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Teaching Cheminformatics through a Collaborative Intercollegiate Online Chemistry Course (OLCC)

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ABSTRACT: While cheminformatics skills necessary for dealing with an ever-increasing amount of chemical information are considered important for students pursuing STEM careers in the age of big data, many schools do not offer a cheminformatics course or alternative training opportunities. This paper presents the Cheminformatics Online Chemistry Course (OLCC), which is organized and run by the Committee on Computers in Chemical Education (CCCE) of the American Chemical Society (ACS)'s Division of Chemical Education (CHED). The Cheminformatics OLCC is a highly collaborative teaching project involving instructors at multiple schools who teamed up with external chemical information experts recruited across sectors, including government and industry. From 2015 to 2019, three Cheminformatics OLCCs were offered. In each program, the instructors at participating schools would meet face-to-face with the students of a class, while external content experts engaged through online discussions across campuses with both the instructors and students. All the material created in the course has been made available at the open education repositories of LibreTexts and CCCE Web sites for other institutions to adapt to their future needs.



KEYWORDS: *Upper-Division Undergraduate, Graduate Education/Research, General Public, Cheminformatics, Interdisciplinary/Multidisciplinary, Computer-Based Learning, Internet/Web-Based Learning, Professional Development*

INTRODUCTION

Cheminformatics^{1–6} is an emerging scientific discipline that uses computers and informatics techniques to perform various tasks with vast amounts of chemical data such as data collection, storage, search, retrieval, transformation, analysis, visualization, and many others. While cheminformatics techniques are commonly used in the process of drug discovery in the pharmaceutical industry, they are also used in many other industries that deal with chemical data. Computer and informatics skills in analyzing chemical data are considered an important requisite that employers look for in job-seeking students.^{7–10} In a broader sense, this represents a long-perceived gap in the chemistry curriculum. While today's employers emphasize informatics, previous generations pleaded for job candidates more proficient in the use of printed reference works. The more than century-long history of employer appeals of this sort, emphasizing the need for job candidates better trained in the use of chemistry's information base (once paper, now digital), underscores the long-term value of filling the demand for cheminformatics instruction.^{11–13} Therefore, cheminformatics education is increasingly important within the chemical education community,^{14–19} as exemplified in the publication of a special issue on "Chemical Information"¹⁹ in this Journal. Despite workforce need, many chemistry departments do not offer a cheminformatics course

or alternative training opportunities that provide students with the informatics skills that would be an asset in their future science and employment endeavors.

Teaching cheminformatics for chemistry majors presents several major challenges. First, many chemistry departments do not have a faculty member who can teach cheminformatics. This is partly because cheminformatics is a highly interdisciplinary area that involves a wide range of scientific fields, including not only chemistry, but also informatics, database administration, computer science, library science, statistics, and pharmaceutical sciences. As a result, it can be difficult to find instructors who have sufficient knowledge and expertise to teach courses in cheminformatics. Second, there is no cheminformatics textbook or course materials tailored for chemistry majors at the undergraduate level. While several textbooks^{20–23} are available, they are more appropriate for those who already have some informatics backgrounds (e.g.,

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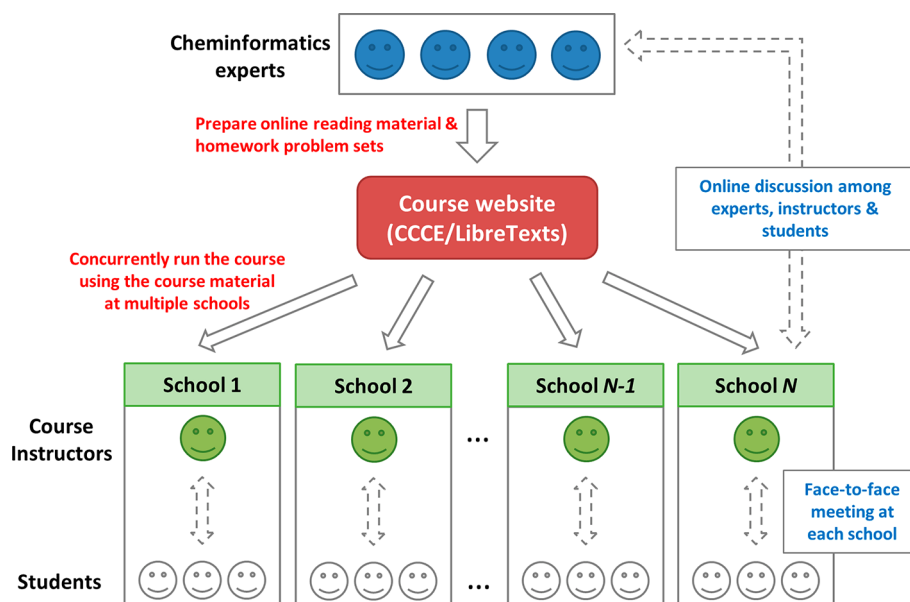


Figure 1. Instructional approaches of Cheminformatics OLCC.

computer science or informatics majors with programming skills or graduate students working on cheminformatics research projects). Third, as evident from the lack of materials, cheminformatics has traditionally been considered a research technique for industrial application rather than a core chemistry skill set and very little activity has been reported to develop appropriate curricula for undergraduate programs.

