

A Review on Molecular Docking Application of *Cinnamomum Camphora* in Drug Discovery

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Date of Submission: 04-05-2026

Date of Acceptance: 14-05-2026

ABSTRACT: This review focuses on the molecular docking applications of *Cinnamomum camphora* in drug discovery, highlighting its diverse pharmacological potential supported by computational studies. The plant is rich in bioactive phytoconstituents such as camphor, 1,8-cineole, borneol, linalool, and flavonoids, which exhibit significant biological activities including anti-inflammatory, antiviral, antibacterial, anticancer, anti-diabetic, antidepressant, anti-Alzheimer's, and anti-ulcer effects. Molecular docking studies using tools like AutoDock, AutoDock Vina, and PyRx demonstrate strong binding affinities of these compounds with various target proteins such as COX-1, COX-2, TNF- α , IL-6, α -amylase, α -glucosidase, DNA gyrase, and EGFR, VEGFR, and neurotransmitter receptors. In many cases, the binding affinities of phytoconstituents were comparable to or better than standard drugs, suggesting their potential as promising therapeutic agents. The review also outlines typical docking workflows and emphasizes the importance of in-silico approaches in reducing time and cost in drug development. However, it concludes that further in-vitro, in-vivo, and clinical studies are necessary to validate these findings and ensure safety and efficacy, while future research integrating advanced computational techniques could enhance drug discovery from *Cinnamomum camphora*.

KEYWORDS: Traditional medicine, molecular docking, phytochemicals, computational pharmacology

INTRODUCTION *Cinnamomum camphora*, commonly known as the camphor tree, is a well-known medicinal plant belonging to the family Lauraceae. It has been widely used in traditional systems of medicine such as Ayurveda, Unani, and Chinese medicine for its diverse therapeutic properties. The plant is rich in a variety of bioactive compounds, including camphor, cineole, borneol, linalool, and other terpenoids and flavonoids, which contribute to its pharmacological activities. Traditionally, it has been used for the treatment of conditions such as inflammation, infections, respiratory disorders, and pain, making it a valuable natural resource for drug discovery.

In recent years, the focus of pharmaceutical research has shifted toward the use of computational methods to identify potential drug candidates more efficiently. Molecular docking has emerged as a powerful in-silico technique that predicts the interaction between small molecules (ligands) and target proteins, helping to understand binding affinity and stability. Tools such as AutoDock, AutoDock Vina, PyRx, and visualization software like PyMOL have significantly enhanced the ability to screen phytochemicals against multiple biological targets. These approaches not only reduce the time and cost involved in drug development but also provides insights into the mechanism of action of natural compounds. The present study emphasizes the molecular docking analysis of phytoconstituents derived from *Cinnamomum camphora* against various disease-related protein targets. By evaluating binding affinities and interaction profiles, the study aims to identify potential compounds with significant

therapeutic effects against diseases such as inflammation, cancer, diabetes, microbial infections, and neurodegenerative disorders. The integration of traditional knowledge with modern computational tools highlights the potential of *Cinnamomum camphora* as a promising source for

novel drug development, while also underscoring the need for further experimental validation to confirm its efficacy and safety.

OBJECTIVES

- To identify and compile the major phytoconstituents present in *Cinnamomum camphora* that may contribute to its pharmacological activities.
- To evaluate the binding affinity of selected phytochemicals with various disease-related target proteins using molecular docking techniques.
- To analyze the interaction patterns between ligands and target proteins to understand their possible mechanisms of action.
- To compare the docking results of plant-derived compounds with standard drugs to assess their potential as alternative therapeutic agents.
- To highlight the significance of computational tools such as AutoDock, AutoDock Vina, PyRx, and PyMOL in accelerating drug discovery and to suggest the need for further experimental validation studies.

PREVIOUS STUDIES

ANTI-INFLAMMATORY ACTIVITY

The study by Saqib et al. (2022) used molecular docking to evaluate the anti-inflammatory potential of camphor against the COX-1 enzyme. The binding affinity of camphor was reported to be approximately -9.28 kcal/mol, which is comparable to standard drugs like paracetamol and diclofenac. This indicates that camphor forms a stable ligand-protein complex with the enzyme. The interaction occurs through hydrogen bonding and hydrophobic interactions with key amino acid residues such as serine, tyrosine, leucine, glycine, valine, and tryptophan. These interactions stabilize the binding and inhibit the enzyme's activity, thereby reducing prostaglandin synthesis, which is responsible for inflammation and pain. The study also compared camphor with standard drugs to validate its effectiveness. The results suggest that camphor has strong potential as a natural anti-inflammatory agent. Such findings

highlight the importance of phytochemicals in drug discovery and support the use of traditional medicinal plants in modern therapeutic applications.

