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Calotropis procera flower extract for the synthesis of double edged octahedral α-Fe_2O_3 nanoparticles *via* a greener approach: an insight into its structure property relationship for *Escherichia coli*†

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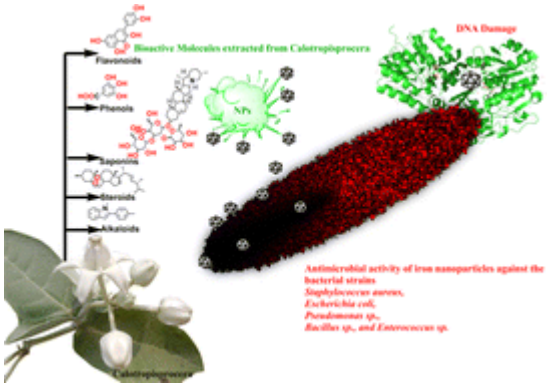
Abstract

Urinary tract infection caused by *Escherichia coli* (*E. coli*) is regarded as one of the most serious issues confronting humans worldwide. However, the antibacterial mechanism and process are time-consuming

and inconclusive. To address this issue, iron oxide-based antibacterial agents were synthesized in a more environmentally friendly greener approach using an Indian traditional flower extract from the *Calotropis procera* plant, which contains several bioactive secondary metabolic moieties. Powder X-ray diffraction (PXRD) techniques confirm the formation of α-Fe_2O_3 crystal packing in green synthesized nanoparticles (NPs) from its crystal planes (012, 104, 110, 113, 024, 116, 018, 214, and 300). High-resolution scanning electron microscopy (HR-SEM) was used to examine the morphology of α-Fe_2O_3 NPs, which revealed a double layer edge-octahedral (DLE-Oh) shape with an average edge length of ~4.0 nm, corresponding to surface area ~55.42 nm^2, and volume ~221.70 nm^3 as calculated. The synthesized α-Fe_2O_3 DLE-OH NPs have effective antibacterial activity against *E. coli*, with a high rate of inhibition observed. Furthermore, the various iron oxide hierarchal structures for *E. coli* membrane proteins were optimized using density functional theory. Molecular docking studies show that the lowest inhibition constant (K_i) values, such as 33.40 and 2.24 μM for 2MEQ and 6ZHP membrane proteins, effectively inhibit bacterial replication.



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