

Introducing the *Journal of Chemical Education's* "Special Issue: Chemical Information"

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ABSTRACT: How chemical information is produced, distributed, discovered, managed, shared, and preserved has changed significantly in the past two decades. The number of publications continues to grow exponentially, and most of the core chemistry literature is now available online. Understanding how to navigate this digital landscape is essential for students, educators, and researchers. Similar to calibrating and learning how to use lab instruments, developing information literacy skills enables researchers to use their time more effectively and efficiently. In response to an open call for papers, this issue contains 26 papers that are grouped into three broad subject areas: Information Skills, Prototypes and Best Practices, and Discovery. Papers in this special issue aim to be a resource for ideas and a catalyst for expanding communication and collaboration between chemists and information professionals. Because some areas of chemical information are not included in this issue, topics for future issues of the *Journal of Chemical Education* are suggested at the end of this editorial. Note: Papers in the *Journal of Chemical Education* Special Issue: Chemical Information have a designation that they are part of the collection published in this issue.

KEYWORDS: High School/Introductory Chemistry, Graduate Education/Research, Chemoinformatics, Undergraduate Research, Communication/Writing, Inquiry-Based/Discovery Learning, Problem Solving/Decision Making, Testing/Assessment

Understanding how chemical information is published, discovered, and managed are key skills needed by students, educators, and researchers. Similar to learning laboratory methods and instruments, developing information literacy skills enables researchers to use their time more effectively and efficiently. Answering an open call for articles, this *JCE* special issue on chemical information contains perspectives, practices, and programs of potential use to educators and librarians in higher education and high school. This special issue aims to provide ideas, inspiration, and to be a catalyst for more collaboration and conversations between chemistry educators and information professionals.

■ CHEMICAL INFORMATION SKILLS

At the undergraduate level, focusing on a core set of tools and skills helps students establish a solid foundation they can build on as they progress in their academic careers. For advanced researchers, developing a strong repertoire of knowledge and skills helps them use their time more effectively and efficiently and enables them to be more competitive in the job market. To help chemistry educators and librarians, the American Chemical Society (ACS) Division of Chemical Information has created a Chemical Information Literacy¹ page that contains key resources and guidelines.

■ CHEMICAL EDUCATION RESEARCH

Zane and Tucci² surveyed secondary education chemistry teachers in the United States to learn about the perceived value of information literacy (IL), potential difficulties in embedding information literacy skills in the curriculum, and the type of resources available to high school chemistry teachers and students. Survey results show that there is an opportunity to equip secondary education chemistry majors with an IL pedagogy they are able to use in the future with their students.

Shultz and Li³ studied how students in a college undergraduate organic chemistry lab course apply information literacy skills to complete problem-based learning assignments. With the use of discourse analysis and evaluation of student-generated artifacts, the evidence suggests that students do not develop information literacy skills without explicit instructions.

■ CHEMICAL INFORMATION LITERACY FOR UNDERGRADUATES

Common elements in teaching chemical information skills include the structure and organization of the literature; methods for performing database searches by searching topics, author, chemical substances; and exporting citations from search results into a reference manager and using these citations in papers. Some courses include searching the patent literature and physical properties. Courses may include how to read a scientific article and practice doing peer review. Either in a literature course or in follow-up courses, students learn how to prepare proposals, write papers, and give presentations. Some instruction is embedded in chemistry courses, yet many examples in this issue are separate courses that are team-taught by faculty, taught by a librarian–faculty team, or via online tutorials.

The paper by Yeagley et al.⁴ is noteworthy because information skills needed by undergraduates are infused throughout the curriculum. Students learn how to review the scientific literature, design experiments, collect and analyze data, and how to disseminate their findings in both written and oral formats.

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Greco's⁵ article covers teaching chemical information literacy in a one-credit, sophomore-level course at a liberal arts college. Students learn about the literature, database searching, managing references, searching the patent literature and physical properties, and using a structure drawing program. Students learn how to read a paper on an unfamiliar topic. They prepare an annotated bibliography on a topic of interest that is used in a subsequent course where they write a review paper.

Danowitz et al.⁶ team-taught a course for undergraduates in their third year that helps students develop skills needed to prepare and present a research proposal. They learn how to search the literature and how to evaluate safety and research ethics of projects. Students then use their proposals as research plans for the remaining part of their undergraduate career.

Jones and Seybold's paper⁷ covers chemical information literacy, ethics, communication skills, and career preparation in a team-taught, semester-long course for undergraduates. Coursework includes writing a term paper, participating in a peer-review exercise, giving an oral presentation, learning about résumé writing, and participating in professional ethics discussions. A highlight of the course is hearing presentations by alumni who work in a broad spectrum of chemistry-related positions.

