Teaching Chemical Literature, Databases, and Chemical Informatics

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The 2003 ACS guidelines document states that a well-prepared student should emerge from a program in chemistry with (among other things) “experience with computers, including an ability to use word processors, spreadsheets, numerical and non-numerical algorithms, simulations and computation, data acquisition, and databases for information handling and retrieval.”1 Furthermore, the guidelines note that “chemical computation of the properties of molecular and macromolecular systems has become a familiar and important part of chemical laboratories, and such experiences may count toward the laboratory requirement for certified majors.”2 It was in part to broaden the formal opportunities for both undergraduate and graduate students to enhance their chemical computation and other computer-based skills that Indiana University developed a series of chemical informatics courses.

Chemical informatics is the application of computer technology to chemistry in all of its manifestations. Cheminformatics techniques are heavily used in the pharmaceutical industry, but chemical informatics is also being applied to problems across the full range of chemistry. Indeed, the various codes for chemical structures that let us both view and search chemical structures via the computer were developed by chemical informaticians.

Undergraduate informatics majors at Indiana University must select a cognate area in which to apply the informatics skills they develop. Courses were created both for the undergraduate chemistry cognate requirement for the BS in Informatics and for a specialized MS in the Chemical Informatics program. The BS in Informatics degree with a cognate requirement for the BS in Informatics and the BS degree with a cognate requirement for the BS in Chemistry must each have two one-hour chemical informatics courses. These are C371 Chemical Informatics I (basic concepts) and C372 Chemical Informatics II (molecular modeling).

Students are also encouraged to take two related courses from the information science side of the curriculum, C471 Chemical Information Sources and Services (1 credit) and C472 Computer Sources for Chemical Information (1 credit).3 We tend to view the material covered in C471 and C472 as specialized areas in the broader field of chemical informatics. Many of the topics in those courses are likely to be presented in any course that introduces undergraduates to the chemical literature. C472 delves into more complex searching in Chemical Abstracts, Beilstein and Gmelin, and the Cambridge Structural Database.

In recent years, the Web has had an incredible impact on students' perceptions of how best to find chemical information, including integration with existing courses.4 Students preparing for professional work in chemistry must learn how to retrieve specific information from the enormous and rapidly expanding chemical literature. The complexity of this task is such that one can no longer easily acquire the necessary skills without some formal instruction. An excellent means for doing so is with a specific course, which usually would not qualify for the advanced course requirement. Other means for imparting these skills involve coordinated instruction integrated into individual courses. Library and computer exercises should be included in such instruction. In departments requiring undergraduate research, instruction in information organization and retrieval may be a part of the introduction to research. It should be recognized that adequate presentation of the subject, including an understanding of the use of Chemical Abstracts, Science Citation Index, Current Contents, PubMed, and other compilations, will generally require formal instruction. It is essential that students gain experience with online, interactive database searching, which can

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In recent years, the Web has had an incredible impact on students’ perceptions of how best to find chemical information. For any question, the great majority of students at the beginning of the C471 course (typical enrollment: 60 students) want to "google" it. At the end of the course, it is satisfying to read the positive comments from the great majority of students whose eyes have been opened to the wealth of chemical information sources available beyond Google.

How should an instructor who has been given the task of satisfying the ACS requirements in the chemical information area proceed? First, despite what is said above, don’t ignore the Web. There are many reliable sources out there that can be accessed for free. Even structured searching can be incorporated with a free tool such as NLM’s ChemIDplus. If time is limited, concentrate on the computer-based material at the expense of the printed resources. Purdue University’s chemistry librarian, Bartow Culp, has put together a small list of free or cheap essential tools of which undergraduate chemistry librarians, chemists, and others by joining the Chemical Information Sources Discussion List, a listserv that has been around since 1991 and currently has over 1400 subscribers.

Be sure to find out the deadline for getting software installed on your campus computer and library system so that students will be able to access it from the first day of class. It may take some convincing of appropriate personnel that plug-ins such as Chimera are essential for visualization of chemical structures and other chemical graphics on the Web. If your institution is not a subscriber to SciFinder Scholar, an alternative and relatively inexpensive way of searching the Chemical Abstracts service is to use STN on the Web through STN’s Academic Program. Even that service will require plug-ins if you want to be able to do structure or sequence searching.

Chemical Abstracts Service has developed a Web page for the academic community that contains links to basic and intermediate training and information about SciFinder Scholar, STN on the Web, and other CAS and STN products and services.

A good resource is the Clearinghouse for Chemical Information Instructional Materials (CCIIM). With pages for Chemical Abstracts, Science Citation Index, and other major tools and topics, the CCIIM connects you to many useful sites for developing chemical information instructional materials and exercises. One page is devoted to "How to Teach Chemical Information," where you will find a link to the "Teaching Chemical Information" workshop that is frequently offered at ACS and other meetings. With some advance planning, the task of creating a chemical information instructional program need not be as daunting as it may seem at first. The resources listed in this brief survey will get you started in the right direction.

