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Original Article

In Silico Exploration of Natural Antioxidant Candidates: Capsaicin Compounds from Cayenne Pepper Leaves (*Capsicum frutescens* L.) as Potential Inhibitors of the COX-2 Enzyme (PDB ID:5IKQ)

Eksplorasi In Silico Kandidat Antioksidan Alami: Senyawa Capsaicin dari Daun Cabai Rawit (*Capsicum frutescens* L.) sebagai Inhibitor Potensial Enzim COX-2 (PDB ID:5IKQ)

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Abstract

Exposure to free radicals caused by oxidative stress is a major factor in cellular damage and contributes to the development of degenerative diseases, highlighting the need for safe and effective natural antioxidants. Oxidative stress is triggered by excessive production of Reactive Oxygen Species (ROS), in which cyclooxygenase-2 (COX-2) plays a key enzymatic role in ROS formation. Cayenne pepper leaves (*Capsicum frutescens* L.) are known to possess antioxidant potential, with capsaicin identified as an important secondary metabolite. The antioxidant potential of capsaicin was evaluated using an *in-silico* approach by analyzing its binding affinity and molecular interactions with the COX-2 enzyme. This research aimed to assess capsaicin from cayenne pepper leaves as a potential natural antioxidant candidate through *in silico* interaction analysis with COX-2. Molecular docking was performed using AutoDock software to determine binding affinity values and optimal ligand conformations at the active site of COX-2. Interaction visualization and amino acid residue analysis were conducted using Discovery Studio Visualizer. The docking results were compared with the native ligand based on binding affinity and inhibition constant (Ki) values to evaluate inhibitory potential. Capsaicin exhibited a binding affinity of −7.41 kcal/mol and a Ki value of 3.73 µM, indicating stable interaction with COX-2. Although its binding affinity was lower than that of the native ligand, capsaicin demonstrated sufficient interaction strength to be classified as a potential natural COX-2 inhibitor. These findings suggest that capsaicin derived from cayenne pepper leaves may possess natural antioxidant activity based on *in silico* analysis.

Abstrak

Paparan radikal bebas akibat stres oksidatif merupakan faktor utama terjadinya kerusakan sel dan berkontribusi terhadap perkembangan penyakit degeneratif, sehingga menegaskan perlunya antioksidan alami yang aman dan efektif. Stres oksidatif dipicu oleh produksi Reactive Oxygen Species (ROS) yang berlebihan, di mana siklooksigenase-2 (COX-2) berperan sebagai enzim kunci dalam pembentukan ROS. Daun cabai rawit (*Capsicum frutescens* L.) diketahui memiliki potensi antioksidan, dengan kapsaisin sebagai salah satu metabolit sekunder penting. Potensi antioksidan kapsaisin dievaluasi menggunakan pendekatan in silico melalui analisis afinitas ikatan dan interaksi molekuler dengan enzim COX-2. Penelitian ini bertujuan untuk menilai kapsaisin dari daun cabai rawit sebagai kandidat antioksidan alami melalui analisis interaksi in silico dengan COX-2. Docking molekuler dilakukan menggunakan perangkat lunak AutoDock untuk menentukan nilai afinitas ikatan dan konformasi ligan yang optimal pada sisi aktif COX-2. Visualisasi interaksi dan analisis residu asam amino dilakukan menggunakan Discovery Studio Visualizer. Hasil docking dibandingkan dengan ligan asli berdasarkan nilai afinitas ikatan dan konstanta inhibisi (Ki) untuk mengevaluasi potensi penghambatan. Kapsaisin menunjukkan afinitas ikatan sebesar −7,41 kcal/mol dan nilai Ki sebesar 3,73 µM, yang mengindikasikan adanya interaksi yang stabil dengan COX-2. Meskipun afinitas ikatannya lebih rendah dibandingkan ligan asli, kapsaisin menunjukkan kekuatan interaksi yang cukup untuk diklasifikasikan sebagai inhibitor COX-2 alami yang potensial. Temuan ini menunjukkan bahwa kapsaisin yang berasal dari daun cabai rawit berpotensi memiliki aktivitas antioksidan alami

berdasarkan analisis in silico.

