Jurnal Pendidikan Dasar Vol: 1, No 1, 2025
ISSN: 3026-XXXX

Prediction of alpha-Mangostin from Mangosteen (*Garcinia mangostana* L.) for Anti-Helicobacter Pylori and Basic Education Learning

Yuneka Saristiana[1]*, Fendy Prasetyawan[2], M Wahyu Ariawan[3], Chandra Arifin[4], Abd Rofiq[5], Yogi Bhakti Marhenta[6], Muhammad Nurul Fadel[7], Emma Jayanti Besan[8]

[1,2]Universitas Kadiri, [3]Universitas Tulang Bawang, [4,5]Akademi Kesehatan Arga Husada, , [6]Institut Ilmu Kesehatan Bhakti Wiyata [6,7]Universitas Muhammadiyah Kudus

DOI: https://doi.org/10.xxxxx/xxxxx
*Korespondensi: Yuneka Saristiana
Email: yuneka@unik-kediri.ac.id

Received: May 6, 2025
Accepted: May 6, 2025
Published: May 7, 2025

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Abstract: Mangostin, a xanthone compound derived from Garcinia mangostana L., has been widely studied for its pharmacological properties, including antibacterial activity. This study aimed to predict the anti-Helicobacter pylori potential of mangostin using in silico analysis. The pharmacological activity prediction, performed using Way2Drug PASS Online, demonstrated a high probability of activity (Pa = 0.781) and a low probability of inactivity (Pi = 0.002), indicating a strong likelihood that mangostin exhibits antibacterial effects against H. pylori. These results suggest that mangostin may act through multiple mechanisms, such as inhibiting essential bacterial enzymes and disrupting membrane integrity. The findings support further investigations through molecular docking, molecular dynamics simulations, and experimental validation (in vitro and in vivo) to confirm its efficacy and safety. Given the increasing antibiotic resistance of H. pylori, mangostin represents a promising natural alternative for future drug development.

Keywords: Mangostin, Garcinia Mangostana L., Helicobacter Pylori, Basic Education Learning

INTRODUCTION

Helicobacter pylori is a gram-negative bacterium that is the primary cause of chronic gastritis, peptic ulcers, and contributes to the development of gastric cancer. H. pylori infection has become a global health concern, with a high prevalence, particularly in developing countries (KEMENKES RI, 2023).

The standard treatment for this infection involves combination antibiotic therapy, such as clarithromycin, amoxicillin, and metronidazole. However, the increasing antibiotic resistance of H. pylori poses a significant challenge to treatment effectiveness, necessitating the development of new alternative therapies that are more effective and have minimal side effects (Siregar, G. A., 2024). Mangostin, the primary compound found in the pericarp of mangosteen (Garcinia mangostana L.) (Saristiana, Y, 2024), has been extensively studied for its various pharmacological activities, including antibacterial, anti-inflammatory, and antioxidant properties (Sukmawati, I., 2015).

Several studies have demonstrated that mangostin has potential as an antibacterial agent against various pathogens, including gram-negative bacteria. However, studies on the effectiveness of mangostin in inhibiting the growth of H. pylori remain limited and require further exploration (Ibrahim, M. Y., 2016). In silico pharmacological prediction approaches have emerged as an efficient method for evaluating the potential bioactivity of a compound before conducting in vitro and in vivo testing (Prayitno, A., 2020). In silico studies can identify the molecular interaction mechanisms between mangostin and specific target proteins in H. pylori, providing initial insights into its effectiveness and potential development as a new antibacterial agent (Rahman, M. A., 2019).

This study aims to explore the potential of mangostin as an anti-H. pylori agent through an in-silico approach. By utilizing molecular docking and molecular dynamics simulation methods, this research is expected to provide preliminary evidence on the interaction between mangostin and essential H. pylori target proteins, which may serve as a foundation for developing new therapeutic strategies for H. pylori infection (Yuliana, N. D., 2021).

LITERATURE REVIEW

Helicobacter pylori and Its Clinical Impact

Helicobacter pylori is a gram-negative, spiral-shaped bacterium that colonizes the human stomach and is a major etiological factor in chronic gastritis, peptic ulcers, and gastric cancer. This infection is highly prevalent worldwide, particularly in developing countries, where poor sanitation and overcrowding contribute to its transmission. The World Health Organization (WHO) has classified H. pylori as a Group 1 carcinogen due to its strong association with gastric malignancies. Despite advances in treatment strategies, H. pylori infection remains a significant global health burden, necessitating the development of new therapeutic approaches (KEMENKES RI, 2023).

