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Development of computer skills in the Organic Chemistry discipline

Desarrollo de habilidades informáticas en la disciplina Química Orgánica

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ABSTRACT
The objective of this work is to describe the realization of an extra class exercise that link the contents of the disciplines Organic Chemistry and Computer Science and Computing in the third year of the Radiochemistry specialty that is being studied at the Higher Institute of Technologies and Applied Sciences . The methods that allowed the basic study were those of the theoretical and empirical level, such as the historical-logical, analysis and synthesis, induction and deduction, systemic-structural, modeling, observation and documentary analysis.The experience was developed during five consecutive courses. An integrating extra class work was carried out every year. Extra class work was titled: «TICs applied to organic chemistry». As a result, the students presented in the report the structures and properties requested in an accurate manner and evidenced clearly having understood the different types of structures and softwares.

Keywords: Organic chemistry; interdisciplinary; computing.

RESUMEN
El presente trabajo tiene como objetivo describir la realización de un trabajo extraclase que vincula los contenidos de las disciplinas Química Orgánica e Informática y Computación en el tercer año de la carrera de Radioquímica que se cursa en el Instituto Superior de Tecnologías y Ciencias Aplicadas. Los métodos que permitieron el estudio de base fueron los del nivel teórico y empírico, tales como el histórico-lógico, análisis y síntesis, inducción y deducción, sistémico-estructural, la modelación, la observación y el análisis documental. La experiencia fue desarrollada durante cinco cursos consecutivos. Se realizó, cada año, un trabajo extraclase integrador. El trabajo extraclase se tituló: «TICs aplicadas a la disciplina química orgánica». Como resultado, los estudiantes presentaron en el informe las estructuras y propiedades solicitadas de forma certera y evidenciaron con claridad haber comprendido los diferentes tipos de estructuras y softwares.

Palabras clave: Química orgánica; interdisciplinariedad e informática.

INTRODUCTION

In order to achieve a more comprehensive and complex representation of reality, attempts are made to establish interdisciplinary relationships, that is, between the knowledge of different sciences fostered by the progressive production of scientific results.

Some authors have pointed out the importance of interdisciplinary relationships. Fernández de Alaiza, (2001) considered it essential to take into account the interdisciplinary relationships established through cognitive nodes, considered as those contained in a subject of a discipline or subject, which includes knowledge, skills and the values associated with it, which are based on an interdisciplinary articulation process in a given university career, to achieve the most complete training of the graduate, that is, the professional future.

Recently, Lau- Gonzalez, Hernández Garcés, Corona, Ruiz and Zamora (2015) presented examples of learning activities aimed at the independent work of the students of Radiochemistry of the Higher Institute of Technologies and Applied Sciences (InSTEC) that allow to achieve systemically coherent link between the disciplines of General and Inorganic Chemistry and the Preparation for Defense on the study of toxic substances of different nature and the risks that, during their handling and use, may arise for human health, economic resources and the environment ; aspects to take into account within the dimensions of National Security.

In the same career Hernández-Garcés, Lau- Gonzalez, Avilés-Rodríguez, Jauregui- Haza and Guzmán-Martínez (2015) reported the results of the application of a didactic strategy for linking the contents of the Organic Chemical and Preparation disciplines for the defense. Then, Hernández-Garcés, Lau- Gonzalez, Grueiro- Cruz, Aviles-Rodriguez, Jauregui- Haza and Guzmán-Martínez (2016) linked the Organic Chemistry discipline with the Professional Practice of Radiochemistry. Subsequently, Hernández-Garcés and Avilés (2017a) published their experiences in linking Organic Chemistry with history through the seminars. Later, Hernández-Garcés and Avilés (2017b) applied the same methodology to link the subjects Chemical Analysis and Preparation for the Defense of the Chemical Engineering degree.

