

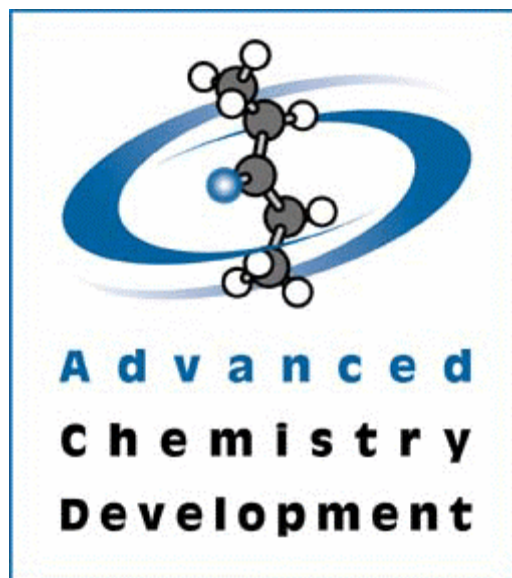
# ACD/ChromManager

Version 5.0 for Windows

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## Technical Note

### Forming an Applications Database



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# Forming an Applications Database with ACD/ChromManager

## Introduction

In the typical chemical organization, a huge number of chromatographic separations are developed each year. Unfortunately, several different laboratories within the organization may perform these separations on the same sample or the same compound. This often means duplication of effort due to the inability to easily share chromatographic information. Several attempts have been made to solve this problem by creating applications databases to archive successful separations and to make the information available throughout the organization.

ACD/ChromManager has been designed to provide an ideal, easy-to-use, and vendor-independent applications database. Its substructure search capability, interface to prediction in ACD/LC Simulator, and ability to simultaneously search several databases make it an essential tool for chromatography. This Technical Note provides instructions on how to easily build an effective, consistent Applications Database within an organization.

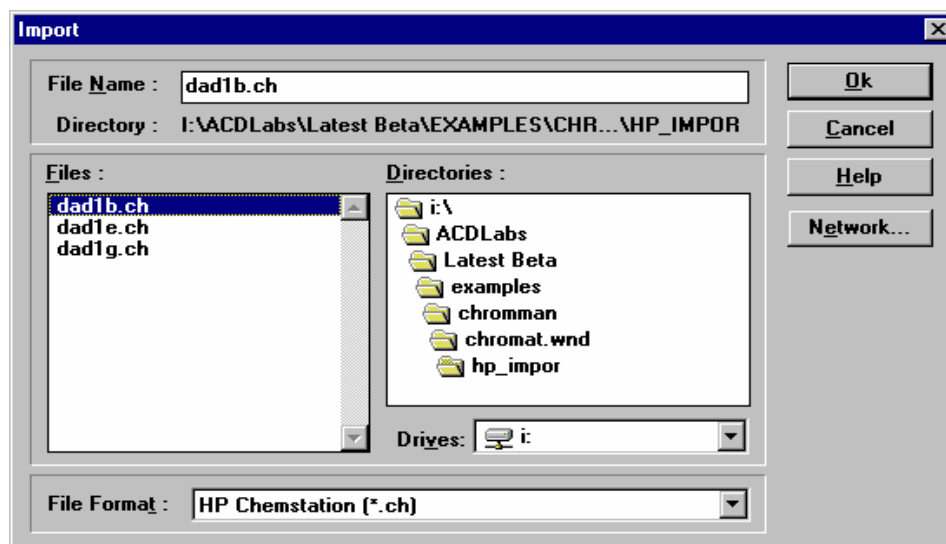
## The Process

### The Tools Involved

ACD/ChromManager databases are fully searchable archives containing chromatograms in the .esp format. Using the .esp file format provides the chemist with access to the original chromatogram with assigned structures, full data collection parameters, column information, and other user-defined data. This user-customized information can include the original sample number as well as method-specific data such as storage or cleanup specifications of a column. All of this information is fully searchable.

