ChemBioOffice Enterprise

Chem & Bio Office Enterprise 2010
Decision Support Platform
Enterprise 11

User Guide

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Contents

ChemBioOffice Enterprise User Guide

Overview

ChemBioOffice Enterprise is a suite of online applications that enable multiple users to manage and share a vast resource of chemical and biological information. Users retrieve the information from an extensive set of databases with an easy-to-use Web-based work area.

This help is designed to provide users with general information and tips for using the ChemBioOffice Enterprise applications. This guide is available in print (this file) and Web-based format. The print format of this guide is available in the Documentation Library.

Global login

ChemBioOffice Enterprise uses a global login interface to manage user related information. Once you login with your username and password, you can access all the ChemBioOffice Enterprise applications to which you have the necessary permissions.

When you log into ChemBioOffice Enterprise, a cookie is written to your machine. This cookie holds login information. Therefore, login information is recognized even after a browser is closed.

NOTE: The cookie expires if you do not perform any action for 25 minutes.

Logging in

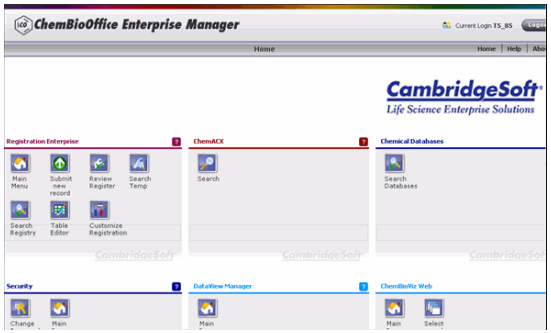
To log into the ChemBioOffice Enterprise suite of products:

1. Type the following address in the address bar of your Web browser: **http://servername**. The ChemBioOffice Enterprise application's User Login page appears:

NOTE: In the specified address, 'servername' is the name of the server where ChemBioOffice Enterprise is installed. Contact your server administrator for this name

2. Enter a valid username and password.

3. Click **OK**. The ChemBioOffice Enterprise homepage appears:



NOTE: The links visible on the homepage depend on the permissions of the user who is logged in. The homepage includes links to all the ChemBioOffice Enterprise applications to which the logged-in user has access rights.

4. Click a link to open an application.

Performing searches

All the ChemBioOffice Enterprise applications incorporate a system of forms, which allow you to search databases containing chemical and biological information. In order to search a database and retrieve results, you need to use a form and enter information within its fields. The information entered makes up a search query.

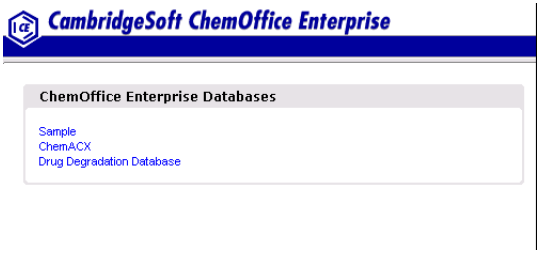
To search a database:

1. Log into the ChemBioOffice Enterprise suite of products and open an application.
2. Choose the appropriate search form.
3. Enter your search criteria and click the **Search** button.

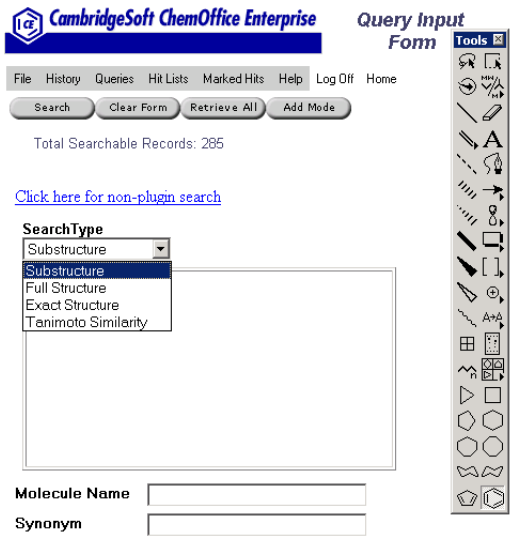
Starting applications

To start an application:

1. Open the homepage of the ChemBioOffice Enterprise application. For more information, see "Logging in" on page 1.
2. Click the link for the desired application. For example, click the **Search Databases** link within the **Chemical Databases** section. The following page appears.



