

# **PathFinder**

Welcome to PathFinder - the tool for visualization of signaling and metabolic pathways.

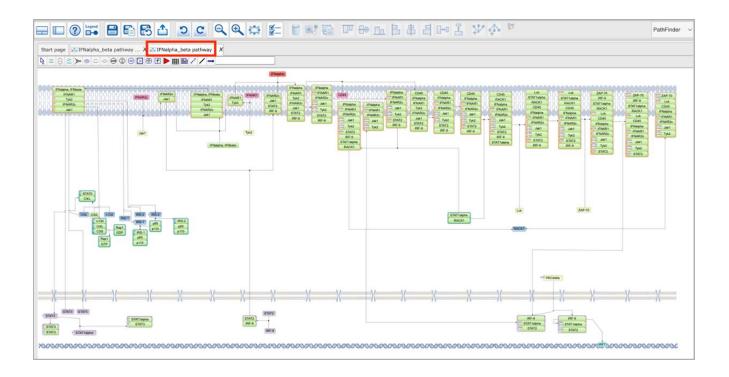
# **Getting started**

The PathFinder tab automatically opens in your browser after you have selected to visualize any of the pathways in the geneXplain database interface by clicking on the **PathFinder** link:

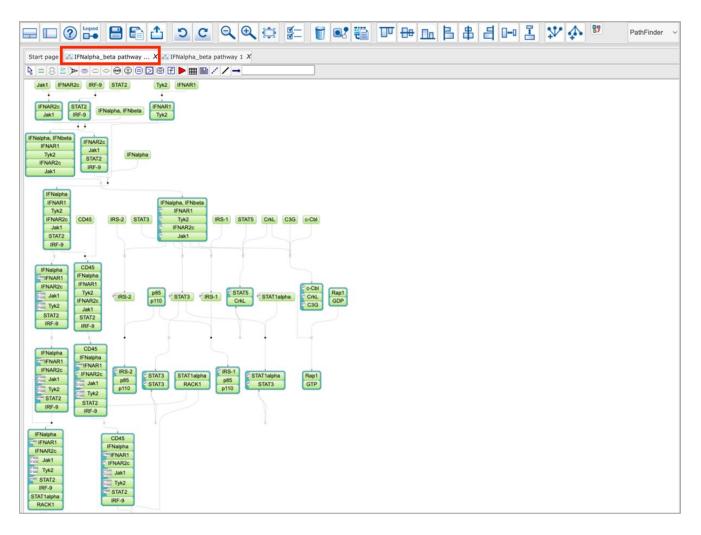
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The selected pathway will be opened in two independent tabs inside the PathFinder interface on your screen:

First tab will contain the auto-layouted pathway in respect to the intracellular compartments its elements belong to:



The second tab will contain the pathway without compartments:



The pathway without compartments is subject to user-selected layout via the layout buttons at the top menu panel on PathFinder (all described below).

If several pathways were selected for visualization in geneXplain portal interface, they will be opened inside independent tabs in the PathFinder interface.

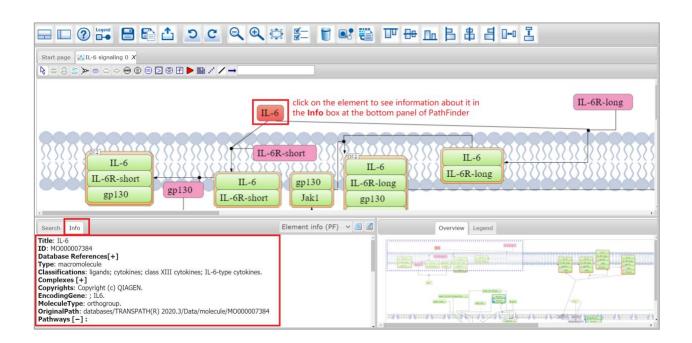
To see the whole diagram at once, you can use the **Fit to screen** button, available at the top menu

panel of PathFinder. For changing the scale of the diagram manually, you can use the **Zoom in** 

Legend

To view information about any element on the pathway diagram, as well as to view the full diagram overview, click on the **Toggle UI mode** button on the top menu panel of PathFinder, which will open the bottom panel.

