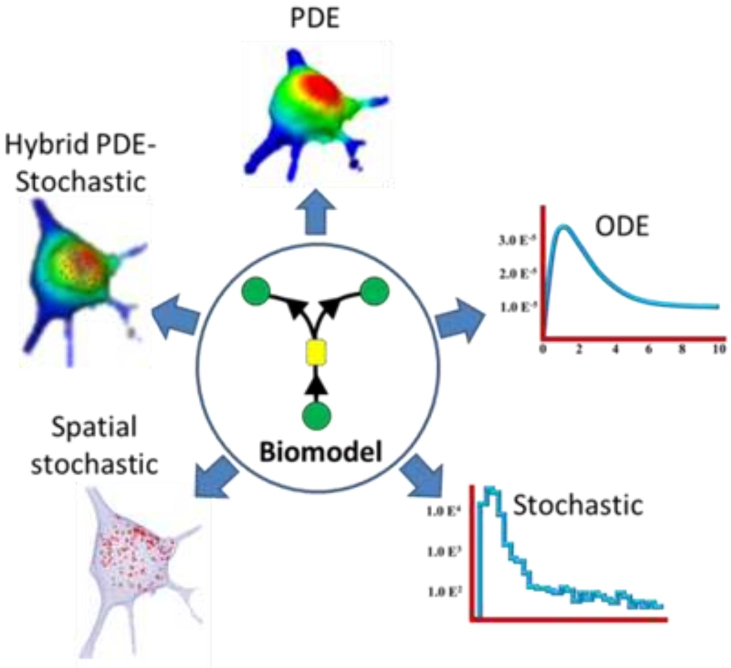
Virtual Cell Tutorials

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)

VCell Tutorial

VCell Pathway Commons Tutorial

Using external pathway databases to construct a biomodel

In this tutorial…

- Use the database navigator to interact with pathway databases such as Biomodels.net, Pathway Commons or SabioRK
- Import pathways or components of pathways into the VCell workspace
- Edit pathway links in VCell models and annotate links
- Use tips for working with large network models in VCell

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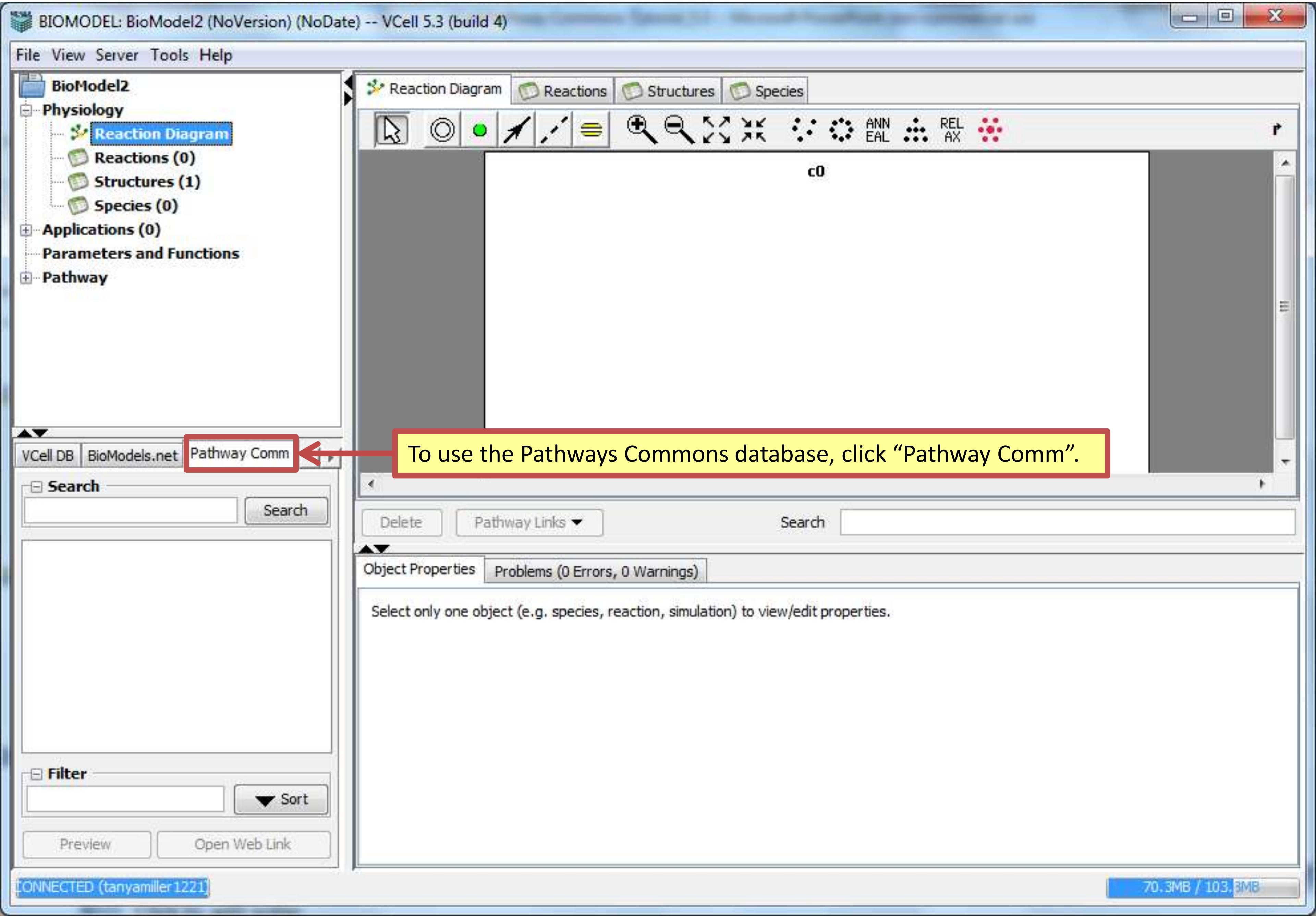
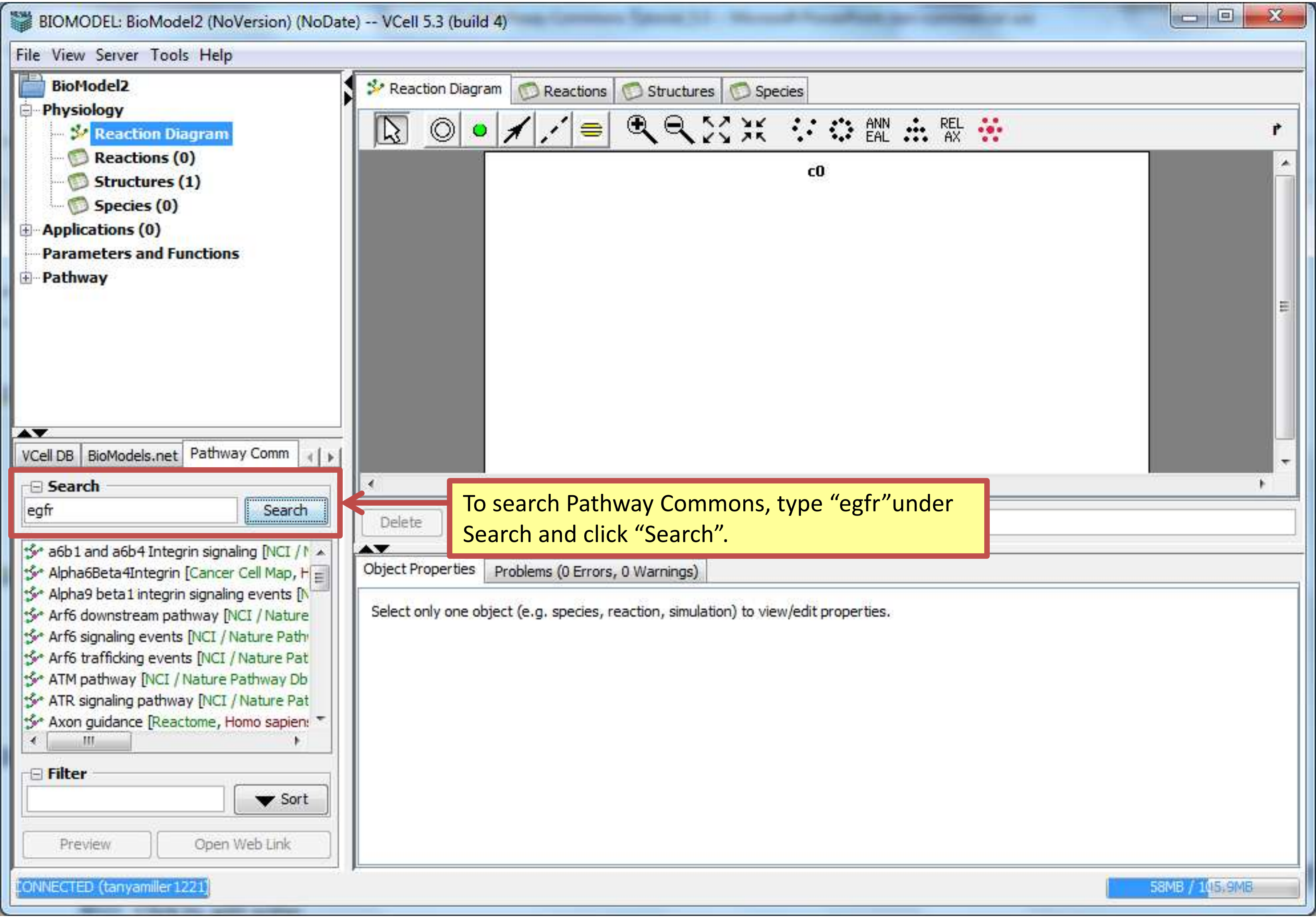


Select only one object (e.g. species, reaction, simulation) to view/edit properties.

To use the Pathways Commons database, click “Pathway Comm”.



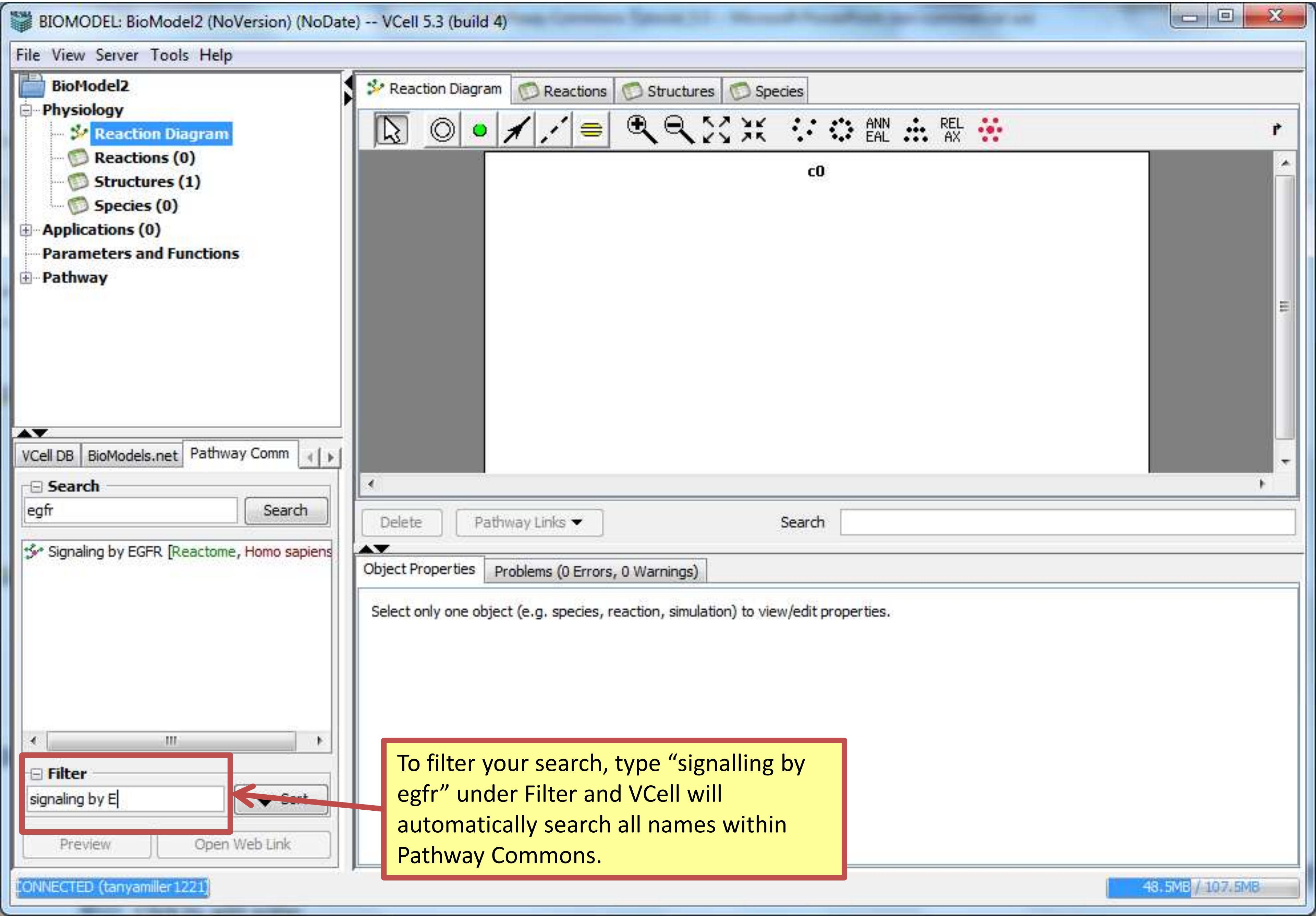
Search: egfr

- a6b1 and a6b4 Integrin signaling [NCI / N
- Alpha6Beta4Integrin [Cancer Cell Map, H
- Alpha9 beta1 integrin signaling events [N
- Arf6 downstream pathway [NCI / Nature
- Arf6 signaling events [NCI / Nature Path
- Arf6 trafficking events [NCI / Nature Pat
- ATM pathway [NCI / Nature Pathway Db
- ATR signaling pathway [NCI / Nature Pat
- Axon guidance [Reactome, Homo sapien

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

CONNECTED (tanyamiller1221)

To search Pathway Commons, type “egfr”under Search and click “Search”.



Search: egfr

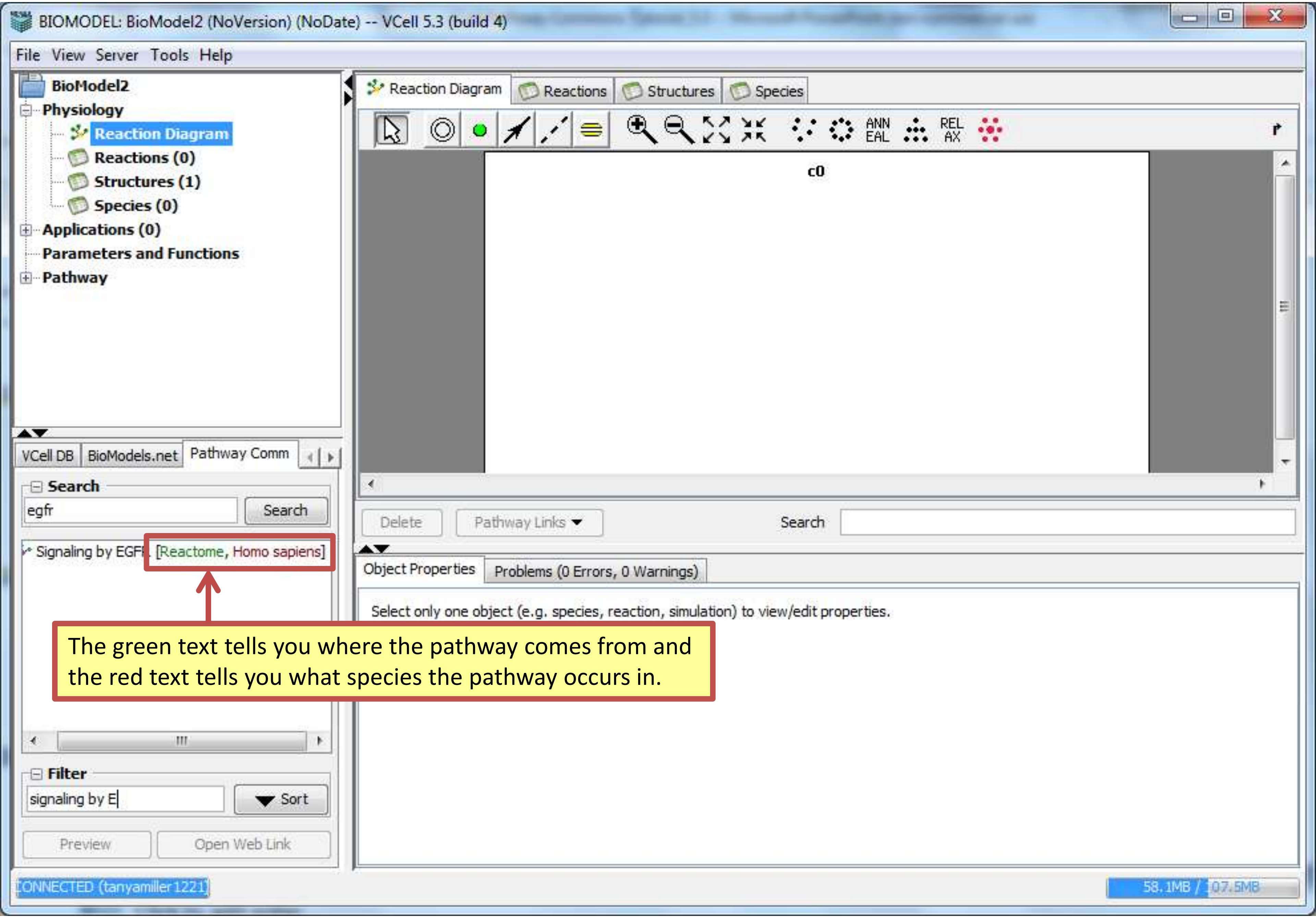
Signaling by EGFR [Reactome, Homo sapiens

Filter: signaling by E

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

To filter your search, type “signalling by egfr” under Filter and VCell will automatically search all names within Pathway Commons.

Contents



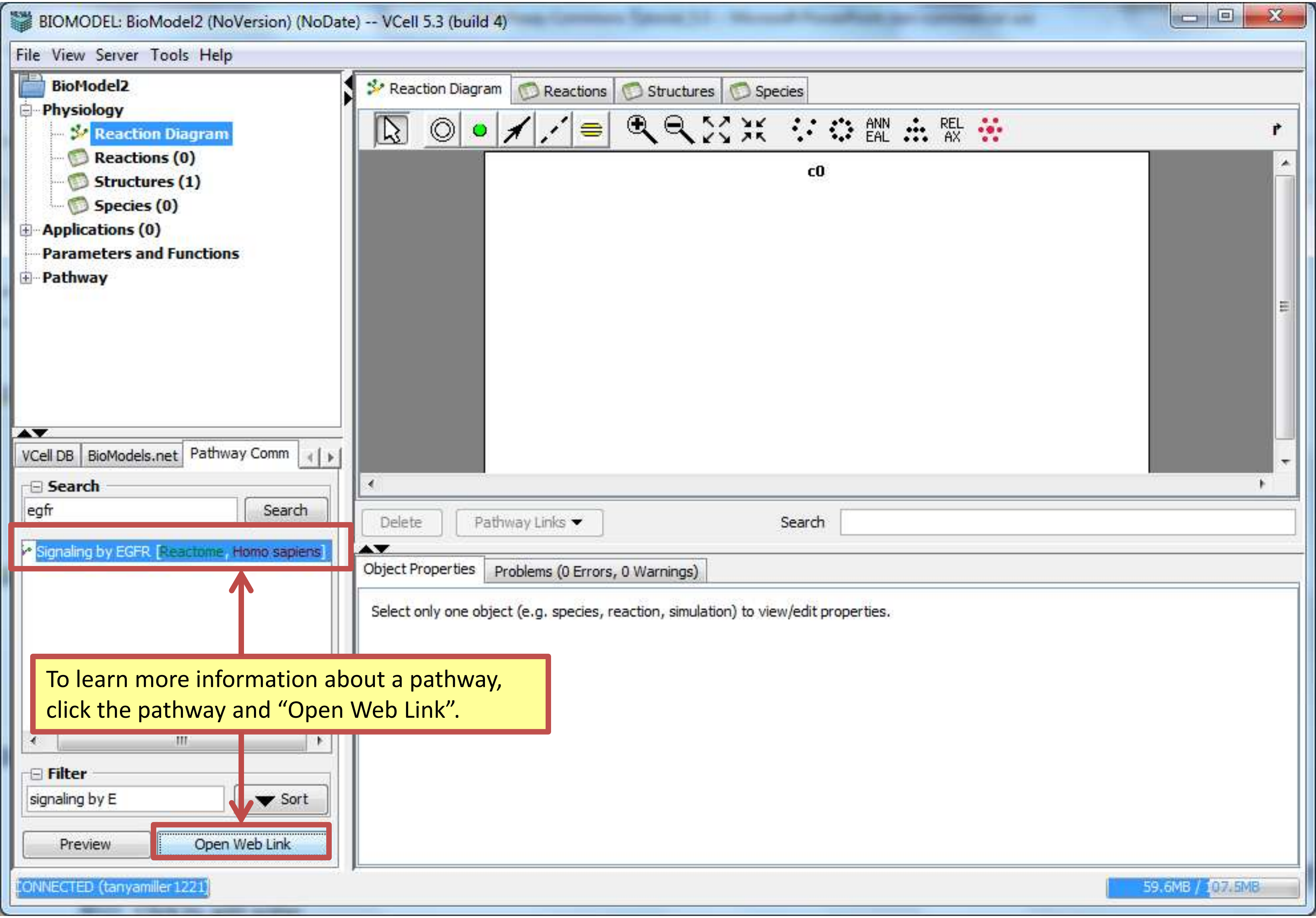
Search: egfr

Signaling by EGFR [Reactome, Homo sapiens]

Filter: signaling by E

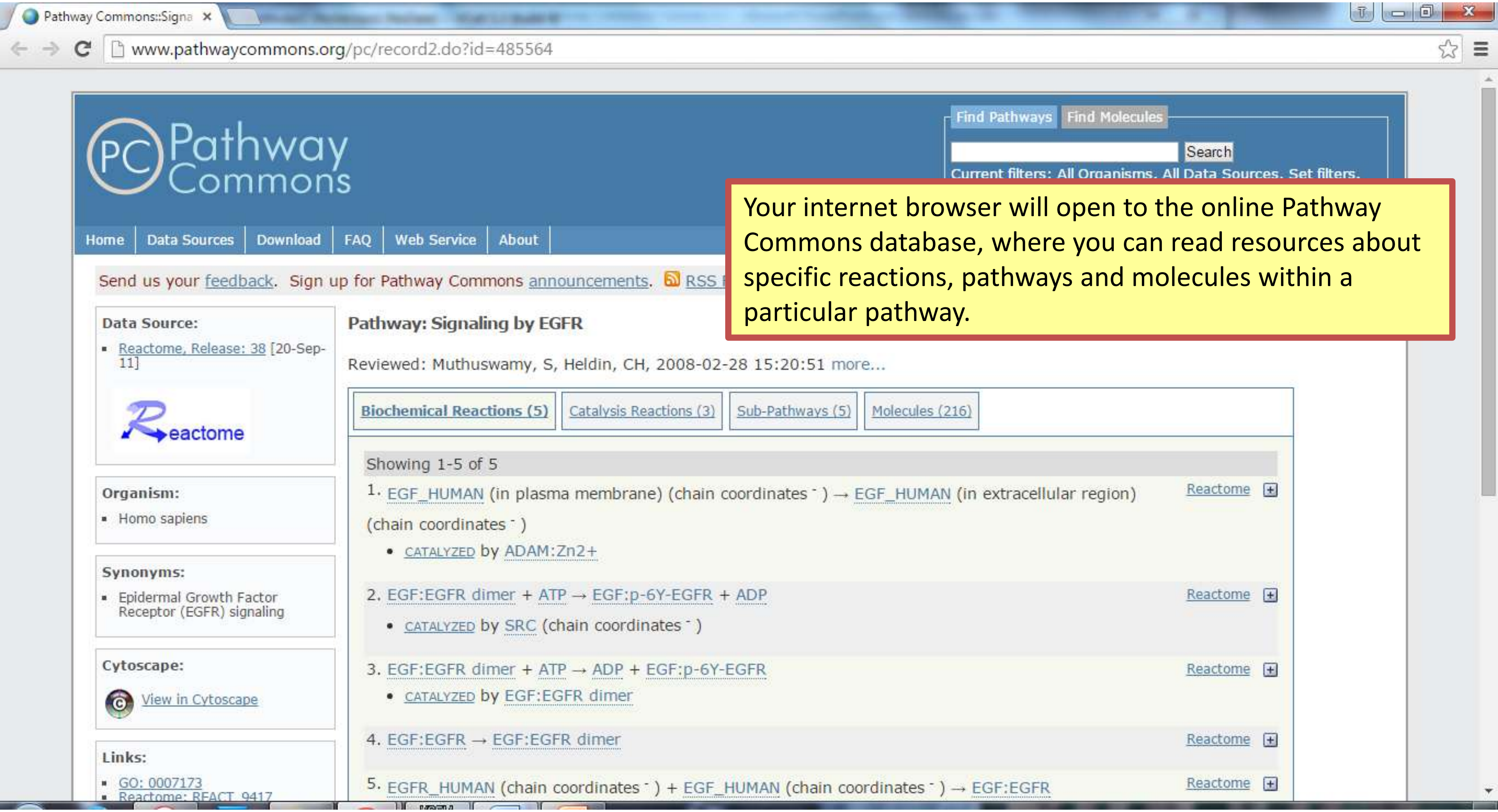
Select only one object (e.g. species, reaction, simulation) to view/edit properties.

