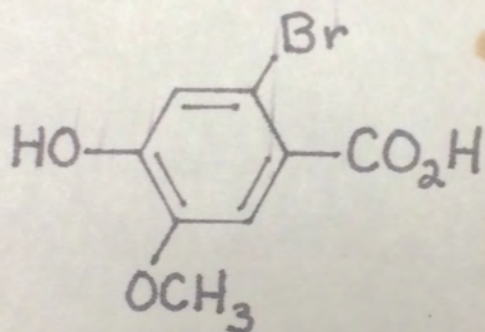


Reaxys (Beilstein) Assignment

- Preliminary Report Due: October 12th
- Final Report Due: November 16th

Sample Beilstein Card

B103



Needles (with 1 H₂O)
mp 192-3

Reaxys (Beilstein) Assignment

- Preliminary Report Includes:
 - 1) Your name
 - 2) Your section number
 - 3) Your Beilstein assignment number (B=???)
 - 4) Reaxys registry number
 - 5) IUPAC name of compound
 - 6) May be handwritten, on a full size sheet of paper (may be on the same sheet as the CAS preliminary report)

Reaxys (Beilstein) Assignment

- Final Report Includes:
 - 1) Your preliminary report and all of its data typed
 - 2) The original journal reference in modern JACS format {*ex* Smith, J.; Jones, T., *J. Org. Chem.*, **61**, 820 (1996)}
 - 3) A brief synthesis of the compound by the method used by the correct author
 - 4) May NOT be handwritten

Reaxys (Beilstein) Assignment

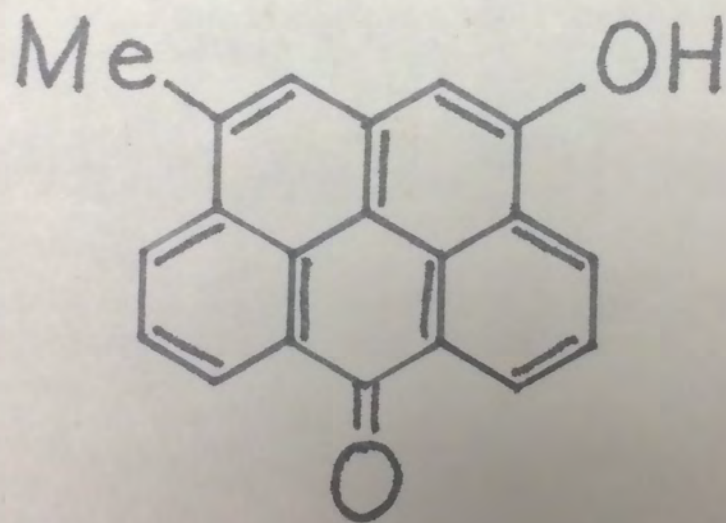
- Website: www.reaxys.com
- You must be using a computer on campus for it to work
- You have to register for it to work
- Proxies might work, DON'T depend on them

Sci-Finder (Chemical Abstracts) Assignment

- Preliminary Report Due: October 12th
- Final Report Due: November 16th

Sample Chem Abstracts Card

C-14



Sci-Finder (Chemical Abstracts) Assignment

- Preliminary Report Includes:
 - 1) Your name
 - 2) Your section number
 - 3) Your Chemical Abstracts assignment number (C=???)
 - 4) CAS registry number
 - 5) IUPAC name of compound
 - 6) May be handwritten, on a full size sheet of paper (may be on the same sheet as the CAS preliminary report)

Sci-Finder (Chemical Abstracts)

Assignment

- Final Report Includes:
 - 1) Your preliminary report and all of its data typed
 - 2) The original journal reference in modern JACS format {*ex* Smith, J.; Jones, T., *J. Org. Chem.*, **61**, 820 (1996)}
 - 3) A diagram of the synthesis of the final product, continuing backwards until a purchasable compound is found, each step must be referenced
 - 4) Price, grade, and supplier for ALL reagents used in the synthesis, scaled appropriately.
 - 5) Melting/boiling points of all isolated organic intermediates, with references
 - 6) May NOT be handwritten

Sci-Finder (Chemical Abstracts)

Assignment

- Website: scifinder.cas.org don't use this until you register go through the library
- You must be using a computer on campus for it to work
- You must register and login for it to work
- Go through the MSU library website to do this <http://er.lib.msu.edu/subject.cfm?cat=0&type=All&Subject=Chemistry>
- Proxies might work, DON'T depend on them!

Citation Format Issues

- There are many formats that the various scientific journals use for citations. In order to ensure that you fully understand which part of the citation refers to what part of the journal, the citation in the final report must be done in the manner specified, which is very often different from the one used by the journal itself.
- This format is:
 - Author(s) Name (telephone directory fashion), *Journals name in italics*, **volume number in bold (subvolumes too)**, page number in plain font (year in parentheses)
 - Smith, Joan; Jones, Emma; Salt, Verucca, *Journal of Org. Chemistry*, **23(1)**, 276-285 (1998)

- Note, all punctuation is in plain font except the sub volume number (If applicable)
- Not all journals {the Journal of the Chemistry Society (London) is the best example} have volume numbers.
-
- Smythe, John; Wallingford, Abigail, *J. Chem. Soc (London)*, 2765-2768 (1923)
-
- Part of the reason great care must be taken here is that in many cases the page number and occasionally the volume number could be confused with the year and *vice versa*. Remember to take extra care when requesting librarian assistance, they will certainly obtain the journal you asked for—you need to make sure it is the one you actually wanted.

