

# UM-BBD Pathway Prediction System (PPS) Tutorial

Mark Fischbach, John Schrom, Lynda Ellis,  
Jennifer Chiantello, Junfeng Gao, Michael Turnbull  
Version 5.1 – October 28, 2011

Web version of this Tutorial:

<http://umbbd.msi.umn.edu/predict/aboutPPS.html>

## Table of Contents

Overview.....	2
Demonstration.....	3
* Start the Demo.....	3
* Status Page.....	5
* Pathway Prediction Results.....	5
* MarvinView.....	7
* Change Default Options.....	8
* Aerobic Likelihood.....	8
* Show Levels.....	8
* Show Products Containing "C".....	11
* Show Products on a Level.....	13
* Rule Button.....	14
* Cpd Button.....	16
* Next Button.....	18
* Green Next or Cpd Button.....	19
* Remove Products.....	20
* Variable Aerobic Likelihood.....	22
* Super Rules.....	22
Drawing Structures.....	23
Entering SMILES Strings.....	25
For Further Information or To Leave Comments.....	26
Bibliography.....	26

## OVERVIEW

The UM-BBD Pathway Prediction System (PPS) predicts microbial catabolic reactions using substructure searching, a rule-base, and atom-to-atom mapping. The PPS recognizes organic functional groups found in a compound and predicts transformations based on biotransformation rules. These rules are based on reactions found in the UM-BBD database or the scientific literature. The pathway prediction system can be accessed at the UM-BBD Pathway Prediction page, which can be reached from the **"Pathway Prediction"** link on the UM-BBD home page, or by using the URL: <http://umbbd.msi.umn.edu/predict/>. The PPS predicts biodegradation of user compounds. Users can choose if they will view all or only the more likely aerobic transformations. The PPS uses Chemaxon's MarvinSketch and MarvinView Java applets as plugins. A user enters a compound into the system by one of two methods: **"Drawing the Structure and Generating SMILES"** or **"Entering SMILES Directly"**.

UNIVERSITY OF MINNESOTA  
BIOCATALYSIS/BIODEGRADATION DATABASE

Home  
Search  
About  
UM-BBD | PPS | BPT  
What's New  
FAQs  
Join E-mail List  
Contributors  
Publications  
Links  
Acknowledgements  
Contact Us

Pathway Prediction System | PredictBT Workshops | Biochemical Periodic Tables

### UM-BBD Pathway Prediction System

#### Purpose and Scope

The PPS predicts plausible pathways for microbial degradation of chemical compounds. Predictions use biotransformation rules, based on reactions found in the UM-BBD database or in the scientific literature. A [list of all rules](#) is available.

PPS predictions are most accurate for compounds that are:

- similar to compounds whose biodegradation pathways are reported in the scientific literature;
- in environments exposed to air, in moist soil or water, at moderate temperatures and pH, with no competing chemicals or toxins; and
- the sole source of energy, carbon, nitrogen, or other essential element for the microbes in these environments, rather than present in trace amounts.

Biodegradation of [some types of compounds](#) should not be predicted. [More information](#) is available.

#### Use

First, either draw the compound whose degradation is to be predicted (click ? for drawing help) and click "Write SMILES", or enter a SMILES string. Next, click "Continue".

This system uses Chemaxon's [MarvinSketch](#) Java applet as its chemical drawing plugin. SMILES string format is described on the [SMILES Home Page](#) from Daylight Chemical Information Systems, Inc. For example, a SMILES string for Benzyl Alcohol is "OCc1ccccc1". Other example SMILES strings are found on the [Aerobial s-Transomes](#) page.

Choose to see all predicted biotransformations, or only those more likely to occur exposed to air (aerobic likelihood "neutral" or above). Biotransformations are assigned aerobic likelihood by two or more biodegradation experts. Standard conditions assumed for aerobic biotransformations are: exposed to air, in moist soil or water, at neutral pH, 25°C, with no competing or toxic other compounds.

Show BioTransformations: ☒ Aerobic ☐ All

File Edit View Insert Atom Bond Structure Tools Help

100%

Write SMILES

SMILES string:

Continue Clear Demo

Powered by ChemAxon

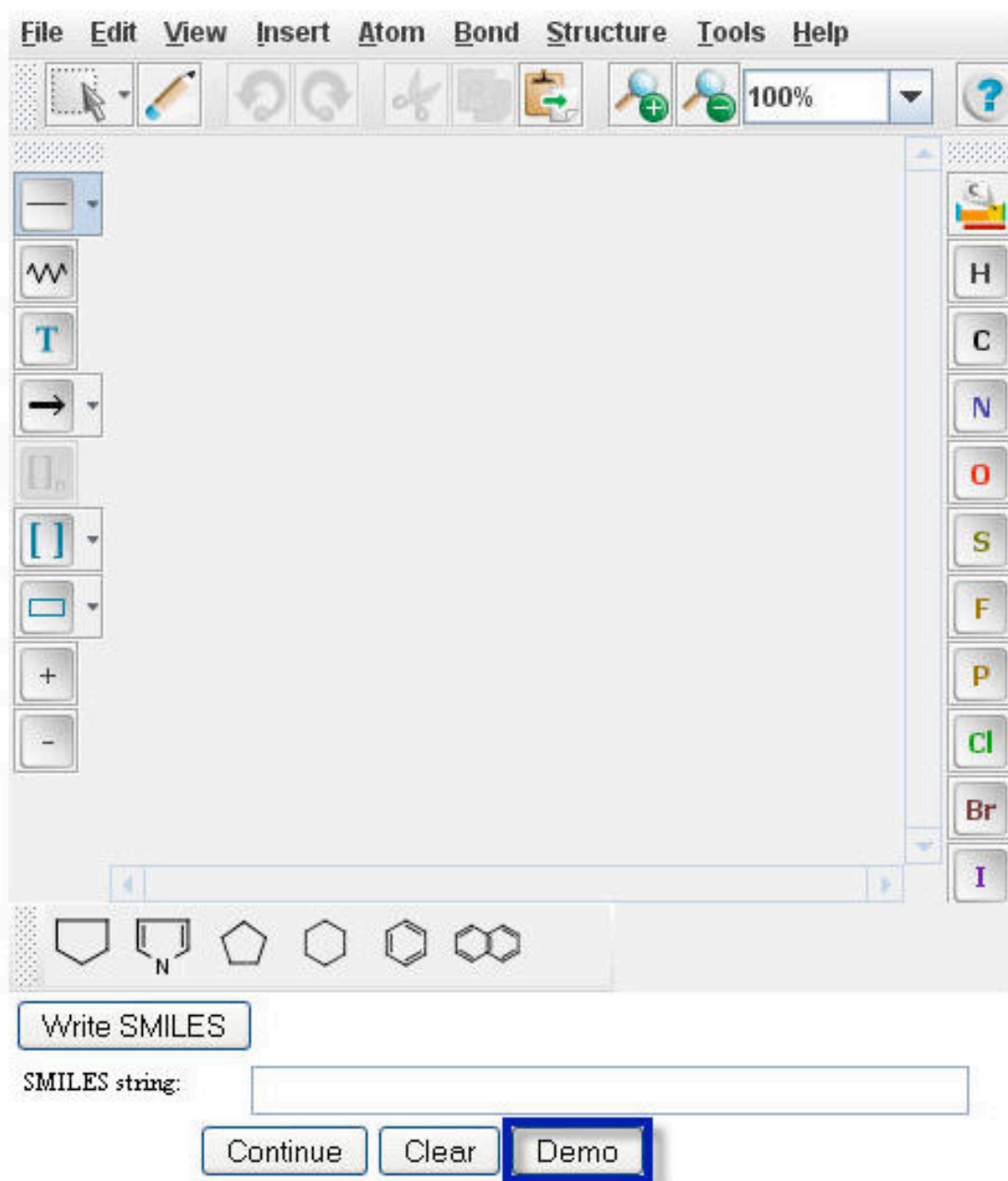
Powered by APACHE

MySQL

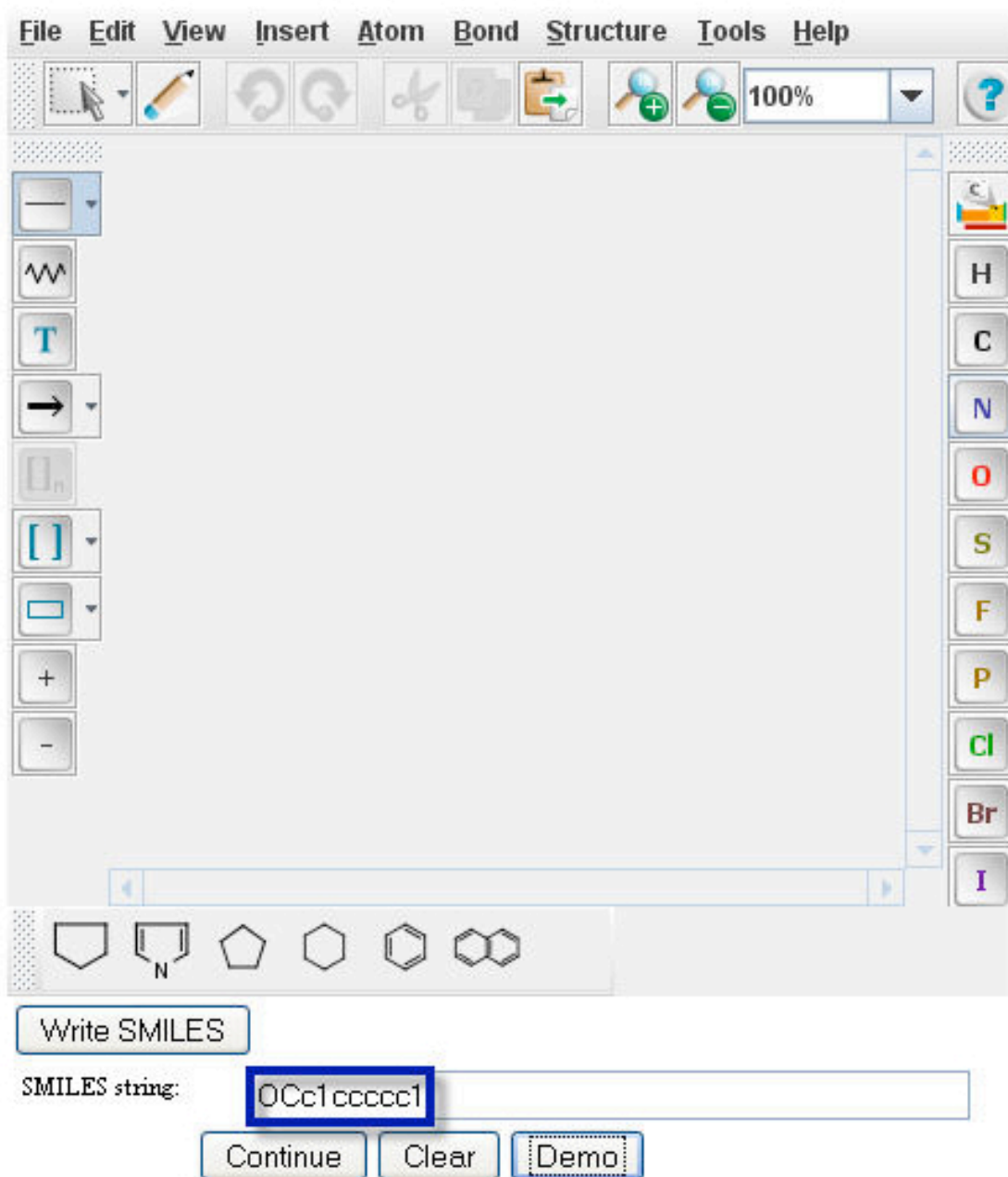
## DEMONSTRATION

### *Start the Demo*

The PPS provides a demonstration of how the system works using the compound Benzyl Alcohol. To access the demo, click on the **"Demo"** button located under the MarvinSketch window of the UM-BBD Pathway Prediction Page.



The Smiles string of Benzyl Alcohol will appear in the "**Smiles string**" box.



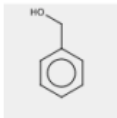
## Status Page


A user will be automatically taken to a prediction status page after clicking on the **"Demo"** button as shown above, or otherwise submitting a query compound, and clicking on the **"Continue"** button.

**UM-BBD: Pathway Prediction Results**

[[About](#)] [[Tips](#)] [[Not Predicted](#)] [[All Rules](#)]

---

Query:  Submitted: 2010.04.20 at 05:23:52 CDT  
In Progress: 4 seconds

 → Aerobically very likely transformation.

---

[[About](#)] [[Tips](#)] [[Not Predicted](#)] [[All Rules](#)]

This page was generated on 2010.04.20 at 05:23:52 CDT. (Job ID: 2010.04.20-05.23.39-56)

The query compound is shown in a grey square in upper left of the status page. The query submission time and the prediction run-time are shown next to the compound square. The prediction run-time is refreshed once a second. A system usage tip is displayed under the compound square. Different random tips are shown every five seconds. A list of all tips is available at: <http://umbbd.msi.umn.edu/servlets/ppstips.jsp>. A unique job id is shown at the bottom of the status page.

When the initial prediction on the query compound is finished, the system will bring a user to the Pathway Prediction Results page.

## Pathway Prediction Results

The Pathway Prediction Results page for Benzyl Alcohol is shown below using default prediction options. Each numbered grey square contains one compound. The default options are changeable throughout the prediction process as described under **Change Default Options** below.

From the Pathway Prediction Results page, a user is able to see the more likely aerobic transformations of Benzyl Alcohol based on the biotransformation rules found in the UM-BBD. The Navigation Bar "BBD Home > PPS Home > 1" permits quick navigation back to previous prediction steps and the PPS and BBD home pages. The Zoom feature to the right of the Navigation Bar allows the user to resize the prediction results as described in the Viewing and Printing page at: <http://umbbd.msi.umn.edu/predict/resize.html>. The prediction run-time is shown in the "Elapsed time" at the bottom of the results page.

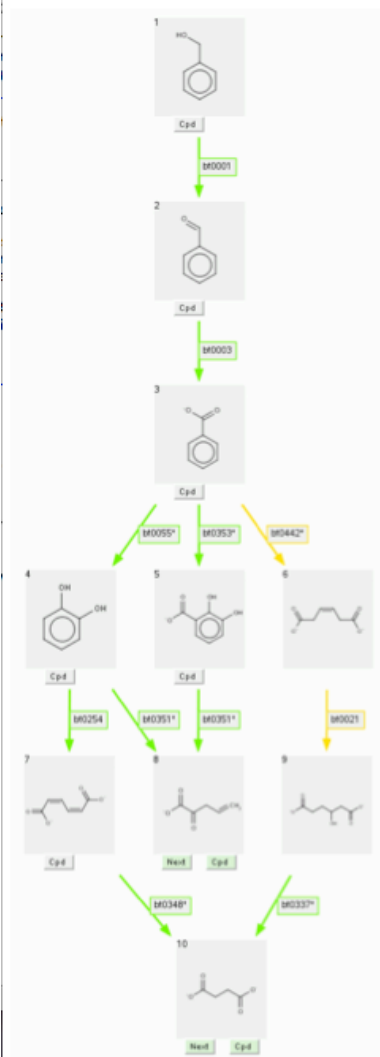
## UM-BBD: Pathway Prediction Results

[\[About\]](#) [\[Tips\]](#) [\[Not Predicted\]](#) [\[All Rules\]](#)

[BBD Home](#) > [PPS Home](#) > 1

[\[Zoom In\]](#) [\[Zoom Out\]](#) [\[Clear\]](#) [\[PDF\]](#) [\[?\]](#)

### The predicted pathway:



### Aerobic Likelihood:

■ Very likely ■ Likely ■ Neutral

### Prediction Options:

#### Show Biotransformations:

☒ Aerobic ☐ All

Show Levels:

Show Products in a Level:

Show Products containing "C":

#### Remove Products:

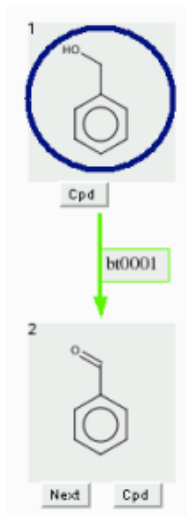
Enter compound numbers, separated by commas. [\(More\)](#)

Elapsed time: 13 seconds

## MarvinView

The user can click on any grey compound square in "The predicted pathway".

