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CHEMISTRY TEACHERS' AWARENESS, UNDERSTANDING, AND CONFIDENCE TOWARD COMPUTATIONAL TOOLS FOR MOLECULAR VISUALIZATION

F. Z. Saudale*[1], R. I. Lerrick[2], A. A. Parikesit[3], F. Mariti[4,5]

[1,2]Department of Chemistry, Faculty of Science and Engineering, University of Nusa Cendana, Kupang, Eastern Nusa Tenggara, 85001
[3]Department of Bioinformatics, School of Life Sciences, Indonesia International Institute for Life Sciences, Pulomas, Eastern Jakarta, 13210
[4]Public High School 8, Alak, Kupang, Eastern Nusa Tenggara, 85231
[5]High School Teacher Organization for Chemistry Subject (MGMP), Kupang, Eastern Nusa Tenggara

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ABSTRACT

Recent advances in cheminformatics and bioinformatics research have generated software and computational tools for molecular modeling and visualization that can be incorporated to improve chemistry teaching and learning in high school. Nevertheless, there have never been any study simultaneously reporting chemistry teachers' awareness, understanding, and confidence toward contemporary computer-aided molecular modeling and visualization tools. This study examined 32 high school chemistry teachers' knowledge, understanding and confidence toward nine new computational programs on molecular modeling and visualization namely ChemDraw, HyperChem, UCSF Chimera, Marvin Sketch, PsiPred, MBC (PS2), Rampage, Vienna RNA Package and Mode RNA following two days of professional workshop-based training. After completing the training and assessments, the teachers showed an enhancement in awareness, understanding, and confidence toward those nine computational programs. Intensive activities consisting of theoretical lectures, hands-on practices, assignments, and case study presentations seem to provide valuable resources to the increase in teachers' knowledge, understanding, and skill that incorporates computational technology. Hence, the impact of this research pointed toward the value of teachers' professional development that creates a platform to reduce the barriers of access, resources, knowledge, and skills. This study is expected to help improving teachers' awareness, understanding, and confidence necessarily required for further implementation of available technology for instructional purposes.

Keywords: chemistry, computational, modeling, teacher, visualization

INTRODUCTION

Digitalization and the internet of things (IoT)-based technologies have become the driving force of industrial revolution 4.0 that has a profound impact not only in the social endeavor and economic life but also in the education community (Puncreobutr, 2016; Schwab, 2016). The science education system has adopted contemporary technology tools and computational platforms to improve the quality of teaching, learning, and assessment (Neumann & Waight, 2019). The last two decades demonstrate the use of specialized learning software applications

*Correspondence Address
E-mail: fredy_saudale@staf.undana.ac.id

that have been expanded and integrated, ranging from interactive visualization to computational modeling tools and e-learning media in science teaching and learning environment (Krajcik & Mun, 2014). This progress is also facilitated by the characteristics of elementary to high school students in this millennial era, known as digital natives, who are already very familiar with digital modes such as smartphones, iPads, or devices connected to the Internet (Keengwe & Georgina, 2013). This digital ecology and technology have tremendous potentials to transform science teaching and learning to be more attractive, interactive and personal, supporting the recent campaign on integrating computational thinking in education and promoting digital as well as visual literacy of science (Bucchi & Saracino, 2016; García-Peñalvo & Mendes, 2018; Jarrahi et al., 2019).

