The Biophysicist

No Experience Required: Inclusive Undergraduate Research in Computational Biophysical Chemistry

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ABSTRACT Undergraduate research is a key tool for recruitment and, more importantly, retention of science, technology, engineering, and math students. Unfortunately, many students are not aware of or do not take advantage of these opportunities and, at best, often wait until late in their college careers. For my undergraduate computational biophysical chemistry research lab I have established a no-experience-required policy that allows me to recruit and mentor more research students. It also allows me to be more inclusive and expand the pool of students who have access to research. This also results in a more diverse research group, which is particularly important at a primarily undergraduate institution that has a diverse population with a high percentage of first-generation students. Here, I lay out the procedures I use to recruit and train students of all levels for my research lab, as well as the research products produced by students and myself.

KEY WORDS undergraduate research; inclusion; computational; biophysical chemistry

I. INTRODUCTION

The last thing on most general chemistry or introductory biology students' minds is joining a research laboratory. The same would have been said of myself as an undergraduate. I would not have thought to start research until my junior or senior year—and said as much to my introduction to biology professor when he asked me if I would like to do an independent study the next semester. I am still grateful that he asked me, and I got so much research experience as an undergrad due to that early start.

Early exposure to research experiences, including independent studies and course-based undergraduate experiences (CUREs), have been shown to improve student retention in science, technology, engineering, and math (STEM) courses and fields of study (1–4). Being involved with research also helps students build relationships with other students and with faculty mentors. These relationships help students build a sense of belonging and improve retention in college (5). My approach builds on previous research in this area, as cited above, along with many others.

At a small, primarily undergraduate institution (PUI), student retention is more important than ever and is often a key institutional success metric for majors and departments. At the same time, we all want to make our programs more diverse, more equitable, and more inclusive. Programs that accomplish this are also more likely to retain their students. Improving undergraduate student access to scientific research is therefore helpful for students and faculty on multiple fronts.

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My research lab is no-experience-required in order to recruit more, and more diverse, undergraduate research students at my small PUI. As discussed previously, most students are not thinking about research when they start college, particularly those who are first generation like myself. These students make up ∼50% of our student population based on institutional data, so it is important to make sure I bring research to them rather than expecting them to know to come to me. These students might also be intimidated about approaching a professor in their first year on campus, or they might lack confidence in their ability to be successful at research.

I start recruitment on the first day of my class each semester, when I let my general biochemistry class know that I am looking for research students for that semester as well as future semesters. I also explain that there is no experience required and that I will teach them everything they need to know. I do the same when I teach a general chemistry course or lab. I also recruit students for my lab at our new student welcome event. Other ways that I have found to recruit students include encouraging current lab members to invite their friends or classmates to join, attending student club meetings to promote my research, and posting a research flier outside my office saying "No Experience Required." Additionally, my department colleagues and I regularly recommend research to our academic advisees, whether that is our own or each other's labs.

The only thing a student must do to join the lab is submit the independent study forms before the university's deadline. I have also developed a computational biochemistry CURE that is no-experience-required and has no prerequisites. I will focus mostly on my research lab in this paper, but it is worth noting that similar practices can be successfully used in a CURE setting as well.

II. METHODS

The sample size for this study is limited to the number of students I have personally supervised since Fall 2018. My goal is always to take as many students as possible, so these numbers represent the maximum possible number of students I was able to support. The final number each semester depends on student interest, how their schedules overlap with mine, and my other university commitments for each semester (e.g., teaching overload and extra service).