3. Click the **Sample** link. The Query Input Form page appears:



The Query Input Form

Use the Query Input Form page to enter the criteria you want to use to search the database. You can search by type, text, and structure.

Total searchable records

The number next to this image specifies the total number of records that are being searched in the database.

File menu

The File menu contains three menu options, which are:

- Preferences: Enables you to accesses the Preferences dialog box, where you can set search preferences for your current session.
- Print: Prints the current window (equivalent to using the browser's print button).
- Export Hits: Exports hits to a SD or RD File.

History menu

The History menu contains two menu options, which are:

- Queries: Allows you to retrieve a query, which was executed in the current session, even if the query was not saved.
- Hit lists: Allows you to retrieve a hit list which was created in the current session, even if the query was not saved.

Queries menu

The Queries menu contains three menu options, which are:

- Restore: Displays the last query entered in the Query Input Form page, or one of the saved queries.
- Save: Saves the current query.
- Manage: Lets you manipulate (restore, edit, and delete) saved queries and queries in the current history.

Hit Lists menu

The Hit Lists menu contains three menu options, which are:

- Restore: Displays the last hit list created, or one of the saved hit lists.
- Save: Saves the current hit list.
- Manage: Allows users to manipulate (restore, edit, and delete) saved hit lists and hit lists in the current history.

Marked Hits menu

The Marked Hits menu contains two menu options, which are:

- Show Marked: Displays all marked records.

- Clear Marked: Clears the marked hits.

Help menu

The Help menu contains two menu options, which are:

- Contents: Accesses the online Help.
- About: Provides information about the version of the ChemBioOffice Enterprise software and the database being searched.

LogOff menu

The LogOff menu ends the current session and clears any resources used by the user.

Home menu

The Home menu opens the ChemBioOffice Enterprise homepage.

SEARCH BUTTON

Starts a search.

CLEAR FORM

Deletes all information in the input form.

RETRIEVE ALL

Performs a search that retrieves all records in the database.

ADD MODE

Switches to Add mode, which gives you the ability to add records to the database.

Query Input Form

The Query Input Form page includes three major components: the SearchType drop-down list, ChemDraw plug-in, and search fields.

SearchType list

The SearchType drop-down list allows you to specify the type of search to perform. The choices are Substructure, Full Structure, Exact Structure and Tanimoto Similarity.

ChemDraw plug-in

The ChemDraw plug-in allows you to draw a structural query in the blank area using the tools of the ChemDraw Plug-in. This structure is used like all other search parameters. For more information on drawing structures, see the ChemDraw documentation.

Search fields

On the Query Input Form page, the additional fields that you can search are: Molecule name, Formula, Molecular Weight, Synonym, and Entry Date. The fields that you can search may change depending on the ChemBioOffice Enterprise database that you are searching.

Performing a simple search

To perform a simple search:

1. Open a query input form.
2. Draw the chemical structure of benzene in the ChemDraw Plug-in area using the toolbar available in the **Query Input Form** page.
3. Click the **Search** button. The results of the search appear in the **Results List View** page.

NOTE: Search results are displayed according to the Preferences dialog box.

Search results

Performing a search within an application results in a list of items matching your query. All result forms in the ChemBioOffice Enterprise applications have similar formats, but the nature of display varies according to the search criteria and returned values.

This section describes the results obtained when searching the sample database. In order view a result, log into the sample database and perform the search described in “Performing a simple search” on page 4.