In science education, computational modeling, simulation, and dynamic visualization are among the emergent technologies that have been applied in teaching and learning (Oliveira et al., 2019). Computational and internet-based digital learning modes that display interactive models and dynamic visualization have been reported to increase students' understanding and learning (Chang, 2013). The strength of computational modeling is its effectiveness to concretize, simplify, and visualize abstract concepts and phenomena that cannot be visually observed through experiments and are limited to be explained by teaching or textbooks (Smetana & Bell, 2012). Thus, molecular modeling in science education can be an enabler for students' mental transformation from two-dimensional (2D) to three-dimensional (3D) representation (Stieff, 2017). Another important value of modeling and models in science education is its contribution to the formation of students' spatial abilities through visualization of complex ideas, processes, and systems that are difficult for students to comprehend through limited 2D space (Lindgren & Schwartz, 2009; Oliver-Hoyo & Babilonia-Rosa, 2017). Herewith computational modeling, simulation, and 3D visualization might reduce the cognitive burden of students on which, in that way, helping them focusing more on understanding and analysis. Hence, modeling, simulation, and 3D visualization with computers can stimulate students to think critically by asking further questions that go beyond visible phenomena to formulate hypotheses that can be experimentally examined to produce new knowledge and findings. From this point of view, modeling can be a starting point that encourages discoveries and computer-aided innovation (Leon, 2009). With this computational modeling in learning, chemistry can be an intellectual tool that stimulates students' conceptual abilities, which will also form their imaginative, intuitive, and innovative characters. These characters are proven to have paved the way for further research in the field of chemistry that has contributed and produced a breakthrough, including winning Nobel prizes in computational chemistry in 1998 and 2013 (Schlick, 2013). In 1998, John A. Pople was awarded the Nobel Prize for developing computational methods in quantum chemistry (NobelPrize, 2019a). Furthermore, in 2013, Martin Karplus, Michael Levitt, and Arieh Warshel shared the Nobel Prize in chemistry for their research efforts in developing and applying computational molecular modeling to understand complex biological systems (NobelPrize, 2019b). Many internet-based computational programs and software are widely available and can be freely accessed to support chemistry teaching and learning such as PyMOL and Jmol (Craig et al., 2013). Visualization programs and/or computational chemistry simulation software such as ChemSketch and PhET have also been used as learning methodologies that are reported to be able to reduce student learning difficulties (Silva et al., 2015). ChemDraw and HyperChem are two popular computational chemistry software products that have been widely utilized by the educational community both in high schools and universities. However, the shortcomings of ChemDraw and HyperChem are the option to purchase the software or to renew the license annually.

Thanks to the rapid advance of computational technology in the cheminformatics and bioinformatics research community. Software and internet-based programs for modeling, simulating, and visualizing chemical molecules can now be accessed free of charge. Some of the cheminformatics programs include UCSF Chimera and Marvin Sketch. Moreover, the progress in Omics research such as genomics, transcriptomics, proteomics, and metabolomics has generated an explosion of big biological data that requires computing assistance to analyze, store and share, which further accelerates the advancement of the field study of bioinformatics (Kovarik et al., 2013). Several bioinformatics computational programs used by scientists, including PsiPred, MBC (PS2), Rampage, Vienna RNA Package, and Mode RNA, are also freely available and can be easily implemented in high school environments (Form & Lewitter, 2011). These computational programs are generally employed in the university research and pharmaceutical industry for modeling RNA and protein as well as designing new chemical compounds as potential drugs. With the increased demand for biological data sciences in the job market, bioinformatics has been introduced and taught since high school (Kovarik et al., 2013; Machluf & Yarden, 2013). Therefore, to be scientifically literate in this 21st digital century, chemistry teachers must be aware of and able to utilize available computational tools in their classroom activities appropriately.

Unfortunately, there is a gap between the availability of technology for teaching/learning and the use of technology by teachers for instructional purposes. The National Center has reported that Education Statistics, on which less than half of the 3000 teachers surveyed using technology for non-instructional tasks such as administration, assessment, attendance, and teaching preparation, some barriers were found to cause low use of technology by teachers in the classroom. These barriers included the lack of knowledge, skills, access, and resources (Gray et al., 2010; Kopcha, 2012; Lawrence & Tar, 2018).

