

# CoLab: A Workshop-Based Undergraduate Research Experience for Entering College Students

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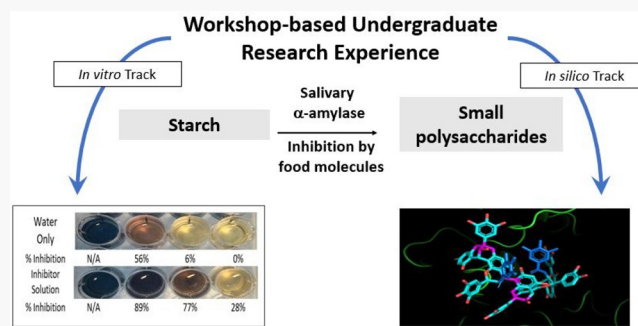
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Supporting Information

**ABSTRACT:** The goal of undergraduate chemistry laboratories is to allow students to learn about chemical systems and key laboratory skills. They should then apply this knowledge to solve problems and connect macroscopic observations in the laboratory with those occurring at the submicroscopic level. Unfortunately, these needs are not met through traditional confirmation laboratories. Therefore, many chemistry instructors are turning toward research-based laboratories and course-based undergraduate research experiences (CUREs). There are also many cases where summer workshops, often with nontraditional pedagogy, are used for students. This article describes the STEM CoLab Program, a novel type of summer workshop that seeks to build student chemistry knowledge and skills in research and presentation at the beginning of their college work. This program uses the principles of CUREs for students who are just entering the university, mostly as freshmen. Several different phenomena have been investigated during the program. In this paper, we report the overall work of the program from 2016 through 2021 and provide additional details on the program's implementation in 2020 and 2021 when students conducted their work from home, using a combination of a take home research kit for studying salivary amylase “in vitro” and computer-based visualizations of amylase-inhibitor interactions “in silico” using PyMOL and online docking tools.

**KEYWORDS:** General Public, General Education, Curriculum, Decision Making, Applications of Chemistry, Distance Learning, Enzymes



## INTRODUCTION

A significant challenge for college-level science, technology, engineering, and mathematics (STEM) education is the need to provide engaging and authentic science experiences to students early in their studies. Given the empirical, lab-oriented practices of chemistry, undergraduate chemistry laboratories should enable students to learn about these practices and about chemical systems, including through the use of key laboratory skills. Using these skills, they should then solve problems and connect macroscopic observations in the laboratory with those occurring at the submicroscopic level, enabling them to better understand authentic science in an open-ended fashion.<sup>1</sup> Ideally this could happen as early as their first days in college so as to better shape their understanding of the scope and purpose of their studies. One place where these goals could be met is in workshops conducted in many institutions just before students start their college work. However, programs that focus on open-ended lab activities in workshop settings have not been reported. Here, we present a program that addresses this challenge with a chemistry-focused research project, which has a well-defined path to contributing new findings toward science and serves a wide variety of STEM majors.

## Precollege Workshops

The use of precollege workshops is now an important part of the college entry experience at many institutions, during which students improve their skills through summer workshop sessions that typically last several weeks. This is especially important for students who may not know what to expect in college or from a STEM degree, including first-generation college students who may not have scientists as role models. The time before the first formal classes may be important to shape their identity that they too can “do” science without the pressure of traditional grading. Remarkably, we are only aware of a single report of such a workshop aimed at students who are not yet matriculated at a four-year institution, reported from Occidental College in 1991.<sup>2</sup> In addition, such summer workshops provide an opportunity for female and minority students to enter the

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sciences, including in workshops that target high school students<sup>3</sup> and engage them in community-oriented outreach work.<sup>4,5</sup>

There are certainly many examples of content-oriented summer bridge programs, especially between the end of high school and the beginning of college. In some cases, these are aimed at preparatory work and mirror traditional courses.<sup>6</sup> However, these preparatory approaches have the drawback of repeating and even reinforcing traditional approaches to content as students learn the material through standard lecture and discussion components. An example of an alternative approach to this is a program at Bridgewater State University (BSU) where students participated in a writing-intensive seminar alongside working with faculty members on a research project and then discussed their research progress with peer mentors. Over 80% of the participants in this program stated they would graduate from BSU with a bachelor's degree in a STEM field.<sup>7</sup> More recently, a report on the *Science Academy in Chemistry Program* at the University of Chicago emphasized connecting chemistry concepts to cultural, personal, and geographic experiences. This approach resulted in significant shifts in overall student confidence, preparation for general chemistry, and the sense of belonging in STEM.<sup>5</sup>

