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Antibacterial efficacy of an Unexplored species of Gentianaceae- *Exacum pedunculatum* on *Escherichia coli* by a Substantial Computational

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Urinary tract infection is one of the most common problem often found in Diabetic patients caused by bacterial infections. The Extended Beta Spectrum lactamases (EBSLs) possess antibiotic resistance mechanism in the face of the introduction of new antimicrobial agents consequently limiting the therapeutic options. Due to these reasons, plant derived compounds or phytomedicines having antimicrobial action are tested by both wet lab and dry lab methods in the present study. In vitro and in silico antibacterial potential of the unexplored species *Exacum pedunculatum* belonging to Gentianaceae family was evaluated. The ethanol extract of *Exacum pedunculatum* was purified to obtain a saturated fatty acid. Qualitative structure analysis of the bioactive compound by IR, NMR and GC-MS techniques revealed the presence of compound. Further, structure was generated using CHEMSKETCH software and PASS PREDICTION software to predict the biological activity. The drugreceptor interaction was simulated by Computer-Aided Drug Design (CADD) method to understand the mechanism of anti-bacterial activity. The protein-ligand interaction plays a significant role in the structural based drug designing. Autolysin, a bacteriolytic enzyme and the compound were docked using HEX docking software and SWISS online docking software and the docking score was very significant with minimum energy value. The result explains that the compound can inhibit the activity of autolysin as it forms a strong atomic interaction with the active site residues. Hence the compound can be used as a drug for bacterial infections. Revitalization of the traditional medicine through Computer-Aided Drug Design (CADD) approach for acceptance as an alternative treatment in the medicinal science is necessary.

Biography

Ms.Lakshmi H V has completed her Master's degree in Biotechnology from Kuvempu University, Karnataka and presently pursuing doctoral studies in the Department of Biotechnology in Karnatak University, Dharwad, India. Worked as Senior Research Fellow in a DBT project on "Comparative Analysis of Functional and Anonymous SNP Diversity in Legumes : PCR based direct (gene based) and indirect (marker-based) tools for Legume Genome Analysis", in Marker Assisted Selection Laboratory, Gandhi Krishi Vignana Kendra, University of Agricultural Sciences, Bangalore, Karnataka, India.

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