COMPUTATIONAL TOXICOLOGY FOR DRUG SAFETY AND A SUSTAINABLE ENVIRONMENT

Editors:
Tahmeena Khan
Saman Raza

Bentham Books

CHAPTER 9

Computational Nanotoxicology and its Applications

Sabeeha Jabeen[1,2], Vasi Uddin Siddiqui[3], Shashi Bala[2], Abdul Rahman Khan[1], Saman Raza[4] and **Tahmeena Khan[1,*]**

[1] *Department of Chemistry, Integral University, Lucknow, U.P., India*

[2] *Department of Chemistry, University of Lucknow, Lucknow, Uttar Pradesh, India*

[3] *Faculty of Engineering, Universiti Putra Malaysia, Serdang, Selangor, Malaysia*

[4] *Department of Chemistry, Isabella Thoburn College, Lucknow, U.P., India*

Abstract: The trial on non-testing approaches for nanostructured materials and the prediction of toxicity that may cause cell disruption is needed for the risk assessment, to recognize, evaluate, and categorize possible risks. Another tactic for examining the toxicologic characteristics of a nanostructure is using *in silico* methods that interpret how nano-specific structures correlate to noxiousness and permit its prediction. Nanotoxicology is the study of the toxicity of nanostructures and has been broadly functional in medical research to predict the toxicity in numerous biotic systems. Exploring biotic systems through *in vivo* and *in vitro* approaches is affluent and time-consuming. However, computational toxicology is a multi-discipline ground that operates *In silico* strategies and algorithms to inspect the toxicology of biotic systems and also has gained attention for many years. Molecular dynamics (MD) simulations of biomolecules such as proteins and deoxyribonucleic acid (DNA) are prevalent for considering connections between biotic systems and chemicals in computational toxicology. This chapter summarizes the works predicting nanotoxicological endpoints using (ML) machine learning models. Instead of looking for mechanistic clarifications, the chapter plots the ways that are followed, linking biotic features concerning exposure to nanostructure materials, their physicochemical features, and the commonly predicted conclusions. The outcomes and conclusions obtained from the research, and review papers from indexing databases like SCOPUS, Web of Science, and PubMed were studied and included in the chapter. The chapter maps current models developed precisely for nanostructures to recognize the threat potential upon precise exposure circumstances. The authors have provided computational nano-toxicological effects with the collective vision of applied machine learning tools.

Keywords: Biomedical, Computational nanotoxicology, *In silico* approaches, Molecular dynamics, Machine learning, Nanostructures.

[*] **Corresponding author Tahmeena Khan:** Department of Chemistry, Integral University, Lucknow, U.P., India; E-mail: tahminakhan30@yahoo.com

Tahmeena Khan & Saman Raza (Eds.)
All rights reserved-© 2023 Bentham Science Publishers