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Chemistry Teachers' Awareness, Understanding and Confidence Toward Computational Tools for Molecular Visualization

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 studies simultaneously reporting chemistry teacher's awareness, understanding and confidence toward contemporary computer-aided molecular modeling and visualization tools. This study examines 32 high school chemistry teachers' knowledge, understanding and confidence toward nine modern 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, teachers showed a gain in awareness, understanding and confidence toward those nine computational programs. Intensive activities consisting of theoretical lectures, hands-on practices, assignments and case study presentation seem provide valuable resources to the increase in teachers' knowledge, understanding and skill that incorporates computational technology. Hence, the impact of this research points toward the value of teachers' professional development that creates a platform to reduce the barriers of access, resources, knowledge and skills. From our study, it helps improve teachers' awareness, understanding and confidence essentially required for further implementation of available technology for instructional purpose.

Keywords: chemistry, teacher, modeling, visualization, computational

INTRODUCTION

Digitalization and internet of things (IoT)-based technologies have become the driving force of industrial revolution 4.0 that has a profound impact not only in social endeavor and economic life but also in education community (Puncreobutr, 2016; Schwab, 2016). Science education system has adopted contemporary technology tools and computational platforms for the purpose of improving the quality of teaching, learning and assessment (Neumann & Waight, 2019). The last two decades demonstrate the use of specialized learning software applications 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 potential to transform teaching and learning of science to be more attractive, interactive and personal, supporting the recent campaign on integrating computational thinking in education and promoting digital and visual literacy of science (Bucchi & Saracino, 2016; Garcia-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/or 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 to focus 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 new 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 new 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). And 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 teaching and learning chemistry 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 of popular computational chemistry software that have been widely utilized by the educational community both in high schools and universities. However, the shortcomings of ChemDraw and HyperChem are the necessity to purchase the software and/or to renew the license annually. Thanks to the rapid advance of computational technology in cheminformatics and bioinformatics research community, several software and/or internet-based programs for modeling, simulating and visualizing chemical molecules can now be accessed free of charge. Some of cheminformatics programs include UCSF Chimera and Marvin Sketch. Moreover, the progress in Omics research such as genomics, transcriptomics, proteomics, and metabolomics have generated an explosion of biological big 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 are also freely available and can be easily implemented in high school environments (Form & Lewitter, 2011). Some of them are PsiPred, MBC (PS2), Rampage, Vienna RNA Package and Mode RNA. These computational programs are generally used 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 scientists in 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, it is necessary for chemistry teachers to be aware of and able to appropriately utilize available computational tools in their classroom activities.

Unfortunately, there is a gap between the availability of technology for teaching and learning and the use of that technology by teachers for instructional purposes. It has been reported by the National Center for Education Statistics on which less than half of the 3000 teachers surveyed actually using technology for non-instructional tasks such as administration, assessment, attendance and teaching preparation (Gray et al., 2010). Several studies have reported some barriers that have caused low use of technology by teachers in the classroom such as lack of knowledge, skills, access, and resources (Kopcha, 2012; Lawrence & Tar, 2018). It has been argued that teachers' awareness and understand toward technology at the first place are fundamental requisites before implementing its usefulness to education (Cavaz et al., 2009). Findings from various studies show that training programs are very important for the development of teachers' pedagogical beliefs in combining technology with teaching. When teachers are given the chance to experience the benefits of using technology, they are more likely to adapt their classroom instructions (Koh et al., 2017; Mupita et al., 2018; Ottenbreit-Leftwich et al., 2010; Aldunate & Nussbaum, 2013). Technology professional training provides teachers with 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 mentorship program along a certain amount of time have been employed to monitor the implementation of the technology use by teachers at school. However, it has raised a number of 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). In addition, it tends to be more focused toward teachers' attitudes and practices on technology over period of time 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 complement alternative through its short period of time with intensive training and low cost while remaining reliant on objective assessments by teachers and instructors. However, to the best of our knowledge, there is no study reporting how standalone professional development changes and improves teachers' awareness, understanding and confidences toward contemporary computational tools for chemistry teaching. Therefore, the objective of this study is to examine teachers' awareness, understanding and confidence after completing two days of professional workshop-based training on available computational tools for molecular modeling and visualization programs. The training consists of theoretical lectures, hands-on practices, homework assignments and presentation of case studies. Pre and post survey was employed as tools to measure teachers' knowledge, understanding and confidence.

