

# Creating a New Metabolika Pathway File

Use the Metabolika module to visualize metabolic pathways and to create, store, export, and process Metabolika drawing files.

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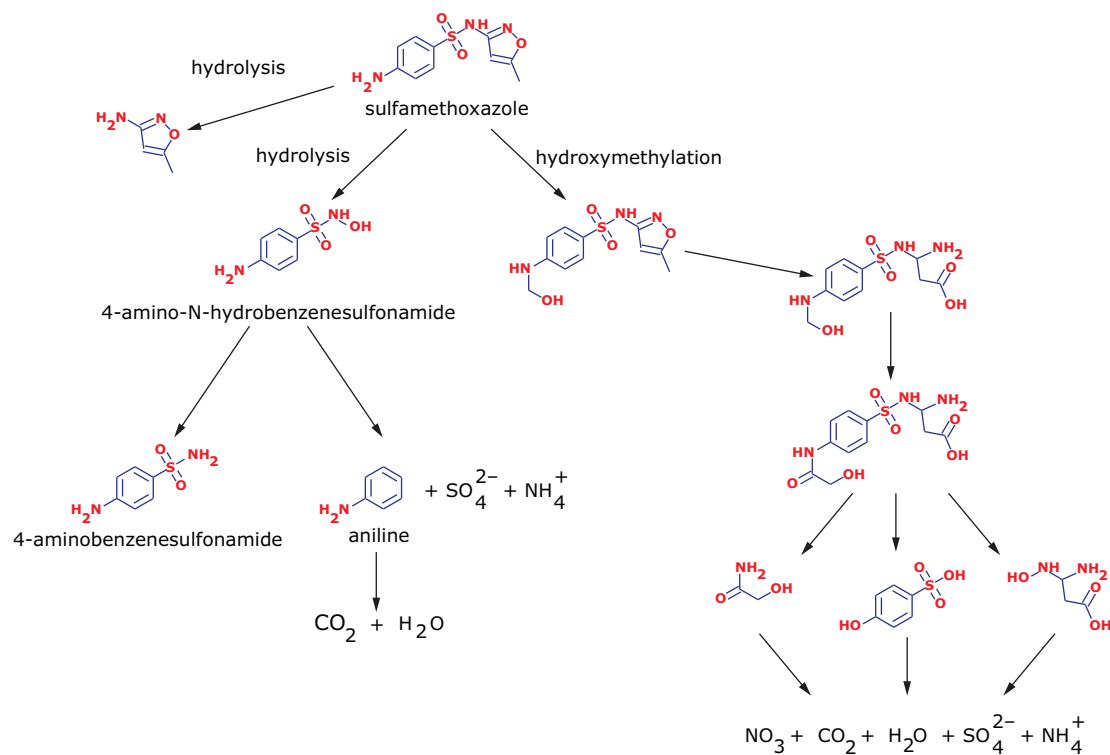
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- [Saving the Drawing as a Metabolika File](#)

## Overview

A Metabolika drawing file consists of chemical structures interconnected by arrows and represents a metabolic reaction or a series of reactions. You can send the pathway structures individually or in a batch to other Mass Frontier modules where they are used for data curation, substructure searches, fragment generation, and so on.

In the Metabolika module, you can add and edit chemical structures, connect them with various arrow types, and annotate them with custom text and labels. You can import structures from supported file types or create them by using the internal structure editor. You can export the pathway structures to structure grids and use them in other Mass Frontier modules. For example, you can use the structures in a structure grid to generate a set of XIC chromatograms in the Chromatogram Processor module.

This tutorial shows you how to draw the metabolic pathway for the bacterial decomposition of the antibiotic sulfamethoxazole by *Pseudomonas psychrophila* HA-4<sup>1</sup> and save the drawing as a Metabolika drawing file.



<sup>1</sup> Jiang, B., Li, A., Cui, D., Cai, R., Ma, F., & Wang, Y. (2014). Biodegradation and metabolic pathway of sulfamethoxazole by *Pseudomonas psychrophila* HA-4, a newly isolated cold-adapted sulfamethoxazole-degrading bacterium.


## Drawing a Metabolic Pathway

### Opening a New Pathway Document

To draw the metabolic pathway for the bacterial decomposition of sulfamethoxazole, follow these topics in order:

1. [Opening a New Pathway Document](#)
2. [Adding Structures to the Pathway](#)
3. [Labeling Structures](#)
4. [Adding Directional Arrows to the Pathway](#)
5. [Adding Arrow Captions](#)
6. [Adding Elemental Formulas](#)

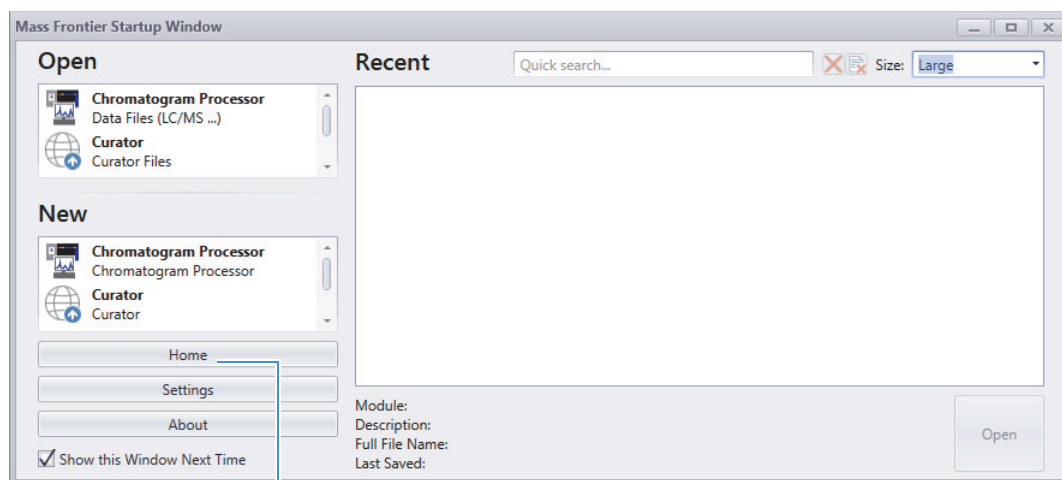
#### ❖ To open a New Pathway document

1. Open the Mass Frontier application by double-clicking its desktop icon, , or by choosing **HighChem Mass Frontier 8.0 > Mass Frontier 8.0** from the Windows™ Start menu.

