Performance Optimization and Recovery: Molecular Docking Validation of Indonesian Herbal Compounds for Mitigating Physiological Fatigue in Athletes

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Abstract. Exercise-induced fatigue remains a critical factor limiting athletic performance and recovery. Indonesia's phytopharmaceutical tradition, particularly Jamu, represents a valuable source of bioactive compounds with potential anti-fatigue properties. This study presents a systematic scientific review combined with in silico molecular docking analysis to examine the mechanisms underlying the anti-fatigue effects of selected Indonesian herbal compounds. The review synthesizes current evidence on the pathophysiology of fatigue, including metabolic, oxidative, inflammatory, and neurophysiological pathways, and identifies key medicinal plants such as Curcuma longa, Zingiber officinale, Centella asiatica, and Andrographis paniculata. Major bioactive constituents, including curcumin, gingerol, asiaticoside, and andrographolide, were evaluated for their binding interactions with fatigue-related protein targets. Molecular docking results revealed strong binding affinities (−7.6 to −9.5 kcal/mol) toward key regulators such as TNF-α, Keap1, AMPK, and 5-HT1A. These interactions indicate multiple complementary mechanisms, including modulation of inflammatory responses, attenuation of oxidative stress, regulation of energy metabolism, and stabilization of neurotransmitter activity. The findings highlight the potential of Indonesian herbal compounds as evidence-based candidates for the development of functional nutraceuticals aimed at enhancing athletic performance and accelerating recovery. This integrative approach strengthens the scientific foundation for the application of traditional herbal medicine within contemporary sport science.

Keywords: Exercise-induced fatigue; Molecular docking; Indonesian herbal compounds; Jamu; Athletic performance; Recovery; Anti-fatigue mechanisms.

1 Introduction

Exercise-induced fatigue constitutes a major physiological constraint on performance, limiting an athlete's capacity to sustain optimal intensity and delaying

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effective recovery processes [1]. This condition arises from a complex interaction of central and peripheral mechanisms, including metabolic depletion, accumulation of fatigue-related metabolites, oxidative stress, inflammatory responses, and alterations in neurotransmitter activity [2]. Beyond its immediate impact on performance, fatigue can impair training adaptation and increase susceptibility to injury, thereby necessitating effective, safe, and sustainable recovery strategies [3].

In recent years, growing attention has been directed toward natural and plant-based interventions as alternatives to synthetic ergogenic aids. Indonesia possesses a long-standing phytopharmaceutical tradition, widely recognized through Jamu, which comprises diverse herbal formulations used to promote vitality, endurance, and recovery [4]. These traditional preparations are valued not only for their empirical efficacy but also for their relatively favorable safety profiles, making them promising candidates for integration into modern sport science and functional nutrition [5].

However, despite their widespread use, the scientific basis underlying the anti-fatigue effects of Indonesian herbal medicines remains insufficiently characterized. In particular, there is limited mechanistic evidence linking specific bioactive compounds to physiological pathways associated with fatigue mitigation. Addressing this gap requires a systematic and evidence-based approach that integrates traditional knowledge with contemporary biomedical analysis [6].

This study aims to provide a comprehensive scientific review of exercise-induced fatigue and to evaluate the potential of selected Indonesian herbal compounds in mitigating its effects. The review synthesizes current understanding of fatigue-related mechanisms, encompassing both central and peripheral pathways, and identifies key medicinal plants such as Curcuma longa, Zingiber officinale, Centella asiatica, and Andrographis paniculata. Particular attention is given to their dominant bioactive constituents, including curcumin, gingerol, asiaticoside, and andrographolide, which are associated with antioxidant, anti-inflammatory, and metabolic regulatory functions [7].

To strengthen mechanistic insights, this study incorporates in silico molecular docking analysis to examine the interaction between selected phytochemicals and key protein targets implicated in fatigue, including TNF-α, Keap1, AMPK, and 5-HT1A. These targets play critical roles in regulating inflammation, oxidative balance, energy metabolism, and neurotransmitter activity. The integration of computational validation with literature-based evidence provides a more robust framework for understanding the therapeutic potential of these compounds [8].

