

A Review on In Silico Approaches to *Centella asiatica*'s Therapeutic Potentials

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ABSTRACT This review explores the therapeutic potential of *Centella asiatica* (Gotu kola) through modern *in silico* computational approaches, which provide a highly efficient, cost-effective, and data-driven pathway for drug discovery by bridging the gap between traditional herbal medicine and modern pharmacology. Traditionally valued for its diverse medicinal properties, the plant's complex phytochemical profile rich in triterpenoid saponins like asiaticoside, asiatic acid, madecassic acid, and madecassoside is analyzed using specialized bioinformatics tools and databases such as PubChem, ChEMBL, AutoDock, and PyRx to predict molecular interactions and binding affinities with high precision. By simulating interactions between these bioactive compounds and specific biological targets, studies validate their potent multi-target efficacy in addressing various modern medical conditions, including Alzheimer's disease, gastric ulcers, cancer, and diabetes. These simulations often identify natural compounds that outperform standard pharmaceutical drugs, while tools like SwissADME facilitate early-stage assessment

of drug-likeness and toxicity. Ultimately, while these findings identify *Centella asiatica* as a significant source of multi-target therapeutic leads and provide a robust theoretical foundation for its traditional uses, they serve as a critical precursor for necessary subsequent *in vitro* and *in vivo* clinical validation.

KEYWORDS: In silico drug discovery, Traditional medicine, Molecular docking, Phytochemicals, computational pharmacology.

INTRODUCTION Medicinal plants have served as the foundation of traditional healthcare for centuries, offering a vast array of bioactive compounds for modern drug discovery. However, traditional experimental methods like *in vitro* and *in vivo* testing are often labour-intensive, costly, and time-consuming. To address these challenges, *in silico* approaches utilizing computational and bioinformatics-based methods have emerged as powerful tools to analyze, predict, and model the molecular interactions between plant compounds and biological targets. These digital methods facilitate virtual screening for

rapid identification of phytochemicals, assessment of toxicity profiles, and prediction of pharmacokinetic properties, effectively bridging the gap between traditional medicine and modern pharmaceutical science^[1].

A wide variety of software tools are employed in these computational studies to evaluate medicinal plants. “AutoDock and AutoDockVina” are widely used to predict how a plant-derived ligand binds to a target protein receptor, helping researchers understand molecular binding mechanisms and identify potential drug candidates. Other essential tools include “PyRx”, an open-source screening tool that can efficiently rank large numbers of phytochemicals based on their binding affinity, and “UCSFChimera or PyMOL”, which allow for the 3D visualization and analysis of these molecular structures. Advanced commercial suites like the “SchrodingerSuite” provide even deeper analysis through molecular dynamics simulations and lead optimization^[2].

Centellaasiatica, also known as Gotukola or Indian pennywort, is a primary subject of these in silico investigations due to its rich history in Ayurveda and Traditional Chinese Medicine as a "brain tonic" and rejuvenating herb^[3]. Its therapeutic benefits are primarily linked to bioactive triterpenoid saponins, including asiaticoside, madecassoside, madecassic acid and asiaticacid^[4]. Computational research has successfully validated many of its traditional uses, showing significant potential in treating Alzheimer's disease through the inhibition of BACE1 and AChE enzymes, as well as demonstrating strong anti-cancer, anti-ulcer, anti-diabetic, anti-inflammatory, wound-healing, cardioprotective, neuroprotective and anti-aging activities. These findings suggest that the plant's phytochemicals could serve as

effective multi-target therapeutic candidates for various modern medical conditions^[5].

Objectives:

- Select and identify traditional medicinal herbs with proven or reported therapeutic potential, using knowledge from ethnopharmacology and published literature.
- Use molecular docking to study how plant-based compounds (phytochemicals) interact with specific protein targets, predicting their binding strength and possible interactions.
- Gather or extract details of bioactive compounds from selected plants using online phytochemical databases such as, PubChem, and ChEMBL.
- Carry out molecular docking experiments to confirm predicted binding affinities and interaction patterns between phytochemicals and target proteins.
- Evaluate the drug-likeness and ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) profiles of selected phytochemicals using in silico tools like SwissADME^[6].