METHODS

This study employed a quantitative method with non-experimental research design through the surveys. It consisted of three stages which were data collection, analysis and interpretation. To collect data, pre-survey and post-survey were conducted through 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 Department of Chemistry at the University of Nusa Cendana and Department Bioinformatics at Indonesian International Institutes of Life Sciences (I3LS) in Jakarta with High School Chemistry Teacher Organization (MGMP) in Kupang city of Eastern Nusa Tenggara (NTT) province in Indonesia. Our roles are in organizing workshop, designing questionnaires, delivering training material, evaluating and analyzing teachers' answers in post and pre survey. The subjects of this study are 32 high school chemistry teachers from 21 public senior high schools located in Kupang city of NTT province. All participating teachers have an undergraduate degree in education. A total of 12.5% are male teachers. And 87.5% are female teachers. The average age of the teacher participants is 37.4 ± 9.6 years old. These participating 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

33 fulness

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 with their state of knowledge before and after the workshop. The same question was given to another type of software and internet-based programs by simply 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 I). 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. There were three sessions in the workshop that proceeded as planned with instructors presented their respective material. In Session I on ChemDraw and HyperChem 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, teachers were trained on how to construct 2D sketches from the input of molecule name, structure, to build isomers and to set the dynamic movement of chemical molecules. Teachers were also trained on how to save the results of chemical molecular sketches in appropriate structural file formats such as SMILES, SDF, MOL2, PDB, which can then be used as input file to be converted into 3D representation using UCSF Chimera. In session III on PsiPred, MBC (PS2), Rampage, Vienna RNA Package, and Mode RNA, 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 teachers to practice to implement the computational tools they learned on the setting of classroom teaching. The assignments were then presented on the next day as a case study. After all the sessions of the workshop were accomplished, a post survey was conducted to determine the percentage of and the gain in awareness, understanding and confidence.

The data analysis stage was

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

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 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 precondition for more complex understanding. On data analysis, Teachers are said to have awareness if they choose answer (B) and (C) irrespective of their given explanation. In other words, teachers get acquainted with the computational programs and its functions regardless of their description of its function. Teachers are said to have understanding and confidence if they choose answer (C). We counted the number of teachers that chose choice A, B, C and measured the percentage related with corresponding computational tool being examined on pre and post survey.

In data analysis, we also wanted to investigate the level of understanding based on instructors' assessment on answer (C) provided by participants. The level of understanding of teachers was dividied into four categories which are (i) Not Demonstrated (C-ND), where they do not specify the answer or give the answer but incorrect, (ii) Emerging (C-E), their answer is half correct or partly illogical, (iii) Satisfactory (C-S), they are able to show one function or able to provide a general explanation and (iv) Exceptional (C-EX), 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 II.

Further, we also measured the percentage of teachers experiencing a gain in awareness, understanding and confidence. Teachers are said to experience a gain in awareness if their answer moves from (A) to (B), or (A) to (C) from pre to post-survey. Teachers are said to experience a gain in understanding if there is a movement from answer (A), or (B), or (C - ND), to answer (C - E), or (C - S), or (C-EX) from pre to post survey. And teachers are said to have increased confidence if there is a movement from answer (A) to (C) or (B) to (C), from pre to post survey. We counted 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

We had conducted a computational professional development in the form of

Table 2 - Example of instructor evaluation of teachers' survey responses to answer (C)

	Not Demonstrated	**Emerging**	**Satisfactory**	**Exceptional**
Criteria	Answer not given or present but incorrect	The answer is partly true or partly illogical	Able to show one purpose or be able to give a general explanation	Elaborate more than one correct use of the modeling tools in question
ChemDraw	Used to make chemical formulas	To describe complicated molecular shapes	To illustrate 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	To see the structure of molecules and macromolecules	3D molecular depiction and visualization	To make 2D sketches and make 3D models, can read the type of atoms and design and create shapes of molecular dynamics
Marvin Sketch	Make text related to the visualization of an atom, ion, molecule including chemical bonds that occur therein	Download software, save and edit chemical structures, save structure files	Describes 2D and 3D structures and confirms the molecular dynamics	Displays molecular structure in the form of 2D / 3D images and animations, displays IUPAC names and structures made and vice versa, displays isomers, free electron pairs, also includes validation and molecular structures created
UCSF Chimera	Formulation and physical and chemical stability test	Describing macromolecules	Visualization of 3D molecular shapes	Convert molecules from 2D to 3D, display 3D molecules from SMILES, SDF, Protein Data Bank files
PsiPred	To investigate the structure of proteins	To see the detailed structure of the molecular structure	Knowing the secondary structure of proteins	Translating the amino acid code so that we can know the secondary structure of the protein is dominated by for example coil, helical, strand
MBC (PS2)	To know the order of protein composition	To find out the structure of biomolecules	Prediction of 3D protein structure	To display, predict and illustrate the modeling of a protein or biomolecule
Rampage	To see the residue of a	Knowing the validity of	Knowing protein stability with	Know the validity of the position of amino

