

# **CHEMICAL AND BIOPHARMACEUTICAL TECHNOLOGIES IN 2025**

**Collection of abstracts**



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## **CHEMICAL AND BIOPHARMACEUTICAL TECHNOLOGIES IN 2025**

Collection of abstracts of the VII International scientific and practical conference "KyivLvivPharma-2025. Pharmaceutical technology and pharmacology in ensuring active longevity", dedicated to the 95<sup>th</sup> anniversary of the foundation of KNUTD and specialised XIII scientific and practical conference with international participation of the school of young scientists of Farmak JSC "Science, innovation and quality in modern pharmaceutical manufacture", dedicated to the 100<sup>th</sup> anniversary of the Farmak company

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3. The market for combination preparations (13 TN) is divided into two main segments: vaginal, dominated by imports (69%) in the middle-high price segment, and dental, where Ukrainian manufacturers (31%) hold leading positions in the low-middle price segment. Ukrainian companies are competitive in dental gels and ointments due to their affordable price.
4. Price ranges within each dosage form reflect the balance between local production (economy segment) and foreign manufacturers (middle/premium), determining different scenarios for rational pharmacotherapy.
5. The analysis shows a trend towards an increase in the number of combination drugs but a limitation in dosage forms, indicating the need to create new dosage forms with improved characteristics.
6. A promising direction is the development of modern local delivery systems (e.g., for topical use), including nanostructured carriers and controlled release, to increase the effectiveness of metronidazole therapy in order to reduce systemic exposure and the profile of adverse reactions, as well as expanding the range of vaginal forms (import substitution), and dental gels with flavor modifications and pediatric indications.

## **QSAR PREDICTION OF HEPATIC METABOLIC CLEARANCE OF ORGANIC DRUG-LIKE COMPOUNDS**

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Hepatic metabolic clearance is one of the key pharmacokinetic parameters determining the bioavailability, safety and therapeutic efficacy of drug candidates. Accurate prediction of this parameter is essential in modern pharmaceutical and biotechnological research, as it enables the identification of compounds with optimal metabolic stability at the early stages of drug discovery. Traditional experimental determination of hepatic clearance is time-consuming, resource-intensive and requires the use of biological materials. Therefore, the development of computational approaches such as Quantitative Structure–Activity Relationship (QSAR) modeling provides a powerful alternative that integrates chemical informatics, molecular design and pharmacokinetic analysis. In the context of pharmaceutical biotechnology, QSAR-based prediction supports the rational design of new bioactive molecules, minimizes experimental workload and enhances the efficiency of bioprocesses involved in drug development and optimization. This approach aligns with global trends toward sustainable, data-driven and cost-effective drug discovery.

**Aim of study:** to develop a QSAR model for predicting the hepatic metabolic clearance of organic drug-like compounds based on their structural characteristics.

**Materials and methods.** The dataset for modeling hepatic metabolic clearance included 41 organic drug-like compounds. To describe these compounds, a set of 15 electronic, physicochemical and topological descriptors was used. The following methods were applied in this study: multiple linear regression; correlation analysis and statistical analysis. 41 organic drug-like compounds were randomly divided into a training set (35 compounds) and a test set (6 compounds). The computational work was carried out using Matlab R2024b (trial license) and Microsoft Excel 2010.

**Results.** The evaluation of physicochemical, electronic and topological descriptors allowed the identification of key parameters contributing most significantly to the prediction of hepatic metabolic clearance values: the energy of the lowest unoccupied molecular orbital, the energy of the highest occupied molecular orbital, torsional energy, the number of hydrogen bond acceptors and the total molecular dipole moment.

**Conclusions.**

1. A QSAR model for predicting hepatic metabolic clearance was developed and validated, demonstrating high statistical significance.
2. The proposed mathematical approach enables the prediction of hepatic metabolic clearance based on molecular descriptors, facilitating the optimization of new drug development and the assessment of metabolic stability at early stages of pharmaceutical research.

## **FEATURES OF REGULATORY POLICY AND USE OF BIOSIMILARS**

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Lack of access to medicines remains a major obstacle to the successful treatment of diseases. Modern biotechnological drugs provide new therapeutic opportunities, but their complex production technologies make them highly expensive. The expiration of patent protection for numerous original biotechnological products has become a key factor in the development of so-called biosimilars (BS) - reproduced versions of original biotechnological medicines.

A biosimilar is a biological medicinal product that contains a version of the active substance of an already approved original biological product (the “reference medicine”) and, based on comprehensive comparability studies, demonstrates similarity to the reference product in terms of quality, biological activity, safety, and efficacy.