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In Silico Study of Bioactive Compounds from *Moringa oleifera* Extract as Anti-Inflammatory Candidates Targeting the Inflammatory Mediator PGD2

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Abstract

Conventional anti-inflammatory drugs may cause serious adverse effects, creating a need for safer plant-derived therapeutic candidates. Although *Moringa oleifera* has recognized biological potential, computational evidence regarding the anti-inflammatory activity of its phytoconstituents against prostaglandin D_2 11-ketoreductase (AKR1C3; PDB ID: 1S2A) remains limited. This *in silico* study evaluated 12 bioactive compounds from an ethanolic extract of *M. oleifera* as potential inhibitors of this molecular target. Pharmacokinetic properties and oral bioavailability were predicted using SwissADME according to Lipinski's rule of five. Molecular docking was subsequently performed using Molecular Operating Environment 2019 to evaluate ligand–receptor binding affinities based on Gibbs free energy (ΔG) and root-mean-square deviation (RMSD). The physicochemical assessment showed that 11 compounds had favorable predicted membrane permeability and systemic absorption, whereas rutin violated Lipinski's criteria. Docking analysis identified quercetin, apigetrin, chlorogenic acid, ellagic acid, and naringenin as the most promising candidates. These compounds exhibited the lowest ΔG values and stable binding

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conformations, with RMSD values below 2.0 Å. The findings indicate that these five phytoconstituents have favorable predicted interactions with AKR1C3 and may possess potential anti-inflammatory activity associated with PGD_2 metabolism. Accordingly, they represent promising lead compounds for developing selective plant-derived anti-inflammatory agents. This study provides a computational foundation for future molecular dynamics simulations and clinical validation.

Keywords: Anti-Inflammatory Activity; Molecular Docking; *Moringa oleifera*; Pharmacokinetics; Prostaglandin D_2 11-Ketoreductase

INTRODUCTION

Inflammation is the body's defense mechanism against foreign agents that enter the body (Mardianingrum et al., 2021). Inflammation can be caused by tissue injury resulting from trauma, exposure to chemicals, heat, and other factors. As a result of this inflammation, the affected tissue releases various substances, which can cause significant changes in the surrounding normal tissue (Robby et al., 2022). Inflammation serves to destroy, reduce, or limit a substance that can cause damage or damaged tissue. It is characterized by symptoms such as swelling, redness, heat, pain, and changes in organ function (Manurung & Sumiwi, 2016). This has led to the development of various anti-inflammatory drugs.

Anti-inflammatory drugs are medications that work to suppress or reduce inflammation. Commonly used anti-inflammatory drugs often have many side effects, including a weakened immune response to infections, osteoporosis, stomach problems, kidney disorders, and anemia; they can also cause hyperglycemia (high blood sugar levels), which has spurred the development of anti-inflammatory agents derived from various plants (Hasim et al., 2019). One plant that can be used as an anti-inflammatory remedy is the moringa tree (*Moringa oleifera*).

Moringa (*Moringa oleifera*) is a plant that offers numerous benefits, both as a food source and for health. Moringa (*Moringa oleifera*) belongs to the Moringaceae family, which comprises 13 species. The moringa plant is reported to be full of health benefits because it contains many nutrients. All parts of the moringa plant possess biological activities such as hypoglycemic, anti-inflammatory, antioxidant, anticancer, antidiabetic, and antimicrobial properties (Riyanti et al., 2024). Moringa plants contain secondary metabolites such as flavonoids. The flavonoids in moringa may have anti-inflammatory effects, which work by

inhibiting the lipoxygenase and cyclooxygenase pathways and by accumulating histamine and leukocytes (Fadhilah et al., 2024).

The bioactive compounds in moringa leaves (*Moringa oleifera*) reported by (Hamdy, 2024) which were extracted with 80% ethanol and analyzed by HPLC are rich in phenolic acids and flavonoids, as shown in (Figure 1)

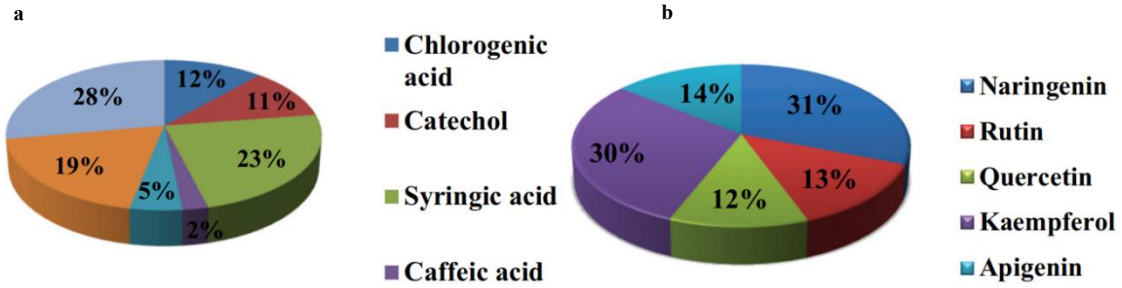


Figure 1. Composition of *Moringa oleifera* leaf extract (a) Phenolic acids; (b) Flavonoids (%) (Hamdy, 2024)

