

POC via CHEMnetBASE for Identifying Unknowns

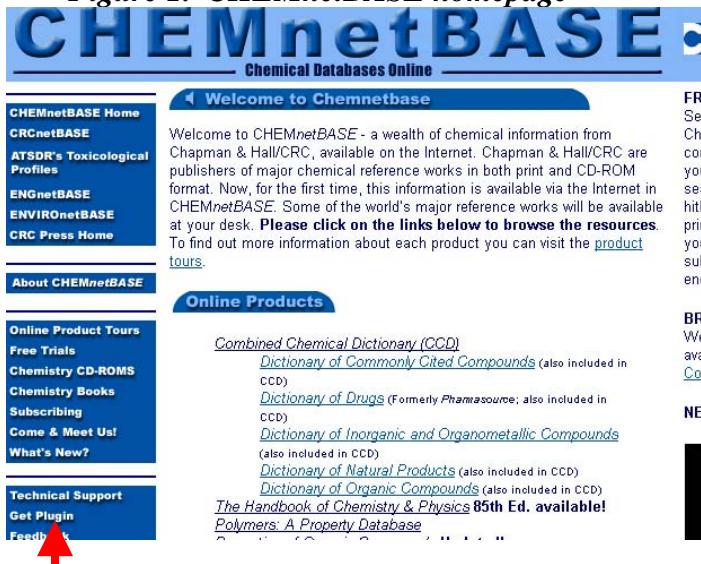
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Note: A red arrow is used to identify where buttons and functions are located in CHEMnetBASE.

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Figure 1. CHEMnetBASE homepage



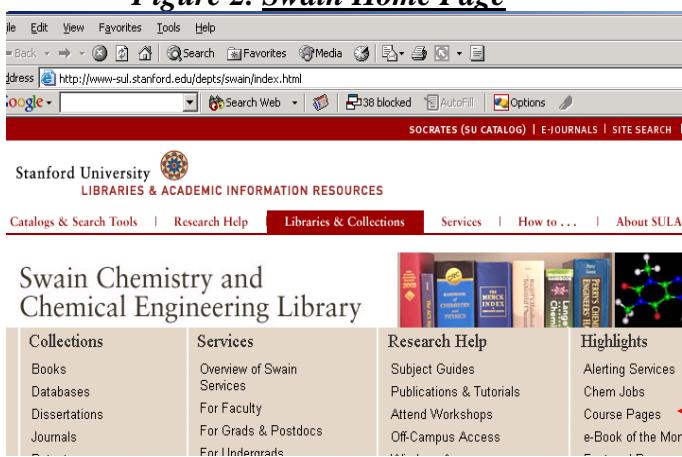
The screenshot shows the CHEMnetBASE homepage. The main content area is titled 'Welcome to Chemnetbase' and discusses the availability of chemical information from Chapman & Hall/CRC. Below this, there is a section titled 'Online Products' listing various chemical dictionaries and databases. The sidebar on the left contains links for 'CHEMnetBASE Home', 'CRCnetBASE', 'ATSDR's Toxicological Profiles', 'ENGnetBASE', 'ENVIRONetBASE', 'CRC Press Home', 'About CHEMnetBASE', 'Online Product Tours', 'Free Trials', 'Chemistry CD-ROMS', 'Chemistry Books', 'Subscribing', 'Come & Meet Us!', 'What's New?', 'Technical Support', 'Get Plugin' (with a red arrow pointing to it), and 'Feedback'.

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.

- You must have a SUNetID and password to fully use any of the databases.

Figure 2. Swain Home Page



The screenshot shows the Swain Home Page. The top navigation bar includes links for 'File', 'Edit', 'View', 'Favorites', 'Tools', and 'Help'. The main content area is titled 'Swain Chemistry and Chemical Engineering Library' and features a grid of links for 'Collections', 'Services', 'Research Help', and 'Highlights'. The 'Highlights' section includes links for 'Alerting Services', 'Chem Jobs', and 'Course Pages' (with a red arrow pointing to it). The bottom navigation bar includes links for 'Catalogs & Search Tools', 'Research Help', 'Libraries & Collections', 'Services', 'How to...', and 'About SULA'.

Action:

- Go to the Swain Library home page: [Swain Library homepage](http://www-sul.stanford.edu/depts/swain/) at www-sul.stanford.edu/depts/swain/

Click on Course Pages, then click on the [Chemistry 130: Library Resources for Identifying Unknowns](#).