To address some of these issues, the Cheminformatics OLCC (Online Chemistry Course) was launched by a group of chemical educators and chemical information experts. OLCCs are one of the oldest ongoing online courses in existence,^{24,25} which have been organized and run by the Committee on Computers in Chemical Education (CCCE) of the American Chemical Society (ACS)'s Division of Chemical Education (CHED) since 1996.²⁶ OLCCs evolved out of the CCCE's ConfChem online conference,²⁷ which dates back to 1993. In a ConfChem conference, authors share papers about their work and discuss them online with other faculty. In an OLCC, students from participating schools are brought into the discussion of papers written by experts in a subject that is not taught in a typical undergraduate chemistry curriculum. An OLCC is a collaboratively taught hybrid course where an expert interacts online with students and instructors from multiple schools, while the instructor at each school interacts face-to-face with the students, is responsible for all assignments, and awards the students their grade for the course. Subjects previously covered in OLCCs included: Environmental and Industrial Chemistry (spring 1996, spring 1998, spring 2000); Pharmaceuticals, Their Discovery, Regulation and Manufacture (fall 1998); and Chemical Safety: Protecting Ourselves and Our Environment (fall 2004).²⁸

The Cheminformatics OLCC is a community effort to introduce cheminformatics content into the undergraduate chemistry curriculum. The goal was not only to offer an online cheminformatics course on multiple campuses, but also to use that process to develop cheminformatics open education resources (OERs) that could be reused once the courses were over. Three cheminformatics OLCCs were held in the Fall 2015, Spring 2017, and Fall 2019 semesters, resulting in three sets of resources that are now available for educators through

LibreTexts,²⁹ a free online textbook Web site (<https://libretexts.org>), and the CCCE Web site (<http://olcc.ccce.divched.org/>). Herein, we describe the instructional approaches of the Cheminformatics OLCC project and the lessons learned from this community effort. We also discuss future directions for this project as well as cheminformatics education in general, including pedagogy, resources, and course content.

INSTRUCTIONAL APPROACHES OF CHEMINFORMATICS OLCC

The Cheminformatics OLCC is a collaborative teaching project by external cheminformatics experts from government, industry, and academia and instructors at multiple schools (Figure 1). External experts develop course materials (texts and homework problems) that cover the topics of their expertise. These materials are freely available through a Web site and used in a cheminformatics course concurrently run at multiple participating schools. During the course, instructors at each school have weekly face-to-face meetings with the students in the classroom while the external experts engage in online discussion with the instructors and students (for more details, see the "Online Discussion Platform" and "Challenges in Intercollegiate Course Delivery" subsections.). The overall enrollment data for the three Cheminformatics OLCCs are summarized in Table 1. While all three OLCCs followed the instructional approaches illustrated in Figure 1, there were differences between them in the course contents as well as the technologies used, which are detailed below.

Course Content

The three Cheminformatics OLCCs covered various cheminformatics topics: chemical data management, chemical information literacy, chemical data formats, line notations for chemical structures, how to interactively use public chemical databases and free online tools, and programmatic access to chemical data (Figure 2). Each OLCC had different areas of focus on core skills. The first OLCC considered basic data management as a core skill set that is often overlooked in regular chemistry curricula. In subsequent OLCCs, more

Table 1. Enrollment Statistics for Cheminformatics OLCC

Semester	No. of Participating Schools	No. of Enrolled Students	Participating Schools ^a
Fall 2015	4	36	UALR (6), Centre (4), WVU (5), UNF (21)
Spring 2017	9	47	UALR (12), Centre (0 ^b), UHSP (3), IQS (6 ^c), SDSU (4), Potsdam (3), UIS (6), Campbell (12), Rutgers (1)
Fall 2019	5	23	UALR (2), Centre (3), UHSP (4), IQS (9 ^c), Otterbein (5)