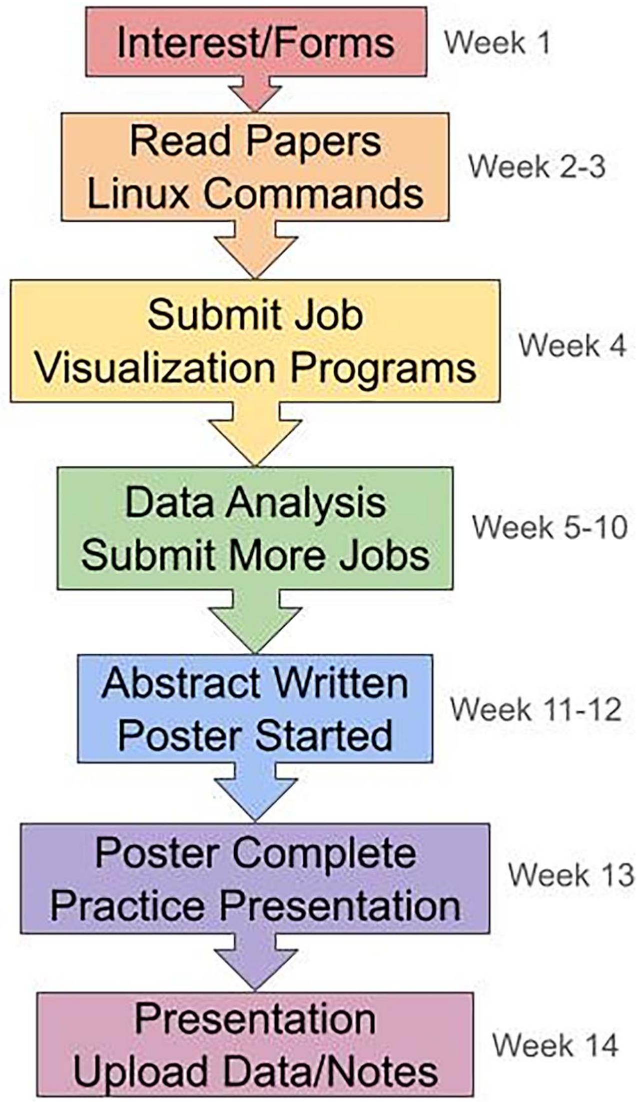

Fig 1. Process of research for undergraduates.

A. Process of research

The process of research mentoring by week in the lab is described below, and the schedule is shown in Figure 1. This schedule is occasionally adjusted for students who work faster or slower, but this is a good overview of my typical schedule. These tasks are completed almost entirely during the students' scheduled 3 h of research per week. Occasionally students need to work on their posters outside of that time, but otherwise, we stick to the scheduled time to respect the students' other commitments. For the computational biochemistry CURE, we do not cover Linux commands because the course is held in a Windows-based computer lab, but the rest of the process is the same.

1. Week 1

Advertise research openings in my classes and contact any students from previous semesters who expressed interest in person or by email. The university requires that independent study forms be submitted by the end of the first week of the semester, so we officially start work in week 2 to make sure everyone starts at the same time. The only requirements to join my lab are that the students are motivated enough to (a) talk to me in person or via email to express their interest in a particular project and (b) to submit the independent study forms on time. This deadline also gives students and myself a week to settle into the semester before starting research.

2. Weeks 2–3

Students are given approximately three key papers on their project's background, and they spend their research time reading these, in the lab if possible. I'm available to answer questions during this time, either one-on-one or with a few students who happen to have the same research time. Students are encouraged to ask lots of questions and reminded that they are not expected to understand everything in the papers yet, particularly the methods sections, which do not usually match the methods we will use in the lab. A key part of building the mentor-mentee relationship is being present during scheduled research times and frequently asking, "What questions do you have so far?" to encourage questions, because I find that some students are hesitant to ask or admit that they don't understand something at first. Depending on the student, they are usually ready to start learning Linux commands in week 3. We go through the basic commands for how to move around the directory structure, copy files, etc., and then continue practicing these throughout the rest of the semester. Docking projects require only a few Linux commands, even on a Linux desktop like in my research lab, although some students want to learn more even if it's not required. Most of the programs we use are free and available for both Windows and Linux; the complete list of programs is available in Section II.A.3.

3. Week 4

By this point, the students are ready to submit their first simulation run. The setup process for this introduces them to the protein and/or small molecule visualization programs that they will also use for data analysis. The students need to visually inspect the protein structure (using VMD [6], PyMOL [7], or a similar program) and then the text of the Protein Data Bank file. For docking, students need to source or construct the ligand molecule as well.

Each student is given their own part of a project to promote a feeling of ownership and agency (e.g., a unique protein–drug combination or a unique protein unfolding simulation setup). If a project is brand new, the students are warned before they select it that there will be a lot of iterations and failure to make sure that they are okay with that. After setting up the input files, they submit the simulation run. The setup process also allows them to practice Linux commands, learn more about their protein, and start learning about the simulation parameters. I do not use practice exercises—we jump right into a real experiment, and I sit with the student throughout the submission process to explain each step.

