Reaxys : Find Chemical Substance Properties and Reactions in Literature

> See the Research Guide from the Shapiro Science Library for tutorials on using Reaxys http://guides.lib.umich.edu/chem216

Organic chemists often search for substance properties and reactions in literature to identify experimental conditions and/or compare results with their own experiments. What is the most efficient way to search these data? Before answering this question, we need to understand the scholarly communication cycle in organic chemistry.

Organic chemists usually publish their original research, such as new substance property data, synthesis methods, and reactions, in original literature and we call them primary sources (See table C-1). The primary source is then indexed and made searchable by various databases and search engines, which are called secondary sources. Data in primary sources can also be extracted from the original publication, organized and even evaluated in review articles, handbooks, and value-added databases etc. We call these value-added publications tertiary sources. Reaxys is one of the tertiary sources widely used in Organic, Inorganic and Organometallic Chemistry fields.
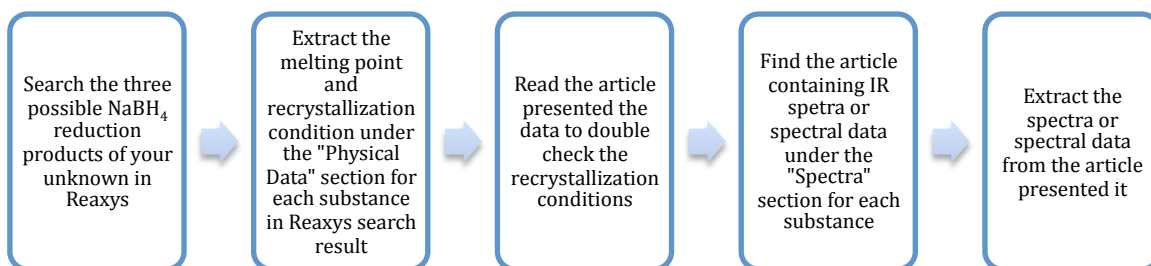
Table C-1 Examples of Primary, Secondary, and Tertiary Sources

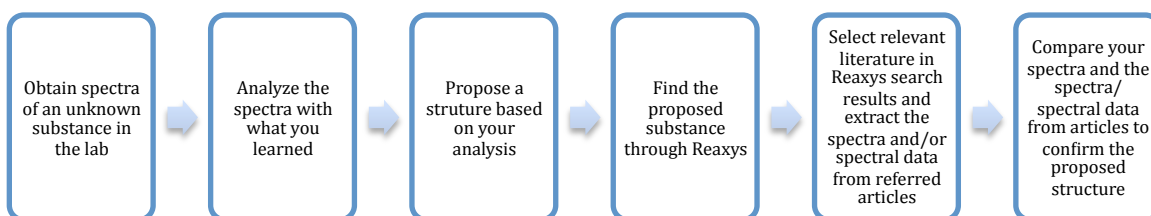| Primary Sources	Secondary Sources	Tertiary Sources
Research articles	Google (Scholar)	Review articles
Lab reports and data sets	Web of Science	Books, handbooks, and textbooks
Patents	PubMed	Wikipedia
Research blogs	Scopus	Reaxys and SciFinder
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When we need to search for substance properties and reactions, we usually start with the tertiary sources and then track back to the primary sources for details if needed. For example, you may look for the melting point of a substance in Reaxys. Once you find the substance, you can read the melting point under the "Physical Data" tab directly. (Remember to cite the source when you write your lab report or paper.) But if you need more details about how the melting point was measured and what solvent was used for recrystallization, you will have to read the reference linked to the melting point. In Reaxys, the blue "MGetIt" link under each reference usually can take you to full text articles subscribed by the University of Michigan Library (See the Research Guide at http://guides.lib.umich.edu/chem216 for details).

Here are a couple of examples on using Reaxys in Chem 216.
1. Find property data and determine experiment conditions (E.g. Experiment 4 Pre-Lab Instructions 4)

| Search the three possible NaBH$_4$ reduction products of your unknown in Reaxys | → | Extract the melting point and recrystallization condition under the "Physical Data" section for each substance in Reaxys search result | → | Read the article presented the data to double check the recrystallization conditions | → | Find the article containing IR spetra or spectral data under the "Spectra" section for each substance | → | Extract the spectra or spectral data from the article presented it |

2. Find spectra or spectroscopic data to confirm proposed structures based on experimental results (E.g. Experiment 8)

| Obtain spectra of an unknown substance in the lab | → | Analyze the spectra with what you learned | → | Propose a struture based on your analysis | → | Find the proposed substance through Reaxys | → | Select relevant literature in Reaxys search results and extract the spectra and/or spectral data from referred articles | → | Compare your spectra and the spectra/ spectral data from articles to confirm the proposed structure |

Q&A

How can I access Reaxys?
The database is available through the following link.
http://proxy.lib.umich.edu/login?url=https://www.reaxys.com

How do I learn to use Reaxys?
Tutorials are available at http://guides.lib.umich.edu/chem216 for you to learn searching substance properties and spectral data through structure search in Reaxys and other means. Please navigate through different topics using the tabs on the top of the page.

Where can I get help?
Chemistry Librarian, Ye Li, is available to answer any questions you may have for finding substance properties and spectral data from Reaxys or other sources. There are three ways for you to ask questions.

1. Come to Ye Li's Office hours at the Science Learning Center (SLC) Alcove 5. She is available 1:00pm-2:00pm on Mondays and 11:00am-12:00pm on Fridays during Winter and Fall semesters. Check the latest schedule at the guide page http://guides.lib.umich.edu/chem216 .
2. Visit Shapiro Science Library Reference Desk (3rd floor Shapiro Library) 10am-5pm M-F or call (734)936-2327.
3. Email Ye Li at liye@umich.edu or call her at (734)615-5694