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INTRODUCTION

Exposure to free radicals induced by oxidative stress is a significant factor contributing to the development of degenerative diseases, such as cancer, atherosclerosis, and premature aging. Oxidative stress arises when the generation of Reactive Oxygen Species (ROS) exceeds the capacity of the body's antioxidant defense systems[1 2]. One of the enzymes involved in the generation of Reactive Oxygen Species (ROS) is cyclooxygenase-2 (COX-2), which catalyzes the conversion of arachidonic acid into prostaglandins and enhances inflammatory processes accompanied by increased free radical production [3]. This research aimed to evaluate the potential of capsaicin derived from *Capsicum frutescens* L. leaves as a natural antioxidant and anti-inflammatory agent through *in silico* analysis of its interaction with cyclooxygenase-2 (COX-2).

Natural products have long been utilized as sources of bioactive compounds with diverse pharmacological effects, including antioxidant activity. One plant with such potential is cayenne pepper (*Capsicum frutescens* L.), which is known to contain capsaicin as its major secondary metabolite[4]. This compound has been reported to exhibit antioxidant, anti-inflammatory, and chemopreventive activities through multiple molecular mechanisms, including inhibition of NF-κB activation and downregulation of COX-2 gene expression[5]. Nevertheless, studies investigating the specific interactions between capsaicin and the COX-2 enzyme remain limited, highlighting the need for preliminary analysis using a computational (*in silico*) approach.

The *in silico* approach is an effective and efficient method in the early stages of drug discovery, as it enables the prediction of the biological activity potential of compounds through molecular interaction analysis between ligands and target receptors. Molecular docking techniques allow visualization of binding modes and calculation of binding affinity values to predict the strength of ligand interactions at the enzyme's active site. Accordingly, this study aimed to explore the potential of capsaicin derived from cayenne pepper leaves as a natural COX-2 inhibitor through *in silico* analysis, thereby providing a scientific basis for the development of natural product–based antioxidant and anti-inflammatory candidates.

METHODS

Research Procedure

This research was conducted using an *in silico* approach employing molecular docking methods. The three-dimensional structure of the COX-2 enzyme (PDB ID: 5IKQ) was retrieved from the Protein Data Bank (PDB), while the ligand structure of capsaicin was obtained from the PubChem database in SDF format and subsequently converted to PDBQT format using Open Babel software. Protein preparation involved removal of water molecules and co-crystallized ligands, followed by the addition of polar hydrogen atoms using AutoDockTools version 1.5.7. The grid box center coordinates were defined based on the position of the native ligand at the active site of the COX-2 enzyme.

Data Analysis

Molecular docking was performed using AutoDock version 4.2 with the Lamarckian Genetic Algorithm (LGA). Docking parameters were set to generate 100 ligand conformations with high exhaustiveness to ensure reliable results. Following docking, binding affinity values of each conformation were analyzed and compared with those of the native ligand. Interaction visualization and amino acid residue identification were carried out using Discovery Studio Visualizer to examine non-covalent interactions, including hydrogen bonding, hydrophobic interactions, and π–π stacking, formed between capsaicin and the COX-2 enzyme.

RESULT AND DISCUSSION

The molecular docking in this research was conducted to evaluate the inhibitory potential and molecular interactions of capsaicin derived from cayenne pepper leaves against the COX-2 enzyme (PDB ID: 5IKQ) using AutoDockTools. AutoDockTools was selected due to its widespread use in molecular docking studies and its availability as an open-source platform, allowing free access for both academic and industrial applications[6].

Table 1. COX-2 Protein Information (Oxidoreductase)

Protein ID	Protein Parameters	
pdb : 5IKQ	▪ Method : X-Ray Diffraction ▪ Resolution : 2.41 Å ▪ Ramachandran Plot Statistics : 90.2 % ▪ G-Factors : 0.26	

The selection of proteins for molecular docking simulations must be based on several critical parameters, as presented in Table 1, including the protein determination method (X-ray crystallography), a resolution of 2.41 Å, an RPS value of 90%, and a G-factor of 0.26. These criteria were applied to optimize the reliability and accuracy of the molecular docking results. Protein preparation of the COX-2 enzyme involved separation of the native ligand from the receptor and removal of water molecules to prevent interference during the docking process. In addition, polar hydrogen atoms were added to approximate physiological pH conditions and to ensure appropriate docking interactions[7]. Additionally, hydrogen atoms were added back to the macromolecule to enable the observation and analysis of hydrogen bond interactions formed during the docking process [8].