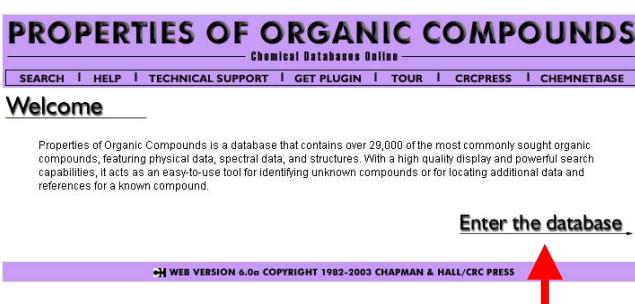
Action:

- Click on [Properties of Organic Compounds \(POC\)](#). 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. Properties of Organic Compounds Database



The screenshot shows the Properties of Organic Compounds Database homepage. The main title is 'PROPERTIES OF ORGANIC COMPOUNDS' and the subtext is 'Chemical Databases Online'. The top navigation bar includes links for 'SEARCH', 'HELP', 'TECHNICAL SUPPORT', 'GET PLUGIN', 'TOUR', 'CRCPRESS', and 'CHEMNETBASE'. The 'Welcome' section provides a brief description of the database. At the bottom of the page, there is a large red button with the text 'Enter the database' (with a red arrow pointing to it).

Action:

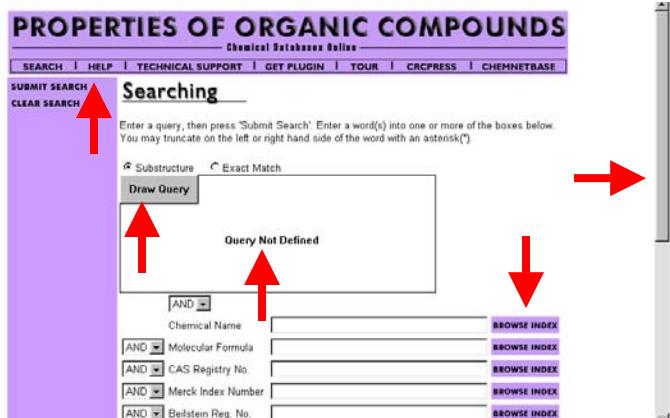
- Click on **Enter the Database** (bottom right of page) to go to the main search page (Fig 4).

Note:

- Use navigation buttons within POC rather than the back button of browser.
- Be sure to logoff after finishing searching in the library so that others cannot use your account.

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Figure 4. Properties of Organic Compounds Main Search Page



Actions:

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

Note:

- The structure drawing workspace is a box near the top of the page that states *Query Not Defined* in the center, if no structural data have been entered.
- A structure drawing plug-in is needed in order to search using structural data.
 - 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.
 - A link to download the plug-in has already been given above.
- The most common types of data entered in POC by Chem. 130 students are:
 - *Melting point or boiling point*
 - *Equivalent Weight*
 - *Spectral Peak values*
 - *Molecular formula information*
 - *Substructure information*
 - *CAS Registry number*
- See “Help” for POC for information about additional search options, such as:
 - *Specifying a range of occurrence for certain elements*
 - *Isolating a ring*
 - *PKa*
 - *Refractive Index*
- Read on to see step-by-step instructions for doing the most common types of searches.

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Figure 5. Melting Point and Boiling Point Search Fields

AND
Chemical Name | BROWSE INDEX
AND Molecular Formula | BROWSE INDEX
AND CAS Registry No. | BROWSE INDEX
AND Merck Index Number | BROWSE INDEX
AND Beilstein Reg. No. | BROWSE INDEX
AND Molecular Weight | BROWSE INDEX
AND Melting Point | BROWSE INDEX
AND Boiling Point | BROWSE INDEX
AND Density | BROWSE INDEX

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 Melting Point Range

AND CAS Registry No. | BROWSE INDEX
AND Merck Index Number | BROWSE INDEX
AND Beilstein Reg. No. | BROWSE INDEX
AND Molecular Weight | BROWSE INDEX
AND Melting Point | 110-120 | BROWSE INDEX
AND Boiling Point | BROWSE INDEX
AND Density | BROWSE INDEX
AND Refractive Index | BROWSE INDEX
AND Specific Rotation | BROWSE INDEX

Action:

- Enter a **melting point range** (+/- 5 deg C from the measured value). Confirm with a TA that you are within the correct range for your unknown before trying to find your unknown in the databases.

