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VIRTUAL SCREENING, AND ADMET EVALUATION OF HERBAL CONSTITUENTS AS POTENTIAL THERAPEUTIC AGENTS FOR POLYCYSTIC OVARY SYNDROME

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ABSTRACT

Polycystic Ovary Syndrome (PCOS) is a common endocrine disorder in women of reproductive age, marked by hormonal imbalance, irregular ovulation, and metabolic issues such as insulin resistance. Existing treatments mainly provide symptomatic relief and may cause side effects, creating a need for safer and more effective alternatives. Herbal constituents, known for their multi-target actions and fewer adverse effects, have gained attention as potential therapeutic agents. With the advancement of computational techniques, virtual screening enables rapid identification of promising bioactive compounds, while ADMET evaluation helps assess their pharmacokinetic and safety profiles at an early stage. Together, these approaches offer an efficient strategy for discovering and validating herbal compounds for the management of PCOS. **Method:** The study involves the identification of key molecular targets associated with Polycystic Ovary Syndrome (PCOS) through literature and database analysis, followed by the selection of herbal constituents reported to have therapeutic relevance. The chemical structures of these compounds are retrieved from standard databases and prepared for analysis. Virtual screening is then performed using molecular docking techniques to evaluate the binding affinity of the selected compounds with the target proteins. Top-ranking compounds are further analysed for interaction patterns and stability. Subsequently, ADMET evaluation is carried out using computational tools to predict their absorption, distribution, metabolism, excretion, and toxicity profiles. Compounds showing strong binding affinity along with favourable ADMET properties are identified as potential therapeutic candidates for PCOS. **Result:** The virtual screening results showed that several herbal constituents had strong binding affinity toward PCOS-related target proteins, indicating good interaction potential. The top compounds demonstrated stable binding with key interactions such as hydrogen bonds. ADMET analysis further revealed that these compounds possess favourable pharmacokinetic properties with low toxicity. Overall, the study identified promising herbal molecules that could be considered for further investigation as potential therapeutic agents for PCOS. **Conclusion:** The study concludes that selected herbal constituents show promising potential as therapeutic agents for the management of PCOS based on their strong binding interactions with target proteins and favourable ADMET profiles. The integration of virtual screening and pharmacokinetic evaluation proved to be an efficient approach for identifying safe and effective candidates. These findings support the potential of plant-derived compounds in PCOS treatment; however, further experimental and clinical studies are necessary to confirm their efficacy and safety.

KEYWORDS: Polycystic Ovary Syndrome (PCOS), Herbal Constituents, Virtual Screening, ADMET Evaluation.

INTRODUCTION

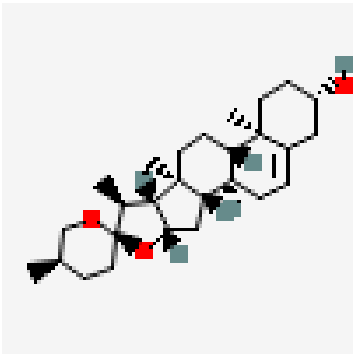
Polycystic Ovary Syndrome (PCOS) is a common hormonal disorder affecting women during their reproductive years, characterized by irregular ovulation, excess androgen levels, and the presence of multiple ovarian cysts. It is frequently linked with metabolic complications such as insulin resistance, obesity, and an increased risk of developing type 2 diabetes and cardiovascular diseases. Due to its complex and multifactorial nature, involving hormonal, genetic, and lifestyle factors, effective management of PCOS remains a significant challenge.

Current treatment strategies mainly aim to control symptoms using hormonal medications and insulin-sensitizing drugs, but these approaches may produce unwanted side effects and are not always effective in the long term. This has increased interest in exploring herbal constituents as alternative therapeutic options, as they are known to possess multiple pharmacological activities with comparatively fewer adverse effects. Many phytochemicals exhibit antioxidant, anti-inflammatory, and endocrine-modulating properties that may help in managing PCOS.

