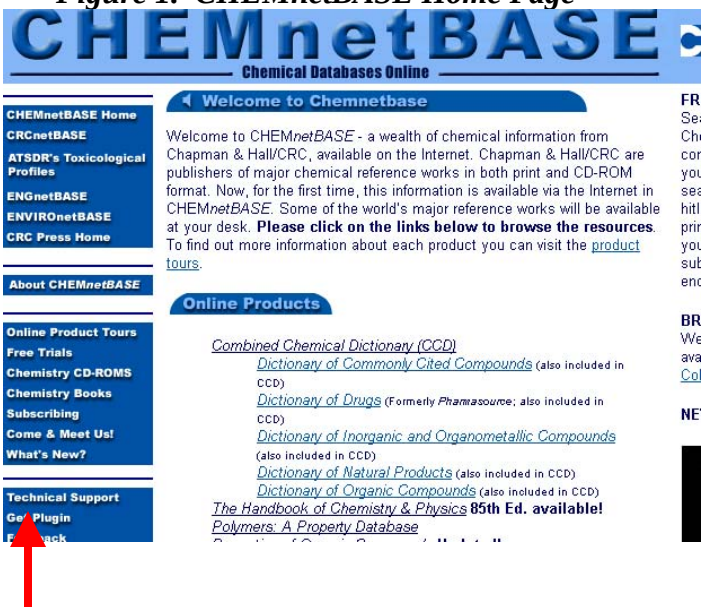
CCD via CHEMnetBASE for Identifying Unknowns

Table of Contents

*Note: A **red arrow** was used to identify where buttons and functions are located in CHEMnetBASE.*

CCD via CHEMnetBASE for Identifying Unknowns

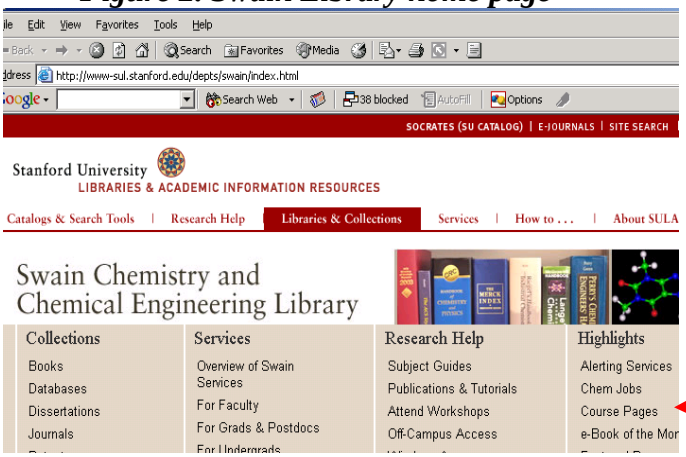
Figure 1. CHEMnetBASE Home Page



Action:

- **Download and install the CHEMnetBASE structure drawing plug-in if you are using your home computer**. This only has to be done once, before using any of the CHEMnetBASE databases for the first time. It has already been done for the computers in the Swain Chemistry library. Go to the CHEMnetBASE homepage (see Fig. 1) at www.**chemnetbase**.com , and click on "Get Plug-in" at the lower left of the page (Structure plug-in), then follow the instructions.

Figure 2. Swain Library home page



Action:

- **Go to the Swain Library home page**: Swain Library homepage at www-sul.stanford.edu/depts/**swain**/

  Click on Course Pages, then click on Chemistry 130: Library Resources for Identifying Unknowns.

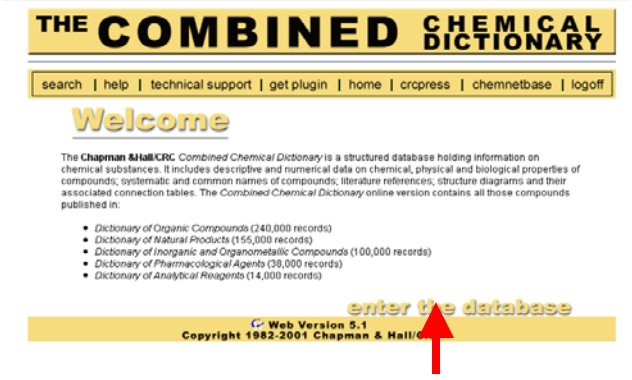
Action:

- Click on Combined Chemical Dictionary (CCD) This will take you to Fig. 3.

