

DOC via CHEMnetBASE for Identifying Unknowns

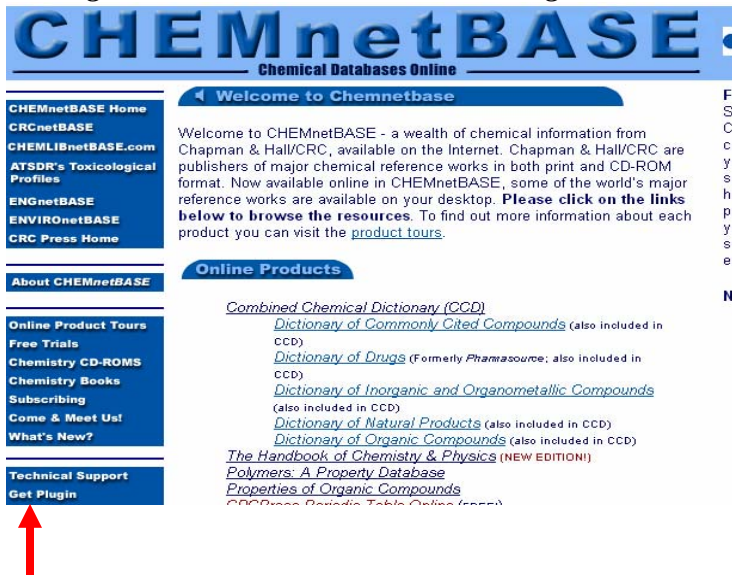
Table of Contents

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

<i>Figure</i>	<i>Description</i>	<i>Page</i>
<i>Entering The Combined Chemical Dictionary (CCD) Database</i>		
1	CHEMnetBASE Home Page	2
2	Swain Library Home Page	2
3	The Dictionary of Organic Compounds Database	2
4	The Dictionary of Organic Compounds Main Search Page	3
<i>Entering Melting Point or Boiling Point Data</i>		
5	Melting Point and Boiling Point Search Fields	4
6	Entering a Range of Melting Points	4
7	Entering a Range of Boiling Points	4
<i>Entering Equivalent Weight Data</i>		
8	Entering Equivalent Weight Data in the Molecular Weight Search Field	5
<i>Entering Molecular Formula Data</i>		
9	Molecular Formula Data: Specifying Heteroatoms	5
10	Browsing the Molecular Formula Index	6
11	Browsing Formula Index Until Seeing Entries that Specify Heteroatoms	6
12	Returning to Main Search Page After Browsing the Molecular Formula Index and Selecting a Search Term	6
13	Viewing Terms Found by Browsing an Index on the Search Page	7
<i>Entering Chemical Name Fragments</i>		
14	Entering Chemical Name Fragments	7
<i>Entering Substructures</i>		
15	Adding a Substructure to a Search	7
16	Main Structure Drawing Screen	8
17	Using the Ring Tool	8
18	Using Functional Groups	8
19	Selecting a Functional Group	9
20	Adding a Functional Group to the Structure Drawing Screen	9
<i>Searching DOC</i>		
21	Performing a Search	9
<i>Displaying Search Results</i>		
22	Viewing Search Results: Brief Display of First Page of Search Results	10
23	Viewing Next Page of Search Results	10
24	Viewing Compound Record in Full Display	11
25	Viewing Hyperlinked Structure of Entry Name Compound in Full Display	11
26	Viewing References in Full Display	11

DOC via CHEMnetBASE for Identifying Unknowns

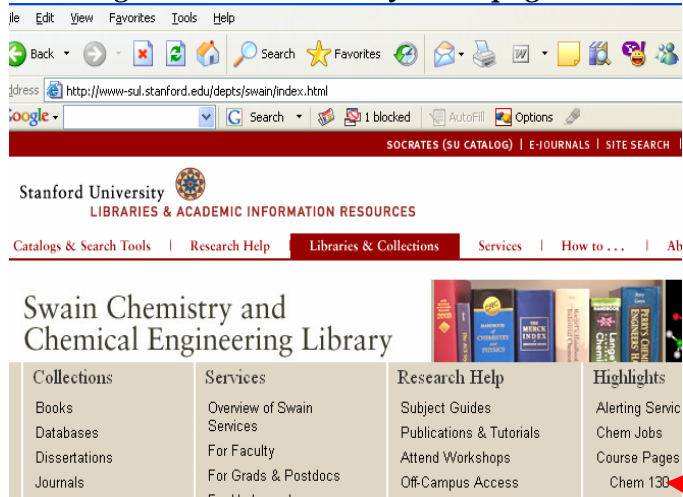
Figure 1. CHEMnetBASE Home Page



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. If you have already downloaded the plug-in for Properties of Organic Compounds, (POC), you do not have to do it again for Dictionary of Organic Compounds (DOC).