The green text tells you where the pathway comes from and the red text tells you what species the pathway occurs in.



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

To learn more information about a pathway, click the pathway and “Open Web Link”.



Send us your feedback. Sign up for Pathway Commons announcements. RSS

Data Source:

- Reactome, Release: 38 [20-Sep-11]

Organism:

- Homo sapiens

Synonyms:

- Epidermal Growth Factor Receptor (EGFR) signaling

Cytoscape:

View in Cytoscape

Links:

- GO: 0007173
- Reactome: REACT_9417

Pathway: Signaling by EGFR

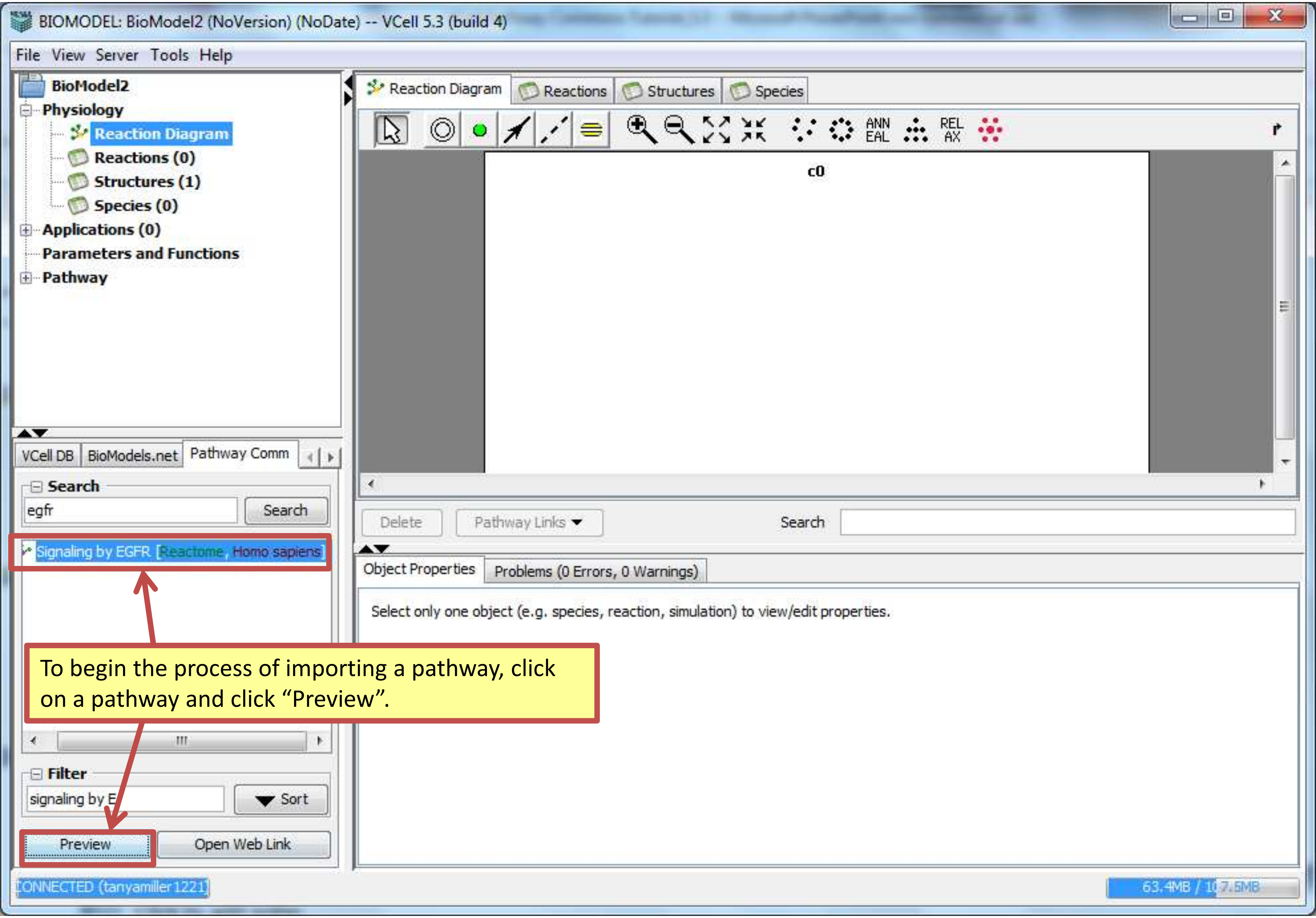
Reviewed: Muthuswamy, S, Heldin, CH, 2008-02-28 15:20:51 more...

Biochemical Reactions (5) | Catalysis Reactions (3) | Sub-Pathways (5) | Molecules (216)

Showing 1-5 of 5

1. EGF_HUMAN (in plasma membrane) (chain coordinates -) → EGF_HUMAN (in extracellular region) (chain coordinates -) — Reactome
   - CATALYZED by ADAM:Zn2+
2. EGF:EGFR dimer + ATP → EGF:p-6Y-EGFR + ADP — Reactome
   - CATALYZED by SRC (chain coordinates -)
3. EGF:EGFR dimer + ATP → ADP + EGF:p-6Y-EGFR — Reactome
   - CATALYZED by EGF:EGFR dimer
4. EGF:EGFR → EGF:EGFR dimer — Reactome
5. EGFR_HUMAN (chain coordinates -) + EGF_HUMAN (chain coordinates -) → EGF:EGFR — Reactome

Your internet browser will open to the online Pathway Commons database, where you can read resources about specific reactions, pathways and molecules within a particular pathway.

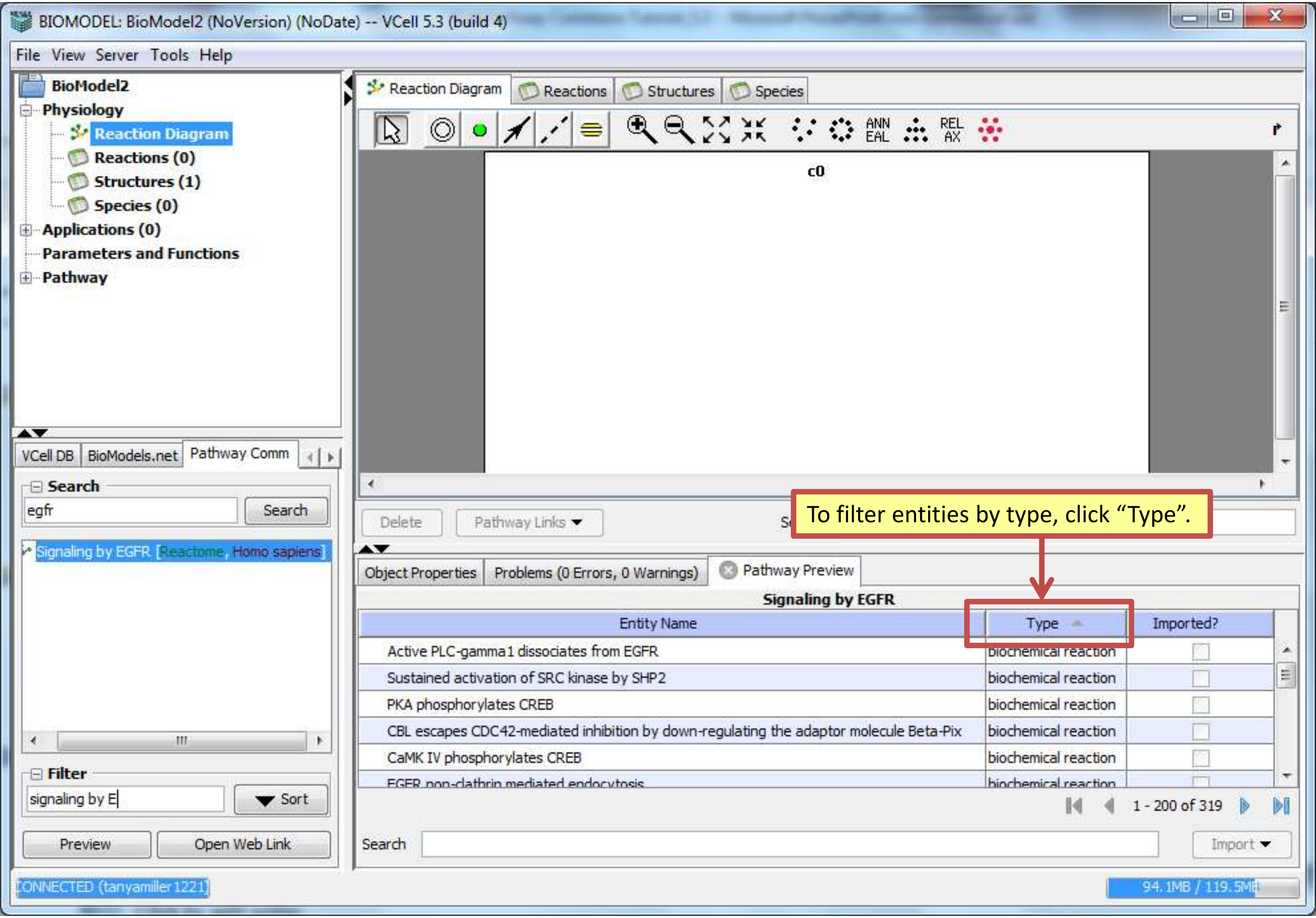


Select only one object (e.g. species, reaction, simulation) to view/edit properties.

To begin the process of importing a pathway, click on a pathway and click “Preview”.

Pathway Commons Tutorial

Contents



Search: egfr

Signaling by EGFR [Reactome, Homo sapiens]

Filter: signaling by E

Signaling by EGFR

Entity Name	Type	Imported?
Active PLC-gamma1 dissociates from EGFR	biochemical reaction	☐
Sustained activation of SRC kinase by SHP2	biochemical reaction	☐
PKA phosphorylates CREB	biochemical reaction	☐
CBL escapes CDC42-mediated inhibition by down-regulating the adaptor molecule Beta-Pix	biochemical reaction	☐
CaMK IV phosphorylates CREB	biochemical reaction	☐
EGFR non-clathrin mediated endocytosis	biochemical reaction	☐

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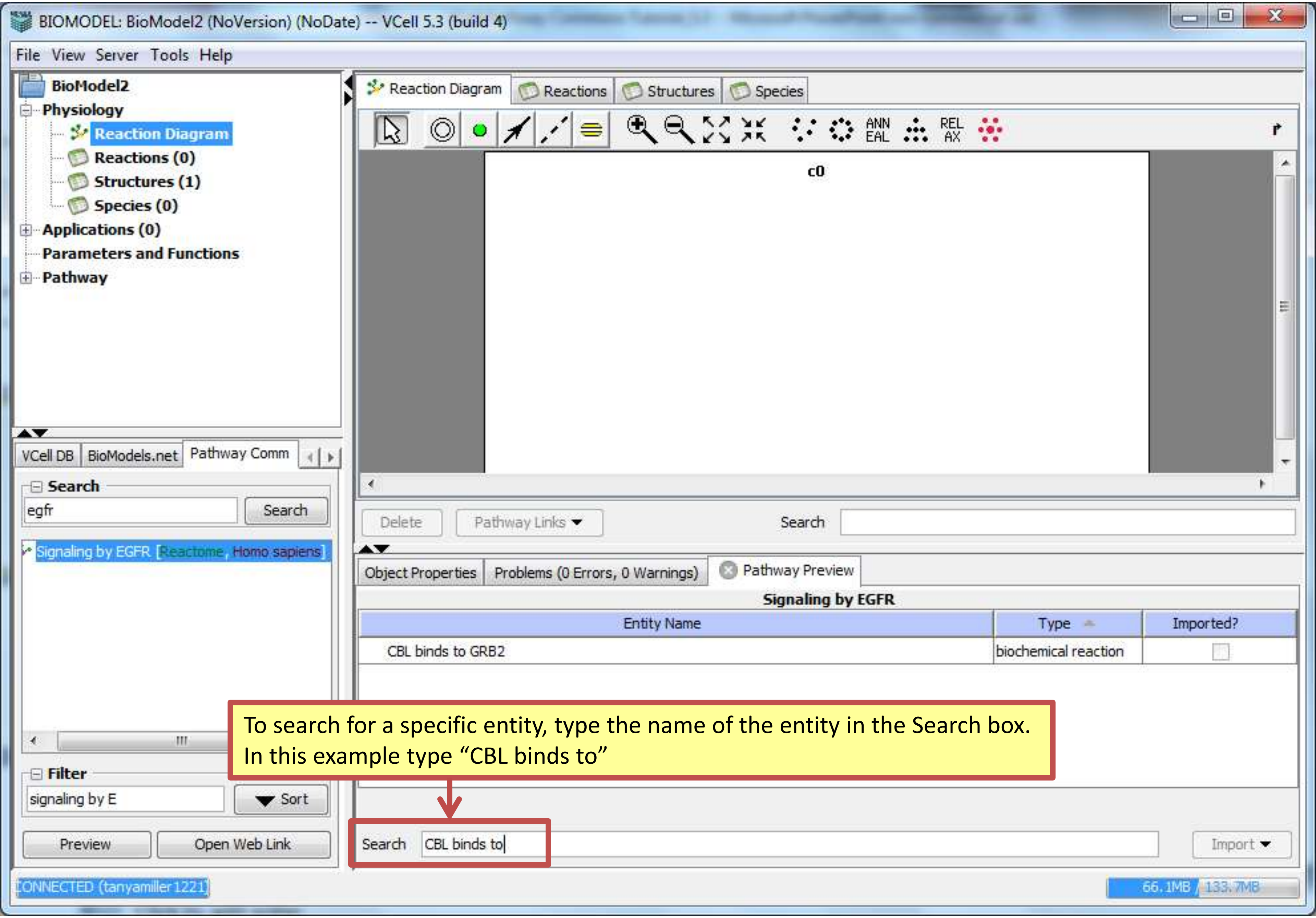
Search

To filter entities by type, click “Type”.



Search: egfr

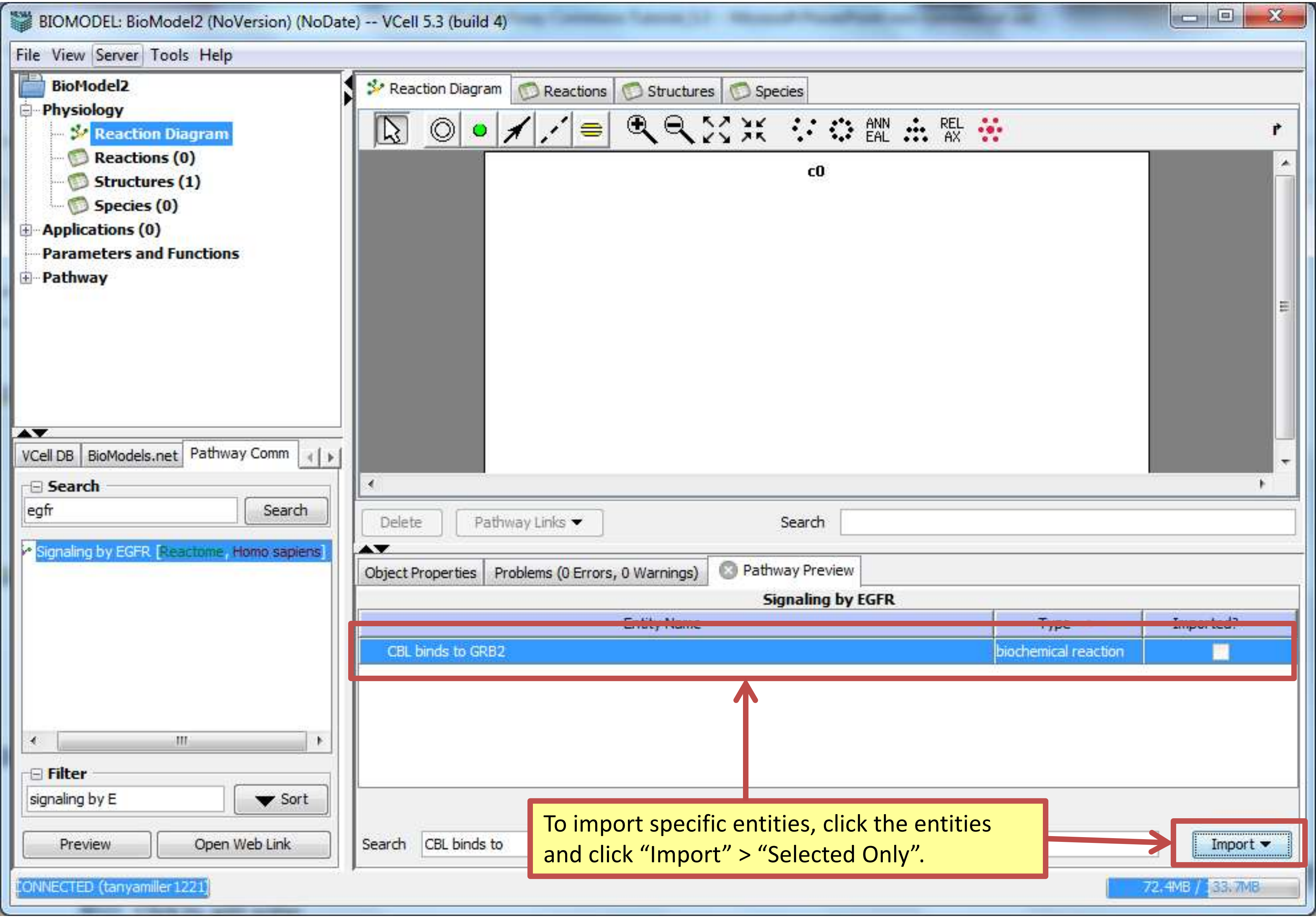
Filter: signaling by E

Signaling by EGFR

Entity Name	Type	Imported?
CBL binds to GRB2	biochemical reaction	☐

To search for a specific entity, type the name of the entity in the Search box. In this example type “CBL binds to”

Search: CBL binds to



BIOMODEL: BioModel2 (NoVersion) (NoDate) -- VCell 5.3 (build 4)

Search: egfr

Signaling by EGFR [Reactome, Homo sapiens]

Filter: signaling by E

Signaling by EGFR

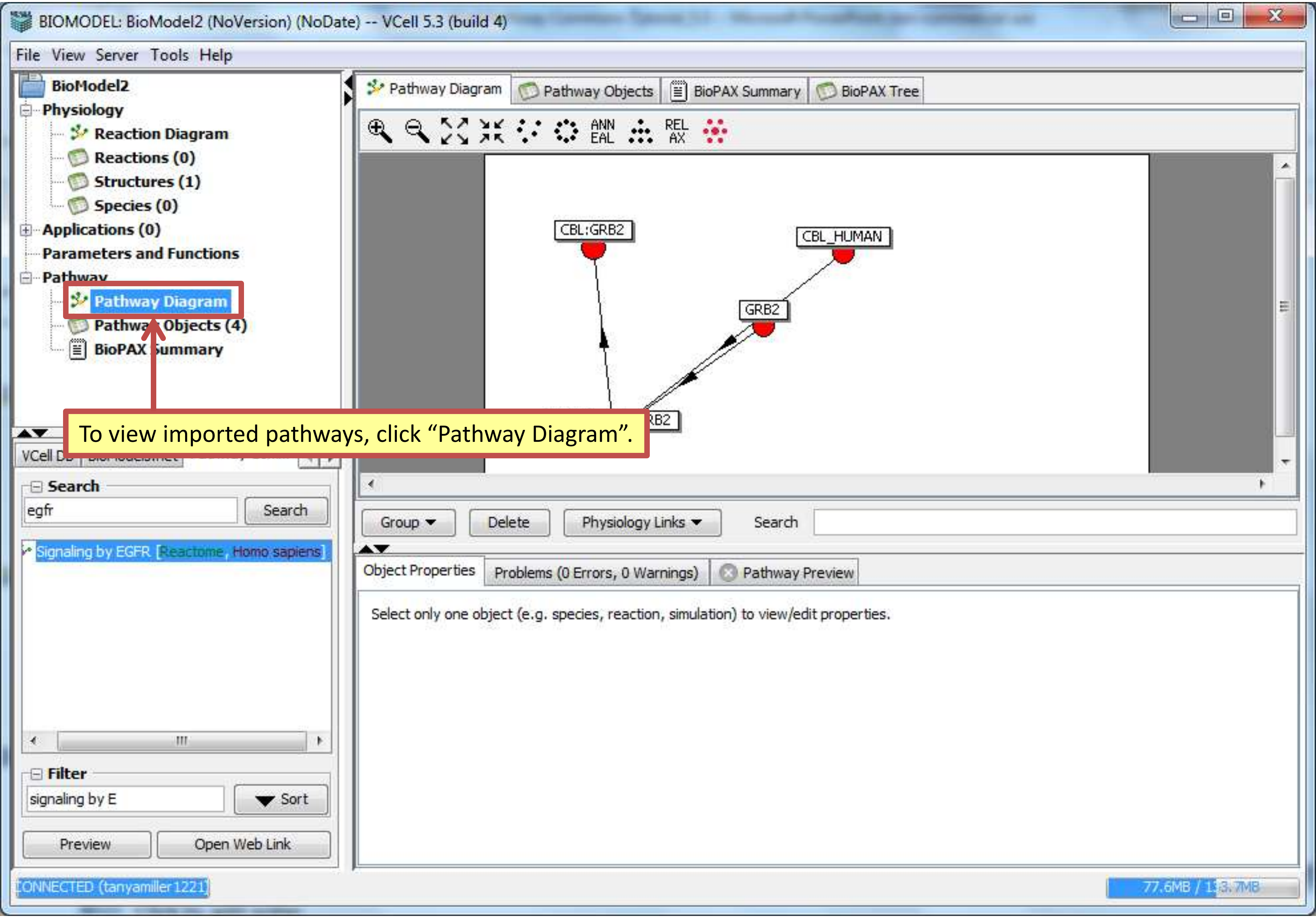
Entity Name	Type	Imported?
CBL binds to GRB2	biochemical reaction	☐

Search: CBL binds to

CONNECTED (tanyamiller1221)

72.4MB / 133.7MB

To import specific entities, click the entities and click “Import” > “Selected Only”.



Search: egfr

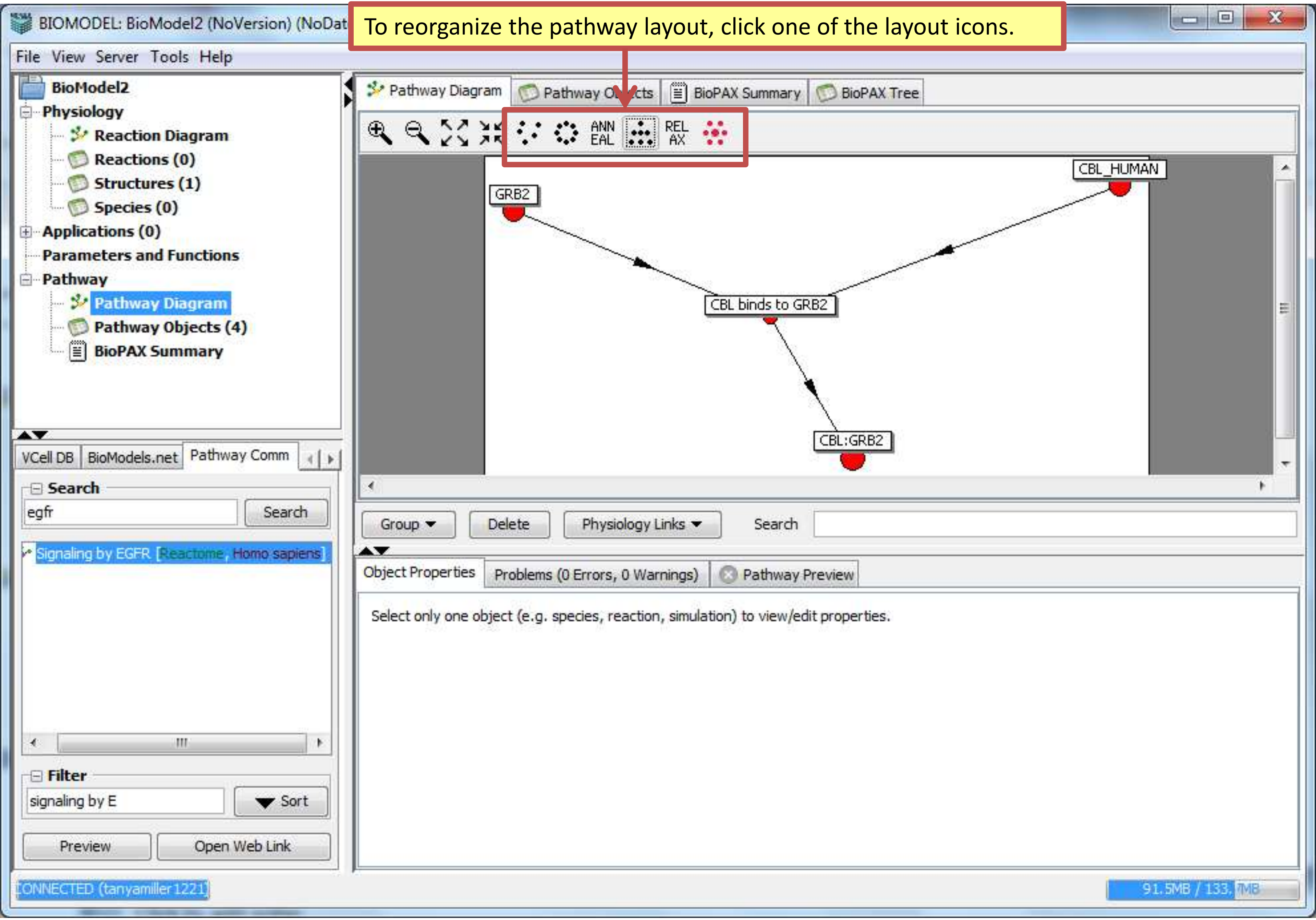
Filter: signaling by E

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

To view imported pathways, click “Pathway Diagram”.