^aNumbers in parentheses are the numbers of enrolled students at individual schools. UALR, University of Arkansas, Little Rock; Centre, Centre College; WVU, West Virginia University; UNF, University of North Florida; UHSP, University of Health Sciences & Pharmacy in St. Louis (formerly, St. Louis College of Pharmacy); IQS, IQS Universitat Ramon Llull (Barcelona, Spain); SDSU, South Dakota State University, Potsdam, State University of New York, Potsdam; UIS, University of Illinois, Springfield; Campbell, Campbell University; Rutgers, Rutgers University; Otterbein, Otterbein University. ^bThe course was taken by three faculty and staff members who participated in a faculty learning circle. No students enrolled. ^cNot formally enrolled as the course was offered as a noncredit seminar.

emphasis was placed on learning skills for programmatic access. Many of the opportunities for using all of these skills have greatly changed with the progress of web-based technology over the time-period between the OLCCs. More detailed content mapping among the three OLCCs is provided as Supporting Information (Table S1).

A core topic area covered in all three OLCCs was chemical structure representations and their use for searching chemical databases. Students learned about common line notations such as Simplified Molecular Input Line Entry System (SMILES)^{30,31} and the IUPAC International Chemical Identifier (InChI),^{32,33} which encode chemical structures into strings, and how to use them as queries to search public

chemical databases, such as PubChem,^{34–36} ChemSpider,^{37,38} NIST Webbook,³⁹ etc., as well as a commercial database, Reaxys⁴⁰ (only for the 2017 OLCC). The students were introduced to various types of structure searches such as identity search, similarity search, and sub- and superstructure searches. These topics were aimed to teach students how to find desired information from public resources in a manner beyond a simple text (keyword/name) search through typical search engines.

Computer Programming Training

Computer programming is an important skill for students to learn because it can be used to automate routine tasks or process a large amount of data.¹⁰ During the 2015 OLCC, students learned how to import chemical data into a spreadsheet (Microsoft Excel or GoogleDocs) from a public database using the representational state transfer (REST) application programming interface (API). This basic skill can be applied to many tasks in laboratory research and all students should be learning it as a preliminary to handling data at larger scales. However, many real-world applications in cheminformatics rely on more comprehensive data processing environments.

The 2017 and 2019 OLCCs covered how to write python scripts to access data from a public database and process them. The 2017 OLCC used trinket (<https://trinket.io/>), which is a web-based interactive coding environment designed for education. A sample code written using trinket can be readily embedded on a web page as an iframe and students can modify and run the code interactively. In the 2019 OLCC, a set of Jupyter notebooks⁴¹ was created, which contain sample Python codes and programming assignments to teach students how to access data in PubChem through its REST interface called PUG-REST^{42–44} and how to perform cheminformatics tasks using open-source software packages such as RDKit,⁴⁵ scikit-learn,^{46,47} and Mordred.^{48,49} Similar materials were also developed for the R language (using JupyterLab and R-Studio). Students could download and run these notebooks on