Viewing results

There are two ways to view search results, which are:

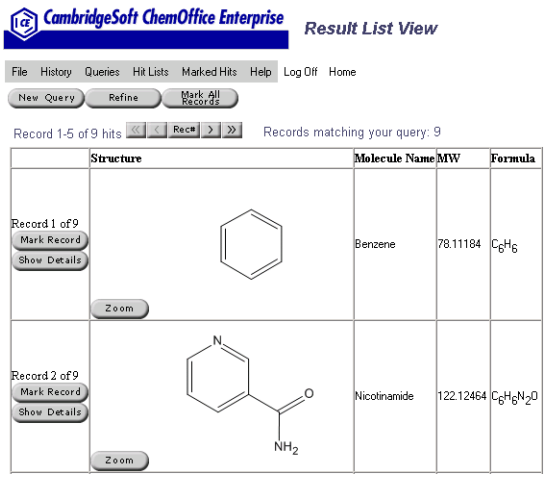
- List View
- Detail View

A default view is set for each ChemBioOffice Enterprise application. You can set the default view in which your results appear, by using the Preferences dialog box. For more information, see “Setting search preferences” on page 16.

List view

The List view lets you view information about multiple records simultaneously. In general, the List view does not display all the fields available for a record. You need to use the Browse buttons to view additional hits.

The display of results in the List view varies depending on the application used. See your application’s user guide for more information. The following figure shows some search results displayed in List view:



Detail view

The Detail view lets you view all the information available in the database about a particular record. The manner of display in the Detail view varies, depending on the application used. See your application’s user guide for more information.

To display a record in Detail view, click the Show Details button corresponding to a record in the Result List View page.

In Detail view, you can scroll through the record set using the Browse buttons to view additional hits.

The following figure shows some search results displayed in Detail view:

To display the record set in List view, click the Return to List button.

Additional hits

The maximum number of hits, which the page, containing the search result, can display at a time is set by the system administrator. Therefore, when the number of hits exceeds this maximum number, you need to browse through the hits using the navigation buttons.

Marking records

Records can be marked (added to a progressive hit list) from both Details and List view. Marked hits are user specific and can be retrieved at any time by using the Show Marked menu option.

To mark a record:

- In List View: Click the **Mark Record** button corresponding to the record that you want to mark.
- In Details View: Click the **Mark Record** button in the upper left hand corner of the record that you want to mark.

NOTE: The record is marked and the button changes to Unmark Record button. To remove the record from the marked records list, click the Unmark Record button.

To view the marked records, select the **Marked Hits** > **Show Marked** menu option. The marked records are loaded into the current hit list and displayed.

To delete marked records, select the **Marked Hits** > **Clear Marked** menu option. The marked records are deleted.

Manipulating queries

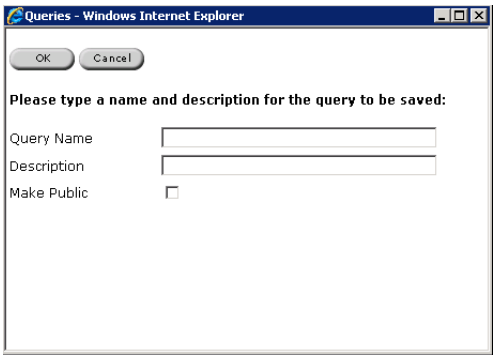
The Queries menu in the menu bar provides menu options using which you can restore, save, and manage queries, which have been used to search data. Saved queries are useful when you need to execute a particular query more than once without going through the process of entering the parameters each time.

Saving queries

You can save a query so that you can use it at a later time. This is often useful when you expect to run the same search more than once.

To save a query:

1. After performing a search, select the **Queries** > **Save** menu option. The **Queries** window appears:



2. Enter a name and description for the query.
3. Select the **Make Public** check box, if you would like other users to access the query.
4. Click **OK** to save your query. For information about retrieving this query, see "Restoring queries" on page 7.

Restoring queries

The Restore Query feature lets you restore a previously entered search criterion to an input query form.

There are two options for restoring a query, which are:

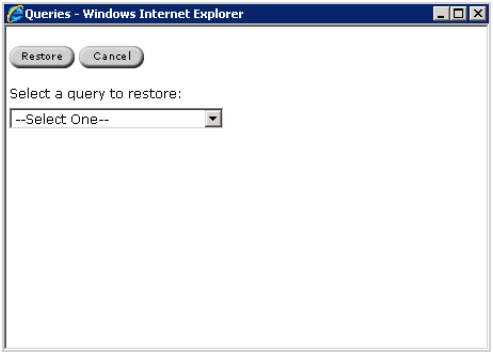
- Restore the last query entered
- Restore a saved query

To restore the last query:

1. Select **Restore** > **Last** from the **Queries** menu. The **Query Input Form** page appears.
2. In the Query Input Form page, edit your criteria, if required, and click the **Search** button. The search results are displayed.