It has been argued that teachers' awareness and understanding toward technology in the first place are fundamental requisites before implementing its usefulness to education (Cavaz et al., 2009). Findings from various studies showed that training programs are significant for the development of teachers' pedagogical beliefs in combining technology with teaching. When teachers are given a chance to experience the benefits of using technology, they are more likely to adapt their classroom instructions (Aldunate & Nussbaum, 2013; Koh et al., 2017; Mupita et al., 2018; Ottenbreit-Leftwich et al., 2010). Information technology professional training provides teachers with the first-hand experience that helps them change their traditional pedagogical beliefs to be more open to the contribution of technology in education (Baran et al., 2019; Funkhouser & Mouza, 2013). For example, situated professional development like a mentorship program along a certain amount of time has been employed to monitor the implementation of the technology used by teachers at school. However, it has raised several methodological problems because of its dependence on self-reports made by teachers, which tends to be biased and overestimate teachers' actual attitudes and practices toward technology (An & Reigeluth, 2011; Hixon & Buckenmeyer, 2009). Besides, it tends to be more focused on teachers' attitudes and practices on technology over a while rather than on assessing the gains in their knowledge and conceptual understanding, which are necessary for changing their concepts toward technology (Mouza, 2009; Rienties et al., 2013). Katic (2008) has also argued that that approach may lead to mere utilitarian use of technology rather than to its transformative potentials for teaching and learning. Therefore, compared with situated professional development, we propose that standalone professional development like workshop-based training on technological tools can still be a complementing alternative. Its short period with intensive training and low cost while remaining reliant on objective assessments by teachers and instructors are among of the advantages of this training.

Nonetheless, to the best of our knowledge, there is no study reporting how standalone professional development changes and improves teachers' awareness, understanding, and confidence toward contemporary computational tools for chemistry teaching. Therefore, the objective of this study is to examine teachers' awareness, understanding, and confidence after completing two-day professional workshop-based training on available computational tools for molecular modeling and visualization programs. The training consisted of theoretical lectures, hands-on practices, homework assignments, and presentation of case studies. Pre and post-survey were employed as tools to measure teachers' knowledge, understanding, and confidence.

METHODS

This study employed a quantitative method with a non-experimental research design through surveys consisting of three stages, data collection, analysis, and interpretation. Pre-survey and post-survey were conducted to collect data by filling in questionnaires by high school chemistry teachers given at the beginning and end of our workshop activity. The workshop is a form of community service project provided by the joint program between the Chemistry Department, University of Nusa Cendana and Bioinformatics Department, Indonesian International Institutes of Life Sciences (I3LS) in Jakarta with High School Chemistry Teacher Organization (*Musyawarah Guru Mata Pelajaran*/MGMP) in Kupang city, Eastern Nusa Tenggara (NTT) province, Indonesia. Our roles include organizing a workshop, designing questionnaires, delivering training materials, evaluating and analyzing teachers' answers in post and pre-survey. The subjects of this study were 32 high school chemistry teachers from 21 public senior high schools located in Kupang city, NTT province. A total of 12.5% are male teachers, and 87.5% are female teachers. All participating teachers have an undergraduate degree in education. The average age of the teacher participants is ± 37.4 years old. These teachers completed our 2-day professional workshop on computational tools for molecular visualization. The questions for both pre-survey and post-survey were the same as shown below:

INSTRUCTION: Choose just one answer that best represents you.

1. CHEMDRAW
   a. I have never heard of this software
   b. I've heard of this software, but I don't know its usefulness
   c. I've heard of this software and know its usefulness for (write your answer below)

Teachers chose only one answer from choice (A), (B), and (C), relevant to their state of knowledge before and after the workshop. The same question was given to another type of software and internet-based programs by merely swapping the name of the computational tool being inspected. In total, nine contemporary computational tools were surveyed, such as ChemDraw, HyperChem, Marvin Sketch, UCSF Chimera, PsiPred, MBC (PS2), Rampage, Vienna RNA package, and Mode RNA (Table 1). The workshop was opened with a pre-survey to find out the baseline of acquaintance, knowledge, and confidence level toward contemporary computational programs associated with molecular modeling and visualization.