Before to the simulation, method validation was first performed to assess the accuracy of the docking protocol[9]. Method validation was carried out through a redocking procedure of the native ligand into the COX-2 protein (PDB ID: 5IKQ). The native ligand was initially separated from the protein crystal structure, subsequently prepared, and then re-docked using the same docking parameters applied to the test compounds with AutoDock 4.2[10]. The results and interaction visualizations of the molecular docking validation are presented in Table 2 and Figure 1. The most critical step in molecular docking method validation is the definition of the grid box. Grid box determination is necessary to identify the coordinate points of the protein binding site, which serve as a reference for subsequent docking simulations of the test compounds[6]. The grid box was defined based on the coordinates of the native ligand at the active site of the protein, with dimensions of 40 × 40 × 40 grid points and a grid spacing of 0.375 Å. Docking

simulations were performed using the Lamarckian Genetic Algorithm (LGA). Acceptance of the docking validation was evaluated based on the Root Mean Square Deviation (RMSD) value, with a threshold of < 2.0 Å[11]. The redocking results yielded an RMSD value of 0.54 Å, which is well below the acceptable limit of < 2.0 Å. This low RMSD value indicates that the docking method is capable of accurately reproducing the native ligand's binding pose and orientation within the protein active site[12].

Table 2. Docking Validation Parameters Based on Native Ligand–COX-2 Redocking (PDB ID: 5IKQ)

Native Ligand	Number Grid Point			Coordinate Grid Point			Spacing Grid Point	RMSD
	X	Y	Z	X	Y	Z	0.375 Å	0.54 Å
Native Ligan	40	40	40	22.518	51.524	17.635		

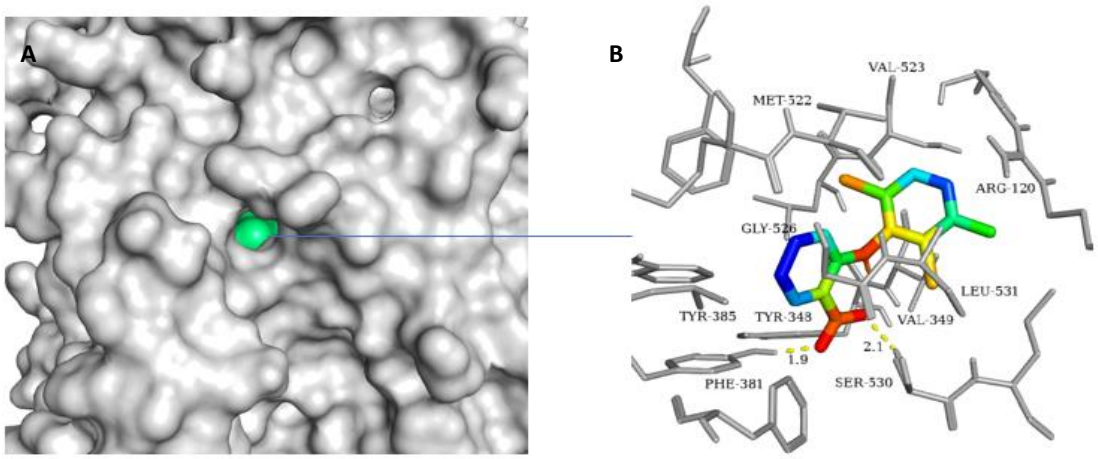


Figure 1. Visualization of molecular docking interactions between the native ligand and the COX-2 protein

Figure 1A illustrates the binding site or active site of chain A of the 5IKQ protein, which represents the region where the ligand adopts a specific conformation through interactions with amino acid residues within the active site. Meanwhile, Figure 1B shows the interactions between the native ligand and the 5IKQ protein, indicating the formation of polar contacts with bond distances of 1.9 Å at the Phe281 residue and 2.1 Å at the Ser530 residue. Shorter interaction distances indicate stronger binding interactions[11]. Based on these results, the docking parameters employed can be considered valid, thereby allowing subsequent docking simulations of the test compound, namely capsaicin derived from *Capsicum frutescens* leaves, to be reliably performed.

