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Determination and Optimisation of Descriptor Values of Safrole by Gas-Liquid Chromatographic Methods and Liquid-Liquid Partition Systems

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Abstract

In recent years, accumulation of harmful organic chemicals in various environmental and biological compartments causes regrettable harmful effects to humans and ecosystems. Therefore, determining their distribution levels and controlling their risks in these compartments is important for environmental risk assessment procedures. However, experimental determination of their distribution for dose-response and exposure assessments needs a large amount of economical, technical, and human resources. Moreover, such requirements are difficult to afford by developing countries like Sri Lanka. As a solution to this problem, Quantitative-Structure Property Relationship (QSPR) method can be used to establish a quantitative relationship between the structures of the compounds and their chemical and physical properties. In this study, Abraham's solvation parameter model, was used as the QSPR together with experimental values to determine descriptor values for safrole. Safrole is a harmful organic chemical which is used as a flavouring agent, a fragrance agent, and a raw material in many industries including the drug and perfumery. Because sufficient levels of safrole were identified as a carcinogen, the use of safrole was prohibited by United States Food and Drug Administration (US FDA) since 1970. According to the food additive regulations, safrole in soft drinks, beverages, and food must be lower than 1 μg ml-1 .Safrole is a constituent compound of some spices which are being used for commercial beverage productions and is also used widely in the perfumery industry. Here, descriptor values for safrole were determined using gas-liquid chromatographic retention factors combined with liquid-liquid partition coefficients. Isothermal retention factors were determined at 20^{o} C intervals over the temperature range of 60^{o} C to 160^{o} C for poly (cyanopropylphenyldimethylsiloxane) stationary phase with 14% cyanopropylphenyl monomer. Previously measured retention factors for poly (dimethyldiphenylsiloxane) stationary phase with 5% diphenylsiloxane monomer were optimized in this research study, over the temperature range of 80^{o} C to 280^{o} C. Partition coefficients of safrole were determined using eight different totally organic partition systems (n-heptane-formamide, n-heptane-methanol, n-heptane-n,n-dimethyl formamide, n-heptanetrifluoroethanol, n-heptane-dimethyl sulfoxide, isopentyl ether-ethylene glycol, isopentyl ether-dimethylsulfoxide, and n-hexane-acetonitrile). Then the descriptor values were determined using Solver Algorithm in excel using the measured retention factors and partition coefficients. Solver is an algorithm which assigns the values for the descriptors such that the standard deviation between the experimental solute property and the calculated solute property would be minimum. Determined descriptor values for safrole using these stationary phases and solvent systems are E=1.108, S=1.123, A=0.000, L=5.340, B=0.174, B (0)=0.365 and V=1.246. Validity of the descriptors were tested with theoretical models. The determined descriptor values have a small standard deviation (0.068). Therefore, the determined descriptor values will be useful in determining the distribution level of safrole in environmental compartments.

Keywords: QSPR, Solvation parameter model, Safrole, Gas-liquid chromatography, Liquid-liquid partition systems