Chemical Literature Search

“An hour in the library is worth at least a day in the laboratory”

REFERENCE: This experiment was adapted from Introduction to Organic Laboratory Techniques, A Microscale Approach, by Pavia, Lampman, Kriz, Engel, 3rd edition and North Carolina State University.


We will be meeting in the library for this lecture. Room 4214

This following list will provide you with several possible sources of information for the literature search assignment. All chemicals will be different, and will require you to look in various places, both online and in print reference books. More ideas for sources can be through the library’s web site at http://www.shoreline.edu/library/ and specifically on the Chem 271 library web page at http://shoreline.libguides.com/index.php - click on science.

I. Chemical Abstracts (CA), published by the American Chemical Society, is a survey of the entire literature of chemistry and is the most complete source of information on chemistry in the world. CA condenses the content of articles into abstracts and indexes the abstracts.

Chemical Abstract Services (CAS), the publishers of Chemical Abstracts, provides a number of databases. Whenever possible, use the compounds CAS Number (also known as the Registry Number), NOT a synonym or common name, to look up your chemical. Even if they do, they may use a different name than you. Reference books and websites may not have name indexes. Some chemicals have dozens of synonyms. CAS Numbers are unique for each chemical and constant in all sources. http://www.cas.org/

➢ use CAS numbers to locate

• literature references to the substance
• experimental and predicted property data (boiling and melting points, etc.)
• commercial availability
• preparative methods
• spectra
• regulatory information from international sources

II. Don’t expect Google to work. and some free websites aren’t going to have all the information you need. Online resources are available through the library’s web site, but many are subscription-based.

III. Don’t neglect print reference books! Believe it: not everything is online. Using a good reference book can save you hours of fruitless internet searching. Print resources for this assignment are also available in the Library Reference area. When you do use reference books, use their indexes. The index volumes may be separate from the main volumes in multi-
volume encyclopedias. Also look for “legend” pages to describe the information each entry contains.

**Literature search outline:**

1. Start with Chemical and Engineering News and find an article on an organic chemical.

2. *They must also be in Aldrich: Advancing Science*, better known as *Aldrich’s Handbook of Fine Chemicals* (and usually simply called *Aldrich*). The chemical MUST be in *Aldrich*—if it’s not, you cannot use this chemical for this assignment. (This is also a good time to ensure that you have an organic chemical!) There is a copy *Aldrich* in the reference stacks. Also available online at http://www.sigmaaldrich.com/.

<table>
<thead>
<tr>
<th>Information usually available:</th>
<th>Sometimes available:</th>
</tr>
</thead>
<tbody>
<tr>
<td>CAS No. (this is the most important piece of data to get).</td>
<td>Density (g/cm³)</td>
</tr>
<tr>
<td>It looks like this: 58-08-2.</td>
<td>Refractive Index (nD)</td>
</tr>
<tr>
<td>Synonyms</td>
<td>Hazards</td>
</tr>
<tr>
<td>Molecular formula</td>
<td>M. Pt. (melting point)</td>
</tr>
<tr>
<td>Cost</td>
<td>B. Pt. (boiling point)</td>
</tr>
</tbody>
</table>

In addition to *Aldrich*, several other resources contain chemical property data.

- **CRC Handbook of Chemistry and Physics** use the CAS No. index. Also includes Beilstein reference numbers.

- **Merck Index** Usually includes a structure, sometimes gives a synthesis reference.


- (NCBI) National Center for Biotechnology Information  

**Hazardous Properties**

- **MSDS** found on your courses blackboard and many online sources.

- **TOXNET** (at http://toxnet.nlm.nih.gov/)

Alternatively, information might be available through above sources such as *Aldrich* and the *Merck Index*. Another option is the *Sigma-Aldrich Library of Chemical Safety Data*

1. **Synthesis**

   The *Merck Index* might provide a reference.

   After finding your chemical, note any journal citations ending in (synth).  

   NOW
a. Use the Journals link on the library website to locate the journal title listed in the synthesis citation (searching by abbreviation is OK here). If no results, try the library Catalog, search by Journal Title (no abbreviations; ask for librarian help if your title is abbreviated).

b. Most syntheses are old, so the journal article may only be available in print, not online

c. Many synthesis references will be to the Collective or Annual volumes of *Organic Syntheses* at [http://www.orgsyn.org/](http://www.orgsyn.org/)
   (Don’t start your search here—it probably won’t work well—but definitely use the site if you have a reference to these from steps above. You can browse right to the volume and page number in that case.)

2. **Spectra** Can be found in the Bio/Chem Learning Center room 2717
   - Aldrich Library of FT-IR Spectra: Use the CAS No. index in Vol. 3 to find your chemical. It will tell you the volume and page number for your chemical.

   **Some online options:**
   2. SDBS, spectral database system. [http://riodb01.ibase.aist.go.jp/sdbs/cgi-bin/cre_index.cgi?lang=eng](http://riodb01.ibase.aist.go.jp/sdbs/cgi-bin/cre_index.cgi?lang=eng)

3. **Some SCC Library texts:**
   Gordon, Arnold J. *The chemist's companion: a handbook of practical data, techniques, and references.*
   Smith, Michael. *March’s advanced organic chemistry : reactions, mechanisms, and structure.*

**LITERATURE SEARCH REPORT FORM**

*(Be sure to show the source for each piece of data reported)*

**Student’s Name**

**Lab Day/Time**

**Name of Compound**

**CAS No.**
Synonym(s)________________________________________________________

Structural Formula

Mpt. ___________________________ bpt. ___________________________ density ____________

Refractive Index \( (n_D) \)_________________ Cost of 100 g________________________

Unusual Hazards_______________________________________________________

Hazardous Biological Activity____________________________________________

Method of Synthesis (include reference)

**IR Spectrum** (interpret at least 4 peaks and attach spectra)

**1H NMR Spectrum** (interpret all peaks and attach spectra)

Attach extra pages as needed. Give references for each piece of data reported.