



Determination of the solute descriptors for ethyl cinnamate by gas chromatography and liquid-liquid partition systems

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Ethyl cinnamate is a naturally occurring ester found in cinnamon oil extracts. Due to its fruity and balsamic odor, it is used in the preparation of artificial flavours of strawberry, raspberry and cherry and used in oriental oil perfumes. Being an ingredient in consumer products, toxicological studies and flavour chemistry are required to quantify its properties that vary with the type of application. Solely experimental quantification needs significant amounts of human, technical and monetary resources, difficult to afford for Sri Lanka. As a solution to the above problem, a quantitative structure-property relationship Abraham's solvation parameter model ($\log SP = c + eE + sS + aA + bB + vV$, where, SP: Free energy related solute property, c: system constant, V: McGowan's Characteristic Volume, E: excess molar refraction, S: dipolarity/polarizability, L: gas-liquid partition coefficient for solute in n-hexadecane where L is used instead of V in the equation for the transfer between gas and condensed phase mass transfer, for the gas-condensed phase systems, A: hydrogen-bond acidity, B: hydrogen-bond basicity) can be used to estimate the environmental distribution of a compound by determining physicochemical and structural properties. The above task was accomplished for ethyl cinnamate by determining its solute descriptors experimentally using a gas chromatographic technique with poly(dimethyldiphenylsiloxane) and poly(cyanopropylphenyldimethylsiloxane) stationary phases and organic biphasic partition systems. The stationary phases were calibrated and isothermal retention factor values were determined at 20 °C intervals from 80 °C to 260 °C. Ethyl cinnamate was equilibrated in nineteen totally organic biphasic systems and the partition coefficients were determined. The descriptor values were then determined using the Solver algorithm in excel such that the standard deviation would be minimum. The determined descriptor values for ethyl cinnamate were, $E = 1.0950$, $S = 1.0749$, $A = 0.0000$, $L = 6.3045$, $B = 0.6290$, and $V = 1.4523$. The determined descriptor values can be used to estimate the distribution of ethyl cinnamate in environmental and industrial partition compartments.

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