Preparatory chemistry classes are another type of summer workshop. Some are designed for students who do not place in general chemistry after completing a chemistry placement exam; others teach students concepts for a class often viewed as a gatekeeper toward student advancement, such as organic chemistry. At-risk students, i.e., low income or first-generation students, particularly benefit from such programs.<sup>6</sup> By enrolling in these workshops, students may avoid having to take the preparatory course itself and still receive better grades in subsequent classes than their peers who did not need the workshop.<sup>8</sup> In some cases, the workshops are offered with credit in the context of a "bridging course".<sup>9</sup>

In some less frequent cases, precollege experiences do not cover traditional material and instead focus on student engagement with experiences that present chemistry in a more authentic fashion. For example, through the Global Learning and Observation to Benefit the Environment (GLOBE) program, students participate in completing chemical tasks directly related to the environment, such as finding the pH of a soil sample or the salinity of a water sample.<sup>10</sup> Aside from teaching students various laboratory techniques beyond those found in a traditional chemistry course, summer workshops could give students opportunities to learn more about career options in chemistry as well as other services available to them at universities, such as advising.<sup>11</sup>

### Course-Based Undergraduate Research Experiences (CUREs)

There is ample evidence that traditional, confirmation-style lab instruction does not show a strong correlation with improvement in content knowledge in the lecture portion of the class.<sup>12,13</sup> Students frequently simply follow steps in a laboratory manual without reflecting on their purpose. Moreover, students often do not connect what they observe in the lab to processes occurring at the atomic/molecular level<sup>14–16</sup> and do not connect properties about chemical systems with chemical principles. Instead, students may focus on psychomotor and procedural issues<sup>17,18</sup> and struggle to connect the laboratory to learning.<sup>19</sup>

To address the challenge of making laboratory learning more relevant to chemistry education and to overcome the deficiencies of confirmation laboratories, several initiatives have investigated replacing traditional laboratory instruction with course-based research experiences (CUREs) that both develop student skills and engage them in more authentic science practices.<sup>1,20–23</sup> Students may also learn about the technical language used in the sciences as well as the nature of science, especially what science is, who does it, and how it is done.<sup>24</sup> By having students engage in research-based laboratories early in their studies, they may gain a greater appreciation for the nature of science. CUREs also emphasize having students collaborate more frequently with peers than students enrolled in traditional confirmation laboratories.<sup>21</sup> Students who participate in CUREs are exposed to a wider variety of chemical instrumentation beyond the basic equipment typically found in a traditional general chemistry laboratory. Furthermore, CUREs are often iterative with multiple designs refining prior versions of work.<sup>20,21,23,25</sup> In this way, CUREs are similar to the design-based research that science and science education researchers engage in. CUREs also play an important role in altering student attitudes toward science by fostering their interest in science and increasing their self-efficacy. Often, the conclusion of a CURE activity is in the form of a final project synthesizing all the knowledge that students have acquired throughout the experience. This may be in the form of a poster session, paper, or a conference presentation. Having even a limited experience of research in this manner—from asking questions to communicating results—may be important in having students complete undergraduate degrees in the sciences.<sup>21</sup>

How and when to institute CUREs is an important question. There are several examples of CUREs that target the general and organic chemistry courses. Indeed, this was a key goal of the NSF in its initial support of the first CUREs, such as the Center for Authentic Science Practice in Education (CASPiE),<sup>20,23,25</sup> the University of Texas' Freshman Research Experience Program,<sup>26</sup> and the multi-institution chemistry CURE initiative, the Ohio Center for Undergraduate Research—Research Experiences to Enhance Learning.<sup>1</sup> CUREs are generally introduced within course settings (hence, their name) and often include skill-building or related activities that match the learning goals of actual college courses.<sup>21,25</sup>

Another challenge of CUREs is how to ensure that the work is scientifically appropriate. In open-ended inquiry laboratories,<sup>12</sup> the outcome of the laboratory is not known to either the instructor or the students. As a result, one important aspect of a CURE is how it defines and develops new findings to the scientific community that have not been explored before.<sup>20</sup> Therefore, an important aspect of CUREs is that the work done by students directly contributes to an authentic research question. Authentic research is defined as the type of research that professionals in the field would engage in. As such, it involves discovery, collaboration, and iteration. And there are many examples now of how work in CUREs ultimately results in conventional journal publications, as was done in CASPiE in the context of biomedical research.<sup>27</sup> Results from CUREs can also provide background and exploratory components that can be used in more focused investigations.<sup>28,29</sup> Finally, the detailed exploration of a phenomenon has also led to the development of innovative instructional laboratories for more conventional use, including in this Journal.<sup>30</sup>