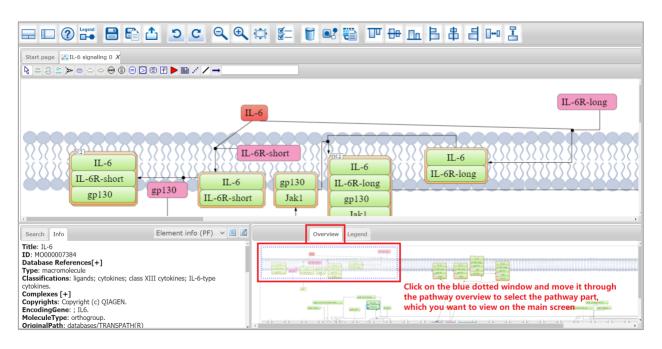
In the left part of the bottom panel you will find the **Info** tab. In this tab available information about the currently selected object is viewed. You can click on any element of the diagram to see its info:



To see information about a complex, click on its colored frame or double click on any of the elements of the complex. Single click on any element of the complex will open information about the selected element itself.

In the right part of the bottom panel you will find the **Overview** tab, which displays the whole pathway diagram in miniature. The blue dotted window highlights the part of the pathway which is currently

viewed in the main window of PathFinder. You can click on the blue dotted window and move it around the whole pathway preview to select the part of the pathway, which you would like to currently look into:



# **Saving diagrams**

By default the pathways you have selected to view in the geneXplain portal interface are opening in PathFinder interface as follows: the pathway with compartments is opened directly from the TRANSPATH database diagrams folder and thus is not editable; the pathway without compartments is subject to modification by user and thus is automatically copied to a temporary folder of your personal project in PathFinder interface. When you will close PathFinder tab in your browser or when your current session will be timed out, the temporary folder will be emptied and the pathway diagram stored in the temporary folder **tmp** will be deleted from your project. If you would like to save the diagram or its

modified version inside your project in PathFinder permanently, please click on the **Save** button on the top menu panel of PathFinder and select the respective path for saving the current diagram. You should select:

#### (1) your project:

Save a copy		×
Folder: PathFinder/Projects	Up +	
Your project name Double click on your project name		
Name:		
	Ok Cancel	

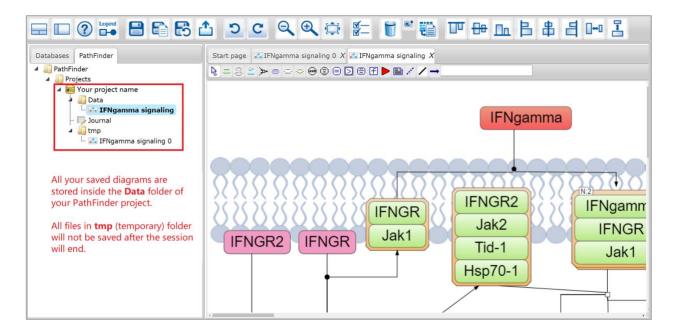
(2) the Data folder inside your project:

Save a copy	,		×
Folder: Path	Finder/Projects/ your project name	•	Up +
Data Journal	Double click on the Data folder		
Name:			
			Ok Cancel

Then specify the name of the diagram that you would like to save and click on the **Ok** button:

Save a copy	×
Folder: PathFinder/Projects/ your project name/Data	Up +
Name: Specify the name of your diagram here	
	Ok Cancel

You will find all data stored inside your own project in PathFinder by opening the left navigation panel of PathFinder using the **Toggle repository** button on the top menu panel of PathFinder:



You can modify any of your locally saved pathways as well as pathways opened directly from TRANSPATH® database (pathways with compartments) inside PathFinder interface and save the

resulting diagram in your local project using the **Save a copy** button the top menu panel of PathFinder.

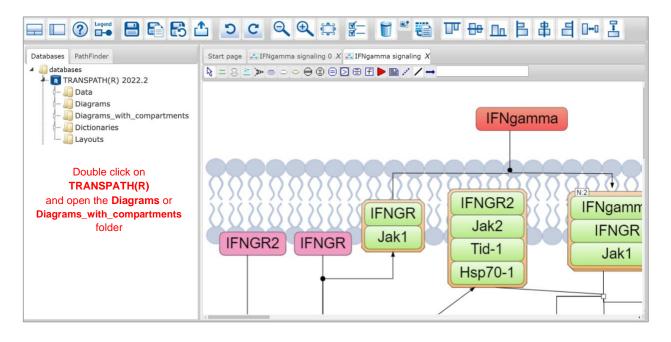
The Export button allows you to save any PathFinder diagram on your local computer in a number of available formats:

Export	locument	×
Format:	Scalable Vector Graphics(*.svg) 🗸	
	Scalable Vector Graphics(*.svg)	
	Antimony JPEG file (*.jpg) Bitmap file(*.bmp) Portable Network Graphics (*.png) BioUML format(*.dml) Pair graph file(*.txt) SBGN-ML SBML GraphML(*.graphml) Cytoscape (*.cx) Generic file COMBINE archive (*.sbex)	1.

