

Chem 228 WS/2007
Synthesis Project-Library Assignment

Name _____ Section _____ StdntNo _____

The following searches are to locate needed information about compounds involved in your synthesis project and to familiarize you with some of the standard reference sources for organic compound information.

I would suggest working in groups for efficiency in obtaining information, however you should actually be present to see how SciFinder works, where the reference books are located, how they are indexed, etc. These reference sources are useful for all reagents and intermediates produced in your synthesis. You might want to assign a different intermediate to each member of a team and make copies for the others.

Q #1 & 2 use the web.

Q #3-5 require a trip to the library.

Q #6 requires ChemDraw, found in CLC rm. 120 or 305 of chemistry.

1. Using SciFinder, do "Chemical Substance or Reaction" searches for p-nitrophenol (228A) or p-nitrotoluene (228C) as the "Substance Identifier". Determine the CAS #, structure and display a list of names and properties by clicking on the microscope icon to the right of the citation. Print out and attach.
2. Using a web browser, go to the SDBS spectral database site at

<http://www.aist.go.jp/RIODB/SDBS/menu-e.html>

Find the KBr disc IR spectrum, ¹H NMR and ¹³C NMR for p-nitrophenol (228A) or p-nitrotoluene (228C).
Print out each and attach, along with the tables of peak positions.
3. Go to "The Purification of Laboratory Chemicals", TP 156.P83 P47 (in hardcopy only, at the UMR library in the reference section) and find purification information for p-nitrophenol (228A) or p-nitrotoluene (228C). Xerox and attach.
4. Go to "The Dictionary of Organic Compounds", QD246.D5 (in hardcopy only, at the UMR library in the reference section) and find the information for p-nitrophenol (228A) or p-nitrotoluene (228C). Use the CAS# in the CAS# index to locate. Xerox and attach.
5. Go to "The Handbook of Data on Organic Compounds", QD 257.7 H36 (in hardcopy only, at UMR library in the reference section) and find the information for p-nitrophenol (228A) or p-nitrotoluene (228C). Use the CAS# index to locate. Xerox and attach.

6. ChemDraw: Go to one of the chemistry CLC's in rm 120 or 305 of chemistry.
(Note: The printer in rm 305 is currently having problems)

Rm 120 Macs: Use the Finder to locate and start the program CS ChemDrawUltra, or follow this path:

MacCLC(hard drive)/ChemistryApplications/CS ChemOffice 2005/CS ChemDrawUltra

Rm 305 PCs: Follow this path:

Start/Programs/Chem Office 2005/Chem Draw Ultra 9.0

In Chem Draw, From the **Structure** menu, select "**Convert Name to Structure**".

Type "p-nitrophenol (228A) or p-nitrotoluene (228C)", hit return.

From the **View** menu, select "**Show Analysis Window**".
Select the Formula and Mol. Wt. boxes and hit Paste to add this to the structure.

From the **Structure** menu, select "**Predict 1H NMR shifts**".
A new window containing the spectrum will appear.
Print and attach.

Copy and paste the formula and MWt from the previous page on the NMR.

If you need to resize anything to make it fit, just grab the lower rt. corner of the selection border, hold down the mouse button and drag the corner diagonally toward the upper left to make it smaller.

Compare the ^1H NMR peak positions calculated via this program to the actual ^1H NMR peak positions tabulated on the spectral database in Q #5.
Calculate % error in the calculated shift values.
Attach a table of this info.