The outputs of molecular docking consist of a docking score and binding pose. The docking score represents the binding free energy (ΔG_{bind}), where lower free energy values indicate more stable ligand–receptor interactions and, consequently, stronger ligand affinity toward the receptor. The binding pose refers to the optimal structural conformation of the ligand when interacting with amino acid residues at the receptor binding site[12]. Various types of interactions can occur between ligands and receptors; however, hydrogen bonding is particularly important as it represents one of the most stable interactions. Hydrogen bond interactions occur between atoms that are not covalently bonded and constitute one of the most common molecular interactions in biological systems. The presence

of hydrogen bonds can influence physicochemical properties, such as boiling point, melting point, aqueous solubility, and chelation capability. These alterations may subsequently affect biological activity, including inhibition of the COX-2 enzyme[13].

Molecular docking analysis revealed that the native ligand exhibited a binding affinity (ΔG) of −8.30 kcal/mol with an inhibition constant (Ki) of 830.53 nM. These values indicate that the native ligand possesses strong and stable binding capability toward the COX-2 enzyme[14]. At the active site of the COX-2 protein, the native ligand interacted with the amino acid residues Ser530 and Tyr385 through hydrogen bonds, which play a crucial role in the catalytic activity of the COX-2 enzyme. In addition, other interactions were observed with the residues Trp387, Val532, Val349, Leu531, and Ala527 through π–π T-shaped and π–alkyl interactions, which represent hydrophobic interactions. The combination of hydrogen bonding and hydrophobic interactions plays a significant role in enhancing the stability of the ligand–receptor complex[16] thereby reinforcing the role of the native ligand as a reference compound in the evaluation of COX-2 inhibitory potential.

Molecular docking analysis revealed that capsaicin exhibited a binding affinity of −7.41 kcal/mol with an inhibition constant (Ki) of 3.73 µM. These values indicate that the interaction between capsaicin and COX-2 is relatively strong, suggesting its potential as a natural inhibitor. Compared to the native ligand, capsaicin showed a slightly lower binding affinity; however, the values remain within a range that indicates the possibility of significant biological activity[17]. A lower binding affinity value indicates that a compound requires less energy to bind or interact with the receptor, thereby exhibiting a greater potential to interact with the target protein[12]. Free binding energy (ΔG) analysis was performed to evaluate the spontaneity of the interaction and the stability of the ligand–receptor complex. The stability of the ligand–receptor interaction is reflected by a lower (more negative) ΔG value. Experimentally, ΔG is directly related to the inhibition constant (Ki), as described by the equation $\Delta G = -RT \ln Ki$. Therefore, the ΔG value can be used to predict the inhibitory potential of a compound against the target protein.[19]. In addition to the ΔG and Ki values, evaluation of ligand–receptor binding modes and interactions with amino acid residues at the receptor active site is also required as a reference for determining the ligand–protein binding characteristic[19].

At the active site of the COX-2 protein, capsaicin interacted with the amino acid residues *Tyr355* and *His90* through hydrogen bonds, which play an important role in stabilizing the ligand–receptor complex. In addition, other interactions were observed with the residue *Val523* via sigma bonds, as well as with *Leu352* and *Val349* through alkyl interactions, representing hydrophobic interactions. The combination of these interactions contributes to the stability of capsaicin binding at the COX-2 active site, thereby supporting its biological activity as an inhibitor of the enzyme[20].

