

VCell Pathway Commons Tutorial

Using an external database

BioModel1

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

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

The main workspace displays a reaction diagram with a single species 'c0' in the center. The diagram area is mostly blank, indicating a simple model.

Pathway Comm

To use the Pathways Commons database, click "Pathway Comm".

VCCell DB | BioModels.net | Pathway Comm | |

Search

Filter

Delete | Pathway Links | Search

Object Properties | Problems (0 Errors, 0 Warnings)

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

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- Pathway

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

c0

To search Pathway Commons, type under Search and click "Search".

- a6b1 and a6b4 Integrin signaling [NCI / Natu
- Alpha6Beta4Integrin [Cancer Cell Map, Homc
- Alpha9 beta1 integrin signaling events [NCI /
- Arf6 downstream pathway [NCI / Nature Pat
- Arf6 signaling events [NCI / Nature Pathway
- Arf6 trafficking events [NCI / Nature Pathwa
- ATM pathway [NCI / Nature Pathway Db, Ho
- ATR signaling pathway [NCI / Nature Pathwa
- Axon guidance [Reactome, Homo sapiens]
- Beta1 integrin cell surface interactions [NCI /
- Class I PI3K signaling events [NCI / Nature P
- Class I PI3K signaling events mediated by Ak

Object Properties | Problems (0 Errors, 0 Warnings)

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

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VCell DB BioModels.net Pathway Comm Sabio

Search
egfr

Signaling by EGFR [Reactome, Homo sapiens]

Filter
signaling by E

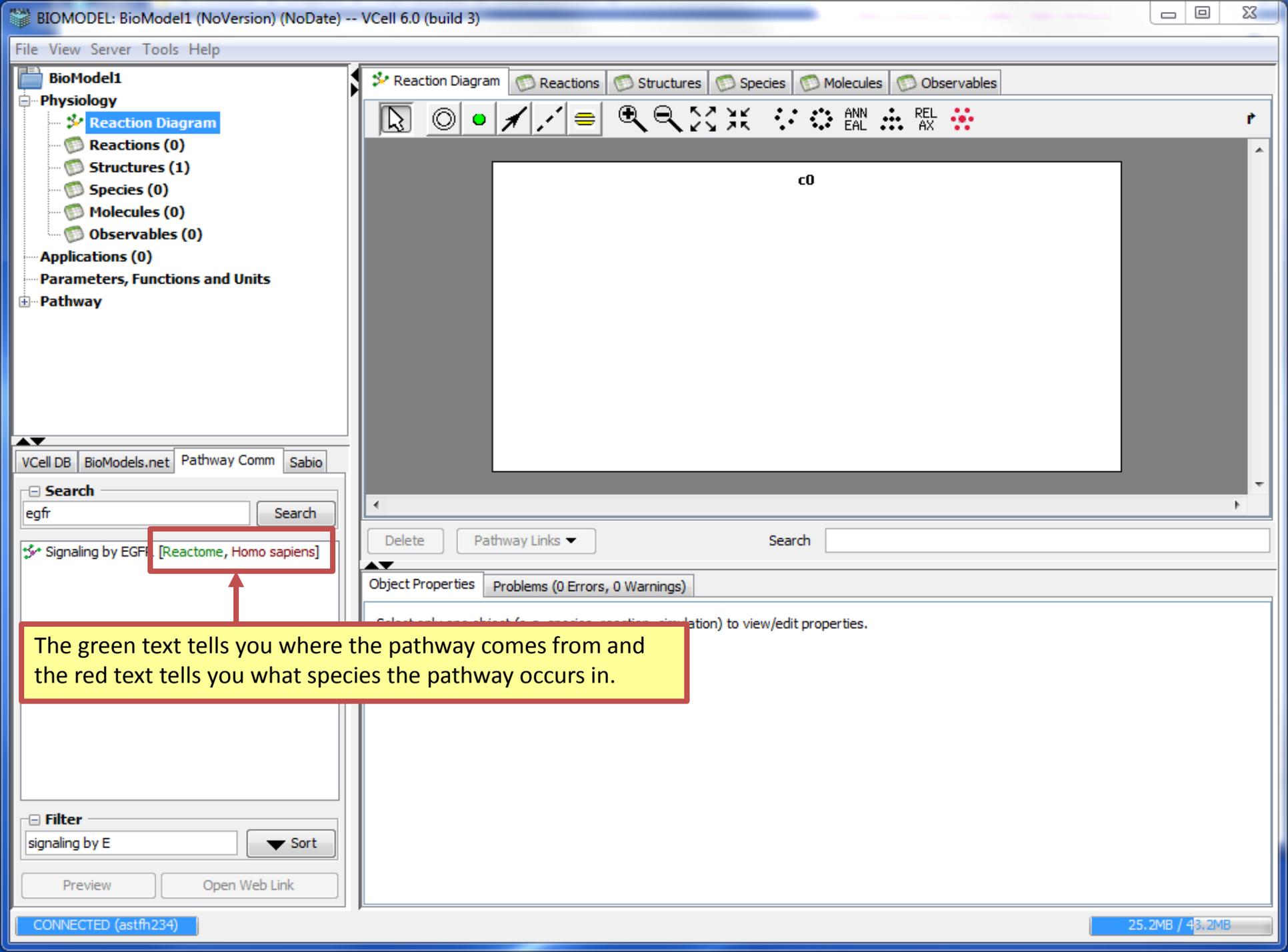
Reaction Diagram Reactions Structures Species Molecules Observables

c0

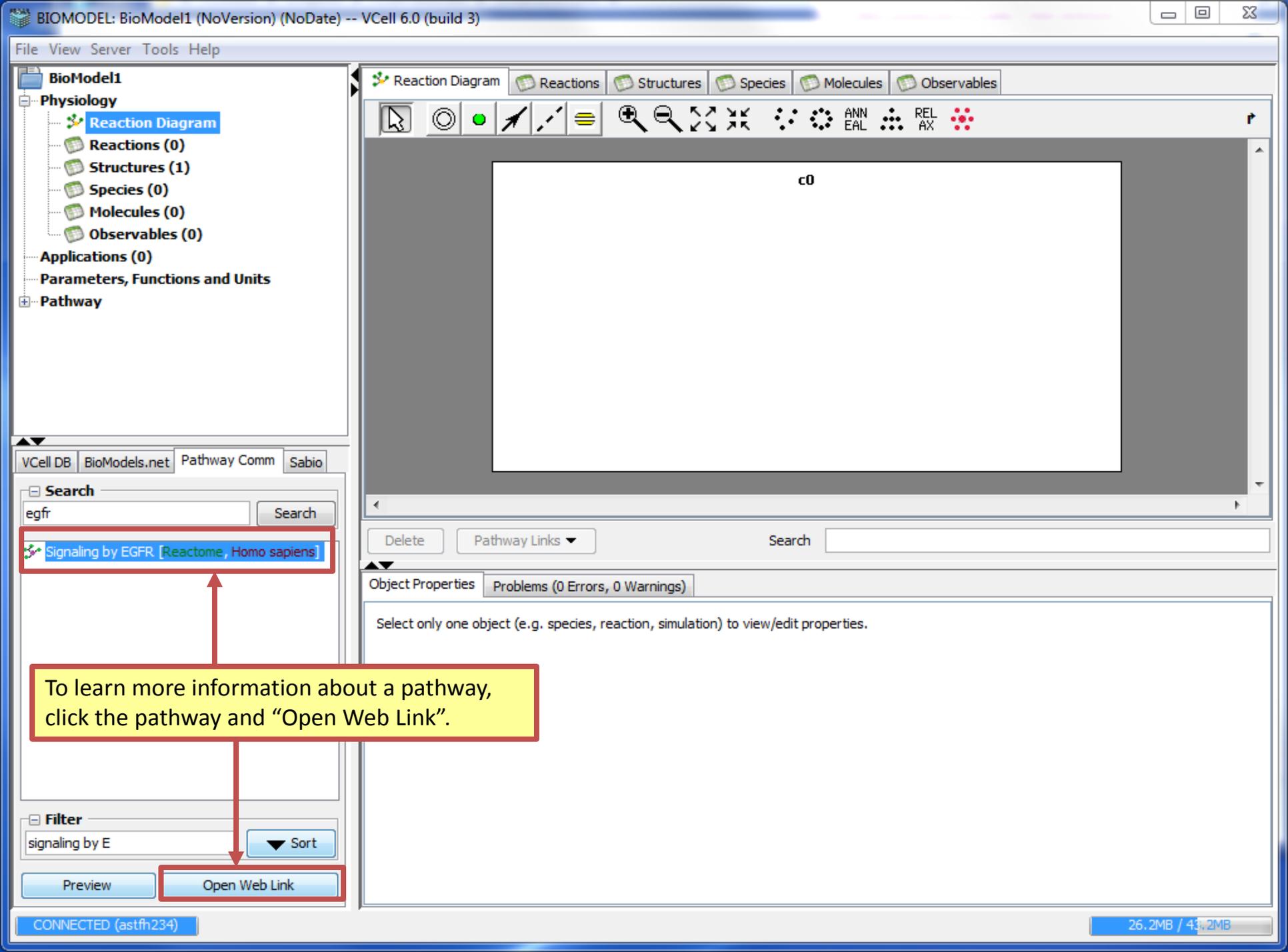
Object Properties Problems (0 Errors, 0 Warnings)

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

To filter your search, type under "Filter" and it will automatically search all names within Pathway Commons.



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



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



Find Pathways Find Molecules

Search

Current filters: All Organisms, All Data Sources. Set filters.

Home Data Sources Download FAQ Web Service About

Send us your [feedback](#). Sign up for Pathway Commons at [Pathway Commons](#)

Data Source:

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



Organism:

- Homo sapiens

Synonyms:

- Epidermal Growth Factor Receptor (EGFR) signaling

Cytoscape:



Links:

Pathway: Signaling by EGFR

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

Biochemical Reactions (5)

Catalysis Reactions (3)

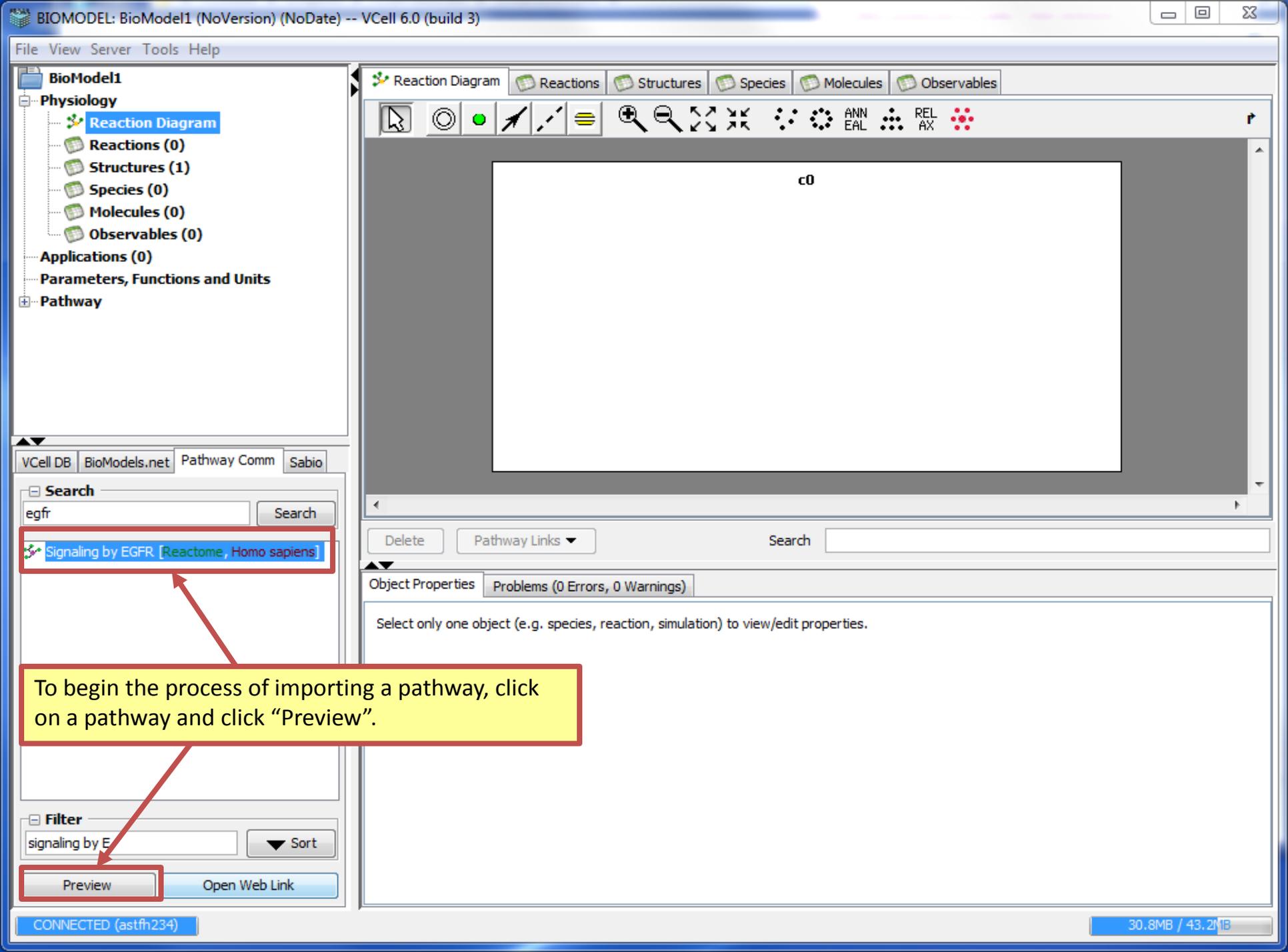
Sub-Pathways (5)

Molecules (216)

Showing 1-5 of 5

- EGF_HUMAN (in plasma membrane) (chain coordinates ^) → [Reactome](#) +
EGF_HUMAN (in extracellular region) (chain coordinates ^)
 - CATALYZED by ADAM:Zn2+
- EGF:EGFR dimer + ATP → EGF:p-6Y-EGFR + ADP [Reactome](#) +
 - CATALYZED by SRC (chain coordinates ^)
- EGF:EGFR dimer + ATP → ADP + EGF:p-6Y-EGFR [Reactome](#) +
 - CATALYZED by EGF:EGFR dimer
- EGF:EGFR → EGF:EGFR dimer [Reactome](#) +
- EGFR_HUMAN (chain coordinates ^) + EGF_HUMAN (chain coordinates ^) [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.