Note:

- CHEMnetBASE provides access to several databases, including the Combined Chemical Dictionary (CCD) and the Properties of Organic Compounds (POC).

Figure 3. The Combined Chemical Dictionary Database



You must have a SUNetID and password to fully use any of the databasesAction:

Action:

- Click on **Enter the Database** (bottom right of page) to go to the main search page.

Note:

- Use navigation buttons within CCD rather than the back button of the browser.

- Be sure to logoff when finished searching so others cannot use your account.

CCD via CHEMnetBASE for Identifying Unknowns

Figure 4. The Combined Chemical Dictionary Main Search Page

Actions:

- **Use Scroll bar on right** to view search options.
- **Click on Browse Index** to see values stored in an index.
- **Click on Help Button** at top to view information about searching the CCD.

Note:

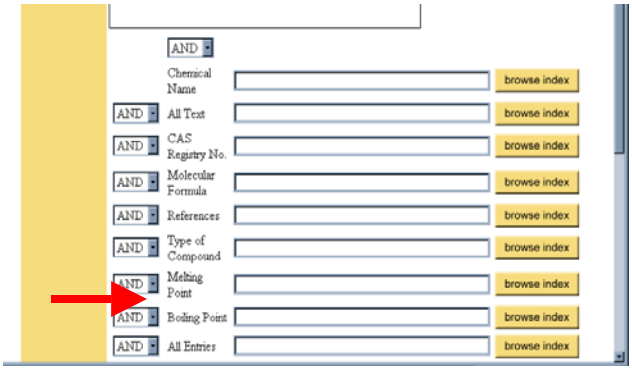
- This is the main search page that you see after entering the CCD.
- The structure drawing workspace is a box near the top of the page that states *Query Not Defined* if no structural data has been entered.
- A structure drawing plug-in is needed in order to do structure searches.
    - If the plug-in has been installed on your workstation, the upper left corner of the structure searching workspace will have a gray box that is labeled *Draw Query*.
    - If the plug-in has not been installed, the upper left corner of the structure searching workspace will have a small box with an x in it.

Note:

- The most common types of searches performed in CCD by Chem. 130 students:
    - *Melting point* or *boiling point*
    - *Molecular Weight*
    - *Molecular formula*
        - *Specifying heteroatoms*
    - *Structural fragments*
    - *CAS Registry number*
    - *Color, appearance, smell*
- While *Type of Compound* is a search option, none of the compound classes you might expect to see are listed. (Click on Browse Index to see what values are present.)
- See FAQ for CCD for information about additional search options, such as:
    - *Specifying range of occurrence for certain elements*
    - *Isolating a ring*
    - *PKa*
    - *Refractive Index*
    - *Physical description such as color or odor*
- Read on to see step-by-step instructions for doing the most common types of searches.

CCD via CHEMnetBASE for Identifying Unknowns

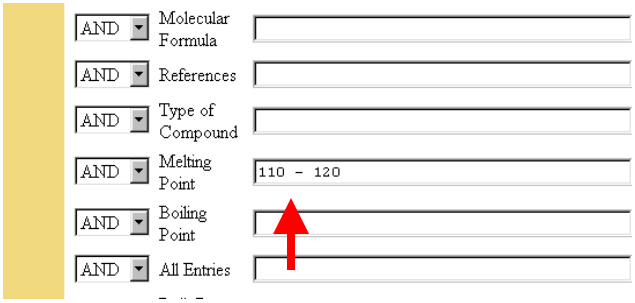
Figure 5. Melting Point and Boiling Point Search Fields



Action:

- To conduct a search based on melting point or boiling point, **use side scroll bar on the right to scroll down until the search boxes for the Melting Point or Boiling Point Search Fields are visible**

Figure 6. Entering a Range of Melting Points



Action:

- **Enter melting point range** (+/- 5 deg C from the measured value). Confirm with a TA you are within range before entering.

