A Usability Study of an Interactive Auditory Display for Supporting Learning of Molecular Structure

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Abstract: Some students have difficulty analyzing physio-chemical properties of molecular structures from molecular models. This analysis has been highly visual, posing some challenges such as occlusion. Auditory display techniques, especially earcons (using musical sounds that represent meaningful information) have been positively used for supporting the analysis and learning of molecular information. We developed earcons that represent the molecular property of hydrophobicity from amino acids (the building blocks of molecules such as proteins) for supporting molecular analysis, along with the visualization of a molecular model. The insulin molecule was used as a test bed due to its suitability for educational purposes. In a preliminary user study, undergraduate students evaluated the usability of the earcons. We found that the sounds efficiently and effectively mapped the phobicity molecular property, and participants perceived the sounds as pleasant and melodic. This was useful for complementing the visualization of insulin's molecular structure.

Introduction

Chemistry and biology students often have hard time learning and analyzing molecular structures. A molecule can be defined as a group of two or more atoms joined by covalent bonds together, representing the smallest unit of a chemical compound. Organic molecules such as amino acids (the "building blocks" of proteins, which are larger molecules) are very important in chemical reactions of living organisms (Hart et al., 2011). Over the past decades, molecular analysis has been highly visual, posing some challenges such as students reaching a proper spatial perception of molecular structures (Zurn, Piotto & Nesper, 2003). Other difficulties arise regarding students' reasoning about the extremely small size and scale of molecular structures in real life, and other difficulties related to interactions of complex molecular systems, where some students are unable to discriminate important molecular information and recognize patterns and relationships among parts of a molecular structure (Tibell & Rundgren, 2010).

Students generally learn molecular structure using physical models made of plastic and other materials, and utilize molecular visualization software with mixed results. Both types of didactic materials present advantages, such as portability and easy manipulation and support for understanding molecular interactions. However, some of those didactic materials and software present some disadvantages, where students cannot properly visualize some molecular parts occluded by their complex structure (Dori & Barak, 2001). In addition, students have difficulties mastering different molecular diagramming representations (Stull, Gainer, Padalkar & Hegarty, 2016).

Scientific sonification (the application of non-speech sound to represent and convey meaningful scientific information) has been used to support analysis of complex data that can be difficult to perceive and understand using visualization alone (Supper, 2012). Sonification takes advantage of the human ear to detect temporal and spatial changes and patterns, relying on audio properties such as pitch, amplitude and rhythm for analyzing and understanding information (Hermann & Hunt, 2011). Another auditory display technique that also relies on auditory properties for representing information is called earcons. Earcons are abstract non-speech messages representing useful data, composed of one or more musical notes called motives. Because earcons do not have a semantic association to the data being represented, their mappings must be learned before using them. One of the earcons' advantages is that they sound melodic and also may sound pleasant the the listener (Hermann & Hunt, 2011). Earcons can be used as mnemonics for memorizing and learning pieces of information. Sonification, earcons and other auditory display techniques can be useful for supporting scientific visualization, helping students with auditory learning style and visually-impaired students by complementing molecular visualization (Garcia-Ruiz & Gutierrez-Pulido, 2006).

The objective of this paper is to describe a preliminary user study on testing an interactive molecular visualization model with auditory display to support learning of amino acid properties. Our research question is as follows: Can earcons (musical motives) be usable enough for complementing interactive molecular visualization? Nielsen (2012) defines usability as a quality attribute that analyzes how efficient, effective and pleasant to use a computer interface is (our molecular visualization software+interactive auditory display). Previous studies such as MacFarlane et al. (2005) found that computer software with high usability facilitates learning. In addition, highly usable educational software should not hinder students' intrinsic motivation (Safadel & White, 2018).

Related Work

Auditory display techniques such as sonification and earcons have been studied as human-computer interactions for supporting molecular analysis for some decades. An early example was done by Hayashi & Munakata (1984), using a computerized system assigning musical notes with different pitches to the four bases (A, C, G and T) that form the DNA molecule (it contains instructions needed by living organisms to develop, reproduce and live) based on their thermal stability data. The researchers found that their musical auditory display helped them to uncover the meaning of specific DNA sequences, and also helping them remembering particular DNA patterns easier. A related application is Project Muse conducted by Dunn & Clark (1999), where they created an artistic rendition of data sonification of the DNA molecule sequences. Ballweg, Bronowska & Vickers (2016) developed a computer program for the sonification of macromolecules using spatialized sound (a sound-rendering technique that simulates playing the sound source in 3D). The researchers conducted a user study where participants successfully perceived feedback sounds while interacted with a molecular visualization software while docking molecular drug compounds. Olson (2018) considered the importance of sonification of molecular structure as an important support of molecular visualization of ever-complex molecular structures.

