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Technology Report

ATRP Kinetic Simulator: An Online Open Resource Educational Tool Using Jupyter Notebook and Google Colaboratory

Yu Wang,* Manyu Li,* Xiang-Sheng Wang, Amanda Gildersleeve, and Nadia Turki

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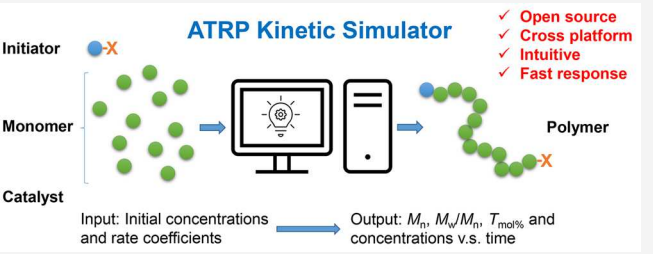
ABSTRACT: This study reported the application of an interactive Open Education Resource, namely, an open virtual experiment simulator education tool (OVESET), in teaching the kinetics of atom transfer radical polymerization (ATRP) in a polymer science classroom. The OVESET ATRP kinetic simulator aims at improving students' inductive reasoning skills. Students were encouraged to perform virtual experiments to systematically examine the influence of each parameter, e.g., type of polymerization and concentrations of reagents, and to observe and make logical explanations of the general trends behind each series of experiments. The tool was designed to maximize accessibility and flexibility through open licensing. The simulator runs under the Jupyter Notebook environment, which is free to use, modify, and redistribute; therefore, instructors can adapt the simulator based on their teaching contexts. The simulator can be applied in a classroom setting without requiring any software installation and can be used across different operating systems. Assessment of the implementation demonstrated that students' learning outcomes and STEM and polymer science identity were improved. Students also rated the tool as useful in increasing their understanding and inductive reasoning. The quick and in-place response of the notebook makes it ideal for both in-class demonstrations and after-class practices. The tool is freely available at https://bit.ly/ATRP-Simulator.



KEYWORDS: *Atom Transfer Radical Polymerization, ATRP, Kinetics, Radical Polymerization, Open Virtual Experiment Simulator Education Tool, OVESET, Jupyter Notebook, Google Colaboratory*

INTRODUCTION

The development of Open Education Resources (OERs) within chemistry has flourished in recent years. Specifically, the application of OERs in chemistry classrooms, such as general chemistry[1,2] and organic chemistry textbooks,[3] has been found to be effective teaching approaches. This study aims to contribute to affordable chemistry OERs beyond the widely available introductory-level resources by developing a kinetic simulator, an open virtual experiment simulator education tool (OVESET) for teaching atom transfer radical polymerization (ATRP) in undergraduate polymer science education. As past research in polymer science education showed, a simulation approach could provide added benefits over traditional learning.[4] This study also aims to implement the tool in undergraduate settings with the pedagogical goal of enhancing students' inductive reasoning in polymerization kinetics. At the end of the kinetic simulator learning experiences, it is expected students will be able to (1) describe parameters that are relevant to the polymerization process (i.e., ATRP), and (2) inductively analyze the outcomes of the polymerization process (i.e., ATRP).

ATRP is a powerful tool for the synthesis of polymers with well-defined molecular structures and functionalities.[5−10] The abundant applications have made this technique widely accepted as part of the polymer chemistry curricula in undergraduate education.[11] It can be challenging to help students understand the detailed kinetics of ATRP through inductive reasoning, e.g., what to expect when the reaction condition is changed and why. Some universities may offer ATRP experiments to help students to gain hands-on experiences as well as a better understanding of this technique.[12−15] However, one or two experiments certainly do not suffice the requirements for students to get enough understanding to perform independent research. Performing virtual experiments is a good solution,[4] but there are no convenient tools available. For example, Predici is widely used for polymerization kinetic simulation, but the high price limits its availability to students.[16] An open-source Monte Carlo polymerization kinetic simulation package, mcPolymer,[17] is available but it is quite challenging to teach students to compile the codes and run the program on their computers.

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Besides, Monte Carlo simulations usually take a long time to finish one virtual experiment and are not suitable for students to practice.