The application opens to the Mass Frontier Startup Window or the Modules & Tools toolbar.

2. If the Mass Frontier Startup Window opens, click **Home** (Figure 1).

**Figure 1.** Mass Frontier Startup Window

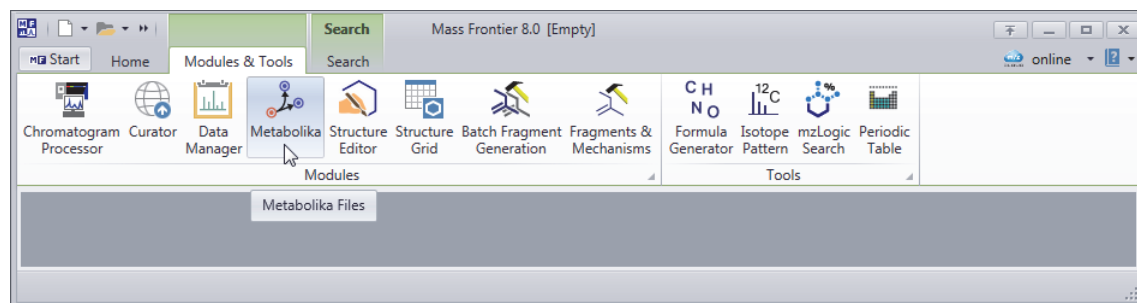


Opens the Modules & Tools toolbar

**Note** If you clear the Show this Window Next Time check box, the next time you open the application, it opens to the Modules & Tools toolbar.

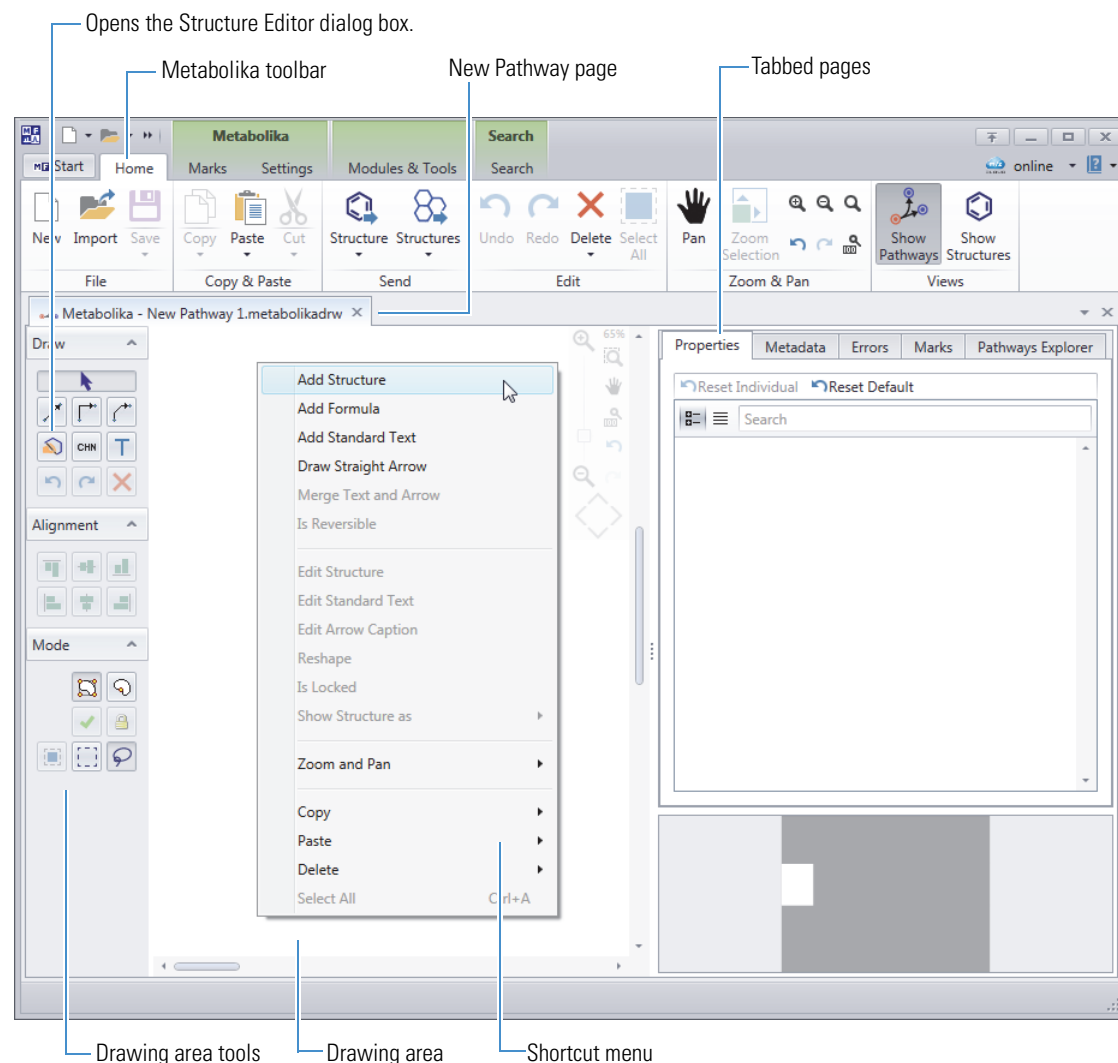
3. In the Modules & Tools toolbar, click **Metabolika**.

