

Article

High School Biology Students Use of Visual Molecular Dynamics as an Authentic Tool for Learning About Modeling as a Professional Scientific Practice

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Abstract

Modeling is a practice of science that is underemphasized in biology classrooms in comparison to its central focus in the physical sciences. Visualizations of the submicroscopic world of molecules are becoming increasingly sophisticated with the evolution of new technologies. With this in mind, we introduced high school biology classrooms to a professional molecular modeling software program used by research biochemists to visualize proteins and other macromolecules. Analysis of surveys completed before and after the use of the program revealed significant student gains in their understandings of the nature of models. Student and teacher perceptions of the program showed an appreciation

for the real/authentic nature of the program, and its affordances when utilizing the three-dimensional rendering of proteins. The teachers did report a general level of frustration regarding their lack of experience with the program and their inability to unlock its full potential due to not being able to access all of the program's features. However, we believe that the evidence at hand indicates that the value of introducing students to authentic molecular modeling tools in high school science classrooms outweighs the potential limitations. © 2018 by The International Union of Biochemistry and Molecular Biology, 00:000–000, 2018..

Keywords: *molecular graphics and representations; molecular visualization; assessment of educational activities; computers in research and teaching; high school*

Introduction

Biological macromolecules are complex systems with intricate three-dimensional structures, which can be difficult for learners to visualize. In the high school science classroom, proteins are basically portrayed through textbook pictures, which limit the students' ability to observe and subsequently interpret and comprehend their three-dimensional characteristics. As a result, high school students who learn about protein structure and function in biology classrooms likely

struggle to visualize these molecules in three-dimensional terms. The ability to visualize and perhaps even perform mental maneuvering of proteins is essential for students to help them develop a sophisticated perspective of the relationship between molecular structure and function within the cell. Rather than merely talking about concepts or using simplified schematics and drawings to discuss complex molecular processes, high school science teachers can employ technological tools to model them in their classrooms. In particular, these programs can allow for students to rotate the molecule in three-dimensional space as well as to choose multiple representations for specific protein models. Especially with the increased ubiquity of technologies capable of running downloaded software in the secondary classroom, such a suggestion is far from impractical. Computer-based modeling is, therefore, not only useful for authentic biochemistry research but also in the biology classroom for the learning about protein structure and function.

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A stated goal of the Next Generation Science Standards that are currently guiding K-12 science instruction in much of the United States is to engage students in the actual methods used by professional scientists [1]. Modeling is one of these authentic practices employed by biochemists in particular, and the resulting models are one of many forms of scientific knowledge [2]. Various software programs have been developed over the last several decades to allow scientists to visualize structures of proteins that have been structurally characterized, for example, using X-ray crystallography. The reported three-dimensional structures of proteins can be visualized through these programs in a variety of ways. Different representations can highlight a variety of features of a particular protein's structure with the possibility of new discoveries and/or scientific understandings of that protein's function. Therefore, since scientists often construct and use models as they engage in scientific inquiry, this practice ought to extend to the science classroom [3].

Additionally, science educators have argued for "model-based scientific practices" as a means to explicitly teach about the nature of science in instructional settings [4]. This is important given that the empirical research confirms that both teachers and students often hold less than adequate conceptions of the nature of science [5]. By extension, when researching and learning about the nature of models, one would be simultaneously learning about broader ideas within the nature of science such as the uncertainty of scientific knowledge. Treagust, Chittleborough, and Mamiala [6] specifically identified five distinct factors related to the nature of models that ought to be understood by secondary science students. They are the changing nature of models, models as exact replicas, models as explanatory tools, models as multiple representations, and the uses of scientific models.

Much of the research into modeling in science education involves the use of models in physical sciences such as chemistry and physics [3, 7]. Coll and Lajium specifically identify a genuine need for additional research on the teaching and learning of modeling practices in life sciences to establish a firm empirical grounding for its importance in biology [3]. Modeling in chemistry is often divided into three levels; macroscopic, microscopic or submicroscopic, and symbolic [8, 9]. It is at the submicroscopic level where proteins are too small to be observed through microscopy [10] that the macromolecules of biochemistry could be modeled in the context of life science/biology education. While symbolic and molecular representations of simple molecules can be exhibited with physical molecular modeling kits, the modeling of macromolecules such as proteins are impractical without the use of computer-based molecular modeling software tools. These tools have been used in secondary classrooms to increase the authenticity of student involvement in the practice of modeling molecules [10, 11].