Contents

To reorganize the pathway layout, click one of the layout icons.



Search: egfr

Signaling by EGFR [Reactome, Homo sapiens]

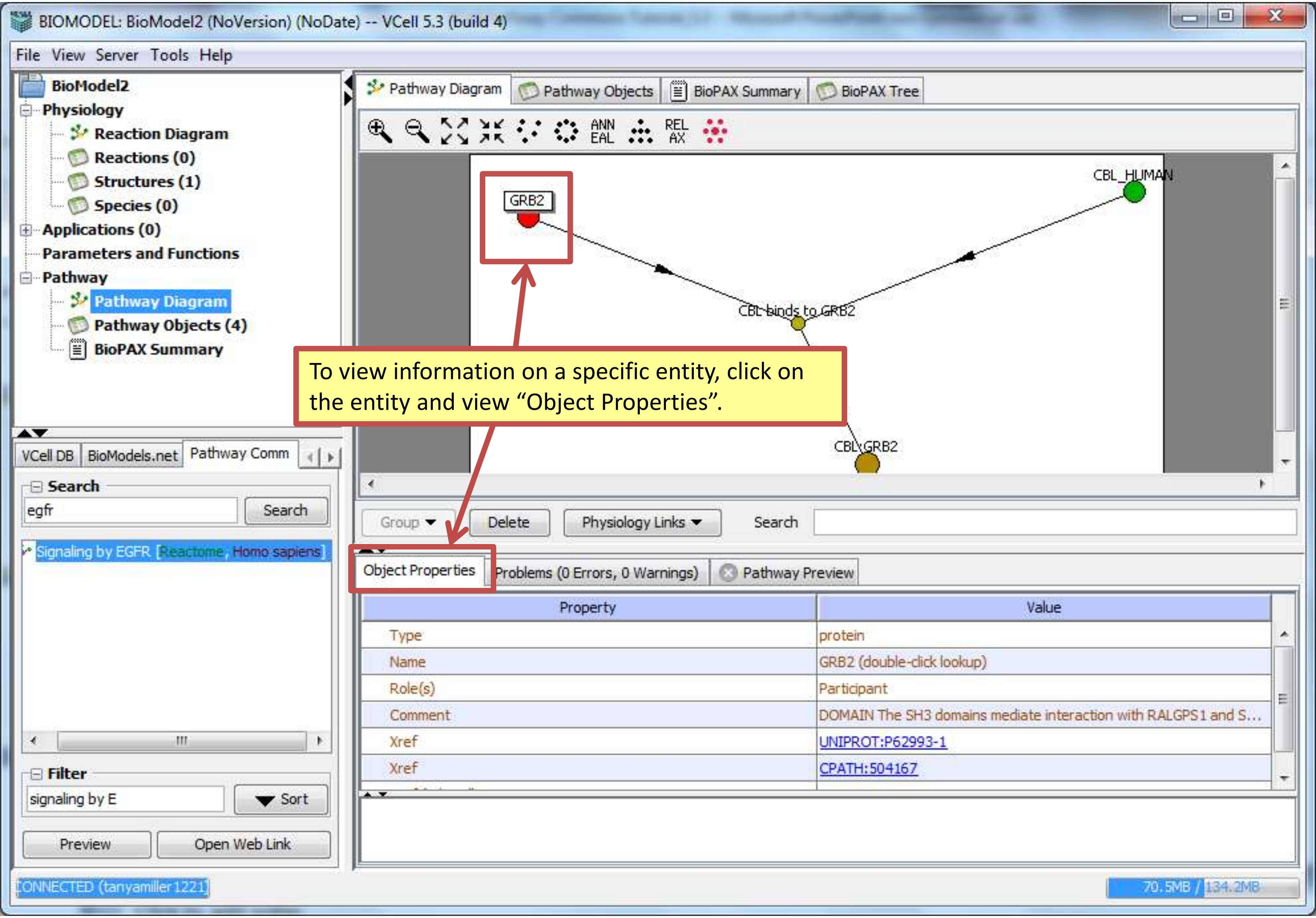
Filter: signaling by E

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

CONNECTED (tanyamiller1221)

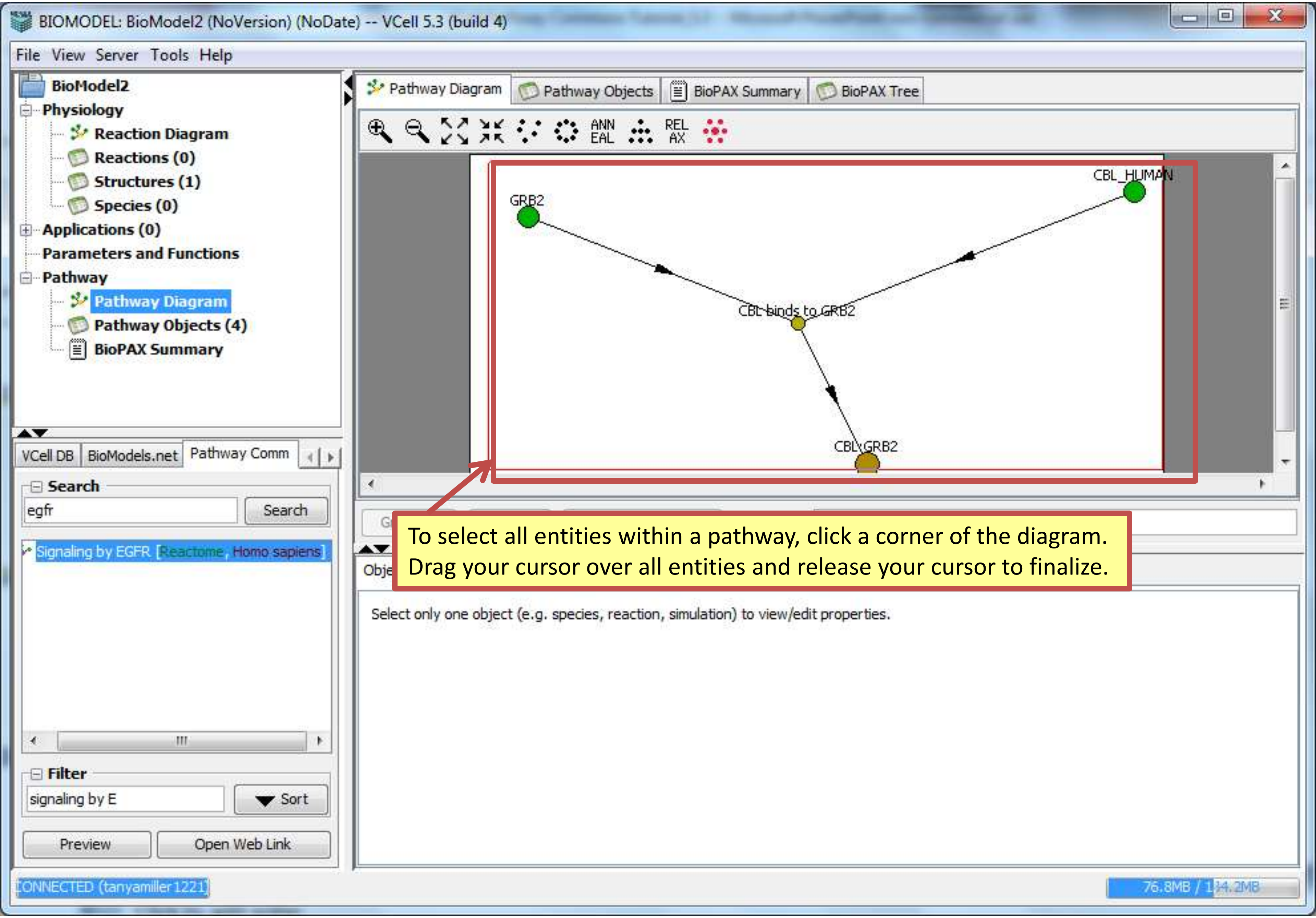
Pathway Commons Tutorial

Contents

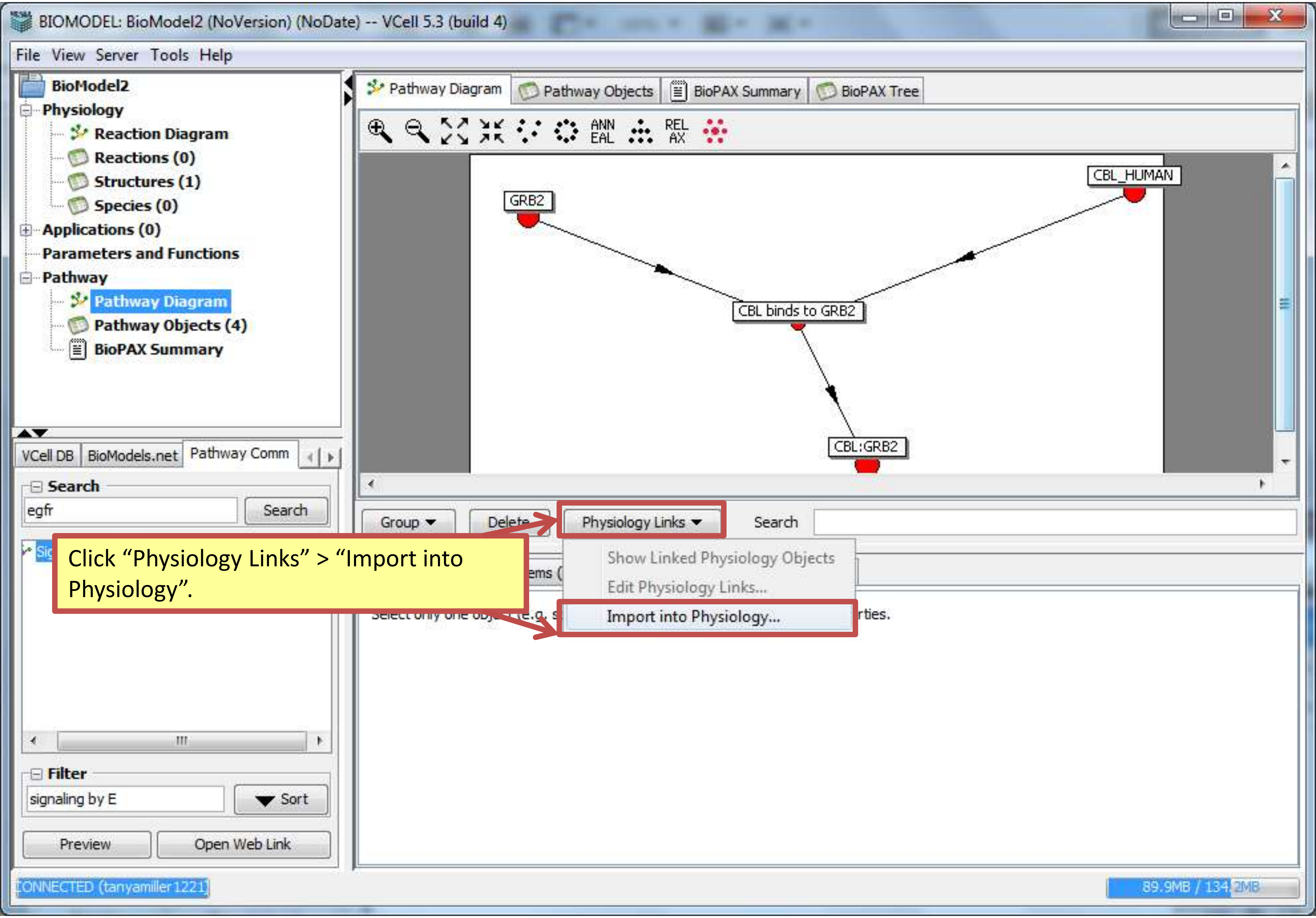


To view information on a specific entity, click on the entity and view “Object Properties”.

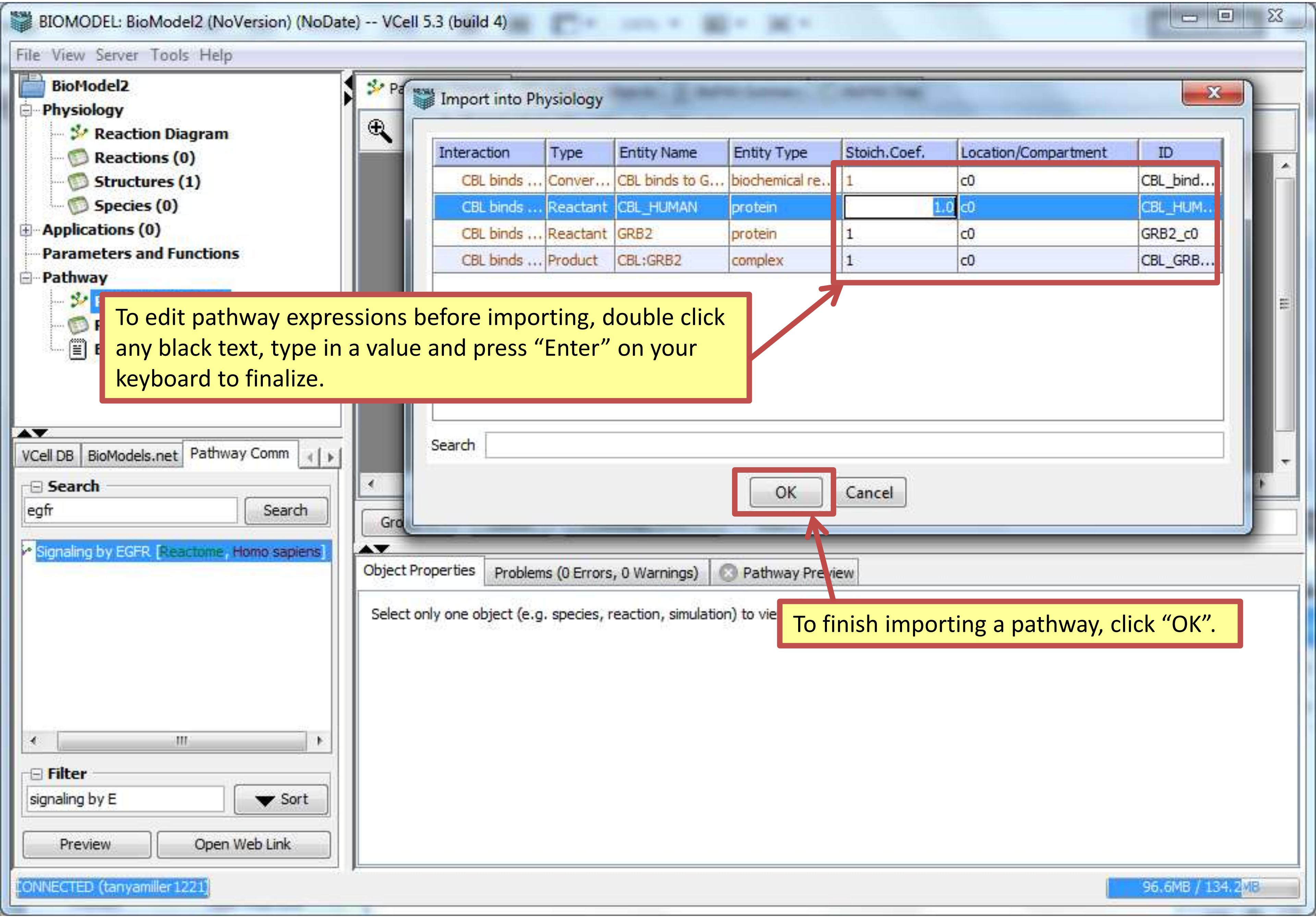
Property	Value
Type	protein
Name	GRB2 (double-click lookup)
Role(s)	Participant
Comment	DOMAIN The SH3 domains mediate interaction with RALGPS1 and S…
Xref	UNIPROT:P62993-1
Xref	CPATH:504167



To select all entities within a pathway, click a corner of the diagram. Drag your cursor over all entities and release your cursor to finalize.



Click “Physiology Links” > “Import into Physiology”.



Search: egfr

Signaling by EGFR [Reactome, Homo sapiens]

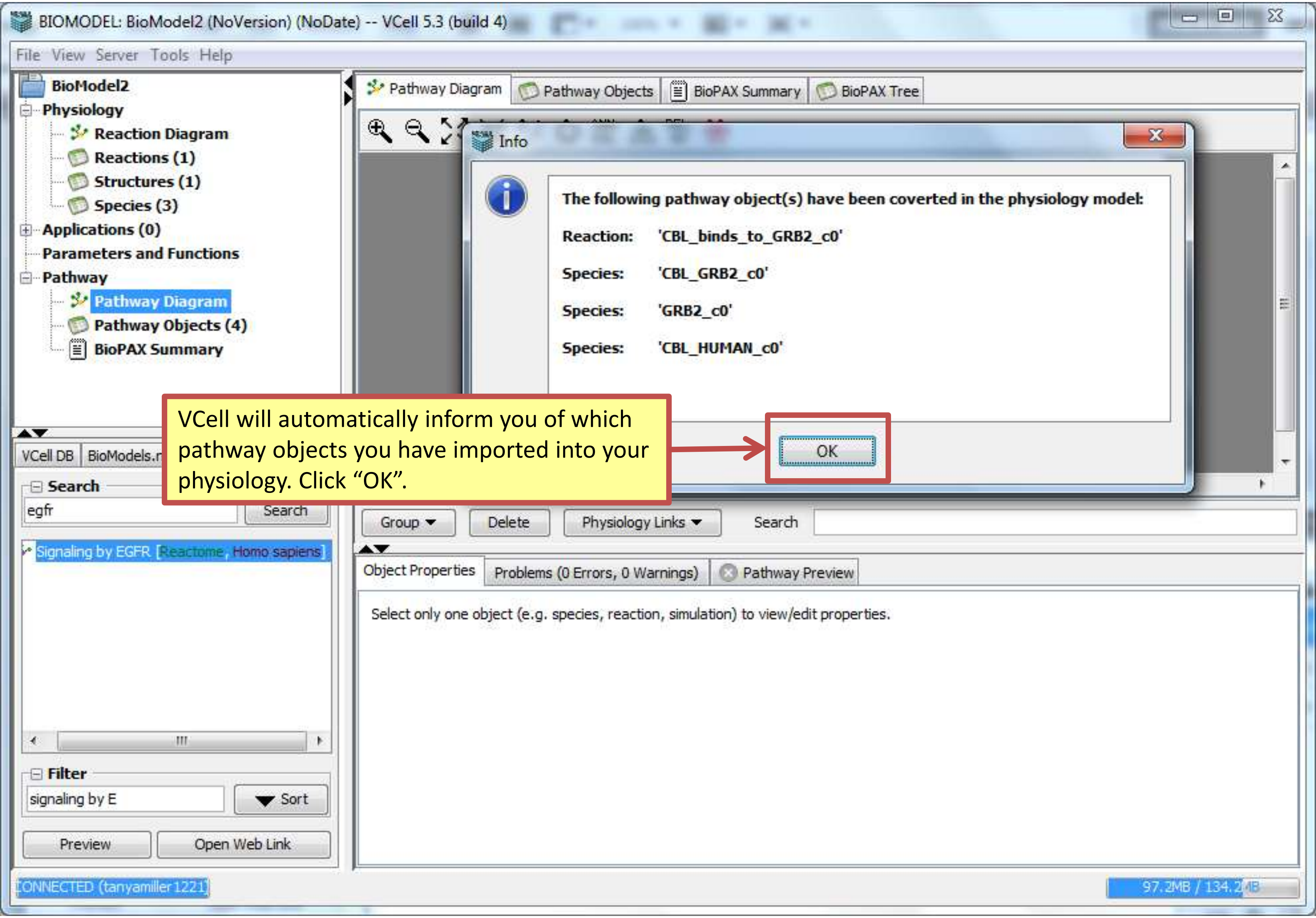
Filter: signaling by E

Interaction	Type	Entity Name	Entity Type	Stoich.Coef.	Location/Compartment	ID
CBL binds ...	Conver...	CBL binds to G...	biochemical re...	1	c0	CBL_bind...
CBL binds ...	Reactant	CBL_HUMAN	protein	1.0	c0	CBL_HUM...
CBL binds ...	Reactant	GRB2	protein	1	c0	GRB2_c0
CBL binds ...	Product	CBL:GRB2	complex	1	c0	CBL_GRB...

Select only one object (e.g. species, reaction, simulation) to vie

To edit pathway expressions before importing, double click any black text, type in a value and press “Enter” on your keyboard to finalize.

To finish importing a pathway, click “OK”.



Search: egfr

Filter: signaling by E

The following pathway object(s) have been coverted in the physiology model:

Reaction: 'CBL_binds_to_GRB2_c0'

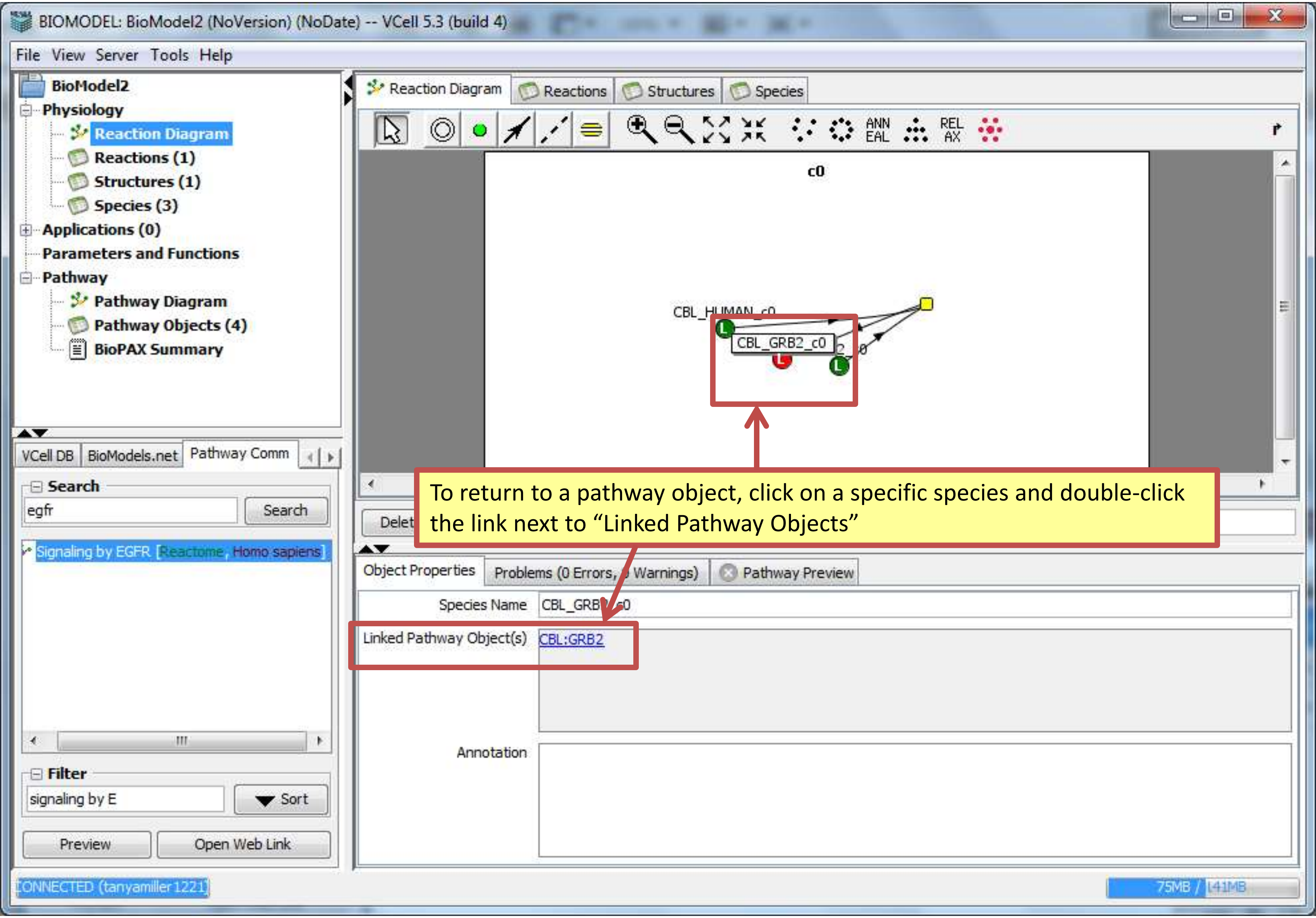
Species: 'CBL_GRB2_c0'

Species: 'GRB2_c0'

Species: 'CBL_HUMAN_c0'

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

VCell will automatically inform you of which pathway objects you have imported into your physiology. Click “OK”.



