Chapter 1: ChemOffice WebServer

About ChemOffice WebServer

ChemOffice WebServer is a World Wide Web (web) chemical information server. Through a web browser, you can use the ChemOffice WebServer web applications to search databases for chemical and biological information.

ChemOffice WebServer is the basis for CambridgeSoft's enterprise applications.

Installation and Administration

Installation instructions, configuration options, and other administration tips can be found in the Admin guide for the ChemOffice Webserver and each of its applications.

Please see the application's readme file and Administrator's Guide (if applicable) for more information.

Global Login and Security

The ChemOffice WebServer uses a global login interface to manage user information for most applications (Sample not included). After logging in once with your user name and password, users have access to all WebServer applications that they have permissions to, without having to login to each application separately.

After logging in, a cookie is written to the client machine, holding login information. The cookie expires after 25 minutes of inactivity. Therefore, login information is recognized even after a browser is closed.

Logging In

To login to the ChemOffice WebServer suite of products:

1. Access the ChemOffice WebServer homepage and click on the **Global Login** link.

   A login box appears.

2. Login with a valid username and password and click OK.

   The Global Login page appears.

   NOTE: *The links visible on this page depend on the permissions of the user who is logged in.*

   This page includes links to all of the applications the logged in user has access to.

3. Click on a link to enter a particular application.

Manage Users and Roles

Users and Roles are managed universally for all ChemOffice WebServer applications. Links to User Management is available from each application as well as from the main global login page, if the user has the correct privileges.

Users

To access the Manage Users interface:

- From the Global Login homepage, click **Manage Users**.

The Manage Users interface appears.

To make changes to the users in the system:

1. Select the application in which the user exists from the **View Users From** drop down menu.

   NOTE: *Selecting* ***All CS Applications*** *will list all users.*

2. Click **Refresh**.
3. Click **Add User** (to add a new user) or highlight a user name and click **Update User** (to edit an existing user).

   A page allowing you to enter user details appears.
4. Enter user details as desired. Fields highlighted in red are required.
5. Select the roles for the user. To select more then one role at once, hold down the CTRL key while highlighting.
6. Click **OK**.

Roles

To access the Manage Roles interface:

- From the Global Login homepage, click **Manage Roles**.

  The Manage Roles interface appears.

To make changes to the roles in the system:

1. Select the application in which the role exists from the **View Roles From** drop down menu.

   NOTE: *Selecting* ***All CS Applications*** *will list all roles.*

2. Click **Refresh**.
3. Click **Add Role** (to add a new role) or highlight a role name and click **Update Role** (to edit an existing role).

   A page allowing you to enter role details appears.
4. Enter role details as desired. Fields highlighted in red are required.
5. Select the roles for the role. To select more then one role at once, hold down the CTRL key while highlighting.
6. Click **OK**.

Searching ChemOffice WebServer Applications

ChemOffice WebServer applications are accessible from any remote computer that has access to the server machine with the ChemOffice WebServer and its applications installed.

ChemInfo is a collection of databases which can be used with the ChemOffice WebServer. For more information about the ChemInfo Databases, please see “ChemInfo Databases” on page 261.

All of the ChemOffice WebServer applications incorporate a system of forms which allow the user to search a database of information. Searches are performed by entering information in fields on a search form. The information entered makes up a search query.

Before beginning a search you must take the following steps:

1. Login to and open a WebServer application.
2. Choose the appropriate search form.
3. Enter your search criteria and click Search.

Due to the similarities between applications, in this chapter, the Sample application is used to illustrate the basic functionality of the available WebServer

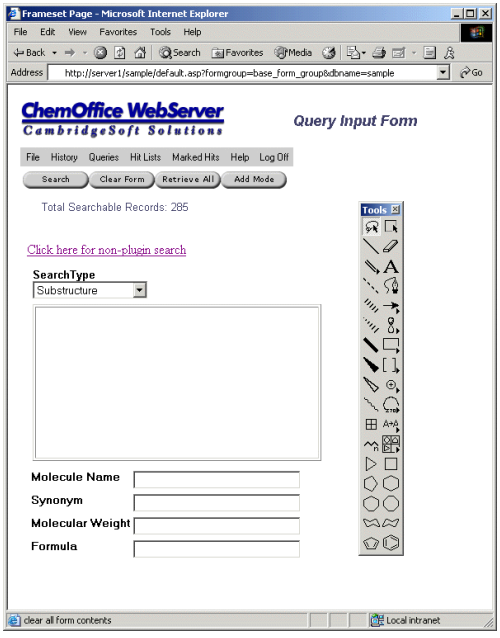
applications. For more detailed information about a particular application, please see, its chapter in this section.

