

POC via CHEMnetBASE for Identifying Unknowns

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

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Figure 1. Swain Home Page



Action:

- Go to Swain Library home page: library.stanford.edu/depts/swain/index.html
- Click on CHEM 130/132 which contains *Library Resources for Identifying Unknowns* library.stanford.edu/depts/swain/chem130/chem130.html
- Download and install CHEMnetBASE structure drawing plug-in (HDS.exe). A link to download it is available in CHEMnetBASE. Go to "get plug-in" in CHEMnetBASE or go to *Searching Resources* section of the library page for Chem 130/132.
- To enter CHEMnetBASE, you can either select it from the Chem 130/132 page, use the pull down menu under *Chem & ChemE Databases* on the Swain Home Page and press **Go** button, or enter the url directly in your web browser www.chemnetbase.com

Figure 2. CHEMnetBASE Home Page



Action:

- Select **Properties of Organic Compounds (POC)** from the *CHEMnetBASE* home page (button is at top of page).

Note:

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

Figure 3. Properties of Organic Compounds Database



Action:

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

Note:

- Use navigation buttons within POC rather than back button of browser.
- Be sure to logoff when finished searching.

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Figure 4. Properties of Organic Compounds
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 POC.

Note:

- This is the main search page that you see after entering the POC.
- 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 blue 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 benzene ring.
- A link to download the plug-in is given in the *Searching Resources* section of the library page for Chemistry 130/132 and on CHEMnetBASE Home Page.

- Most common types of searches performed in POC by Chem. 130/132 students:
 - *Melting point or boiling point*
 - *Molecular formula*
 - *Specifying heteroatoms*
 - *Equivalent Weight*
 - *Spectral Peaks*
 - *Structural fragments*
- See FAQ for POC 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.

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Figure 5. Melting Point and Boiling Point Search Fields

The screenshot shows a search interface with a vertical purple bar on the left. The search fields are listed on the right, each with a dropdown menu and a search button. The fields are: Chemical Name, CAS Registry No., Molecular Formula, Molecular Weight, Melting Point, Boiling Point, Density, Refractive Index, and Specific Rotation. A red arrow points to the 'Melting Point' and 'Boiling Point' 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

The screenshot shows the search interface with the 'Melting Point' field containing the text '110 - 120'. A red arrow points to the 'Boiling Point' field.

Action:

- Enter melting point range (+/- 5 deg C from the measured value). Consult a Library TA for help.

Note:

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

Example:

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

Figure 7. Entering a Range of Boiling Points

The screenshot shows the search interface with the 'Boiling Point' field containing the text '185 - 195'. A red arrow points to the 'Boiling Point' field.

Action:

- Enter boiling point (+/- 5 deg C from the measured value). Consult a Library TA for help.

Note:

- There must be a space before and after the hyphen.
- For a small number of compounds in POC, boiling point data is reported at reduced boiling point pressure (via superscript notation). Consult library TA for help.

Example:

- For example, if the measured boiling point were 190 deg C, the maximum range you would enter is 185 - 195

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

AND	Molecular Formula	
AND	Molecular Weight	(197-203) OR (397-403)
AND	Melting Point	
AND	Boiling Point	

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.

Note:

- The molecular weight may be one or two times the equivalent weight for a compound.
- Add +/- 3 from the measured value. Consult Library TA for help for help.

Example:

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

Figure 9. IR Spectral Peak Data

AND	Melting Point	
AND	Boiling Point	
AND	Density	
AND	Refractive Index	
AND	Specific Rotation	
AND	IR	(2780-2820) AND (1380-1420)
AND	¹³ C NMR	
AND	¹ H NMR	
AND	UV	
AND	MASS SPEC	

Action:

- **Enter a range for a few significant spectral peaks** (maximum of +/- 20 wave numbers max. from the measured value).
- Place a **hyphen with a space on both sides** of range for peak.
- **Surround range in parentheses if searching more than one range. Use AND between ranges.**

Note:

- When searching spectral peaks, just input a few key peaks. Don't just search one value for each peak; search a range. Remember if you get too detailed you may limit yourself too much and miss what's in the database.
- Warning: do not be misled by published spectral data. Your IR and NMR spectral data will not be identical to literature values obtained in different solvents or physical states or under different instrumental conditions.

