Predicting The Solubility of Pesticide Compounds in Water Using QSPR Methods

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Abstract

Pesticide contamination of surface water and groundwater due to agricultural activities has been of concern for a long time. Water solubility indicates the tendency of a pesticide to be removed from soil by runoff or irrigation and to reach surface water. The experimental procedures determining the solubility in water of pesticides are always time-consuming, expensive and it is difficult to accurately distinguish species with similar physicochemical properties. A highly effective tool depending on a quantitative structure-property relationship (QSPR) can be utilized to predict physical properties such as bio-concentration factor and solubility in water for those pesticide compounds with no literature values. QSPR models were developed using multiple linear regression, partial least squares (PLS) and principal component neural networks analyses (PC-ANN) for 219 different pesticide compounds. The PLS and PC-ANN give good regression models with good prediction. The optimal models obtained by PC-ANN are better than those obtained by PLS analyses from the statistical point of view. The results obtained offers excellent regression models that hold good prediction ability. The descriptors used in these models are in consistence with the suggested experimental factors to affect the solubility of pesticides compounds in water.