## CONTEXT

### University Setting

This article describes a type of structured research experience implemented in the context of a summer precollege workshop. The STEM CoLab (where “CoLab” stands for Cohort-building Laboratory research experience) is for incoming university students at a large Midwestern public research university. CoLab aims to strengthen their skills in critical thinking, scientific reasoning, and scientific experimentation. It is a key component of the STEM Initiative, a special success program supported by the university. The STEM Initiative, modeled on the Meyerhoff Scholars Program at the University of Maryland, Baltimore County (UMBC),<sup>31</sup> was established in 2015 under the umbrella of the President’s Award Program (PAP), one of the most prestigious scholarships offered by the University System for this setting. Since 1985, this scholarship has been awarded to students graduating from in-state high schools who have demonstrated outstanding academic performance and who represent the rich diversity of the state. In addition to first-year STEM majors within the PAP, the STEM Initiative is also open to high-achieving transfer students from the City Colleges of Chicago.

The STEM Initiative is designed to address identified pipeline issues at the national level<sup>32</sup> by increasing the number of students earning undergraduate STEM degrees. Special emphasis is placed on retaining and graduating underrepresented minorities in these disciplines. Through structured activities and engagement with STEM faculty, the STEM Initiative aims to promote high academic achievement and persistence to graduation for students seeking to attain Masters, Ph.D., and M.D./Ph.D. in STEM fields. CoLab offers an opportunity to build cohesion, teamwork, and friendships among an entering cohort of students prior to their matriculation. Additionally, the program builds laboratory skills and self-efficacy, laying a solid foundation that will support their progress in STEM disciplines at the college level. It is a required summer research program for students entering the STEM Initiative. It is also an optional program for students in certain other scholarship and training programs, such as NSF S-STEM and the NIH Bridges to the Baccalaureate training program, that are present at the institution. Students foster new connections with other incoming freshmen that serve as their entryways into the world of building connections within the scientific community. These connections are forged during the lab activities of the CoLab as well as during supplemental programming, including workshops that introduce students to various campus resources, peer support from STEM upperclassmen, and supplemental academic advising. These programs are conducted in hopes that students will be retained in the STEM track and complete a science or engineering degree during their undergraduate studies at the University of Illinois at Chicago.

This institution itself is a large Midwestern urban research university that is also a federally designated Hispanic-Serving Institution as well as an Asian American and Native American Pacific Islander-Serving Institution. No racial or ethnic group has a majority among student demographics. The university has large programs in multiple STEM disciplines. Students from many different majors participate in the program, including natural sciences, computer science, engineering, and integrated health studies.

### Program Outline

The STEM CoLab Program builds on prior work done with support from an NSF STEP grant,<sup>33</sup> a successor program, the *Latino Health Science Program* of the UIC Hispanic Center for Excellence, and, most recently, direct funding from the UIC Office of Academic and Enrollment Services that also engaged students in the Guaranteed Admissions Transfer (GAT) program between the City Colleges of Chicago and UIC. On average, 50 students from different STEM pathways as varied as computer science and integrated health sciences enroll in the STEM CoLab each summer. Students work over the course of 6 weeks, for three and a half hours 1 day per week, on an open-ended exploration of an important phenomenon.

The CoLab is designed on the basis of innovations from CASPIE.<sup>20,25</sup> The first half of the program focuses on skill-building. During this time, students learn to use the appropriate techniques as well as how to perform skills critical for research, such as literature searches using databases. The second half of the program allows students to explore a research topic of their interest related to the phenomenon at large with the knowledge they acquired during the first half of the CoLab.

The research topics that students have engaged with vary across the years. All involve students with an important chemical system that provides multiple ways for them to engage, including with evocative phenomena, direct measurement of properties of interest, and questions with important social import. The topics range from chemical studies of coumarin-102 fluorescence<sup>34,35</sup> to modeling of the reactions of extracellular electron transfer by bacteria<sup>36,37</sup> (see Table 1). These research topics were chosen

**Table 1. Overview of CoLab Topics, 2016–2021**

year	topic	title of key literature reference
2016	Coumarin-102	Coumarins as environmentally sensitive fluorescent probes of heterogeneous inclusion systems. <sup>34,35</sup>
2017	Propidium iodide binding to DNA	Energetics of DNA intercalation reactions. <sup>38</sup>
2018	Kautsky effect	Teaching laser-induced fluorescence of plant leaves. <sup>39</sup>
2019	Chemistry of electric bacteria	A flavin-based extracellular electron transfer mechanism in diverse Gram-positive bacteria. <sup>36,37</sup>
2020	SARS-CoV-2 and amylase protease modeling	Pharmacologic treatments for coronavirus disease 2019 (COVID-19). <sup>40,41</sup>
2021	Starch inhibition experiment and modeling	Grape seed extract and other food inhibitors of $\alpha$ -amylase. <sup>42,43</sup>

for their potential to allow students to have an engaging experience for the participants, allowing them to investigate novel aspects of a phenomenon that can be understood through direct interaction with measurements, usually visual, that they can relate to with their own senses. In general, the topics are associated with larger curriculum and chemical education research studies to have more contemporary phenomena in the undergraduate curricula, meeting the goal for a CURE to have direct application to practice. Students engage in research to document how specific phenomena can be studied in a way that either generates a conventional course-based CURE or uses procedures that can be used in conventional lab instruction.