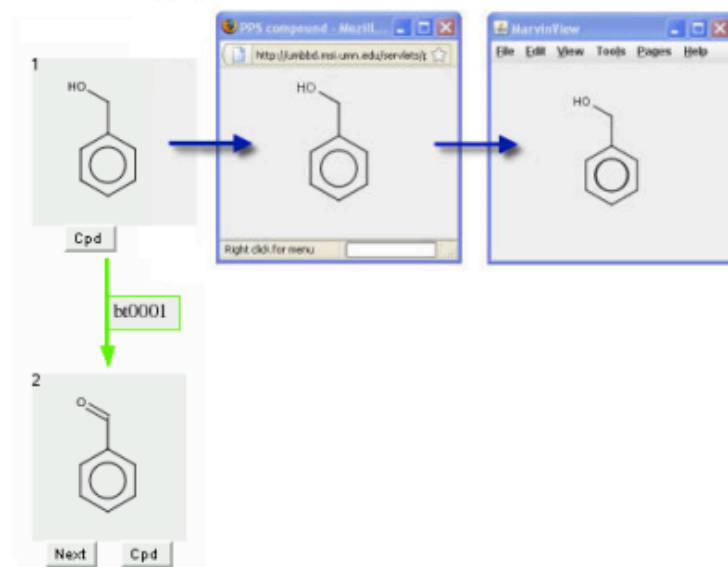
### The predicted pathway:



Clicking on a grey compound square will show the compound in a new window. The compound can be rotated in this window. The window can also be increased in size, to better view larger compounds. Double clicking in this new window will produce a MarvinView window. The MarvinView window can provide much additional information on the compound. Information on how to use it is available at:

<http://www.chemaxon.com/marvin/help/view/view-index.html>.

### The predicted pathway:



## Change Default Options

### Prediction Options:

Show Biotransformations:

☒ Aerobic ☐ All

Show Levels: 6 ▼

Show Products in a Level: 10 ▼

Show Products containing "C": 3+ ▼

Go!

By default, the PPS will show "Aerobic" biotransformations, show up to 6 levels, display compounds containing 3 or more carbon atoms, and stop before any level where there are more than 10 compounds. These default options are changeable throughout the prediction process, as described below.

### Aerobic Likelihood

Aerobic Likelihood is the likelihood that the reaction will occur under aerobic conditions, exposed to air, in soil (moderate moisture) or water, at neutral pH, 25°C, with no competing or toxic other compounds. Rules are assigned aerobic likelihood by two or more biodegradation experts. More information is available, <http://umbbd.msi.umn.edu/predict/rulepriority.html>.

The aerobic likelihood of a transformation is indicated by a color of an arrow that starts from one substrate to one or two products. Users are able to choose, before or after a compound undergoes transformation, if they will view all or only the aerobic likely transformations of a compound by selecting the appropriate button.

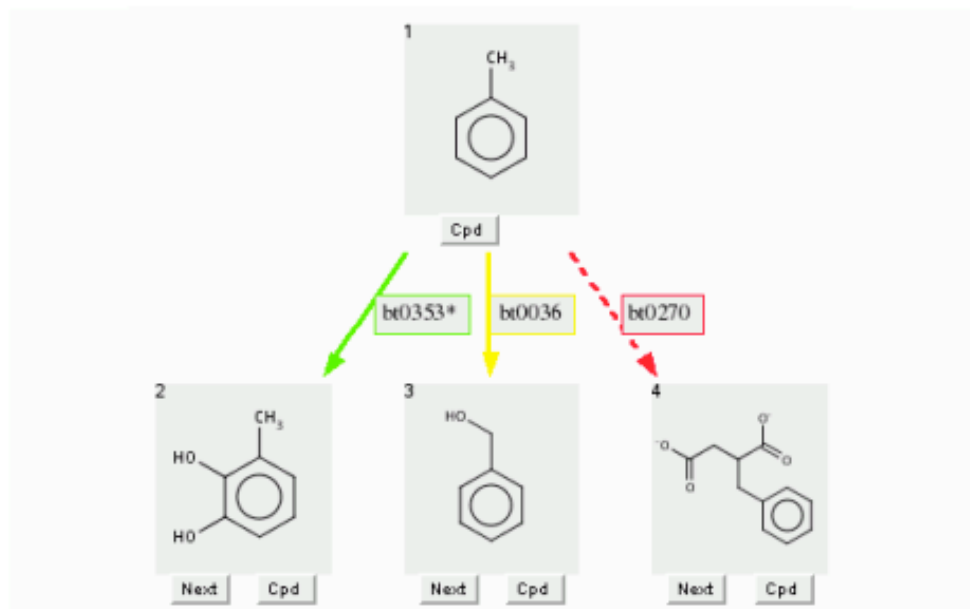
If the aerobic setting is chosen, and no very likely, likely, or neutral transformations, but some unlikely and/or very unlikely transformations, are found, the setting is automatically changed to "**All**" and these transformations are shown.

### Show Levels

By default, the system will predict up to 6 levels in the first step. The "**All**" choice is shown below for toluene, an immediate precursor of the benzyl alcohol used in the above examples, in a prediction set to 1 level. If "**Aerobic**" were chosen, only the first two choices (3-methylcatechol and benzyl alcohol) would be shown. When "**All**" is chosen, a third choice, succinate addition to the toluene methyl side chain, is displayed.



## The predicted pathway:



## Aerobic Likelihood:

■ Very likely 
 ■ Likely 
 ■ Neutral 
 ■ Unlikely 
 ■ Very unlikely 
 ■ Unknown

## Prediction Options:

Show Biotransformations:

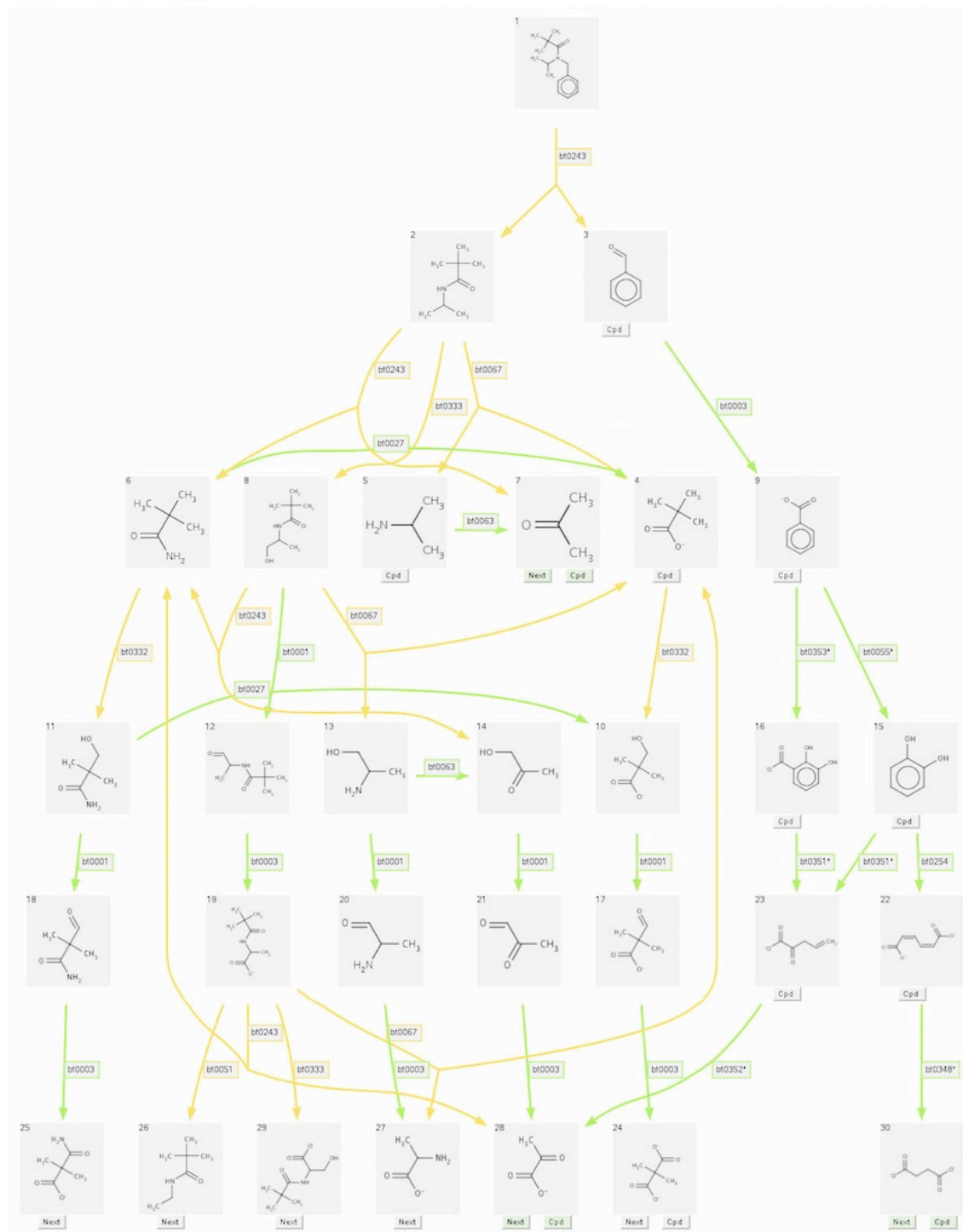
☐ Aerobic 
 ☒ All

Show Levels: 1

Show Products in a Level: 10

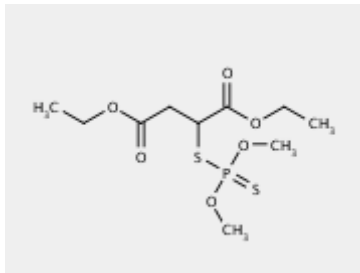
Some predictions are too complex to be displayed. If this occurs, the prediction is rerun with a decreased number of levels, and a message is displayed under the last compound row as shown below.

