Guest Editorial Preface

Special Issue on QSPR in Nanotechnology

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Innovations in nanotechnology and nanomaterial design are rapidly changing the landscape of industrial and consumer products, with promising application prospects in numerous areas (e.g.: health, technology, energy, etc.). With a great number of new nanoparticles introduced into commercial use every day, there is a need of developing new computational tools to support designing of new nanoparticles and nanomaterials. The application of virtual screening methods can significantly reduce time and cost of experimental trials. Moreover, many more potential solutions can be considered when the computer supports or even sometimes replaces traditional laboratory instruments. In this special issue, we present three case studies illustrating the current state-of-the-art in the area of Quantitative Structure-Property Relationships (QSPR) modeling in nanotechnology.

The authors of the first paper, Sabine van Miert et al., present the results of mining a nanoparticle data set derived within the European MODENA COST action. Since, in most cases, the paucity of publicly available experimental nanotoxicity data are arguably the greatest roadblock in their widespread use for modeling purposes, every attempt of combining the existent sources of data should be appreciated.

In the second paper, Sizochenko et al. present the results of predicting thermal conductivity of selected nanofluids with the QSPR approach. This is a good illustrative example, how to use QSPR methodology for designing materials having the required physical-chemical property.

Possessing high efficacy is not the only challenge to be faced when nanomaterials are designed. Newly produced nanoparticles must be safe for human and the environment. The third paper by Kuz'min et al. illustrates the idea of applying QSPR for predicting cytotoxicity of metal oxides nanoparticles.

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