The activities listed in Table 1 were presented to students who all read one or more of the associated papers from the chemistry research literature and did some preliminary experiments to introduce them to the phenomenon. They then developed and



Table 2. Schedule of 2021 UIC STEM Initiative CoLab Program

week	description	skill-building activities (see Supporting Information)
1	Introduction to CoLab, download of PyMOL, and completion of preliminary activity (all students).	A Brief Introduction to PyMOL
2	Demo of amylase lab, introduction to HDOCK/PatchDock, library presentation on literature searches (all students).	Solution preparation, Procedure for working with HDOCK/PatchDock
3	Introduction to ImageJ (Track 1), introduction to Python scripting (Track 2), Office of Undergraduate Research Presentation (all students).	Photo analysis: Determining percent reaction for amylase reaction, A brief introduction to PyMOL
4	Amylase lab completion with selection of own food sample as inhibitor (Track 1), modeling of selected inhibitor (Track 2).	Procedures to check amounts of starch, amylase, and iodine, including iodine and inhibitor (Track 1); Procedures to code a script for molecular modeling in PyMOL and use docking software independently (Track 2)
5	Data analysis (all students).	Interpreting the inhibition data (Track 1); Interpreting the molecular modeling data (Track 2)
6	Poster presentation (all students).	Creating a visually appealing poster

refined procedures to allow that phenomenon to be studied in ways that could be used in lower-division lab settings. The systems studied could be as simple as how a sample fluoresced (2016, 2017, or 2018) or demonstrating the way that ferrozine could be used to characterize the concentration of the iron(II) ion formed in reactions that modeled extracellular electron transfer processes. The students were then tasked with developing a research plan and given an opportunity to carry out the project. Their work was as open-ended as possible, with specific attention to ensuring safety. For students with an engineering and computer science focus, this often involved working through various methods for image processing, programming measurement devices, or coding visualization software. The project provided the students with an experience of answering questions that they generated and often resulted in novel insights into how to work with the phenomenon in specific and exciting ways. These results then contributed to other materials development and research work.

An example of the outcome of this is that the coumarin-102 CoLab resulted in a fluorescence experiment for undergraduate students,<sup>44</sup> as has occurred with the outcomes of other CURES.<sup>30</sup> Similarly, results from 2017 (propidium iodide binding to DNA<sup>38</sup>) are also in development for undergraduate biology and chemistry settings. On the other hand, the results from the study of the Kautsky effect,<sup>39</sup> where the fluorescence of leaves increases after a period in the dark, did not yield preliminary results that could be developed further, as sometimes happens in authentic research. In 2019, student work focused on modeling the fundamental chemistry of extracellular electron transfer, both in terms of practical routes to conducting air-free chemistry in a teaching lab using nitrogen glove bags and to study the electrochemistry of solutions of relevant bacteria (*L. innocua*) models.<sup>36</sup>

As a specific example relevant to the current challenges of teaching laboratory online,<sup>45,46</sup> this paper focuses on the activities for the 2020 and 2021 CoLab programs. In 2020, we implemented an entirely online set of activities using molecular visualization with PyMOL 2.5 to observe interactions of small molecules bound to proteins (elaborating on the work of Acuna et al.<sup>47</sup>). Students employed docking programs to examine the binding of inhibitors to the main protease of SARS-CoV-2<sup>40,41</sup> (PDB ID: 6y2g) and to  $\alpha$ -amylase. For the latter, students were provided with a PDB file of the coordinates of  $\alpha$ -amylase. These coordinates were obtained by removing the ligands and water from the human salivary  $\alpha$ -amylase structure,<sup>48</sup> PDB ID: 1smd, using Discovery Studio 3.1 Visualizer. As an alternative, PyMOL could also be used to extract relevant coordinates. To make the inquiry appropriate for the allocated time frame, structures of relevant ligands (inhibitors in this case) were also provided to

