

## Library Assignment Fall 2015

The assignment below is the library assignment for the Fall quarter 2015. The assignment aims to improve your skills to locate relevant information in the literature using Reaxys, which is a standard platform in chemistry. Since some of the students will perform the synthesis of the phenytoin as an extra credit project this quarter as well, please look at this assignment as an exercise to write your formal report for this project later. If you have problems, please consult with your teaching assistant or instructor.

The assignment is a required assignment and is worth 15 points. The assignment is due by **Friday, October 16, 2015 at 12:00 pm** in YH 3077 E (instructor's office) as hardcopy (only page 2 and page 3 have to be turned in and can be printed double-sided). **Like always, no late assignments will be accepted.**

Name:

TA:

Section:

Score: /15

Go to <http://www.library.ucla.edu/sel>

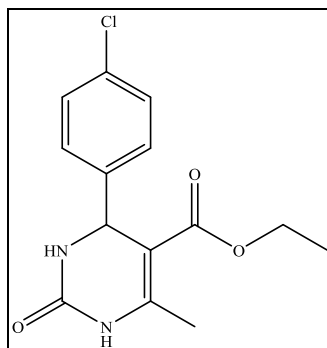
Click on *Journal Articles and Conference Papers*. Then click on *Reaxys*.

(If you are off-campus, make sure you have the proxy server or VPN client set up to access library resources: <http://www.library.ucla.edu/use/computers-computing-services/connect-campus>)

(If you get an intro screen, choose “Start Search with... Structures and Reactions”)

Searching in *Substances*, double click on the white box to open the Structure Editor.

Draw the following **Dihydropyrimidinone derivative**:



Click on "**Transfer Query**" when you are finished to move the structure into the search box from the Structure Editor. Then, click the "**Search Substances**" button.

Click on “Show Details” for the compound above (Reaxys Registry Number 679348) and answer the following questions:

1. What is IUPAC name of the compound?
2. What is its CAS Registry Number (unique identifier)?
3. What is its molecular formula?
4. Under physical data, what is the melting point observed by Xia at al. (2015)?
5. In what journal can you find this article? Provide the exact citation.

Find the full text of the same article (click on full text, the DOI link, and then open the PDF) and answer the following question.

6. What are the specific reagents and catalyst used to form the compound here?
7. Which solvent is used for the actual synthesis?
8. What are the exact condition for the reaction of this compound?
9. What is the final step of the purification of the crude (be specific)?
10. What is the observed yield?

Using the following reference (Liberto et al. *Tetrahedron* **2013**, 69(38), 8245), answer the following questions.

11. Where are the N-H stretching frequencies located in the infrared spectrum for this compound?
12. What are the chemical shifts of the amide protons?
13. What are the chemical shifts of the benzylic proton?
14. Which solvent is used to acquire the  $^1\text{H}$ -NMR spectrum of the compound?
15. Which frequency was used to acquire the  $^1\text{H}$ -NMR spectra in this paper?
16. *Extra Credit*: What is used as catalyst in the Liberto et al. paper?