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 all of the webserver applications.

System Requirements

ChemOffice WebServer requires the following minimum configuration for Windows systems:

Server

- WinNT Option Pack 4.0 (IIS 4); sp6a; Microsoft Data Access Components 2.5sp2 or later service pack, Windows2000 Server OR Windows 2002 Advanced Server SP2
- IIS and IE security patches
- CambridgeSoft ChemDraw Pro Plugin/ActiveX Control 7.01
- Oracle ODBC Driver 8.01.07 AND/OR Oracle OLEDB Driver 8.17.00

Client

- Internet Explorer 5.x or higher, or Netscape 4.x or higher
- CambridgeSoft ChemDraw Pro Plugin/ActiveX Control 7.01

Some individual applications have additional software requirements. For system requirements specific to an application, please see that application's Administrators Guide or Readme file.

Installation

Installation instructions for ChemOffice WebServer applications differ from application to application. Please see the application's readme file and Administrators Guide (if applicable) for detailed installation instructions.

Logging In

Opening a ChemOffice Web Application

All ChemOffice WebServer applications can be accessed from the WebServer homepage found at **http://*servername***.

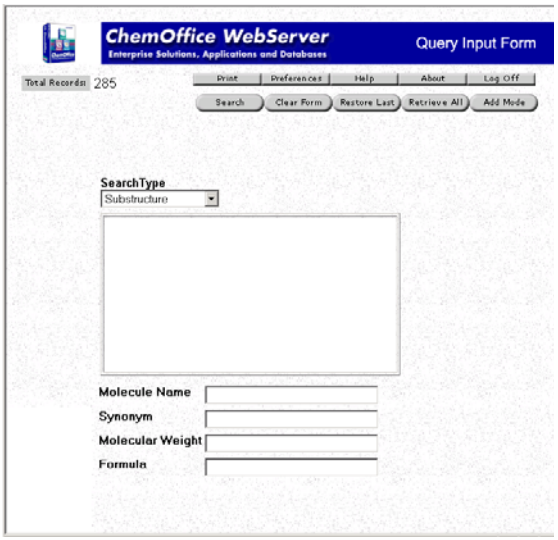
NOTE: *Servername is the name of the ChemOffice WebServer. Please contact your system administrator for information about your server.*

To open the ChemOffice Sample web application:

- Type **http://*servername*** into your web browser. The main ChemOffice WebServer window appears.
- Click on **Sample**.

NOTE: *To access a different WebServer application from the main ChemOffice Window, click on the name of the appropriate application name.*

The Query Input Form appears for the Sample application.



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 incorporates its web applications with numerous databases. Information stored in the databases can be accessed through the use of web forms in the applications. For example, if you want to find information stored in the bucky balls database, you would submit a query using the Bucky Base web application. The query searches the Bucky Base database for the information desired.

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 321.

ChemOffice Webserver applications have many similarities. Although sometimes the different applications have a distinct look, most allow searching and viewing of results in basically the same way. For this reason, 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.

Using The Query Input Form

The first step to searching a database with the ChemOffice WebServer is to create a query. A search query is simply a list of parameters and the values for those parameters that the resulting records should have.

Each web application has slightly different search forms, but the same basic steps apply to creating a query and browsing search results.

Navigation Toolbar

The navigation toolbar appears at the top of most search forms in the ChemOffice WebServer. The buttons available in the Sample application are listed:

Feature	Description
Total Records:	The **Total Records** in the database being searched is listed next to the Total Records block.
Preferences	Opens the **Preferences** dialog box. For more information, see "Setting Your Display and Search Preferences" on page 17.
Help	Opens the online help for the application
About	Displays information about the ChemOffice WebServer and the currently open database.
Log Off	Ends the current searching session and clears all forms or data views.
Search	Starts a search.
Clear Form	Clears all information in the search form
Restore Last	Displays the last query entered through the search form
Retrieve All	Retrieves the first n records in the database, where n is a number set in the application INI file. The default for Sample is 100.

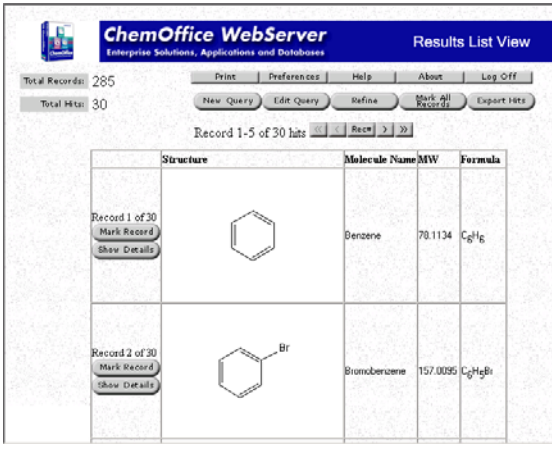
Creating a Simple Query

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 17.
using results for other searches.	"Search Results" on page 12.
searching with other types of queries.	"Sample Application Search Fields" on page 9.