the students. These were obtained by the faculty either from PubChem or by removing all other atoms from structures from the Protein Data Bank<sup>49,50</sup> that included the respective ligands. Specifically, the coordinates of acarbose were obtained from PubChem (3D conformer, CID: 41774) and the coordinates of several acarbose analogues (available in the Supporting Information) were extracted from complexed structures obtained from the Protein Data Bank (PDB IDs: 1xcw, 1xdo, and 1xd1)<sup>51</sup> using Discovery Studio 3.1 Visualizer. In the event that ligand structures are unavailable, PyMOL can be used to build the ligands and minimize them energetically to remove clashes between atoms. We employed this approach to generate a starting point for the docking simulations performed by the students in the 2021 CoLab (see details below). It is important to note that in recent years, flexible ligand docking algorithms have become the standard in predicting ligand binding sites in proteins. Therefore, minimizing the ligand prior to docking is not critical when the ligand does not exhibit clashes among its atoms (e.g., when the ligand is extracted from a structure from the Protein Data Bank).

During the summer of 2021, we engaged students in activities involving a combination of wet chemistry and online work on modeling the binding of drugs and food molecules to salivary  $\alpha$ -amylase. Students worked for approximately three and a half hours once per week. While some activities involved all students, in the fourth week the students were divided into two tracks for other activities (see Table 2). Specifically, Track 1 (designated as in vitro to reflect the use of laboratory equipment in experiments) was set up to allow students to do research on actual foods. Track 2 (designated as in silico to reflect the focus on computer programming for the research) was a computer science and engineering major track (see Table 2). For the first 3 weeks of the program, students worked on the sample amylase inhibition and PyMOL activities provided in the Supporting Information. After being introduced to both the in vitro and in silico components of the CoLab in the first 3 weeks as well as completing activities pertaining to both tracks, students chose the Track they wanted to work in (Track 1 or Track 2) for the final 3 weeks. Track 1 continued using procedures developed in a report in the Journal by Maqsood et al. on at-home amylase experiments<sup>52</sup> in an advanced biochemistry lab. At the same time, Track 2 built on materials developed from the report by Acuna et al. on the use of online docking in evaluating protein-drug interactions<sup>47</sup> and programmed scripts to control the display of visualizations in PyMOL. The final materials presented and used by students in the 2021 year and the set of PDB files prepared for 2020 and 2021 are provided in the Supporting Information. In January of 2022, the CoLab activities were fit into a condensed schedule with 5 h of work for 3 days, with all

students doing the in vitro track. The modified schedule only included a brief introduction to *PyMOL* on the first day.

An important part of developing a CURE in any setting is to provide activities in a form that is both accessible for students, given their background and prior experience, and that permits new investigations. The Maqsood et al. procedure already documented how to use smartphone images to study amylase activity solutions of starch prepared at home (in their case, using crackers or toast).<sup>52</sup> It also described how to use commercially available tincture of iodine to prepare starch-iodine complexes to characterize starch concentrations and enzyme activity.<sup>52</sup> In this method, iodine is used to detect the presence of starch in assays using its characteristic blue color, based on a  $\lambda_{\text{max}}$  of 620 nm. When amylase degrades the starch, there is a reduction in the blue color and a decrease in the amount of red light absorbed.

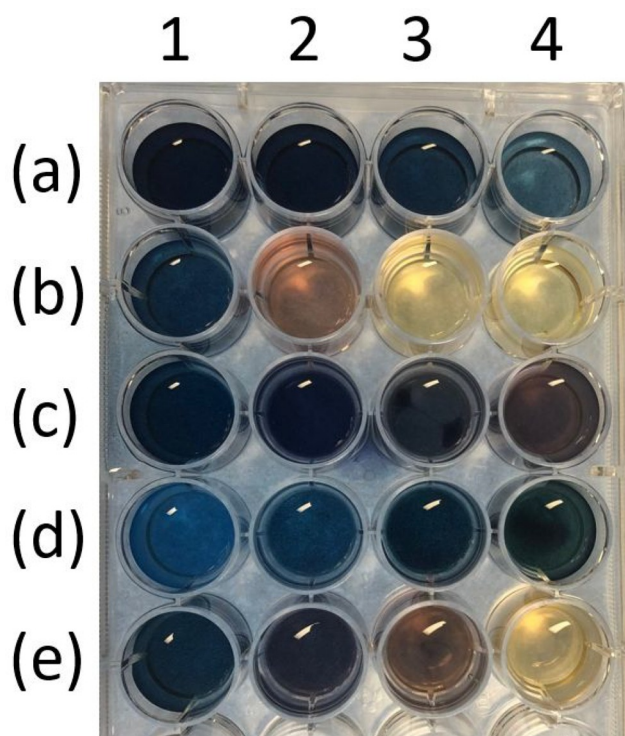
In our setting, we wanted students to investigate inhibition using different foods. We further adapted this method to make it possible for incoming university freshmen to carry out inhibition studies of the enzyme and use a standard source of starch. Tapioca starch was found to be optimal for this, and it was distributed as part of the research materials. Students were given procedures to learn about the basic chemistry of the reaction through skill building procedures by carrying out the following steps:

1. Prepare solutions of starch using commercially available samples of tapioca starch.
2. Prepare and determine the activity of solutions of amylase using saliva.
3. Check on the potential interference of the food extract with the iodine.
4. Determine the inhibition of the amylase by a food extract, using grape seed extract marketed as a nutritional supplement, to follow on a related research paper report.<sup>42</sup>

Figure 1 shows a photo of a set of experiments done in a typical procedure, described in more detail in Table 3. Students assessed the amount of light based on image analysis using *ImageJ*,<sup>53</sup> either as a Java app or using the online version.<sup>54</sup> They were directed to split the image into RGB channels and use the gray scale image of the red channel for analysis (see Supporting Information for detailed procedures using the image in Figure 1 as a template).

Calculations of the % reaction and % inhibition were carried out by comparing actual yield to theoretical yield and subtracting inhibited activity from normal measured activity, dividing by normal activity, and multiplying by 100%, respectively. We note that these methods are far less quantitative than could be obtained using a spectrophotometer. However, for our workshop process, this approach provided clear results on both  $\alpha$ -amylase activity and inhibition.

For their research, students investigated food combinations that had not yet been reported in the literature using this simple starch-iodine assay, so that they may contribute new information to the currently existing body of knowledge. UIC research librarians introduced students to how to find articles that cite the grape seed research paper.<sup>42</sup> The librarians showed how to locate citations to that work (more than 210 as of Summer 2021). The students themselves identified foods in the literature that included red rice bran,<sup>55</sup> raspberries,<sup>56,57</sup> strawberries,<sup>56</sup> and models of tannins from persimmons, and used them to conduct the amylase inhibition experiments. Specifically, one



**Figure 1.** Well plates showing the progression of different experiments. All rows except (d) contained fixed amounts of iodine. (a) Screening for starch amount. (b) Determining amylase impact. (c) Determining inhibitor impact on amylase (high inhibitor concentration). (d) Determining inhibitor impact on iodine. (e) Determining inhibitor impact on amylase (low inhibitor concentration). Deeper blue color due to increased absorption of light in the red channel indicates more starch.

group used strawberries as their food extract, a second group also used strawberries but compared fresh with fermented strawberries to add an additional element to their research, a third group used raspberries and rice bran, and a fourth group used red rice bran.

Two important challenges arose because of side reactions with the food extracts. These created additional authentic research experiences associated with the need to solve problems during the design and conduct of scientific investigations. First, many foods have antioxidant capacity. As noted by Maqsood et al.,<sup>52</sup> this interferes with the starch-iodine complex, presumably due to reduction of the iodine by antioxidants in the food in a side reaction. To prevent this interference, students increased the concentration of iodine until a strong blue solution formed in the well plates (compare rows c and d in Figure 1). Second, students who studied red rice bran had to contend with the presence of starch from the rice product. This was addressed by decreasing the amount of starch extract.

The visualization portion of the program built on previous reports on the use of computer modeling of proteins and drugs, in particular the work of Acuna et al.<sup>47</sup> During the COVID-19 pandemic, online work using such programs allowed the students to gain real world experience and collaborate with their peers while staying safe.<sup>58</sup> In our case, students were provided with a PDB file with a model of the salivary  $\alpha$ -amylase prepared for the 2020 CoLab. Potential inhibitors were constructed by the faculty members using the Builder tools in *PyMOL*.

Table 3. Description of Experiments in a Typical Procedure (Figure 1)

figure row/procedure step	design of procedure	outcome of procedure (for results in Figure 1)
(a) Starch determination	Different amounts of water and starch are treated with a constant amount of iodine to determine the ideal amount for a starch solution.	Well 3 is selected as the amount of starch to use.
(b) Amylase determination	Using the amount of starch from (a), different amounts of amylase solution are added. Well "1" is a control.	All wells with amylase show some iodine remaining, indicating that the amylase concentration is appropriate
(c) Inhibitor determination (high concentration)	Using the starch and amylase amounts from (b), add a constant amount of inhibitor solution in place of water. Well "1" is a control.	Wells 2 and 3 show very little or no amylase activity. Conclude that the inhibitor concentration is too high.
(d) Check inhibitor/iodine ratio	Using starch and iodine amounts from well a3, add different amounts of inhibitor to ensure that the inhibitor does not destroy the iodine.	All wells continue to show starch iodine complex, indicating that the antioxidant behavior of the inhibitor does not compromise the assay.
(e) Inhibitor determination (low concentration)	Using the starch and amylase amounts from (b), add a constant amount of diluted inhibitor solution in place of water. Well "1" is a control.	All wells with inhibitor show decreased but not zero amylase activity, permitting determination of inhibition.