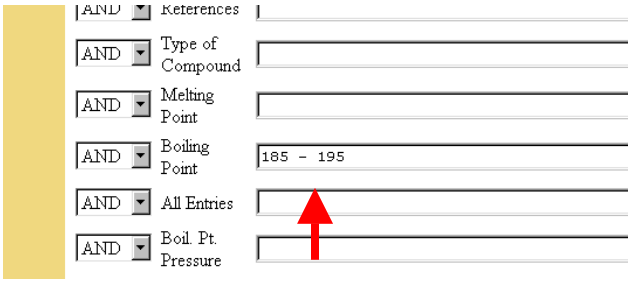
Note:

- There must be a space before and after the hyphen.

Example:

- For example, if the measured melting point were 115 deg C, the range you would enter would be 110 – 120.

Figure 7. Entering a Range of Boiling Points



Action:

- **Enter boiling point range** (+/- 5 deg C from the measured value). Confirm with a TA you are within range before entering.

Note:

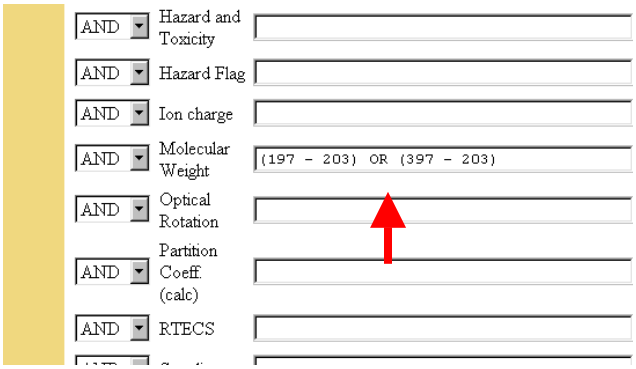
- There must be a space before and after the hyphen.
- For some compounds in CCD, boiling point data are reported at reduced pressure (via subscript notation). For example**:** $Bp_{0.4}$ 120° would be the boiling point at 0.4 mm of mercury. The normal boiling point at 1 atm (=760mm mercury) would appear without any subscript.

Example:

- If the measured boiling point was 190 deg C, the range you would enter is 185 – 195.

CCD via CHEMnetBASE for Identifying Unknowns

Figure 8. Entering Equivalent Weight Data in the Molecular Weight Search Field



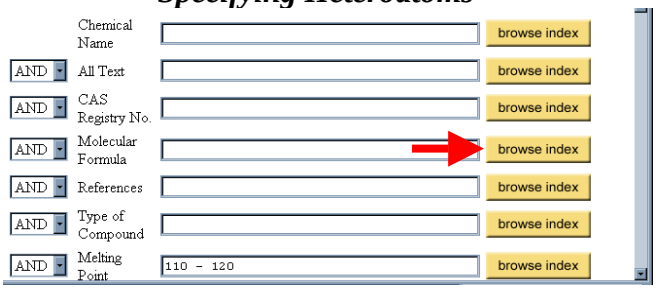
Action:

- **Convert equivalent weight into possible molecular weights and enter values into molecular weight search field.**
  - Multiply equivalent weight by one and by two to get the two possible molecular weights for your unknown.
  - Add +/- 3 grams to each equivalent weight in order to create a range for searching each equivalent weight value.
  - Enter a range for each equivalent weight,
    - There must be a space before and after the hyphen.
    - Surround numbers of each range in parentheses.
    - Put an OR between each range.

Example:

- Equivalent weight in lab was 200. Thus, the search strategy to cover all the mono and diacid possibilities is: (197 – 203) OR (397 – 403)

Figure 9. Molecular Formula Search: Specifying Heteroatoms



Action:

- Click on **Browse Index** button for Molecular Formula.

Note:

- If you have molecular formula information, such as knowing that the compound has only C, H, and O atoms present, you can use this information to narrow down a search.