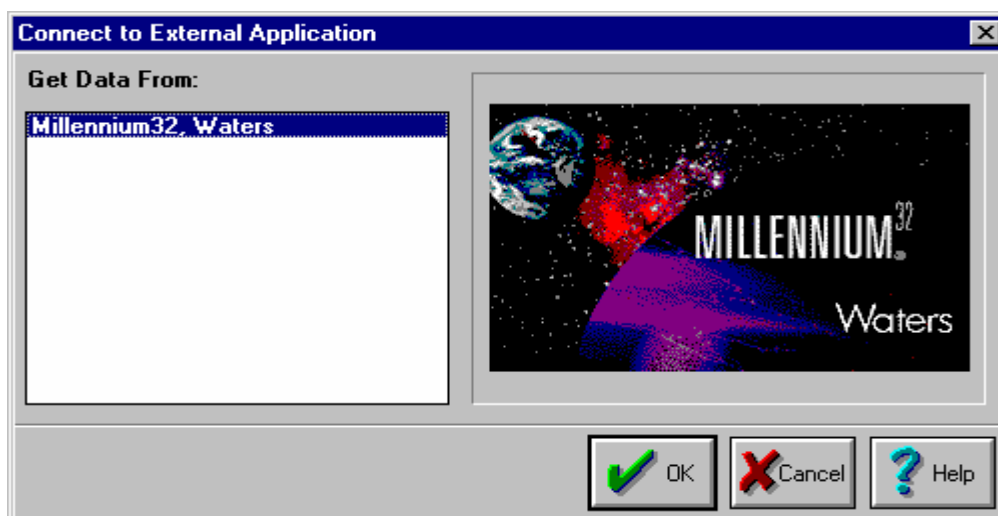
## Preparing the Chromatogram

The first step in building an Applications Database in ChromManager is to import a chromatogram into the chromatogram window. Figure 1 shows the import window using a ChemStation .ch file as an example.



**Figure 1. Importing a ChemStation HPLC Dataset Using the File/Import Menu Item.**



Certain external applications, such as Millennium, allow direct transfer of data to ACD/ChromManager as shown in Figure 2. Choose **Connect to...** from the **File** menu, and select the external application. Proceed as outlined in the ChromManager User Guide.

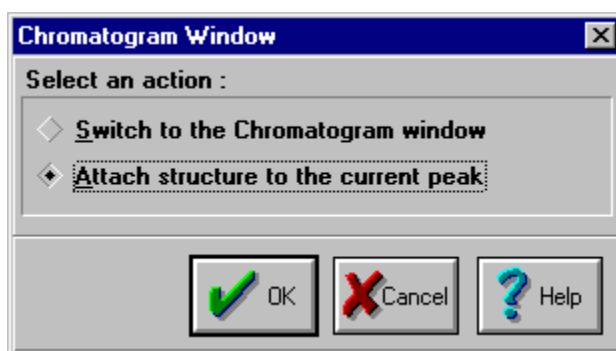


**Figure 2. Opening a Connection to an External Application Using the File/Connect to... Menu Item.**

Once the data has been imported and processed as desired (processing instructions may be found in the ACD/ChromManager User Guide), one may begin the process of assigning structures to their respective chromatographic peaks.

To assign a structure to a peak:

1. Open the **Peak Table** using the **Show Table of Peaks** button 
2. Select the peak of interest.
3. Now click the **Attach Molecular Structure** button 
4. In the ChemSketch window that appears, draw or import the molecular structure corresponding to that peak.
5. Then click **Chromatogram** on the Window Switching Bar. The **Chromatogram Window** dialog box will appear (see Figure 3).



**Figure 3. The Chromatogram Window Dialog Box.**

6. Select the **Attach structure to the current peak** option.
7. Perform this operation for every known peak; this information will be used later in searches and predictions.

## Entering Chromatographic Parameters

ACD/ChromManager may not extract all of the desired parameters from the raw vendor data file. Table 1 lists all parameters recommended in order to obtain the best possible results with LC Simulator. When adding a chromatogram to the database, it is strongly recommended that values for each of these parameters be entered.

**Table 1. Chromatographic Parameters Used by ACD/LC Simulator.**

Sample Name	Instrument Name	Extracolumn Volume
Injection volume	* Dwell Volume	Wave length (nm)
Time constant (or sampling rate)	Detector type	* Solvent A
* Temperature	* Flow rate	Column Name
* Solvent B	* Gradient program	* Particle size
* Column Length	* Column Diameter	* Bonded phase
Pore diameter	Plate number	* Observed t <sub>0</sub> (or V <sub>0</sub> )
Endcapped	% carbon	Observed pressure

Note: Values may be left blank when unknown; however missing values may prevent LC Simulator from performing certain predictions.

