

Molecular Docking, Cytotoxicity and Antioxidant Evaluation of Bioactive Compounds from *Capparis zeylanica* Linn, Stem.

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Doi: <https://doi.org/10.5281/zenodo.17909106>

Received: 10 September 2025

Accepted: 14 September 2025

Abstract:

The present study investigates the phytochemical composition and pharmacological potential of *Capparis zeylanica* Linn stem, a medicinal plant traditionally employed in Ayurveda and Unani medicine. Phytochemical screening confirmed the presence of alkaloids, flavonoids and phenolic compounds, which were subsequently isolated and characterized using chromatographic and spectroscopic techniques. Molecular docking studies revealed strong binding affinities of the isolated compound with both wild-type and mutant forms of epidermal growth factor receptor (EGFR) kinase, suggesting significant anticancer potential.

Pharmacological evaluation through the MTT assay demonstrated notable cytotoxicity of the ethanolic extract against HCC827, H1975 and HT-29 cancer cell lines. Western blot analysis further confirmed the inhibition of EGFR autophosphorylation, validating its mechanistic role in suppressing tumor growth and progression. Furthermore, antioxidant activity, assessed by the DPPH radical scavenging assay, demonstrated marked free-radical neutralizing capacity, underscoring its potential to alleviate oxidative stress.

Overall, the findings establish *C. zeylanica* stem as a valuable source of bioactive compounds exhibiting dual pharmacological properties—anticancer and antioxidant. This study not only provides scientific evidence supporting its traditional applications but also highlights its importance in modern drug discovery, particularly for the development of targeted anticancer therapeutics and antioxidant-based formulations.

Keywords: *Capparis zeylanica* (L), Molecular docking Study, Anticancer activity, Antioxidant activity

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