Computerized Molecular Modeling as Means for Enhancing Students' Understanding of Protein Structure and Function

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Abstract

Computerized molecular models (CMM) and computerized visualization of chemical processes are powerful tools for manipulating and predicting molecular spatial structures. These capabilities opened the way for advanced research in chemistry as well as advanced instructional methods for teaching and learning. Our presentation focuses on a new biochemistry learning unit that aimed at promoting in-depth understanding of 3D structure and function of proteins and nucleic acids, via CMM. Our goal was to examine whether, and to what extent, learning via CMM affect students' understanding of biochemistry and their ability to transfer across the four levels of chemistry understanding: microscopic, macroscopic, symbolic and process. The research population included 234 grade 12 students from Jewish, Arab and Druze sectors, divided into three comparative groups: (a) traditional curriculum without the use of CMM, (b) new curriculum with student's hands-on practice of CMM, (c) new curriculum with teacher's demonstrations of CMM. The research included also five chemistry teachers who integrated CMM as part of their teaching. In our talk we will present the research findings and discuss the benefits and barriers of CMM and visualization in the context of high school teaching and learning.

Keywords: Computerized molecular models, chemical education, spatial structures, visualization.

Introduction

Recent research on technology-enhanced instruction identified the need for providing learners with knowledge representation tools (Barak, Harward & Lerman, 2007; Jackson, Krajcik, & Soloway, 2000) and inquiry experience (Linn, Davis, & Bell, 2004, Songer, Lee, & Kam, 2002). Technology can provide tools that enable students to manipulate representations of spatial structures. Enabling 3D manipulation is one of many design principles that emphasize making scientific phenomena visible (Kali, 2006). Visualizations of spatial structures can enable students to rotate objects being studied and thus view them from various directions (Barak & Dori, 2005; Hsi, Linn & Bell, 1997).

Chemistry understanding relies on making sense of the invisible and untouchable. A good understanding of chemistry requires the ability to navigate properly between four levels of understanding: macroscopic, microscopic, symbolic and process levels (Dori & Hameiri, 2003; Dori, Barak & Adir, 2003). However, research has shown that many students find it difficult to properly link between the different levels of understanding (Gable, 1998; Dori & Barak, 2001; Chandrasegaran, et al., 2007). These difficulties, combined with difficulties in understanding the spatial structures of molecules, obstruct students' ability to solve questions and problems in chemistry (Gabel, 1998; Coll & Treagust, 2003). The use of computerized molecular models (CMM) provides a solution to these problems. Indeed, research has shown that visual aids and the use of CMM may enhance students' chemical understanding and spatial ability (Barak & Dori, 2005; Williamson & Abraham, 1995).

In light of the importance of integrating visualization tools and connecting the learning material to students' daily living experiences, the Chemistry Committee of the Israeli Ministry of Education initiated in 2003, a reform in high school chemistry curriculum. As result, new learning units were developed, introducing inquiry-based leaning, interdisciplinary connections, and the use of advanced technologies such as computer-based laboratories and CMM. One of the novel learning units is: "*Biochemistry: the Chemistry of Proteins and Nucleic Acids*". The learning unit aimed at deepening students' understanding of chemical processes within the context of the human body. The uniqueness of this learning unit lies in its interdisciplinary approach and the use of CMM for illustration of biopolymers' structure and function.

The goal of this research was threefold. First goal was to examine whether learning biochemistry via CMM affects students' conceptual understanding and their ability to transfer across the four levels of chemistry understanding. Second goal was to examine students' learning process as they carried out the CMM assignments. Third goal was to examine technology-enhanced instruction, in the eyes of the teachers.

Research Design and Procedure

The research participants included a representative sample of 234 grade twelve students from Jewish, Arab and Druze sectors. All research participants studied proteins for their matriculation examination. They were divided into three groups: (a) traditional curriculum without the use of CMM (N=85), (b) new curriculum with student's hands-on practice of CMM (N=52), (c) new curriculum with teacher's demonstrations of CMM (N=97). The research included also five chemistry teachers who integrated CMM as part of their teaching. All of the teachers had more than 10 years experience in teaching chemistry.