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

File View Server Tools Help

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Reaction Diagram Reactions Structures Species Molecules Observables

Reaction Diagram

c0

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Search

egfr Search

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Filter

signaling by E Sort

Preview Open Web Link

To filter entities by type, click "Type".

Delete Pathway Links Search

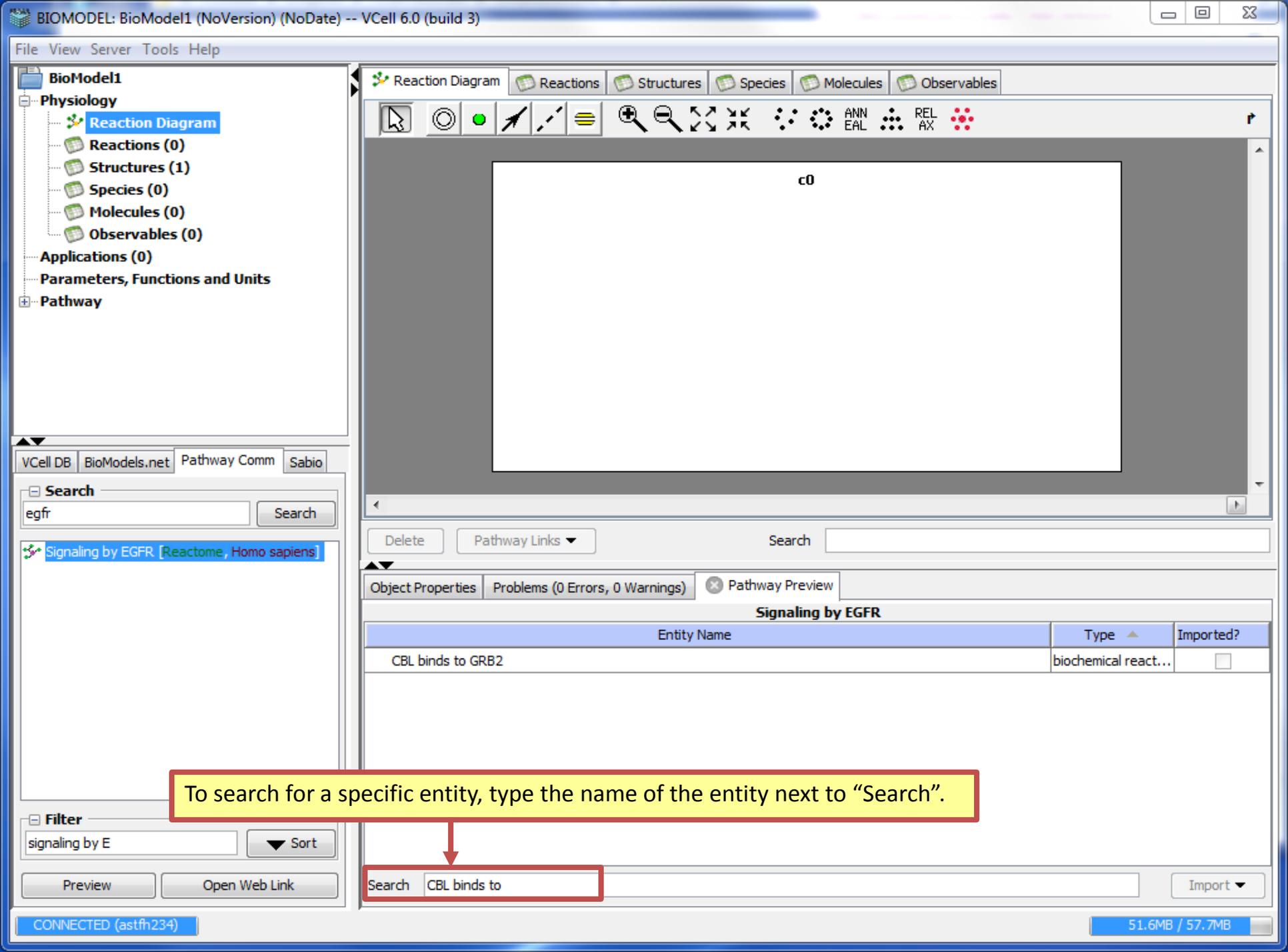
Object Properties Problems (0 Errors, 0 Warnings) Pathway Preview

Signaling by EGFR

Entity Name	Type	Imported?
Gab1:Grb2 binds to EGF:Phospho-EGFR	biochemical reac...	<input type="checkbox"/>
Stabilisation of RAF by further phosphorylation	biochemical reac...	<input type="checkbox"/>
CBL binds to GRB2	biochemical reac...	<input type="checkbox"/>
Sprouty lures cytosolic CBL away from EGFR	biochemical reac...	<input type="checkbox"/>
Dephosphorylation of PAG by SHP2	biochemical reac...	<input type="checkbox"/>
AKT phosphorylates BAD	biochemical reac...	<input type="checkbox"/>
IP3 binds to the IP3 receptor, opening the endoplasmic reticulum Ca2+ channel	biochemical reac...	<input type="checkbox"/>

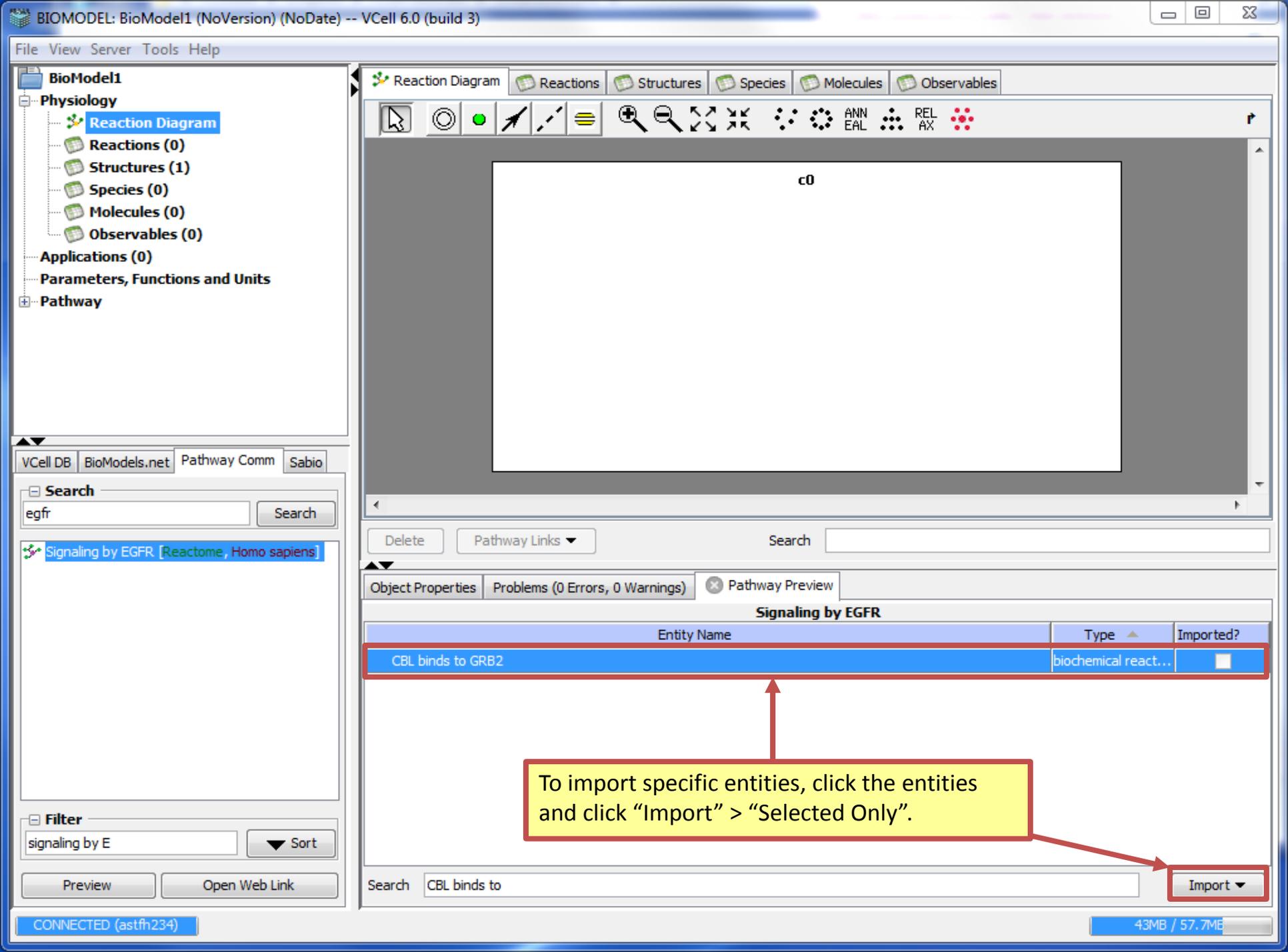
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Search Import



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

Search CBL binds to



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Search
egfr Search

Signaling by EGFR [Reactome](#) [Homo sapiens](#)

Filter
signaling by E Sort

Preview Open Web Link

Reaction Diagram toolbar with icons for selection, zoom, and editing.

Diagram content: c0

Delete Pathway Links Search

Signaling by EGFR		
Entity Name	Type	Imported?
CBL binds to GRB2	biochemical react...	<input type="checkbox"/>

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

Search CBL binds to Import

File View Server Tools Help

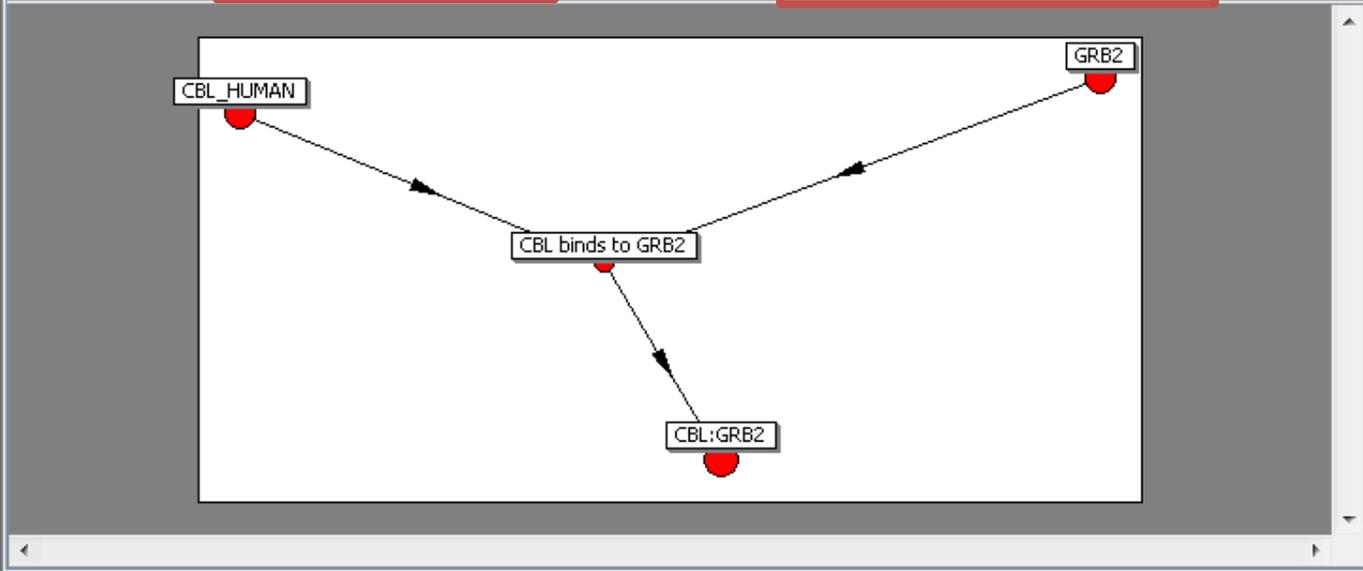
BioModel1

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- Applications (0)
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- Pathway
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 - Pathway Objects (4)
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Pathway Diagram Pathway Objects BioPAX Summary BioPAX Tr

Navigation icons: zoom in, zoom out, pan, zoom reset, and icons for ANN EAL, REL AX.

