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Didactic Strategy Based on Molecular Modeling Tools for Teaching About the Chemistry Present in Food

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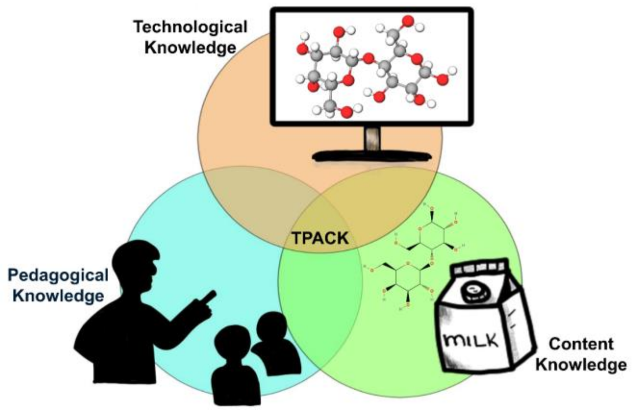
Many students struggle to understand chemistry due to the complexity of the content and abstract concepts. Teachers' mediation based on technological, pedagogical, content knowledge (TPACK) and the contextualization of the content with everyday life may help in this process. In this study, molecular modeling was used as a tool to help teach chemistry integrated with biology. An observational, qualitative and quantitative study was conducted with 136 high school students and 167 undergraduate students. We carried out a mini course named "Is there chemistry in food" and some of the examples approached were water, sodium chloride, sucrose, lactose, oleic acid, collagen, capsaicin receptor and others. An increase in correct answers was observed by comparing the answers after the two-hour mini-course and the correct answers before the activity, reaching 46.30% in some questions. When asked about the efficiency of the method, most of the students answered positively and detached the contributions to learning, the innovative, fun, interactive or dynamic character, the visualization of the molecules, and the practice itself. Thus, molecular modeling tools can be an interesting strategy to be explored in chemistry and biology classes, especially in high school.

Graphical abstract



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1. Introduction

In the 21st century, the use of technology in educational environments has become increasingly common. The importance of using Digital Information and Communication Technologies (DICTs) is notable in the academic environment. According to Souza and Carvalho (2023), their use can promote the interaction between practice and theory in chemistry teaching, in which new practices can emerge that bring technology and education closer together. In addition, it

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can also promote the formation of critical citizens who are active in society [1, 2]. However, technology alone is not enough for the educational process. Qualified support is needed to develop activities for the new generation to improve their ability to read, interpret, and explore various educational content and to search for information in digital media [3, 4]. In addition, schools should have a structure to incorporate new technologies and integrate the spaces of leisure and study [5]. In 2001, Prensky created the term 'Digital natives' to refer to the generation of people born of people born around 1980, who have lived with technologies since the beginning of their lives and for whom interacting with computers is a common day-to-day task [6]. Digital natives are believed to possess sophisticated technical skills and learning preferences for which traditional education is unprepared [7].

Chemistry teachers face several problems that are not restricted to Chemistry but to all Science teaching. Teaching centered on the teacher, the lack of contextualization, the absence of experimentation, and the deficient structure of laboratories and reagents are obstacles to be overcome [8–12]. Although some teachers develop teaching plans based on experimentation and daily practice, they generally reflect personal beliefs and previous experiences, with a simplified view of teaching prevailing, centered on the transmission of content and assessment through tasks and grades [13].

In addition, students' difficulty in understanding theoretical content is also an obstacle to being overcome by teachers of this discipline, and in this regard, the various methodologies can be the path to didactic transposition. At the same time, in the teaching of Chemistry, diversified methodologies have been successfully used by providing a better understanding of theoretical contents, which are commonly described by students as abstract, thus facilitating the didactic transposition of contents. For Garcez and collaborators (2012), the teacher, when taking over a classroom, should seek alternative methodologies to facilitate learning about the contents and collaborate with the awareness of the importance that Chemistry presents to everyday life [14].

In this context, Molecular Modeling (MM) has been recognized as an interesting tool in teaching subjects such as medicinal chemistry, biochemistry, biology, chemistry, and physics [15–18]. This tool may help in the understanding of chemical contents since it allows the visualization of molecules as well as properties that physical models normally cannot show [19]. Thus, the abstract structures, that are generally shown as immovable figures, take shape, and can be visualized dynamically, which promotes the student's interaction with the object of the study and facilitates the learning of concepts and their applicability [20–23]. There are several options for free or paid software of molecular modeling that provide much more than just the visualization of molecules in a three-dimensional space. In addition, they offer a set of calculated property values, such as the potential energies of the molecules, the orbital contour coefficients, and the electrostatic potential map, among other information. These tools are important to develop visuospatial skills in students, fundamental aspects for understanding different chemical concepts [24, 25].

Thus, this study aimed to evaluate the use of molecular modeling tools for visualizing structures and teaching chemistry and biology in an integrated manner. The mini-course named "Is there chemistry in food?" last two hours and was carried out with high school and undergraduate students.

