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Teaching and Learning of PCM 2000 Phytochemistry - Utilizing the Molecular Models and PC Software for Chemical Structures

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Abstract

"Phytochemistry PCM 2000" is a core course in the full-time Bachelor of Pharmacy (Hons) in Chinese Medicine programme. The chemical structures and properties of organic compounds in Chinese medicinal herbs are the major teaching content of this course. It is very important for students to memorize and understand the chemical structures in Chinese Materia Medica (CMM) and hence their physico-chemical properties, structural elucidation and biological activities. This is the main objective in teaching the course "Phytochemistry". This project focused on teaching the students to draw 2D and 3D chemical structures of the constituents in CMM by using several pieces of PC chemical software, and to make stereo-molecular models by employing Molecular Model Kits. Some of the resulting models and graphics were used in PowerPoints for the teaching of this course.

Key words

Chinese medicine, phytochemistry, chemical structures

Introduction

Phytochemistry PCM 2000 is a core course in Hong Kong's first full-time Bachelor of Pharmacy (Hons) in Chinese Medicine Programme, launched in Hong Kong Baptist University in 2001. The educational content of this course includes chemical structures, physico-chemical properties, isolation and separation methods, structural analyses and elucidation, and biosynthesis of active constituents in Chinese Materia Medica (CMM). The chemical constituents in CMM usually possess structural diversities, complex skeletons and particularly have much more chiral centers forming special 3D stereo-structures compared with synthesized organic compounds. The stereo-structures of the CMM components

are closely related to their pharmacological activities. Therefore, the chemical structures in Chinese herb are very important for grasping their physico-chemical properties, structural elucidation and biological activities.

This project aimed at training students to draw 2D and 3D chemical structures of the constituents of CMM by using several pieces of PC chemical software, and to make stereo-molecular models by utilizing two kinds of Molecular Model Kits. Through these activities, students' understanding of the chemical structures and their properties was enhanced and strengthened. In addition, one common and typical pharmacologically-active compound of CMM was selected for measurement of its 1D- and 2D-NMR spectra for the purpose of elucidating the stereo-structure in solution. The stereo-structures derived from modeling and NMR measurement were compared. The students were required to search the chemical references of the constituents in CMM, to draw the chemical structures, and to establish molecular models. This improved their ability to analyze and solve problems they encounter, and trained them in the use of chemical software and molecular model kits which are necessary for their future study and work. Moreover, 3D stereo-structures in the PowerPoints generated by this project were attractive and vivid, and thus could stimulate students' learning enthusiasm and increase their understanding of the chemical constituents in CMM.

Aims and Objectives

This project was designed to teach the students how to draw 2D and 3D chemical structures and make stereo-models of the organic compounds in Chinese herbal medicines. Students learned:

1. To draw 2D and 3D structures of organic compounds employing ChemDraw software
2. To make molecular models of chiral compounds using Dreiding Model Kit and HGS Molecular Model
3. To measure the ^{1}H-NMR spectrum of common natural products. A solution structure obtained from NMR data was compared with those of the models drawn from software by the students.
4. To establish a database of the organic compounds in some common Chinese herbal medicines

Methodology

This project ran from January, 2003 to December, 2004. The project consisted of :

1. The chemical structures of several types of compounds, such as alkaloids, flavonoids, tannins, lignans, saponins, which are very common in CMM, were drawn using chemical software "ChemOffice".
2. Using the chemical software "Chime" and "Rasmol", downloaded from websites, the stereo-structures of CMM constituents were viewed.
3. Molecular models were hand-made using Dreiding Model Kit and HGS

Molecular Model. The models were photographed.

4. One compound which is a typical active constituent of CMM was selected. Students measured the NMR spectra, particularly the NOESY and ROESY spectra, in order to clarify its stereostructure in solution.
5. Based on the above achievements, PowerPoints were made for effective and qualified teaching of the course *Phytochemistry*.

Results/Findings

We have made the following progress in the teaching and learning of *Phytochemistry (PCM 2000)*:

1. The students were taught to use ChemDraw and Chem3D software for drawing, observing and calculating 2D and 3D molecular structures of the active components in Chinese medicines. Students showed in assignments that they could skillfully use the software and their understanding of the stereochemistry of organic compounds improved greatly.
2. A free software named ISIS Draw, similar to ChemDraw, was installed in the PCs in the CM library and the students' own PCs so that they could study chemical structures in the library or at home.
3. In the teaching section of the Chapter "Monosaccharides and Glycosides", HGS Molecular Models were employed in the lecture to give the students a better understanding of the concepts of conformation and configuration of natural organic compounds.
4. In the students' project reports and oral presentations arranged in the course, students were found to have fully grasped the use methods of the drawing software and HGS molecular model.
5. 1D and 2D-NMR spectra of quercetin, a common flavonoid in Chinese herbal medicines, were measured with Varian Inova NMR (400 MHz) in the Department of Chemistry. The 3D conformation of quercetin based on the NMR data and molecular modeling were compared in the class.
6. Some students took part in the compiling of two books on Chinese medicines (see the references) using the knowledge they grasped in course *Phytochemistry*.

Enhancement on Teaching and Learning

Through this project, it was observed that:

- Students learnt how to use several items of chemical software which are necessary for research work in the field of phytochemistry and phytochemical analysis.
- Students were trained to better understand and observe the 3D stereostructures, conformation and configuration of the organic compounds in CMM. They became able to analyze and elucidate the characteristics and physico-chemical properties of organic compounds.

- The structures of the compounds in the PowerPoints of the lecture were presented in a three-dimensional image. Therefore they were more attractive and easier to memorize and understand.
- Students were given assignments on the components of CMM including their 3D structures and stereochemistry. This trained the ability to analyze and solve problems in the organic chemistry of natural products.

Students' feedback on the teaching style was solicited by using a questionnaire. The students' feedback and Teaching Evaluation results showed that this approach was largely welcomed by students. They found that this teaching style greatly helped them learn phytochemistry.

Limitations/Difficulties

In the classes, there were not enough models for the students to use. In addition, as the ChemDraw software was installed in the PC of CM Library, the lecture had to be held in the CM Library so that the teacher could demonstrate how to draw 2D and 3D structures of the compounds using the software. We found that 3D structures of the compounds are somewhat difficult for some students to understand even if the software was used in the lecture. This may be due to the poor stereo-imaginative ability for some students. Another limitation is that the use of ChemOffice software in the SCM Library sometimes became crowded because PG students, RAs and year three and four BPharm students all wanted to use this software in the library.

Conclusion

Employing several PC chemical softwares and two kinds of Molecular Model Kits, the lecturer of subject "Phytochemistry" was successful in teaching the students to draw 2D and 3D chemical structures and further ensured the students understood the stereochemistry, chemical properties and characteristics of the organic compounds in Chinese herbs. These abilities are important for their subsequent subject study, honours project and future work after graduation. Also, using this knowledge, the students could join in the compiling of a Chinese (Zhao, 2003) and an English book (Zhao, 2004) on Chinese herbal medicines by searching and drawing chemical structures. This demonstrated the effectiveness and quality teaching of the course "Phytochemistry".

References

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