Figure 2. Swain Library home page



Action:

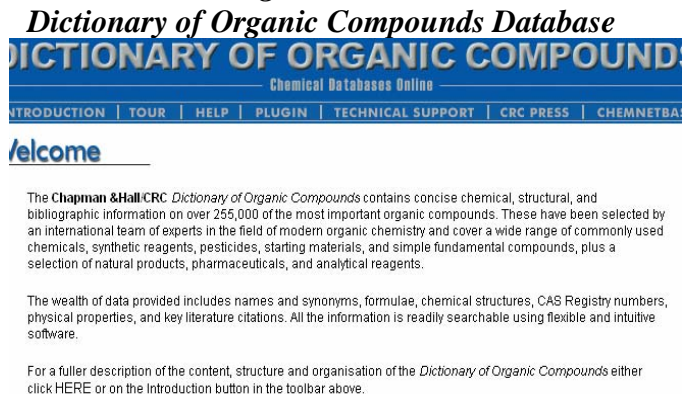
- Go to the Swain Library home page: [Swain Library homepage at www-sul.stanford.edu/depts/swain/](http://www-sul.stanford.edu/depts/swain/)

Click on Chem 130 (see red arrow in lower right corner of Fig. 2).

Action:

- Scroll down, and under Resources, click on [Dictionary of Organic Compounds \(DOC\)](#). This will take you to Fig. 3.

Figure 3. The



Action:

- Click on **Enter the Database** (bottom right of page in Fig. 3) to go to the main search page.

Note:

- Use navigation buttons within DOC rather than the back button of the browser.
- Be sure to logoff when finished searching in Swain Library so others cannot use your account.

➔ [Enter the database](#)

DOC via CHEMnetBASE for Identifying Unknowns

Figure 4. The Dictionary of Organic Compounds Main Search Page



Actions:

- Use Scroll bar on right to view search input variables available.
- Click on Browse Index to see values stored for any given index variable.
- Click on Help Button at top to view additional information about searching the DOC.

Note:

- The structure drawing workspace is a box near the middle 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 include structure elements in 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 with DOC by Chem. 130 students will use one or more of the following variables:
 - *Melting point or boiling point*
 - *Molecular Weight*
 - *Molecular formula*
 - *Specifying heteroatoms*
 - *Structural fragments*
 - *CAS Registry number*
 - *Color, appearance, smell, text*
- 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 DOC Help for information about additional search options, such as:
 - *Specifying range of occurrence for certain elements*
 - *Isolating a ring*
 - *Refractive Index*
- Read on to see step-by-step instructions for doing the most common types of searches.

DOC via CHEMnetBASE for Identifying Unknowns

Figure 5. Melting Point and Boiling Point Search Fields

The screenshot shows a search interface with a header "Query Not Defined". Below it is a list of search criteria, each with a dropdown menu set to "AND" and a text input field followed by a "BROW" button. The criteria listed are: All Entries, Chemical Name, All Text, CAS Registry No., Molecular Formula, References, Type of Compound, Melting Point, and Boiling Point. A red arrow points to the "Melting Point" field.

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 are visible.**

Figure 6. Entering a Range of Melting Points

The screenshot shows the same search interface as Figure 5. The "Melting Point" field now contains the text "110 - 120", with a red arrow pointing to the text. The "Boiling Point" field is empty.

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, and it was confirmed by the TA to be correct within the +/- 5 deg range, you would enter 110 – 120.

Figure 7. Entering a Range of Boiling Points

The screenshot shows the same search interface as Figure 5. The "Boiling Point" field now contains the text "185 - 195", with a red arrow pointing to the text. The "Melting Point" field is empty.

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 DOC, 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, and only these are of interest for Chem 130.