To enter chromatographic parameters:

1. Parameter entry may be performed in the chromatogram window prior to archival, or in the database window afterwards. Make the appropriate window active by clicking in it.
2. Select **Edit/HPLC Parameters** from the menubar.
3. Fill out all of the fields from Table 1 in the **HPLC Parameters** dialog box, pictured in Figure 4.
4. Once these fields have been filled in, click **OK** and they will be updated.
5. The chromatogram is now ready for addition to a database.

**HPLC Parameters**

Save Load OK Cancel Help

**Sample Data:**

Sample Name:

Injection Volume: 5.00 µl Operator Identify:

Save Load

**Instrumental Data:**

Name:

Dwell Volume:  ml

Time Constant:  sec

Extracolumn Volume:  ml

**Detector**

UV λ =  nm

RI

Other

Sensitivity: 1.00

Save Load

**Elution Data:**

**Type of experiment**

Isocratic

Gradient

Temperature: 20.0 °C

Flow rate: 1.00 ml/min

Solvent(s)

Save Load

**Column parameters:**

Column name:

Length:  cm

Diameter:  cm

Particle size:  microns

Pore diameter:  nm

Plate number:

Observed t0:  min

Observed pressure:  psi

at a flow rate of:  ml/min

Endcapped: Yes

% Carbon:

Bonded phase:

Save Load

**Figure 4. The HPLC Parameters dialog box Opened Using the Edit/HPLC Parameters Menu Item.**

## Creating a Database


1. Switch to the **Database** window.
2. Choose **Database/New** from the menu bar.
3. In the **Create New Database** dialog box, locate and open the directory where you want to create the new database.
4. Enter the desired file name for the new applications database.
5. Click **OK**.
6. Choose the level of password protection that you require. If you do not wish to use passwords, leave all fields empty.
7. Click **OK** to return to the **Chromatogram** window.
8. Select **Database/Update Database with Chromatogram** from the menubar.
9. The database now has one record in it. You may add more records by processing additional chromatograms as described above, and then repeating only the previous step (step 8 *only*—the database will remain open until you close it or exit the program).
10. The database is immediately searchable by virtually every data field.