The need to link the content of the Organic Chemistry discipline with those of Computer Science and Computing, in the Radiochemical career, arises from the Professional Model (InSTEC , 2007), where it is stated that computer science becomes, in the case of Radiochemistry, in a consubstantial part of professional training.

The Radiochemical career is structured in 63 subjects organized in 14 disciplines. One of them is informatics and computing where in its conception, it is specified «It is complemented through the computing dimension with the other disciplines of the career» (InSTEC, 2007).

The core curriculum of the informatics and Computing discipline consists of two subjects, Computation I and II, with a total of 112 class hours (InSTEC, 2007) in the first two years of the degree. However, experience has shown that this time is not enough to cover all aspects described in the Professional Model. (Figure).

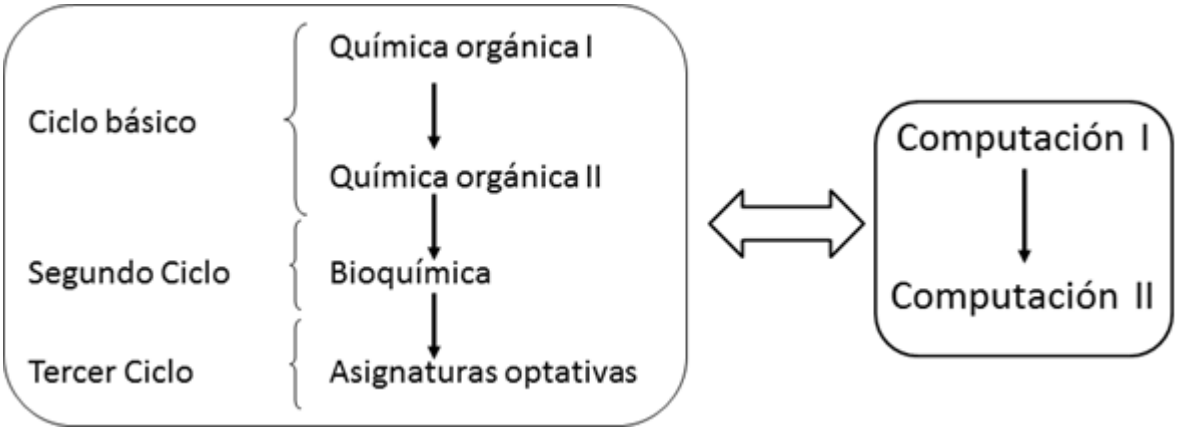

Fig. -Organic Chemical Discipline and its relationship with Computer Science and Computing.

Source: own construction.

Curriculum D (MES, 2003) proposes the transformation of the teaching-learning process with the help of Information and Communication Technologies (ICTs). Addi tionally, it suggests a more interdisciplinary approach to career structures. One of the advantages of Plan D is that it gives the student, within the elective subjects, the possibility of selecting subjects that complement their training in various areas. Computing is one of those declared in the Radiochemical Professional Model (InSTEC , 2007). In this race Gamboa-Carballo, Ferino-Pérez, Lau- Gonzalez, Hernández-Garcés, Corona-Hernández and Jáuregui-Haza (2017) described an essay on the use of ICTs as a tool to visualize molecular structures in chemistry teaching General.

Numerous computer applications have been used in chemistry. One of them, CHEMWIND is a program for drawing and publishing chemical structures developed by Softshell (1992). This software was applied by Amaral and Balcevicz (2012) who included it in an ICT training module for chemistry teachers in five municipalities of the Rio Grande do Sul state in Brazil.

Another example is Hyperchem, (Pazun, 1993); molecular design software that provides special support for the development of molecular models that combines 3D visualization and animation with quantum chemical calculations. Kingsbury (1993) pointed out that this software had the pedagogical value of allowing the molecular geometry of organic compounds to be manipulated graphically in the computer and thus perceive steric interactions due to changes or twists in link angles.

