

# Table of Contents

## International Journal of Quantitative Structure-Property Relationships

Volume 2 • Issue 2 • July-December-2017 • ISSN: 2379-7487 • eISSN: 2379-7479

*An official publication of the Information Resources Management Association*

### GUEST EDITORIAL PREFACE

- v **Special Issue on QSPR Applications in Food and Agricultural Sciences, Part 2**  
Matheus Puggina de Freitas, Department of Chemistry, Federal University of Lavras, Lavras, Brazil

### RESEARCH ARTICLES

- 1 **QSPR Models of  $\beta$ -dihydroagarofuran Derivatives: Exploring Lead Compounds for Pesticides**  
Elaine Fontes Ferreira da Cunha, Laboratory of Computational Chemistry, Department of Chemistry, Federal University of Lavras, Lavras, Brazil  
Daniela Rodrigues Silva, Federal University of Lavras, Lavras, Brazil  
Leticia Santos-Garcia, Federal University of Lavras, Lavras, Brazil  
Letícia Cristina Assis, Federal University of Lavras, Lavras, Brazil  
Tamiris Maria de Assis, Federal University of Lavras, Lavras, Brazil  
Giovanna Cardoso Gajo, Federal University of Lavras, Lavras, Brazil  
Teodorico Castro Ramalho, Federal University of Lavras, Lavras, Brazil
- 16 **Multi-Objective Modeling of Herbicidal Activity from an Environmentally Friendly Perspective**  
Joyce K Daré, Department of Chemistry, Federal University of Lavras, Lavras, Brazil  
Stephen J Barigye, Universidad de Las Américas (UDLA) - Quito, Ecuador  
Matheus P Freitas, Department of Chemistry, Federal University of Lavras, Lavras, Brazil
- 27 **Predicting Degradation Half-life of Organophosphorus Pesticides in Soil Using Three-Dimensional Molecular Interaction Fields**  
Maryam Salahinejad, Nuclear Science and Technology Research Institute, Tehran, Iran  
Ehsan Zolfonoun, NFCRS, Nuclear Science and Technology Research Institute, Tehran, Iran  
Jahan B. Ghasemi, Chemistry Faculty, University of Tehran, Tehran, Iran
- 36 **The History and Development of Quantitative Structure-Activity Relationships (QSARs): Addendum**  
John C. Dearden, School of Pharmacy & Biomolecular Sciences, Liverpool John Moores University, Liverpool, UK
- 47 **Identification of Pharmacophore for Wild and T877A Mutant Androgen Receptor Antagonist: Challenges in Designing 3D-QSAR For Mutant Protein**  
Divakar Selvaraj, Department of Pharmacology, PSG College of Pharmacy, Coimbatore, India  
Sivaram Hariharan, Department of Chemistry, PSG College of Pharmacy, Coimbatore, India  
Ramanathan Muthiah, Department of Pharmacology, PSG College of Pharmacy, Coimbatore, India
- 62 **Path Pendeccentric Connectivity Indices: Detour Matrix Based Molecular Descriptors for QSAR/QSPR Studies, Part 1: Development and Evaluation**  
Naveen Khatri, Faculty of Pharmaceutical Sciences, Pt. B. D. Sharma University of Health Sciences, Rohtak, India  
Harish Jangra, Department of Pharmacoinformatics, National Institute of Pharmaceutical Education and Research, Mohali, India  
A. K. Madan, Faculty of Pharmaceutical Sciences, Pt. B. D. Sharma University of Health Sciences, Rohtak, India
- 75 **Path Pendeccentric Connectivity Indices: Detour Matrix Based Molecular Descriptors for QSAR/QSPR Studies, Part 2: Development of Models for TTK Inhibitory Activity of Acetamide/Carboxamide Analogs**  
Naveen Khatri, Faculty of Pharmaceutical Sciences, Pt. B. D. Sharma University of Health Sciences, Rohtak, India  
A. K. Madan, Faculty of Pharmaceutical Sciences, Pt. B. D. Sharma University of Health Sciences, Rohtak, India
- 90 **Quantitative Structure-Activity Relationship Studies of Anticancer Activity for Isatin (1H-indole-2,3-dione) Derivatives Based on Density Functional Theory**  
Samir Chtita, MCNS Laboratory, Faculty of Science, University Moulay Ismail, Meknes, Morocco  
Mounir Ghamali, MCNS Laboratory, Faculty of Science, University Moulay Ismail, Meknes, Morocco  
Majdouline Larif, Separation Process Laboratory, Faculty of Science, University Ibn Tofail, Kenitra, Morocco  
Rachid Hmamouchi, MCNS Laboratory, Faculty of Science, University Moulay Ismail, Meknes, Morocco  
Mohammed Bouachrine, High School of Technology, University Moulay Ismail, Meknes, Morocco  
Tahar Lakhliifi, MCNS Laboratory, Faculty of Science, University Moulay Ismail, Meknes, Morocco

### Copyright

The *International Journal of Quantitative Structure-Property Relationships (IJQSPR)* (ISSN 2379-7487; eISSN 2379-7479), Copyright © 2017 IGI Global. All rights, including translation into other languages reserved by the publisher. No part of this journal may be reproduced or used in any form or by any means without written permission from the publisher, except for noncommercial, educational use including classroom teaching purposes. Product or company names used in this journal are for identification purposes only. Inclusion of the names of the products or companies does not indicate a claim of ownership by IGI Global of the trademark or registered trademark. The views expressed in this journal are those of the authors but not necessarily of IGI Global.

The *International Journal of Quantitative Structure-Property Relationships* is indexed or listed in the following: Cabell's Directories; Google Scholar; Ulrich's Periodicals Directory