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 Boiling Point Range

AND Merck Index Number | BROWSE INDEX
AND Beilstein Reg. No. | BROWSE INDEX
AND Molecular Weight | BROWSE INDEX
AND Melting Point | BROWSE INDEX
AND Boiling Point | 185 - 195 | BROWSE INDEX
AND Density | BROWSE INDEX
AND Refractive Index | BROWSE INDEX
AND Specific Rotation | BROWSE INDEX

Action:

- Enter **boiling point range** (+/- 5 deg C from the measured value). Confirm the range with a TA before searching for an unknown.

Note:

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

Example:

- For example, if the measured boiling point was found to be 190 deg C, the range entered would be 185 – 195.

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

Chemical Name
AND Molecular Formula
AND CAS Registry No.
AND Merck Index Number
AND Beilstein Reg. No.
AND Molecular Weight (197 - 203) OR (397 - 403)
AND Melting Point
AND Boiling Point
AND Density
AND Refractive Index
AND Specific Rotation
BROWSE INDEX
BROWSE INDEX

Action:

- Convert equivalent weight into possible molecular weights and enter values into molecular weight search field.
 - To allow that you might have a diacid, multiply the equivalent weight by 1 and by 2 to get the two possible molecular weights.
 - Add +/- 3 grams to each equivalent weight in order to create a range for searching each equivalent weight.
 - Enter the range for each equivalent weight,
 - There must be a space before and after the hyphen.
 - Surround numbers of each range with parentheses.
 - Put an OR between each range.

Example:

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

Action:

POC can accept data from 6 different kinds of spectral methods. IR AND HNMR entries are used for illustration here. **Enter a range for a few significant spectral peaks** (use ~ +/- 20 wave numbers from the measured value for IR, and remember to put a space on both sides of the hyphen). Surround the ranges in parentheses if searching more than one range. Use AND between ranges. See Fig. 9.1.

Note:

- If you narrow the range too much, you may miss your compound.
- **Warning:** do not be misled by published spectral data. Your IR and NMR spectral data may not be identical to literature values, if obtained in different solvents or physical states and/or under different instrumental conditions.

Example:

- For an IR spectrum with peaks at 2800 and 1400, search 2 ranges of ~ +/- 20 wave numbers, ie.
 - (2780 – 2820) AND (1380 – 1420)
- For an HNMR spectrum with peaks at 1.4 and 7.2 ppm, search 2 ranges of ~ +/- 0.2 ppm, ie
 - (1.2 – 1.6) AND (7.0 – 7.4)

Figure 9.1 Enter IR Spectral Peak Data

AND Density
AND Refractive Index
AND Specific Rotation
AND Mass Spectral Peaks
AND Infrared Peaks (2780 - 2820) AND (1380 - 1420)
AND Raman Peaks
AND Ultraviolet Peaks
AND ¹H NMR Peaks
AND ¹³C NMR Peaks
AND All Entries
BROWSE INDEX
BROWSE INDEX

Figure 9.2 Enter HNMR Spectral Peak Data

AND Beilstein Reg. No.
AND Molecular Weight
AND Melting Point
AND Boiling Point
AND Density
AND Refractive Index
AND Specific Rotation
AND Mass Spectral Peaks
AND Infrared Peaks
AND Raman Peaks
AND Ultraviolet Peaks
AND ¹H NMR Peaks (1.2-1.6) AND (7.0-7.4)
AND ¹³C NMR Peaks
BROWSE INDEX
BROWSE INDEX

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Figure 10. Molecular Formula Data: Specifying Heteroatoms

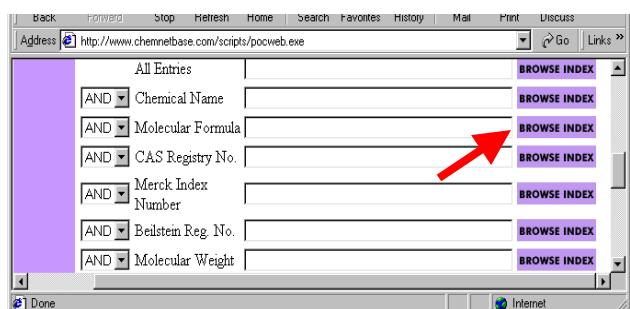


Figure 11. Browsing the Molecular Formula Index, Selecting a Term, and Returning to Main Search Page