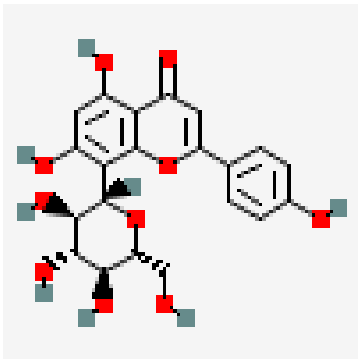
Advancements in computational drug discovery have introduced techniques such as virtual screening and molecular docking, which allow rapid evaluation of bioactive compounds by predicting their interaction with specific targets. Furthermore, ADMET analysis helps in assessing the pharmacokinetic and toxicity profiles of these compounds at an early stage. Combining these approaches provides a systematic and efficient method for identifying potential herbal candidates for the treatment of PCOS.

Drug Molecules

(1) Androgen Binding Drug Molecules

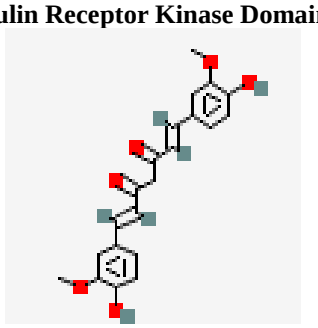


DIOSGENIN

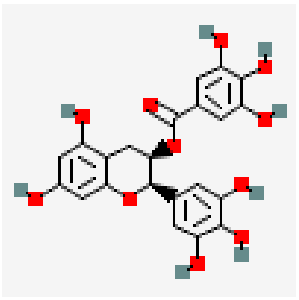


VITEXIN

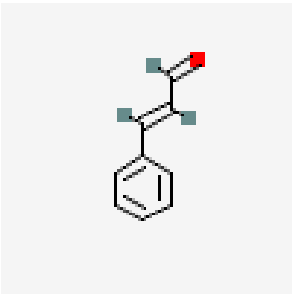
(2) Insulin Receptor Kinase Domain Drugs



CURCUMIN

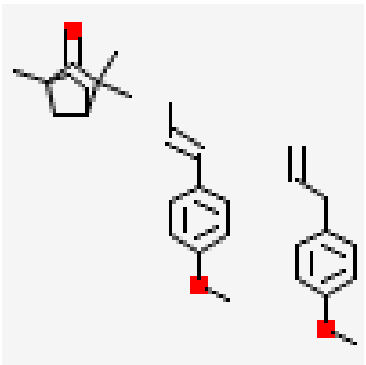


EPIGALLOCATECHIN



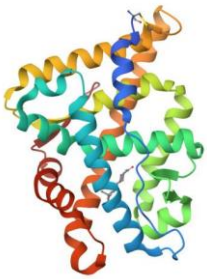
CINNAMALDEHYDE

(3) Reproductive Health Enhancer



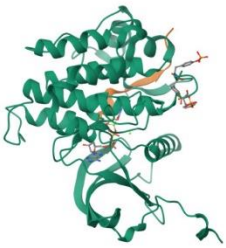
FOENICULUM VULGARE (FENNEL)

Receptors



ANDROGEN RECEPTOR

FSH RECEPTOR



INSULIN RECEPTOR

METHADOLOGY

Study Design and Approach

The present research was conducted using a computational (in silico) drug discovery approach to identify potential herbal constituents for the treatment of Polycystic Ovary Syndrome (PCOS). This approach integrates virtual screening, ADMET analysis to evaluate both the biological activity and safety profile of selected compounds. The overall workflow was designed to systematically filter and identify promising lead molecules from a pool of phytochemicals.

2. Identification of Therapeutic Targets

Proteins involved in the development and progression of PCOS were identified through an extensive literature survey of research articles and scientific databases. These targets were selected based on their roles in key pathological processes such as insulin resistance, androgen excess, follicular development, and ovarian dysfunction. Selecting appropriate targets is critical to ensure that the screened compounds are relevant to disease management.

3. Retrieval and Selection of Protein Structures

The three-dimensional structures of selected target proteins were retrieved from the RCSB Protein Data Bank (PDB). Preference was given to structures determined by X-ray crystallography with high resolution and completeness. Proteins lacking missing residues or structural errors were prioritized to enhance the reliability of docking results.