Search: egfr

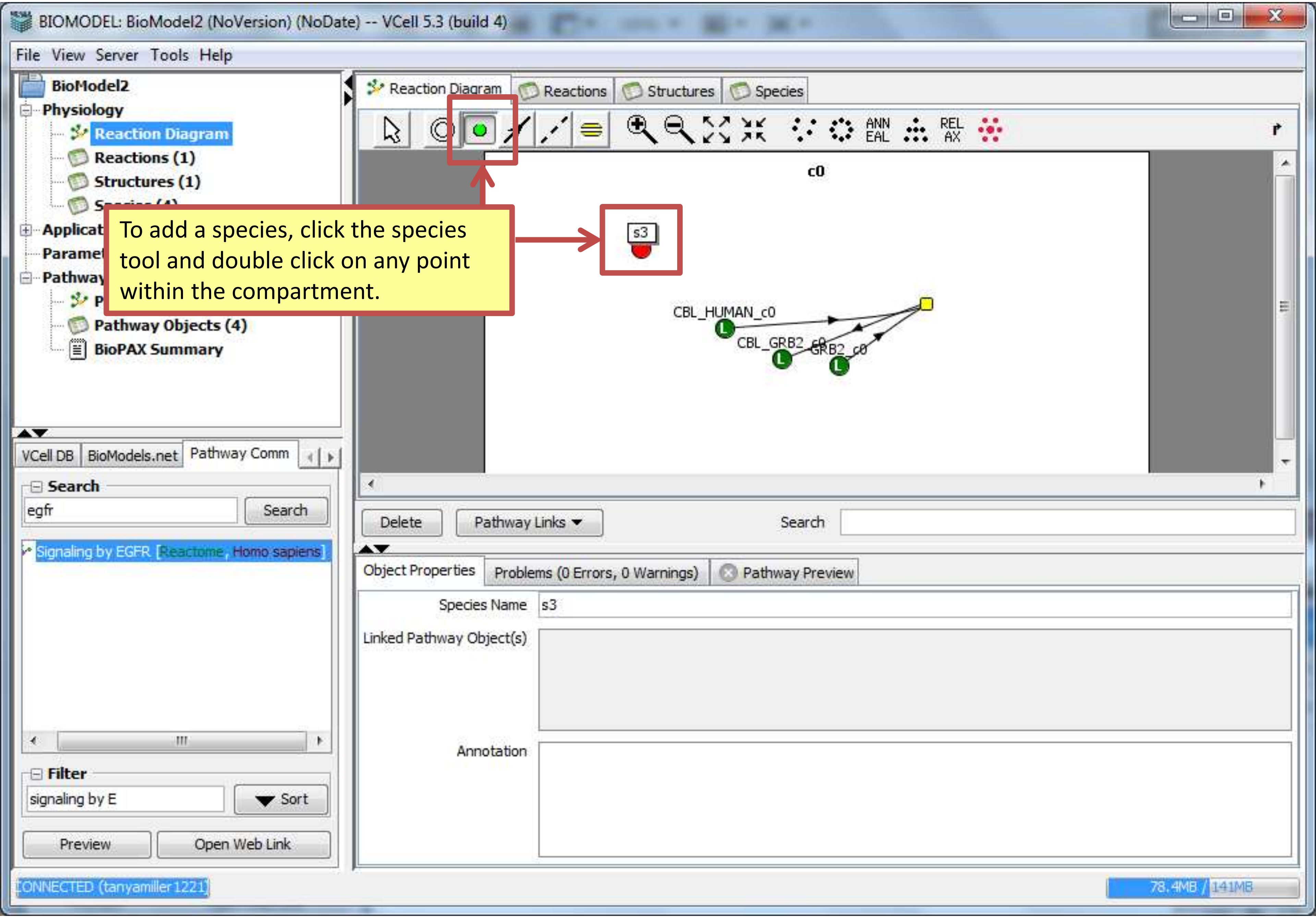
Filter: signaling by E

Species Name: CBL_GRB2_c0

Linked Pathway Object(s): CBL:GRB2

To return to a pathway object, click on a specific species and double-click the link next to “Linked Pathway Objects”

Contents



To add a species, click the species tool and double click on any point within the compartment.

Search: egfr

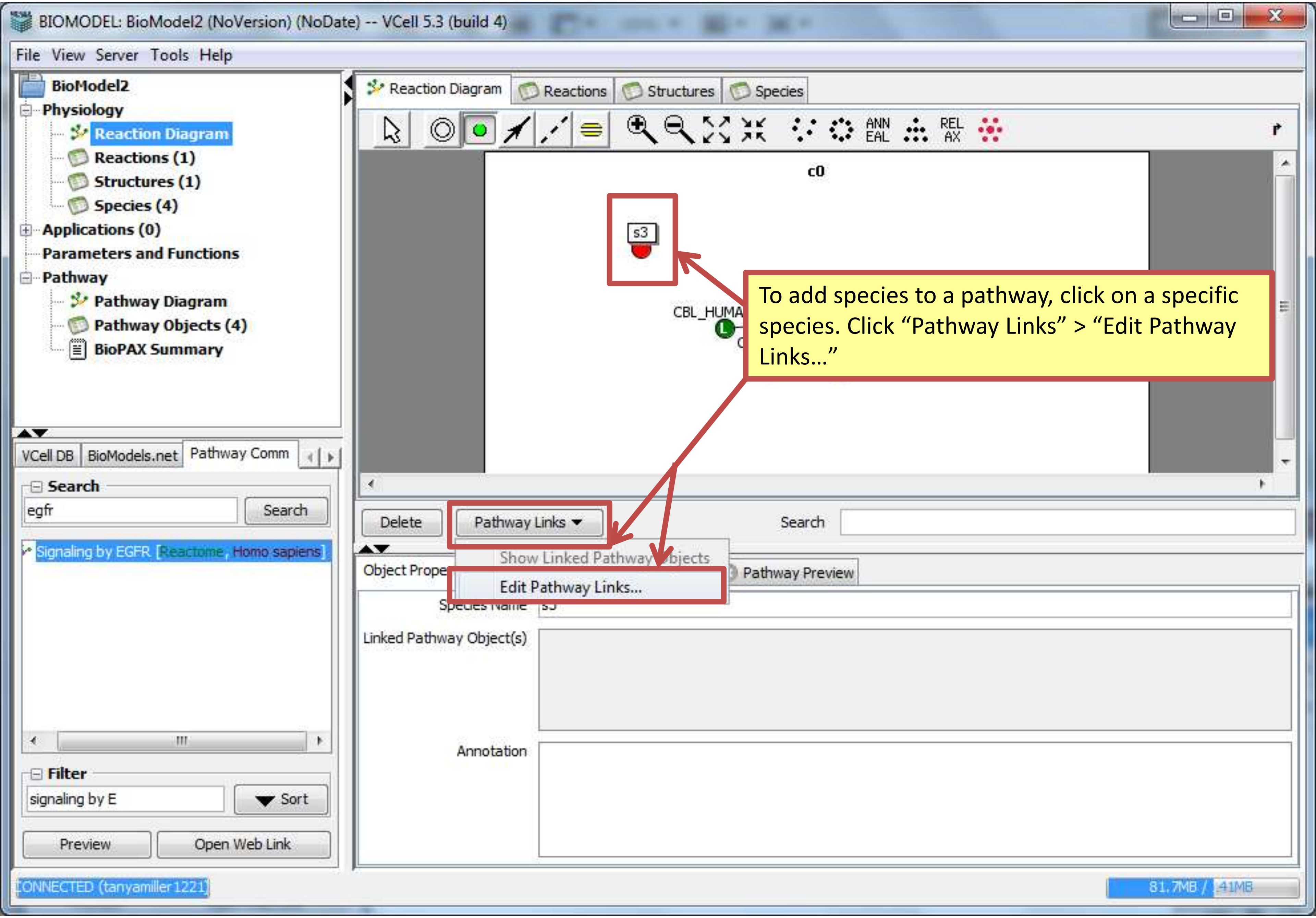
Signaling by EGFR [Reactome, Homo sapiens]

Filter: signaling by E

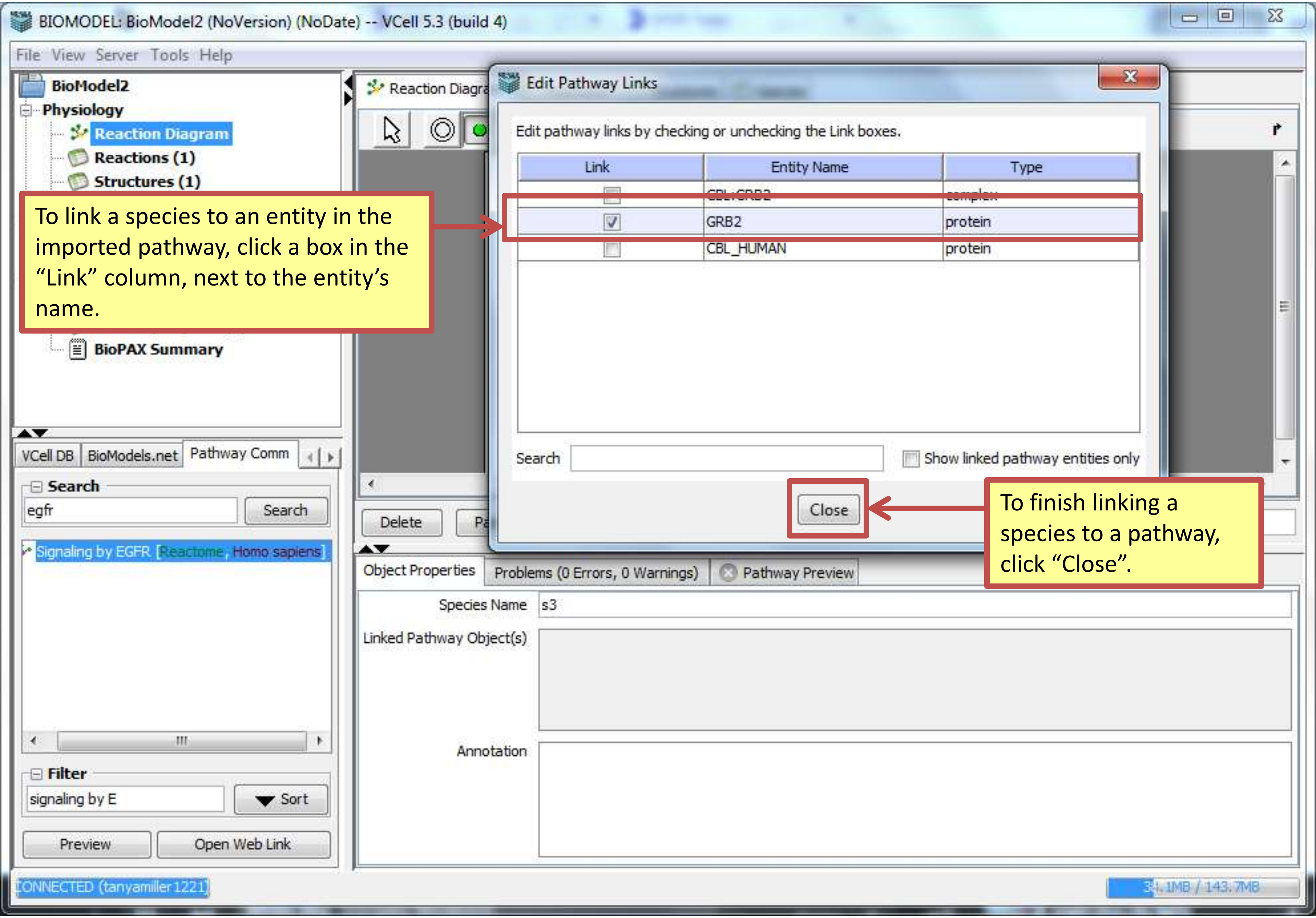
Species Name: s3

CONNECTED (tanyamiller1221)

78.4MB / 141MB



To add species to a pathway, click on a specific species. Click “Pathway Links” > “Edit Pathway Links…”



Edit Pathway Links

Edit pathway links by checking or unchecking the Link boxes.

Link	Entity Name	Type
☐	CBL:GRB2	complex
☑	GRB2	protein
☐	CBL_HUMAN	protein

Search

☐ Show linked pathway entities only

Close

Search: egfr

Signaling by EGFR [Reactome, Homo sapiens]

Filter: signaling by E

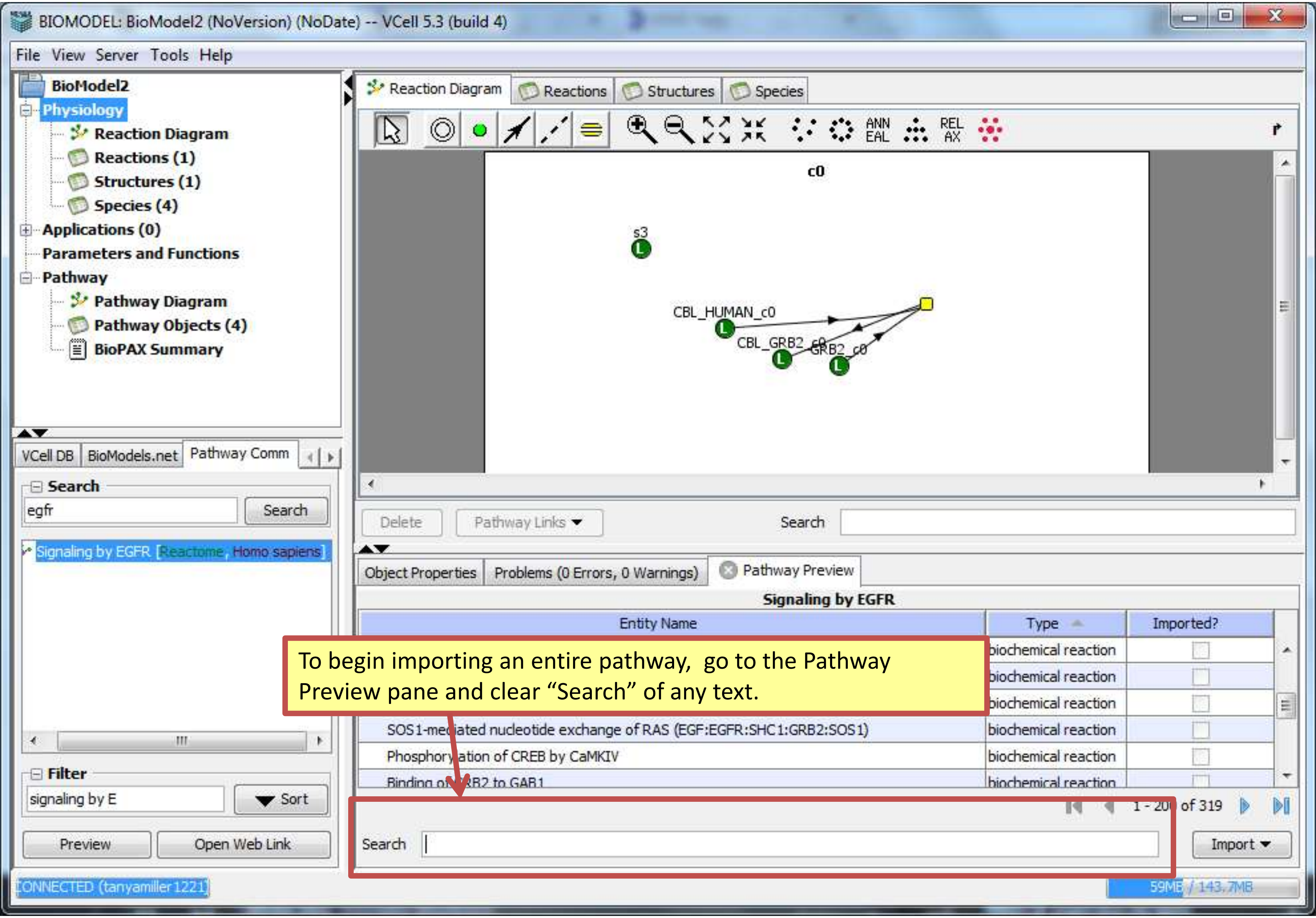
Species Name: s3

Linked Pathway Object(s)

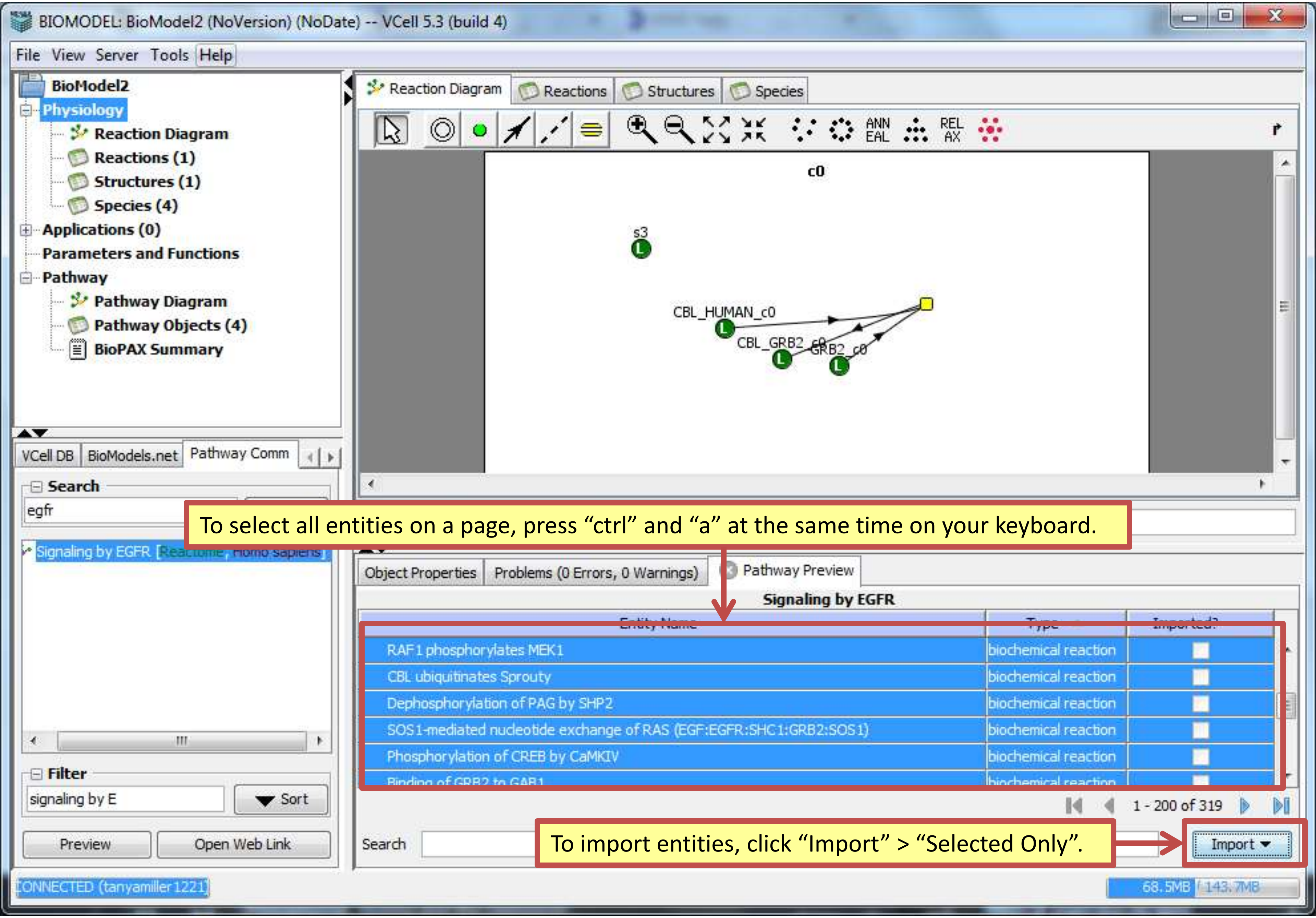
Annotation

To link a species to an entity in the imported pathway, click a box in the “Link” column, next to the entity’s name.

To finish linking a species to a pathway, click “Close”.



To begin importing an entire pathway, go to the Pathway Preview pane and clear "Search" of any text.



Search: egfr

Signaling by EGFR [Reactome, Homo sapiens]

Filter: signaling by E

Signaling by EGFR

Entity Name	Type	Imported?
RAF1 phosphorylates MEK1	biochemical reaction	☐
CBL ubiquitinates Sprouty	biochemical reaction	☐
Dephosphorylation of PAG by SHP2	biochemical reaction	☐
SOS1-mediated nucleotide exchange of RAS (EGF:EGFR:SHC1:GRB2:SOS1)	biochemical reaction	☐
Phosphorylation of CREB by CaMKIV	biochemical reaction	☐
Binding of GRB2 to GAB1	biochemical reaction	☐

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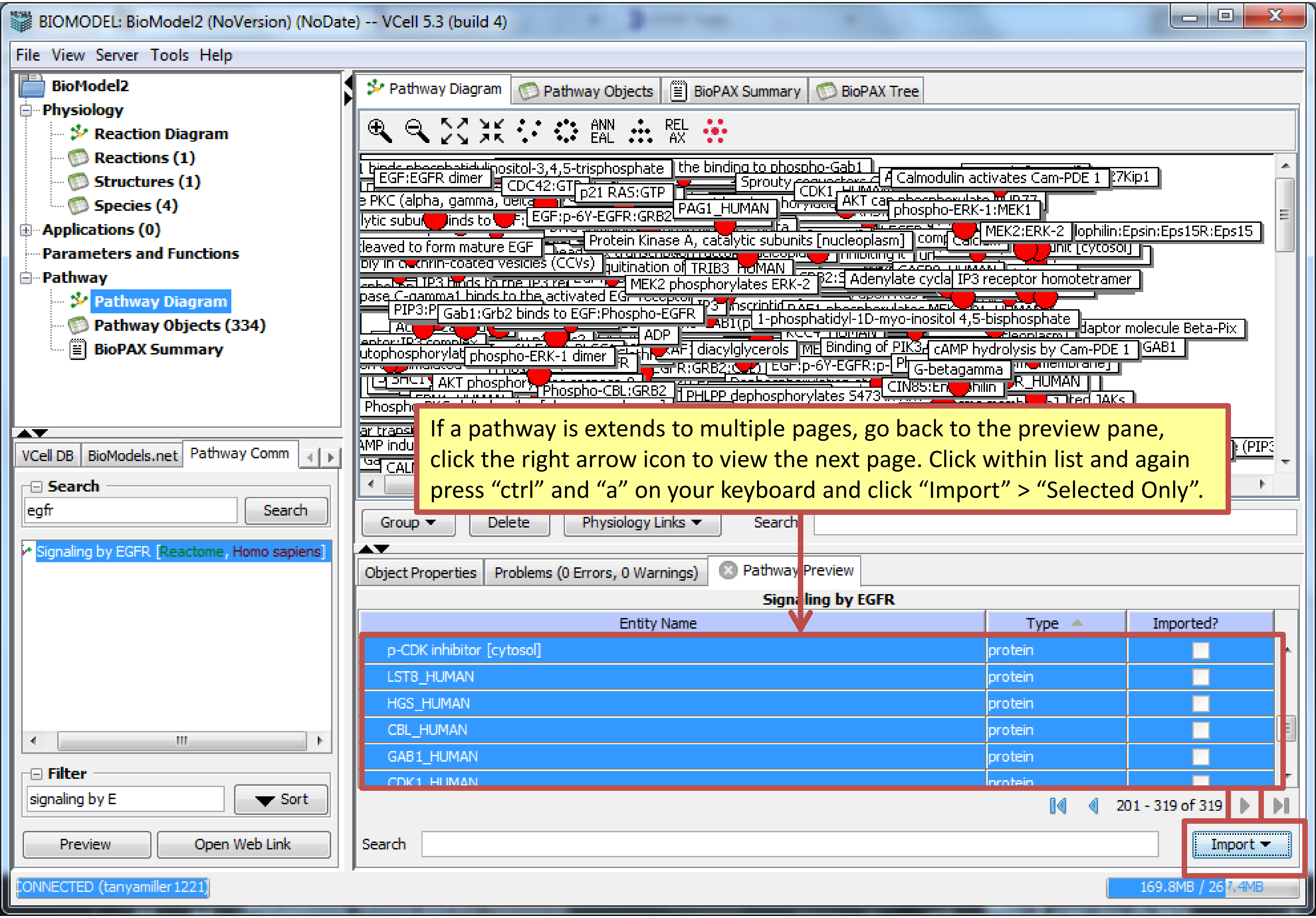
To select all entities on a page, press “ctrl” and “a” at the same time on your keyboard.