Sample Application Search Fields

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, or Tanimoto Similarity. For more information about structure types, see "Searching With Structures" on page 10.
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.
Formula	Enter a molecular formula. For more information, see "Searching With Molecular Formulas" on page 11.

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 17.

Searching With Text

A text field is any field in which text is entered. For example, 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 three 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
- **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 17.

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.
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

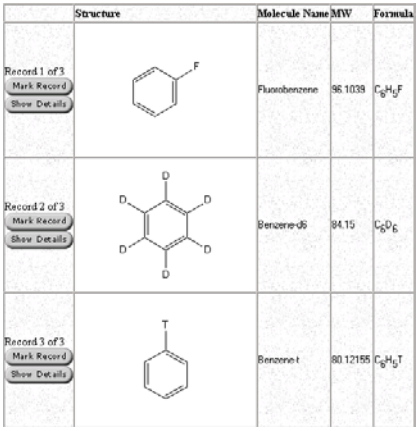
Combining the types of searches described above allows the user to really take advantage of the searching power of the ChemOffice WebServer. The WebServer searching applications implicitly support combination searching as a Boolean AND search, but does not support OR and NOT searches.

To perform a simple combination query:

1. From the Sample Application Query Input Form, enter **benz*** in the **Molecule Name** box.
2. Enter **80-100** in the **Molecular Weight** box.
3. In the **Structure** box, draw a benzene ring.
4. From the **Search Type** list, choose **Substructure**.
5. Click **Search**.

   The Results List View window appears.

   ChemOffice WebServer finds 3 records that match your query.



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

Search Results

Viewing Serch 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 17.

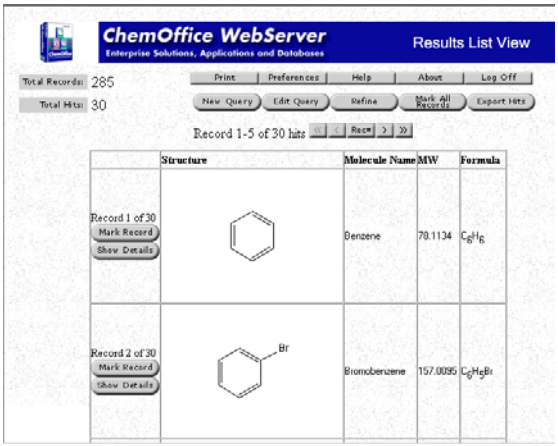
Viewing Results in List View

List View allows the user to view abbreviated entries for several records at one time.

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.



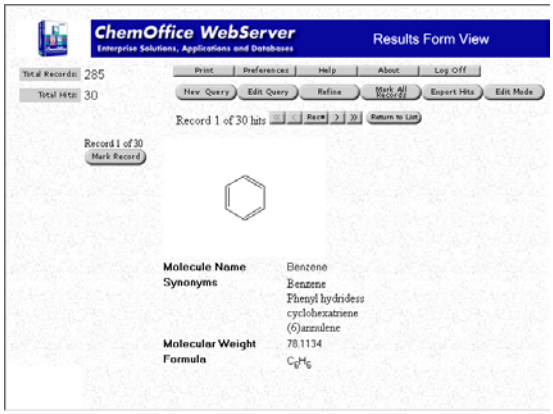
Viewing Results in Form View

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, search 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 17.*

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** 

If you want to see	Then click
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 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 100records:

- 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. Form 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.

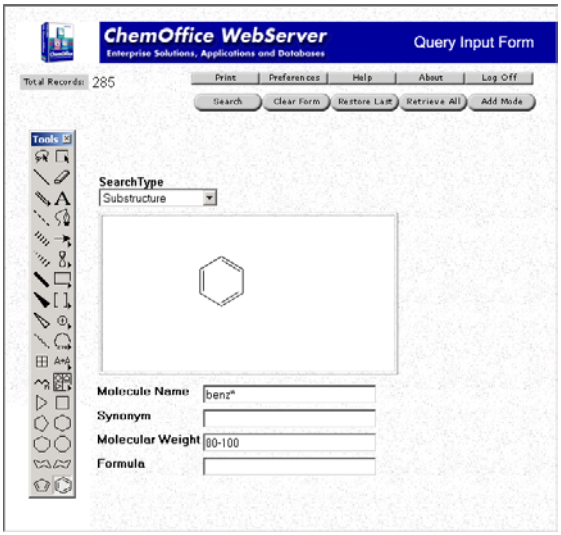
Editing Queries

If search results are returned and you would like to broaden or narrow the results further, it is usually beneficial to edit the current search rather then start a new search. This will allow you to view the search just performed and edit those values rather then having the enter the criteria again.