Theoretical framework

The theoretical basis of Technological Pedagogical Content Knowledge (TPACK) is centered on the fact that teaching requires more than just content or pedagogical knowledge in isolation, and it is up to the teacher to understand how to integrate it with technology to enhance learning [26–30].

Developed by Mishra and Koehler (2005; 2006), TPACK expands on Shulman's concept of Pedagogical Content Knowledge (PCK), which states that effective teaching requires more than mere expertise in a subject area but also requires a nuanced understanding of how to present content in ways that make it accessible and engaging for students [31, 32]. Building on PCK, Mishra and Koehler considered the increasingly vital role of technology in education, leading to the inclusion of technology as a central component to help teachers navigate digital tools and platforms [26, 30].

In addition, the TPACK framework draws on constructivist theories of learning, which emphasize that knowledge is constructed by students, highlighting the importance of aligning content with students' experiences and the context of learning in which students are immersed in their daily lives. Through it, teachers can create learning environments that support active engagement by combining technologies with pedagogical approaches that allow students to question and explore content in meaningful ways [29]. Saubern et al. (2020) emphasize the relevance of TPACK to educational technology research but also suggest the need to focus on how teachers can bring this integrated knowledge into practical applications in the classroom [27]. Meanwhile, Albeta et al. (2023) suggest that TPACK-based blended learning, where technology allows flexibility and promotes student engagement through multimedia formats. This approach favors adaptive and forward-thinking teaching practices, promoting innovative learning experiences, with the student at the center of their learning process, aligning with the skills enabled in the 21st century [28]. The framework encourages teachers to offset old and ineffective teaching practices by allowing them to incorporate tools that promote interactive, personalized, and differentiated learning. By understanding TPACK, educators can customize learning experiences that are not only content-rich but also engaging students through technological tools. Although TPACK has been widely adopted, there are ongoing debates about its theoretical and practical challenges. Some researchers, such as Graham (2011), highlight the "fuzzy boundaries" of TPACK, making it difficult for teachers to clearly distinguish between TPACK components when applied in real-world scenarios [26]. To alleviate these limitations, the researchers recommend refining the definitions of TPACK components and focusing on developing tools that measure how effectively teachers integrate technology, pedagogy, and content into their instructional practices. This will enable teachers to meaningfully integrate technology into their teaching practices, meeting the diverse needs of students, and preparing them for today's technology-driven world [26–29].

2. Results and Discussion

A total of 303 students participated in the course, 136 students (44.9%) from High School (HS) and 167 (55.1%) from undergraduate (UG) courses. Most of the HS students were female (n = 70; 55.5%) and aged between 15 and 26 years. Most UG students were also female (n = 138; 82.6%), aged from 17 to 48 years and participants (58.1%) were from the

Pharmacy course, 67 (40.1%) from the Biological Sciences course, and 3 (1.8%) from other undergraduate courses.

Among UG students, 154 answered they use the computer to study, 11 of them did not use it and 2 did not respond. When asked if they struggled with using computers, 138 answers were negative, and 29 were positive. Among HS students, 113 said they use a computer to study, one of them uses it occasionally, 21 did not use it, and 2 students did not respond. Also, 125 HS students answered that they are not struggling with using a computer, 10 reported having some difficulty and one of them answered that it depends.

Regarding the survey on the interest level in chemistry and biology, HS students declared greater interest in chemistry than in biology, while UG students showed greater interest in biology (Table 1).

Before the practical class, we asked the opinion of the students about having practical classes related to chemistry or biology using the computer. The answers were grouped into 8 mutually exclusive categories that emerged according to the analysis of their content (Table 2).

Table 1. Level of interest in Chemistry and Biology contents. HS = High school; UG = Undergraduate.

Interest Level	Interest in Chemistry		Interest in Biology	
	Number of Students		Number of Students	
	HS	UG	HS	UG
High	25,74% (35)	35,93% (60)	27,94% (38)	82,63% (138)
Moderate	55,88% (76)	48,50% (81)	43,38% (59)	14,97% (25)
Little	13,24% (18)	13,17% (22)	20,59% (28)	2,4% (4)
None	5,15% (7)	1,80% (3)	7,35% (10)	0%
No answer	0%	0,60% (1)	0,73% (1)	0%

Table 2. Categorizing students' opinions about carrying out practical classes related to chemistry or biology using the computer.

Groups	HS	UG
Positive opinion without justification	55	45
Emphasis on the practice itself	8	5
Emphasis on innovative, fun, interactive, or dynamic character	10	14
Contributions to learning	47	38
Visualization of molecules or other images	10	9
Participants who showed no interest or conditioned it to something	22	15
Others	10	7
No answer	5	3

Most of the students (100) had a positive opinion but did not justify their answers. Of those who justified their answers, 85 reported the importance and contributions to learning, and 24 students stated that it may be innovative, fun, interactive, or dynamic. Also, among the positive opinions, 13 students reported the issue of practice as the main reason, and 19 participants said that the main justification was the possibility of viewing molecules or images. On the other hand, 37 students did not show interest in or condition it (Table 2).

Considering that teaching chemistry in both HS and Higher Education is seen as demotivating, new alternatives and methodologies are increasingly needed for students to understand the content studied [33].

