

NEUROPROTECTIVE POTENTIAL OF HESPERIDIN AGAINST BENZO(A)PYRENE-INDUCED CEREBRAL PALSY

Surajit Bhattacharjee^{a*}, Shubhadeep Chakraborty^b and Ankush Sharma^c

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ABSTRACT

This study investigates the link between cigarette smoke, specifically benzo(a)pyrene (BaP), and cerebral palsy, focusing on BaP's neurotoxicity. It also examines the neuroprotective potential of hesperidin, a citrus-derived compound, by assessing its binding affinity with the $\beta 4$ subunit of Adapter Protein Complex 4 (AP-4). Molecular docking analyses using Discovery Studio and PyRx were performed with the $\beta 4$ subunit of AP-4 as the protein and benzo(a)pyrene and hesperidin as ligands. The results showed that hesperidin had a higher binding affinity ($-7.2 \text{ kcal mol}^{-1}$) compared to BaP ($-6.5 \text{ kcal mol}^{-1}$), establishing multiple interactions, including van der Waals, hydrogen, and pi-alkyl bonds. Key receptor residues for hesperidin binding were identified. These findings highlight hesperidin's potential neuroprotective role, suggesting it may help to prevent BaP-induced neurotoxicity in cerebral palsy. The study emphasizes the promise of hesperidin, encouraging further *in vivo* and clinical investigations.