Guest Editorial Preface

Special Issue on Computational Modeling Approaches in Health, Food, Environment, and Materials Sciences

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Computational modeling is a process to solve critical science problems with the help of computational resources employing mathematics, data science, physics, and chemistry. Many interdisciplinary fields are considered under computational approaches. The noted ones are cheminformatics and bioinformatics. A series of chemometrics algorithms as well as machine learning approaches allow the interdisciplinary exploration of knowledge on chemical compounds covering the aspects of chemistry, physics, biology, and toxicology. It provides a formalism for developing mathematical correlations between the chemical features and the behavioral manifestations of structurally homogenous/heterogenous compounds. Among chemometric approaches, quantitative structure-activity/property relationship (QSAR/QSPR) is one of the strongest mathematical algorithms, and it provides a reasonable basis for establishing a predictive correlation models (Roy et al., 2015a, 2015b). Apart from providing a mathematical correlation, QSAR technique also enables the exploration of chemical features encoded within descriptors. The QSAR technique proves to be a valuable alternative method in this perspective and is encouraged for the design and development of biologically active molecules, especially drugs (Ambure et al., 2014), food and agrochemicals (Loso et al., 2016), property prediction (Wu et al., 2015) as well as in predictive toxicology analysis of environmental pollutants (Kar et al., 2020). On the other hand, machine learning models can handle big data in no time and can predict a huge population of data efficiently. Again, bioinformatics deals with omics and biology data to solve the problems and understand the critical biological problems.

The first article of this special issue, entitled "First QSTR Report on Allium Cepa Phytotoxicity of Pesticides: QSTR Phytotoxicity Models of Allium Cepa," contributed by Murmu et al., introduces the first QSTR models for onion toxicity of pesticides. The QSTR models were developed based on EC_{25} and NOEL endpoints which can be used for the prioritization of the pesticides as well as useful for the determination of phytotoxicity of existing and upcoming pesticides for the benefit of the ecosystem and society. The second article, "De-Novo Design of Hits Against New Delhi Metallo-β-Lactamase Enzyme," authored by Sardar et al., presents a fragment-based and knowledge-based approach to design drug-like molecules against New Delhi Metallo-β-lactamase 1 (NDM-1) enzyme. The study reported one ligand Gen-15-48 which exhibits stable binding with this enzyme, confirmed by molecular docking and 100ns molecular dynamics simulation. The third article, "Classification of Parkinson's Disease Using Motor and Non-Motor Biomarkers Through Machine Learning Techniques," by

Cingireddy et al., focuses classification of Parkinson's disease (PD) patients, scans without evidence for dopaminergic deficit (SWEDD) patients, and healthy controls by considering motor and non-motor biomarkers supervised and unsupervised machine learning algorithms and identified random forest can predict with 98% accuracy among the studied algorithms. The next article, entitled "2D-QSAR Modeling of Quinazolinone Derivatives as Angiotensin II Type 1a Receptor Blocker," authored by Shah et al., carried out QSAR analysis on a large set of structural datasets of 114 quinazolinone derivatives with AT-1a receptor blocking activity. The authors reported that the multiple QSAR models successfully identified that increase in surface area of negatively charged carbon atom within four bonds from N atom, presence of tetrazole substituents and sp3 N atoms governs the AT-1a receptor blocking activity. The fifth and final paper of the issue, "Exploring Quantitative Structure-Activity Relationships (QSARs) for Urea-Based Dual FAAH and sEH Inhibitors," authored by Jaswanthi et al., deals with QSAR modeling study to investigate the molecular features that favor potency towards fatty acid amide hydrolase (FAAH) enzyme and soluble epoxide hydrolase (sEH) enzyme inhibition. The authors have successfully developed and validated two distinct QSAR models for capturing FAAH and sEH inhibitory activity. The reported QSAR models should be helpful in the identification and/or screening of novel anti-inflammatory and antinociceptive agents.

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REFERENCES

Ambure, P., Kar, S., & Roy, K. (2014). Pharmacophore Mapping-Based Virtual Screening Followed by Molecular Docking Studies in Search of Potential Acetylcholinesterase Inhibitors as Anti-Alzheimer's Agents. *Bio Systems*, *116*, 10–20. doi:10.1016/j.biosystems.2013.12.002 PMID:24325852

Kar, S., Sanderson, H., Roy, K., Benfenati, E., & Leszczynski, J. (2020). Ecotoxicological assessment of pharmaceuticals and personal care products using predictive toxicology approaches. *Green Chemistry*, *22*(5), 1458–1516. doi:10.1039/C9GC03265G

Loso, M. R., Benko, Z., Buysse, A., Johnson, T. C., Nugent, B. M., Rogers, R. B., Sparks, T. C., Wang, N. X., Watson, G. B., & Zhu, Y. (2016). SAR studies directed toward the pyridine moiety of the sap-feeding insecticide sulfoxaflor (Isoclast™ active). *Bioorganic & Medicinal Chemistry*, *24*(3), 378–382. doi:10.1016/j.bmc.2015.11.022 PMID:26706115

Roy, K., Kar, S., & Das, R. N. (2015a). *Understanding the Basics of QSAR for Applications in Pharmaceutical Sciences and Risk Assessment*. Academic Press.

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

Wu, W., Zhang, C., Lin, W., Chen, Q., Guo, X., Qian, Y., & Zhang, L. (2015). Quantitative Structure-Property Relationship (QSPR) Modeling of Drug-Loaded Polymeric Micelles via Genetic Function Approximation. *PLoS One*, *10*(3), e0119575. doi:10.1371/journal.pone.0119575 PMID:25780923