Jacobs et al.^{8,9} wrote two articles about integrating chemical information instruction into the chemistry and biochemistry curriculum at an undergraduate institution. The first article focuses on collaborative efforts of a chemistry professor and science librarian to devise online tutorials for searching SciFinder. Created using simple, user-friendly software, the tutorials have developed into a set of 14 modules that are narrated by the professor. The first article also describes development of the tutorial, feedback-driven revisions, and assessment of learning outcomes.⁸ The second companion article covers the execution and assessment of a semester-long capstone project for Organic Chemistry II.⁹ In the six years since this information literacy program was implemented, technology changes, student feedback, and learning outcomes were used to revise the tutorials and research report assignment.

Cowden and Santiago's paper¹⁰ is another collaborative effort between a chemist and a librarian who worked to improve student research and critical thinking skills for interdisciplinary research by using problem-based learning in an advanced biochemistry class. Initial findings for this pilot project suggest that the combination of using a problem-based approach to searching for information coupled with multidisciplinary thinking may give students a more holistic view of chemical research.

Baykoucheva et al.¹¹ offers methods for integrating chemical information literacy instruction into many undergraduate and graduate courses at a research university. A collaborative effort between a chemistry librarian and course instructors, this article focuses on two small classes (40–60 students) and one large class (380–460 students). Using face-to-face methods with online tutorials, they teach students how to search key databases and how to manage citations in EndNote. An online assignment to assess student learning was designed using SurveyMonkey.

Zwicky and Hands¹² use peer review in a writing project of an upper-level chemistry literature course as a way to help improve student performance. Students were asked to find articles on a topic and write a brief paper that was anonymously peer-reviewed by classmates and then revised. The papers and

the reviews were then evaluated using a rubric based on information literacy competency standards.

■ CHEMICAL INFORMATION LITERACY FOR GRADUATE STUDENTS

Scalfani et al.¹³ introduced a new graduate-level course on literature and communication in chemistry, replacing a literature seminar requirement. Course topics included chemical information resources, critical analysis, scientific writing and presentations, and peer review. This change was well received by chemistry faculty and chemistry graduate students. This article covers implementation, content covered, and potential revisions.

A leading educator in chemical information, Currano¹⁴ reviews how a graduate-level chemical information course has changed during the past two decades at her research institution. The course evolved from being a series of workshops to a more holistic examination of the chemical literature and the research process. The course includes group assignments, a term project, and a final exam, all of which test students' ability to navigate the literature effectively and efficiently, helping them to develop skills they will need to be successful in their academic and professional careers.

Gozzi and colleagues¹⁵ cover changes for teaching students at their three-year graduate-level program in chemical engineering. While understanding how to search the literature remains important, the type of searching skills needed has been integrated into the curriculum so that students now learn information skills at the point they need to use them.

■ PROTOTYPES AND BEST PRACTICES

Kamijo et al.¹⁶ developed a prototype called CLeArS (Chemical Literature Extraction and Aloud-Reading System) that reads names of chemical compounds to help visually impaired chemists recognize chemical structures. CLeArS uses IUPAC nomenclatural rules. Experimental results on 450 images comprising both simple and complex chemical structures showed a 90% recognition rate among subjects with visual disabilities.

Pence and Williams¹⁷ review the rapid and pervasive growth of big data. They define big data as being a combination of volume, variety, velocity, and veracity of computerized data that is being processed. As big data tools are already having an impact on industry and research, they discuss whether an introduction to these developments should be included in undergraduate chemical education.

Walker and Li,¹⁸ a chemistry professor and a chemistry librarian, respectively, provide an excellent overview about the chemistry content in Wikipedia. They address how students can use Wikipedia effectively as an information source, to critically evaluate content, and to learn key information literacy skills. By having a class assignment to edit Wikipedia articles, students move from being consumers to producers of chemical information that is shared in the real world.

Stuart and McEwen,¹⁹ an environmental, health, and safety professional, and a chemistry librarian, respectively, identified significant synergies between the skill sets needed for lab safety and chemical information by the ACS Committee on Professional Training (CPT) guidelines for undergraduate chemistry programs.^{20,21} By the integration of emerging tools in the laboratory safety field into information literacy frameworks, a strong foundation can be established for developing skills

identified by the CPT. This paper describes strategies and provides examples of how these concepts can be implemented in both the chemistry teaching and research laboratory settings.

