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# Incorporating Research-Based Problems from the Primary Literature into a Large-Scale Organic Structure Analysis Course

Jiahai Ma*

School of Chemistry and Chemical Engineering, University of Chinese Academy of Sciences, Beijing 100049, China

*Supporting Information*

**ABSTRACT:** Problems are an important part of teaching and important for achieving the creative education targets for graduates and upper-division undergraduates. Besides classical problems in textbooks, problems from recent research should be involved in class, too. This article reports how literature-based problems were incorporated in a scalable manner in a large-scale graduate course of organic structure analysis with widely varying levels of student preparedness at the University of Chinese Academy of Sciences. Two literature based problem designing cases were detailed, aiming at bringing possibilities and challenges to the students that are highly welcomed by them, and more such problems were provided further. The implications for both students and teachers were discussed to guide the future designing of more effective problems. These problems give students experience in modern scientific research in a large-scale class and build upon a habit that strongly emphasizes research-style thinking.

[1]Problem *noun* \ˈprä-bləm, -bəm, -ˌblem\

Definition of PROBLEM

1 *a* : a question raised for inquiry, consideration, or solution
*b* : a proposition in mathematics or physics stating something to be done

2 *a* : an intricate unsettled question
*b* : a source of perplexity, distress, or vexation
*c* : difficulty in understanding or accepting <I have a *problem* with your saying that>

**KEYWORDS:** *Upper-Division Undergraduate, Graduate Education/Research, Inquiry-Based/Discovery Learning, Testing/Assessment*

## ■ INTRODUCTION

Test and exam problems play important and indispensable roles in the whole education process including the spectrum of learning and thus successful application of knowledge. A good problem can greatly enhance a lecture. Thus, effective problems are invaluable sources to both students and teachers.

There are many excellent problems in outstanding textbooks for university curricula. These textbook problems are somewhat artificial and specifically designed to teach basic concepts to build the foundation of knowledge; they are crucial in the very beginning due to their systematic and logical approaches. However, capstone courses, especially for some chemistry or biology majors, are usually descriptive and qualitative; thus, upper-division undergraduates and graduates are easy to ignore the appended textbook problems. More important, classic textbooks are written behind the speed of literature publication. Furthermore, teaching problems to pass standardized testing is a pedagogy that does not prepare students for research achievements or the real world. Thus, besides outstanding textbooks, much more real research cases should be involved in class. Problems borrowed from research articles are much more complex and consist of raw data (complex spectra, etc.); these research-based problems are absolutely essential due to the big gap between a textbook and real research.

Over the recent decades, there has been an increasing drive to incorporate research experiences into the undergraduate curriculum, and significant efforts and improvements have been made in various areas of chemistry education to increase student motivation and engagement by exposing them to current research.[1−10] However, most of these works focused on research-based lab experiences[1,2,4] or writing assignments;[3,7−9] moreover, these works were designed for small groups rather than large-scale classes. Thus, despite the acknowledged pedagogical value of integrating research into the laboratory curriculum, this approach has not been widely adopted for large-scale classes, especially in organic chemistry, due to the high activation barrier to this change.[11] Incorporating research-based activities into a large-scale class can be challenging considering the high enrollments and different backgrounds typically associated with such courses. Moreover, few studies have focused on innovative problem design, especially for large-scale class. For the graduate and upper-division undergraduate courses, there is a vast and constant need for updated problems that are closely related to active research areas.

This article presents some problem-designing cases used in the classroom at the University of Chinese Academy of Sciences (UCAS) for a large-scale organic structure analysis course.[5] Organic structure analysis is considered an essential course in the training not only of chemists, but also of many other specialists. In addition, the concepts, models, theories, methods, and tools of this course permeate all college and postcollege chemistry courses. As a large-scale fundamental graduate course, it offers a good chance to bring the possibilities and challenges to graduates by effectively designed problems. Problems are important for students to learn both the spectra interpretations and "utilizing" literacy. This article further demonstrated incorporating research cases as an integral part of the chemistry curriculum and discussed related issues to help

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improve undergraduate or graduate students' engagement, motivation, and interest in chemistry.