Non-speech sounds have been also studied for supporting learning of molecular information. Garcia-Ruiz & Gutierrez-Pulido (2006) reviewed a comprehensive list of research projects and applications of molecular audifications with educational purposes. For example, Miner & Della Villa (1997), along with their students, made computerized musical compositions mapping musical notes from instruments such as a harp and a saxophone onto the sequences of the four DNA bases. The researchers found that many of their students found the compositions melodic and were motivated to learn about DNA molecule. Garcia-Ruiz (2001) mapped musical notes (earcons) and sound effects of water (also called auditory icons) to the physical property of hydrophobicity of amino acids. A brief user study with university students found that many of them could identify the right amino acid when playing its respective audification. Larsen (2016) developed an algorithm to make musical compositions loosely inspired in jazz genre, based on sonifications of large datasets of microbial DNA. University students applied his algorithm to generate musical compositions based on human gut microbiome data and had their compositions performed by a choir composed of primary school students. Larsen pointed out that "biology educators can sonify complex data in a fun and interactive format, making it easier to communicate both the importance and the excitement of exploring the planet earth's largest ecosystem" (p. 129). A recent project was focused on sonification of biochemical structures intended for blind students, with positive results (Arce & McMullen, 2017).

Motivation

Our motivation in pursuing auditory display of molecular information is that previous audification/sonification research has been positively conducted in the sciences, and in particular for helping understanding physio-chemical phenomena. This can support learning of molecular structure, leveraging the human sense of hearing, including musical properties for enhancing intrinsic motivation and curiosity of students.

Materials and Methods

We used the molecular model visualization tool PyMOL(TM) (PyMOL, 2019) for displaying the molecular model of human insulin (a molecule that the human body utilizes for regulating blood glucose levels). We chose this molecule because it is considered useful for educational purposes (PDB-101, 2001). The molecular model of human insulin was obtained from Insulin (2019) and was opened in PyMOL. PyMOL has been used for teaching molecular structure with success (e.g. Rigsby & Parker, 2016). The first author developed a script in Python programming language that identified which amino acid the student is selecting with the computer mouse from the molecular model displayed on PyMOL. Then, the program played the earcon that was mapped onto the selected amino acid and the program visually displayed the selected amino acid. The earcons' musical notes represented the selected amino acids' type of hydrophobicity, that is, how soluble an amino acid is in water (Sigma-Aldrich, 2019). Tab. 1 shows the mappings. The Musical Instrument Digital Interface (MIDI) protocol format was used to pre-record the earcons. They were made with four different musical instruments (percussion, string and woodwind) to ease hydrophobic groups' identification. Each earcon was made of 3 musical notes played at different pitches to make them more melodic. Each earcon was recorded at 60 beats per minute (BPM) with a duration of approximately 1.8 seconds.

Hydrophobicity type:	Earcon's musical instrument:	Musical notes:	Amino acids:
very hydrophobic	vibraphone	F#5, G5, G#5 (ascending notes)	Leu, Ile, Phe, Trp, Val, Met
hydrophobic	xylophone	D#5, E5, F5 (ascending notes)	Cys, Tyr, Ala
neutral	acoustic grand piano	C4,C4,C4 (equal notes)	Thr, Glu, Gly, Ser, Gln, Asp
hydrophilic	flute	G#5,G5,F#5 (descending notes)	Arg, Lys, Asn, His, Pro

Table 1: Mappings of earcons and amino acids (Sigma-Aldrich, 2019).

Fig. 1 shows PyMOL displaying the molecular model of insulin. An amino acid was selected with the mouse and its corresponding earcon was played.

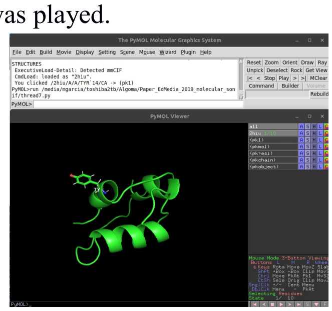

Figure 1: The molecular model of insulin showing a selected amino acid (encircled).

PyMOL and the earcons were displayed on a gaming laptop with a 13.3-inch screen running Linux Ubuntu O.S. version 18.10.

Study Participants

Eight computer science undergraduate students (7 males and 1 female, with an age average of 20 years old) participated in our test. They were recruited using a hallway testing set-up (we invited students passing by the hallway to evaluate our system). Only three students reported learned molecular biology or related areas in previous courses, but they did not recall the hydrophobicity property, used in our testing.