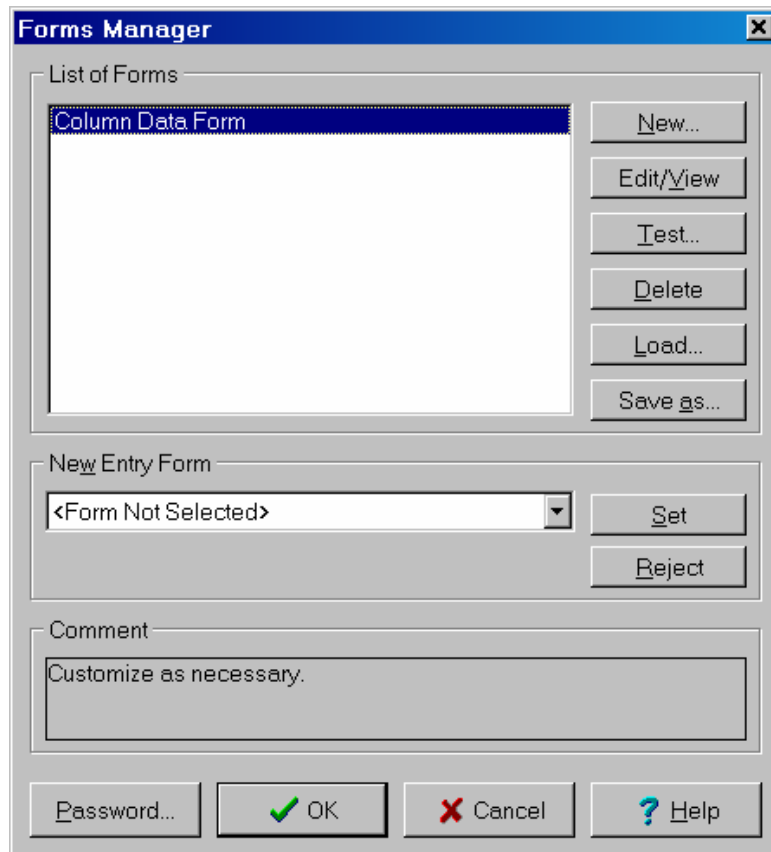
## User Data Forms

One of the main challenges with having multiple users building databases is that the same data can easily be entered multiple times in different ways. Such inconsistencies in the database may make certain searches unreliable or impossible. For example, a search for all “reversed phase” experiments, will not cull data from experiments entered as “reverse phase”. Even worse, some users may forget to include key information. To help avoid these difficulties, we recommend that a standard User Data Form be created to direct users to include all key information in each record. User Data Forms can be invoked each time an entry is added to the database. Dropdown menus, checkboxes, and other tools are available to help ensure standardized descriptions and spellings, and certain entries can be made “mandatory” so that these fields will never be blank.

A demonstration example is provided here to illustrate the creation and use of a User Data Form. It describes the addition of a field to column.frm, the form used for the internal ACD Applications Database. This form contains fields specific to the column used in a separation. The example illustrates the procedure used to add a field called “**Chromatographic Type**”.

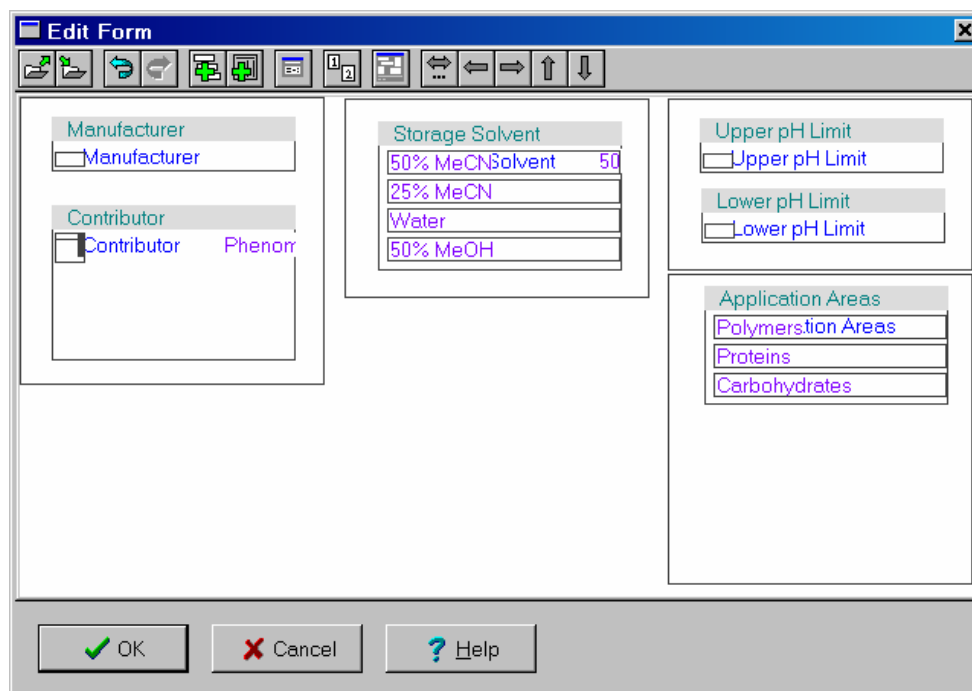
To add the field “Chromatographic Type” to a User Database Form:

1. Open a user database; the one created in the previous example is fine, and if it is still open it can be used as is.
2. Select the **Switch User Database to Update Mode** button  on the toolbar if it is not already selected (“depressed” in appearance).
3. Select the **Options/Database Forms Manager...** command from the menubar. This will cause the database **Forms Manager** dialog box to appear. (This dialog box is shown in Figure 5, although at this point the List of Forms may be empty).




