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Synthesis and functionalization of gold nanoparticles and investigation of their bioactivity and biocompatibility *in vivo*

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Inorganic nanoparticles are frequently functionalized with biopolymers to improve their physicochemical properties, bioactivities, and biocompatibilities. Gold nanoparticles (Au NPs) are frequently used in the field of biomedical engineering for the purpose of diagnosis as well as therapeutics purposes. The as-synthesized concave cube shaped gold (CCAu) nanoparticles was synthesized via seed-mediated approach and functionalized with a thiol-group containing polymer, alpha lipoic acid (-LPA) which is a natural antioxidant, to generate CCAuLPA nanoparticles. Both the as-synthesized (CCAu) and CCAuLPA nanoparticles were characterized through UV-Vis spectroscopy, FTIR spectroscopy, surface-enhanced Raman spectroscopy (SERS), scanning electron microscopy, transmission electron microscopy, and zetasizer. Both the UV-Vis spectroscopy and SERS confirm the synthesis of CCAu and their functionalization with LPA. The SEM and TEM images confirm the synthesis of monodispersed Au NPs. The zeta potential of CCAu and CCAuLPA were +49 and +16 mV, respectively. The antibacterial activity was investigated against 10 pathogenic and nonpathogenic bacteria in dose-dependent manner. The CCAuLPA nanoparticles showed the highest antibacterial activity against *B. subtilis* at 4000 g/ml and the zone of inhibition was 20 mm. Moreover, the CCAuLPA nanoparticles showed the lowest minimum inhibitory concentration value (i.e., 21 g) against *B. subtilis*. The dead bacteria were observed through trypan blue dye exclusion assay as well as propidium iodide assay under phase contrast and fluorescence microscope, respectively. Lipid peroxidation assay confirms the damage of bacterial cell wall due to their interaction with the AuNPs. Furthermore, the formation of malondialdehyde-thiobarbituric acid adduct revealed that Au nanoparticles oxidize the fatty acids of bacterial cell membrane. Biocompatibility was determined in male Wistar rats. The level of hematological parameters as well as serum biomarkers of liver, kidney and heart was determined and no significant toxicity was found. Furthermore, the histopathology of liver, kidney, brain, spleen, heart and lung did not show any toxicity as well.