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Application of 3D Modeling Methods to Study the Spatial-Temporal Distribution of Drugs

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ABSTRACT

Physiologically based pharmacokinetic modeling (PBPK) of drugs is a promising area of research in pharmacology. It is based on mathematical transformations of real anatomical structures and physiological processes, making it easier to interpret the results. However, there are limitations to PBPK modelling, particularly in the way it describes the transfer of substances between different parts of the body. Specifically, the use of differential equations to describe this transfer does not take into account hemodynamic properties such as blood flow and diffusion rates, which can lead to inaccurate results and make it difficult to interpret. Therefore, it is essential to develop more accurate and detailed models that take these factors into account. The aim of our study was to develop a universal, multidimensional model that could describe in detail the distribution and transformation of metabolites, while taking into account the transfer of substances between different components of a system. Our approach is based on simulating real physical processes, such as hemodynamics and diffusion within a closed system, which allow us to create a more accurate representation of matter movement between compartments. Unlike traditional PBPK (physiologically based pharmacokinetic) models, our approach takes into account the first-pass effect and the non-Newtonian properties of blood, as well as its incompressibility. Using this model, we were able to thoroughly investigate the distribution and metabolism of paracetamol. The results confirmed the high accuracy and practical usefulness of our model. The developed model is a powerful tool for studying pharmacokinetics and predicting the distribution and metabolism of drugs. This opens up new possibilities for optimizing pharmacotherapy and reducing the risks associated with drug use.

Keywords: liver, 3d modelling, pharmacokinetic, first-pass effect

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