### Browsing all pathways and reactions

To browse all TRANSPATH® pathways and reactions directly from PathFinder interface first open the

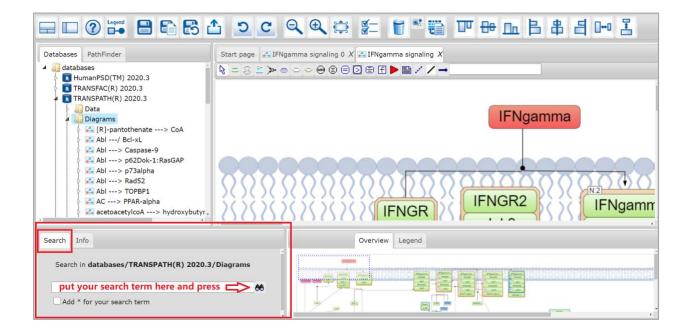
left panel of PathFinder by clicking on the **Toggle repository** button on the top menu panel of PathFinder, then switch to the **Databases** tab inside the left panel of PathFinder, double click on **TRANSPATH®** database and open the **Diagrams** or **Diagrams\_with\_compartments** folder:



Databases PathFinder
4- 🔃 TRANSPATH(R) 2022.2
🛄 Data
🗕 🔐 Diagrams
🕬 🛃 [R]-pantothenate> CoA
þ 🚰 Abl/ Bcl-xL
b 🛃 Abl> Caspase-9
here and the second sec
∲… 🚰 Abl> p73alpha
} ≥ Rad52
∲ 🚰 AbI> TOPBP1
P Z- AC> PPAR-alpha
🗁 🛃 acetoacetylcoA> hydroxybutyrate
ectyl-CoA> malonyl-CoA
Image: Image
acetyl-CoA, acetoacetyl-CoA> cholesterol, fatty acid
acetyl-CoA, malonyl-CoA> lignoceric acid
acidic hexose derivatives and inositol
₽ 🛃 activin A> Smad2
ŀ… 🚰 activin A> Smad3
ŀ 🚰 ActR-I> Smad3
> Smad3
> fatty acyl-CoA, malonyl-CoA> fatty acyl-CoA
> free fatty acid
🗁 🚰 adenine, alpha-D-5-P-ribosyl-PP> inosine, ammonia
🤄 🚣 Adiponectin> AMPK
ADP> dATP

To search for pathways or reactions of your interest open the bottom panel of PathFinder by clicking on

the **Toggle UI mode** button on the top menu panel of PathFinder and navigate to the **Search** tab inside this panel:



Interactive search results will open in the newly accessible **Search result** tab on the right side of the bottom panel of PathFinder:

Search Info		🗅 🗖 🗟 Overview Legend Search res	ult			
Search in databases/TRANSPATH(R) 2020.3/Diagrams/CH0000004485	First	Previous 1 Next Last Path	Showing 1 to 36 o	f 36 entries SI Components	how 50 v en	ntries
egf 🔬	0	EGF> c-Fos	EGF> c- Fos	MEK1{p} + MP1 + ERK <==> MEK1{p}:MP1		com read edg
Add * for your search term	1	C EGF> ERK1, ERK2	EGF> ERK1, ERK2	Shc-1> Grb-2, MEK1 -> ERK1, MEK1> E		com read edg
	2	EGF> PAK1	EGF> PAK1	ErbB1> Grb-2, Grb-2 -> PAK1, EGF> Er	CH00000052	com reac

The pathway of your interest can then be easily accessed by clicking on the respective search result:

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acetoacetylcoA> hydroxybutyrate	×					
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Search in databases/TRANSPATH(R) 2020.3/Diagrams	First	Previous 1 Next Last	Showing 1 to 36 o		Show 50	✓ entries
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egf search term	0	EGF> c-Fos	EGF> c- Fos	MEK1{p} + MP1 + ERK1 <==> MEK1{p}:MP1	CH000000999	reactions:13 edges:35
	1	Z EGF> ERK1, ERK2	EGF> ERK1, ERK2	Shc-1> Grb-2, MEK1 - -> ERK1, MEK1> E	CH00000030	components reactions:10 edges:20
	2	Z EGF> PAK1	EGF> PAK1	ErbB1> Grb-2, Grb-2 - -> PAK1, EGF> Er	CH000000052	components reactions:3, edges:6

PathFinder is integrated with HumanPSD<sup>™</sup>+TRANSPATH® and TRANSFAC® databases and holders of respective subscriptions can perform direct searches in these databases inside the PathFinder interface similar to how the search through TRANSPATH® diagrams was described above.

