

NEW INSIGHTS INTO THE PREDICTION OF POTENTIAL PHYTOCOMPOUNDS OF *PIMENTA DIOICA* STEM VIA DETAILED COMPUTATIONAL INVESTIGATIONS: GCMS STUDIES, NETWORK PHARMACOLOGY, MOLECULAR DOCKING ANALYSIS ON PCOS TARGET PROTEINS

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ABSTRACT

Polycystic ovarian syndrome (PCOS) is an endocrine disorder affecting women during their fertile years, marked by hormonal imbalance, cystic ovaries and irregular menstruation. *Pimenta dioica*, a traditional medicinal plant, was evaluated for its therapeutic potential against PCOS using *in silico* approaches. GC-MS analysis identified key phytochemicals, which were further assessed through network pharmacology, drug-likeness, ADMET analyses and molecular docking studies. Network analysis revealed five crucial PCOS-associated targets: Insulin receptor substrate-1 (1QQG), Androgen receptor (1E3G), Follicle-stimulating hormone (1XWD), Leptin receptor (3V60), and CYP17 (3RVK). Among the identified compounds, eugenol exhibited strong binding affinity towards these targets. ADMET profiling and PASS prediction confirmed its favourable pharmacokinetics, non-toxicity, and non-carcinogenic properties. These findings suggest that *Pimenta dioica*, particularly eugenol, holds promise as a potential lead compound for developing novel early-stage therapeutics for PCOS management.