An increasing demand and a commensurate advancement of nanotechnology have witnessed the advent of nanomaterials as the emerging candidates for diverse biomedical applications. In this thesis, first, the effect of a chemical denaturant on the agglomeration behavior of a citrate stabilized Au NP–protein composite has been demonstrated. The observations reported indicated that the interaction between the cit–Au NP and protein leading to agglomeration is dependent on the conformation of protein.

The potential applications of nanomaterials in biomedical field include improvement in diagnostic therapy, i.e., theranostic. In recent years, multifunctional systems have been developed by combining drugs, molecular targeting and imaging agents into a single system. Interestingly, nowadays, metal NCs have been widely used as an imaging agent due to their low toxicity, chemical stability, excitation wavelength tunability, pH dependent emissive properties, and lower toxicity than the Q-dots.

Therefore, water soluble copper nanoclusters (Cu NCs) with an average diameter of <3 nm were synthesized by biomolecule bovine serum albumin (BSA), lysozyme and PVP as the stabilizing agent with bright fluorescent property under UV light. Finally, theranostic applications were carried out by using Cu NCs such as antibacterial activity, bioimaging and biolabeling and drug delivery. It was found that Cu NCs have an excellent antibacterial activity having minimum inhibitory concentration (MIC) which was much less than Cu NPs. Similarly, Cell viability studies indicated their noncytotoxic nature, making the NCs ideal for biological applications. The Cu NCs were found to be hemocompatible. Thus, blood compatibility assay supported the potential of composites (thus Cu NCs) for applications in vivo. Fascinatingly, Cu NCs were found to generate ROS in cancer cells which increased the efficacy of cisplatin in killing the cancer cells by providing the synergy of action.