**The predicted pathway:**



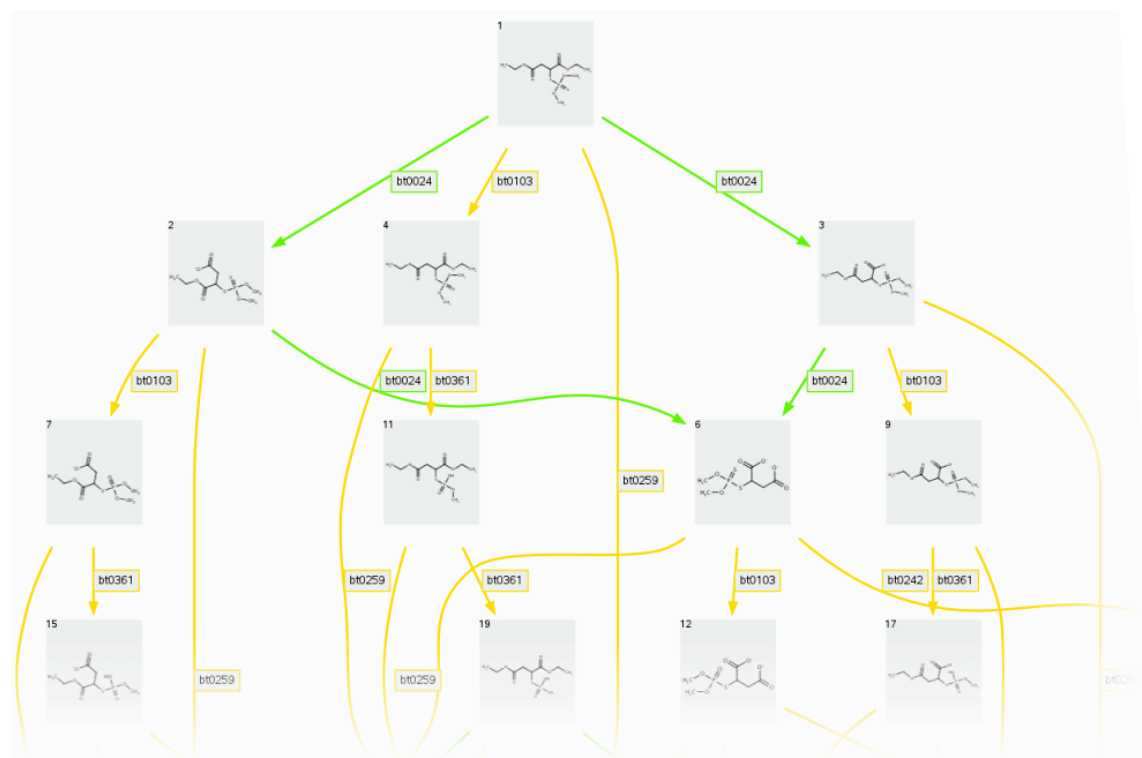
### Show Products Containing "C"

The next examples show predictions for the herbicide malathion [CCOC(=O)CC(C(=O)OCC)SP(=S)(OC)OC], a compound with many organic functional groups, including two ethyl esters.



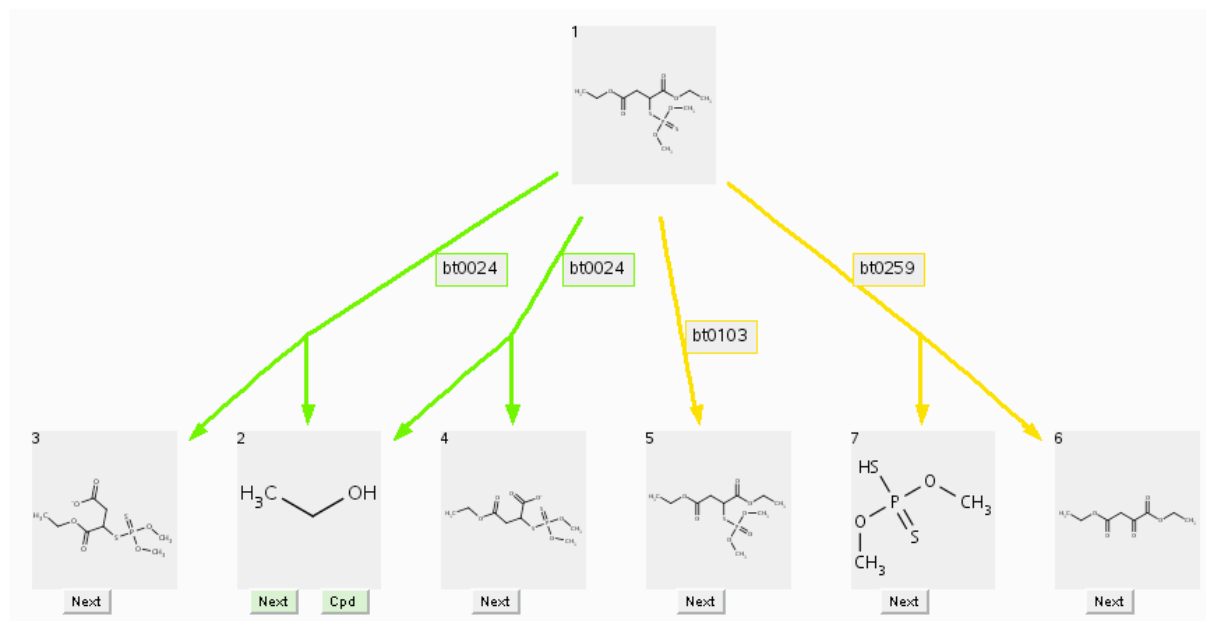
The first three levels of the prediction for malathion are shown below using default prediction options.

#### The predicted pathway:



By default, the system will only display compounds containing 3 or more carbon atoms. A user can change this minimum number of carbon atoms to view more or fewer compounds. In the malathion prediction shown above, the ethanol cleaved by bt0024 are not displayed using the default settings. The 1-level prediction for malathion with an option to show 2 or more carbon atoms, which does show the missing ethanol, is shown below.

### The predicted pathway:



Cleavage compounds (Compounds 2 and 3, Compounds 2 and 4, Compounds 6 and 7) are indicated by two tailed arrows. Duplicate compounds (ethanol in this example) are removed and only one (Compound 2) is left, pointed to by multiple arrows.

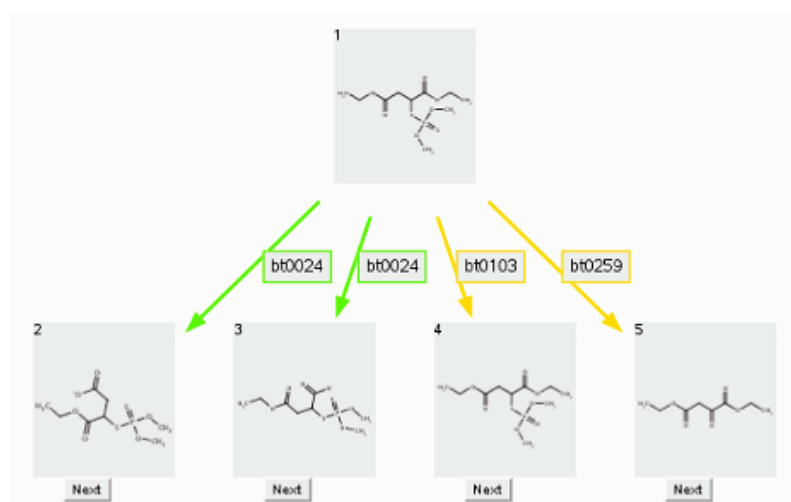
An exception to “Show compounds containing above a threshold number of carbon atoms” occurs when the parent compound is one carbon or less above the threshold. In those cases, compounds with one or more carbons are shown.

