

Library Assignment Spring 2016

The assignment below is the library assignment for the Spring quarter 2016. The assignment aims to improve your skills to locate relevant information in the literature using Reaxys, which is a standard platform in chemistry. For those of you that perform the synthesis of the dihydropyrimidinone derivative as an extra credit project later this quarter, it will help you writing the formal report because it provides you with resources to locate the literature data. 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, April 15, 2016 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>

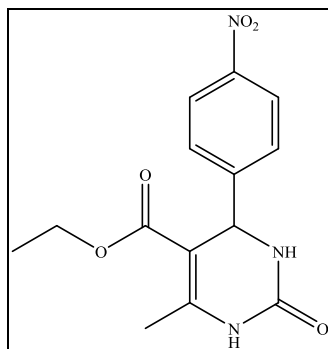
Click on *Journal Articles and Conference Papers*. Then click on *Reaxys*.

(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** (it can be drawn in the editors that come 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.

1. What is Reaxys Registry Number 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 reported by Xia at al. (2015)?
5. In what journal can you find this article? Provide the exact citation (Hint: Which information do you need to locate this article?).

Find the full text of the Xia et al. 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?

Reagents:

Catalyst:

7. Which solvent is used for the actual synthesis?

8. What are the exact reaction conditions 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 for this compound?

Using the following reference (Liberto et al. *Tetrahedron* **2013**, 69(38), 8245), answer the following questions. *Include units in your answers.*

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

16. *Extra Credit:* Farhadi et al. reports the UV-Vis data for the compound. Where do they observe the absorbances (include the molar extinction coefficients)?