THEORETICAL ASSESSMENT OF PMMA'S POTENTIAL TO REMOVE BETA-BLOCKERS FROM THE AQUATIC ENVIRONMENT USING ATOMISTIC CALCULATIONS

Svetlana Pelemiš[1], Andrijana Bilić[2,3], Dušica Krunić[4], Sanja J. Armaković[2,3*], Stevan Armaković[3,4]

[1]*University of East Sarajevo, Faculty of Technology Zvornik, Karakaj 34a, Zvornik, Republic of Srpska, Bosnia and Herzegovina*
[2]*University of Novi Sad, Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental Protection, Trg Dositeja Obradovića 3, Novi Sad, Serbia, sanja.armakovic@dh.uns.ac.rs**
[3]*Association for the International Development of Academic and Scientific Collaboration (AIDASCO), Sutjeska 2, Novi Sad, Serbia*
[4]*University of Novi Sad, Faculty of Sciences, Department of Physics, Trg Dositeja Obradovića 4, Novi Sad, Serbia*

Abstract

Water stress is a significant issue globally, with many regions experiencing water scarcity. The main challenge in achieving effective wastewater treatment is maximizing the overall efficiency of treatment systems. Polymers play a significant role in environmental applications, particularly in water treatment systems. Certain pharmaceuticals, such as β-blockers like salbutamol and atenolol, are emerging contaminants commonly found in water sources. These substances pose considerable risks due to their persistence and bioactivity. Polymethyl methacrylate (PMMA) is a polymer with excellent mechanical, optical, and electrical properties. It is also economical, non-toxic, and insoluble in water, making it an ideal material for water remediation. Understanding the molecular interactions between these pharmaceuticals and PMMA is essential for optimizing filtration and purification technologies. The atomic calculations provide a detailed understanding of the interaction between molecules without the need for expensive equipment. This study presents a computational analysis of how the polymethyl methacrylate interacts with salbutamol and atenolol. Geometrical optimizations were performed using semiempirical and density functional theory (DFT) calculations. To identify significant interactions between PMMA and pharmaceuticals, we employed the reduced density gradient (RDG) approach, providing insight into intramolecular noncovalent interactions between PMMA's atoms and pharmaceutical molecules. These findings illuminate the fundamental mechanisms of PMMA interactions with pharmaceuticals, offering valuable insights for its use in the environmental remediation of pharmaceutical pollutants.

Keywords: *water purification, salbutamol, atenolol, polymers, DFT, RDG*