Another molecular design software applied to teaching is Spartan (Casanova, 1993). Miller and Ellison (2015) used it to describe Computational Chemistry exercises to be applied in Physical Chemistry courses and thus link the theory of molecular orbitals and molecular structure.

Taking into account these antecedents, this work aims to describe the realization of an integrative extraclass work between the Organic Chemistry and informatics and Computer disciplines to cover the training requirements of the Radiochemical career in the area of computing.

MATERIALS AND METHODS

In order to achieve the objective in the research, the general dialectic-materialist method was considered as a general method of science, as a basis and guide for the integral study of objects, their functioning and the logic that favors the application of the methods. From the theoretical level the historical-logical method, analysis and synthesis, induction and deduction, systemic-structural and modeling were used.

The historical-logical method was used to know the history of the phenomenon under investigation and what concerns the ICTs applied to Chemistry, to determine the theoretical-methodological aspects, as well as principles, concepts, theories and research, regarding the use of the potentials offered by ICTs.

Meanwhile, the method of analysis and synthesis made it possible to break down the phenomenon that is discussed in the components and their multiple relationships and arrive at synthesized reasoning about the exploitation of the potential of ICTs.

On the other hand, induction and deduction facilitated the interpretation of the results that allow reaching conclusions and generalizations of a theoretical and empirical nature, in relation to the potential of ICTs.

The systemic-structural method allowed the general orientation in the construction of the strategy for the exploitation of the potential of ICTs, by determining the relationships between its components that reveal its internal logic.

For the same purpose the modeling method was used, which favors the approximation to the social reality that one wants to transform and shape the scientific product that is proposed.

The empirical level methods used were documentary analysis and observation.

In this case, the documentary analysis allowed the collection, processing and study of the entire bibliography on the use of ICTs, based on determining their potential, their use in the educational process and their characterization. It led to the review of documents referring to ICTs and the written press, as well as to view related audiovisual programs that arrive from different media of this type.

As a fundamental method the observation allowed to verify the level of preparation that the students have for the use of the potentials of the TICs, which contributes to determine the strengths and limitations according to the potentials offered by these programs.

Within the Organic Chemistry discipline of the Radiochemical career, the study of organic compounds, their structure, physical chemical properties, their fundamental reactions and reaction mechanisms are taught and addressed. The link with the knowledge of the informatics and Computing discipline can then be achieved, with the construction of structures in relevant software.

In order to fulfill the objective of the study, it was proposed to carry out an extraclass work so that students could identify, relate, describe, characterize, argue and explain organic substances and their structure. The extraclass work was entitled: « ICTs applied to the organic chemical discipline».

For the conception of the extraclass work, the content of the Organic Chemistry discipline corresponding to the characteristics of the organic substances, their properties and structure and the Computer and Computing related to the use of scientific software and content and communications applications were taken into account.

The didactic method to be used in extraclass work was independent work, bibliographic search, internet review, interviews with specialists on the subject, work with the textbook, explanation, inductive and conversation; and the means to review were the basic text of the Organic Chemistry II discipline, digital information on the internet, the CHEMWIND Software, the Hyperchem software, the Spartan software and the user manuals of the corresponding softwares (Table).

Students were distributed in four teams. Students were given a list with the name of organic compounds. Each semigroup should choose only one compound from the list. The report should contain an image with the structure of the compound made in CHEMWIND, another image with the optimized construction and the table with the properties of the compound obtained from Hyperchem and another image of the 3D structure and the table with the result of the calculation of the loads partially made in Spartan.

Table - Description of the extraclass job.

Work extraclase	ICTs applied to the organic chemical discipline
goals	Link knowledge of the informatics and Computing disciplines and Organic Chemistry discipline
Content	Knowledge of the Organic Chemistry discipline Knowledge of the applied computing discipline
Methods	Independent work Bibliographic search Internet review Interviews with specialists on the subject Working with the textbook Explanation Inductive Conversation
Form of organization / Type of class	work extraclase
Media	Basic text of the Organic Chemistry discipline II Digital information on the Internet CHEMWIND Software Hyperchem

	Software Spartan Software Software User Manual
Evaluation	Work in digital format Coherence of the exhibition Degree of fulfillment of the objectives Clarity of the communication of knowledge

The task systems used to expand the areas of near development contain tasks of activity and communication (Fariñas, 2005). In this sense, the exercise was oriented to extraclass the students through an explanation in class. In addition, they were given a guide with the details of it. The students performed the work independently.