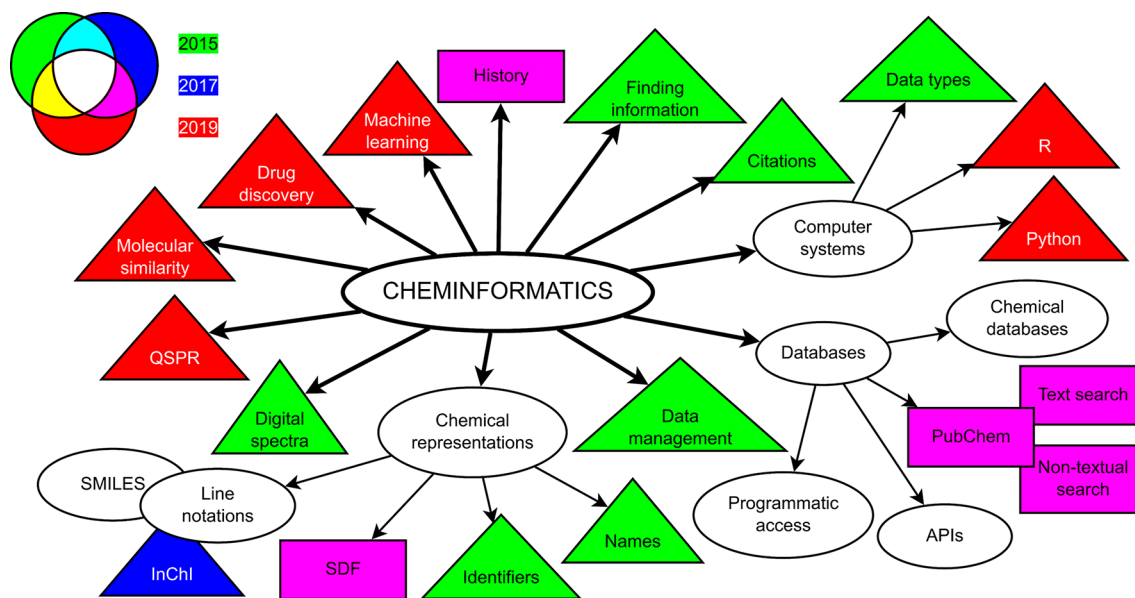


Figure 2. Course content map for the Cheminformatics OLCCs, offered in Fall 2015, Spring 2017, and Fall 2019. The triangles, rectangles, and ovals indicate the topics covered in one, two, and three Cheminformatics OLCCs, respectively. The colors of the shapes represent the year(s) in which the corresponding topics were covered (see the Venn Diagram at the top-left).

their own computers. Alternatively, they could run the notebooks on JupyterHub⁵⁰ available through LibreTexts. Because computer programming activities were implemented in each module, students were exposed to computer programming as early in the semester as possible, which gave them more time to practice these skills.

Student Projects

During the 2015 and 2017 OLCCs, students were required to work on small projects for the last 2 to 4 weeks of the semester. They were allowed to work in groups and external experts advised them in the projects as a mentor. Chemical information experts and instructors suggested potential projects that exploited the skill sets acquired through the course and students selected one of these. A wide variety of projects were offered, ranging from the development of an Android app to the creation of educational video tutorials. A list of the videos created by students is provided as a supporting material (Table S2). During the 2015 OLCC, some students participated in the Reference Data Challenge,⁵¹ organized by the U.S. National Institute of Standard and Technology (NIST), a competition in which participants developed apps that use NIST Standard Reference Data (SRD) with mobile devices. One of the students won the second place of this competition.⁵²

Select students had opportunities to give oral presentations about their projects^{53–63} at a special symposium at the Spring 2016 ACS National Meeting in San Diego. In addition, some student projects evolved into more formal, long-term projects,^{64–66} which were also presented at the Division of Chemical Health and Safety (CHAS) symposia at ACS National Meetings. One student's project eventually became the basis of a master's thesis, "Monadal approach to 2D binary chemical safety fingerprints",⁶⁷ and the data sets resulted from this project were made freely available to the public on Figshare.⁶⁸

Setting aside 4 weeks out of one semester for student projects made it difficult to cover a broad area of cheminformatics with the remaining time. Therefore, inclusion of student projects in the 2019 OLCC was up to the discretion of the instructor at each participating school, and students at one school did complete small projects in the last 2 weeks of the semester in lieu of a final exam.

Course Websites

For the 2015 and 2017 OLCCs, the course materials were hosted at the CCCE Web site (<http://olcc.ccce.divched.org/>) (see Table 2). After the courses were completed, all materials

Table 2. Course Websites for Cheminformatics OLCC

OLCC	Course Websites
2015	<ul style="list-style-type: none"> •http://olcc.ccce.divched.org/Fall2015OLCC •https://chem.libretexts.org/link?50598
2017	<ul style="list-style-type: none"> •http://olcc.ccce.divched.org/Spring2017OLCC •https://chem.libretexts.org/link?83678
2019	<ul style="list-style-type: none"> •https://chem.libretexts.org/link?143689

were archived at LibreTexts (<https://libretexts.org>), which provides online textbooks free of charge. Materials used during the third Cheminformatics OLCC were directly hosted on LibreTexts for use during and after the course. The transition to LibreTexts is intended to make the materials more accessible and reusable. Importantly, LibreTexts provides

authoring tools that assist instructors to readily modify the existing materials or add new content on top of them. This will allow the education community to work together to update and improve the materials.

Online Discussion Platform

During the 2015 and 2017 OLCCs, online discussion among students, instructors, and external experts was done through comment sections available at the bottom of each web page. The hypothes.is web annotation service⁶⁹ was introduced in the 2017 OLCC as an alternative online discussion approach, and solely used in the 2019 OLCC. Hypothes.is allows one to annotate a web page based on the annotation standards for digital documents developed by the W3C Web Annotation Working Group.⁷⁰ Using hypothes.is, one can make comments on text on a web page, which can be kept private or shared with peers or the public for discussion. This service can be used to facilitate online discussion between instructors and students in classrooms.^{71–74}

DISCUSSION

Collaborative Teaching Strategies

As indicated in Figure 1, online discussion occurs between experts, instructors, and students. Critical to the success of each OLCC were weekly online Zoom or Skype meetings between experts and instructors prior to instructors meeting with students. The goals for each meeting were to provide an expert walk-through of the next week's activity with the instructors, to clarify questions instructors had while working through the activity before sharing with students, and to improve content based on instructors' pedagogical expertise. Time was also set aside to review individual questions that came up from student work in the previous week. As some of the technologies being used were nascent and unfamiliar to students (e.g., hypothes.is), as well as students not feeling completely comfortable asking questions directly to experts, weekly meetings allowed faculty to ask the experts questions the students had or issues that came up in their classrooms, and experts were able to guide instructors on how to best answer student questions in subsequent classroom settings.

