

### **2012 Laboratory Research Project Part 1: Literature Search**

This session will be held during the week of March 5<sup>th</sup>, in a smart classroom in the library, most likely the LTEC classroom near to Minerva's Cafe. The purpose is to identify a viable laboratory procedure in the chemical literature, to use for the conversion of *p*-anisaldehyde to *p*-anisyl alcohol in the laboratory.

#### **Schedule of activities**

The schedule is very tight, but this is necessary if we are to achieve the goal of the project in a manageable amount of time. The timetable will be enforced strictly.

13:00 Assemble, log into laptops

13:05 Science librarian Carol Franck presents on information sources and searching.

13:45 Elect a task manager, who then helps the group choose a moderator and scribes assigns tasks.

13:55-14:00 Search your assigned literature source (start as soon as assigned).

14:20 Compile useful results into a summary, give these to the instructor.

14:30 Your instructor will summarize everyone's results, and scribes post key information. The group agrees on a shortlist of 5-10 top choice methods.

15:00 Find full-text information for all shortlisted methods.

15:15 Agree on a first and second choice procedure, and give these to the instructor.

15:30 Complete any remaining parts of experiment 5 (nitration experiment).

#### **Special roles**

All people will participate in the literature searching and the discussions, unless specifically excluded. In addition, certain leadership roles will be needed in order to expedite the work:

Task manager (1)

- Once chosen by the group, this person ensures that a discussion moderator and scribes are picked quickly, and that search tasks are selected and begun quickly.
- Walks around the group while searching is being done, to find out how each person is doing and what they are finding.
- With the discussion moderator, make the final "call" on the shortlist and final choices.

### Discussion moderator (1)

- Runs the initial and final discussions of the search results, using the board to summarize opinions, and moving the group towards consensus.
- During the initial search period, helps work through the “STN Easy” output.
- With the task manager, makes the final “call” on the shortlist and final choices.

### Scribes (2)

- During the initial search period, the scribes work through the Chemical Abstract “STN Easy” search results with the instructor, and summarize the different methods on the wiki.
- Work with the task manager and instructor to post the summaries, shortlist and final procedures into the wiki quickly, so that all students can see the search results during discussions.

### Literature sources

We will use primary sources (journals and dissertations) as well as secondary/tertiary sources such as books and web databases. There are two main types of chemical procedure you will look for – *generic* methods (for reducing aldehydes in general to the corresponding alcohol) and *specific* methods (for carrying out the exact reaction you want to try). We will look for both, because the generic methods (in italics) may sometimes identify a superior process, or at least help us choose a specific method.

The literature sources are given in priority order. Your task manager will assign one of these sources to you. Once your task has been assigned, begin searching immediately.

1. Chemical Abstracts “STN Easy” search results (done by scribes + moderator)
2. ACS Journal database: One person to search before 1999, another 2000-present.
3. Science Direct: One person to search before 1999, another 2000-present.
4. *Organic Syntheses*: One person to search for reduction on aromatic aldehydes to the corresponding alcohol
5. *Books*: As supplied by the library staff and the instructor. These will mostly provide generic information. No. of people to be assigned on the day.
6. Google Scholar: One person to search for the specific reaction
7. Web search: One person to search on the given InChIKeys in Google and at least one other major search engine.
8. ChemSpider: One person to search anisaldehyde and anisyl alcohol literature
9. *WebReactions*: ([www.webreactions.net](http://www.webreactions.net)) One person to search for reduction on aromatic aldehydes to the corresponding alcohol

## Reaction to be searched



### Reactant

Common name: *p*-anisaldehyde

IUPAC name: 4-methoxybenzaldehyde

CAS No: [123-11-5]

InChI: InChI=1S/C8H8O2/c1-10-8-4-2-7(6-9)3-5-8/h2-6H,1H3

InChIKey: ZRSNZINYAWTAHE-UHFFFAOYSA-N

### Product

Common name: *p*-anisyl alcohol, *p*-methoxybenzyl alcohol

IUPAC name: (4-methoxyphenyl)methanol

CAS No: [105-13-5]

InChI: InChI=1S/C8H10O2/c1-10-8-4-2-7(6-9)3-5-8/h2-5,9H,6H2,1H3

InChIKey: MSHFRERJPWKJFX-UHFFFAOYSA-N

## The literature search

As you search, you will mostly be compiling summary information from the data source, such as bibliographic information (a journal name, with authors, year and page nos. etc.), as well as a method description (a reaction scheme and/or abstract). Be sure to compile this information by copying and pasting into a Word document or similar. You will normally keep moving onto the next search result, but if you uncover what looks like an ideal method, you may download the full text while you have it to hand.

Be realistic with your search results. The final procedure needs to be run in one afternoon by undergraduates using common chemicals. Any process that is far from meeting those criteria can be disregarded. For procedures that suggest a longer reaction time, perhaps up to 5 hours, you may still note the procedure in your list, but move it to a lower ranking when reporting your results.

If you are finding more generic methods, be selective: Is the reaction being described similar to the one we plan to carry out? (For example, is it an aromatic aldehyde that is being reduced?) If it is much different, it should be disregarded.

## **Literature report** (worth 90 points)

Two weeks after you participate in this session, you will be submitting your written literature report. This will include the following

- The overall purpose of the group's literature search
- The specific search that you performed, and the specific goals you had for that search.
- A complete list of your useful search results, with a ChemDraw reaction scheme for each reaction that is different. You must include at least three results; if you fail to find enough useful results, you may include some of the less useful ones that you initially discarded, or you may perform further searches at a later date.
- A discussion of the various methods. You **MUST** begin by grouping the various methods into a handful of general approaches. For example, you may find that half of the procedures used sodium borohydride as a reagent – these should be summarized and discussed together. Do not discuss every search result individually unless you only have three or fewer, though you may highlight distinctive features of specific search results (e.g., one sodium borohydride method that works within 10 minutes). Compare the pros and cons of the various approaches, including the following:
  - ease of procedure (short reaction time, simple apparatus, etc)
  - good yield
  - low E-factor or high atom economy
  - low cost materials
- A conclusion about which procedure you would recommend, from just the procedures you found within your own search.

Note: The task manager will be responsible for writing up an overview of the whole group's results.

## **Online assignment**

This will include some questions on the presentation by the librarian, and on some of the search methods and literature sources used,

## **Main paper**

In April you will submit a final paper, in two drafts. This paper will include a section describing the main synthetic approaches found by the group, and the basis of the group's final procedure selection.