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Title: Prediction of Solubility of Solid Biomolecules in Supercritical Solvents Using Group Contribution Methods and Equations of State

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Abstract: The purpose of this study is to present a method to estimate the solubility of solid solutes in supercritical fluids when only the molecule structure is known. The solubility of solid solutes in a supercritical fluid is an important thermo-physical property that needs to be determined if one is to develop a generic supercritical fluid extraction model. Due to the general lack of solubility data and/or pure component property data needed to estimate solubility, a need exists to develop methods to estimate the solubility of solid solutes in a supercritical solvents using limited information. Group contribution methods were used to estimate pure component properties, equations of state (Lee-Kesler-Plocker (LKP) and Mohsen-Nia-Moddaress-Mansoori (MMM) were then used to estimate the PVT behaviour of the solvent and the fugacity coefficient of solute in the solute-solvent mixture. The solubilities of β-carotene, cholesterol, nimodipine and nimbin in supercritical solvents were determined. Our results show that the LKP model provides the best fit for β-carotene and nimodipine in $SCCO_2$ and the MMM model is best for cholesterol in $SCCO_2$ and SCC_2H_6 and for nimbin in $SCCO_2$. The Aromaticity Index (AI) seems to be an important parameter for determining which model will perform best; based on the systems analysed here, one should use the LKP EOS when AI > 0.3, otherwise use the MMM EOS.

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