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NanoSAR: Structure Activity Model for the Toxicity of Nanoparticles

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There are increasing number of engineered nanomaterials (ENMs) that have to be hazard tested before they are allowed to be used in commercial and industrial applications. This requires new methodologies to be explored and implemented to rapidly and effectively screen and evaluate ENM toxicity. Data-driven models of nanostructure-biological activity relationships are becoming increasingly important as the hazard testing lags further behind innovation in nanotechnology. Although the use of non-testing quantitative structure-activity relationship ((Q)SAR) methods for predicting adverse effects of ENMs has gained more and more attention over the past several years, there exist a number of limitations that influence the quality and generalizability of nano-(Q)SAR models. This study reviews (Q)SAR-related nano-aspects, from nanostructure characterization to (Q)SAR modelling tools, in order to improve the understanding of the (Q)SAR modelling of ENM toxicity. It provides a critical assessment of previously published nano-(Q)SAR studies as well as the available nanostructure-nanotoxicity data. Moreover, the study aims to identify the issues that complicate the implementation of (Q)SAR approaches in nanotoxicology, in addition to the main challenges ahead. In conclusion, we believe that this study can provide valuable insights into the current status and future potential of (Q)SAR modelling in nanotoxicology.

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