To restore a saved query:

1. Select **Restore** > **Saved** from the **Queries** menu. The **Queries** window appears:

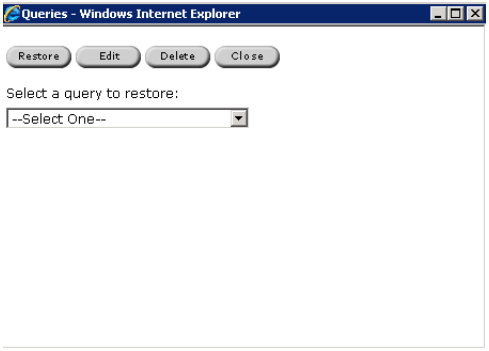


2. Select the appropriate query from the drop-down list appearing in the **Queries** window.
3. Click **Restore**. The **Query Input Form** page appears.
4. Edit the search criteria, if required. and click the **Search** button.

Managing queries

The Queries window allows you to restore, edit, and delete queries in the current history and saved queries. Saved queries are user specific.

To start managing your queries, select **Manage** from the **Queries** menu. The **Queries** window appears:



Restoring queries

To restore a query through the Queries window:

1. Select the appropriate query from the **Select One** drop down list.
2. Click the **Restore** button. The query input form appears.

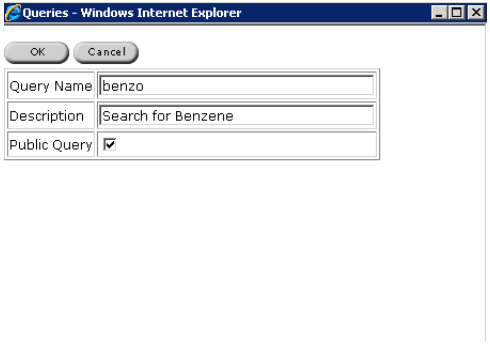
NOTE: For more information about restoring queries, see "Restoring queries" on page 7.

Editing queries

Editing a query allows you to enter new identifier information for the query, such as a new name and description, or make the query public. Making a query public makes your query accessible to any other user of the system.

To edit a query:

1. Select the appropriate query from the **Select One** drop down list.
2. Click **Edit**. The following window appears:



3. Enter appropriate information and click **OK** to save the changes.

Deleting queries

Only saved queries can be deleted. History queries remain in the query list until the history is cleared. To schedule history clearance, consult your system administrator.

To delete a query:

1. Select the appropriate saved query from the **Select One** drop down list.
2. Click **Delete**. A confirmation message box appears.
3. Click **OK**. The query is deleted from the list.

Managing hit lists

The Hit Lists features let you restore, save, and manage hit lists that have been generated.

Saving hit lists

To save a hit list:

1. Perform a search and obtain the result. For more information, see "Performing searches" on page 2.
2. Select **Save** from the **Hit Lists** menu. The **save hitlist** window appears.
3. 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.

4. Click **OK** to save the hit list. For information about retrieving this hit list, see "Restoring hit lists" on page 8.

Restoring hit lists

There are two options for restoring a hit list, which are:

- Restore the last hit list generated
- Restore one of the saved hit lists

To restore the last hit list generated, select **Restore** > **Last** from the **Hit Lists** menu in the menu bar. The hit list is displayed in List view.

To restore a saved hit list:

1. Select **Restore** > **Saved** from the **Hit Lists** menu.The **restore hitlist** window appears.

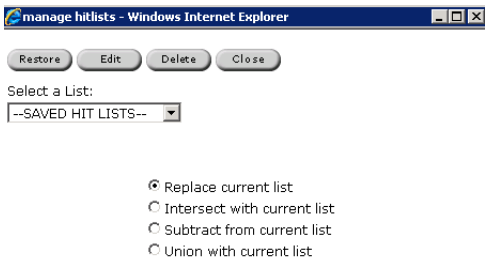
2. Select the appropriate hit list from the drop-down list available in the **restore hitlist** window.
3. Click **Restore**. The hit list is displayed in List view.