Example:

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

DOC via CHEMnetBASE for Identifying Unknowns

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

ND	Hazard Flag		BROWSE INDEX
ND	Ion charge		BROWSE INDEX
ND	Metabolism		BROWSE INDEX
ND	Molecular Weight	(197 - 203) OR (397 - 403)	BROWSE INDEX
ND	Optical Rotation		BROWSE INDEX
ND	Partition Coeff. (calc)		BROWSE INDEX
ND	Percent Composition		BROWSE INDEX

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 (to allow for mono and di acids).
 - Add +/- 3 grams to each equivalent weight in order to create a range.
 - Enter a range for each equivalent weight,
 - There must be a space before and after the hyphen.
 - Put parentheses around each range.
 - Put an OR between each range.

Example:

- Equivalent weight from 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

AND	All Text		BROWSE INDEX
AND	CAS Registry No.		BROWSE INDEX
AND	Molecular Formula		BROWSE INDEX
AND	References		BROWSE INDEX
AND	Type of Compound		BROWSE INDEX
AND	Melting Point	110 - 120	BROWSE INDEX
AND	Boiling Point		BROWSE INDEX
AND	Accurate Mass		BROWSE INDEX
AND	Biological Source		BROWSE INDEX
	Biological		

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, as shown below, to help narrow results.

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Figure 10. Browsing the Molecular Formula Index

Chemical Databases Online

INTRODUCTION | TOUR | HELP | PLUGIN | TECHNICAL SUPPORT | CRC PRESS | CONTACT

RETURN TO SEARCH
FIRST ENTRY
PREVIOUS ENTRY
NEXT ENTRY
LAST ENTRY

Browsing Molecular Formula

Search Terms:

In the **Index Stem** box below, type in as many letters of your search term as possible. Press the 'Go To' button to browse the relevant part of the index. Select your term on it and it will automatically be transferred to the **Search Terms** box above.

All-Elements | Only-C H X | A | B | C | D | E | F | G | H | I | J | K | L | M | N | O | P | Q | R | S | T | U | V | W | X | Y | Z

Action:

- After pressing the Browse Index button, **click on Only-C H X**, to view some useful molecular formula shortcuts.

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

ARCHIVE

Browsing Molecular Formula

Search Terms:

In the **Index Stem** box below, type in as many letters of your search term as possible. Press the 'Go To' button to browse the relevant part of the index. Select your term on it and it will automatically be transferred to the **Search Terms** box above.

All-Elements | Only-C H X | A | B | C | D | E | F | G | H | I | J | K | L | M | N | O | P | Q | R | S | T | U | V | W | X | Y | Z

Index Stem: **GO TO**

#	INDEX
8565	-ONLY-C H
13819	-ONLY-C H N
79827	-ONLY-C H N O
13514	-ONLY-C H N O X
4692	-ONLY-C H N X
168615	-ONLY-C H O
17291	-ONLY-C H O X
1251	-ONLY-C H P
903	-ONLY-C H P X
2408	-ONLY-C H S
640	-ONLY-C H S X
5588	-ONLY-C H X
12	**

Action:

- Note the choices which begin with -ONLY .
- **Click on the appropriate general formula for your compound to copy it to the Search Terms box (shown by red arrow in Fig. 11).**

Note:

- 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, and it will be pasted to the Search Terms box.

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

RETURN TO SEARCH
FIRST ENTRY
PREVIOUS ENTRY
NEXT ENTRY
LAST ENTRY

Browsing Molecular Formula

Search Terms: "-ONLY-C H O"

In the **Index Stem** box below, type in as many letters of your search term as possible. Press the 'Go To' button to browse the relevant part of the index. Select your term on it and it will automatically be transferred to the **Search Terms** box above.

All-Elements | Only-C H X | A | B | C | D | E | F | G | H | I | J | K | L | M | N | O | P | Q | R | S | T | U | V | W | X | Y | Z

Index Stem:

#	INDEX
8565	-ONLY-C H
13819	-ONLY-C H N
79827	-ONLY-C H N O
13514	-ONLY-C H N O X
4692	-ONLY-C H N X
168615	-ONLY-C H O
17291	-ONLY-C H O X
1251	-ONLY-C H P

Action:

- After pasting molecular formula choice, eg "-ONLY C H O", to Search Terms box, **click on Return to Search in upper left corner of the screen (shown by red arrow).**

Note:

- Before clicking on Return to Search, check Search Terms box to make sure that only one copy of selected term, "-ONLY C H O", is in the Search Terms box.