## THE COURSE AND ITS PARTICIPANTS

Organic structure analysis (also known as spectral identification of organic compounds) is a fundamental course for the autumn term at the School of Chemistry and Chemical Engineering that covers the content of UV, IR (and Raman), NMR, and MS materials. Because of the importance of the course, it has a high enrollment. From 2009−2014, the course had more than 300 students every year. The students came from more than 30 research institutes, covering more than 25 subdisciplines in chemistry, biology, materials, and environmental sciences. The students' background knowledge is quite varied because cross-disciplinary learning is an important characteristic of UCAS. Some participants from earth or physics majors had taken only general chemistry courses at the undergraduate level, which they had completed two or three years prior to taking this course.

## PROBLEM ORIGIN

Today, the teachers of higher education are facing the challenge of bridging the gaps between delivering basic knowledge and truly achieving the graduate classroom goals, that is, to produce qualified future researchers. To address this, the author's teaching philosophy in designing the problems was to strongly increase the relevance of this course to current trends in academia while maintaining attention to the basic the spectra interpretations. Thus, problems coming from both sources of textbook and research are complementary and applicable for different levels of preparedness and backgrounds of students.

Table 1 shows the comparison of two sources of possible problems for the classroom. The first is from the textbooks; problems of this type are convenient for teachers but potentially out-of-date. For example, for $^{13}C$ NMR, the off-resonance techniques have been replaced by DEPT series experiments, while the problems based on off-resonance data are still popular in Chinese textbooks. On the other hand, the problems from textbooks usually have definite conditions (given information), and students must use all of these given information; if not, the right answer could not be worked out, so it is good at evaluating student's knowledge, but clearly it is very different from the real-world research. In real-world research, scientists need to try their best to use various experimental methods to find enough evidence to directly or indirectly support or test their conclusion or hypothesis. The second problem is that problems from research articles always give more than enough information to work out the problem; and at this point, students need to select information. Thus, problems from research articles move away from the "cook-book" exercises to more open-ended and investigative processes.

**Table 1. Comparison of Two Sources of Inquiry Problems Used in a Large-Scale Organic Structure Analysis Course**

| | Sources for Inquiry Problems Used with Students | |
|---|---|---|
| Comparison Dimensions | Textbooks (Emphasis on Knowledge) | Research Articles (Emphasis on Evaluation and Application) |
| Purpose | Teach basic concepts to build a foundation of knowledge | Report research findings, bridging the gap between textbook learning and real-world research |
| Approach | Remove distractions and simplify topics | Present raw and often imperfect data (complex spectra, etc.) |
| Advantages | Systematic and logical presentation of topics | Up-to-date presentation of topics |
| | Easy to obtain | Provide research circumstances |
| | Mature ideas presented | Novel topics presented increase students' interest in chemistry |
| | Convenient for teacher | Helpful for future research |
| | Allow evaluation of students' knowledge | Allow evaluation of researchers' abilities |

From Table 1, the first type problems emphasize knowledge, and the second type problems push students to evaluate and apply corresponding information. The problems coming from research articles demand more for teachers' efforts; in turn, teachers benefit from literature-based problems by gaining an "educational" view and understanding research in more depth.

Could we design effective research-based problems that highlight current research? The answer is definitely "yes", but where and how to find novel "practical" examples? Of course, it is not optimal to design the problems based solely or mainly on the teacher's personal special background or limited research experience; further, if so, it may unconsciously lead to biased opinion for designing problems that are only centered in the teacher's personal research fields or interests. Luckily, there are inexhaustible resources in literature, and scientists are creating more every day. The rapid growth in recent years of literature makes this goal of designing effective research-based problems much more realistic and achievable.

## RESEARCH-BASED PROBLEMS BRIEF

To some extent, the major barrier to including problems from the literature in class is the amount of time required to find example problems that students can reasonably be expected to solve; this is particularly true for combined spectra, which are often far too complex (or too low quality) for students to analyze in detail. Table S1 summarized the literature-based problems used in the class,[12−29] and the detailed information such as target and expansion could be found in the table, too. Furthermore, how does one select a problem from a research article and adopt it for the students? The following points derived from Table S1 (Supporting Information) are helpful to other teachers with similar goals to design efficient literature-based problems:

(1) Have corresponding high-quality spectra.
(2) Have no demand of special knowledge backgrounds (and have energy, environment. or life science backgrounds), and thus they could be readily incorporated in a scalable manner in a large-scale class with widely varying levels of student preparedness.
(3) Additionally, some problems are related with daily life to stimulate student interest; though not typically necessary, it is a definite plus.
(4) Articles published on higher-rank journals are preferred; more important, it is perfect if the article itself is landmark research.