	macromolecule	biomolecules	Ramachandran plot	acids geometrically with Ramachandran's diagram
Vienna RNA package	See detailed RNA examples	To predict 2D structures	Predict the secondary structure of RNA	Predict and analyze validation of secondary RNA structures
Mode RNA	Look at RNA data	Know the structure and data from RNA	Describe the structure of RNA in 3D	Predict and visualize RNA structures in 3D

standalone workshop-based training for high school chemistry teachers in Kupang city at NTT province of Indonesia that sought to introduce and assist them 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 of HyperChem was only 9.4%. The high level of teachers' experiences with ChemDraw and HyperChem suggests their familiarity with the software which are quite popular and commonly used in chemistry instruction from high school to university level (Haworth & Martin, 2018).

On the other hands, teachers never heard and knew the use of PsiPred, MBC (PS2) and Vienna RNA. Interestingly, 6.3% and 12.5% of teachers had heard of Rampage and Mode RNA, respectively, but did not know their usefulness. And the rests do not have knowledge and confidence in Marvin Sketch, UCSF Chimera, Rampage, PsiPred, MBC (PS2), Vienna RNA and Mode RNA. Teachers' ignorance of the computational program such as Mode RNA, Marvin Sketch, UCSF Chimera, Rampage, PsiPred, MBC (PS2) and Vienna RNA indicates that they have never been exposed and informed on the availability of those tools. In part, it could be because cheminformatics and bioinformatics software are mostly used for modeling and analyzing 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 free of charge from ChemAxon website for high school educators, teachers were not aware of this advantage. It is almost likely that they are not cognizant about the free availability and usefulness of those computational programs. English language constraints may also be a reason for teachers to then perceive that those computational tools are difficult to learn and not easy to use. In line with this, previous study has reported that lack of access and knowledge is among several contributing factors that hamper teachers' adoption and integration 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

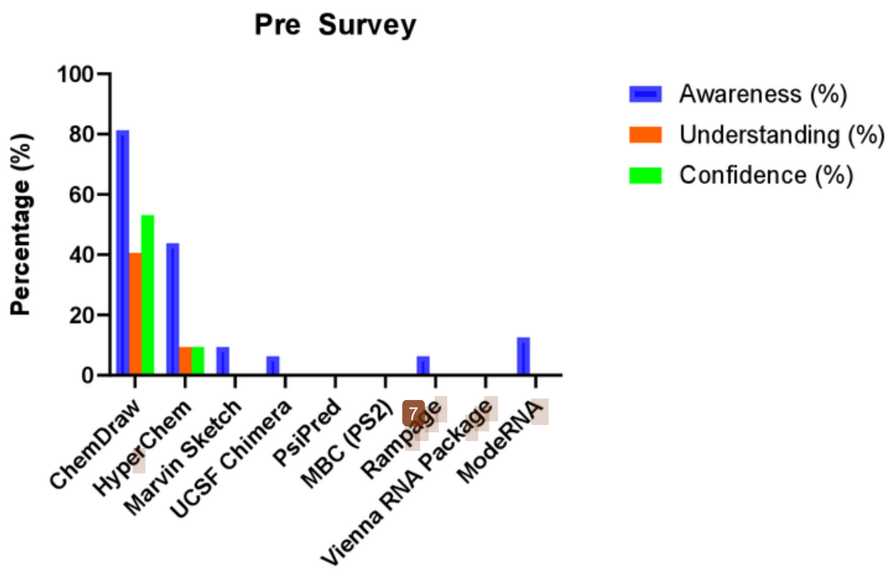

Figure 1. Pre-survey result. It shows percentage of high school chemistry teachers on awareness, understanding and confidence toward nine computational tools for molecular visualization before completing the workshop (N=32).

