Evaluation of the Predictive Retention Factor of Phenolic Compounds by QSPR Equations

노경호*, 이승기[1], Yulia Polyakova[1]
인하대학교 생명화학공학부; [1]인하대학교 화학공학과
(rowkho@inha.ac.kr*)

Evaluation of the predictive retention factor of phenolic compounds from their physico-chemical and structural properties can be made successfully in terms of QSPR researches. Correlation relationships between retention factors of sixteen phenolic compounds reported in bibliography and various descriptors including binding energy (E_b), hydrophobicity ($log\ P$), hydrophilic-lipophilic balance (HLB), molecular refractivity (MR), polarizability (α), water solubility ($log\ S$), connectivity index ($^0\chi$) of zero order and wiener index (w) were established. The empirical equations were expressed in a linear and multiple-linear form. The results of theoretical calculations are in good agreement with experimental data. The empirical equation can be applied for prediction of the various chromatographic properties, identification of the substances having a similar structure.