

# Editorial Preface

## Inaugural Issue, Part 2

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The inaugural special issue of the *International Journal of Quantitative Structure-Property Relationships (IJQSPR)* (<http://www.igi-global.com/journal/international-journal-quantitative-structure-property/126552>) continues in the current issue (Volume 1, Issue 2). While four articles have been published in Issue 1, the current issue includes five more articles.

Ramon Carbo-Dorca and Silvia González have authored the fifth article of the inaugural issue (Article 1 of Issue 2), entitled “Molecular Spaces Quantum Quantitative Structure-Properties Relations (QQSPR): A Quantum Mechanical Comprehensive Theoretical Framework”, which deals with quantum QSPRs and their applications in computing complex molecular properties. The sixth article (Article 2 of Issue 2) entitled “Can toxicity for different species be correlated? The concept and emerging applications of interspecies Quantitative Structure-Toxicity Relationship (i-QSTR) modeling” authored by Supratik Kar, Rudra Narayan Das, Kunal Roy and Jerzy Leszczynski highlights the importance of interspecies quantitative structure-activity relationship (QSAR) in order to overcome the cost of multiple toxicity tests, improve the understanding of the mechanism of toxic action of chemicals for different organisms and endpoints and fill the data gaps where toxicity value for a particular compound is absent for a specific endpoint. Alla P Toropova and Andrey A Toropov have contributed the seventh article (Article 3 of Issue 2) entitled “Evolution of optimal descriptors-solved, unsolved, and unsolvable tasks”, which demonstrates the perspectives and limitations of the optimal descriptors computed from the CORAL software. The eighth article (Article 4 of Issue 2) entitled “QSPR-modeling for the Second Virial Cross-coefficients of Binary Organic Mixtures” contributed by Elena Mokshyna, Pavel Polishchuk, Vadim Ivanovich Nedostup and Victor Kuz'min reports quantitative structure-property relationship (QSPR) models for analysis and prediction of the second virial cross-coefficient using intermolecular interaction based descriptors. The last article of the inaugural special issue (Article 5 of Issue 2) entitled “A QSAR Study of Human Thymidine Phosphorylase Inhibitors with SMILES-based Descriptors: QSAR Study of Human TP Inhibitors” has been contributed by Adriana Santos Costa and Eduardo Borges de Melo. This article discusses a QSAR analysis of a set of uracil derivatives as thymidine phosphorylase inhibitors using SMILES-based descriptors. The authors have used multiple strategies for theoretical validation of their QSAR model which was also used for prediction of some compounds from the ZINC database selected by similarity search. All these articles are available for free download from the IGI Global site.

I hope that the collection of nine articles of the inaugural special issue will be of interest to the researchers in the field of QSPR/QSAR/QSTR studies. I also hope that this publication platform will be able to attract a good number of high quality manuscripts reporting new research findings and/or review of the literature within the scope of the Journal. I look forward to hearing from the readers on any issues in connection with further development of the Journal.

Kunal Roy  
Editor-in-Chief  
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