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Simulations of pharmacokinetics and pharmacodynamics in virtual populations to enhance understanding of toxicology in humans

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Abstract

An understanding of the pharmacokinetic (PK) and pharmacodynamic (PD) behavior of pharmaceutical and environmental compounds is essential to optimize their beneficial effects and minimize their toxicity. Although clinical studies have the potential to provide useful information on the toxicity of these compounds, studies on all compounds, doses and other relevant variables may not be feasible. Simulations and predictions of PK and PD in virtual subjects provide a useful tool during drug development and toxicity screening of environmental compounds. Simcyp is a physiologically-based population pharmacokinetic (PBPK) simulator used in such applications. Using in vitro-in vivo extrapolation techniques to predict absorption, distribution, metabolism, excretion and their associated variability in populations, this user-friendly software supports applications relevant to environmental toxicology, drug development and regulatory assessments. PBPK models linked to PD models are useful for simulation and prediction of responses to compounds based on plasma concentrations of the compound as well as predicted concentrations at the target site within the body, where measurement of the drug concentration may not be practical. Case studies illustrating the use of these PBPK models linked to PD models for prediction of the potential for toxicity of compounds, exploring mechanisms of drug toxicity and identifying populations that may present with a greater risk of toxicity are presented in this talk.

Biography

After training as a pharmacist, Manoranjenni Chetty obtained a PhD in Pharmacology. She has extensive lecturing experience in Pharmacology and Pharmacokinetics at universities in Australia and South Africa. She is currently a Principal Scientist at Simcyp Ltd, based in Sheffield in the United Kingdom. More than 35 papers on pharmacokinetics, pharmacodynamics and biologics have been published in reputed journals by her.