عنوان مقاله:

Insights on the interaction mechanism of a new Cu(II) complex of Lidocaine Drug to calf thymus DNA by multispectral techniques and molecular docking

محل انتشار:

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خلاصه مقاله:

In the present research, the feasibility of a new copper(II) complex (Cu(II) complex) containing the lidocaine (LC) drug for affinity with the target calf thymus DNA (ct-DNA) is demonstrated. To investigate the molecular interaction between the synthesized complex and ct-DNA, some multi-spectroscopic approaches associated with molecular docking were employed in the physiological buffer (pH ۷.۴). The ct -DNA binding properties of Cu(II) complex exhibit that it binds to ct -DNA through a groove binding mode, and the binding constant values were computed employing the emission spectral data. The thermodynamic profile exhibited the spontaneous formation of ct-DNA-Cu(II) complex system via hydrogen bonds and van der Waals forces. Meanwhile, the results of docking simulation confirmed our spectroscopic findings

کلمات کلیدی:

Interaction; Copper complex; DNA binding; Fluorescence; Docking; Spectroscopy