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COX-2 as a therapeutic target: A computational approach to indole alkaloids for analgesic design

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Medicinal plants provide natural compounds that aid in biological processes, including the treatment of inflammation-related disorders. These have been connected to a direct inhibitory binding mechanism, particularly on the COX-2 protein. The present work describes an *in silico* analysis of chosen alkaloids for COX-2. The goal is to analyze the structural and conformational characteristics of these selected indole alkaloids to determine its inhibitory properties and demonstrate its binding manner in the COX-2 active site. The compounds exhibit distinct interactions, involving both hydrogen bonding and van der Waals forces, with specific amino acid residues within the COX-2 binding site. Trigonoliimine C forms hydrogen bonds with Met 522 and Val 523, accompanied by van der Waals interactions with key residues such as Val 116 and Trp 387. Trigonoliimine A demonstrates hydrogen bonding with Tyr 355 and van der Waals interactions with Pro 84 and Phe 518. Flinderole C engages in hydrogen bonding with Phe 381 and Ser 353, coupled with van der Waals interactions with Val 89 and Tyr 385. Ramiflorine B exhibits hydrogen bonding with Tyr 355 and van der Waals interactions with Thr 85 and Ser 530. Ramiflorine A, forming hydrogen bonds with Tyr 355 and engaging in van der Waals interactions with Pro 84 and Phe 518, showcases a remarkable specificity in molecular recognition. These findings provide valuable insights into the potential therapeutic applications of these compounds, offering a foundation for further experimental validations and the development of novel anti-inflammatory agents targeting COX-2.

Keywords: Molecular docking, COX-2 interaction, Hydrogen bonding, Van der Waals forces, Anti-inflammatory agents