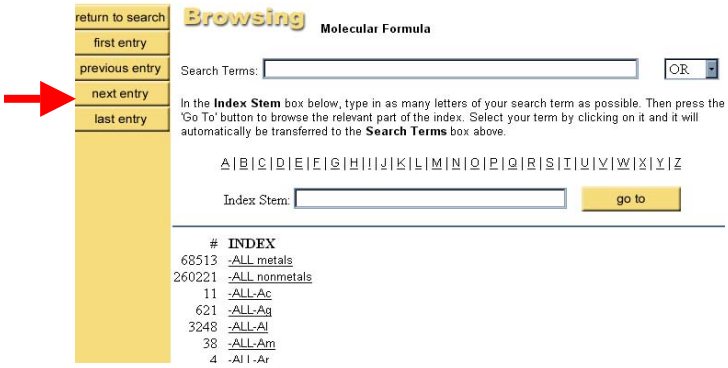
- Element symbols in the Molecular Formula index are case-sensitive.

Example:

- Using the example above of melting point in the range of 110 - 120 deg C, one can add molecular formula information to help narrow results.

CCD via CHEMnetBASE for Identifying Unknowns

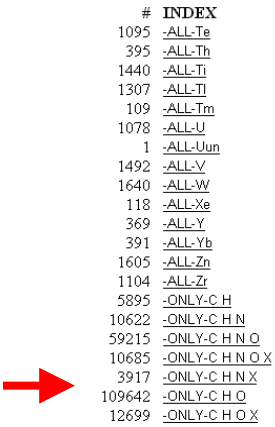
Figure 10. Browsing the Molecular Formula Index



Action:

- After pressing the Browse Index button, **click on next entry** to view the next "page" in the Molecular Formula Index.

Figure 11. Browsing Formula Index Until Seeing Entries that Specify Heteroatoms



Action:

- After pressing *next entry* button, **scroll down to the middle of the second page** until you see entries that specify all heteroatoms present in a formula.
- **Click on an entry to copy it to the Search Terms box**.

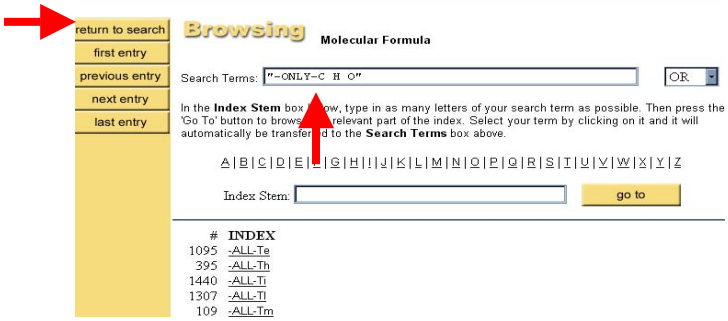
Note:

- If you browse the Molecular Formula Index, you will discover that it begins by listing all compounds that contain a certain element. Next in the list are compounds that only contain certain heteroatoms. Entries containing exact formulas follow entries for heteroatoms.
- In the entries for heteroatoms, the symbol X is used to denote a Halogen.

Example:

- If you are trying to limit a search to substances that only contain Carbon, Hydrogen, and Oxygen, then click on - ONLY-C H O.

Figure 12. Returning to Main Search Page After Browsing the Molecular Formula Index and Selecting a Search Term



Action:

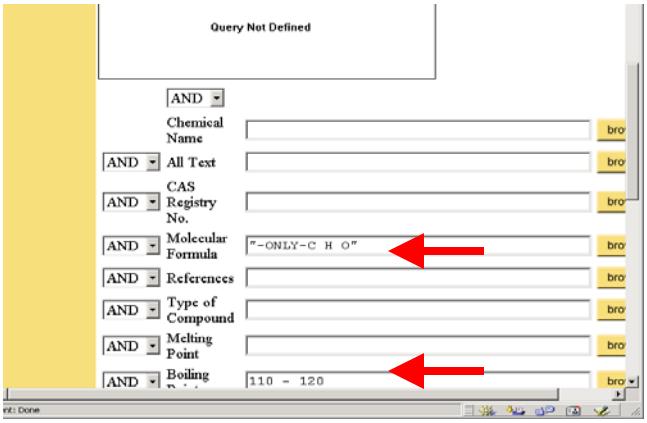
- **Scroll up to top of Browsing an Index page and click on Return to Search button in upper left corner of the screen**.