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Figure 13. Viewing Terms Selected from Molecular Formula and Melting Point

All Entries		BROW
AND	Chemical Name	BROW
AND	All Text	BROW
AND	CAS Registry No.	BROW
AND	Molecular Formula	"-ONLY-C H O" ←
AND	References	BROW
AND	Type of Compound	BROW
AND	Melting Point	110 - 120 ←
AND	Boiling Point	BROW
AND	Accurate Mass	BROW
AND	Biological Source	BROW

- After clicking on Return to Search, make sure values in search term boxes are correct.

Figure 14. Chemical Name Fragment Searching

AND	Chemical Name	BROW
AND	All Text	*acid ←
AND	CAS Registry No.	BROW
AND	Molecular Formula	"-ONLY-C H O" BROW
AND	References	BROW
AND	Type of Compound	BROW
AND	Melting Point	110 - 120 BROW
AND	Boiling Point	BROW

Action:

- Enter name fragment and add 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

ARCH
ARCH

Searching

Enter a query, then press 'Submit Search'. Enter a word(s) into one or more of the boxes. You may truncate on the left or right hand side of the word with an asterisk(*).

Substructure Exact Match

Draw Query

↑
Query Not Defined

AND

All Entries BROW

Action:

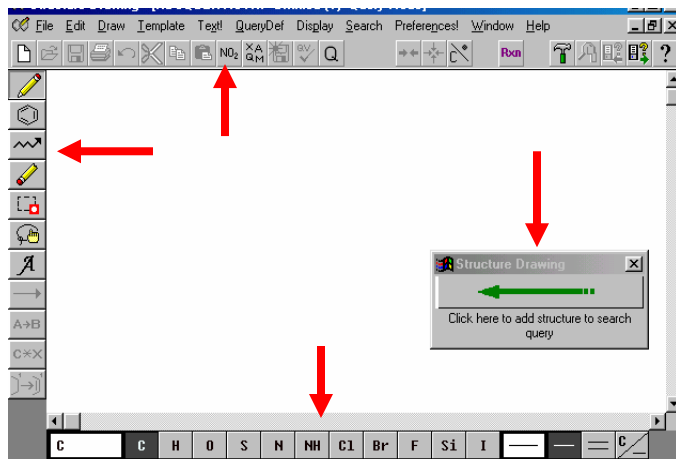
- Click on the **Draw Query** button.

Note:

- If a small box with an x in it is present where the Draw Query box is shown, get the plug-in (as explained for Fig. 1).

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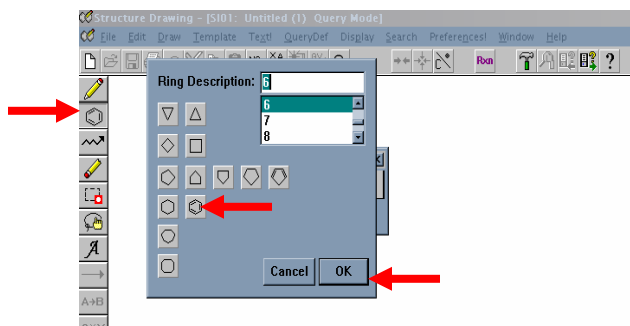
Figure 16: Main Structure Drawing Screen



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 having finished entering structural data, press the green arrow (in box on workspace) to return to main search page.

Figure 17. Using the Ring Tool



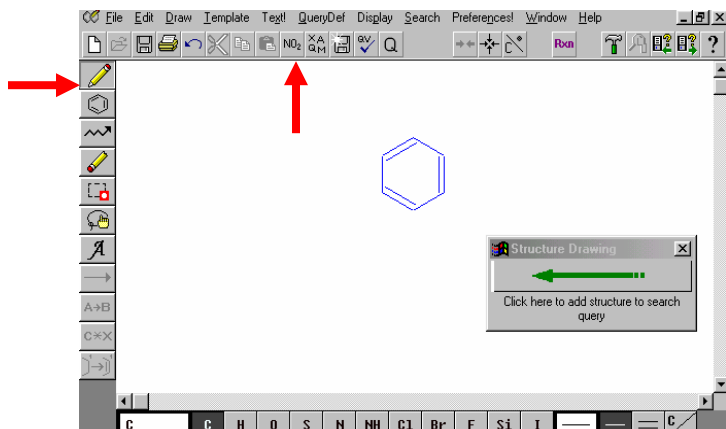
Example:

- Add a benzene ring to your search.

