



# Using SDBS Database for Identifying Unknowns

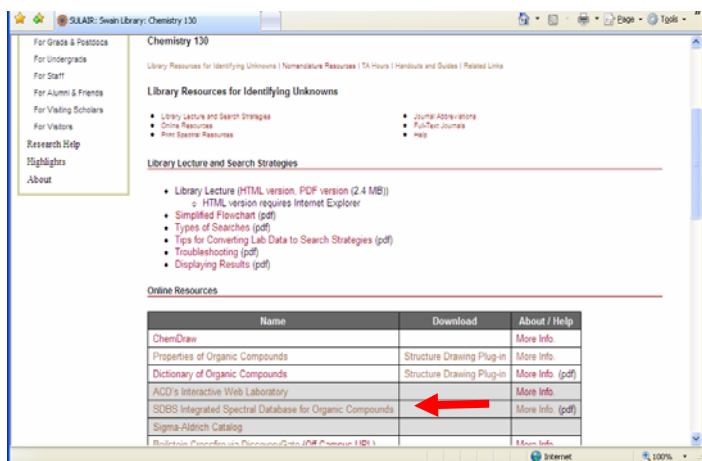
Figure 1. Swain Home Page



Action:

- Go to the Swain Library home page: <http://www-sul.stanford.edu/depts/swain/index.html>
- This will take you to Fig. 1.
- Under Highlights, go to Course Pages, and click on Chem 130. That will take you to a page with a heading “Chemistry 130” in the left middle of the page.
- Scroll down on this page until you see what is shown in Fig. 2.

Figure 2. Chemistry 130 Page



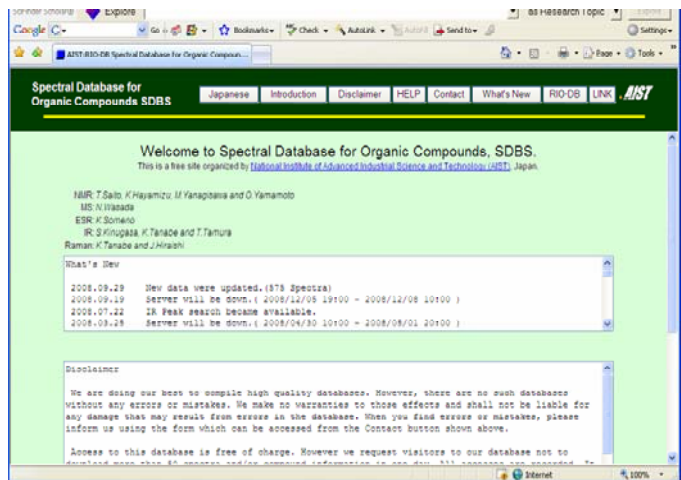
Action:

- Click on [SDBS Integrated Spectral Database for Organic Compounds](#).

Note:

- This will take you to Fig. 3.

Figure 3. SDBS Database Homepage

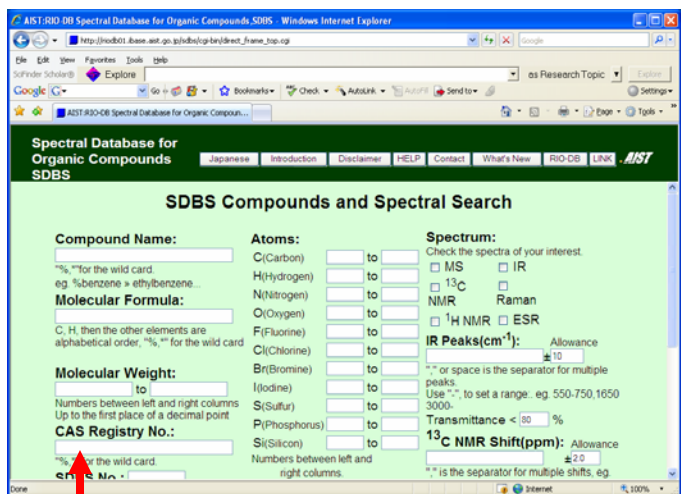


Action:

- Scroll to the bottom of the page and accept the disclaimer.
- This will take you to Fig. 4.

