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## SCHEDULED MAINTENANCE

**Maintenance work is planned from 09:00 BST to 12:00 BST on Saturday 28th September 2024.**

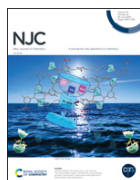
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Issue 24, 2023

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From the journal:

**New Journal of Chemistry**

### ***Calotropis procera* flower extract for the synthesis of double edged octahedral $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> nanoparticles via a greener approach: an insight into its structure property relationship for *Escherichia coli*<sup>†</sup>**



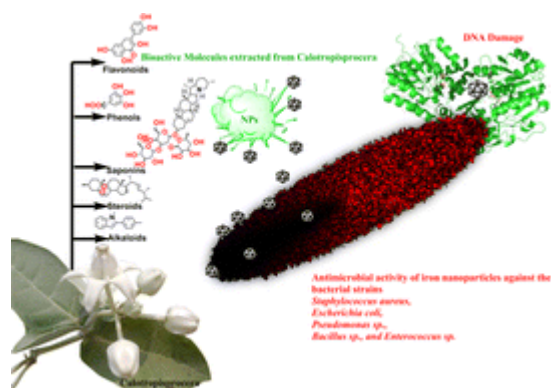
[Karavelan Murugan](#),  <sup>\*ab</sup> [Rajakannu Subashini](#), <sup>a</sup> [Udayadasan Sathiskumar](#) <sup>c</sup> and [Greeshma Odukkathil](#) <sup>d</sup>

[Author affiliations](#)

## 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  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> 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  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> NPs, which revealed a double layer edge-octahedral (DLE-Oh) shape with an average edge length of  $\sim$ 4.0 nm, corresponding to surface area  $\sim$ 55.42 nm<sup>2</sup>, and volume  $\sim$ 221.70 nm<sup>3</sup> as calculated. The synthesized  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> 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  $\mu$ M for 2MEQ and [6ZHP](#) membrane proteins, effectively inhibit bacterial replication.

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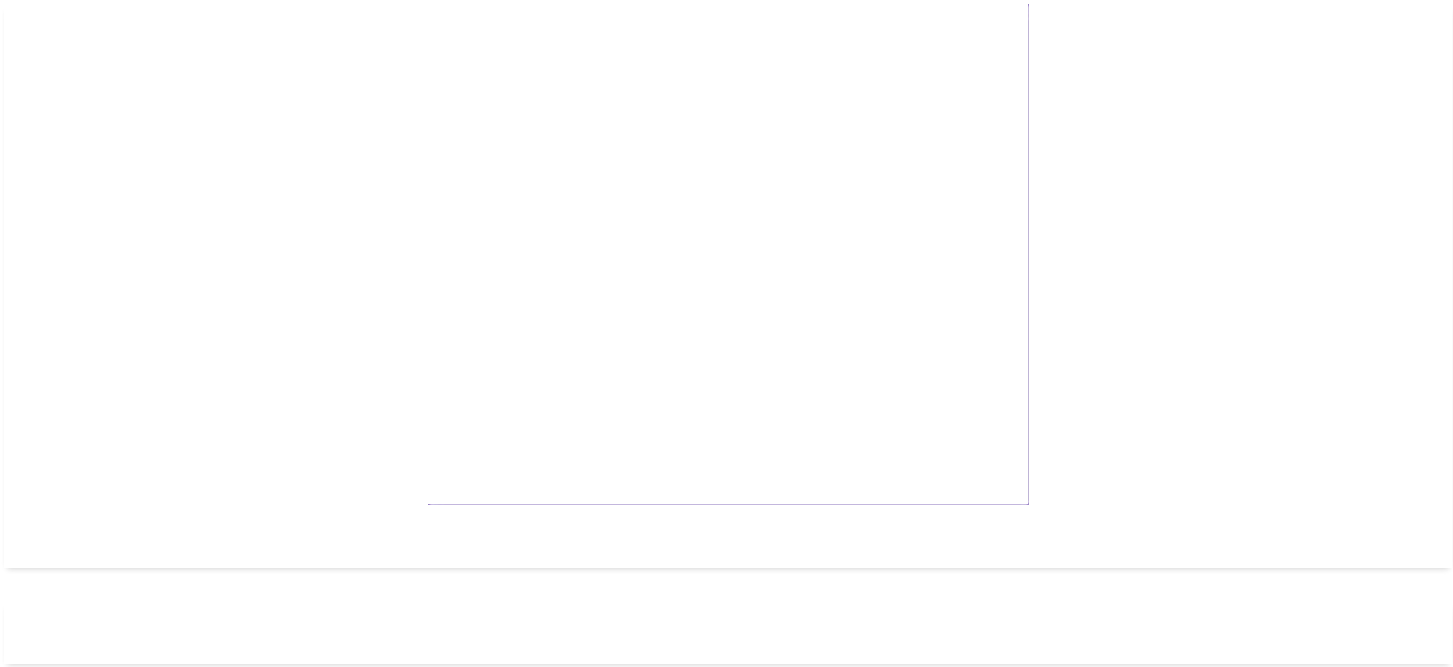
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