Example:

- For lab measurements of 2800 and 1400, search a range that includes +/- 20 wave numbers.
 - (2780 – 2820) AND (1380 - 1420)

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Figure 10. Molecular Formula Data: 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.

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

Action:

- **Click on an entry** to copy it to the Search Terms box.
- Make sure that only **one copy of selected term is in the Search Terms box.**
- Click on **Return to Search** button in upper left corner of the screen.

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

Action:

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

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Figure 13. Entering Chemical Name Fragments



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 14. Adding a Substructure to a Search



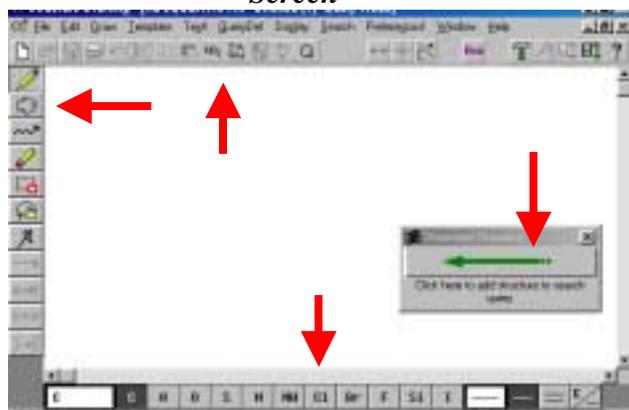
Action:

- Click on **Draw Query** button.

Note:

- Get CHEMnetBASE structure drawing plug-in if a 6-membered ring is present rather than a Draw Query button.

Figure 15. Main Structure Drawing Screen

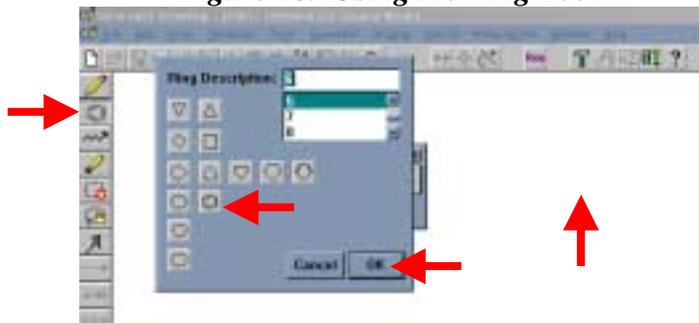


Note:

- 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



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.

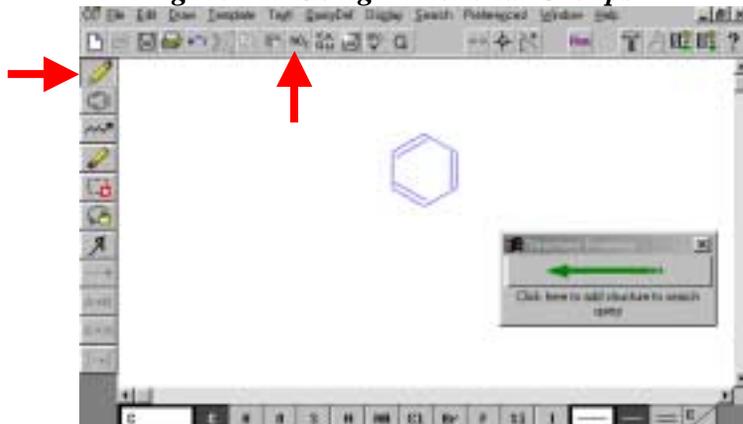
Note:

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

Example:

- Draw benzene ring.

Figure 17. Using Functional Groups



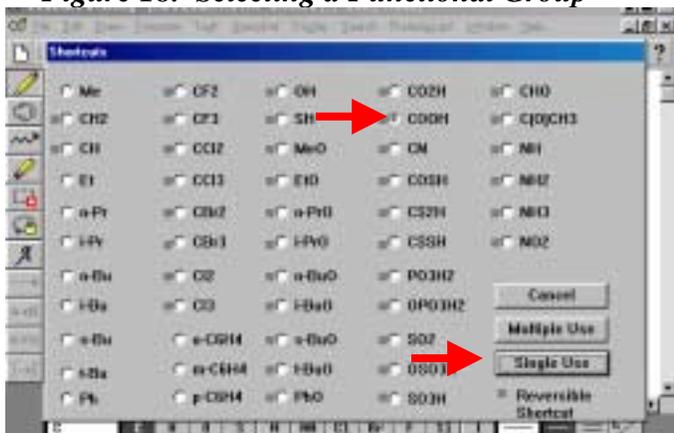
Action:

- 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

Figure 18. Selecting a Functional Group



Action:

- Click on **desired shortcut for functional group**.
- Click **Single Use** to place one copy of functional group on drawing screen.