Note:

- Check search term box to make sure that one copy of selected term is in the Search Terms box.

CCD via CHEMnetBASE for Identifying Unknowns

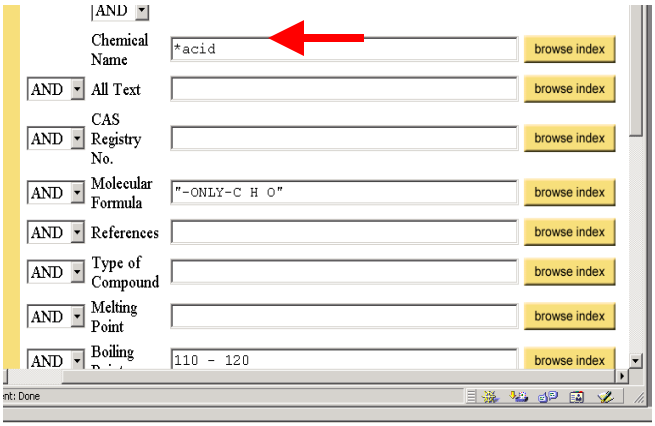
Figure 13. Viewing Terms Found by Browsing an Index on the Search Page



Action:

- **Make sure values in search term boxes are correct**.

Figure 14. Chemical Name Fragment Searching



Action:

- **Enter name fragment adding wild card characters as needed**.

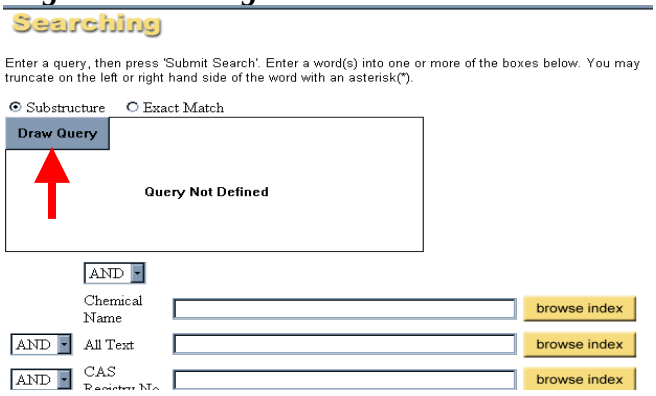
Note:

- You may use ***** as a wild card to indicate any number of characters and a **?** to indicate only one character.
- The * can be used at the beginning, anywhere in the middle, or at the end of a search term.
- Only use name fragment searching for identifying unknowns in cases where the nomenclature is consistent for a class of compounds.

Example:

- Enter ***acid** to find compounds that have “acid” as part of their name.

Figure 15: Adding a Substructure to a Search



Action:

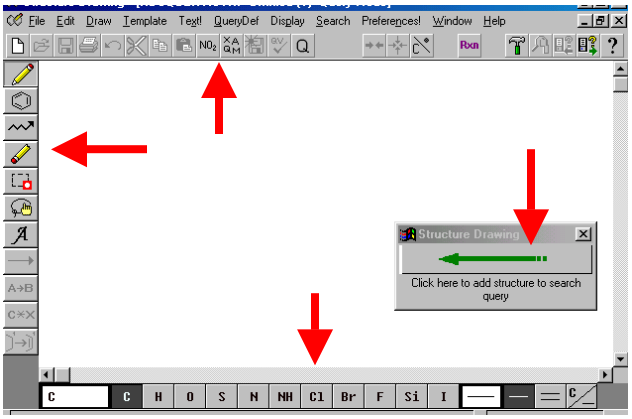
- Click on **Draw Query** button.

Note:

- Get CHEMnetBASE structure drawing plug-in if a small box with an x in it is present rather than a Draw Query button.

