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AI-Guided Molecular Profiling and Experimental Validation of *Gymnema sylvestre* Derived AgO Nanoparticles Targeting Quorum Sensing in *Escherichia coli* Associated with Type 1 Diabetes

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ABSTRACT

Bacteria associated with Type-1 Diabetes Patients often develop complications due to polymicrobial infections and their tendency to form biofilms. The virulence of *Escherichia coli*. bacteria could also be enhanced due to their ability to "sense" the presence of other bacteria within a community (quorum sensing) which may help inform alternative antibacterial strategies that would target these mechanisms to prevent/reduce bacterial pathogenicity and thus, potential resistance to standard antibiotics. The aims of this project were to determine if silver oxide nanoparticles (AgONPs) produced from the leaf extract of *Gymnema sylvestre* were able to inhibit *E. coli* quorum sensing using integrated wet and dry laboratory techniques. The viability and stability of AgONPs were examined by characterisation studies using various physicochemical approaches. The interactions between phytochemical functionalised AgONP surfaces and proteins involved in the *E. coli* quorum sensing system were predicted using AI-assisted molecular modelling and in-silico docking. Overall, AgONPs inhibited biofilm formation in *E. coli* (due to quorum sensing) without affecting overall growth, indicating their promise as anti-virulence agents. Additionally, by combining the use of AI technology with traditional experimental validation resulted in a greater prediction accuracy and reduced the uncertainty encountered when comparing experimental data against predictions.

Keywords: *Gymnema sylvestre, silver oxide nanoparticles, Quorum sensing, Escherichia coli, Type 1 Diabetes*

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