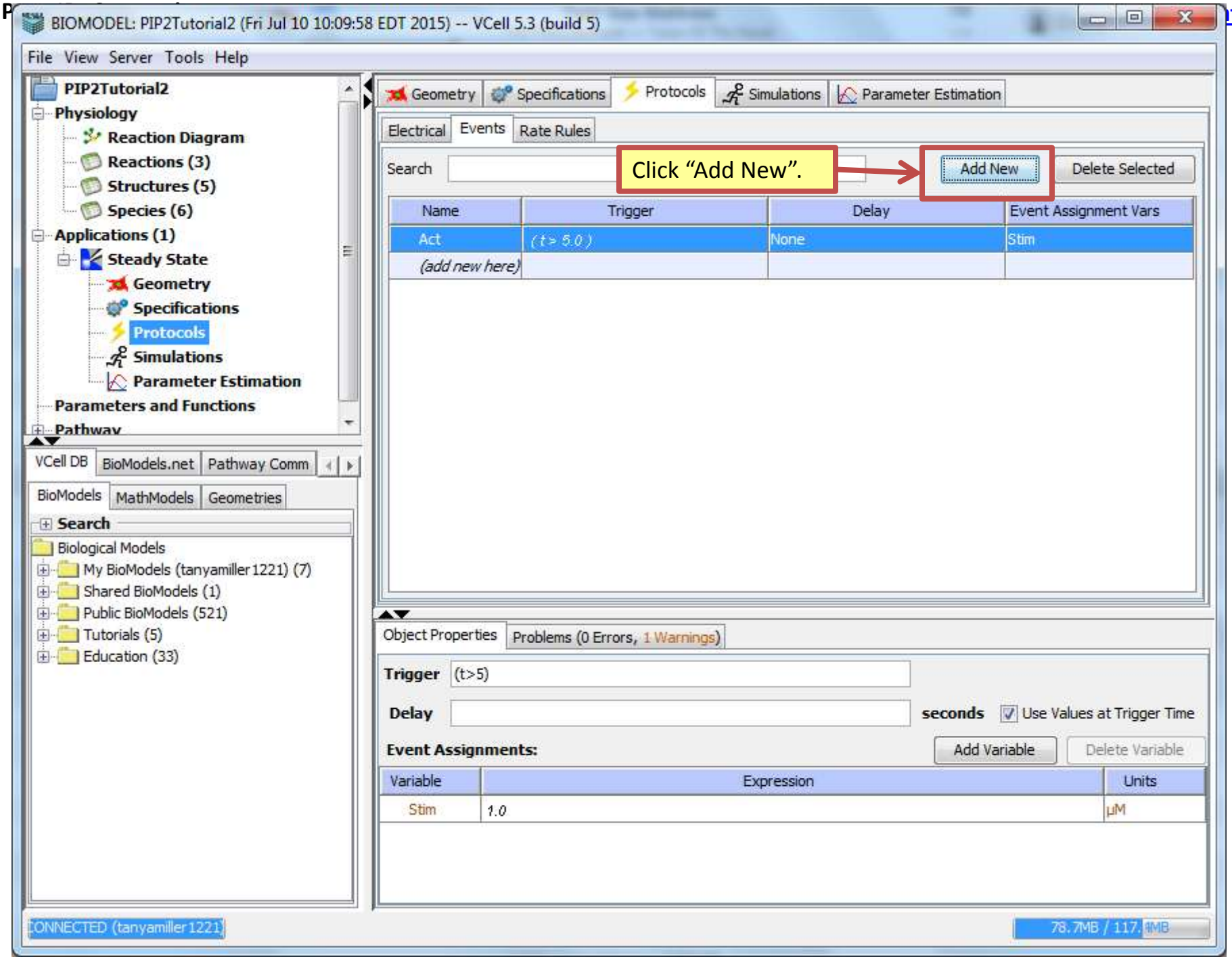
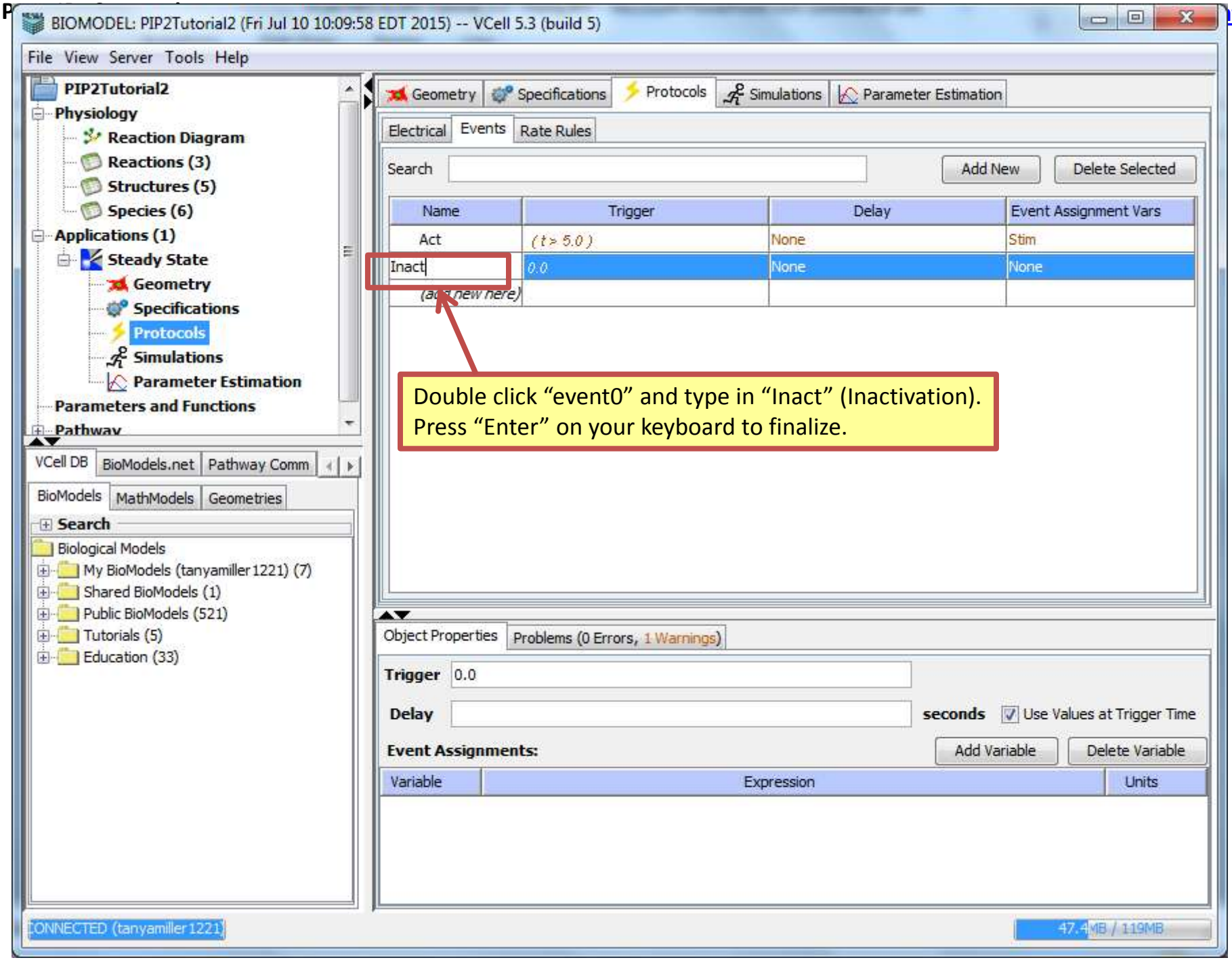
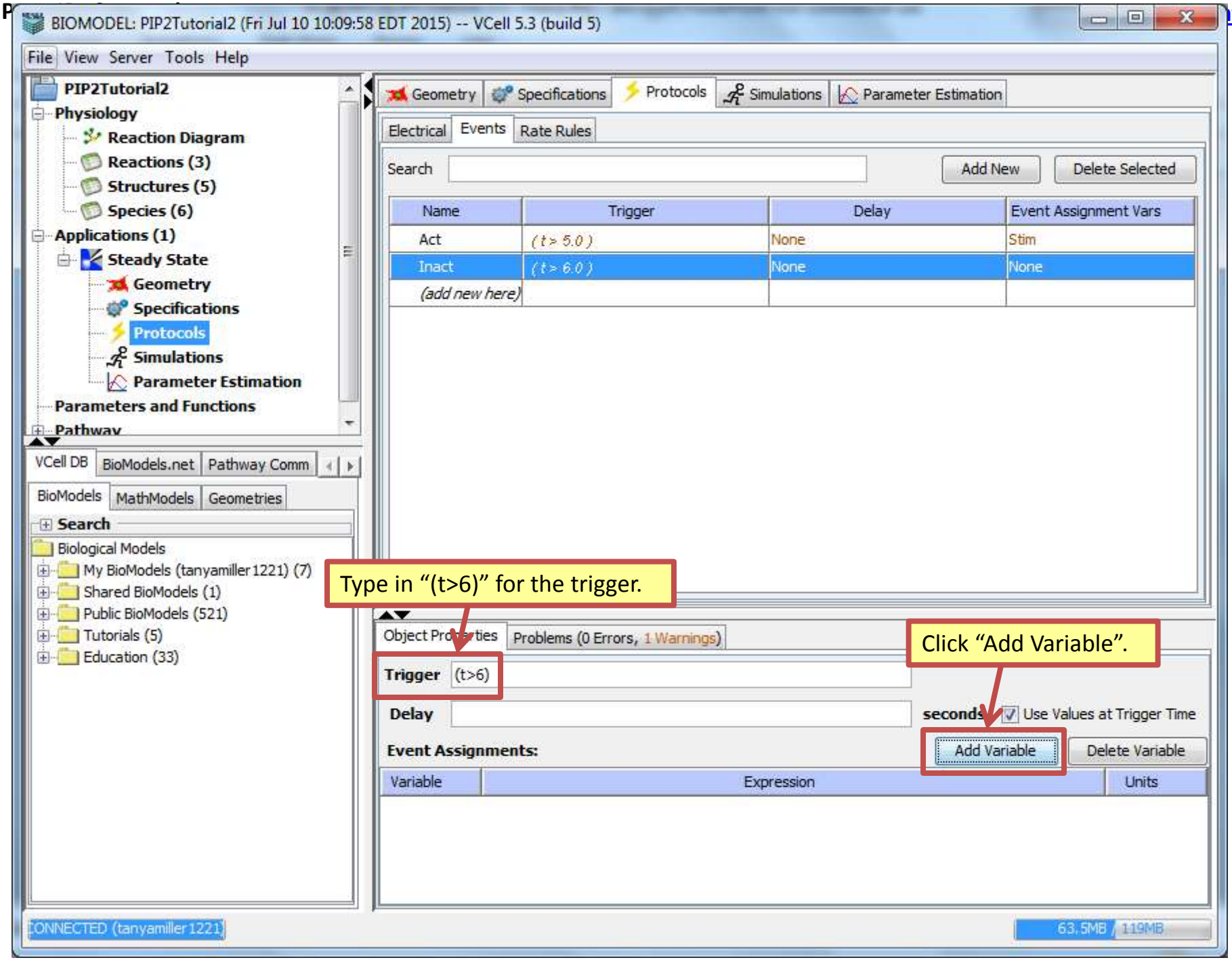
Simulations
Parameter Estimation
Parameters and Functions
Pathway
VCell DB
BioModels.net
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (tanyamiller1221) (7)
Shared BioModels (1)
Public BioModels (521)
Tutorials (5)
Education (33)
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Electrical
Events
Rate Rules
Search
Add New
Delete Selected
Name
Trigger
Delay
Event Assignment Vars
Act
0.0
None
None
Double click “event0” and type in “Act” (Activation).
Press “Enter” on your keyboard to finalize.
Object Properties
Problems (0 Errors, 1 Warnings)
Trigger
0.0
Delay
seconds
Use Values at Trigger Time
Event Assignments:
Add Variable
Delete Variable
Variable
Expression
Units
CONNECTED (tanyamiller1221)
91.4MB / 123.2MB

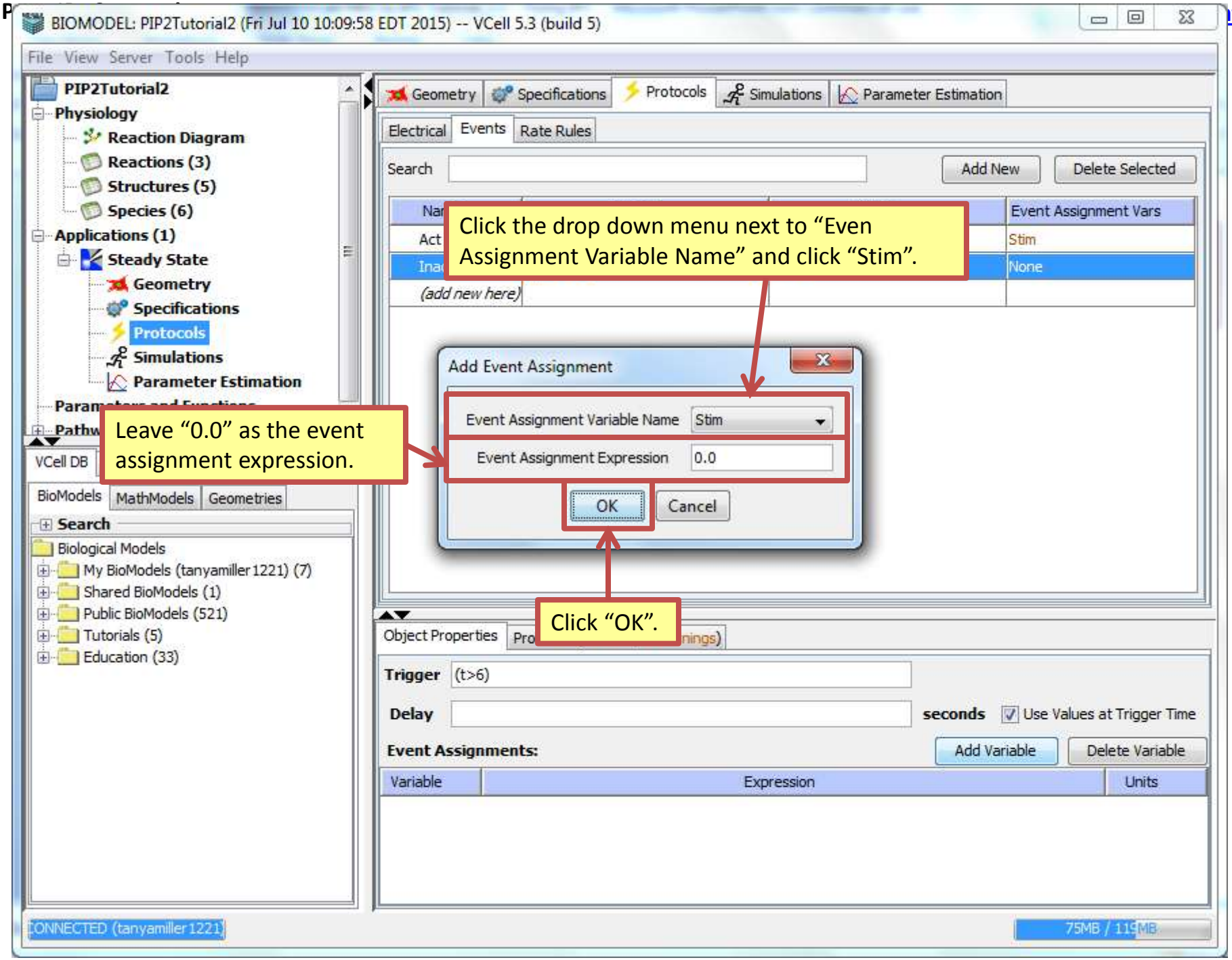

BIOMODEL: PIP2Tutorial2 (Fri Jul 10 10:09:58 EDT 2015) -- VCell 5.3 (build 5)
File View Server Tools Help
PIP2Tutorial2
Physiology
Reaction Diagram
Reactions (3)
Structures (5)
Species (6)
Applications (1)
Steady State
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Parameters and Functions
Pathway
VCell DB
BioModels.net
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (tanyamiller1221)
Shared BioModels (1)
Public BioModels (521)
Tutorials (5)
Education (33)
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Electrical
Events
Rate Rules
Search
Add New
Delete Selected
Name
Trigger
Delay
Event Assignment Vars
Act
(t > 5.0)
None
None
(add new here)
Type in "(t>5)" for the trigger.
Object Properties
Problems (0 Errors, 1 Warnings)
Trigger
(t>5)
Delay
seconds
Use Values at Trigger Time
Event Assignments:
Add Variable
Delete Variable
Variable
Expression
Units
Click "Add Variable".
CONNECTED (tanyamiller1221)
57.2MB
117.4MB

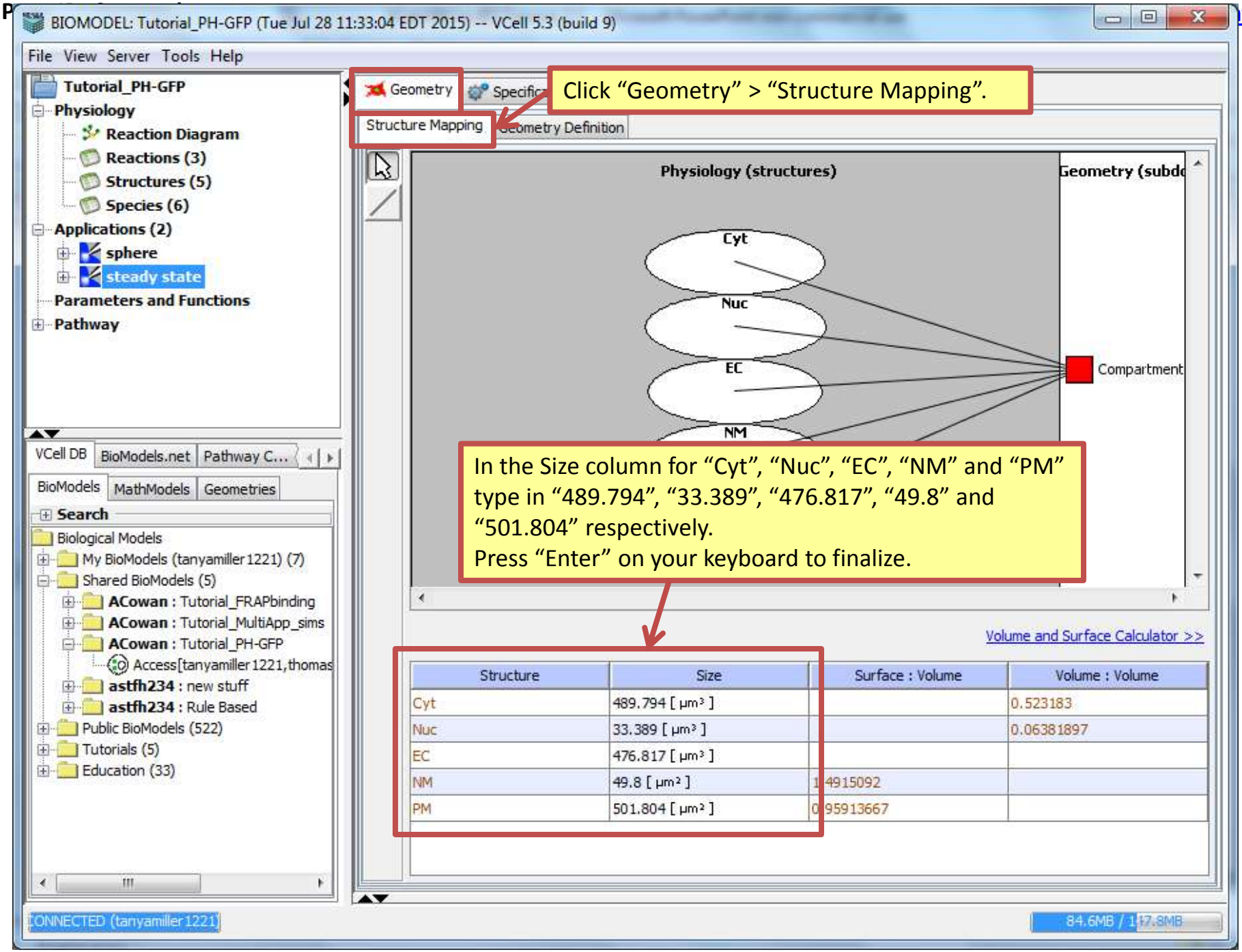

BIOMODEL: PIP2Tutorial2 (Fri Jul 10 10:09:58 EDT 2015) -- VCell 5.3 (build 5)
File View Server Tools Help
PIP2Tutorial2
Physiology
Reaction Diagram
Reactions (3)
Structures (5)
Species (6)
Applications (1)
Steady State
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Parameters and Functions
Pathway
VCell DB
BioModels.net
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (tanyamiller1221) (7)
Shared BioModels (1)
Public BioModels (521)
Tutorials (5)
Education (33)
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Electrical
Events
Rate Rules
Search
Add New
Delete Selected
Name
Trigger
Delay
Event Assignment Vars
Act
(add new here)
Click the drop down menu next to “Even Assignment Variable Name” and click “Stim”.
Add Event Assignment
Event Assignment Variable Name
Stim
Event Assignment Expression
1
OK
Cancel
Type “1” for the event assignment expression.
Click “OK”.
Object Properties
Problems (0 Errors, 1 Warnings)
Trigger
(t>5)
Delay
seconds
Use Values at Trigger Time
Event Assignments:
Add Variable
Delete Variable
Variable
Expression
Units
CONNECTED (tanyamiller1221)
65.3MB / 17.4MB

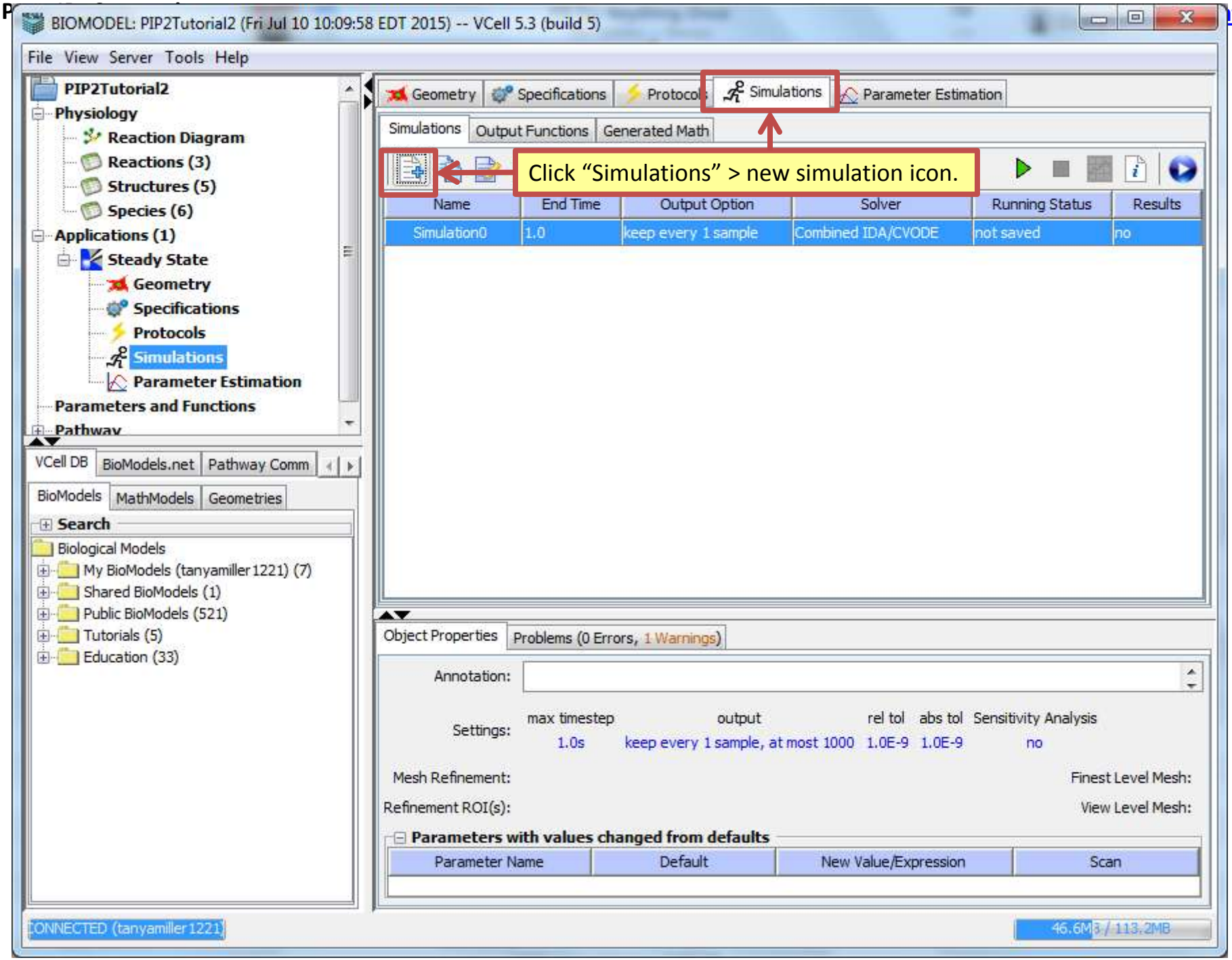

BIOMODEL: PIP2Tutorial2 (Fri Jul 10 10:09:58 EDT 2015) -- VCell 5.3 (build 5)
File View Server Tools Help
PIP2Tutorial2
Physiology
Reaction Diagram
Reactions (3)
Structures (5)
Species (6)
Applications (1)
Steady State
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Parameters and Functions
Pathway
VCell DB
BioModels.net
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (tanyamiller1221) (7)
Shared BioModels (1)
Public BioModels (521)
Tutorials (5)
Education (33)
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Electrical
Events
Rate Rules
Search
Click “Add New”.
Add New
Delete Selected
Name
Trigger
Delay
Event Assignment Vars
Act
(t > 5.0)
None
Stim
(add new here)
Object Properties
Problems (0 Errors, 1 Warnings)
Trigger
(t>5)
Delay
seconds
Use Values at Trigger Time
Event Assignments:
Add Variable
Delete Variable
Variable
Expression
Units
Stim
1.0
µM
CONNECTED (tanyamiller1221)
78.7MB / 117.4MB

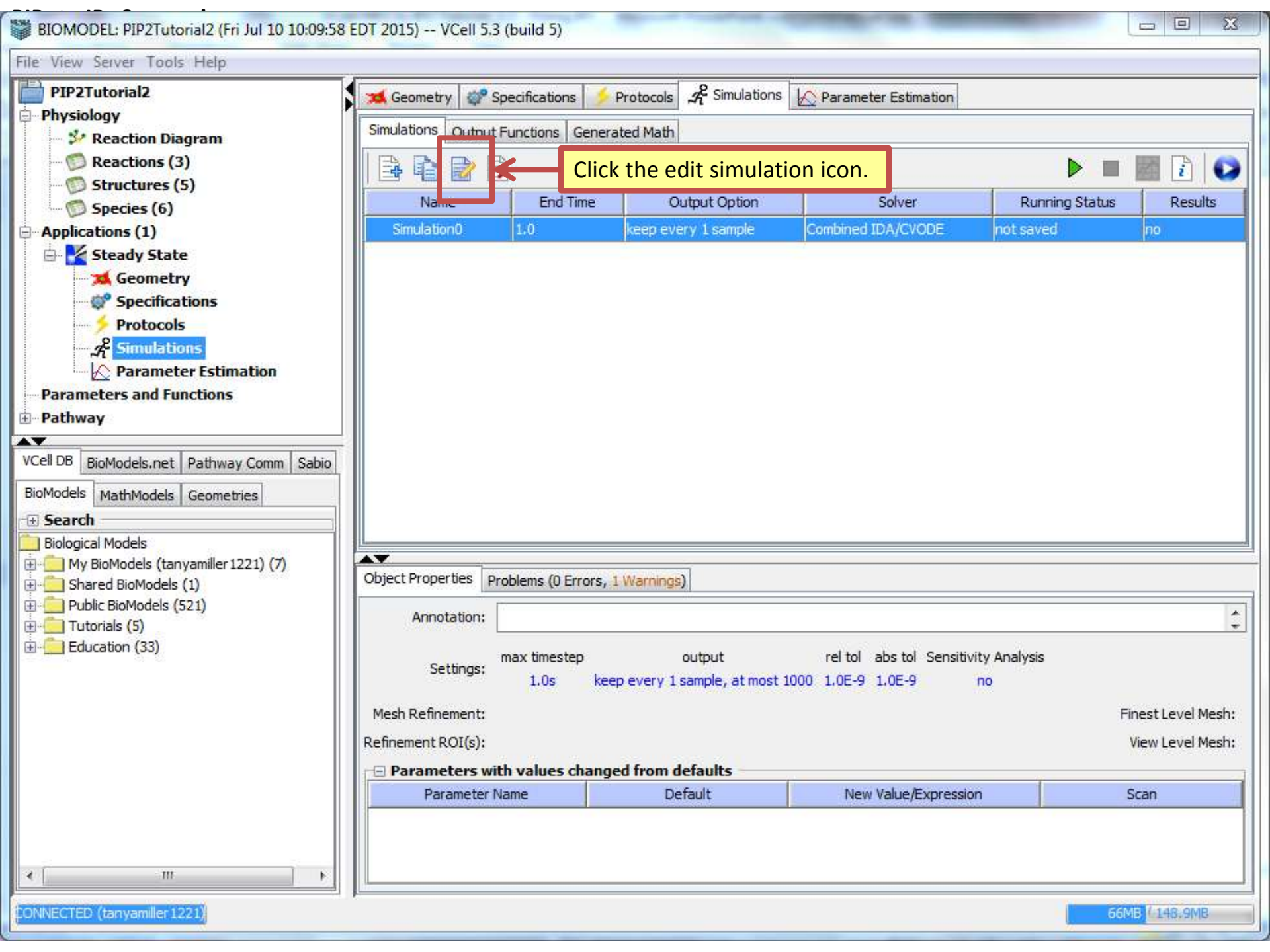

BIOMODEL: PIP2Tutorial2 (Fri Jul 10 10:09:58 EDT 2015) -- VCell 5.3 (build 5)
File View Server Tools Help
PIP2Tutorial2
Physiology
Reaction Diagram
Reactions (3)
Structures (5)
Species (6)
Applications (1)
Steady State
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Parameters and Functions
Pathway
Geometry Specifications Protocols Simulations Parameter Estimation
Electrical Events Rate Rules
Search
Add New
Delete Selected
Name Trigger Delay Event Assignment Vars
Act (t > 5.0) None Stim
Inact 0.0 None None
(add new here)
Double click “event0” and type in “Inact” (Inactivation).
Press “Enter” on your keyboard to finalize.
VCell DB BioModels.net Pathway Comm
BioModels MathModels Geometries
Search
Biological Models
My BioModels (tanyamiller1221) (7)
Shared BioModels (1)
Public BioModels (521)
Tutorials (5)
Education (33)
Object Properties
Problems (0 Errors, 1 Warnings)
Trigger 0.0
Delay
seconds
Use Values at Trigger Time
Event Assignments:
Add Variable
Delete Variable
Variable Expression Units
CONNECTED (tanyamiller1221)
47.4MB / 119MB