CCD via CHEMnetBASE for Identifying Unknowns

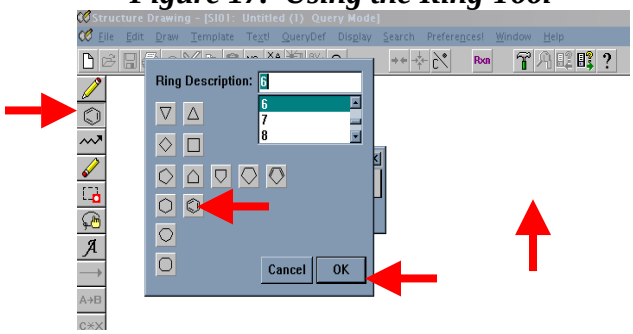
Figure 16: Main Structure Drawing Screen



Note:

- The structure drawing screen consists of :
  - Drawing workspace (large white interior area of screen)
  - Drawing palette (on left of screen) that contains tools for drawing structures (pencil, ring tool, chain tool, eraser, highlighter, lasso)
  - Common atoms and bonds (on bottom of screen)
  - Toolbar for frequently used functions and commands (at top of work space)
  - Menu bar for drawing, filing, editing, and displaying a structure (at top of structure drawing screen)
- After finished drawing structure, press green arrow (in box on workspace) to return to main search page.

Figure 17. Using the Ring Tool



Example:

- Add a benzene ring to your search.

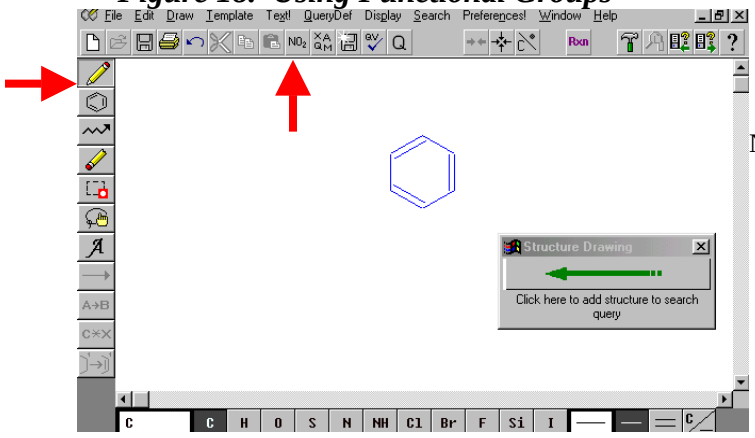
Action:

- Click on **Ring Tool**. Screen at left will appear.
- **Choose image of ring** desired or scroll down window in upper right to choose size of ring.
- Click the **OK** button.
- Next, move cursor (which has turned into hexagon with a + sign in center) to work space and **click again** to paste the ring into drawing workspace.

Note:

- See *Ring Isolation* in FAQ for CCD if you need to search a ring that is not fused to another ring.

Figure 18. Using Functional Groups



Action:

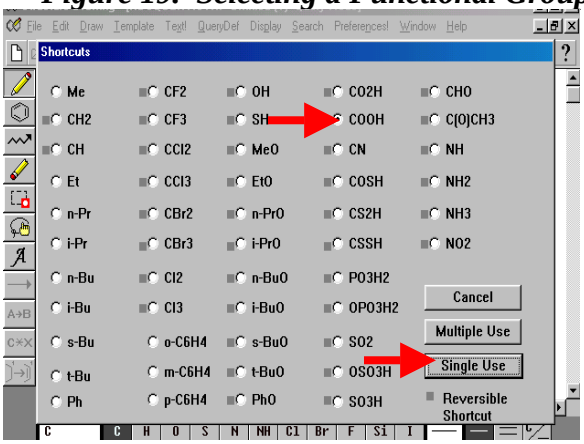
- Click on **Pencil tool** (at left of screen).
- Click on **NO2 icon** (at top of screen) to add a functional group to your search.