The mini-course "Is there Chemistry in Food?" presents the contents of chemistry and biology in an integrated manner and work themes from the daily lives of students, which incites their interest in the class. Additionally, the use of computational tools promotes greater freedom for students to explore the resources and creates a familiar environment for their learning. Most participants (n = 268) say they have the habit of using computers to help in their studies, and 263 said they had no difficulties in using it.

The first molecule explored in the activity was water. We showed the dynamic three-dimensional (3D) structures as well as the vectors of each covalent bond and the resulting vector, called dipole moment, and the electrostatic potential map. In a traditional theoretical class, these water's properties would be taught using mathematical calculations that are abstract and barely noticeable. In the water molecule, hydrogens are less electronegative than oxygen, so they have positive partial charges, and due to the angular geometry of water, its dipole moment is different from zero, meaning it is polar. In the minicourse taken, the water molecule was presented with the dipole vectors, showing the electrostatic potential map and its geometry in a more interactive way that makes understanding these subjects easier (Figure 1). Likewise, while the students observed the 3D molecule, the characteristics of water, such as its solubility and its intermolecular and intramolecular interactions, were explained.

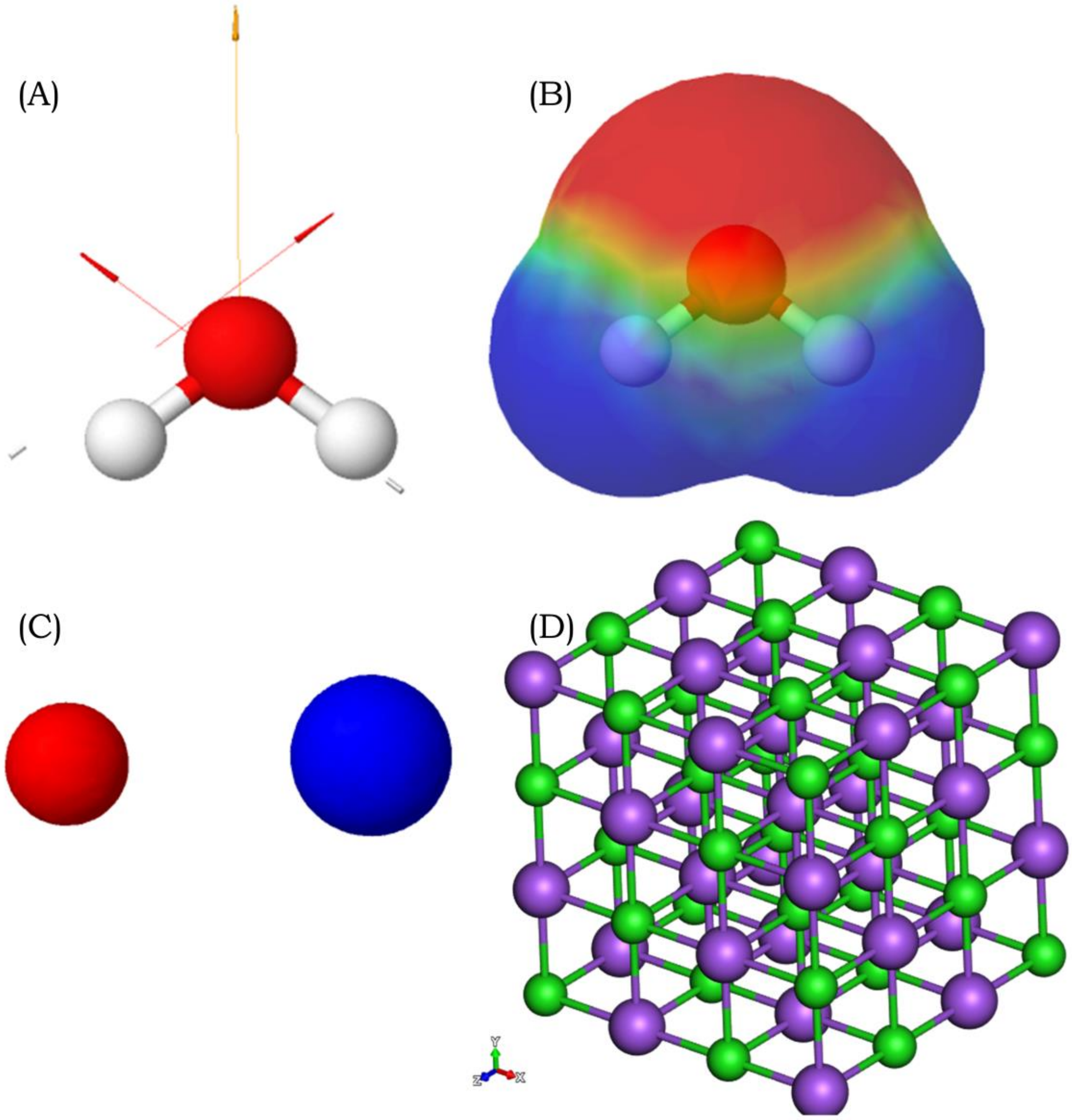

Fig. 1. Water and salt. A) 3D structure of water molecule with the dipole vectors and the resulting vector (overall dipole moment); B) Electrostatic potential map for the water molecule (in red is the most electronegative region and in blue the most electropositive region); C) Representation of the ions Na and Cl; D) Structural representation of the sodium chloride crystal. MolView online server was used for 3D visualization.