PREVIOUS STUDIES:

Centellaasiatica as a nutraceutical^[5]

Centella asiatica, widely known as a potent nutraceutical, owes its therapeutic versatility to a rich profile of bioactive compounds, including asiaticoside, madecassoside, and various flavonoids. These constituents provide comprehensive health benefits by acting as antioxidant, anti-inflammatory, and neuroprotective agents that reduce oxidative stress and modulate inflammatory pathways. Beyond its internal benefits, such as cardioprotection and anxiety management, the

herb is highly effective in wound healing and skin rejuvenation due to its ability to stimulate collagen synthesis and tissue regeneration. In the tradition of Ayurveda, where it is referred to as *Mandukaparni*, the herb is a cornerstone of "MedhyaRasayana" formulations designed to enhance memory and cognitive function. It is frequently combined with other nootropic herbs in classical preparations like *Brahmi Ghrita* to treat neurological disorders and improve mental clarity. Today, its pharmacological value is reflected in a wide array of commercial products, ranging from cognitive enhancers and cardiac supplements by The Himalaya Drug Company to specialized dermatological creams and metabolic teas produced globally.

Anti-Alzheimer's Activity

Nala Mawaddani et al. (2020) conducted an insilico study showing that *Centella asiatica* phytochemicals such as sitosterol, flavanol, and germacrene B exhibit strong binding affinity toward the BACE1 enzyme, with sitosterol showing the highest binding energy (-239.7 kcal/mol). These ligands interact with key amino acid residues at or near the active site, potentially reducing amyloid- β formation, although they may not completely inhibit enzymatic activity [7]. Similarly, Ekka et al. (2026) demonstrated that compounds like asiaticoside, madecassoside, asiatic acid, and madecassic acid show significant binding affinity with both BACE1 and acetylcholinesterase (AChE). Asiaticoside, in particular, exhibited strong interactions (around -9.1 kcal/mol with BACE1), suggesting stable ligand-protein binding through hydrogen bonds and hydrophobic interactions, indicating promising multi-target therapeutic potential for Alzheimer's disease, though further experimental validation is needed [8].

Anti-Cancer Activity

ChaiwatMonmai et al. (2025) investigated the anticancer activity of asiatic acid and asiaticoside against EGFR in non-small cell lung cancer (NSCLC). Asiatic acid showed superior inhibitory activity with strong binding affinity (-8.8 kcal/mol for wild-type EGFR) and lower IC₅₀ values, outperforming standard drugs such as erlotinib. The compound interacts with the ATP-binding pocket through hydrogen bonding and hydrophobic interactions, leading to reduced cancer cell viability and induction of apoptosis [9]. In another study, Temkar et al. (2024) identified phytoconstituents like isoquercetin, quercetin, and 9H-fluorene-2-carboxylic acid as effective aromatase inhibitors with binding affinities around -8.4 kcal/mol. These compounds demonstrated stable binding even in SNP-mutated proteins, indicating their potential use in breast cancer therapy with consistent efficacy across genetic variations [10].

Anti-Ulcer Activity

Kolageri et al. (2025) evaluated the anti-ulcer potential of *Centella asiatica* phytoconstituents using molecular docking against gastric H⁺/K⁺-ATPase. The results showed that asiaticoside B exhibited the highest binding affinity (-17 kcal/mol), followed by madecassic acid (-14.6 kcal/mol), both of which showed stronger interactions than the standard drug omeprazole (-7.2 kcal/mol). These compounds interact with important amino acid residues such as tyrosine, arginine, and asparagine within the active site, suggesting their ability to effectively inhibit gastric acid secretion and act as potent natural anti-ulcer agents [11].

Anti-Inflammatory Activity

Legiawati et al. (2018) conducted an *in silico* docking study demonstrating that phytoconstituents such as asiaticoside, madecassic acid, and terminolic acid show strong binding affinity with pro-inflammatory cytokines like IL-1 α , IL-1 β , and IL-6, as well as anti-inflammatory cytokine IL-4. Asiaticoside showed the highest affinity (-14.4 kcal/mol with IL-1 α), indicating its ability to inhibit inflammatory mediators while enhancing anti-inflammatory pathways [12]. Additionally, PiriyaChonsut et al. (2024) reported that asiatic acid, madasiatic acid, and madecassic acid exhibit strong binding with glucosyltransferase C (-10 kcal/mol), surpassing standard drugs such as chlorhexidine, and also demonstrated antibiofilm and anti-inflammatory effects [13]. Furthermore, Musfiroh et al. (2023) showed that asiatic acid forms a stable complex with COX-2 enzyme (-7.37 kcal/mol), supported by molecular dynamics simulations, indicating its potential as a natural anti-inflammatory agent [14].

Anti-Malarial Activity

Susmitha Yadav et al. (2025) investigated the antimalarial potential of *Centella asiatica* phytochemicals targeting the falcipain enzyme of *Plasmodium falciparum*. Among the screened compounds, campesterol showed the highest binding affinity (-8.6 kcal/mol), followed by ursolic acid and rutin. These compounds demonstrated stronger binding interactions than the standard drug chloroquine (-5.5 kcal/mol), suggesting their potential to inhibit haemoglobin degradation in the parasite and serve as promising candidates for antimalarial drug development [15].

