IN SILICO TOXICOLOGICAL PREDICTION OF POLYCYCLIC AROMATIC HYDROCARBONS FROM SUGARCANE BIOMASS BURNING

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INTRODUCTION: Polycyclic aromatic hydrocarbons (PAH) are toxic compounds released during incomplete combustion processes, including sugarcane straw burning, a practice still used to enable manual harvesting in Brazil. This exposes sugarcane cutters and nearby populations to airborne pollutants such as particulate matter and carcinogenic substances. Environmental monitoring in Araraquara and São Paulo has identified elevated concentrations of these compounds during harvest seasons. Given the socioeconomic importance of sugarcane agriculture in Pernambuco and the occupational vulnerability of rural workers, evaluating the toxicological risks of these exposures is essential. **OBJECTIVE:** To assess the toxicological potential of polycyclic aromatic hydrocarbons associated with sugarcane biomass burning through predictive modeling and molecular interaction analysis. **MATERIALS AND METHODS:** Nine compounds were analyzed: Fluorene, Benzo[a]pyrene, Benzo[a]fluoranthene, Benzo[b]fluoranthene, Pyrene, Benzo[a]anthracene, Anthracene, Naphtalene, and Retene. Toxicokinetic and toxicodynamic predictions were performed using DeepPK and ProTox 3.0 platforms to evaluate systemic and organ-specific risks. Protein–protein interactions were analyzed using STRING to identify toxicologically relevant targets, followed by gene enrichment analysis in R (org.Hs.eg.db) using Kyoto Encyclopedia of Genes and Genomes pathways. Based on these results, molecular docking was performed with AutoDock Vina to evaluate interactions between the selected compounds and five proteins: PPARγ, acetylcholinesterase, cytochrome P450, Toll-like receptor 4, and p53. Structures were retrieved from public databases and prepared using standard protocols. Visual inspection and interpretation were conducted using Discovery Studio. **RESULTS AND CONCLUSION:** Predictions identified relevant toxicity indicators, including hepatotoxicity, mutagenicity, immunotoxicity, and endocrine disruption. STRING analysis highlighted interactions among CYP1A1, p53, and PPARγ. The enrichment analyses confirm that the molecular network is involved in xenobiotic metabolism, DNA damage response, inflammatory regulation, and metabolic modulation. Docking results revealed interactions exclusively with PPARγ at chain A, showing binding affinities below –6 kcal/mol and RMSD values under 2.0, indicating stable and specific ligand binding. These findings reinforce the potential health risks associated with occupational exposure to PAH in sugarcane burning areas and emphasize the need for targeted toxicological monitoring and preventive strategies.

KEYWORDS: Polycyclic aromatic hydrocarbons; Biomass burning; Ocupational exposure.

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