

### **Library Assignment (Summer 2015)**

The assignment aims to improve your skills to locate relevant information in the literature using Reaxys, which is one of the standard search platforms in chemistry. Since some of the students will perform the synthesis of the dihydropyrimidinone 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, August 21, 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). Place the handwritten answers in the boxes provided. Include the proper units where is needed. **Like always, no late assignments will be accepted.**

Name:

TA:

Section:

Score: /15

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

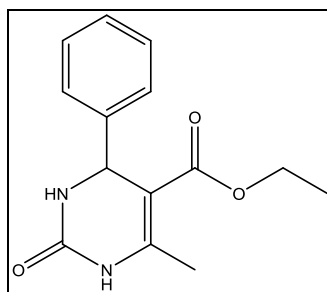
Click on *Journal Articles and Conference Papers*. Then click on *Reaxys*.

(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 248367) and answer the following questions:

1. What is IUPAC name of the compound?

2. What are its CAS Registry Numbers?

3. What is its molecular formula?

4. Under physical data, what is the melting point observed by Ramos et al.?

5. In what journal can you find this article? Provide the exact citation.

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?

11. Which solvent is used to acquire the  $^1\text{H-NMR}$  spectrum of the compound?

12. Where are the carbonyl stretching frequencies located in the infrared spectrum for this compound?

13. What are the chemical shifts of the amide protons?

14. Which frequency was used to acquire the  $^1\text{H-NMR}$  spectra in this paper?

15. Which program/software was used to perform the DFT calculations in this paper?

16. *Extra Credit:* Provide the structure of the solvent used in this reaction.