

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

GREEN ALTERNATIVES WIZARD HELP GUIDE

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1. PURPOSE OF THE DATABASE

The Green Alternatives Wizard is a database designed to provide easy and quick access to information about available chemical alternative to hazardous solvents. It was designed with the understanding that finding the ideal, green drop-in replacement for hazardous solvents does not work for every situation. The alternatives provided, however, do present a starting point for researchers to consider alternative methods to their own research that would reduce, if not eliminate, the use of a particular hazardous solvent. In many instances, the alternative chemicals or processes provided still have their own disadvantages that need improvements—as such, information about the advantages and disadvantages of chemical alternatives are also provided.

2. SEARCH CATEGORIES

A user can search by Chemical to Replace, Process to Replace (or modify), Alternative Chemical, or Alternative Process.

Chemical to Replace: By initially choosing a *Chemical to Replace*, clicking *Continue*, selecting a chemical from the drop-down menu, and clicking *Continue*, the database returns a result list of possible alternative chemicals and/or alternative processes that can be used to eliminate or reduce the use of the chosen chemical.

- For example, choosing carbon tetrachloride as a *Chemical to Replace* would return a list of alternative chemicals or processes that could be used to reduce, if not eliminate, the use of carbon tetrachloride.

Process to Replace: By initially choosing *Process to Replace*, clicking *Continue*, selecting a process from the drop-down menu, and clicking *Continue*, the database returns a result list of possible alternative chemicals and/or alternative processes that can be used to avoid or modify the process to avoid hazardous conditions or reduce the use of hazardous chemicals.

- For example, choosing flash chromatography as a *Process to Replace* would return a list of alternative chemicals or process that could be used to either avoid the use of flash chromatography or reduce the generation of hazardous wastes from flash chromatography.

Alternative Chemical: By initially choosing *Alternative Chemical*, clicking *Continue*, selecting a chemical from the drop-down menu, and clicking *Continue*, the database returns a search list of the chemicals and/or processes that can be replaced or modified by the chosen *Alternative Chemical*.

- For example, choosing ionic liquids as an *Alternative Chemical* would return of a list of the chemicals and processes that can be replaced or modified by ionic liquids to reduce, if not eliminate, the use of hazardous chemicals.

Alternative Process: By initially choosing *Alternative Process*, clicking *Continue*, selecting a process from the drop-down menu, and clicking *Continue*, the database returns a search list of the chemicals and/or processes that can be replaced or modified by the chosen *Alternative Process*.

- For example, choosing solvent-free reactions as an *Alternative Process* would return a list of the chemicals and processes that can be replaced or modified by a solvent-free reaction to reduce, if not eliminate, the use of a hazardous solvent.

3. HOW THE DATABASE WORKS

Information in this database is inputted based on the reference information available for a certain chemical or process. All references associate a chemical or process with an alternative. As such, a search starting at *Chemical to Replace* or *Alternative Chemical* may return the same references.

Drop-down menus: Information for alternatives for a certain chemical or process, are predetermined and accessed through a drop-down menu. The drop-down menu appears after choosing a method to search, i.e. *Chemical to Replace*, *Process to Replace* (or modify), *Alternative Chemical*, or *Alternative Process*. When a chemical or process is selected, click *Continue*.

Search results list: The *Search Results* page returns a list of chemicals and processes that have been associated through the chosen chemical/process through a reference. Choosing a chemical or process from a drop-down menu in a search by *Chemical to Replace* or *Process to Replace* returns a search results list of possible alternatives identified through one or more references. Choosing a chemical or process from a drop-down menu in a search by *Alternative Chemical* or *Alternative Process* returns a search results list of the chemicals or processes that the chosen alternative can be used to replace.

Descriptions: By clicking on the chemical or process within the *Search Results* list, the descriptions of the chemical or process appear in the right-side window. The pros and cons of alternative chemicals are also included in the description.