Accessing a ChemOffice WebServer Application

To access a ChemOffice WebServer application:

1. Access the following URL: http://servername/chemoffice.asp where servername is the name of the server where ChemOffice WebServer 2003 is installed. Contact your server administrator for this name.
2. Click the ChemOffice WebServer application link you want to search. For this example, click Sample.

   The Query Input Form appears. Click on the image below for more information about its function.



The Query Input Form User Interface

The Navigation Toolbar

The navigation toolbar appears at the top of most search forms in the ChemOffice WebServer. It consists of a menubar and a series of buttons. The actions available in the Sample application are listed:

Feature	Description
Total Records:	**Total Records** The number next to this image indicates the total number of records in the database being searched.
File Preferences... Print Export Hits...	**File Menu** *Preferences* - Accesses the Preferences dialog box, where you can set search preferences for the session you are currently in. For more information, see “Setting Your Display and Search Preferences” on page 20. *Print* - Prints the current window (equivalent to using the browser's print button). *Export Hits* - Exports hits to a SD or RD File.

Feature	Description
	**History Menu** *Queries* - Allows users to retrieve a query which was executed in the current session (does not require having saved the query). *Hit lists* - Allows users to retrieve a hit list which was created in the current session (does not require having saved the hit list).
	**Queries Menu** *Restore* - Displays the last query entered in the Query Input Form, or one of the saved queries. *Save* - Saves the current query. *Manage* - Allows users to manipulate (restore, edit, and delete) saved queries and queries in the current history.

Feature	Description
	**Hit Lists Menu** *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** *Show Marked* - Displays all marked records. *Clear Marked* - Clears the marked hits.
	**Help Menu** *Contents* - Accesses the online Help. *About* - Provides information about the version of the ChemOffice WebServer software and the database being searched.
	**LogOff Menu** Ends the current session and clears any resources used by the user.

Feature	Description
	**Search Button** Starts a search.
	**Clear Form** Deletes all information in the input form.
	**Add Mode** Switches to Add Mode which gives users the ability to add records to the database.
	**Retrieve All** Performs a search that retrieves all records in the database.

Search Input Form

The following is a list of fields found in the Sample application. For more information about a field in another WebServer application, please see the application's chapter in the "ChemOffice Desktop to Enterprise Solutions" Manual.

Search Field	Action
Search Type pull-down menu.	Select the type of structure search for your query: Substructure, Exact Structure, Identity Search, or Tanimoto Similarity. For more information about structure types, see "Searching With Structures" on page 9.
Structure box and **ChemDraw Tools** toolbar	Draw a structure. For more information about drawing structures, see the ChemDraw User's Guide.
Molecule Name	Enter a molecular name or a portion of a molecular name.
Synonym	Enter a synonym for a molecular name.
Molecular Weight	Enter a molecular weight or a range of molecular weights. For more information, see "Searching With Numerical Ranges" on page 11.

Search Field	Action
Formula	Enter a molecular formula. For more information, see “Searching With Molecular Formulas” on page 10.

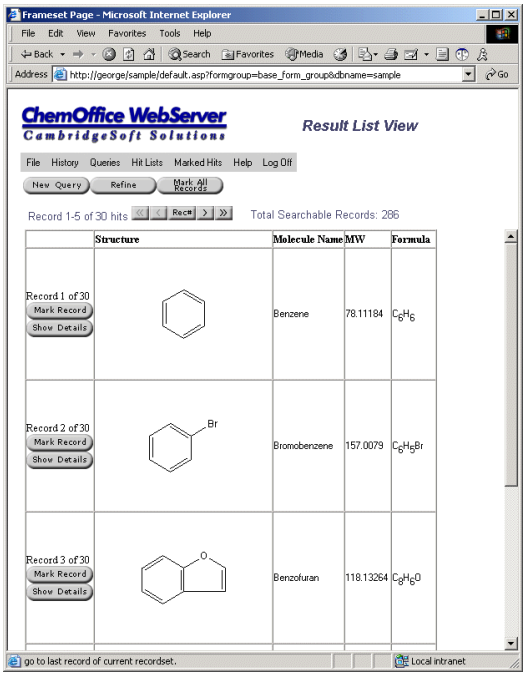
Performing a Simple Search

Queries are used to search for information in databases. Queries can contain different types of information and can be simple or complex, depending on the database you want to search. This example shows how to create a simple text query for searching the Sample database.

To create a simple text query:

1. In the **Molecule Name** box, type **benz**.
2. Click **Search**.

The Results List View window appears.



ChemOffice WebServer finds 30 records that match your query. These results can also be called hits.