Overall, this research is intended to bridge traditional phytotherapy and modern sport science by offering a scientifically grounded perspective on the use of Indonesian herbal medicines for performance optimization and recovery. The findings are expected to support the development of evidence-based nutraceuticals and to inform future preclinical and clinical investigations aimed at enhancing athletic performance through safe and sustainable interventions [9].

2 Material and Methods

This systematic scientific review was conducted to comprehensively analyze the current literature on exercise-induced fatigue, traditional Indonesian *Jamu* and herbal remedies, their bioactive constituents, and their potential molecular mechanisms of action in mitigating fatigue and enhancing athletic performance. The methodological approach encompassed a rigorous multi-stage process of literature search, selection, data extraction, and synthesis, designed to ensure the objectivity and scientific robustness of the review's findings[12].

2.1 Literature Search Strategy

A systematic search of peer-reviewed scientific literature was performed across several major electronic databases, including PubMed, Scopus, Web of Science, Google Scholar, and ScienceDirect. The search strategy employed a combination of relevant keywords and Medical Subject Headings (MeSH) terms, both individually and in combination, to maximize the identification of pertinent studies[13]. Keywords included, but were not limited to: "exercise-induced fatigue," "athletic performance," "Jamu," "traditional Indonesian medicine," "herbal remedies Indonesia," "phytopharmaceuticals," "bioactive compounds," "molecular mechanisms," "central fatigue," "peripheral fatigue," "energy metabolism," "oxidative stress," "inflammation," "HPA axis," "neurotransmitters," "polysaccharides," "terpenoids," "flavonoids," "polyphenols," "molecular docking," "RMSD," and "similarity indices." The search was primarily focused on publications up to the current date (November 2025 - January 2026), with no date restrictions for seminal or highly cited historical works. Indonesian-language publications were also considered, particularly those detailing traditional Jamu formulations, where appropriate and when translated into English[14].

2.2 Inclusion and Exclusion Criteria

Studies were selected for inclusion based on the following criteria: (1) original research articles, review articles, and book chapters published in English or validated Indonesian translation; (2) studies investigating the pathophysiology of exercise-induced fatigue in humans or animal models; (3) studies identifying *Jamu* or Indonesian herbal remedies and their efficacy in mitigating fatigue or enhancing recovery; (4) studies elucidating the chemical composition and bioactive compounds of these remedies; (5) studies exploring the molecular mechanisms of action of these compounds relevant to fatigue, performance, and recovery (antioxidant, anti-inflammatory, energy metabolism modulation, neuroendocrine regulation); and (6) *in silico* or *in vitro* studies that provided data on compound-target interactions (molecular docking scores, RMSD values, similarity indices) with relevance to muscle fatigue markers[15], [16].

Studies were excluded if they: (1) were abstract-only presentations, conference proceedings without full text, or non-peer-reviewed articles; (2) did not involve

Indonesian *Jamu* or traditional herbal remedies; (3) focused on synthetic drugs without herbal components; (4) lacked clear methodological descriptions; or (5) pertained to types of fatigue unrelated to physical exercise[17].

2.3 Data Extraction and Synthesis

Data extracted from the selected literature included: (1) characteristics of exercise-induced fatigue (central vs. peripheral mechanisms); (2) specific *Jamu* formulations and traditional herbal remedies identified for anti-fatigue properties; (3) the primary botanical sources and parts used; (4) identified bioactive compounds (e.g., polysaccharides, terpenoids, flavonoids, polyphenols); (5) proposed molecular mechanisms of action (enhanced energy metabolism, elimination of metabolites, neutralization of oxidative stress, modulation of inflammation, HPA axis regulation, neurotransmitter system harmonization); (6) relevant preclinical and clinical study outcomes pertaining to performance and recovery markers; and (7) any reported *in silico* data (RMSD, docking scores, similarity indices) linking herbal compounds to muscle fatigue pathways[18], [19].