Rossiere (2020) reflects on how chemical language is complex, with difficult names, shapes, and symbols that are important and necessary, but that can contribute to the teaching of chemistry being considered far from the reality of the student, who does not connect with the daily life and may lose interest in the discipline [34].

To approach the reality of the student with the content offered in the course, sodium chloride was mentioned referring to table salt. It was also interesting to hear from them regarding the solubility of the salt after the explanation of how water acts on the crystal, as they were able to relate the topic addressed with their own experience.

During the activity, several types of sugars and their respective classifications were addressed. The students were able to visualize the structure of the sugars (Figure 2) such as glucose, sucrose, lactose and amylopectin and they calculated their hydrophilic character.

According to Gonçalves and Goi (2020), the cause of students' lack of interest in Natural Sciences may be because they are unable to relate the content studied in the classroom with their daily activities, then, the students memorize what they have learned and quickly forget it [35]. To make the activity even closer to the student's social context, and make the learning process more enjoyable, lipids were also included. After all, who has never wondered why vegetable oils are liquid and butter, also a lipid, is solid? And this was one of the examples addressed in the activity.

During the explanation about lipids, melting points, saturation, and unsaturation of fatty acids were addressed. Using the MolView Program, students could visualize the structures of oleic and stearic acids (Figure 3) and analyze the possible existing intermolecular interactions.

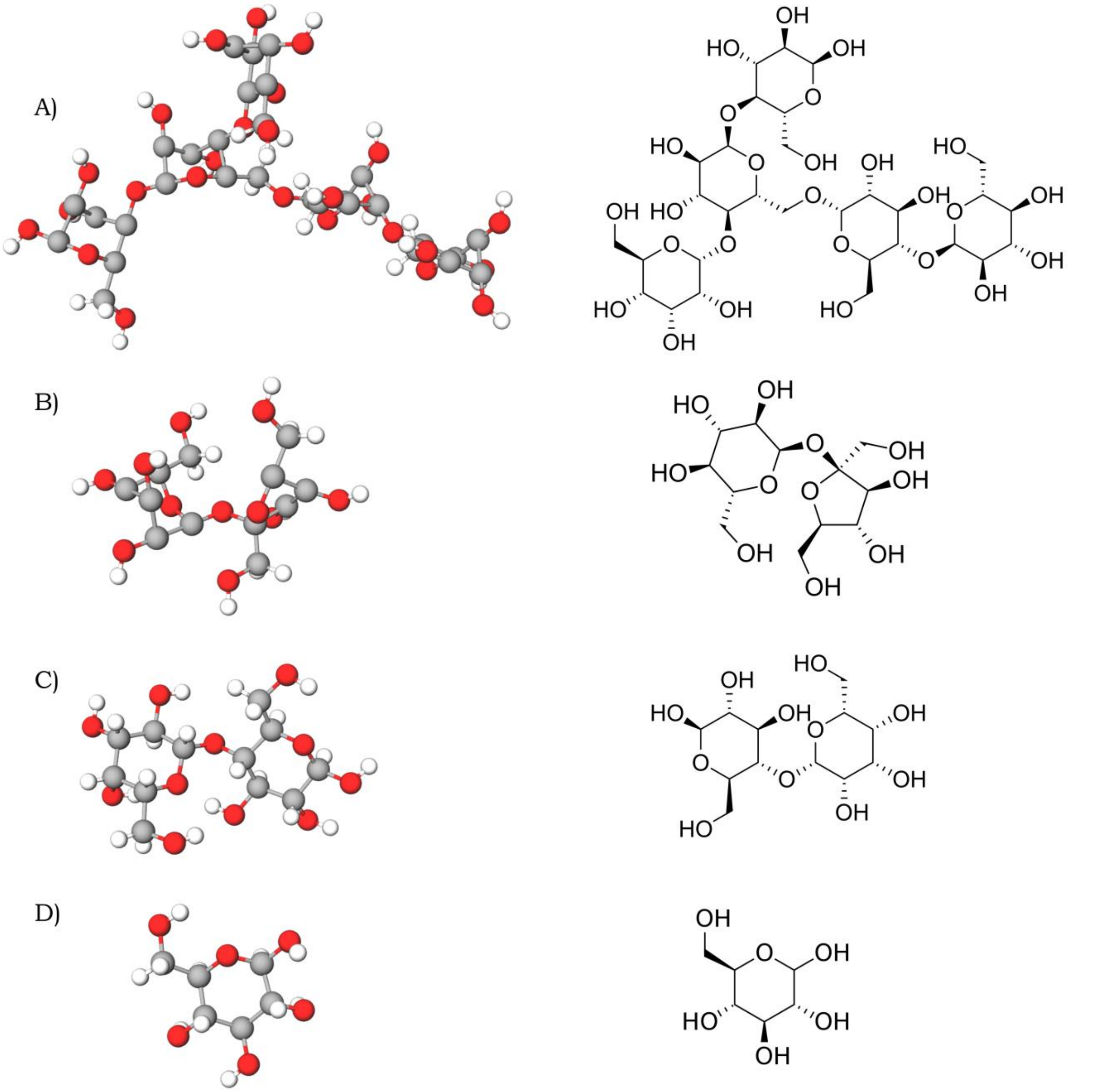

Fig. 2. 3D and 2D structure of carbohydrates A) amylopectin; B) sucrose; C) lactose; D) glucose. MolView online server was used for visualization.