Figure 1a shows that twelve compounds were identified in the 80% ethanol extract of Moringa oleifera. Seven of these belong to the phenolic acid compound group, including benzoic acid (28%), syringic acid (23%), ellagic acid (19%), chlorogenic acid (12%), catechol (11%), gallic acid (5%), and caffeic acid (2%). Figure 1b shows the identification of five flavonoid compounds, including naringenin (31%), kaempferol (30%), apigenin (14%), rutin (13%), and quercetin (12%) (Hamdy, 2024).

These data indicate that the bioactive compounds in moringa leaves can provide a deeper understanding of the use of moringa leaves for human health, particularly as an anti-inflammatory agent. These results can serve as a preliminary basis for molecular docking studies, thereby improving the efficiency of active compound design and enabling the examination of intermolecular interactions (Men et al., 2024) related to anti-inflammatory effects through in silico studies of bioactive compounds from M. oleifera. Although the bioactive compounds in M. oleifera have been identified, computational studies on M. oleifera's anti-inflammatory effects against the inflammatory mediator PGD2 remain limited and have not been reported; therefore, PGD2 was selected as the inflammatory mediator.

Prostaglandin D2 (PGD2) is a pro-inflammatory lipid mediator of the arachidonic acid pathway that is predominantly released by mast cells and macrophages during tissue injury (Domingo et al., 2018). PGD2 also acts as a ligand for two receptors: the prostanoid D (DP) receptor and the chemotactic receptor homolog expressed on Th2 cells (CRTH2);

therefore, PGD2 can exert either pro-inflammatory or anti-inflammatory effects in different biological systems (Mishima et al., 2021). Increased PGD2 production plays a direct role in triggering vasodilation, swelling, pain, and cartilage degradation in inflammatory bone conditions such as osteoarthritis (Jang et al., 2020). Therefore, inhibiting the PGD2 signaling pathway (PDB ID: 1S2A) represents a selective and promising strategy for suppressing the inflammatory cascade while avoiding the side effects associated with conventional anti-inflammatory drugs; consequently, this study employed molecular docking using the inflammatory mediator PGD2.

The objective of this study was to conduct molecular docking analyses of all bioactive compounds in the ethanol extract of M. oleifera as a potential anti-inflammatory agent using the target protein PGD2 (PDB ID: 1S2A) (Figure 2). The results of this study are expected to provide new insights into the anti-inflammatory potential of bioactive compounds from M. oleifera and to identify promising candidate compounds for the development of new anti-inflammatory agents to address the problem of inflammatory resistance.



Figure 2. 3D structure of the PGD2 target protein (PDB ID: 1S2A)

Figure 2 shows the 3D structure of the inflammatory mediator PGD2 (PDB ID: 1S2A), which has a sequence length of 331, belongs to the species *Homo sapiens*, is classified as an oxidoreductase, is expressed in *Escherichia coli*, and has no mutations according to data from the Protein Data Bank (PDB).

METHODS

This computational study was conducted using a computer equipped with an Intel® Celeron® N4000 CPU running at 1.10 GHz, 1101 MHz, and 4 GB of RAM. The software used was Molecular Operating Environment (MOE) 2019, with ligands sourced from PUBCHEM (https://pubchem.ncbi.nlm.nih.gov/) and target proteins obtained from the Protein Data Bank (https://www.rcsb.org/). An 80% ethanol extract of Moringa oleifera was prepared by (Hamdy, 2024), who reported the phytochemical analysis using High-Performance Liquid Chromatography (HPLC), identifying twelve major active compounds in Moringa oleifera. These compounds were selected as representative bioactive molecules that are potentially responsible for the biological activity of Moringa oleifera and can subsequently be used as ligands for further computational analysis. These twelve ligands will be obtained from PUBCHEM and evaluated using Lipinski's rules, with predictions made using SwissADME (http://www.swissadme.ch/index.php).