BIOMODEL: PIP2Tutorial2 (Fri Jul 10 10:09:58 EDT 2015) -- VCell 5.3 (build 5)
File View Server Tools Help
PIP2Tutorial2
Physiology
Reaction Diagram
Reactions (3)
Structures (5)
Species (6)
Applications (1)
Steady State
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Parameters and Functions
Pathway
VCell DB
BioModels.net
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (tanyamiller1221) (7)
Shared BioModels (1)
Public BioModels (521)
Tutorials (5)
Education (33)
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Electrical
Events
Rate Rules
Search
Add New
Delete Selected
Name
Trigger
Delay
Event Assignment Vars
Act
(t > 5.0)
None
Stim
Inact
(t > 6.0)
None
None
(add new here)
Type in "(t>6)" for the trigger.
Object Properties
Problems (0 Errors, 1 Warnings)
Click "Add Variable".
Trigger
(t>6)
Delay
seconds
Use Values at Trigger Time
Event Assignments:
Add Variable
Delete Variable
Variable
Expression
Units
CONNECTED (tanyamiller1221)
63.5MB / 119MB


BIOMODEL: PIP2Tutorial2 (Fri Jul 10 10:09:58 EDT 2015) -- VCell 5.3 (build 5)
File View Server Tools Help
PIP2Tutorial2
Physiology
Reaction Diagram
Reactions (3)
Structures (5)
Species (6)
Applications (1)
Steady State
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Geometry Specifications Protocols Simulations Parameter Estimation
Electrical Events Rate Rules
Search
Add New
Delete Selected
Event Assignment Vars
Stim
None
(add new here)
Click the drop down menu next to “Even Assignment Variable Name” and click “Stim”.
Add Event Assignment
Event Assignment Variable Name
Stim
Event Assignment Expression
0.0
OK
Cancel
Leave “0.0” as the event assignment expression.
Click “OK”.
VCell DB
BioModels MathModels Geometries
Search
Biological Models
My BioModels (tanyamiller1221) (7)
Shared BioModels (1)
Public BioModels (521)
Tutorials (5)
Education (33)
Object Properties
Trigger
(t>6)
Delay
seconds
Use Values at Trigger Time
Event Assignments:
Add Variable
Delete Variable
Variable
Expression
Units
CONNECTED (tanyamiller1221)
75MB / 119MB


BIOMODEL: Tutorial_PH-GFP (Tue Jul 28 11:33:04 EDT 2015) -- VCell 5.3 (build 9)
File View Server Tools Help
Tutorial_PH-GFP
Physiology
Reaction Diagram
Reactions (3)
Structures (5)
Species (6)
Applications (2)
sphere
steady state
Parameters and Functions
Pathway
Geometry
Specifi
Structure Mapping
Geometry Definition
Click “Geometry” > “Structure Mapping”.
Physiology (structures)
Geometry (subdc
Cyt
Nuc
EC
NM
Compartment
In the Size column for “Cyt”, “Nuc”, “EC”, “NM” and “PM” type in “489.794”, “33.389”, “476.817”, “49.8” and “501.804” respectively.
Press “Enter” on your keyboard to finalize.
Volume and Surface Calculator >>
Structure
Size
Surface : Volume
Volume : Volume
Cyt
489.794 [µm³]
0.523183
Nuc
33.389 [µm³]
0.06381897
EC
476.817 [µm³]
NM
49.8 [µm²]
4915092
PM
501.804 [µm²]
95913667
VCell DB
BioModels.net
Pathway C...
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (tanyamiller1221) (7)
Shared BioModels (5)
ACowan : Tutorial_FRAPbinding
ACowan : Tutorial_MultiApp_sims
ACowan : Tutorial_PH-GFP
Access[tanyamiller1221,thomas
astfh234 : new stuff
astfh234 : Rule Based
Public BioModels (522)
Tutorials (5)
Education (33)
CONNECTED (tanyamiller1221)
84.6MB / 147.8MB


BIOMODEL: PIP2Tutorial2 (Fri Jul 10 10:09:58 EDT 2015) -- VCell 5.3 (build 5)
File View Server Tools Help
PIP2Tutorial2
Physiology
Reaction Diagram
Reactions (3)
Structures (5)
Species (6)
Applications (1)
Steady State
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Parameters and Functions
Pathway
VCell DB
BioModels.net
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (tanyamiller1221) (7)
Shared BioModels (1)
Public BioModels (521)
Tutorials (5)
Education (33)
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Simulations
Output Functions
Generated Math
Click “Simulations” > new simulation icon.
Name
End Time
Output Option
Solver
Running Status
Results
Simulation0
1.0
keep every 1 sample
Combined IDA/CVODE
not saved
no
Object Properties
Problems (0 Errors, 1 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
Mesh Refinement:
Finest Level Mesh:
Refinement ROI(s):
View Level Mesh:
Parameters with values changed from defaults
Parameter Name
Default
New Value/Expression
Scan
CONNECTED (tanyamiller1221)
46.6M


BIOMODEL: PIP2Tutorial2 (Fri Jul 10 10:09:58 EDT 2015) -- VCell 5.3 (build 5)
File View Server Tools Help
PIP2Tutorial2
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Species (6)
Applications (1)
Steady State
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Pathway
VCell DB
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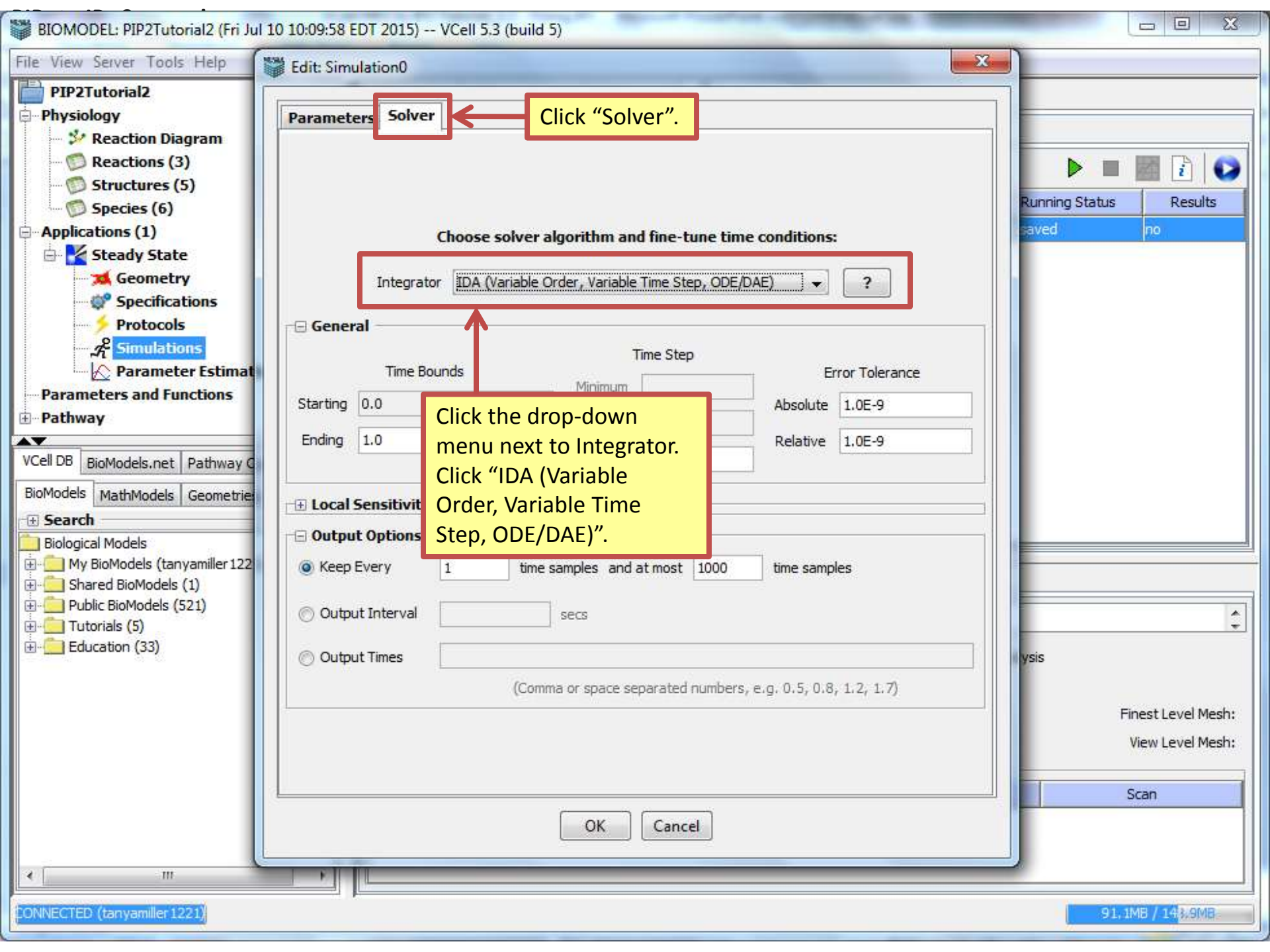
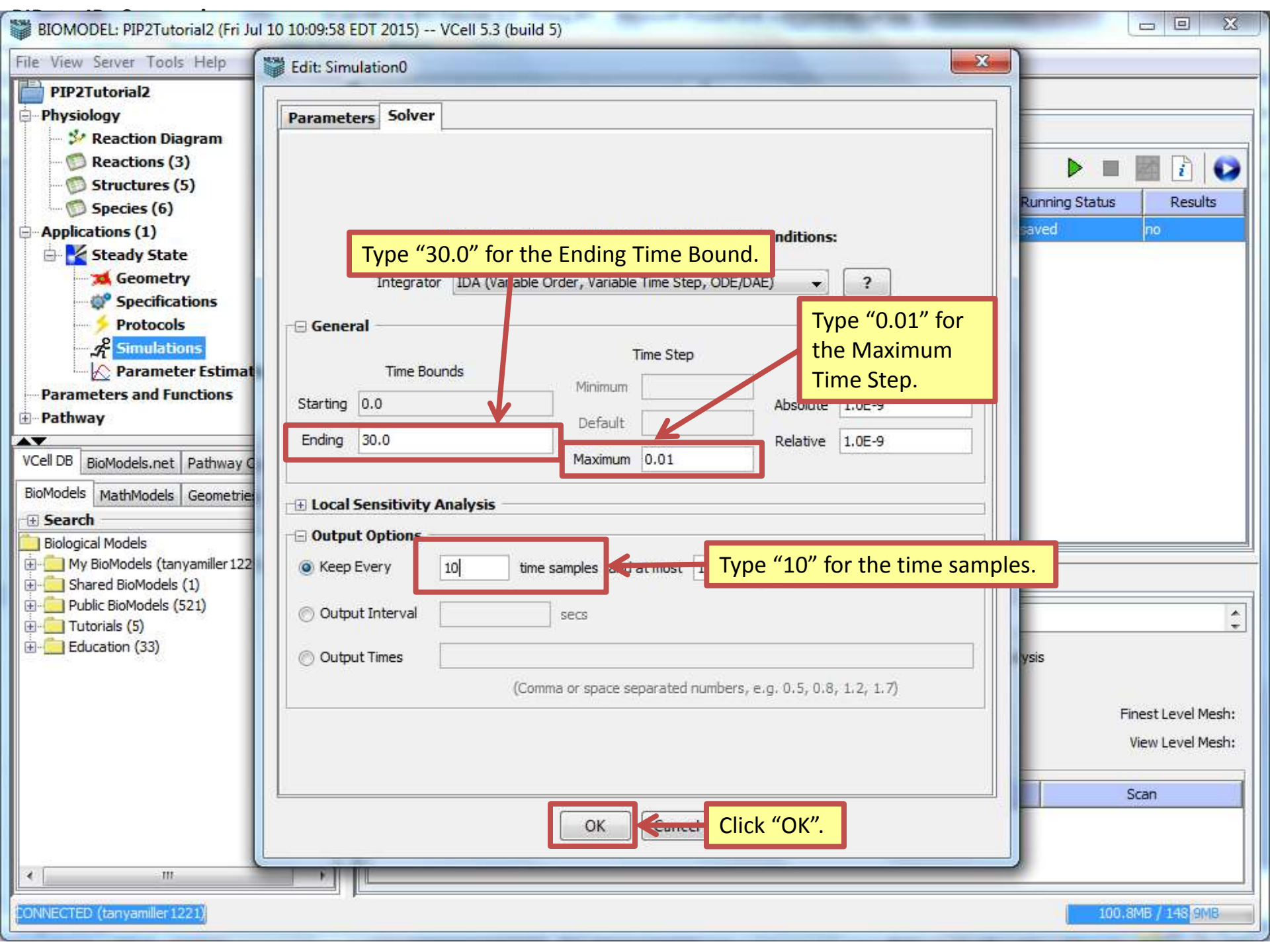
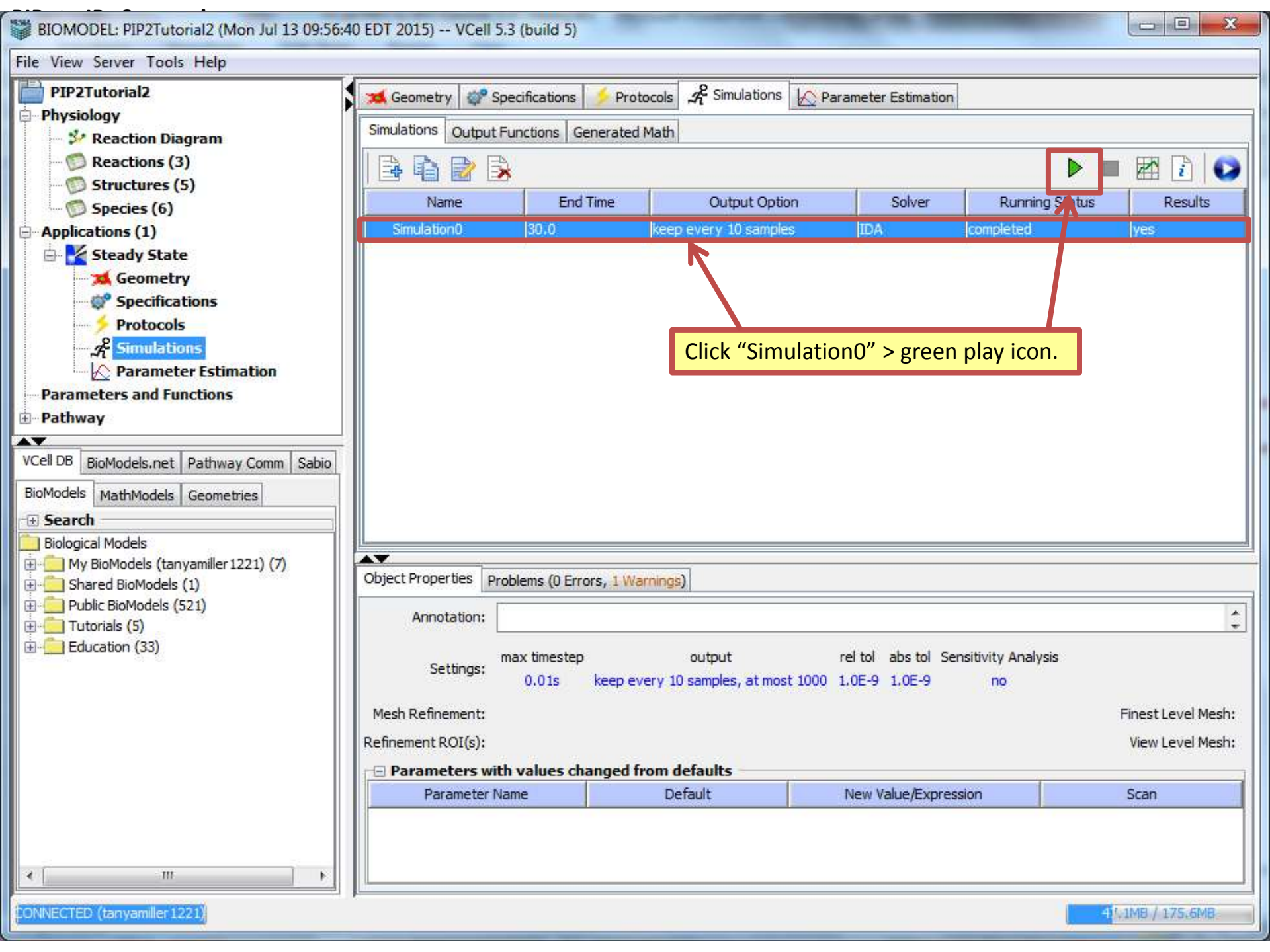
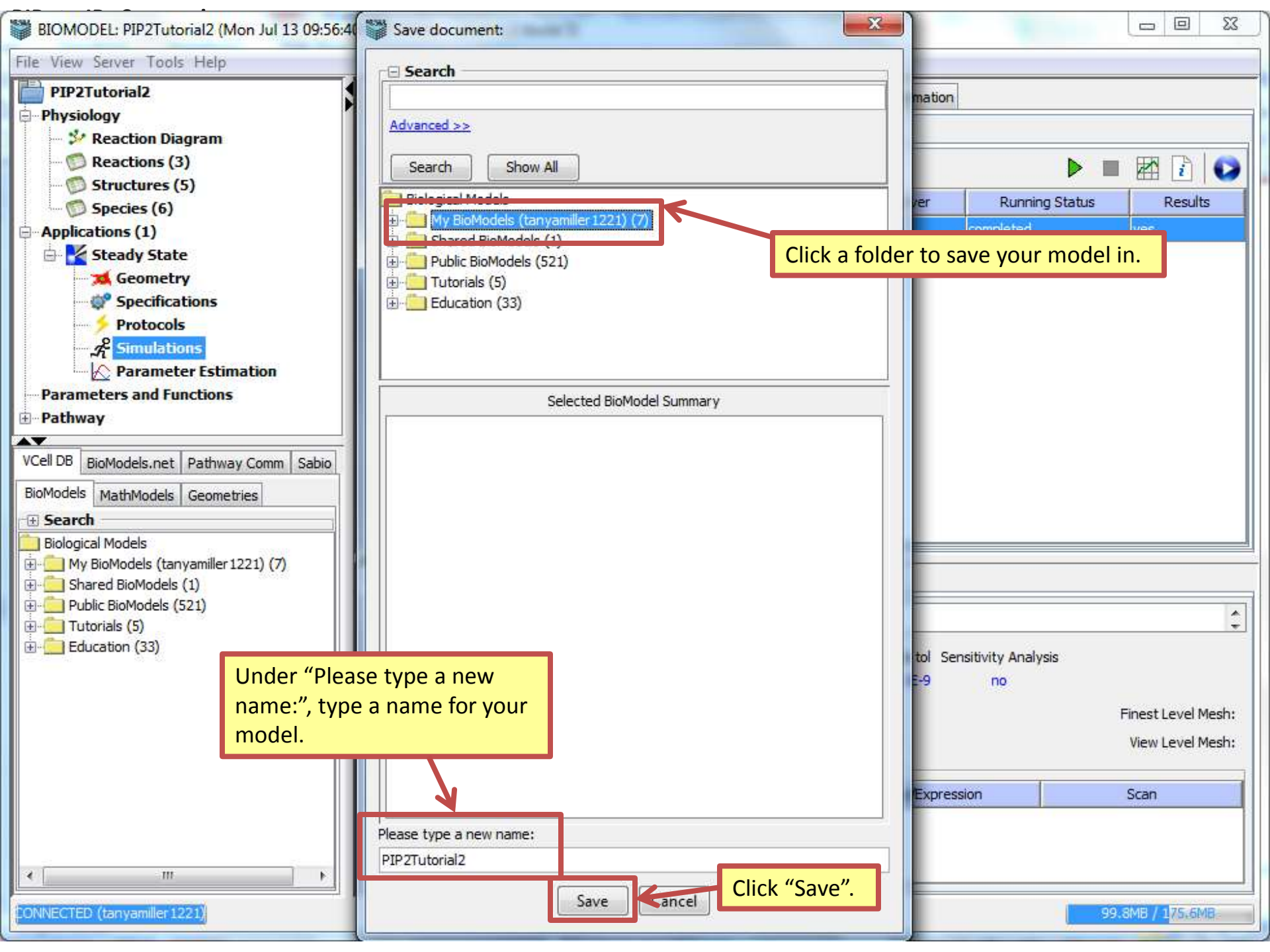
Sabio
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (tanyamiller1221) (7)
Shared BioModels (1)
Public BioModels (521)
Tutorials (5)
Education (33)
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Simulations
Output Functions
Generated Math
Click the edit simulation icon.
Name
End Time
Output Option
Solver
Running Status
Results
Simulation0
1.0
keep every 1 sample
Combined IDA/CVODE
not saved
no
Object Properties
Problems (0 Errors, 1 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
Mesh Refinement:
Finest Level Mesh:
Refinement ROI(s):
View Level Mesh:
Parameters with values changed from defaults
Parameter Name
Default
New Value/Expression
Scan
CONNECTED (tanyamiller1221)
66MB / 148.9MB


BIOMODEL: PIP2Tutorial2 (Fri Jul 10 10:09:58 EDT 2015) -- VCell 5.3 (build 5)
File View Server Tools Help
PIP2Tutorial2
Physiology
Reaction Diagram
Reactions (3)
Structures (5)
Species (6)
Applications (1)
Steady State
Geometry
Specifications
Protocols
Simulations
Parameter Estimat
Parameters and Functions
Pathway
VCell DB
BioModels.net
BioModels
MathModels
Search
Biological Models
My BioModels (tanyamiller122
Shared BioModels (1)
Public BioModels (521)
Tutorials (5)
Education (33)
CONNECTED (tanyamiller1221)
Edit: Simulation0
Parameters
Solver
Click “Solver”.
Choose solver algorithm and fine-tune time conditions:
Integrator
IDA (Variable Order, Variable Time Step, ODE/DAE)
?
General
Time Bounds
Starting
0.0
Ending
1.0
Time Step
Minimum
Error Tolerance
Absolute
1.0E-9
Relative
1.0E-9
Local Sensitivit
Output Options
Keep Every
1
time samples and at most
1000
time samples
Output Interval
secs
Output Times
(Comma or space separated numbers, e.g. 0.5, 0.8, 1.2, 1.7)
Click the drop-down menu next to Integrator. Click “IDA (Variable Order, Variable Time Step, ODE/DAE)”.
OK
Cancel
Running Status
Results
saved
no
Finest Level Mesh:
View Level Mesh:
Scan
91.1MB / 14


BIOMODEL: PIP2Tutorial2 (Fri Jul 10 10:09:58 EDT 2015) -- VCell 5.3 (build 5)
File View Server Tools Help
PIP2Tutorial2
Physiology
Reaction Diagram
Reactions (3)
Structures (5)
Species (6)
Applications (1)
Steady State
Geometry
Specifications
Protocols
Simulations
Parameter Estimat
Parameters and Functions
Pathway
VCell DB
BioModels.net
Pathway C
BioModels
MathModels
Geometrie
Search
Biological Models
My BioModels (tanyamiller122
Shared BioModels (1)
Public BioModels (521)
Tutorials (5)
Education (33)
CONNECTED (tanyamiller1221)
Edit: Simulation0
Parameters
Solver
Type "30.0" for the Ending Time Bound.
nditions:
Integrator
IDA (Variable Order, Variable Time Step, ODE/DAE)
?
General
Time Bounds
Starting
0.0
Ending
30.0
Time Step
Minimum
Default
Maximum
0.01
Absolute
Relative
1.0E-9
Type "0.01" for the Maximum Time Step.
Local Sensitivity Analysis
Output Options
Keep Every
10
time samples
Type "10" for the time samples.
Output Interval
secs
Output Times
(Comma or space separated numbers, e.g. 0.5, 0.8, 1.2, 1.7)
OK
Cancel
Click "OK".
Running Status
Results
saved
no
Finest Level Mesh:
View Level Mesh:
Scan
100.8MB / 148.9MB


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 09:56:40 EDT 2015) -- VCell 5.3 (build 5)
File View Server Tools Help
PIP2Tutorial2
Physiology
Reaction Diagram
Reactions (3)
Structures (5)
Species (6)
Applications (1)
Steady State
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Parameters and Functions
Pathway
VCell DB
BioModels.net
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (tanyamiller1221) (7)
Shared BioModels (1)
Public BioModels (521)
Tutorials (5)
Education (33)
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Simulations
Output Functions
Generated Math
Name
End Time
Output Option
Solver
Running Status
Results
Simulation0
30.0
keep every 10 samples
IDA
completed
yes
Click “Simulation0” > green play icon.
Object Properties
Problems (0 Errors, 1 Warnings)
Annotation:
Settings:
max timestep
output
rel tol
abs tol
Sensitivity Analysis
0.01s
keep every 10 samples, at most 1000
1.0E-9
1.0E-9
no
Mesh Refinement:
Finest Level Mesh:
Refinement ROI(s):
View Level Mesh:
Parameters with values changed from defaults
Parameter Name
Default
New Value/Expression
Scan
CONNECTED (tanyamiller1221)


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 09:56:4
File View Server Tools Help
PIP2Tutorial2
Physiology
Reaction Diagram
Reactions (3)
Structures (5)
Species (6)
Applications (1)
Steady State
Geometry
Specifications
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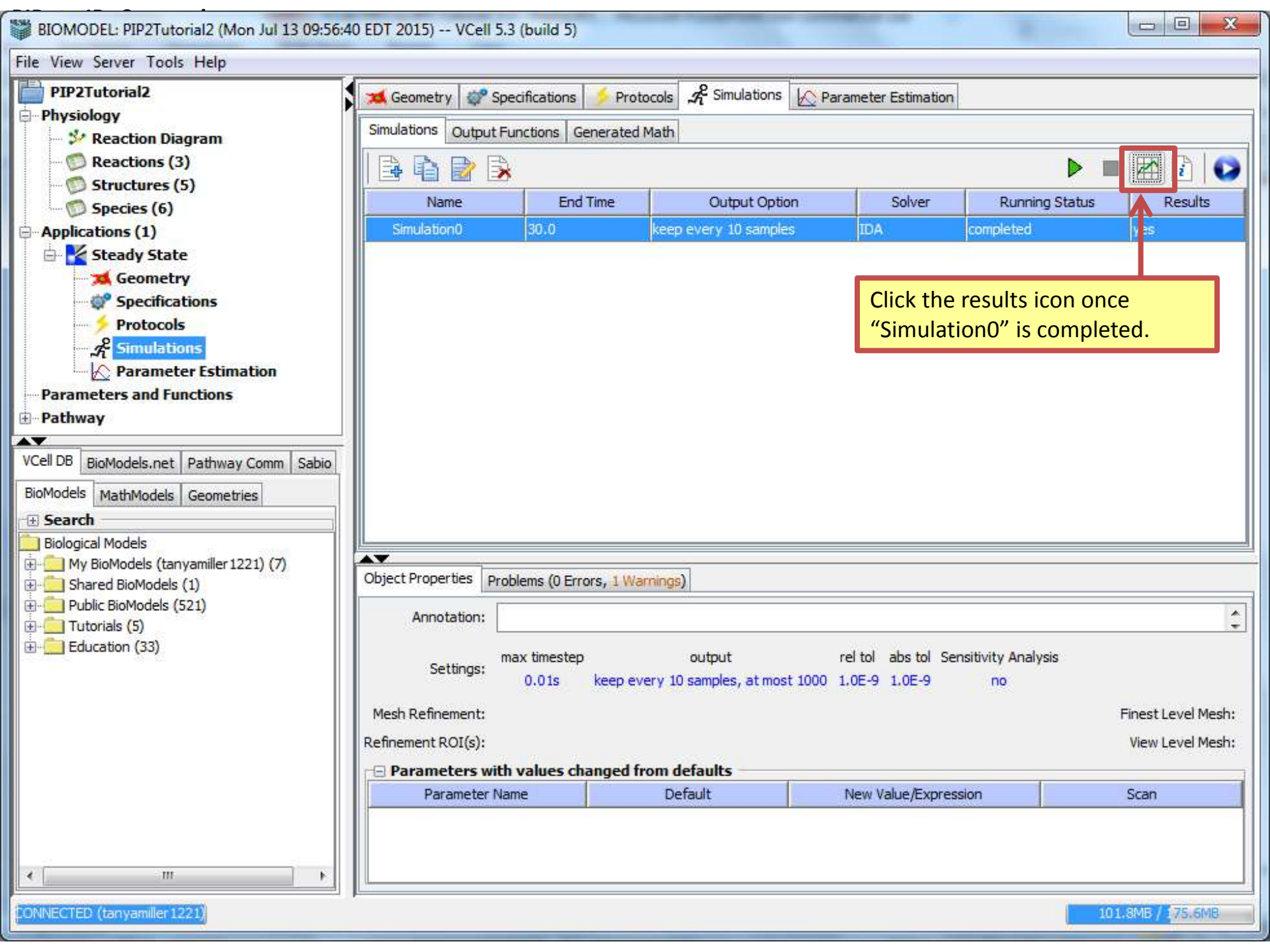
Parameter Estimation
Parameters and Functions
Pathway
VCell DB
BioModels.net
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (tanyamiller1221) (7)
Shared BioModels (1)
Public BioModels (521)
Tutorials (5)
Education (33)
CONNECTED (tanyamiller1221)
Save document:
Search
Advanced >>
Search
Show All
Biological Models
My BioModels (tanyamiller1221) (7)
Public BioModels (521)
Tutorials (5)
Education (33)
Selected BioModel Summary
Please type a new name:
PIP2Tutorial2
Save
Cancel
Click a folder to save your model in.
Under “Please type a new name:”, type a name for your model.
Click “Save”.
Running Status
Results
Sensitivity Analysis
no
Finest Level Mesh:
View Level Mesh:
Expression
Scan
99.8MB / 175.6MB


