# SCIENTIFIC AND PRACTICAL CONFERENCE «INNOVATIONS IN MEDICINE AND PHARMACY: CONTRIBUTION OF YOUNG SCIENTISTS»

**Date: February 28, 2025** 

# НАУКОВО-ПРАКТИЧНА КОНФЕРЕНЦІЯ «ІННОВАЦІЇ В МЕДИЦИНІ ТА ФАРМАЦІЇ: ВНЕСОК МОЛОДИХ ВЧЕНИХ»

Дата проведення: 28 лютого 2025 р.





## НАУКОВО-ПРАКТИЧНА КОНФЕРЕНЦІЯ «ІННОВАЦІЇ В МЕДИЦИНІ ТА ФАРМАЦІЇ: ВНЕСОК МОЛОДИХ ВЧЕНИХ»

#### 28 лютого 2025 р.

influence on this process is VEGF-A. Its production is regulated by several factors, including the oncogenes E6 and E7, which are encoded by human papillomavirus genes. When it binds to VEGFR2-receptor on a blood vessel, the process of angiogenesis starts. Cervical cancer is characterized by a dense capillary network and neovascularization. Moreover, there is a direct connection between VEGF synthesis and the level of dysplasia. That is why VEGF-targeted therapy is an important field for development. For example, bevacizumab is a recombinant antibody that neutralizes VEGF and prevents it from binding with its receptor. According to the phase III trial, simultaneous administration of bevacizumab and chemotherapy showed higher overall survival, progression-free survival and response rate compared to chemotherapy alone. However, the negative side of using bevacizumab includes many side effects and contraindications, with the most important being that tumor cells can become resistance to the effects of this drug. That is why searching for more effective anti-angiogenic medicine should be a priority for scientists. For instance, integrin alpha 5 plays a significant role in signal transmission between cells. However, research has shown that it is also produced by tumor cells and influences the activation of the VEGF pathway of angiogenesis. It means that reducing integrin alpha 5 expression could possibly become a new target for researchers involved in seeking treatment for cervical cancer.

**Conclusions:** to sum up, finding more effective medicine for cervix cancer curation is crucial to decrease the number of women's deaths and give them an ability to live long, happy lives. Ukrainian government has to pay more attention on implementing new methods of cervix cancer therapy and update local protocols. Additionally, it would be remarkably to participate in drug production and contribute to overcoming this disease.

Keywords: cervical cancer, pharmacotherapy, angiogenesis inhibitors.

## PROBABILISTIC NEURAL NETWORK MODELS FOR PREDICTING METABOLISM OF TABLETED MEDICINES ACCORDING TO BIOPHARMACEUTICAL DRUG DISPOSITION CLASSIFICATION SYSTEM

## Kaouthar Bouaalam

Scientific advisor: candidate of chemical sciences, associate professor Y. Pushkarova Department of analytical, physical and colloid chemistry Head of department: candidate of chemical sciences, associate professor G. Zaitseva Bogomolets National Medical University

Kyiv, Ukraine

Actuality: the accurate prediction of drug metabolism is crucial in pharmaceutical research, as it influences drug efficacy, safety, and regulatory approval. The Biopharmaceutics Drug Disposition Classification System provides a framework for understanding drug absorption, distribution, metabolism, and excretion based on solubility and permeability. However, traditional experimental approaches for assessing metabolism are time-consuming and resource-intensive. Probabilistic neural network offers a promising alternative by enabling rapid and reliable predictions of drug metabolism, particularly for solid dosage forms.

**Aim:** to develop a predictive model for classifying drug metabolism (poor or extensive) within the Biopharmaceutics Drug Disposition Classification System using the Kruskal-Wallis test and a probabilistic neural network.

Methods of research: a set of compounds (n = 220) was investigated. Compounds were divided into a training subset (n = 176) and a testing subset (n = 44). Eleven physical-chemical descriptors were studied. The combination of the Kruskal-Wallis test and a probabilistic neural network was used to determine the informativeness of descriptors for predicting metabolism according to the Biopharmaceutics Drug Disposition Classification System (software: ChemOffice 2020, Matlab R2024b).