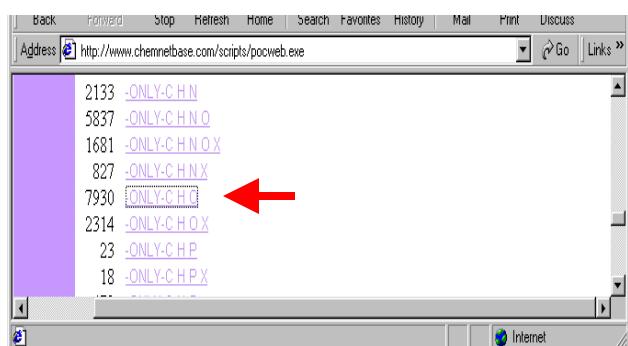
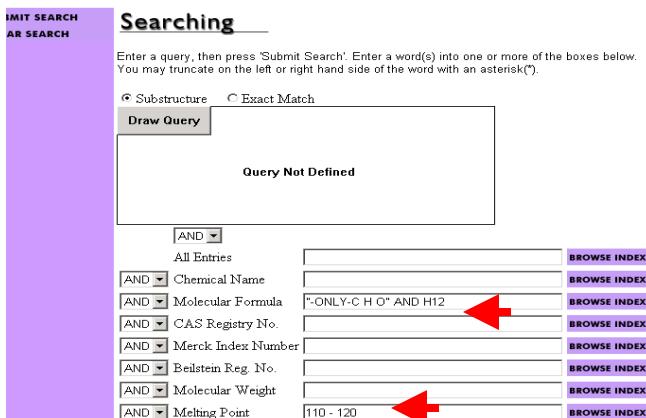


Figure 12. Viewing Terms Found by Browsing an Index on Search Page



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

Note:

- If you have molecular formula information, such as knowing that only C, H, and O atoms are present, you can use this information to narrow down the search.
- Element symbols in the Molecular Formula index are case sensitive.

Example:

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

Action:

- After clicking on Browse Index, scroll down until you can read entries starting with -ONLY. If your unknown compound has only C, H, and O, click on -ONLY-C H O. Scroll back to the top of the page, and make sure only that entry is copied to the Search Terms box.
- Then click **RETURN TO SEARCH**.

Note:

- In the entries for molecular formula, the symbol X is used to denote a Halogen, such as Br.

Note:

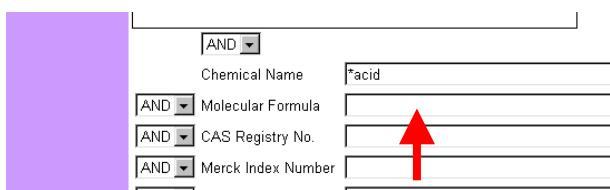
- If you also have information such as the number of Hydrogens in your unknown (from HNMR), you can enter this information into the molecular formula field as well. For example, if your unknown was known to have 12 Hydrogens you would put the cursor after the -ONLY-C H O, then hit space, and type in **AND H12**. It should look as shown in Fig. 12.

Action:

- Make sure the entries in the search term boxes are correct.

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Figure 13. Entering Chemical Name Fragments



- 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.

Action:

- Click on **Draw Query** button.

Note:

- Get CHEMnetBASE structure drawing plug-in if a box with an x in it is present rather than a Draw Query button (see page 2).

Figure 14. Adding a Substructure to a Search

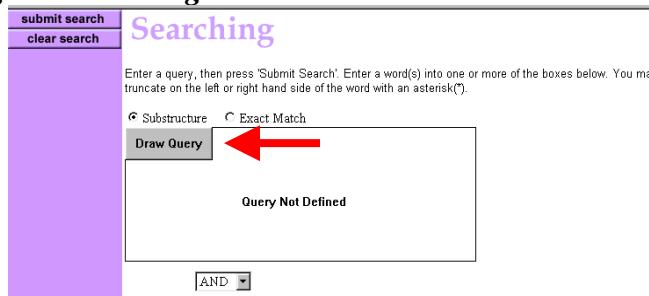
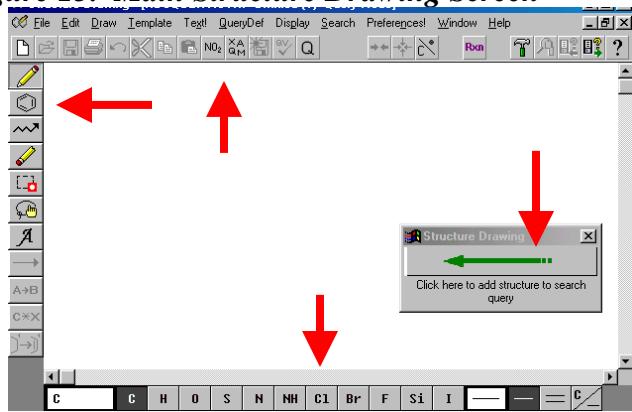