The above literature lays the framework for this study in which we propose to use an authentic professional

molecular modeling software program created by and for research biochemists in the context of a high school biology classroom; that classroom being an underserved population when it comes to participating in the scientific practice of modeling. One of our aims was to engage students in analyzing models through the use of a highly authentic tool with the goal of positively impacting their understandings of the nature of models. Another objective we had was to promote the interest of high school students regarding what exactly it is that professional biochemists use in their research. We hoped they would be excited by the prospect of using the same tool authentically employed by biochemists to model proteins.

Context for This Study

Two biology teachers in a large urban public high school in the southern United States agreed to participate with us in this project and additionally serve as coauthors on this manuscript. The lead author of this article is an assistant professor of science education. Through conversations with an assistant professor in chemistry who has a specialization in the molecular modeling of biochemical structures, and is an additional author of this report, we became aware of the availability of a free molecular visualization software program that the chemistry professor uses to model large macromolecules, mainly proteins, in his professional work. These two professors then went to the high school teachers and trained them on the use of the program: Visual Molecular Dynamics [12]. The program is used primarily as a tool for viewing and analyzing the results of molecular dynamics simulations. The teachers, in coordination with instructional technology personnel at their school, installed the software on school laptop computers. The teachers subsequently designed an activity (to be described below) that would engage their students in the use of the program. It should be noted that a version of this program has been used in high school biology and chemistry classrooms and was well received by the student participants [13].

We would be remiss not to explicitly address our rationale for choosing Visual Molecular Dynamics over a more user-friendly and high school appropriate molecular modeling software program such as Jmol [14] or Protopedia [15], which could have afforded similar opportunities for the visualization of proteins. The chief reason for our choice was we wanted to provide an opportunity for students to use the actual tools employed by professional biochemists and subsequently allow for a potentially more in-depth level of authentic involvement in the practices of science. It was important to us that the students were aware their work was not conducted by using a simulated tool designed for instructional purposes but instead was conducted using the professional software package. We do not mean to suggest that there is no place for these other visualization tools

in educational contexts, but rather just to emphasize that we wanted students to use a highly authentic modeling tool in this experience. Students, by retrieving a protein structure from a database and then rendering it through Visual Molecular Dynamics, would be performing some of the same tasks conducted by scientists in their work. In this case, the high school from which our population was drawn is a short distance from a research university, thus it would be motivating for the students to be working with a program that they knew that their local community uses. A comparison has been made between learning science and participating in athletic events that is useful in explaining the use of Visual Molecular Dynamics. Learning to play a sport would be rather dull if all one did was practice drills and memorize a rulebook without ever actually playing a game. Similarly, in science learning, we often have the students work with simple examples, rather than participate in genuine and authentic forms of scientific practice [16]. We were hoping to allow for a higher level of participation in the practice of modeling by using the software package we chose. We also wanted to examine both teacher and student attitudes and impressions about the use of the program to potentially explore different and perhaps more effective uses of it in the future.

In the teacher-developed activity, students (all biology students in grade nine or grade 10, 14–16 years of age) worked in small groups on an in-class project (one extended class period lasting approximately one and a half hours). They researched a genetic disease or disorder and the associated protein that is impacted by that condition. The students then searched the Protein Data Bank [17] to find and download a digital file of the protein that could be rendered in three-dimensions using the program. Students were encouraged to observe and manipulate/rotate multiple representations of the proteins they were investigating with the objective of them learning about the nature of models in general and protein structure in particular. The activity was conducted within a unit of instruction that centered on the biochemistry of proteins and was accompanied by discussions and videos that instructed the students about the role of X-ray crystallography in the development of these structures. Before this unit, to the knowledge of the classroom teachers, students had not participated in molecular modeling using computer software. The extent of the students' modeling experiences would have involved physical models of small molecules (e.g., H₂O). We believed that by students interacting with Visual Molecular Dynamics to visualize proteins they would develop more sophisticated understandings of critical aspects of modeling such as the need for multiple representations and that models are not exact replicas.

