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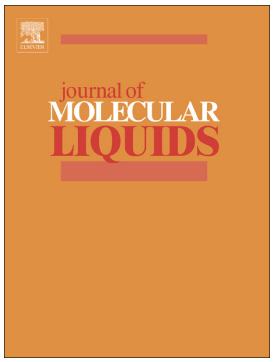

Assessment for multi-endpoint values of carbon nanotubes: Quantitative nanostructure-property relationship modeling with norm indexes

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Assessment for multi-endpoint values of carbon nanotubes: quantitative nanostructure-property relationship modeling with norm indexes

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Abstract

Carbon nanotubes (CNTs) have important role in ecological environment owing to their ability of the adsorption of organic contaminants which might greatly affect the dispersibility of CNTs in aquatic environments. Thus in this work, quantitative nanostructure-property relationship modeling studies were performed with the norm indexes descriptors our group proposed to predict the adsorption data (represented by $\log K_{\infty}$ and $\log K_{\mathrm{SA}}$) of organic compounds by multi-walled CNTs and the dispersibility (represented by $\log C_{\max}$) of single-walled CNT in various organic solvents. Calculation results showed that the three models could provide accurate and satisfactory predictions with the squared correction coefficient for the training set and the test set of 0.9500 and 0.9792 for $\log K_{\infty}$, 0.9258 and 0.9770 for $\log K_{\mathrm{SA}}$, 0.9511 and 0.9956 for $\log C_{\max}$ respectively. Validation results containing cross validation, Y-randomized test and applicability domain analysis together with the comparison with other works demonstrated that our models were stable, robust and reliable. These satisfactory results showed that the norm indexes descriptors our group proposed might have extensive and promising applications in nanotechnology.

Keywords: carbon nanotubes; quantitative nanostructure-property relationship; adsorption; dispersibility; norm indexes

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