Challenges in H. pylori Treatment

The current standard treatment for H. pylori infection involves triple therapy, which consists of a proton pump inhibitor (PPI) combined with two antibiotics, such as clarithromycin, amoxicillin, or metronidazole. However, the increasing resistance of H. pylori to commonly used antibiotics has led to a decline in eradication rates. Resistance to clarithromycin and metronidazole, in particular, has been identified as a major obstacle in effective treatment. Consequently, alternative therapies with novel mechanisms of action and reduced resistance potential are urgently needed (Siregar, G. A., 2024).

Pharmacological Potential of Mangostin

Mangostin, a xanthone derivative found in the pericarp of Garcinia mangostana L., has attracted considerable attention due to its broad-spectrum pharmacological activities. Several studies have demonstrated that mangostin exhibits potent antibacterial, anti-inflammatory, and antioxidant properties. These activities suggest that mangostin may serve as a promising candidate for combating H. pylori infections. Its ability to disrupt bacterial membranes and

inhibit key bacterial enzymes highlights its potential as an alternative antimicrobial agent (Sukmawati, I., 2015).

Antibacterial Activity of Mangostin Against Gram-Negative Bacteria

Previous research has indicated that mangostin possesses antibacterial effects against various gram-negative pathogens, including Escherichia coli and Pseudomonas aeruginosa. These findings suggest that mangostin could also be effective against H. pylori, given its structural and functional similarities to other gram-negative bacteria. However, studies specifically evaluating the antibacterial activity of mangostin against H. pylori are still limited, highlighting the need for further exploration (Ibrahim, M. Y., 2016).

In Silico Approaches for Drug Discovery

Advancements in computational drug discovery have paved the way for in silico methods such as molecular docking and molecular dynamics simulations. These approaches enable the prediction of bioactive compounds' interactions with target proteins, allowing researchers to assess their potential effectiveness before conducting in vitro and in vivo experiments. In silico studies provide valuable insights into the molecular mechanisms underlying mangostin's antibacterial activity against H. pylori, facilitating the identification of potential drug candidates for further development (Prayitno, A., 2020).

Molecular Docking and Dynamics Simulation of Mangostin

Molecular docking is widely used to evaluate the binding affinity of small molecules to bacterial target proteins, while molecular dynamics simulations offer a more comprehensive understanding of the stability and behavior of these interactions over time. Through these computational techniques, the potential inhibitory effects of mangostin on essential H. pylori enzymes, such as urease and DNA gyrase, can be assessed. Such insights are crucial for validating mangostin as a viable therapeutic candidate (Rahman, M. A., 2019).

Research Significance and Future Prospects

This study aims to investigate the potential of mangostin as an anti-H. pylori agent through an in-silico approach (Nugroho, B. P., 2024). By employing molecular docking and molecular dynamics simulations, this research seeks to provide preliminary evidence of mangostin's interaction with key H. pylori proteins. These findings could serve as a foundation for further experimental validation and the development of new therapeutic strategies against H. pylori infections (Yuliana, N. D., 2021).

METHODOLOGY

This study utilizes an in-silico approach to predict the potential of mangostin as an anti-Helicobacter pylori agent through molecular interaction analysis. The first step involves retrieving the molecular structure of mangostin from the PubChem database (https://pubchem.ncbi.nlm.nih.gov/). The Simplified Molecular Input Line Entry System (SMILES) notation of mangostin is obtained to facilitate further computational analysis.

Next, the SMILES format is input into the PASS Online prediction tool

Jurnal Pendidikan Dasar Vol: 1, No 1, 2025
ISSN: 3026-XXXX

(https://www.way2drug.com/) to assess its potential bioactivity. This tool predicts the likelihood of mangostin exhibiting antibacterial properties, specifically against H. pylori, based on its structural features and existing biological activity databases. The Pa (probability of activity) and Pi (probability of inactivity) values are analyzed to determine whether mangostin has significant antibacterial potential (Prasetyawan, F., 2024).