The benefits of the collaborative sessions between experts and faculty appear to be critical in the success of the OLCC. Not all faculty were versed in the topic and were able to learn new skills, as indicated in instructor feedback comments:

"Cheminformatics was a new topic for me. I would not have been able to offer this course without the weekly Zoom meeting with the other facilitators and course content creators. This format allowed me to both learn and teach a new topic for students."

"I could not have offered this course without the external support—my background is just too limited and we don't have the resources in a small department like ours. Having the weekly Zoom meetings was critical in keeping me up-to-date and helped reassure me that what we were doing was similar to other schools."

Another benefit of the collaboration was faculty could explore ideas with their students in ways that were appropriate for their institution. Students enrolled in the classes had different backgrounds in programming from no experience to facility in multiple languages. Content experts were able to help faculty to develop content specific to various student needs.

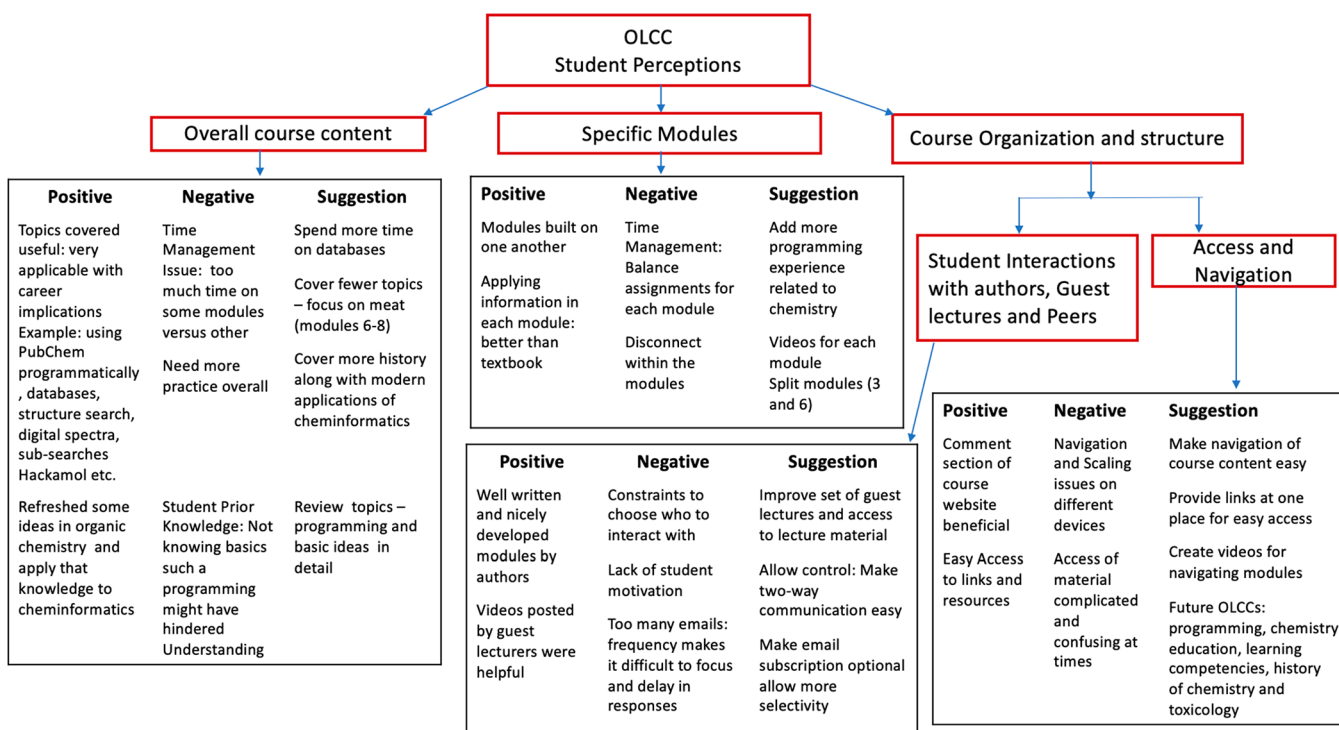


Figure 3. Student perceptions of OLCC in relation to the specific aspects of the course.