For more information about hit lists, see "Managing hit lists" on page 9.

Managing hit lists

Managing hit lists involves restoring, editing, and deleting hit lists, which were made by the current user. Saved hit lists are user specific.

To start managing your hit lists, select **Manage** from the **Hit Lists** menu. The **manage hitlists** window appears:



Restoring a hit list

When restoring a hit list from the **manage hitlists** window, saved hit lists can be merged in specific ways to generate a new hit list. The following table lists the options when restoring a hit list:

Restore Option	Result
Replace current list	The saved list is displayed in list view as it was saved.
Intersect with current list	A hit list is displayed, which contains only the hits found in both the saved list and the current list.
Subtract from current list	A hit list is displayed, which contains all the hits in the current list, not including hits of the saved list.
Union with current list	A hit list is displayed, which contains all the hits in the saved list as well as those in the current list.

To restore a hit list:

1. Select the appropriate hit list from the drop-down list available in the **manage hitlists** window.
2. Click the appropriate radio button to indicate how you would like the list to be restored.
3. Click the **Restore** button. The hit list is displayed in List view.

NOTE: For more information about restoring hit lists, see "Restoring hit lists" on page 8.

Editing a hit list

Editing a hit list allows you to enter new identifier information for the hit list, such as a new name and description.

To edit a hit list:

1. Select the appropriate hit list from the drop-down list available in the **manage hitlists** window.

2. Click **Edit**. The **edit hitlist** window appears.
3. Edit the fields as per your requirements.
4. Click **OK** to save the changes.

Deleting a hit list

Only saved hit lists can be deleted. Hit lists in the history remain until the history is cleared. To learn more about clearing the history, contact your system administrator.

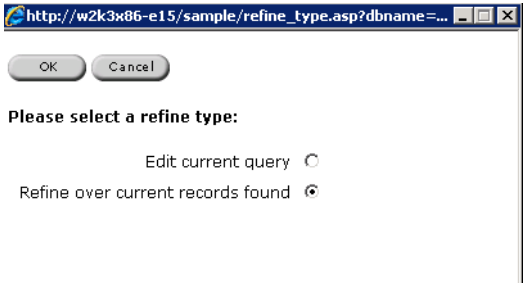
To delete a hit list:

1. Select the appropriate hit list from the drop-down list available in the **manage hitlists** window.
2. Click **Delete**. A message box appears, prompting you to confirm the deletion.
3. Click the **OK** button to delete the hit list.

Refining search results

In a large data set, you may want to modify your search criteria and search over the current results set. To refine your search:

1. Click the **Refine** button while viewing a current result set. The following window appears:



2. Select an option. The available options are described below:

If you want to...	Click...
Re-run the original query, and then apply the refinement query.	Edit current query. See Edit Queries within the topic, “Managing queries” on page 7.
Apply the refinement query to the current record set.	Refine over current records found.

3. Click **OK**. The following page appears:

4. Enter the search criteria.
5. Click the **Search** button to display the search results.

Refining over current records found

In a large data set, you may want to modify your search criteria to search over the current result set rather than the entire database.

To refine over the current records:

1. Perform a search and access the query input form for refining your query.
2. Enter your query. For example, if you want to refine the search to only compounds that have a hydroxyl attached:
   a. Draw methanol.
   b. Choose **Substructure** from the **Search Type** drop-down list.
3. Click the **Apply** button. Results from the refined search contain all the compounds in the data set which include the hydroxyl group. Records in the database which were not hit in the original search will not be part of the refined search.

Undoing a refined search

To return to results obtained before refining a search:

1. Perform a search operation and refine it.
2. Click the **Undo Refine** button to display the results from the previous search.

Exporting search results

It is possible to save a hit list as a 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. Choose the type of templates from **Export Templates** drop-down list.
3. Select the additional fields under **Templates** by enabling the check box corresponding to the appropriate field name.
4. 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.
5. Click **OK**. A new window opens.
6. 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.
7. Click the **Save** button to display the **Save As** dialog box.
8. Select a location.
9. 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.