Get References: Clicking on *Get References* returns a list of the titles of references under the *Relevant References* window on the left side of the screen. These references specifically associate an alternative with a chemical or process.

Reference Description: By clicking on a reference title listed under *Relevant References*, full reference details appear in the right-side window. This window includes all or some of the following:

- Author
- Journal Reference (or citation for patents, white papers, etc.)
- URLs to information available online
- Article summary of the reference that explains how an alternative can be used to reduce or eliminate the use of a hazardous chemical or process.

Filtering: On the screen of the *Search Results* page, a filtering option is available in the bottom right hand corner of the wizard. By inputting terms to in the filter and clicking on *Filter Further*, the database searches through the descriptions, reference titles, and article summaries associated with each chemical or process in the search result list. The chemicals

or processes that had the filter term appear in its description, its associated reference titles, or the article summaries of its associated reference titles are returned.

Emailing: On the *Search Results* page, an *Email Results List* button in the bottom right hand corner of the screen can be clicked to email the URL for that page to an email address. On the *Relevant References* page, an *Email References* button in the bottom right hand corner of the screen can be clicked to email the URL for that page to an email address.

Printing: On the *Search Results* or *Relevant References* page, a *Print* button appears on the bottom right hand side of the screen. This can be used to print either the search results on the *Search Results* list or the references on the *Relevant References* page.

Ordering: By clicking on a chemical or process returned in the search results list on the *Search Results* page, a *Go to Ordering* button appears in the bottom right hand corner of the screen. Clicking on this button returns links to the chemical ordering process through SciQuest, VWR, or SAPweb.

4. TUTORIAL

This tutorial leads you through a search by *Chemical to Replace* for an alternative for dichloromethane, also called methylene chloride.

SCREEN 1 : Choose 'Chemical to Replace' and click 'Continue'

The screenshot shows a Microsoft Internet Explorer browser window displaying the "Green" Alternatives Wizard. The browser's address bar shows the URL <http://web.mit.edu/environment/academic/wizard/greenChemWiz5.html>. The page title is "Green" Alternatives Wizard. On the left, there is a logo of a flask with a blue liquid and green leaves. The main content area is titled "Choose your starting point" and "Start searching by:". There are four radio button options: "Chemical to Replace" (which is selected), "Process to Replace", "Alternative Chemical", and "Alternative Process". Below these options is a "Continue" button. To the right of the options, there is explanatory text: "The purpose of this database is to provide information on alternatives to hazardous chemicals or processes." followed by three paragraphs of examples for each option. At the bottom of the page, there is a "Help?" button and a line of text: "If you have any comments, questions, and/or are interested in participating in this project please email us at greenchem@mit.edu."

input - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Forward Stop Home Search Favorites Refresh Print Mail News RSS Feeds

Address <http://web.mit.edu/environment/academic/wizard/greenChemWiz5.html>

Google Search 0 blocked Check AutoLink AutoFill Options

"Green" Alternatives Wizard X Exit



Choose your starting point
Start searching by:

- Chemical to Replace
- Process to Replace
- Alternative Chemical
- Alternative Process

The purpose of this database is to provide information on alternatives to hazardous chemicals or processes.

If you are looking to replace a chemical, click **Chemical to Replace**.
e.g. Replacing carbon tetrachloride with cyclohexane.

If you are looking to modify or replace a process, click **Process to Replace**.
e.g. Avoiding the use of flash chromatography with polymer immobilized solvents.