Procedure

First, participants were explained our study purpose and the mappings between the earcons and the amino acids' hydrophobicity types (shown in Tab. 1). Participants listened to the earcons through Sennheiser headphones (model HD 428). This was considered as a training session. Then, participants tested the usability of our earcons played along the visualization of the insulin molecular model on PyMOL. The participant's task was to select with the mouse any amino acid of the insulin molecular model and to identify the hydrophobicity type of the selected amino acid according to its corresponding earcon that was played. The participants were asked to select four different amino acids from the molecular model. After the testing, participants filled out the System Usability Scale (SUS) questionnaire (Brooke, 1996), a software industry standard instrument that evaluates the usability of an interactive digital product, and it is scored with a value from 0 (very bad usability) to 100 (excellent usability), and has ten Likert scales. It is shown in Tab. 2.

1. I think I would like to use this molecular audification frequently	Strongly disagree (1)...Strongly agree (5)__
2. I found the molecular audification unnecessarily complex.	Strongly disagree (1)...Strongly agree (5)__
3. I thought the molecular audification was easy to use.	Strongly disagree (1)...Strongly agree (5)__
4. I think I would need the support of a technical person to be able to use this molecular audification.	Strongly disagree (1)...Strongly agree (5)__
5. I found the various functions in this molecular audification were well integrated.	Strongly disagree (1)...Strongly agree (5)__
6. I thought there was too much inconsistency in this molecular audification.	Strongly disagree (1)...Strongly agree (5)__
7. I would imagine that most people would learn how to use this molecular audification very quickly.	Strongly disagree (1)...Strongly agree (5)__
8. I found the molecular audification very cumbersome (complicated) to use.	Strongly disagree (1)...Strongly agree (5)__
9. I felt very confident using the molecular audification.	Strongly disagree (1)...Strongly agree (5)__
10. I needed to learn a lot of things before I could get going with this molecular audification.	Strongly disagree (1)...Strongly agree (5)__

Table 2: The SUS questionnaire.

Fig. 2 shows a student interacting with PyMOL and listening to the earcons.

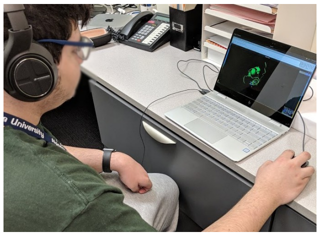

Figure 2: A student testing the molecular visualization + audification.

Results

Fig. 3 shows the median of each of the SUS questionnaires' Likert scales.

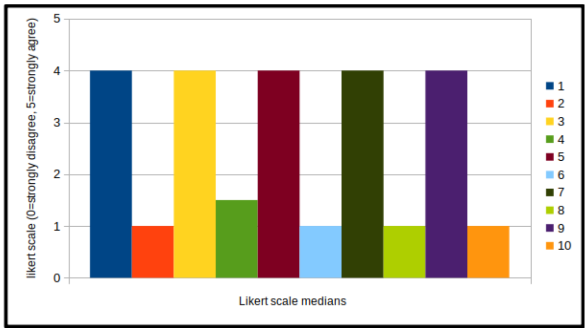

Figure 3: Medians of the ten SUS questionnaire's Likert scales.

The SUS questionnaires filled out by the students were scored according to Brooke (1996), where a usability score was obtained (0=very bad usability, 100=excellent usability). The average of the usability scores from the SUS questionnaires filled out by the eight students was 81.75, which is deemed as high (Sauro, 2011). About 85% of the students correctly identified the mappings between the earcons and the phobicity types. These results are by no means definitive. More research is needed regarding the usability of the earcons, for example, testing the earcons with more biology undergraduates.

Conclusions

This brief test indicated that the designed earcons can be useful for representing a type of physio-chemical property along the interactive visualization of a complex molecular model such as insulin. It seems that the earcons positively complemented the molecular visualization of each amino acid from the molecular model of insulin, freeing up the students' visual channel. However, we will need to confirm this in further tests. This evaluation is in line with our previous findings on positively representing molecular data with earcons described in Garcia-Ruiz (2001). Our Python program can be customized for the audification of any molecular model that contains amino acids making it versatile, and can be adapted according to the needs of molecular biology educators and students. In a future study, we will play spatialized earcons (sound sources played in 3D) to see if this will support identification of the 3D position of amino acids. Future work includes the preparation of chemistry/biology in-class activities with biology educators integrating our audifications and molecular model visualizations.

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