From Data to Decisions: Computational Tools for Evaluating the Ecotoxicological Effects of Nanomaterials

Kabiruddin Khan*, Mahmoud Bousily, Farhad Dovlatov, Agnieszka Gajewicz-Skrętna*

Laboratory of Environmental Chemoinformatics, Faculty of Chemistry, University of Gdansk, Gdansk, Wita Stwosza 63, 80-308 Gdansk Poland

Nanomaterials and advanced materials are gaining traction across industries due to their unique properties and wide-ranging applications. However, concerns about their environmental impact, particularly ecotoxicity, necessitate effective assessment methods. Here, we discuss the use of Quantitative Structure-Activity Relationships (QSARs) and Species Sensitivity Distributions (SSDs) in addressing these concerns. QSARs provide a computational approach to predicting chemical toxicity based on physicochemical properties and structural characteristics. By establishing quantitative relationships between molecular descriptors and ecotoxicological endpoints, QSAR models enable the estimation of potential environmental risks associated with these materials. Concurrently, SSDs offer a statistical framework for integrating toxicity data from multiple species and deriving ecotoxicity thresholds for environmental risk assessment. Analyzing the distribution of species sensitivities, SSDs facilitate the estimation of hazardous concentrations affecting a given proportion of species in an ecosystem. In summary, this work highlights the advantages and limitations of various computational tools in ecotoxicity assessment, along with current challenges and future directions. Case studies demonstrate the practical implementation of these approaches in environmental risk assessment, supporting informed decision-making and sustainable development practices in nanotechnology and materials science.

Reference

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