Action:

- Click on **Ring Tool (benzene ring just under pencil on left side)**. Screen at left will appear.
- **Choose image of ring** desired or scroll down window on upper right to choose size of ring. Here we have selected benzene ring.
- Click the **OK** button.
- Next, move the cursor (which has turned into a hexagon with a + sign in center) to work space and **click once** to paste the ring into the drawing workspace. The result is shown in Fig. 18.

Figure 18. Using Functional Groups



Action:

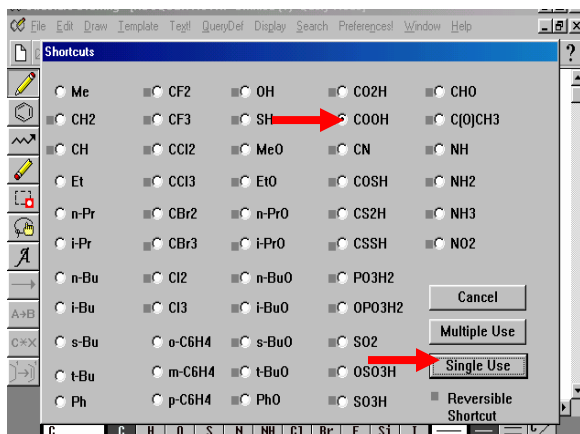
- Click on the **Pencil tool** (at left of screen).
- Click on **NO2 button** (at top of screen) to add a functional group to your search.

Note:

- The NO2 link lists many common functional groups, such as Me (methyl), Et (ethyl), COOH (carboxylic acid), NH (secondary amine), MeO (methoxy), etc.

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Figure 19. Selecting a Functional Group



Example:

- Search for carboxylic acids.

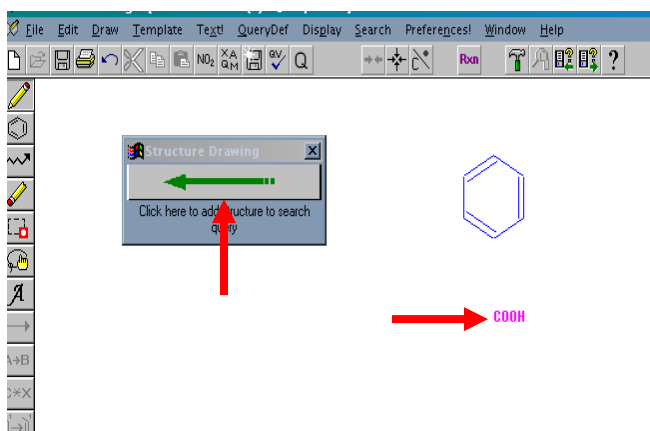
Action:

- Click on **white dot in front of COOH**.
- Click **Single Use**, which will cause the list of functional groups to disappear.

Note:

- Using one copy of a functional group in your search will retrieve substances that have one or more occurrences of that functional group present in the 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 COOH to your search strategy.
- After finishing drawing structural fragments, **click on large green arrow** to return to main search screen.

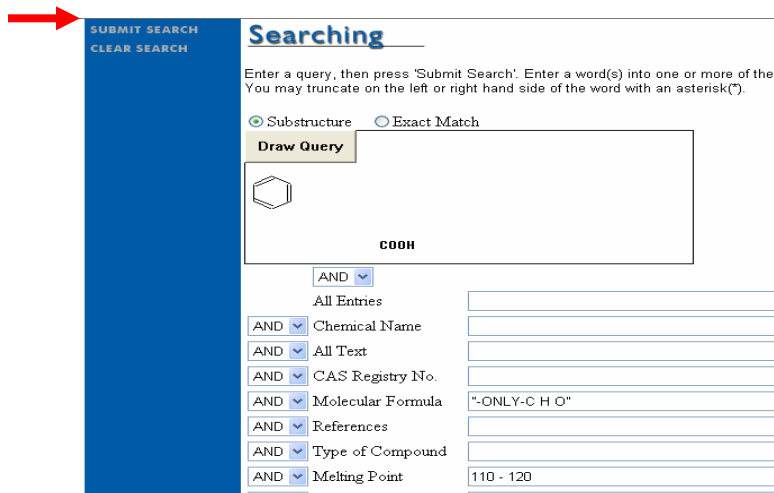
Note:

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

Example:

- Screen shown in Figure 20 will search for carboxylic acids which contain benzene ring(s), but the acid group does not necessarily have to be on the ring.