Different CMM applications, free on the Internet were used as platforms for the students' activities. Specially designed assignment (written in Hebrew or Arabic) encouraged students to manipulate 3D molecular models of amino acids, proteins, DNA, and RNA. The students responded to questions focusing on connections between a molecule's 3D structure and its function in the human body.

The 'mixed methods research' model (Johnston & Onwuegbuzie, 2004) was employed by using both quantitative and qualitative methodologies in the analysis and interpretation of data. The research included three research tools: special designed pre- post-questionnaires, class observations, and semi-structured interviews. The questionnaires were designed for indicating students' conceptual understanding and their ability to transfer across the four levels of chemistry understanding. They were administrated to the students before and after they studied *Proteins* either by using traditional, teacher-centered, handbook-based curriculum, or by using the new biochemistry curriculum via CMM. The quantitative data were analyzed using GLM statistical procedures, paired sample t-tests and ANCOVA tests, to compare between the research groups.

Class observations were conducted in order to examine students' behavior while engaged in CMM activities. The class observations were conducted once a week, in a computer laboratory, focusing on students' reaction to the use of CMM and their interactions with their peers. The data was collected by using a researcher logbook, documenting special events and students discussions. Semi-structured interviews were conducted among chemistry teachers who integrated CMM in order to learn about their opinion on the new curriculum. The teachers were interviewed once, after they completed teaching the learning unit. Each interview was about 30-40 minutes long, documented in researcher logbooks. The qualitative data were gradually analyzed from a constructivist and interpretative perspective. The data from the researchers' logbooks were read, reread, and analyzed by three experts in science education. Only then, the data was collaboratively categorized establishing 100% consent among researchers.

Findings

Mean scores and standard deviations of the pre-and post-questionnaires, by research groups are presented in Table 1.

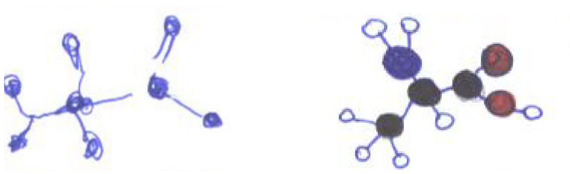
Table 1. Mean scores and standard deviations of pre-and post-questionnaires, by research groups

Research group	N	Pre		Post	
		Mean*	SD	Mean*	SD
Biochemistry learning via hands-on CMM	52	4.79	1.98	6.08	2.23
Biochemistry learning via teacher's demonstration of CMM	97	4.00	1.47	5.09	2.13
Traditional learning without CMM	85	4.55	1.60	4.60	2.25

* The mean score was calculated out of 10 points.

Table 1 shows that students who belonged to the 'biochemistry learning via hands-on CMM' group achieved the highest mean scores on the post-questionnaire. ANCOVA test comparing between groups indicated statistically significant difference ($F_{(2,154)}=25.56$, $p<0.01$). Post Hoc Sidak test showed that the post-questionnaire mean score of the 'traditional learning' group was lower than that of the other two research groups. Meaning that learning biochemistry via CMM improved students' conceptual understanding and ability to transfer across the foul levels of chemistry understanding.

Analysis of students' drawings of amino acids (as part of their post-questionnaire) showed that those who studied biochemistry via CMM drew more accurate representations (Figure 1).



(a) *(b)*

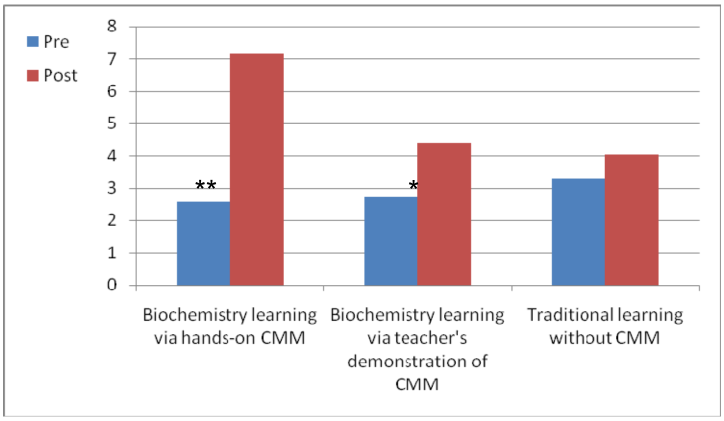
Figure 1. Drawings of Alanine molecule by: a) a student that was not exposed to CMM b) a student that used CMM as part of her learning

