Applications of Physiologically Based Pharmacokinetic (PBPK) Modeling in Nanomedicine and Food Safety Assessment and Roles of Artificial Intelligence (AI) Approaches in these Areas

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Abstract

Physiologically based pharmacokinetic (PBPK) modeling is a computational simulation process that describes the absorption, distribution, metabolism, and excretion of a chemical and/or its metabolites in the body based on the interrelationships among key physiological, physicochemical, and biochemical determinants using mathematical equations. It is a scientifically-sound tool in the prediction of internal dose metrics of a chemical in the target organ, in vitro to in vivo extrapolation (IVIVE) of kinetic and toxicity data, and interspecies species from animals to humans. It is a useful tool in different areas, such as drug discovery and development, and chemical risk assessments on human health, environmental health and animal health. In this presentation, I will introduce how we develop PBPK models of drugs, environmental chemicals and nanoparticles for applications in nanomedicine, food safety, and human health risk assessments. I will present our recent studies to illustrate each application. I will also introduce a new physiological parameter database for PBPK modeling in food-producing animals, including cattle, swine, sheep, goats, chicken, and turkey. In addition, I will share our experience and my perspective on the roles of artificial intelligence (AI) in these areas and how PBPK and AI approaches can be integrated to support each other.