Using the history

The application history can be used to retrieve queries and hit lists, which had been executed earlier, but were not saved. The history is cleared periodically, based on the application configuration. Consult your system administrator for more information about history clearance.

To restore a query in your history:

1. Select **Queries** from the **History** menu. The **Queries** window appears.
2. Select the appropriate query or hit list from the **Select One** drop down list.
3. Click the **Restore** button.

Types of searches

ChemBioOffice Enterprise forms contain various types of fields, and you can search data based on any of the fields.

The various types of searches that you can perform in ChemBioOffice Enterprise are:

- Text
- Structure
- Formula
- Numeric
- Combination

NOTE: You can further customize your search forms using the Preferences dialog box to allow or disallow valence modifications during the search. For more information on setting preferences, see "Setting search preferences" on page 16.

Text searching

In text searching, information can be entered using wildcard ("*") characters to broaden the search results or "=" to narrow to exact wording.

NOTE: You cannot enter "AND", "OR", or "NOT" into the text searches.

The following table lists examples of text queries:

Text Entered	Results Found
ben	Retrieves records that start with "ben", but may have any characters after. For example, the search returns benzene and benzofuran, but not bromobenzene.
*ben	Retrieves records that have any character before "ben" and any character after "ben" in the name field. For example, the search returns benzene, bromobenzene, and benzofuran.
=Benzene	Retrieves the exact text typed. For example, the search returns Benzene.
Ben*chl	Retrieves compounds with "ben" at the beginning, any character after "ben" and before "chl" and any character after "chl". For example, the search returns Benzyl Chloride.

Structure searching

Structure searching allows you to search for chemicals based on their chemical structures, which can be drawn using the ChemDraw plug-in. For more information on using ChemDraw, see the ChemDraw documentation.

ChemBioOffice Enterprise provides four options for searching chemicals by structure. These options are:

- Substructure

- Full Structure
- Exact Structure
- Tanimoto Similarity.

Substructure searching

Substructure search is the default search type for structure searching. Substructure searching returns structures that meet the following criteria:

- Match the basic chemical structure specified in the query form.
- Contain additional attachments at the open bond positions.

In order to perform a narrower or broader search, you can attach different features, such as atom lists and variable bond types to a structure using ChemDraw plug-in.

For more information about the available query features and their effect, see the following:

- Appendix A of the ChemDraw manual.
- ChemDraw Quick Reference Guide.

To perform a substructure search:

1. Click the **New Query** button in a search result.
2. Draw a chemical structure using the ChemDraw plug-in.
3. Select **Substructure** in the **Search Type** drop-down list.
4. Click the **Search** button to obtain the results.

Full structure searching

Full structure searching retrieves structures that match the structure drawn in the query input form, without considering additional attachments. Isotopes are recognized as hits.

To perform a Full Structure search:

1. Click the **New Query** button to display a blank search form.
2. Draw a structure.
3. Select **Full Structure** in the **Search Type** drop-down list.
4. Click the **Search** button. The records including isotopes are retrieved.

Exact structure searching

Exact searching retrieves only those structures that exactly match the structure you draw in the query input form. When matching structures, exact searching takes stereochemistry into account and does not recognize isotopes as hits.

To perform an exact structure search:

1. Click the **New Query** button to display a blank search form.
2. Draw a structure.
3. Select **Exact Structure** in the **Search Type** drop-down list.
4. Click the **Search** button. The records excluding isotopes are retrieved.

Similarity (Tanimoto) searching

Tanimoto Similarity searching retrieves chemicals having structural features that correspond to those specified in the query input form. Similarity searches are by nature, "fuzzy". Tanimoto Similarity searches are useful if you have a general idea of the types of compounds you are looking for, but do not know the precise target compound.

Tanimoto Similarity searching matches general structural features and not specific atoms or bonds. Therefore, you need not specify particular bonds when searching compounds based on Tanimoto similarity.

ChemBioOffice Enterprise uses a Tanimoto calculation to determine if compounds are similar. You can specify the degree of similarity in the Preferences dialog box. For more information on setting preferences, see “Setting search preferences” on page 16.