Table 1. Cheminformatics and Bioinformatics Software and Web-Based Computational Programs Used in the Workshop and Survey

Software and URL Address	Function
ChemDraw https://www.perkinelmer.com/category/chemdraw	Sketching 2D chemical molecules, chemical reactions, stereochemistry
HyperChem http://www.hyper.com/	Drawing and simulating 2D chemical molecules
Marvin Sketch https://chemaxon.com/products/marvin	Drawing 2D and 3D chemical structures quickly and accurately
UCSF Chimera https://www.cgl.ucsf.edu/chimera/	Interactive visualization and analysis of the structure of chemical molecules, DNA, RNA, and proteins
PsiPred http://bioinf.cs.ucl.ac.uk/psipred/	Prediction and visualization of secondary structures of proteins
MBC (PS2) http://ps2.life.nctu.edu.tw/	Template-based prediction of protein structure
Rampage http://mordred.bioc.cam.ac.uk/~rapper/rampage.php	Visualizing the area energetically permitted from the angle of the main protein chain dihedral
Vienna RNA https://www.tbi.univie.ac.at/RNA/	Prediction and analysis of secondary RNA structures
Mode RNA http://genesilico.pl/moderna/	Comparative modeling of 3D RNA structures

Three sessions in the workshop proceeded as planned by the instructors. In Session I on ChemDraw and HyperChem, the teachers were presented on how to make 2D sketches and isomers of chemical compounds. Some forms of chemical molecular representation that display chemical bonds, free electron pairs, as well as 3D shapes of chemical bonds that approach and move away from the planar field were also given. In session II on Marvin Sketch and UCSF Chimera, the teachers were trained on how to construct 2D sketches from the input of molecule name and structure to build isomers and to set the dynamic movement of chemical molecules. The teachers were also trained on how to save the results of chemical molecular sketches in proper structural file formats such as SMILES, SDF, MOL2, PDB, which can then be used as input files to be converted into 3D representation using UCSF Chimera. In session III on PsiPred, MBC (PS2), Rampage, Vienna RNA Package, and Mode RNA, the teachers were presented with the topics on modeling and predicting secondary and 3D structures of RNA as well as on exploring 3D protein structures.

The homework assignments were also given for the teachers to implement the computational tools they learned in the setting of classroom teaching. The assignments were then presented on the next day as a case study. After all of the sessions were accomplished, a post-survey was conducted to determine the percentage and improvement in awareness, understanding, and confidence. The data analysis stage was carried out based on the pre and post-survey data. It heavily relied on a method developed by Terrell & Listenberger (2017).

In this research stage, we modified the data analysis by targeting high school chemistry teachers through measuring their awareness, understanding, and confidence toward a computational program for molecular modeling and visualization. Awareness is defined as familiarity whether teachers have previously heard of the computational programs or not. Awareness perceived as a basic form of knowledge as well as a precondition for a more sophisticated understanding. On data analysis, the teachers are said to have awareness if they choose answer (B) and (C) irrespective of their given explanation. In other words, the teachers got acquainted with the computational programs and their functions regardless of their description of its function. The teachers are said to understand and be confident if they choose answer (C). We counted the number of teachers that chose choice A, B, C, and measured the percentage related to the corresponding computational tool being examined on pre-and post-survey.

In data analysis, we also wanted to investigate the level of understanding based on the instructors' assessment on the answer (C) provided by the participants. The level of teachers' understanding was divided into four categories which are (i) Not Demonstrated (C-ND), if they do not specify the answer or give the answer but incorrect; (ii) Emerging (C-E), if the answer is half correct or partly illogical, (iii) Satisfactory (C-S), if they are able to show one function or provide a general explanation and (iv) Exceptional (C-EX), if they explain more than one correct use and gain new knowledge. As an example of answer (C) provided by chemistry teachers and evaluated by workshop instructors based on those four categories can be seen in Table 2.

Table 2. The Example of Instructors' Assessment on the Participants' Answer (C)

