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Development and evaluation of PBPK model of perfluorodecanoic acid: Application to human exposure assessment

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The aim of present study was to develop a physiologically-based pharmacokinetic (PBPK) model of perfluorodecanoic acid (PFDA) in rats for applying its human exposure assessment. We constructed the PBPK model based on *in vivo* study after the oral or intravenous administration of PFDA in female rats (at dose of 1 mg/kg). The biological samples consisted of plasma, nine tissues (kidney, liver, lung, heart, spleen, adipose tissue, muscle, GI tract, and brain), urine, and feces were analyzed using UPLC-MS/MS with liquid-liquid extraction after protein precipitation. The PBPK model was fitted and simulated as changing the key parameters such as the transporter maximum (T_m), the transporter affinity constant (K_t), the rate constant to storage compartment (K_{st}), and the urinary elimination rate constant (K_u). The tissue-plasma partition coefficient was the highest in the liver (0.607), followed by kidney (0.233), lung (0.100), and spleen (0.052). The model simulation was fitted well with the observed values. The parameters of T_m , K_p , K_{st} , and K_u were 199.5 $\mu\text{g}/\text{h}$, 201.5 $\mu\text{g}/\text{L}$, 0.19 h^{-1} , and 0.13 h^{-1} , respectively. A PBPK model was extrapolated to humans by taking the interspecies differences in physiological parameters into account. The reference dose of 22.98 $\mu\text{g}/\text{kg}/\text{day}$ and external dose of 5.54 $\text{ng}/\text{kg}/\text{day}$ for human risk assessment were estimated using Korean biomonitoring values. The developed PBPK model in rats can be a foundation for the development of human model for PFDA and used as a tool in assessing human exposure of PFDA.

Biography

Yong Bok Lee is currently a Professor of the College of Pharmacy, the former Vice-President of Chonnam National University and the Ex-President of The Korean Society of Pharmaceutical Sciences and Technology. He received his PhD degree in Pharmaceutics from Seoul National University. His research interests are focused on the lymphatic delivery of immunosuppressants and the application of population PK/PD models associated with genetic differences in drug transporters and enzymes. He won many prestigious awards and honors including the KSPs Progress Prize and Academic Prize, the KFDC Academic Prize, the CNU Yongbong Academic Prize and the MEST official commendation.

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