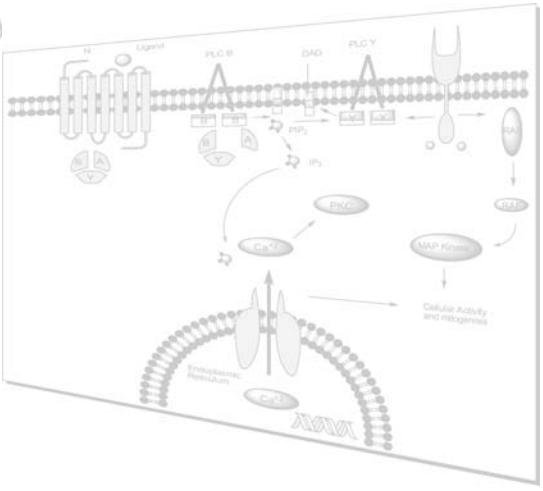
ChemACX Enterprise

Chem & Bio Office Enterprise 2008
Decision Support Platform
Enterprise 10

User Guide



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ChemACX

About this Guide

Welcome to the ChemACX User Guide. Inside this guide, you will find a full description of ChemACX, its features, and complete instructions on how to use them. This guide is available in print (this file), CHM, and Web-based format.

Overview

ChemACX (Available Chemicals Exchange) is a vast database of chemical products that are currently available from chemical manufacturers and distributors. The database featuring complete catalogs of major world suppliers of fine research, specialty, and industrial chemicals.

Opening ChemACX

1. To open ChemACX, type *http://servername* into your Web browser. The main ChemOffice Enterprise window appears.

NOTE: Servername is the name of the Chem Office Enterprise sever. For more information about your server, contact your system administrator.

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2. Click **ChemACX**. The ChemACX Query Input Form appears.

Searching ChemACX Catalogs

ChemACX is your guide to commercially available chemicals worldwide. Whether you are planning a bench synthesis, scale-up, or a commercial process, you can search these databases to determine the availability and sources for the chemicals you need.

You can search ChemACX by one or more of the following criteria:

- Chemical structure
- Chemical substructure
- Substance Name (text search)
- CAS Registry Number
- ACX Number
- Molecular Formula
- MolWeight Range
- Catalog Number

To search for information from ChemACX vendors:

1. Open **ChemACX**.
2. Enter the desired search criteria.
3. Select the appropriate search:

- If you would like to search over all of the vendors in ChemACX, select **Search all vendors**.
- If you would like to search over a previously generated list of favorite vendors, select **Search your favorite vendors**.
- If you want search results to include chemicals that do not have a vendor associated with them, select **Display all substances even if no vendors are found**.
- Click the **Search** button. The Search Results page appears.

For information about searching, see the ChemFinder section in the manual *Chem &*

Bio Office: Chem & Bio 3D, Finder, and Bio-Viz.

Searching Without the Plug-in

A ChemDraw plug-in is available from the ChemACX Query Input Form. With the plug-in installed, you can draw or paste a substructure drawings as a query parameter. If you do not need to use a substructure in you searches, you can simplify your query using only a chemical name or a CAS number.

To search without the plug-in:

1. In the advanced ChemACX query input form, click the **Click for Non-Plugin Search** button. The Non-Plug-in Search page appears.
2. Do one of the following:

If you want to search	Then
by chemical name	in the text box, enter a chemical name.
by CAS number	in the text box, enter a CAS number.
with the full query page, including structures and other criteria	click **Advanced Query with Plugin**.

1. Click the **Search** button. The Search Results page appears.

Favorite Vendors

You can also search for substances under a shorter list of preferred vendors. This shorted list helps to limit search results to include products from only your favorite vendors.

To create or edit a list of favorite vendors available to search under:

1. In the advanced ChemACX Query input form, click the **Edit Favorite Vendors List** button. The Vendor Selector box appears.

   NOTE: Your browser settings must allow pop-up windows to be displayed for the Vendor List to appear.

2. Select the checkbox next to any vendor that you want to include in the favorite list. To remove a vendor, deselect the checkbox.
3. Click the **Save as Preferred List** button. Your list of favorite vendors is saved and the Vendor Selector box closes.