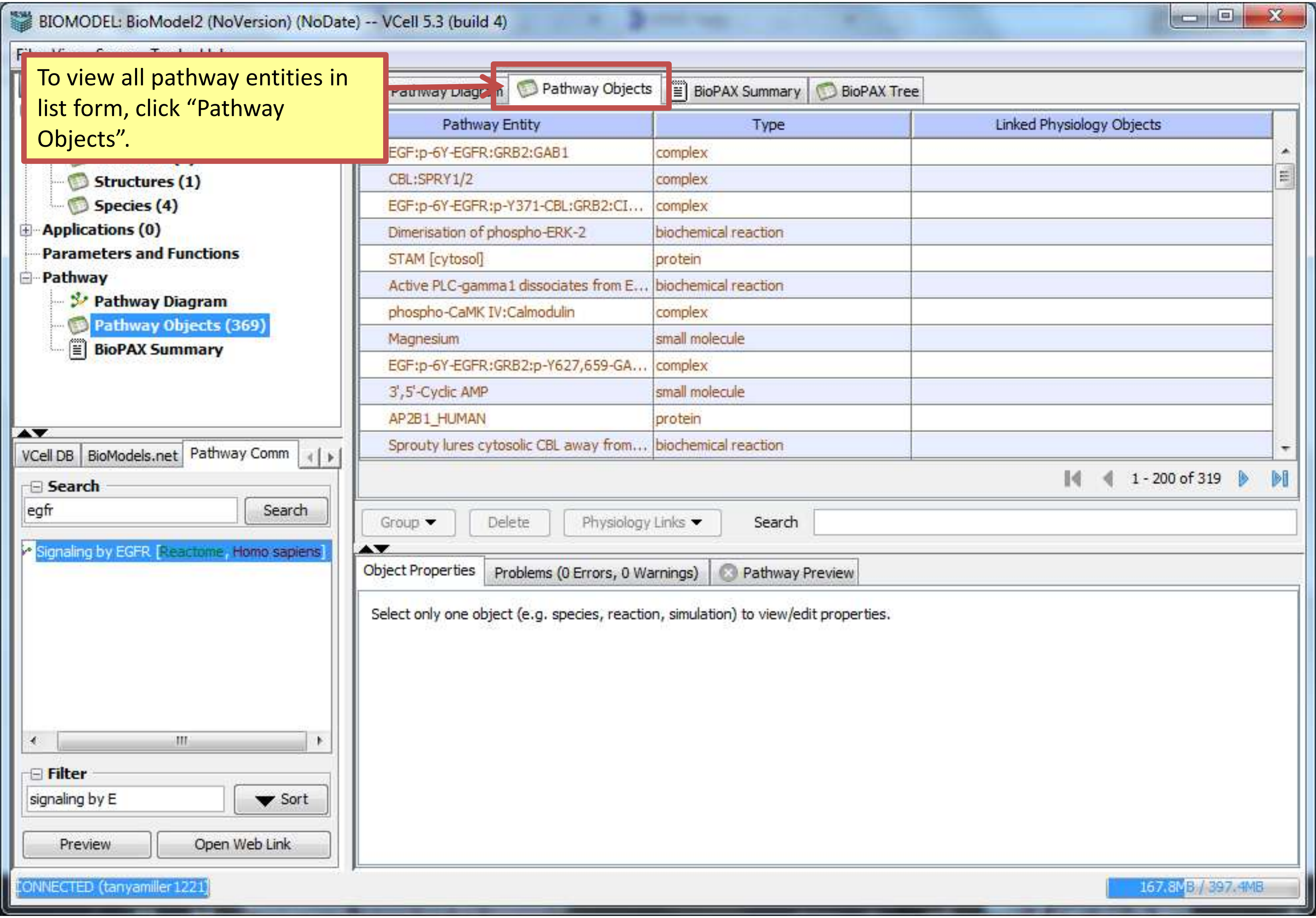
To import entities, click “Import” > “Selected Only”.

Pathway Commons Tutorial Contents



Entity Name	Type	Imported?
p-CDK inhibitor [cytosol]	protein	☐
LST8_HUMAN	protein	☐
HGS_HUMAN	protein	☐
CBL_HUMAN	protein	☐
GAB1_HUMAN	protein	☐
CDK1_HUMAN	protein	☐

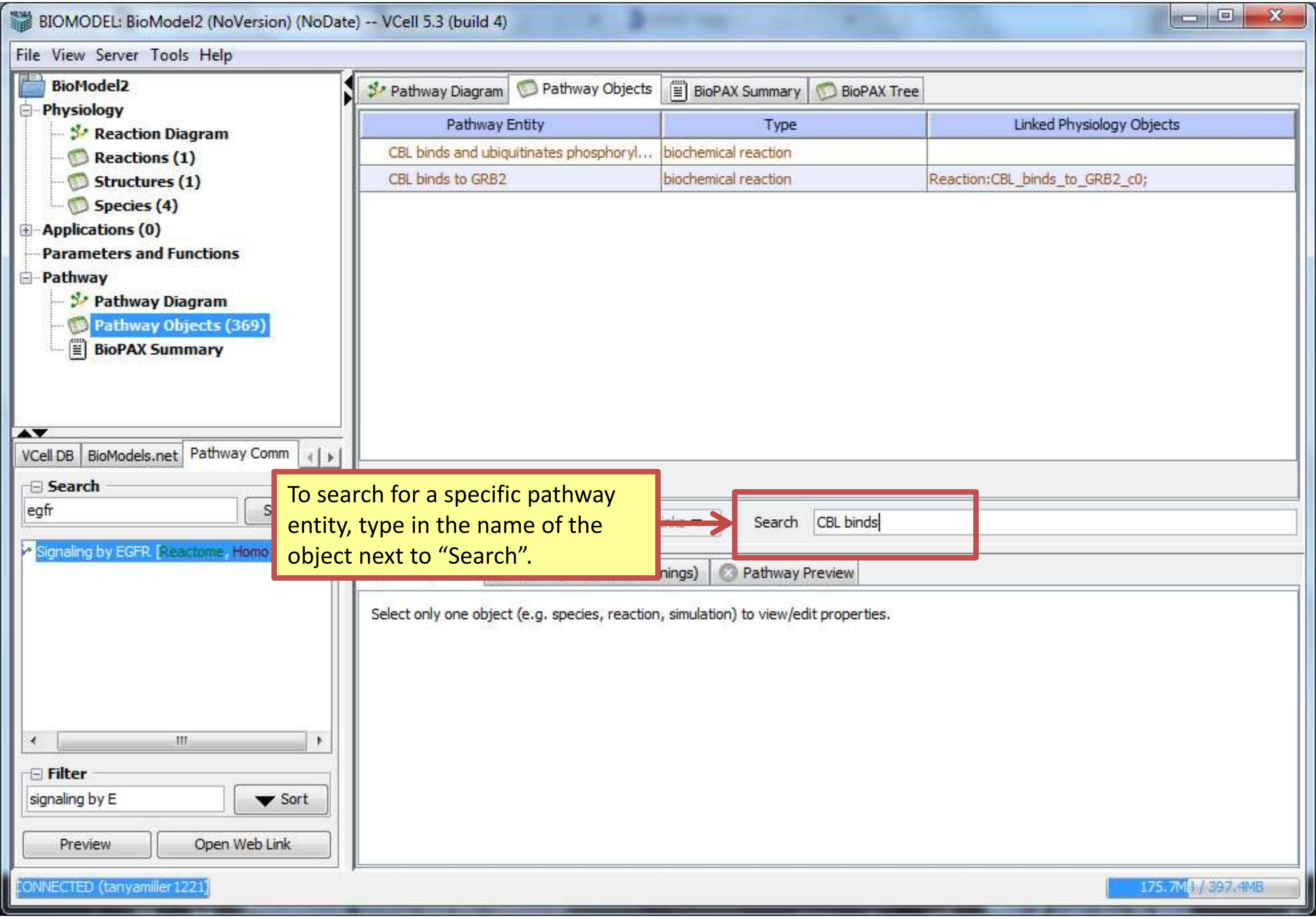
If a pathway is extends to multiple pages, go back to the preview pane, click the right arrow icon to view the next page. Click within list and again press “ctrl” and “a” on your keyboard and click “Import” > “Selected Only”.



To view all pathway entities in list form, click “Pathway Objects”.

Pathway Entity	Type	Linked Physiology Objects
EGF:p-6Y-EGFR:GRB2:GAB1	complex	
CBL:SPRY1/2	complex	
EGF:p-6Y-EGFR:p-Y371-CBL:GRB2:CI…	complex	
Dimerisation of phospho-ERK-2	biochemical reaction	
STAM [cytosol]	protein	
Active PLC-gamma1 dissociates from E…	biochemical reaction	
phospho-CaMK IV:Calmodulin	complex	
Magnesium	small molecule	
EGF:p-6Y-EGFR:GRB2:p-Y627,659-GA…	complex	
3',5'-Cyclic AMP	small molecule	
AP2B1_HUMAN	protein	
Sprouty lures cytosolic CBL away from…	biochemical reaction	

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



Pathway Entity	Type	Linked Physiology Objects
CBL binds and ubiquitinates phosphoryl...	biochemical reaction	
CBL binds to GRB2	biochemical reaction	Reaction:CBL_binds_to_GRB2_c0;

Search: egfr

Signaling by EGFR [Reactome, Homo

Filter: signaling by E

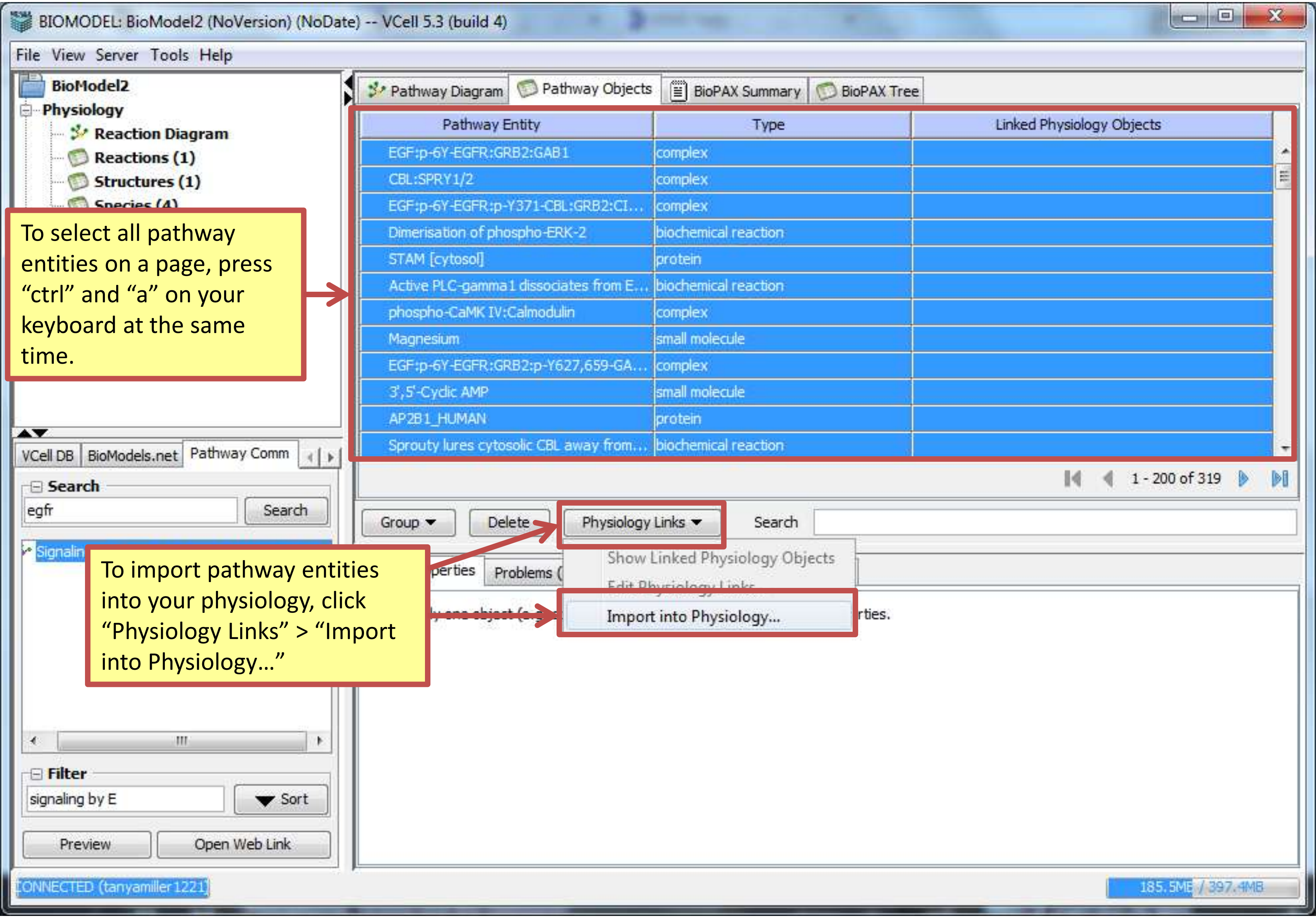
Search: CBL binds

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

CONNECTED (tanyamiller1221)

175.7MB / 397.4MB

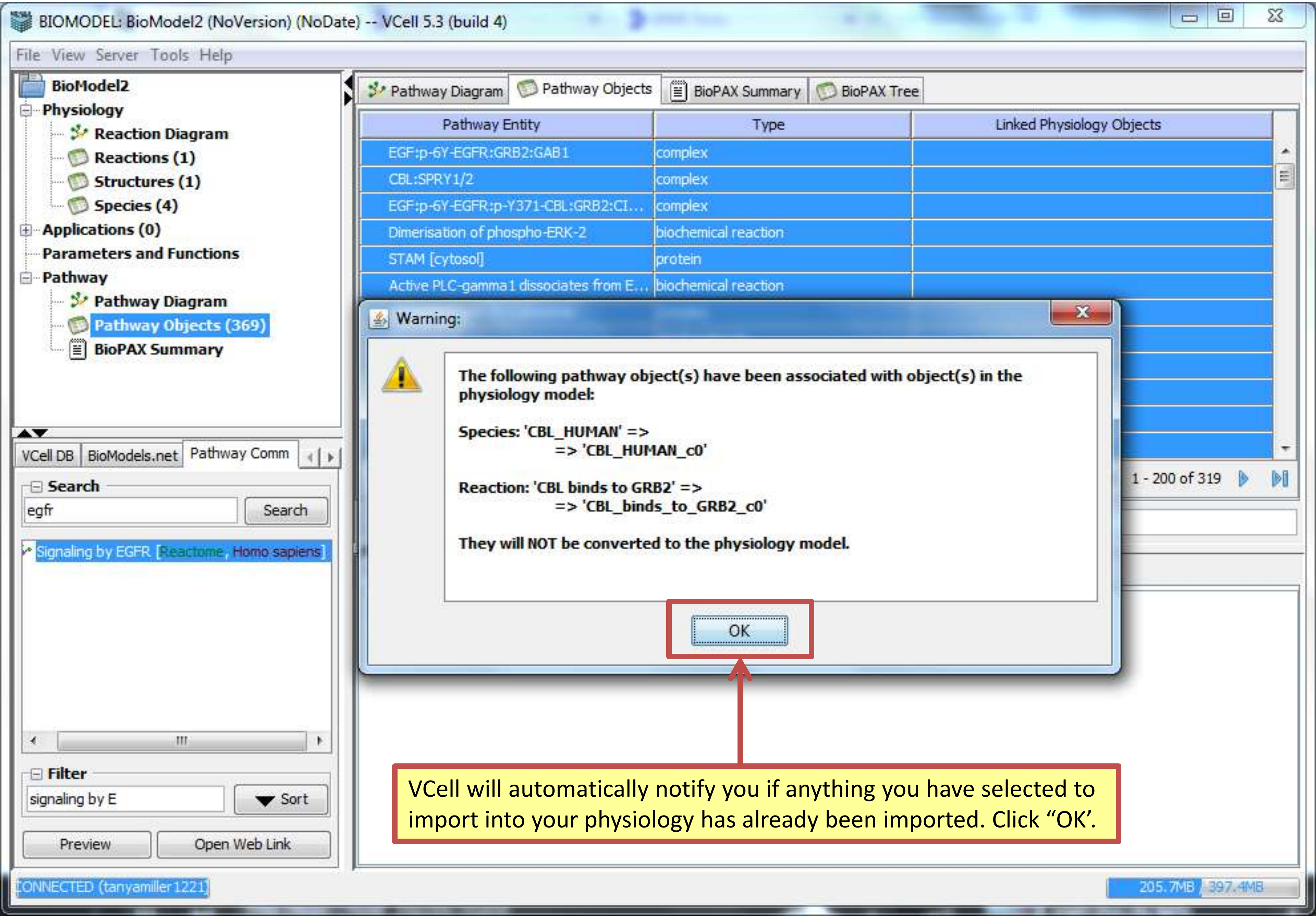
To search for a specific pathway entity, type in the name of the object next to "Search".



Pathway Entity	Type	Linked Physiology Objects
EGF:p-6Y-EGFR:GRB2:GAB1	complex	
CBL:SPRY1/2	complex	
EGF:p-6Y-EGFR:p-Y371-CBL:GRB2:CI...	complex	
Dimerisation of phospho-ERK-2	biochemical reaction	
STAM [cytosol]	protein	
Active PLC-gamma1 dissociates from E...	biochemical reaction	
phospho-CaMK IV:Calmodulin	complex	
Magnesium	small molecule	
EGF:p-6Y-EGFR:GRB2:p-Y627,659-GA...	complex	
3',5'-Cyclic AMP	small molecule	
AP2B1_HUMAN	protein	
Sprouty lures cytosolic CBL away from...	biochemical reaction	

To select all pathway entities on a page, press “ctrl” and “a” on your keyboard at the same time.

To import pathway entities into your physiology, click “Physiology Links” > “Import into Physiology…”



Pathway Entity	Type	Linked Physiology Objects
EGF:p-6Y-EGFR:GRB2:GAB1	complex	
CBL:SPRY1/2	complex	
EGF:p-6Y-EGFR:p-Y371-CBL:GRB2:CI…	complex	
Dimerisation of phospho-ERK-2	biochemical reaction	
STAM [cytosol]	protein	
Active PLC-gamma1 dissociates from E…	biochemical reaction	

The following pathway object(s) have been associated with object(s) in the physiology model:

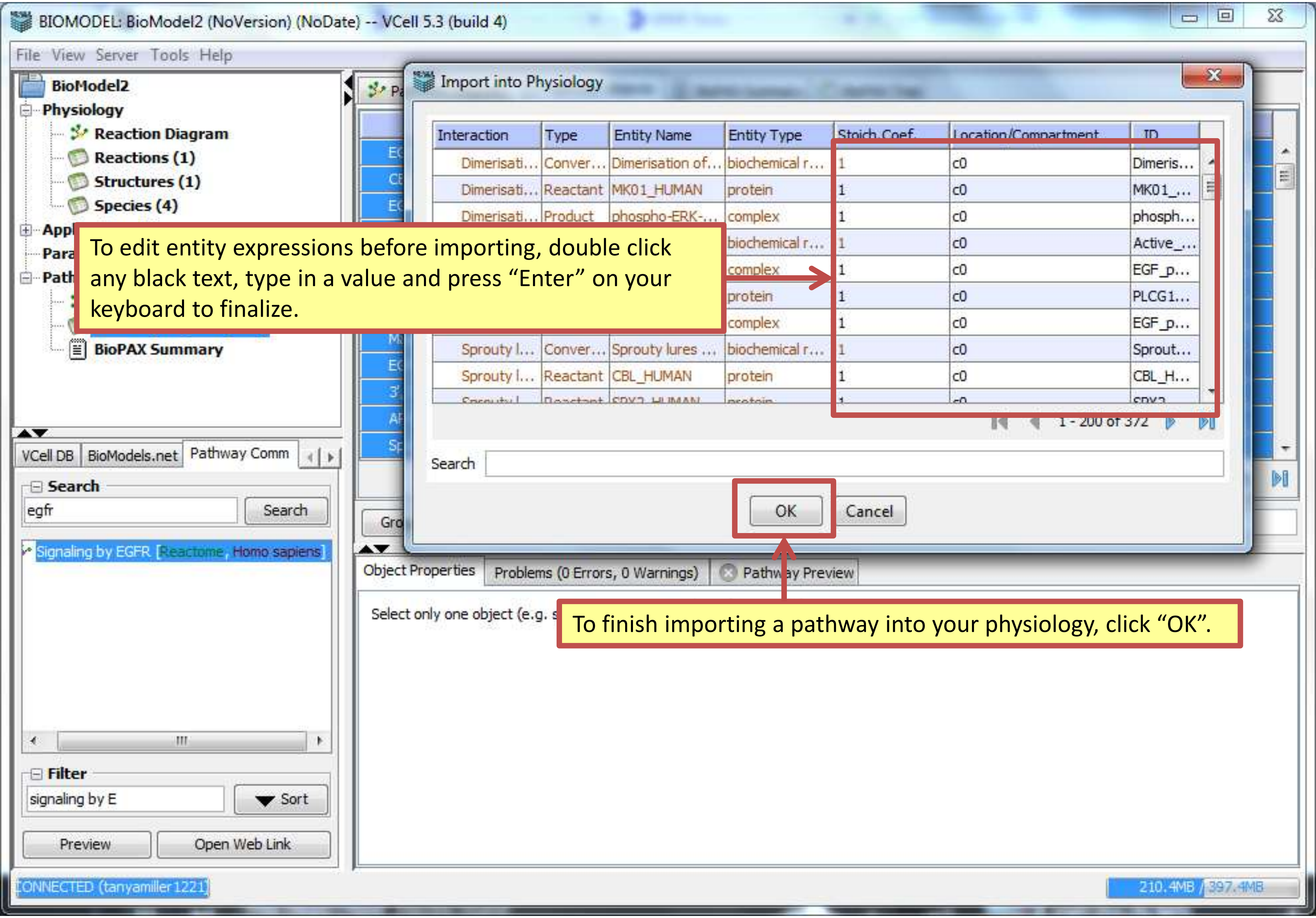
Species: 'CBL_HUMAN' =>
=> 'CBL_HUMAN_c0'

Reaction: 'CBL binds to GRB2' =>
=> 'CBL_binds_to_GRB2_c0'

They will NOT be converted to the physiology model.

VCell will automatically notify you if anything you have selected to import into your physiology has already been imported. Click “OK’.

Contents



Search: egfr

Signaling by EGFR [Reactome, Homo sapiens]

Filter: signaling by E

Import into Physiology

Interaction	Type	Entity Name	Entity Type	Stoich.Coef.	Location/Compartment	ID
Dimerisati…	Conver…	Dimerisation of…	biochemical r…	1	c0	Dimeris…
Dimerisati…	Reactant	MK01_HUMAN	protein	1	c0	MK01_…
Dimerisati…	Product	phospho-ERK-…	complex	1	c0	phosph…
			biochemical r…	1	c0	Active_…
			complex	1	c0	EGF_p…
			protein	1	c0	PLCG1…
			complex	1	c0	EGF_p…
Sprouty l…	Conver…	Sprouty lures …	biochemical r…	1	c0	Sprout…
Sprouty l…	Reactant	CBL_HUMAN	protein	1	c0	CBL_H…

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Search

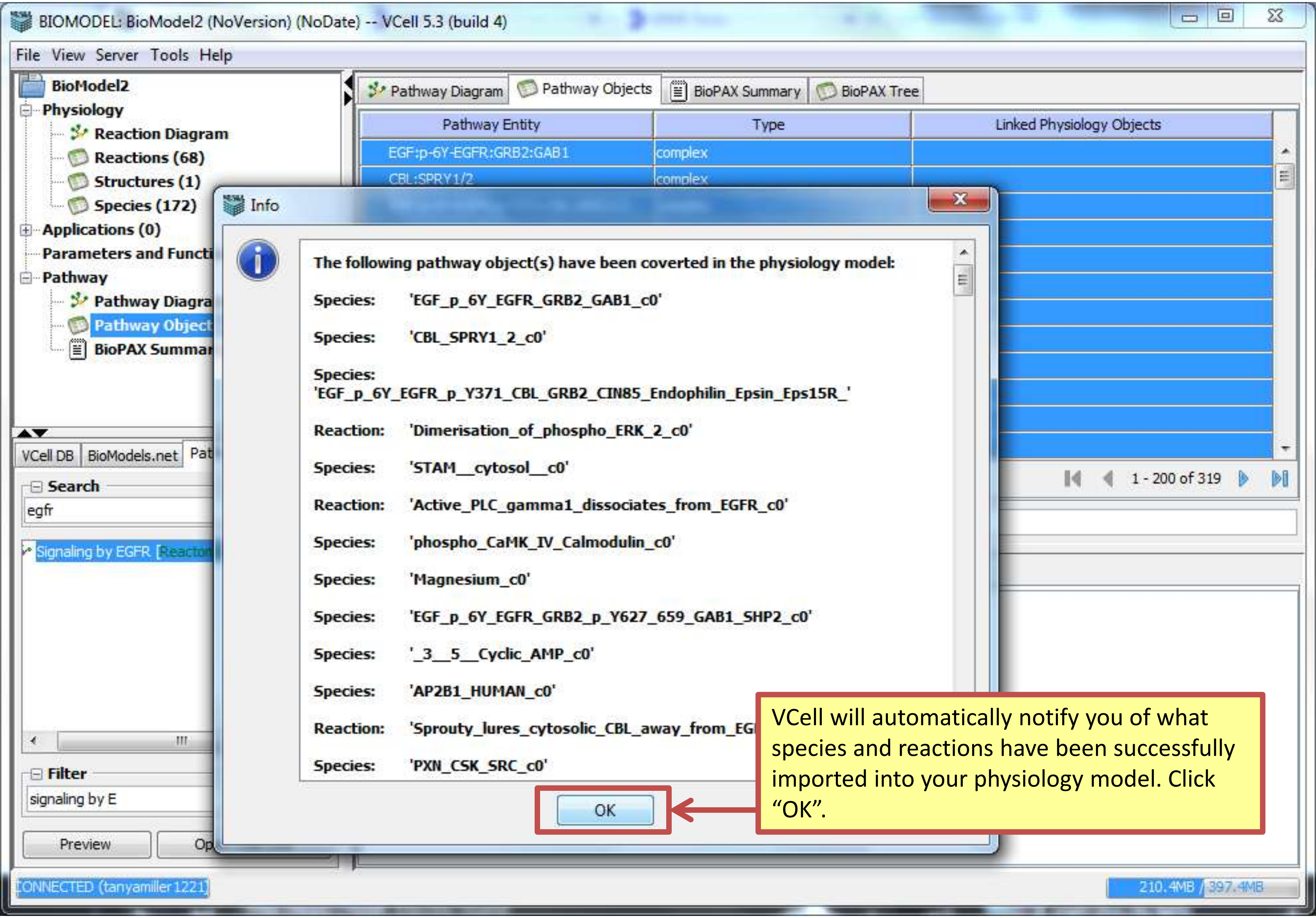
OK Cancel

Select only one object (e.g. s

To edit entity expressions before importing, double click any black text, type in a value and press “Enter” on your keyboard to finalize.

