Prediction of toxicological effects of ionic liquids to fish Danio rerio using in silico calculated linear free energy relationship descriptors

조철웅, 한민희[1], 윤영상[1,†]
전남대학교 바이오에너지공학과; [1]전북대학교 화학공학부
(ysyun@jbnu.ac.kr†)

Ionic liquids (ILs) are one class of the most interesting solvents in chemical industries because they are likely to be applied in a variety of research area. However, their environmental characteristics have not been sufficiently investigated; in particular, their toxicological information is needed to forcast their environmental risk. Here, fish toxicity test method, designated as one of the standard toxicity indicators, are applied to identify toxicological characteristics. However, since the toxicity values of ILs to fish are rarely presented, the gap of toxicological information should be filled. In order to solve this problem, quantitative structure-activity relationship approach, especially linear free energy relationship model, is desirable because it provides high predictability, high structural accessibility, and understanding of the chemical meaning at the molecular level. For the prediction, ILs' common toxic effects by comprehensive toxicity prediction model was calculated and correlated with the experimental values. The results show that the calculated values could be used to correlate the experimentally determined fish toxicity in R^2 of 0.94-0.95.