

Interrelation of Retention Factor of Amino-Acids by QSPR and Linear Regression

노경호*, 이승기¹, Yulia Polyakova¹
인하대학교 생명화학공학과; ¹인하대학교 화학공학과
(rowkho@inha.ac.kr*)

Interrelation between retention factors of several L-amino acids and their physico-chemical and structural properties can be made successfully in chromatographic researches. In this paper we have described the prediction for retention factor in various properties of the L-amino acids. Eighteen L-amino acids were included in the study, and the retention factors were measured experimentally by RP-HPLC. Binding energy (E_b), hydrophobicity ($\log P$), molecular refractivity (MR), polarizability (α), total energy (E_t), water solubility ($\log S$), connectivity index (χ) of different orders and wiener index (w) were theoretically calculated. Relationships between these properties and retention factors are established, and their predictive and interpretive ability are evaluated. The equation between retention factors and various descriptors of L-amino acids was suggested as $k = a + b(P)$, and the correlation coefficients estimated were relatively higher than 0.90.