## CASE I

Because of the rapidly increasing competition and space limitations, many journals are offering Supporting Information (SI) for detailed figures and results (usually free), and thus SI can accommodate almost any detailed supplementary figures or data (e.g., reproductions of spectra, tabulated data, and expanded discussion of peripheral findings). For example, the



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SI of the instructor's one article provided complete absorption and emission spectra of many model quinones and hydroquinones, which are not readily collected elsewhere and very useful for related research.[30] Further, the teachers could compose their unique problems based on careful selection and recombination of the SI of journal articles.

The recent decades are clearly identifiable as the age of mass spectrometry (MS); "soft" ionization techniques (such as electrospray ionization (ESI), and matrix-assisted laser desorption ionization (MALDI)), targeting molecular ion peak while not fragment peak, have enabled bold advances in many directions. Further, for routine analysis, GC-MS with ever-expanding database usually could directly present the molecular structure. Thus, students are showing declining interest in learning detailed MS interpretation. However, in the instructor's opinion, the structure-solving strategy is unchanging and needs to be emphasized more. Case I was designed from the SI of an article to deepen the basic structure-solving strategy of MS. Figure 1 showed the problem: Diclofenac, an anti-inflammatory drug, is one of the commonly detected pharmaceuticals in sewage treatment plant effluents; the following MS was from the transformation of Diclofenac by manganese oxides. (1) Why do the main peaks have a difference of 2? (2) Deduce the pathway to fragment ions of ②, ③, and ④.

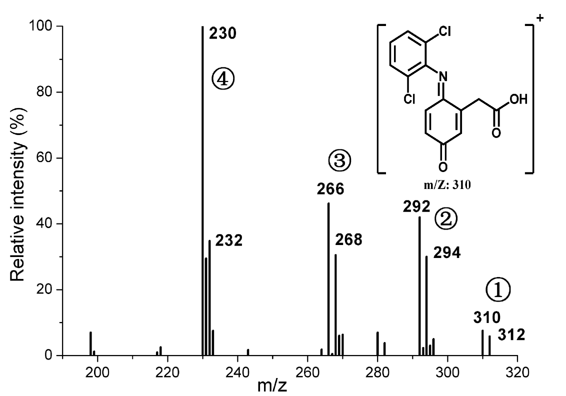


**Figure 1.** Higher-end MS of the shown molecule. The figure was revised based on the SI of the original research paper of ref 26.

The problem here clearly examined the basic strategy of MS interpretation. First, it reminded the isotopic abundances. Second, it emphasized one important skill to find which fragment is lost, such as common loss of $H_2O$, $CO_2$, H, and Cl, which corresponded to pathways to the fragments. Indeed, some students who only memorize mechanically were confused by the relatively large molecule and could not correlate the spectra with the knowledge of isotopic abundances. Thus, this problem differs from those centering on memorized knowledge and is not just the "textbook stuff".

## ■ CASE II

The instructor's one favorite problem source is "JACS (*Journal of American Chemistry Society*) Image Challenges"; many of these image challenges are spectral problems and well designed, providing a good balance of the necessary background materials as well as summaries of up-to-date research, and are suitable for capstone-type courses. To some extent, this source is born for organic structure analysis and thus should appeal to students from different disciplines for touching current chemical research.