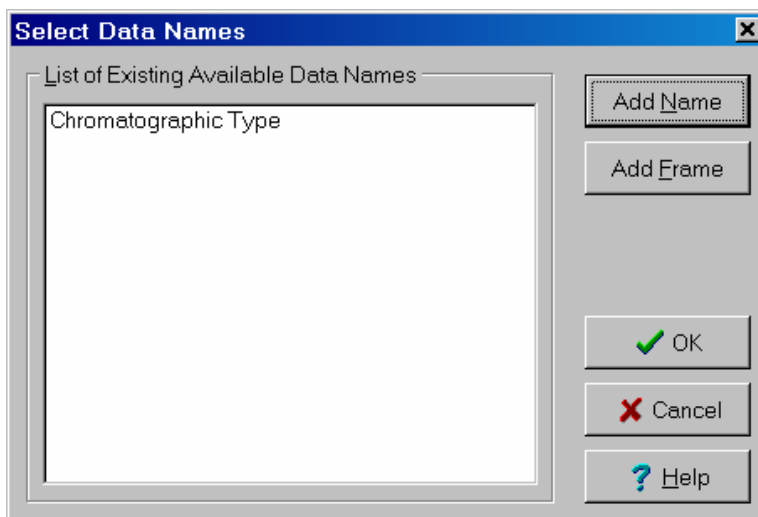
**Figure 5. The Database Forms Manager Dialog Box**

4. To open column.frm, click **Load**. In the dialog box that appears, locate column.frm and click **OK**. (To locate this file, Browse to the ACD software folder [usually C:\ACD... or C:\Program Files\ACD...], then open Examples\ChromMan. The file should be in the ChromMan folder.)
5. To avoid making undesired changes in a supplied template, immediately save the form to a new name: Click **SAVE AS** and enter "C:\Temp\example", or any other folder and filename you prefer, then click **OK**.
6. Click once on the currently displayed "Column Data Form" and then click the **DELETE** button (yes, do it! This button only deletes the form from the form list, NOT from the file system. You can reload it at any time.)
7. Load the new form by clicking **LOAD**, browsing to the new file location, and double-clicking the file.
8. To preview the form:
  - a. Click once on its name in the list.
  - b. Click **Test**. (This same functionality is available from within the form editor.)
  - c. Click **OK** when you get tired of looking at the form.
9. To edit the new form:
  - a. If it is not already selected, click once on the name of the form to select it.
  - b. Click the **Edit/View** button. You will see the blank Edit Form dialog box shown in Figure 6.



**Figure 6. The Edit Form GUI Opened Using the Forms Manager Edit/View Button.**

- c. Click the Add Data Name button 
- d. In the Select Data Names dialog box select: Add New Name. Enter “Chromatographic Type” in the Add New Data Name box (see Figure 7), followed by **OK** twice.




**Figure 7. The Select Data Names Dialog Box.**

- e. To specify or edit the properties of the new Data Name, double-click the “Chromatographic Type” box in the Edit Database Form window. This will open the Form Item Properties dialog box, pictured in Figure 8, as it should look once the steps below are completed.

**Figure 8. The Form Item Properties Dialog Box. This box is used to customize each component of the form interface.**

- f. The Edit Type list contains the possible types of the form items that control the way they will be represented in the finished form. For the current example of the data field “Chromatographic Type,” in the Edit Type list choose DropDownListBox. List boxes have two advantages over text boxes. The first is that it is faster to select than to type. Second—and more importantly—the data entries will always be consistent. Note that there are several other controls available, and each has its own rich set of customizable parameters.
- g. This will activate the List of Values field. To specify the list of possible values for this item, click the Edit button **Edit...** in the List of Values field. This will display the following dialog box:
- h. Click New Value... to add a value (in this case, a chromatographic type) to the list. This will cause the Enter New Value dialog box appear. Enter “Reversed Phase”. Click OK to make the label appear in the list. Repeat this action several times, adding “Normal Phase”, “CE”, and “Other”.
- i. Select “Reversed Phase” from the Default Value picklist.
- j. Click **OK** to save and close the ListBox control’s properties.
- k. Click and drag the “Chromatographic Type” control to whatever position you desire. Figure 9 shows an example of what the finished form may look like.

**Figure 9. The Edit Form Display of the Customized Column Form.**

- l. To observe the behavior of this new control, click the test button  on the editor toolbar, then click the down arrow on the side of the “Chromatographic Type” list box.
  - m. When you are done playing with the form, click **OK** to exit the Test mode, then click **OK** again to exit the editor (answer “Yes” when it asks if you want to save the form.)
10. To use the new form:
- a. Open a chromatogram from the example files.
  - b. Click Update Database, and the form will be invoked prior to updating our database with the new chromatogram.
  - c. Fill out the fields and click **OK**. The User Data Fields will be automatically updated.