To finish importing a pathway into your physiology, click “OK”.

Contents



The following pathway object(s) have been coverted in the physiology model:

Species: 'EGF_p_6Y_EGFR_GRB2_GAB1_c0'

Species: 'CBL_SPRY1_2_c0'

Species: 'EGF_p_6Y_EGFR_p_Y371_CBL_GRB2_CIN85_Endophilin_Epsin_Eps15R_'

Reaction: 'Dimerisation_of_phospho_ERK_2_c0'

Species: 'STAM__cytosol__c0'

Reaction: 'Active_PLC_gamma1_dissociates_from_EGFR_c0'

Species: 'phospho_CaMK_IV_Calmodulin_c0'

Species: 'Magnesium_c0'

Species: 'EGF_p_6Y_EGFR_GRB2_p_Y627_659_GAB1_SHP2_c0'

Species: '_3__5__Cyclic_AMP_c0'

Species: 'AP2B1_HUMAN_c0'

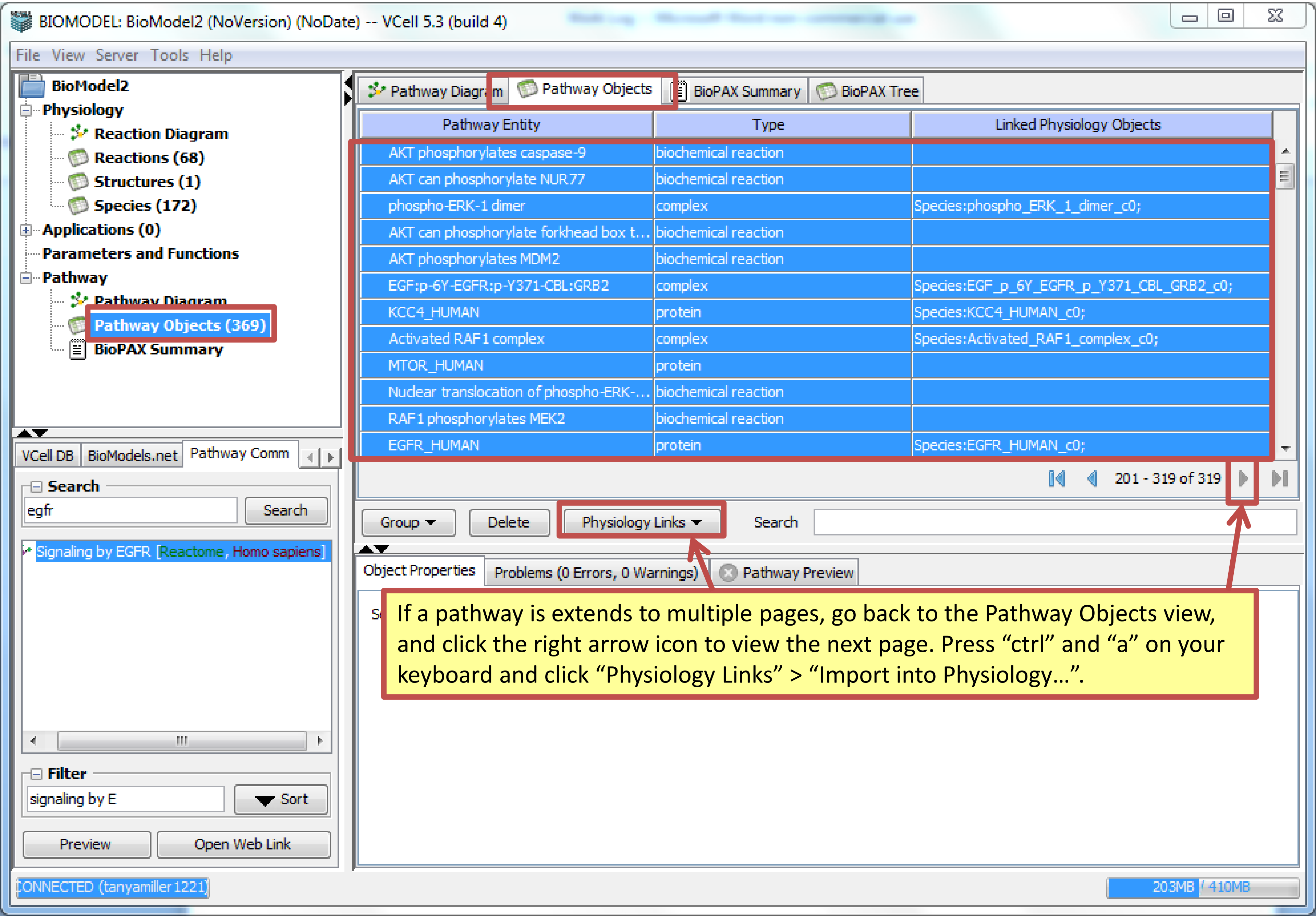
Reaction: 'Sprouty_lures_cytosolic_CBL_away_from_EG

Species: 'PXN_CSK_SRC_c0'

VCell will automatically notify you of what species and reactions have been successfully imported into your physiology model. Click “OK”.

Pathway Commons Tutorial

Contents



BIOMODEL: BioModel2 (NoVersion) (NoDate) -- VCell 5.3 (build 4)

Search: egfr

Signaling by EGFR [Reactome, Homo sapiens]

Filter: signaling by E

Pathway Entity	Type	Linked Physiology Objects
AKT phosphorylates caspase-9	biochemical reaction	
AKT can phosphorylate NUR77	biochemical reaction	
phospho-ERK-1 dimer	complex	Species:phospho_ERK_1_dimer_c0;
AKT can phosphorylate forkhead box t...	biochemical reaction	
AKT phosphorylates MDM2	biochemical reaction	
EGF:p-6Y-EGFR:p-Y371-CBL:GRB2	complex	Species:EGF_p_6Y_EGFR_p_Y371_CBL_GRB2_c0;
KCC4_HUMAN	protein	Species:KCC4_HUMAN_c0;
Activated RAF1 complex	complex	Species:Activated_RAF1_complex_c0;
MTOR_HUMAN	protein	
Nuclear translocation of phospho-ERK-...	biochemical reaction	
RAF1 phosphorylates MEK2	biochemical reaction	
EGFR_HUMAN	protein	Species:EGFR_HUMAN_c0;

201 - 319 of 319

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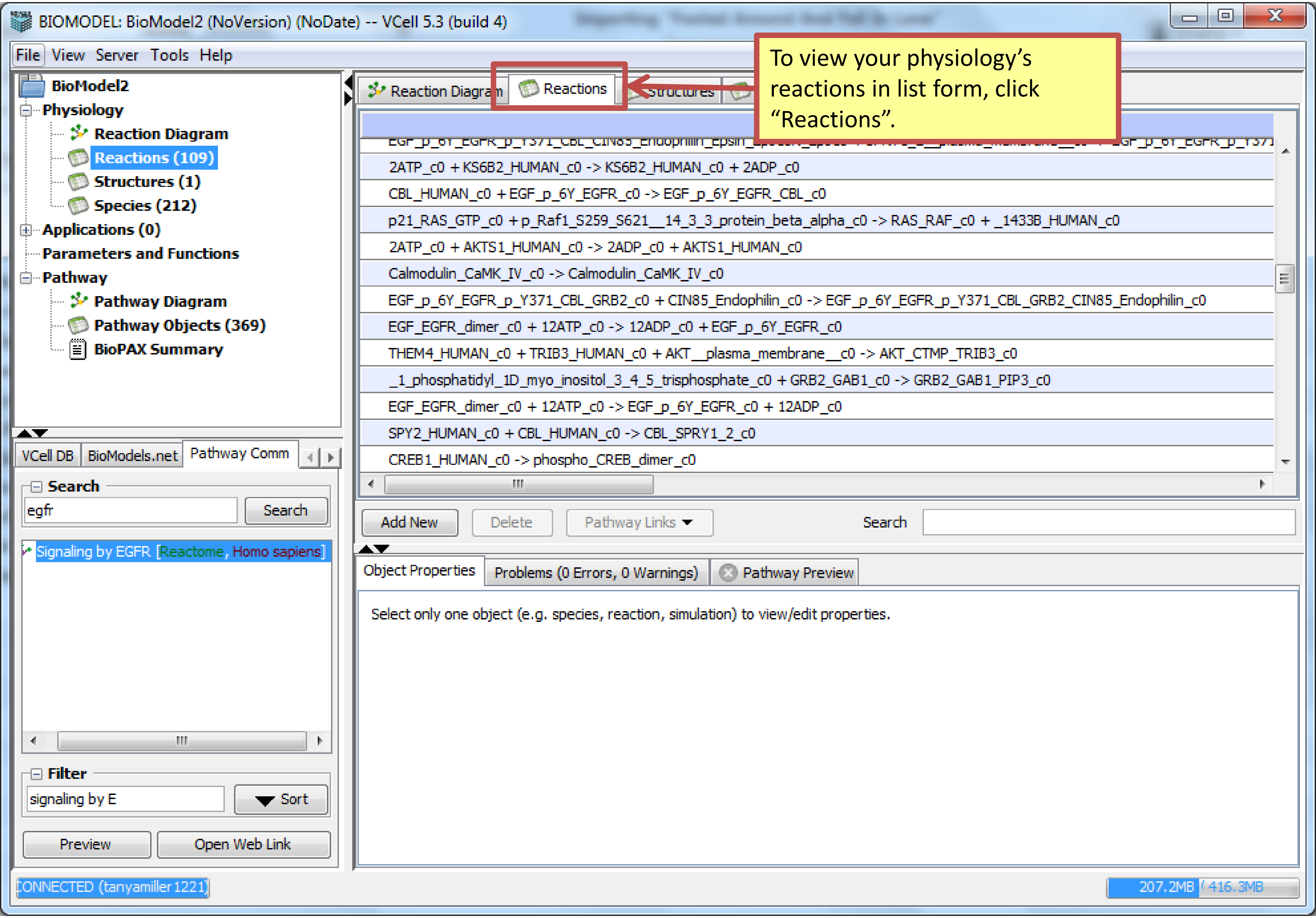
203MB / 410MB

If a pathway is extends to multiple pages, go back to the Pathway Objects view, and click the right arrow icon to view the next page. Press “ctrl” and “a” on your keyboard and click “Physiology Links” > “Import into Physiology…”.



To view your physiology's reactions in list form, click "Reactions".

BIOMODEL: BioModel2 (NoVersion) (NoDate) -- VCell 5.3 (build 4)

- BioModel2
  - Physiology
    - Reaction Diagram
    - Reactions (109)
    - Structures (1)
    - Species (212)
  - Applications (0)
  - Parameters and Functions
  - Pathway
    - Pathway Diagram
    - Pathway Objects (369)
    - BioPAX Summary

2ATP_c0 + KS6B2_HUMAN_c0 -> KS6B2_HUMAN_c0 + 2ADP_c0

CBL_HUMAN_c0 + EGF_p_6Y_EGFR_c0 -> EGF_p_6Y_EGFR_CBL_c0

p21_RAS_GTP_c0 + p_Raf1_S259_S621__14_3_3_protein_beta_alpha_c0 -> RAS_RAF_c0 + _1433B_HUMAN_c0

2ATP_c0 + AKTS1_HUMAN_c0 -> 2ADP_c0 + AKTS1_HUMAN_c0

Calmodulin_CaMK_IV_c0 -> Calmodulin_CaMK_IV_c0

EGF_p_6Y_EGFR_p_Y371_CBL_GRB2_c0 + CIN85_Endophilin_c0 -> EGF_p_6Y_EGFR_p_Y371_CBL_GRB2_CIN85_Endophilin_c0

EGF_EGFR_dimer_c0 + 12ATP_c0 -> 12ADP_c0 + EGF_p_6Y_EGFR_c0

THEM4_HUMAN_c0 + TRIB3_HUMAN_c0 + AKT__plasma_membrane__c0 -> AKT_CTMP_TRIB3_c0

_1_phosphatidyl_1D_myo_inositol_3_4_5_trisphosphate_c0 + GRB2_GAB1_c0 -> GRB2_GAB1_PIP3_c0

EGF_EGFR_dimer_c0 + 12ATP_c0 -> EGF_p_6Y_EGFR_c0 + 12ADP_c0

SPY2_HUMAN_c0 + CBL_HUMAN_c0 -> CBL_SPRY1_2_c0

CREB1_HUMAN_c0 -> phospho_CREB_dimer_c0

Search: egfr

Signaling by EGFR [Reactome, Homo sapiens]

Filter: signaling by E

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

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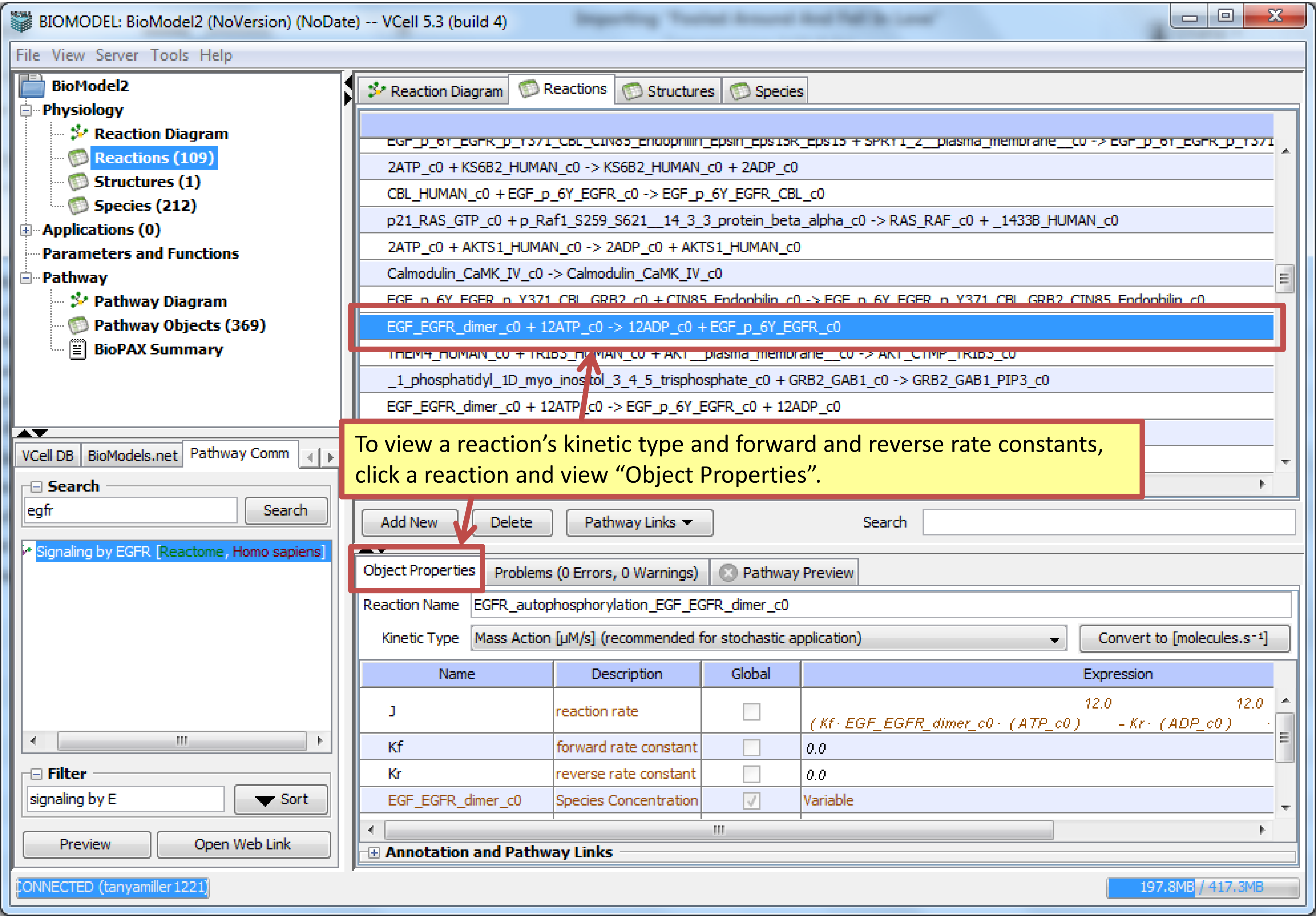
207.2MB / 416.3MB

Contents



To view a reaction's kinetic type and forward and reverse rate constants, click a reaction and view "Object Properties".

BIOMODEL: BioModel2 (NoVersion) (NoDate) -- VCell 5.3 (build 4)

Search: egfr

Signaling by EGFR [Reactome, Homo sapiens]

Filter: signaling by E

- EGF_p_6Y_EGFR_p_Y371_CBL_CIN85_Endophilin_Epsin_Eps15R_Eps15 + SPRY1_2__plasma_membrane__c0 -> EGF_p_6Y_EGFR_p_Y371
- 2ATP_c0 + KS6B2_HUMAN_c0 -> KS6B2_HUMAN_c0 + 2ADP_c0
- CBL_HUMAN_c0 + EGF_p_6Y_EGFR_c0 -> EGF_p_6Y_EGFR_CBL_c0
- p21_RAS_GTP_c0 + p_Raf1_S259_S621__14_3_3_protein_beta_alpha_c0 -> RAS_RAF_c0 + _1433B_HUMAN_c0
- 2ATP_c0 + AKTS1_HUMAN_c0 -> 2ADP_c0 + AKTS1_HUMAN_c0
- Calmodulin_CaMK_IV_c0 -> Calmodulin_CaMK_IV_c0
- EGF_p_6Y_EGFR_p_Y371_CBL_GRB2_c0 + CIN85_Endophilin_c0 -> EGF_p_6Y_EGFR_p_Y371_CBL_GRB2_CIN85_Endophilin_c0
- EGF_EGFR_dimer_c0 + 12ATP_c0 -> 12ADP_c0 + EGF_p_6Y_EGFR_c0
- THEM4_HUMAN_c0 + TRIB3_HUMAN_c0 + AKT__plasma_membrane__c0 -> AKT_CTMP_TRIB3_c0
- _1_phosphatidyl_1D_myo_inositol_3_4_5_trisphosphate_c0 + GRB2_GAB1_c0 -> GRB2_GAB1_PIP3_c0
- EGF_EGFR_dimer_c0 + 12ATP_c0 -> EGF_p_6Y_EGFR_c0 + 12ADP_c0

Reaction Name: EGFR_autophosphorylation_EGF_EGFR_dimer_c0

Kinetic Type: Mass Action [µM/s] (recommended for stochastic application)

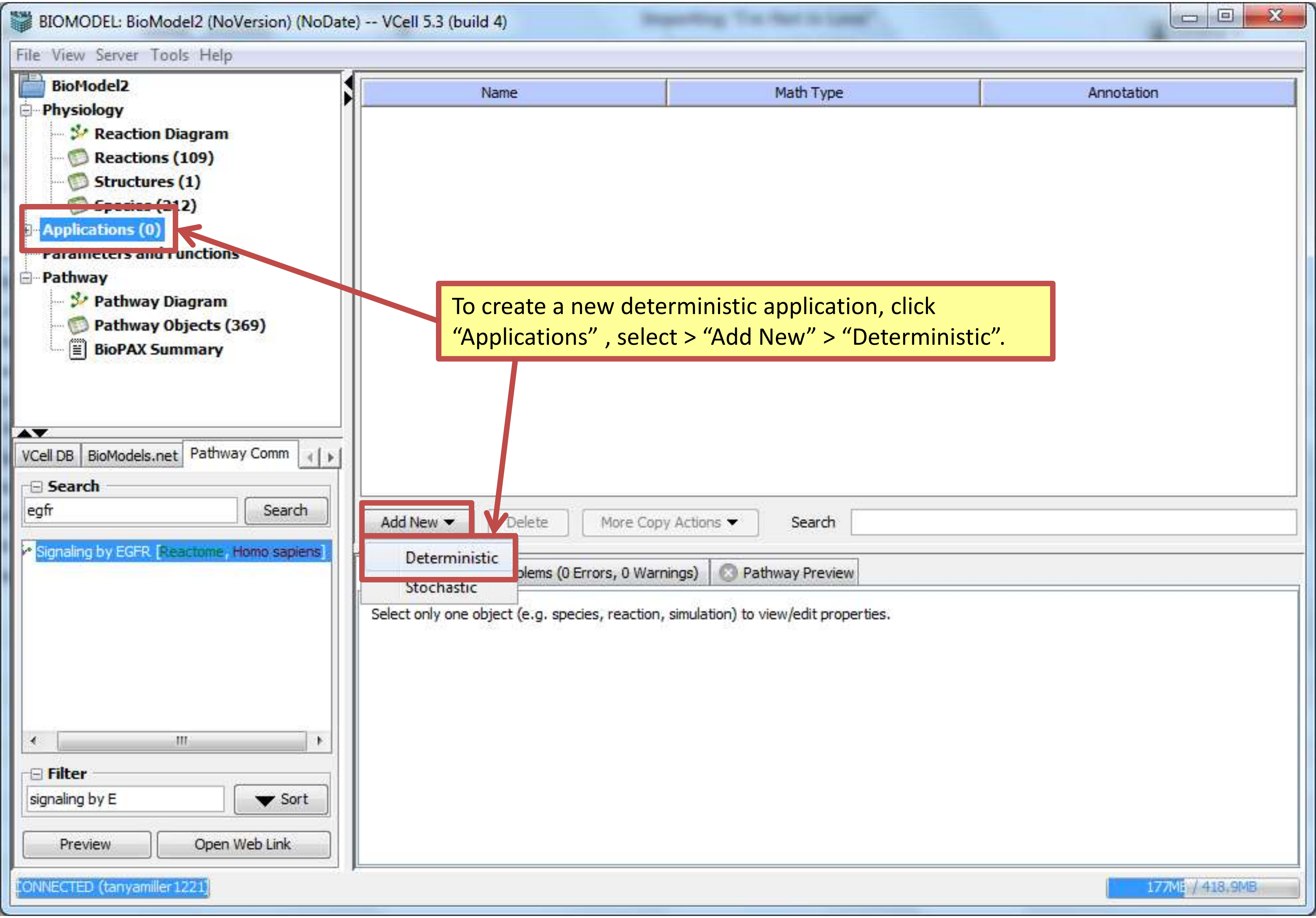
Convert to [molecules.s⁻¹]

Name	Description	Global	Expression
J	reaction rate	☐	$(Kf \cdot EGF\_EGFR\_dimer\_c0 \cdot (ATP\_c0)^{12.0} - Kr \cdot (ADP\_c0)^{12.0}$
Kf	forward rate constant	☐	0.0
Kr	reverse rate constant	☐	0.0
EGF_EGFR_dimer_c0	Species Concentration	☑	Variable

CONNECTED (tanyamiller1221)

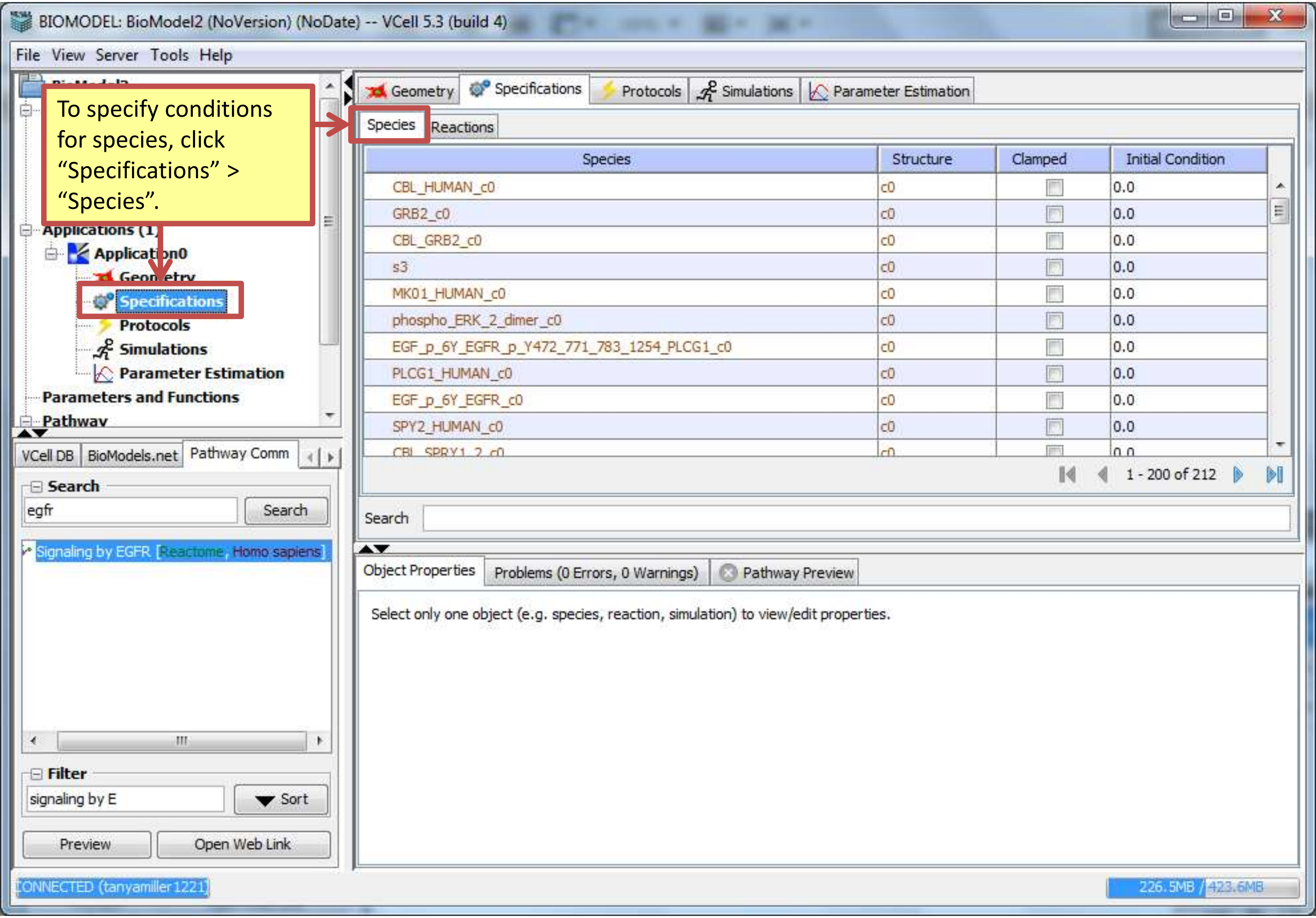
197.8MB / 417.3MB

Contents



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

To create a new deterministic application, click "Applications" , select > "Add New" > "Deterministic".