Footnotes

ACS Academic Employment Initiative

The ACS is running an experimental program to support the academic hiring process through activities at its 2004/5 national meetings. The program, known as the Academic Employment Initiative (AEI), aims to broaden the faculty recruitment process by making it easier for faculty recruiters to meet and interact with more candidates seeking faculty positions than is possible under the current system. Normally, departments meet only the few candidates selected for campus interviews on the basis of their paper portfolios. The idea of AEI is to open the process by encouraging personal contact between faculty recruiters and job seekers prior to campus interviews and in a relatively informal and noncommittal setting, namely through the venue of the popular SciMix poster sessions at national meetings. The first AEI-SciMix poster event will be held at the fall 2004 ACS meeting in Philadelphia where job candidates are invited to present posters on their accomplishments and objectives in research or teaching or both. As of this printing, over 100 posters have been submitted. The event is open to the entire range of colleges and universities, and is expected to be of interest to candidates for positions at institutions where faculty responsibilities include both teaching and research as well as undergraduate colleges where teaching is the primary focus. The success of this experiment will depend on the participation of both job candidates and faculty from departments with open positions. It is a welcome opportunity for candidates to reach a wider audience and for faculty to meet more potential young colleagues than would otherwise be possible. As ACS President Charles Casey states in his commentary in C&EN (March 1, 2004) “Few matters are more important to departments of chemistry than the hiring of excellent faculty…Through this process (AEI), we expect to create a more inclusive system of faculty recruitment that will ultimately strengthen research and teaching in the chemical sciences.” The upcoming ACS SciMix session in Philadelphia is the first step in this direction and will be the first of many with the support of the academic community.
Life After Graduate School

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M ost people would agree that the current doctoral education system in the United States does a very good job of preparing chemists to do independent research. However, doctoral programs are generally not as good at imparting some of the ancillary skills that are necessary to obtain a job and to enjoy a successful career in chemistry: communication skills, both written and oral; team skills; and navigating the political waters. To quote a respondent to the Committee on Professional Training’s Surveys of Programs and Participants (Graduate Education in Chemistry, American Chemical Society, 2002), the Ph.D. experience “really did not prepare us very well for life after graduate school.”

To help address this outage, the Department of Chemistry at the University of Cincinnati has initiated a course entitled, appropriately enough, “Life After Graduate School.” This course is offered pass-fail to students in their third year or beyond in the doctoral program. It is taught by Joel Shulman, an adjunct professor with 31 years of industrial experience, and Assistant Professor Anna Gudmundsdottir, and makes liberal use of outside speakers. Because 60% of Ph.D. chemists are employed by industry, this is a main focus of the course. However, teaching at universities and four-year colleges as well as working for the government are also covered. The course is built around three main topics:

- what chemists do in the “real world,”
- what skills and knowledge are needed to succeed after graduate school, and
- honing the skills needed to find a job.

What Chemists Do

The course begins with a comparison of careers in industrial and academic research: solving illustrated by the case study and get a real appreciation of the value of approaching a problem as a multidisciplinary team.

Some Skills and Knowledge Needed To Succeed

The emphasis here is on communication, both written and oral. Differences between academic and industrial presentations are discussed. Particularly important is a writing exercise on advocating a position—something that is very different from the technical writing to which students are exposed in graduate school. Grant writing is discussed, as well.

A nother key aspect of this section of the course is a discussion of ethics in science (using, in part, the A A A S video vignettes on Integrity in Scientific Research). The issues arising when academic research is sponsored by industry, including the intellectual-property questions that can arise from such arrangements, form an important part of the ethics discussion.

The final portion of this part of the course discusses postdoctoral positions as a means to refine a person’s skills: why do a postdoc and how to go about finding the best position for you.

Finding a Job

Landing a job consists of three steps: targeting potential employers, getting through initial screening, and receiving an offer after visiting the employer. Many aspects of the job search are different between academic and industry; these differences are discussed and strategies for finding each type of job are covered. The skills important to each step of the industrial job search are emphasized, especially developing an effective resume, preparing an industrial seminar, and learning interviewing skills.

All students are given a mock interview to practice their skills. They learn a lot about themselves during these mock interviews as they think about questions that may never have occurred to them before. Many students see a dramatic improvement in their interviewing ability simply by knowing the types of questions to expect.

The course completed its third iteration in the fall of 2003. Past participants have given very positive feedback on the course, which continues to evolve to meet the needs of students. A student summed up his experience, “the topics taught in this course are some of the most important for students preparing to enter the workforce; however, they’re rarely taught anywhere else.”

Certificates for ACS-Certified Graduates

Chemistry majors who receive a baccalaureate degree from an ACS-approved program and complete a curriculum described in the ACS guidelines may be certified to the Society for membership purposes by the head or chair of the approved institution. We will be happy to send certificates to certified graduates. When requesting certificates, please include the students’ current mailing addresses. If you would like to have certificates available for presentation to your certified graduates, please let us know the number of certificates that you would like and the date that you need them. Send all requests to the Office of Professional Training, American Chemical Society, 1155 Sixteenth St., N.W., Washington, D.C. 20036 or by email to cpt@acs.org.