For more information about:

This subject	See
changing the way results appear.	“Setting Your Display and Search Preferences” on page 20.
using results for other searches.	“Search Results” on page 12.
searching with other types of queries.	“Searching by Different Query Methods” on page 9.

Searching by Different Query Methods

The following is a list of the basic types of searches or query methods utilized in ChemOffice WebServer applications:

- Text
- Structure
- Molecular Formula
- Numeric (e.g. Molecular Weight)
- Combination (a combination of the above types)

Each of the above methods include distinct features which, when used correctly, can help to manipulate a search.

In addition, search preferences can be modified to allow valence modifications. For more information on setting preferences, see "Setting Your Display and Search Preferences" on page 20.

Searching With Text

One example of a text field, in the Sample Application, both **Molecule Name** and **Synonym** are text fields.

When entering search criteria into a text field, use the following rules:

- Use wildcard characters (*) to broaden search results.
- Use equals (=) to narrow search results.
- A regular text field is not a free text search so do not use **AND**, **OR**, or **NOT** for queries.

For example, the following searches actually mean:

Text entered	Search Results include
ben	Records that start with "ben," with any combination of characters following. Matches include benzene and benzofuran, but not bromobenzene.
***ben**	Records that include "ben" anywhere within the field. Other characters can be found before or after "ben". Matches include benzene, benzofuran, and bromobenzene.
=Benzene	Records that include "Benzene" with no other characters in the field's entry.
Ben*chl	Records that have "ben" as the first three letters of the entry, followed by any number of characters, followed by "chl" and any number of characters to end the entry. A match would include Benzyl chloride but not Benzene.

Searching With Structures

Searching by chemical structure is greatly simplified by using a ChemOffice WebServer structure search. There are four types of structure searches. The type of search is indicated by the choice made in the structure pull-down menu found above the structure box.

The following is a list of types of structure searching found in the Structure pull-down menu:

- **Substructure** - identical to the structure drawn in addition to any records with other attachments at open positions of the structure
- **Exact Structure** - identical to the structure drawn (hits isotopes)
- Identity - identical to the structure drawn (does not find isotopes) including equivalent stereochemistry
- **Tanimoto Searching** - similar to the structure drawn

Drawing a structure in the box provided is facilitated by the ChemDraw toolbar. The ChemDraw toolbar makes particular pieces of a structure available with one mouse click. For more information about using the ChemDraw toolbar, please see "Drawing Chemical Structures" in the ChemDraw Manual.

If the ChemDraw toolbar is not visible when you are ready to start drawing:

1. Right click anywhere inside the structure box.
2. Go to **View>Main Tools.**

   The ChemDraw Toolbar appears

Similarity (Tanimoto) Searching

The Tanimoto Similarity option finds structures that have structural features that generally correspond to those in the query. Similarity searches are usually indistinct. In a full structure similarity search, the results are guaranteed to include all those you would obtain from a substructure search with the same query and usually some additional hits. 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. Similarity searching matches general structural features and not specific atoms and bonds.

The application uses a Tanimoto calculation to determine if compounds are similar. How similar the results should be can be specified in the Preferences dialog box. For more information on setting preferences, see "Setting Your Display and Search Preferences" on page 20.

Searching With Molecular Formulas

Searching for molecular stoichiometry is accomplished with the inclusion of a formula query method. Formula queries consist of element symbols and element counts or ranges.

When searching by formula, use the following rules:

- Capitalize the symbols properly.
- Use symbols that are one or two letters, and upper or lower case.
- Use element counts that are single integers or ranges (two integers separated by a hyphen). If a count is omitted, it is assumed to be 1.
- Note that formula searches are completely non-structural. The formula CH3CH2OH matches dimethyl ether and ethyl alcohol because both compounds have the same molecular formula: C2H6O.

For example, the following searches really mean:

Formula	Results
C6H6*	Entries with 6 carbons and 6 hydrogens, plus any number of other elements in the formula field. Matches include C6H6, C6H6N2O.
CH3CH3	2 carbons and 6 hydrogens.
(CH2)3	3 carbons and 6 hydrogens.

Formula	Results
C6*	6 carbons plus any number of other elements.
C6 N1-3*	6 carbons and between one and three nitrogens, plus any number of other elements. Matches include C6H7N and C6H5NO2.

Searching With Numerical Ranges

All numeric fields allow the inclusion of one particular number or a range of numbers. The **Molecular Weight** field is an example of a numeric range field found in the Sample Application.

If a numeric search is performed with one number, the application will interpret the number as a range. For example, if 78 is entered, the range used spans .5 above and .5 below the number (77.5-78.5).