	Not Demonstrated	**Emerging**	**Satisfactory**	**Exceptional**
Criteria	No answer is given; or presented but incorrect	Partly correct or partly illogical	Could show one purpose or a general explanation	Elaborating more than one correct use of the modeling tools in question
ChemDraw	Used to make chemical formulas	Describing complicated molecular shapes	Illustrating the structure of 2D and 3D molecules	Describing 2D and 3D structures of a compound, knowing the physical and chemical properties of compounds, knowing the prediction of NMR compounds, knowing the structure based on the name of the compound and vice versa
HyperChem	Visualization model from ChemDraw	Seeing the structure of molecules and macromolecules	3D molecular depiction and visualization	Making 2D sketches and making 3D models, can read the type of atoms, and designing as well as creating shapes of molecular dynamics
Marvin Sketch	Making text related to the visualization of an atom, ion, molecule including chemical bonds that occur therein	Downloading software, saving and editing chemical structures, saving structure files	Describing 2D and 3D structures and confirming the molecular dynamics	Displaying molecular structure in the form of 2D / 3D images and animations, displaying IUPAC names and structures made and vice versa, displaying isomers, free electron pairs, also including validation and molecular structures created
UCSF Chimera	Formulation and physical and chemical stability test	Describing macromolecules	Visualization of 3D molecular shapes	Converting molecules from 2D to 3D, displaying 3D molecules from SMILES, SDF, Protein Data Bank files

Further, we also measured the percentage of teachers experiencing a gain in awareness, understanding, and confidence. The teachers are said to experience an improvement in awareness if their answer moves from (A) to (B), or (A) to (C) from pre to post-survey. The teachers are said to experience a gain in understanding if there is a movement from the answer (A), or (B), or (C - ND), to answer (C - E), or (C - S), or (C-EX) from pre to post-survey. The teachers are declared to increase confidence if there is a movement from the answer (A) to (C) or (B) to (C), from pre to post-survey. We counted the total teachers that showed such trends and measured in percentage (%). The data were compiled, analyzed, and visualized using GraphPad Prism software version 8.2.1 (San Diego, CA).

RESULTS AND DISCUSSION

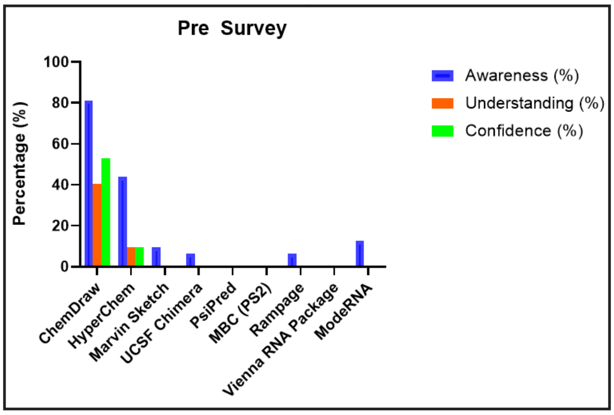

Figure 1. The Pre-Survey Result (N=32)

The workshop conducted intended to introduce and assist chemistry teachers to current molecular modeling and visualization tools that may improve their pedagogical activities in chemical structure instruction. From the pre-survey, it was known that the awareness of chemistry teachers to ChemDraw was already very high (81.3%), followed by HyperChem (43.8%), Mode RNA (12.5%), Marvin Sketch (9.4%), UCSF Chimera (6.3%), Rampage (6.3%) (Figure 1). This high familiarity with ChemDraw was also accompanied by a moderate level of knowledge (40.6%) and confidence in using the software (53.1%).

Meanwhile, the percentage of knowledge and confidence in HyperChem was only 9.4%. The high level of teachers' experiences with ChemDraw and HyperChem suggests their familiarity with the software, which are quite famous and commonly used in chemistry instruction from high school to university level (Haworth & Martin, 2018).