Figure 21: Performing a Search



Action:

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

Note:

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

Example:

- The 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 group.

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Figure 22. Viewing Display of Search Results



DICTIONARY OF ORGANIC COMPOUNDS
Chemical Databases Online

INTRODUCTION | TOUR | HELP | PLUGIN | TECHNICAL SUPPORT | CRC PRESS | CHEMNET

RETURN TO SEARCH | Estimated 88 of 507226 documents matched query. Hits 1 to 10
PRINT PREVIEW
FIRST ENTRY
PREVIOUS ENTRY
NEXT ENTRY
LAST ENTRY

Name	CAS Registry Number	Molec Form
2-Acetoxybenzoic acid	50-78-2	C ₉ H ₈ O ₄
2-Acetylbenzoic acid, ecr	577-56-0	C ₉ H ₈ O ₃
1,3-Benzenedicarboxylic acid, ecr; Mono-Et ester		C ₁₀ H ₁₀ O ₄
Benzenehexacarboxylic acid, ecr; Tetra-Me ester		C ₁₆ H ₁₄ O ₁₁
1,2,4-Benzenetricarboxylic acid, ecr; 1,2-Di-Me ester	54699-35-3	C ₁₁ H ₁₀ O ₆
4-Benzoylbenzeneacetic acid, ecr	26077-80-5	C ₁₅ H ₁₂ O ₃
2-Benzoyloxypropanoic acid, ecr; (±)-form		C ₁₀ H ₁₀ O ₄

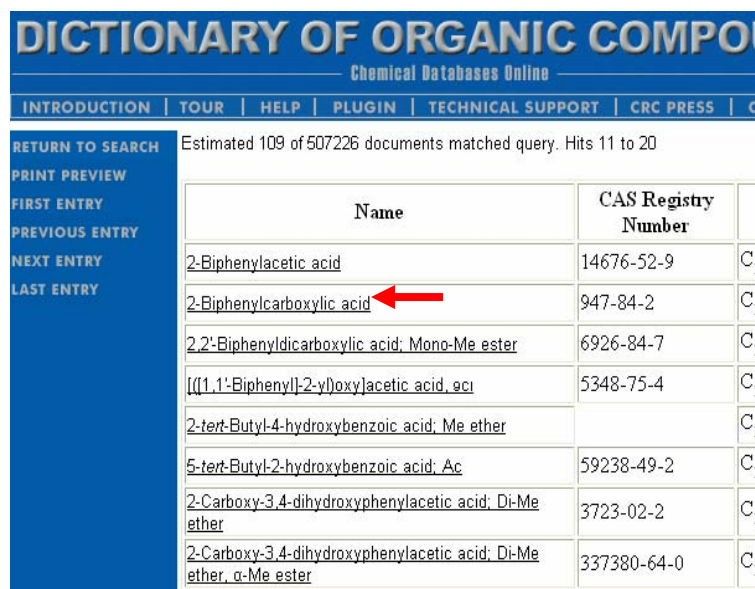
Action:

- After clicking on **Submit Search**, you will see the screen shown in Fig. 22. Click on **“NEXT ENTRY”** (on the left side) to view the 2nd page of search results (Fig. 23).

Note:

- Total “estimated” number of records retrieved in a given search is shown at the top of the list. This number may change as you start viewing the next pages or individual records.
- Navigation buttons for viewing answer set are at left side of screen.
- Brief display for each record includes substance name, CAS (Chemical Abstracts) Registry Number, and molecular formula.
- Substance names are hypertext linked to a full record for each name.