**Figure 2.** Modules & Tools toolbar



A new document named New Pathway 1.metabolikadrw opens as a tabbed page with a toolbar on the left, a drawing area in the middle, and a set of tabbed pages on the right that are opened to the Properties page. Right-clicking the drawing area opens a shortcut menu (Figure 3).

**Figure 3.** New pathway page opened in the Metabolika module



Leave the New Pathway page open and go to the next topic “[Adding Structures to the Pathway.](#)”

## Adding Structures to the Pathway

There are several ways to add structures to the pathway. You can load a structure from a 2D structure file, draw a structure by using the Structure Editor, or copy a structure from a structure grid or another .metabolikadrw file.

To add the structures and some of the other pathway objects to the drawing area, follow these procedures in order:


1. [Adding a Structure from a MOL File](#)
2. [Copying a Structure from a Structure Grid](#)
3. [Copying a Metabolika Pathway](#)

**Note** To show you how to add arrows and text to a metabolic pathway, this topic instructs you to copy only the structures from an existing Metabolika drawing file instead of all the pathway elements.

### Adding a Structure from a MOL File

To add the parent compound—sulfamethoxazole—to the pathway, use the MOL file provided in the Demo Data folder.

#### ❖ To add a structure from a MOL file to the pathway

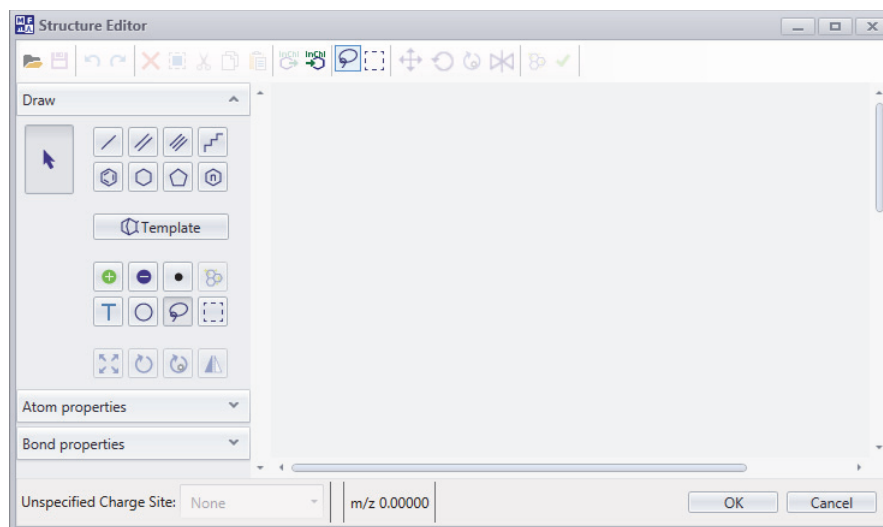
1. In the New Pathway document, do either of the following:
  - In the Draw toolbar at the left, click the **Add/Edit Structure** icon,  (Figure 3).


—OR—

- Right-click the drawing area and choose **Add Structure** (Figure 3).

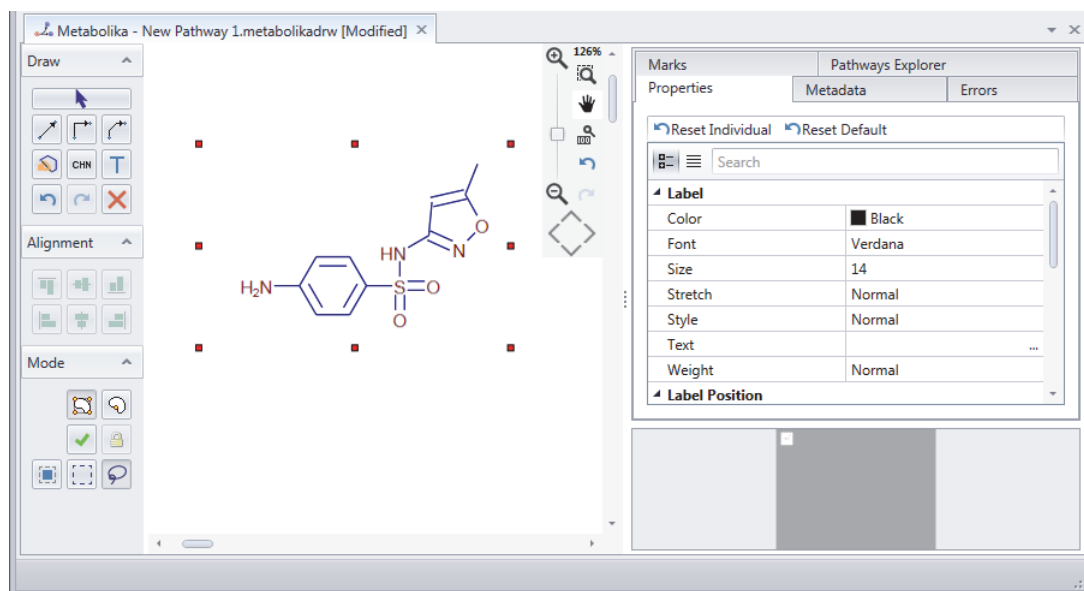
The Structure Editor opens as a dialog box with a general toolbar at the top and three structure-specific toolbars at the left.

**Figure 4.** Structure Editor dialog box



2. In the toolbar at the top of the Structure Editor, click the **Open** icon, .
3. Browse to the following folder:  
*drive:\Users\Public\Public Documents\HighChem\Mass Frontier 8.0\Demo Data\Structures*
4. Select the following 2D structure file—**sulfamethoxazole.mol**.  
The structure for sulfamethoxazole appears in the Structure Editor's drawing area.
5. Click **OK**.  
The Structure Editor closes and the structure appears as a structure object in the drawing area of the New Pathway page.
6. Use the left mouse button to move the structure in the drawing area.

**Figure 5.** Sulfamethoxazole added to the drawing area of a New Pathway page



Leave the New Pathway page open and go to the next topic, “Copying a Structure from a Structure Grid.”