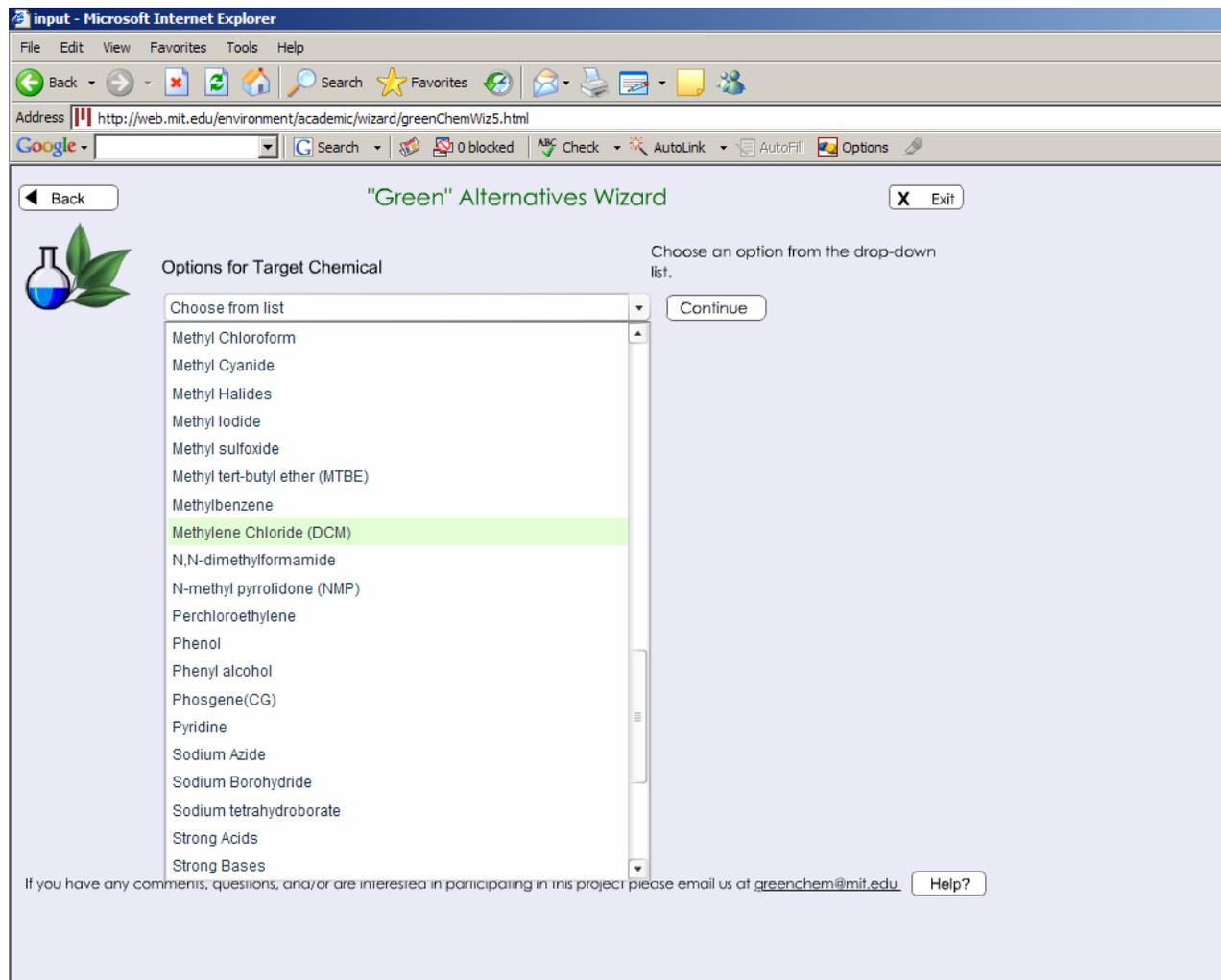
If you want more information about less hazardous, alternative chemicals, click **Alternative Chemicals**.
e.g. Learning more about supercritical fluids.

If you want more information about less

If you have any comments, questions, and/or are interested in participating in this project please email us at greenchem@mit.edu

TUTORIAL

SCREEN 2: Use the drop-down menu to choose dichloromethane and click 'Continue'



The screenshot shows a web browser window titled "input - Microsoft Internet Explorer". The address bar displays the URL: <http://web.mit.edu/environment/academic/wizard/greenChemWiz5.html>. The page content is titled "'Green' Alternatives Wizard" and includes a "Back" button and an "Exit" button.

