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Modelling Of POP Environmental Persistence And Long Range Transport By QSAR And Chemometric Approaches

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Abstract: The Long Range Transport (LRT) potential of chemicals is due to the combination of their persistence in the environment and their inherent tendency towards mobility, and is an undesirable property of POPs (Persistent Organic Pollutants). Finding the best combination of chemical properties to minimize LRT is a multicriteria problem that can be approached by MultiCriteria Decision-Making (MCDM) techniques. Utility functions have been applied to two proposed indexes, the “global persistence index” and the “mobility index”, allowing a ranking of the studied chemicals according to their LRT potential. The “global persistence index” was obtained by linear combination, by Principal Component Analysis of the half-life data in various environmental compartments. Half-life data are commonly used as persistence indicators, but the availability of such data is limited to only a few organic compounds, thus QSAR (*Quantitative Structure-Activity Relationships*) models were used to predict such data starting from molecular structure information. Validated OLS regression models were realised using different theoretical molecular descriptors able to predict half-life values; all the regression models were strongly validated for their prediction power by the *leave-one-out* and *leave-more-out* procedure ($Q^2=70-90\%$). Analogously the “mobility index” was ascertained by Principal Component Analysis of different physico-chemical properties relevant to the determining of LRT, for instance, volatility, water solubility and different sorption coefficients. The final application of QSAR regression models and classification models (CART) on the obtained MCDM scores allows a fast screening and ranking of existing chemicals for their inherent tendency towards LRT. This approach could be usefully applied also to new chemicals, even those not yet synthesized, as it is based simply on the knowledge of the molecular structure.

Keywords: POPs; LRT; QSAR; classification; Multicriteria.