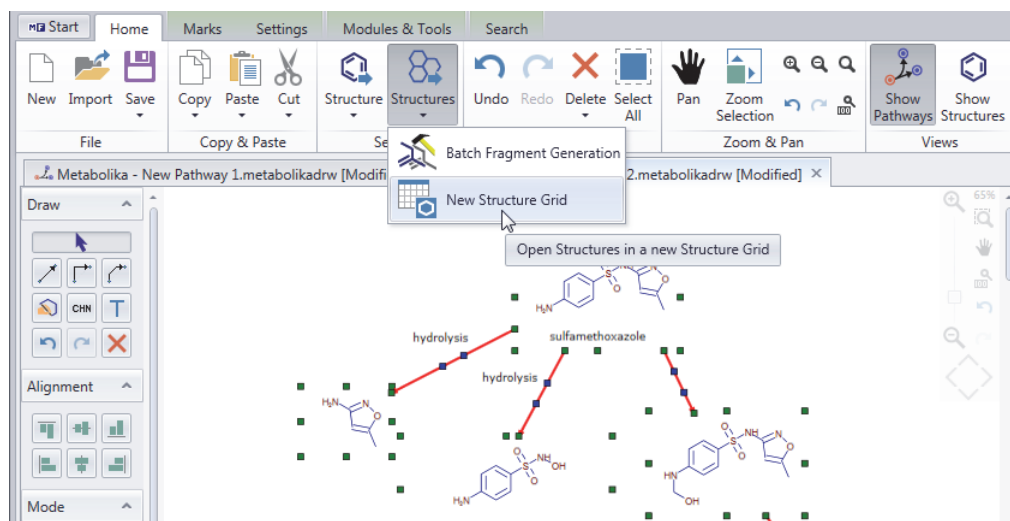
## Copying a Structure from a Structure Grid

The SMX Decomposition.metabolikadrw file in the Demo Data folder contains the metabolic pathway for sulfamethoxazole. In this topic, you send the structures in the demonstration drawing to a Structure Grid page, and then copy one of the structures to the New Pathway page where you are creating the new drawing.

**Note** You can copy all or part of a Metabolika drawing to another Metabolika drawing or send one or more structures in a Metabolika drawing to a Structure Grid page.

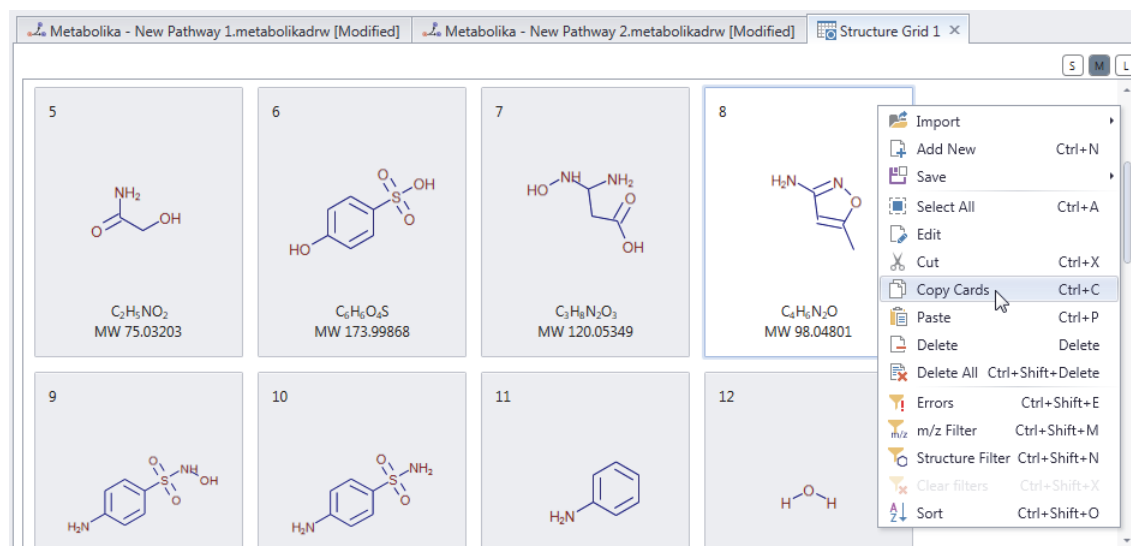
### ❖ To send structures from a Metabolika drawing file to a structure grid

1. Open the example Metabolika drawing that contains the pathway of interest as follows:
  - a. In the Metabolika toolbar, click **New**.  
A second New Pathway page opens to the right of the current New Pathway page.
  - b. In the Metabolika toolbar, click **Import**.
  - c. Browse to the following folder, select **SMX Decomposition.meabolikadrw**, and click **Open**.  
*drive:\Users\Public\Public Documents\HighChem\Mass Frontier 8.0\Demo Data\Metabolika*
2. To send the structures on the second New Pathway page to a structure grid, click **Structures**, and then click **New Structure Grid** in the Send Group of the Metabolika toolbar.



