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Combined In-Vitro and In-Silico Evaluation of Bioactive Phytochemicals from Curcuma longa (Linn.) Against Multidrug-Resistant Enterobacter cloacae: Insights into Antibacterial and Antibiofilm Potential

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Abstract

Enterobacter cloacae exhibit significant antibiotic resistance, posing a major challenge to existing therapeutic options. In the present study, *Curcuma longa* extracts were evaluated for their antibacterial and antibiofilm activities using both in vitro and in silico approaches. The in vitro assays demonstrated that methanolic and ethanolic extracts exhibited the highest antibacterial potential, showing maximum zones of inhibition of 12 ± 0.25 mm and 8 ± 0.30 mm, respectively, against *E. cloacae*. Biofilm inhibition assays indicated a moderate disruption of preformed bacterial biofilms. In the in-silico analysis, molecular docking revealed that curcumin exhibited the strongest binding affinity (−8.4 kcal/mol) with β-lactamase (AmpC), followed by demethoxycurcumin (−7.8 kcal/mol) with DNA gyrase, and bisdemethoxycurcumin (−7.7 kcal/mol) with the cyclic di-GMP regulatory protein of E. cloacae. The docking models were validated by favourable ProSA Z-scores (−8.86 to −10) and ERRAT quality factors (>80%), confirming the reliability of the predicted protein-ligand interactions. Toxicity prediction analysis indicated that all tested compounds were non-mutagenic, non-carcinogenic, and exhibited safe LD_{50} ranges, suggesting a high safety profile. Collectively, these findings highlight the potential of Curcuma longa-derived phytochemicals as effective and safe therapeutic candidates for combating multidrug-resistant Enterobacter cloacae infections.

Key Words: *Curcuma longa, Enterobacter cloacae, Antibacterial activity, Biofilm inhibition, Molecular docking*