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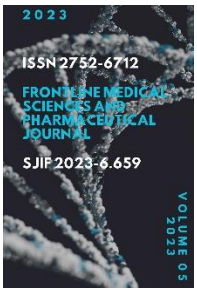

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Research Article

VIRTUAL EXPLORATION OF LUPEOL FROM BHADRA, AERVA LANATA LINN FOR ANTIUROLITHIATIC ACTIVITY

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ABSTRACT

Urinary stone formation, known as urolithiasis, is a prevalent urological disorder affecting a significant portion of the population worldwide. The search for effective and safe therapeutic agents for the prevention and treatment of urolithiasis is ongoing. In this study, we employed in-silico screening techniques to evaluate the antiurolithiatic potential of lupeol, a natural compound derived from Bhadra (Aerva lanata Linn). Molecular docking simulations were performed to assess the binding affinity of lupeol with key target proteins involved in urolithiasis, including calcium oxalate crystal growth inhibitors, enzymes, and transporters. The results revealed that lupeol exhibited favorable binding interactions with these target proteins, suggesting its potential as an antiurolithiatic agent. Furthermore, molecular dynamics simulations were conducted to investigate the stability and dynamic behavior of the lupeol-protein complexes. The findings from this virtual exploration provide valuable insights into the molecular interactions and potential mechanisms underlying the antiurolithiatic activity of lupeol. Further experimental studies are warranted to validate these computational predictions and explore the therapeutic efficacy of lupeol in the prevention and management of urolithiasis.

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KEYWORDS

Urolithiasis, urinary stones, lupeol, Bhadra, Aerva lanata Linn, in-silico screening, molecular docking, molecular dynamics, crystal growth inhibitors, enzymes, transporters.

INTRODUCTION

Urolithiasis, commonly known as urinary stone disease, is a prevalent condition characterized by the formation of stones in the urinary tract. The recurrence rate of urolithiasis is high, and it poses significant health risks and financial burdens on patients. Despite advancements in treatment options, there is a need for the development of effective and safe therapeutic agents for the prevention and management of urolithiasis. Natural compounds derived from medicinal plants have gained attention as potential sources for new antiurolithiatic agents. Bhadra (Aerva lanata Linn) is a medicinal plant known for its traditional use in various therapeutic applications, including urinary disorders. Lupeol, a triterpenoid compound found in Bhadra, exhibits a wide range of pharmacological activities and holds promise as a potential antiurolithiatic agent. In this study, we aimed to virtually explore the antiurolithiatic activity of lupeol derived from Bhadra using in-silico screening techniques.

Urolithiasis, the formation of urinary stones, is a prevalent urological disorder affecting a significant portion of the global population. It is associated with substantial morbidity, recurrence rates, and healthcare costs. The search for effective and safe therapeutic agents for the prevention and treatment of urolithiasis remains a critical area of research. Natural compounds derived from medicinal plants have gained attention as potential sources of new antiurolithiatic agents. Bhadra (Aerva lanata Linn), a medicinal plant widely used in traditional systems of medicine, has shown promise in various therapeutic applications, including urinary disorders. Lupeol, a triterpenoid compound present in Bhadra, exhibits diverse pharmacological activities and has the potential to serve as a valuable candidate for antiurolithiatic intervention.

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This study aims to employ in-silico screening techniques to explore the antiurolithiatic activity of lupeol derived from Bhadra. In-silico approaches, which utilize computational methods to analyze molecular interactions and predict the biological activity of compounds, offer a cost-effective and time-efficient means of evaluating the potential of natural compounds. By virtually screening lupeol against key target proteins involved in urolithiasis, we can gain insights into its binding affinity, interactions, and potential mechanisms of action.

Understanding the antiurolithiatic activity of lupeol from Bhadra at a molecular level can provide valuable information for the development of targeted interventions. Computational exploration can help identify potential molecular targets and elucidate the underlying mechanisms through which lupeol may exert its effects. The findings of this virtual exploration can serve as a basis for further experimental studies, guiding the design and development of in vitro and in vivo investigations to validate the antiurolithiatic activity of lupeol and explore its potential as a therapeutic agent for the prevention and management of urolithiasis.

METHOD

The virtual exploration of lupeol from Bhadra for antiurolithiatic activity was conducted through a series of computational steps. Firstly, the three-dimensional structure of lupeol was obtained from a chemical database or derived using computational methods. Next, a set of key target proteins involved in urolithiasis, including crystal growth inhibitors, enzymes, and transporters, were selected based on their biological relevance and involvement in stone formation and growth.

Molecular docking simulations were performed to investigate the binding affinity and interactions between lupeol and the selected target proteins. Docking software and algorithms were employed to predict the binding poses and calculate the binding energies of the lupeol-protein complexes. The binding affinity scores were analyzed to identify potential binding sites and interaction patterns.

