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Molecular structure, spectroscopy, molecular docking, and molecular dynamic studies of tetrahydroneoprzewaquinone as potent cervical cancer agent

- Aniekan E. Owen , Ernest C. Agwamba , Mathias E. Gideon , Kelechi Chukwuemeka , Emmanuel U. Ejiofor , Innocent Benjamin , Eze F. Ahukwe , Festus O. Ogungbemiro , Kube T. Maxwell , Amanda-Lee E. Manicum and Hitler Louis

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Abstract

Cervical cancer is one of the most prevalent cancer-related diseases, causing accelerated morbidity and mortality rates in low-income countries and African states. This study explores the potential of (3*R*,3′*R*)-2,2′,3,3′-tetrahydroneoprzewaquinone (TDN) as a treatment for cervical cancer by investigating its structural and molecular properties using molecular modelling technique, which include; DFT, molecular docking, molecular dynamic

simulation. The results are promising, with TDN demonstrating exceptional stability in the energy gap (E_g) as well as through natural bond order analysis (NBO). $\pi \rightarrow \sigma^*$ electronic transitions were found to contribute mainly to the molecule's stability, with an outstanding total stabilization energy ($E^{(2)}$). Docking exercises showed that TDN binds more favorably to the pro-apoptotic receptor 4s0o with a stronger H-bond compared to the conventional DOX drug, which interacted less effectively with TDN and more strongly with the anti-apoptotic protein, forming an outstanding strong H-bond. Molecular dynamics simulations also revealed that TDN's interaction with the pro-apoptotic protein (TDN_4S0o) was more stable than the standard DOX drug (DOX_4s0o). The H-bond plot indicated that TDN could effectively interact with both anti and pro-apoptotic receptors, forming approximately 1 to 4 hydrogen bonds between TDN_1g5M with respect to each picosecond (ps) ranging from 0 to 1000 ps. In contrast, the number of hydrogen bonds fluctuated when DOX interacted with the anti-apoptotic protein (1g5M), ranging from 1 to 5 H-bonds. Overall, these results suggest that TDN may be a promising drug candidate for cervical cancer treatment.

Keywords: DFT; molecular docking; molecular dynamics; cervival cancer; tetrahydroneoprzewaquinone

Corresponding authors: Ernest C. Agwamba, Computational and Bio-Simulation Research Group, University of Calabar, Calabar, Nigeria; and Department of Chemistry, Covenant University, Ota, Ogun, Nigeria, E-mail: agwamba.ernest@gmail.com; and **Innocent Benjamin**, Computational and Bio-Simulation Research Group, University of Calabar, Calabar, Nigeria, E-mail: benjamininnocent53@gmail.com

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