The guide communicated the following:

Work extraclase. ICTs applied to the organic chemical discipline

Delivery Date: May 1st

(Each student chooses only one compound from each list)

They must send in digital format a file compacted with:

1. Drawing (cw2) made in CHEMWIND of:

- Benzaldehyde 2,4-dinitrophenylhydrazone
- β-carotene
- caffeine
- NBS
- Thiamine Chloride
- Chlorodiacepotoxic
- Orange II

2. An image (jpg) with the properties window and a file (mol) with the optimized Hyperchem construction of:

- benzene
- pyridine
- furan
- toluene
- pyrrole
- thiophene
- pyrimidine

3. A file (Spartan) with the structure and calculation of partial loads (partial loads must be included separately in a txt) of:

- methanal
- ethanal
- propanone
- 2 butanone
- Methanoic acid
- Ethanoic acid
- Methyl methanoate

4. A text document (MS Word) with a report that groups all the previous information. You must include the student's name.

This experience was developed during five consecutive courses from 2010 to 2014, with 64 students in the third year of the Radiochemistry career, whose knowledge of ICTs was considered high after having studied them in the two semesters of the first year.

RESULTS

The task systems used to expand the areas of near development include activity and communication tasks (FarinÞas, 2005). In this sense, the students performed the exercise individually without the collaboration of the teachers.

As it was the first time they faced the softwares they had to use time creatively, one of the most important manifestations of the development of organizational skills (FarinÞas, 2005). The skills exercised by students in this research have the function of generating widespread effectiveness, particularly for learning to learn.

Students reviewed the sources individually and selected the substances independently without the participation of the teachers.

Within the software used, it was decided to use the English language versions, granting a greater degree of complexity to the extraclass work and trying to integrate the English language discipline.

The evaluation was carried out by email (another dimension of the use of ICTs by students) of a report in digital format of the work done, which took into account the content, coherence, degree of compliance with the objectives, clarity of the communication of results and teamwork.

DISCUSSION

During the five years of the experience, the extraclass work had satisfactory results. The students presented in the report the structures and properties requested accurately and clearly showed that they understood the different types of structures and software.

Students had to make a creative use of time, one of the most important manifestations of the development of organizational skills (Fariñas, 2005), since they had to perform the exercise independently integrating for the first time knowledge of two disciplines. The skills exercised by the students in this study have the function of generating widespread effectiveness, particularly for learning to learn.

When carrying out activities with a higher level than the one required by the routine tasks that these types of students usually execute, they are motivated with a stimulation superior to the usual one. It is a challenge that requires a higher level of independence and self - organization, in keeping with the concept of "zone of near development" developed by Vygotsky (1982), in which the central aspect for all instructional psychology is base don the possibility to rise, through collaboration, to an intellectually superior degree, and that is the basis of all the importance of instruction, in the development of professional and personal skills and abilities.

This activity tributed to the development of three of the shaping skills of personality development: the understanding and search for information, communication and the temporal organization of life.

With this activity, it was possible to link the contents of the Organic Chemistry discipline with those of Computer Science and Computing, and elements of English were included.

There were problems with the timely delivery of reports in some cases, which evidenced a bad planning and temporary organization of the students.

In addition, they presented difficulties with the delivery format proving that they are more skilled with scientific software and content and communications applications.

The students were motivated to give more importance to the subjects of the nformatics and Computer discipline by showing them the link they have with the subjects of the curriculum of the career they chose by vocation.

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