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 09:56:40 EDT 2015) -- VCell 5.3 (build 5)
File View Server Tools Help
PIP2Tutorial2
Physiology
Reaction Diagram
Reactions (3)
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Steady State
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Parameter Estimation
Parameters and Functions
Pathway
VCell DB
BioModels.net
Pathway Comm
Sabio
BioModels
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Geometries
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Biological Models
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Public BioModels (521)
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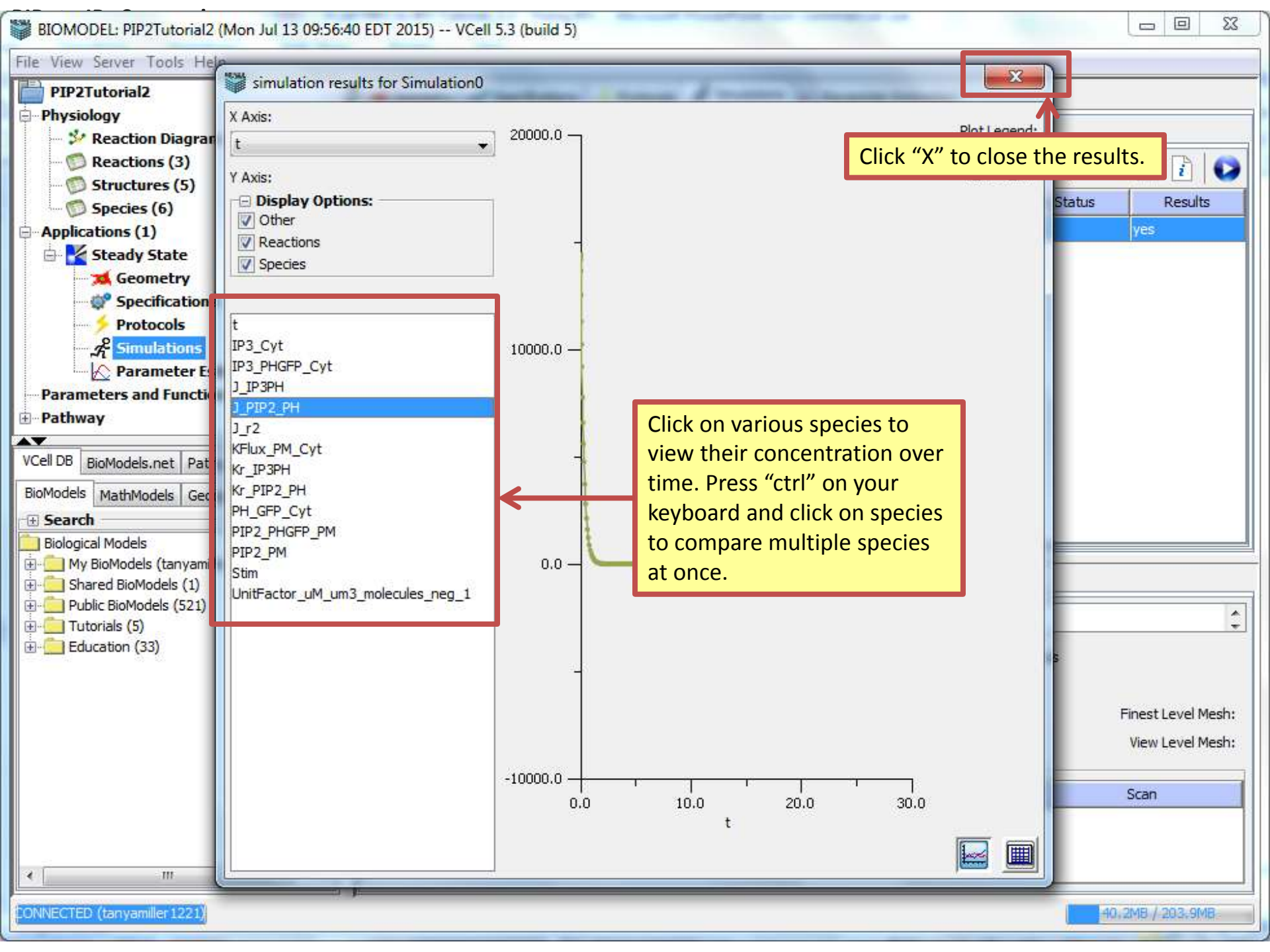
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Simulations
Output Functions
Generated Math
Name
End Time
Output Option
Solver
Running Status
Results
Simulation0
30.0
keep every 10 samples
IDA
completed
yes
Click the results icon once "Simulation0" is completed.
Object Properties
Problems (0 Errors, 1 Warnings)
Annotation:
Settings:
max timestep
output
rel tol
abs tol
Sensitivity Analysis
0.01s
keep every 10 samples, at most 1000
1.0E-9
1.0E-9
no
Mesh Refinement:
Finest Level Mesh:
Refinement ROI(s):
View Level Mesh:
Parameters with values changed from defaults
Parameter Name
Default
New Value/Expression
Scan
CONNECTED (tanyamiller1221)
101.8MB / 175.6MB


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 09:56:40 EDT 2015) -- VCell 5.3 (build 5)
File View Server Tools Help
PIP2Tutorial2
Physiology
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Parameter Estimation
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MathModels
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Biological Models
My BioModels (tanyami
Shared BioModels (1)
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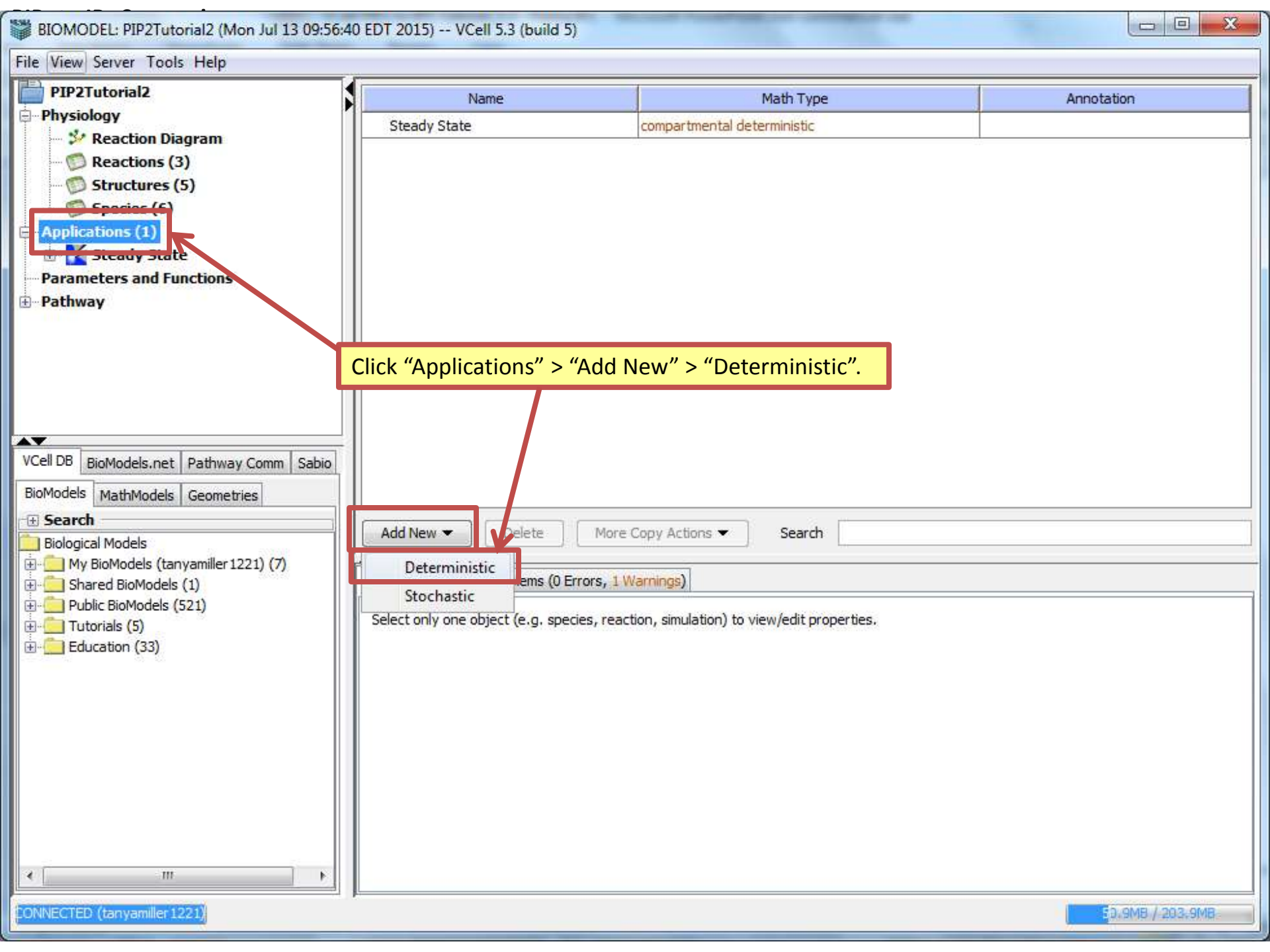
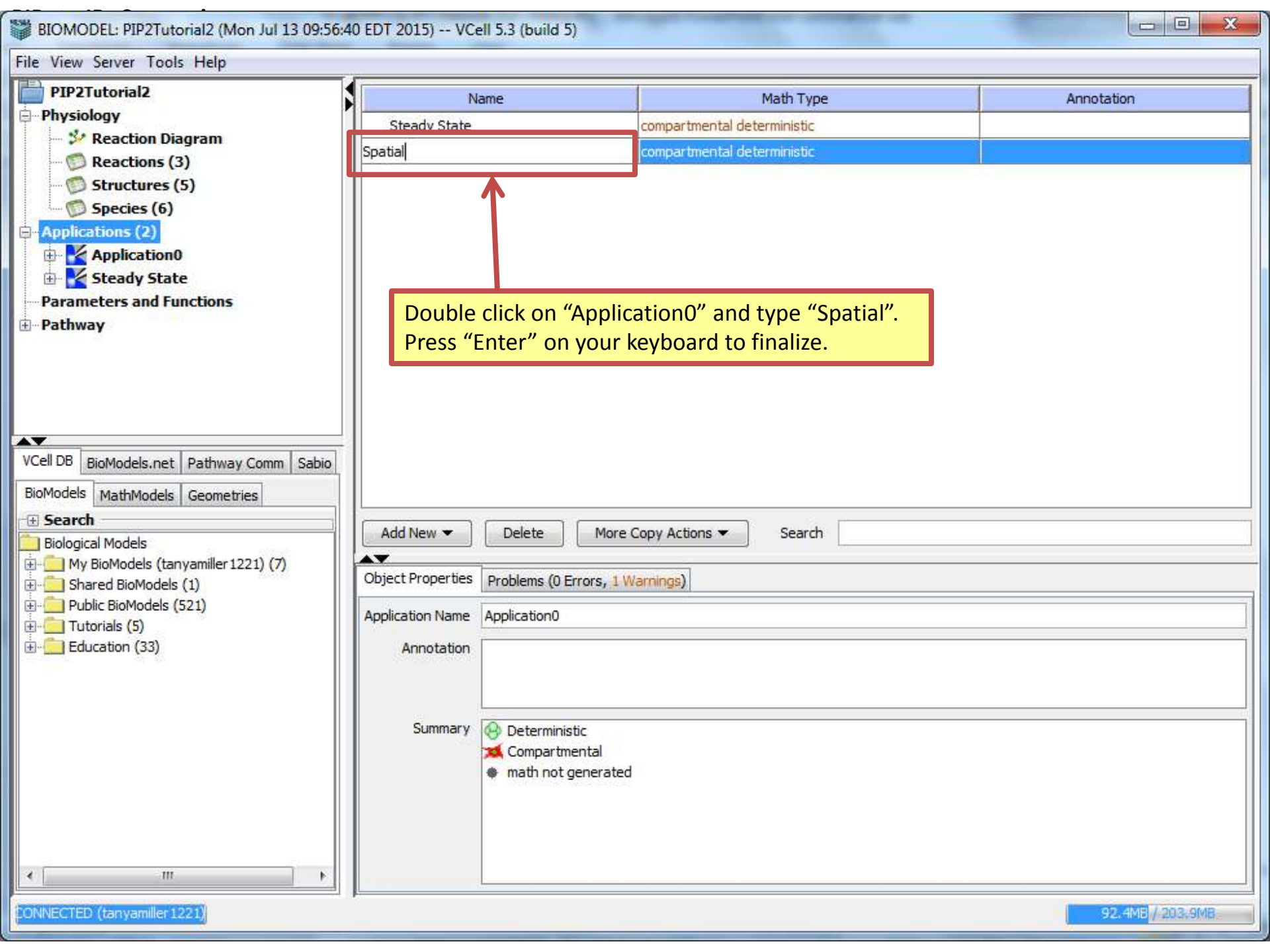
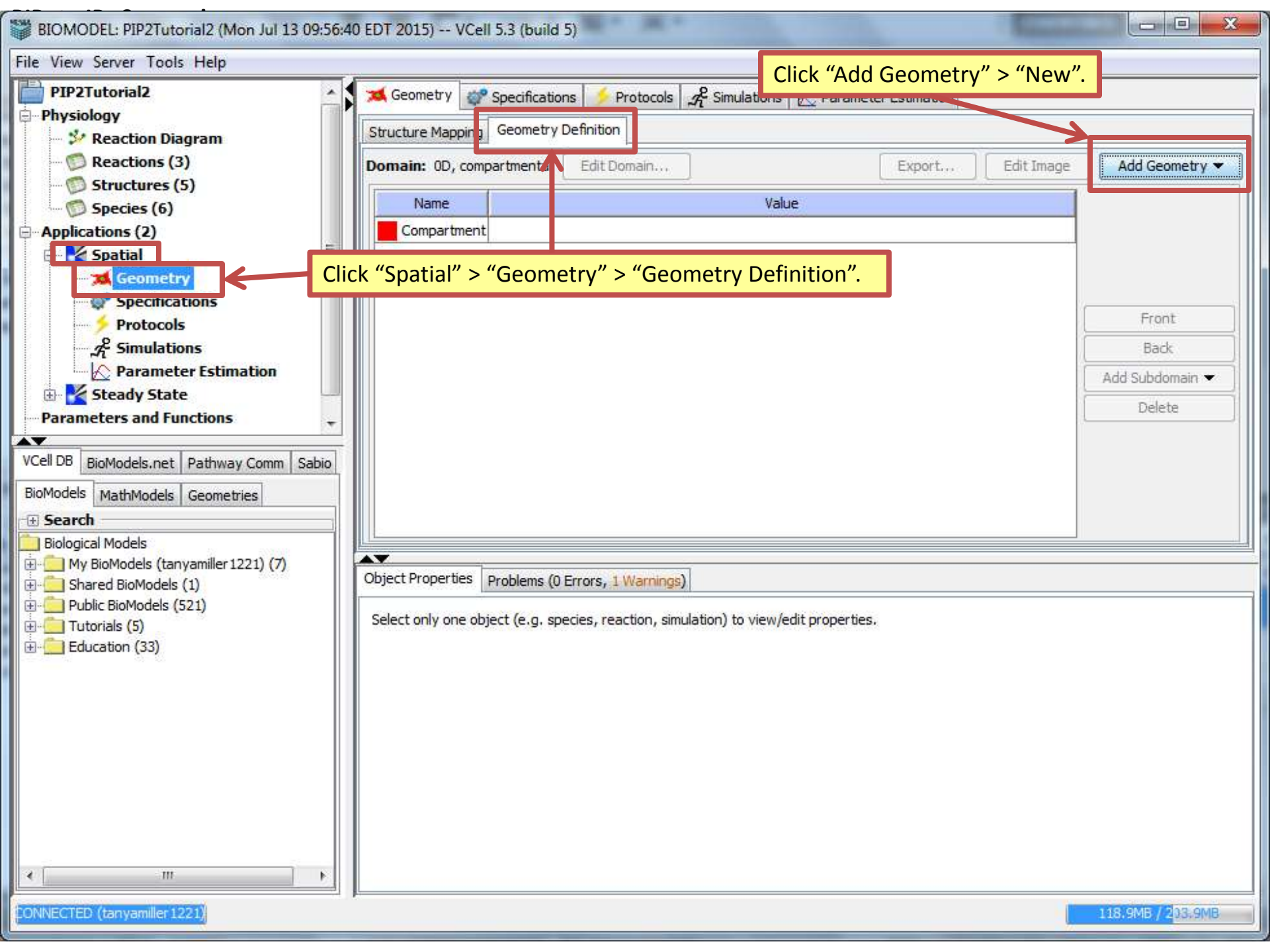
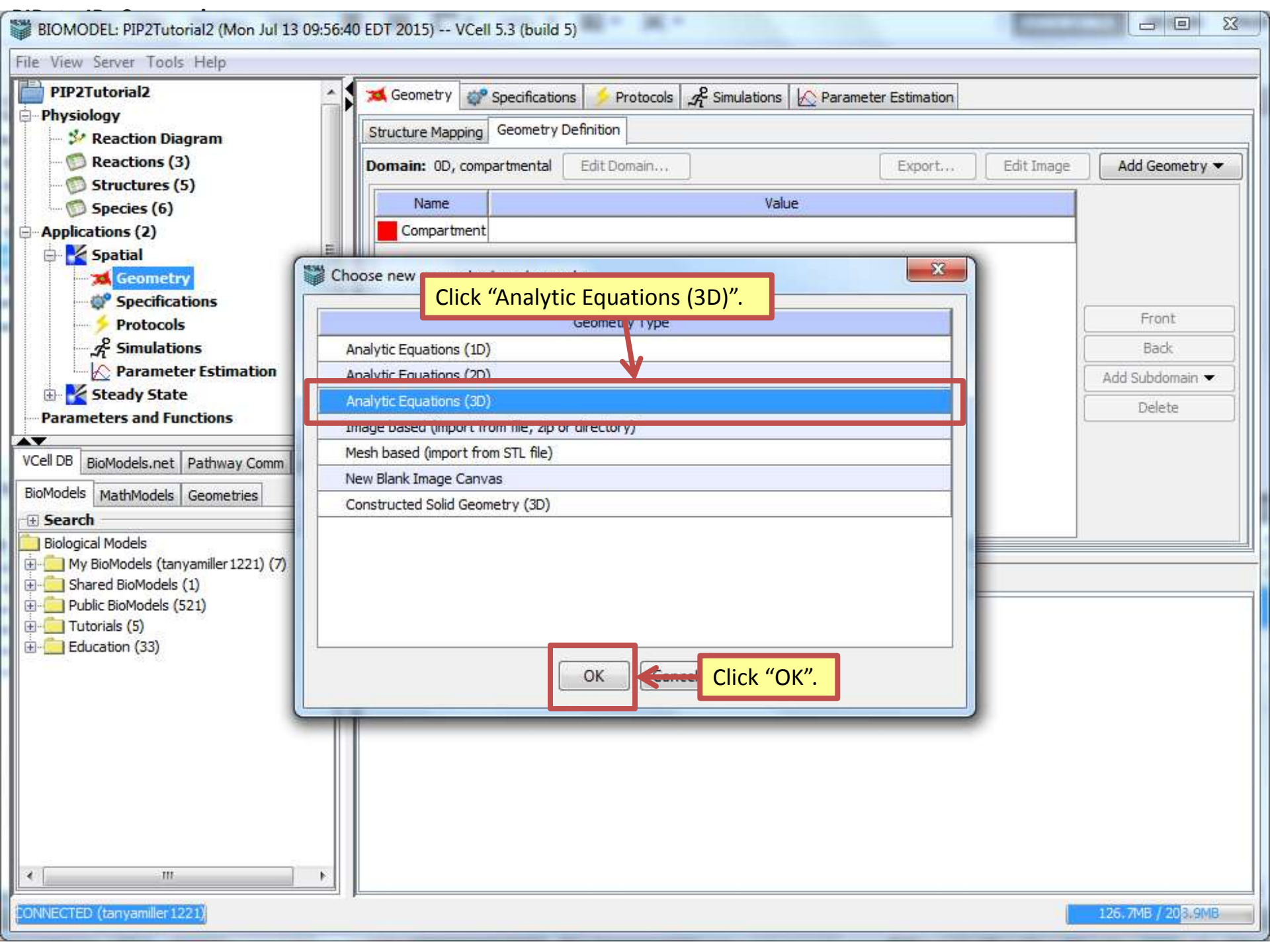
Education (33)
simulation results for Simulation0
X Axis:
t
Y Axis:
Display Options:
Other
Reactions
Species
t
IP3_Cyt
IP3_PHGFP_Cyt
J_IP3PH
J_PIP2_PH
J_r2
KFlux_PM_Cyt
Kr_IP3PH
Kr_PIP2_PH
PH_GFP_Cyt
PIP2_PHGFP_PM
PIP2_PM
Stim
UnitFactor_uM_um3_molecules_neg_1
20000.0
10000.0
0.0
-10000.0
0.0
10.0
20.0
30.0
t
Plot Legend:
Click "X" to close the results.
Click on various species to view their concentration over time. Press "ctrl" on your keyboard and click on species to compare multiple species at once.
Status
Results
yes
Finest Level Mesh:
View Level Mesh:
Scan
CONNECTED (tanyamiller1221)
40.2MB / 203.9MB


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 09:56:40 EDT 2015) -- VCell 5.3 (build 5)
File View Server Tools Help
PIP2Tutorial2
Physiology
Reaction Diagram
Reactions (3)
Structures (5)
Applications (1)
Parameters and Functions
Pathway
Name
Math Type
Annotation
Steady State
compartmental deterministic
Click “Applications” > “Add New” > “Deterministic”.
Add New
Delete
More Copy Actions
Search
Deterministic
Stochastic
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
VCell DB
BioModels.net
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (tanyamiller1221) (7)
Shared BioModels (1)
Public BioModels (521)
Tutorials (5)
Education (33)
CONNECTED (tanyamiller1221)


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 09:56:40 EDT 2015) -- VCell 5.3 (build 5)
File View Server Tools Help
PIP2Tutorial2
Physiology
Reaction Diagram
Reactions (3)
Structures (5)
Species (6)
Applications (2)
Application0
Steady State
Parameters and Functions
Pathway
Name
Math Type
Annotation
Steady State
compartmental deterministic
Spatial
compartmental deterministic
Double click on “Application0” and type “Spatial”.
Press “Enter” on your keyboard to finalize.
Add New
Delete
More Copy Actions
Search
VCell DB
BioModels.net
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (tanyamiller1221) (7)
Shared BioModels (1)
Public BioModels (521)
Tutorials (5)
Education (33)
Object Properties
Problems (0 Errors, 1 Warnings)
Application Name
Application0
Annotation
Summary
Deterministic
Compartmental
math not generated
CONNECTED (tanyamiller1221)
92.4MB / 203.9MB


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 09:56:40 EDT 2015) -- VCell 5.3 (build 5)
File View Server Tools Help
PIP2Tutorial2
Physiology
Reaction Diagram
Reactions (3)
Structures (5)
Species (6)
Applications (2)
Spatial
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Steady State
Parameters and Functions
Click “Spatial” > “Geometry” > “Geometry Definition”.
Click “Add Geometry” > “New”.
Geometry
Specifications
Protocols
Simulations
Structure Mapping
Geometry Definition
Domain: 0D, compartment
Edit Domain...
Export...
Edit Image
Add Geometry
Name
Value
Compartment
Front
Back
Add Subdomain
Delete
VCell DB
BioModels.net
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (tanyamiller1221) (7)
Shared BioModels (1)
Public BioModels (521)
Tutorials (5)
Education (33)
Object Properties
Problems (0 Errors, 1 Warnings)
Select only one object (e.g. species, reaction, simulation) to view/edit properties.
CONNECTED (tanyamiller1221)
118.9MB / 203.9MB


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 09:56:40 EDT 2015) -- VCell 5.3 (build 5)
File View Server Tools Help
PIP2Tutorial2
Physiology
Reaction Diagram
Reactions (3)
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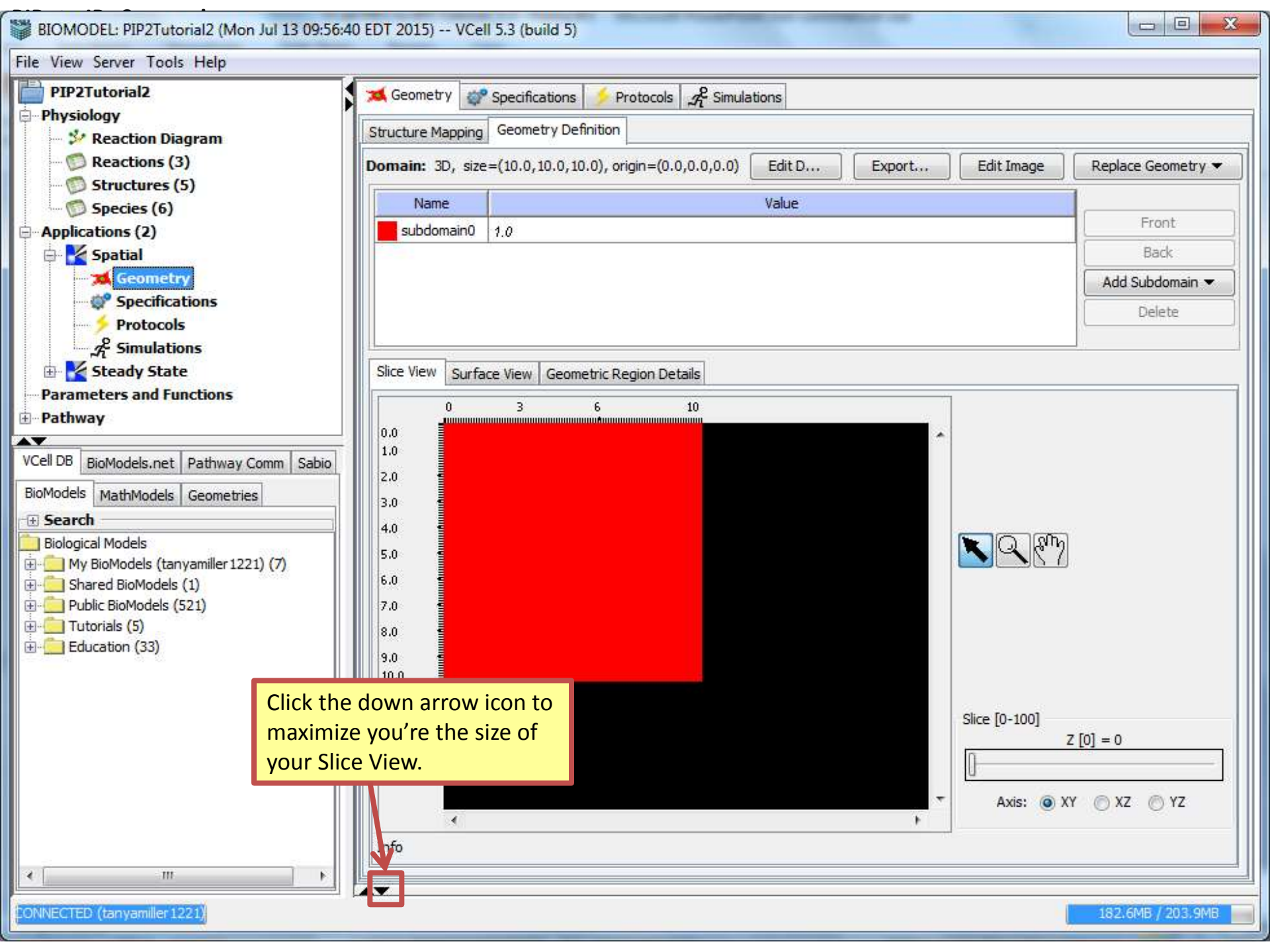
Species (6)
Applications (2)
Spatial
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Steady State
Parameters and Functions
Geometry
Specifications
Protocols
Simulations
Parameter Estimation
Structure Mapping
Geometry Definition
Domain: 0D, compartmental
Edit Domain...
Export...
Edit Image
Add Geometry
Name
Value
Compartment
Front
Back
Add Subdomain
Delete
Choose new
Click “Analytic Equations (3D)”.
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)
OK
Click “OK”.
VCell DB
BioModels.net
Pathway Comm
BioModels
MathModels
Geometries
Search
Biological Models
My BioModels (tanyamiller1221) (7)
Shared BioModels (1)
Public BioModels (521)
Tutorials (5)
Education (33)
CONNECTED (tanyamiller1221)
126.7MB / 203.9MB


