

# Table of Contents

## International Journal of Quantitative Structure-Property Relationships

Volume 6 • Issue 2 • April-June-2021 • ISSN: 2379-7487 • eISSN: 2379-7479

### Research Articles

- 1 **Monte Carlo Optimization-Based QSAR Study of Some Indole-Based Mcl-1 Inhibitors**  
Sudipta Nandi, Dr. Harisingh Gour University, India  
Kalyan Ghosh, Dr. Harisingh Gour University, India  
Anju Rathore, Dr. Harisingh Gour University, India  
Adarsh Sahu, Dr. Harisingh Gour University, India  
Shovanlal Gayen, Dr. Harisingh Gour University, India
- 19 **QSAR Modeling and Prediction of Triptan Binding Affinities**  
Lucas Alland, Newark Academy, USA  
Solomon H. Jacobson, Ashland, LLC, USA
- 29 **Application of Artificial Intelligence and Machine Learning Techniques in Classifying Extent of Dementia Across Alzheimer's Image Data**  
Robin Ghosh, Department of Computational and Data-Enabled Science and Engineering, Jackson State University, Jackson, USA  
Anirudh Reddy Cingreddy, Department of Computational and Data-Enabled Science and Engineering, Jackson State University, Jackson, USA  
Venkata Melapu, Department of Electrical and Computer Engineering and Computer Science, Jackson State University, Jackson, USA  
Savanthi Joginipelli, Department of Electrical and Computer Engineering and Computer Science, Jackson State University, Jackson, USA  
Supratik Kar, Interdisciplinary Center for Nanotoxicity, Department of Chemistry, Physics and Atmospheric Sciences, Jackson State University, Jackson, USA
- 47 **Alternative QSAR Study for Unsymmetrical Aromatic Disulfide Anti-SARS Inhibitors**  
Pablo Roman Duchowicz, Instituto de Investigaciones Fisicoquímicas Teóricas y Aplicadas (INIFTA), Argentina  
Silvina Fiorelli, CONICET, Universidad de Belgrano, Argentina  
Gustavo Romanelli, CINDECA, Argentina  
Daniel E. Babelo, CONICET, Universidad de Belgrano, Argentina

### Open Access Article

- 58 **Identification of Potential Mpro Inhibitors for the Treatment of COVID-19 by Targeted Covalent Inhibition: An In Silico Approach**  
Dushyant V. Patel, Faculty of Pharmacy, The Maharaja Sayajirao University of Baroda, India  
Divya M. Teli, Department of Pharmaceutical Chemistry, L. M. College of Pharmacy, India  
Ashish M. Kanhed, Shobhaben Pratapbhai Patel School of Pharmacy and Technology Management, SVKM's NMIMS University, India  
Nirav R. Patel, Faculty of Pharmacy, The Maharaja Sayajirao University of Baroda, India  
Bhavik S. Shah, Faculty of Pharmacy, The Maharaja Sayajirao University of Baroda, India  
Amisha K. Vora, Shobhaben Pratapbhai Patel School of Pharmacy and Technology Management, SVKM's NMIMS University, India  
Mahesh T. Chhabria, Department of Pharmaceutical Chemistry, L. M. College of Pharmacy, India  
Mange Ram Yadav, Parul University, India

### COPYRIGHT

The **International Journal of Quantitative Structure-Property Relationships (IJQSPR)** (ISSN 2379-7487; eISSN 2379-7479), Copyright © 2021 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; UGC-CARE List (India)