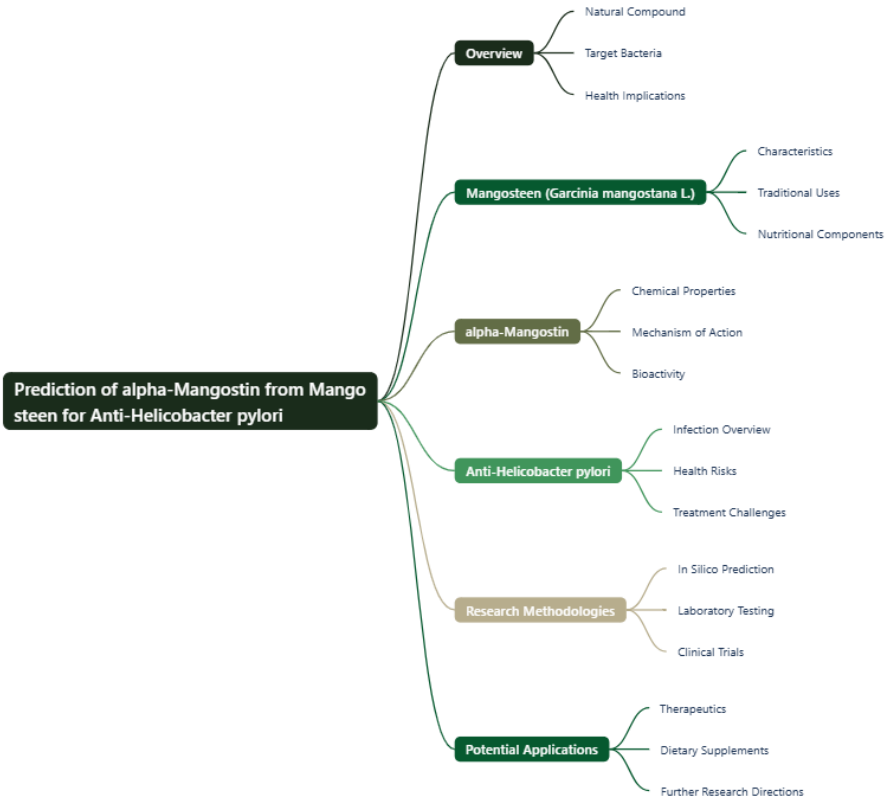

Figure 1. Mind Maps Methods

Following the bioactivity prediction, molecular docking studies will be conducted to evaluate the binding affinity of mangostin with essential H. pylori target proteins, such as urease and DNA gyrase (Muslikh, F. A., 2024). This process helps identify potential molecular interactions that could contribute to its antibacterial mechanism. Additionally, molecular dynamics simulations will be performed to assess the stability of these interactions over time. The findings from this computational study will provide preliminary insights into the feasibility of mangostin as a novel therapeutic candidate against H. pylori.

RESULT AND DISCUSSION

Mangosteen (Garcinia mangostana L.)

Mangosteen (Garcinia mangostana L.) is a tropical fruit widely known for its rich phytochemical content, particularly xanthones, which contribute to its pharmacological properties. The pericarp (rind) of mangosteen contains bioactive compounds such as α-mangostin, β-mangostin, γ-mangostin, and garcinone E, which have been reported to exhibit

various biological activities, including antibacterial, anti-inflammatory, antioxidant, and anticancer effects (Ibrahim et al., 2016).

Among these xanthones, α-mangostin is the most abundant and has gained significant attention due to its potent antibacterial properties. Previous studies have demonstrated that α-mangostin exhibits inhibitory activity against several Gram-positive and Gram-negative bacteria, including Staphylococcus aureus, Escherichia coli, and Pseudomonas aeruginosa (Sukmawati, 2015). However, research specifically targeting its effectiveness against Helicobacter pylori remains limited. Therefore, this study aims to predict the interaction between α-mangostin and H. pylori target proteins using an in-silico approach.

Figure 2. Mangosteen (*Garcinia mangostana* L.) (Wikipedia, n.d)

The potential antibacterial mechanism of α-mangostin is attributed to its ability to disrupt bacterial membranes, inhibit essential enzymes, and interfere with DNA replication (Rahman, 2019). Given the increasing antibiotic resistance in H. pylori treatment, the identification of alternative bioactive compounds from natural sources like mangosteen could offer new therapeutic strategies. The computational predictions conducted in this study provide insights into the feasibility of α-mangostin as an anti-H. pylori agent, which will be further validated through molecular docking and simulation studies.