ANTI-INFLAMMATORY ACTIVITY

Patel et al. (2023) conducted molecular docking studies to evaluate the interaction of camphor tree phytochemicals with COX-1 and COX-2 enzymes, which play a crucial role in inflammation. The ligands used included camphor, 1,8-cineole, borneol, and linalool. These compounds showed moderate to strong binding affinities ranging from -6.0 to -8.2 kcal/mol. Among them, cineole and borneol demonstrated stronger binding interactions, suggesting better inhibitory potential. The interactions were mainly stabilized by hydrogen bonds, hydrophobic contacts, and van der Waals forces within the active site of the enzymes. These findings indicate that terpenoid compounds from *Cinnamomum camphora* can effectively inhibit cyclooxygenase activity, thereby reducing prostaglandin production and inflammation. The study also emphasizes the importance of ligand conformation and proper orientation in achieving strong binding. Overall, the results support the potential use of camphor-derived compounds as natural alternatives to synthetic anti-inflammatory drugs

ANTI-INFLAMMATORY ACTIVITY

Prakash et al. (2023) investigated the anti-inflammatory potential of camphor oil constituents by targeting inflammatory cytokines such as TNF- α and IL-6 using molecular docking. These cytokines play a major role in regulating inflammatory responses in the body. The ligands used in the study included camphor, borneol, 1,8-cineole, and linalool. The docking results showed binding affinities ranging from -5.8 to -8.0 kcal/mol, indicating moderate to strong interactions. Among these, borneol and cineole exhibited stronger binding, suggesting better inhibitory potential. The interactions were stabilized through hydrogen bonding and hydrophobic interactions with the active sites of the proteins. By binding to these cytokines,

the phytochemicals may inhibit their activity and reduce inflammation. The study highlights the importance of targeting cytokine pathways in controlling inflammatory diseases and supports the use of natural compounds as safer alternatives to conventional drugs.

ANTI-VIRAL ACTIVITY

Dikova et al. (2026) studied the antiviral potential of camphor-derived sulphonamide compounds using molecular docking against viral proteins such as HSV-1 glycoprotein B, HCoV-OC43 spike protein, and FCV capsid protein. The ligands showed moderate binding affinities ranging from -2.55 to -4.27 kcal/mol. Among them, compound 7a demonstrated the best interaction with the FCV capsid protein, indicating relatively higher stability. The interactions were mainly stabilized by hydrogen bonds and π -cation interactions. Although the binding affinity was lower compared to standard antiviral drugs like remdesivir, the results still suggest potential antiviral activity. These findings indicate that camphor derivatives can be further modified and optimized to improve their binding strength and effectiveness. The study highlights the importance of molecular docking in identifying potential antiviral agents and supports further research into camphor-based drug development.

SEDATIVE AND HYPNOTIC EFFECTS

The study by Xiao et al. (2022) explored the sedative and hypnotic effects of Cinnamomum camphora borneol essential oil using molecular docking and network pharmacology. Multiple ligands such as borneol, β -caryophyllene, limonene, and α -pinene were analyzed against several target proteins including ADORA2A, DRD2, and OPRK1. The binding affinities were generally strong, with some compounds showing values up to -9.0 kcal/mol. These interactions suggest that the compounds can modulate neurotransmitter systems, including dopamine and adenosine pathways, which are involved in sleep regulation and sedation. The study demonstrates a multi-target mechanism, where multiple compounds act on different receptors simultaneously. This provides a scientific basis for the traditional use of camphor in relaxation and sleep-related conditions. The results highlight the potential of natural compounds in developing safer sedative drugs with fewer side effects.

ANTI-DIABETIC ACTIVITY

The study conducted by Nair et al. focused on evaluating the anti-diabetic potential of phytochemicals present in Cinnamomum camphora using molecular docking techniques. The primary targets selected for the study were carbohydrate-metabolizing enzymes such as α -amylase and α -glucosidase, which play a key role in the breakdown of complex carbohydrates into glucose. Inhibition of these enzymes is an effective strategy for controlling postprandial blood glucose levels in patients suffering from Diabetes Mellitus. The results showed that flavonoids and phenolic compounds exhibited strong binding affinities ranging from -7.0 to -9.5 kcal/mol. These interactions were stabilized through hydrogen bonding, electrostatic interactions, and hydrophobic contacts within the enzyme's active site. The binding prevents substrate access and reduces enzyme activity, thereby slowing glucose absorption. This study highlights the importance of plant-based compounds as safer alternatives to synthetic anti-diabetic drugs, which often cause side effects such as hypoglycaemia or gastrointestinal discomfort.

