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Creation and evaluation of a two/three dimensional molecular database for drugs used to target the respiratory system

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Introduction: Healthcare students and professionals could benefit greatly from using a holistic drug database as a reference point for clinical, physiochemical and structural information. Advancements in technology have enabled the creation of visual aids which cater for various learning styles in terms of presenting an abstract idea in a more tangible form.

Aims: To compile an electronic molecular database with constructions of drug structures used in the management of respiratory diseases in two and three dimension, representations of key drug interactions as well as drug clinical parameters and physiochemical properties. Furthermore, to assess its utility by carrying out a randomized control study comparing the pharmacy students' performance prior to and post introducing an intervention lecture using the database.

Method: A thorough literature review about teaching practices, the design and content of the database was carried out. The third section of the BNF 64 was used to identify drugs acting to the respiratory system. Structures were constructed in two dimension using Symyx® and in three dimension using Sybyl®. Symyx® was also used to generate physiochemical properties of the drugs. OCA browser® was utilized to identify protein data bank entries of drugs pertaining to this section. Interactions occurring between drugs and their cognate receptor were highlighted through depictive representations using Visual Molecular Dynamics® (VMD). Jmol® was used to create and embed interactive properties to three dimensional structures and protein data bank entries. The structures, representations and information were compiled in a searchable database framework using Zoho.com®. The database was uploaded onto the university's website. Phase three involved the creation of pre and post test questionnaires and the conduction of a randomized control study on a student cohort. The questionnaires were formulated and validated by a panel of experts. The pretest questionnaire was disseminated to first, second and third year pharmacy students. A randomly selected group of students were asked to attend the intervention lecture which focused on learning through the use of the database. The post test questionnaire was then disseminated to the entire cohort. Statistical results using SPSS® version 17 were generated.

Results: Forty six structures were constructed in 2D and interactive 3D formats. Twenty one interactive representations of the seven protein data bank entries identified were created. The compilation of information and visual aids together with an inbuilt search function lead to the completion of the online database. The latter was then uploaded on the university's website. Out of the one hundred twenty pharmacy students who took part in the study ninety two students had never used a molecular database. A positive trend in student knowledge was identified in all four years, with students performing better (p=0.000) after being exposed to the database during the intervention lecture. Moreover a significant improvement in the final marks was attained in the experimental group with respect to the control group for the first (p=0.018), second (p=0.000), third and fourth (p=0.000) year students.

Conclusion: Student understanding and knowledge is enhanced when teaching practices take on an innovative approach. In fact, the majority of the students (86%) deemed the electronic database to be a relevant reference point for information during the undergraduate course.

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