4. Weeks 5–10

Once the results of the first simulation come back, data analysis can start. At this point, the students learn about the meaning of their data and how the simulation works through the data analysis. We cover visualizing the results with both visualization software and graphing software. Any calculations needed are also covered at this point and recording data and notes are discussed. It is typically easier to have students take notes digitally because they can share their file with me at the end of the semester. They also often like to add screenshots of Linux commands or software menu options to their notes, and digital notes are more convenient for that as well. This is also a good time to answer questions about biochemistry or biophysics concepts with which they do not have prior experience, because I find they engage with the material more effectively by looking at their own results.

Part of this explanation covers how experiments can go wrong or not work at all. Students can often get discouraged or think that they are at fault when their experiments do not work out. When this happens, we discuss that this is how research goes, even for professors and other experienced researchers. Keep in mind that students will probably need repeat instructions during their first semester, forget key steps, and make mistakes. I have found that part of being a good research mentor is to demonstrate a growth mindset and to assure students that asking repeat questions and making mistakes are a normal part of the learning process and not something to apologize for or feel bad about. They are not graduate students who can spend all day mastering their research, so it will take them longer to become proficient, but they can do it with practice.

After the first round of data analysis, more jobs are submitted, and the new data sets are analyzed. This can be repeated several times depending on the project, ideally finishing with the last round of analysis done or nearly done in week 10. For example, students can usually complete two to three rounds of unfolding or docking simulations in this time.

5. Weeks 11–12

At this point in the semester, a call for abstracts has usually gone out for our campus end-of-semester poster session, and each research student writes and submits their own abstract. Students then start working on the poster by using a template file. I help with edits, but they always write the first drafts themselves. The first drafts help me to see their current understanding level, so I know what to cover with each student while they make their posters. Successive drafts and making changes with feedback also help them build a growth mindset and mimic the process of scientific peer review. Developing the abstract and poster also requires the student to compare their work to previous and other current students' results, as well as to refer back to the literature they read during week 2, reinforcing how much they have learned over the semester.

I prefer to have students present a poster instead of presenting at a group meeting for a few reasons. First, we have a relatively small group and number of projects, and the students usually know the basics of what everyone is working on already. Second, the poster session gives them practice telling people who are not experts in our field about their research and builds general communication skills and confidence. Finally, it is something they can put on their resumes as a professional development event. During the COVID-19 pandemic when we did remote research, we held group meetings until virtual conferences started up, and it was not as valuable an experience based on my observations.

6. Week 13

During this week the students finalize their poster, and I arrange to print them. There is also time for practice presentations. This can be as simple as having the student show their poster on their desktop and walk through their elevator pitch. More experienced students might not need this for a poster. For students giving a talk at the symposium, we do a full run through of their talk with the group so they can practice and receive feedback from myself and the group. Practice sessions are another tool to build a growth mindset and self-confidence for students. Local conferences are a great venue for undergraduate research presentations because students are able to practice with very low stakes.

7. Week 14

The last week of the semester is when poster sessions are typically scheduled, so this takes up most of the students' research time for the week. This is a good time to take pictures of the students with their posters. During that week, students are responsible for uploading all of their files and notes to Google Drive so that I have easy access to them. One of the final things I do is remind them that they should ask for a recommendation letter, and that they should keep in touch if they are graduating.

B. Programs and computers used

Due to the constraints of working at a small PUI, I decided when I set up my lab to rely on free programs as much as possible. The list of programs and their main purposes is provided below. Note that there are many options for these types of programs with various advantages and disadvantages, and of course, many programs that are not free and might have additional useful features are also available. We were able to obtain a site license for PyMOL (7) this year as well, so that will be great experience for the students while we have it (8).

1. Protein Visualization: VMD (6), UCSF Chimera (9), RasMol (10), POCASA (11).
2. Small Molecule Drawing: Marvin Sketch (12).
3. Graphing: Xmgrace (13), Veusz (14).
4. Simulations: SOP-GPU (15), SwissDock (16), Phyre2 (17).