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 09:56:40 EDT 2015) -- VCell 5.3 (build 5)
File View Server Tools Help
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Pathway Comm
Sabio
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Biological Models
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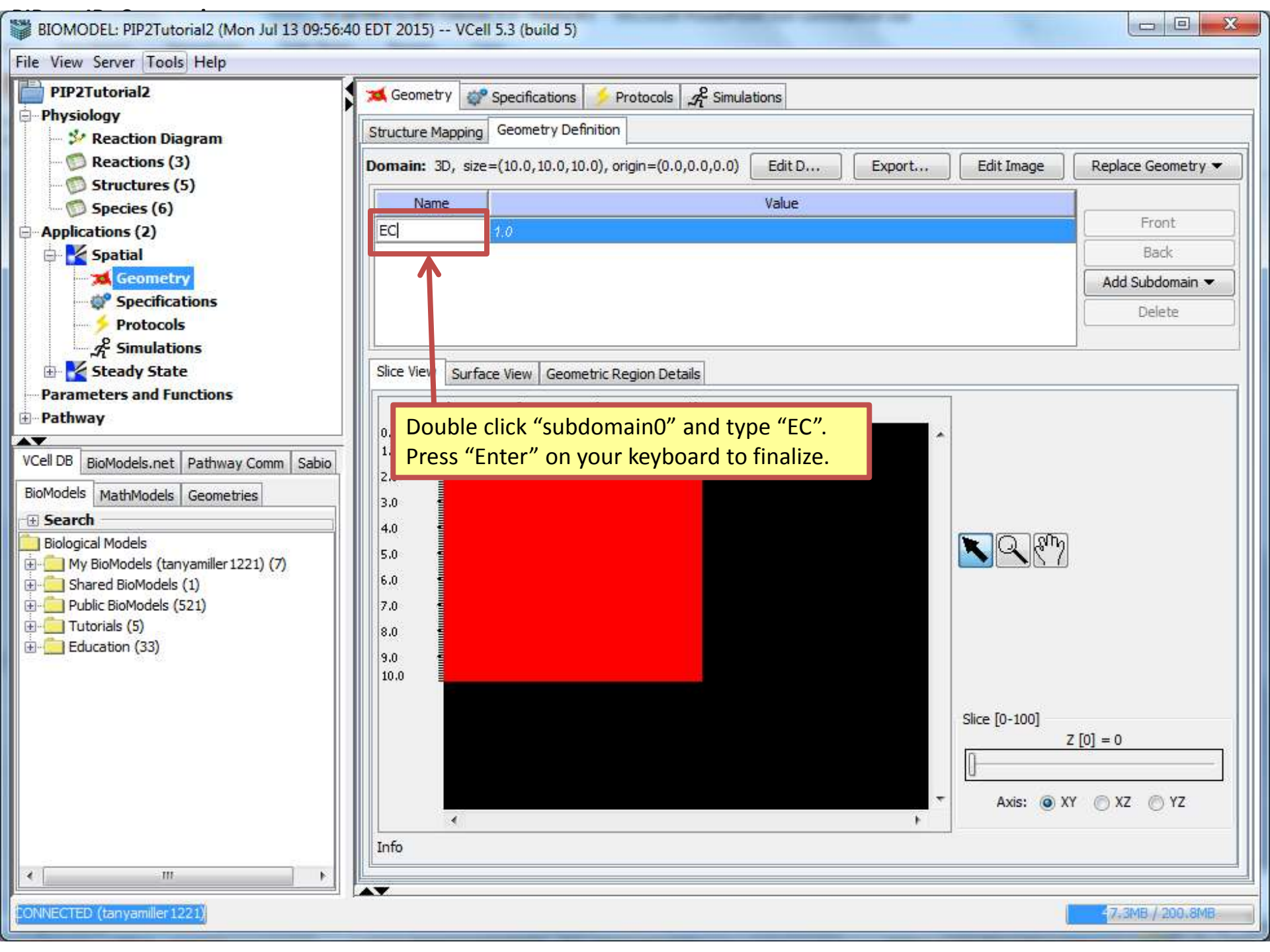
Tutorials (5)
Education (33)
Geometry
Specifications
Protocols
Simulations
Structure Mapping
Geometry Definition
Domain: 3D, size=(10.0,10.0,10.0), origin=(0.0,0.0,0.0)
Edit D...
Export...
Edit Image
Replace Geometry
Name
Value
subdomain0
1.0
Front
Back
Add Subdomain
Delete
Slice View
Surface View
Geometric Region Details
0
3
6
10
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
Slice [0-100]
Z [0] = 0
Axis: XY XZ YZ
Click the down arrow icon to maximize you're the size of your Slice View.
CONNECTED (tanyamiller1221)
182.6MB / 203.9MB


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 09:56:40 EDT 2015) -- VCell 5.3 (build 5)
File View Server Tools Help
PIP2Tutorial2
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Reaction Diagram
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Specifications
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VCell DB
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Pathway Comm
Sabio
BioModels
MathModels
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Search
Biological Models
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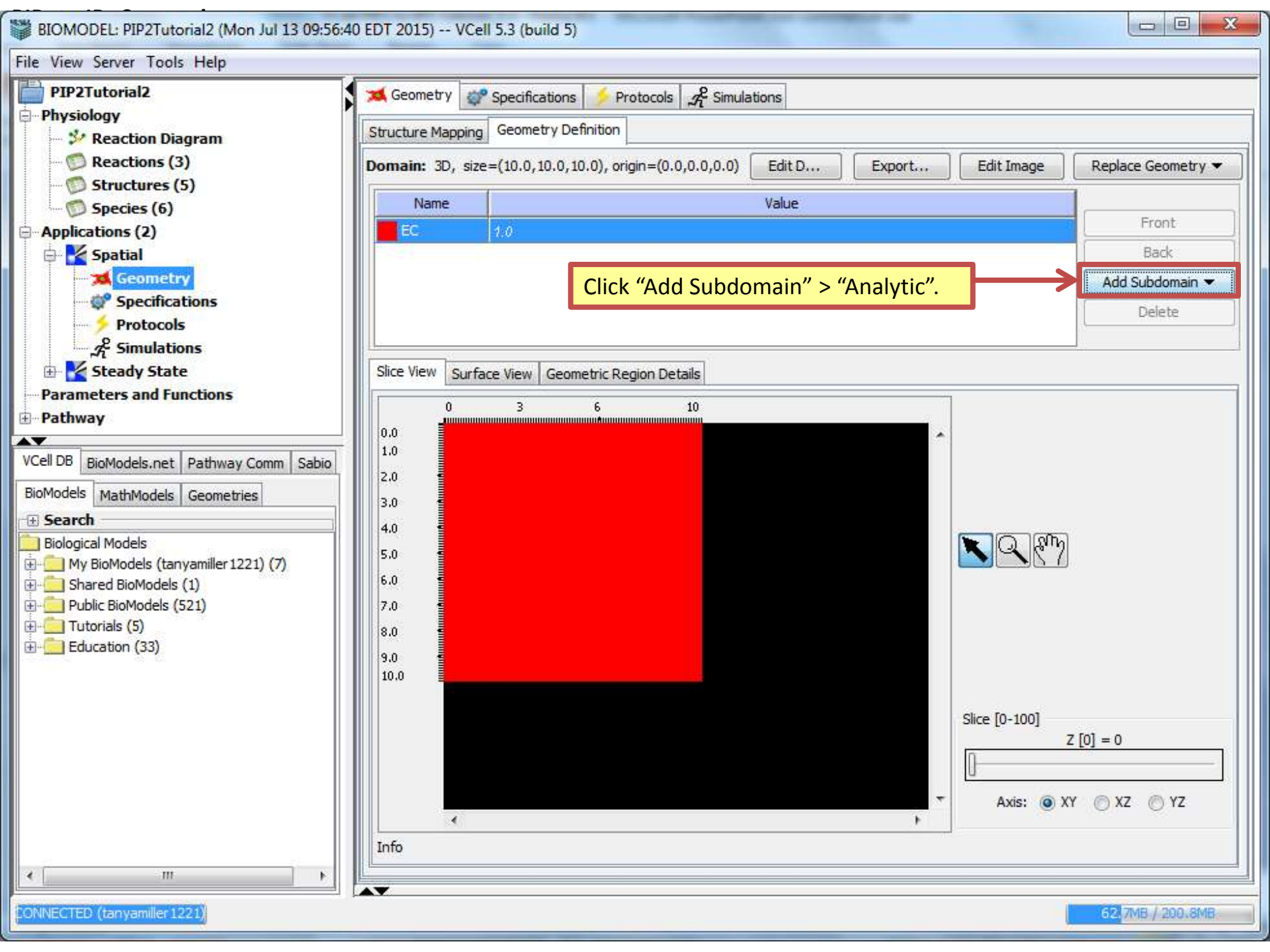
Shared BioModels (1)
Public BioModels (521)
Tutorials (5)
Education (33)
Geometry
Specifications
Protocols
Simulations
Structure Mapping
Geometry Definition
Domain: 3D, size=(10.0,10.0,10.0), origin=(0.0,0.0,0.0)
Edit D...
Export...
Edit Image
Replace Geometry
Name
Value
EC
1.0
Front
Back
Add Subdomain
Delete
Slice View
Surface View
Geometric Region Details
Double click “subdomain0” and type “EC”.
Press “Enter” on your keyboard to finalize.
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
Slice [0-100]
Z [0] = 0
Axis: XY XZ YZ
Info
CONNECTED (tanyamiller1221)
7.3MB / 200.8MB


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 09:56:40 EDT 2015) -- VCell 5.3 (build 5)
File View Server Tools Help
PIP2Tutorial2
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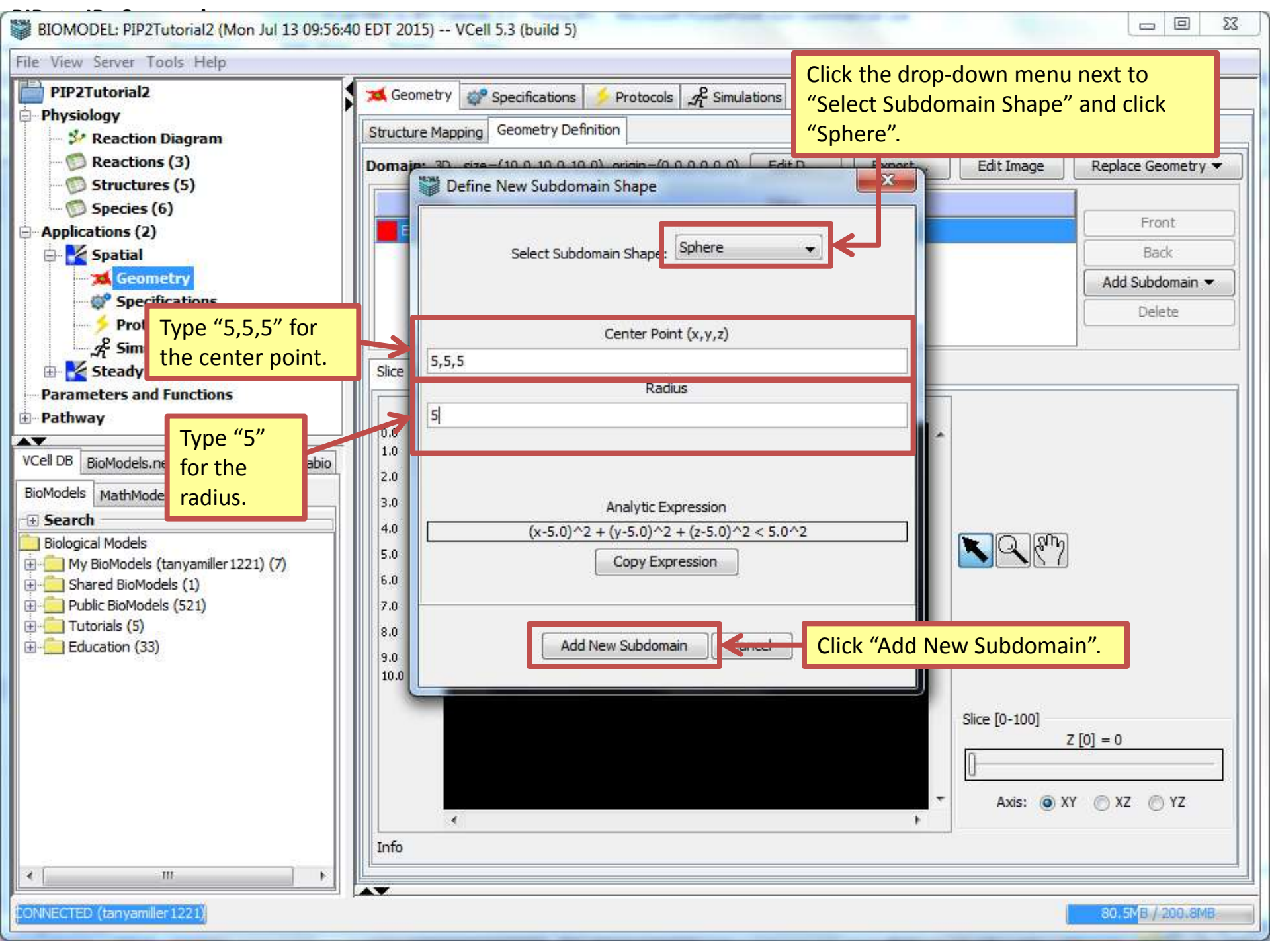
Specifications
Protocols
Simulations
Structure Mapping
Geometry Definition
Domain: 3D, size=(10.0,10.0,10.0), origin=(0.0,0.0,0.0)
Edit D...
Export...
Edit Image
Replace Geometry
Name
Value
EC
1.0
Front
Back
Add Subdomain
Delete
Click “Add Subdomain” > “Analytic”.
Slice View
Surface View
Geometric Region Details
0
3
6
10
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
Slice [0-100]
Z [0] = 0
Axis: XY XZ YZ
Info
CONNECTED (tanyamiller1221)
62.7MB / 200.8MB


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 09:56:40 EDT 2015) -- VCell 5.3 (build 5)
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Spatial
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Parameters and Functions
Pathway
Geometry
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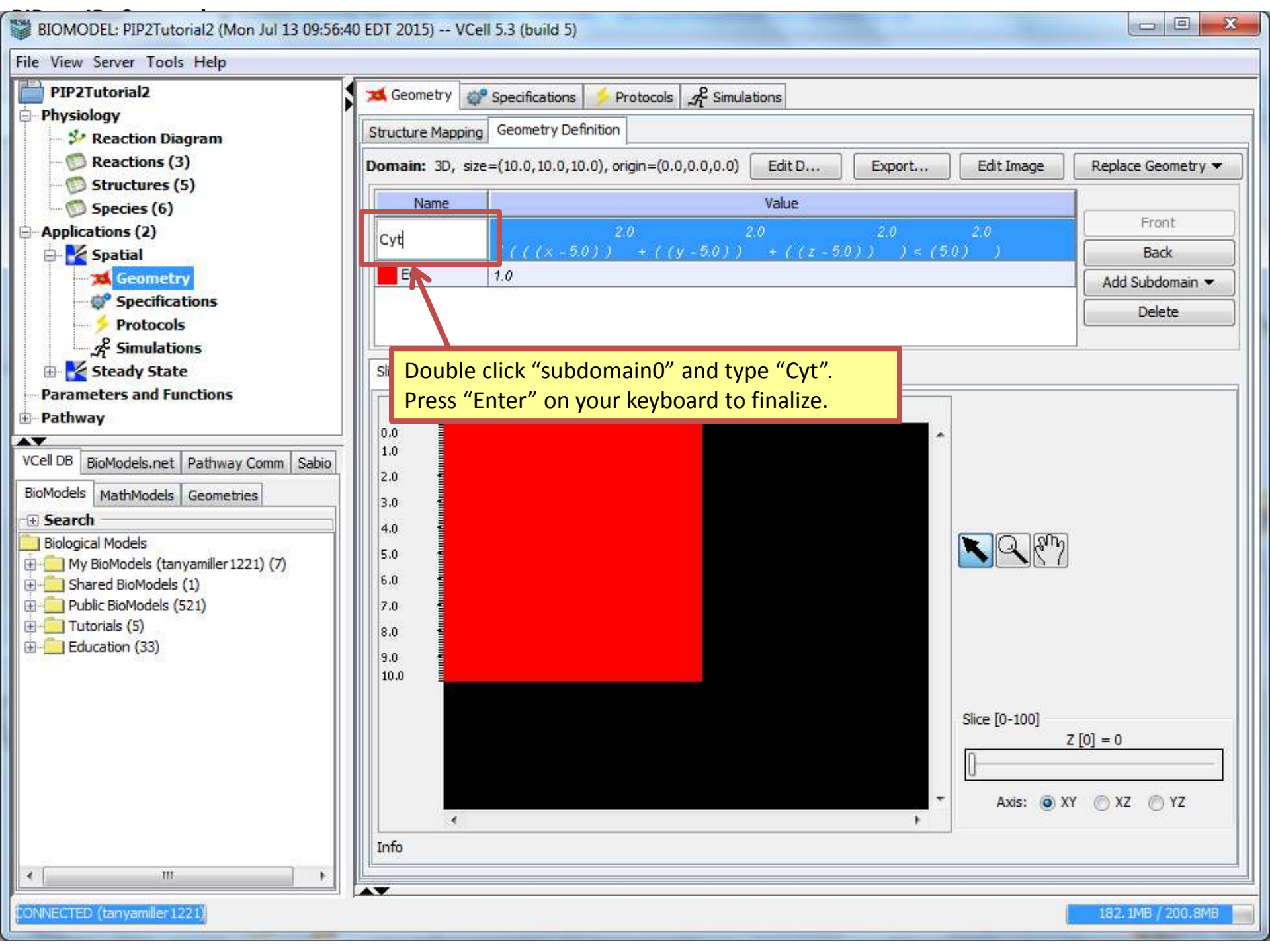
Simulations
Structure Mapping
Geometry Definition
Edit Image
Replace Geometry
Front
Back
Add Subdomain
Delete
Slice
Define New Subdomain Shape
Select Subdomain Shape:
Sphere
Center Point (x,y,z)
5,5,5
Radius
5
Analytic Expression
(x-5.0)^2 + (y-5.0)^2 + (z-5.0)^2 < 5.0^2
Copy Expression
Add New Subdomain
Cancel
Click the drop-down menu next to "Select Subdomain Shape" and click "Sphere".
Type "5,5,5" for the center point.
Type "5" for the radius.
Click "Add New Subdomain".
VCell DB
BioModels
Search
Biological Models
My BioModels (tanyamiller1221) (7)
Shared BioModels (1)
Public BioModels (521)
Tutorials (5)
Education (33)
Slice [0-100]
Z [0] = 0
Axis: XY XZ YZ
Info
CONNECTED (tanyamiller1221)
80.5MB / 200.8MB


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 09:56:40 EDT 2015) -- VCell 5.3 (build 5)
File View Server Tools Help
PIP2Tutorial2
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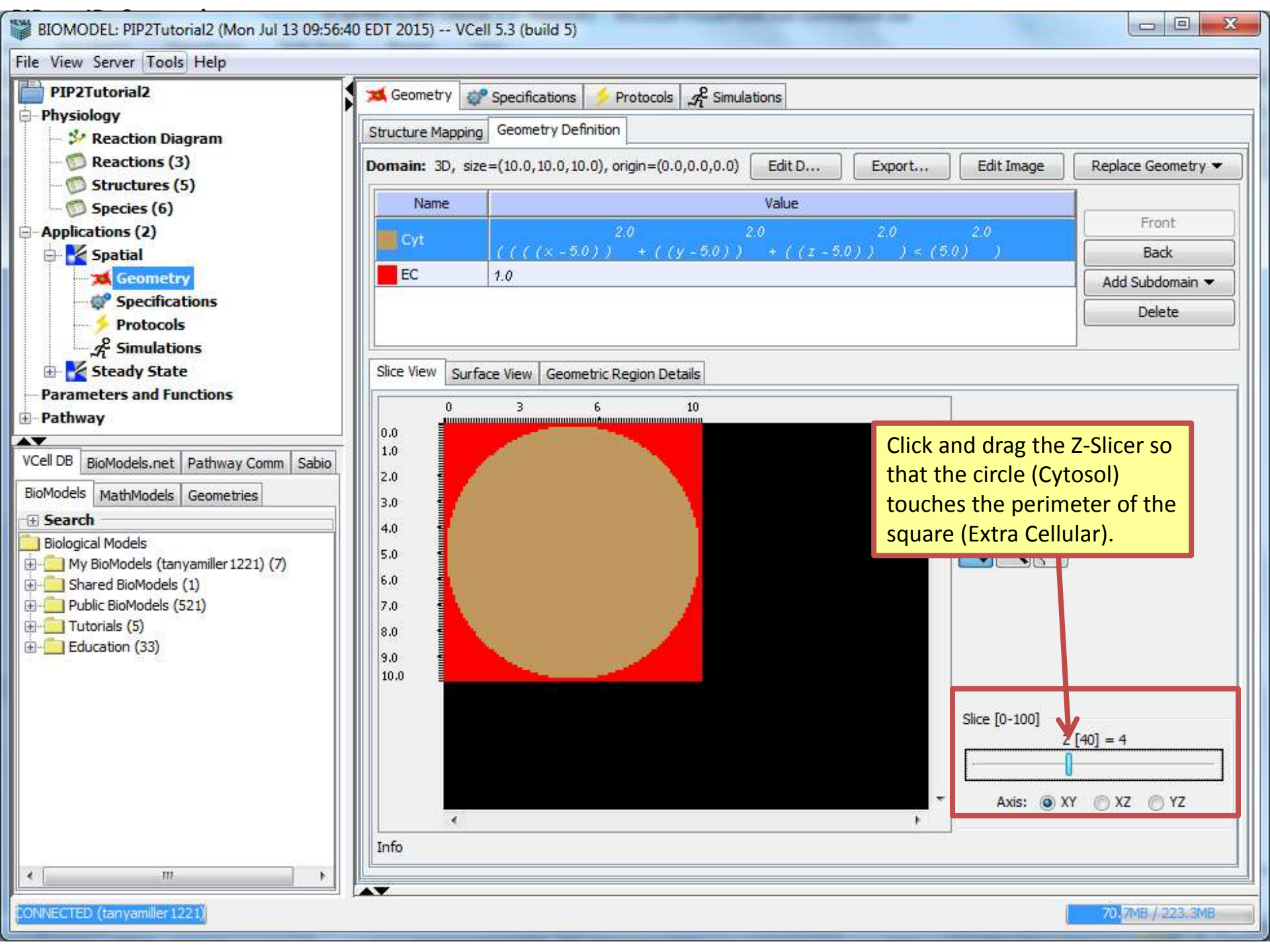
Geometry
Specifications
Protocols
Simulations
Structure Mapping
Geometry Definition
Domain: 3D, size=(10.0,10.0,10.0), origin=(0.0,0.0,0.0)
Edit D...
Export...
Edit Image
Replace Geometry
Name
Value
Cyt
1.0
Front
Back
Add Subdomain
Delete
Double click “subdomain0” and type “Cyt”.
Press “Enter” on your keyboard to finalize.
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
Slice [0-100]
Z [0] = 0
Axis: XY XZ YZ
Info
CONNECTED (tanyamiller1221)
182.1MB / 200.8MB


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 09:56:40 EDT 2015) -- VCell 5.3 (build 5)
File View Server Tools Help
PIP2Tutorial2
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Sabio
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Search
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Public BioModels (521)
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Education (33)
Geometry
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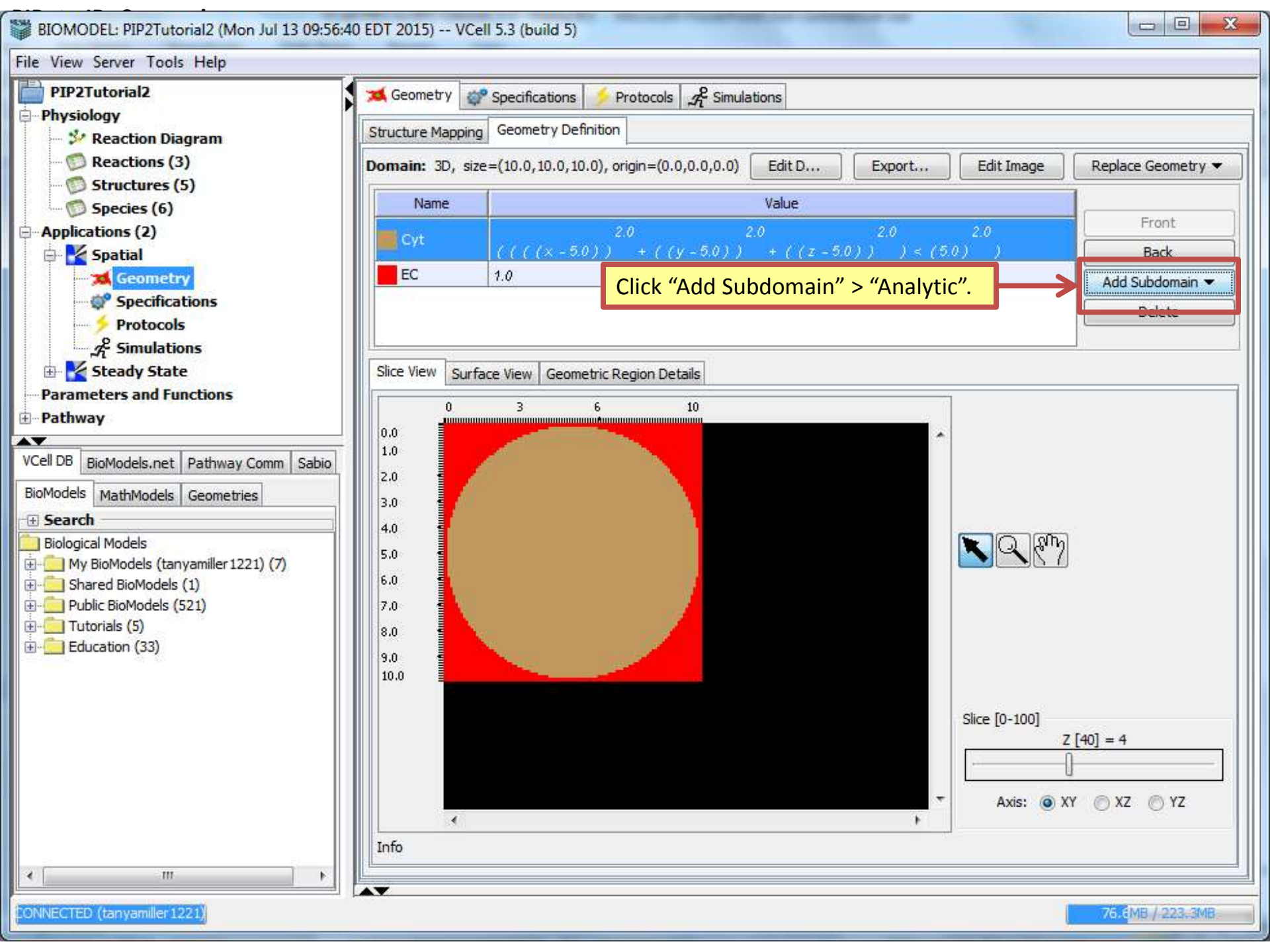
Protocols
Simulations
Structure Mapping
Geometry Definition
Domain: 3D, size=(10.0,10.0,10.0), origin=(0.0,0.0,0.0)
Edit D...
Export...
Edit Image
Replace Geometry
Name
Value
Cyt
EC
1.0
Front
Back
Add Subdomain
Delete
Slice View
Surface View
Geometric Region Details
Click and drag the Z-Slicer so that the circle (Cytosol) touches the perimeter of the square (Extra Cellular).
Slice [0-100]
Z [40] = 4
Axis: XY XZ YZ
Info
CONNECTED (tanyamiller1221)


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 09:56:40 EDT 2015) -- VCell 5.3 (build 5)
File View Server Tools Help
PIP2Tutorial2
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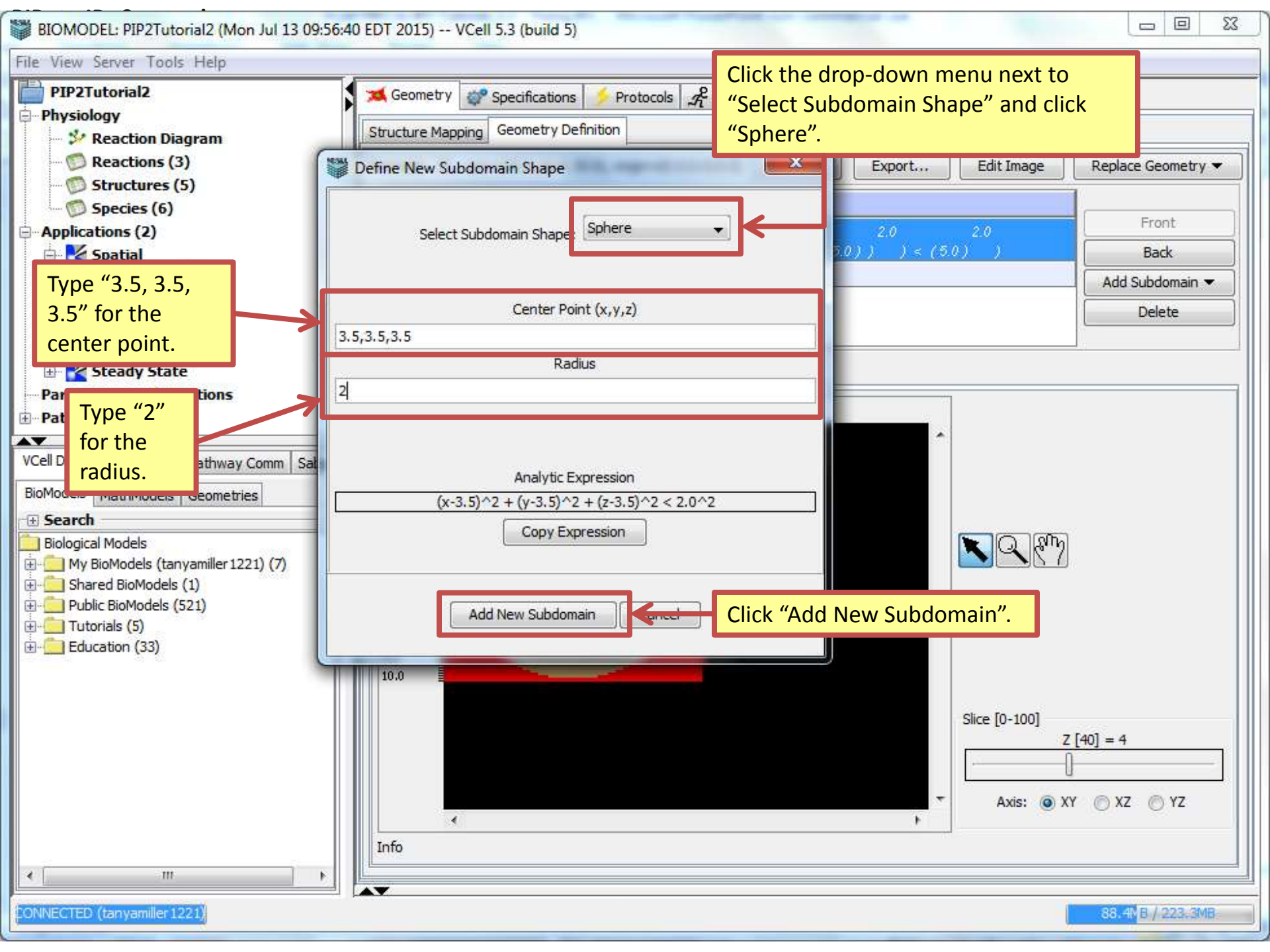
Education (33)
Geometry
Specifications
Protocols
Simulations
Structure Mapping
Geometry Definition
Domain: 3D, size=(10.0,10.0,10.0), origin=(0.0,0.0,0.0)
Edit D...
Export...
Edit Image
Replace Geometry
Name
Value
Cyt
EC
1.0
Front
Back
Add Subdomain
Delete
Click “Add Subdomain” > “Analytic”.
Slice View
Surface View
Geometric Region Details
Slice [0-100]
Z [40] = 4
Axis: XY XZ YZ
Info
CONNECTED (tanyamiller1221)