Wide access to the use of technologies has given teachers the chance to reorganize curricula and make the most of this technological potential, creating new ways of teaching, questioning, and visualizing [36]. In traditional teaching, the functions of proteins are usually taught, but their structure and how they are formed are rarely shown. New computational tools aimed at research and teaching emerged to facilitate this learning and visually show the composition of macromolecules, such as proteins, more dynamically and interactively, which was not possible through textbooks.

To understand more about proteins, collagen was shown as the famous gelatin, either colorless or full of colors and flavors. This part of the course started with the following questions: "How do you make gelatin? In hot or cold water? Have you tried doing it in ice water?" These questions stimulate curiosity. The 3D structure of collagen was shown (Figure 4), in which the triple helix could be observed. They also form collagen fibers that are present in the skin.

The other protein shown was hemoglobin, with their four chains, and the HEME groups present (RCSB PDB 1GZX) [37]. The importance of iron and oxygen was also addressed (Figure 5). They are also able observe the 3D structures of DNA with its double helix correctly linked to adenine and thymine, cytosine and guanine, and the mutation induced by a fungus toxin, named aflatoxin (RCSB PDB 1MK6) [38].

Regarding the 16 specific questions of Chemistry and Biology, the average number of correct answers before the course was 43.66% for HS students and 63.51% for UG students. After carrying out the proposed activities, the average number of correct answers increased for both HS and UG students, 62.14% and 80.50%, respectively (Table 3).

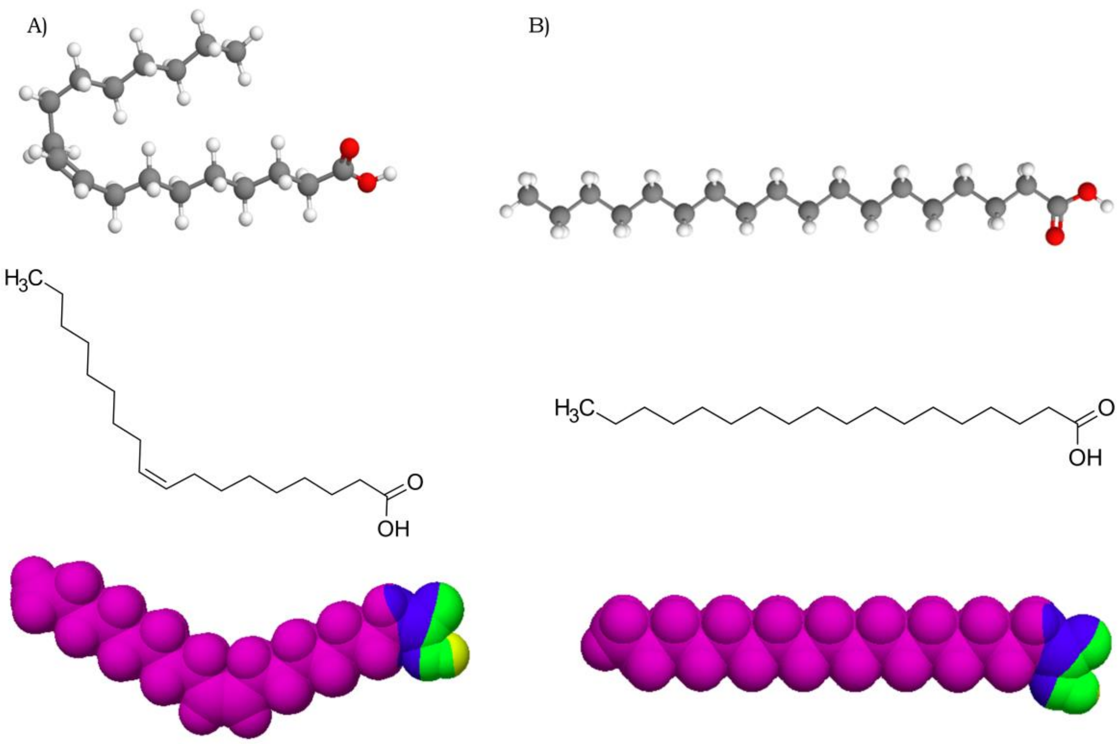

Fig. 3. 3D and 2D structure and molecular lipophilicity potential map (MLP) of the lipids A) oleic acid; B) stearic acid. MolView online server was used for 3D visualization, and Molinspiration server was used for MLP maps.