Anti-Fibrotic Activity

Gayathri et al. (2024) explored the antifibrotic potential of *Centella asiatica* compounds using network pharmacology and molecular docking. Compounds such as bayogenin, isothankunicacid, and madasiatic acid showed strong binding affinity toward fibrosis-related targets like MAPK-1, SRC, SMAD-3, and TGF- β 1. Bayogenin exhibited the highest binding affinity (-9.7 kcal/mol), and molecular dynamics studies confirmed the stability of these interactions. These findings suggest that the phytochemicals can regulate fibrosis pathways, including inflammation and collagen deposition, making them promising therapeutic agents [16].

Anti-Aging and Wound Healing Activity

Khotimah et al. (2021) studied the interaction of *Centella asiatica* phytoconstituents with proteins involved in skin aging and wound healing, such as collagenase and elastase. Compounds like asiaticoside and madecassoside showed strong binding affinities ranging from -7.0 to -10.5 kcal/mol. These interactions are stabilized by hydrogen bonding and hydrophobic interactions, which help inhibit collagen degradation and promote tissue regeneration, supporting their use in anti-aging and wound healing applications [17].

Anti-Diabetic Activity

Vineet Mehta et al. (2016) demonstrated that *Centella asiatica* extract exhibits significant antidiabetic activity through inhibition of α -amylase and α -glucosidase enzymes. Molecular docking studies revealed that compounds like centellasaponin-C (-181.7 kcal/mol) and asiaticoside show strong binding affinity toward the insulin receptor, indicating their role in improving insulin signalling and glucose metabolism [18]. Additionally, Singh

and Bharadvaja (2024) reported that multiple phytochemicals, including asiaticoside and quercetin, interact with various diabetes-related targets such as FBP1 and ACE, showing better binding affinity than the standard drug metformin and supporting a multi-target therapeutic approach^[19]

Neuroprotective Activity

Ekka et al. (2026) reported that *Centella asiatica* phytoconstituents exhibit significant neuroprotective potential through strong interactions with multiple neurological targets. These compounds demonstrate stable binding affinities and may help in reducing oxidative stress, inflammation, and neuronal damage, thereby supporting their potential role in managing neurodegenerative disorders, although further experimental studies are required for confirmation^[20].

Cardioprotective activity

RangkiAstiani et al. (2023) explored the role of triterpenoid saponins of *Centella asiatica* as renin inhibitors targeting the renin-angiotensin-aldosterone system (RAAS). Molecular docking results demonstrated good binding affinity of these compounds with renin, which plays a key role in blood pressure regulation. By inhibiting renin activity, these phytochemicals may help control hypertension and improve overall cardiovascular function, highlighting their potential as natural cardioprotective agents^[21]. Ajani et al. (2023) investigated asiatic acid and asiaticoside against Cathepsin S enzyme using both in silico and in vitro methods. The compounds showed strong binding affinity and stable interactions with key amino acid residues, indicating their role in inhibiting enzyme activity involved in atherosclerotic plaque

formation. This suggests that these phytoconstituents may help prevent cardiovascular diseases by reducing inflammation and lipid accumulation in blood vessels^[22].

Anti Cholera activity

Hossain et al. (2023) conducted a pharmacoinformatics and molecular docking study to evaluate the anti-diarrheal potential of *Centella asiatica* against *Vibrio cholerae*. The phytochemicals showed strong binding affinity with bacterial target proteins, indicating their ability to interfere with toxin production and bacterial survival. Molecular dynamics simulations further confirmed the stability of ligand-protein complexes. These findings suggest that *Centella asiatica* compounds may act as effective natural agents in controlling cholera by reducing bacterial activity and fluid loss associated with diarrheal conditions^[23].

Antibacterial Activity

SeptyanAndriyanto et al. (2025) evaluated the antibacterial potential of *Centella asiatica* leaf bioactive compounds using both in vitro and in silico approaches. The study demonstrated that phytochemicals from the plant exhibited strong inhibitory activity against fish pathogenic bacteria, with molecular docking revealing effective binding interactions with bacterial target proteins such as DNA gyrase. These interactions suggest that the compounds can interfere with bacterial DNA replication, leading to antimicrobial effects. Additionally, the study confirmed that the plant-derived ligands showed stable binding affinity and could act as promising natural antibacterial agents, supporting the traditional use of *Centella asiatica* in treating infections^[24].