# **Editing diagrams**

To edit the diagrams in PathFinder you can use the tools available at the top panel of PathFinder interface, the context menu that opens with a right-click on a selected diagram element or by simple mouse 'click and move' interactive operation available on all diagrams.

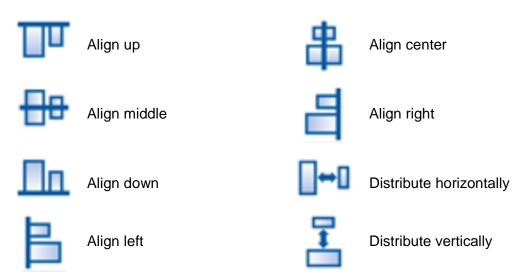
All elements on the diagram are clickable. If you have opened the bottom panel of PathFinder using the

**Toggle UI mode** button on the top menu panel of PathFinder, you will see the element info upon clicking on any molecule, reaction or complex on the diagram. Once you have clicked on the element and it was highlighted, you can move the element with your mouse to any other location or delete it

using the **Remove selected** button on the top menu panel of PathFinder. To select a complex, you need to either click on its colored frame or double click on any of its elements. Clicking on any element of the complex only once will select just the element itself. You can check what exactly was selected by looking into the element information, provided in the info box at the bottom panel of PathFinder. To select multiple elements, hold *Ctrl* and click through the needed elements. You can save the selected

elements as a new diagram by clicking on the **Save selected subset** button on the top menu panel of PathFinder. Make sure <u>not to save the new diagram in the temporary **tmp** folder of your project, as this file <u>will not be kept after your session has ended</u>. Please <u>save the new diagram to the **Data** folder of your project</u>. For further guidance on how to save and manage your PathFinder diagrams please refer to the **Saving diagrams** section of this guide (see above).</u>

Automatic layouting can be applied to selected elements of the diagram using the following buttons on the top menu panel of PathFinder:

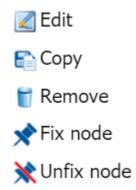


Any of these auto layout options will layout the selected elements in respect to the selected layout type, relative to each other and to the size of the functional cell compartment they belong to.



The **Adjust reactions nodes** button on the top menu panel of PathFinder fixes all nodes of the diagram, except of reactions, and launches the auto layout procedure. This function becomes very useful when you have manually moved some elements (molecules) on the diagram and now the automatic re-layouting of the diagram edges is needed.

A right mouse click on any of the selected elements of the diagram will open the following context menu:



The **Edit** menu item will open the options of the selected element, that specify the position, type, name and database reference of the element.

The **Copy** menu item will copy the selected element(s) of the diagram and will automatically paste the copied elements on the current diagram in the place to which you will point and click with your mouse.

The **Remove** menu item will delete the selected element(s) from the diagram.

The **Fix node** menu item will pin the selected element(s) to their current locations and these elements will not be moved by any of the auto layouters you might apply later.

The **Unfix node** menu item will unpin the selected element(s) and they will again become movable in the automatic layout procedures.

Any of the performed actions can be rolled back or repeated using the **Undo** and **Redo** buttons on the top menu panel of PathFinder. All changes made to the diagram in comparison with its last saved version can be cancelled by using the **Revert to saved** button.

The **Diagram view options** button on the top menu panel of PathFinder allows you to change the overall appearance of the diagram. You can change colors, element positions, fonts, and other general appearance options with this function.

### All buttons denotations

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**Toggle UI mode** - this button opens the bottom panel of PathFinder, which enables search and info tabs in the left section of the panel and diagram overview and navigation window in the right section of the panel.

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**Toggle repository** - this button opens the left panel of PathFinder, which gives access to the PathFinder tab, containing all your saved data inside a respective project, and to the Databases tab, which provides access to the databases you have an active license for.



Help - this button opens the PathFinder user guide.



Legend - this button opens the PathFinder legend.



**Save document** - this button saves the currently opened diagram. Please make sure to save all diagrams to the <u>Data</u> folder inside your own project in PathFinder.