Figure 15. Main Structure Drawing Screen

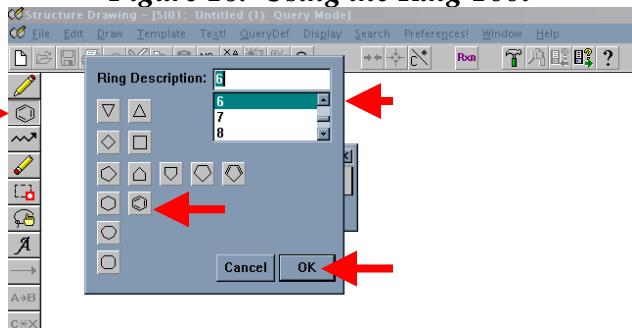


Note:

- The structure drawing screen consists of :
 - Drawing workspace for structure (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.

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Figure 16. Using the Ring Tool



Example:

- Add a benzene ring to drawing workspace.

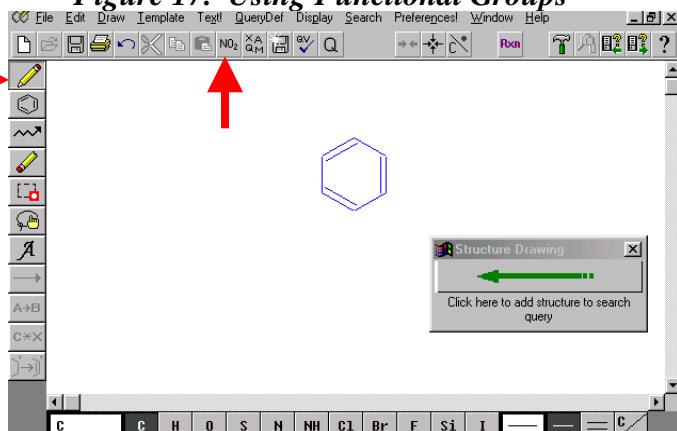
Action:

- Click on **Ring Tool** (on toolbar at left). Box will open that contains Ring Descriptions.
- 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 POC if you need to search a ring that is not fused to another ring.

Figure 17. Using Functional Groups



Example:

- Add a carboxylic acid group to drawing workspace.

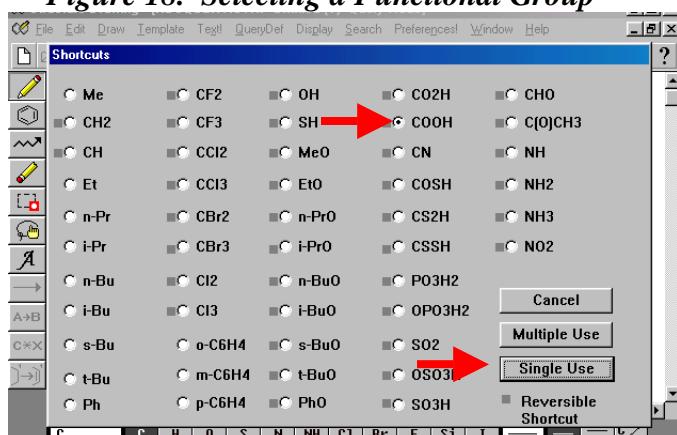
Action:

- 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

Figure 18. Selecting a Functional Group



Action:

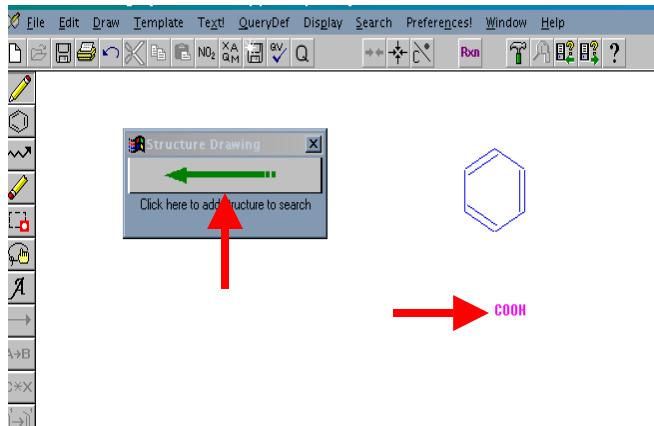
- Click on **white dot in front of COOH**.
- Click **Single Use** to place one copy of functional group on drawing screen.