4. Protein Preparation and Optimization

The obtained protein structures were prepared using AutoDock Tools. Preparation involved several steps, including removal of crystallographic water molecules, addition of polar hydrogen atoms, correction of bond orders, and assignment of Kollman charges. These steps are essential to ensure proper interaction between the protein and ligands during docking simulations.

5. Selection of Herbal Compounds

A diverse set of herbal constituents was selected based on their reported biological activities relevant to PCOS, such as antioxidant, anti-inflammatory, anti-diabetic, and endocrine-modulating effects. The selection was supported by ethnopharmacological data and published scientific studies, ensuring that the chosen compounds have potential therapeutic significance.

6. Ligand Retrieval and Structural Preparation

The chemical structures of selected phytochemicals were obtained from the PubChem. These structures were subjected to energy minimization and structural optimization to achieve stable conformations. Using Open Babel, the compounds were converted into appropriate file formats (such as PDBQT) compatible with docking software. Proper ligand preparation ensures accurate prediction of binding interactions.

7. Active Site Identification

The active sites of target proteins were identified based on available literature, co-crystallized ligands, or computational prediction methods. Defining the active site is crucial for guiding the docking process, as it determines the region where ligands are most likely to bind and exert their biological effect.

8. Virtual Screening

Virtual screening was performed using AutoDock Vina to evaluate the binding affinity between ligands and target proteins. A grid box was set around the active site to restrict the docking search space. Multiple docking simulations were conducted, and binding energies were calculated for each ligand–protein interaction. Lower binding energy values indicate stronger and more stable interactions.

9. Post-Docking Analysis and Visualization

The docking results were further analysed using Discovery Studio Visualizer. Interaction analysis included identification of hydrogen bonds, hydrophobic interactions, electrostatic interactions, and van der Waals forces. Visualization of ligand–protein complexes helped in understanding the binding orientation and stability of the compounds within the active site.

10. ADMET Prediction and Drug-Likeness Evaluation

To assess the pharmacokinetic properties and safety of the selected compounds, ADMET analysis was performed using SwissADME and pkCSM. Parameters such as gastrointestinal absorption, blood–brain barrier permeability, metabolic stability, excretion rate, and

toxicity (including hepatotoxicity and carcinogenicity) were evaluated. Drug-likeness criteria, such as Lipinski's Rule of Five, were also considered to determine the suitability of compounds as oral drugs.

11. Lead Identification and Selection Criteria

Based on docking scores, interaction patterns, and ADMET profiles, the most promising compounds were selected as lead candidates. Compounds showing strong binding affinity, stable molecular interactions, good bioavailability, and low toxicity were prioritized for further study.

RESULT

The virtual screening of selected herbal constituents against key protein targets associated with Polycystic Ovary Syndrome (PCOS) produced a range of binding affinities, indicating varying degrees of interaction between the ligands and target proteins. Among the screened compounds, a group of phytochemicals demonstrated comparatively lower binding energy values, suggesting a stronger and more stable interaction within the active sites of the selected proteins. These results indicate that certain herbal constituents have a higher likelihood of modulating the activity of proteins involved in PCOS pathophysiology.

Further examination of the docking poses revealed that the top-ranking compounds were well accommodated within the binding pockets of the target proteins. These compounds formed multiple stabilizing interactions, including hydrogen bonds with key amino acid residues, as well as hydrophobic and van der Waals interactions that contributed to the overall stability of the ligand–protein complex. The spatial orientation and alignment of these ligands within the active site suggested a favourable binding conformation, which is essential for effective biological activity.

LIGAND	RECEPTOR	BINDING AFFINITY (Kcal/mol)	MODE	RMSD lower bound	RMSD upper bound
Berberine	Androgen	-7.8	0	0.0	0.0
Vitexin	Androgen	-8.2	0	0.0	0.0
Diosgenin	Androgen	-8.1	0	0.0	0.0
Curcumin	Insulin receptor kinase domain	-7.2	0	0.0	0.0
Epigallocatechin	Insulin receptor kinase domain	-7.5	0	0.0	0.0
Cinnamaldehyde	Insulin receptor kinase domain	-5.5	0	0.0	0.0
Trigonelline	Insulin receptor kinase domain	-5.0	0	0.0	0.0
Foeniculum vulgare	FSH Receptor Extracellular domain	-4.4	0	0.0	0.0

Comparative analysis among the screened compounds showed that only a limited number consistently exhibited strong binding across multiple targets, indicating their potential as multi-target agents. This is particularly important in a complex disorder like PCOS, where multiple biological pathways are involved. The ability of certain phytochemicals to interact with more than one target enhances their therapeutic relevance.