The extracted data were then systematically synthesized and categorized. The pathophysiology of central and peripheral fatigue was thoroughly reviewed and summarized, followed by an in-depth analysis of traditional *Jamu* formulations[20], [21]. These formulations were classified according to their historical and perceived regulatory functions across organ systems and emotional states, as described in the literature. Bioactive compounds were correlated with specific traditional remedies, and their proposed molecular mechanisms were cross-referenced with established pathways of fatigue mitigation. *In silico* data were critically reviewed to identify promising compounds based on their predicted interaction with biological targets relevant to muscle fatigue, providing a scientific rationale for their therapeutic potential[22]..

2.4 Quality Assessment and Bias Mitigation

The methodological quality and potential risk of bias of the included studies were assessed critically. For *in vivo* and *in vitro* studies, criteria such as experimental design, sample size, control groups, and statistical analyses were considered. For *in silico* studies, the validation methods and relevance of the computational models were evaluated. Reviewers independently extracted and analyzed data, with discrepancies resolved through discussion and consensus. The comprehensive nature of the search strategy and the rigorous inclusion/exclusion criteria were designed to minimize publication and selection bias.[23].

3 Result and Discussions

The findings of this study integrate evidence from a systematic literature review and in silico molecular docking analysis, providing a comprehensive understanding of the mechanisms underlying exercise-induced fatigue and the therapeutic potential of Indo-

nesian herbal compounds. The results demonstrate that fatigue is a multifactorial condition involving interconnected pathways, including inflammation, oxidative stress, energy metabolism, and neurotransmitter regulation. The combined analytical approach offers a robust framework for evaluating traditional herbal remedies within a modern scientific context.

3.1 Characterization of Traditional Anti-Fatigue Formulations

The ethnopharmacological analysis identified several widely used Indonesian herbal formulations with established roles in enhancing endurance and recovery. Frequently reported plant sources include Curcuma longa, Zingiber officinale, Centella asiatica, and Andrographis paniculata. These botanicals are commonly administered as decoctions or infusions and are traditionally associated with improvements in circulation, reduction of inflammation, and stabilization of physiological and psychological functions.

Phytochemical profiling indicates that these plants are rich in bioactive constituents such as flavonoids, terpenoids, polysaccharides, and polyphenols. These compounds are recognized for their capacity to interact with multiple biological systems, suggesting a multi-target mode of action that aligns with the complex nature of exercise-induced fatigue [24].

3.2 Molecular Docking Analysis of Bioactive Compounds

The in silico molecular docking analysis evaluated the interaction between key phytochemicals—curcumin, gingerol, asiaticoside, and andrographolide—and selected protein targets implicated in fatigue mechanisms, including TNF-α, Keap1, AMPK, and 5-HT1A.

The docking results (Table 1) demonstrate consistently strong binding affinities, ranging from −7.6 to −9.5 kcal/mol, indicating favorable ligand–protein interactions. Furthermore, all Root Mean Square Deviation (RMSD) values were below 2.0 Å, confirming the structural stability and reliability of the predicted docking conformations. These findings suggest that the evaluated compounds possess significant potential to modulate key biological pathways associated with fatigue.

Comparative analysis with reference ligands, such as anakinra (TNF-α inhibitor), omaveloxolone (Keap1 modulator), metformin (AMPK activator), and buspirone (5-HT1A agonist), further supports the pharmacological relevance of these phytochemicals, as their binding affinities are within comparable ranges.

