

COMPUTATIONAL TOXICOLOGY FOR DRUG SAFETY AND A SUSTAINABLE ENVIRONMENT



Editors:
Tahmeena Khan
Saman Raza

Bentham Books

Computational Toxicology Studies of Chemical Compounds Released from Firecrackers

Alfred J. Lawrence¹, Nikita Tiwari² and Tahmeena Khan^{3,*}

¹ Department of Chemistry, Isabella Thoburn College, Lucknow, U.P., India

² Department of Chemistry, Sri Ramswaroop Memorial College of Engineering and Management, Lucknow, Uttar Pradesh, India

³ Department of Chemistry, Integral University, Lucknow, U.P., India

Abstract: Customary firework burning during different festivals and occasions have been reported from different parts of the world. The pollutants emitted from fireworks exert toxicological effects on human health and the environment. A virtual study was performed to assess the extent of binding of sixteen important components of fireworks including Al_2O_3 , $\text{Ba}(\text{NO}_3)_2$, C_6H_6 , CO , Ethylbenzene (C_8H_{10}), $\text{Fe}_2\text{O}_3 \cdot \text{H}_2\text{O}$, KClO_3 , KClO_4 , KNO_3 , $\text{Na}_2\text{C}_2\text{O}_4$, NH_3 , NO , o-Xylene (C_8H_{10}), SO_2 , $\text{Sr}(\text{NO}_3)_2$ and Toluene (C_7H_8) with human superoxide dismutase (SOD), human serum albumin (HSA), and estrogen related receptor gamma (ERR-gamma) proteins. AutoDock 4.2.6 was employed to perform rigid docking. Against HSA, NH_3 exhibited the least binding energy *i.e.* -5.19 kcal/mol. Against ERR-gamma, Al_2O_3 showed the least binding energy *i.e.*, -4.08 kcal/mol. With SOD, ethylbenzene exhibited binding energy of -4.62 kcal/mol. A molecular dynamics simulation of 10 ns was performed on the ERR-gamma-o-xylene complex at 300K at the molecular mechanics level using GROMACS 5.1.2., showing conformational changes within the protein due to the o-xylene binding. The average Root Mean Square Fluctuation of the complex was 0.0821 nm. The results can be further elaborated and may guide future research for the intervention of protein targets for chemical toxins.

Keywords: Air pollution, Health, Hazard, Virtual screening, Protein.

INTRODUCTION

Fireworks burning are reported from all over the world during the festival of Deepawali in India [1], Chinese Spring Festival [2], 4th of July, the Independence Day in the USA [3], Lantern Festival in Taiwan [4], and Guy Fawkes in the United Kingdom [5] (Table 1).

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