Guest Editorial Preface

Special Issue on QSPR Applications in Food and Agricultural Sciences, Part 1

Matheus Puggina de Freitas, Department of Chemistry, Federal University of Lavras, Lavras, Brazil

While most QSPR applications have been focused on medicinal chemistry (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.

This special issue aims at covering the advances of QSPR in food and agricultural sciences, given the economical relevance of food and agriculture to many countries, besides the health and environmental benefits of improving products to use with this end.

In the first short review paper, Prof. Fujita reports an overview on the applications of classical QSAR to agrochemical research, emphasizing on the consequences from these analyses: the building of models to design and synthesize new bioactive compounds, and the mechanistic rationalization of the biological action.

In the second paper of this special issue, Halder, Saha and Jha describe the quantitative structure-toxicity relationship on avian toxicity of some pesticides using Monte Carlo based analyses, focusing on the building of a predictive QSTR model, as well as to define the domain of applicability of the proposed model, validate and interpret the model.

The third paper by Duarte, Freitas and Nunes shows that simple descriptors based on the size of the carbon chain, as well as the number, position and stereochemistry of double bonds in fatty acid derivatives are capable of providing accurate estimations of retention times.

Matheus Puggina de Freitas
Guest Editor
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Matheus Puggina de Freitas is a PhD in Organic Chemistry. He is associate professor at the Department of Chemistry of the Federal University of Lavras, Brazil. His research interests are conformational analysis and QSPR modeling.