To reorganize pathways, click the circle icons.



VCell DB BioModels.net Pathway Comm Sabio

Search egfr Search

Signaling by EGFR [Reactome](#) [Homo sapiens](#)

Filter signaling by E Sort

Preview Open Web Link

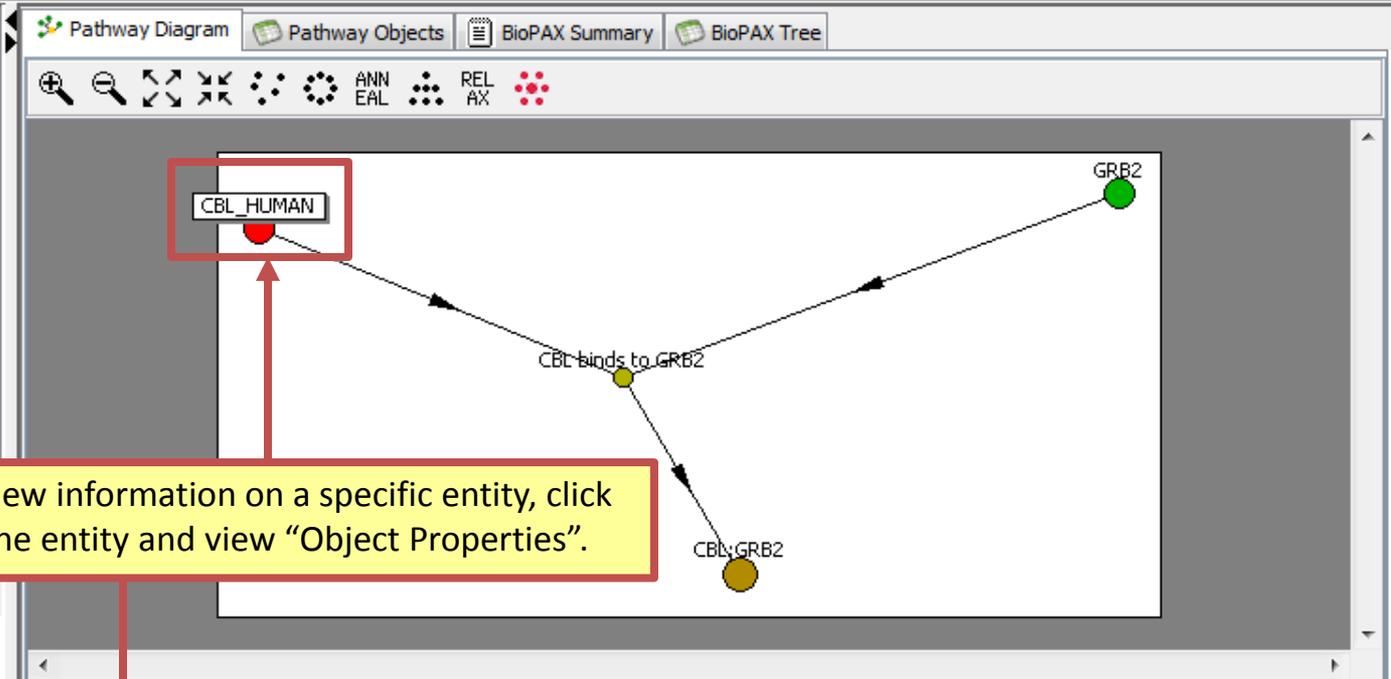
Group Delete Physiology Links Search

Object Properties Problems (0 Errors, 0 Warnings) Pathway Preview

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

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

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Search

egfr Search

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Filter

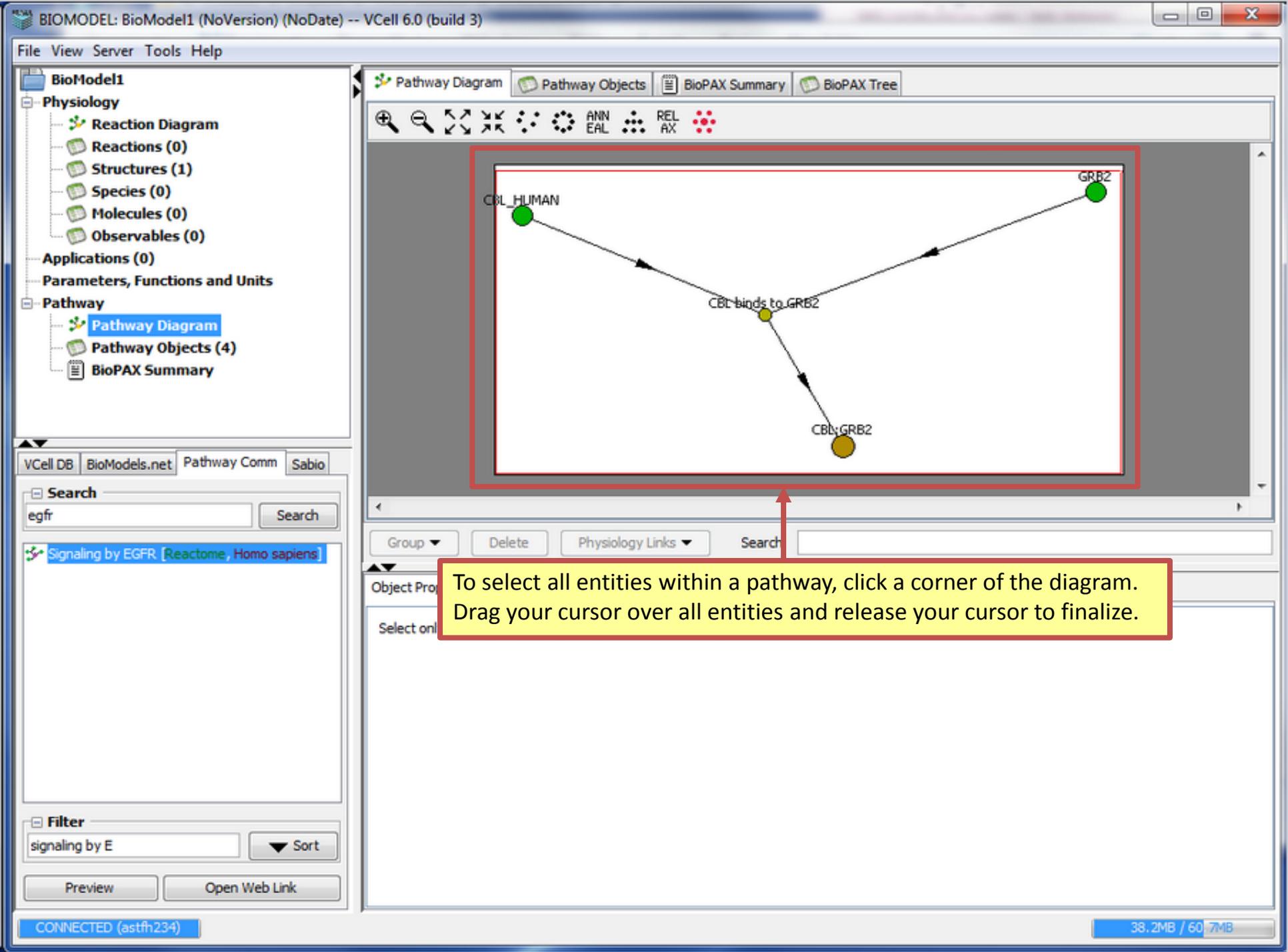
signaling by E Sort

Preview Open Web Link

Group Delete Physiology Links Search

Object Properties Problems (0 Errors, 0 Warnings) Pathway Preview

Property	Value
Type	protein
Name	CBL_HUMAN (double-click lookup)
Role(s)	Participant
Comment	FUNCTION: Participates in signal transduction in hematopoietic cells. ...
Xref	UNIPROT:A3KMP8
Xref	UNIPROT:P22681



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egfr Search

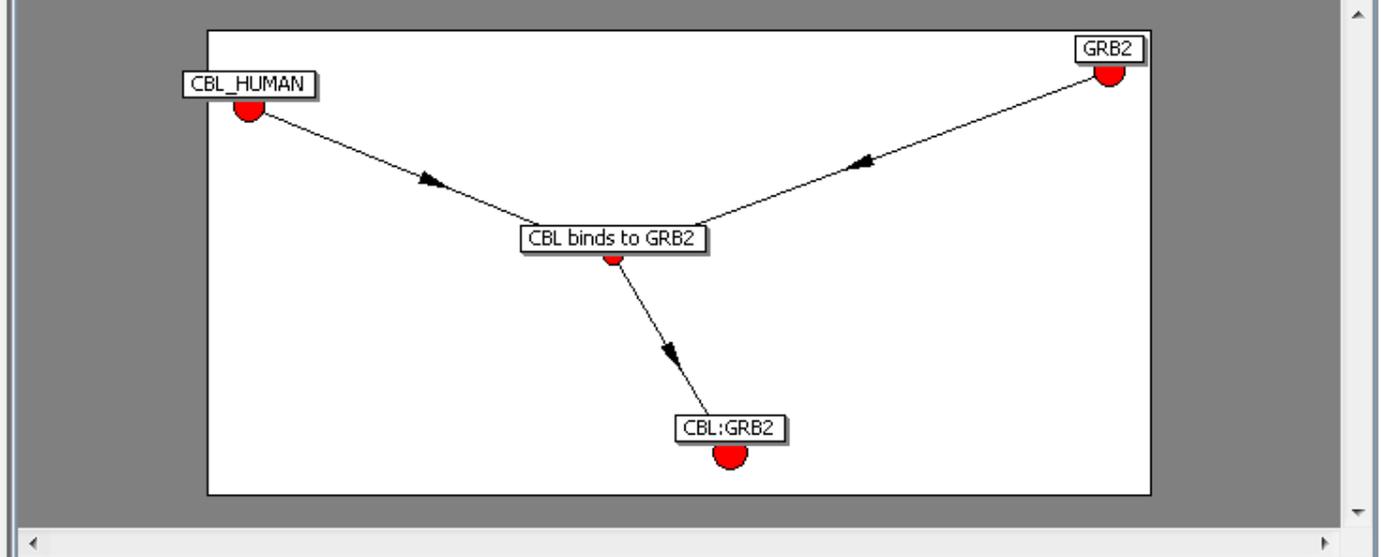
Signaling by EGFR [Reactome](#) [Homo sapiens](#)

Filter
signaling by E Sort

Preview Open Web Link

Pathway Diagram Pathway Objects BioPAX Summary BioPAX Tree

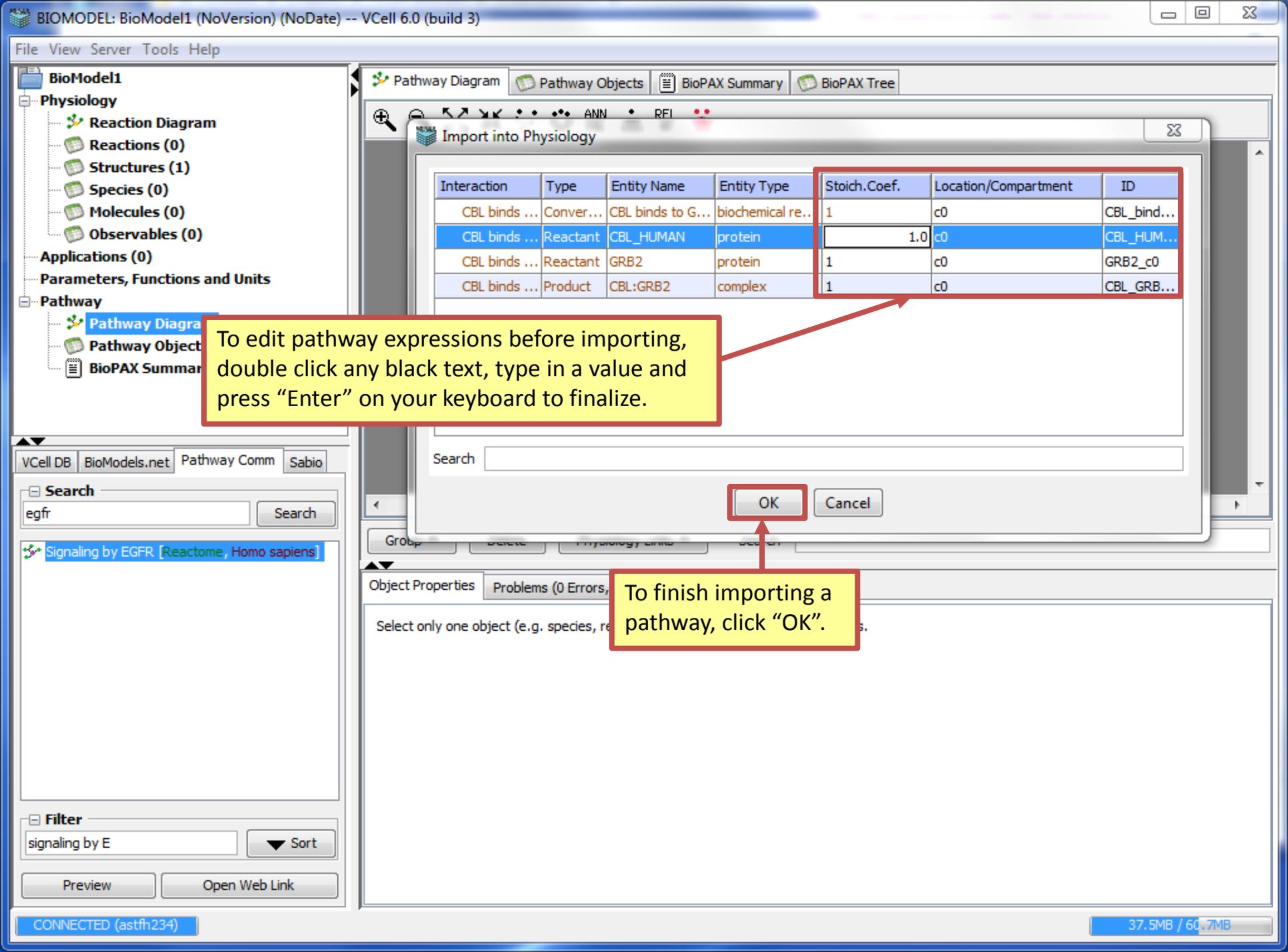
Navigation icons: zoom in, zoom out, pan, fit, reset, refresh, ANN EAL, REL AX, and a red cluster icon.