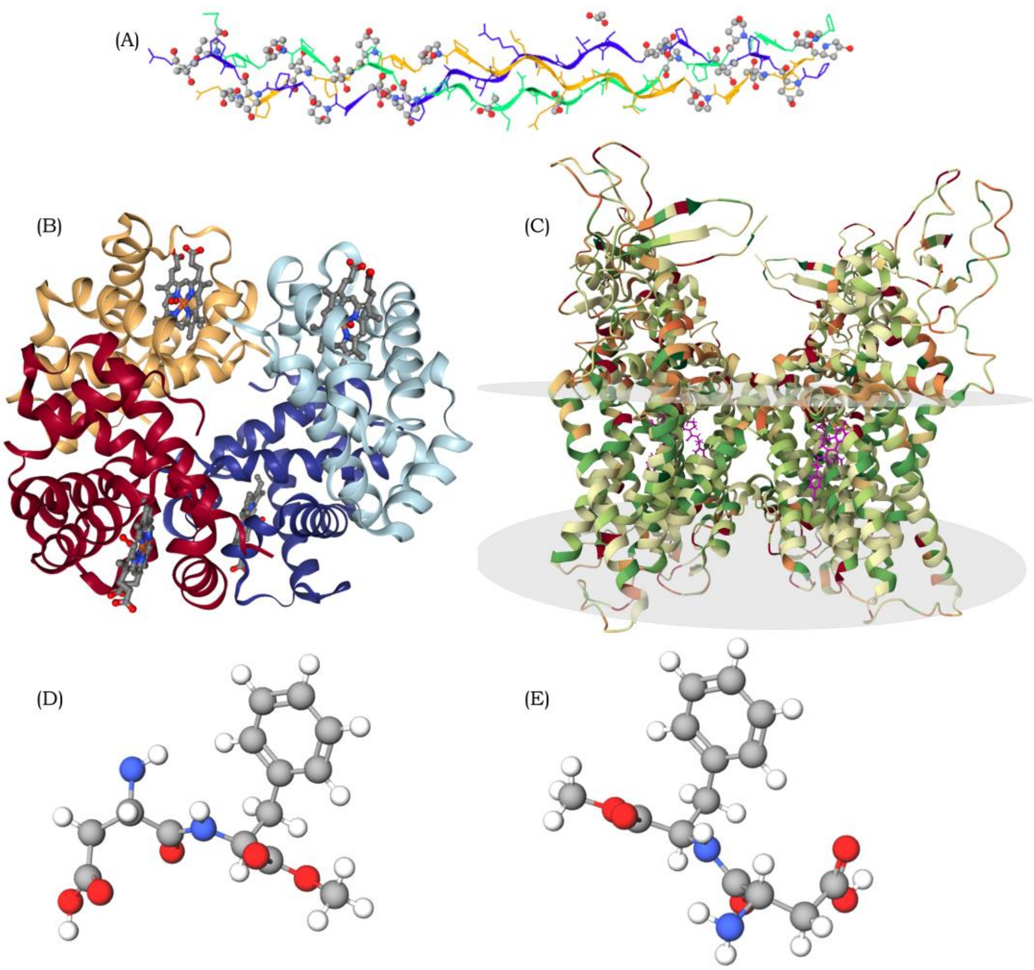

Fig. 4. Structural representation of proteins and amino acids. A) collagen; B) hemoglobin (PDB ID 1GZX); C) receptor TRPV1 in complex with capsazepine (PDB ID 5IS0); D) aspartame molecule; E) L-aspartyl-D-Phenylalanine methyl Ester. MolView online server was used for 3D visualization.