Table 1. *In Silico* Molecular Docking Scores for Selected Bioactive Compounds with Key Fatigue-Related Protein Targets

Plant Origin	Bioactive Compound	Target Protein	RMSD (Å)	Binding Affinity (kcal/mol)	Reference Ligand Binding Affinity (kcal/mol)
Curcuma longa (Turmeric)	Curcumin	TNF-α	0.87	-9.2	-9.8 (Anakinra)
	Curcumin	Keap1	0.95	-8.5	-9.1 (Omaveloxolone)
Zingiber officinale (Ginger)	Gingerol	AMPK	1.12	-7.8	-8.5 (Metformin)
	Gingerol	TNF-α	1.03	-8.1	-9.8 (Anakinra)
Centella asiatica (Gotu Kola)	Asiaticoside	5-HT1A	0.79	-8.9	-9.5 (Buspirone)
	Asiaticoside	Keap1	1.01	-7.6	-9.1 (Omaveloxolone)
Andrographis paniculata	Andrographolide	TNF-α	0.98	-9.5	-9.8 (Anakinra)
	Andrographolide	AMPK	1.21	-8.2	-8.5 (Metformin)

Table 2. Proposed Mechanism of Action (related to target)

Plant Origin	Bioactive Compound	Proposed Mechanism of Action (related to target)
Curcuma longa (Turmeric)	Curcumin	Modulating inflammation (via TNF-α inhibition)
	Curcumin	Activating Nrf2 antioxidant pathway
Zingiber officinale (Ginger)	Gingerol	Enhancing energy metabolism (via AMPK activation)
	Gingerol	Anti-inflammatory effects
Centella asiatica (Gotu Kola)	Asiaticoside	Modulating neurotransmitter systems (central fatigue)
	Asiaticoside	Antioxidant defense enhancement
Andrographis paniculata	Andrographolide	Potent anti-inflammatory action
	Andrographolide	Energy regulation and anti-fatigue

3.3 Mechanistic Interpretation of Anti-Fatigue Activity

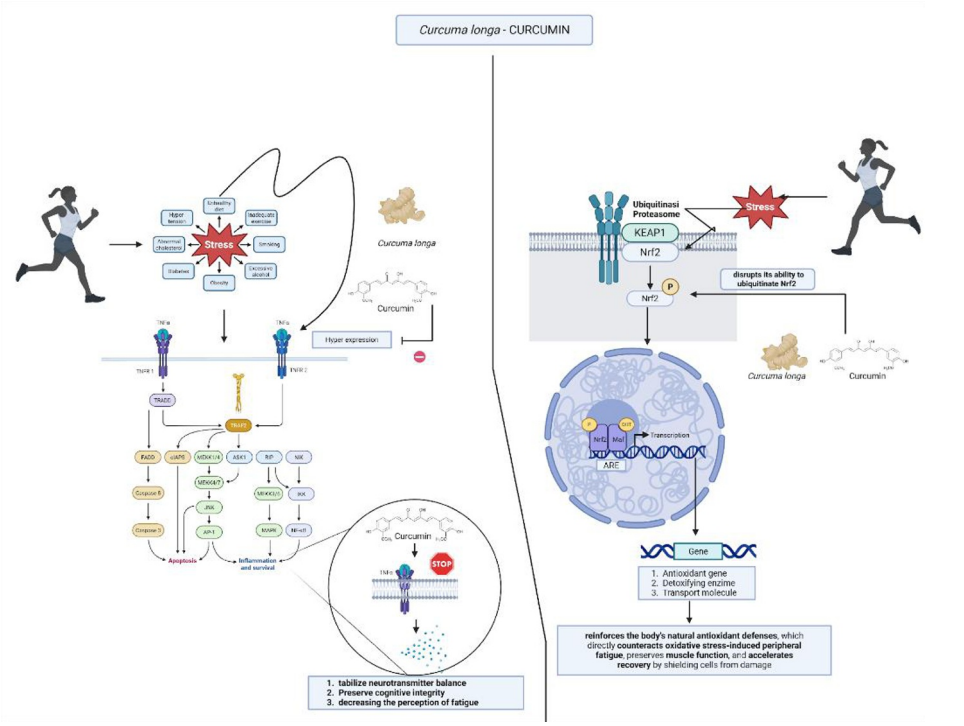

Fig 1. Curcuma longa and Molecular Fatigue Mechanism (Created in Biorender. Armansyah Maulana Harahap. (2026). https://biorender.com (accesed 01 January 2026))