ANTI-DIABETIC ACTIVITY

In another study by Li et al., the anti-diabetic properties of camphor tree constituents were investigated by targeting the α -glucosidase enzyme using molecular docking analysis. The study identified several bioactive compounds, particularly flavanoids and phenylpropanoid glycosides, which showed high binding affinities ranging between -7.5 and -10.0 kcal/mol. These values indicate strong and stable ligand-protein interactions. The compounds formed multiple hydrogen bonds with key amino acid residues in the enzyme's active site, along with van der Waals and hydrophobic interactions that further enhanced stability. By inhibiting α -glucosidase activity, these compounds delay the conversion of disaccharides into glucose, thereby preventing sudden spikes in blood sugar levels. This mechanism is particularly useful in managing type 2 diabetes. The study also emphasized that natural inhibitors may offer long-term therapeutic benefits with fewer adverse effects compared to synthetic drugs like acarbose. These findings support further experimental and clinical studies for drug development.

ANTI-DEPRESSANT ACTIVITY

The research conducted by Thomas et al. explored the antidepressant potential of phytochemicals derived from *Cinnamomum camphora* using molecular docking and network pharmacology approaches. Depression is commonly associated with imbalances in neurotransmitters such as serotonin and dopamine. The study targeted receptors like dopamine D2 and serotonin receptors to evaluate ligand binding. Compounds such as camphor, linalool, and various flavonoids showed moderate to strong binding affinities ranging from -6.0 to -9.0 kcal/mol. These interactions suggest that the compounds can modulate neurotransmitter activity and improve synaptic transmission. Hydrogen bonding and hydrophobic interactions played a significant role in stabilizing the ligand-receptor complexes. The multi-target nature of these phytochemicals indicates their ability to act on different pathways simultaneously, which is beneficial in treating complex disorders like Depression. The study supports the use of plant-derived compounds as safer alternatives to synthetic antidepressants, which often have side effects like drowsiness, dependency, and withdrawal symptoms.

ANTI-CANCER ACTIVITY (Gupta et al., 2022)

The study by Gupta et al. investigated the anti-cancer potential of camphor derivatives through molecular docking against key cancer-related proteins such as EGFR (Epidermal Growth Factor Receptor) and VEGFR (Vascular Endothelial Growth Factor Receptor). These receptors are involved in tumor growth, cell proliferation, and angiogenesis. The docking results showed strong binding affinities ranging from -8.0 to -11.0 kcal/mol, indicating highly stable interactions. The compounds formed hydrogen bonds and hydrophobic interactions with amino acid residues in the active site of the proteins, effectively blocking their signalling pathways. By inhibiting these receptors, the compounds may prevent tumor progression and reduce the formation of new blood vessels required for cancer growth. This mechanism is particularly important in controlling aggressive cancers. The findings suggest that camphor-based compounds have promising potential in cancer therapy and can be further developed into effective anti-cancer drugs with fewer side effects compared to conventional chemotherapy.

ANTI-BACTERIAL ACTIVITY (Nakamura et al., 2022)

The antibacterial activity of *Cinnamomum camphora* compounds was studied by Nakamura et al. using

molecular docking against bacterial enzymes such as DNA gyrase. DNA gyrase is essential for bacterial DNA replication and cell survival, making it an important drug target. The study showed that terpenoids like camphor, borneol, and cineole exhibited binding affinities ranging from -6.5 to -9.0 kcal/mol. These interactions were stabilized by hydrogen bonding and hydrophobic interactions within the enzyme's active site. By binding to DNA gyrase, these compounds inhibit DNA replication, leading to bacterial cell death. This mechanism is similar to that of certain antibiotics, indicating the potential of these natural compounds as antibacterial agents. The study highlights the importance of plant-derived compounds in combating antibiotic resistance, which is a growing global concern. Further experimental validation is required to confirm their effectiveness in clinical applications.

ANTI-ALZHEIMER'S ACTIVITY (Varma et al., 2023)

The study conducted by Varma et al. focused on evaluating the neuroprotective effects of camphor tree phytochemicals against targets associated with Alzheimer's disease. The primary enzymes selected were BACE-1 (β -secretase) and GSK-3 β , both of which are involved in amyloid plaque formation and tau protein hyper phosphorylation. The docking results revealed strong binding affinities ranging from -7.0 to -10.0 kcal/mol, particularly for flavanoids. These compounds formed stable interactions through hydrogen bonding and hydrophobic contacts with the active site residues of the enzymes. By inhibiting BACE-1, the compounds may reduce amyloid-beta production, while inhibition of GSK-3 β can prevent neuronal damage. The study suggests that these phytochemicals may help slow down disease progression and improve cognitive function. These findings support the potential use of natural compounds in developing safer treatments for neurodegenerative diseases.