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 09:56:40 EDT 2015) -- VCell 5.3 (build 5)
File View Server Tools Help
PIP2Tutorial2
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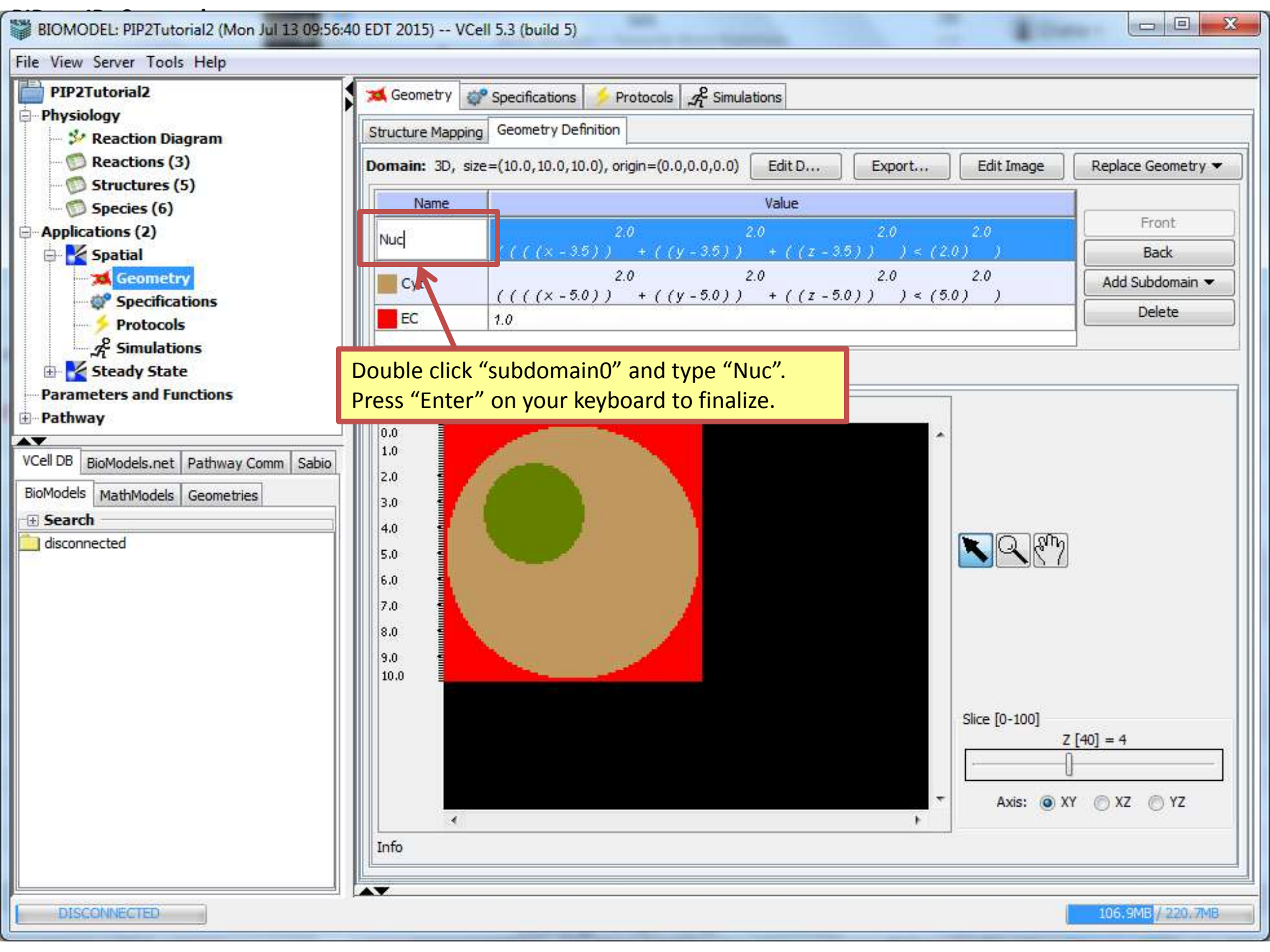
Structure Mapping
Geometry Definition
Export...
Edit Image
Replace Geometry
Front
Back
Add Subdomain
Delete
Define New Subdomain Shape
Select Subdomain Shape
Sphere
Center Point (x,y,z)
3.5,3.5,3.5
Radius
2
Analytic Expression
(x-3.5)^2 + (y-3.5)^2 + (z-3.5)^2 < 2.0^2
Copy Expression
Add New Subdomain
Cancel
Click the drop-down menu next to "Select Subdomain Shape" and click "Sphere".
Type "3.5, 3.5, 3.5" for the center point.
Type "2" for the radius.
Click "Add New Subdomain".
Search
Biological Models
My BioModels (tanyamiller1221) (7)
Shared BioModels (1)
Public BioModels (521)
Tutorials (5)
Education (33)
Slice [0-100]
Z [40] = 4
Axis: XY XZ YZ
Info
CONNECTED (tanyamiller1221)


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 09:56:40 EDT 2015) -- VCell 5.3 (build 5)
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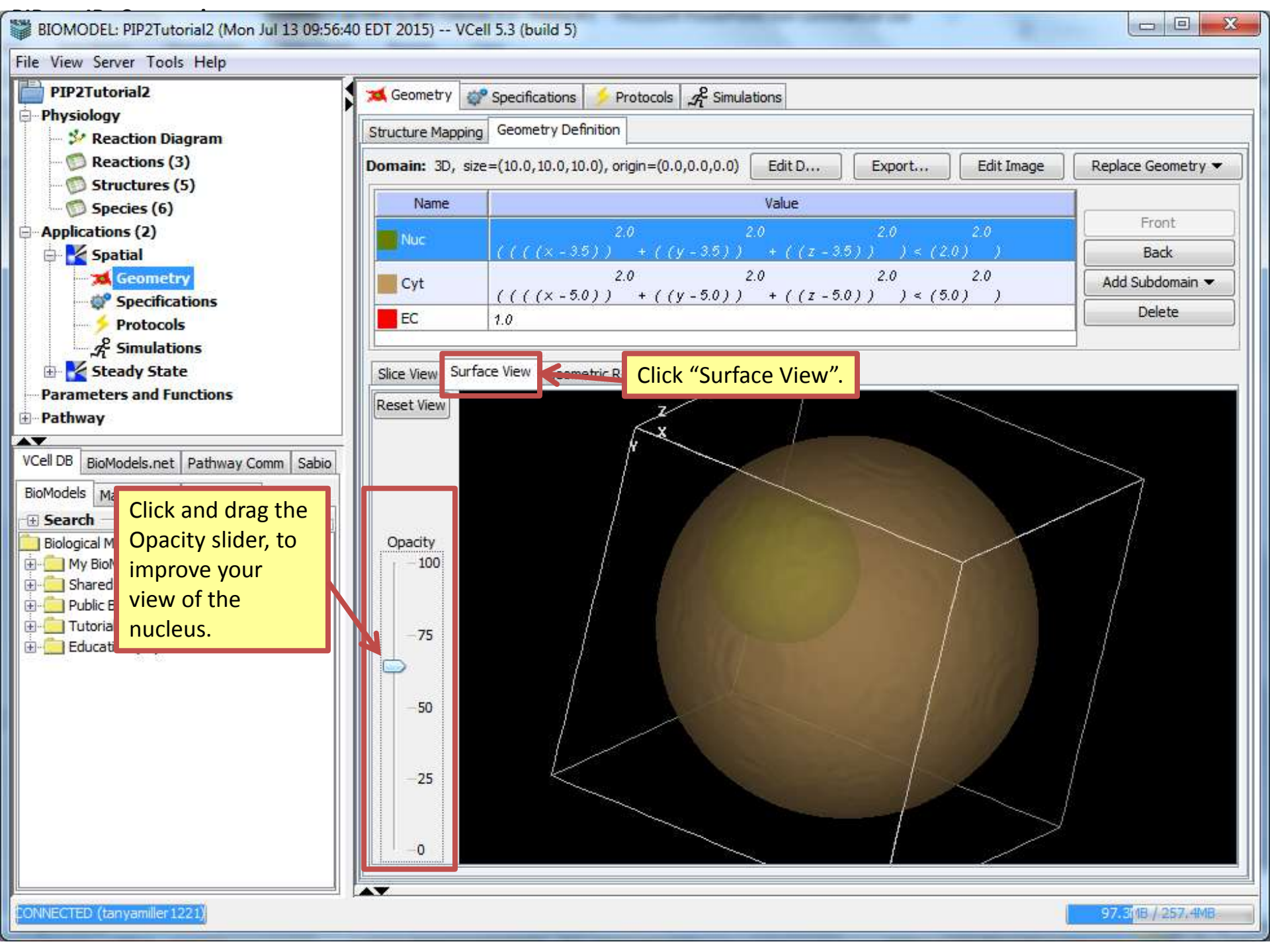
Structure Mapping
Geometry Definition
Domain: 3D, size=(10.0,10.0,10.0), origin=(0.0,0.0,0.0)
Edit D...
Export...
Edit Image
Replace Geometry
Name
Value
Nuc
Cyt
EC
1.0
Front
Back
Add Subdomain
Delete
Double click “subdomain0” and type “Nuc”.
Press “Enter” on your keyboard to finalize.
Slice [0-100]
Z [40] = 4
Axis: XY XZ YZ
Info
VCell DB
BioModels.net
Pathway Comm
Sabio
BioModels
MathModels
Geometries
Search
disconnected
DISCONNECTED
106.9MB / 220.7MB


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 09:56:40 EDT 2015) -- VCell 5.3 (build 5)
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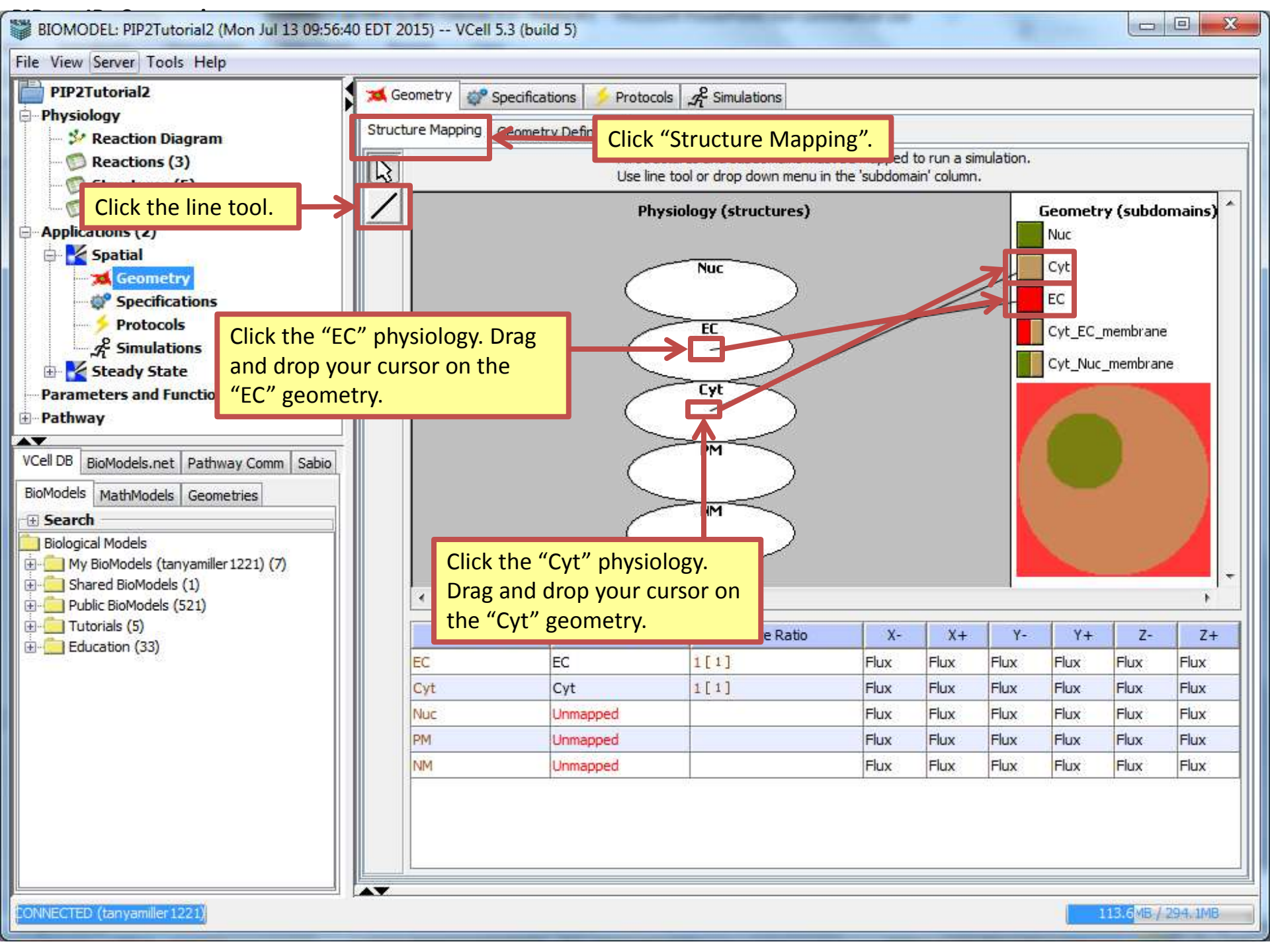
Pathway
Geometry
Specifications
Protocols
Simulations
Structure Mapping
Geometry Definition
Domain: 3D, size=(10.0,10.0,10.0), origin=(0.0,0.0,0.0)
Edit D...
Export...
Edit Image
Replace Geometry
Name
Value
Nuc
Cyt
EC
1.0
Front
Back
Add Subdomain
Delete
Slice View
Surface View
Click “Surface View”.
Reset View
Opacity
100
75
50
25
0
Click and drag the Opacity slider, to improve your view of the nucleus.
VCell DB
BioModels.net
Pathway Comm
Sabio
BioModels
Search
CONNECTED (tanyamiller1221)


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 09:56:40 EDT 2015) -- VCell 5.3 (build 5)
File View Server Tools Help
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BioModels
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Geometry
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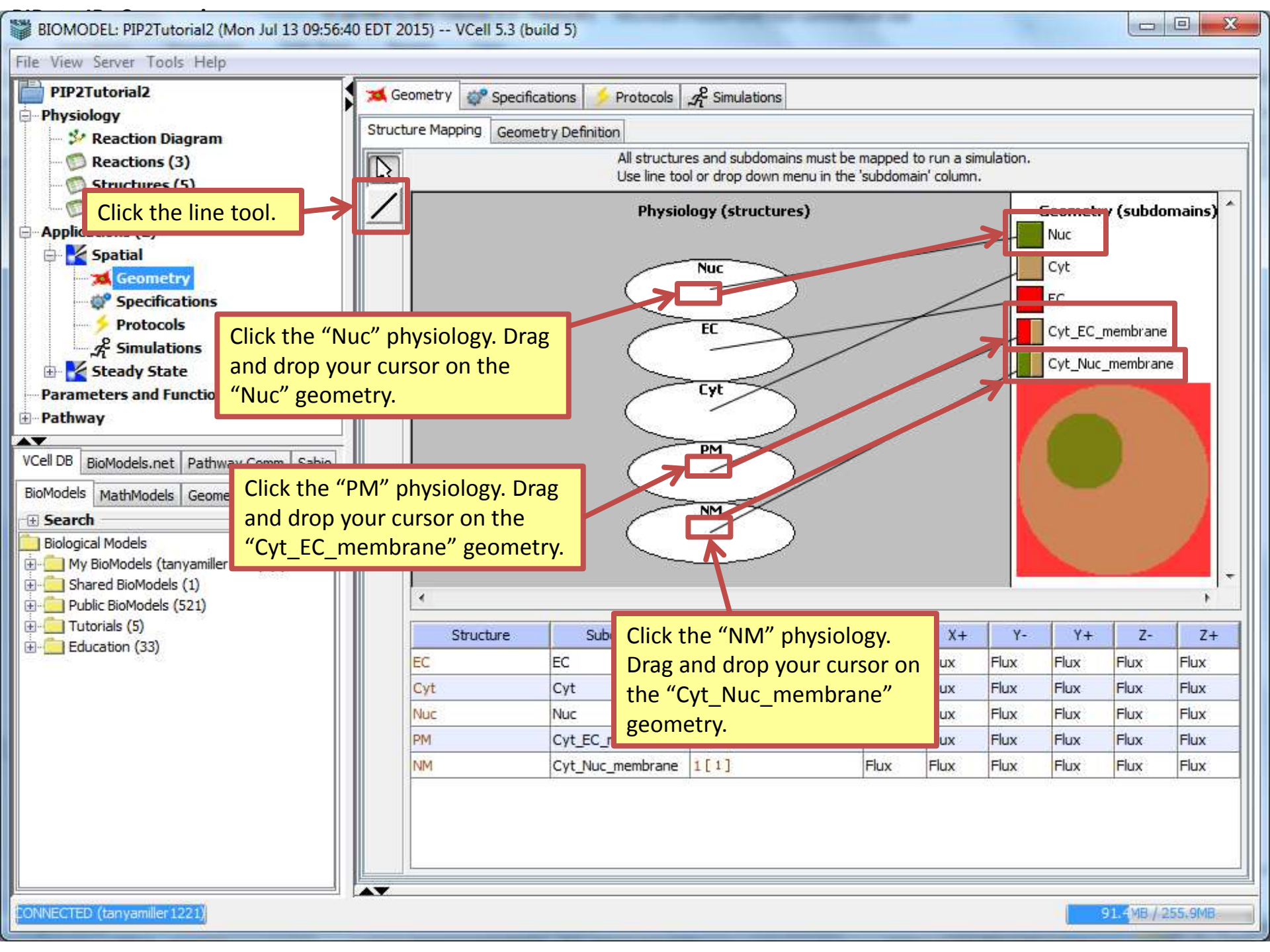
Simulations
Structure Mapping
Click "Structure Mapping".
Use line tool or drop down menu in the 'subdomain' column.
Click the line tool.
Physiology (structures)
Nuc
EC
Cyt
PM
NM
Geometry (subdomains)
Nuc
Cyt
EC
Cyt_EC_membrane
Cyt_Nuc_membrane
Click the "EC" physiology. Drag and drop your cursor on the "EC" geometry.
Click the "Cyt" physiology. Drag and drop your cursor on the "Cyt" geometry.
X- X+ Y- Y+ Z- Z+
EC EC 1 [1] Flux Flux Flux Flux Flux Flux
Cyt Cyt 1 [1] Flux Flux Flux Flux Flux Flux
Nuc Unmapped Flux Flux Flux Flux Flux Flux
PM Unmapped Flux Flux Flux Flux Flux Flux
NM Unmapped Flux Flux Flux Flux Flux Flux
CONNECTED (tanyamiller1221)
113.6MB / 294.1MB


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 09:56:40 EDT 2015) -- VCell 5.3 (build 5)
File View Server Tools Help
PIP2Tutorial2
Physiology
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Reactions (3)
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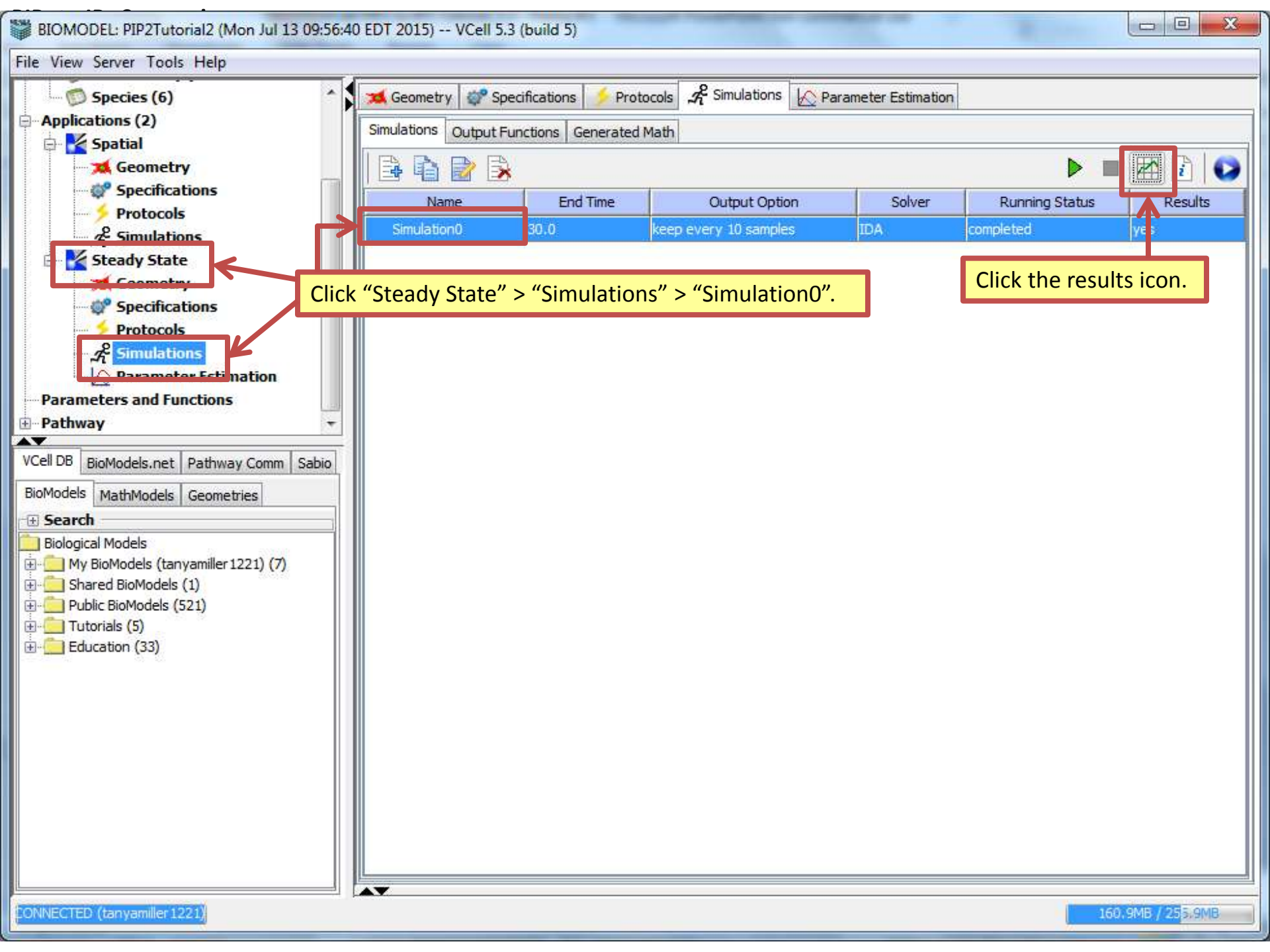
Simulations
Structure Mapping
Geometry Definition
All structures and subdomains must be mapped to run a simulation.
Use line tool or drop down menu in the 'subdomain' column.
Physiology (structures)
Nuc
EC
Cyt
PM
NM
Geometry (subdomains)
Nuc
Cyt
EC
Cyt_EC_membrane
Cyt_Nuc_membrane
Structure
EC
Cyt
Nuc
PM
NM
Cyt_Nuc_membrane
X+
Y-
Y+
Z-
Z+
Flux
CONNECTED (tanyamiller1221)
91.4MB / 255.9MB
Click the line tool.
Click the “Nuc” physiology. Drag and drop your cursor on the “Nuc” geometry.
Click the “PM” physiology. Drag and drop your cursor on the “Cyt_EC_membrane” geometry.
Click the “NM” physiology. Drag and drop your cursor on the “Cyt_Nuc_membrane” geometry.


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 09:56:40 EDT 2015) -- VCell 5.3 (build 5)
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Applications (2)
Spatial
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Simulations
Steady State
Geometry
Specifications
Protocols
Simulations
Parameters and Functions
Pathway
Geometry Specifications Protocols Simulations Parameter Estimation
Simulations Output Functions Generated Math
Name End Time Output Option Solver Running Status Results
Simulation0 30.0 keep every 10 samples IDA completed yes
Click "Steady State" > "Simulations" > "Simulation0".
Click the results icon.
VCell DB BioModels.net Pathway Comm Sabio
BioModels MathModels Geometries
Search
Biological Models
My BioModels (tanyamiller1221) (7)
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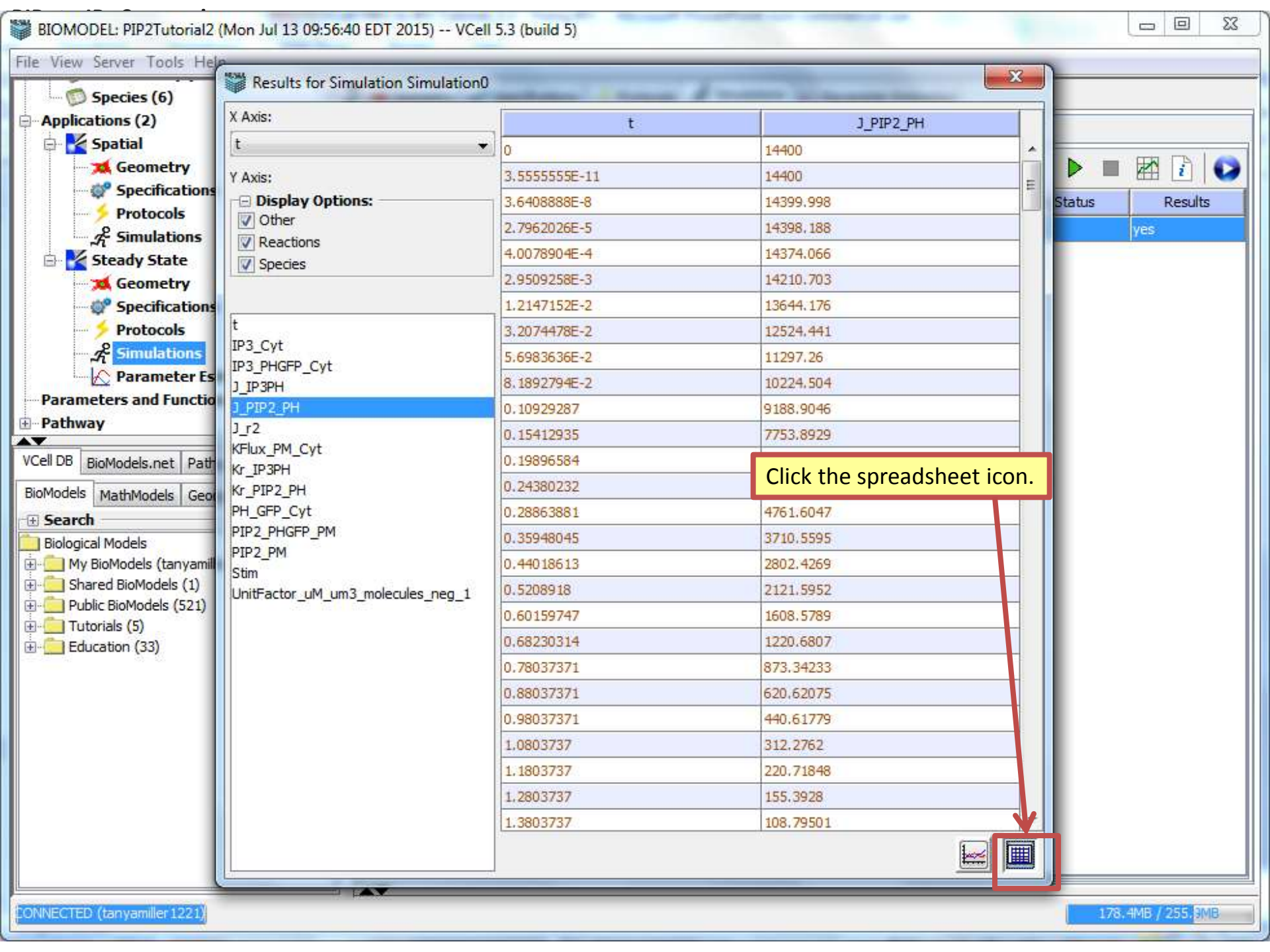
Public BioModels (521)
Tutorials (5)
Education (33)
CONNECTED (tanyamiller1221)
160.9MB / 255.9MB


