Linear Solvation Energy Relationships in the Application to Prediction of Chromatographic and Some Physicochemical Properties of Phenolic Compounds

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Quantitative structure-property relationships (QSPR) belong to the most often studied manifestations of the linear solvation energy relationships (LSER). In this study, LSER methodology was proposed for evaluation the retention factors and some others chromatographic significant and important parameters of phenolic compounds.
A LSER approach has been developed to predict the retention factors k and acid dissociation constant pKa for a published collection of data of phenolic compounds. Other dependent variables (n-octanol-water partition coefficient logP, molar refraction MR, dipole moments m, energy hydration EH, and total energy Etot were calculated by itself and estimated also with LSER. The independent variables in these models are empirically determined descriptors (Abraham's descriptors) of the solute and solvent molecules. Results suggest that retention and other types of properties in may be modeled using a LSER approach. All obtained equations showed acceptable correlation coefficients ($r2 > 0.9$) and demonstrated their adequate predicting ability.