Table 3. Molecular Docking Analysis of the Native Ligand and Capsaicin with COX-2

Ligand/Compound	Binding Affinity (ΔG)	Inhibition Constant (Ki)	Amino Acid Residues	Binding Interactions
Native ligan	-8.30 kcal/mol	830.53 nM	Ser530, Tyr385 Trp387 Val532,349, Leu531, Ala527	H-Bond Pi-pi T-Shaped Pi-Alkyl
Capsaicin	-7.41 kcal/mol	3.73 µM	Tyr355, His90 Val523	H-Bond Pi-Sigma

	Leu352, Val349	Alkyl

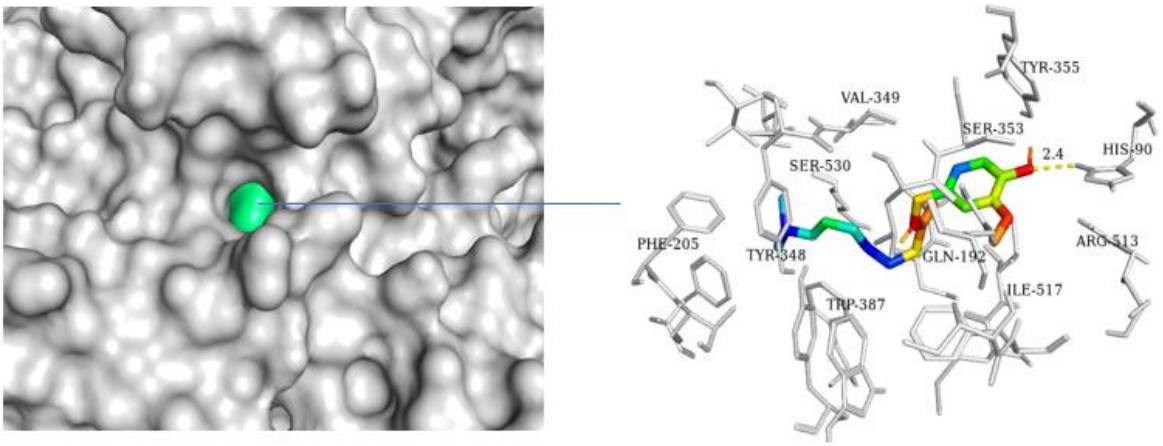


Figure 2. Molecular docking visualization of capsaicin with the COX-2 protein (5IKQ)

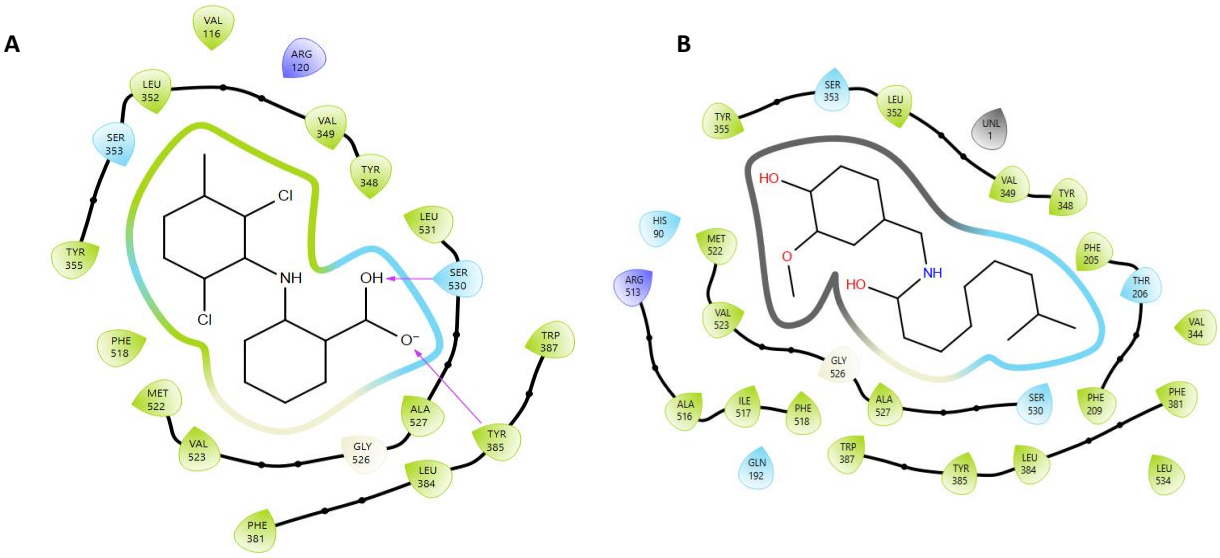


Figure 3. Visualization of molecular docking analysis: (A) native ligand and (B) capsaicin compound with the 5IKQ protein