To perform a Tanimoto Similarity search:

1. Select **Tanimoto Similarity** in the **Search Type** drop-down list of a query input form.
2. Draw a structure.
3. Click the **Search** button.

Formula searching

Formula searching allows you to search molecular stoichiometry, either exactly or in the range that you specify. Formula queries consist of element symbols and element counts or ranges. The following table lists a few examples of Formula search:

Formula Entered	Results Found
C6H6	Compounds with 6 carbon and 6 hydrogen atoms, plus any number of other elements. Finds C6H6, C6H6N2O.
=C6H6	Compounds with exactly 6 carbon atoms, 6 hydrogen atoms, and no other elements.
C6	Compounds with 6 carbon atoms plus any number of other elements.
C6 N1-3	Compounds with 6 carbon atoms, one to three nitrogen atoms, plus any number of other elements.

In Formula searching, various rules apply, which are:

- Symbols may be one or two letters. Symbols may be in upper or lower case. If there are ambiguities, the program resolves them according to a set of rules. To avoid ambiguities:
  - Capitalize the symbols properly.
  - Insert spaces between symbols.
  - Use the Periodic Table to enter formulas.
- Element counts are single integers or ranges between two integers, which are separated by a hyphen. If a count is omitted, it is assumed to be 1.
- If the formula query contains no wild card character, such as '*****', it is assumed to be an Exact search. The search requires an exact formula match, containing no elements other than those indicated. If there is an asterisk (*) anywhere in the string then the search is a partial match and other elements may be present in the hits. Symbols may be repeated. For example, CH3CH3 is interpreted as C2H6.

NOTE: Formula searches are completely non-structural: CH3CH2OH will match both dimethyl ether and ethyl alcohol because both compounds have the same molecular formula: C2H6O.

- Parentheses may be used to group elements and apply a count to the entire group. For example, (CH2)3 is interpreted as C3H6.
- Spaces or non-alphanumeric characters other than parentheses are ignored.
- If a symbol is properly capitalized (first letter upper case, followed by zero, one, or two lower-case letters) then the longest valid symbol which matches is preferred. For example, "Phe" matches phenylalanine rather than phosphorus; "Co" matches cobalt.
- If symbols are not properly capitalized then the shortest symbol which matches is preferred. For example, 'co' is interpreted as carbon-oxygen instead of cobalt. However, there is an exception. The exception is that if two characters represent a valid two-letter symbol and also a valid one-letter symbol followed by an invalid one, then the two-letter symbol is favored. cl is interpreted as chlorine and not as carbon followed by the invalid symbol L.

Numerical searching

Searching numerical data allows you to find information, such as boiling points and molecular weights. When performing a numerical search, you can specify the range using a hyphen between the values at either end of the range. Ranges may also be indicated using inequality operators (<, >) together with the AND operator.

In numerical searching, you provide a decimal value or range in your the query. If you provide a single value, the number of significant digits determines the precision of the search. A hit is any value that rounds off to the value specified in your query.

The following table lists a few examples of numerical queries:

Entry in a Numerical Field	Results Found
78.15	Values from 78.15 and greater, inclusive.
78	Values from 78 and greater inclusive.
89.5-90.5	Values from 89.5 to 90.5.
90.05-91.05	Values from 90.05 to 91.05.
90-100	Values from 90 through 100, inclusive.
>90 and <100	Values from 90 through 100, exclusive.

Combination searching

You can perform a search that is a combination of the search types mentioned earlier and obtain a boolean AND search result.

For a complete list of types of searches, see “Types of searches” on page 12.

NOTE: OR and NOT searches are not supported in the ChemBioOffice Enterprise.

To perform a sample combination search:

1. Open a query input form.
2. Type *ene in the **Molecule Name** text box and 100-200 in the **Molecular Weight** text box.

