Prediction of Solubility Parameters and Miscibility of Drugs with Pure Alcohols by Molecular Dynamics Simulations

임준혁, 신문삼[1], 김병헌, 김화용*
서울대학교; [1]을지대학교
(hwayongk@snu.ac.kr*)

The objective of this study was to develop a computational model based on molecular dynamics technique to predict the miscibility of drugs with pure alcohols. Molecular dynamics (MD) simulations were performed using the COMPASS force field and the cohesive energy density and the solubility parameters were determined for the model compounds. The magnitude of difference in the solubility parameters of drugs and pure alcohols is indicative of their miscibility. The MD simulations predicted drugs (triclosan, IPBC, salicylic acid, triclocarban, and climbazole) are miscible with pure alcohols (ethanol, 1-propanol, 1-butanol, 1-pentanol, 1-hexanol, and 1-heptanol). This is consistent with our experimental results and the solubility parameter values obtained using the MD simulations values were in reasonable agreement with those calculated using group contribution methods. The findings demonstrate that molecular modeling is a powerful technique for determining the solubility parameters and predicting miscibility of drugs.