Group Delete Physiology Links Search

Object Properties Problems (0 Errors, 0 Warnings) Pathway Preview

Click "Physiology Links" > "Import into Physiology".



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".

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Search
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Filter
signaling by E

Pathway Diagram Pathway Objects BioPAX Summary BioPAX Tree

Info

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

- Species: 'GRB2_c0'
- Species: 'CBL_GRB2_c0'
- Species: 'CBL_HUMAN_c0'
- Reaction: 'CBL_binds_to_GRB2_c0'

Group Delete Physiology Links Search

Object Properties Problems (0)

Select only one object (e.g. species)

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

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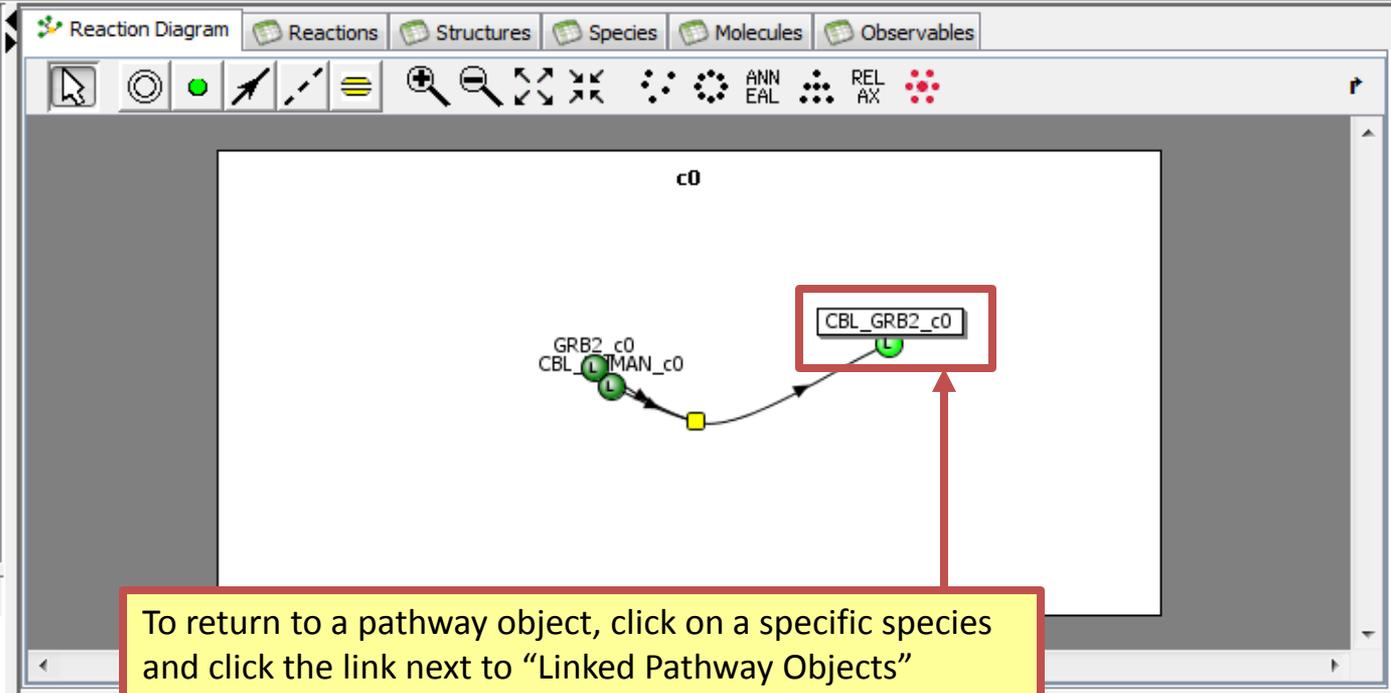
Search

egfr

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Filter

signaling by E



To return to a pathway object, click on a specific species and click the link next to "Linked Pathway Objects"

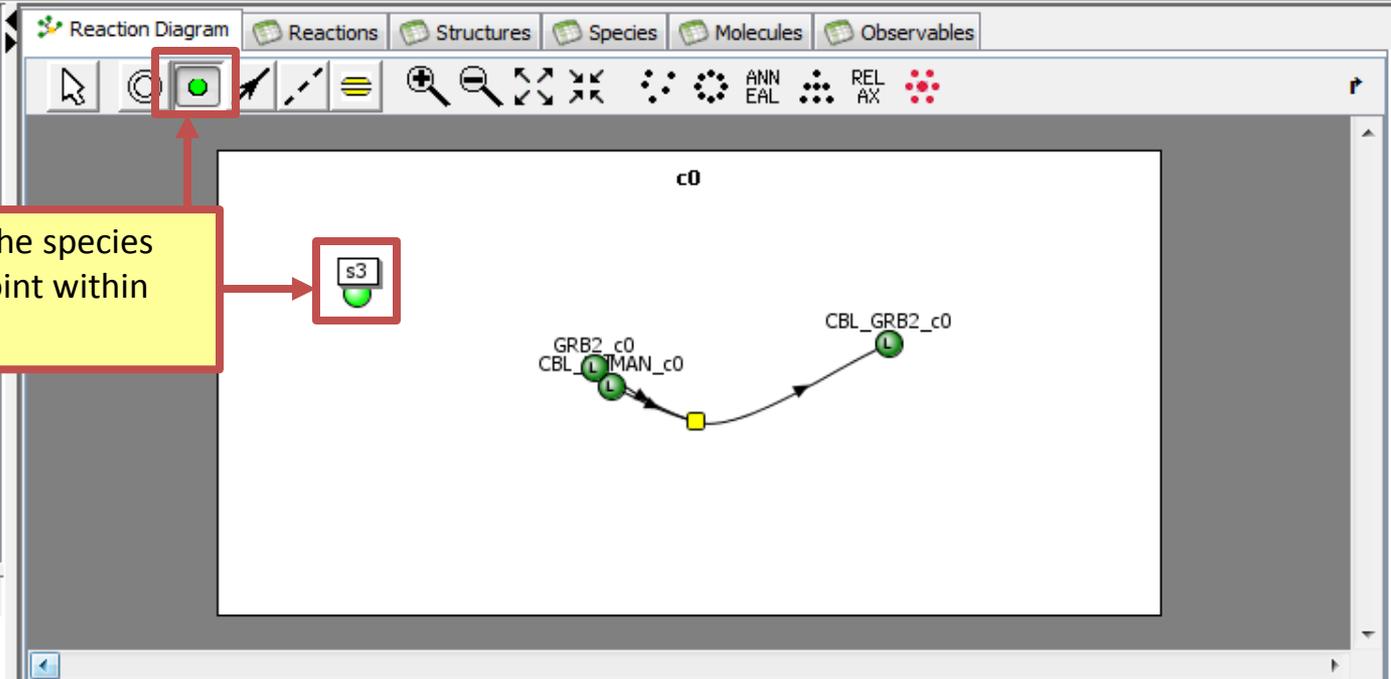
Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings) Pathway Preview

Species Name	CBL_GRB2_c0	Species: CBL_GRB2_c0
Linked Pathway Object(s)	CBL:GRB2	
Annotation		

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

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Search

egfr Search

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Filter

signaling by E Sort

Preview Open Web Link

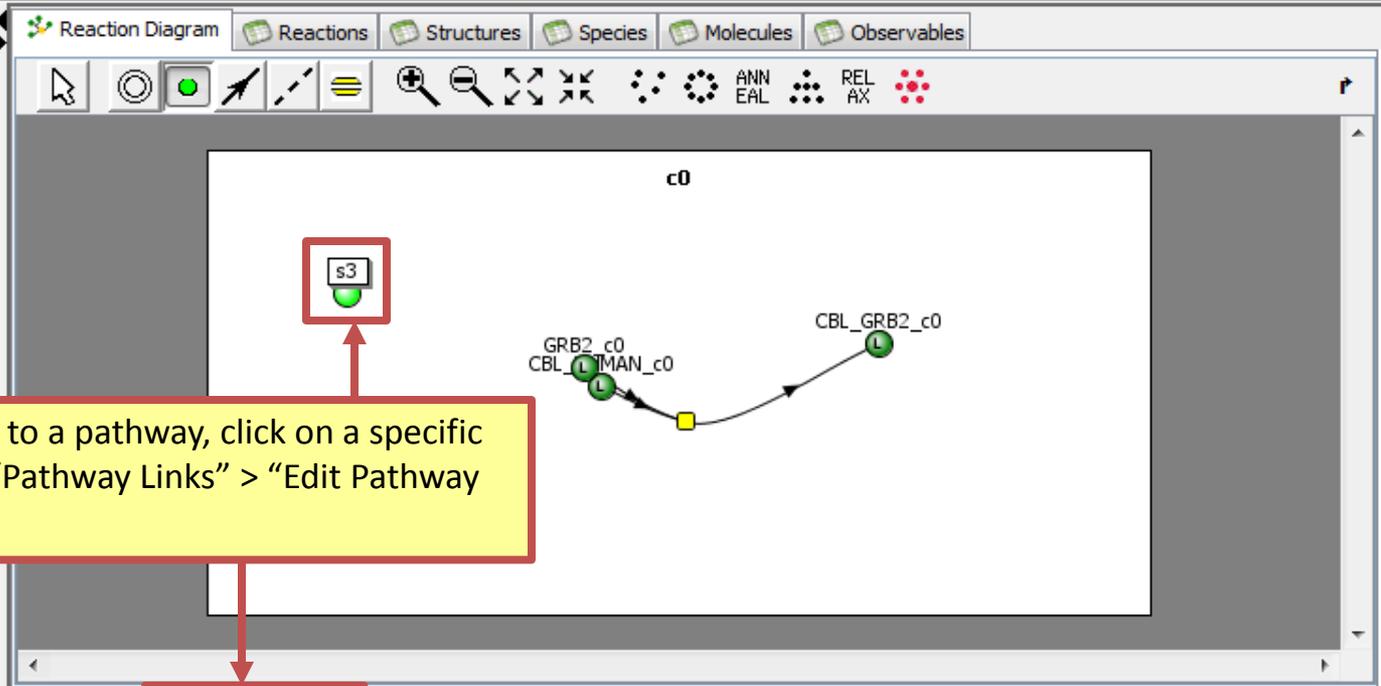
Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings) Pathway Preview

Species Name	s3	Species: s3
Linked Pathway Object(s)		
Annotation		

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

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Search

egfr

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Filter

signaling by E

Delete | **Pathway Links** | Search

Object Properties | Problems (0 Errors, 0 Warnings) | Pathway Preview

Species Name	s3	Species: s3
Linked Pathway Object(s)		
Annotation		

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Search:

Signaling by EGFR [Reactome](#) [Homo sapiens](#)

Filter:

Edit Pathway Links

Edit pathway links by checking or unchecking the Link boxes.

Link	Entity Name	Type
<input checked="" type="checkbox"/>	GRB2	protein
<input type="checkbox"/>	CBL:GRB2	complex
<input type="checkbox"/>	CBL_HUMAN	protein

Search: Show linked pathway entities only

To link a species to an entity, check a box in the "Link" column, next to the entity's name.

To finish linking a species to a pathway, click "Close".