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**Save a copy** - this button saves a copy of the currently opened diagram into a new location. Please make sure to save all diagrams to the <u>Data</u> folder inside your own project in PathFinder.



**Revert to saved** - this button cancels all changes you have made to the currently opened diagram in comparison to its last saved version.



**Export** - this button allows you to save the currently opened diagram to your local computer in a number of formats.

**Undo** - this button rolls back the last performed modification of the currently opened diagram.



**Redo** - this button repeats the last performed and then cancelled modification of the currently opened diagram.



**Zoom out** - this button zooms out the currently opened diagram in the main window of PathFinder.



**Zoom in** - this button zooms in the currently opened diagram in the main window of PathFinder.



Fit to screen - this button fits to screen the currently opened diagram in the main window of PathFinder.



**Diagram view options** - this button allows changing of the overall appearance of the diagram (colors, element positions, fonts, grid and other general appearance options of the diagram can be changed with this function).



**Remove selected** - this button deletes the selected element(s) from the currently opened diagram.



Adjust reactions nodes - this button fixes all nodes of the diagram, except of reactions, and launches the auto layout procedure. This function can be used for automatic layouting of edges after manually changing the positions of various elements (molecules) on the diagram.



**Save selected subset** - this button allows to save the selected elements of the currently opened diagram as a new diagram. Please make sure to save all diagrams to the <u>Data</u> folder inside your own project in PathFinder.



**Align up** - this button performs automatic layout of the selected elements of the currently opened diagram. The selected elements are aligned to the top relative to each other and to the sizes of corresponding functional cell compartments that they belong to.

Align middle - this button performs automatic layout of the selected elements of the currently opened diagram. The selected elements are aligned to the center relative to each other and to the sizes of corresponding functional cell compartments that they belong to.

**Align down** - this button performs automatic layout of the selected elements of the currently opened diagram. The selected elements are aligned to the bottom relative to each other and to the sizes of corresponding functional cell compartments that they belong to.

Align left - this button performs automatic layout of the selected elements of the currently opened diagram. The selected elements are aligned to the left relative to each other and to the sizes of corresponding functional cell compartments that they belong to.

**Align center** - this button performs automatic layout of the selected elements of the currently opened diagram. The selected elements are aligned to the center relative to each other and to the sizes of corresponding functional cell compartments that they belong to.

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**Align right** - this button performs automatic layout of the selected elements of the currently opened diagram. The selected elements are aligned to the right relative to each other and to the sizes of corresponding functional cell compartments that they belong to.



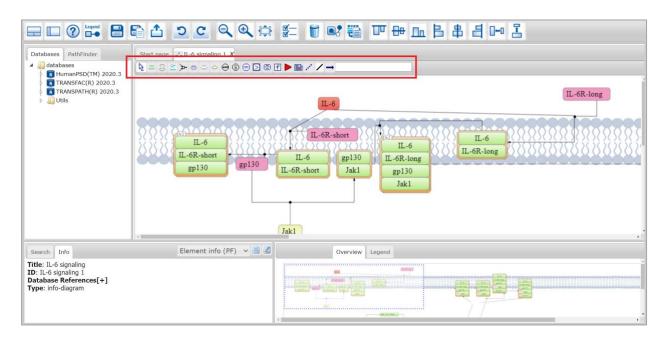
**Distribute horizontally** - this button performs automatic layout of the selected elements of the currently opened diagram. The selected elements are distributed horizontally relative to each other and to the sizes of corresponding functional cell compartments that they belong to.



**Distribute vertically** - this button performs automatic layout of the selected elements of the currently opened diagram. The selected elements are distributed vertically relative to each other and to the sizes of corresponding functional cell compartments that they belong to.

# Additional menu

All PathFinder diagrams have a standard SBGN and SBML operations menu (toolbar) available on the top of the diagram:



This menu allows adding new elements to the currently opened diagram. A mouseover infotip will appear when you navigate to any element of this toolbar.

Once you have selected the desired button (type of the new element) on the toolbar, simply click on the respective place of the diagram for this new element to appear.

You can edit the properties of the newly created diagram elements by selecting the respective element, right-clicking on it and pressing on the **Edit** menu item.

The blank field on the right side of the toolbar is a search input window:



It can be used for searching for certain elements in the currently opened diagram. The search term should be submitted in the format of MO ID (e.g. ErbB1 ID: MO000016681). Enter the needed MO ID in the blank field and press *Enter*. If the currently opened diagram contains the respective element, the diagram will be repositioned on the screen in such a way that the searched element will be placed in the center of the main PathFinder window.