### Show Products on a Level

By default, the system will display up to 10 compounds on a level and stop before any level where the number of compounds exceeds this threshold. If a prediction is stopped due to the threshold, a message will be shown under **"The predicted pathway"**. All compounds in the very first level of any prediction step will be shown, even if they exceed the threshold.

A user can decrease or increase the threshold value. Shown below is the prediction for malathion, limited to no more than 5 compounds.

### The predicted pathway:

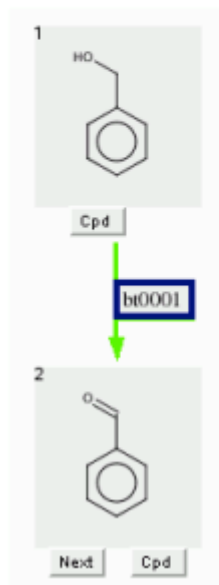


\* Predicted products not shown at level 2 (14 products). No more than 5 products are allowed to continue the prediction.

## Rule Button

The demo provides the user with the ability to click up to three buttons for each transformation. One of these, always shown, is the "**Rule**" button. The "**Rule**" button is found as the label of an arrow that represents a predicted transformation.

## The predicted pathway:



Clicking the "**Rule**" button will open a new browser window containing the rule page of the biotransformation rule associated with the specific reaction. The Biotransformation rule page provides a user with links to the PPS, a list of All BTrules, and the UM-BBD Main Menu. It also provides one or more descriptions of the type(s) of reactions handled by the rule, the likelihood the reaction will occur under aerobic conditions, a list of UM-BBD reactions that exemplify the rule, staff comments, similar biotransformation rules (if any), and a way for the user to provide comments. A list of all rules the system uses is available. More information about rules is available in "**About the BBD**," <http://umbbd.msi.umn.edu/aboutBBD.html#btrule>

## Rule bt0001

[\[Pathway Prediction Engine\]](#) [\[All Rules List\]](#) [\[BBD Main Menu\]](#)



primary Alcohol -> Aldehyde

**Aerobic Likelihood:**  Likely

### UM-BBD Reaction(s):

[Benzyl alcohol -----> Benzaldehyde \(reactID# r0267\)](#)  
[cis-3-Chloro-2-propene-1-ol -----> cis-3-Chloroallyl aldehyde \(reactID# r0691\)](#)  
[trans-3-Chloro-2-propene-1-ol -----> trans-3-Chloroallyl aldehyde \(reactID# r0690\)](#)  
[2-Chloroethanol -----> Chloroacetaldehyde \(reactID# r0002\)](#)  
[2,2-bis\(4'-Chlorophenyl\)ethanol \(DDOH\) -----> bis\(4'-Chlorophenyl\)acetate \(DDA\) \(reactID# r0518\)](#)  
[Citronellol -----> Citronellal \(reactID# r1155\)](#)  
[p-Cumic alcohol -----> p-Cumic aldehyde \(reactID# r0393\)](#)  
[2,3-Dihydroxy-2-methyl propionate -----> 2-Hydroxy-2-methyl-1,3-dicarbonate \(reactID# r0620\)](#)  
[1-Dodecanol -----> Dodecanal \(reactID# r0603\)](#)  
[Ethanol -----> Acetaldehyde \(reactID# r0172\)](#)  
[Geraniol -----> Geranial \(reactID# r1163\)](#)  
[1-Hydroxy-4,4-dimethylpentan-3-one -----> 4,4-Dimethyl-3-oxopentanal \(reactID# r1308\)](#)  
[3-Hydroxybenzyl alcohol -----> 3-Hydroxybenzaldehyde \(reactID# r0400\)](#)  
[6-Hydroxyhexanoate -----> 6-Oxohexanoate \(reactID# r0174\)](#)  
[1-Hydroxymethylnaphthalene -----> 1-Naphthaldehyde \(reactID# r0786\)](#)  
[2-Hydroxymethylnaphthalene -----> 2-Naphthaldehyde \(reactID# r0771\)](#)  
[2,2-bis\(4-Hydroxyphenyl\)-1-propanol -----> 2,2-bis\(4-Hydroxyphenyl\)-propanoic acid \(reactID# r0863\)](#)  
[4-Hydroxytoluene -----> 4-Hydroxybenzaldehyde \(reactID# r0272\)](#)  
[Methanol -----> Formaldehyde \(reactID# r0238\)](#)  
[Methyl fluoride -----> Formaldehyde \(reactID# r0344\)](#)  
[2-Methyl-2-hydroxy-1-propanol -----> 2-Hydroxyisobutyrate \(reactID# r0616\)](#)  
[2-Methylbenzyl alcohol -----> 2-Methylbenzaldehyde \(reactID# r0221\)](#)  
[3-Methylbenzyl alcohol -----> 3-Methylbenzaldehyde \(reactID# r0213\)](#)  
[p-Methylbenzyl alcohol -----> p-Tolualdehyde \(reactID# r0176\)](#)  
[Myrtenol -----> Myrtenal \(reactID# r0710\)](#)  
[1-Octanol -----> 1-Octanal \(reactID# r0022\)](#)  
[Perillyl alcohol -----> Perillyl aldehyde \(reactID# r0729\)](#)  
[Pivalate -----> Dimethylmalonate \(reactID# r1038\)](#)  
[4-Sulfobenzyl alcohol -----> 4-Sulfobenzaldehyde \(reactID# r0291\)](#)  
[Trichloroethanol -----> Trichloroacetate \(reactID# r0489\)](#)  
[2,4,4-Trimethyl-1-pentanol -----> 2,4,4-Trimethylpentanal \(reactID# r1270\)](#)  
[Vanillyl alcohol -----> Vanillin \(reactID# r0651\)](#)

### Comments:

Does NOT handle alcohols when the vincinal carbon is halogenated. Rule is blocked from acting on CoA.

### Similarities:

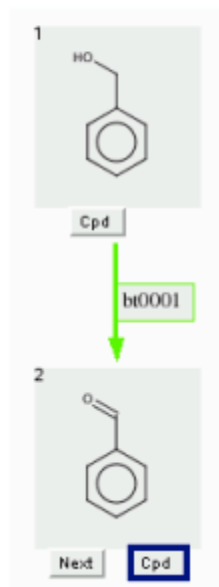
[bt0002](#): secondary Alcohol -> Ketone

[bt0314](#): primary Alcohol with halogen on the same carbon -> Aldehyde

### ***Cpd Button***

Another button is the "**Cpd**" button, located in the bottom of an individual compound square. The "**Cpd**" button does not appear on every transformation (only on compounds found in the UM-BBD).

### **The predicted pathway:**

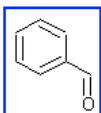




Clicking the "**Cpd**" button will open a new browser window containing the compound page of a biotransformation. The compound page provides a user with a graphic image of the compound, its chemical formula, molecular weight, SMILES string, and links to reaction pages in the UM-BBD where the compound is either the substrate or product. More information about compound pages is available in "**About the BBD.**"

<http://umbbd.msi.umn.edu/aboutBBD.html#compound>

## Benzaldehyde



- Formula: C<sub>7</sub>H<sub>6</sub>O
- MW: 106.12
- SMILES String: O=Cc1ccccc1
- CAS Reg. 100-52-7
- [PubChem Substance Entry](#)
- [National Toxicology Program](#)
- UM-BBD reactions whose *product* is **Benzaldehyde**
  - [Benzoylformate](#) -----> [Benzaldehyde \(reacID# r1049\)](#)
  - [Benzyl alcohol](#) -----> [Benzaldehyde \(reacID# r0267\)](#)
  - [Benzyl sulfide](#) -----> [Benzaldehyde + Benzyl mercaptan \(reacID# r1013\)](#)
- UM-BBD reactions whose *substrate* is **Benzaldehyde**
  - [Benzaldehyde](#) -----> [Benzoate \(reacID# r0269\)](#)