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Figure 4. SDBS Data Entry Page



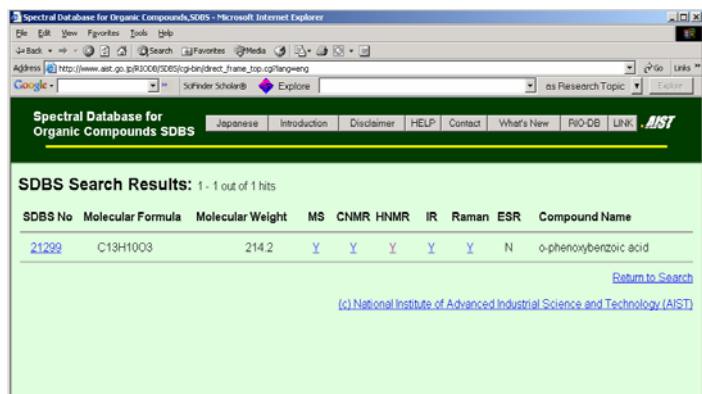
Action:

- You will typically enter either 1) a CAS Registry Number, and click on Search to see if your compound is in the database, or 2) enter  $^{13}\text{C}$  &/or  $^1\text{H}$  NMR &/or IR spectral data, plus elemental data, if known and needed, and then click on Search to see if the list of compounds generated contains your compound of interest.
- We will now give an example of each of the 2 types of searches mentioned above.

Action:

- Enter the CAS Registry No. 2243-42-7 into the field just below **CAS Registry No.:** (at the lower left of the page), and click on Search at the bottom of the page (or hit "Enter" on keypad).

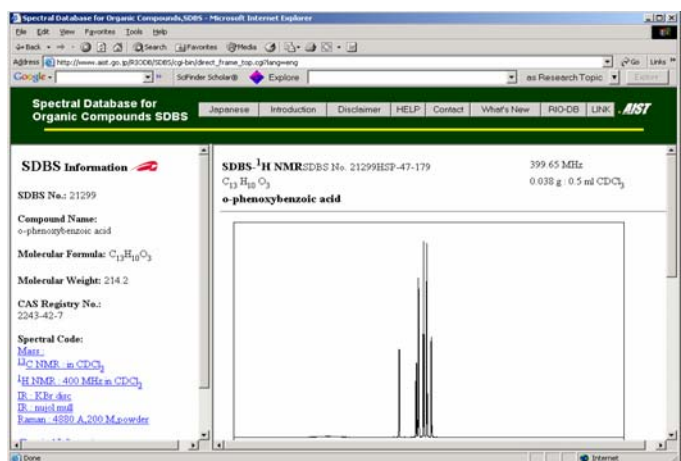
Figure 5. Results of CAS Registry No. Search



Note:

- This will take you to Fig. 5. You will see a Y for Yes, under MS (Mass Spec), CNMR ( $^{13}\text{C}$  NMR), HNMR ( $^1\text{H}$  NMR), IR (Infra Red), and Raman, and an N for No under ESR (Electron Spin Resonance). Each Y is linked to an actual spectrum. So if one clicks on Y under HNMR, one would see Fig. 6.

Fig. 6.  $^1\text{H}$  NMR plot for o-phenoxyacetic acid

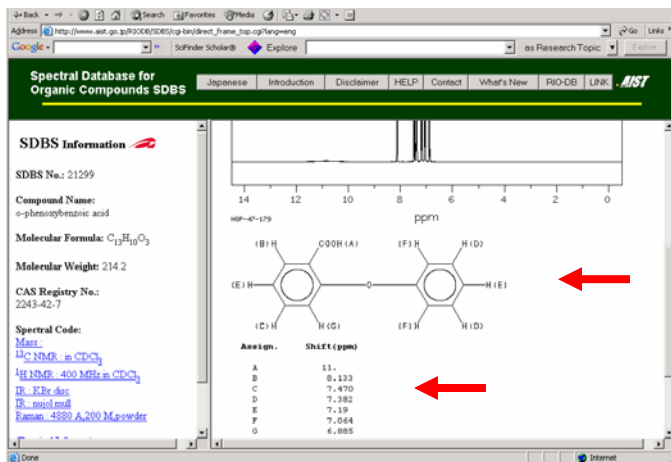


Note:

- You will see the actual spectrum in the middle of the page, and on the left are links to other spectral data such as  $^{13}\text{C}$  NMR, and IR.
- If you scroll down you will see Fig. 7.

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Figure 7. Peaks assigned to Hydrogens



Note:

- Each hydrogen is labeled and assigned to a peak with a given chemical shift in ppm (parts per million).