## 7. User Notes

There is a field for User Notes in addition to the User Data Fields. This is useful for “non-routine” entries such as special procedures, etc. This field is searchable based on any text string.

## 8. The ACD Internal Applications Database (AIADatabase)

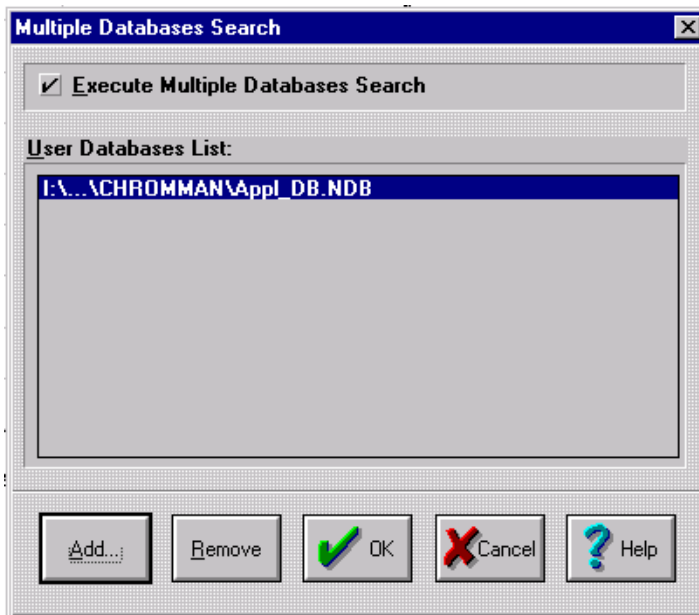
Every ACD/ChromManager user has access to a ready-made Applications Database. This database is the result of collaboration between ACD and a growing list of column vendors that makes available a large number of chromatographic methods. For a complete list of the contributors please see [www.acdlabs.com](http://www.acdlabs.com).

Due to ACD/ChromManager’s capability to search multiple databases at the same time, it is possible to search a number of organizational databases at the same time as the ACD Internal Applications Database. To open the database, move to the database and select **Open...**

**App\_Database.ndb.** You can now scroll through the current Database. Note that substructure and structure search function exactly as they do for User Databases.

## 9. Searching More than One Database at a Time

We will now specify searching our organizational Applications Database at the same time as the AIADatabase. From the database window, choose **Search**, and **Define Multiple Databases List**. Select the ACD Internal Applications Database (App\_Database.ndb) and our new Database (ACMEADatabase.ndb).

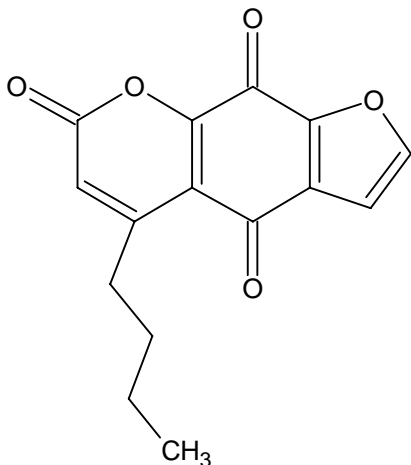


We can now perform searches across both databases at the same time.

## 10. Using the Database

The exact procedure for retrieving an appropriate separation method from the database will depend on a number of factors. The most valuable search technique is the substructure search, but other criteria that are important as well. For example, one may already know the column to be used, e.g. reversed phase, and this information can be used to limit the search to those records using this type of column. Searches are performed in iterative fashion until the number of potential methods is manageable.

As an example, let's consider a new method for with the following substance:

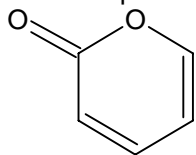


First, a structure search is performed to see if this structure has been part of another separation developed earlier.

