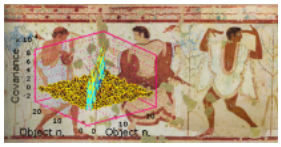

A QSPR for Prediction of Solubilization of Hazardous Compounds Using GA-Based MLR in CTAB Micellar Media

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Abstract

QSPR studies for estimating the incorporation organic hazardous compounds in cationic surfactant (CTAB) were developed by application of the structural descriptors and MLR method. A simple model with low standard errors and high correlation coefficients was selected. It was also found that MLR method could model the relationship between solubility and structural descriptors perfectly. The proposed methodology was validated using full cross validation and external validation using division of the available data set into training and test sets. The proposed model can be used adequately for the prediction and description of the solubility of organic compounds in micellar solutions**.** The statistical parameters root mean squares error of prediction (RMSEP) relative error of prediction (REP)% and standard error of prediction (SEP) were 0.169, 9.561 and 0.176 respectively for proposed MLR model.

Introduction

The micellar-enhanced ultrafiltration (MEUF) and cloud-point procedure have been applied for preconcentration and removal of several organic pollutants including pesticides, herbicides, aromatic hydrocarbons, PCB's, aliphatic alcohols, aromatic amines, phenols and chlorophenols from aqueous samples [1]. Surfactants can solubilize materials into solvents other than water. Even when surfactant aggregation does not occur or the aggregation number is small in a particular solvent in the absence of other material, the addition of solvent-insoluble material, such as water, may give rise to aggregation with consequent solubilization of the additive [2]. In this way, surfactant micelles can enhance the sensitivity and can bring about changes in solubility, pKa, chemical equilibria, reaction rates and mechanisms, spectral distributions and intensities and the stereoselectivity of some chemical processes [3, 4]. One of the most successful approaches for the prediction of chemical properties, starting solely with molecular structural information, is modelling of quantitative structure–activity/property relationships (QSAR/QSPR). The QSPR model provides significant additional insight into the relationship between the molecular structure and fundamental processes and phenomena in chemistry. Such a data processing strategy is useful in describing the relationship between chemicals molecular structures and analytical parameters. One of main striking advantage of QSPR method is prediction of seeking property that can't be measured in real matrix due to interference effect of other matrix components.

Materials & Methods

The experimental data utilized in this work consists of the micellar solubility (K_s), for 40 solutes in CTAB were reported by Frank Quina et.al. [1]. The data set is heterogeneous, and includes practically all the principal functional groups present in pesticides, herbicides and various organic pollutants. The data set is heterogeneous, and includes practically all the principal functional groups present in pesticides, herbicides and various organic pollutants. The standard experimental conditions adopted for the K_s values were ambient temperature (20-30 ^{o}C) at low extents of solute

incorporator in the absence of significant amounts of added electrolyte or other additives. Some of the chemicals in the literature database have more than one K_s value and the result of being derived from different sources; in these cases were randomly selected. The modelled data were expressed in logarithmic units (log K_s), for chemicals with a log K_s range of -0.39 to 4.06.

Results

The MLR technique was performed on the molecules of the training set. The result obtained from the multivariate combinations is shown in equation 1.

$$\log K_s = -1.1522(\pm 0.2901) + 0.0070(\pm 0.0015)\,MP + 0.8089(\pm 0.0897)\,LogP - 0.1262(\pm 0.0454)\,DPLL \quad (1)$$

Increasing the DPLL will decrease log K_s and increasing the Log P and MP increases extent of log K_s of the organic compounds. Fig. 1 shows the effect of Log P, MP and DPLL for the QSPR study of organic solutes in CTAB.

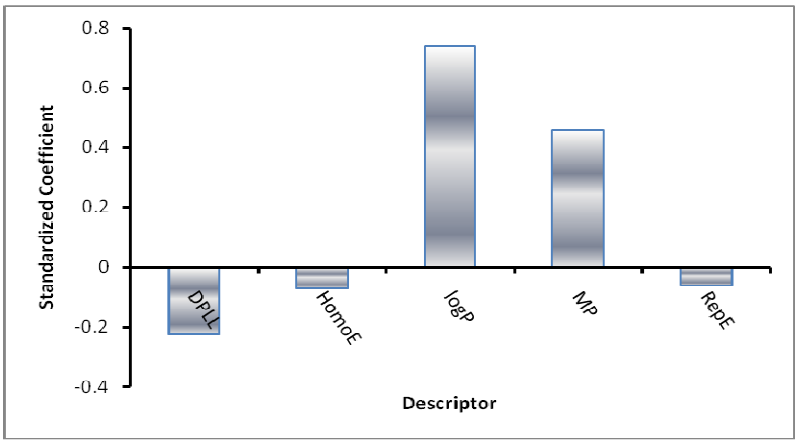

Fig. 1 Standardized coefficients of descriptors in MLR.

The model obtained is quite successful, bearing in mind the great variety of functionality: amino, alkyl, hydroxyl, carbonyl, carboxyl groups and aromatic rings of the applied compounds. Furthermore, this data have been measured by different groups in the diverse methodology and the lack of rigorous identity of experimental conditions. Methods include solubilization at saturation (SOL), cmc depression (CMC), micellar liquid chromatography (MLC), ultrafiltration (UF) and solute vapour pressure techniques (SVP) [1]. The QSPR developed indicated that lipophilicity (Log P) of the solutes, melting point (MP) of the molecules and Dipole length (DPLL) of the solutes; the factors that influence the solubility of each species and satisfactorily describes the solubility of structurally different solutes.

Conclusion

A successful description of the micellar solubility presented with a few physicochemical significant molecular descriptors for diverse chemical compounds in a cationic surfactant (CTAB). These are simple to calculate, providing a rapid and accurate method for estimation and description of solubility behaviour in micellar solutions. The descriptors involved in the correlations reflect both the intermolecular and intramolecular interactions

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