---

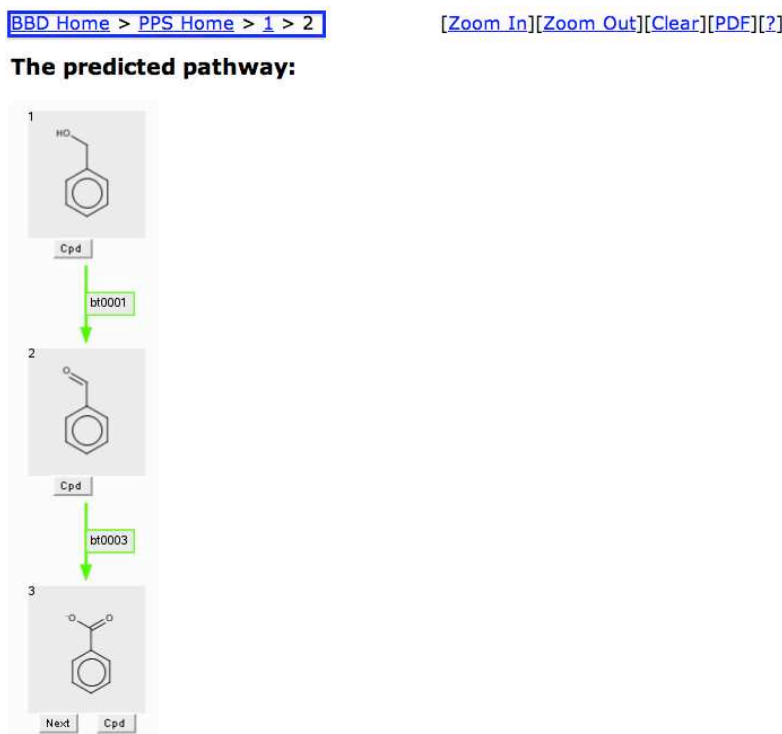
[\[Toluene\]](#) [\[Benzyl Sulfide\]](#) [\[Mandelate\]](#) [\[BBD Main Menu\]](#)

## Next Button

The **"Next"** button is also located in the bottom of an individual compound square, to the left of the **"Cpd"** button if one is present.



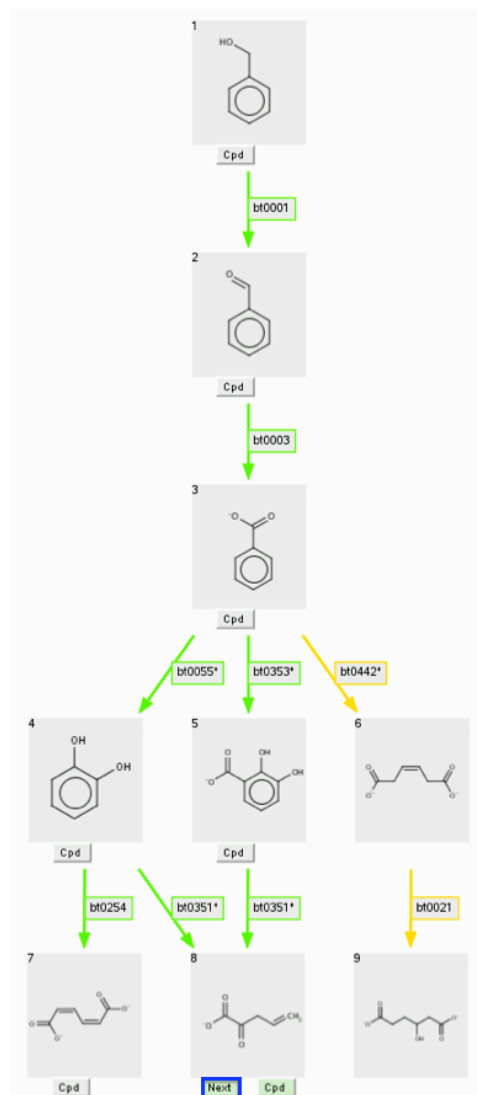
To continue the pathway, select the **"Next"** button to start another transformation cycle. The **Navigation Bar** will then expand to "BBD Home > PPS Home > 1 > 2" for easy navigation to previous PPS prediction pages, or BBD or PPS Home pages. The product selected will appear as an intermediate compound in the predicted pathway starting from the original compound. The colored arrow indicates the aerobic likelihood of the biotransformation that connects two compounds.



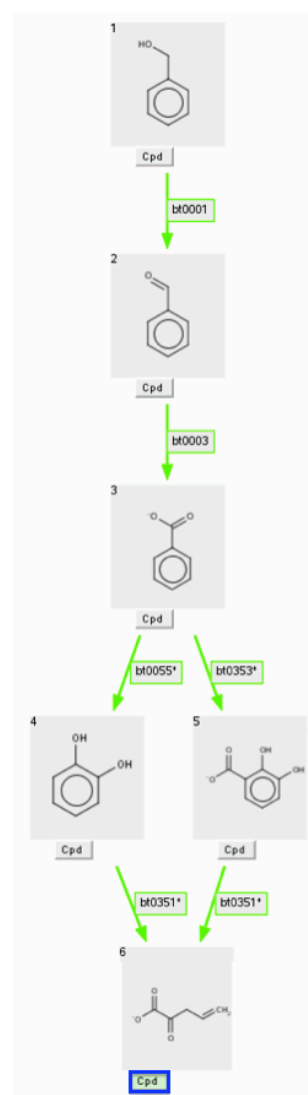
### Green Next or Cpd Button

After several cycles of the prediction process, you might see a green-shaded version of the “**Next**” button (left below) or “**Cpd**” button (right below).

The predicted pathway:



The predicted pathway:



Clicking on the “**Green Next**” button will redraw the prediction showing only the selected branch (above left → above right). The “**Green Cpd**” button indicates that this compound is found in a KEGG pathway. Clicking the “**Green Cpd**” button brings a user to a KEGG pathway web page. Alternatively, a user may choose to continue prediction by clicking on a non-green “**Next**” button, if one is present.

## Remove Products

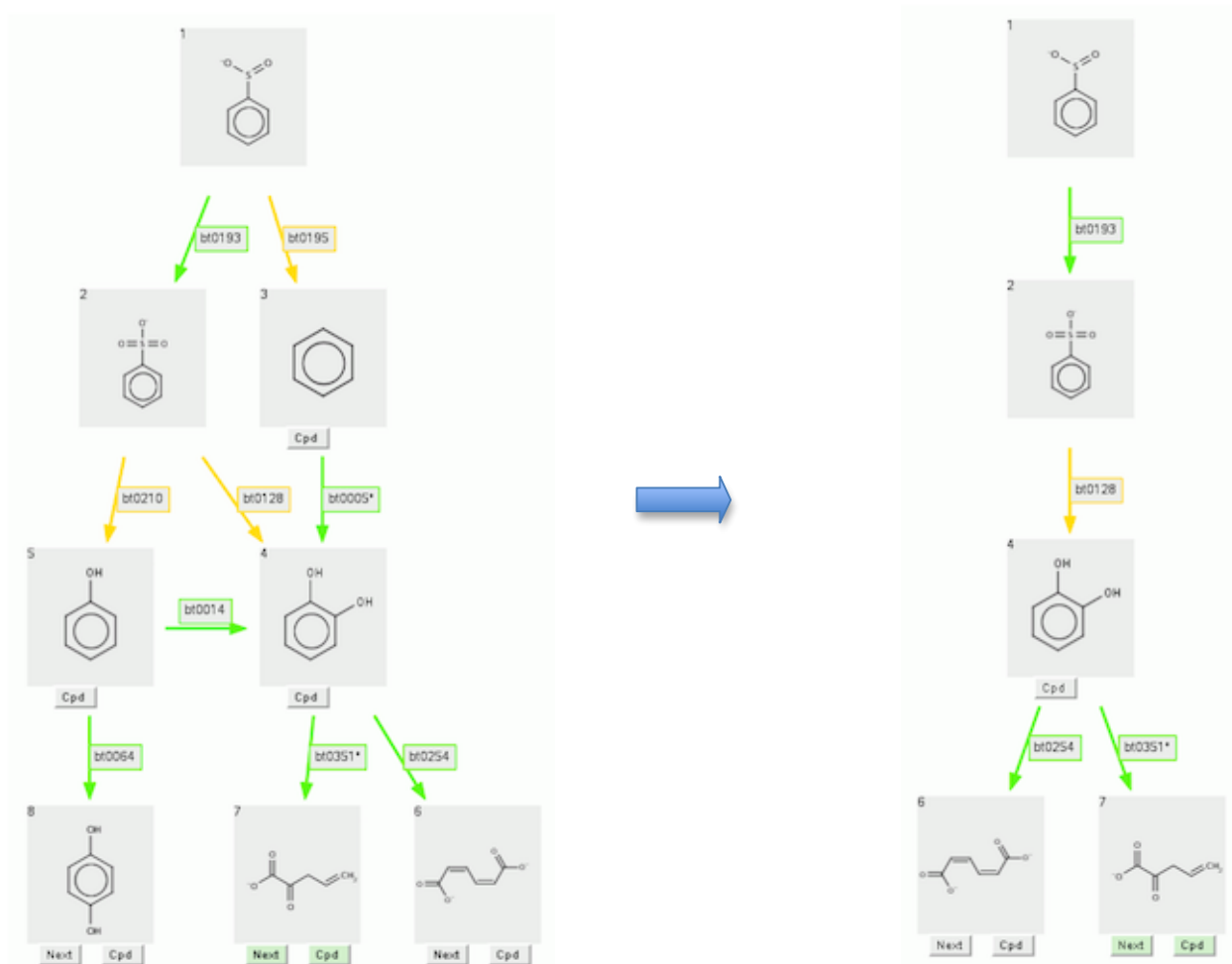
As shown above, when the Next button is clicked, the new pathway contains that compound and the pathway branch or branches that produced it. That is, other predicted compound squares and rule arrows are removed. The “Remove Products:” option, at the bottom of a prediction, allows more control over compound removal.