“The seminar following the Fall 2019 OLCC took advantage of the assignments developed in Python and R. The course, which was a curious experience, got moving between both languages as we offered the students the opportunity to follow the course in the programming language of their choice. This wouldn’t have been possible without the collaborative effort behind the course materials.”

A key outcome of the OLCC was providing a mechanism to bring content experts to campuses with small departments that may not have significant experience in cheminformatics. It is worth comparing the OLCC mechanism with other collaborative teaching approaches. Many small liberal arts colleges have joined online course or degree consortia^{75,76} to provide course offerings to students enrolled without having to hire new specialized faculty. However, in these consortia, students enroll in an online course taught by a faculty member at another institution. Massive open online courses (MOOCs) provide another mechanism to bring content expertise to any individual seeking it, but few MOOCs can be taken for college credit, have high attrition rates, and offer little interaction between course instructor and student due to autograded assignments.⁷⁷ The OLCC model provided here combines the best parts of MOOCs, online courses, and traditional in-person courses. Institutions do not need to have all the specialized faculty resources to teach a course as experts are generating peer-reviewed content and developing learning activities that are rigorously tested. The home institution faculty provide the accountability and instructor availability of a traditional on campus course. In this model, faculty and students at the home institution can participate in a shared learning experience both gaining knowledge by interacting with experts in the field. As one faculty member indicated:

“The design of this course was so useful for our students since I am part of a small department that does not have anyone with significant experience in Cheminformatics. It brought valuable information from experts in the field to better prepare our students for current job demands. It was also highly beneficial for me to learn along with my students as I facilitated the class. I worked through all the material in advance of the class in order to better understand the usefulness of each section of material and plan my course requirements accordingly.”

Sustainability Issues of the Cheminformatics OLCCs

In the long run, a cheminformatics course should be offered periodically as a regular part of the undergraduate chemistry program curriculum at individual schools, because students need information skills necessary to deal with an ever-increasing amount of data. The collaborative teaching strategy taken by the Cheminformatics OLCC is one suitable way to achieve this goal, but will rely upon the continued collaboration. Absent continued free server space through the CCCE Web site or LibreTexts, and commitment of our academic, industrial, and governmental partners, securing necessary funding will be an ongoing issue for long-term sustainability of the project.

It is noteworthy that the Cheminformatics OLCCs provide learning opportunities for chemical educators who do not have prior knowledge of cheminformatics. Through the Cheminformatics OLCCs, they build cheminformatics expertise necessary to teach their own cheminformatics courses later without the support from external experts. In addition, all course materials created from the Cheminformatics OLCCs are freely available to the public through the CCCE Web site and LibreTexts (see Table 2). Since the OLCC has been offered multiple times, there are a wide array of topics that can be brought together and remixed as deemed best for the home institution’s instructor. This has allowed faculty members to

not only participate in the OLCC, but also develop their own courses and bring materials back to the group, as reflected in the following testimony from one of the authors:

"After participating in the 2017 OLCC, I decided to offer my own course at my institution in 2018. I noticed that there was material in the 2015 course that was available online, but was not specifically used in 2017. It was great to be able to reuse material from both offerings, and create a course for my student's needs. I also developed my own materials in 2018 that made their way into the 2019 course, indicating the power of the collaborative nature of this platform."

While a majority of the materials developed from Cheminformatics OLCC was reusable, some materials have become obsolete since they were first released. Many covered how to use public databases, which continuously change the web interfaces to keep up with technological advances or often discontinue some services for various reasons (e.g., due to lack of sufficient funding). Materials that contain the screenshots of the old web interfaces required updating, and materials that covered discontinued services could not be used anymore. Therefore, when developing cheminformatics education materials in the future, it will be necessary to consider separating the "static" content from others which will be subject to change.

Students' Perception of the Course

The goal of the Cheminformatics OLCC was not that of chemical education research but of enabling schools to offer a course in cheminformatics that targeted the needs of undergraduate chemistry majors. In addition to the normal course evaluations that were administered at each school, a link to an online survey was sent out to students after the 2015 and 2017 OLCCs, but only 11 students responded, with eight of those responses coming from the same school. The questions in the surveys focused on overall course content, specific modules, and the intercollegiate course organization and structure.

It was often observed that when students were asked a particular question, their response would often allude to a different aspect of the course. For example, when asked about strengths of a course, students often made suggestions to improve the course. Likewise, when asked about a specific module, some students provided information about the overall course in addition to the module. Nonetheless, from students' responses, we were able to identify three basic types of responses (positive, negative, and suggestions) and these are summarized in Figure 3.