When searching by molecular weight, use the following rules:

- To search over a range of weights, use a hyphen between the values at either end of the range. Ranges may also be indicated using inequality operators (<, >) together with the AND operator.
- Note that the number of significant digits determines the precision of the search. A hit is any value that rounds off to the query.

For example, the following searches really mean:

Molecular Weight	Results
78.15	78.145 to 78.155.
78	77.5 to 78.5.
89.5–90.5	89.5 to 90.5.
90.05–91.05	90.05 to 91.05.
90–100	90 to 100.
>=90 and <=100	90 to 100.
>90 and <100	90 through 100, exclusive.

Combination Searching

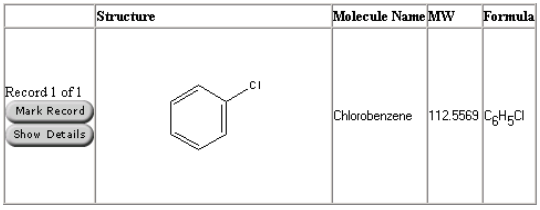
Combining the types of searches described above allows the user to really take advantage of the searching power of the ChemOffice WebServer. The WebServer searching applications implicitly support combination searching as a Boolean AND search, but does not support OR and NOT searches.

To perform a simple combination query:

1. From the Sample Application Query Input Form, enter ***ene** in the **Molecule Name** box.
2. Enter **100-200** in the **Molecular Weight** box.
3. In the **Structure** box, draw a chlorobenzene.
4. From the **Search Type** list, choose **Substructure**.
5. Click **Search**.

   The Results List View window appears.

   The ChemOffice WebServer finds 1 record that matches your query.



Notice that if the molecular weight range (for example) was not included, more results would have been returned.

Search Results

Performing a search within an application results in a list of items matching your query. All result forms in the WebServer applications have similar formats, but vary according to what you are searching for, and what is returned.

This section describes the results obtained when searching the Sample Database. In order to follow along, login to the Sample Database and perform the search described in Performing a Simple Search.

Viewing Search Results

There are two result formats available:

- List View
- Form View

The appearance of search results can be changed in the Display Preferences. For more information about Preferences, see “Setting Your Display and Search Preferences” on page 20.

Viewing Results in List View

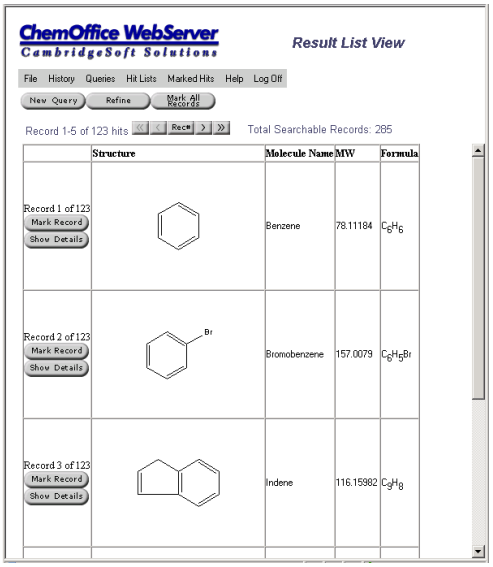
The List View allows the user to view information about multiple records at once. In general, List View does not display all the fields available for a record.

Use the browse buttons to view additional hits.

To change from Form View to List View:

- In a **Results Form View** window, click **Return to List**.

  The record you want to see appears in the Results List View window, along with the other search results.



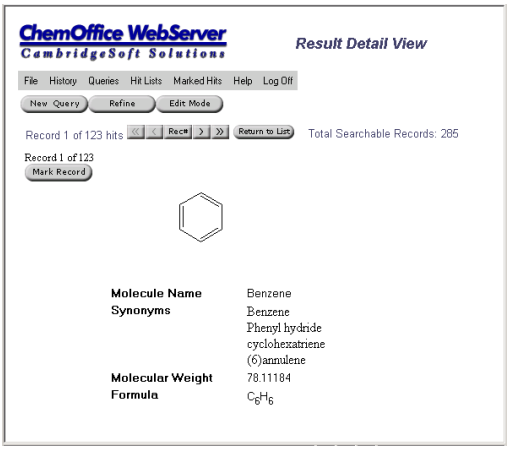
Viewing Results in Form View

Form View allows the user to view all of the information available in one record.

To change from List View to Form View:

1. In a **Results List View** window, go to the record you want to see in Form View.
2. Click **Show Details**.

   The record you want to see appears in the Results Form View window.



Browsing Other Records

After the ChemOffice WebServer completes a search, the results appear in a Results window. Sometimes, not all the records returned from the search appear in the Results window.

