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OPTIMIZATION OF THE SOLUTE DESCRIPTORS FOR CITRONELLAL BY GAS CHROMATOGRAPHY AND LIQUID-LIQUID PARTITION SYSTEMS

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Citronellal is a naturally occurring monoterpenoid aldehyde that has an intense lemon aroma. It is the main compound found in citronella oil that is often used as a natural insect repellant, antifungal agent, flavouring agent, and fragrance in the cosmetic industry. Despite their natural origin, the long-term use of these essential oil compounds can result in considerable health and environmental hazards. To assess such effects, the available conventional methods are costly and require significant human and technical resources. Instead, the Abraham solvation parameter model can be used. This model is based on quantitative structure-property relationships. This has become popular in estimating solute properties and environmental distribution with significantly lower costs by using fewer resources. The model is expressed as $log\,\mathrm{SP} = c + e\mathrm{E} + s\mathrm{S} + a\mathrm{A} + b\mathrm{B} + v\mathrm{V}$ for transfers between two condensed phases. Here, SP is a Free energy-related solute property; lowercase letters are system constants, and uppercase letters are solute descriptors. V: McGowan's Characteristic Volume, E: excess molar refraction, S: dipolarity/polarizability, A and B: hydrogen-bond acidity and basicity. The determination of solute descriptors for citronellal was carried out using the gas chromatographic technique with six stationary phases including (14% cyanopropyl-phenyl)-methylpolysiloxane, (88% Cyanopropyl)aryl-polysiloxane, and diphenyldimethyl polysiloxane stationary phases. Also, Citronellal was equilibrated in 17 organic biphasic systems, and the partition coefficients were determined. The obtained solute descriptor values and partition coefficient values were then utilized to optimize the descriptor values using the Solver algorithm in MS Excel® such that the standard deviation is minimal. The optimized descriptor values for citronellal are E = 0.279, S = 0.703, A = 0, L = 5.045, B = 0.454, and V = 1.490, respectively, with a standard deviation of 0.049. These descriptor values can be used to estimate the distribution of citronellal in environmental and industrial partition compartments and in toxicological data.

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Keywords: Citronellal, Descriptors, Solvation parameter model, Gas chromatography