Viewing Search Results

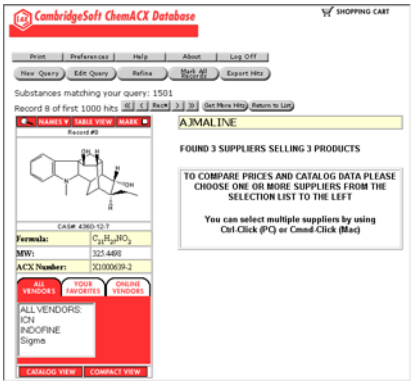
Similar to other ChemOffice Enterprise applications, search results can be viewed in two major formats: List View and Details View.

- List View lists all results in a compact manner, giving only summary information for each result. You are able to register and look up MSDX data from this view.
- Details view lets you view all information in the selected record. You can register and look up MSDX data from this view as well as add items to your shopping cart.

To view a record entry:

1. Search for a chemical.

2. To view vendors for a specific record, click its corresponding **Details** button. The detailed view appears.



3. Select one of the tabs: **All Vendors**, **Your Favorites**, or **Online Vendors**.
4. Highlight a vendor name in the list found in the tabs to display a catalog listing to the right. To display more then one vendor, hold down CTRL when highlighting vendor names.
5. Click **Catalog View** or **Compact View** to modify how the vendor information is displayed.
6. In the list, select the checkbox next to **add to cart** and enter a quantity. The order is added to your Shopping Cart.

7. To view the full catalog listing for a specific vendor, select **Catalog View** and click **Catalog Details**. A new window will appear displaying the catalog entry for the chemical you selected.
8. In the list, select the checkbox next to Add to Cart and enter a quantity. The order is added to your Shopping Cart.

List View

Results of a search are returned in list view by default. The maximum total number of records returned and the number of records returned on each page is controlled by user preferences.

The following functions can be performed from this view:

- Zoom in on the structure.
- List all Synonyms for the substance.
- Access the record in details view.
- Mark the record.
- Register the compound in Registration Enterprise.
- Access the MSDX data for the compound.

To view results in list view, perform a search. Use the browsing buttons to browse through the pages of result.

Details View

Details view makes available all of the tools to browse through vendor catalogs and add products to your shopping cart. Click the **Details** button for a search result in the List view to return additional information on that compound.

In the Details View, you can do any of the following:

- Zoom in on the structure.
- List all synonyms for the substance.
- Return the List View.
- Mark the record.
- Register the compound in Registration Enterprise.
- Access the MSDX data for the compound.
- Browse for vendors.
- Add products to your shopping cart.

Browsing for Vendors

Records in details view are displayed with both structure and vendor information.

To find a vendor catalog:

1. Select one of the tabs: **Online Vendors**, **Your Favorite Vendors**, or **Other Vendors,** depending on your preference.
2. Highlight a vendor name in the list found in the tabs to display a catalog listing to the right.

NOTE: To compare more then one vendor, hold down CTRL and select two or more vendors.

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3. Select the appropriate viewing option by clicking one of the following buttons:

Catalog View

To view the full catalog listing, click Catalog Details, and a new window will appear displaying catalog information.

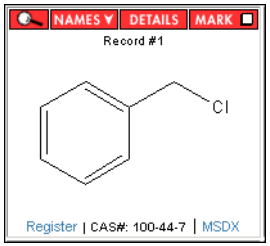
Compact View

For details about using the shopping cart, please see “Using the Shopping Cart” on page 4.

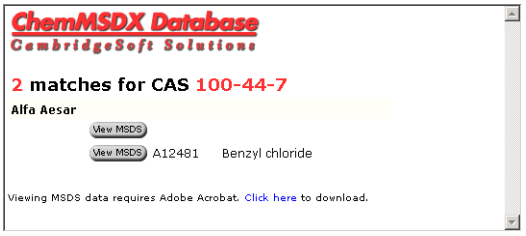
Accessing MSDX Data

MSDX Data, when available, can be accessed from the MSDX link found in list and details view on a substance's record. MSDX data is not available for all substances. By default, when the data is not available, the MSDX link will appear greyed out.

To access a substance's MSDX data, click the **MSDX** link in list or details view.



If there is more then one data sheet for the substance, an option window appears.



If there is only one data sheet available, or as a result of selecting one of the options, the datasheet appears in PDF format.

Using the Shopping Cart

The Shopping Cart is a convenient way to save a list of chemicals that you want to order. For more information, about ordering the chemicals in your shopping cart, see “Saving your Shopping Cart List” on page 5.

You can add items in the shopping cart from Details View of any record.

To view a record entry:

1. Open a record in Details View.
2. In the vendor list, select one or more vendors to browse.

3. In the list, select the checkbox next to **add to cart** and enter a quantity. The order is added to your Shopping Cart.