One basic knowledge point in UV spectra is the absorption of disubstituted benzene: when electronically complementary groups are suited *para* to each other, such as 4-nitroaniline, due to the extension of the chromophore from the electron donating group (D) to the electron accepting group (A) through the benzene ring ($\pi$), the disubstituted benzene has profound shift in the main absorption band. The instructor highlighted that such D−$\pi$−A molecules form the basis of organic molecule devices; further, the instructor introduced the topic of visual detection of ultratrace amount of TNT using an easy-to-read paper to broaden the students' view of D−A interaction.[31] Moreover, the instructor recommended more recent achievements in this field.[32,33] A problem (from "JACS Image Challenge" #176) was presented to evaluate the learning result of the D−A interaction topic.[15] Figure 2 showed the problem: When $C_{60}$ powder was suspended in $CH_3CN$ solution of the molecular capsule at 80 °C, the color of the solution changed from pale-yellow to red−purple due to the encapsulation. Which of the following interactions is the main driving force for the encapsulation of $C_{60}$?

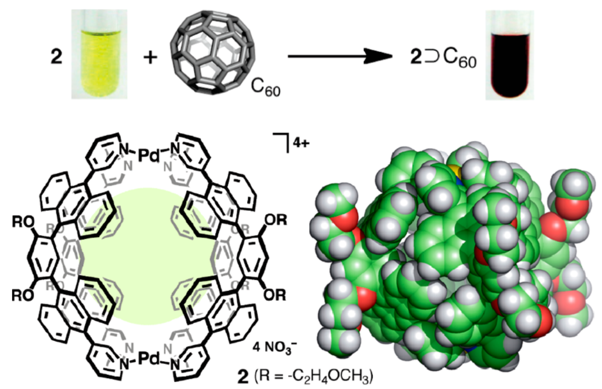


**Figure 2.** Molecular capsule has an aromatic anthracene shell, which provides a cavity with a diameter of ~1 nm that could encapsulate $C_{60}$. The figure is from "JACS Image Challenge" #176 (used with ACS Copyright permission) and the original research paper of ref 15.

(1) Hydrophobic interactions
(2) CH-$\pi$ interactions
(3) $\pi$-Stacking interactions
(4) Electrostatic interactions

The correct answer is $\pi$-Stacking interactions. Students who learned the D−$\pi$−A interactions the teacher lectured above would work out this problem easily, though it is likely beyond the traditional UV knowledge coverage. Indeed, more than 90% of the class chose the correct answer. For classroom use, this explanation based on D−A rule maybe better than the provided answer at the Web site. From their answer: the key is "A UV−vis spectrum of the $C_{60}$-encapsulated complex showed a broadened absorption band corresponding to a typical charge-transfer band for $C_{60}$ due to $\pi$-stacking interactions. Therefore, the main driving force for the encapsulation is $\pi$-stacking interactions between $C_{60}$ and the anthracene rings of the capsule." Students need to finish reading the original article to understand the Web site answer. Furthermore, there is another interesting image challenge (#46) that was recommended to students for colorimetric detection of $Hg^{2+}$ using


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DNA and nanoparticle conjugates, although it needed background knowledge that base thymine (T) binds Hg readily.[16]

Worthy of note, case II is a multiple-choice problem, which is not common for upper-level courses where students are usually expected to explain their reasoning; however, if used in a moderate and rational way, a multiple-choice problem is efficient for in-classroom learning assessment for a large-scale course and is helpful for stimulating after-class self-study, too.

## FLEXIBILITY OF LITERATURE-BASED PROBLEMS

Literature-based problems are flexible. First, according to the different audiences of lower-division undergraduates, upper-division undergraduates, or graduates, the instructor could appropriately choose to provide related background knowledge or not, disclose more spectroscopic data or not, or make the structural problem easier or not for a better learning result. Second, the instructor could readily use the literature-based problems in lecture, in exam, or as homework. Third, literature-based problems should not only be used for the course (in class and in exam), but also in the future, the author would like to extend them to the important graduate entrance exam of organic chemistry for UCAS (if so, about 1000 graduates per year would be exposed to such literature-based problems), hoping to effectively distinguish potential MS. and Ph.D. candidates, and the grade results could be used to guide the future designing of more effective problems.