There are five student Linux desktops in my lab, and, as mentioned previously, the CURE is held in a campus student computer classroom that runs Windows. I also have a GPU workstation in the lab, which is required for our unfolding simulations and was purchased with my start-up funds. The process described here could also use students' personal computers if they have laptops or desktops, which were used during the COVID-19 pandemic by my lab and many others (18). Cloud computing and web-based programs are also excellent resources for resource-limited labs. It is important to note that many programs do not work on tablets, Chromebooks, etc., which many students rely on now, so providing students with desktops in the lab is more equitable and inclusive when the resources are available.

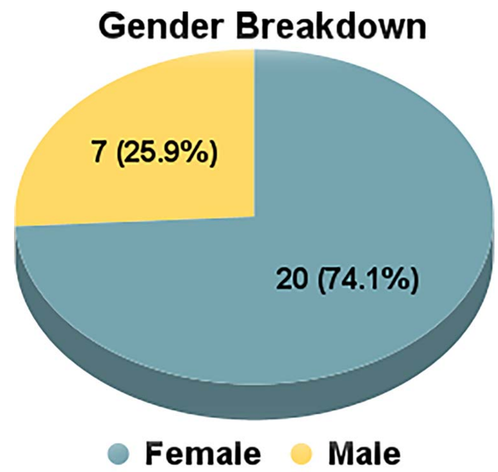

Fig 2. Research student gender breakdown for Fall 2018 to Fall 2023.

III. RESULTS AND DISCUSSION

A. Student demographics

Figure 2 shows the gender breakdown of research students in my lab from August 2018 to the present. Of the students, 74% (20 of 27) were female. Additionally, 52% (14) were either Black/African American, Hispanic/LatinX, Asian/Asian American, or from another minoritized group. Many students were first-generation students and/or grew up or still lived in the local community. There were many overlapping identities as well; for example, a student who was first generation could also be female or from a minoritized group. To protect student privacy, a more detailed breakdown of these demographics is not possible. The current overall demographics for my university are as follows: 63% female, 37% male; 66% white, 11% Black, 13% Hispanic, 2% Asian, and 8% any other ethnicity. In Fall 2021, ∼49% of the incoming freshman class self-identified as a first-generation student.

Table 1 shows that my research students come from a wide variety of majors, with biomedical sciences being the most common. The course I teach every semester is nonmajors biochemistry, so that is where most of my students are recruited.

Table 1. Research student undergraduate majors.

Undergraduate major	Number of students (%)
Biomedical sciences	9 (33.3)
Biology	6 (22.2)
Biochemistry	4 (14.8)
Nutrition	3 (11.1)
Chemistry	2 (7.4)
Medical Technology	2 (7.4)
Pre-Dental	1 (3.7)

Table 2. Research products from Fall 2018 to Fall 2023.

Research product type	Number
Accepted student presentation	21
Accepted PI presentation	13
Invited PI presentation	2
Research paper (accepted)	1
Research paper (submitted)	1
Research paper (in-preparation)	1
Grant application (internal)	2
Grant application (external)	3

PI, Principal Investigator.

B. Research products

Table 2 shows the research products from Fall 2018 to the present for my research lab. The submitted and in-preparation research papers all have multiple student coauthors, comprising everyone who has worked on the project. All the grant applications relied on student-generated preliminary data as well. It is important to obtain an additional form of contact for students who graduate beyond their university email, such as an alternate email or LinkedIn connection. When publishing, coauthors are required to approve manuscripts when submitted to most major journals.

C. Student feedback on the process of research

The feedback presented here is from three of my recent undergraduate research students. They were asked if they would like to contribute feedback on their research experience for this paper and consented to their feedback being used if they did provide it. Their feedback was entirely voluntary, and not all students chose to participate. Those that did typed their responses; no survey was used. Student 1 was in their second semester in the lab, student 2 was new, and student 3 first took my CURE course before joining the lab for two semesters.