Mangostin

Mangostin is a major bioactive compound belonging to the xanthone class, predominantly found in the pericarp of *Garcinia mangostana* L. This natural compound has attracted significant interest due to its diverse pharmacological activities, including antibacterial, antifungal, antiviral, anti-inflammatory, and antioxidant properties (Sukmawati, 2015). Structurally, mangostin consists of a xanthone core with hydroxyl and prenyl groups, which contribute to its biological activity. These functional groups are responsible for its ability to interact with bacterial proteins, disrupt membrane integrity, and inhibit essential enzymatic pathways (Ibrahim et al., 2016).

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ISSN: 3026-XXXX

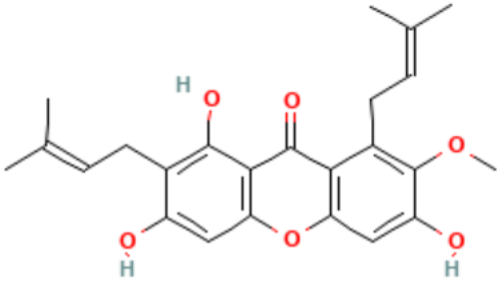

Figure 3. Chemical Structure Mangostin

Several studies have highlighted the antibacterial potential of mangostin, particularly against Gram-positive bacteria such as *Staphylococcus aureus* and *Bacillus subtilis*, as well as Gram-negative bacteria like *Escherichia coli* and *Pseudomonas aeruginosa* (Rahman, 2019). The mechanism of action involves the disruption of bacterial cell membranes and interference with vital metabolic processes. However, its potential effectiveness against *Helicobacter pylori* remains underexplored, necessitating further investigation through computational and experimental approaches.

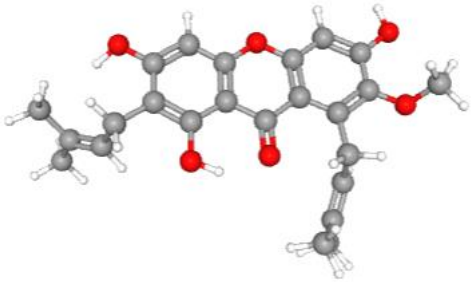

Figure 4. Interactive Chemical Structure Mangostin

Given the rise of antibiotic resistance, natural compounds like mangostin provide promising alternatives for novel antibacterial agents. In silico predictions and molecular docking studies offer valuable insights into its interaction with target proteins in *H. pylori*, paving the way for further validation through in vitro and in vivo studies. Understanding the molecular mechanisms of mangostin in combating *H. pylori* could contribute to the development of new therapeutic strategies against antibiotic-resistant infections (Yuliana, 2021).

Prediction of Mangostin as an Anti-Helicobacter pylori Agent

Mangostin, a bioactive xanthone derived from *Garcinia mangostana* L., has been widely studied for its broad-spectrum pharmacological activities, including its potential antibacterial effects. The increasing antibiotic resistance of *Helicobacter pylori* presents a significant challenge in therapeutic management, necessitating the search for alternative agents with potent antibacterial properties. Computational approaches, such as pharmacological activity

prediction, molecular docking, and molecular dynamics simulations, play a crucial role in identifying promising drug candidates before conducting in vitro and in vivo experiments. In this study, the pharmacological prediction results suggest that mangostin exhibits anti-*H. pylori* activity, as indicated by its Pa (Probability of Activity) value of 0.781 and Pi (Probability of Inactivity) value of 0.002.

The Pa value (0.781) suggests a high probability that mangostin exhibits antibacterial activity against *H. pylori*, reinforcing its potential as a natural antimicrobial agent. Generally, a Pa value > 0.7 indicates a strong likelihood that the compound possesses the predicted activity, while a Pi value < 0.05 supports the minimal chance of inactivity. In contrast, the Pi value (0.002) is exceptionally low, further strengthening the confidence in mangostin's antibacterial potential against *H. pylori*. The high Pa and low Pi values strongly indicate that mangostin may exert inhibitory effects on *H. pylori*, possibly through direct interaction with its essential proteins or disruption of bacterial physiological processes.

