# Guest Editorial Preface

# Special Issue on QSPR/QSAR in Materials and Toxicological Sciences

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Among many computational techniques, quantitative structure-property/activity relationship (QSPR/QSAR) modeling holds a special status. It is a technique that allows the interdisciplinary exploration of knowledge on chemical compounds covering the broad aspects of chemistry, physics, biology, and toxicology (Roy et al., 2015a, 2015b). It provides a formalism for developing mathematical correlations between the chemical features and the behavioral manifestations of structurally similar compounds. The tool is developed based on a robust mathematical algorithm, and it provides a reasonable basis for establishing a predictive correlation model. Apart from providing a mathematical correlation, QSPR technique also enables the exploration of chemical features encoded within descriptors (Todeschini and Consonni, 2008). The QSPR technique proves to be a valuable alternative method in this perspective and is encouraged for the design and development of biologically active molecules as well as in predictive toxicology analysis (Kar et al., 2016). The QSPR formalism is also widely employed to serve different purposes of materials science toward the design and development of purpose-specific novel and/or alternative materials It may be very interesting to note that historically the earliest inception for the ideology of QSPR modeling emerged from the simple concept of a correlation between response and chemical nature of molecules which remains the same even today after various developments and nourishments in the QSAR algorithms (Kar et al., 2017). In this special issue, we present four case studies and one review illustrating the current state-of-the-art in the area of QSPR modeling in Materials and Toxicological Sciences.

The first article of this special issue, entitled "QSPR models for predicting of the melting points and refractive indices for inorganic substances - components of the optical film-forming materials" contributed by Kuz'min et al., introduces 1D-QSPR descriptor system for analysis of the properties of various inorganic compounds and showed the effectiveness of the proposed approach to model the refractive indices and melting points of the target compounds. The second article entitled "QSAR-models, validation, and IIC-paradox for drug toxicity: QSAR, validation and IIC-paradox for drug toxicity" was contributed by Toropova et al. It discusses the index of ideality of correlation as a useful criterion for estimation of the predictive potential of QSAR models of drug toxicity. "Risk Assessment of Cosmetic Preservatives using QSAR: QSAR of Cosmetic Preservatives" is the third article contributed by Bhardwaj et al. It elaborates a detailed view on cosmetic preservatives, regulatory aspects and application of computational strategies for toxicity predictions. The next article entitled "A quantitative structure-activity relationship study on the antimalarial activities of 4-aminoquinoline, febrifugine and artemisinin compounds" contributed by Ou and Chang investigates the antimalarial activities of 4-aminoquinoline, febrifugine, artemisinin and their derivatives against the chloroquine-resistant *Plasmodium*

*falciparum* W-2 strain. The fifth and final paper of the issue titled "QSAR/QSPR in Polymers. Recent Developments in Property Modeling" contributed by Casanola-Martin and Rasulev discusses main applications of QSPR/QSAR methods in polymers along with the clues that could lead to the improvement in the efficient computational design and/or optimization of new polymers with enhanced properties/activities.

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