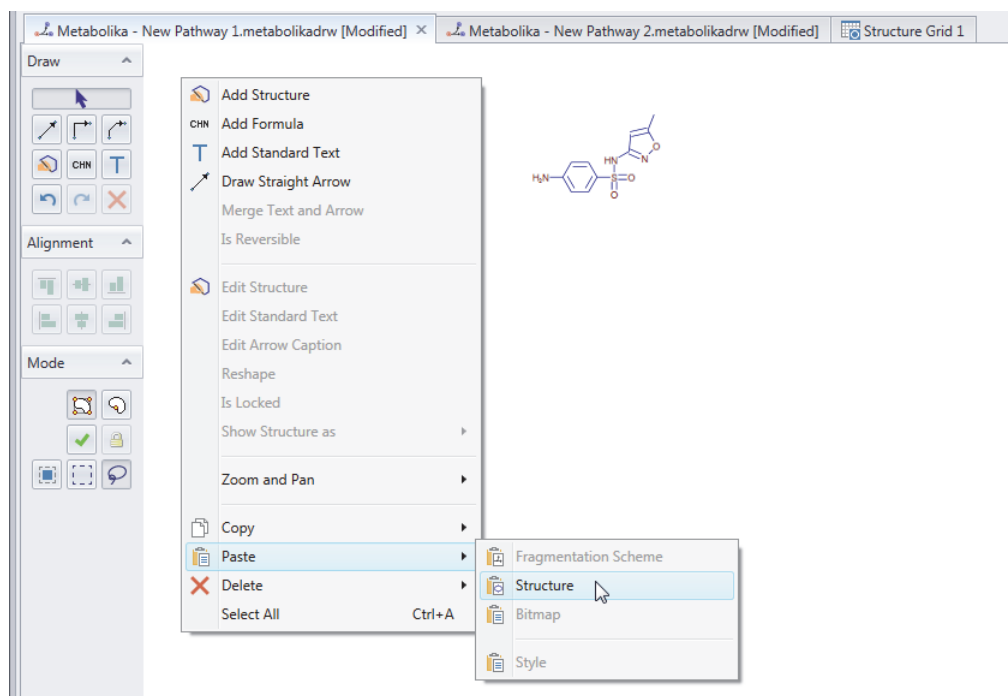
A new Structure Grid page with 25 cards opens to the right of the second New Pathway page.

3. Right-click **Card 8** (MW 98.04801) and choose **Copy Cards**.



**Note** You can copy and paste only one structure at a time from a Structure Grid page to a New Pathway page.



- To return to the first New Pathway page where you are creating the new drawing, click its tab.
- Right-click the New Pathway page and choose **Paste > Structure** (or press CTRL+V).



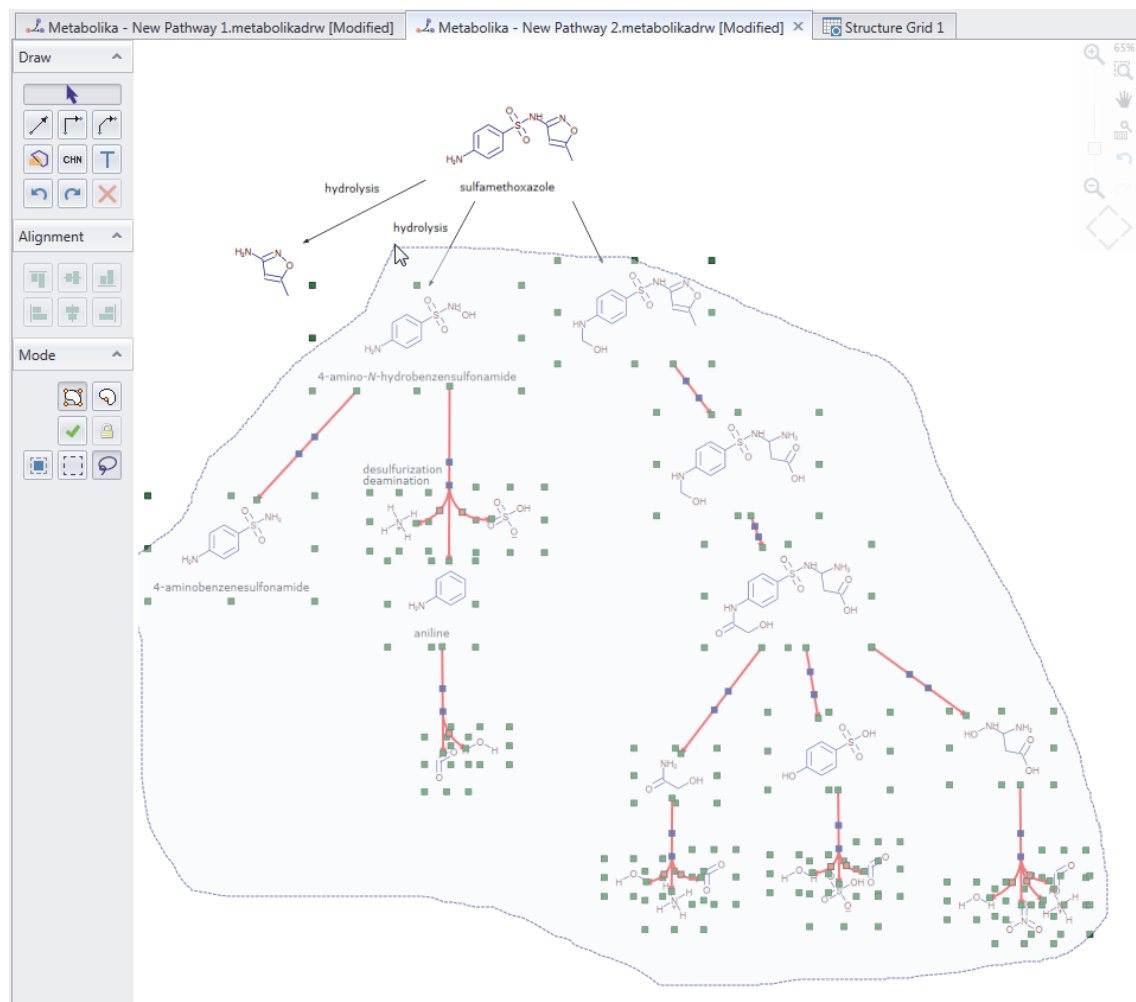
You now have two structures on the New Pathway page where you are creating the new drawing. Leave the New Pathway page open and go to the next topic, “[Copying a Metabolika Pathway](#).”

