COMPUTATIONAL TOXICOLOGY FOR DRUG SAFETY AND A SUSTAINABLE ENVIRONMENT

Editors:
Tahmeena Khan
Saman Raza

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CHAPTER 5

Adverse Environmental Impact of Pharmaceutical Waste and its Computational Assessment

Tuba Siddiqui[1], Saima Arif[2], Saman Raza[3] and **Tahmeena Khan[4,*]**

[1] *Department of Biochemistry, Integral Institute of Medical Sciences and Research, Lucknow-226026, Uttar Pradesh, India*

[2] *Toxicokinetics Laboratory, CSIR- Indian Institute of Toxicology Research (IITR), Lucknow-226001, Uttar Pradesh, India*

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

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

Abstract: Pharmaceuticals are necessary products that have indubitable benefits for people's health and way of life. Following their use, there is a corresponding increase in the production of pharmaceutical waste. We need to figure out how to lessen the production of pharmaceutical waste and prevent its release into the environment, which could eventually pose major health risks to the rest of the living world. If handled incorrectly, pharmaceutical waste increases the danger, which is inversely correlated with the active concentration of chemical components in various environmental compartments. As a result, when drugs and their unaltered metabolites are dispersed into the environment through several sources and channels, they may influence both animals and humans. Finding the sources and points of entry of pharmaceutical waste into the ecosystem is the first step in understanding pharmaceutical ecotoxicity. Several techniques, like the Structure-Activity Relationship (SAR) and Quantitative Structure-Activity Relationship (QSAR) models, help assess and manage environmental risks caused by pharmaceutical waste. The persistency, mobility, and toxicity (PMT) of pharmaceutical compounds have been predicted computationally using QSAR models from OPERA QSAR, VEGA QSAR, the EPI Suite, the ECOSAR, and the QSAR toolbox. *In silico* predictions have been made for molecular weight, STP total removal, sewage treatment plant, Octanol-water partition coefficient (KOW), ready biodegradability, soil organic adsorption coefficient, short- and long-term ecological assessments, carcinogenicity, mutagenicity, estrogen receptor binding, and Cramer decision tree. The adverse effects of medications on the living world, as well as risk assessment and management, have been covered in this chapter. Several computational methods that are employed to counteract the negative consequences of pharmaceutical waste have also been addressed. The goal is to better understand how to minimize the concentration of pharmaceutical waste in our environment.

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

Tahmeena Khan & Saman Raza (Eds.)