

Abstract Submitted
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Study on the Dynamics and Stabilities of DNA Intercalating Agents Using Computer Analysis RICHARD KYUNG, ETHAN HAN, CRG-NJ — In this paper, a computational gene editing software which is an open-source molecular editing program equipped with an auto-optimization feature was used. In the DNA intercalation, guanine benzopyrene intercalates in the array to form an adduct. The binding causes an alteration of the structure and replication proceeds to gene mutation. To assess the activity, dipole moment was calculated and checked how different values of electronegativity of different atoms in a molecule affect the stability of the system. This difference in electronegativity causes the shared pair of electrons to shift towards one atom, creating a slight difference in charge and activity. Also, electrostatic potential maps were found to show active parts of the molecule. Through this map, users can discover electron density, proton acidity, and how those affect the overall electron density and stability.

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