Activity	Best Ligand
Anti-Alzheimer's	Sitosterol
Anti-Alzheimer's (dual)	Asiaticoside
Anti-Cancer	Asiatic acid
Aromatase	Isoquercetin
Anti-Ulcer	Asiaticoside B
Anti-Inflammatory	Asiaticoside
Anti-Biofilm	Asiatic acid
COX-2	Mefenamic acid
Anti-Malarial	Campesterol
Anti-Fibrotic	Bayogenin
Wound Healing	Madecassoside
Anti-Diabetic	Centellasaponin-C
Multi-target diabetes	Asiaticoside
Neuroprotective	Asiaticoside
Cardioprotective	Asiaticoside
Anti-Cholera	Viridiflorol
Antibacterial	13-Hexyloxy compound
Atherosclerosis	Asiaticoside

Target	Binding Affinity	Compared Standard
BACE1	-239.7	Lanabecestat
BACE1/AChE	-9.6	Donepezil
EGFR	-8.8	Erlotinib
CYP19A1	-8.4	Letrozole
H ⁺ /K ⁺ ATPase	-17.0	Omeprazole
IL-1 α	-14.4	No standard
GtfC	-10.0	Chlorhexidine
COX-2	-8.9	Aspirin
Falcpain	-8.6	Chloroquine
MAPK-1	-9.7	Corticosteroid
TNF- α	-10.7	No standard
Insulin receptor	-181.7	No standard
FBP1	-8.9	Metformin
Fyn kinase	-9.1	Saracatinib
Renin	-9.6	Aliskiren
ToxT	-8.7	Virstatin
DNA gyrase	-7.4	Ciprofloxacin
Cathepsin S	-7.08	LY3000328

Table :1

Computational Tools and Techniques in Drug Discovery

researchers used the computational software for the determination of ligands, target proteins, ligand binding site and ligand binding affinity. Most of them used the “AutoDock 4, AMDock with AutoDock Vina”, for molecular docking studies. Their docking result was analyzed by using the software “PyMOL v2.5 (PyMOL LiGPlot +2.2.4)”. Most of them retrieved the ligand structure from public chemical database such as “PubChem” and the selected ligands were made using “PyRx's” Open Babel program. They drew the chemical structure of the ligands using “ChemDraw Ultra 9.0”. Common tools: AutoDock, PyRx, SwissDock, Schrödinger Glide.

Database and software used

The *in silico* research outlined in the document utilizes several key computational tools and biological databases to evaluate the medicinal potential of *Centella asiatica*. Researchers primarily retrieve the 2D and 3D chemical structures of phytochemical ligands from public databases such as **PubChem** and the **ZINC database**. For molecular docking and screening, common software includes **AutoDock/AutoDock Vina**, **PyRx** (which integrates AutoDock Vina), and **SwissDock** to predict how compounds like asiaticoside bind to target proteins. Advanced analysis and visualization are performed using **Schrodinger Suite** for molecular dynamics, **UCSF Chimera** or **PyMOL** for 3D structural mapping, and **ChemDraw** for chemical structure editing. Additionally, **ArcGIS** is mentioned as a tool for mapping the environmental distribution and suitable habitats of the medicinal plant^[25].

AI and machine learning in *in silico* drug design

The use of *in silico* approaches encompassing AI and machine learning drastically enhances drug design by replacing expensive and time-consuming *in vitro* and *in vivo* trials with efficient, data-driven computational methods. These tools allow researchers to rapidly screen thousands of phytochemicals, such as those from *Centella asiatica*, to predict their biological activity, molecular interactions, and binding energies with high precision. Furthermore, *in silico* modelling facilitates early-stage assessment of a compound's pharmacokinetic properties and toxicity (ADMET profiling), which significantly improves the efficiency of lead selection and bridges the gap between traditional herbal medicine and modern pharmacology^[25].

Conclusion

In silico computational approaches provide a highly efficient, cost-effective, and data-driven pathway for drug discovery by bridging the gap between traditional herbal medicine and modern pharmacology. By utilizing a diverse array of specialized software and databases such as **PubChem** and **ChEMBL** for structure retrieval, **AutoDock**, **AutoDock Vina**, and **PyRx** for molecular docking, and **PyMOL** or **UCSF Chimera** for 3D visualization researchers can predict molecular interactions and binding affinities with high precision. Studies on *Centella asiatica* validate that its bioactive triterpenoid saponins, including asiaticoside, madecassoside, and asiatic acid, demonstrate potent multi-target therapeutic potential for conditions such as Alzheimer's disease, cancer, diabetes, and gastric ulcers. These simulations often identify natural compounds that outperform standard pharmaceutical drugs such as asiaticoside-B

showing higher affinity than omeprazole or campesterol exceeding the performance of chloroquine while tools like **SwissADME** facilitate the early-stage assessment of drug-likeness and toxicity. Ultimately, while these computational findings provide a robust theoretical foundation for the plant's traditional medicinal uses, they serve as a critical precursor for necessary subsequent in vitro and in vivo clinical validation.

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