### Remove Products:

Enter compound numbers, separated by commas. [\(More\)](#)

Go!

Compounds are removed by entering their numbers (the small number shown in the upper left of each grey compound square), separated by commas, in the “Remove Products:” box, and then clicking on the “Go!” button below the box. The starting compound (compound 1) cannot be removed. The [\(More\)](#) link will open this section of the UM-PPS help webpage in a separate window.



For example, above left is the 3-level prediction for benzenesulfinate. If it is desired to remove the product benzene in level 1 (product 3) and phenol in level 2 (product 5), these products and all compound boxes and rule arrows following them are removed by entering “3,5” (or “5,3”) in the “Remove Products:” box, and clicking the “Go!” button.

**Remove Products:**  
 Enter compound numbers, separated by commas. [\(More\)](#)

The partial prediction is shown above right. To return to the original prediction, click on the “Show Original” button, to the right of the “Go!” button after a partial prediction has been made.

**Remove Products:**  
 Enter compound numbers, separated by commas. [\(More\)](#)

Once back at the original, you can return to the partial prediction by clicking on the “Show Partial” button, in the same position as the “Show Original” button. Compounds in a partial prediction retain the same numbers as in the original prediction. Since some compounds were removed, there are gaps in the number sequence.

Removing compounds can be done in multiple steps, without returning to the original prediction. In the above example, you can get to the same result by first choosing to remove compound 3 (or 5), and, after reviewing the result, choosing to remove compound 5 (or 3). If you return to the original prediction, you can remove different compounds to create a new partial prediction. If a previous partial prediction exists, the new one overwrites it.

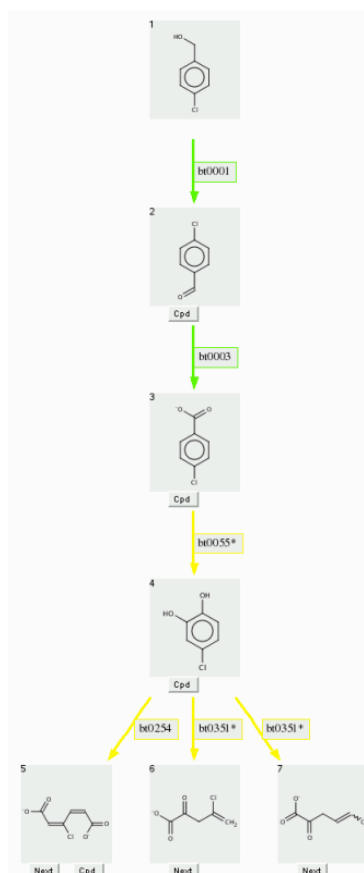
Zoom In, Zoom Out, and PDF buttons work in a partial prediction the same way as in the original. Clicking the Clear button in a partial prediction returns to the original. Compound, Rule and Next buttons work in a partial prediction as in the original. If the Next button is clicked in a partial prediction, the Next step in the prediction will be that of the original, not the partial, prediction.

## Variable Aerobic Likelihood

Some rules handle a wide range of compounds, and a single aerobic likelihood is not appropriate for all of them. Thus structure-based variable aerobic likelihood has been added to the PPS. For aerobically likely aromatic ring monooxygenation, dioxygenation, cleavage, and decarboxylation rules, when the substrate contains one or more halogens, the aerobic likelihood for the transformation is changed to "neutral".

Compare the previous predicted pathway for benzyl alcohol, with the pathway below for *p*-chlorobenzyl alcohol. The aerobic likelihoods for the first three transformations are likely, as above. However when the ring is oxygenated and cleaved, the aerobic likelihoods are neutral for the chlorinated compound, rather than the likely found for the non-halogenated compound.

The predicted pathway:



A second use of variable aerobic likelihood is for nitro groups. Aerobically likely or neutral rules for oxidation of aliphatic carbons have been changed to unlikely when the chain contains one or more nitro groups.

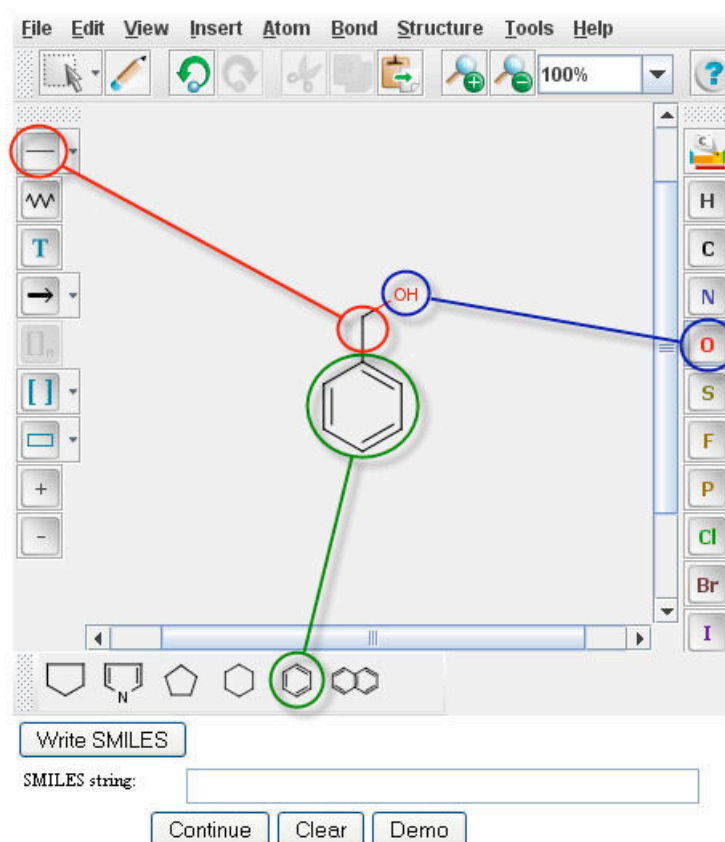
## Super Rules

Super rules include two or more contiguous biotransformation rules that form a small pathway of their own. They are indicated with asterisk. For example, bt0055 and bt0351 are super rules shown on the Figure in **Variable Aerobic Likelihood** section above.