Object Properties Problems (0 Errors, 0 Warnings) Pathway Preview

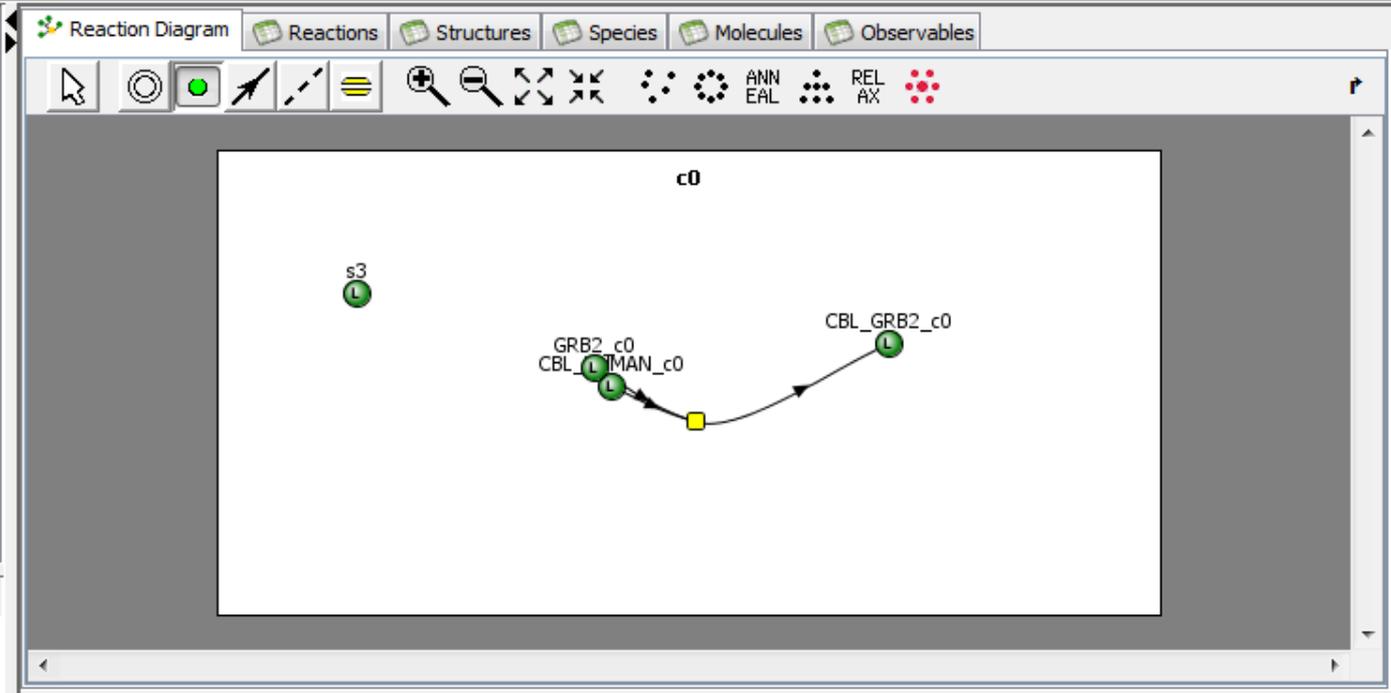
Species Name: Species: **s3**

Linked Pathway Object(s):

Annotation:

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Search
egfr Search

Signaling by EGFR [Reactome](#) [Homo sapiens](#)

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

Filter
signaling by E Sort

Preview Open Web Link

Signaling by EGFR

Entity Name	Type	Imported?
Gab1:Grb2 binds to EGF:Phospho-EGFR	biochemical reac...	<input type="checkbox"/>
Stabilisation of RAF by further phosphorylation	biochemical reac...	<input type="checkbox"/>
CBL binds to GRB2	biochemical reac...	<input checked="" type="checkbox"/>
Sprouty lures cytosolic CBL away from EGFR	biochemical reac...	<input type="checkbox"/>
Dephosphorylation of PAG by SHP2	biochemical reac...	<input type="checkbox"/>
AKT phosphorylates BAD	biochemical reac...	<input type="checkbox"/>
IP3 binds to the IP3 receptor, opening the endoplasmic reticulum Ca2+ channel	biochemical reac...	<input type="checkbox"/>

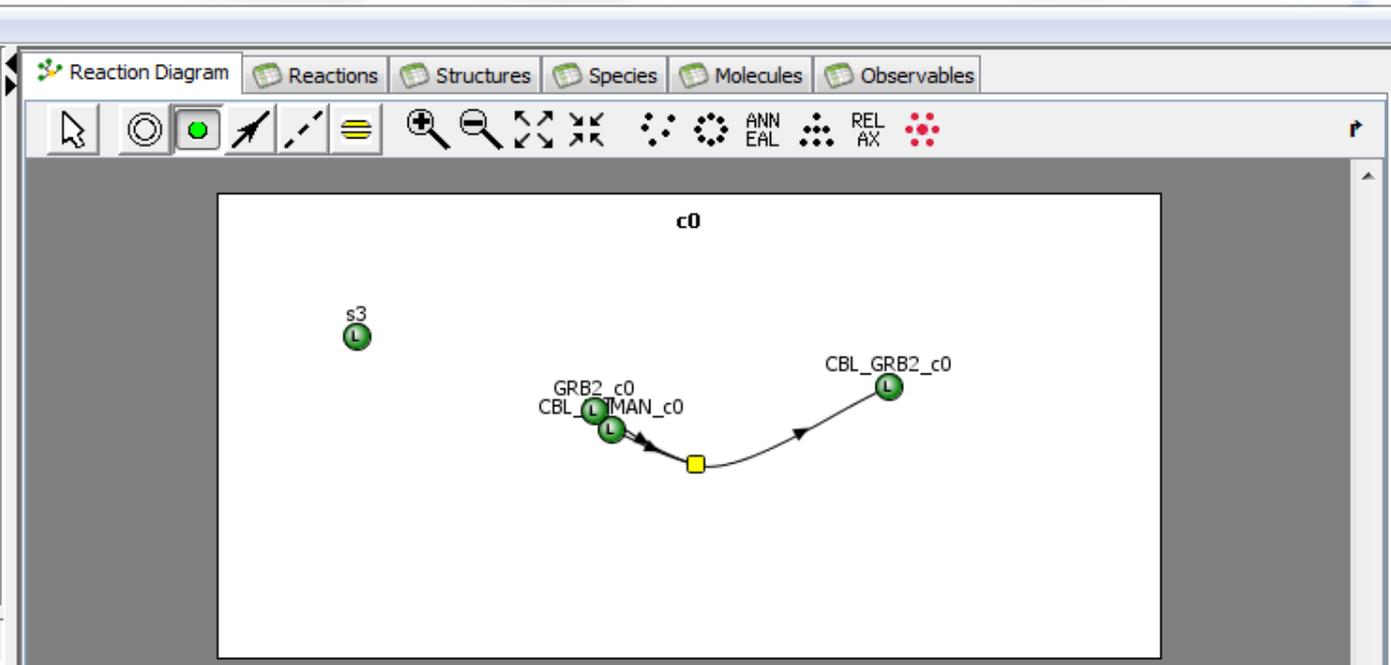
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Search Import

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To select all entities on a page, hit "ctrl+a".

Object Properties Problems (0 Errors, 0 Warnings) Pathway Preview

Signaling by EGFR

Entity Name	Type	Imported?
Gab1:Grb2 binds to EGF:Phospho-EGFR	biochemical reac...	<input type="checkbox"/>
Stabilisation of RAF by further phosphorylation	biochemical reac...	<input type="checkbox"/>
CBL binds to GRB2	biochemical reac...	<input checked="" type="checkbox"/>
Sprouty lures cytosolic CBL away from EGFR	biochemical reac...	<input type="checkbox"/>
Dephosphorylation of PAG by SHP2	biochemical reac...	<input type="checkbox"/>
AKT phosphorylates BAD	biochemical reac...	<input type="checkbox"/>
IP3 binds to the IP3 receptor, opening the endoplasmic reticulum Ca2+ channel	biochemical reac...	<input type="checkbox"/>

To import entities, click "Import" > "Selected Only".

Search

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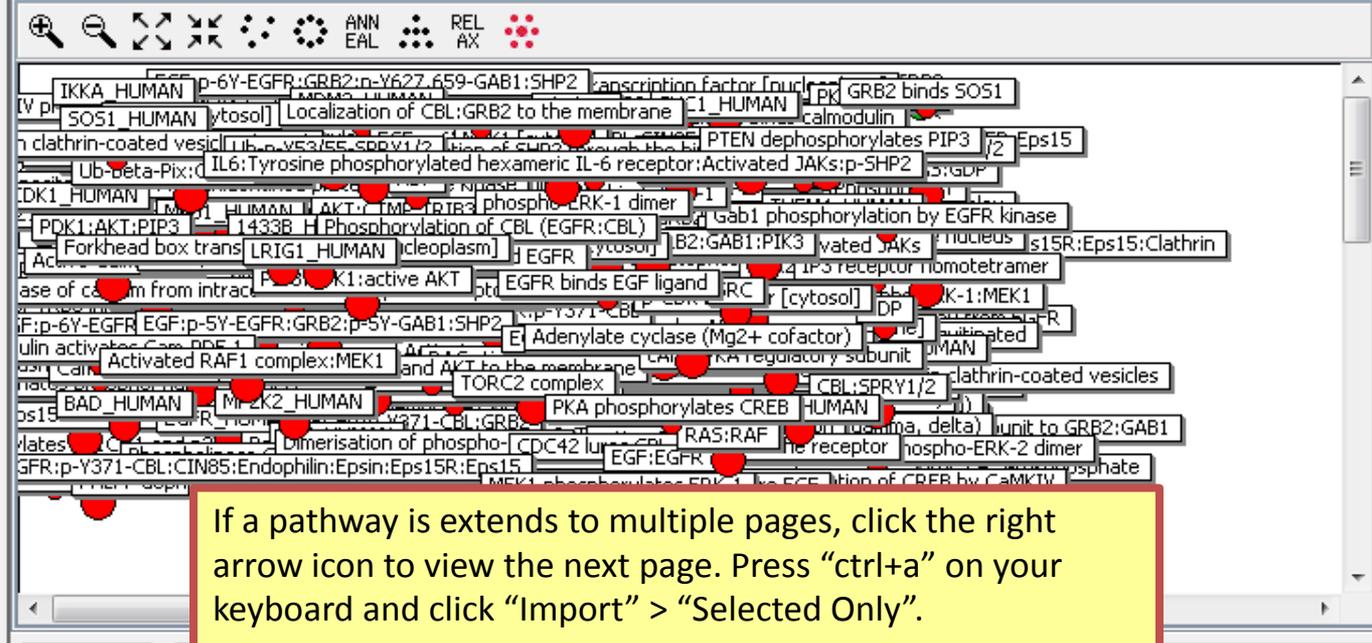
Search
egfr Search

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Filter
signaling by E Sort

Preview Open Web Link

Pathway Diagram Pathway Objects BioPAX Summary BioPAX Tree



Group Delete Physiology Links Search

Object Properties Problems (0 Errors, 0 Warnings) Pathway Preview

Signaling by EGFR

Entity Name	Type	Imported?
EGF:Phospho-EGFR	complex	<input type="checkbox"/>
EGF:p-6Y-EGFR;p-Y371-CBL:CIN85:Endophilin:Epsin:Eps 15R:Eps 15	complex	<input type="checkbox"/>
cAMP:PKA regulatory subunit	complex	<input type="checkbox"/>
GRB2:Phospho-GAB1	complex	<input type="checkbox"/>
Adenylate cyclase (Mg2+ cofactor)	complex	<input type="checkbox"/>
RAS:RAF	complex	<input type="checkbox"/>
DNA	physical entity	<input type="checkbox"/>

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Filter
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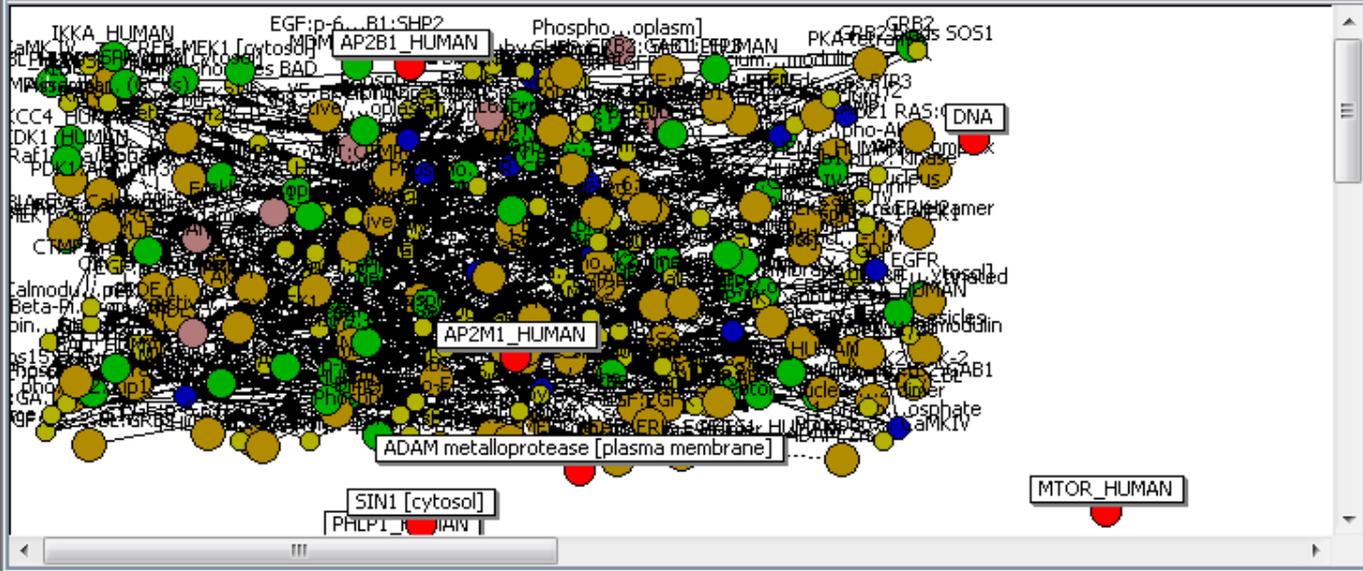
Preview Open Web Link

Pathway Diagram Pathway Objects BioPAX Summary

Click "Pathway Objects" to organize the entities into list form

Navigation icons: zoom in, zoom out, pan, rotate, etc.