On the other hand, the teachers never heard and knew the use of PsiPred, MBC (PS2), and Vienna RNA. Interestingly, 6.3% and 12.5% of the teachers had heard of Rampage and Mode RNA, respectively, but did not know their usefulness. Furthermore, the rests did not have knowledge and confidence in Marvin Sketch, UCSF Chimera, Rampage, PsiPred, MBC (PS2), Vienna RNA, and Mode RNA. Their ignorance of the computational program such as Mode RNA, Marvin Sketch, UCSF Chimera, Rampage, PsiPred, MBC (PS2), and Vienna RNA indicated that they have never been exposed and informed on the availability of those tools. In part, it could be because cheminformatics and bioinformatics software products are mostly used for modeling and analyzing the 3D structure of protein and RNA in research universities. This then creates a gap that causes teachers' lack of access and knowledge. For example, although Marvin Sketch software can be downloaded for free from the ChemAxon website for high school educators, the teachers were not aware of this advantage. It was almost likely that they were not cognizant about the free availability and usefulness of those computational programs. English language constraints may also be a reason for teachers to perceive that those computational tools are challenging to learn and not easy to use. In line with this, the previous study has reported that lack of access and knowledge is among several contributing factors that hamper teachers' adoption and integration of Information Communication Technology (ICT) in teaching and learning (Lawrence & Tar, 2018). These circumstances motivated us to introduce bioinformatics, cheminformatics software and computational tools for modeling and visualization as a part of professional development workshop for chemistry teachers.

Cheminformatics is a relatively new development of chemistry that applies the use of computers and information techniques in management, database, and analysis of chemical molecule structures specifically related to recently rapid advances of research in computational design and discovery (Wild, 2013). Bioinformatics deals with the application of computational techniques to manage and analyze biological information and biomolecule structures such as DNA, RNA, and proteins generated from research in genomics, transcriptomics, proteomics, and metabolomics (Patel et al., 2019). The past decade has shown increasing efforts to introduce cheminformatics and bioinformatics to teaching and learning chemistry in high school (Kovarik et al., 2013; Machluf & Yarden, 2013; Wild, 2013). This is due in part to the growing demand of cheminformaticians, bioinformaticians, and biological data sciences in the job market (Attwood et al., 2017). Another reason is that the integration of the use of cheminformatics software has been reported to improve students' visual and spatial abilities (Lohning et al., 2019). It has also been reported that the perception of secondary school students towards the integration of bioinformatics in the curriculum is also very positive in improving their learning (Machluf et al., 2016). Hence, to be scientifically literate with the fast demand of 21st digital century, it is such a necessity for high school chemistry teachers to upgrade their professional qualifications related to computing technology through professional development on modeling, visualization and application of chemistry and bioinformatics databases in supporting teaching and learning pedagogy (Tuvi-Arad & Blonder, 2019). After the workshop, an increase in awareness, knowledge, and confidence were seen, which could be observed in Figure 2.

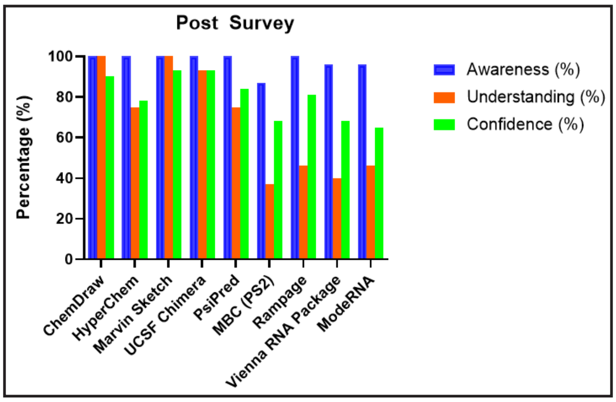

Figure 2. The Post Survey Result (N=32)

