

Abstract Submitted  
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**Study on the Gene Mutations Caused by Intercalation of 4-Aminobiphenyl Compound and BaP Diol-Epoxyde in DNA** JANA CHOE, CRG-NJ — Polycyclic aromatic hydrocarbons such as benzo[a]pyrene (B[a]P) and 4-aminobiphenyl (4-ABP) which alter the levels of Reactive Oxygen Species(ROS) in the lung epithelial cells cause lung and bronchus cancer via DNA mutations. In this research, biochemical and computational simulations were performed to figure out how vaping affects the metabolic conversions of 4-Aminobiphenyl(4-ABP) to 4-ABPdG and benzo[a]pyrene (BaP) to BaP diol-epoxyde(BPDE) respectively. Both are chemical carcinogens identified in electronic cigarettes. For computational and biochemical analysis, molecular gene-editing programs were used. The programs enable us to determine the theoretical values of a certain structures atomic properties through the Density Functional Theory (DFT). The programs also allow users to build virtually any molecule and optimize its geometry according to various force field options. The Auto Optimize Tool was used for each molecule modeled in this project to determine its optimization energy. The Universal Force Field (UFF) option was selected for each molecule modeled.

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