Findings indicated that students who experienced hands-on CMM, their drawings were scientifically correct (no atoms were missing), they had a 3D perspective (using angles and shadows for illustration), and they differentiated atoms by colors and/or proportional dimensions. Examples for students' answers to one of the questions that examined their conceptual understanding are presented in Table 2.

Table 2. Examples for students' answers about the amphoteric properties of amino acids

Students' answers Amino acids are amphoteric substances because:	Score	Levels of chemistry understanding
*They **can react both as acids and basis**. Amino acids have an amino group (-NH2) that may attract a proton (H +) due to a pair of non-bounding electrons on the nitrogen atom, thus acting as a base. They also have a carboxylic group (-COOH) that may release a proton, thus acting as an acid.*	10	**Macro**, Micro, Symbol and Process
They consists of both an amino group *(-NH2) and a carboxylic group (-COOH).*	5	Micro, Symbol
They consist of a hydrophilic group and a hydrophobic group.	0	-

Pre- post-questionnaire mean scores of students' conceptual understanding are presented in Figure 2. Paired t-test showed statistically significant difference between pre- and post-scores for students who studied biochemistry via CMM either by hands-on manipulation or teacher's demonstration.



*p<0.05 ** p<0.01

Figure 2. Students' scores of 'conceptual understanding' in the pre- and post-questionnaires

The analysis of class observations revealed five major claims. Data suggests that CMM-enhanced learning may:

a) Enable personal and close relationships among the students and between them and their teacher.
b) Encourage learning strategies such as question posing, conceptualization and reflection.
c) Advance students' ability to transfer the four level of chemistry understanding.
d) Enable the understanding that CMM serve as knowledge representation tools and, if used properly, may assist in "figuring things out".
e) Enable a pleasant, relaxed, and informal learning climate.

The analysis of teachers' interviews presented positive opinions regarding the integration of CMM, indicating that CMM assisted students in understanding abstract chemical concepts, in enhancing their ability to transfer across the levels of chemistry understanding, and in promoting motivation to learn chemistry. However, they also presented some concerns about CMM usability and accessibility, and the time allocated for such activities.

Conclusions

Successful technology-enhanced instruction often takes advantage of models, simulations, or visualizations to introduce new ideas (Barak & Dori, 2005; Hsi, Linn, & Bell, 1997). Based on this idea, the novice biochemistry learning unit introduced technology-enhanced learning via CMM manipulation. In accordance to previous studies, our study strengthens the claim that CMM is an effective tool for representing complex molecular structures and enhancing students' conceptual understanding and learning achievements (Barak & Dori, 2005; Williamson & Abraham, 1995).

The integration of CMM as part of the students' learning environment enhanced students' ability to transfer across the four levels of chemistry understanding, and improved their understanding of biochemical molecules, their spatial structure, and function. It is important to note that although the results of the students who were exposed to CMM via teacher's demonstration improved (relative to their peers in the traditional classrooms) their scores were lower than those of the students who actively manipulated CMM. Our findings suggest that an effort should be made to allow individual use of CMM, even if the school lacks resources.

The presented research is innovative in embedding knowledge representation tools, i.e., CMM enabling 3D manipulation, within technology-enhanced instruction of biochemistry. The new curriculum, as oppose to traditional teacher-centered curriculum, adopts the 'investigative-approach' to biochemistry studies. In addition, the research is unique in its interdisciplinary nature, focusing on students' conceptual understanding, both from the chemical and biological aspects. Our study contributes to the body of knowledge on CMM usage as knowledge representation tools (Jackson, Krajcik, & Soloway, 2000) for teaching and learning.

In our talk we will present the research findings and discuss the benefits and barriers of integrating CMM into the context of biochemistry learning. We will also present instructional strategies and lessons-to-learn from the students and teachers perspectives.

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