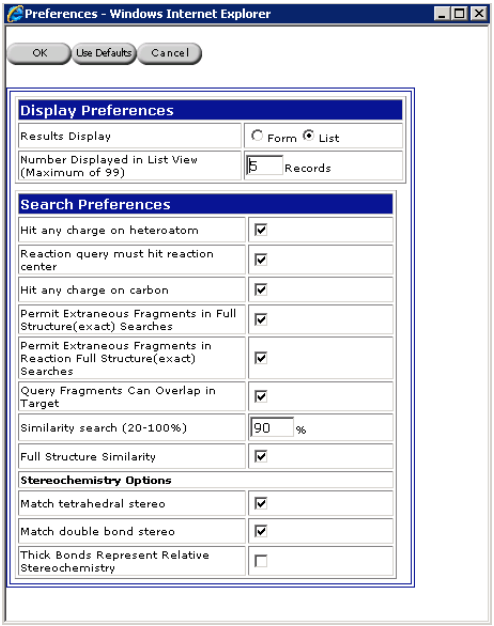
3. Draw a bond with a chloride using the ChemDraw plug-in.
4. Select **Substructure** in the **Search Type** drop-down list.
5. Click the **Search** button. The result of combination search that matches the entered criteria is displayed.

Setting search preferences

The Preferences dialog box allows you to specify the search preferences and control the manner in which results are displayed. These settings are global for a user throughout an application. The settings can be different in different applications.

To access the Preferences dialog box:

1. Select **File** > **Preferences** from the menu bar of a query input form. The **Preferences** dialog box appears:



2. In the **Preferences** dialog box, do one or more of the following, based on your requirements:

- Specify whether results are displayed in Detail view or List view by clicking the appropriate radio button in the **Display Preferences** frame.
- Specify the number of records displayed in List View by typing a value in the **Records** text box within the **Display Preferences** frame.
- Specify whether charges or radicals specified on atoms in the query must match those in the target by selecting one of the following options:
  - Hit any Charge on Heteroatom: Allows uncharged atoms in the query to match charged atoms in the target.

NOTE: Charged atoms in the query must always match charged atoms in the target regardless of this setting.

  - Hit any Charge on Carbon: Allows uncharged carbon atoms in the query to match charged carbon atoms in the target.

NOTE: Charged carbon atoms in the query must always match charged carbon atoms in the target regardless of this setting. The valence of a charged atom is taken to be the valence of the isoelectronic neutral atom.

- Specify that the reaction centers in the query must overlap the reaction centers in the target by selecting the **Reaction query must hit reaction center** check box.
- Specify Exact structure searching options by selecting the **Permit Extraneous Fragments in Full Structure (exact) Searches** check box or **Permit Extraneous Fragments**

in Reaction Full Structure (exact) Searches check box.

- Specify whether query fragments will be used to identify targets by selecting the **Query Fragments Can Overlap in Target** check box.
- Specify the degree of similarity when performing a similarity search, by typing a percentage value in the **Similarity search** check box. A lower value requires the target to be less similar. Select the **Full structure Similarity** check box, if you want to search for completely similar compounds.
- Reset all values, if required, by clicking the **Use Defaults** button.
- Specify whether or not you want a structure search to consider stereochemistry by selecting on of the following check boxes:
    - Match Tetrahedral Stereo: To recognize tetrahedral chirality.

    NOTE: Keeping this flag ON greatly decreases the speed of searching the registry. If this type of duplicate checking is not important to you then it is recommended that you keep it turned OFF.

    - Match Double Bond Stereo: To recognize cis/trans double-bond geometry.

NOTE: When either of these options are selected, the search includes any stereo-chemistry indicated.

- Thick Bonds Represent Relative Stereochemistry: To specify whether thick bonds will represent relative stereochemistry.

NOTE: Stereochemistry is perceived in the query from: hashed or wedged bonds at a tetrahedral center and unsymmetrical substitution at a C=C double bond.

Retrieving server information

For information about the server software and the database being currently used:

1. Select **Help** > **About** from the menu bar to display the required information in a new window.
2. Click **OK** to close the window.

Logging off

When you access a ChemBioOffice Enterprise application, a session starts with the server. Although the server times out after a period specified by the administrator, it is recommended that you log out when your session is finished.

To log off from a ChemBioOffice Enterprise application, click Log Off in the menu bar of the application. When you log off, the server resources being used are cleared.

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