The receptor (target protein) uses PGD2 as an inflammatory mediator, obtained from the Protein Data Bank (PDB) with PDB ID: 1S2A (Fardhani et al., 2020). The protein was prepared by removing the native ligand and water (H_2O) both of which are unnecessary chains and then optimized. The docking process was performed using the Triangular Matcher algorithm with standard settings. In this docking process, the ligand was positioned at the active site of the target protein. The docking results were evaluated using the Root Mean Square Deviation (RMSD) value; values below 2 Å and increasingly negative ΔG values were considered indicators of good docking results. The research was conducted from April 16, 2026, to May 18, 2026. Data collection for the upcoming docking will utilize phytochemical data from a natural compound to be used as a ligand, and a receptor with anti-inflammatory potential is required.

RESULTS

Pharmacokinetic Predictions for *Moringa oleifera* Ethanol Extract

The physicochemical properties were analyzed based on Lipinski's rules, which specify the following criteria: molecular weight (MW) less than 500 g/mol, fewer than 5 proton donors, fewer than 10 electron acceptors, log P less than 5, Polar Surface Area (PSA) less than 140 Å, and fewer than 10 rotatable bonds (Bitew et al., 2021). The physicochemical

properties of twelve compounds found in *Moringa oleifera* were examined to determine whether they comply with Lipinski's rules; these are presented in Table 1.

Table 1. Pharmacokinetic Predictions of Phytoconstituents in an Ethanol Extract of *Moringa oleifera*.

Compound Name	Parameter					
	Molecular Weight	Proton Donor	Proton Acceptor	Polar Surface Area	Rotable Bond	Log P
	<500 g/mol	<5	<10	<140 Å	<10	<5
Gallic acid (PubChem CID: 370)	170.12	4	5	97.99	1	0.21
Benzoic acid (PubChem CID: 243)	122.12	1	2	37.30	1	1.44
Catechol (PubChem CID: 289)	110.11	2	2	40.46	0	0.97
Syringic acid (PubChem CID: 10742)	198.17	2	5	75.99	3	0.99
Naringenin (PubChem CID: 439246)	272.25	3	5	86.99	1	1.84
Caffeic acid (PubChem CID: 689043)	180.16	3	4	77.76	2	0.93
Chlorogenic acid (PubChem CID: 17944427)	354.31	6	9	164.75	5	-0.39
Quercetin (PubChem CID: 5280362)	382.30	5	10	183.11	3	0.83
Apigetrin (PubChem CID: 5280704)	432.38	6	10	170.05	4	0.52
Rutin (PubChem CID: 5280805)	610	10	16	-	-	-1.87
Ellagic acid (PubChem CID: 5281855)	302.19	4	8	141.34	0	1.00
Kaemferol (PubChem CID: 10095180)	448.38	7	11	190.28	4	0.10

Table 1 shows the pharmacokinetics of twelve compounds found in Moringa oleifera. Based on these physicochemical properties, the compound that does not meet Lipinski's rules is rutin, as none of its physicochemical properties satisfy Lipinski's rules.

The result of the interaction between the ligand and the target protein

Docking results between the target protein and secondary metabolites in *Moringa oleifera* extract

The docking interactions of the eleven ligands yielded RMSD values; a favorable RMSD is considered to be less than 2 Å, accompanied by a low (negative) ΔG. The table below presents the interaction values specifically RMSD and binding energy resulting from the molecular docking of the ligands with the receptor, The docking results are shown in Table 2.

Table 2. Docking results between the target protein (PDB ID: 1S2A) and phytoconstituents in *Moringa oleifera* leaf extract.

No	Name	ΔG	RMSD
1.	Gallic acid (PubChem CID: 370)	-12.1468	3.1139
2.	Benzoic acid (PubChem CID: 243)	-8.0604	2.2098
3.	Catechol (PubChem CID: 289)	-8.5853	-1.9307
4.	Syringic acid (PubChem CID: 10742)	-11.9881	0.5321
5.	Naringenin (PubChem CID: 439246)	-12.8355	0.9736
6.	Caffeic acid (PubChem CID: 689043)	-11.6715	2.2358
7.	Chlorogenic acid (PubChem CID: 17944427)	-15.3543	1.6425
8.	Quercetin (PubChem CID: 5280362)	-17.7259	1.2621
9.	Apigetrin (PubChem CID: 5280704)	-17.6748	1.5273
10.	Rutin (PubChem CID: 5280805)	-15.4914	2.4183
11.	Ellagic acid (PubChem CID: 5281855)	-13.2178	0.7844
12.	Kaemferol (PubChem CID: 10095180)	-12.5454	3.2772

Table 2 shows the docking results for twelve ligands in *Moringa oleifera* extract with the inflammatory mediator PGD2. These docking results present the free energy values and RMSD of the ligand-receptor interactions.