For example, if a search was performed in the Sample application to find the molecule named "benz", although the application returns 13 records, only one through five of the 13 appear in the current Results List View window.

NOTE: *The maximum number of records displayed on one page in Results List View is set in the Preferences box. The default is five records. For more information, see "Setting Your Display and Search Preferences" on page 20.*

The following buttons are available at the top of the results form to allow the user to view additional records:

If you want to see	Then click
the next group of records.	**Next Record** 
the last record of all the records returned from the search.	**Last Record** 
the group of records you saw most recently.	**Previous Record** 
the first record of all the records returned from the search.	**First Record** 
a specific record.	**Record Number**  Type a number in the box, within the given range. Click **OK**.

Viewing All Records

ChemOffice WebServer retrieves a set number of records at a time, and these records are displayed several at a time in the Results View window (the number of records displayed depends on user preferences). The number of records retrieved depends on a setting in the application's INI file. For information about the maximum number of hits retrieved for your application, please see your system administrator. The default number of maximum hits for Sample is 100.

To retrieve the first 100 records of a database:

1. From the Query Input Form, click **Retrieve All**.

   The Results List View appears, showing records 1–5 of 100 hits.

To see the next 100 records:

- In a **Results Form View** window, click **Get More Hits**.

  The Results List View changes, showing records 101–105 of 200 hits.

Marking and Unmarking Records

Records retrieved from a search can be marked to allow viewing later without repeating the search.

To mark a record to view again later:

1. From the Query Input Form, in the **Molecule Name** box, type **benz**.
2. From the **Search Type** menu, choose **Substructure**.
3. Click **Search**.

   The Results List View window appears.

   The Sample Application finds 13 records that match your query.
4. Click **Mark Record** for records #1 and #3.

   The Mark Record button changes to the Unmark Record button for records #1 and #3 only.

   The Show Marked and Clear Marked buttons appear on the left side of the window.

To see the records marked in a List View:

- From the **Results Form View** or the **Results List View**, click **Show Marked**.

  Records 1–2 of 2 hits appear in the Results List View window.

  The Show Last List button appears on the left side of the window, below the Clear Marked button.

To see the most recent Results List View:

- From the **Results List View**, click **Show Last List**.

  The most recent Results List View appears.

To remove a record from the marked records list:

- From the **Results Form View** or the **Results List View**, click **Unmark Record**.

  The Unmark Record button changes to the Mark Record button for the records you unmarked.

To remove all of the marked records from the marked records list:

- From the **Results Form View** or the **Results List View**, click **Clear Records**.

  The Unmark Record button changes to the Mark Record button. No records remain marked.

Manipulating Queries

The **Queries** menu gives users access to tools, which allow you to restore, save, and manage queries which have been performed. This is especially useful to users interested in using a particular query more than once without going through the process of entering the parameters each time.

Restoring Queries

Restore Query allows the user to restore previously entered search criteria to an input form.

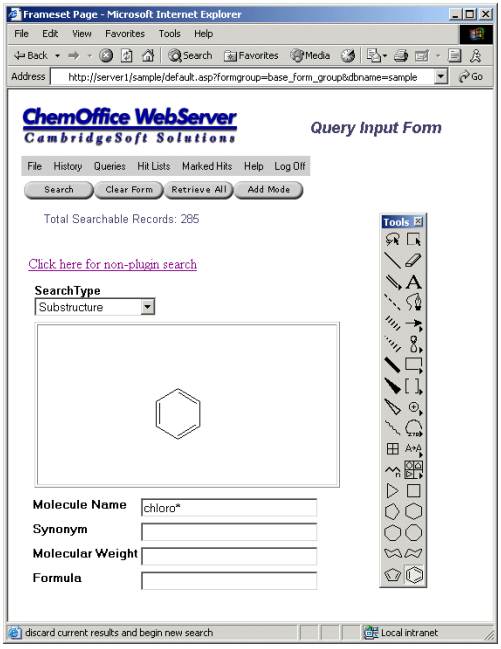
There are two options when restoring a query:

- Restore the last query entered
- Restore a saved query

To Restore the Last Query:

1. Select **Restore > Last** from the **Queries** Menu.

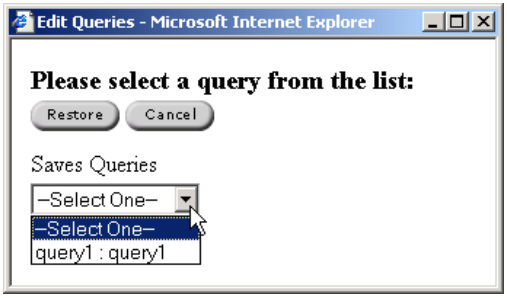
   The query input form appears:



2. Edit your criteria and click **Search**.

To Restore a Saved Query:

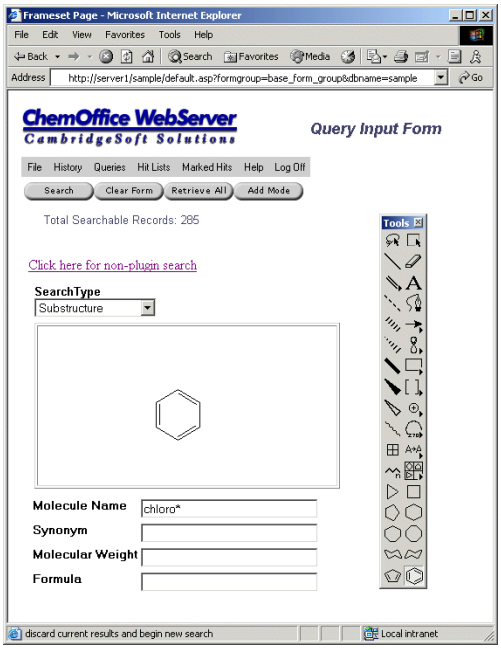
1. Select **Restore > Saved** from the **Queries** Menu.



2. Select the appropriate query from the listbox.

3. Click **Restore**.

   The query input form appears:



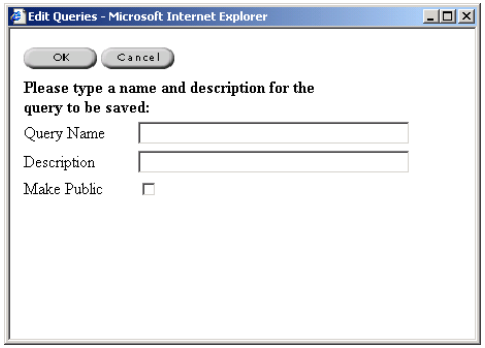
4. Edit your criteria and click **Search**.

Saving Queries

Users can save a query to be recalled 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 **Save** from the **Queries** Menu.



2. Enter a name and description for the query.
3. Select the **Make Public** checkbox if you would like other users to be able to access the query.
4. Click OK.

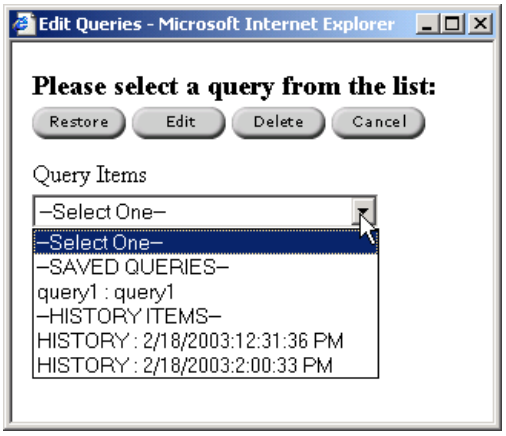
   Your query is saved. For information about retrieving this query, please see “Restoring Queries” on page 14.

Managing Queries

The Manage Queries dialog box allows users 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 Manage Queries dialog appears.



Restoring Queries

For information about restoring queries, please see “Restoring Queries” on page 14.

To Restore a Query from the Manage Queries dialog:

1. Select the appropriate query from the listbox.
2. Click **Restore**.

   The query input form appears.

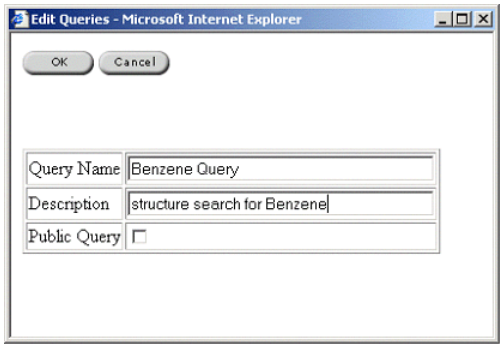
Editing Queries

Edit Query allows the user 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 by any other user of the system.

To edit a query:

1. Select the appropriate query from the listbox.
2. Click **Edit**.

The edit query window appears:



3. Enter the appropriate information and click **OK**.

   The query information has been edited and you are returned to the Manage Query window.

Delete Queries

Only saved queries can be deleted. History queries remain in the query list until the history is cleared. To change when the history is cleared, please see your system administrator.

To delete a query:

1. Select the appropriate saved query from the listbox.
2. Click **Delete**.

   The query is deleted from the list.