These *in silico* findings support previous experimental studies reporting strong antioxidant activity of *Capsicum frutescens* extracts, as demonstrated by both DPPH and FRAP assays [16] [17]. The antioxidant mechanism of capsaicin is believed to involve two primary pathways: direct electron donation to neutralize free radicals and inhibition of COX-2–mediated inflammatory pathways[18]. These findings indicate that molecular docking can provide preliminary insights into the pharmacological potential of a compound prior to further *in vitro* and *in vivo* evaluations [19].

In addition, the application of *in silico* methods offers advantages in terms of research time and cost efficiency, as well as the ability to screen potential compounds prior to more complex experimental stages[20]. However, *in silico* predictions are subject to limitations due to their dependence on protein model accuracy and the algorithms used [21]. Therefore, further experimental researches are required to validate the biological potential of capsaicin as a COX-2 inhibitor.

Overall, this research reinforces the position of capsaicin as a promising bioactive compound derived from Indonesian natural resources with potential for development as a natural antioxidant and anti-inflammatory candidate. The application of molecular docking methods not only provides insights into binding strength but also enables detailed visualization of molecular interactions, serving as a rational basis for natural product–based drug design.

Limitation

This research has several limitations that should be considered when interpreting the results. First, the research was conducted exclusively using a computational (*in silico*) approach through molecular docking without experimental validation using *in vitro* or *in vivo* methods. Therefore, the findings are predictive in nature and may not fully represent the biological activity of the compound within complex biological systems.

Second, the scope of this research was limited to a single bioactive compound, namely capsaicin, as the primary metabolite investigated from cayenne pepper leaves (*Capsicum frutescens* L.), without considering the potential contributions of other compounds that may exert synergistic effects.

Third, the molecular target investigated in this research was limited to the cyclooxygenase-2 (COX-2) enzyme with the crystal structure PDB ID: 5IKQ; therefore, the findings cannot be generalized to other isoenzymes, such as COX-1, or to other molecular targets involved in inflammation and oxidative stress.

Fourth, the docking simulations were performed using AutoDock 4.2 with the Lamarckian Genetic Algorithm (LGA) and specific parameter settings, which may lead to variations in results if different computational methods, algorithms, or parameters are applied.

Fifth, the ligand–receptor interaction analysis was limited to the identification of interaction types and amino acid residues involved in non-covalent interactions based on docking visualization results, without performing molecular dynamics simulations to evaluate the temporal stability of the ligand–protein complex.

Finally, this research did not include evaluations of the pharmacokinetic properties, toxicology, or ADMET profile of capsaicin; therefore, the safety and therapeutic potential of the compound cannot be comprehensively concluded.

CONCLUSION

The results of this research indicates that capsaicin from cayenne pepper leaves (*Capsicum frutescens* L.) has potential as a natural COX-2 enzyme inhibitor, with a binding affinity of −7.41 kcal/mol and a Ki of 3.73 µM. The interactions involve key residues at the COX-2 active site, suggesting possible antioxidant and anti-inflammatory biological activity. This *in silico* approach provides a scientific basis for the development of capsaicin as a safe and effective natural antioxidant candidate derived from Indonesian natural resources.

AUTHOR CONTRIBUTION STATEMENT

Esti Febri Fatwami: *conceptualization* of the research and the development of the scientific framework. Dian Islamiyati: *methodology*, *data curation*, and *formal analysis*, as well as manuscript preparation through *writing – original draft* and *visualization*. Ryan Syahputra: *validation*, *writing – review & editing*, and *supervision* of the overall research process. All authors have read and approved the final version of the manuscript.

CONFLICT OF INTEREST DECLARATION

The authors declare no conflict of interest

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