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**Abstract**

The interactions of natural drug functionalized metal nanoparticles with DNA plays a pivotal role in developing effective therapeutic agents having a wide range of potential biomedical applications. The focus of this study was to decipher the binding mechanism of diosmin capped gold nanoparticles (DM-AuNPs) with calf thymus DNA (ctDNA) through a combination series of spectroscopic and calorimetric studies. The gold nanoparticles were successfully synthesized by the facile one-pot synthesis using DSM as a capping and reducing agent. The DM-AuNPs were characterized using UV-Visible spectroscopy, XRD, FTIR, DLS and HRTEM analysis confirming the formation of stable AuNPs with an average size of  $30\pm 3$  nm. A series of experiments such as UV-Vis absorbance, fluorescence dye displacement studies, temperature melting and viscosity analysis unravelled the binding mode of DM-AuNPs by establishing a typical groove binding mode upon its complexation with ctDNA. The CD and FTIR measurements provided clear-cut evidences regarding the

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