1. Student 1: “I really liked how you taught me how to do things and what they meant as we were going on through the simulations. I think if you were to teach me everything before, I would have felt overwhelmed and that I was not ‘smart’ enough or had enough experience to do this type of research. You gave me confidence and reinstated that I did not need to have a strong background in this field to do this kind of research. I appreciate it a lot, and it has given me the opportunity to learn new things that do not particularly come across my specific major of nutrition.”
2. Student 2: “I found the information I was learning to be very different from how I had approached science before. I essentially had to learn a whole new language when using Linux. Although it was all completely new to me, I found the environment in which I was learning to be very welcoming and open. I felt comfortable asking questions and was able to grasp a solid understanding on what I was doing in my research within the first couple weeks.”
3. Student 3: “[The] research [is] undergrad friendly and step by step taught and guided me into conducting research. Having us conduct the simulations and after we conduct them [going] through and help[ing] us understand what we are seeing [was helpful]. I feel like this is important because it helps create more of a hands-on learning experience for a lab that’s computational and since the data we are collecting is essentially new, it encourages us as students to want to understand more of the

data we collected. [Your process is good] for students who are intimidated about doing research."

The quotes below are from my CURE course in spring 2022 and spring 2024 and illustrate how students perceived their research experience overall. The student responses to this survey were Institutional Review Board–exempt as an in-class activity.

1. "What I liked about the course is that it helped me to understand the full process of doing scientific research and I actually understood what it was that I did my research on."
2. "I feel like I am actually doing something that can potentially make a difference, so I feel it is pretty cool."
3. "To me I don't think it settled in that the research that I've done helps to contribute to a larger scientific cause. But if I'm being honest, overall, it's a thrilling feeling."
4. "Contributing to the body of scientific knowledge feels like I'm finally able to call myself a scientist."
5. "Honestly [this experience was] pretty special. I always stayed away from research because it seemed scary but I really enjoyed this. I felt accomplished to see all my work on a poster and able to present it."
6. "I'm so glad to be a part of solving a world issue and helping the world in some sort of way."

IV. CONCLUSIONS

My main goal for my research lab is to make undergraduate research as inclusive and accessible as possible by removing barriers to participation. Encouraging students with no experience to join the lab results in a slightly larger time commitment upfront for faculty and can slow down the data collection and analysis process slightly. In my experience, the work of several students over many semesters adds up to a publication, which is different from how a lab with graduate students would operate. For example, my most recently submitted publication has 15 student coauthors and covers eight semesters of research. However, these policies allow me to mentor more research students and to provide research experience to many students who might not have considered research otherwise. Given the benefits of undergraduate research, it is my belief that this trade-off is well worth it.

Table 3. Research student postgraduation outcomes.

Postgraduation outcomes	Number (%)
Health care or related areas	7 (29.2)
Laboratory, research technician, scientist	6 (25.0)
STEM graduate school	5 (20.8)
Writing or related areas	1 (4.2)
Unknown	5 (20.8)

In one semester of three hours of work per week, a student can generate enough data for a poster: either several rounds of unfolding simulations that can be compared or a similar number of docking simulations. Students will gain communication skills and a concrete product for their resume by presenting their work at a local symposium. If all goes well, students also end up with a good recommendation letter for summer research programs, graduate school, or jobs. Table 3 shows postgraduation outcomes for my research students, where known. A large majority of them are in health care fields, research labs, or graduate school.

Students will hopefully gain a sense of accomplishment and an appreciation of the process of science through participation in research, as demonstrated by the student feedback above, and a mentor through the rest of their college career and beyond. All of this is in addition to the conceptual skills of Linux commands, protein visualization, and molecular simulations. I have also found that more experienced students gain leadership experience by helping new students in the lab, which reinforces their own knowledge while decreasing some of the training required from me. Each student's understanding level will vary by the end of the semester, which is okay. It is still a worthwhile experience for the student even if they do not develop deep knowledge of computational simulations; they are not graduate students, so we cannot and should not expect them to have the same time commitment and understanding level. Nor should we relegate them to solely doing dishes or other upkeep tasks when they are capable of real contributions to science.

I hope to contribute to the current efforts promoting that undergraduate research should be inclusive and accessible to all students, and to continue to change the perceptions of what undergraduate researchers can accomplish.

AUTHOR CONTRIBUTIONS

KET designed the lab policies, practices, and research projects described here; collected and analyzed the student data; and wrote the paper. This is a single-author publication.

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