ANN EAL REL AX



Group Delete Physiology Links Search

Object Properties Problems (0 Errors, 0 Warnings) Pathway Preview

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

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Pathway Entity	Type	Linked Physiology Objects
AKT phosphorylates p21Cip1 and p27Kip1	biochemical reaction	
AKTS1_HUMAN	protein	
IKKA_HUMAN	protein	
Sprouty lures membrane-bound CBL aw...	biochemical reaction	
Active AKT [plasma membrane]	protein	
Phosphorylation of EGFR by SRC kinase	biochemical reaction	
THEM4_HUMAN	protein	
EGF:p-6Y-EGFR:GRB2:p-5Y-GAB1:SH2	complex	
PDK1:AKT:PIP3	complex	
Phospho-AKT [plasma membrane]	protein	
AKT phosphorylates IKKalpha	biochemical reaction	
CBL binds and ubiquitinates phosphoryl...	biochemical reaction	
MEK1:ERK-1	complex	
IP3 receptor [endoplasmic reticulum me...	physical entity	

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egfr Search

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Group Delete Physiology Links Search

Object Properties Problems (0 Errors, 0 Warnings) Pathway Preview

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

Click a Pathway Object to find more Object Properties

Filter
signaling by E Sort

Preview Open Web Link

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

Search
egfr

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Filter
signaling by E Sort

Preview Open Web Link

Use "Search" to find a specific pathway entity, type in the name of the object next to "Search".

Search CBL binds

Pathway Preview

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

File View Server Tools Help

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To select all pathway entities on a page, press "ctrl+a"

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Pathway Entity	Type	Linked Physiology Objects
CBL:SPRY1/2	complex	
CDC42:GTP	complex	
Gab1:Grb2 binds to EGF:Phospho-EGFR	biochemical reaction	
Stabilisation of RAF by further phospho...	biochemical reaction	
Protein kinase C (alpha, gamma, delta) ...	protein	
CBL binds to GRB2	biochemical reaction	Reaction:CBL_binds_to_GRB2_c0;
MEK2:ERK-2	complex	
Sprouty lures cytosolic CBL away from ...	biochemical reaction	
GRB2:GAB1:PIK3R1	complex	
TRIB3_HUMAN	protein	
Active AKT [cytosol]	protein	
CBL:Beta-Pix	complex	
KCC4_HUMAN	protein	
NR4A1_HUMAN	protein	

Group Delete Physiology Links Search

Object Properties Problems (0 Errors, 0 Warnings) Pathway Preview

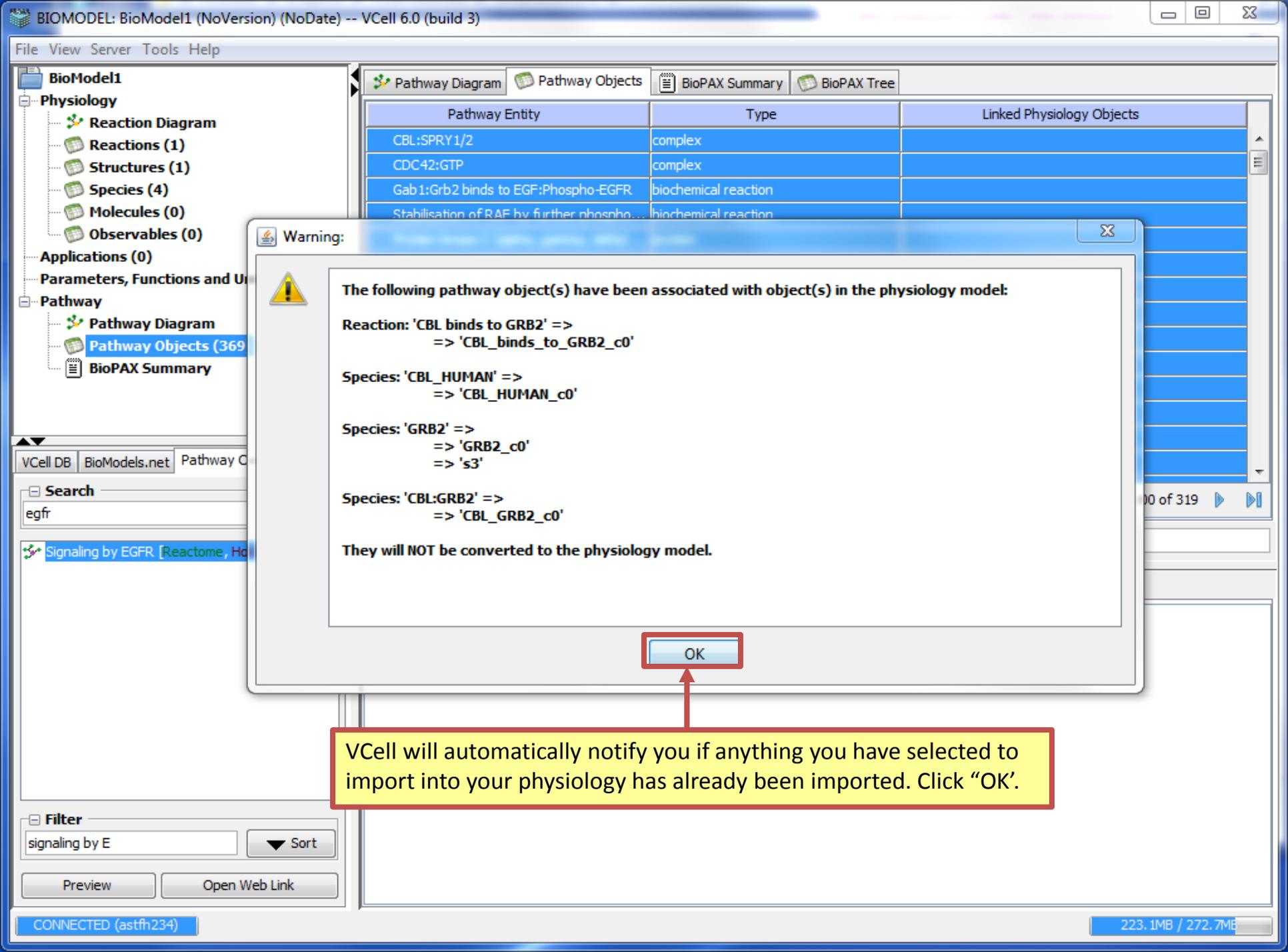
Select only one object (e.g. species, reaction, simulation) to view/edit properties.

To import pathway entities into your physiology, click "Physiology Links" > "Import into Physiology..."

Filter

signaling by E Sort

Preview Open Web Link



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Pathway Entity	Type	Linked Physiology Objects
CBL:SPRY1/2	complex	
CDC42:GTP	complex	
Gab1:Grb2 binds to EGF:Phospho-EGFR	biochemical reaction	
Stabilisation of RAF by further phospho...	biochemical reaction	

Search
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Filter
signaling by E Sort

Preview Open Web Link

BioModel1

- Physiology
 - Reaction Diagram
 - Reactions (1)
 - Structures (1)
 - Species (4)
 - Molecules (0)
- App...
- Para...
- Path...
- Pathway Objects (369)
- BioPAX Summary

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

Import into Physiology

Interaction	Type	Entity Name	Entity Type	Stoich. Coef.	Location/Compartment	ID
Gab1:Grb...	Conver...	Gab1:Grb2 bin...	biochemical r...	1	c0	Gab1_...
Gab1:Grb...	Reactant	GRB2:GAB1:PIP3	complex	1	c0	GRB2_...
Gab1:Grb...	Reactant	EGF:n-6Y-EGFR	complex	1	c0	EGF_p...
		F...	complex	1	c0	EGF_p...
		tyl...	small molecule	1	c0	_1_pho...
		or...	biochemical r...	1	c0	Stabilis...
			small molecule	2	c0	ATP_c0
Stabilisati...	Reactant	RAS:RAF:14-3-3	complex	1	c0	RAS_R...
Stabilisati...	Product	Activated RAF...	complex	1	c0	Activat...
Stabilisati...	Product	ADD	small molecule	2	c0	ADD_c0

Search

OK Cancel

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

VCCell DB BioModels.net Pathway Comm Sabio

Search Search

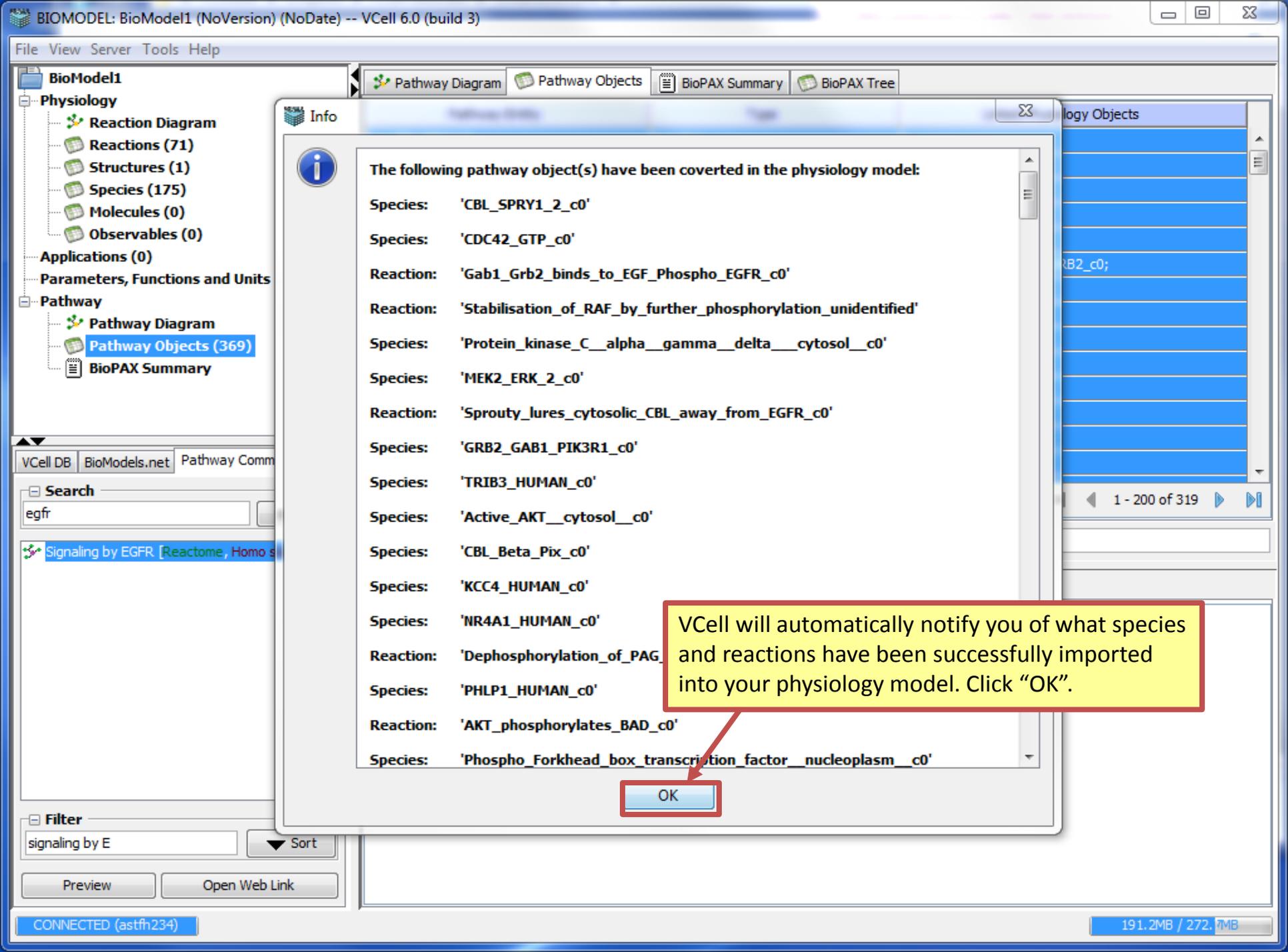
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Filter Sort