Note:

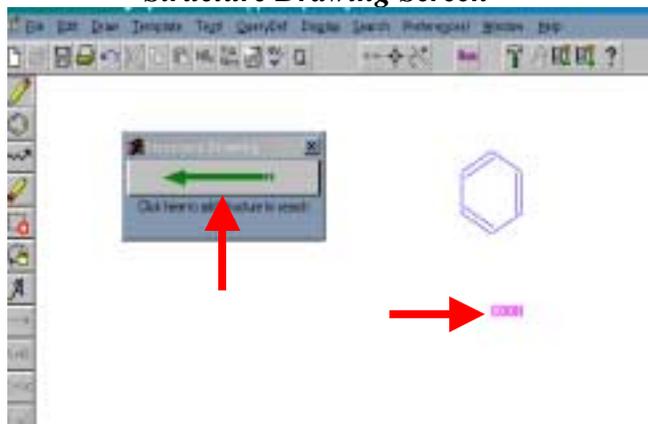
- Using one copy of a functional group in your search will retrieve substances that have one or more occurrences of the functional group present in a structure.
- Shortcuts for some functional groups are ambiguous, e.g. CHO. Completely draw functional group if this problem occurs.

Example:

- Search carboxylic acid.

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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



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:

- 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.

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Figure 21. Viewing Search Results: Brief Display

Name	CAS Registry Number	Molecular Formula
1,1'-Diphenyl-4-butanecarboxylic acid	5857-60-9	C ₁₉ H ₁₈ O ₂
1,1'-Diphenyl-2-carboxylic acid	947-34-2	C ₁₇ H ₁₄ O ₂
2-Naphthylacetic acid, 2,4-dihydroxy-	22490-38-6	C ₁₁ H ₁₀ O ₃
Propionic acid, 2-phenyl-	1972-21-6	C ₉ H ₁₀ O ₂
Propionic acid, 2-phenyl-	949-31-8	C ₉ H ₁₀ O ₂

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.

Figure 22. Viewing Record in Full Display

Name: 1,1'-Diphenyl-2-carboxylic acid
Synonyms: 2-Diphenylacetic acid; 2-Carboxyphenyl Diphenyl-2-carboxylic acid; 2-Phenylbenzoic acid; o-Phenylbenzoic acid
Molecular Formula: C₁₇H₁₄O₂
Line Formula: 2-(HO₂C)C₆H₄-C₆H₅
CAS Registry Number: 947-34-2
Beilstein Registry Number: 974073
Beilstein Reference: 4-18-18-42472
Molecular Weight: 198.217
Color/Crystalline Form: E (solid)
Melting Point (°C): 114.3
Normal Boiling Point (°C): 343.5
Solubility in Common Solvents: H₂O: 1, BOE: 4, to 4, HOAc: 4
Solution Properties: pH = 2.46 @ 25°C
Infrared Peaks (cm⁻¹): 3460, 2830, 1700, 1620, 1590, 1570, 1500, 1480, 1450, 1440, 1410, 1400, 1390, 1260, 1140, 1090, 1070, 1010, 920, 800, 770, 730, 690, 638, 618, 588, 548, 518, 410, 291
Ultraviolet Peaks (nm): 228(1070), 260(8000)
¹H NMR Peaks (ppm): 7.7, 7.5, 7.3, 7.1, 6.8, 6.6, 6.4, 6.2, 6.0, 5.8, 5.6, 5.4, 5.2, 5.0, 4.8, 4.6, 4.4, 4.2, 4.0, 3.8, 3.6, 3.4, 3.2, 3.0, 2.8, 2.6, 2.4, 2.2, 2.0, 1.8, 1.6, 1.4, 1.2, 1.0, 0.8, 0.6, 0.4, 0.2

Action:

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

Note:

- Clicking the benzene ring to left of the name will display the structure for the compound.
- Selected physical properties, 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 another database as the way a name is entered into a database varies.

Figure 23. Viewing Hyperlinked Structure for Compound in Full Display

A 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.