



Molecular Modeling as a Didactic Tool in Organic Chemistry Teaching on Some Abuse Drugs Thematic

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Authors' contributions

This work was carried out in collaboration between all authors. All authors read and approved the final manuscript.

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ABSTRACT

Aims: Chemistry is a complex science, due it theories explain the phenomena at the microscopic level, making the concepts of it difficult to understand, which restrict students perception. This work demonstrates the importance of Information and Communication Technologies (ICTs) to the organic chemistry teaching with a thematic approach on drugs using molecular modeling as a didactical tool in the teaching and learning process.

Place and Duration of Study: The research was conducted in Amapá State University (UEAP), located in the city of Macapá-AP, Brazil.

Study Design: The population sample consisted of randomly academics degree course in the

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second chemical semester and the data were collected through questionnaires.

Methodology: The research presents quantitative characteristics and the sample group consisted of 24 undergraduate students from UEAP, equally divided into two groups: Control Group (CG) and Intervention Group (IG). In the first part the questionnaires were applied to students of both groups to check the perceptions, conceptions about drugs and molecular modeling. In a second part was held a class lecture to the academic groups, which were showed concepts about drugs, classification, law, chemistry drug-related, and study for molecular modeling, followed by questionnaires. In the third part, an introductory course in molecular modeling to 12 students of the intervention group (IG), using the ChemSketch software, being treated together, the theme drugs and application of molecular modeling by applying the questionnaire to the intervention group after the course. The answers from both groups were compared and observed the level of knowledge of students before and after the inclusion of the introductory course in molecular modeling.

Results: The study revealed a considerable difference in the results obtained after three different parts, the first two times were simultaneously experienced by both groups (CG and IG) and the third time only the IG participated of the introductory course in molecular modeling. After evaluate the data obtained by the students on the theme of drugs, molecular modeling and their approach on organic chemistry respectively, was possible to notice in the proposal questions the growth of the hit rate and therefore the reducing errors. Regarding the concept drugs and the differences between the terms medicines and pharmaceuticals, Issue 1, Part 1 (62.50%), Part 2 (83.33%) and Part 3 (91.67%). In this question the errors were related to difficulties in distinguishing academic terms: drug, remedy and medicine, as well as its relationship to the body. Regarding the complexity of molecular modeling as a tool, Issue 3, said "no" respectively, Part 1 (37.50%), Part 2 (71.00%) and Part 3 (83.33%). The assimilation of basic information on modeling and later the performance of the course contributed to increase the hits. About the potential offered by molecular modeling software when inserted into the chemistry teaching, question 8, it was found the following rates of correct answers, Part 1 (29.17%), Part 2 (62.50%) and Part 3 (75.00%). The lack of in-depth knowledge on the subject was dominant for the low rate at the beginning, but after the theoretical explanations and further the practice classes, which selected IG had the opportunity to combine theory with practice and explore the chemical potential offered by modeling molecular organic chemistry as a facilitator of this drug, the indices were reversed.

Conclusion: The dynamism of the teaching and its constant changes require both, the professor and the institution, different strategies in an attempt to provide a more meaningful education. From this perspective, we observe that professors should always seek skills and training in order to improve their teaching methodology, diversifying their classes, creating other learning environments, contextualizing with the academic daily, providing greater interaction and understanding their science, these characteristics have been acquired and well accepted by the inclusion of molecular modeling in organic chemistry teaching focused on drugs, making learning more meaningful.

Keywords: Molecular modeling; didactical tool; organic chemistry teaching; drugs.

1. INTRODUCTION

To become the complex process of learning more effective, the professor as the mediator of knowledge plays an important role. To that, beyond knowledge that is inherent, they need to develop some skills and abilities to involve their students, allowing them to assimilate the concepts in the best way. Therefore, the search, improvement and adaptation of didactic tools can become a differential attempt to reach a quality education, which also emphasizes the compromise of the superior Institution providing the whole necessary structure, resources and training to promote a more effective human progress. The scientific evolution enabled the

development of diverse sectors of society, as an education, health, industry and technology, among others, which offers to the educational area the Information and Communication Technologies (ICTs), tools that are responsible to transmit the information to contribute to the innovative teaching practices and encourage the learning of disciplines [1,2].

The ICTs can be understood as the combination of information technology (IT), which term replaced in the late 1980 the computers when the data processing, started to give more emphasis on ability to store and retrieve information with other related technologies, specifically, the communication technology [3].

The ICTs are essential and important technology tools that make possible the representation, communication and knowledge of information, which is able to help the knowledge construction through participation, creation and interactivity between students and professor, these characteristics are look for the institution to training the individuals as critics and good professionals. To reach it, they employ since the simplest technological resource as a pen, but also computers, Internet, educational software's, among others [2].

