Computational Study of the Effects of Polycyclic Aromatic Hydrocarbons on Human Health and the Environment

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Abstract
Industrialization and urban expansion have accelerated pollution from human activities, including the release of polycyclic aromatic hydrocarbons (PAHs), which pose significant environmental and health risks. This study aims to computationally assess the physicochemical properties, pharmacokinetic and pharmacodynamic profiles, and correlations among these factors for a set of 9 PAH compounds. Utilizing the PubChem database, we retrieved SMILES files and physicochemical properties for these compounds. In silico analysis of absorption, distribution, metabolism, excretion, and toxicity (ADMET) profiles was conducted using the pkCSM, ProTox II, and admetSAR 2.0 databases. Additionally, ecotoxicity predictions were made with admetSAR 2.0, while bioactivity was assessed using Molinspiration software. Correlations between physicochemical properties and biological activities were established to develop a mathematical model, with Excel used for calculations. Molecular targets were predicted using the SuperPred database. PAHs, characterized as small, hydrophilic molecules with negative partition coefficients, demonstrate moderate water solubility. They adhere to Lipinski and Veber's drug-likeness rules but not the Muegge rule. PAHs exhibit high gastrointestinal absorption and easily penetrate the blood-brain barrier, impacting central nervous system function. They undergo rapid metabolism and function as both substrates and inhibitors, with concentration playing a crucial role. Most compounds display low total clearance, indicating challenges in elimination. PAHs have adverse effects on human health, including skin and eye issues, mutagenicity, carcinogenicity, and immunotoxicity, though they do not induce cytotoxic or hepatotoxic effects according to databases. Naphthalene shows the lowest bioactivity score for various drug targets. Ecotoxicity assessments reveal toxicity to certain organisms but low biodegradability overall. The best statistics of univariate correlation are shown by the partition coefficient correlated with blood-brain barrier permeability. DNA-(apurinic or apyrimidinic site) lyase is the predicted target for these compounds. Computational methods offer efficient avenues for designing safer compounds and decreasing existing toxic effects compared to traditional analyses.

Keywords: Bioinformatics; Polycyclic aromatic hydrocarbons; Human health; Environment