The ADMET analysis provided additional insights into the pharmacokinetic behaviour and safety profile of the selected compounds. Most of the top-performing molecules demonstrated good predicted gastrointestinal absorption, indicating their potential for oral bioavailability. Distribution parameters suggested an acceptable ability to reach target tissues, while metabolism predictions indicated moderate stability with a lower likelihood of rapid degradation. Excretion profiles were found to be within acceptable limits, supporting their suitability for further development.

Toxicity assessment revealed that the majority of the selected compounds are likely to be non-toxic, with low risk of hepatotoxicity, mutagenicity, or carcinogenicity. Furthermore, drug-likeness evaluation indicated that several compounds complied with established criteria such as Lipinski's Rule of Five, suggesting that they possess favourable physicochemical properties for drug development.

In summary, the integrated analysis of molecular docking and ADMET profiling identified a subset of herbal constituents with strong binding affinity, stable interaction patterns, and promising pharmacokinetic and safety characteristics. These findings suggest that the identified compounds may serve as potential lead molecules for the development of novel therapeutic agents for PCOS, warranting further validation through experimental studies.

DISCUSSION

The present study employed an in-silico approach to explore the therapeutic potential of herbal constituents against key targets involved in Polycystic Ovary Syndrome (PCOS). The results of virtual screening and molecular docking indicated that several phytochemicals possess strong binding affinity toward selected proteins, suggesting their ability to modulate pathways associated

with hormonal imbalance and metabolic dysfunction. These findings are significant, as PCOS is a multifactorial disorder requiring multi-target therapeutic strategies.

The interaction analysis revealed that the top-performing compounds formed stable complexes with target proteins through hydrogen bonding and hydrophobic interactions. Such interactions are crucial for maintaining ligand stability within the active site and enhancing biological activity. The ability of certain compounds to exhibit strong binding across multiple targets highlights their potential as multi-functional agents, which is particularly advantageous in managing complex conditions like PCOS that involve interconnected biological pathways.

The ADMET evaluation further supported the suitability of these compounds by demonstrating favourable pharmacokinetic properties, including good absorption and acceptable metabolic stability. Additionally, the predicted low toxicity profiles suggest that these herbal constituents may offer safer alternatives compared to conventional therapies, which are often associated with side effects and long-term complications. This aligns with the growing interest in plant-based compounds for safer and more sustainable drug development.

Despite these promising findings, it is important to acknowledge the limitations of the study. Since the analysis is entirely computational, the predicted interactions and pharmacokinetic properties require validation through experimental methods. In vitro and in vivo studies are necessary to confirm the biological activity, efficacy, and safety of the identified compounds in real biological systems.

Overall, the study demonstrates that combining virtual screening with ADMET analysis is an effective strategy for identifying potential herbal therapeutics for PCOS. The results provide a strong foundation for further research and support the potential role of phytochemicals in the development of novel, multi-target treatment options for this complex disorder.

CONCLUSION

The present study demonstrates that selected herbal constituents possess promising potential as therapeutic agents for the management of Polycystic Ovary Syndrome (PCOS). Through virtual screening and molecular docking, several compounds showed strong and stable interactions with key target proteins, indicating their ability to influence important pathways involved in the disorder. The ADMET analysis further supported these findings by revealing favourable pharmacokinetic properties and low predicted toxicity, suggesting their suitability as drug candidates.

Overall, the integration of computational techniques proved to be an efficient and cost-effective approach for identifying potential lead molecules from natural sources. While the results are encouraging, further experimental validation through in vitro and in vivo studies is necessary to confirm their efficacy and safety. These findings provide a valuable basis for future research aimed at developing safe, effective, and plant-based therapies for PCOS.

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