Abstract No: 2025_287

Chitosan-Stabilized Silver Nanoparticles: Molecular Dynamics Simulation on the Stability and *in-vivo* Interactive Toxicity with Cadmium on an Aquatic Model *Moina macrocopa*

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Silver nanoparticles (AgNPs) are a significant innovation in nanoscience, particularly for their potential applications in biological systems. In this study, silver nanoparticles were synthesized using chitosan acting as both reducing and capping agent, and characterized by UV-visible spectroscopy, Transmission Electron Microscopy (TEM), Fourier-Transform Infrared Spectroscopy (FTIR), and X-Ray Diffraction (XRD). The surface plasmon resonance peak of CS-AgNPs was identified at 440 nm. TEM revealed spherical particles with an average of 12nm in size. XRD patterns confirmed crystalline silver with a face-centered cubic structure. Molecular docking revealed weak non-bonding interactions with a +0.03 kcal/mol binding energy. In a water simulation model, molecular dynamics simulations were performed to predict the stability of CS-AgNPs compared to bare AgNPs. Radius of gyration (Rg) and Root Mean Square Deviation (RMSD) indicated the stabilization of CS-AgNPs throughout the 50 ns simulation length. The toxicity of CS-AgNPs and their interactive effects with Cd were evaluated *in-vivo* using the freshwater zooplankton, *Moina macrocopa* (age <24 hours). Acute toxicity tests revealed a notable change in 24-hour LC_{50} values upon exposure to $AgNO_3$, CS-AgNPs, $CdSO_4$, and combined (CS-AgNPs + Cd), which were 0.005, 0.056, 0.057, and 0.036 mg/L, respectively. Chronic toxicity tests revealed a significant reduction in body length, population size, and the total reproductive output of the exposed individuals to the chemical mixtures for 7 days ($p < 0.05$). Synergistic toxicity was observed in the combined exposure to both acute and chronic toxicity studies. In conclusion, CS-AgNPs demonstrated significantly reduced toxicity compared to their Ag+ counter concentrations, and molecular dynamics revealed the better stability of AgNPs when they were coated with chitosan, highlighting their applications in nanomedicine and industries. The interactive toxicity of CS-AgNPs with Cd metal ions on *M. macrocopa* highlights the need to optimize their safe concentrations for ecological safety.

Keywords:

Silver nanoparticles, CS-AgNPs, *Moina macrocopa,* toxicity, molecular dynamics

Acknowledgment:

This research is funded by the Department of Chemistry, University of Kelaniya & Department of Zoology and Environmental Management, University of Kelaniya.