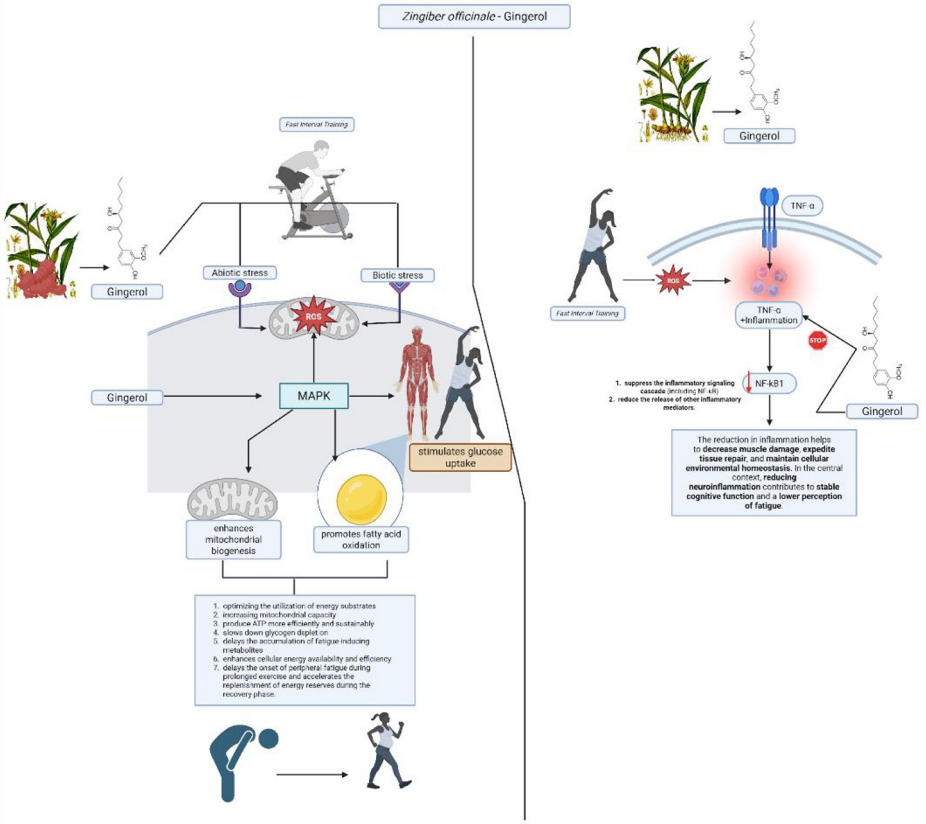

Fig 2. *Zingiber officinale* and Molecular Fatigue Mechanism (Created in Biorender. Armansyah Maulana Harahap. (2026). https://biorender.com (accesed 01 January 2026))

3.3.1 Anti-Inflammatory Pathways (TNF-α Modulation)

Curcumin and andrographolide exhibited strong binding affinities to TNF-α, suggesting potent anti-inflammatory activity. Chronic inflammation is a key contributor to both central and peripheral fatigue, as pro-inflammatory cytokines impair muscle function, disrupt mitochondrial activity, and alter neurotransmitter balance. By inhibiting TNF-α signaling, these compounds may reduce muscle damage, alleviate soreness, and facilitate recovery. The additional interaction of gingerol with TNF-α highlights the synergistic anti-inflammatory potential of combined herbal formulations [25].

3.3.2 Antioxidant Defense (Keap1–Nrf2 Pathway)

Curcumin and asiaticoside demonstrated notable interactions with Keap1, indicating a potential role in activating the Nrf2 antioxidant pathway. Activation of this pathway

enhances the expression of endogenous antioxidant enzymes, thereby mitigating oxidative stress induced by intense physical activity. This mechanism is particularly relevant in preserving mitochondrial integrity and improving muscle recovery, which are critical factors in sustained athletic performance [26].