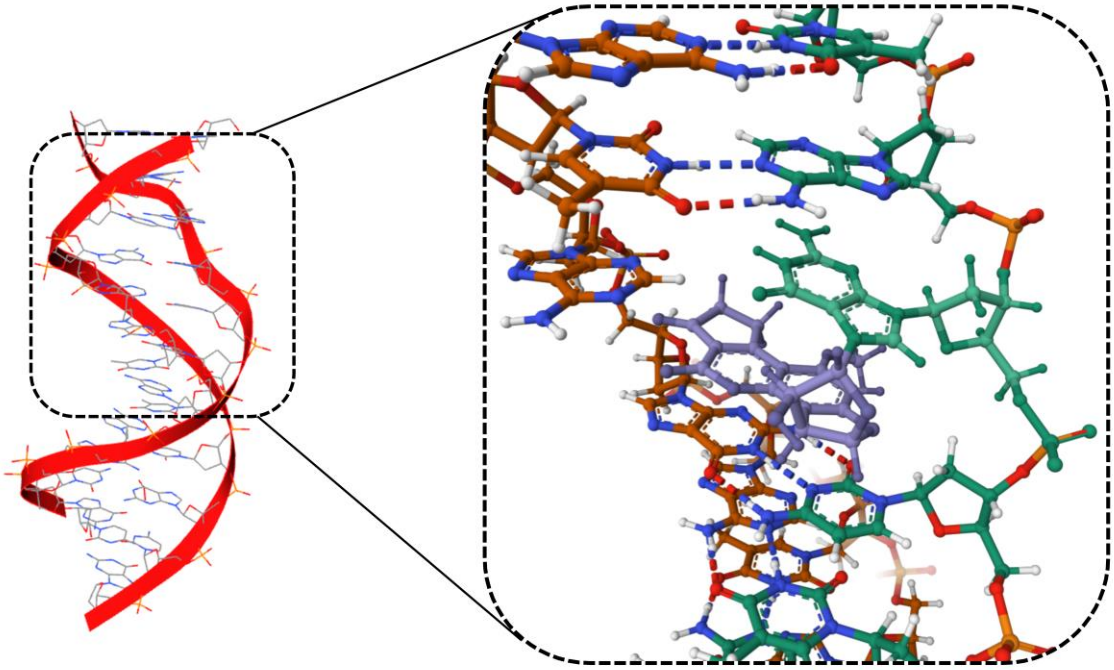

Fig. 5. Structural of the aflatoxin intercalated into the DNA strand (PDB 1MK6).

Table 3. Percentage of correct answers before and after the activities performed by HS and UG students.

	Questions	HS			UG		
		Before	After	IH	Before	After	IH
1	What kind of molecule is water?	72.80%	89.70%	16.90%	94.00%	98.20%	4.20%
2	What type of interaction/bond occurs between oxygen and hydrogens to form a water molecule?	55.20%	66.20%	11.00%	32.90%	75.20%	42.30%
3	What are the basic units that makeup proteins?	69.90%	79.40%	9.50%	95.20%	94.60%	-0.60%
4	Which mineral present in food is important to form the heme group of hemoglobin, and it lack is related to a type of anemia?	50.70%	75.70%	25.00%	81.40%	93.40%	12.00%
5	What type of interaction/bonding occurs to form sodium chloride?	48.50%	62.50%	14.00%	63.50%	74.30%	10.80%
6	Amylopectin, the main component of starch, is a polysaccharide, which means it is made up of several units of:	26.50%	25.70%	-0.80%	62.30%	64.10%	1.80%
7	Are there toxic substances that when ingested in food can cause DNA mutation?	34.60%	80.90%	46.30%	48.50%	85.60%	37.10%
8	Comparing natural long-chain fatty acids, which generally have a higher melting point and therefore are generally solid at room temperature?	23.50%	44.10%	20.60%	34.70%	61.10%	26.40%
9	The sucrose molecule is a sugar that has more regions:	44.10%	72.80%	28.70%	67.70%	86.20%	18.50%
10	Is collagen from food used directly as it is ingested to form the skin and other body tissues?	30.90%	42.70%	11.80%	40.70%	76.10%	35.40%
11	What are the basic units that make up deoxyribonucleic acid (DNA)?	44.90%	61.80%	16.90%	86.20%	94.60%	8.40%
12	Can mutations that occur in DNA lead to the formation of defective proteins?	52.20%	78.70%	26.50%	82.60%	91.00%	8.40%
13	Stearic acid is an 18-carbon fatty acid present in animal and vegetable oils and fats. In its structure are present more regions:	33.10%	72.10%	39.00%	73.10%	87.40%	14.30%
14	From the breakdown of lactose, glucose can be obtained, which is a molecule that provides energy to the body:	61.00%	79.40%	18.40%	71.30%	88.60%	17.30%
15	Proteins have the same three-dimensional structure despite having different functions.	22.10%	27.90%	5.80%	41.90%	55.70%	13.80%
16	Oils like soy and canola that we use in the kitchen have more fatty acids of what kind?	26.70%	34.60%	7.90%	40.10%	64.70%	24.60%

IH = incremental hits

Regardless of schooling, students in general showed an increase in correct answers after the mini-course class, indicating that the activities contributed to the understanding of the concepts covered. For HS students, the number of correct answers increased by 18.5%, except for question 6, and for UG students, this increase was 17%, except for question 3.

Even with the practical activity lasting only 2 hours it already promoted an increase in the performance of the students and greater learning about the issues were addressed.

Regarding the difficulty level of activities for HS students, 106 participants did not have difficulties in understanding the contents covered in the practical class, 4 did not respond, and 26 said they had difficulties. Among UG students, 118 had no difficulties, 47 had some, and 2 did not respond.

The students carried out an evaluation of the activities developed. Of HS students, 133 (98%) considered the activities positive, one said that at first, the activity was interesting but then it became tiring, and another rated it as reasonable. For UG students, one did not answer, and all others evaluated positively, demonstrating good acceptance of the methodology applied in the course.

Finally, when asked if they thought molecular modeling could contribute to the teaching of chemistry and biology, all UG and HS students responded affirmatively, except for one HS student who did not answer this question.

The general analysis of this work revealed that the course applied to HS and UG students, working with computational tools, helped the understanding of chemistry and biology content, which is usually difficult to understand because it involves structures and interactions that cannot be visualized in isolation. This positive evaluation also occurred with other authors that applied this tool to the teaching of chemistry to basic education students young people and adults [12, 33–36, 39–44]. These authors revealed a significant improvement in learning when they used some unusual educational resources such as experimentation, educational games, or software, as well as education in non-formal spaces and playfulness.