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 09:56:40 EDT 2015) -- VCell 5.3 (build 5)
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Biological Models
My BioModels (tanyamill
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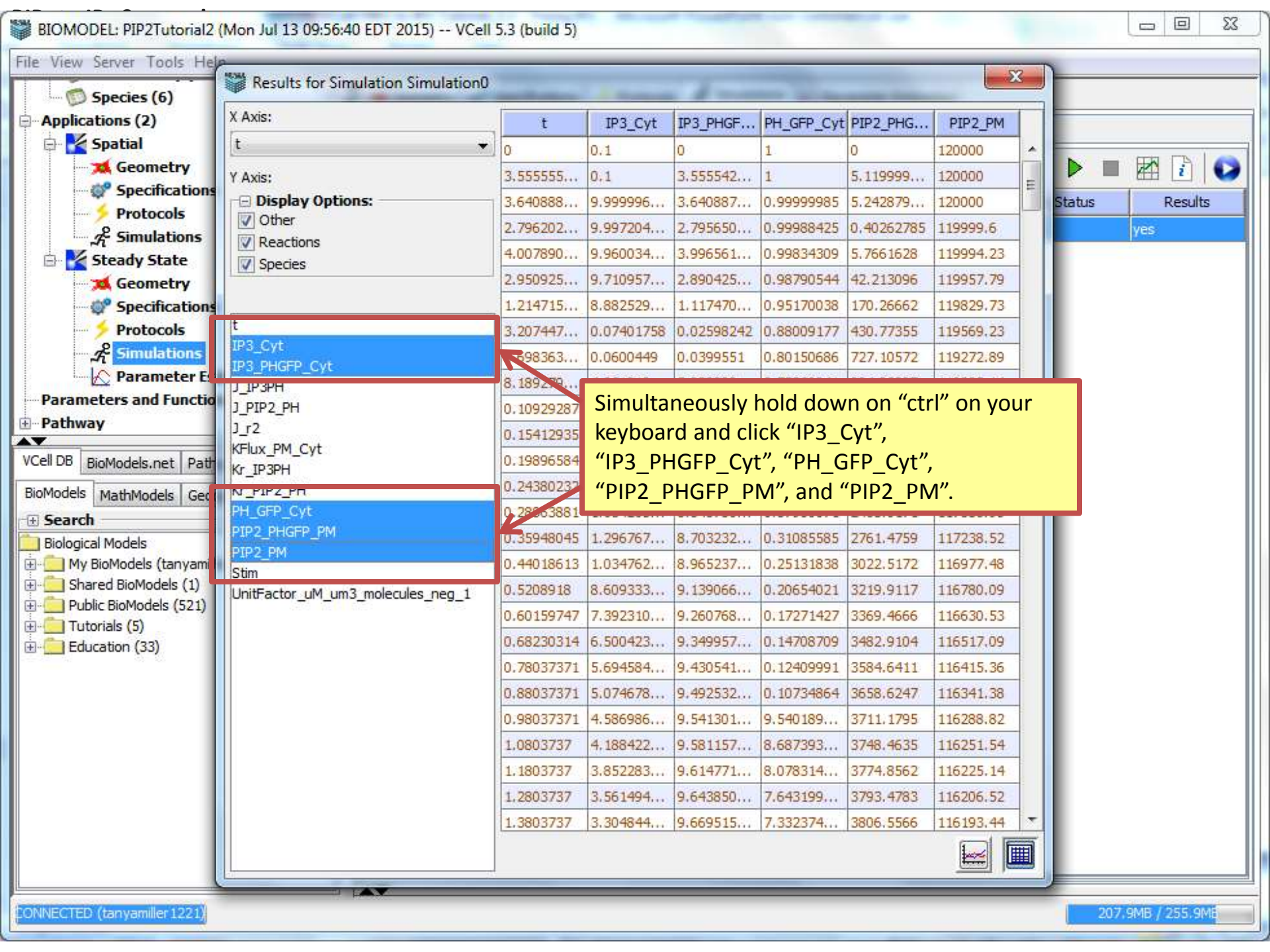
Results for Simulation Simulation0
X Axis:
t
Y Axis:
Display Options:
Other
Reactions
Species
t
IP3_Cyt
IP3_PHGFP_Cyt
J_IP3PH
J_PIP2_PH
J_r2
KFlux_PM_Cyt
Kr_IP3PH
Kr_PIP2_PH
PH_GFP_Cyt
PIP2_PHGFP_PM
PIP2_PM
Stim
UnitFactor_uM_um3_molecules_neg_1
t
J_PIP2_PH
0
14400
3.5555555E-11
14400
3.6408888E-8
14399.998
2.7962026E-5
14398.188
4.0078904E-4
14374.066
2.9509258E-3
14210.703
1.2147152E-2
13644.176
3.2074478E-2
12524.441
5.6983636E-2
11297.26
8.1892794E-2
10224.504
0.10929287
9188.9046
0.15412935
7753.8929
0.19896584
0.24380232
0.28863881
4761.6047
0.35948045
3710.5595
0.44018613
2802.4269
0.5208918
2121.5952
0.60159747
1608.5789
0.68230314
1220.6807
0.78037371
873.34233
0.88037371
620.62075
0.98037371
440.61779
1.0803737
312.2762
1.1803737
220.71848
1.2803737
155.3928
1.3803737
108.79501
Click the spreadsheet icon.
Status
Results
yes
CONNECTED (tanyamiller1221)
178.4MB / 255.3MB


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 09:56:40 EDT 2015) -- VCell 5.3 (build 5)
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Public BioModels (521)
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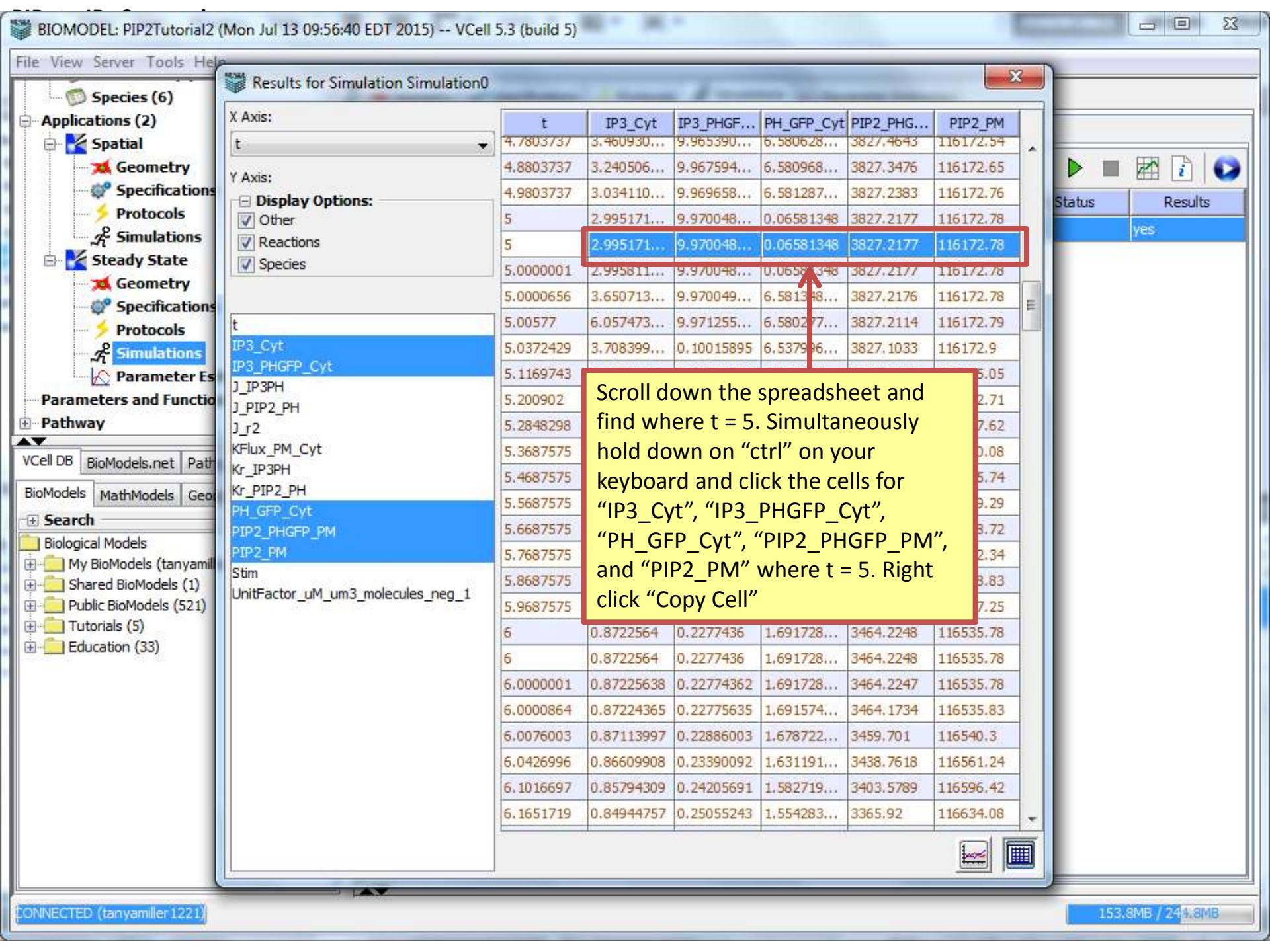
Results for Simulation Simulation0
X Axis:
t
Y Axis:
Display Options:
Other
Reactions
Species
t
IP3_Cyt
IP3_PHGFP_Cyt
J_IP3PH
J_PIP2_PH
J_r2
KFlux_PM_Cyt
Kr_IP3PH
PH_GFP_Cyt
PIP2_PHGFP_PM
PIP2_PM
Stim
UnitFactor_uM_um3_molecules_neg_1
t | IP3_Cyt | IP3_PHGF... | PH_GFP_Cyt | PIP2_PHG... | PIP2_PM
0 | 0.1 | 0 | 1 | 0 | 120000
3.555555... | 0.1 | 3.555542... | 1 | 5.119999... | 120000
3.640888... | 9.999996... | 3.640887... | 0.99999985 | 5.242879... | 120000
2.796202... | 9.997204... | 2.795650... | 0.99988425 | 0.40262785 | 119999.6
4.007890... | 9.960034... | 3.996561... | 0.99834309 | 5.7661628 | 119994.23
2.950925... | 9.710957... | 2.890425... | 0.98790544 | 42.213096 | 119957.79
1.214715... | 8.882529... | 1.117470... | 0.95170038 | 170.26662 | 119829.73
3.207447... | 0.07401758 | 0.02598242 | 0.88009177 | 430.77355 | 119569.23
698363... | 0.0600449 | 0.0399551 | 0.80150686 | 727.10572 | 119272.89
0.10929287
0.15412935
0.19896584
0.35948045 | 1.296767... | 8.703232... | 0.31085585 | 2761.4759 | 117238.52
0.44018613 | 1.034762... | 8.965237... | 0.25131838 | 3022.5172 | 116977.48
0.5208918 | 8.609333... | 9.139066... | 0.20654021 | 3219.9117 | 116780.09
0.60159747 | 7.392310... | 9.260768... | 0.17271427 | 3369.4666 | 116630.53
0.68230314 | 6.500423... | 9.349957... | 0.14708709 | 3482.9104 | 116517.09
0.78037371 | 5.694584... | 9.430541... | 0.12409991 | 3584.6411 | 116415.36
0.88037371 | 5.074678... | 9.492532... | 0.10734864 | 3658.6247 | 116341.38
0.98037371 | 4.586986... | 9.541301... | 9.540189... | 3711.1795 | 116288.82
1.0803737 | 4.188422... | 9.581157... | 8.687393... | 3748.4635 | 116251.54
1.1803737 | 3.852283... | 9.614771... | 8.078314... | 3774.8562 | 116225.14
1.2803737 | 3.561494... | 9.643850... | 7.643199... | 3793.4783 | 116206.52
1.3803737 | 3.304844... | 9.669515... | 7.332374... | 3806.5566 | 116193.44
Simultaneously hold down on “ctrl” on your keyboard and click “IP3_Cyt”, “IP3_PHGFP_Cyt”, “PH_GFP_Cyt”, “PIP2_PHGFP_PM”, and “PIP2_PM”.
Status
Results
yes
CONNECTED (tanyamiller1221)
207.9MB / 255.9MB


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 09:56:40 EDT 2015) -- VCell 5.3 (build 5)
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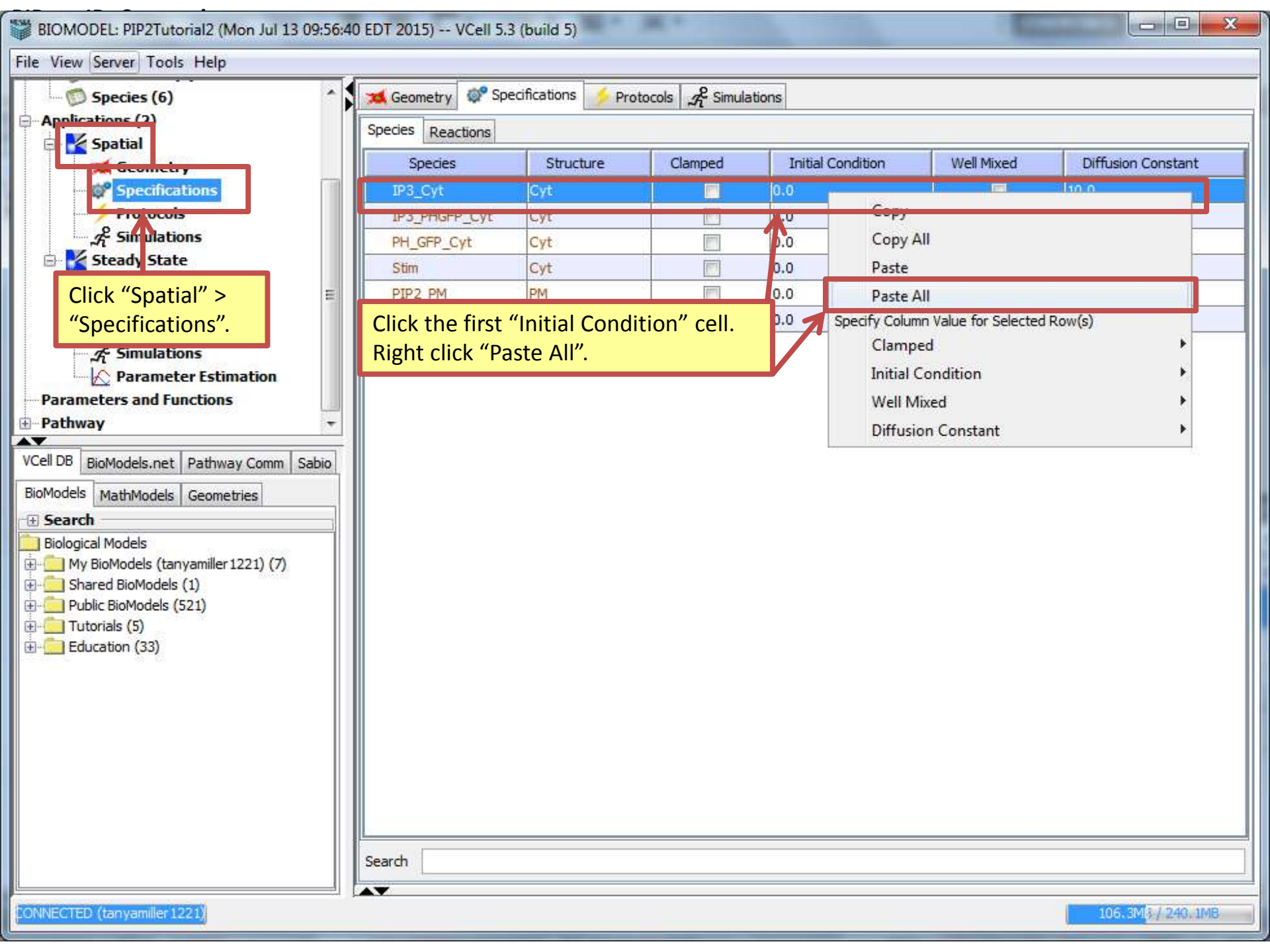
Education (33)
Results for Simulation Simulation0
X Axis:
t
Y Axis:
Display Options:
Other
Reactions
Species
t
IP3_Cyt
IP3_PHGFP_Cyt
J_IP3PH
J_PIP2_PH
J_r2
KFlux_PM_Cyt
Kr_IP3PH
Kr_PIP2_PH
PH_GFP_Cyt
PIP2_PHGFP_PM
PIP2_PM
Stim
UnitFactor_uM_um3_molecules_neg_1
t
IP3_Cyt
IP3_PHGF...
PH_GFP_Cyt
PIP2_PHG...
PIP2_PM
4.8803737 3.240506... 9.967594... 6.580968... 3827.3476 116172.65
4.9803737 3.034110... 9.969658... 6.581287... 3827.2383 116172.76
5 2.995171... 9.970048... 0.06581348 3827.2177 116172.78
5 2.995171... 9.970048... 0.06581348 3827.2177 116172.78
5.0000656 3.650713... 9.970049... 6.581348... 3827.2176 116172.78
5.00577 6.057473... 9.971255... 6.580277... 3827.2114 116172.79
5.0372429 3.708399... 0.10015895 6.537996... 3827.1033 116172.9
6 0.8722564 0.2277436 1.691728... 3464.2248 116535.78
6 0.8722564 0.2277436 1.691728... 3464.2248 116535.78
6.0000001 0.87225638 0.22774362 1.691728... 3464.2247 116535.78
6.0000864 0.87224365 0.22775635 1.691574... 3464.1734 116535.83
6.0076003 0.87113997 0.22886003 1.678722... 3459.701 116540.3
6.0426996 0.86609908 0.23390092 1.631191... 3438.7618 116561.24
6.1016697 0.85794309 0.24205691 1.582719... 3403.5789 116596.42
6.1651719 0.84944757 0.25055243 1.554283... 3365.92 116634.08
Scroll down the spreadsheet and find where t = 5. Simultaneously hold down on “ctrl” on your keyboard and click the cells for “IP3_Cyt”, “IP3_PHGFP_Cyt”, “PH_GFP_Cyt”, “PIP2_PHGFP_PM”, and “PIP2_PM” where t = 5. Right click “Copy Cell”
Status
Results
yes
CONNECTED (tanyamiller1221)
153.8MB / 244.8MB


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 09:56:40 EDT 2015) -- VCell 5.3 (build 5)
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Pathway
Click "Spatial" > "Specifications".
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Pathway Comm
Sabio
BioModels
MathModels
Geometries
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Shared BioModels (1)
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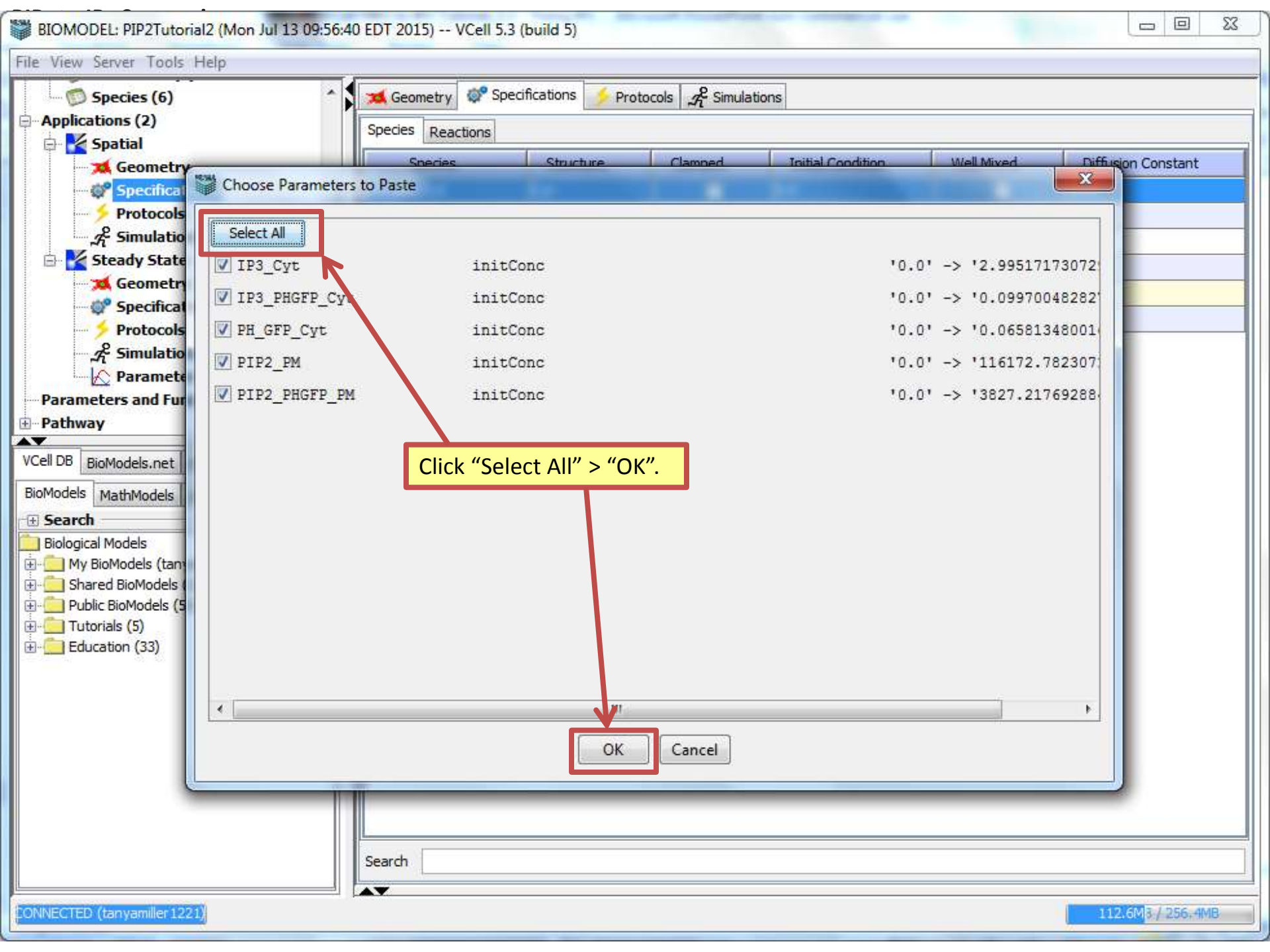
Reactions
Species
Structure
Clamped
Initial Condition
Well Mixed
Diffusion Constant
IP3_Cyt
Cyt
0.0
PH_GFP_Cyt
Stim
PIP2_PM
PM
Copy All
Paste
Paste All
Specify Column Value for Selected Row(s)
Clamped
Initial Condition
Well Mixed
Diffusion Constant
Click the first "Initial Condition" cell.
Right click "Paste All".
Search
CONNECTED (tanyamiller1221)


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 09:56:40 EDT 2015) -- VCell 5.3 (build 5)
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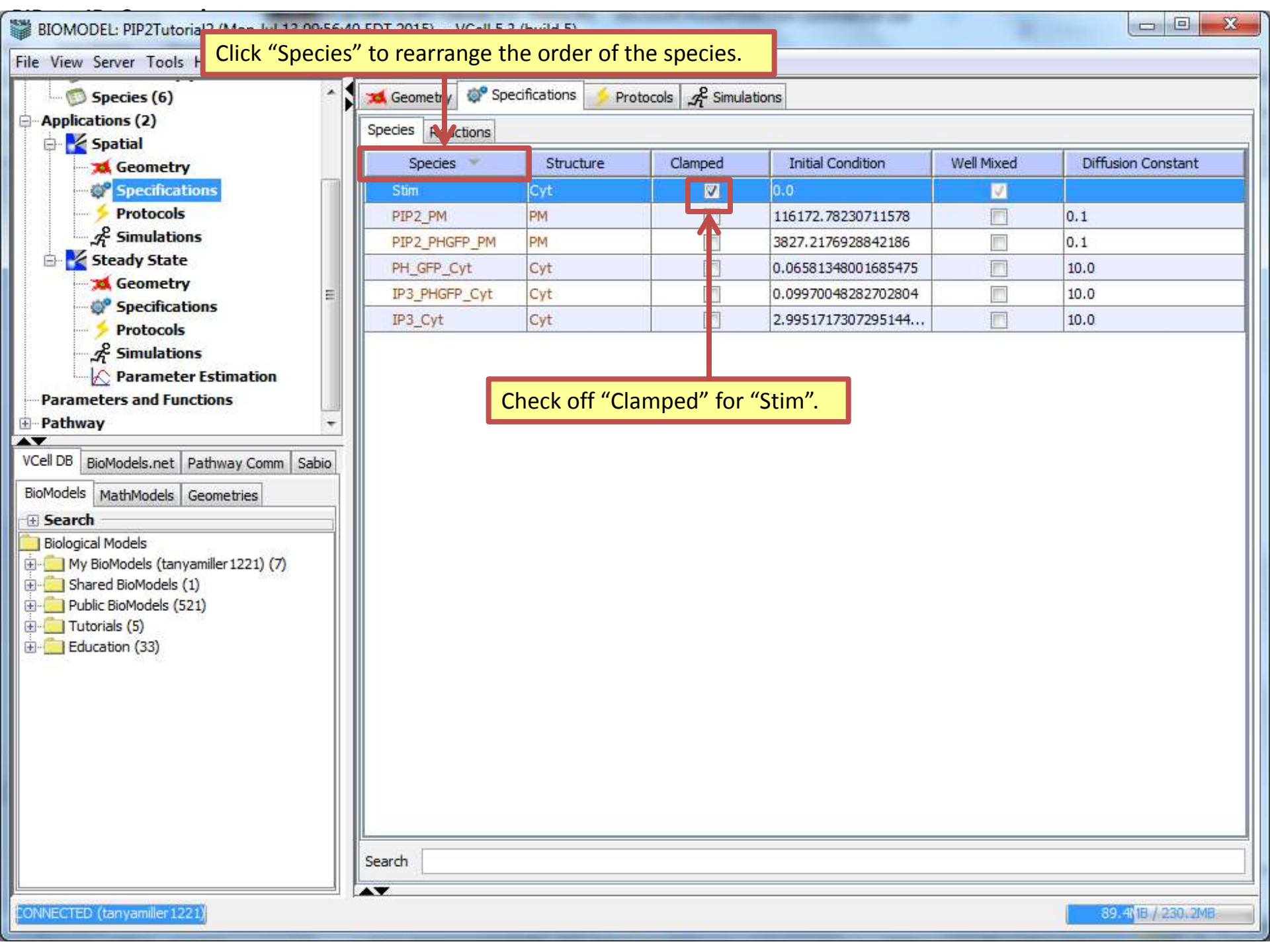
Steady State
Parameters and Fu
Pathway
Species
Reactions
Structure
Clamped
Initial Condition
Well Mixed
Diffusion Constant
Choose Parameters to Paste
Select All
IP3_Cyt initConc '0.0' -> '2.99517173072
IP3_PHGFP_Cyt initConc '0.0' -> '0.09970048282
PH_GFP_Cyt initConc '0.0' -> '0.06581348001
PIP2_PM initConc '0.0' -> '116172.782307
PIP2_PHGFP_PM initConc '0.0' -> '3827.21769288
Click “Select All” > “OK”.
OK
Cancel
VCell DB
BioModels.net
BioModels
MathModels
Search
Biological Models
My BioModels (tan
Shared BioModels
Public BioModels (5
Tutorials (5)
Education (33)
Search
CONNECTED (tanyamiller1221)
112.6MB / 256.4MB


Click “Species” to rearrange the order of the species.
Check off “Clamped” for “Stim”.
BIOMODEL: PIP2Tutorial2
File View Server Tools
Species (6)
Applications (2)
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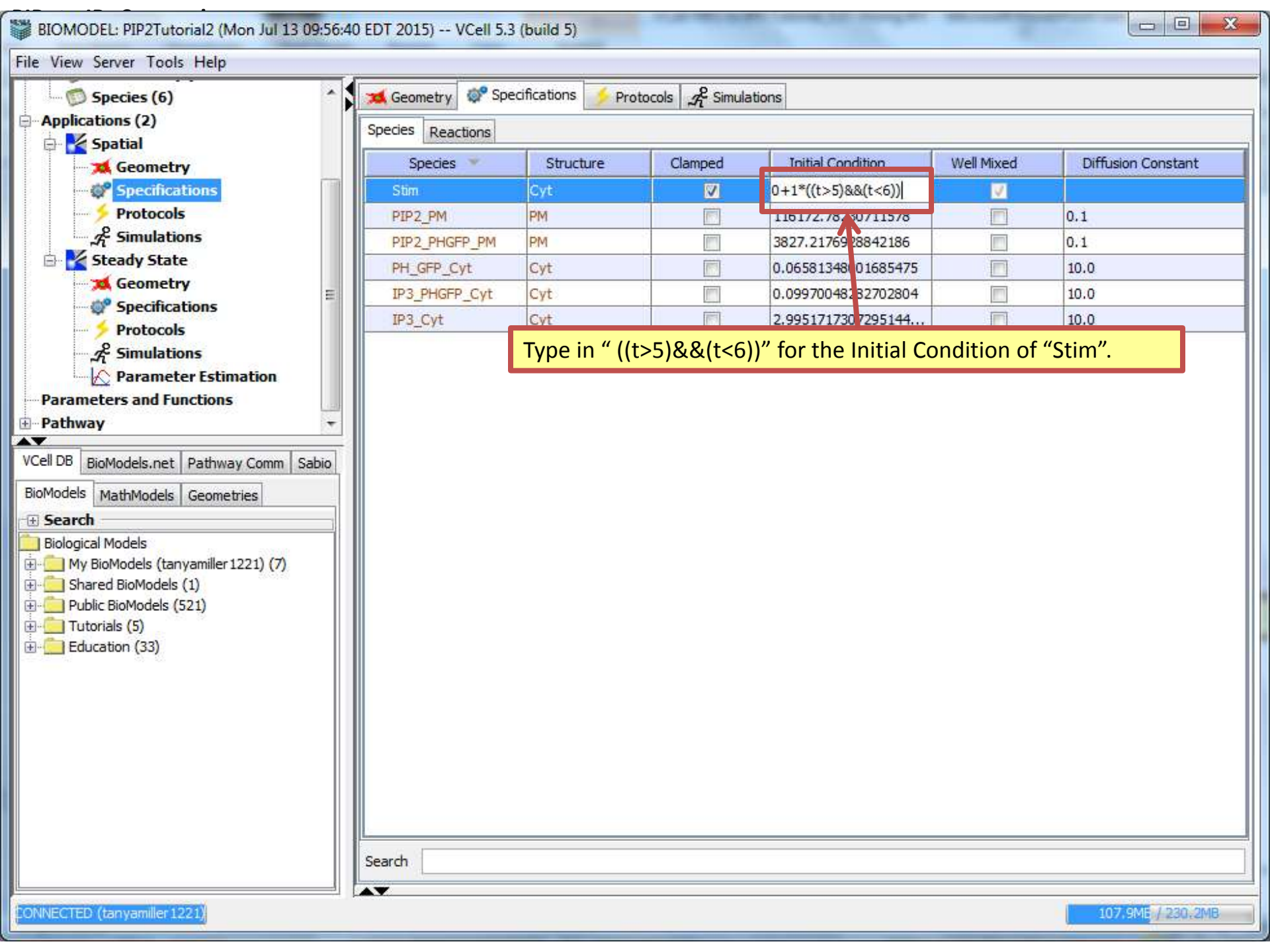
Species
Reactions
Species
Structure
Clamped
Initial Condition
Well Mixed
Diffusion Constant
Stim
Cyt
0.0
PIP2_PM
PM
116172.78230711578
0.1
PIP2_PHGFP_PM
PM
3827.2176928842186
0.1
PH_GFP_Cyt
Cyt
0.06581348001685475
10.0
IP3_PHGFP_Cyt
Cyt
0.09970048282702804
10.0
IP3_Cyt
Cyt
2.9951717307295144...
10.0
Search
CONNECTED (tanyamiller1221)