To fill the gap in affordable educational materials in polymer science, an ATRP kinetic simulation package was developed in Python employing the method of moments.[18,19] The OVESET ATRP kinetic simulator is an OER that runs under the Jupyter Notebook environment, which is an open-source programming platform that combines professional formatting of notes, images, videos, symbols, equations, etc. Jupyter Notebook has a user-friendly interface which is critical for lowering the learning curve. After the Jupyter Notebook simulator was deposited on GitHub, it can be run online through the service of Google Colaboratory, see the screenshot Figure 1. Anyone who has a Google account can run this simulator in a browser without installation or configuration on the local computer.

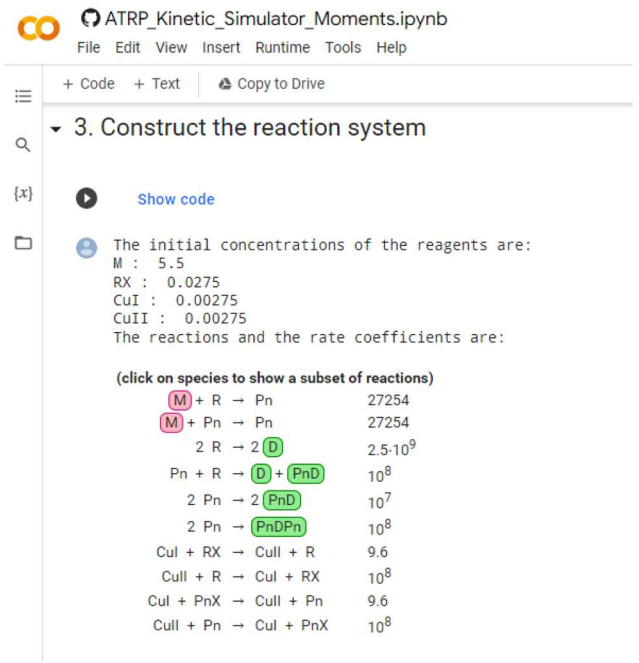

Figure 1. Screenshot of the ATRP kinetic simulator.

In this study, students brought their own laptops to the classroom and performed the virtual experiments simply with a link to the OVESET ATRP kinetic simulator provided by the instructor. In the Jupyter Notebook file, it is straightforward to find where to edit the initial experimental conditions; then, the simulation can be triggered simply by "one-click". The results are shown as plots in the notebook presenting the information on concentration changes of all species, the number-average molecular weight (M_n) of the obtained polymers, molecular weight distribution (M_w/M_n), and the mole percent of the loss of the chain end functional groups ($T_{mol\%}$). After the setup of the initial conditions, the simulation takes only a few seconds to run. Thus, this simulator is ideal for both in-class demonstrations and after-class practices.

HOW TO USE THE ATRP KINETIC SIMULATOR

Using the link https://bit.ly/ATRP-Simulator, users are directed to OVESET ATRP kinetic simulator, presented in the format of a notebook under the Google Colab environment. By default, the notebook is preloaded with the reaction conditions of a normal ATRP of methyl acrylate (MA) at 60 °C. Under the dropdown menu "Runtime", click "Run all", and the simulator will perform a simulation with the preloaded parameters. Under section "3. Construct the reaction system", the initial concentrations of the reagents and the reactions with the rate coefficients should be shown. In section "4. Simulation", the differential equations used for the simulation are listed. The results of the simulation are plotted in section "5. Results" including the changes in concentrations of the reagents, the monomer conversion vs time, and the information on the average molecular weights. In the left panel, under the tab "Files", the results are exported as a CSV file and figures. A more detailed explanation of this example can be found in the Supporting Information.

To run a different simulation, simply go to section "2. Reaction conditions" and edit the parameters in place, and then rerun all cells. New results will be shown as plots in the notebook and will be exported. Some examples of polymerizations under various conditions can be found in the Supporting Information as well.

Some instructors may want to modify the program and deploy the modified version to their students. This can be achieved easily by saving the modified simulator in one's Google Drive or on GitHub and open it with Google Colaboratory (i.e., similar to other Google Documents). Then, instructors can share the link of the modified simulator with their students. When the Internet is not available or for any other reason the users want to run the simulator on their own computers, an easy option is to install Anaconda, a program that includes Jupyter Notebook by default. To use the ATRP kinetic simulator, the users would also need to install a package called "chempy".[20] After the installation, the ATRP kinetic simulator can be opened under the Jupyter Notebook environment.