Since 1998, the National Curricular Parameters (PCN) highlight the teacher's role to know the realities that their students are inserted in order to adapt them in the process of teaching and learning at various levels and curriculum areas, and one of the teaching strategies to be used are come from the development of sciences and technological, to help them in the search for a more meaningful learning [4,5].

National Curriculum Standards of high school, in accordance with the Law of Guidelines and Bases of National Education (LDB 9.394/96), were designed by educators from all the country at the request of the Ministry of Education (MEC) with the purpose of promoting curricular reorganization in knowledge areas and support the teachers in the search for new approaches and methodologies, these objectives aimed to filling the gaps of an educational previously, compartmentalized and based on memorizing of informations. Therefore, the document gives more meaning to knowledge by contextualization, avoiding fragmentation through interdisciplinary and thus enable the further development of student cognition, so that the knowledge is constructed in an integrated and significantly way [6].

Despite the validity of the parameters, its objectives are still far from being materialized, as the current teaching of chemistry developed in high school is still predominantly traditional, which means theoretical, fragmented, disconnected from content with each other and the social student [7]. The teaching of organic chemistry, mostly practiced in high schools comes down only to the theoretical way, which knowledge is delivered to you ready and finished without carrying out practices and their proper correlation with the student daily life, limiting them to simply memorizing names, formulas and concepts, restricting the scientific knowledge and hence the full exercise of citizenship [8]. This practice still exists and highlights the contrast

between what the parameters exalt and which is performed in the classroom.

The relevant thematic approach for school in society context, as the chemical education in the case of drugs, it is a teaching strategy used by professors in attempt to Acquiring Scientific Knowledge through the problems experienced by students day-by-day, so giving them the sense in chemical, social, cultural and economic aspects, expanding their vision field about the world that they live and put them close to science using teaching tools, such as newspapers, magazines, documentaries, internet and other technologies [9,10].

The chemical knowledge is indispensable for understanding the world, the individual will have a limited view without ownership from the fundamental principles of chemical science, which provides a critical vision, the ability to analyze and intervene in their daily lives in order to contribute to their quality of life [11]. However, to happen it in a satisfactory way, the study of chemistry cannot be restrict to theories that limit the imagination of students, it is important some specific features that help interpret, understand and represent the chemical phenomenas, as three different levels: Macroscopic, microscopic and symbolic. While in macroscopic state the chemical phenomena are observable and measurable, in microscopic, they are explained in terms of particles, atoms, ions and molecules, both are represented symbolically by: formulas, equations, numbers, graphics, symbols and coefficients [12,13].

One of the main challenges faced nowadays by chemistry professors, is the great complexity of understanding and representation of chemical concepts by students. This is because of the complexity of this science, whose studies are based on the explanation of macroscopic phenomenas, and mostly studies aimed at the microscopic level, making it difficult to understand the concepts, restricting the student's perception. Although with the advent of science technology in the last decades, allowed the development in this scenario, professors already have computer tools and modeling to be adapted in their pedagogical approaches, which improve his representative capacity at molecular level phenomena. In this way, the integration of it into chemistry curriculum can make a difference in the conceptual understanding of certain chemical phenomena [13,14]. Through the computer, you can transform two-dimensional images into

three-dimensional books, making them to move, providing within the teaching-learning process that the described theory can be simulated, visualized and thus better assimilated [15,16].

The use of learning resources from technological advances in education, such as the computer, arise from the search for innovative and effective alternative that enables a good integration in teaching practice, providing opportunities to create new learning environments, allowing the relationship between theory and practice, that overcome the barriers imposed by the traditional method of teaching, combined with the real problems faced by society, making the science more exciting and thus the learning process occurs naturally [14].

Lately, it has been disseminated and introduced in undergraduate chemistry courses, the use of molecular modeling as a teaching tool, highlighting the importance of computer technology innovation as a resource for educators develop cognitive skills in their students, making these information producers, rather than merely passive consumers. This tool is transforming the way of seeing and thinking about chemistry ,since then, " it has never been so easy to see graphically the properties and behavior of chemical systems, exploring the chemistry integrated, interactive, attractive in totally new way" [17].

Due to the big scientific knowledge acquired and propagated during different times, what allowed the chemist unlock the secrets of material, their physicochemical properties, conducting them to develop theoretical models based on concepts of atoms and molecules able to reproduce, control, studying the chemical reactions and develop new materials, so appeared the molecular modeling [18]. Molecular modeling is a branch of chemistry that uses the computer as a tool to build and manipulate models. Through the models is possible to represented briefly some physical and real objects phenomenas, to that it is employed the chemical and theoretical studies of computer graphics, to facilitate the visualization, manipulation, analysis and a reporting about the molecule [19].

