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A QUANTITATIVE STRUCTURE ACTIVITY RELATIONSHIP FOR BIOCONCENTRATION OF ALCOHOL ETHOXYLATES

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Alcohol Ethoxylates (AE) are a subtype of nonionic surfactants which consist of a hydrophilic ethoxylate chain and a hydrophobic alkyl chain. Most AEs contain a hydrophobic alkyl chain attached to a hydrophilic ethylene oxide (EO) chain via an ether linkage. This study attempted to build a Quantitative Structure Activity Relationship (QSAR)-based toxicity model for bioconcentration factor (BCF) of a selected group of AEs and predict the BCF of another independent group of AEs with respect to the generated model.

A group of twenty one AEs of general use was selected for the study. AEs were converted to SMILE (Simplified Molecular Input Line Entry System) formulas, which is a typographical line notation of the basic chemical structure of a compound. The conversion was achieved by EPIWEB® 4.1 developed by Unites States Environmental Protection Agency (USEPA). LogBCF values were generated by a USEPA-developed estimation program: BCFBAF®. A molecular descriptor is the final numerical result of a mathematical procedure which transforms chemical information encoded within a molecular structure. 560 molecular descriptors were calculated for each AE by DRAGON® 1.0 molecular modeling program developed by the Milano Chemometrics and QSAR Research Group. An initial Principal Component analysis (PCA) was conducted. The multivariate statistical software package, SIMCA-P® was used to fit molecular descriptor data (X-variable matrix) and LogBCF (Y-response factor) into a linear relationship using Orthogonal Partial Least Squares (OPLS). The QSAR was internally cross validated for the best fit possible. The predictor group consisted of five separate AE compounds.

The PCA analysis indicated three AEs incongruous with the QSAR model. They were identified as structurally dissimilar from the rest, hence were excluded from further analysis. Remaining AEs were observed in two clusters with the first group governed by 2-dimensional molecular descriptors such as the average reciprocal squared distance between atoms and cumulative molecular eigenvector coefficients. The second group was governed more by ones such as the octanol-water partition coefficient and sum of eigenstates of methyl groups. The developed QSAR model exhibited a goodness fit (R^2) of 0.89 and a goodness of prediction (Q^2) of 0.60. Peer-studies had presented QSARs with R^2 ranging between 0.90-0.99 and Q^2: 0.59-0.85. Predicted LogBCF values for the external AE group were cross compared with values estimated by the EPI® toxicology estimation program. Highest and lowest percentage differences of predicted values were 10% and 37% respectively.

The possibility of QSAR approach for modeling environmental behaviour of AEs at a fully empirical level was demonstrated by this study. A significant relationship between bioconcentration and molecular descriptors for AEs was exhibited. This type of QSAR models may help predict toxicities as well as chemical characteristics and behaviour of new AE surfactants in the environment.