Figure 23. Viewing 2nd Page of Search Results



DICTIONARY OF ORGANIC COMPOUNDS
Chemical Databases Online

INTRODUCTION | TOUR | HELP | PLUGIN | TECHNICAL SUPPORT | CRC PRESS | C

RETURN TO SEARCH | Estimated 109 of 507226 documents matched query. Hits 11 to 20
PRINT PREVIEW
FIRST ENTRY
PREVIOUS ENTRY
NEXT ENTRY
LAST ENTRY

Name	CAS Registry Number	Molec Form
2-Biphenylacetic acid	14676-52-9	C ₁₅ H ₁₂ O ₂
2-Biphenylcarboxylic acid	947-84-2	C ₁₅ H ₁₀ O ₂
2,2'-Biphenyldicarboxylic acid; Mono-Me ester	6926-84-7	C ₁₆ H ₁₂ O ₄
[(1,1'-Biphenyl)-2-yloxy]acetic acid, ecr	5348-75-4	C ₁₆ H ₁₄ O ₂
2-tert-Butyl-4-hydroxybenzoic acid; Me ether		C ₁₆ H ₁₈ O ₃
5-tert-Butyl-2-hydroxybenzoic acid; Ac	59238-49-2	C ₁₆ H ₁₈ O ₃
2-Carboxy-3,4-dihydroxyphenylacetic acid; Di-Me ether	3723-02-2	C ₁₅ H ₁₂ O ₅
2-Carboxy-3,4-dihydroxyphenylacetic acid; Di-Me ether, α-Me ester	337380-64-0	C ₁₆ H ₁₄ O ₆

Action:

- Click on name of any compound to view full record (Eg., clicking on 2-biphenylcarboxylic acid will retrieve record shown in Fig 24).

DOC via CHEMnetBASE for Identifying Unknowns

Figure 24. Viewing Record in Full Display

Chemical Databases Online
ELP | PLUGIN | TECHNICAL SUPPORT | CRC PRESS | CHEMNETBASE

Hit 12 of 109 (estimated)

Entry Name: 2-Biphenylcarboxylic acid

Synonym(s): *o*-Phenylbenzoic acid
Chapman & Hall Number: DVR75-C
CAS Registry Number: 947-84-2
Molecular Formula: C₁₃H₁₀O₂
Molecular Weight: 198.221
Accurate Mass: 198.06808
Percentage Composition: C 78.77%; H 5.08%; O 16.14%
Melting Point: Mp 114°
Boiling Point: Bp 343-344°
pKa Value: pK_a 5.03 (EtOH aq.)
Aldrich: B3470-2
Fluka: 14418

Derivative: Me ester
Chapman & Hall Number: DVR76-D
CAS Registry Number: 16605-99-5
Molecular Formula: C₁₄H₁₂O₂

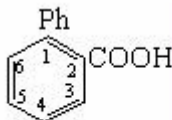
Action:

- View the 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 unknown compound is listed as a derivative in DOC. The name of the specific substance your search matched on is highlighted in blue.
- The small benzene ring to the left of a chemical name is a hypertext link to the structure for that substance.
- Selected physical properties are listed for each compound.
- The 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.

Figure 25. Viewing Hyperlinked Structure of Entry Name Compound in Full Display



Action:

- Click on the benzene ring icon in Fig. 24, to show the structure of the compound, given in Fig. 25.

Web Version 2004 (2)

Figure 26. Viewing References in Full Display

Synonym(s): *o*-Phenylbenzoic acid
Melting Point: Mp 35-37°
Rare Chemicals Library: S5714-3

References:
Aldrich Library of FT-IR Spectra, 1st edn., 1985, 2, 236A, (ir)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, 2, 1160A, (nmr)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, 3, 1333C, (ir)
Drapala, T. et al., Pol. J. Chem. (Rocz. Chem.), 1960, 34, 1371 1972, 46, 9, (uv)
Kenner, G.W. et al., J.C.S., 1962, 1756, (synth)
Sheley, C.F., Org. Mass Spectrom., 1974, 9, 731, (ms)
DiBiase, S.A. et al., J.O.C., 1978, 43, 447, (synth, ir, pmr)
Sain, B. et al., J.O.C., 1990, 55, 2545, (nitrile, synth)
Hattori, T. et al., Bull. Chem. Soc. Jpn., 1993, 66, 3035, (synth)
Dobson, A.J. et al., Acta Cryst. C, 1998, 54, 795-798, (cryst struct)
Hattori, T. et al., J.O.C., 2003, 68, 2099-2108, (diethylamide, synth, ir, pmr, cmr)

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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.