In the perspective to seek improvements in organic chemistry teaching, as well as become it more significant, trying to ameliorate the concepts in drug thematic was offered the resources from development of ICT, which is still little explored by Amapá state education. The Work was focused on chemistry academic

degree students in Amapá State University, to verify the perceptions and conceptions on drugs and molecular modeling using the ChemSketch program [20] as a didactic tool to make the teaching-learning process easier.

2. MATERIALS AND METHODS

2.1 Research Place and Target Audience

The research was conducted in Amapá State University (UEAP) located in the city of Macapá - AP, Brazil. Initially 24 students of the full degree in chemistry course from second semester were randomly selected. These students were divided into two groups: Control Group (CG) and Intervention Group (IG), each group consisting of 12 academics.

2.2 Construction of the Questionnaires

The research presented experimental qualitative character, with the application of closed-ended questionnaires. The questionnaires had objective to evaluate the level of understanding of academic full degree course in chemistry UEAP on the differences between the terms remedies and drugs; verify if the academics know the themes classifications; the organism targets and its effects; identify if the academic students know this tool and its practicality; identify the level of academic students information related to the use of molecular modeling software; establish a theory based on the theme drugs, like: Classifications, effects and its relation to organic chemistry, assess the level of information related to the molecular modeling potential before and after the course, identify how conceptions of academics on using this tool and make them aware about the role of teacher to develop skills and abilities, evaluate how the academics understand the potential offered by a molecular modeling software when inserted into the chemistry teaching.

2.3 Methodological Parts

This work was developed in three methodological parts.

2.3.1 First part

In this part, the questionnaire was applied to students of both groups to check the perceptions and conceptions that they know about drugs and molecular modeling.

2.3.2 Second part

In the second part, there was a lecture to students of both groups, addressing in context the topic drug under the following aspects: social (crime, traffic accidents and contamination with the AIDS virus), chemical-biological (concepts, classification, site of action in the body, effects and its relation to organic chemistry) and about the legislation (Law No. 8.069/90 of the Children and Adolescents, Article 81 and Law No. 11.343/06, establishing the National System Public Policy on Drugs (SISNAD), Article 2° and 28). A theoretical exhibition was held on the applications of molecular modeling in chemistry of drugs. After that was applied again the questionnaire to both groups.

2.3.3 Third part

On the third part, the introductory course in molecular modeling was taught only to the students of the intervention group (IG) using the software ChemSketch 12.00 as a facilitating tool in the teaching and learning process. In the IG was emphasized the use of the programs based on three-dimensional (3D) simulations of the molecules studied (ethyl alcohol, nicotine, Δ^9 -tetrahydrocannabinol and cocaine), i.e., the teacher helped the construction of the chemical structures attempting to lead an alternate reality with the use of the software in order to motivate students in the teaching and learning process. The ChemSketch 12.00 is a software advanced freeware program with simple layout and easy to handle, focused on the chemical modeling, so based on theories such as the octet rule, valence bond theory (VBT) and theory of molecular orbital. Allowing to calculate automatically the valence of each atom, the construction of chemical structures, may be used to put name in the compounds according to IUPAC, calculate the molecular properties (e.g., molecular weight, density, molar volume), and also presents a large database with different structures of molecules and lab materials [20].

After the course was applied again to the standard IG questionnaire to evaluate the teaching and learning process capabilities with the use of software focused on chemistry.

2.4 Collection and Evaluation of Data

Data collection was carried out in three (03) distinct steps by the application of a survey with closed-ended questions, which were applied before and after the expositive classes (CG and

IG) and course+intervention (IG) for both groups. The professors were present to inhibit interaction between the academics during the survey. Then, the responses of CG and IG were compared considering the content studied, in order to evaluate the student's learning level and their conceptions about the use of ICT's and ChemSketch 12.00 software in chemistry classes.

2.5 Ethical Aspects

The participants were instructed that there would be assurance of anonymity, because their ID's in their respective evaluation activities were treated in a respectful and confidential manner, and aimed to defend the interests of research participants in its dignity of contribute to the development of research within ethical standards [21].

3. RESULTS AND DISCUSSION

In this section is explained the perceptions and conceptions of academics related to drugs theme (concept, differences between the terms medicine and drug, ratings, body target, effects and its correlation to organic chemistry) and molecular modeling (practicality, the academic information to the use of the software and the potential of the tool before and after the introductory of molecular modeling, teacher's role in developing skills and abilities).

3.1 Perceptions and Conceptions of Academics Related to the Drug and Molecular Modeling Themes

The data presented below are intended to discuss the perceptions and conceptions of academics in related to drug and molecular modeling. Question 1 "What are drugs?" it led to evaluate the level of prior understanding of academics regarding the concept drugs and the differences between the terms medicines and drugs.

