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Prediction of Systemic Concentrations of Sensitizing Compound Using TKTD Simulation Model

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To investigate the safe handling of an industrial product, *phenyl vinyl sulfone* (PVS), which has an extremely high potential for dermal sensitization at low concentrations and positive mutagenicity, the maximum no-effect concentration for dermal deposits was obtained from dermal sensitization experiments. The systemic concentrations in the liver, which is considered to be a target tissue of mutation, were monitored using the TKTD (Toxico Kinetics Toxico Dynamics) model by inputting the maximum no-effect concentration of sensitization. The predicted highest concentration in the liver was compared with the no-effect level of mutation in the same tissue, which was derived from an in vitro mutagenicity study. The results showed that when this product is handled at lower concentrations, which may not induce dermal sensitization, the systemic concentrations that prevent dermal sensitization caused by PVS could also protect against the mutagenicity of this compound.

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