Students utilizing PyMOL gained a basic understanding of the Python programming language and an appreciation of how computer coding finds use in the sciences. As with the amylase activity, it was important to design methods to introduce students to the visualization software, including coding, without any assumptions of prior coding experience.

To evaluate protein–ligand interactions, students were introduced to the docking programs HDOCK<sup>59,60</sup> and PatchDock.<sup>61,62</sup> Docking programs search for the best fit between the ligand and the protein, and through this process, identify possible orientations (poses). The results are then ranked according to the degree of binding affinity between the protein and the ligand. Using the results produced by HDOCK<sup>59,60</sup> and PatchDock,<sup>61,62</sup> students were able to visualize multiple poses of a ligand and its target. Examples of work done in the in silico research track (Track 2) included providing efficient scripts to highlight particular parts of a bound ligand or to report on systematic trends observed in putative binding sites predicted by multiple "hits" from the docking simulation. One group of students in this track visualized the likely active parts of green tea, epigallocatechin gallate (EGCG) and (–)-epicatechin gallate (ECG), as their selective inhibitors.<sup>63</sup> A second group used a model of a persimmon tannin with multiple types of intermolecular linkages and pendent catechol and galloyl side groups (Figure 2).<sup>43,64</sup>

Faculty members and graduate chemistry students checked in with students throughout both the wet chemistry (in vitro) and modeling (in silico) tracks to make sure that students were making sufficient progress and to answer any questions they may have. At the conclusion of the program, students presented their work to faculty members and other students from UIC in a

poster session. Aside from learning about the findings of other groups within their respective track, students from Track 1 (in vitro) also learned about the results obtained by students in Track 2, and students from Track 2 (in silico) also learned about the observations made by students in Track 1. This poster session was done electronically via Zoom, and each student had a chance to go over their group's poster at least once. This poster session gave students the opportunity to emulate scientists presenting their work to their peers at scientific conferences. Additionally, it provided an authentic assessment approach as students attempted to answer questions about their work asked by faculty members outside of the CoLab as well as by other students.<sup>65</sup>

## STUDENT OUTCOMES AND FUTURE DIRECTIONS

A long-term goal of the CoLab program is to increase student retention and graduation in college, especially in the STEM majors that they are initially interested in. We can see the impact of this through tracking data with the 2016–2019 cohorts. During that period, 202 total students participated in the full CoLab program. As of the end of the Fall, 2021 semester, 173 (86%) of these have graduated (86 students) or are still enrolled (87 students). Of the 202 total participants, 165 (82%) are graduated or enrolled in STEM majors (including health sciences). While we do not have a control group, we note that the overall numbers are well above the average rates for the university at large, which reported a six-year graduation rate of 62% for the entering class just before this group, in 2015. Though we are not collecting demographic data on the students, we note that the vast majority of students have been in the President's Award Program, which is issued to first-year candidates who are from an Illinois county that sends few students to the university, families in need of financial assistance, or from groups that are traditionally underrepresented at the university.<sup>66</sup> The distribution of these students is shown in Figure 3, with red-hued sections for natural sciences, mathematics, and health sciences (50%), blue-hued sections for engineering (32%), green for non-STEM (4%), and gray for those who have left without graduating (14%).

We have also begun to collect direct interview data on the experiences of the students. A total of six students (two from the summer of 2021, four from January of 2022) consented to participate in an interview following completion of the CoLab program. Two of these students are chemistry majors, one is a chemical engineering major, another is a computer science major, and two are transfer students enrolled in the RN to BSN program who work as nurses. The interview focused on the nature of science, the affective domain, preparing and presenting a poster, and past research experiences of the students as well as