Overall student responses indicate several benefits of OLCC for students. Students found the Cheminformatics OLCC helpful in applying their knowledge and skills to research projects and thought that it would be of value for their future careers. There are also some areas of improvement in OLCCs, specifically with respect to the amount of time spent on modules, course access and navigation, and communication among students and the instructor to foster intercollegiate collaborative learning through the OLCCs.

Balancing the Depth and Breadth of Course Contents

Cheminformatics is a highly interdisciplinary area, covering chemistry, data management, computer science, information technology, and related skills. This discipline requires not only working with data, but also understanding the types of analysis that becomes possible at this scale. Data management involves

essential skills that all chemists should be familiar with but are neither taught regularly in the curriculum and are often not evident in practice. Such skills as how to clean and handle data to avoid information loss and misinterpretation by downstream users (human and machine) are just one component of the objectives of these courses.

Designing a one-semester course that combines content across all of these areas is impractical, especially if students had no prior programming experience, and thus each iteration of this OLCC had a different focus. Each was dependent upon the expertise and interests of the external chemical information experts who contributed. The 2015 OLCC had the broadest range of topics, including chemical information literacy in traditional search systems and basic data management skills as referenced in the ACS guidelines for Bachelor's degree programs in chemistry.^{78,79}

Since cheminformaticians deal with large amounts of data, they often automate routine tasks through programming. Subsequent iterations focused more predominantly on skills associated with automating common tasks to handle chemical data using computer programs. The 2017 OLCC focused on the use of computational services provided by PubChem, while the 2019 OLCC required the students to use either R or Python and focused on the use of open-source software programs such as RDKit,⁴⁵ scikit-learn,^{46,47} Pandas^{80,81} and Numpy,^{82,83} which the students ran on their local computers or in the LibreText JupyterHub⁵⁰ out of UC Davis. Thus, each iteration of the OLCC had a different focus and provides a unique contribution to the depth and breadth of cheminformatics educational resources.

It is noteworthy that no prior computer programming skills were required as prerequisites for the Cheminformatics OLCC. If we did, we could have run the course at a faster pace and covered more advanced topics. However, it would have made the course less accessible to students, considering that most chemistry undergraduates do not take an introductory computer programming course, because it is not a part of a typical chemistry curriculum. While there was a discussion among some instructors and external experts, we decided not to have a computer programming prerequisite to reach out to a larger audience.

Challenges in Intercollegiate Course Delivery

Offering an intercollegiate course involves a multitude of challenges, ranging from basic scheduling to web technologies for communication across institutions. Central to the idea of an OLCC is that students across campuses communicate with each other, faculty, and external experts. While this required a synchronized course delivery, variance in academic calendars required the development of ancillary material that was used by campuses that were in session when other campuses were not. For example, in the spring 2017 OLCC, some schools started in early January while others the first week of February. Likewise, variances in spring break were almost a month, which was dealt with by having connected modules that were taught for longer than a week.

Another challenge was managing the course expectations across institutions. Course offerings ranged from a three-credit special topics course to a one-credit independent study or undergraduate research, to integration into existing seminar/capstone experience courses, and even a credit-less offering taken by faculty at one school. Therefore, in the OLCC model, all grading policies and standards were determined by the

instructor at each institution, making it difficult to standardize students' expectations across schools. In addition, the nature of the shared instruction in the OLCC presents challenges in identifying who is responsible for the course expectations: the expert who was teaching across campuses or the local instructor who graded their work. With that said, one way to better understand the pedagogical model of the OLCC is to view the outside experts as those who play a similar role as textbook authors in a traditional course. In essence, the external experts develop online materials (the textbook). The course instructors at individual schools use the materials and have full control of the course (e.g., the number of credit hours, assignments, and grading, etc.), just like the way they teach a traditional course. However, one notable difference is that, in the OLCC model, students and instructors have direct and facilitated communication with the authors of their textbook (i.e., external experts), which is not usually feasible in a typical course. This communication also benefits the expert in their development of the course content because the feedback from instructors and students are used to improve the material.

