Guest Editorial Preface

Special Issue on QSPR Applications in Food and Agricultural Sciences, Part 2

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While most quantitative structure-property relationship (QSPR) applications have been focused on medicinal chemistry (quantitative structure-activity relationship or QSAR), food and agricultural sciences have emerged as interesting fields to explore the relationship of chemical structures with flavor, maintenance/protection of food against microorganisms, soil sorption, bioconcentration, pesticide activity and so on. In addition, a variety of QSPR methodologies have been proposed - despite not employed as widely as in medicinal chemistry - then offering a broad spectrum of possibilities to interpret the outcomes and, consequently, to design improved compound candidates. In this second part of the Special Issue on "QSPR Applications in Food and Agricultural Sciences", three papers were devoted to contribute for the development of QSPR models, aiming at targeting prospective compounds useful either as pesticides or in view of a better environmental perspective.

In the first paper of this special issue by da Cunha and coworkers, the mortality rates of a series of β-dihydroagarofuran derivatives were modeled using a four-dimensional QSPR approach, and based on the insights provided, seven chemical analogs were then proposed as novel pesticide candidates.

In the second paper, Daré, Barigye and Freitas developed a double-objective QSPR model multivariate image analysis (MIA) descriptors, in which information on herbicidal activity and soil sorption of some triazines were captured simultaneously by using pIC_{50}/$logK_{OC}$ values as dependent variables.

The third paper by Salahinejad, Zolfonoun and Ghasemi describes the development of a robust 3D-QSAR model for the prediction of the degradation half-life of organophosphorus pesticides in soil, which has been further interpreted in terms of molecular interaction fields.

It is our hope that this special issue will be interesting to the researchers in QSAR/QSPR field.

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IJQSPR

Matheus Puggina de Freitas studied Chemistry (BSc and PhD) at the State University of Campinas (UNICAMP), following a postdoctoral stay at the same University. He worked as a researcher in two pharmaceutical companies and, in 2005, he started as Adjunct Professor at the Federal University of Lavras (UFLA). He is currently Associate Professor of Organic Chemistry at UFLA, where he has research interests in conformational analysis of small molecules, NMR spectroscopy, computational chemistry and QSAR/QSPR.