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 the structure of chemical molecules specifically related to recently rapid advances of research in computational drug 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 in 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 scientists 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).

Following the workshop, it was shown that there was an increase in awareness, knowledge and confidence (Figure 2). The percentage of awareness to ChemDraw software was 100%, 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%, 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%. And the percentage of teachers' confidence in using ChemDraw software was 90.6%, Hyperchem78.1%, 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 presentation within 2-day workshop contributes to accomodate fast development of teachers' theoretical knowledge and skills on those programs. On the hands-on practice, we gave teachers real examples of problems in sketching the molecular structures that often students found difficult to comprehend. On homework assignment, we gave teachers an opportunity to find a problem themselves on chemical structures and try to solve it with computational tools they have learned. And on case study presentation, 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 help

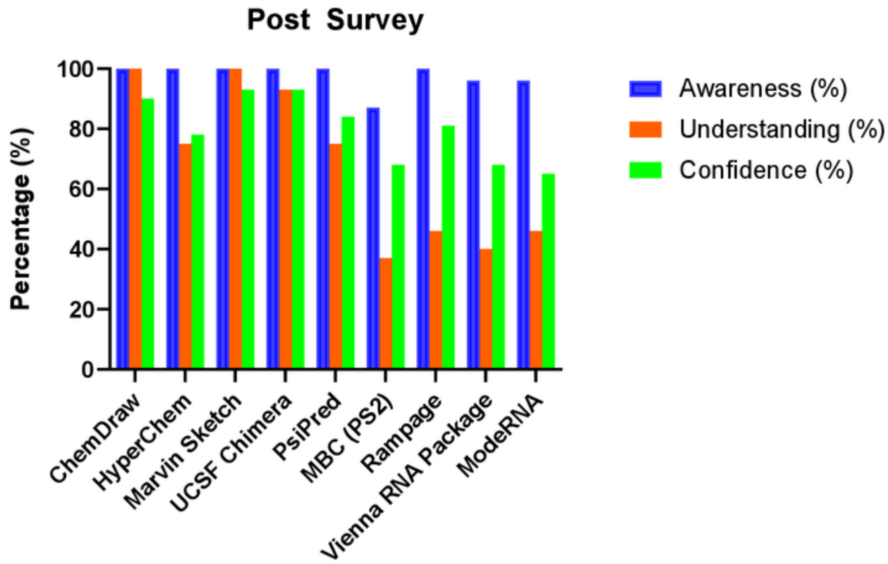

Figure 2. Post survey result. It shows percentage of high school chemistry teachers on awareness, understanding and confidence toward nine computational tools for molecular visualization after completing the workshop. (N=32).

increase teachers' knowledge, understanding and confidence. Although the percentage of teachers' awareness to protein and RNA modeling software has increased, their understanding and confidence are lower than ChemDraw, HyperChem and Marvin Sketch. This could be that the amount of time that teachers spend to learn that programs during workshop and/or homework assignment was less than ChemDraw, HyperChem and Marvin Sketch Sketch. This may be also because the material on protein and RNA is not given a high proportion in chemistry curriculum at high school, which is only briefly taught in the class XII.

We also aspired to explore teachers' gain in awareness, understanding and confidence (Figure 3). This aimed to trace the progress of individuals' awareness and understanding from pre to post survey that may reflect their change in knowledge, perception and attitude toward computational technology for molecular visualization that can be integrated in teaching and learning process. In ChemDraw, the percentage of teachers' gain in awareness seemed only 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 improvement to those teachers who had already choose 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 who at the beginning of the training did not know ChemDraw had experienced a gain in awareness with the software. Likewise, there was a gain in understanding of ChemDraw, which was 90.6% and 43.8% in confidence. There was also a gain in awareness above 50% in HyperChem, Marvin Sketch, UCSF Chimera, PsiPred, MBC (PS2), Rampage, Vienna RNA, and Mode RNA. On understanding, there was a high increment on ChemDraw (90.6%), HyperChem (71.9%), Marvin Sketch (100%), UCSF Chimera (91.8%), and PsiPred (75%). Meanwhile a gain in understanding of MBC (PS2), Rampage, Vienna RNA, and Mode RNA was notwithstanding below 50%. This suggests that teachers need to spend more time to digest new materials on RNA and Protein as well as its related computational tools. For a gain on confidence, there were an increase above 60% on HyperChem, Marvin Sketch, UCSF Chimera, PsiPred, MBC (PS2), Rampage, Vienna RNA, and Mode RNA.