### Copying a Metabolika Pathway

#### ❖ To copy a pathway from another New Pathway page

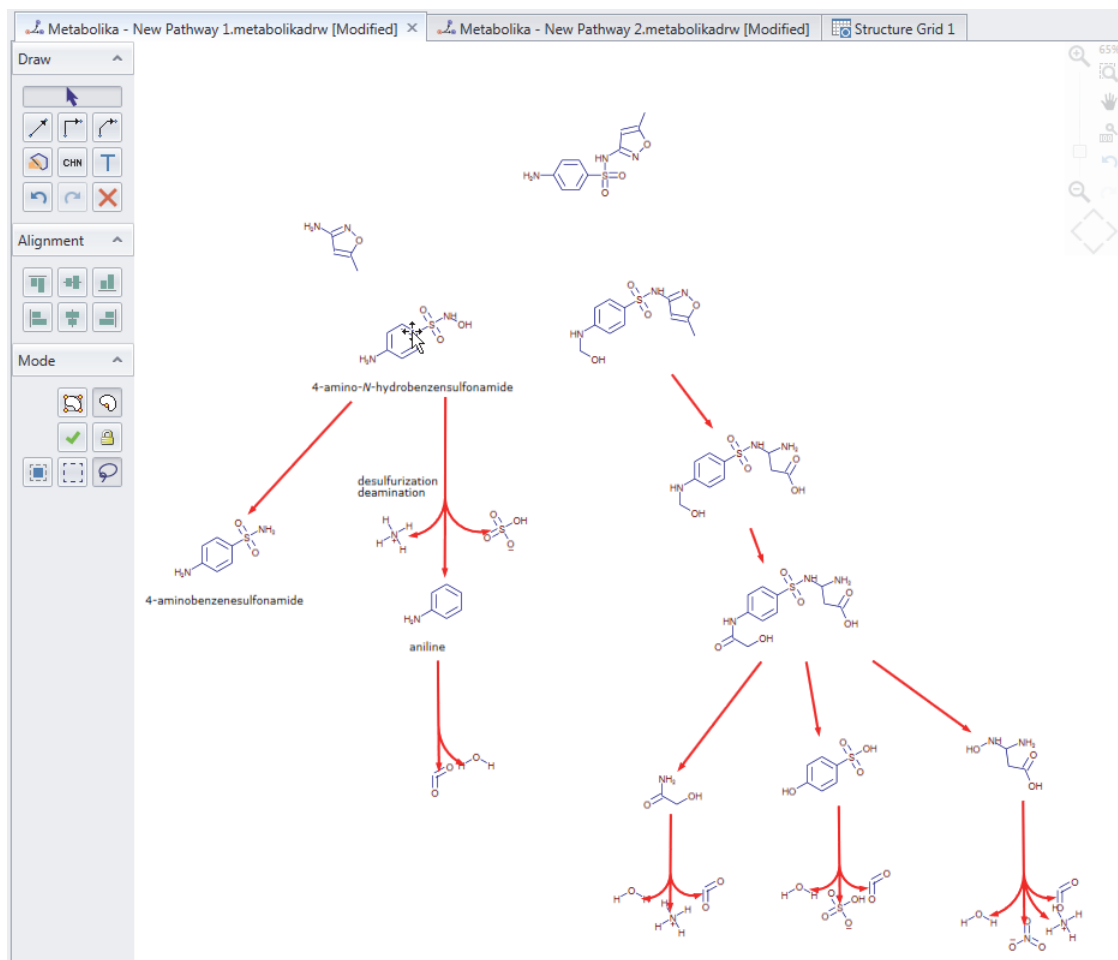
- To open the New Pathway page that contains the full metabolic pathway for sulfamethoxazole, click the **New Pathway 2** tab.
- At the left of the drawing area, under Mode, click the **Rectangular Selection** tool, , or the **Lasso Selection** tool, , and then drag the pointer across or around the structures in the pathway that you have not already copied to the first New Pathway page ([Figure 6](#)).

**Figure 6.** Portion of pathway selected by dragging the Lasso Selection tool around the structures

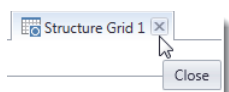


3. On the computer keyboard, press **CTRL+C**.
4. To return to the New Pathway 1 page where you are creating the new drawing, click its tab.
5. On the computer keyboard, press **CTRL+V** to paste the selection to the New Pathway 1 page.
6. Use the left mouse button to move the selection below the two existing structures (Figure 7).

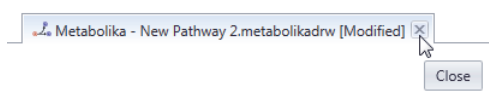
**Figure 7.** Pasting the selection to the New Pathway 1 page



7. Close the Structure Grid page.



8. Close the New Pathway 2 page.



Leave the New Pathway 1 page open and go to the next topic, “Labeling Structures.”