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 09:56:40 EDT 2015) -- VCell 5.3 (build 5)
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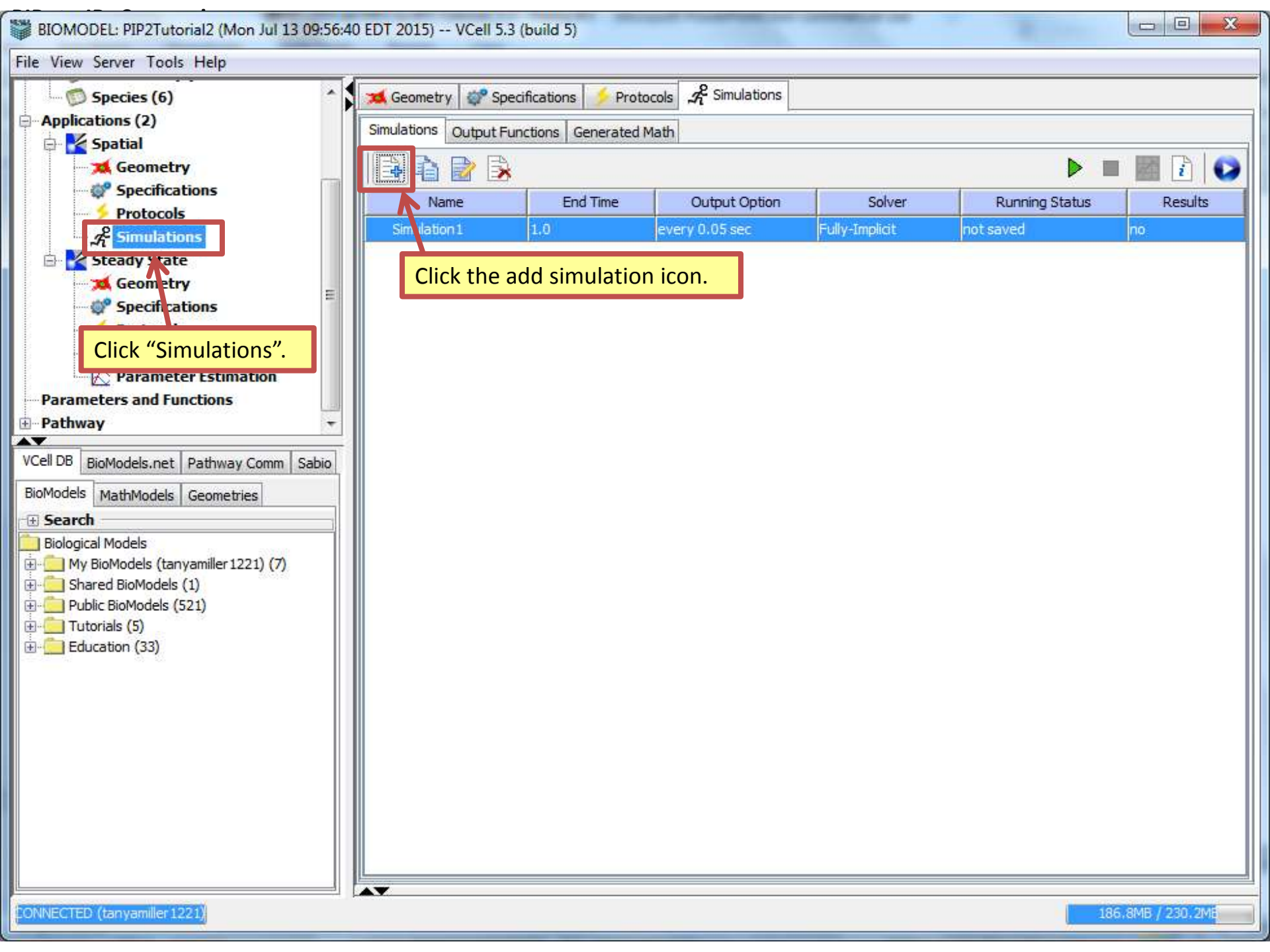
Species
Structure
Clamped
Initial Condition
Well Mixed
Diffusion Constant
Stim
Cyt
0+1*((t>5)&&(t<6))
PIP2_PM
PM
0.1
PIP2_PHGFP_PM
PM
3827.21769
0.1
PH_GFP_Cyt
Cyt
10.0
IP3_PHGFP_Cyt
Cyt
10.0
IP3_Cyt
Cyt
10.0
Type in " ((t>5)&&(t<6))" for the Initial Condition of "Stim".
Search
CONNECTED (tanyamiller1221)
107.9MB / 230.2MB


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 09:56:40 EDT 2015) -- VCell 5.3 (build 5)
File View Server Tools Help
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Pathway
Click "Simulations".
Geometry
Specifications
Protocols
Simulations
Simulations
Output Functions
Generated Math
Name
End Time
Output Option
Solver
Running Status
Results
Simulation1
1.0
every 0.05 sec
Fully-Implicit
not saved
no
Click the add simulation icon.
VCell DB
BioModels.net
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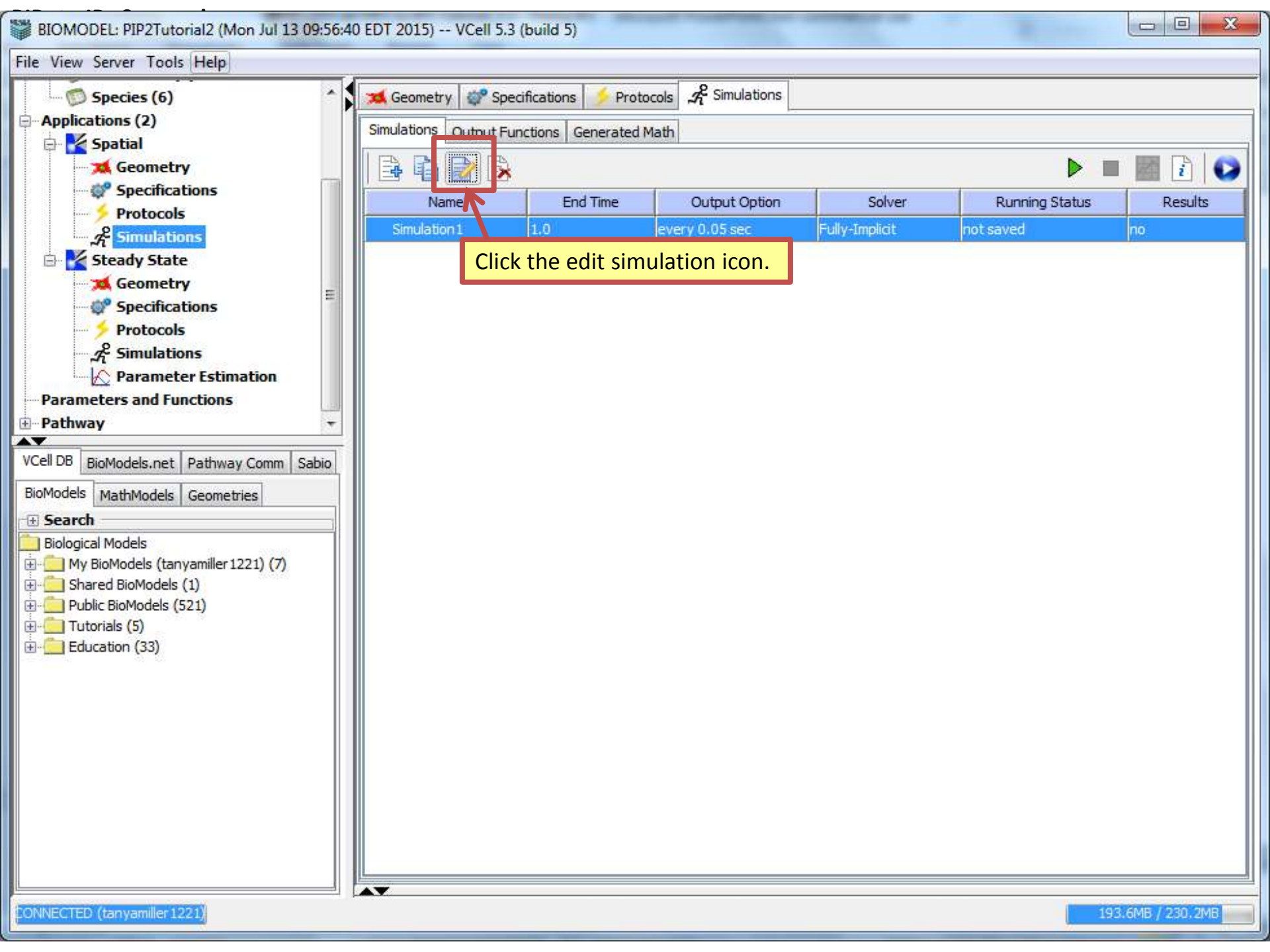
CONNECTED (tanyamiller1221)
186.8MB / 230.2MB


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 09:56:40 EDT 2015) -- VCell 5.3 (build 5)
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Simulations
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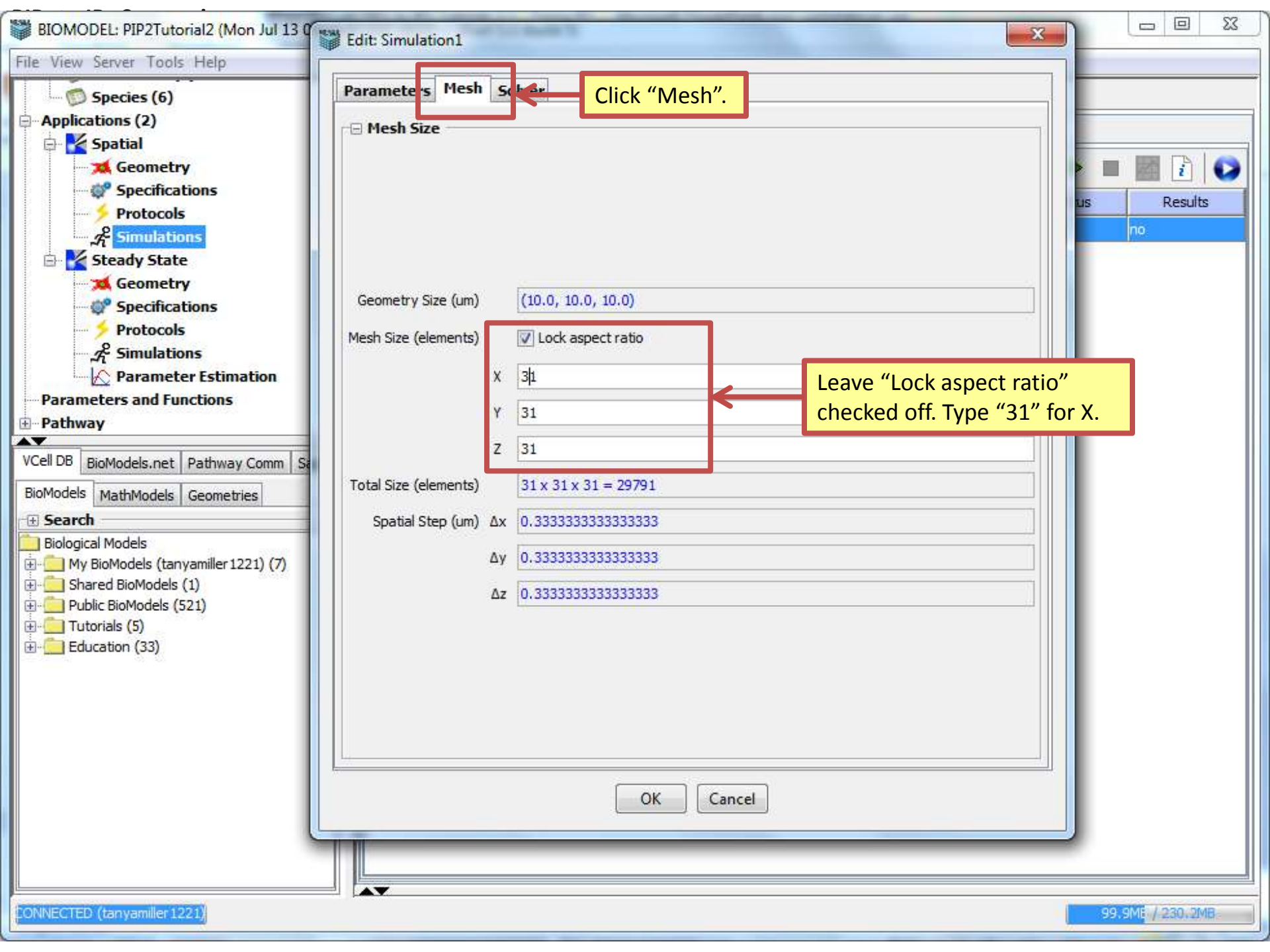
Generated Math
Name
End Time
Output Option
Solver
Running Status
Results
Simulation1
1.0
every 0.05 sec
Fully-Implicit
not saved
no
Click the edit simulation icon.
CONNECTED (tanyamiller1221)
193.6MB / 230.2MB


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 0
File View Server Tools Help
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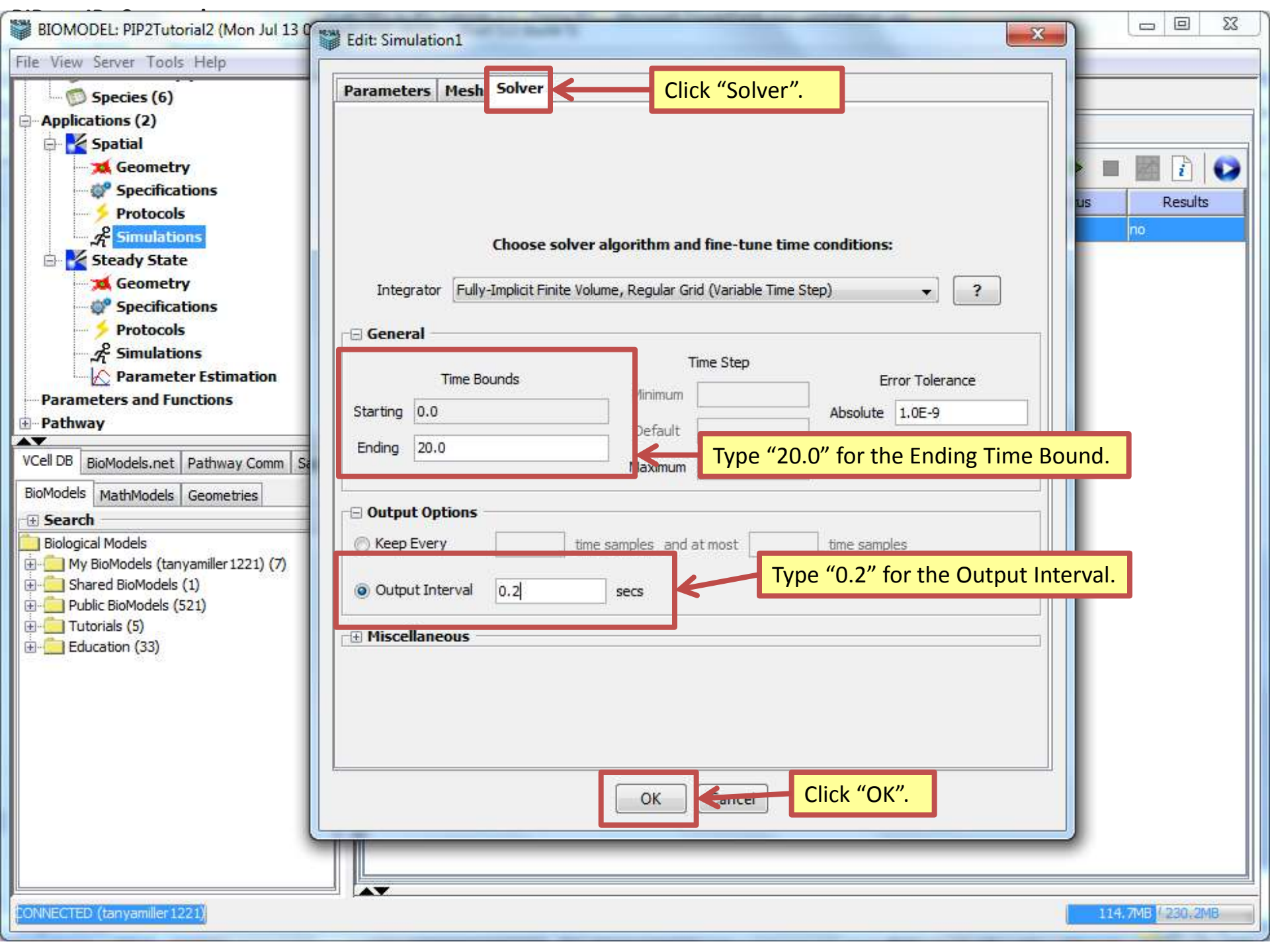
Education (33)
CONNECTED (tanyamiller1221)
Edit: Simulation1
Parameters
Mesh
Solver
Click “Mesh”.
Mesh Size
Geometry Size (um)
(10.0, 10.0, 10.0)
Mesh Size (elements)
Lock aspect ratio
X
31
Y
31
Z
31
Leave “Lock aspect ratio” checked off. Type “31” for X.
Total Size (elements)
31 x 31 x 31 = 29791
Spatial Step (um)
Δx
0.3333333333333333
Δy
0.3333333333333333
Δz
0.3333333333333333
OK
Cancel
Results
no
99.9MB / 230.2MB


BIOMODEL: PIP2Tutorial2 (Mon Jul 13
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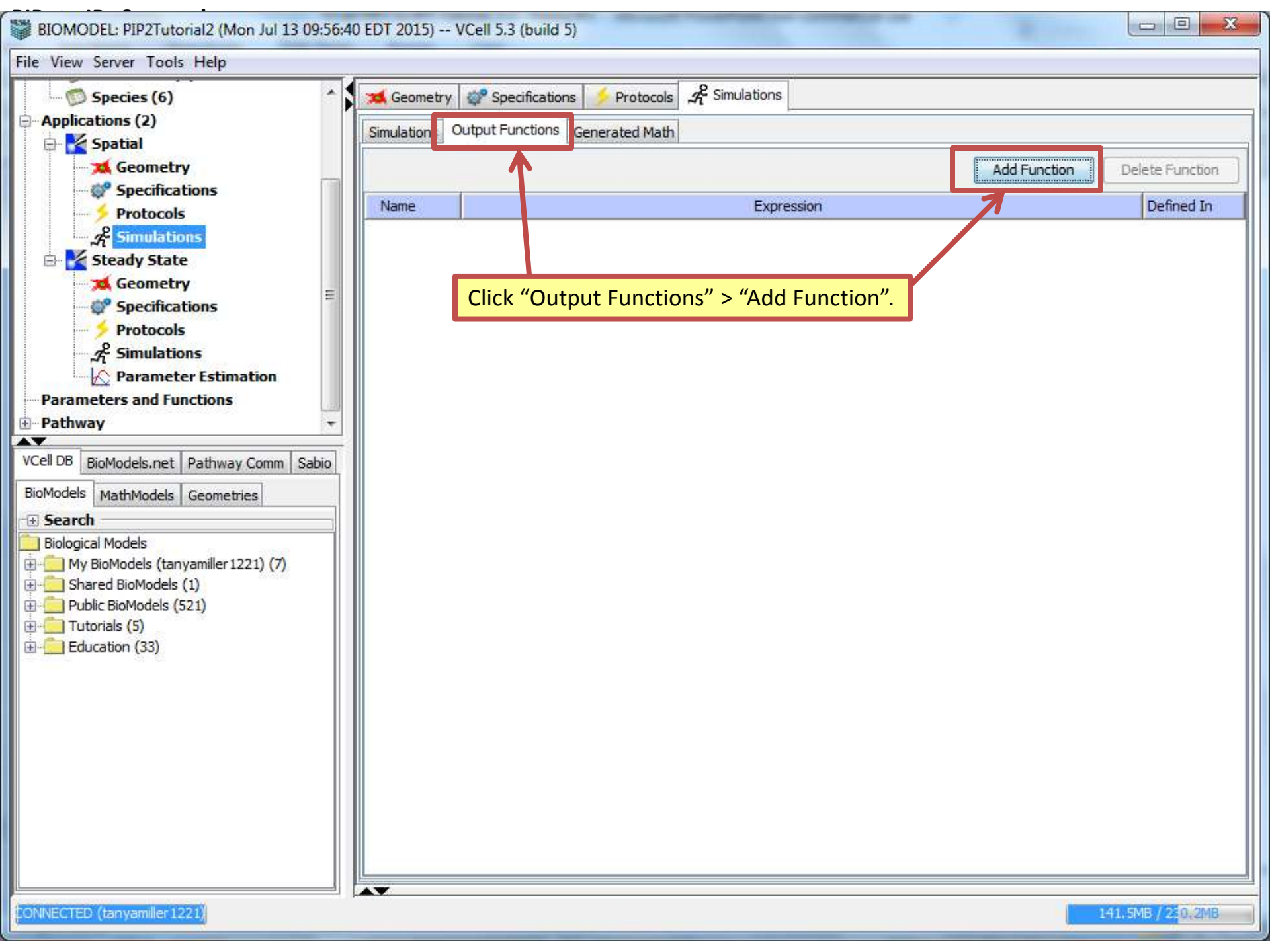
CONNECTED (tanyamiller1221)
Edit: Simulation1
Parameters
Mesh
Solver
Click “Solver”.
Choose solver algorithm and fine-tune time conditions:
Integrator
Fully-Implicit Finite Volume, Regular Grid (Variable Time Step)
?
General
Time Bounds
Starting
0.0
Ending
20.0
Time Step
Minimum
Default
Maximum
Error Tolerance
Absolute
1.0E-9
Type “20.0” for the Ending Time Bound.
Output Options
Keep Every
time samples and at most
time samples
Output Interval
0.2
secs
Type “0.2” for the Output Interval.
Miscellaneous
OK
Cancel
Click “OK”.
Results
no
114.7MB
230.2MB


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 09:56:40 EDT 2015) -- VCell 5.3 (build 5)
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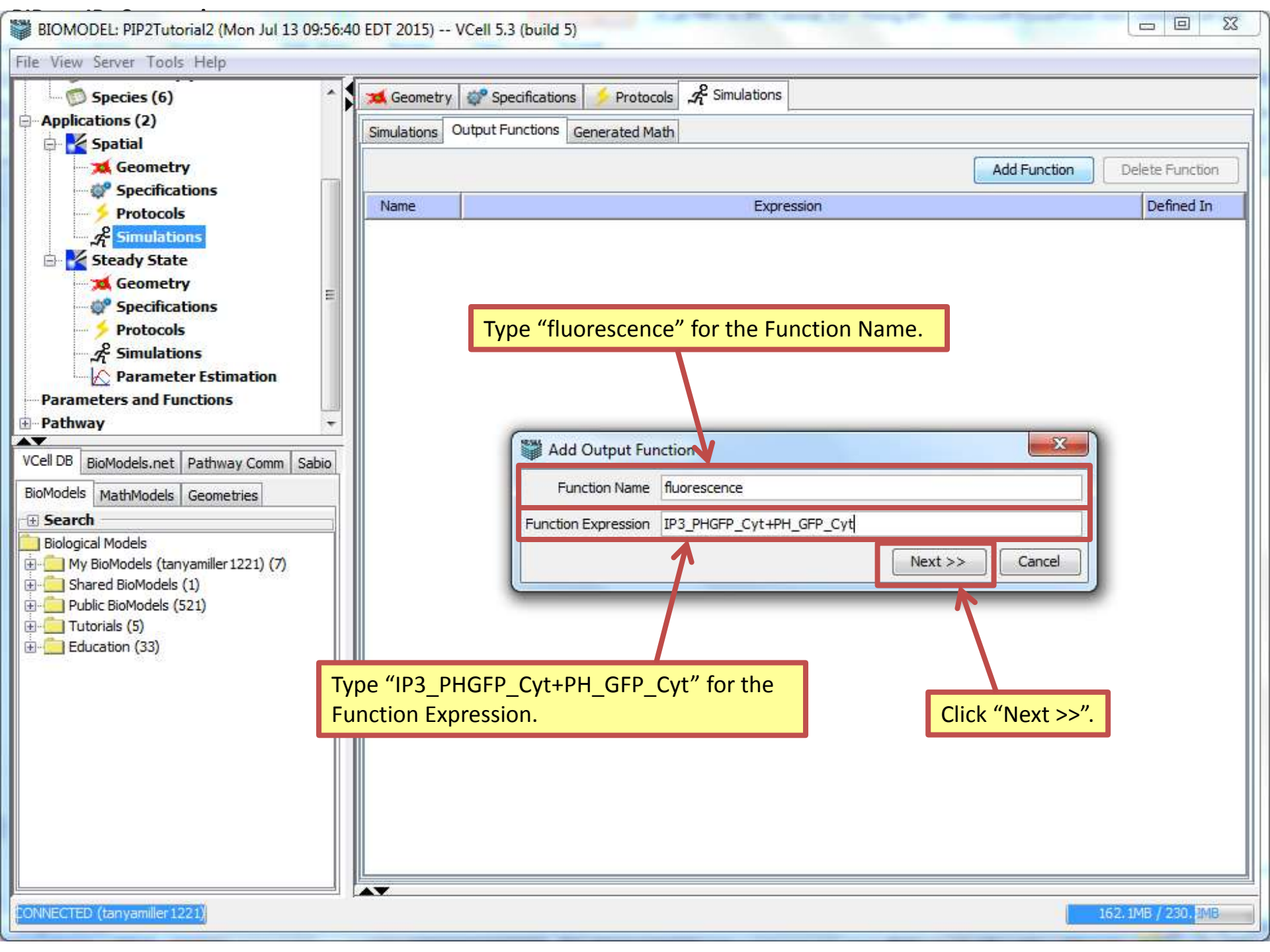
Simulation
Output Functions
Generated Math
Add Function
Delete Function
Name
Expression
Defined In
Click “Output Functions” > “Add Function”.
CONNECTED (tanyamiller1221)
141.5MB / 230.2MB


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 09:56:40 EDT 2015) -- VCell 5.3 (build 5)
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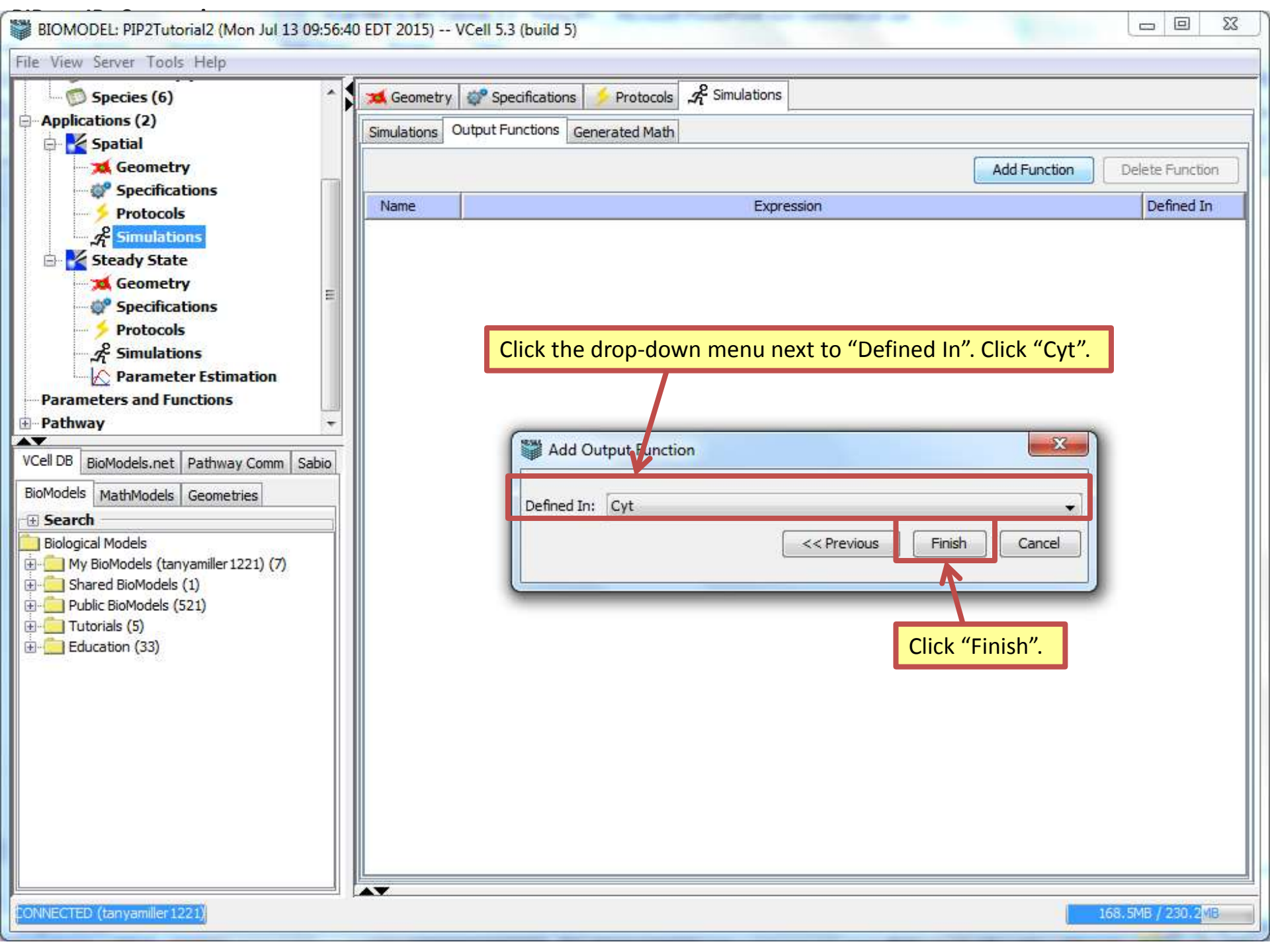
Simulations
Output Functions
Generated Math
Add Function
Delete Function
Name
Expression
Defined In
Type “fluorescence” for the Function Name.
Add Output Function
Function Name
fluorescence
Function Expression
IP3_PHGFP_Cyt+PH_GFP_Cyt
Next >>
Cancel
Type “IP3_PHGFP_Cyt+PH_GFP_Cyt” for the Function Expression.
Click “Next >>”.
CONNECTED (tanyamiller1221)
162.1MB / 230.