Action:

- Return to the SDBS data entry page shown in Figure 4, using the “Back” arrow or as shown above.
- We are now going to search for a compound which has only one peak in its <sup>13</sup>C NMR spectrum, at 49 +/- 2 ppm, and has only C, H, and O atoms.

Figure 8. Entering Spectral Data

Action:

- In the field just under the phrase <sup>13</sup>C NMR Shift(ppm):, enter 49. The default range (allowance) is +/- 2, and we will accept that.
- In the field to the right of the phrase **No Shift Regions:**, enter the ranges where there are no peaks (ie from 250 to 52, and 46 to 5). These are entered as 250 52,46 5 (note there is a space between the beginning and end of a range, and note there is NO space after the comma if 2 or more ranges are entered).

Action:

- Then click Search at the bottom of the page. This will generate a list of 15 hits. One can narrow that down further by entering atom data if available. Here it is known that the compound has only C, H, and O atoms.

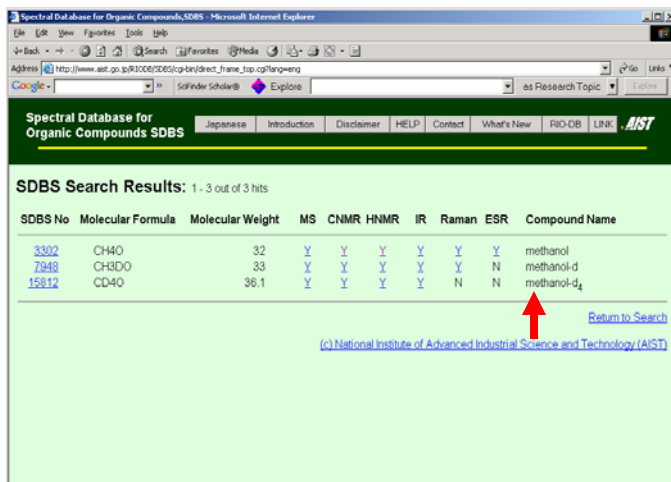
Figure 9. Entering Atom Data

Action:

- If it is not known how many C, H, and O atoms there are in the molecular formula, one can leave those boxes blank, or put in a range if known. However one can enter zeroes for the elements which are known to be absent. For each atom one must specify a range, using the left and right hand columns. If an atom is absent, one must still put in the range as 0 to 0, as shown in Fig. 9. Then click on Search, or hit Enter. The results are shown in Fig. 10.

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Figure 10. Results of a spectral-plus-atom data search using SDBS



SDBS No	Molecular Formula	Molecular Weight	MS	CNMR	HNMR	IR	Raman	ESR	Compound Name
3302	CH4O	32	Y	Y	Y	Y	Y	Y	methanol
7946	CH3DO	33	Y	Y	Y	Y	Y	N	methanol-d
15812	CD4O	36.1	Y	Y	Y	Y	N	N	methanol-d <sub>4</sub>

[Return to Search](#)  
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Action:

- One can see that the compounds which meet the search criteria are 3 different forms of methanol. If  $^1\text{H}$  NMR data had been used as well, one would have obtained only a single compound, ie the non-deuterated form of methanol.
- $^1\text{H}$  NMR data are entered in the same way as the  $^{13}\text{C}$  NMR. However, as shown, the default range (allowance) is  $\pm 0.2\text{ppm}$ , which is normally accepted. If multiple peaks are entered, they are separated by a comma with NO space after the comma.
- IR data can be entered as either peaks or ranges, in the box under **IR Peaks ( $\text{cm}^{-1}$ )**: , per the format shown under the box. One can accept the "allowance" of  $\pm 10$ , or change it to a lower value such as 5 to reduce the size of the hit list, although be aware that if only one peak differs from SDBS by greater than the allowance, the compound will be dropped from the hit list. Also be aware that if the hit list is large, one can reduce its size by entering the hetero atom data given by the lab TA, for all elements except C, H, & O, and then one can often estimate ranges for C & H & O, using spectral data, eg. a range for H from HNMR integrals, a range for C from the number of C13 peaks, and a range for O from C=O, C-O peaks in IR, plus chemical test data.
- One should not use the small IR peaks because the "transmittance" is set by default to  $< 80\%$  and small peaks usually have a transmittance of  $> 80\%$ . If one wants to use small peaks, one can set the transmittance to 90 for example, but then the hit list grows considerably as well.
- When viewing spectra or entering data, be aware that solvents can add peaks or shift peaks, both for H & C13 NMR. The values for the more common solvents are given in the course text.