IMPLEMENTATION IN UNDERGRADUATE SETTINGS AND RESULTS

Learning Setting of the Implementation

The kinetic simulator was implemented in an upper-level undergraduate introduction to polymer science course during the spring semester of 2022 at a predominantly White institution (PWI) 4-year university in the Southern United States. Among the 12,041 undergraduates enrolled, 57% were females and 43% were males. The two largest groups were students identified as Black/African (22%) and White (62%). There were 121 students enrolled as chemistry majors during the semester of implementation. A total of 25 students enrolled in the course. The course has two prerequisites: (1) completion of the general chemistry sequence, and (2) completion of the introduction to organic chemistry. The course was taken by students majoring or minoring in chemistry or engineering. The course is only required for students seeking an ACS-certified Bachelor of Science in Chemistry degree, but not other students. Students met three times per week for 50 min per session.

On the first class day of the implementation, students were given a lecture that introduced the basic concepts of ATRP polymerization. Mainly, compared to conventional radical polymerization, ATRP uses Cu catalysts and alkyl halide (RX) type initiators to introduce a reversible deactivation process and thus lead to controlled polymer chain length with active halogen chain ends. However, normal ATRP usually requires

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Table 1. Virtual Experiments Performed by Students: Series I and II

Series	Parameter(s)	Range (mol/L)	Polymerization rate	Polymer concentration	M_n[a]
I	c0_CuI	0−0.0275	positive	none	none
I	c0_CuII	0−0.0275	negative	none	none
I	keep the ratio between c0_CuI and c0_CuII constant, change both values	0−0.0275	none	none	none
II	c0_RX	0.0055−0.135	positive	positive	negative

[a]The average molecular weight at the same monomer conversion.

high-concentration Cu catalysts. In order to reduce the amount of Cu, initiators for continuous activator regeneration (ICAR) ATRP were introduced. After the basic concepts were explained, students were asked to open the kinetic simulator app using their own devices (laptops or mobile phones). The instructor also demonstrated the kinetic simulator using the classroom projector, explained the default example, and discussed any questions students had.

In the next class (i.e., the second class meeting during the implementation), students were asked to work together in 2−3 person groups and perform virtual experiments following instructions as stated below in Series I to IV. All four series were completed during one class meeting. To fit in a 50 min class time, the students were asked to change only a few parameters in the simulator, while the majority of the input remained unchanged with default values. Four series of experiments were performed to help students inductively reason the influences of concentrations of Cu catalyst, RX type initiator, and azobis(isobutyronitrile) (AIBN) on the polymerization rate, the concentration of polymers, the average molecular weights of the polymers in normal ATRP and ICAR ATRP, and compared to conventional radical polymerization. Students were asked to conclude general trends in each series of experiments through observation and discuss the explanations of the phenomena. Finally, the instructor helped to clarify the findings.

Every time the students started a new series of experiments, they were asked to close the simulator and reopen it to reset to the default values of parameters. The first two series of experiments were designed to help students to understand normal ATRP. The parameters to be evaluated and the expected outcomes are summarized in Table 1.

Series I: Influence of Cu Catalyst Concentrations in Normal ATRP

In the first series of experiments, the students were asked to change the values of c0_CuI and c0_CuII while keeping all other parameters with their default values. After performing this series of experiments, it was observed that the concentrations of the Cu catalyst had no influence on the polymer concentration or the average molecular weight of the polymers. The polymerization rate increased with Cu(I) concentration and decreased with Cu(II) concentration. If the concentrations of both Cu(I) and Cu(II) increased or decreased simultaneously by the same factor, the polymerization rate would keep constant because the influences of Cu(I) and Cu(II) canceled each other. Thus, the conclusion is that the ratio between Cu(I) and Cu(II) determined the polymerization rate. Each of the group students was able to observe and summarize those trends. The students were able to explain that the reason was that Cu(I) reacted with RX to produce radicals which were responsible for the polymerization process, i.e., more Cu(I) led to more radicals and thus faster polymerization; while Cu(II) reacted with radicals thus having a negative effect on the polymerization rate. The instructor further explained the ATRP equilibrium and the correlation between the radical concentration and the Cu(I) and Cu(II) ratio.