On the left side, there is a logo of a flask with a green leaf. The main heading is "Options for Target Chemical". To the right of this heading, there is a prompt: "Choose an option from the drop-down list." Below this, there is a drop-down menu with the text "Choose from list" and a "Continue" button to its right.

The drop-down menu is open, showing a list of chemical alternatives. The following table represents the items in the list:

Chemical Alternative
Methyl Chloroform
Methyl Cyanide
Methyl Halides
Methyl Iodide
Methyl sulfoxide
Methyl tert-butyl ether (MTBE)
Methylbenzene
Methylene Chloride (DCM)
N,N-dimethylformamide
N-methyl pyrrolidone (NMP)
Perchloroethylene
Phenol
Phenyl alcohol
Phosgene(CG)
Pyridine
Sodium Azide
Sodium Borohydride
Sodium tetrahydroborate
Strong Acids
Strong Bases

At the bottom of the page, there is a footer text: "If you have any comments, questions, and/or are interested in participating in this project please email us at greenchem@mit.edu." and a "Help?" button.

TUTORIAL

SCREEN 3: Search results for alternatives for dichloromethane are listed. Processes are listed in blue; chemicals are listed in orange.

input - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Forward Stop Home Search Favorites Refresh Print Mail News RSS Options

Address <http://web.mit.edu/environment/academic/wizard/greenChemWiz5.html>

Google Search 0 blocked ABC Check AutoLink AutoFill Options

Back New Search "Green" Alternatives Wizard X Exit

Chosen Chemical or Process:
Methylene Chloride (DCM)

Click on found item to view full description.

Search Results

- Alumina Support
- Benzotrifluoride (BTF)
Also known as: Trifluorotoluene
- Catalytic Systems
- d-Limonene
- Dibasic Esters (DBE)
- Diethoxymethane (DEM)
Also known as: Formaldehyde diethylacetal
- Ethanol
- Ionic Liquids
- Lactate Esters
Also known as: Ethyl lactate

Legend: ■ =Process ■ =Chemical

Email Result List Print

Input information below to filter found data:

Filter Further

If you have any comments, questions, and/or are interested in participating in this project please email us at greenchem@mit.edu Help?

TUTORIAL

SCREEN 3: Click on the search result benzotrifluoride to view its description. Included in the description are pros and cons of the alternative and a link to 'Get References' appears. Click on 'Get References.'

input - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Address <http://web.mit.edu/environment/academic/wizard/greenChemWiz5.html>

Google Search 0 blocked ABC Check AutoLink AutoFill Options

Back New Search "Green" Alternatives Wizard X Exit

Chosen Chemical or Process:
Methylene Chloride (DCM)

Click on found item to view full description.

Search Results

- Alumina Support
- Benzotrifluoride (BTF)**
Also known as: Trifluorotoluene
- Catalytic Systems
- d-Limonene
- Dibasic Esters (DBE)
- Diethoxymethane (DEM)
Also known as: Formaldehyde diethylacetal
- Ethanol
- Ionic Liquids
- Lactate Esters
Also known as: Ethyl lactate

Description: Benzotrifluoride (BTF)

Benzotrifluoride (BTF, C₇H₅F₃) is a less toxic and more environmentally friendly alternative to tetrahydrofuran and methylene chloride.

Pros

- Less volatile
- Lower toxicity
- Relatively inert
- Stable in strongly basic conditions
- Non-ozone depleter
- Polarity between methylene chloride and ethyl acetate
- Dissolves organic compounds
- Miscible with organic solvents

Cons

- Prepared industrially from toluene

Email Result List Print Get Reference Go to Ordering

Input information below to filter found data:

Filter Further

Legend: ■ =Process ■ =Chemical

If you have any comments, questions, and/or are interested in participating in this project please email us at greenchem@mit.edu Help?