Note:

- NO2 icon lists common functional groups.
- XAQM icon lists common system defined variables.
  - X = Halogen
  - A = Any element except Hydrogen
  - Q = Any element except Carbon or Hydrogen
  - M = Any Metal

CCD via CHEMnetBASE for Identifying Unknowns

Figure 19. Selecting a Functional Group



Example:

- Search for carboxylic acids.

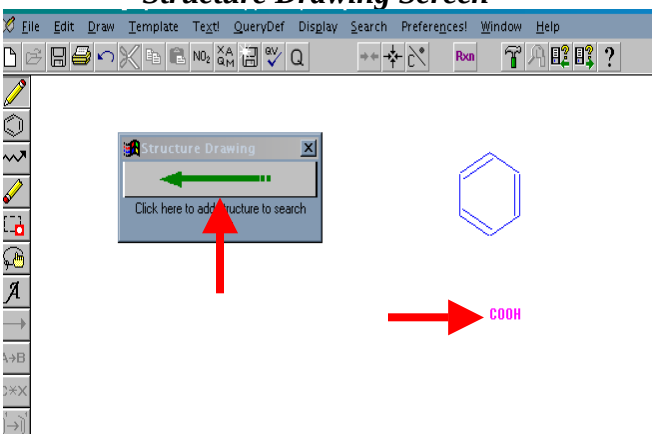
Action:

- Click on **white dot in front of COOH.**
- Click **Single Use** to place one copy of functional group on drawing screen.

Note:

- Using one copy of a functional group in your search will retrieve substances that have one or more occurrences of functional group present in structure.
- Some shortcuts for functional groups are ambiguous, e.g. CHO. Completely draw functional group if this problem occurs.

Figure 20. Adding a Functional Group to the Structure Drawing Screen



Action:

- **Next, click on drawing workspace** to add functional group to your search strategy.
- After finishing drawing structural fragments, **click on large green arrow** to return to main search screen.

Note:

- Do not attach fragments together unless you are sure that they are connected to one another.
- Searching disconnected structural fragments will retrieve compounds that have all fragments in them.

Example:

- Screen shown in Figure 20 will search for carboxylic acids which contain benzene ring(s).

Figure 21: Performing a Search

Action:

- **Press Submit Search** button to perform search. This will produce a list of "hits".

Note:

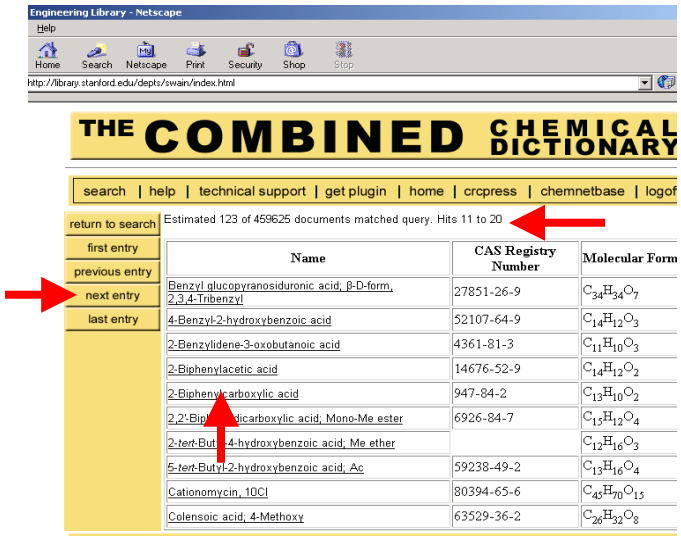
- Before submitting search, verify that all terms and structures that you want to be included in the search appear on the screen.

Example:

- Screen in Figure 21 will search for compounds that melt between 110 - 120 degrees C., only have elements C, H, and O present in the molecular formula, and contain at least one benzene ring and one carboxylic acid.