Series II: Influence of RX Concentrations in Normal ATRP

In this series of experiments, the students were asked to change the values of c0_RX and keep the default values of all other parameters. It was found that the concentration of RX influenced the polymerization rate, the polymer concentration, and the average molecular weight of polymers. The students were able to find that the polymer concentration essentially equaled the initial concentration of RX because in normal ATRP every RX initiator converted into one polymer chain. With the same amount of Cu(I), more RX would produce more radicals and lead to faster polymerization. The instructor further explained the ATRP equilibrium and derived the equation to calculate the radical concentration which determines the polymerization rate, eq 1.

$$[R^{\bullet}] + [R{-}P_n^{\bullet}] = K_{ATRP}([R{-}X] + [R{-}P_n{-}X])\frac{[Cu^{I}X/Ligand]}{[Cu^{II}X_2/Ligand]} \quad (1)$$

where $R^{\bullet}$ means the primary radicals, $R{-}P_n^{\bullet}$ means the polymeric radicals, K_{ATRP} is the ATRP equilibrium constant, R−X and $R{-}P_n{-}X$ are the RX initiator and the polymers with halogen chain ends.

At the same monomer conversion, the average number of monomer units in each polymer should equal the number of monomers that have reacted divided by the number of polymers. Thus, a higher initial concentration of RX, i.e., more polymers, would lead to a lower average molecular weight of polymers. Some students had difficulty getting the quantitative correlation between M_n and the initial concentration of RX. The equation to calculate M_n was given by the instructor, eq 2. After the explanation, all students were able to understand the correlation.

$$M_n = \frac{[M]_0}{[R - X]_0} \times \text{conv} \times M_M \quad (2)$$

where M_n is the number-average molecular weight of the polymers, $[M]_0$ and $[R{-}X]_0$ are the initial concentrations of the monomer and RX, conv is the monomer conversion, and M_M is the molecular weight of the monomer.

Series III: Influence of AIBN Concentrations in ICAR ATRP and Comparison with Conventional Radical Polymerization

The students were asked to change the polymerization type, i.e., Poly_type, from "normal" to "icar", change the values of both k_a_0_atrp and k_a_atrp from 9.6 to 96, and change the values of both c0_CuI and c0_CuII from 0.00275 to 0.000138. The concentration of AIBN, i.e., c0_TI, was set to values in a range as indicated in Table 2. After each simulation of ICAR

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Table 2. Virtual Experiments Performed by Students: Series III

Series	Poly_type	Parameter	Range (mol/L)	Polymerization rate	Polymer concentration	M_n[a]
III	"icar"	c0_TI	0.00069−0.0069	positive	none	none
III	"conven"	c0_TI	0.00069−0.0069	positive	positive	negative

[a]The average molecular weight at the same monomer conversion.

ATRP, the students were asked to change the polymerization type from "icar" to "conven" and to run the simulation of conventional radical polymerization. The results of ICAR ATRP and conventional radical polymerization were compared.

Students had learned the kinetics of conventional radical polymerization and understood how would the concentration of AIBN affect the polymerization rate and polymer concentration, as well as the average molecular weight of polymers. This series of experiments showed that in ICAR ATRP the concentration of AIBN had little influence on the polymer concentration and the average molecular weight. Instead, in ICAR ATRP the concentration of polymers depended on the initial concentration of RX which was the same as in normal ATRP. The average molecular weight of polymers could also be calculated by eq 2, which was the same as in normal ATRP as well. Concerning the polymerization rate of ICAR ATRP, it was close to that of conventional radical polymerization with the same concentration of AIBN. With relatively low AIBN concentrations, ICAR ATRP was slightly faster than conventional radical polymerization, while with high AIBN concentrations the polymerization rates of ICAR ATRP and conventional radical polymerization were nearly the same.