## IMPLICATIONS FOR STUDENTS

Needless to say, spectra theory and techniques have always been the principal dimensions in the teaching of the course and are very important for training students. However, there is a third dimension that is equally (if not more) important in teaching the course; this dimension is "problem-solving" thinking, which enables students to attack problems efficiently and conclusively using both theory and techniques.[34] Implementing research-based problems is not difficult, as the basic knowledge does not need to change; what changes are the way the problem is set up and how the actual research background is introduced. Rather than following a step-by-step knowledge evolution procedure, the research-based problems have general guidelines for the corresponding research topic, enabling students to develop research-based problem thinking and solving procedures of their own. The module introduces students to a research topic, presents fundamental spectra concepts in an applied context, and exposes students to potential research opportunities. Indeed, many students told the author that they were very interested in the visual detection and wanted to do some research in this field.

Especially in the thinking and solving and after-thinking process, students entered into the simulated research scenario very closely, looked at the spectra (data), and generally reproduced the ways in which the actual research was done. Students must identify essential questions and draw and integrate relevant information from the provided background; this process requires more original intellectual contribution on the part of the student, and therefore, to some extent, solving the research-based problem becomes an inquiry-based project. In a word, such problems have a greater potential to engage students and develop their scientific thinking and solving skills. By continually exposing them to research-based problems, students were treated as researchers at such a large-scale course readily; thus, even at this early stage in their careers, students appreciated that the problems made them think about chemistry and how it can be applied to real-life situations. In addition to related spectra concepts or knowledge, students may learn:

(1) Why the scientists do such experiments.
(2) Where to begin.
(3) What is key to successful solving.
(4) What implications and thus further questions the problem brought to them.
(5) Whether the reported results were worth further digging and how to do it, or what spectral experiments could be done to further confirm or disprove it.
(6) If novel spectra methods worked, were they universal? What other reaction system could be applied by these methods?

In addition to the engagement of the students in the "research" activity in the classroom, the result of this approach has been the development of students who are capable of formulating hypotheses, moreover, sound thinking styles and solving procedures to test these hypotheses.

The author also combined the research-based problems with traditional problems from textbooks into the exam paper with a ratio of 1:1. From the grades analysis, some students are not used to the research-based problems and basically have nothing to do with it. However, for most students, once they left the "real-world fear" behind, or more accurately, once they looked through the "real-world disguise", they could solve the problem.

## IMPLICATIONS BEYOND THE COURSE

The author's teaching experience suggests that the best approach is utilizing literature-based problems carefully to fit the level of the course that requires students to make connections between basic principles and special research. In addition, teachers should not abandon those excellent textbook problems; instead, the teacher should combine the two origins together in such a format that students having different knowledge backgrounds could gain more with less pain.

The instructor would emphasize that, whether for problems from old textbooks or from current research, the target of the course is analyzing organic molecular structures; the only way to become proficient in this area is to practice. A mix of memorization and discovery (based on literature-based problems) could be a good approach and provide students with the benefits inherent in both modalities.

Literature-based problems have been shown to promote students' independent thinking and encourage students to look beyond both textbooks and faculty for answers. Indeed, one of the fundamental features of learning this course and chemistry is that students need to have robust molecular-level images of molecular structures, and reactions and to be able to connect those molecular-level images to what observed (the macroscopic), and what is represented (the spectra symbolic). From a big view, getting the "sense" of chemical research requires the capacity, which is learned and practiced through literature-based problems in this course, to develop mental habits that picture invisible chemical images in the molecular world; thus, it is more rewarding than teaching students only to solve organic structural questions.

Further, confirmatory laboratories usually could not provide sufficient opportunities for students to experience the cycles of failure and recovery that real-world scientists experience as an ordinary part of their work. Indeed, learning how to deploy


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efficient thinking and solving is a critical part of becoming a scientist yet is rarely reflected in most textbook problems and lab curricula. If we truly want to cultivate a world of problem-solvers, we must allow students opportunities to wrestle with literature-based problems and be rewarded for conceiving efficient strategies for solving them. Our students have shown us they are ready for the challenge.

## ■ ASSOCIATED CONTENT

### Supporting Information

The Supporting Information is available on the ACS Publications website at DOI: 10.1021/ed5008662.

Overview of real-world inquiry problems used in the course (PDF, DOCX)

## ■ AUTHOR INFORMATION


### Corresponding Author

*E-mail: majia@ucas.ac.cn.


### Notes

The authors declare no competing financial interest.

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