DISCUSSION

SwissADME analysis (Table 1) reveals that among the 12 evaluated *Moringa oleifera* derivatives, six compounds fully comply with Lipinski's rules, five meet three to four criteria, and one fails to meet any criteria. Specifically, the compound rutin (PubChem CID: 5280805) violates these parameters due to its large molecular size and an excessive number of proton donors and donor-acceptor pairs (Singh et al., 2022). An excessive number of hydrogen

bonds between proton donors and acceptors increases the thermodynamic energy required for adsorption, thereby significantly slowing the systemic absorption of these compounds within the body (Rajesham et al., 2025). Physicochemical evaluation is crucial for predicting a compound's suitability as a drug and the oral bioavailability of candidate compounds, particularly through the application of Lipinski's Rule of Five (Bakchi et al., 2022).

Ligands that comply with Lipinski's rules proceed to molecular docking analysis targeting the inflammatory mediator PGD2 (PDB ID: 1S2A). Molecular docking provides predictive insights into binding affinity and intermolecular interactions between pharmacological ligands and target receptors, serving as a foundation for modern drug discovery (Tharun et al., 2025). The mechanism involves the binding of a ligand a small molecule to the receptor's active site, thereby forming a ligand-receptor complex (Pratama et al., 2017). PGD2 (PDB ID: 1S2A) is an inflammatory mediator specifically a lipid mediator secreted primarily by mast cells and immune cells (Johnsson et al., 2021). PGD2 plays a central role in driving inflammatory pathways, particularly in pathological conditions such as asthma and osteoarthritis (OA) (Gress et al., 2024), consequently, it was selected as the inflammatory mediator for this study.

Based on the docking results in Table 2, *quercetin*, *apigetrin*, *chlorogenic acid*, *ellagic acid*, and *naringenin* indicate the lowest binding energy and optimal RMSD metrics. The RMSD value is a parameter that measures the positional difference between the docked ligand and its original position (Miller et al., 2021). A higher RMSD value indicates a greater positional deviation of the docked ligand compared to the original ligand (Alamsyah, 2024). Ligand-receptor complex stability was evaluated using Gibbs free energy (ΔG) and Root Mean Square Deviation (RMSD). A lower (more negative) ΔG value indicates a spontaneous binding interaction with high affinity, while an RMSD value < 2.0 Å reflects the accuracy of the docked ligand's position relative to its original conformation (Rendi et al., 2021).

Naringenin demonstrated an excellent docking score, however, it exhibited limited structural interaction, forming only a single hydrogen bond with the tryptophan residue at position 227 of the 1S2A protein. This limited interaction profile is likely attributable to a highly specific binding pose, which restricts the conformational sampling capabilities of the MOE docking algorithm (Li et al., 2025). Conversely, *syringic acid* failed to achieve a stable conformation within the 1S2A binding pocket. This anomaly indicates a structural or

electronic mismatch, likely stemming from conflicting hydrophobic or hydrophilic characteristics that hinder effective ligand-receptor binding (Nurfadhila et al., 2023).

Overall, the robust structural interactions of *quercetin*, *apigenin/apigetrin*, *chlorogenic acid*, *ellagic acid*, and *naringenin* with the 1S2A protein demonstrate a potent ability to inhibit the PGD2 signaling pathway. Inhibition of this specific pathway effectively suppresses the inflammatory response, positioning these bioactive constituents of *Moringa oleifera* as promising candidates for the development of novel anti-inflammatory therapies (Chis et al., 2024). However, this study is subject to limitations, as the MOE software predicts ligand-protein interactions based on a single static conformational state. The method does not fully account for protein structural fluctuations, binding dynamics over time, or the influence of solvent dynamics (water and ions) under actual *in vivo* biological conditions.

CONCLUSION

Based on docking simulation results involving phytochemicals from the *Moringa oleifera* ethanol extract and the inflammatory mediator PGD2 (1S2A), the extract demonstrated promising potential for inhibiting inflammation. *Quercetin*, *apigenin*, *chlorogenic acid*, *ellagic acid*, and *naringenin* showed potential as anti-inflammatory agents, exhibiting RMSD values of less than 2 Å. These docking results are expected to provide new insights into the potential of *Moringa oleifera* as an anti-inflammatory agent, particularly for asthma and osteoarthritis. Future studies could involve molecular dynamics simulations to evaluate protein-ligand complex stability, as well as *in vitro* and *in vivo* testing to clinically confirm the anti-inflammatory activity of the bioactive compounds found in *Moringa oleifera*.

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