

Editorial Preface

Inaugural Issue: Part 1

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The principles of quantitative structure-property/activity/toxicity relationships (QSPR/QSAR/QSTR) have been in use in diverse disciplines such as medicinal chemistry, agricultural science, ecotoxicology, material science, pharmacokinetics etc. for about fifty years (Roy et al., 2015a, b). QSAR/QSPR models have received an increased importance in the pharmaceutical and chemical industries in recent years due their regulatory applications. There are many emerging areas of applications of QSAR/QSPR/QSTR which include modeling of properties and toxicities of nanoparticles, properties and toxicities of ionic liquids, mixture toxicity, safety and risk assessment of cosmetics, interspecies toxicity, etc. Though QSAR related papers are currently published in different journals specialized in specific fields of application, there has been a requirement of a common platform of presenting research findings on diverse and important applications of QSAR/QSPR/QSTR. The International Journal of Quantitative Structure-Property Relationships (IJQSPR) (<http://www.igi-global.com/journal/international-journal-quantitative-structure-property/126552>) is a new journal that will explore the latest research surrounding the topic of QSAR/QSPR/QSTR models and the applications of these models across the fields of materials science, chemical engineering, pharmaceutical and medicinal chemistry, pharmacokinetics, toxicology (including ecotoxicology), and agricultural sciences, among others. The Journal has a strong Editorial Board, and the board members have proven expertise in QSAR/QSPR/QSTR modeling with applications in diverse fields. With the help of the Editorial Review Board members and selected external reviewers, the journal aims to set a high standard for the published articles.

The inaugural special issue of the Journal is a compilation of nine articles highlighting the concept, evolution, salient features, tools and different applications of QSPR/QSAR/QSTR. This special issue has been split into two parts: Issues 1 and 2 of Volume 1 of the Journal.

The first article of issue 1, entitled “The History and Development of Quantitative Structure-Activity Relationships (QSARs)” contributed by John Dearden, introduces the concept and historical evolution of QSAR and also briefly mentions its different applications and recent developments. The second article entitled “Applicability Domain For QSAR Models, Where Theory Meets Reality” contributed by Domenico Gadaleta, Giuseppe Felice Mangiardi, Marco Catto, Angelo Carotti and Orazio Nicolotti discusses different approaches used to build applicability domain of QSAR models with some practical examples. “Ten Years of the MIA-QSAR Strategy: Historical Development and Applications” is the third article contributed by Stephen Jones Barigye and Matheus Puggina de Freitas. This article discusses the historical evolution and successes achieved by the Multivariate Image Analysis applied to QSAR. The fourth article entitled “A New QSPR Study on Relative Sweetness” contributed by Cristian Rojas, Piercosimo Tripaldi and Pablo R. Duchowicz reports

QSPR of natural and synthetic sweeteners in order to predict relative sweetness of un-evaluated and un-synthesized sweeteners.

The second part of the inaugural special issue will be published as Issue 2 of Volume 1 of the Journal. All papers published in the Special Inaugural Issue of IJQSPR (Volume 1, Issues 1 and 2) will be available online for free download in order to ensure the maximum dissemination, and I hope that the readers will be benefitted from the free access provided by the Publisher.

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REFERENCES

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Roy, K., Kar, S., & Das, R. N. (2015b). *A Primer on QSAR/QSPR Modeling: Fundamental Concepts (SpringerBriefs in Molecular Science)*. Heidelberg: Springer. doi:10.1007/978-3-319-17281-1