Manipulating Hit Lists

The **Hit Lists** menu gives users access to tools, which allow you to restore, save, and manage hit lists which have been generated by the current user.

Restoring Hit Lists

Restore Hit List allows the user to restore a hit list which was previously generated.

There are two options when restoring a hit list:

- 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.

  The hit list is displayed in list form.

To Restore a Saved Hit List:

3. Select **Restore > Saved** from the **Hit Lists** Menu.
4. Select the appropriate hit list from the listbox.
5. Click **Restore**.

   The hit list is displayed in list form.

Saving Hit Lists

Save Hit List allows a user to save a hit list and recall it at a later time.

To Save a Hit List:

1. After performing a search, select **Save** from the **Hit Lists** Menu.
2. Enter a name and description for the hit list.
3. Click **OK**.

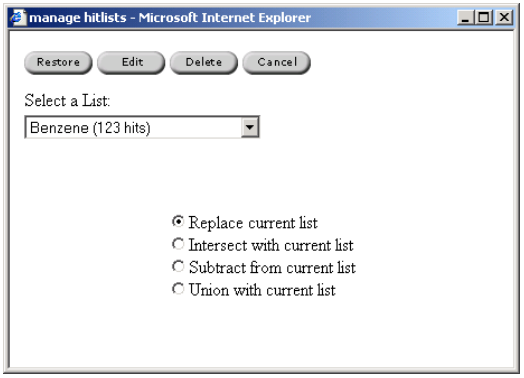
   Your hit list is saved. For information about retrieving this hit lists, please see “Restoring Hit Lists” on page 17.

Managing HIt Lists

The Manage Hit Lists dialog box allows users to restore, edit, and delete hit lists in the current history and saved hit lists. Saved hit lists are user specific.

To start managing your hit lists, select **Manage** from the **Hit Lists** Menu.

The Manage Hit Lists dialog appears.



Restoring a Hit List

When restoring a hit list from the Manage Hit Lists dialog box, saved hit lists can be merged in specified ways to generate a new hit list. The options when restoring a hit list are:

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 of the hits in the current list, not including any hits also found in the saved list.
Union with Current List	A hit list is displayed which contains all of 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 listbox.
2. Select the appropriate radio button (to indicate how you would like the list restored).
3. Click **Restore**.

   The hit list is displayed in list view.

Editing a Hit List

Edit Query allows the user 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 by any other user of the system.

To edit a query:

Edit Hit List allows the user to enter new identifier information for the hit list, such as a new name and description.

1. To edit a hit list:
2. Select the appropriate hit list from the listbox.
3. Click **Edit**.

   The edit hit list window appears:
4. Enter the appropriate information and click **OK**.

   The hit list information has been edited.

Delete a Hit List

Only saved hit lists can be deleted. Hit lists in the history remain in the hit list until the history is cleared. To change when the history is cleared, please see your system administrator.

To delete a hit list:

1. Select the appropriate saved hit list from the listbox.
2. Click **Delete**.

   The hit list is deleted from the list.

Refining Search Results

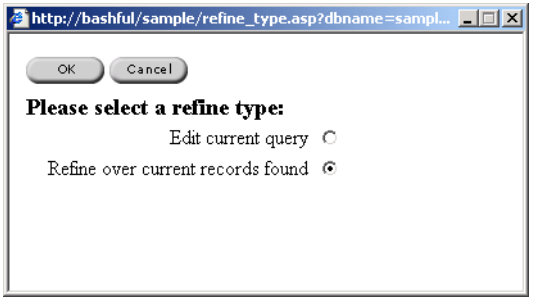
A query can be changed to narrow search results. This can be accomplished by either editing the current query and searching over the records that have already been retrieved, or by editing the current query and searching over the whole database again.

To refine a search over the current records:

1. Create a query.
2. Click **Search**.

   The Results View window appears.
3. Click **Refine**.

   The **Refine Query** box appears.



4. Click **Refine over current records found**.
5. Click **OK**.

   The Refine Query Input Form appears.
6. Change the query.
7. Click **Apply**.

   The Results View window appears.

Refining Over Current Records Found

In a large dataset, 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. In the Refine Query Input Form, enter your query.

- For example, if you want to refine the search to only compounds that have a hydroxyl attached:

  a. Draw methanol.

  b. From the Search Type list, choose Substructure.

2. Click Apply.

   Results from the example refined search (above), contain all of the compounds in the dataset which include the hydroxyl group. Records in the database which were not hit in the original search will likewise, not be part of the refined search.

Undoing a Refined Search

To return to results obtained previous to a refined search:

- Click Undo Refine.

  The results from the previous search appear.