The percentage of awareness to ChemDraw software was 100%, then HyperChem (100%), Marvin Sketch (100%), UCSF Chimera (100%), PsiPred (100%), MBC (PS2) (87.5%), Rampage (100%), Vienna RNA (96.8%) and Mode RNA (96.9%). Moreover, the percentage of teachers' knowledge on ChemDraw software was 100%, followed by Hyperchem (75%), Marvin Sketch (100%), UCSF Chimera (93.8%), PsiPred (75%), MBC (PS2) (37.5%), Rampage (46.9%), Vienna RNA (40.6%) and Mode RNA (46.9%). On the other hand, the percentage of teachers' confidence in using ChemDraw software was 90.6%, followed by Hyperchem (78.1%), Marvin Sketch (93.8%), UCSF Chimera (93.8%), PsiPred (84.4%), MBC (PS2) (68.8%), Rampage (81.3%), Vienna RNA (68.8%) and Mode RNA (65.6%). The combination of lectures, hands-on, homework assignments, and presentations within the 2-day workshop contributes to accommodate the fast development of teachers' theoretical knowledge and skills on those programs. On the hands-on practice, we gave the teachers real examples of problems in sketching the molecular structures that students usually find it difficult to comprehend. On homework assignments, we allowed the teachers to find a problem themselves on chemical structures and try to solve them with computational tools they have learned. Moreover, on the case study presentation, the teachers were given a chance to present their knowledge and skills in showing the usefulness of the programs to sketch the structure they have picked with the setting that mimics classroom instruction. We found these methods helpful in increasing teachers' knowledge, understanding, and confidence. Although the percentage of teachers' awareness of protein and RNA modeling software has increased, their understanding and confidence were lower than ChemDraw, HyperChem, and Marvin Sketch. This could be that the amount of time that the teachers spent to learn that programs during the workshop and/or homework assignment were less than ChemDraw, HyperChem, and Marvin Sketch Sketch. This may also be because of the small portion of protein and RNA materials in the high school chemistry curriculum, which are only taught briefly in class XII.

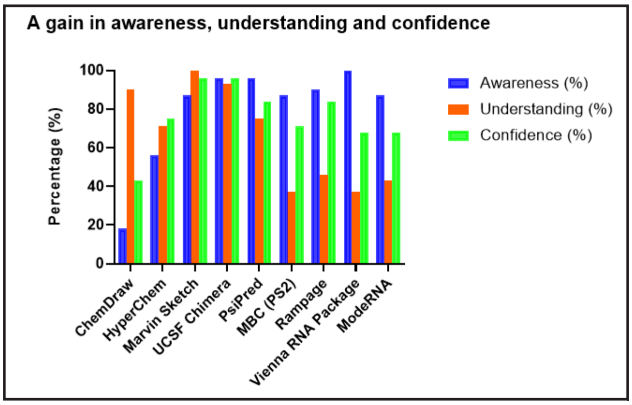

Figure 3. The Gain Analysis from Pre- to Post-Survey

We also aspired to explore the teachers' enhancement in awareness, understanding, and confidence (Figure 3). This aimed to trace the progress of the teachers' awareness and understanding from pre to post-survey that may reflect their change in knowledge, perception, and attitude toward computational technology for molecular visualization. In ChemDraw, the percentage of teachers' increase in awareness seemed low, which was 18.7%. However, those were the small number of teachers who were not familiar with the software before the workshop took place. We did not count on the improvement of those who had already chosen answer (B) and/or (C) on the pre-survey simply because they had already been accustomed to the software. Nevertheless, it showed that some of the teachers, whom at the beginning of the training did not know ChemDraw, had experienced an advancement in awareness of the software. Likewise, there was an increase in understanding of ChemDraw, which was 90.6% and 43.8% in confidence. Moreover 50% enchancement was recorded on the awareness of HyperChem, Marvin Sketch, UCSF Chimera, PsiPred, MBC (PS2), Rampage, Vienna RNA, and Mode RNA. On the understanding, there was a high increment on ChemDraw (90.6%), HyperChem (71.9%), Marvin Sketch (100%), UCSF Chimera (91.8%), and PsiPred (75%). Meanwhile, an improvement in the understanding of MBC (PS2), Rampage, Vienna RNA, and Mode RNA was notwithstanding below 50%. This suggested that the teachers need to spend more time to digest new materials on RNA and Protein as well as their related computational tools. Furthermore, 60% increase was seen on confidence of utilizing HyperChem, Marvin Sketch, UCSF Chimera, PsiPred, MBC (PS2), Rampage, Vienna RNA, and Mode RNA.