TUTORIAL

SCREEN 4: A list of reference titles appears. Click on a reference title to view reference description. Reference description includes authors, citation, URL (if applicable), and an article summary.

(Other options include clicking on 'Email References' to email a list of references to yourself, 'Print' to print the references, and 'Go to Ordering' to directly enter the purchasing system at MIT.)

input - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Forward Stop Refresh Home Search Favorites

Address <http://web.mit.edu/environment/academic/wizard/greenChemWiz5.html>

Google Search 0 blocked Check AutoLink AutoFill Options

Back New Search "Green" Alternatives Wizard X Exit

 Chosen Chemical or Process:
Methylene Chloride (DCM)

Found Chemical or Process:
Benzotrifluoride (BTF)

Click on Reference title to view full description.

Relevant References

Benzotrifluoride and derivatives: useful solvents for organic synthesis and fluorous synthesis

Benzotrifluoride: A Useful Alternative Solvent for Organic Reactions Currently Conducted in Dichloromethane and Related Solvents

Solvent Replacement for Green Processing

Details for: Benzotrifluoride: A Useful Alternative ...

Author: Ogawa, A. and Curran, D. P.

Journal Reference: J. Org. Chem. 1997, 62(3), 450-451.

URL:
http://pubs3.acs.org/acs/journals/doilookup?in_doi=10.1021/jo9620324

Article Summary: Benzotrifluoride has been used as a less volatile, low toxicity replacement for dichloromethane with similar yields. Three potential limitations for its use, however, its relatively high freezing point, sensitivity to electron transfer reductions, reactivity with strong Lewis acids, and sensitivity to hydrolysis by strong acids at high temperatures.

Email References Print Go to Ordering ►

If you have any comments, questions, and/or are interested in participating in this project please email us at greenchem@mit.edu Help?

5. FREQUENTLY ASKED QUESTIONS

How should I start my search?

Please read the description on the right of the first screen. Choose a search method and click *Continue*. If you are unsure of what to search by, see section 2.

Why can't I find what I'm looking for?

Make sure to scroll-down in the drop-down menus. Different search categories have different chemicals or processes listed in the drop-down menus. If what you are looking for still does not appear, it is probably not in the database. Please email greenchem@mit.edu so that this information can be inputted in the future.

What if the filter doesn't work?

Filters search through the text of chemical or process descriptions, reference titles, and article summaries. Exact word matches need to be made in order for a filtered result to appear; try synonyms.

What are the color codes?

In the *Search Results* list, blue results are processes; orange results are chemicals.

How come I can't see any descriptions?

Click on an item in the *Search Results* list to view descriptions.

How come I can't see any reference details?

Click on the reference titles to get more information.

How come I can't see the *Go to Ordering* button?

Click on an item in the *Search Results* list; the button should appear in the bottom right hand of your screen.

Why are there so many results but so few references?

Many references are associated with more than one chemical and/or process. Therefore, in many cases only one reference is returned for multiple chemicals or processes listed in the *Search Results* list.

Where do the references come from?

The references typically come from the scientific literature. A few references are from the United States Patent and Trademark Office, white papers, industrial cases studies, MIT case studies, and chemical vendors.

How were these references evaluated?

The references were reviewed for their direct applicability to our goal: reducing the generation of hazardous wastes.

Can a *Chemical to Replace* also be an *Alternative Chemical*?

Yes, hazardous chemicals that can be greener alternatives for even more hazardous chemicals are listed in the database. For example, toluene can be used to replace benzene.

What if my chemical has more than one name?

Multiple names of chemical compounds should all appear in the drop-down menus of the database. If not, please email greenchem@mit.edu.

CONTACT INFORMATION

Please contact greenchem@mit.edu with your comments, questions, or suggestions.

This database was created to be launched in June 2006.