

Scrutinizing Potential Phytoconstituents from *Bauhinia variegata* in Mitigating the Symptoms of Polycystic Ovarian Syndrome: A Computational Approach

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ABSTRACT

Background: Polycystic ovarian syndrome is a metabolic disorder majorly caused by the hormonal fluctuations in female and the current scenario explains that adolescents remain predominantly affected with this disorder. *Bauhinia variegata* assist in the treatment of various ailments and are used as an ingredient in targeting uterine disorders, yet the exact constituent that contributes on activity remains unknown. **Aim:** The main aim of our study is to determine the potent phytoconstituent of *Bauhinia variegata* to fight against the symptoms of PCOS through computational techniques. **Materials and Methods:** Five *in silico* techniques like Molecular docking analysis, Pharmacokinetics, toxicity prediction of the compounds, Biological activity and Molecular dynamics simulation studies were performed to identify the potent phytoconstituent. **Results and Discussion:** Molecular docking studies show that the major constituent lupeol had a good binding interaction and high docking score of -10.31 Kcal/mol and -11.52 Kcal/mol with both the proteins 3RUK and 1E3K. Pharmacokinetics, toxicity and biological activity studies reveal that it had ideal drug likeliness properties with proper biological activity values and were found to non-toxic in the analysed parameters. Lupeol complex was found to be potentially stable throughout the molecular dynamic's simulation for 100 ns. **Conclusion:** Thus, through *in silico* analysis it is evident that from the list of phytoconstituents of *Bauhinia variegata*, lupeol possess potent activities in mitigating the symptoms of PCOS. Further *in vitro* and *in vivo* analysis on PCOS model is expected to yield favourable results.

Keywords: *Bauhinia variegata*, Molecular docking, Molecular dynamics, Pharmacokinetic analysis, Toxicity prediction.

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INTRODUCTION

Women of reproductive age majorly possess metabolic abnormalities which results in the prevalence of polycystic ovarian syndrome.¹ Worldwide diagnostic report from National Institutes of Health (NIH) denotes 4-10% of reproductive women are affected with PCOS. One among ten women of the world population are diagnosed with the disorder and many are left out without proper diagnosis.^{2,3} Though the women of reproductive age are predominantly affected, prevalence of the disorder is seen in late adults even after the child bearing age.⁴ The factors that play a wide role in the occurrence includes, hyperandrogenism, hereditary, excessive stress, anxiety and atypical sleep patterns.⁵

The precise pathophysiology of PCOS is yet to be determined, however few factors like chronic low grade inflammation that leads to excessive oxidative stress,⁶ increase of prolactin and decline of melatonin levels, imbalance in the Hypothalamic-Pituitary-Ovarian (HPO) axis which leads to the excessive secretion of GnRH and Insulin resistance remain as contributing elements (Figure 1).⁷

PCOS likewise termed as Stein-Leventhal syndrome is mainly diagnosed with the help of a criteria called Rotterdam criteria which was introduced in the year 2003⁸ and underwent few amendments at recent times. In accordance to the criteria, women with positive results for two among the three conditions are referred to be categorized under PCOS. The conditions include, presence of ≥ 20 antral follicles in either of the ovaries with accumulation of ovarian volume greater than 10 cm³, Oligo anovulation characterized by less than 8 menstrual cycle per year and hyperandrogenism determined through ideal clinical and biochemical methods.^{9,10} PCOS is often diagnosed with the



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