The medicine expression is a very popular name used to refer to scientifically drugs, however, there are differences in terms of words, while the medicine seeks to alleviate symptoms of a disease or pain, the drug refers to substances with an active principle able to act in the body and in fact cure rather than just remedy. Therefore, it can be said that every drug or medicine is a remedy, but the remedy term is limited, and it is not necessarily a drug [22,23].

The changes caused in the functions of human body by natural or synthetic substances are considered drugs. Therefore, drugs are substances that produce effects on people's behavior, be it physical, emotional or psychological [24].

Based on histogram data of Fig. 1, it was possible to observe that the level of students understanding related to the concept of drugs, is positive, even the current chemistry teaching still held in schools being rooted to the traditional method, the conceptions and perceptions of academics regarding the concept increased significantly, part 1 (62.50%), part 2 (83.33%) and part 3 (91.67%), respectively.

This growth in the number of correct answers is due to the fact that in the part 1 was tried to observe only prior knowledge of academics. In the part 2 after the lectures, there were a considerable change in their views and perceptions, since the mistakes were related to difficulties in distinguishing academic terms: Drug, medicine, and remedy, as well as its relationship to the body. The result obtained in part 3, after the introductory molecular modeling course administered to IG, was observed a growth of 29.17% when compared the part 1 and 8.34% compared the part 2. This fact is the course result, with the best assimilation of the concepts by students from IG.

Question 2, "About abuse drugs are correct to say" with this kind of question was possible to verify if the academics know about the

classifications, body target and the drugs effect. The histogram in Fig. 2 presents the data of Question 2.

Nowadays, the use of abuse drugs is one of the serious problems faced by humanity, which represent a big challenge for public health. Among the various types of drugs inserted in daily life, we could highlight cocaine, which is directly related to the crime, too much alcohol, causing numerous accidents and deaths and the use of injectable drugs such as heroin, a potential cause of contamination with the AIDS virus [23].

According to the Fig. 2, it is possible to see in the first part that the preliminary knowledge required in question was below average, with 54.17% of the students that answered wrong and 45.83% that were correct. After the theoretical explanation in the second part, it showed a reversal in rates, reducing by 25.00% the number of errors in relation to the first part, and the number of hits increased to 70.83%, so the theoretical explanation was satisfactory to promote the change of perceptions and conceptions. In the third part, the hits rate increased 37.50% compared to the part 1 and 12.50% over the part 2, this fact can be linked to the introductory course in molecular modeling.

To show the teaching chemistry more comprehensive, significant and present in the students' lives, teachers plan their lessons trying to relate the theory with the day-by-day of the students, to that, they combine scientific knowledge with relevant facts of society, hoping

