Molecular docking approach to elucidate potential genotoxic impact of copper engineered nanoparticles (CuO NP) upon red blood cells

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Abstract

Although copper-based nanoparticles (CuO-NPs) are widely used as anti-fungal and antibacterial agents and it is known that copper complexes have clastogenic effects by binding to minor and major grooves in DNA, there is no adequate information about the interaction mode and affinity of CuO-NPs with DNA [1]. In this study, docking simulations were performed to model the binding mode and interaction of CuO-NPs with its possible intracellular target, DNA, as well as to calculate its binding affinity against this target receptor. CuO-NPs significantly induced specific erythrocyte DNA damage (micronucleated cells), as well as an alteration in intracellular oxidative stress response (CAD, SOD and GST) in *Carassius carassius* used as model organism [2]. The docking results showed that the DNA damage induced by CuO-NPs could possibly be a direct damage rather than secondary ROS-induced event, that is, DNA damage induced by CuO-NPs is likely to be bimodal [3]. Ecophysiological studies on nano-bio interfaces combined with molecular docking can offer a powerful approach to better predict the effects of nanoparticles on animal and human cells and tissues.

References

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[3] Baildya, N., Dey, I., Bagchi, A., & Chattopadhyay, A. P. 2020. Interaction of copper nanoparticles with DNA: structural and docking studies. *Journal of Biomolecular Structure and Dynamics*, *38*(4), 1256-1261

Figures

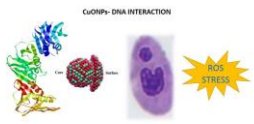

Figure 1: Copper nanoparticles-DNA interaction