Correlation Linear Equation for Retention Factor of Nucleic acid using QSPR

<u>정금주</u>, 노경호*, 한순구

인하대학교 화학공학과

(rowkho@inha.ac.kr*)

The retention time of sample in column was determined by various parameters. To predict the accuracy retention time, the study that predicting retention time based on different structures of samples is performed. Quantitative structure property relationships (QSPR) relate physicochemical properties. And it was quantified the connection between the structure and retention property of molecules and allow the prediction retention parameters of solute using molecular structure parameters. In this study, the retention factor of nucleic acid were assumed to be governed by their several descriptor such as water solubility, polarizability, solvation free energy, wiener index, molar refractivity etc. The effect of retention factor was estimated with calculated values, and the results showed that each descriptor with different molecular structure has different effect. The empirical equation was estimated from two to seven types of descriptors, respectively. When seven types of descriptor were used, a higher value of correlation coefficient of the empirical equation was obtained. Furthermore, the experimental data and the theoretical values have good agreement.