Overall we observe a gain in teachers' awareness, understanding and confidence toward computational software for modeling and visualization after two days of 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 teaching practice and learning science in the classroom (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). In addition, the conceptual belief of the teachers who perceive that technology is too complex also impedes the acceleration of the integration of the technology (Mishra et al., 2019). It was evident from our

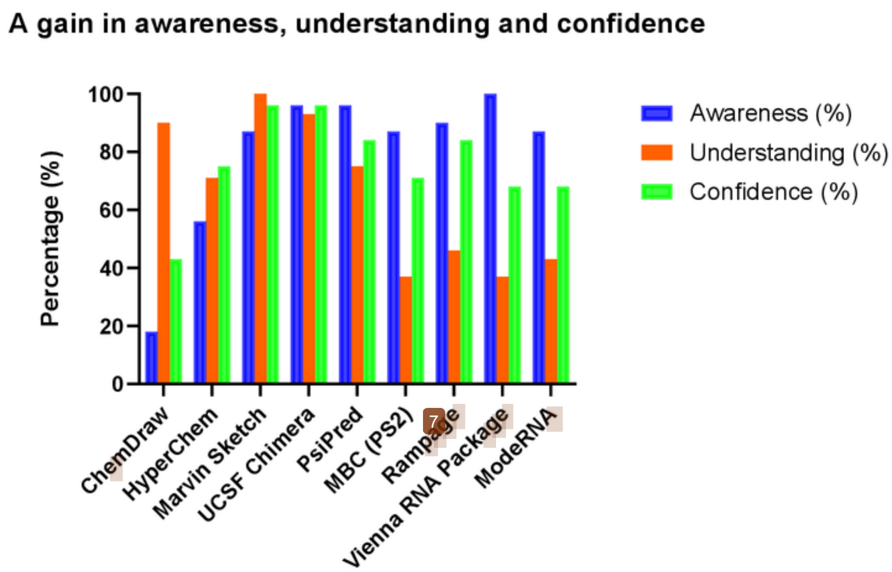

Figure 3. A gain analysis from pre to post survey. Percentage of teachers who experienced an increase in terms of awareness, understanding and confidence after participating a 2-day workshop (N=32).

study that 2-day computational professional development comprising of theories, hands-on practice and individual assignments was found beneficial to improve teachers' understanding on the functions and applications of computational program for modeling and visualization. In line with our study, An & Reigeluth (2011)suggests that conducting professional development is one among 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 a long period of time, a large cost, and the problem of methodological bias because it depends on the teacher's self-report that tends to exaggerate their actual practice with technology, standalone professional workshops can be done in a short period of time through intensive training. It could be conducted with a reachable cost by remaining reliant employing objective assessments of the teachers' knowledge and understanding combined with the assessments from the instructors. Terrell & Listenberger (2017) developed an inquiry-based molecular visualization project for several weeks for students of Biochemistry. They found that there was an increase in student knowledge and confidence in using online databases and computing tools. Our study results show that their method can be applied for professional development program toward high school chemistry teachers within shorter period of time (e.g. two days) on which we found a comparable increase of awareness, understanding and confident in using computational tools.

In addition, we argue 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 as well.

Nonetheless, we are aware of the limitation of our study that this increase in teachers' acquaintance, knowledge and confidence on contemporary computational tools on molecular visualization does not necessarily imply that teachers will incorporate it into their pedagogical teaching and learning in the classroom. Research has shown that several important factors also play a key role in complex implementation of ICT on teaching and learning such as 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' attitude 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 to choose and use according to their needs and conditions as well as the learning objectives in the classroom. For example, Marvin Sketch software from ChemAxon can be a complement 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 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. With the hope that this course will make learning chemistry specifically the molecular structure more attractive, interactive, dynamic and personal for students. From there, 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 21st century job market with highly required skills such as analytical, spatial and conceptual thinking aided by computational skills for solving complex problems in real world (Barr et al., 2011; Yadav et al., 2017).

CONCLUSION

Our study showed an improvement of high school chemistry teachers' awareness, understanding and confidence after following 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 a gain in awareness, understanding and confidence on 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 regards, it has been shown to help improve teachers' awareness, understanding and confidence which are essentially required for further use of available technology for instructional purpose. 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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