Figure 1 displays several different representations of the same protein rendered through the Visual Molecular Dynamics program. The protein structure shown in Fig. 1 is one of several crystal structures associated with the Huntington's

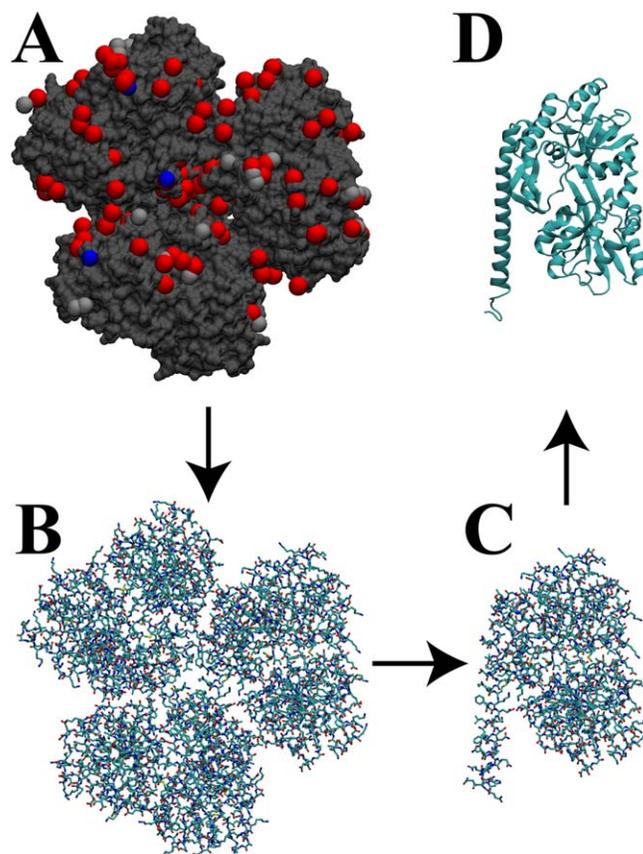


FIG 1

Model of Huntington protein's N-terminal region (Protein Data Bank entry: 4FEB) rendered through Visual Molecular Dynamics using different Selections and Drawing Methods. (a) Surface representation of the protein, water, zinc, and sodium. (b) Licorice representation of protein. (c) Licorice representation of one of the three protein chains. (d) Cartoon representation of the protein chain shown in b. Please confirm whether the color figures should be reproduced in color or black and white in the print version. If the color figures must be reproduced in color in the print version, please fill the color charge form immediately and return to Production Editor. Or else, the color figures for your article will appear in color in the online version only. [Color figure can be viewed at wileyonlinelibrary.com]

disease that has been deposited in the Protein Data Bank. Huntington's disease was one of 12 illnesses caused by "altered or missing proteins" that students could have selected to model.

Method

The following research questions guided this investigation:

1. How do students' perceptions of models change after instruction that includes the use of a professional molecular modeling software program?



TABLE I

Results of t-test analysis of prepost surveys reported by aspect of the nature of models

	<i>Pre avg</i>	<i>Post avg</i>	<i>p-Value</i>	<i>Cohen's d</i>
Changing nature of models	4.08	4.23	0.022 ^a	0.24
Models as exact replicas	2.73	2.62	0.133	-0.15
Models as explanatory tools	4.20	4.32	0.050 ^a	0.23
Models as multiple representations	3.77	3.95	0.001 ^a	0.34
Use of scientific models	3.77	3.91	0.011 ^a	0.24

Note: n = 115; a score of 5 on any aspect represents an informed perspective.

^aSignificant at the 0.05 level.

2. What are the perceptions of students and teachers regarding the use of the molecular modeling software program?

We used a survey, created by Treagust et al., before and after the instructional use of the program to investigate any changes in understandings of the nature of models in science [6]. The survey is a Likert scale instrument consisting of a series of statements about models and their uses in science (Appendix). Each of these statements is aimed at measuring understandings of one of the five aspects of the nature of models that we previously described. The pre-survey was administered approximately one month before the instructional use of the program, and the post-survey was administered nearly two months after its use in the curriculum. The rationale for this was that we could potentially make claims regarding the persistence of changed views on the nature of models over time. The limitation to this approach is that a variety of classroom influences in addition to the use of the specific software program could have played a role in the development of students' understandings of models. To accommodate for this limitation, we specifically asked students on the post-survey, through an open-ended free response item, to tell us if they believed that they learned anything about models specifically as a result of using the Visual Molecular Dynamics software.