■ DISCOVERY

The chemical information ecosystem has changed significantly over the years.^{22,23} The number of publications has grown exponentially^{24,25} and English has become the dominant language used in scientific publications.²⁶ Over the past two decades, virtually all databases and most journals have migrated from print to online. Excluding some textbooks and popular works, new monographs and an increasing number of older books are also available online. Chemistry journals have the highest average cost of all disciplines.²⁷ A small yet growing number of chemistry articles are becoming openly accessible to readers.^{28,29} Understanding the challenges, opportunities, and impact this publication landscape has on chemistry students, instructors, and researchers is important.

While search interfaces have evolved rapidly and strive to be user-friendly, most chemistry databases are large and complex. It is easy to drown in a sea of data while missing core materials on a topic. Annual Reviews has a white paper on the role of the critical review article in alleviating information overload.³⁰ Fortunately, resources such as books, online help, tutorials, and webinars, plus library workshops and consultations with information professionals or information providers, are available to help users learn essential searching and information management skills.

Several articles published in this special issue include information about the content in databases and methods that can be used for searching them.

Tomaszewski³¹ covers the concept of the “imploded” Boolean search with undergraduate chemistry students. He shows how combining different types of data as search terms, for example, a chemical substance or reaction plus keywords plus numeric values (e.g., physical properties) enables users to quickly refine searches to highly relevant items.

Härtinger and Clarke's paper³² shows how to use patent classification for discovering chemical information in a free patent database. Patents are a rich source of chemistry information. Using graphene as an example, the authors provide step-by-step instructions for using patent classification to quickly focus search results.

Glasser³³ provides an overview of crystallographic information resources, many of which are freely available. He summarizes the content available and methods for searching them.

Rzepa³⁴ covers how to do 3D chemical information searches in the Cambridge Structural Database to demonstrate core concepts in organic and inorganic chemistry (e.g., connecting the regiochemistry of aromatic electrophilic substitution with the geometrical properties of hydrogen bond interactions to the ring).

Mendez and Cerda³⁵ identify the challenges of finding reliable biochemical thermodynamic data. Some biochemical thermodynamic data does not include the state (reference or biochemical), and without this information, students can reach an incorrect conclusion. Reliable resources for biochemical thermodynamic data are included.

Buntrock³⁶ reviews citation searching that enables users to move forward in time, finding a more recent publication that includes an interesting article in its bibliography. This paper

also describes how bibliometrics and alternative metric methods are being used to evaluate publications, authors, and journals.

Love and Bennett³⁷ describe an activity they are using to introduce first-semester organic chemistry lab students to searching electronic resources. Using SciFinder, students are required to determine the structures of three compounds plus the synthetic route for one of the substances listed in the ingredients of a consumer product label.

Zardecki et al.³⁸ offer a technology report about the RCSB Protein Data Bank (PDB), an essential resource studying the shape and interactions of biological molecules. The RCSB PDB is available for free. This article includes information about depositing, searching, visualizing, and analyzing PDB data. Educational resources are also available for free and unrestricted use in the classroom.

■ LOOKING AHEAD

Despite the broad array of topics covered in this special issue, a number of additional areas might be of interest to chemical educators. Perhaps future efforts and research could investigate these topics:

- Productivity software tools and mobile apps
- Research services to support best practices for activities such as managing information and meeting funder requirements for sharing research data
- Preservation of digital content
- Metadata and discovery services
- Scholarly communication issues such as author's rights and copyright guidelines
- New and renovated library spaces to better support current academic and research needs
- Information about library materials (publishing trends, economics, use) plus an assessment to determine whether a collection is meeting local programmatic needs

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Notes

Views expressed in this editorial are those of the author and not necessarily the views of the ACS or Stanford University.

Grace Baysinger serves as the Head Librarian and Bibliographer of the Swain Chemistry and Chemical Engineering Library at Stanford University, where her responsibilities include building and managing the collection as well as providing reference and instructional services to faculty and students. Her current professional activities include being the Chair of the Education Committee for the ACS Division of Chemical Information, a member of the ACS Committee on Chemical Abstracts Service, an Editorial Advisory Board member for the *Journal of Chemical Education*, an Editorial Advisory Board member for the *CRC Handbook of Chemistry and Physics*, an Advisory Board member for the *Science of Synthesis*, and a Trustee for the CSA Trust. Projects at Stanford include being a lead for xSearch, a search service that allows users to search up to 275 resources at one time; and being a project team member who is focused on publication data for Stanford Profiles [<https://profiles.stanford.edu/grace-baysinger>] (accessed Feb 2016)].

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