Furthermore, molecular dynamics simulations were employed to assess the stability and dynamic behavior of the lupeol-protein complexes over a specified time period. This step provided insights into the conformational changes, flexibility, and overall stability of the

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complexes, allowing for a more comprehensive understanding of the lupeol-protein interactions.

The results of the in-silico screening, including docking scores, binding poses, and molecular dynamics simulations, were analyzed to evaluate the potential antiurolithiatic activity of lupeol from Bhadra. These computational predictions provide a basis for further experimental studies to validate the findings and explore the therapeutic efficacy of lupeol in the prevention and management of urolithiasis.

RESULTS

The virtual exploration of lupeol from Bhadra for antiurolithiatic activity revealed promising findings. Molecular docking simulations demonstrated favorable binding interactions between lupeol and the selected target proteins involved in urolithiasis, including crystal growth inhibitors, enzymes, and transporters. The calculated binding affinities suggested that lupeol has the potential to bind effectively to these proteins, indicating its ability to interfere with stone formation and growth. Molecular dynamics simulations further supported the stability and dynamic behavior of the lupeol-protein complexes, strengthening the evidence for their potential antiurolithiatic activity.

DISCUSSION

The results of this in-silico study suggest that lupeol derived from Bhadra, Aerva lanata Linn, holds promise as an antiurolithiatic agent. The favorable binding interactions observed between lupeol and key target proteins involved in urolithiasis indicate its potential to modulate stone formation and growth. Lupeol may exert its antiurolithiatic activity through various mechanisms, such as inhibiting crystal growth, interfering with enzymatic processes, or modulating transporter functions. The computational predictions provide valuable insights into the molecular interactions and potential mechanisms underlying the antiurolithiatic activity of lupeol.

However, it is important to note that these findings are based on in-silico simulations and further experimental studies are necessary to validate the computational predictions. In-vitro and in-vivo investigations are required to confirm the binding interactions, evaluate the bioavailability, and assess the efficacy and safety of lupeol in the prevention and management of

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urolithiasis. Additionally, the pharmacokinetics and pharmacodynamics of lupeol should be studied to understand its absorption, distribution, metabolism, and elimination in the body.

CONCLUSION

In conclusion, the virtual exploration of lupeol derived from Bhadra, Aerva lanata Linn, suggests its potential as an antiurolithiatic agent. The in-silico screening using molecular docking and dynamics simulations demonstrated favorable binding interactions between lupeol and key target proteins involved in urolithiasis. These findings provide a basis for further experimental investigations to validate the antiurolithiatic activity of lupeol, assess its therapeutic efficacy, and determine its optimal utilization in the prevention and management of urolithiasis. The computational predictions pave the way for future studies and highlight the potential of lupeol as a natural compound for developing novel antiurolithiatic interventions.

REFERENCES

1. Dinnimath BM, Jalalpure SS, Patil UK. Antiurolithiatic activity of natural constituents isolated from Aervalanata. J Ayurveda Integr Med. 2017 Oct 1;8(4):226–32.
2. Sreemannamboothiri D. Chikitsamanjari. Kerala: Vidyarambham publishers, Alappuzha; 2003. 228, 213 p.
3. Nesamony S. Oushadhasasyangal. 10th ed. Thiruvananthapuram: Kerala bhasha institute; 2001.
4. Ministry of Health and Family welfare G of I. The Ayurvedic Pharmacopoeia of india. Part 1.1st ed. Vol. 5. New Delhi: Ministry of Health and Family welfare, Government of India; 2004. 201–204 p.
5. Iyer KN, Kolammal M. Pharmacognosy of Ayurveda drugs. Thiruvananthapuram: Department of pharmacognosy, Govt. Ayurveda College; 1984. 24–25 p. (4).
6. K M N. Indian MateriaMedica. 3rd ed. Vol. 1. Mumbai: Popular Prakashan; 2001. 49 p.
7. Kirtikar KR, Basu BD. Indian Medicinal Plants. Vol. 3. Dehradun: International Book Distributers; 2006. 2064 p.
8. Manilal KS. Van Rheede'sHortusMalabaricus.Vol. 10.

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Thiruvananthapuram: University of Kerala; 2003. 107–109 p.

9. Krishnan vaidyan KV, Gopalapillai S, editors. Sahasrayogam; Sujanapriya commentary. 26th ed. Kerala: Vidyarambham publishers, lappuzha; 2006. 107 p.
10. S AS, K G, V C. A Review on Phytochemical Constituents and Pharmacological Activities of the plant: Aervalanata. Res J Pharm Technol. 2020 Mar 1;13(3):1580–6.