To specify conditions for species, click "Specifications" > "Species".

BIOMODEL: BioModel2 (NoVersion) (NoDate) -- VCell 5.3 (build 4)

Search: egfr

Signaling by EGFR [Reactome, Homo sapiens]

Filter: signaling by E

Species	Structure	Clamped	Initial Condition
CBL_HUMAN_c0	c0	☐	0.0
GRB2_c0	c0	☐	0.0
CBL_GRB2_c0	c0	☐	0.0
s3	c0	☐	0.0
MK01_HUMAN_c0	c0	☐	0.0
phospho_ERK_2_dimer_c0	c0	☐	0.0
EGF_p_6Y_EGFR_p_Y472_771_783_1254_PLCG1_c0	c0	☐	0.0
PLCG1_HUMAN_c0	c0	☐	0.0
EGF_p_6Y_EGFR_c0	c0	☐	0.0
SPY2_HUMAN_c0	c0	☐	0.0

1 - 200 of 212

Search

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

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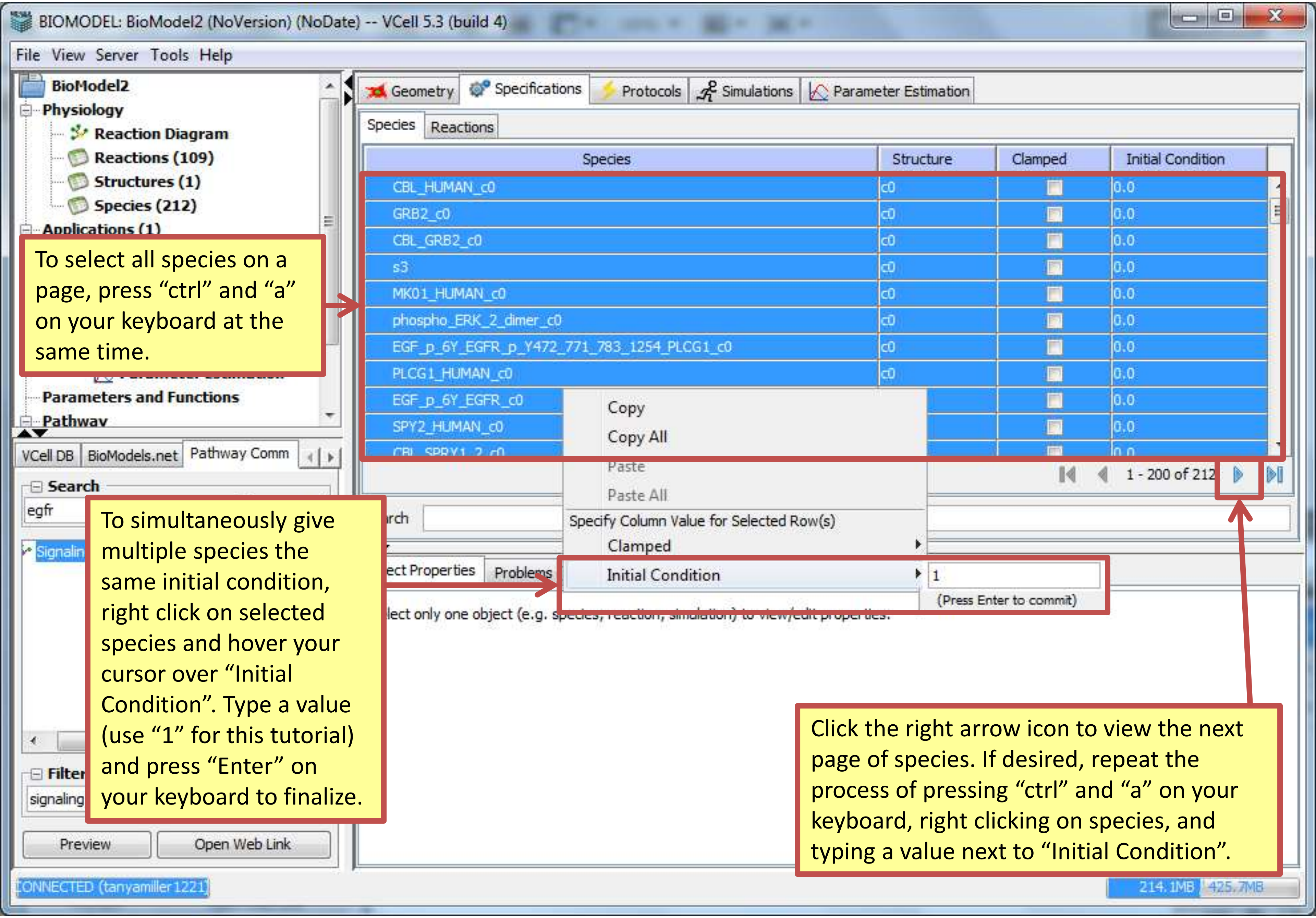
226.5MB / 423.6MB



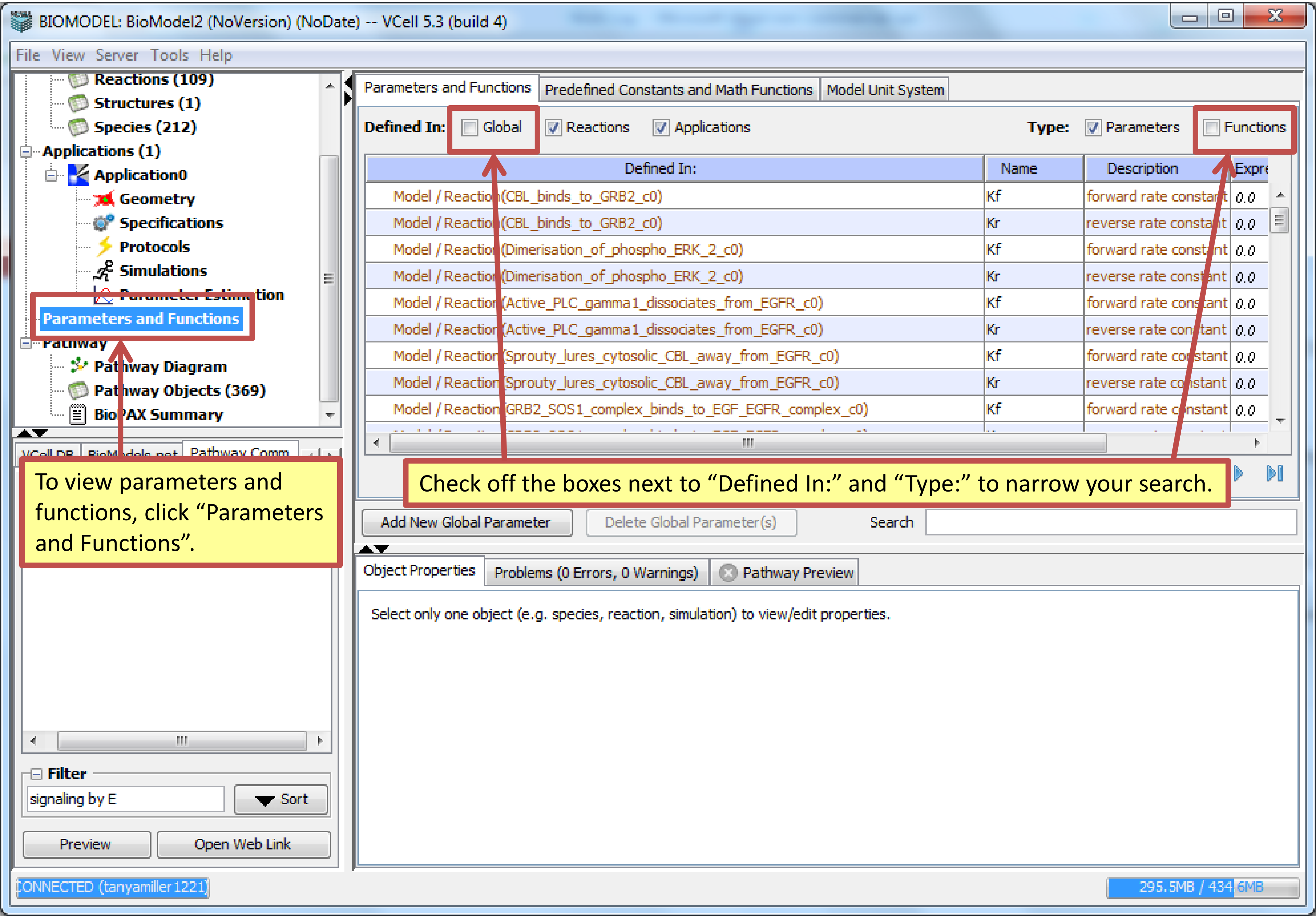
Species	Structure	Clamped	Initial Condition
CBL_HUMAN_c0	c0	☐	0.0
GRB2_c0	c0	☐	0.0
CBL_GRB2_c0	c0	☐	0.0
s3	c0	☐	0.0
MK01_HUMAN_c0	c0	☐	0.0
phospho_ERK_2_dimer_c0	c0	☐	0.0
EGF_p_6Y_EGFR_p_Y472_771_783_1254_PLCG1_c0	c0	☐	0.0
PLCG1_HUMAN_c0	c0	☐	0.0
EGF_p_6Y_EGFR_c0		☐	0.0
SPY2_HUMAN_c0		☐	0.0

To select all species on a page, press “ctrl” and “a” on your keyboard at the same time.

To simultaneously give multiple species the same initial condition, right click on selected species and hover your cursor over “Initial Condition”. Type a value (use “1” for this tutorial) and press “Enter” on your keyboard to finalize.

Click the right arrow icon to view the next page of species. If desired, repeat the process of pressing “ctrl” and “a” on your keyboard, right clicking on species, and typing a value next to “Initial Condition”.

Contents



Defined In: ☐ Global ☑ Reactions ☑ Applications

Type: ☑ Parameters ☐ Functions

Defined In:	Name	Description	Expre
Model / Reaction(CBL_binds_to_GRB2_c0)	Kf	forward rate constant	0.0
Model / Reaction(CBL_binds_to_GRB2_c0)	Kr	reverse rate constant	0.0
Model / Reaction(Dimerisation_of_phospho_ERK_2_c0)	Kf	forward rate constant	0.0
Model / Reaction(Dimerisation_of_phospho_ERK_2_c0)	Kr	reverse rate constant	0.0
Model / Reaction(Active_PLC_gamma1_dissociates_from_EGFR_c0)	Kf	forward rate constant	0.0
Model / Reaction(Active_PLC_gamma1_dissociates_from_EGFR_c0)	Kr	reverse rate constant	0.0
Model / Reaction(Sprouty_lures_cytosolic_CBL_away_from_EGFR_c0)	Kf	forward rate constant	0.0
Model / Reaction(Sprouty_lures_cytosolic_CBL_away_from_EGFR_c0)	Kr	reverse rate constant	0.0
Model / Reaction(GRB2_SOS1_complex_binds_to_EGF_EGFR_complex_c0)	Kf	forward rate constant	0.0

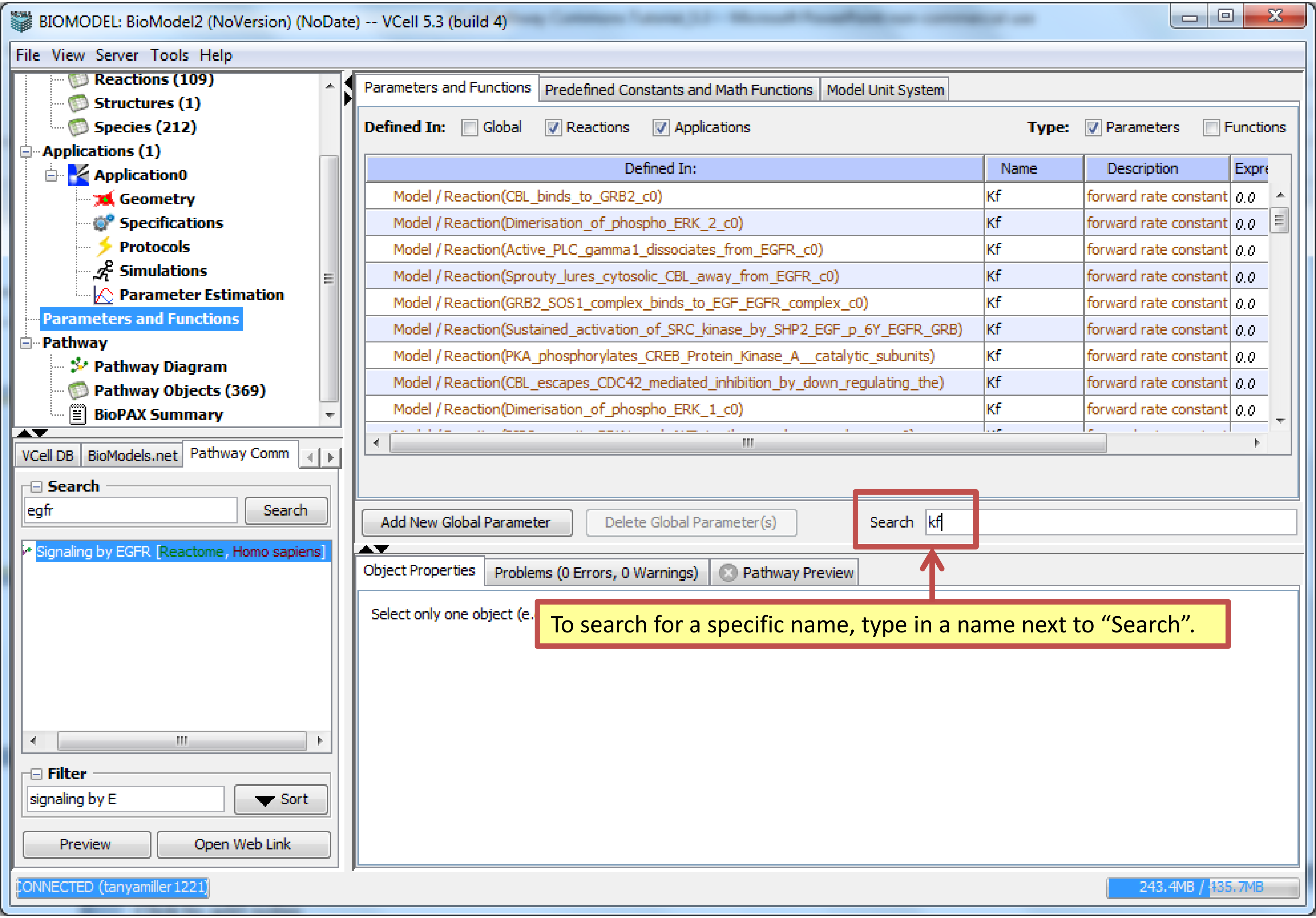
Filter: signaling by E

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

To view parameters and functions, click “Parameters and Functions”.

Check off the boxes next to “Defined In:” and “Type:” to narrow your search.

Contents



Defined In: ☐ Global ☑ Reactions ☑ Applications

Type: ☑ Parameters ☐ Functions

Defined In:	Name	Description	Expre
Model / Reaction(CBL_binds_to_GRB2_c0)	Kf	forward rate constant	0.0
Model / Reaction(Dimerisation_of_phospho_ERK_2_c0)	Kf	forward rate constant	0.0
Model / Reaction(Active_PLC_gamma1_dissociates_from_EGFR_c0)	Kf	forward rate constant	0.0
Model / Reaction(Sprouty_lures_cytosolic_CBL_away_from_EGFR_c0)	Kf	forward rate constant	0.0
Model / Reaction(GRB2_SOS1_complex_binds_to_EGF_EGFR_complex_c0)	Kf	forward rate constant	0.0
Model / Reaction(Sustained_activation_of_SRC_kinase_by_SHP2_EGF_p_6Y_EGFR_GRB)	Kf	forward rate constant	0.0
Model / Reaction(PKA_phosphorylates_CREB_Protein_Kinase_A__catalytic_subunits)	Kf	forward rate constant	0.0
Model / Reaction(CBL_escapes_CDC42_mediated_inhibition_by_down_regulating_the)	Kf	forward rate constant	0.0
Model / Reaction(Dimerisation_of_phospho_ERK_1_c0)	Kf	forward rate constant	0.0

Search: egfr

Signaling by EGFR [Reactome, Homo sapiens]

Filter: signaling by E

Search kf

Select only one object (e.

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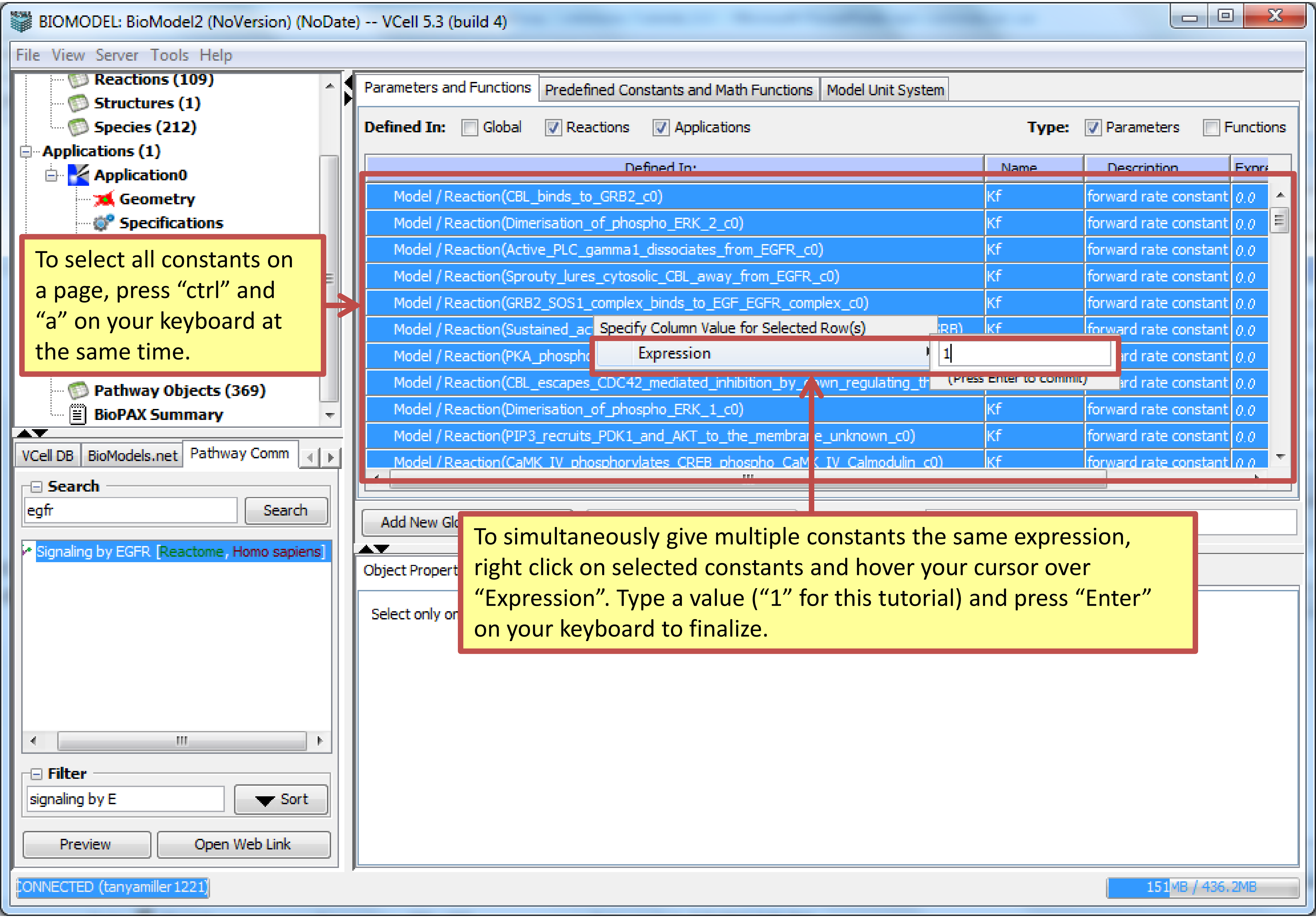
243.4MB / 435.7MB

To search for a specific name, type in a name next to “Search”.

Pathway Commons Tutorial



Search: egfr

Signaling by EGFR [Reactome, Homo sapiens]

Filter: signaling by E

Defined In: ☐ Global ☑ Reactions ☑ Applications

Type: ☑ Parameters ☐ Functions

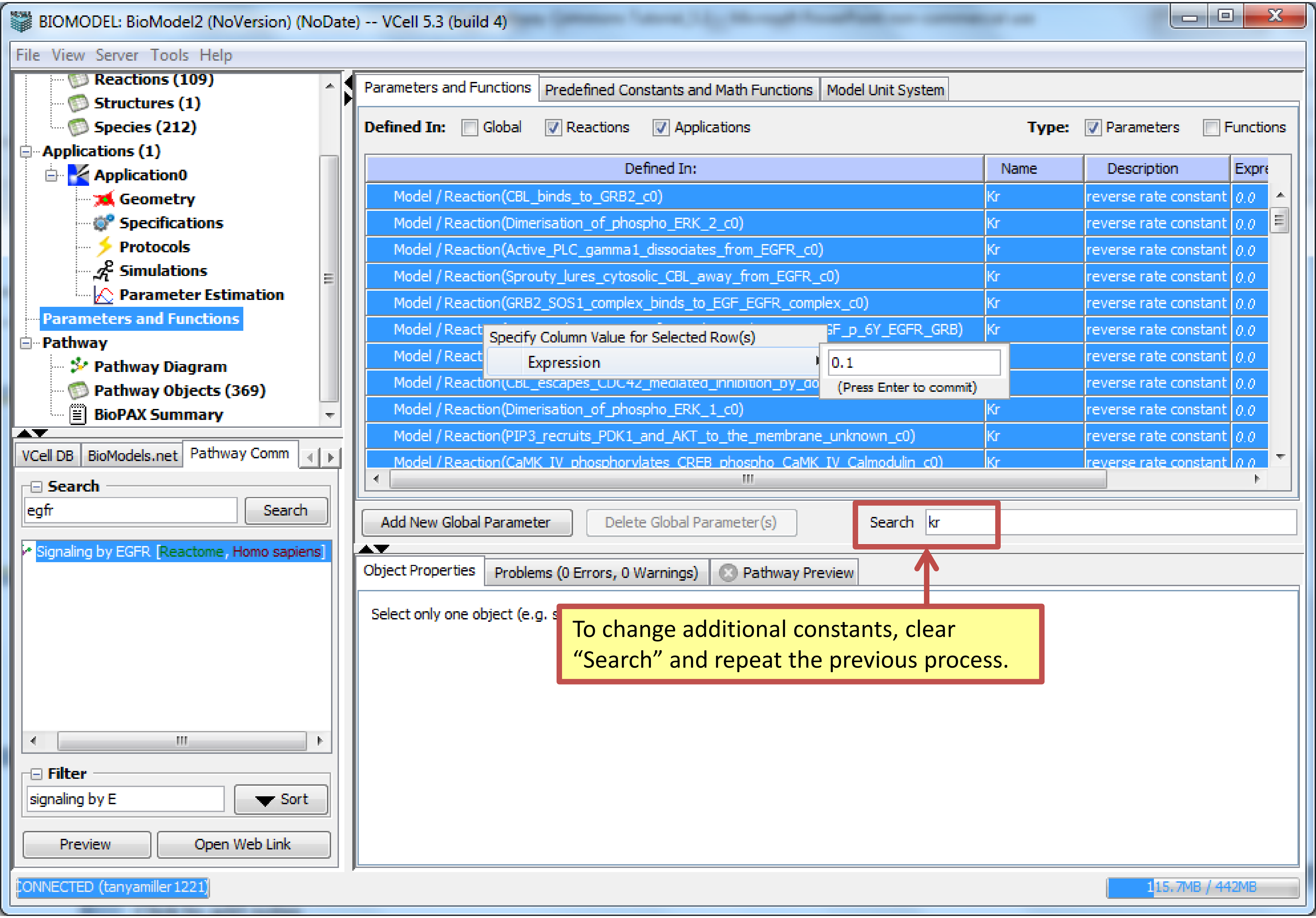
Defined In:	Name	Description	Expre
Model / Reaction(CBL_binds_to_GRB2_c0)	Kf	forward rate constant	0.0
Model / Reaction(Dimerisation_of_phospho_ERK_2_c0)	Kf	forward rate constant	0.0
Model / Reaction(Active_PLC_gamma1_dissociates_from_EGFR_c0)	Kf	forward rate constant	0.0
Model / Reaction(Sprouty_lures_cytosolic_CBL_away_from_EGFR_c0)	Kf	forward rate constant	0.0
Model / Reaction(GRB2_SOS1_complex_binds_to_EGF_EGFR_complex_c0)	Kf	forward rate constant	0.0
Model / Reaction(Sustained_ac … RB)	Kf	forward rate constant	0.0
Model / Reaction(PKA_phospho …		…rd rate constant	0.0
Model / Reaction(CBL_escapes_CDC42_mediated_inhibition_by_down_regulating_th…		…rd rate constant	0.0
Model / Reaction(Dimerisation_of_phospho_ERK_1_c0)	Kf	forward rate constant	0.0
Model / Reaction(PIP3_recruits_PDK1_and_AKT_to_the_membrane_unknown_c0)	Kf	forward rate constant	0.0
Model / Reaction(CaMK_IV_phosphorylates_CREB_phospho_CaMK_IV_Calmodulin_c0)	Kf	forward rate constant	0.0

Expression: 1

To select all constants on a page, press “ctrl” and “a” on your keyboard at the same time.