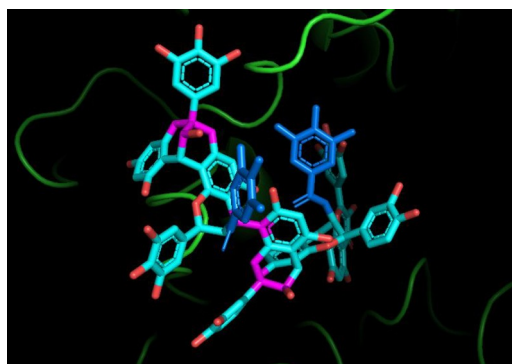
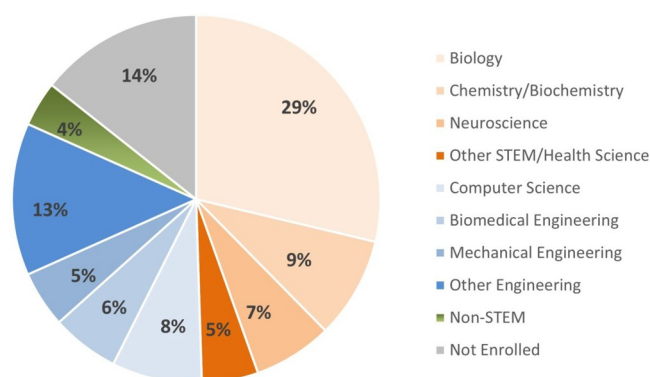


Figure 2. PyMOL model of persimmon Tannin with four flavonoid units. Dark blue shows the galloyl side groups. Purple shows the interunit connections. The protein backbone is shown as a green ribbon diagram.





**Figure 3.** Distribution of 2016–2019 participants, as of Fall 2021, by major or outcome.

their future research interests, and is part of a larger longitudinal study on student belonging and self-identity in science.

For many of the students, the CoLab was the first time they engaged in such a research experience. They had previously only worked on traditional confirmation laboratories in their science classrooms. For example, one student mentioned she had previously participated in literature research using library resources. However, this was the first time she actively participated in a research study that included data collection and analysis. She also noted that through the CoLab program, she was able to better understand the importance of the steps a research process encompasses:

*The CoLab is actually my first like research experience, but I have like my like the other programs. I mean like uh, there's this scholars program like we talk a lot about research and like you know how to find it and things like that. Um, I think I now [after the CoLab] understand more of the aspect of like, you know, collecting data, then interpreting that data to use those results to like you know, proceed and use your hypothesis. And I have more of an understanding of like why we're doing this research and why it's important like the different levels.*

The interview data also showed how students express a desire to continue in STEM and pursue future STEM research. These responses are representative of the students who participated in the interview. One student expressed their wish to explore forensic science or ecology research as a junior or senior:

*I was looking into a little bit like when you use the database and type the topic you're interested in like forensic science is a topic I want to explore and find really interesting or like ecology, so I looked at like a little bit in regards to those subjects, but all the faculty conducting research with regards to those subjects wanted juniors or seniors.*

Another stated that they plan to pursue research as a secondary career in the future:

*So, it was exciting to have the opportunity, first of all, and also to be in a position to learn things that will actually help me in my future career... so that's going to be my secondary career after finishing this next set of degrees and so.*

Besides this work with student outcomes, we note that another goal of the CoLab program is the development of new experiments for undergraduate students. This has already been done, as noted, with the coumarin-102 results from 2016. Results from the 2021 CoLab will be used to adjust the procedure to implement the lab in the general chemistry curriculum. In addition, the CoLab program is now a part of an

NIH “Bridges to the Baccalaureate” grant with a nearby community college. Part of that program is to provide professional development for faculty at the community college in the development of their own CURE program.

In conclusion, the STEM CoLab program allows incoming students to engage in research-based lab experiences that resemble authentic research done under a faculty member but on a much shorter time scale. Students also have the opportunity to interact with other members of their incoming class and potentially build connections that will last throughout their science careers. Many students who participate in the CoLab program are retained in STEM majors and go on to partake in undergraduate research. Additionally, the CoLab program produces new laboratories for the undergraduate curriculum. This was previously demonstrated with the coumarin-102 fluorescence lab and is a major goal of this year's CoLab as well. We expect to return to face-to-face instruction in 2022, which will allow the students to more easily communicate and get in touch with one another to collaborate outside of our weekly meeting time for the CoLab Program. Building on the experience acquired during the COVID-19 pandemic, an online version of the program may also run parallel to the face-to-face CoLab in 2022 and in subsequent years.

## ■ ASSOCIATED CONTENT

### SI Supporting Information

The Supporting Information is available at <https://pubs.acs.org/doi/10.1021/acs.jchemed.1c01290>.

Introduction to scripting using Python for application to PyMOL (PDF)

Folder containing a listing of files of structures referred to in the program and actual files of the structures modified or created for use in the program in 2020 and 2021 (ZIP)

List of materials, guidelines, and directions for instructors and students for amylase activity and inhibition and information on the use of ImageJ for image processing to determine activity and inhibition (PDF) (DOCX)

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## Notes

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