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Object Properties

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



Info

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

- Species: 'CBL_SPRY1_2_c0'
- Species: 'CDC42_GTP_c0'
- Reaction: 'Gab1_Grb2_binds_to_EGF_Phospho_EGFR_c0'
- Reaction: 'Stabilisation_of_RAF_by_further_phosphorylation_unidentified'
- Species: 'Protein_kinase_C_alpha_gamma_delta_cytosol_c0'
- Species: 'MEK2_ERK_2_c0'
- Reaction: 'Sprouty_lures_cytosolic_CBL_away_from_EGFR_c0'
- Species: 'GRB2_GAB1_PIK3R1_c0'
- Species: 'TRIB3_HUMAN_c0'
- Species: 'Active_AKT_cytosol_c0'
- Species: 'CBL_Beta_Pix_c0'
- Species: 'KCC4_HUMAN_c0'
- Species: 'NR4A1_HUMAN_c0'
- Reaction: 'Dephosphorylation_of_PAG_c0'
- Species: 'PHLP1_HUMAN_c0'
- Reaction: 'AKT_phosphorylates_BAD_c0'
- Species: 'Phospho_Forkhead_box_transcription_factor_nucleoplasm_c0'

OK

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

File View Server Tools Help

BioModel1

- Physiology
 - Reaction Diagram**
 - Reactions (71)
 - Structures (1)
 - Species (175)
 - Molecules (0)
 - Observables (0)
- Applications (0)
- Parameters, Functions and Units
- Pathway
 - Pathway Diagram
 - Pathway Objects (369)
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VCell DB BioModels.net Pathway Comm Sabio

Search
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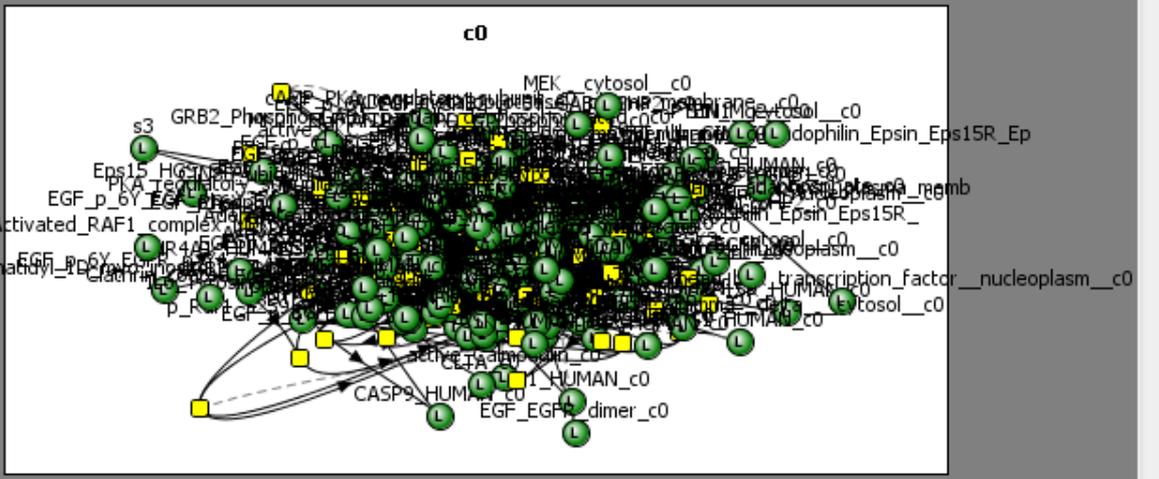
Filter
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Preview Open Web Link

Reaction Diagram Reactions Structures



To view reactions in list form, click "Reactions".



Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings) Pathway Preview

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

File View Server Tools Help

PathwayCommons

- Physiology
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VCCell DB BioModels.net Pathway Comm

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CONNECTED (astfh234) 144.2MB / 289.2MB

Reaction Diagram Reactions Structures Species Molecules Observables

Reaction

ATP_c0 + NR4A1_HUMAN_c0 -> ADP_c0 + NR4A1_HUMAN_c0

KS6B2_HUMAN_c0 + ATP_c0 -> KS6B2_HUMAN_c0 + ADP_c0

ATP_c0 + Forkhead_box_transcription_factor_nucleoplasm_c0 -> Phospho_Forkhead_box_transcription_factor_nucleoplasm_c0 + ADP_c0

BAD_HUMAN_c0 + ATP_c0 -> BAD_HUMAN_c0 + ADP_c0

ATP_c0 + CREB1_HUMAN_c0 -> CREB1_HUMAN_c0 + ADP_c0

GSK3_cytosol_c0 + ATP_c0 -> p_S9_21_GSK3_cytosol_c0 + ADP_c0

MDM2_HUMAN_c0 + ATP_c0 -> MDM2_HUMAN_c0 + ADP_c0

ATP_c0 + AKTS1_HUMAN_c0 -> ADP_c0 + AKTS1_HUMAN_c0

Tuberin_c0 + ATP_c0 -> ADP_c0 + Tuberin_c0

ATP_c0 + CASP9_HUMAN_c0 -> CASP9_HUMAN_c0 + ADP_c0

Active_AKT_cytosol_c0 -> Active_AKT_nucleoplasm_c0

H2O_c0 + 1_phosphatidyl_1D_myo_inositol_4_5_bisphosphate_c0 -> diacylglycerols_c0 + IP3_c0

EGFR_c0

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

Add New Reaction Add New Rule Delete Pathway Links Search

Object Properties Problems (0 Errors, 0 Warnings) Pathway Preview

Reaction Name AKT_phosphorylates_TSC2_inhibiting_it_c0

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

Name	Description	Global	Expression	Units
J	reaction rate	<input type="checkbox"/>	$(K_f \cdot \text{Tuberin_c0} \cdot \text{ATP_c0} - K_r \cdot \text{ADP_c0} \cdot \text{Tuberin_c0})$	$\mu\text{M}\cdot\text{s}^{-1}$
Kf	forward rate constant	<input type="checkbox"/>	1.0	$\text{s}^{-1}\cdot\mu\text{M}^{-1}$
Kr	reverse rate constant	<input type="checkbox"/>	0.1	$\text{s}^{-1}\cdot\mu\text{M}^{-1}$
Tuberin_c0	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM
ATP_c0	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM
ADP_c0	Species Concentration	<input checked="" type="checkbox"/>	Variable	μM

Annotation and Pathway Links

File View Server Tools Help

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 - Applications (0)**
- Parameters, Functions and Units
- Pathway
 - Pathway Diagram
 - Pathway Objects (3)
 - BioPAX Summary

Name	Math Type	Annotation
(Empty table)		

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

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Object Properties Problems (0 Errors, 0 Warnings)

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

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Geometry Specifications Protocols Simulations Parameter Estimation

Species Reaction Network

Species	Structure	Clamped	Initial Condition
CBL_HUMAN_c0	c0	<input type="checkbox"/>	0.0
GRB2_c0	c0	<input type="checkbox"/>	0.0
SPY2_HUMAN_c0	c0	<input type="checkbox"/>	0.0
ATP_c0	c0	<input type="checkbox"/>	0.0
RAS_RAF_14_3_3_c0	c0	<input type="checkbox"/>	0.0
Activated_RAF1_complex_c0	c0	<input type="checkbox"/>	0.0
ADP_c0	c0	<input type="checkbox"/>	0.0
unidentified_protein_tyrosine_kinase_c0	c0	<input type="checkbox"/>	0.0
SPY2_HUMAN_c0	c0	<input type="checkbox"/>	0.0

To specify conditions for species, double click the new application and click "Specifications" > "Species".

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Search

Object Properties Problems (0 Errors, 0 Warnings) Pathway Preview

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

BioModel1

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To select all species on a page, press "ctrl+a" on your keyboard.

Species Reaction Network

Species	Structure	Clamped	Initial Condition
CBL_HUMAN_c0	c0	<input type="checkbox"/>	0.0
GRB2_c0	c0	<input type="checkbox"/>	0.0
CBL_GRB2_c0	c0	<input type="checkbox"/>	0.0
s3	c0	<input type="checkbox"/>	0.0
GRB2_GAB1_PIP3_c0	c0	<input type="checkbox"/>	0.0
EGF_p_6Y_EGFR_c0	c0	<input type="checkbox"/>	0.0
EGF_p_6Y_EGFR_GRB2_GAB1_c0	c0	<input type="checkbox"/>	0.0
_1_phosphatidyl_1D_myo_inositol_3_4_5_trisphosphate_c0	c0	<input type="checkbox"/>	0.0
ATP_c0	c0	<input type="checkbox"/>	0.0
RAS_RAF_14_3_3_c0	c0	<input type="checkbox"/>	0.0
Activated_RAF1_complex_c0	c0	<input type="checkbox"/>	0.0
ADP_c0	c0	<input type="checkbox"/>	0.0
unidentified_protein_tyrosine_kinase_c0	c0	<input type="checkbox"/>	0.0
SPY2_HUMAN_c0	c0	<input type="checkbox"/>	0.0

VCCell DB BioModels.net Pathway Comm Sabio

Search: egfr Search

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Filter: signaling by E Sort

Preview Open Web Link

Select only one o To simultaneously give multiple species the same initial condition, right click on selected species and hover your cursor over "Initial Condition". Type a value and press "Enter" on your keyboard to finalize. For this tutorial, the value "1" was used.

File View Server Tools Help

- Reactions (71)
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 - BioPAX Summary

Parameters, Functions and Units

Parameters and Functions | Predefined Constants and Math Functions | Model Unit System

Defined In: Global Reactions and Rules Applications

Type: Parameters Functions

Defined In:	Name	
Model / Reaction(CBL_binds_to_CRB2_c0)	Kf	forward rate constant
Model / Reaction(CBL_binds_to_CRB2_c0)	Kr	reverse rate constant
Model / Reaction(Gab1_Grb2_binds_to_EGF_Phospho_EGFR_c0)	Kf	forward rate constant
Model / Reaction(Gab1_Grb2_binds_to_EGF_Phospho_EGFR_c0)	Kr	reverse rate constant
Model / Reaction(Stabilisation_of_RAF_by_further_phosphorylation_unidentified)	Kf	forward rate constant
Model / Reaction(Stabilisation_of_RAF_by_further_phosphorylation_unidentified)	Kr	reverse rate constant
Model / Reaction(Sprouty_Jures_cytosolic_CBL_away_from_EGFR_c0)	Kf	forward rate constant
Model / Reaction(Sprouty_Jures_cytosolic_CBL_away_from_EGFR_c0)	Kr	reverse rate constant
Model / Reaction(Dephosphorylation_of_PAG_by_SHP2_c0)	Kf	forward rate constant
Model / Reaction(Dephosphorylation_of_PAG_by_SHP2_c0)	Kr	reverse rate constant
Model / Reaction(AKT_phosphorylates_BAD_c0)	Kf	forward rate constant
Model / Reaction(AKT_phosphorylates_BAD_c0)	Kr	reverse rate constant

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

To view parameters and functions, click "Parameters, Functions and Units".

Add New Global Parameter | Delete Global Parameter(s) | Search

Object Properties | Problems (0 Errors, 0 Warnings) | Pathway Preview

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

Filter: signaling by E Sort

Preview Open Web Link

File View Server Tools Help

- Reactions (71)
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- Observables (0)
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VCell DB BioModels.net Pathway Comm Sabio

Search

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Filter

signaling by E Sort

Preview Open Web Link

Parameters and Functions Predefined Constants and Math Functions Model Unit System

Defined In: Global Reactions and Rules Applications **Type:** Parameters Functions

Defined In:	Name	
Model / Reaction(CBL_binds_to_GRB2_c0)	Kf	forward rate constant
Model / Reaction(Gab1_Grb2_binds_to_EGF_Phospho_EGFR_c0)	Kf	forward rate constant
Model / Reaction(Stabilisation_of_RAF_by_further_phosphorylation_unidentified)	Kf	forward rate constant
Model / Reaction(Sprouty_Jures_cytosolic_CBL_away_from_EGFR_c0)	Kf	forward rate constant
Model / Reaction(Dephosphorylation_of_PAG_by_SHP2_c0)	Kf	forward rate constant
Model / Reaction(AKT_phosphorylates_BAD_c0)	Kf	forward rate constant
Model / Reaction(Transient_dissociation_of_14_3_3_upon_Ras_binding_c0)	Kf	forward rate constant
Model / Reaction(IP3_binds_to_the_IP3_receptor__opening_the_endoplasmic_retic)	Kf	forward rate constant
Model / Reaction(EGFR_activates_PLC_gamma1_by_phosphorylation_EGF_p_6Y_EGFR_P)	Kf	forward rate constant
Model / Reaction(AKT_phosphorylates_PRAS40_c0)	Kf	forward rate constant
Model / Reaction(CBL_mediated_ubiquitination_of_CIN85_EGF_p_6Y_EGFR_p_Y371_CB)	Kf	forward rate constant
Model / Reaction(Inhibition_of_GRK2_by_calmodulin_unknown_c0)	kf	forward rate constant

Add New Global Parameter Delete Global Parameter(s) Search kf

Object Properties Problems (0 Errors, 0 Warnings) Pathway Preview

Select only one object (e

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

- Reactions (71)
- Structures (1)
- Species (175)
- Molecules (0)
- Observables (0)
- Applications (1)
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- Pathway
 - Pathway Diagram
 - Pathway Objects (369)
 - BioPAX Summary

To select all constants on a page, press "ctrl+a".