To simultaneously give multiple constants the same expression, right click on selected constants and hover your cursor over “Expression”. Type a value (“1” for this tutorial) and press “Enter” on your keyboard to finalize.

Pathway Commons Tutorial



Search: egfr

Signaling by EGFR [Reactome, Homo sapiens]

Filter: signaling by E

Defined In: ☐ Global ☑ Reactions ☑ Applications

Type: ☑ Parameters ☐ Functions

Defined In:	Name	Description	Expre
Model / Reaction(CBL_binds_to_GRB2_c0)	Kr	reverse rate constant	0.0
Model / Reaction(Dimerisation_of_phospho_ERK_2_c0)	Kr	reverse rate constant	0.0
Model / Reaction(Active_PLC_gamma1_dissociates_from_EGFR_c0)	Kr	reverse rate constant	0.0
Model / Reaction(Sprouty_lures_cytosolic_CBL_away_from_EGFR_c0)	Kr	reverse rate constant	0.0
Model / Reaction(GRB2_SOS1_complex_binds_to_EGF_EGFR_complex_c0)	Kr	reverse rate constant	0.0
Model / React … GF_p_6Y_EGFR_GRB)	Kr	reverse rate constant	0.0
Model / React		reverse rate constant	0.0
Model / Reaction(CBL_escapes_CDC42_mediated_inhibition_by_do		reverse rate constant	0.0
Model / Reaction(Dimerisation_of_phospho_ERK_1_c0)	Kr	reverse rate constant	0.0
Model / Reaction(PIP3_recruits_PDK1_and_AKT_to_the_membrane_unknown_c0)	Kr	reverse rate constant	0.0
Model / Reaction(CaMK_IV_phosphorylates_CREB_phospho_CaMK_IV_Calmodulin_c0)	Kr	reverse rate constant	0.0

Expression: 0.1

Search: kr

Select only one object (e.g. s

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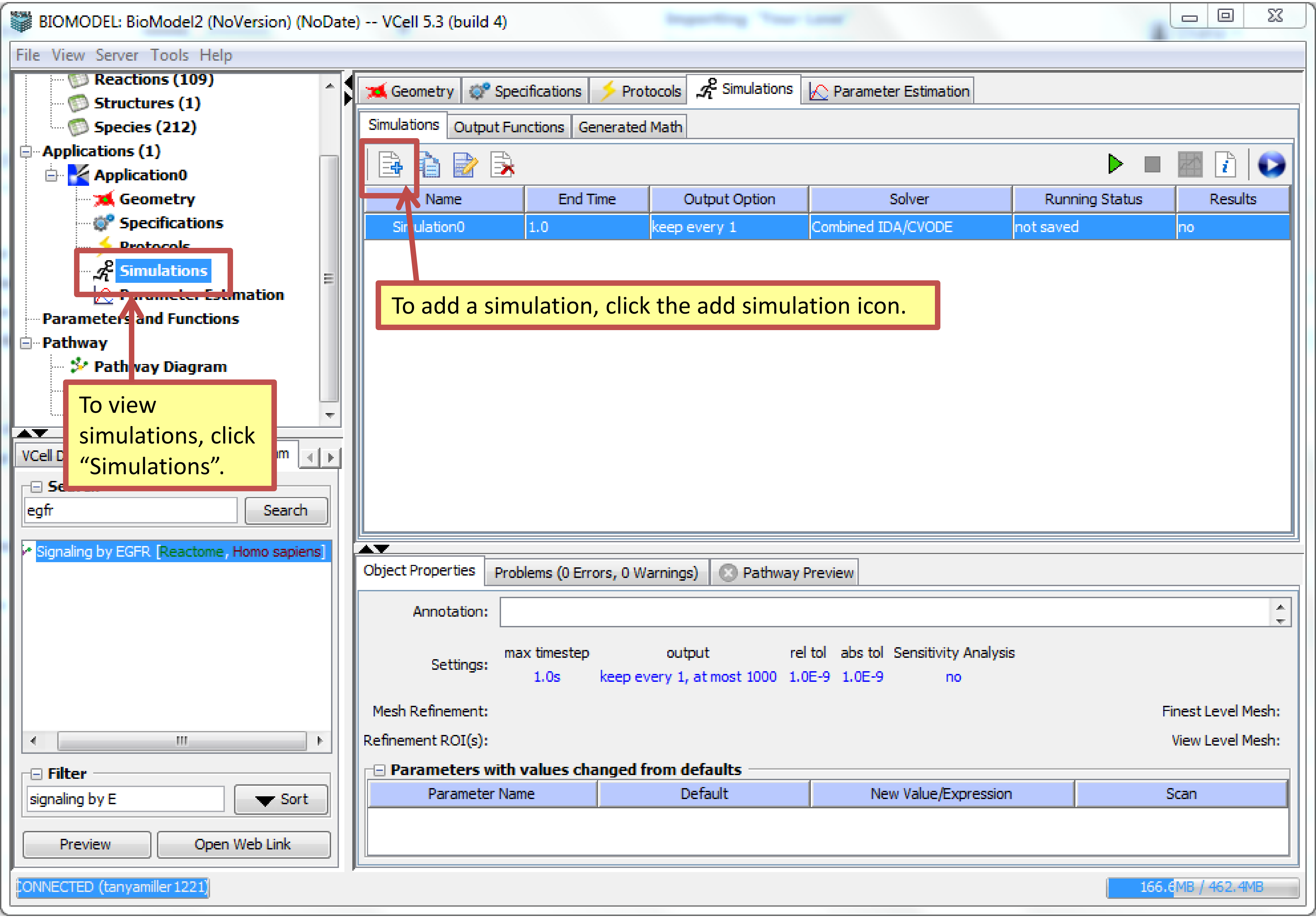
115.7MB / 442MB

To change additional constants, clear "Search" and repeat the previous process.



To add a simulation, click the add simulation icon.

To view simulations, click "Simulations".

Name	End Time	Output Option	Solver	Running Status	Results
Simulation0	1.0	keep every 1	Combined IDA/CVODE	not saved	no

Search: egfr

Signaling by EGFR [Reactome, Homo sapiens]

Filter: signaling by E

Sort

Annotation:

Settings:

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

Mesh Refinement:

Refinement ROI(s):

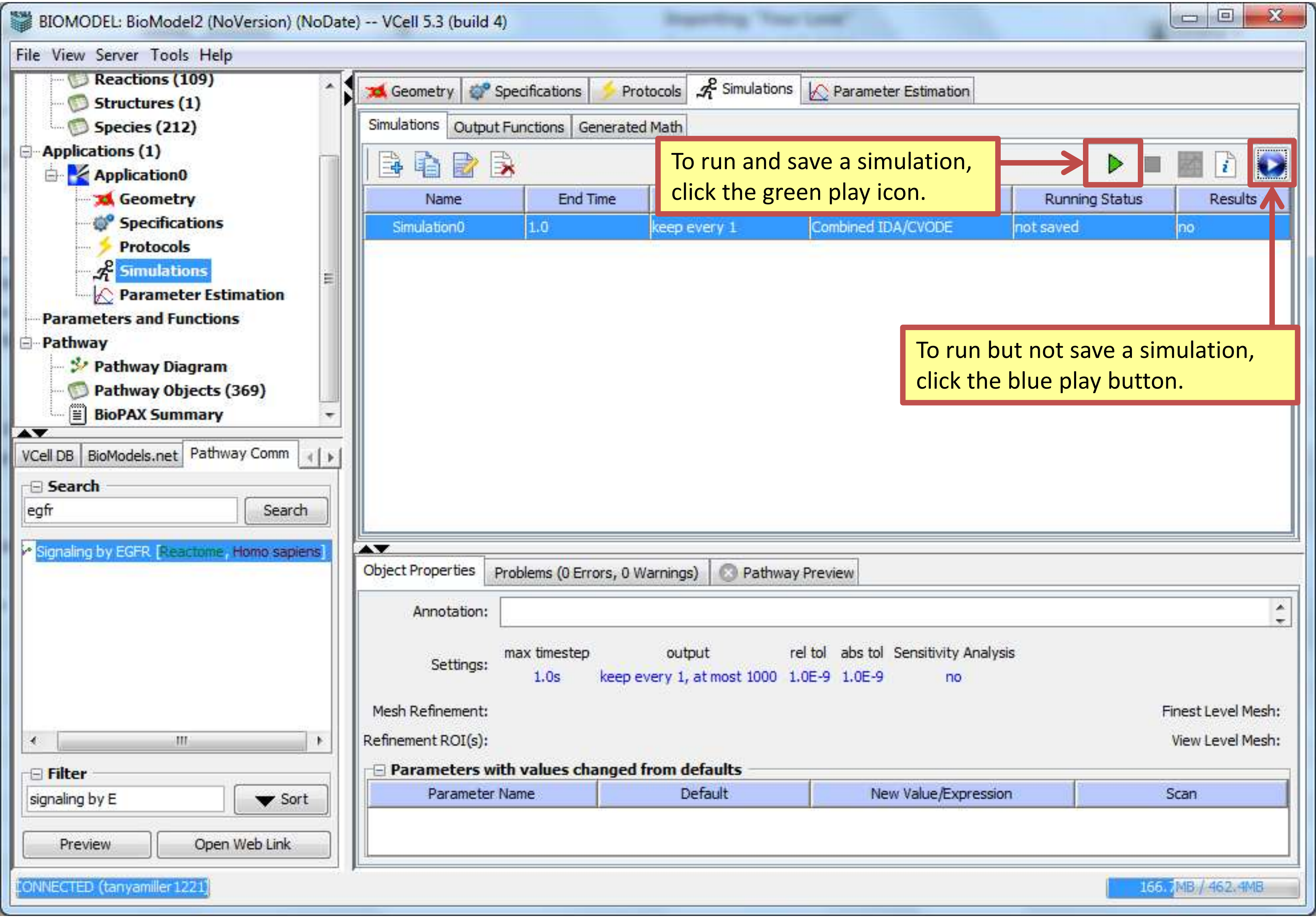
Finest Level Mesh:

View Level Mesh:

Parameters with values changed from defaults

Parameter Name	Default	New Value/Expression	Scan

Contents



BIOMODEL: BioModel2 (NoVersion) (NoDate) -- VCell 5.3 (build 4)

To run and save a simulation, click the green play icon.

To run but not save a simulation, click the blue play button.

Name	End Time			Running Status	Results
Simulation0	1.0	keep every 1	Combined IDA/CVODE	not saved	no

Settings:

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

Search: egfr

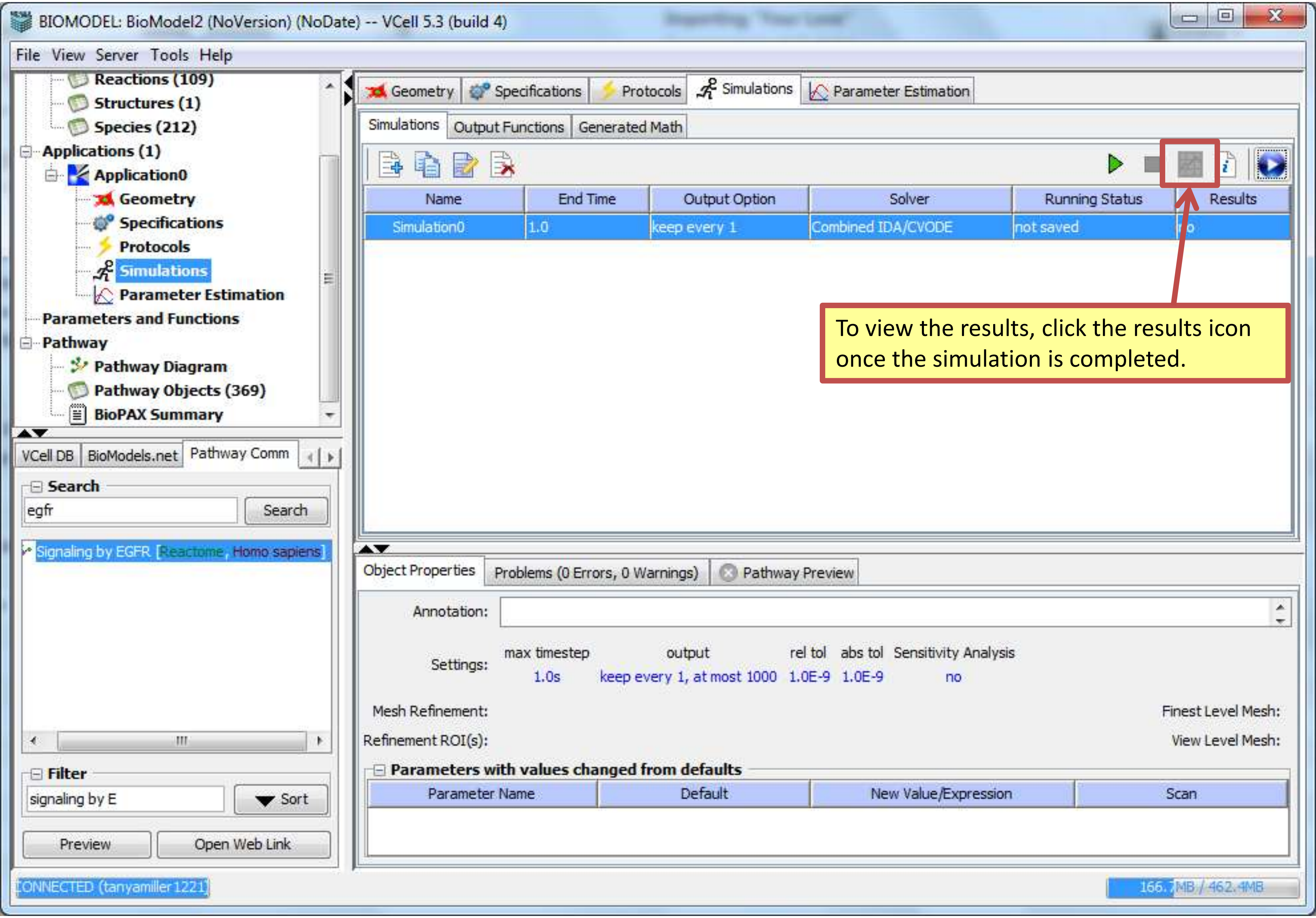
Signaling by EGFR [Reactome, Homo sapiens]

Filter: signaling by E

CONNECTED (tanyamiller1221)

166.7MB / 462.4MB

Contents



Search: egfr

Signaling by EGFR [Reactome, Homo sapiens]

Filter: signaling by E

Name	End Time	Output Option	Solver	Running Status	Results
Simulation0	1.0	keep every 1	Combined IDA/CVODE	not saved	no

To view the results, click the results icon once the simulation is completed.

Annotation:

Settings:

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

Mesh Refinement:

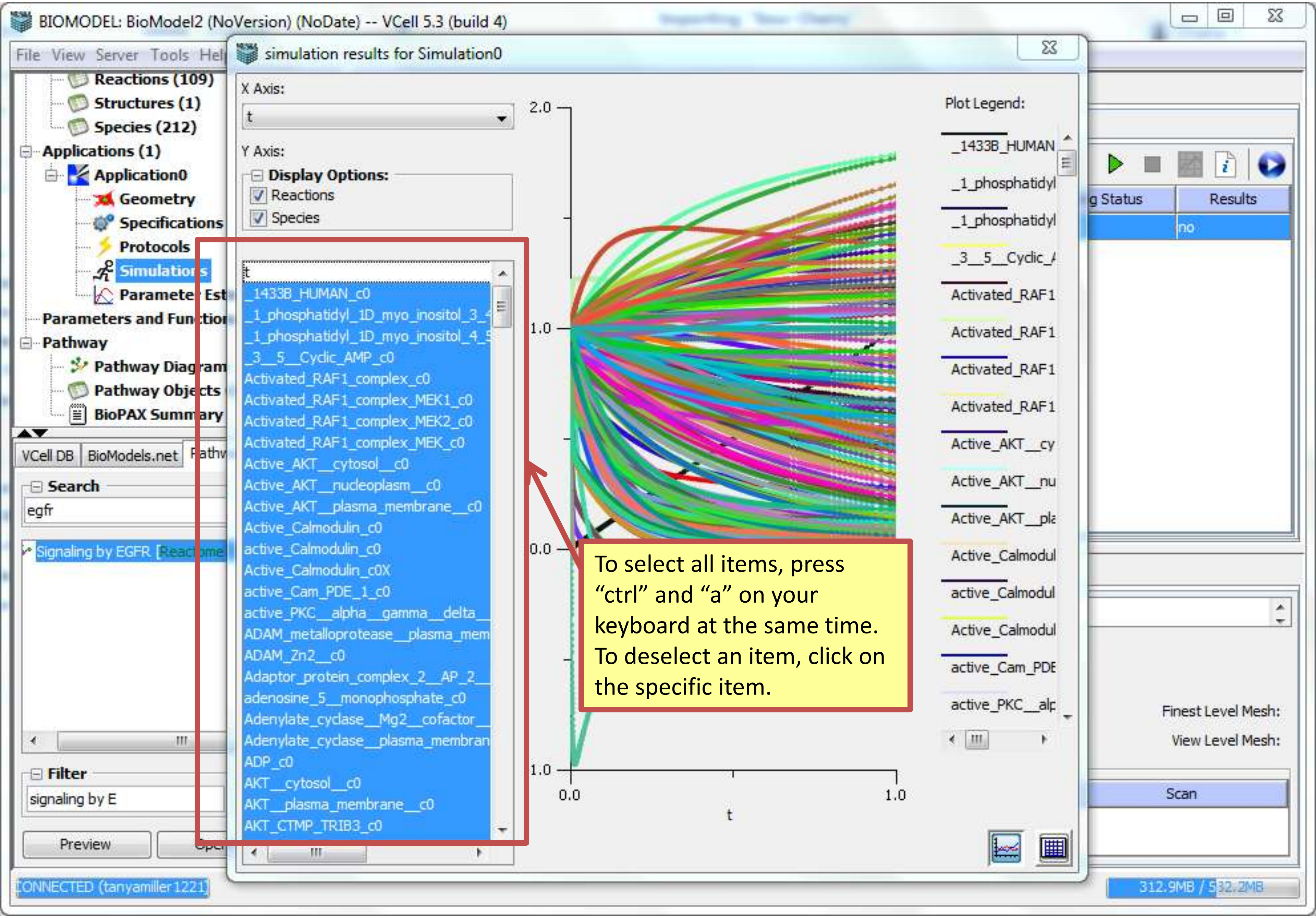
Finest Level Mesh:

Refinement ROI(s):

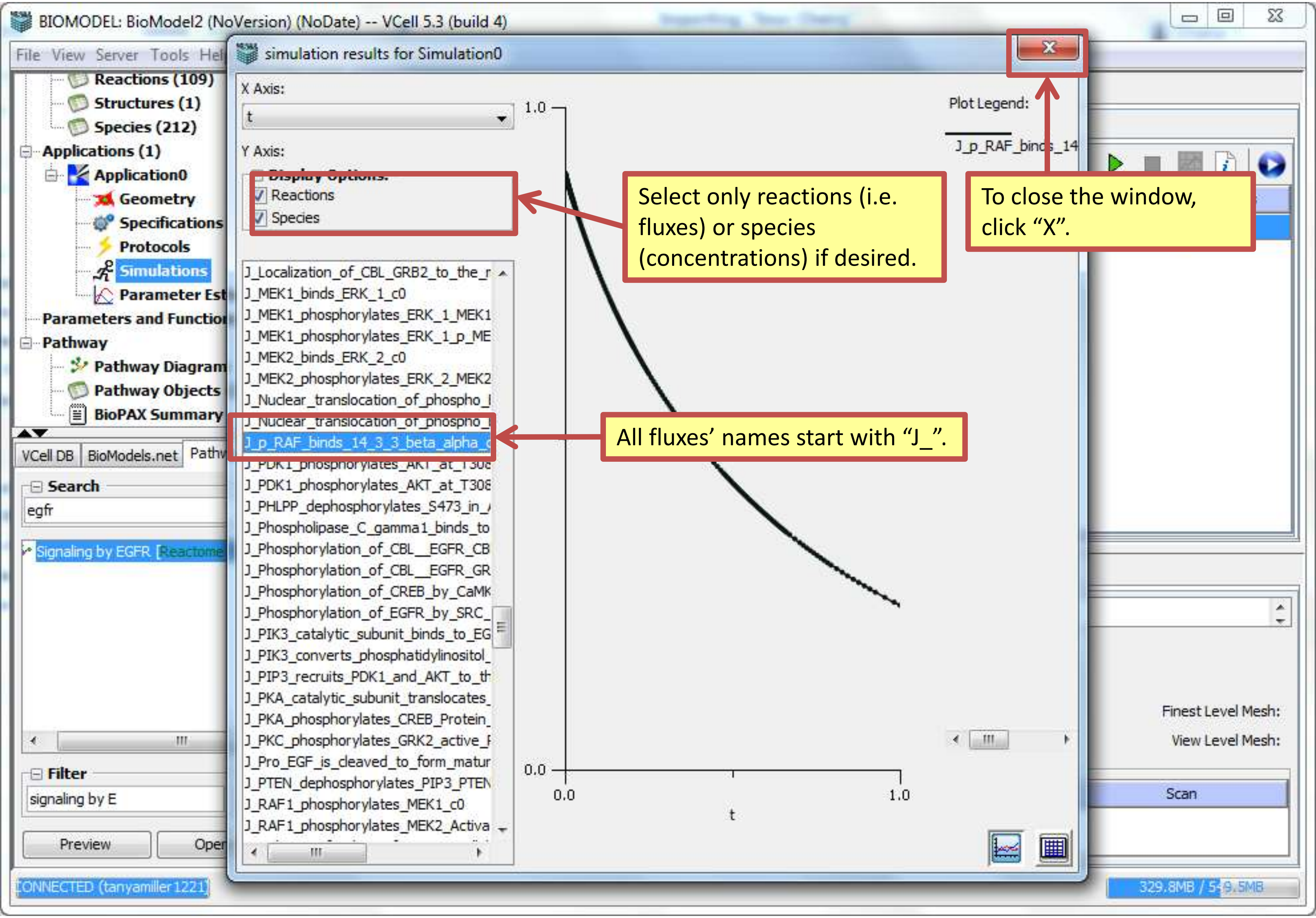
View Level Mesh:

Parameters with values changed from defaults

Parameter Name	Default	New Value/Expression	Scan



To select all items, press "ctrl" and "a" on your keyboard at the same time. To deselect an item, click on the specific item.



X Axis: t

Search: egfr

Filter: signaling by E

Select only reactions (i.e. fluxes) or species (concentrations) if desired.

To close the window, click “X”.

All fluxes’ names start with “J_”.