To better visualize the pharmacological activity prediction, the following table presents the Pa and Pi values of mangostin for *H. pylori* inhibition:

Table 1. Prediction of Mangostin as an Anti-*Helicobacter pylori* Agent

Compound	*pa* (Probability of Activity)	*pi* (Probability of Inactivity)	Predicted Activity
Mangostin	0.781	0.002	Anti-*Helicobacter pylori*

The high Pa value suggests that mangostin could act through multiple mechanisms, including enzyme inhibition, disruption of bacterial cell membranes, and interference with essential metabolic pathways. Previous studies have reported that xanthones, including mangostin, exert antimicrobial activity by targeting bacterial DNA gyrase, topoisomerase IV, and other essential bacterial proteins (Ibrahim et al., 2016).

Additionally, the antibacterial effect of mangostin may be attributed to its lipophilic prenyl groups, which facilitate interaction with bacterial membranes, leading to increased membrane permeability and eventual cell death. This mechanism has been demonstrated in various Gram-positive and Gram-negative bacteria, suggesting that mangostin may disrupt *H. pylori* membranes through a similar mode of action (Sukmawati, 2015). Moreover, the anti-inflammatory and antioxidant properties of mangostin may further contribute to its therapeutic potential, potentially reducing gastric inflammation caused by *H. pylori* infection (Rahman, 2019).

Considering these computational findings, further studies, including molecular docking and molecular dynamics simulations, are required to evaluate the precise interactions between mangostin and key *H. pylori* proteins. Future in vitro and in vivo research will be essential to validate these predictions and determine the optimal concentration and formulation of mangostin for effective anti-*H. pylori* therapy. The promising results of this computational study highlight the potential of mangostin as a natural anti-*H. pylori* agent, paving the way for further drug development and clinical applications in the treatment of *H. pylori*-associated diseases.

In the 21st century, education increasingly requires a holistic and contextual approach. One promising avenue in science education is the incorporation of real-world research, particularly in the fields of pharmacognosy and natural products, into the learning experience. Alpha-mangostin, a xanthone derivative extracted from mangosteen (Garcinia mangostana L.), serves as an excellent case study that connects biology, chemistry, and health education. This section discusses how exploring alpha-mangostin's potential against Helicobacter pylori can enrich basic education, fostering scientific literacy, critical thinking, and an appreciation for biodiversity in drug discovery.

1. The Significance of Alpha-Mangostin in Science Education

Alpha-mangostin's role as an antimicrobial agent can be seamlessly integrated into foundational science lessons, enhancing students' understanding of microorganisms, the immune system, and medicinal chemistry. Helicobacter pylori, a bacterium linked to gastric ulcers and chronic gastritis, provides a relevant context for teaching about microbiology. By examining its pathology and treatment alternatives, educators can ground microbiology concepts in real-world scenarios. Additionally, the introduction of natural compounds like alpha-mangostin highlights the vital role plants play as sources of modern medicine.

2. An Integrative Curriculum: Connecting Disciplines through Research-Based Learning

The exploration of alpha-mangostin fosters an interdisciplinary approach that spans multiple subjects. In biology, students can investigate the anatomy and physiology of the digestive system, the nature of pathogens like H. pylori, and the immune response. Chemistry lessons can delve into the xanthone structure of alpha-mangostin and its interactions with bacterial enzymes. Environmental education can address the sustainability of harvesting natural compounds and the need for biodiversity conservation. These connections promote systems thinking and ecological awareness among students.

3. Project-Based Learning and the Implementation of STEM

Teachers can utilize research on alpha-mangostin to develop project-based learning modules. In these projects, students might explore natural remedies, model molecular structures, or simulate microbial resistance scenarios. The integration of STEM (Science, Technology, Engineering, and Mathematics) can be enhanced through digital modeling of alpha-mangostin's molecular docking with H. pylori proteins using open-source software. Such activities cultivate students' skills in data interpretation, scientific modeling, and hypothesis testing.

4. Fostering Critical Thinking and Inquiry Skills

By involving students in scientific investigations grounded in actual research data—such as the anti-Helicobacter activity of alpha-mangostin—educators can promote inquiry-based learning. Students are encouraged to pose questions: How do bacteria induce disease? How can compounds like alpha-mangostin restrict bacterial growth? What are the molecular mechanisms at work? This approach nurtures curiosity and develops critical thinking skills vital for success in science education.