Patents

- United States and European Patents are cited like this:
- **US 3979508** (1971)
- Any that seem nonstandard, come see me for assistance.

Principle Reference Works

- 1) SciFinder Scholar (Chemical Abstracts)
- 2) Reaxys (Beilstein/Gmelin)

Naming Issues

- CAS indexes were originally intended to be searched by hand and so CAS took steps to use naming conventions that are more logical even than the IUPAC naming system. Also, computer power was very expensive and much, much slower than today. One of the most obvious examples is that CAS calls aniline, aminobenzene. They simply decided to do it. Although this is a perfectly logical name, aminobenzene is not an IUPAC name. Aniline is the IUPAC name.
-
- Another example is using telephone directory naming for esters, acids, and salts. For example ethyl acetate is indexed as acetic acid, ethyl ester. Ethyl acetate is the IUPAC name not acetic acid, ethyl ester. Similarly sodium acetate is indexed as acetic acid, sodium salt.
-
- This is also done for complicated heterocyclic structures. Instead of listing 2-methylpyrrole (the IUPAC name) it is indexed as pyrrole, 2-methyl-. If you see a dangling hyphen at the end of the name it is a telephone directory style name and you must rearrange it properly to obtain the IUPAC name.

Scaling Issues

- Pick an amount (entirely your choice) of the product that you intend to make. Make sure the amounts you quote prices for, for all reagents, are appropriate for this scale.
- Price is not a consideration
- Match purity and grade as specified in the paper(s)
- Equipment does not have to be bought

The Chemist's Library

The Most Useful Reference Materials
for the Chemist

SciFinder Scholar (Chemical Abstracts)

Pros

- Up-to-date
- Comprehensive
- Entirely in English

Cons

- Not error-checked
- Data is in original form

Reaxys (Beilstein/Gmelin)

Pros

- Critically Reviewed
- Listing is by Compound

Cons

- Not up-to-date
- Parts in German

Smaller Reference Works

- 1) Catalogs
- 2) Handbooks, Encyclopedias, and Journals
- 3) Websites
- 4) Search Engines

Catalogs

- 1) Aldrich
- 2) Eastman
- 3) Alfa-Aesar
- 4) Matheson Gas Data Book

Aldrich Catalog

- 1) 37,000+ Products. Organics, Inorganics, Elements, Polymers, Organometallics.
- 2) Arranged by 'product name'
- 3) Includes physical properties, references to Aldrich Library of NMR or FT-IR spectra
- 4) Molecular Formula
- 5) CAS RN indexes
- 6) Online

<http://www.sigmaaldrich.com/Brands/Aldrich.html>

Alfa-Aesar

- 1) Includes physical properties
- 2) CAS RN indexes
- 3) MSDS's embedded in description
- 4) Merck Index references
- 5) <http://www.alfa.com/alf/index.htm>

Eastman Catalog

Item descriptions include applications, MSDS, sales spec sheet, technical data sheets.

<http://www.eastman.com/>

Handbooks and Journals

- 1) Merck Index
- 2) Handbook of Chemistry and Physics (CRC)
- 3) Kirk-Othmer Encyclopedia of Chemical Technology
- 4) Ullmann's Encyclopedia of Industrial Chemistry
- 5) Organic Solvents
- 6) Journal of Physical and Chemical Reference Data
- 7) Fieser and Fieser
- 8) Organic Syntheses
- 9) Combined Chemical Dictionary

Merck Index

- 1) 13th edition 2002
- 2) 4000+ drugs and pharmaceuticals
- 3) 2000+ organics/ reagents
- 4) 2000+ naturally occurring substances
- 5) 1000+ elements/inorganic compounds
- 6) 1000+ agricultural compounds/biological agents
- 7) Name, Formula, CAS RN, and Therapeutic Category and Biological Activity Indexes, Organic Name Reactions, Miscellaneous Useful Tables(Latin Terms, Greek Alphabet, etc.)
- 8) Merck Index Online <http://products.camsoft.com/themerckindex.cfm>

Handbook of Chemistry and Physics

- 1) Huge number of useful data tables for all of the divisions of chemistry
- 2) www.hbcnetbase.com/

Websites

- 1) ChemINDEX
- 2) DIPPR
- 3) Solv-DB
- 4) BRENDA
- 5) NIST Critically Selected Stability Constants of Metal Complexes
- 6) NIST Webbook
- 7) Organic Syntheses

Search Engines

- 1) Google <http://www.google.com>
- 2) Yahoo <http://search.yahoo.com>
- 3) Lycos <http://www.lycos.com/>

Online Chemistry Sites

- 1) www.orgsyn.org
- 2) ChemINDEX chemindex.cambridgesoft.com/
- 3) www.chemfinder.com
- 4) dippr.byu.edu/
- 5) solvdb.ncms.org/index.html
- 6) www.brenda.uni-koeln.de/
- 7) www.syrres.com/esc/