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The Critical Role of Quantitative Structure Activity Relationship in Predicting the Removal of Organic Micropollutants

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Organic micropollutants (OMPs), a group of natural and synthetic organic materials, enter the environment from various domestic, industrial, and agricultural sources and are one of the most pressing environmental challenges[1]. These persistent compounds originate from various pharmaceuticals, personal care products, pesticides, microplastics, and industrial waste[2]. They frequently bypass conventional treatment processes, posing a serious threat to aquatic ecosystems and human health[3]. Although advanced technologies are being developed to remove these compounds, the research community faces a fundamental bottleneck (the cost, time, and enormous resources required for experimental testing) in determining the optimal conditions for new and emerging compounds[4].

To overcome these problems, computational prediction methods are not only useful but also essential. Among these, chemometric modeling methods based on quantitative structure–activity relationships (QSAR) offer a powerful and attractive solution to these problems[5]. QSAR is a powerful method that establishes relationships between molecular descriptors, including the structural, topological, physical, geometric, and electronic properties of a contaminant with physical, chemical, or biological activity. This transforms the process for determining the activity of a new compound from a random, trial-and-error approach to a rational, targeted, and efficient one. Consequently, QSAR serves as a standard and prerequisite tool for decreasing the time, cost, and number of animal testing, thus facilitating green chemical design across various scientific and industrial fields[6].

In this approach, molecular descriptors are first calculated, and then statistical techniques such as multiple linear regression (MLR), artificial neural network (ANN), and mathematical relationships are used to establish the relationship between the experimental values of degradation (dependent data) and the molecular descriptors (independent data). This relationship is expressed as a mathematical equation based on the most significant descriptors[7]. The descriptor most closely related to OMP degradation is considered the most appropriate model for OMP degradation[8].

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The validity of the generated model was tested using the testing set molecules, along with a scatter plot and residual error plot. Once validated, the degradation efficiency of a new OMP can be predicted by inputting its molecular descriptors into the selected model. Furthermore, these models can predict how changes in specific molecular descriptors affect degradation efficiency within a given treatment process[9].

The use of QSAR in research offers the following benefits

1-Screening: Researchers can virtually screen vast chemical libraries to prioritize compounds that are most likely to pose a risk. This allows them to focus their experimental efforts where they are most needed[10].

2-Mechanism prediction: These models do more than predict the outcomes of the degradation process; they help understand why and how a compound is eliminated or degraded. By identifying key molecular descriptors, QSAR reveals the underlying mechanisms governing these processes[11].

3-Green design: QSAR can guide the green design for the removal of future compounds and determine how new compounds should be removed before entering the environment with at least chemicals[10].

However, for QSAR to reach its full potential, the scientific community must produce high-quality, standardized experimental data for model training and validation. This requires interdisciplinary collaboration among chemists, environmental engineers, and scientific computing experts in artificial intelligence. By using QSAR, we can shift from a reactive to a proactive stance and manage the vast universe of OMPs not only by testing a compound at a great time and expense but also through the powerful lens of predictive science[6].

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