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Research

Computer technologies in pharmacy-Filling in the gaps in Ukrainian PharmD curriculum

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Abstract

Objective: To improve the teaching of under-represented medicinal chemistry components (in the field of drug discovery and development) in the PharmD curriculum in Ukraine.
Methods: The differences between Medicinal Chemistry (according to the "Western standards") and Pharmaceutical Chemistry (in the post-soviet countries) were evaluated. The gaps in the Ukrainian PharmD curriculum within drug discovery and development were outlined.
Results: The course "Computer Technologies in Pharmacy" has been introduced to fill in the gaps in training of the pharmacy students in Ukraine. It was designed to help students understand the depth and diversity of the drug design and development processes. The course includes the main principles related to a meaningful literature search, approaches to new drug-candidate design/development, and computerization of pharmaceutical industry. The overall idea is to familiarize students with a more holistic picture of the drug lifecycle: from idea to drug-candidate creation, getting a new drug onto the market, indication extension or withdrawal from the market, or restriction of the label claims.
Conclusion: "Computer Technologies in Pharmacy" course is a step toward unification the educational systems and reduce the gap between European, USA, and post-Soviet educational systems, in particular elimination the differences in the study of medicinal and pharmaceutical chemistry in the spirit of modern drug design/development education.

Keywords: Pharmaceutical/medicinal chemistry; Drug design; Pharmacy education

Drug design study: Ukrainian omissions

Drug discovery has changed enormously over the past few decades. Advances in biomedical science resulted in creation of hundreds of drugs from different pharmacological and chemical classes. However, the increasing demands on quality, efficacy, and safety make development of new molecules particularly difficult, as well as illustrate real advances in medicinal chemistry[1] and its interplay with experimental pharmacology, molecular biology, and medical science in general.[2] The pharmaceutical industry nowadays relies heavily on the use of various computational techniques in all fields and at all stages of the manufacturing and drug discovery/development processes. For instance, the application of virtual screening [quantitative structure–activity (property), QSA(P)R, relationship analyses, molecular docking, ADME/Tox (absorption, distribution, metabolism, elimination, and toxicity properties prediction)], methods of combinatorial chemistry, and

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high-throughput screening allows researchers to synthesize and estimate biological activity of thousands of compounds during a short period of time. These computer-assisted methods often successfully complement classical approaches in the search for biologically active compounds and serendipitous drug discovery that seems to drive the majority of modern research and development (R&D) projects. This enhanced reliance on computation should be considered in the education of pharmacy students.

The typical starting point for every research and educational endeavor is the search for up-to-date specialized information (e.g., information about newly approved drugs, clinical trial results, modern processes in medical/pharmaceutical practice, and chemical information). This information is often beyond the content of classic textbooks and handbooks, especially for non-English speaking students. Searching for this type of information is a common task for experienced R&D professionals; however, it is not a simple assignment for third- or fourth-year professional students. First, a student needs to know the sources of specialized information such as publishers' web sites, databases, electronic libraries, and patents. Students must also be able to ascertain if the information they are reading can be trusted and if it is relevant. But how can a student judge the relevancy of an information source?[3] This task can be thought of as "finding a needle in a haystack."[4] Unfortunately, the current pharmaceutical curriculum in Ukraine and other post-Soviet countries does not include skills related to the search and subsequent analysis of the literature. This issue is even more complicated for students with suboptimal English proficiency. Due to the limited funding, there are no Ukrainian universities, to our knowledge, that have prepaid access to resources such as Scopus or Web of Science. However, some positive changes should be noted. For example, there is an increase in the use of commonly available sources, such as Wikipedia,[5] especially in student self-education. (*Note*: This represents the opinion of this author group and may not reflect the opinion of the members of the *Currents in Pharmacy Teaching and Learning* (CPTL) Editorial Board.) This is reflected in the growing number of specialized articles in Ukrainian.

Currently the main topics related to pharmaceutical R&D (on the way "from molecule to drug") are taught in the Medicinal Chemistry course[1]; however, discussions are underway about the role, tasks, and structure (in the context of students teaching) of this course. In post-Soviet countries and particularly in Ukraine, the relevant pharmaceutical disciplines are sporadically scattered among several courses. This significantly complicates student understanding of the current state of drug design and development. The course "Computer Technologies in Pharmacy" was introduced to address this gap and to help familiarize future pharmacists with the main achievements and methods associated with medicinal chemistry, especially modern drug design methods, tools, and technologies.

Content and pedagogy

Before describing the structure of the course, it is necessary to outline details about the Ukrainian pharmaceutical educational system (five-year PharmD level). The main features are the disconnection of the medicinal chemistry and informational search topics between different years and disciplines. The major responsibility is assigned to pharmaceutical chemistry that is taught over two years (third and fourth years). In fact, instead of "classical" medicinal chemistry[6] being taught, pharmaceutical chemistry is what is being delivered in Ukraine. The goal of pharmaceutical chemistry is to study the synthesis, analysis, and structure–activity relationships of existing drugs. In practice, however, the emphasis is placed on the analysis of drugs (e.g., "Pharmaceutical Analysis"). The study of pharmaceutical chemistry starts with inorganic medicine and organic small molecules and ends with the study of more complex organic molecules (e.g., steroids, glycosides, and heterocyclic compounds). This type of approach makes it difficult to understand drug design methods, especially within certain pharmacological groups (e.g., anti-inflammatory agents) that might involve agents from different chemical classes. Thus, the drug design process is often omitted in pharmaceutical chemistry courses in Ukraine.

In 2000, we faced an urgent need to establish a course that would include subjects on drug design, computational chemistry, as well as the development and marketing of pharmaceutical substances. The course was designed to help students understand the depth and diversity of the process "from an idea to drug" as a holistic and fundamental question of pharmacy as an attempt to fill in the gaps mentioned above.

The course "Computer Technologies in Pharmacy" is at the intersection of pharmaceutical and medicinal chemistry (according to the "western standards"), pharmacology, biochemistry, and computational chemistry and includes limited aspects associated with drug marketing. This course is to be taken during the fourth year of the five-year program (PharmD level).

The exploration of very modern computational technologies and their use by pharmaceutical professionals is the focus of this course. It includes a number of seemingly different tasks: study of literature search; mastery of contemporary strategies/methods/tools in the creation of small "drug-like" molecules (illustrating achievements of modern medicinal chemistry), as well as their development into marketable drugs (assessment of the role and place of a new drug on the market, including analysis of the results of pre-clinical and clinical studies and evidence-based medicine metrics). This can be illustrated by exploration of the development of sildenafil (Viagra®). The following stages include in its development: fundamental study of the role of nitric oxide, establishing the role of the phosphodiesterase family, effective inhibitor design, pre-clinical and clinical trials, introduction of Viagra® for the treatment of erectile dysfunction, introduction of generics and analogues, and