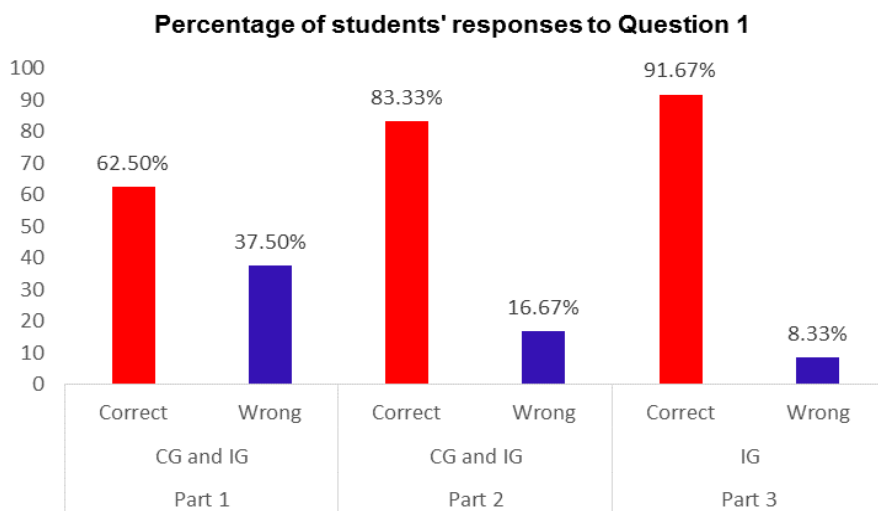


Fig. 1. Histogram of question 1 "what are abuse drugs?" in three distinct parts

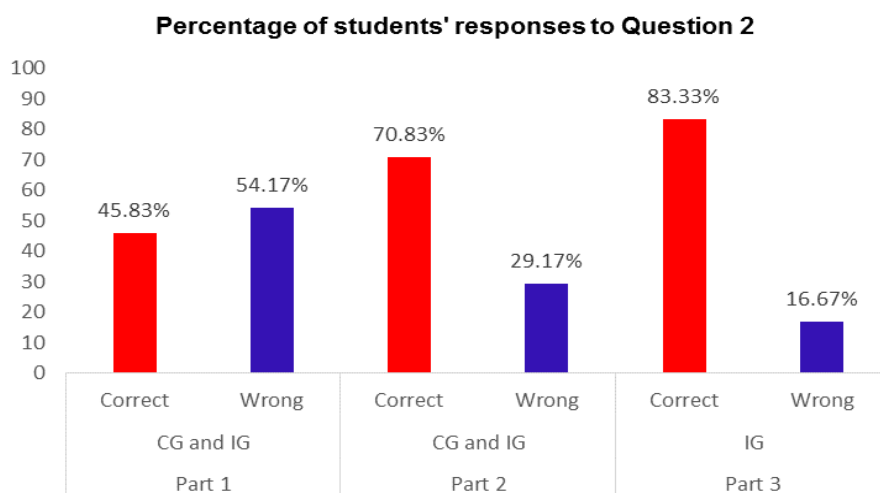


Fig. 2. Histogram of question 2, "about abuse drugs are correct to say?" in three distinct parts

that the student can give them directions in chemical, social, cultural and economic, expand its area to the world we live and getting close of science using didactic tools such as newspapers, magazines, documentaries, internet and other technologies [9,10].

Question 3 is "Molecular modeling is a complex tool to handle?" It was to identify if academics were aware of this tool and its practicality. The histogram in Fig. 3 shows the data of question 3.

The Fig. 3 shows that only 37.50% of intervention participants knew about molecular modeling and its practicality, saying "no" that it is a complex tool, which means, that they already had information or had contact with this type of tool or another similar, but 62.50% of the students answered "yes", therefore, most of them did not know what it was, because they had little knowledge of the subject and, consequently, to little connection to the computer and its basic tools.

Later the theoretical elucidation, part 2, there is a reversal in their opinions, more knowledgeable about the subject became aware that it is a simple tool that can perform various functions in chemistry. In this part, there was a positive increase in the index of those who marked "no" regarding the first part of 41.67% Finally, in carrying out the practice, in third part by the IG, it was found that the molecular modeling software used even being advanced is not an obstacle but an outstanding helper to understand the theory, in this part, there was an increase in the positive responses of academics 45.83% compared to the first part and 4.16% over the second part.

The question 4, "what does molecular modeling use as the primary execution tool?" with this question was possible to evaluate the information level of academics regarding the basic tools to use the molecular modeling software (Fig. 4).

In the part 1, it is noted that 41.67% of the students already had some knowledge about the molecular modeling, because it is a branch of computational chemistry booming, focused on research and teaching, using the computer as the main tool and projector to dissemination of information. However, 58.33% did not know the basic instruments of execution and missed the question. After a theoretical molecular modeling introduction, part 2, there was an increase in the hit rate of 33.33% when compared to the earlier time, reducing the number of errors to 25.00%, thus showing changes in their conceptions. Unlike previous times, the results obtained with the IG were extremely satisfactory, since at this stage they were not in the theoretical and had direct contact with the tool and could also analyze the resources used for intervention, which facilitated their answers, at that time, the right answers grew 50.00% compared to the part 1 and 16.67% compared to the part 2.

The question 5, "Respecting about the following abuse drugs: Alcohol, tobacco, marijuana and cocaine, is it correct to say?" demanded the students a theoretical basis on the theme drugs as: classifications, effects and its relation to organic chemistry (Fig. 5).

From the study of the chemical structures of drugs it is possible to know fundamental

concepts of organic chemistry such as carbon chains and hybridizations, the covalent bonds, nomenclature and the organic functions [9].

Fig. 5 shows that there were a low rate of positive responses at the first part 1, just 8.33% of the students answered right and 91.67% were wrong. These data show that most academics had very little content domain on this theme and its relation to organic chemistry. They had difficulty in classifying the drugs mentioned in the various existing classifications required by the question, and its effects in human after the use of them, the main kind of molecules and their names according to IUPAC. After the theoretical classes, the part 2, there were an increase in the

number of correct answers 33.34%, reducing the error rate to 58.33%, which justifies the theory assimilation, however, the number of wrong answers were not a desired result by any teacher, due the amount of mistakes which were still higher than 16.66% in relation to the number of hits at that time. However, the third part, the molecular modeling course proved to be essential to the IG in understanding the chemistry present in such drugs, expanding its point of view, favoring the understanding of chemistry at the microscopic level, thus being decisive for growth of hits at this stage, there were 58.34% accuracy more than the part 1 and 25.00% higher than the second part, reaching acceptable index.