## Labeling Structures

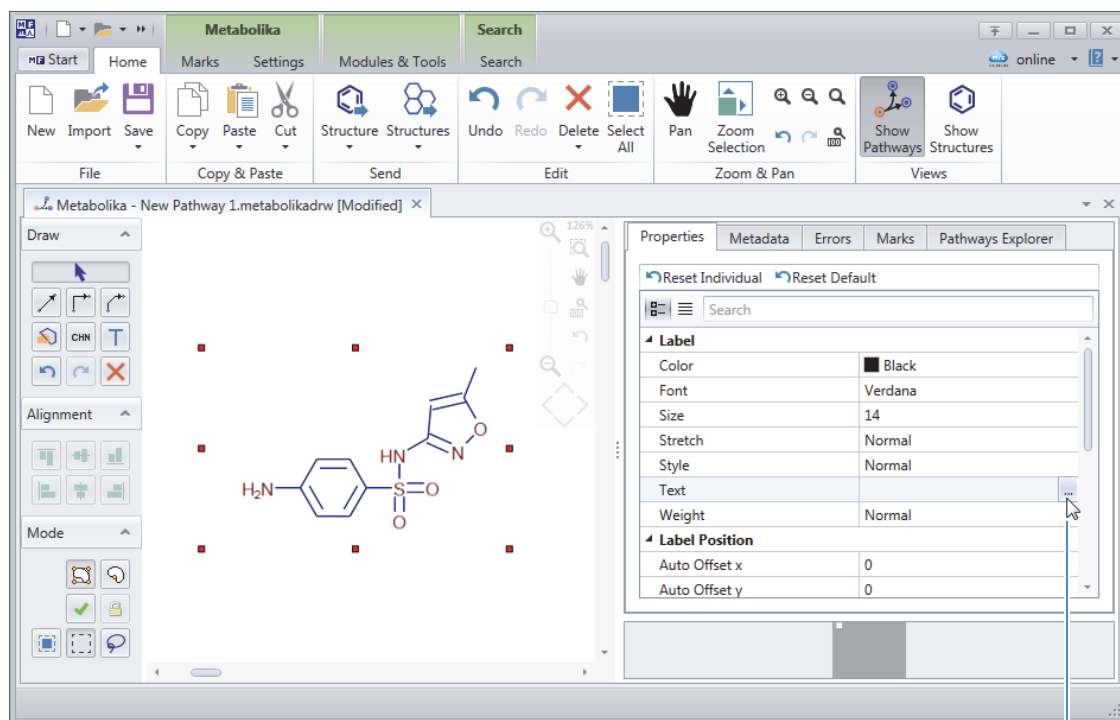
You can annotate a structure by adding standard text or a label—however, if you want the text to be part of the structure object and move together with the structure, annotate the structure by adding a label.

### ❖ To add a label to a structure

1. In the drawing area of the New Pathway page, select the parent structure at the top.
2. On the Properties page to the right, click the browse icon, ..., to the right of the Text box in the Label area (Figure 8).

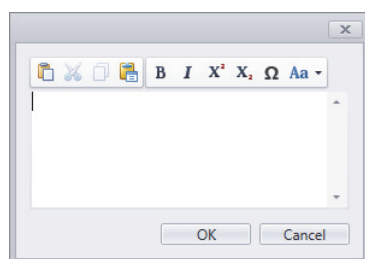


**Figure 8.** Parent compound selected

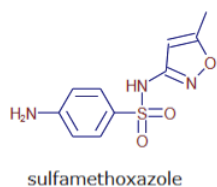


Opens a text entry box  
for creating a label

A text entry box opens.



3. Type the label and click **OK**. For parent structure in this tutorial, type **sulfamethoxazole**.  
The label appears below the structure.




**Note** To change the properties of a label after adding it to a structure object, select the structure object and modify the label's properties on the Properties page.

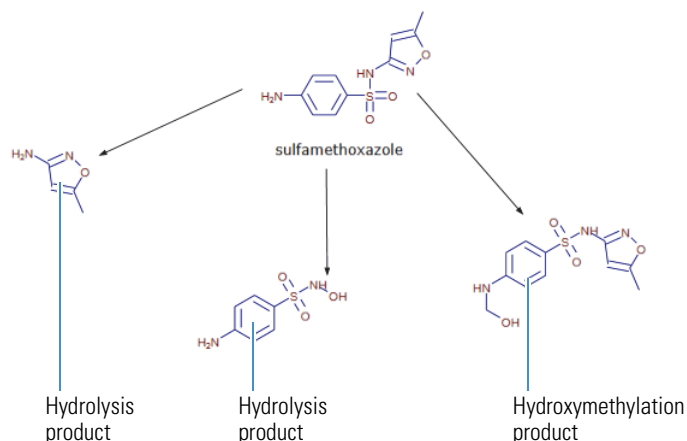
Leave the New Pathway 1 page open and go to the next topic, [“Labeling Structures.”](#)

## Adding Directional Arrows to the Pathway

Arrows indicate the direction between reactants and products. Follow the first procedure to add the three missing directional arrows to the pathway. The remaining procedures are optional.

### ❖ To add the missing directional arrows

1. To draw a straight arrow from the parent compound to the hydrolysis product on the right, under Draw, click the **Add/Connect to Straight/Arc Connector** icon, .
2. Point to the parent structure, and then drag the mouse toward the first hydrolysis product on the right. By default, the arrow is locked to the parent compound, but not the hydrolysis product.
3. Right-click the arrow and choose **Is Locked**.
4. Repeat this procedure for the other hydrolysis product and the hydroxymethylation product.




Leave the New Pathway 1 page open and go to the next topic, “Adding Arrow Captions” on page 11.

(Optional) To modify the arrows in a Metabolika pathway, follow these procedures:

- To move an arrow
- To change an arrow's angle
- To change an arrow's curvature
- To straighten a curved arrow
- To make an arrow bidirectional to represent a reversible reaction
- To merge arrows


### ❖ To move an arrow

1. Select the arrow and hold down the left mouse button to display the move pointer (.




2. Drag the arrow to another location.

### ❖ To change an arrow's angle

1. Select the arrow to display its anchor points, and then point to an end anchor point.
2. When this pointer () appears, drag the end of the arrow up or down as needed.

❖ **To change an arrow's curvature**

1. Select the arrow to display its anchor points, and then point to one of its two internal anchor points.
2. When this pointer () appears, drag the pointer arrow up or down as needed.




❖ **To straighten a curved arrow**

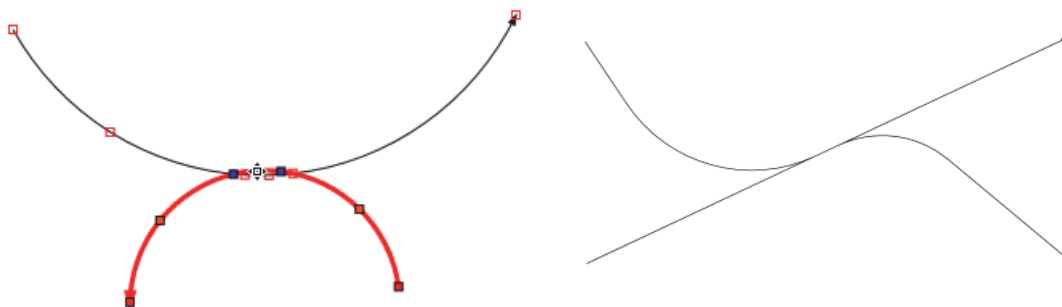
Right-click it and choose **Reshape**.

