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Prediction of cellulose dissolution in ionic liquids using molecular descriptors based QSAR model

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Statement of the Problem: The dissolution of lignocellulose by ionic liquids attracted much attention during the last decade. However, the experimental screening and selection of a large number of potential ionic liquids for biomass processing are challenging tasks.

Methodology & Theoretical Orientation: In this work, the prediction of cellulose dissolution in ionic liquids (ILs) was evaluated by quantitative structure-activity relationship (QSAR) model using the molecular descriptors of ionic liquid's constitutional ions derived from Comprehensive Descriptors for Structural and Statistical Analysis (CODESSA) program. All the structures of individual cations and anions of ILs were optimized without constraint using B3LYP/6-31G(d,p) level in Gaussian 03 package and verified as minima by frequency calculations. The CODESSA package calculates various descriptors such as constitutional, topological, geometrical, electrostatic, quantum-chemical, and thermodynamic from the three-dimensional structures of molecules. 438 molecular descriptors were calculated for 80 different ILS in the data set.

Findings: Two QSAR correlation models for cellulose solubility in ILs with respect to mass and molar percentages were developed. Both models include 13 molecular descriptors and were reliable as indicated by the considerably high R^2 value for both training and test sets. Models based on cellulose molar solubility exhibited better correlation (R^2 of 0.92 vs. 0.88) and predictability (R^2 of 0.89 vs. 0.83) than those based on mass percentage solubility.

Conclusion & Significance: These results indicated that the molecular descriptors of ILs could be effectively used to develop QSAR models for facilitating the in silico and a prior screening/selection of ILs customized for specific applications.

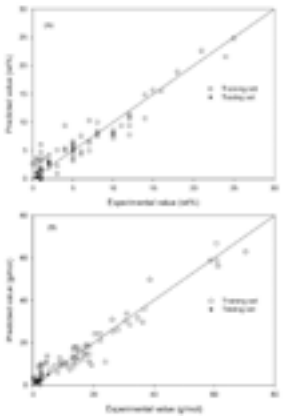

Figure: Scatter plots of predicted vs. experimental values of cellulose solubility in ionic liquids

Biography

Chan Kyung Kim is a Professor and Chairman of the Department of Chemistry, Inha University located in Incheon, Korea. He is an active member of Brain Korea 21 Plus Project supported by the Ministry of Education, Science and Technology. His research is concentrated on the development and application of QSAR/QSPR method including MSEP for high energy density materials. He is also interested in the theoretical organic and inorganic chemistries to understand the structures and reactivity of chemical systems. Recently, his research is oriented on the design of carbon dioxide removal in the presence of N-methylaniline and silyl halides and conversion of carbon dioxide to some useful materials in the zeolite catalysts.

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