To edit the query performed in "Combination Searching" on page 12:

1. From the search results page, click **Edit Query**.

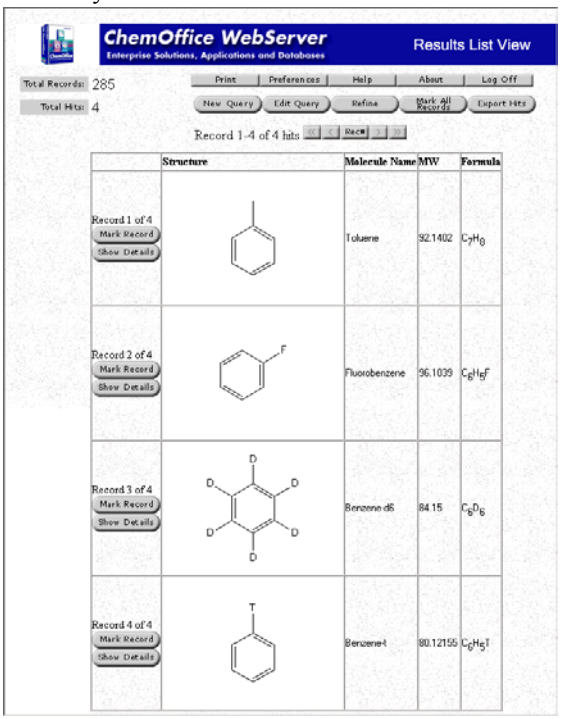
   The Search form returns.



2. In the **Molecule Name** box, enter ***ene** instead of **benz***.
3. Click **Search**.

   The Results List View window appears.

Four records are returned, including the records returned in the pervious search in addition to an entry for Toluene.



Restoring a Query

Restoring a query becomes useful if you want to use the most recent query created without typing all the information again.

To restore the most recently created query:

1. From the Query Input Form, click **Restore Last**.

   The Query Input form changes and the most recently created query appears.

   You can edit the query or run a search without changing the query. For more information about changing your query, see “Search Results” on page 12.

2. Click **Search**.

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.

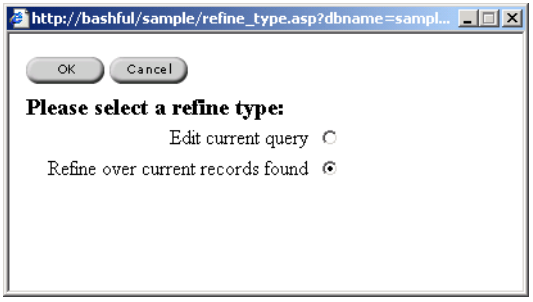
To refine a search over the current records:

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.

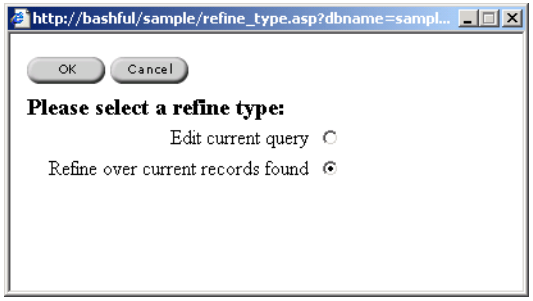
To refine a search over the whole database:

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

   The Results List View or the Results Form View window appears.

3. Click **Refine**.

   The **Refine Query** box appears.



4. Click **Edit current query**.
5. Click **OK**.

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

   The Results List View or the Results Form View window appears.

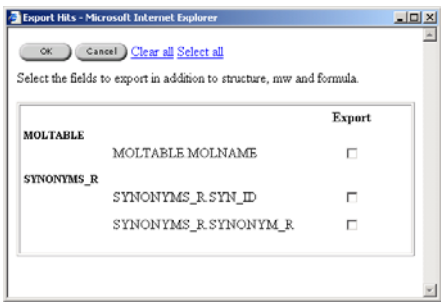
Exporting Search Results

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. 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 **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**.

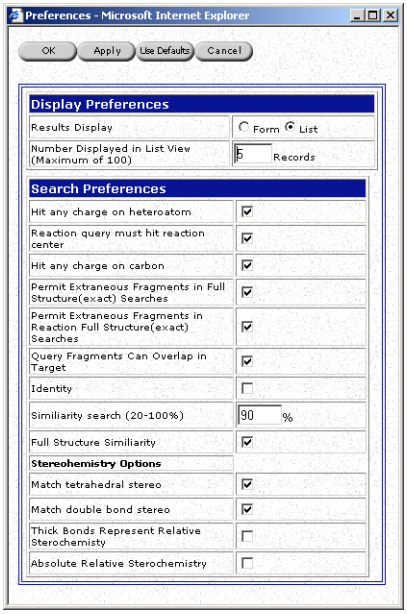
Setting Your Display and Search Preferences

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**.
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.

If you want your search to	Then, in the Search Preferences section
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**.
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.