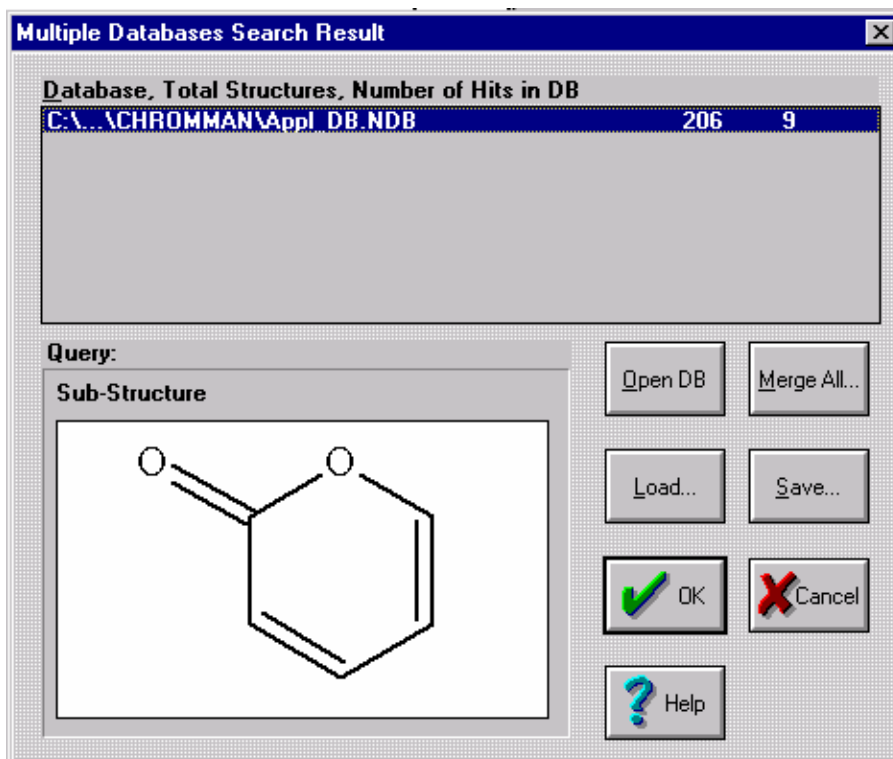
- Draw the structure in the ChemSketch window.
- Click **Search Structure** on the Window Switching Bar. ChromManager will search both the AIADatabase and our database. No hits should be found.

Now we will attempt to find related compounds.

- Delete two portions of the molecule, leaving the characteristic heterocycle. Note that all of the unspecified hydrogens will be treated as "any" atom



- Click **SS Search**. When the search is complete, the dialog box pictured in Figure 10 should appear.





**Figure 10. The Multiple Databases Search Result Dialog Box.**

There are nine hits, all from the AIADatabase. We have two potential separation methods that we can now evaluate. Note that if there were more hits, we could perform a second search to narrow the field further. Click **Open Database** to view the retrieved chromatograms.

## 11. Evaluating Retrieved Methods

Once the substructure search has narrowed the list to a few possible candidates, it is time to consider evaluating in a new way. Provided that at least three peaks have been assigned to structures in the chromatogram, we can predict the retention time of our new compound in each system using another ACD module, LC Simulator.

To predict retention times for a system, first double-click a retrieved chromatogram to transfer it to the chromatogram window. Click on the **Show Table of Structures** button  to verify that three structures have been assigned to peaks. Now click on the **Optimize Chromatogram** button  to carry the chromatogram to ACD/LC Simulator. The directions for predicting retention times can be found in the manual for LC Simulator.

We will now predict the retention time of our compound in that system. Return to ChemSketch, and restore the original compound. Click **Undo** (from the **Edit** menu) in order to remove the deletion steps.

Click Optimizations **Optimizations**, and the retention time of the structure will be predicted and shown with the training set. If we had more compounds to evaluate, we could draw them in ChemSketch and predict in the same manner.

In practice, prediction of retention times depends on a number of different factors, and errors may easily be in the 10% range. This means that predicted co-elution is not necessarily a reason to reject a method. The least desirable scenarios are the situation in which at least one component in the mixture has a very large predicted retention time, suggesting that run times will be much too long, or when multiple components elute very early in the run time. These are unlikely to be viable solutions. This separation method can be rejected, or modified if it appears to be somewhat applicable. Some advice on this can be found in Technical Note #2, *Working with Applications Databases and Chromatographic Prediction*.