❖ **To make an arrow bidirectional to represent a reversible reaction**

Right-click it and choose **Is Reversible**.

❖ **To merge arrows**

1. Reshape the arrows into curves.
2. Overlay the curved arrows, and then select one of the curves.
3. Point to any of the blue squares.
4. When this pointer () appears, drag the selected curve until the red square anchor points appear on the second curve. Then, release the mouse button.



**Note** The shape of your merged curves might differ from those shown above.

5. To straighten one of the merged arrows, right-click it and choose **Reshape**.

Add arrow captions to the two hydrolysis steps at the top of the pathway.

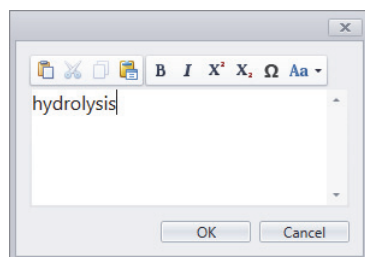
❖ **To add an arrow caption**

1. Right-click the arrow for the first hydrolysis reaction at top left of the pathway, and then choose **Edit Arrow Caption**.

A dialog box opens.

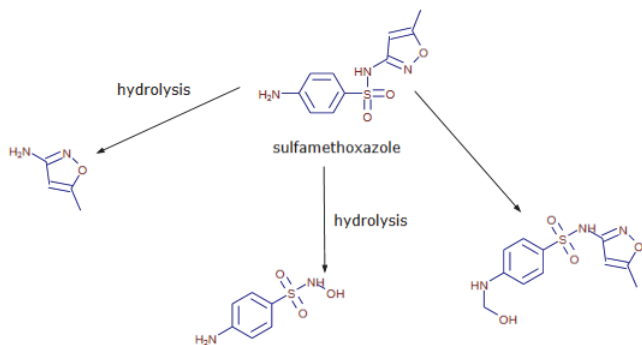
2. Type text and click **OK**.

For this tutorial, type **hydrolysis**.



## Adding Arrow Captions

- Right-click the arrow for the second hydrolysis reaction, choose **Edit Arrow Caption**, type **hydrolysis**, and click **OK**.



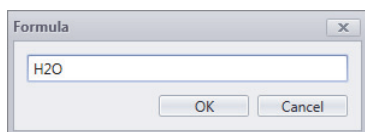
Leave the New Pathway 1 page open and go to the next topic, “[Adding Elemental Formulas](#)” on [page 12](#).

## Adding Elemental Formulas

The metabolic pathway that you copied from the SMX Decomposition.metabolikadrw file contains structures for small molecules, such as water and carbon dioxide. For simplicity, you can replace small structures with elemental formulas.

### ❖ To add elemental formulas to a drawing

- Right-click in the drawing area and choose **Add Formula**.
- Type the Formula in the Formula dialog box.



- Click **OK**.

The formula appears in the drawing area with the numeric value for each element inserted as a subscript, for example, H<sub>2</sub>O.

Leave the New Pathway 1 page open and go to the next topic, “[Saving the Drawing as a Metabolika File](#).”

## Saving the Drawing as a Metabolika File


### ❖ To save the new metabolic pathway drawing

- In the File group of the Metabolika toolbar, click **Save**, and then select **Save As**.
- Browse to an appropriate folder.

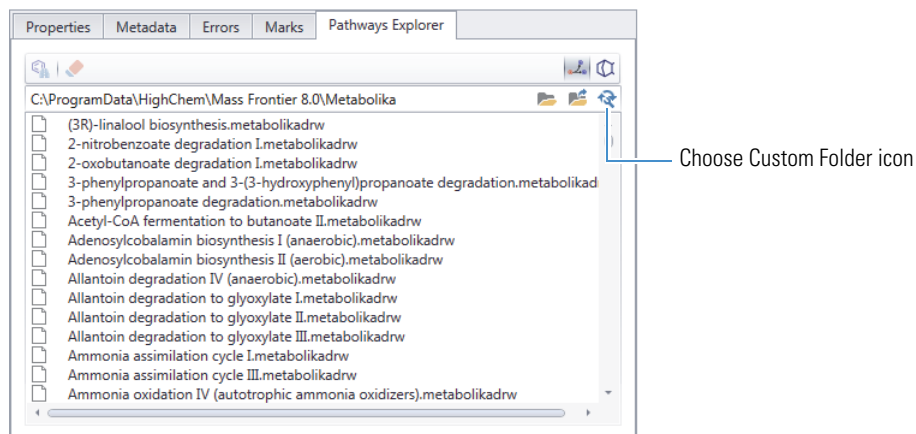
If you have not set already set up folders for your Metabolika pathway files, the Save Metabolika File dialog box opens to the Demo Data\Metabolika folder.

- In the File Name box, type **A New Pathway**.
- Click **Save**.

### ❖ To view a Metabolika pathway from the Pathways Explorer


- In the File group of the Metabolika toolbar, click **New**.
- Close the **A New Pathway** file that you created and saved in this tutorial.
- To the right of a Metabolika New Pathway document, click the **Pathways Explorer** tab (see [Figure 3](#) on [page 3](#)). The Pathways Explorer page appears.
- To view any of the pathways that are provided with the application, click the **Choose Default Folder** icon,  ([Figure 9](#)).

**Figure 9.** List of pathways that come with the application



5. In the pathway list, select a pathway.

The selected pathway opens as a tabbed page.

6. On the Pathway Explorer page, click the **Choose Custom Folder** icon, .

7. Browse for the folder where you saved the **A New Pathway.metabolikadrw** file and click **OK**.

8. In the files list, select the file that you want to view or edit.

The selected pathway opens as a tabbed page.

## Trademarks

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