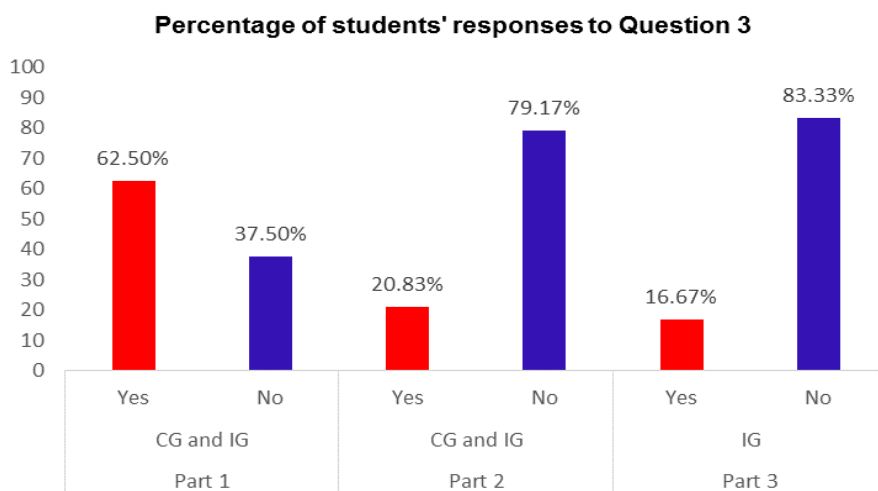


Fig. 3. Histogram of question 3 "Is molecular modeling a complex tool to handle?" in three distinct parts

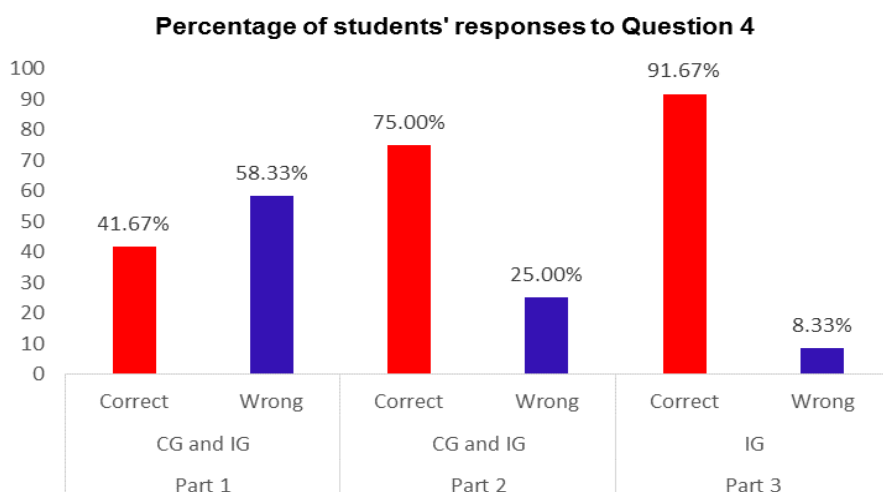


Fig. 4. Histogram of question 4, "what does molecular modeling use as the primary execution tool?" in three distinct parts

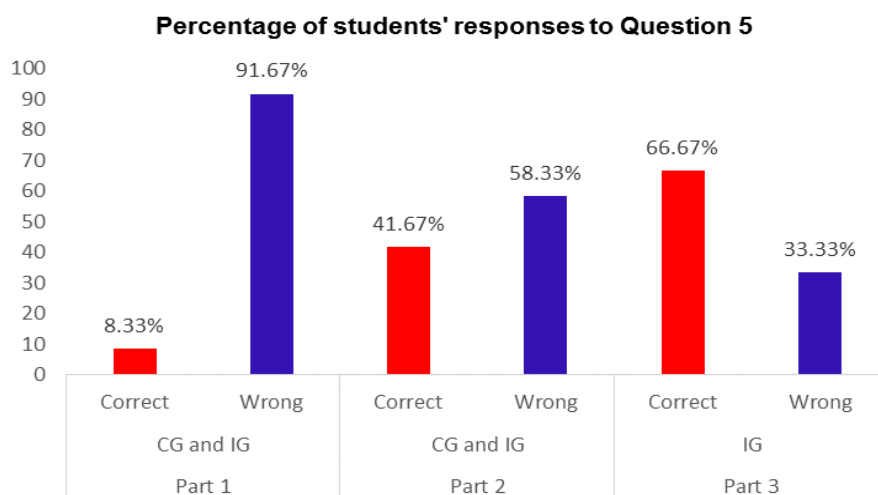


Fig. 5. Histogram of the question 5, "about the following drugs: alcohol, tobacco, marijuana and cocaine, is it correct to say, except?" in three distinct parts