Overall, the researchers observed an enhancement in the teachers' awareness, understanding, and confidence toward computational software for modeling and visualization after two days of a standalone professional workshop. Computational technology in the form of software and internet-based programs has become an indispensable component of life science research and education. However, research has shown that, for reasons of inadequate experience, teachers often do not include the element of technology in science teaching and learning (Koehler & Mishra, 2009). Common barriers to technology have been investigated, including lack of knowledge, skills, confidence, access, and time (Dinçer, 2018; Kopcha, 2012; Lawrence & Tar, 2018). Also, the conceptual belief of the teachers who perceive that technology is too sophisticated impedes the acceleration of the integration of the technology (Mishra et al., 2019). In line with our study, An & Reigeluth (2011) suggested that implementing professional development is one of five strategies that should be conducted to overcome the general barriers such as knowledge and skills of integrating computational technology for instructional purposes in K-12 schools. Compared to continuous and situated professional development, which requires an extended period, a high cost, and methodological bias due to dependence on teachers' self-report that tends to exaggerate their actual practice with technology, standalone professional workshops can be done in a short time through intensive training. It could be conducted with a reasonable cost by remaining to rely on objective assessments of the teachers' knowledge and understanding combined with the instructors' assessments. Terrell & Listenberger (2017) developed an inquiry-based molecular visualization project for several weeks for Biochemistry I students. They found that there was an increase in the students' knowledge and confidence in using online databases and computing tools. The results of this study showed that their method can be applied for professional development programs toward high school chemistry teachers within a shorter period (e.g., two days) on which we found a comparable increase in awareness, understanding, and confident in using computational tools. Besides, we argued that standalone professional development can be held quickly to adjust to the needs and rapid development of information technology that demands fast learning and adaptation.

Nonetheless, we are aware of the limitation of our study that the enhancement in the teachers' acquaintance, knowledge, and confidence in contemporary computational tools on molecular visualization does not necessarily imply that they will incorporate it into their pedagogical teaching and learning in the classroom. Research has shown that several important factors also play a crucial role in the complex implementation of ICT on teaching and learning, which include leadership, institutional support, resources, geographical context, infrastructures, training, and technical support (Lawrence & Tar, 2018). Thus, we consider our study as a preliminary result for further follow-up research on chemistry teachers' attitudes and challenges in applying their knowledge and skills on modern computational tools in classroom settings.

The outcome of our study may harness the motivation and alter the pedagogical beliefs of chemistry teachers toward computational technology. It may also provide chemistry teachers with various software and web-based tools according to their needs, conditions, and the learning objectives in the classroom. For example, Marvin Sketch software from ChemAxon can be a compliment or an alternative to ChemDraw as it is freely accessed, relatively easy and fast to use and apply both for teacher's preparation and classroom applications. The introduction of the UCSF Chimera may equip teachers to transform the representation of 2D molecules into 3D in more interactive ways. The introduction of software and computational tools of bioinformatics such as PsiPred, MBC (PS2), Rampage, Vienna RNA Package, and Mode RNA may also help teachers to grasp more realistic and detailed understanding of 2D and 3D structural models of RNA and Protein biomolecules. From here, computational tools for modeling and visualization may transform the ways of teaching and learning presented to students, hoping that this course will make learning chemistry, especially the molecular structure more attractive, interactive, dynamic, and personal for students. At this point, students may begin to be introduced and informed to the benefits of utilizing computational technology in helping their cognitive, psychomotor, and affective development. As a result, it may equip them well to enter higher education and later on the 21st-century job market with highly required skills such as analytical, spatial and conceptual thinking aided by computational skills for solving complex problems in the real world (Barr et al., 2011; Yadav et al., 2017).

CONCLUSION

This study resulted in an improvement in high school chemistry teachers' awareness, understanding, and confidence after following the 2-day professional workshop on computational tools for molecular modeling and visualization. Through intensive training comprising of theory, practice, and independent assignments and case study presentation and assessed by pre and post-survey, the teachers showed an advancement in awareness, understanding, and confidence in utilizing those tools. The impact of this research points toward the value of standalone professional development that is still relevant and useful in creating a valuable platform to reduce the barriers of access, resources, knowledge, and skills. In that regard, it has been shown to help improve teachers' awareness, understanding, and confidence, which are necessarily required for further use of available technology for instructional purposes. The implication of this study may contribute to a recent campaign and discussion on the need to incorporate computational science and information technology into teaching and learning chemistry in facing and adapting the challenge of industrial revolution 4.0.

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