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DNA interaction studies on the drug sotlol and its Cu(II) complex using viscosity measurements, UV-Vis spectroscopy and molecular docking simulation methods

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Recent years have seen a rejuvenation of interest in studies on the interaction mechanism of deoxyribonucleic acid (DNA) with small molecules, especially in interaction with drugs [1, 2]. In this project, the interaction of the drug sotalol (SOT) and its Cu(II) complex (CuSOT) with calf thymus DNA (ct-DNA) was investigated using viscosity measurements, UV-Vis spectroscopy and molecular docking simulation methods. Viscosity measurement studies indicated that the SOT interacts with ct-DNA via a groove mode of binding. The molecular docking simulation visualized that both the SOT and CuSOT are located in the minor groove of the DNA helix. The binding constant measured from the UV–Vis absorption studies showed that the binding strength of SOT to ct-DNA, compared to the drug cytarabine as a known anticancer agent, is significant [3]. Also, the calculated binding constants (K_b) by AutoDock Vina showed that the affinity of CuSOT for DNA is higher than that of the drug SOT.

Keywords: Sotalol, Copper complex, DNA interaction, Molcular docking.

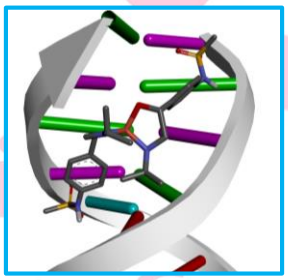


Figure 1. Molecular docking 3D visualization of DNA–CuSOT system which shows the location of CuSOT in DNA (PDB ID: 1BNA).

References

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