Note:

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

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Figure 19. Adding Functional Group to Structure Drawing Screen



Action:

- Next, click on drawing workspace to add functional to your search strategy.
- When 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:

- Search benzene ring and carboxylic acid.

Figure 20. Performing a Search

The screenshot shows the CHEMnetBASE search interface. On the left, there are buttons for 'submit search' and 'clear search'. The main area is titled 'Searching' and contains a 'Draw Query' section. The search query is set to 'AND'. The query consists of a benzene ring and a carboxylic acid group (COOH). Below the query, there are several search criteria listed as 'AND' conditions: Chemical Name, CAS Registry No., Molecular Formula (set to "-ONLY-C H O"), Molecular Weight, Melting Point (set to 110 - 120), and Boiling Point. Each condition has an associated text input field.

Action:

- Press Submit Search button to perform search.

Note:

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

Example:

- A compound that contains at least one benzene ring and one carboxylic acid, has only Carbon, Hydrogen, and Oxygen present in the molecular formula, and melts between 110-120 deg C, would be entered as shown on the left.

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Figure 21. Viewing Search Results: Brief Display

PROPERTIES OF ORGANIC COMPOUNDS

search | help | technical support | get plugin | home | crcpress | chemnetbase | logoff

return to search | 25 of 28873 documents matched query. Hits 21 to 25

Name	CAS Registry Number	Molecular Formula
[1,1'-Biphenyl]-4-butanoic acid	6057-60-9	C ₁₆ H ₁₆ O ₂
[1,1'-Biphenyl]-2-carboxylic acid	947-84-2	C ₁₃ H ₁₀ O ₂
2-Naphthylsuccinic acid, 3,4-dihydro-	22440-38-6	C ₁₁ H ₁₀ O ₂
Propanoic acid, 2-phenoxy-, (±)-	1912-21-6	C ₉ H ₁₀ O ₃
Propanoic acid, 2-phenoxy-	940-31-8	C ₉ H ₁₀ O ₃

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Figure 22. Viewing Record in Full Display

return to search | Hit 22 of 25

Name: [1,1'-Biphenyl]-2-carboxylic acid
 Synonym: 2-Biphenylcarboxylic acid 2-Carboxybiphenyl Diphenyl-2-carboxylic acid
 2-Phenylbenzoic acid *o*-Phenylbenzoic acid
 Molecular Formula: C₁₃H₁₀O₂
 Line Formula: 2-(HO₂)C₆H₄C₆H₃
 CAS Registry Number: 947-84-2
 Beilstein Registry Number: 974075
 Beilstein Reference: 4-09-00-02472
 Molecular Weight: 198.217
 Color/Crystalline Form: lf (dil al)
 Melting Point (°C): 114.3
 Normal Boiling Point (°C): 343.5
 Solubility In Common Solvents: H₂O 1, EtOH 4, bz 4, HOAc 4
 Solution Properties: pK = 3.46 @ 25°C
 Infrared Peaks (cm⁻¹): 3060 2880 1700 1680 1600 1580 1570 1500 1480 1450 1440 1410 1400 1290 1260 1140 1090 1070 1010 920 800 770 750 700 650 610 580 540 510 410 350
 Ultraviolet Peaks (nm): 238(5570) MeOH/KOH
¹H NMR Peaks (ppm): 7.3 7.3 7.9 11.8 CDCl₃

Figure 23. Viewing Hyperlinked Structure for Compound in Full Display

POC Server v6.0 - Netscape

Draw Query

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Action:

- Click on name of compound to view full display.

Note:

- Total number of records retrieved in search results is listed at top of page. Because the total is estimated, the total number of documents retrieved varies with each 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.

Action:

- View record in full display to see if it is of interest, and if the data matches that for your unknown.

Note:

- Clicking the benzene ring to left of the name will display the structure for the compound.
- Selected physical properties, often including spectral peaks, are listed for each compound.
- Solubility in Common Solvents: a relative scale of solubility is used.
 - 1=insoluble
 - 2=slightly soluble
 - 3=soluble
 - 4=very soluble
 - 5=miscible
 - 6=decomposes
- CAS Registry Number is frequently included for a substance. Using this number is an excellent way to find more information about this compound in other databases, as the way a name is entered into a database can vary.

Note:

- After clicking on a structure link (benzene ring icon to left of compound name), a display like the one on the left will appear.
- A link to *Draw Query* enables you to modify the structure for a new structure search.