CCD via CHEMnetBASE for Identifying Unknowns

Figure 22. Viewing Search Results: Brief Display



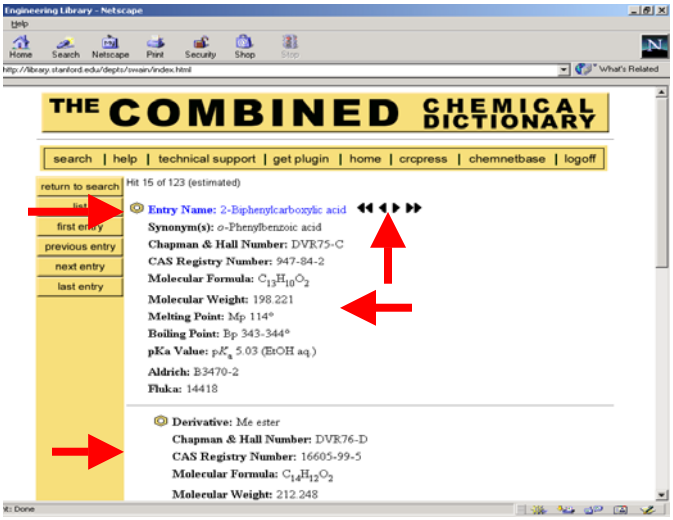
Action:

- **Click on next entry** to view 2nd page of list, and **Click on name** of compound to view full display (Eg., 2-biphenylcarboxylic acid).

Note:

- Total number of records retrieved in search results is listed at top of page.
- Navigation buttons for viewing answer set are at left side of screen.
- Brief display from each record includes substance name, CAS (Chemical Abstracts) Registry Number, and molecular formula.
- Substance names are hypertext linked. Click on name of compound to view full record.

Figure 23. Viewing Record in Full Display



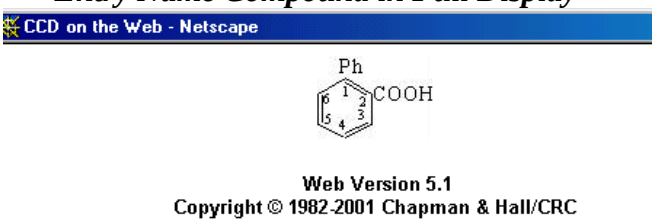
Action:

- **View record in full display** to see if it is of interest.

Note:

- Each record contains a "parent compound" and selected derivatives. It is possible that your parent unknown compound is listed as a derivative in CCD. The name of the specific substance name your search matched on is highlighted in blue.
- Small benzene ring to left of a chemical name is a hypertext link to the structure for that substance.
- Selected physical properties are listed for each compound.
- CAS Registry Number is also frequently included for a substance. Using this number is an excellent way to find more information about this substance in another database.
- Black navigation arrows to right of "hit" chemical name can be used to go to other records in an answer set.

Figure 24. Viewing Hyperlinked Structure of Entry Name Compound in Full Display



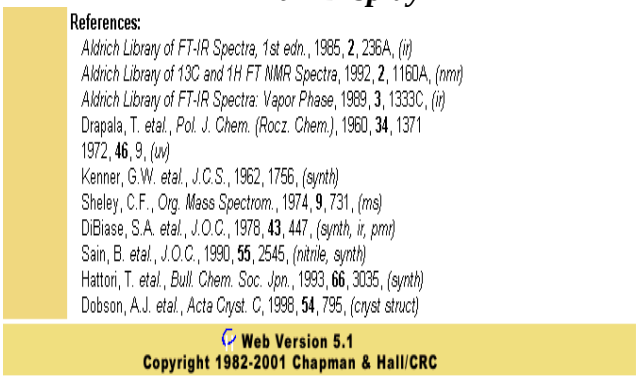
Action:

- **Click on benzene ring icon** to left of a chemical name. A structure display like the one on the left will appear.

- If you click on a structure link for a *Derivative*, not only will the structure appear but also a link to *Draw Query* that would enable you to modify structure for a new substructure search.

CCD via CHEMnetBASE for Identifying Unknowns

Figure 25. Viewing References in Full Display



Action:

- You can look up references to synthesis papers. They frequently give descriptions of substances.

Note:

- Each citation contains: author, abbreviated name of source where research was published, publication year, volume, page, and in parentheses a brief notation as to content of article. Ask Library TA or library staff for help deciphering abbreviations for sources.

- Swain shelves all journals alphabetically by title.