3.3.3 Energy Metabolism Regulation (AMPK Activation)

Gingerol and andrographolide showed favorable binding to AMPK, a key regulator of cellular energy homeostasis. Activation of AMPK promotes glucose uptake, fatty acid oxidation, and mitochondrial biogenesis, all of which contribute to improved energy efficiency during exercise. The similarity of their binding profiles to metformin supports their potential role in enhancing endurance and accelerating post-exercise recovery [27].

3.3.4 Neurotransmitter Modulation (5-HT1A Interaction)

Asiaticoside exhibited strong interaction with the 5-HT1A receptor, suggesting a mechanism for modulating central fatigue. Regulation of serotonin pathways is essential for maintaining motivation, reducing perceived exertion, and sustaining cognitive performance during prolonged exercise. This finding highlights the potential of Centella asiatica in addressing both physical and psychological components of fatigue [28].

3.4 Integrated Multi-Target Mechanisms

The collective findings indicate that Indonesian herbal compounds exert anti-fatigue effects through a multi-target mechanism involving inflammation control, oxidative stress reduction, energy metabolism enhancement, and neurotransmitter regulation. This integrative mode of action reflects the holistic nature of traditional Jamu formulations, where multiple compounds act synergistically across interconnected physiological systems.

The consistently low RMSD values further strengthen the reliability of the molecular docking results, supporting the structural feasibility of these interactions. Together, these findings provide a strong mechanistic basis for the observed empirical benefits of herbal remedies in fatigue management.

3.5 Compound-Specific Insights

Curcuma longa (Curcumin).
Curcumin demonstrated dual activity through TNF-α inhibition and Keap1 modulation, indicating its capacity to simultaneously reduce inflammation and enhance antioxidant defense. This combined mechanism positions curcumin as a key candidate for mitigating peripheral fatigue and supporting muscle recovery.

Zingiber officinale (Gingerol).
Gingerol exhibited interactions with both AMPK and TNF-α, suggesting a dual role in energy metabolism and inflammation control. This profile supports its effectiveness in sustaining endurance and reducing post-exercise muscle fatigue.

Centella asiatica (Asiaticoside).
Asiaticoside showed strong affinity for 5-HT1A and Keap1, indicating its potential to regulate both central fatigue and oxidative stress. This dual action highlights its importance in maintaining cognitive function and physiological resilience.

Andrographis paniculata (Andrographolide).

Andrographolide demonstrated strong binding to TNF-α and AMPK, supporting its role in inflammation suppression and energy regulation. This compound may contribute significantly to both fatigue prevention and recovery processes.

4 Conclusions

This study integrates insights from traditional Indonesian Jamu practices with contemporary molecular analysis to elucidate the anti-fatigue potential of selected herbal compounds. The findings demonstrate that key phytochemicals, including curcumin, gingerol, asiaticoside, and andrographolide, exhibit favorable binding interactions with critical protein targets associated with exercise-induced fatigue, namely TNF-α, Keap1, AMPK, and 5-HT1A.

These interactions suggest a multi-mechanistic mode of action involving the modulation of inflammatory pathways, enhancement of antioxidant defense systems, regulation of cellular energy metabolism, and stabilization of neurotransmitter activity. Such integrative effects are consistent with the complex and multifactorial nature of fatigue, indicating that these compounds may contribute to both peripheral and central fatigue mitigation.

The results provide a scientific basis for the traditional use of Indonesian herbal medicines in supporting athletic performance and recovery. Moreover, the study highlights the relevance of combining ethnopharmacological knowledge with computational approaches to identify promising bioactive candidates for functional and therapeutic applications.

Despite these promising findings, further validation through well-designed preclinical studies and controlled human clinical trials is required to confirm efficacy, safety, and optimal dosage. Future research should also explore formulation strategies and synergistic interactions among compounds to enhance their applicability as evidence-based nutraceuticals in sport science.

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