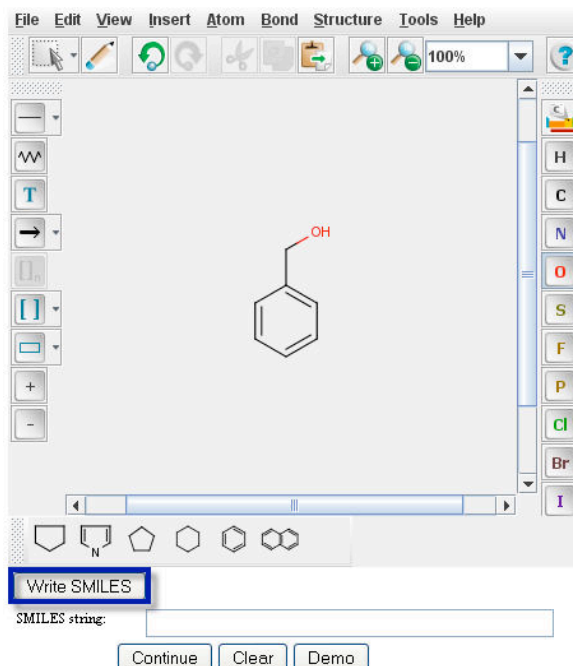
## DRAWING STRUCTURES

The PPS uses Chemaxon's MarvinSketch for drawing compounds. Start from the PPS main page. To draw Benzyl Alcohol in the MarvinSketch window, select the "Benzene Ring" from the lower tool bar menu. Drag the structure to the desired location in the window and click to paste. Next select the "single bond" button from the left tool bar (for more options; e.g., double bond, or single bond up, click and hold the **v** to the right of the "single bond" button). With the "single bond" selected, click a corner of the benzene ring, drag the bond in the desired direction and release to paste. With the "single bond" still selected, click the methyl group, drag in the desired direction, and release to create a two carbon chain. To make the compound an alcohol, select the atomic symbol for oxygen, "O", from the right menu bar. Click on the methyl group to replace it with a hydroxide. A Marvin Sketch tutorial is available at

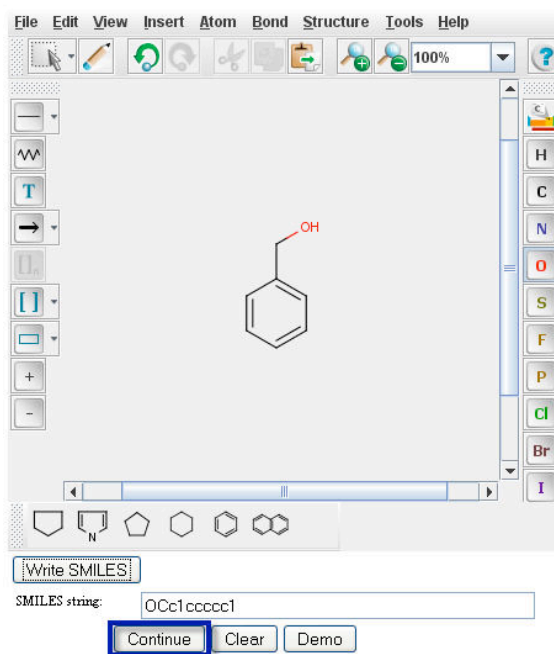
<http://www.chemaxon.com/jchem/marvin/chemaxon/marvin/help/about-sketch.html>.



After creating an image image in the MarvinSketch window, a user next generates the SMILES string for that specific compound, by clicking the **"Write SMILES"** button located beneath the MarvinSketch window.



The SMILES string will appear in the **"Smiles string:"** window directly underneath your structure.



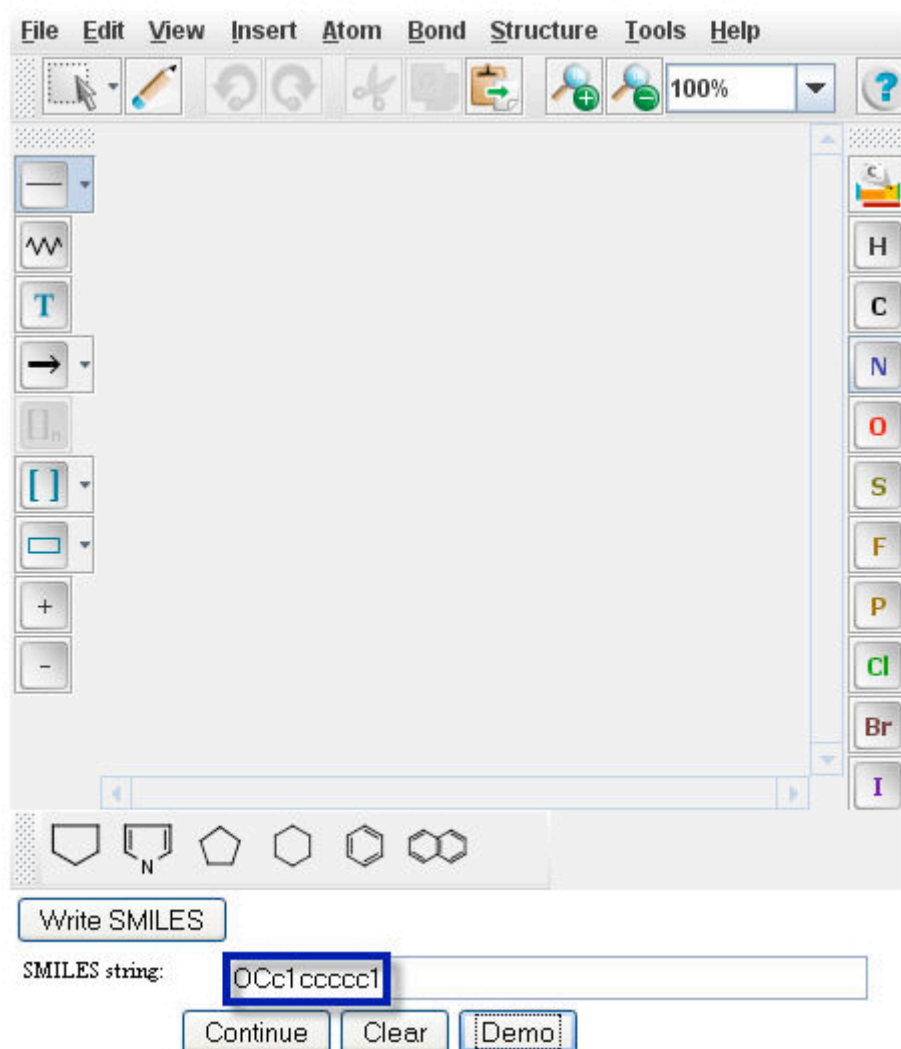
Click on the **"Continue"** button to proceed to **"Pathway Prediction Results"** for Benzyl Alcohol (page 4).



## ENTERING SMILES STRINGS

If you know the SMILES string for your compound, you can instead enter a SMILES string directly. A SMILES string is an alphabetical representation of a compound. The SMILES string format is described on the SMILES Home Page from Daylight Chemical Information Systems, Inc. <http://www.daylight.com/smiles/>

As a demonstration, type or paste the SMILES string of Benzyl Alcohol, OCc1ccccc1, into the "**Smiles string**" window.



Click on the "**Continue**" button to proceed to "**Pathway Prediction Results**" for Benzyl Alcohol (page 4).

## FOR FURTHER INFORMATION OR TO MAKE COMMENTS

To receive periodic progress reports, join the UM-BBD email list.

<http://lists.umn.edu/cgi-bin/wa?SUBED1=um-bbd&A=1>

Comments related to the database are appreciated. Our users are encouraged to contribute compound, reaction, and/or pathway information to the UM-BBD. To make comments or request more information "Contact Us".

<http://umbbd.msi.umn.edu/contact.html>

## BIBLIOGRAPHY

Gao J, Ellis LB, Wackett LP. (2011) "The University of Minnesota Pathway Prediction System: multi-level prediction and visualization." *Nucleic Acids Research*, **39** Suppl 2: W406-11.

Wicker, J., Fenner, K., Ellis, L.B.M., Wackett, L.P., Kramer, S. (2010) "Predicting Biodegradation Products and Pathways: A Hybrid Knowledge-Based and Machine Learning Based Approach" *Bioinformatics*, **26**: 814-21.

Gao, J., Ellis, L.B.M., and Wackett, L.P. (2010) "The University of Minnesota Biocatalysis/Biodegradation Database: improving public access" *Nucleic Acids Research*, **38**: D488-D491.

Fenner, K., Gao, J., Kramer, S., Ellis, L.B.M., Wackett, L.P. (2008) "Data-driven extraction of relative reasoning rules to limit combinatorial explosion in biodegradation pathway prediction." *Bioinformatics*, **24**: 2079 - 2085.

Ellis, L.B.M., Gao, J., Fenner, K., Wackett, L.P. (2008) "The University of Minnesota pathway prediction system: predicting metabolic logic." *Nucleic Acids Research*, **36**: W427-W432.

Ellis, L.B.M., Roe, D., Wackett, L.P. (2006) "The University of Minnesota Biocatalysis/Biodegradation Database: The First Decade" *Nucleic Acids Research*, **34**: D517-D521.

Hou, B.K., Ellis, L.B.M., Wackett, L.P. (2004) "Encoding Microbial Metabolic Logic: Predicting Biodegradation" *Journal of Industrial Microbiology and Biotechnology*, **31**: 261-272.

Hou, B.K., Wackett, L.P., Ellis, L.B.M. (2003) "Predicting Microbial Catabolism: A Functional Group Approach" *Journal of Chemical Information and Computer Sciences*, **43**: 1051-1057.