Analyzing the histogram (Fig. 6), it appears that most of the students at first part did not achieve success in their answers because the limited knowledge they had to the required question. At this part, 37.50% of the students achieved successes and 62.50% missed the question. Subsequently, at part 2, there were change of opinions and values, consequence of theory diffusion, rising the number of correct responses in 29.17% compared to the previous time. At the part 3, run by the IG, in addition to theoretical knowledge assimilated, they had the course of modeling, and they learned to handle the proposed software and explore it potential, they realized that the teaching tool in question does not replace the main teacher's role as mediator of knowledge, but that it can assist in the understanding of theory with practice, helping both teachers and students within the teaching /learning process. At this stage there was an increase of 54.17% compared to the part 1 and 25% over part 2.

The question 7, "What does the professor need to use molecular modeling is his teaching classes?"

Seeks to identify the conceptions of the students on the use of this tool and make them aware about the teacher's role in developing skills and abilities to their students (Fig. 7).

From the histogram (Fig. 7), it is possible to notice that at the beginning, at first moment, undergraduate students had very little information about this new area of chemistry and

so far no contact with anything. This lack of experience in relation to new teaching practices and that both are required by the educational system, eventually inducing them to error, was assigned 16.67% accuracy and 83.33% errors. However, at the second part by theoretical exposition they became aware that teaching is in constant transformation, requiring the educator reformulations in their teaching methodology and go in search of other, more effective, however, to this just the domain of their own knowledge about science is not enough, being necessary to acquire new skills and abilities and put together their knowledge in search of a more meaningful teaching, at that part there was an increase in 58.33% more hits in relation to the moment 1 and a decrease in the error rate to 25.00%. The introductory course in molecular modeling, part 3, was the basis for the IG to reaffirm all the theory previously acquired, which they observed that the use of the modeling software was planned due its capabilities that promote understanding of organic chemistry of drugs but for this it was necessary to go beyond the chemical knowledge and go to computer science area. In this step, the hit rate increased by 75.00% compared to 16.67% at part 1 and relative to the part 2.

Currently, there is technological development which is present in all areas of society, and education is one of them, what highlights the need of teaching institutions to be structured and offer to teachers training and qualification, so they can use ICT effectively in their work environment, enabling the construction of knowledge [1].

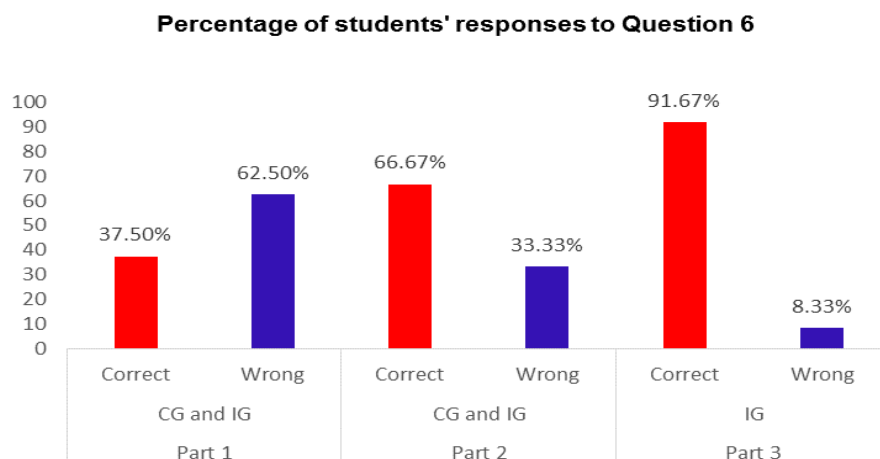


Fig. 6. Histogram of question 6 "in your opinion which is the characteristic of molecular modeling that inserts it as an educational tool?" in three distinct parts

