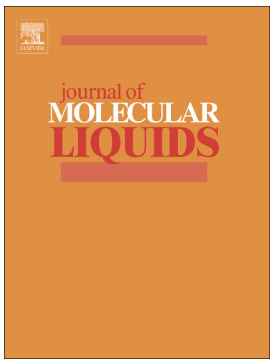

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Solute-solvent and solvent-solvent interactions and preferential solvation of limonin in aqueous co-solvent mixtures of methanol and acetone

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ABSTRACT

Solute-solvent and solvent-solvent interactions of limonin in binary solvent mixtures of methanol + water and acetone + water were investigated from the solubility data by using the linear solvation energy relationships concept. The variation of limonin solubility depended mainly upon the hydrogen bond basicity for methanol (1) + water (2) mixtures, and the cavity term for acetone (1) + water (2) mixtures. The preferential solvation parameters ($\delta x_{1,3}$) of limonin in two solvent mixtures were derived by means of the inverse Kirkwood–Buff integrals method. $\delta x_{1,3}$ values were negative in water-rich mixtures but positive in solvent compositions from 0.24 or 0.20 (0.25) to 1 in mole fraction of methanol or acetone, respectively. It was conjecturable that in water-rich mixtures, the hydrophobic hydration around the nonpolar methyl groups of limonin played a relevant role in the