Series IV: Influence of Cu Catalyst Concentrations in ICAR ATRP

The students were asked to change the polymerization type, i.e., Poly_type, from "normal" to "icar", and change the values of both k_a_0_atrp and k_a_atrp from 9.6 to 96. The concentrations of Cu(I) and Cu(II) were changed in a range as indicated in Table 3. It was found by the students, Cu(I) and Cu(II) concentrations did have influences on the polymerization rates; however, the influences were insignificant. The polymer concentration and the average molecular weight of the polymers did not depend on the Cu(I) and Cu(II) concentrations as long as the overall Cu concentration was not 0. However, if the concentrations of Cu(I) and Cu(II) were both 0, the polymerization was essentially a conventional radical polymerization where the RX initiators remained intact during the polymerization. Using this series of experiments, the instructor explained to the students the important feature of ATRP vs conventional radical polymerization, i.e., in ATRP the majority of polymers grew from an RX type of initiator thus such a polymerization method could be used to make block copolymers or surface initiated polymers while conventional radical polymerization could not.

Table 3. Virtual Experiments Performed by Students: Series IV

Series	Parameter	Range (mol/L)	Polymerization rate	Polymer concentration	M_n[a]
IV	c0_CuI	0−0.000275	positive	none	none
IV	c0_CuII	0−0.000275	negative	none	none

[a]The average molecular weight at the same monomer conversion.

ASSESSMENTS OF UNDERGRADUATE CLASSROOM IMPLEMENTATION

Assessment Questions and Analyses

The implementation and assessment reporting in this manuscript were approved by the Institutional Review Board (IRB) of the authors' institution (IRB-21-068-OTHR-OTHR). Out of the 25 students, 20 students consented to the use of their data for research purposes. The final sample contained 19 students who consented and were present during the learning experiences. After the consent, students were divided into two groups and attended the class meetings separately. Both groups were given a pretest before the presentation of any of the learning materials. Then, one group (n = 11) was taught using the kinetic simulators as described above. The other group (n = 8) was presented with the same concepts and examples but using PowerPoint lectures. Both groups then completed the post-test content assessment questions. Group comparison showed that students who used the kinetic simulators showed higher average scores (M = 0.88, SD = 0.78) than students who had not used the kinetic simulators (M = 0.36, SD = 0.50). It should be noted, however, that the sample size was too small for a well-powered inferential test to compare whether the two groups were significantly different. After the pretest and post-test assessments, for equity reasons, the group that had not received the kinetic simulator learning experiences was given time to learn with the kinetic simulator.

All students were invited to rate the kinetic simulator on a 5-point Likert scale. This brief survey was administered on a separate day after students completed the module exam. This was to allow students sufficient time to explore the tool both in class and at home during their own study. The students who participated in the brief survey (n = 14) agreed that the kinetic simulator was useful in learning new knowledge (M = 4.13, SD = 0.60) and in learning inductive reasoning behind the ATRP process (M = 3.75, SD = 0.83).

In addition to content knowledge, students' STEM and polymer identity were gauged. Particularly, students were asked to rate their perception of STEM and polymer science identity before and after learning with the kinetic simulator. The pretest was administered during Week 4 of the spring 2022 semester, and the post-test was administered during Week 8 of the same semester. The learning materials were presented to the students during Weeks 6−7. STEM and polymer science identity were measured separately by adapting the STEM Professional Identity Overlap measure (STEM-PIO-1)[21] rated on a 7-point scale. Students' ratings on their STEM identity improved slightly after the kinetic simulator learning experience (M = 5.63, SD = 1.65), compared to before (M = 5.00, SD = 1.65). The pretest average is similar to the average obtained by the scale development study[21] in which the authors found an average of 4.70 (SD = 1.68) in hard STEM-major college students in the United States. Students'

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initial polymer science identity was very low (M = 1.75, SD = 0.83), but the post-test score was slightly increased (M = 2.50, SD = 0.87).