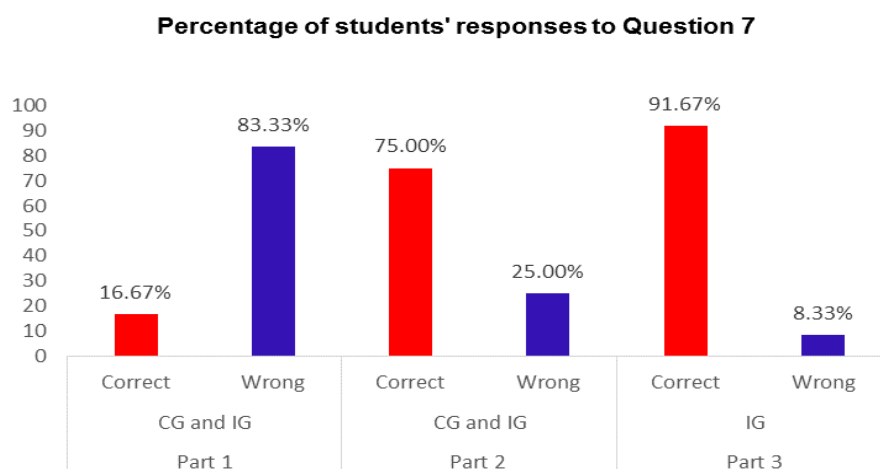


Fig. 7. Histogram of question 7 "what does the professor need to use molecular modeling is his teaching classes?" in three distinct parts

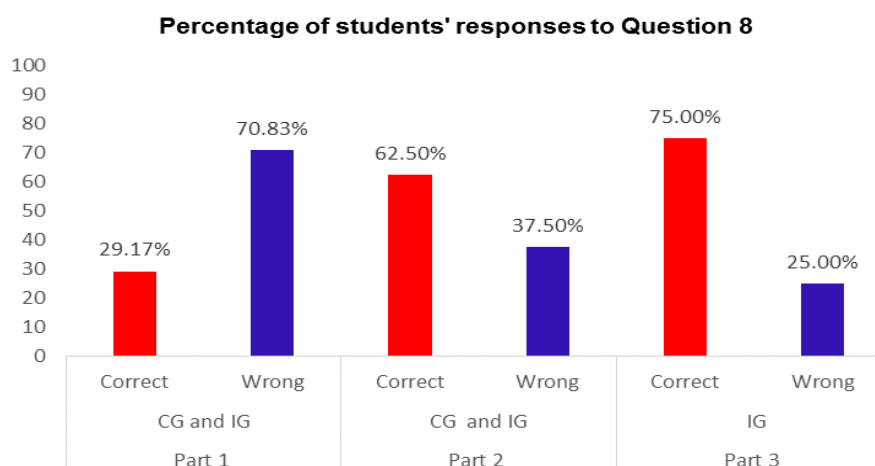


Fig. 8. Histogram of question 8 "what does make possible in molecular modeling to show the concepts and chemical drugs representations?" in three distinct parts

The question 8 "What does make possible in molecular modeling to show the concepts and chemical drugs representations?" Tried to evaluate the ideas of the students regarding the potential offered by molecular modeling software when inserted into the chemistry teaching, (see Fig. 8).

According to the histogram (Fig. 8), it is clear that during the initial phase, the part 1, the lack of in-depth knowledge about the subject was dominant for the low hit rate (29.17%) and the large number of errors (70.83%). Subsequently, the theoretical elucidation, their conception about the subject increased the hit rate (62.50%) and reduced the errors in (33.33%) compared to the part 1. Finally, the part 3, was further differentiated, for it the selected IG group had the opportunity to combine theory with practice and explore the chemical potential offered by molecular modeling as a facilitator of organic chemistry of drugs. At this stage, there was an increase (45.83%) of correct responses relative to part 1 (12.50%) compared to the part 2.

4. CONCLUSION

Since teaching is dynamic, ie, is in constant transformation, always reformulating looking for didactic and methodological innovative alternatives in order to promote quality education, to face it, the professor as a mediator of knowledge, cannot be away of these changes. However, to the things happen in a planned and satisfactorily way, it is essential that the change occurs in its base, ie, the educational institutions responsible for their training, to enable their teaching skills and qualifications, as well as offer the whole physical structure necessary to put into practice the new theories being released, so that their students and future professors can assimilate the theories and acquire resources to help them develop the best of its role as an educator, and that through this training perspective and awareness arise other more effective.

The scientific and technological development has changed the way of thinking and acting of people, as well as their habits and behaviors, these development changes are present in all areas of modern society, and education is among them, however, it falls short. The new and advanced technological features are the result of scientific studies; therefore, they can also promote knowledge of science, thus the chemical search through the computer science offer

innovative and effective tools to assist teachers in their research and teaching learning. In this scenario, emphasis on molecular modeling, computational chemistry branch that emerges as a teaching tool support to be inserted in the teaching of chemistry in understanding the theories and to replace the traditional method of teaching. It is a tool with enormous chemical potential, however, still little explored due to lack of knowledge about or difficulty handling.

The purpose of the study was to proven scientifically that molecular modeling is a differentiated and effective educational tool in organic chemistry teaching within the thematic abuse drug approach, which was confirmed by the results presented by the intervention group when they besides, have learned about drugs, explored the possibilities offered by modeling in getting knowledge about drugs organic chemistry and reaffirmed the widespread theory with practice.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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