Successful examples of the use of molecular modeling for teaching chemistry or biology can be observed, such as Ramos and Serrano (2015), which used molecular modeling to teach Cis/Trans stereochemistry for students in the first semester of the technical course in chemistry at a federal institute [19]. Another study analyzed the possibilities of meaningful learning for Biology Teaching, with the mediation of molecular modeling tools. In this study molecular modeling also allowed a significant improvement in the understanding of the structure and function of DNA, proving once again the importance of the tool [17].

This work matches Paulo Freire´s [45] proposal, who defends questioning learning as a way of “educating and educating oneself” and that criticizes the vertical relationship in education where the teacher is responsible for transmitting all the knowledge it holds, sometimes in an authority way. Rather, the teacher may mediate the learning in a dialogical way to sharpen all curiosity in students, forming questioning and critical students involved with the world in which they live. Several authors [33–36, 40–44] revealed significant improvement in learning when they used some resource educational experience such as experimentation, educational games or software, as well as education in non-formal spaces and playfulness.

3. Material and Methods

This is an observational, quali-quantitative study in which the use of a teaching strategy for chemistry content was evaluated. The Mini-course named “Is there Chemistry in Food?” was carried out in the context of the University extension project named "Virtual world". Practical classes lasted approximately two hours and were carried out in the computer labs of the Federal University of Rio de Janeiro - campus Macaé and in schools from Macaé city, and the target audience was undergraduate and high school students.

In the practical classes, the contents of chemistry and biology were addressed in an integrated way. We showed the structure and function relationship of the components present in food (*e.g.* proteins, carbohydrates, lipids, mineral salts, and water, besides toxic compounds present in foods that can affect DNA).

A tutorial (Supplementary material) was developed containing brief questions about the molecules visualized in the course and the commands and procedures needed to visualize their structures and properties (Table 2). During the practical classes, besides the teacher, there were trained monitors to assist the students in carrying out the tasks.

For the activity, the servers MolView (**https://molview.org/**), RCSB Protein Data Bank visualizer 3D [46, 47] and Molinspiration Galaxy 3D Structure Generator v. 2018.01 beta (**https://www.molinspiration.com/cgi-bin/galaxy**) [48]. These tools are freely available online and allow for the three-dimensional visualization of molecules as well as calculations of some molecular properties.

To assess the potential of molecular modeling as a learning tool, participants answered two questionnaires. The first questionnaire applied before the practical class consisted of general questions such as age, name, education, and 16 multiple-choice questions about chemistry and biology issues that were covered during the practical class. The second questionnaire was applied at the end of the minicourse, with the same 16 multiple-choice questions and open questions asking the students' evaluations about the activity.

The data obtained from the questionnaires were analyzed by descriptive statistics using the Excel program and the effectiveness of molecular modeling tools as a didactic resource and the participant’s opinions were verified by analyzing their responses. Participants agreed to answer the questionnaires, and all participants’ names and any information that could identify them were kept confidential.

4. Conclusions

Learning has been carried out traditionally for a long time, but the reality and behavior of young people have changed significantly with easier access to digital technologies such as smartphones and digital games. New tools in the learning process, such as molecular modeling applied in the present work, motivate students to be interested in the proposed content, in this case, chemistry and biology. In the present study, after participating in the course, students from HS increased the correct answers by 18% and those from UG by 17%. This fact shows the importance of using different alternatives so that the student can be an effective agent of their learning. During the application of the activity, we verified that the students were enthusiastic and very excited about the course, being able to associate the content learned in their daily lives.

Despite this, this study has limitations related to the short time taken to complete the tutorials with the students, as well as the small number of participants. We think these tools could be more efficient if they were used in more classes. Furthermore, knowledge here is not a fully measurable variable, considering that everyone has their own pace and way of learning. However, the data obtained through the questionnaires applied, combined with the enthusiasm demonstrated by the students throughout the mini-course, indicate that the approach adopted contributed to a clearer and more concrete understanding of the concepts of Chemistry.

Thus, we concluded that the methodology proposed was valid to arouse the students' interest and that the computational resources were a useful tool in the teaching-learning process of the proposed themes. Furthermore, the project continues to be carried out in different classes, reaching not only the students but also the teachers who teach in HS.

Supporting Information

MINI-COURSE TUTORIAL: Is there Chemistry in Food? A tutorial containing brief questions about the molecules visualized in the course and the commands and procedures needed to visualize their structures and properties.

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Author Contributions

Study design, PASCHOAL, C.R.S.; de SOUZA, I.G.M.; BARBOSA, N.P.; SILVA, P.L.; VIEGAS, D.J.; ABREU, P.A.; Development, PASCHOAL, C.R.S.; de SOUZA, I.G.M.; BARBOSA, N.P.; SILVA, P.L.; VIEGAS, D.J.; ABREU, P.A.; Analysis and interpretation of data, PASCHOAL, C.R.S.; de SOUZA, I.G.M.; ABREU, P.A.; Final writing, PASCHOAL, C.R.S.; de SOUZA, I.G.M.; BARBOSA, N.P.; SILVA, P.L.; VIEGAS, D.J.; ABREU, P.A.

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