The evolving nature of social web technologies was also a challenge for these OLCCs. All OLCCs prior to the Cheminformatics OLCC (1996–2004) posted material online in static HTML web pages and discussed it through two list servers: one for students and faculty and the other for faculty only. The Cheminformatics OLCCs were the first to use web 2.0 technologies. The 2015 and 2017 OLCCs were hosted on Drupal servers and used the comment feature connected to papers, or sections of papers. During the 2017 OLCC, one school also started to use the hypothes.is social-semantic web annotation service. Students were hesitant to post formal comments directly on papers written by professionals and found it easier to make informal annotations in the hypothes.is overlay, which emulated both note-taking and social media practices. Discussions during the 2019 OLCC were entirely on the hypothes.is web annotation service, which had been integrated into LibreTexts, and was set up to send an email to students and faculty whenever an annotation was created. In future OLCCs, this notification needs to be extended to other types of social media because "email" is often not students' preferred means for online communication, and these communications need to be across web platforms.

Challenges in Student Projects

As indicated above most students had no prior experience with programming, although students at one school (Centre College) during the 2015 and 2019 OLCC did take a prior computer science course. The nature of the student projects was clearly dependent on prior knowledge of computer programming basics and such knowledge would better prepare students to learn sufficient cheminformatics content. It was difficult for students to complete projects during the span of the class. However, multiple students found their projects inspiring and continued to work after the completion of the course. This resulted in multiple presentations at national meetings.^{53–66,84} This shows the value of OLCCs coupling external professional experts to the students' academic experience resulting in increased student engagement and professional development.

One of the goals of the Cheminformatics OLCC was to create projects involving teams of students from across different campuses. As students from different campuses

interact with each other, there is a sharing of ideas and perspectives that go beyond the classroom. Differences in class schedules at the various institutions resulted in limited intercollegiate student interaction as well as added complication to completing projects. Intercollegiate student interactions would be better facilitated by more synchronous schedules between the campuses involved. Further, lessons in remote learning from the coronavirus disease 2019 (COVID-19) pandemic⁸⁵ may increase both student willingness and ability to interact with students at other campuses which in turn may create better conditions for intercollegiate student projects.

Future Directions

Since its inception in 1996 the OLCC model has allowed the CHED CCCE to drive innovation in the chemistry curriculum. Given the success of this OLCC, faculty involved in this project are planning to offer yet another variation of the Cheminformatics OLCC in the 2021–2022 academic year. In addition to the upcoming Cheminformatics OLCC, the CCCE is exploring a new OLCC on the Internet of Chemistry Things (IOCT).^{86–91} This new OLCC will involve students in programming IOCT devices that generate live chemical data streams to the web and enable a variety of citizen science projects.

CONCLUSION

The Cheminformatics OLCC is a highly collaborative teaching effort involving instructors from multiple schools and external cheminformatics experts from various institutions including government, industry, and academia. The external experts developed course materials (texts and homework problems) that cover the topics of their expertise. During the course, the instructor at each school maintained face-to-face meetings with the students in a physical classroom and the external experts engaged in online discussions with the instructors and students across campuses. The Cheminformatics OLCC provided participating instructors expertise in cheminformatics and has already contributed to stand-alone courses in cheminformatics. All the material is freely available online.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available at <https://pubs.acs.org/doi/10.1021/acs.jchemed.0c01035>.

Detailed course mapping information across the three Cheminformatics OLCCs (XLSX)

Educational cheminformatics videos created by students. (PDF, DOCX)

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Author Contributions

The initial draft was written by S.K., L.R.M., E.B., K.D.F., J.L.M., J.C., R.E.B., D.J., and T.G. All authors commented on the manuscript and read and approved the final version. R.E.B. conceived this project, recruited subject matter experts for the project, taught all three sessions, was responsible for the Web sites, and wrote original material for the 2019 OLCC. S.K. developed modules about line notations, public chemical databases, and programmatic access for the three OLCCs. L.R.M. contributed to the original design of the course and developed several modules in 2015 and 2017. E.B. taught with the 2017 and 2019 OLCCs and contributed his own materials for the 2019 OLCC. K.D.F. and D.J. taught with the 2019 OLCC. J.C. developed modules for the three OLCCs and also led face-to-face classes for the 2017 and 2019 OLCCs. J.L.M. led a face-to-face class during the 2015 OLCC. L.A.M. taught a

face to face class for the 2017 OLCC. T.G. participated in the 2017 OLCC and taught this class in hybrid mode that included weekly face-to-face meetings. A.S.I.D.L. developed modules for the 2015 OLCC. Y.L. codeveloped modules about finding information for research in chemistry, collaborative citation management, and data management best practices, and also provided instructional support in the 2015 OLCC. E.H.S. developed modules about representing small molecules and provided instructional support in 2015. A.P.C. helped with the content aspect of the 2017 OLCC and took care of the migration of the course materials from the CCCE Web site to LibreTexts. K.B. codeveloped modules about data management best practices and provided instructional support in the 2015 OLCC.

Notes

The authors declare no competing financial interest.

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