Modelling of quantitative structure activity relationship for predicting toxic effects of ionic liquids

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Ionic liquids (ILs), as molten salts, have been highlighted in various industrial fields due to their excellent properties, e.g., thermal & chemical stability, ignorable volatility, and material dissolution ability. Since ILs are structurally tunable, their physical, chemical, and environmental properties can be appropriately controlled. On the other hand, some of ILs can be potentially hazardous and persistent substance in aquatic environments. In this sense, environmental benign ILs should be designed to fulfill basic green principle for sustainable development. For the purpose, we developed a quantitative structure activity relationship model for predicting biological responses in several toxicity testing methods and understanding the toxicological mechanisms according to solely IL structure. In results, a single linear free energy relationship (LFER) model with sensitivity-related terms was developed, and their combination could be used to predict each of 50 toxicological effects of ILs with R2 of 0.593~0.978, and SE of 0.098~0.699 log unit, and overall dataset was fitted with predicted values in R2 of 0.901 and SE of 0.426 log unit.