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 09:56:40 EDT 2015) -- VCell 5.3 (build 5)
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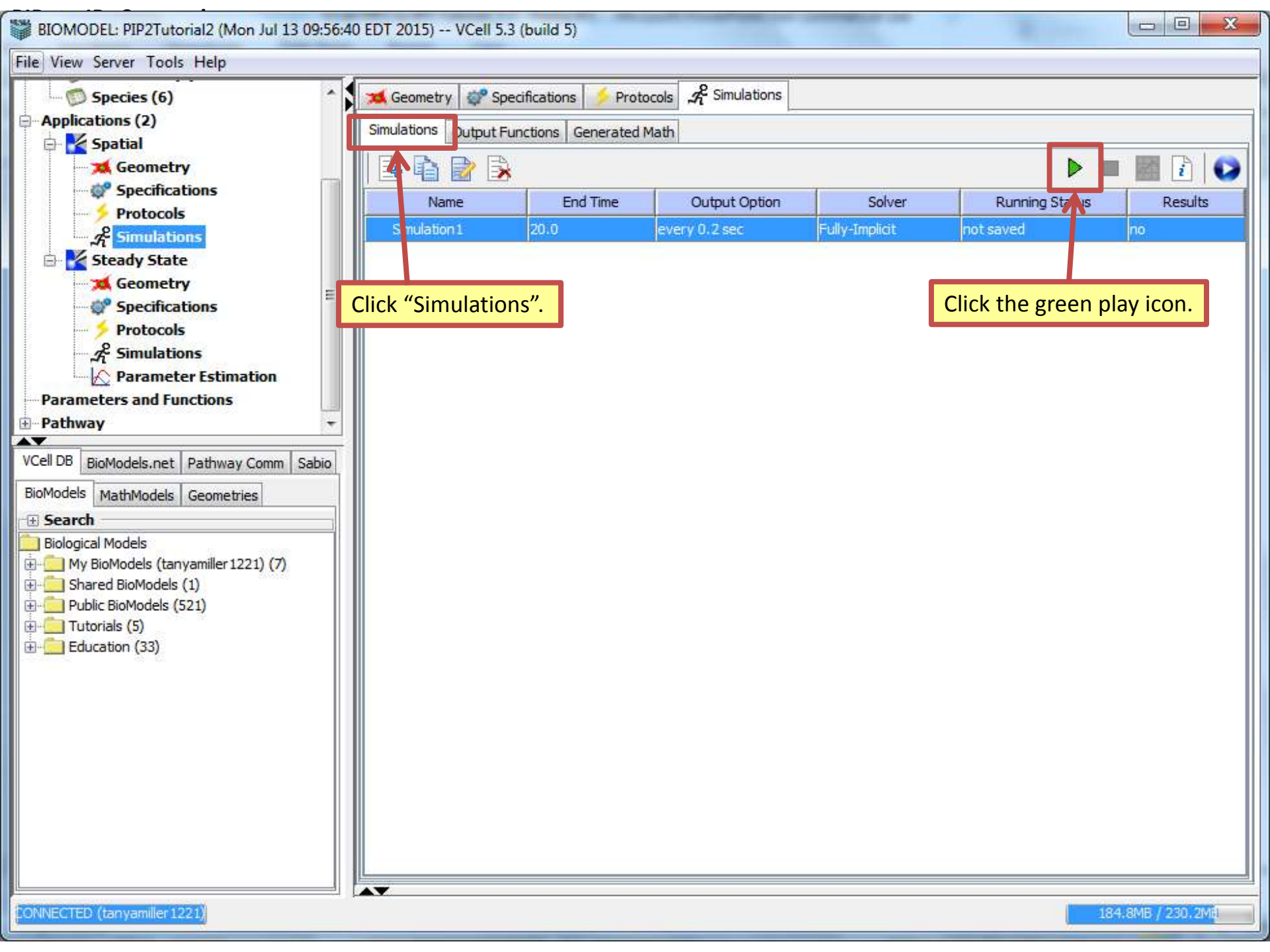
Simulations
Output Functions
Generated Math
Add Function
Delete Function
Name
Expression
Defined In
Click the drop-down menu next to “Defined In”. Click “Cyt”.
Add Output Function
Defined In:
Cyt
<< Previous
Finish
Cancel
Click “Finish”.
CONNECTED (tanyamiller1221)
168.5MB / 230.2MB


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 09:56:40 EDT 2015) -- VCell 5.3 (build 5)
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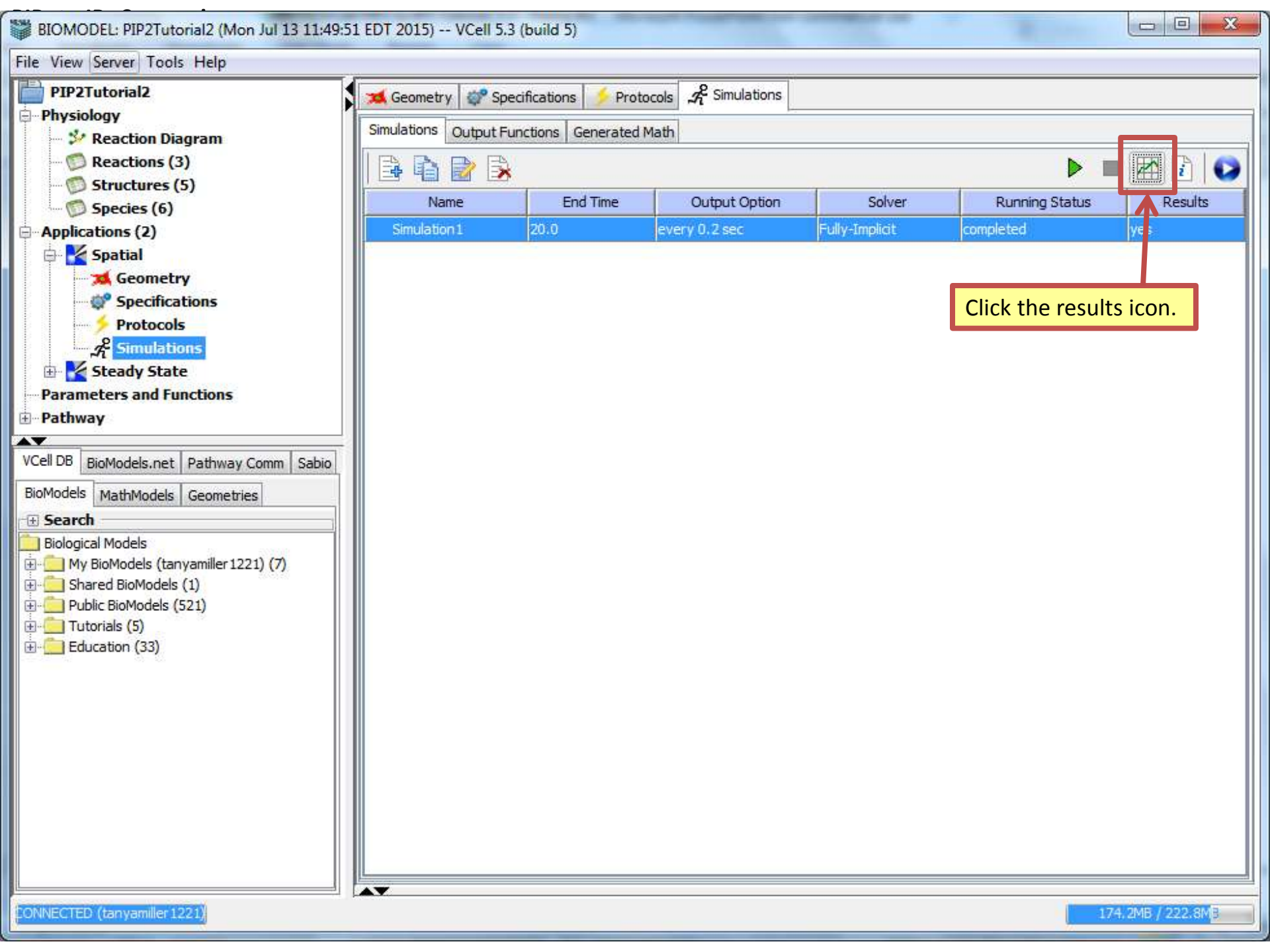
Simulations
Output Functions
Generated Math
Name
End Time
Output Option
Solver
Running Status
Results
Simulation1
20.0
every 0.2 sec
Fully-Implicit
not saved
no
Click "Simulations".
Click the green play icon.
CONNECTED (tanyamiller1221)
184.8MB / 230.2MB


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 11:49:51 EDT 2015) -- VCell 5.3 (build 5)
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Reactions (3)
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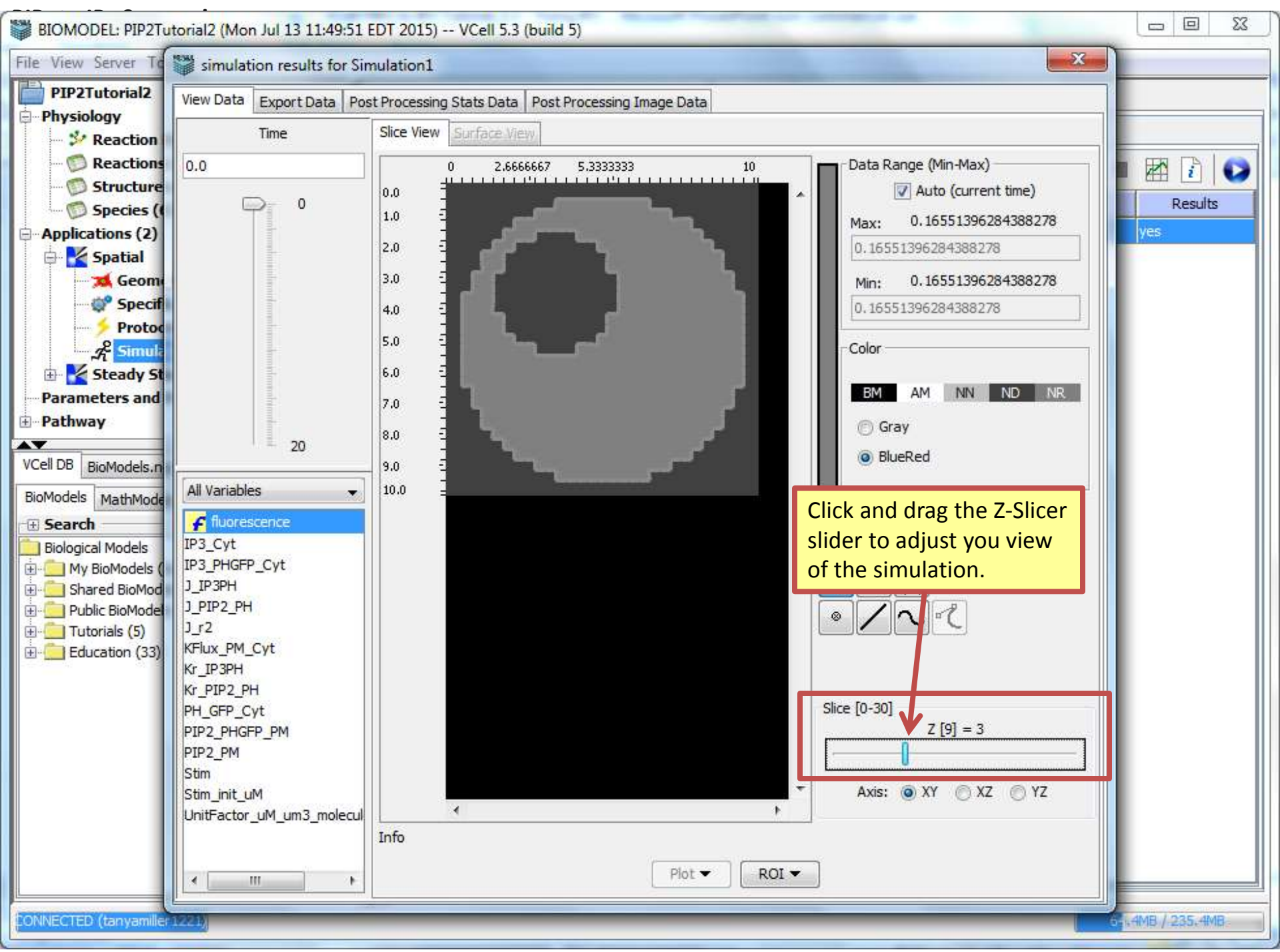
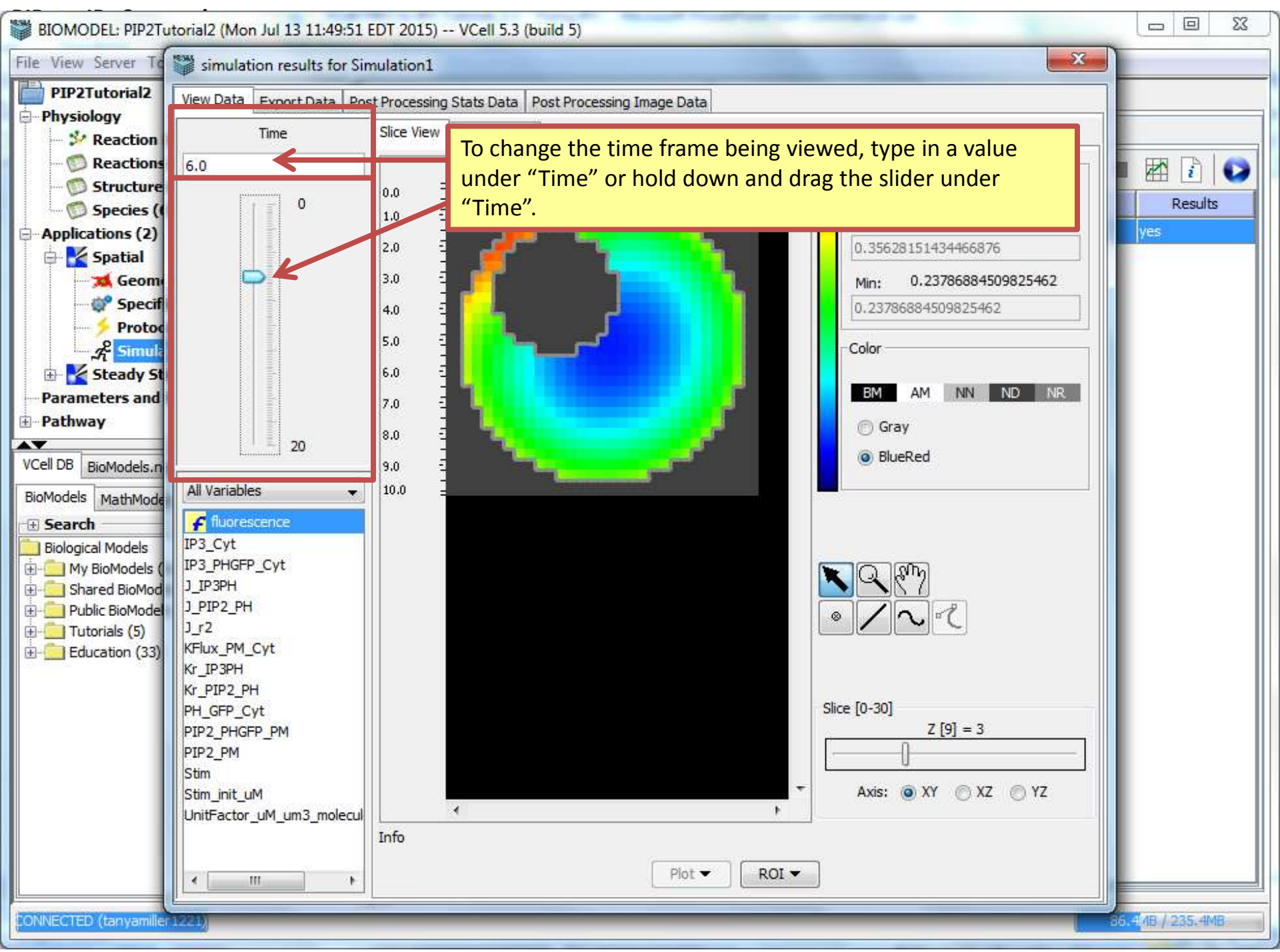
Protocols
Simulations
Simulations
Output Functions
Generated Math
Name
End Time
Output Option
Solver
Running Status
Results
Simulation1
20.0
every 0.2 sec
Fully-Implicit
completed
yes
Click the results icon.
CONNECTED (tanyamiller1221)
174.2MB / 222.8MB


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 11:49:51 EDT 2015) -- VCell 5.3 (build 5)
simulation results for Simulation1
View Data
Export Data
Post Processing Stats Data
Post Processing Image Data
Time
0.0
0
20
Slice View
Surface View
0
2.6666667
5.3333333
10
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
Data Range (Min-Max)
Auto (current time)
Max:
0.16551396284388278
Min:
0.16551396284388278
Color
BM
AM
NN
ND
NR
Gray
BlueRed
All Variables
fluorescence
IP3_Cyt
IP3_PHGFP_Cyt
J_IP3PH
J_PIP2_PH
J_r2
KFlux_PM_Cyt
Kr_IP3PH
Kr_PIP2_PH
PH_GFP_Cyt
PIP2_PHGFP_PM
PIP2_PM
Stim
Stim_init_uM
UnitFactor_uM_um3_molecul
Click and drag the Z-Slicer slider to adjust you view of the simulation.
Slice [0-30]
Z [9] = 3
Axis:
XY
XZ
YZ
Info
Plot
ROI
PIP2Tutorial2
Physiology
Reaction
Reactions
Structure
Species
Applications (2)
Spatial
Steady St
Parameters and
Pathway
VCell DB
BioModels
Search
Biological Models
My BioModels
Shared BioMod
Public BioModel
Tutorials (5)
Education (33)
Results
yes
CONNECTED (tanyamiller 1221)


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 11:49:51 EDT 2015) -- VCell 5.3 (build 5)
simulation results for Simulation1
View Data
Export Data
Post Processing Stats Data
Post Processing Image Data
Time
6.0
0
20
Slice View
To change the time frame being viewed, type in a value under “Time” or hold down and drag the slider under “Time”.
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
0.35628151434466876
Min:
0.23786884509825462
0.23786884509825462
Color
BM
AM
NN
ND
NR
Gray
BlueRed
All Variables
fluorescence
IP3_Cyt
IP3_PHGFP_Cyt
J_IP3PH
J_PIP2_PH
J_r2
KFlux_PM_Cyt
Kr_IP3PH
Kr_PIP2_PH
PH_GFP_Cyt
PIP2_PHGFP_PM
PIP2_PM
Stim
Stim_init_uM
UnitFactor_uM_um3_molecul
Slice [0-30]
Z [9] = 3
Axis:
XY
XZ
YZ
Info
Plot
ROI
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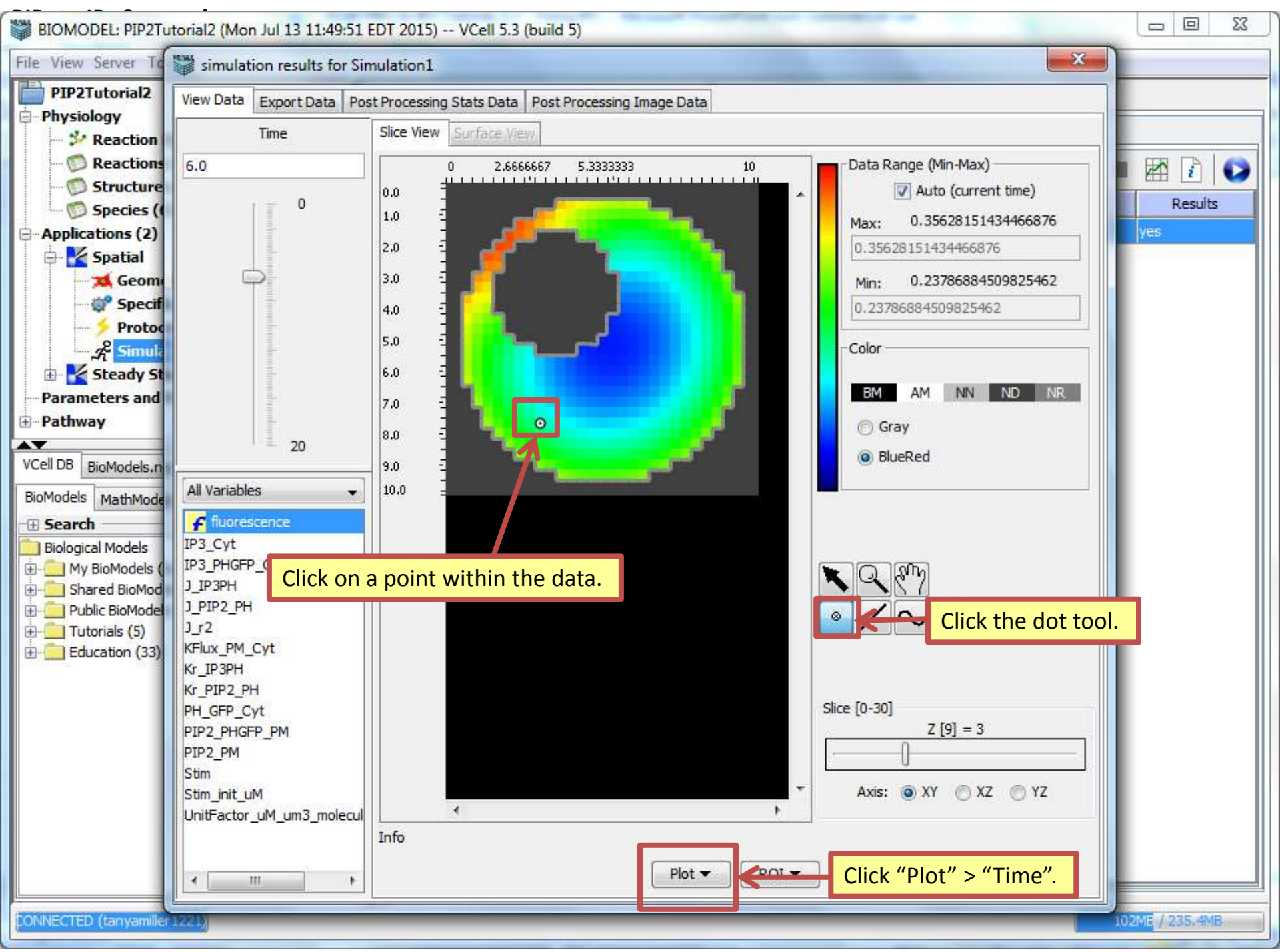
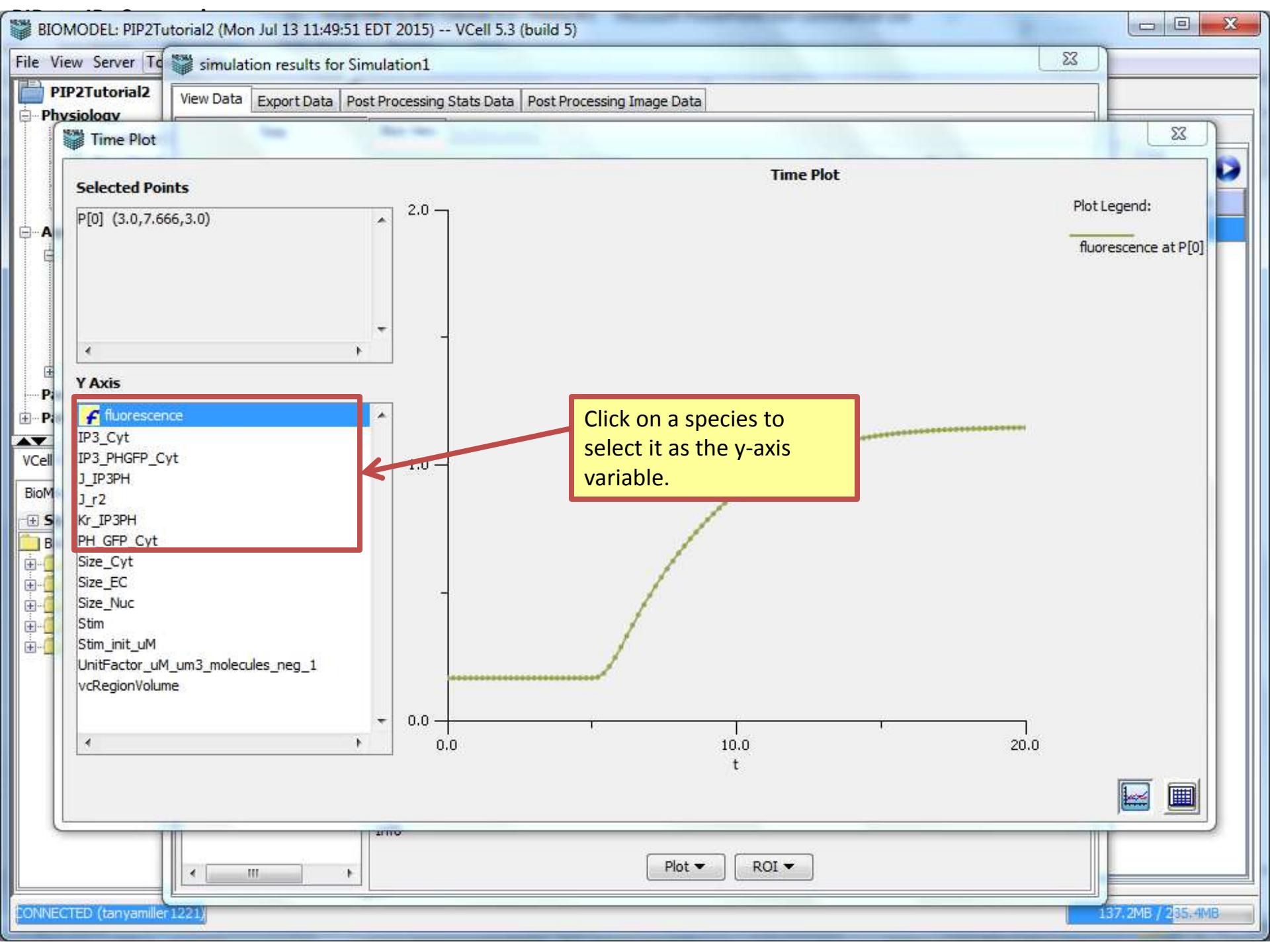
My BioModels
Shared BioMod
Public BioModel
Tutorials (5)
Education (33)
Results
yes
CONNECTED (tanyamiller 122)


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 11:49:51 EDT 2015) -- VCell 5.3 (build 5)
simulation results for Simulation1
View Data
Export Data
Post Processing Stats Data
Post Processing Image Data
Time
6.0
Slice View
Surface View
Data Range (Min-Max)
Auto (current time)
Max: 0.35628151434466876
Min: 0.23786884509825462
Color
BM
AM
NN
ND
NR
Gray
BlueRed
All Variables
fluorescence
IP3_Cyt
J_IP3PH
J_PIP2_PH
J_r2
KFlux_PM_Cyt
Kr_IP3PH
Kr_PIP2_PH
PH_GFP_Cyt
PIP2_PHGFP_PM
PIP2_PM
Stim
Stim_init_uM
UnitFactor_uM_um3_molecul
Slice [0-30]
Z [9] = 3
Axis: XY XZ YZ
Info
Plot
Click on a point within the data.
Click the dot tool.
Click “Plot” > “Time”.


BIOMODEL: PIP2Tutorial2 (Mon Jul 13 11:49:51 EDT 2015) -- VCell 5.3 (build 5)
File View Server
PIP2Tutorial2
Physiology
simulation results for Simulation1
View Data
Export Data
Post Processing Stats Data
Post Processing Image Data
Time Plot
Selected Points
P[0] (3.0,7.666,3.0)
Y Axis
fluorescence
IP3_Cyt
IP3_PHGFP_Cyt
J_IP3PH
J_r2
Kr_IP3PH
PH_GFP_Cyt
Size_Cyt
Size_EC
Size_Nuc
Stim
Stim_init_uM
UnitFactor_uM_um3_molecules_neg_1
vcRegionVolume
Time Plot
Plot Legend:
fluorescence at P[0]
2.0
1.0
0.0
0.0
10.0
20.0
t
Click on a species to select it as the y-axis variable.
Plot
ROI
CONNECTED (tanyamiller1221)
137.2MB / 235.4MB