**Results:** a set of four descriptors was identified as optimal for predicting metabolism: hydrogen bond acidity, octanol-water partition coefficient, distribution coefficient at pH 7.4 and the number of hydrogen bond donors. The classification accuracy was approximately 80% across different spread parameter values. In this study, classification refers to assigning compounds to either extensive metabolism or poor metabolism class.

## SCIENTIFIC AND PRACTICAL CONFERENCE «INNOVATIONS IN MEDICINE AND PHARMACY: CONTRIBUTION OF YOUNG SCIENTISTS»

#### February 28, 2025

**Conclusions:** this study demonstrates the potential of combining the Kruskal-Wallis test and probabilistic neural networks for predicting the metabolism of tableted medicines according to the Biopharmaceutics Drug Disposition Classification System. The predictive model showcases the feasibility of utilizing these computational methods to streamline drug metabolism predictions, thereby reducing the time and resources typically required by traditional experimental approaches.

Keywords: pharmaceutical research, computational modeling, drug metabolism.

## PROSPECTS FOR THE DEVELOPMENT OF SOFT DRUGS FOR THE TREATMENT OF DIAPER DERMATITIS

T. I. Tatyanych-Radkivska, O. M. Hlushchenko

Supervisor: Candidate of Pharmacy, Associate Professor O. M. Hlushchenko Department of Pharmacy and Industrial Technology of Drugs Head of the Department: Doctor of Pharmacy, Professor Zh. Polova Bogomolets National Medical University Kyiv, Ukraine

**Relevance:** diaper dermatitis (DD) is one of the most common skin diseases in children of the first years of life in Ukraine. This disease can occur in any child who needs to wear diapers due to urinary incontinence. Most often, diaper dermatitis affects children aged from one month to two years old, reaching its peak in children aged six months to a year, it also affects 35 to 50% of babies.

With the advent of modern hypoallergenic, breathable disposable diapers the incidence of irritant and allergic contact dermatitis, as well as severe forms of the disease has significantly decreased, diaper dermatitis is still a common dermatological problem. Although it is not life-threatening, it does cause discomfort in newborns, and children, and anxiety for parents and guardians.

The aim of our work is to investigate the problems of emergence and prospects for the development of soft drugs for the treatment of diaper dermatitis.

Methods of research: search, analysis, generalization and systematization of data.

**Results:** world studies have shown that this disease is most often observed in children aged seven months to one year, among infants the prevalence of diaper dermatitis ranges from 7% to 35%.

Based on a study conducted in the United Kingdom involving more than twelve thousand infants, it was found that 25% of infants developed diaper dermatitis in the first four weeks of life. According to the literature, the incidence of diaper dermatitis in Italy is 15.2%, in Nigeria – 7% and in Kuwait – about 4%.

Diaper dermatitis is an inflammatory skin lesion of the perineal and perianal area as a result of several external factors: moisture, prolonged skin contact with urine and feces, and exposure to detergents, antiseptics, and medications. Water with high and salt content can also negatively affect the skin's protective barrier, reducing its resistance to irritants.

The most common causes of diaper rash are fungal infection caused by Candida albicans, which can be both the primary cause of dermatitis and the secondary cause of chronic skin irritation. In neonates, Staphylococcus aureus infection is most common. Staphylococcus aureus, Streptococcus pyogenes may also cause infectious skin lesions.

Insufficient development of sebaceous glands, high skin acidity (6.5-7.0 in infants vs. 5.3 in adults) and an increased tendency to allergic reactions also contribute to the development of inflammation. Mechanical friction of the skin with a diaper, humidity, improper care, antibiotics, and changes in the child's diet can accelerate the development of the disease. Changes in the infants' diet affect the intestinal microbiota and fecal acidity. Breastfeeding is considered a protective factor because it promotes the formation of healthy microflora. Prolonged contact with urine and feces increases the risk of inflammation. Babies who are changed diapers more often are less likely to develop dermatitis.

The main factor in the development of diaper dermatitis is increased due to diaper wear. It promotes friction and maceration of the skin, which makes the skin more susceptible to damage and penetration by microorganisms. Also