DISCUSSION

The OVESET ATRP kinetic simulator is designed for implementation in undergraduate polymer science education with several distinctive features. First, the simulator is an OER, thus allowing anyone to retain, reuse, revise, remix, and redistribute freely. The use of Google Colaboratory and the notebook environment facilitate the open process as the simulator can be easily edited and saved as a new learning tool. Second, the simulator is preloaded with a ready-to-use teaching example. Instructors can simply open the link and start teaching with it. Third, the minimum technical requirement for using the kinetic simulator is only a web browser. The notes and the experimenter are intertwined in the simulator. Therefore, class time is not wasted downloading/installing software or switching across platforms. This makes fitting the kinetic simulator in short class periods possible. Finally, the simulator was developed with a pedagogical goal to teach students inductive reasoning of the complex relationships behind polymerization processes. The kinetic simulator allows students to experiment with different conditions and visualize the outcomes. Overall, the kinetic simulator developed in this study adds to existing polymer science education literature, such as computer-based learning,[22] simulation learning,[4] and visualization.[23]

The assessment of the implementation in an undergraduate classroom showed that students' content assessment scores appeared to have improved after using the kinetic simulator when compared with peers who had not used the kinetic simulator. Students' feedback on the tool was also positive. The assessment results showed evidence that the kinetic simulator is a useful tool to be added to undergraduate introductory polymer science classrooms.

Limitations and Future Directions

The current version of the tool only allows users to experiment with ATRP. More work needs to be done to extend the tool to cover a complete polymer science curriculum. Also, the tool does not require users to have any programming skills, but to update or change the design of the tool, educators may need to have basic python coding knowledge. In terms of the implementation, the tool was implemented in a small classroom. Students might have a more intimate classroom experience than students in a large classroom and might feel more comfortable asking questions. Instructors using the kinetic simulator in large classrooms may want to divide students into small groups and may train teaching assistants to help answer questions. Future research is needed to assess larger classroom implementations and to include a larger sample size for statistical tests on the effectiveness of the tool. In addition, future researchers may explore the pedagogy used. For example, the tool encourages students to learn in small groups of 2−3 students. Researchers may explore if this type of collaborative learning pedagogy promotes inclusiveness and a positive classroom climate. In addition to classroom implementation, future research mentors may also consider using the tool and the implementation suggestions in undergraduate student research experiences (SRE).

Another limitation is that the assessment of the tool was administered about 2 weeks after students were presented with the tool. This allowed students to experience the tool both in class and at home before the exam on the topic. The class meeting (after the exam week) had a low attendance rate; therefore, not all students who participated in the learning experience rated the tool. We also followed the ethical protocol to allow students' voluntary participation. Although the students who rated the tool were generally positive about the tool, other students' perception was unknown.

CONCLUSIONS

The free OVESET ATRP kinetic simulator was developed as a tool for teaching and learning ATRP, particularly, helping students to describe parameters that are relevant to ATRP and teach students to inductively analyze the outcomes of ATRP. The program was written in an open-source platform, Python under Jupyter Notebook environment, and was licensed as an OER to freely use/modify/redistribute. Instructors can modify and deploy a revised version of the simulator to their students. The OVESET ATRP kinetic simulator can be used either online without installing anything or run locally on one's own computer. Students do not need to spend time setting up the system nor do they need to have any background in programming. The simulator is easy to access and fast responding, and thus is ideal for both in-class demonstrations and after-class practices.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available at https://pubs.acs.org/doi/10.1021/acs.jchemed.2c01250.

Example Simulation and Explanation, Evaluation Questions, and Exam Questions Related to this Study (PDF)

AUTHOR INFORMATION

Corresponding Authors

Yu Wang − *Department of Chemistry, University of Louisiana at Lafayette, Lafayette, Louisiana 70504, United States; Institute for Materials Research and Innovation, University of Louisiana at Lafayette, Lafayette, Louisiana 70504, United States;* orcid.org/0000-0002-6066-2634; Email: yuwang@louisiana.edu

Manyu Li − *Department of Psychology, University of Louisiana at Lafayette, Lafayette, Louisiana 70504, United States;* orcid.org/0000-0002-8324-5868; Email: manyu.li@louisiana.edu

Authors

Xiang-Sheng Wang − *Department of Mathematics, University of Louisiana at Lafayette, Lafayette, Louisiana 70504, United States*

Amanda Gildersleeve − *Department of Chemistry, University of Louisiana at Lafayette, Lafayette, Louisiana 70504, United States*

Nadia Turki − *Department of Chemistry, University of Louisiana at Lafayette, Lafayette, Louisiana 70504, United States*

Complete contact information is available at: https://pubs.acs.org/10.1021/acs.jchemed.2c01250

Notes

The authors declare no competing financial interest.

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