Parameters and Functions Predefined Constants and Math Functions Model Unit System

Defined In: Global Reactions and Rules Applications Type: Parameters Functions

Defined In:	Name	
Model / Reaction(CBL_binds_to_GRB2_c0)	kf	forward rate constant
Model / Reaction(Gab1_Grb2_binds_to_EGF_Phospho_EGFR_c0)	kf	forward rate constant
Model / Reaction(Stabilisation_of_RAF_by_further_phosphorylation_unidentified)	kf	forward rate constant
Model / Reaction(Sprouty_lures_cytosolic_CBL_away_from_EGFR_c0)	kf	forward rate constant
Model / Reaction(Dephosphorylation_of_PAG_by_SHP2_c0)	kf	forward rate constant
Model / Reaction(AKT_phosphorylates_BAD_c0)	kf	forward rate constant
Model / Reaction(Transient_dissociation_of_14_3_3_upon_Ras_binding_c0)	kf	forward rate constant
Model / Reaction(IP3_binds_to_the_IP3_receptor_opening_the_endoplasmic_retic)	kf	forward rate constant
Model / Reaction(EGFR_activates_PLC_gamma1_by_phosphorylation_EGF_p_6Y_EGFR_P)	kf	forward rate constant
Model / Reaction(AKT_phosphorylates_PRAS40_c0)	kf	forward rate constant
Model / Reaction(CBL_mediated_ubiquitination_of_CIN85_EGF_p_6Y_EGFR_p_Y371_CB)	kf	forward rate constant
Model / Reaction(Inhibition_of_GRK2_by_calmodulin_unknown_c0)	kf	forward rate constant
Model / Reaction(CamKIV_enters_the_nucleus_c0)	kf	forward rate constant

Add New Global Parameter Delete Global Parameter(s) Search kf

To simultaneously give multiple constants the same expression, right click on selected constants and hover your cursor over "Expression". Type a value and press "Enter" on your keyboard to finalize. For this tutorial, the value "1" was used.

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Search: egfr Search

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- Reactions (71)
- Structures (1)
- Species (175)
- Molecules (0)
- Observables (0)
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 - Parameter Estimation
- Parameters, Functions and Units
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- BioPAX Summary

Click "simulations"

Geometry Specifications Protocols Simulations Parameter Estimation

Simulations Output Functions Generated Math

Simulations toolbar with icons for adding, deleting, and running simulations.

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

To add a simulation, click the add simulation icon.

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Filter signaling by E Sort

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Object Properties Problems (0 Errors, 0 Warnings) Pathway Preview

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

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Geometry Specifications Protocols Simulations Parameter Estimation

Simulations Output Functions Generated Models

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

Name	End Time	Running Status	Results
Simulation0	1.0	keep every 1 sample	Combined IDA/CVODE

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

Object Properties Problems (0 Errors, 0 Warnings) Pathway Preview

Annotation:

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

Parameters with values changed from defaults

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

PathwayCommons

- Physiology
 - Reaction Diagram
 - Reactions (71)
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VCell DB BioModels.net Pathway Comm Sabio

Search

Signaling by EGFR [Reactome](#) [Homo sapiens](#)

Filter

Simulations **Output Functions** Generated Math

Name	End Time	Output Option	Solver	Running Status	Results
Simulation0	1.0	keep every 1 sample	Combined IDA/CVODE	completed	yes

Click to view results.

Object Properties Problems (0 Errors, 0 Warnings)

Annotation:

Settings:

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

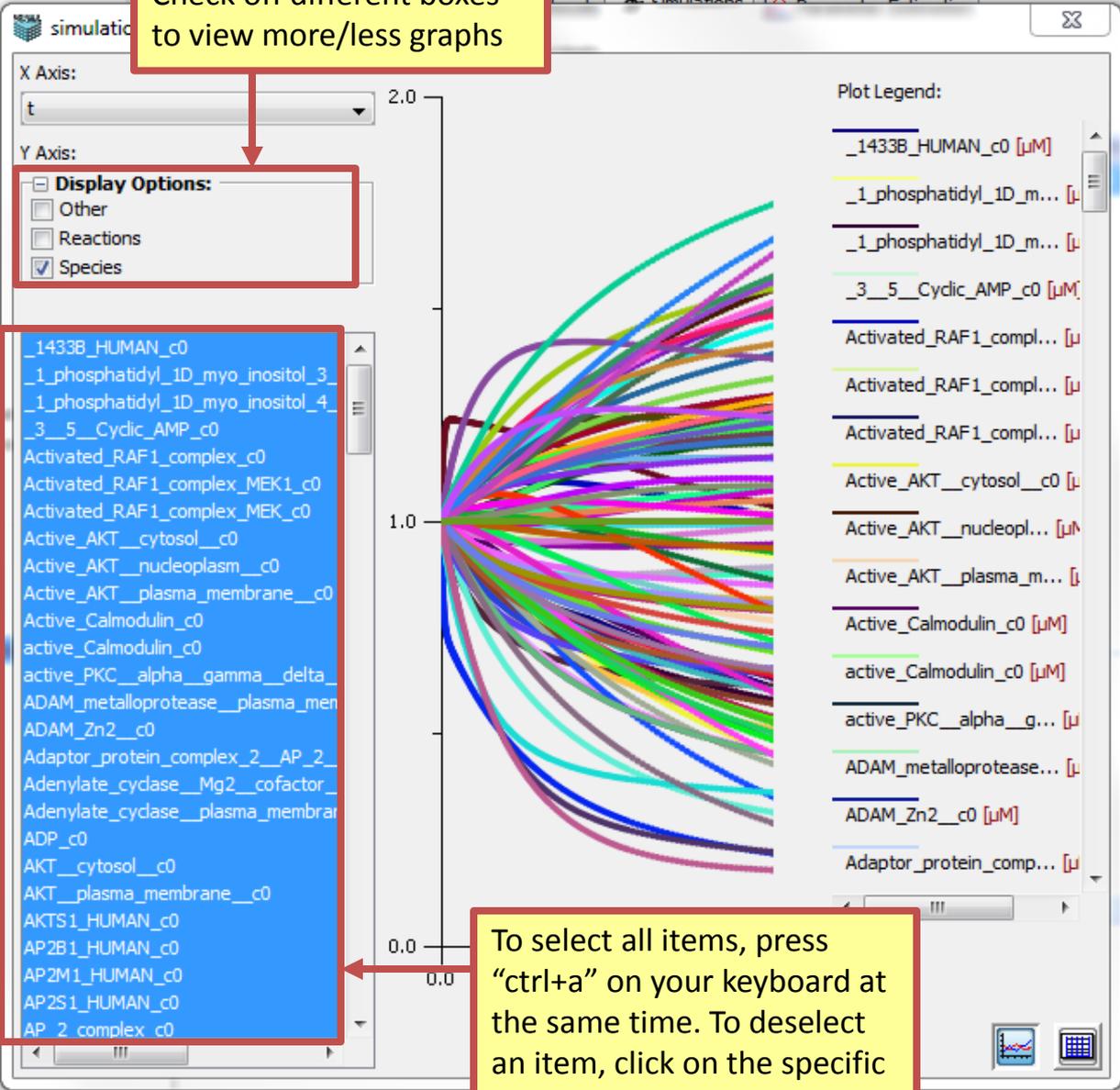
Parameters with values changed from defaults

Parameter Name	Default	New Value/Expression	Scan

PathwayCommons

- Physiology
 - Reaction Diagram
 - Reactions (71)
 - Structures (1)
 - Species (175)
 - Molecules (0)
 - Observables (0)
- Applications (1)
 - Application0
 - Geometry
 - Specifications
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 - Parameter Estimation
- Parameters, Functions and Pathway

Check off different boxes to view more/less graphs



- __1433B_HUMAN_c0
- __1_phosphatidyl_ID_myoinositol_3_4_5_c0
- __1_phosphatidyl_ID_myoinositol_4_5_c0
- __3_5_Cyclic_AMP_c0
- Activated_RAF1_complex_c0
- Activated_RAF1_complex_MEK1_c0
- Activated_RAF1_complex_MEK2_c0
- Active_AKT_cytosol_c0
- Active_AKT_nucleoplasm_c0
- Active_AKT_plasma_membrane_c0
- Active_Calmodulin_c0
- active_Calmodulin_c0
- active_PKC_alpha_gamma_delta_c0
- ADAM_metalloprotease__plasma_membrane_c0
- ADAM_Zn2_c0
- Adaptor_protein_complex_2_AP_2_c0
- Adenylate_cyclase_Mg2_cofactor_c0
- Adenylate_cyclase__plasma_membrane_c0
- ADP_c0
- AKT_cytosol_c0
- AKT_plasma_membrane_c0
- AKTS1_HUMAN_c0
- AP2B1_HUMAN_c0
- AP2M1_HUMAN_c0
- AP2S1_HUMAN_c0
- AP_2_complex_c0

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

Simulation Control Panel

Status: Results

yes

Scan

PathwayCommons

- Physiology
 - Reaction Diagram
 - Reactions (71)
 - Structures (1)
 - Species (175)
 - Molecules (0)
 - Observables (0)
- Applications (1)
 - Application0
 - Geometry
 - Specifications
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 - Parameter Estimation
- Pathways

simulation results for Simulation0

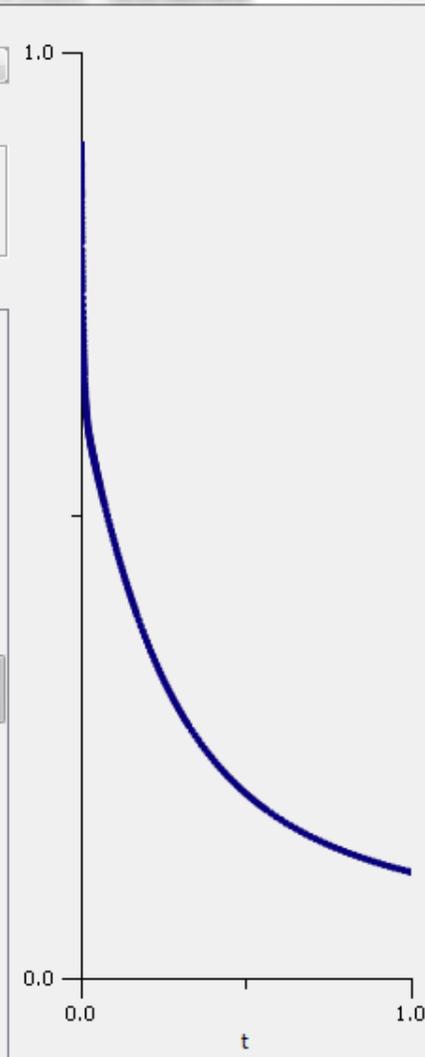
X Axis: t

Y Axis:

Display Options:

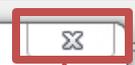
- Other
- Reactions
- Species

- J_Adenylate_cyclase_produces_cAMP_c0
- J_Adenylate_cyclase_produces_cAMP_c0
- J_AKT_can_phosphorylate_forkhead_box_TSC2_c0
- J_AKT_can_phosphorylate_NUR77_c0
- J_AKT_can_phosphorylate_RSK_c0
- J_AKT_can_phosphorylate_RSK_c0
- J_AKT_phosphorylates_CREB_Active_c0
- J_AKT_phosphorylates_GSK3_Active_c0
- J_AKT_phosphorylates_MDM2_c0
- J_AKT_phosphorylates_PRA1810_c0
- J_AKT_phosphorylates_TSC2_inhibitor_c0**
- J_AKT_translocates_to_the_nucleus_c0
- J_Assembly_of_EGFR_complex_in_data_c0
- J_Binding_of_CBL_to_EGFR_c0
- J_Binding_of_GRB2_to_GAB1_c0
- J_Binding_of_PIK3_regulatory_alpha_subunit_to_PDK1_c0
- J_Calcium_binds_calmodulin_c0
- J_Calmodulin_binds_CaMK_IV_c0
- J_CaMK_IV_autophosphorylation_c0
- J_CaMK_IV_phosphorylates_CREB_phosphorylated_c0
- J_CamKIV_enters_the_nucleus_c0
- J_cAMP_induces_dissociation_of_inactivated_CaMKIV_c0
- J_CBL_binds_to_GRB2_c0
- J_CBL_escapes_CDC42_mediated_inhibition_c0
- J_CBL_mediated_ubiquitination_of_CIP1_c0



Plot Legend:

J_AKT_phos



To close the window, click "X".

All of the fluxes start with "J".

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