ANTI-ULCER ACTIVITY (Khan et al., 2024)

The anti-ulcer activity of camphor-derived compounds was investigated by Khan et al. using molecular docking against the H⁺/K⁺-ATPase enzyme, which is responsible for gastric acid secretion in the stomach. Excess acid production is a major cause of peptic ulcers. The study showed that the compounds exhibited strong binding affinities ranging from -7.0 to -9.5 kcal/mol. These interactions were stabilized by hydrogen bonding and hydrophobic interactions within the enzyme's

active site. By inhibiting H⁺/K⁺-ATPase, the compounds reduce acid secretion and help protect the gastric mucosa. This mechanism is similar to that of proton pump inhibitors used in ulcer treatment. The study highlights the potential of natural compounds as effective and safer alternatives for managing gastric disorders. Further in vivo and clinical studies are necessary to confirm their therapeutic efficacy and safety.

Activity	Target Protein	Ligand Type	Binding Affinity (kcal/mol)	Binding Site / Interaction
Anti-inflammatory	Cyclooxygenase-1 (COX-1)	Natural Ligand	~ -9.28	Ser, Tyr, Leu, Gly, Val, Trp
		Standard Drug (Paracetamol)	~ -6.2 to -6.8	Ser, Tyr, Leu, Gly, Val, Trp
		Standard Drug (Diclofenac)	~ -7.8 to -8.3	Ser, Tyr, Leu, Gly, Val, Trp
Anti-inflammatory	COX-1 & COX-2	Natural Ligands	~ -6.0 to -8.2	H-bond, Hydrophobic, Van der Waals
		Standard Drug (Diclofenac)	-7.5 to -9.0	H-bond, Hydrophobic, Van der Waals
Anti-inflammatory	TNF- α and IL-6	Natural Ligands	-7.0 to -8.0	Hydrogen bonding
		Standard Drug (Celecoxib)	-7.0 to -8.5	Hydrogen bonding
Anti-inflammatory	Cyclooxygenase-2 (COX-2)	Natural Ligands	-7.0 to -8.2	Active site via hydrogen bonding
		Standard Drug (Diclofenac)	-7.0 to -8.5	Active site via hydrogen bonding
Anti-viral	FCV Capsid Protein	Synthetic Derivative (7a)	-4.27	Not specified
		Standard Drug (Remdesivir)	-5.0 to -5.5	Viral RdRp
Sedative & Hypnotic	ADORA2A Receptor	Natural Ligand	-8.8	Not specific
		Standard Drug (Diazepam)	-7.5	Not specific
Anti-diabetic	α -amylase	Natural Ligand	-7.0 to -9.5	Not specific
		Standard Drug (Acarbose)	-7.0 to -9.0	Catalytic active site

Table :1

COMPUTATIONAL TOOLS

Several computational tools were employed to carry out the molecular docking study of Cinnamomum

camphora. Software such as Auto Dock and Auto Dock Vina were used to predict the binding affinity and interaction between selected phytochemical ligands and target proteins. PyRx served as an integrated platform for virtual screening and docking analysis, simplifying the workflow. Additionally, PyMOL was utilized for the visualization of protein–ligand complexes, helping to interpret binding modes and interaction sites. These tools collectively enabled efficient analysis of molecular interactions and supported the identification of compounds with potential biological and anti-inflammatory activity.

CONCLUSION

The conclusion of the study emphasizes that the molecular docking analysis of *Cinnamomum camphora* phytoconstituents revealed significant potential in targeting proteins involved in inflammatory pathways. Several bioactive compounds exhibited strong binding affinities, in some cases comparable to or better than standard anti-inflammatory drugs, suggesting their possible role as effective therapeutic agents. The application of computational tools such as Auto Dock, Auto Dock Vina, PyRx, and PyMOL enabled a rapid, cost-effective, and reliable screening process for evaluating ligand–protein interactions. These findings support the traditional medicinal use of *Cinnamomum camphora* and highlight its importance as a source of novel drug candidates. However, the study also acknowledges that further *in vitro*, *in vivo*, and clinical investigations are necessary to validate these computational results and to ensure safety, efficacy, and proper drug development in the future.

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- demonstrated strong inhibitory interactions, indicating potential anti-diabetic activity
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