We analyzed the survey according to the procedures employed by Gobert et al. [18] in their research of students' understandings of scientific models. Each item was scored on a scale from one to five. A score of one corresponded with strongly disagreeing with a given statement, and a score of five corresponded with strongly agreeing with a given statement on the survey. Scores in between these values corresponded with more moderate levels of agreement or disagreement. For all but one of the aspects of the nature of models (models as exact replicas), agreeing with the statements (a score of five) demonstrated a

sophisticated understanding of the nature of models. For analysis, student scores were reversed for the items for this particular aspect to indicate the same score of five for an informed response that would have been indicated for the other aspects. The paired sample *t*-test was chosen to analyze the survey data since there was a pre- and post-survey and the students' two surveys could be matched. The paired sample *t*-test allows for an analysis of the differences between the two measures. A *p*-value of <0.05 is considered to be significant at the 95% confidence level. This indicates that there is a significant chance (95%) that two means are different. The population of students (within multiple biology classes taught by two different teachers) that completed both the pre- and the post-survey, participated in the activity, and turned in all Institutional Review Board consent forms numbered 115.

In addition to the survey, we observed the classroom use of the Visual Molecular Dynamics program in one of each of the teachers' classes, interviewed both of the teachers about their perceptions of the program, and interviewed three students about their opinions of the program. These interviews were conducted at the end of the school year, some months after the use of the program. Interviews were analyzed according to methods of naturalistic inquiry employing a form of constant comparative analysis [19]. Field notes from observations were used to give us further confidence regarding the emergent findings from our interview analysis.

Findings

Table I displays the results of the paired samples *t*-test. Overall, student understandings of four of the five aspects of the nature of models increased pre to post and did so significantly based on an analysis of the survey as can be seen from the difference in means. Understandings of one of the

aspects (models as exact replicas) decreased from pre to post, but not by a significant degree. Models as exact replicas also happened to be the aspect that students understood the least before working with the Visual Molecular Dynamics program. While the differences between mean scores on the survey may have been significant, the magnitude of those differences, as can be seen from the Cohen's *d* effect size, were small. Though these effect sizes were small, they were not so meaningless as to ignore the significant changes in understandings of the nature of models from pre to post [20]. We do want to note that the aspects of the nature of models (models as exact replicas, models as multiple representations, use of scientific models) that were most difficult for students to grasp before using the program were still the most difficult for them to understand afterwards. However, students' understandings of these (models as multiple representations and the use of scientific models) did significantly increase from pre to post.

Of the two biology teachers, both had some positive things to say about the use of the Visual Molecular Dynamics program in their classrooms. Mr. Kaminski told us, "Having the actual tool there might have lit a couple sparks." Additionally, he recognized that the activity allowed him to engage his students in modeling practices and that "modeling in biology and biochemistry is super important from a teacher perspective." Mrs. Stocker similarly found some benefits from the use of the program. Her positive perspective centered primarily on the realism that was allowed through the use of the program. "[The] biggest benefit of the program is that they were able to get more of a realistic picture in their head of what it looks like."

The teachers' chief complaint with the program dealt with the challenges of using it being that its intended purpose was as a professional tool rather than as an educational one. Mr. Kaminski said, "I would do it again [use the Visual Molecular Dynamics program] if we could add a little more of the functions and features. I feel like there is so much more to do with it." Mrs. Stocker told us that she "would have liked to have the ability to give them more guidance." The complicated and multifaceted nature of the program resulted in her feeling unable to help her students as much as she would have preferred. "That program has so many features that even for me, I wasn't familiar with even a fraction of what it is capable of."

The students overall had a positive perception of the use of the Visual Molecular Dynamics program in their classroom. Approximately 70% of the student participants identified on the post-survey free-response item that they had learned something about models and modeling as a result of using the Visual Molecular Dynamics program in particular. For example, one student wrote, "the impact that my interactions with [the] molecular modeling software [had] is that it let me understand that there may be more than one model of an object/process." Approximately 18% of the students thought that they had not benefited

from the use of the program. Their chief complaint was related to the complications of using a professional tool not designed for use in high school science classrooms. "I think it was a bit overkill for high school. Like I love technology and programming, but this is too complicated" (student post-survey written response). Indeed, as we observed the classrooms using the program, we noted some challenges that students were having, mainly when it came to viewing multiple representations of their selected program. At the same time, however, students were engaged and were discussing with each other various features of the proteins as they rotated them and viewed them from many angles and with multiple representations.

