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

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ANALYSIS OF BIOPHARMACEUTICS CLASSIFICATION SYSTEM BY MEANS OF CHEMOMETRIC METHODS

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Actuality: the growing role of data-driven approaches in pharmaceutical research makes this analysis highly relevant. The Biopharmaceutics Classification System classifies drugs based on two main properties: solubility and permeability. The Biopharmaceutics Classification System is crucial in pharmaceutical sciences as it helps predict drug absorption, bioavailability, and the need for bioequivalence studies. Integrating chemometric models with Biopharmaceutics Classification System aligns with modern trends in personalized and computational pharmaceutics, facilitating early-stage drug screening and optimizing formulation strategies. Furthermore, the ability to predict drug behavior more efficiently accelerates the drug development process, reducing time and costs associated with traditional testing.

Aim: to predict compound classes according to the Biopharmaceutics Classification System using the Kruskal-Wallis test and a probabilistic neural network.

Methods of research: a set of compounds (n = 122) was investigated. Compounds were divided into a training subset (n = 102) and a testing subset (n = 20). Eleven descriptors were studied. The Kruskal-Wallis test was used to determine the optimal number of descriptors for the correct classification of compounds according to the Biopharmaceutics Classification System (software: ChemOffice 2020). The probabilistic neural network was used to predict compound classes according to the Biopharmaceutics Classification System (software: Matlab R2024b).

Results: it was established that only three descriptors are sufficient for the correct classification of compounds according to the Biopharmaceutics Classification System: partition coefficient, solubility and polar surface area. It was recommended to use probabilistic neural network with a spread parameter of 0.1. At this spread parameter value the minimum classification error of 10 % was observed, meaning the classification precision was 90%. Additionally, we applied the proposed procedure to 23 compounds, that could belong to different classes due to factors such as intermediate solubility and permeability or variability in physiological conditions that influence drug absorption. The probabilistic neural network successfully assigned these compounds to one of the classes.

Conclusions: the use of both statistical and machine learning approaches provides a robust method for prediction. These findings support the potential of machine learning models in enhancing the accuracy and efficiency of pharmaceutical classification tasks.

Keywords: artificial neural network, drug design, pharmacy, statistics.