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Flavonoid-coated gold nanoparticles as efficient antibiotics against gram-negative bacteria—evidence from *in silico*-supported *in vitro* studies

Hani A Alhadrami
King Abdulaziz University, Saudi Arabia

Flavonoids are a class of bioactive plant-derived natural products that exhibit a broad range of biological activities including antibacterial ones. Their inhibitory activity toward Gram-positive bacterial was found to be superior over that against Gram-negative ones. Accordingly, we designed in the present investigation gold nanoparticles-flavonoids conjugates to enhance the antibacterial effects of chrysin, kaempferol, and quercetin, against a number of Gram-negative bacteria. The prepared GNPs were able to conjugate to these three flavonoids with conjugation efficiency ranged from 41% to 80%, respectively. Additionally, they were able to exert an enhanced antibacterial activity in comparison with the free flavonoids and the unconjugated GNPs. Quercetin-loaded GNPs were the most active nano-conjugate and as able to penetrate the cell wall of *E. coli*. Upon testing of these flavonoids against *E. coli's* DNA gyrase they showed very promising micromolar inhibition. A number of *in silico* experiments (docking, molecular dynamic simulations) were carried out to explain the antibacterial mechanisms of these flavonoids. In conclusion, these bioactive flavonoids-based GNPs are considered very promising antibiotic candidates for further development and evaluation.

Keywords: Gold nanoparticles, flavonoids, Gram-negative bacteria, DNA-gyrase, in silico.