In the student interviews, the three students we interviewed had some positive things to say about using the program. One of the notable things evident was that they tended to appreciate what the computer program allowed them to do that otherwise would not have been possible using physical models. One student said, "in the previous year we built the elements with the sticks and balls. In a physical science class... it would have taken a much longer time to do if you did it by hand. They were so big; it would take a long time to get everything right." Other students were impressed that they were using the same tool used by a professional scientist, rather than some simplified program designed for high school use. "Mrs. Stocker explained it. That it was something that people on campus [professional research scientists on the University campus in town] were using too... It gives it more a sense of this is real. People are actually using it". Another student said, "If I am able to understand... most parts that are used by professionals then I think it can be used in a high school setting... And it is really cool that we actually got to use it because it is like hey we did this, and we are only 9th and tenth graders in class". These positive feelings were supported by the overall level of student engagement and excitement that we observed during the classroom use of the Visual Molecular Dynamics program. A few interesting comments overheard during these observations were "this is like the Dewey decimal system of proteins" and "this program makes me feel like a hacker."

Conclusions

While we observed significant positive changes pre to post in the students' understandings of the nature of models, it is not possible for us to say with certainty that this was a direct result of the use of the Visual Molecular Dynamics program and not some other factor within the teachers' classroom instruction. Both students and teachers had an overall appreciation for the program and understood that they were using an authentic tool to model complex macromolecules that has rarely been used in a high school classroom, and certainly not in their own. The only teacher complaint was an expressed desire to understand and be



able to use more of the capabilities of the program. We are encouraged by this level of enthusiasm and hope to develop more user-friendly instructional materials to support the use of the Visual Molecular Dynamics program in high school settings to unlock the potentials of the program fully. In this first foray into using this program in this specific context, we found more positive impacts and impressions than not and hope to continue to collaborate with these teachers to bring even more authentic uses of the program (such as simulations of protein functions i.e., membrane transport) into their classrooms.

In summary, the students developed a more sophisticated understandings of models during an instructional unit on proteins that employed the use of an authentic modeling tool. The potential for using this program in other high school science classrooms and investigating its impact is substantial especially given the general level of interest in technology that diverse groups of high school students share. Importantly, this research demonstrates that highly authentic molecular modeling software programs can be used to some effect within high school biology classrooms. We encourage high school biology teachers to foster dialogue with professional scientists and to come up with creative ways to engage their students with practices that are closely similar to those that scientists participate in on a recurring basis.

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Appendix

Students' Understandings of Models in Science (SUMS) post-survey [6]

Students selected from the following options for each item: Strongly Disagree, Disagree, Don't Know, Agree, and Strongly Agree.

1. A model is a smaller sized version of an object.
2. Models show ideas.
3. Models are used to make predictions about a scientific object or process.
4. Models show the relationship between ideas.
5. Models are used to test theories about a scientific object or process.
6. A model may be changed if there are new ideas about a scientific object or process.
7. Models are used to help formulate ideas about a scientific object or process.
8. More than one model is used to represent different versions of an object/process.
9. A model may be changed if there are new findings about a scientific object or process.
10. Models are used to explain a scientific object or process.
11. A model may be changed if there are new theories about a scientific object or process.
12. A model is similar to the real thing in every way except for size.

13. Models are used to physically or visually represent something.
14. More than one model is used to show different perspectives about an object/process.
15. A model shows what the real thing looks like.
16. A model has what is needed to show or explain a scientific object/process.
17. More than one model is used to show different sides or features of an object/process.
18. Models are used to test predictions about a scientific object or process.
19. A model is an exact replica of the real thing.
20. There may be more than one model for an object/process because different people may have different perspectives on what it looks like or how it works.
21. A model may be changed if new technology allows us to discover new evidence about an object/process.
22. More than one model may be used if different people interpret the data/evidence in different ways.
23. Briefly describe the impact that you think your interactions with the molecular modeling software had on your responses to these items. Use another sheet of paper if necessary and attach it to this survey.