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Stochastic Approach to Pharmacokinetics vs Principles of Quantum Mechanics

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Statement of the Problem: A stochastic modelling in pharmacokinetics [1,2] is an important method of tracking endo- as well as exogenous substances in the organism. These mechanistic models provide a statistical description of the behaviour of single molecules of the investigated compound. Nanocarriers, which can be viewed as nanocompartments, constitute a very attractive field of application of these models. However, to ensure true mechanistic character of the model, one should be very cautious not to come into conflict with fundamental laws of nature. For instance, Zhao et al. claim: … little research has been done to systematically determine the probability for a drug molecule to follow a specific traveling route [3]. Their paper (and some others [4]) is based on the concept of the probability P_ij for a drug molecule in compartment i at time 0 to end in compartment j after an elapsed time t. The purpose of the present study is: 1. to indicate that this concept becomes meaningless when many identical molecules are present. 2. To suggest a direction in which to search for a solution. Theoretical: As far as one considers a single molecule, it is possible, at least in principle, to watch its trace. However, the number of molecules is of order in range 10 ^17- 10 ^20 and then their tracking is excluded by the principles of quantum mechanics, namely the indistinguishability of identical particles [5]. Findings One therefore cannot say about the route of the molecules or count their visits in particular compartments. This is not necessary, though. An effectiveness of drug action or physiological process can be expressed in other manner, not violating laws of nature. Conclusion: Stochastic modelling can and should be done by means of correctly described quantum states. It is especially important in nanopharmaco¬kinetics [6] which should also become a quantum pharmacokinetics.

Biography

Wojciech Jawień obtained his MS degree in physics from Jagiellonian University in Kraków and PhD in pharmaceutical sciences from Medical Academy (now Medical College JU). His area of interest ranges from application of AI in drug therapy through computational aspects of pharmacokinetic modelling to physical considerations in pharmacokinetics.

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