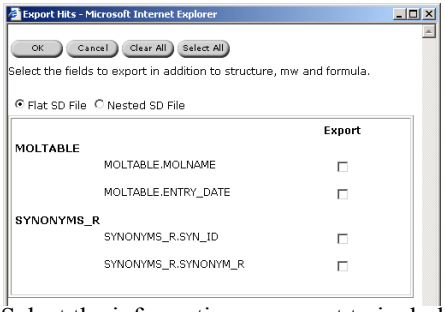
Exporting Search Results

The results of a search can be saved as a .sdf file. A .sdf file can be exported to ChemFinder and other ChemOffice applications. Information such as structure, molecular weight, and formula are automatically exported in the file. Additional information can be selected to be included in the file.

To export search results:

1. After marking his, from a **Results View**, click **Export Hits**.

   The Export Hits dialog box appears.



2. Select the information you want to include in the file.
3. Click **OK**.
4. **Click to Download**.

   The Save As dialog box appears, containing a numerical name for the sdf file, based on the date and time.
5. Select a download location and click **Save**.

Histories

The application history can be used to retrieve queries and hit lists which had been executed earlier, but were not necessarily saved. The history is cleared periodically, according to how the application is configured. Please see your system administrator for more information about when the history is cleared.

Use the **History** menu to restore a query or hit list in your history:

1. Select **Queries** or **Hit Lists** from the **History** Menu.
2. Select the appropriate query or hit list from the list box.
3. Click **Restore**.

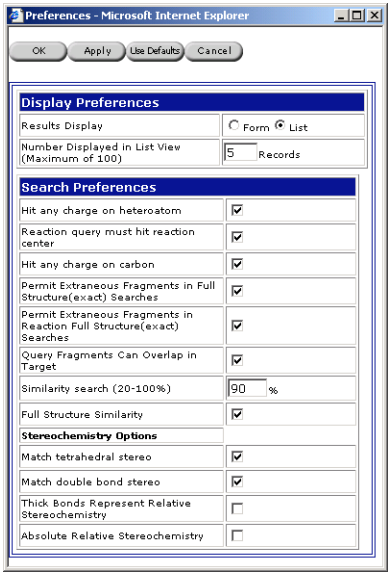
Setting Your Display and Search Preferences

Display and search preferences are set in the ChemOffice WebServer Preferences dialog box.

To set display preferences:

1. From a page in a ChemOffice WebServer application, click **Preferences**.

   The Preferences dialog box appears.



2. Take the appropriate action:

If you want to	Action
see search results one record at a time.	From **Results Display**, click **Form**.
see search results several records at a time.	From **Results Display**, click **List**.

If you want to	Action
specify the number of records you see in List View.	From the **Number Displayed in List View**, type a number in the **Number** box.

3. Click **Apply**.

   The new preferences are applied to your next search.

To set search preferences:

1. Click **Preferences**.

   The Preferences dialog box appears.

2. Take the appropriate action:

If you want your search to	Then, in the Search Preferences section
match the charges or radicals to the heteroatom in your query structure.	Click **Hit any charge on heteroatom**.
match the reaction centers in your query structure.	Click **Reaction query must hit reaction center**.
match the charges or radicals to the carbon in your query structure.	Click **Hit any charge on carbon**.
require that the reaction centers in the query overlap the reaction centers in the target	Click **Reaction Query Hit Reaction Center.**
specify exact structure searching options	Select the appropriate checkbox next to Permit Extraneous Fragments in Full Structure or Reaction searches. If Permit Extraneous Fragments (for structure or reaction searching) is selected, the search wil allow hits to contain molecular fragments in addition to that which was hit by the query.
match the similarity of your query structure by a specific percentage.	From the **Similarity search** box, type a number between 0 and 100. A lower value requires the target to be less similar than your query structure.
match the tetrahedral chirality to your query structure.	Click **Match tetrahedral stereo**.
match the cis/trans double bond geometry to your query structure.	Click **Match double bond stereo**.

If you want your search to	Then, in the Search Preferences section
make thick bonds represent relative stereochemistry	Click **Thick Bonds Represent Relative Stereochemistry**
require absolute relative stereochemistry	Click **Absolute Relative Chemistry**

3. Click **Apply**.

   ChemOffice WebServer applies your preferences to your next search.

Server Information

You can retrieve information about the server software currently in use and the database being searched from the application window.

To get Server information:

- Click the **About** button in the ChemOffice WebServer navigation bar.

To return to the previous page:

- Click **OK**.

Logging Off

When you first access a ChemOffice web application, you start a user session with the server. Although the server times out after a period specified by your administrator, you can log off when you are finished with the session.

To log off:

- Click **Log Off**.

  You are logged off and the server resources that you use are released.