Viewing Your Shopping Cart

Your Shopping Cart list can be retrieved from the ChemACX Query Input form or the Search Results page.

To view your Shopping Cart, click either

- SHOPPING CART OR
- VIEW SHOPPING CART

Your Shopping Cart list appears.

Removing Items

- To remove an item from your Shopping Cart, on the Shopping Cart page, click **REMOVE**.

To remove all items from your Shopping Cart, on the Shopping Cart page, click the **Remove all** button.

Saving your Shopping Cart List

You have three options to save the ChemACX shopping cart information gathered during a session: **Print**, **Export to Excel**, or **Export to Word**.

To print your shopping cart, click Print **Print**.

To export shopping cart data to Excel or Word:

1. Click Export to Excel **Export to Excel** (or **Export to Word**).

NOTE: Exporting to MS Excel or MS Word are options configured by your system administrator. See your system administrator for more details.

The Requisitioner Information Form appears.

2. Enter appropriate information in the space provided.
3. Click Export to Excel **Export to Excel** (or **Export to Word**).

Your shopping Cart information is saved to an Excel workbook or Word Document with one sheet for each vendor.

Registering ChemACX Chemicals

If you have Registration Enterprise, you can register ChemACX chemicals.

NOTE: To configure ChemACX and integrate it with Registration Enterprise, see your system administrator.

To register a ChemACX chemical in Registration Enterprise:

1. Search the required chemical in ChemACX.
2. Click the **Register** link in the compound record. The **Register a compound** dialog box appears.
3. In the **Register a compound** dialog box, click the **OK** button. The chemical gets registered in Registration Enterprise.

Creating Inventory Containers

If you have Inventory Enterprise installed, you can send the ChemACX chemicals to Inventory and creating Inventory containers.

To create containers in Inventory Enterprise from ChemACX chemicals:

1. Open the shopping cart.
2. Click the **Send to Inventory Manager** button. The **Create Inventory Containers from ChemACX** page appears.

   NOTE: Consult your system administrator, if you do not see the Send to Inventory Manager button.

3. Provide the required information and click the **OK** button. A new page will appear.
4. In the new page, click the **Commit** link. Another page will appear.
5. In the next page, click the **View** link to view the newly created containers.

Saving Hit Lists

1. After you perform a search, select **Save** from the **Hit Lists** menu. The save hitlist window appears.
2. Enter a name and description for the hit list.

NOTE: You can mark the saved hit list as a Public, by selecting the Make Public check box.

3. Click the **OK** button to save the hit list.

Exporting Search Results

You can save a hit list as an SD or RD file. The structure, molecular weight, and formulae are automatically exported. Any other fields in the search form used to produce the hit list can be included in the export.

To export search results or hit lists:

1. Select Export Hits from the File menu. The **Export Hits** window appears.
2. Select the additional fields by enabling the check box corresponding to the appropriate field name.
3. Select a type of SD file:
   - Flat: Select this type when multiple results for one field (a record is created for each result).
   - Nested: Select this type when multiple results for one field all appear in one cell.
4. Click the **OK** button. A new window appears.
5. Click the **Click to Download** hyperlink. The **File Download** dialog box appears, containing a numerical name for the file, based on the date and time.
6. Click the **Save** button to display the **Save As** dialog box.
7. Select a location.
8. Click the **Save** button.

The exported file flattens each record so that a compound with sub-form fields, such as multiple batches in the Registration Enterprise is found within a single record in the exported file. All sub-form data is concatenated with '--' between fields. The first line indicate the field names.

Logging Off

You can end your session with ChemACX at anytime. To log off, click the **Log Off** button.

Vendor Participation

CambridgeSoft keeps adding catalogs of new vendors to ChemACX. Therefore, the vendor you are looking for might be in the next release

of ChemACX, or it might already be in the CambridgeSoft's WWW subscription service, ChemInfo Pro.

However, you can also ask your favorite vendor to participate in ChemACX so that you can find your favorite vendor in the next release of ChemACX. To participate, the vendor needs to send their product list to CambridgeSoft. The preferred format for sending the product list is a ChemFinder database containing structure details of the products. Other electronic formats, such as Access databases and Excel spreadsheets can also be used for sending the product list. If the product list is small, it can be sent in the form of brochure. The vendor can send the product list to the following address:

ChemACX Data, CambridgeSoft Corporation, 100 CambridgePark Drive, Cambridge, MA 02140 (USA)

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