

Library Assignment Winter 2016

The assignment below is the library assignment for the Winter quarter 2016. The assignment aims to improve your skills to locate relevant information in the literature using the Reaxys search engine, which is one of the platforms to locate information in chemistry. Since many of the students will probably perform the synthesis of the dihydropyrimidinone derivative as an extra credit project this quarter again, you should look at this assignment as an exercise to find necessary information needed to write a good formal report for this project later. Please locate and read the papers below very carefully before trying to answer the questions below. 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, January 22, 2016 at 12:00 pm** in YH 3077 E (instructor's office or the grey mailbox in the office suite) as hardcopy (only page 3 and page 4 have to be turned in and can be printed double-sided this time). **Like always, no late assignments will be accepted.**

Student Name:

TA:

Section:

Score: /15

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

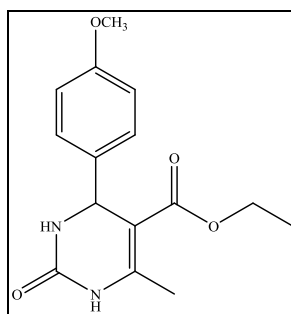
Click on *Journal Articles and Conference Papers*. Then click on *Reaxys*.

(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** (it can be drawn in the editor that comes with the program or with Chemdraw):



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: 292377) 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 Kodape, M. M., et al. (2015)?
5. In what journal can you find this article? Provide the exact citation with proper abbreviations.

Find the full text of the same article (click on full text, then click on *Directory of Open Access Journals*, next type the author's name into the search box) 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 conditions for the reaction of this compound?

9. How was the progress of the reaction monitored (be specific)?

10. What is the observed yield?

Using the following reference (Dhumaskar, K. L. et al. *Bioorg. Med. Chem. Lett.* **2014**, *24*, 2897), answer the following questions (include units).

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. How was the infrared spectrum of the compound acquired?

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 Dhumaskar, K. L. et al. paper?