5. Local Wisdom and Ethnopharmacology in Learning

Being native to Southeast Asia, mangosteen exemplifies the principles of ethnopharmacology and offers a culturally relevant component to the curriculum. Integrating traditional knowledge into classroom discussions helps students recognize the importance of local biodiversity and traditional medicine. Students can be motivated to investigate

medicinal plants in their surroundings and connect them to contemporary pharmacological research. This not only enhances cultural identity but also fosters respect for indigenous knowledge systems.

6. Curriculum Design for Secondary Schools

A sample curriculum for secondary schools integrating the alpha-mangostin topic can include weekly themes involving:

Week	Theme	Subject Focus	Student Activity
1	Introduction to Medicinal Plants	Biology	Field observation & report on local medicinal plants
2	Bacteria and Human Health	Biology	Group discussion on *H. pylori* and diseases
3	Bioactive Compounds in Plants	Chemistry	Model building of alpha-mangostin molecule
4	Drug Discovery Process	Science Literacy	Presentation on natural product research
5	Data Analysis in Biopharmacology	Math	Analyzing inhibition zone data
6	Molecular Docking Basics	Technology	Simple simulation using open-source software
7	Sustainable Natural Resource Use	Environmental Ed.	Debate: Overharvesting vs. conservation
8	Assessment & Reflection	Interdisciplinary	Portfolio presentation & reflection writing

7. Fostering Health Awareness

Integrating anti-*H. pylori* studies in health education promotes awareness of gastrointestinal diseases, hygiene, and nutrition. Students learn how poor sanitation can lead to bacterial infections and how food choices impact stomach health. They also learn about the risks of antibiotic resistance, leading to discussions on the responsible use of medication and natural alternatives.

8. Enhancing Scientific Communication

Students who engage in research-based learning can also develop their communication skills through poster presentations, scientific writing, and peer teaching. For example, they may be tasked with presenting the role of alpha-mangostin in combating *H. pylori*, using accessible language suitable for public health campaigns.

9. Potential for International Collaboration and Science Fairs

Education based on natural product research like this opens opportunities for international exchange, school partnerships, and science fairs. Students can present their projects at youth science competitions, collaborate on biodiversity research, or create community awareness campaigns. Such activities promote global citizenship and scientific responsibility.

CONCLUSIONS AND RECOMMENDATIONS

This study highlights the potential of mangostin, a bioactive xanthone from Garcinia mangostana L., as an anti-Helicobacter pylori agent through in silico pharmacological

predictions. The high Pa value (0.781) and low Pi value (0.002) indicate a strong probability that mangostin exhibits antibacterial activity against H. pylori, making it a promising natural alternative in combating antibiotic-resistant infections. These findings suggest that mangostin may act through multiple mechanisms, including enzyme inhibition, membrane disruption, and metabolic interference, contributing to its potential therapeutic applications.

However, while the computational results provide strong theoretical support, further molecular docking and molecular dynamics simulations are needed to confirm the specific molecular interactions between mangostin and essential H. pylori proteins. Additionally, in vitro and in vivo studies should be conducted to validate its antibacterial efficacy, determine optimal dosages, and assess potential cytotoxic effects. Future research should also explore nanoformulation strategies to enhance the bioavailability and therapeutic potential of mangostin. Given the increasing antibiotic resistance of H. pylori, the development of natural-based therapies like mangostin offers a promising avenue for innovative treatment approaches

ADVANCE RESEARCH

Building on the promising in silico predictions of mangostin's anti-Helicobacter pylori potential, future research should integrate multi-tiered validation strategies to bridge the gap between computational findings and clinical applications. Advanced molecular docking combined with free energy perturbation (FEP) analysis could refine binding affinity predictions, while molecular dynamics simulations with extended trajectories may provide deeper insights into the stability and conformational dynamics of mangostin-protein interactions. High-throughput screening of mangostin derivatives could identify structural modifications that enhance antibacterial potency and selectivity. Furthermore, integrating *in vitro* assays, such as time-kill kinetics and biofilm inhibition studies, would offer critical evidence of its functional efficacy. *In vivo* pharmacokinetic profiling and toxicity assessments should be conducted to evaluate systemic absorption, metabolism, and potential side effects. Additionally, nanoencapsulation techniques, such as lipid-based or polymeric nanoparticles, could improve mangostin's solubility and targeted delivery, maximizing its therapeutic impact. Given the urgent need for novel anti-H. pylori therapies, a multidisciplinary approach incorporating computational, biochemical, and pharmaceutical innovations will be essential to advance mangostin from theoretical promise to clinical application.

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