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Phytochemical, Antioxidant and Antimicrobial Properties of Zinc Oxide Nanocomposites (ZnONCs) on Multidrug-Resistant E. Coli Enzyme: In-Vitro and In-Silico Studies

Authors : Callistus I. Iheme, Kenneth E. Asika, Emmanuel I. Ugwor, Chukwuka U. Ogbonna, Ugonna H. Uzoka, Nneamaka A. Chiegboka, Chinwe S. Alisi, Obinna S. Nwabueze, Amanda U. Ezirim, Judeanthony N. Ogbulie

Abstract : Antimicrobial resistance (AMR) is a major threat to the global health sector. Zinc oxide nanocomposites (ZnONCs), composed of zinc oxide nanoparticles and phytochemicals from Azadirachta indica aqueous leaf extract, were assessed for their physico-chemicals, antioxidant, in silico, and in vitro antimicrobial properties on multidrug-resistant Escherichia coli enzymes. Gas chromatography coupled with mass spectroscope (GC-MS) analysis on the ZnONCs revealed the presence of twenty volatile phytochemical compounds, among which is scoparone. Characterization of the ZnONCs was done using Ultraviolet-visible spectroscopy (UV-vis), energy dispersive spectroscopy (EDX), transmission electron microscopy (TEM), scanning electron microscopy (SEM), and x-ray diffractometer (XRD). The results showed arrays of ZnONCs nanorods with maximal absorption wavelengths of 320 nm and 350 nm and thermally stable at the temperature range of 423.77 to 889.69 ℃. In vitro, the study assessed the dehydrogenase inhibitory properties of the ZnONCs, a conjugate of ZnONCs and ampicillin (ZnONCs-amp), the aqueous leaf extract of A. indica, and ampicillin (standard drug). The findings revealed that at the concentration of 500 µm/mL, 57.89 % of the enzyme activities were inhibited by ZnONCs compared to 33.33 % and 21.05 % of the standard drug (Ampicillin), and the aqueous leaf extract of the A. indica respectively. The inhibition of the enzyme activities by the ZnONCs at 500 µm/mL was further enhanced to 89.74 % by conjugating with Ampicillin. In silico study on the ZnONCs revealed scoparone as the most viable competitor of nicotinamide adenine dinucleotide (NAD+) for the coenzyme binding pocket on E. coli malate and histidinol dehydrogenase. The antioxidant analysis using DPPH indicated that ZnONCs exhibited lower reducing power when compared to the standard (garlic acid). From the findings, it can be concluded that the scoparone components of the nanocomposites in synergy with the zinc oxide nanoparticles inhibited E. coli malate and histidine dehydrogenase by competitively binding to the NAD+ pocket and that the conjugation of the ZnONCs with ampicillin further enhanced the antimicrobial efficiency of the nanocomposite against multidrug-resistant E. coli.

Keywords : antimicrobial resistance (AMR), dehydrogenase activities, E. coli, zinc oxide nanocomposites
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