

In Silico Molecular Docking Studies on the Phytochemicals of *Capparis zeylanica* Linn. for Anti-Hypertensive Activity

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Publication Date: 2026/10/03

Abstract: The present study investigated the phytochemical constituents of the leaves of *Capparis zeylanica* Linn. and evaluated selected constituents for their potential anti-hypertensive activity using an in silico molecular docking approach. The leaves were shade-dried, powdered and subjected to successive Soxhlet extraction using chloroform, ethyl acetate, ethanol and distilled water. Preliminary phytochemical screening indicated the presence of alkaloids in all extracts, while phenolic compounds, flavonoids, cardiac glycosides, saponins and triterpenoids were detected particularly in the ethyl acetate extract. GC-MS analysis of the ethyl acetate extract identified several phytochemical constituents, including pinolenic acid, salicylic acid, 2,4-dihydroxybenzaldehyde and 2,4-diamino-5-butyl-8-hydroxy-5H-chromeno[2,3-b]pyridine-3-carbonitrile. These compounds, together with captopril as the standard, were evaluated against angiotensin-converting enzyme (PDB ID: 1J37) using AutoDock Vina through the Chimera platform. The docking scores were –6.7 kcal/mol for pinolenic acid, –6.4 kcal/mol for salicylic acid, –6.0 kcal/mol for 2,4-dihydroxybenzaldehyde and –8.8 kcal/mol for 2,4-diamino-5-butyl-8-hydroxy-5H-chromeno[2,3-b]pyridine-3-carbonitrile, compared with –6.0 kcal/mol for captopril. The docking results indicate that the selected phytochemicals can interact with the ACE target and provide a in silico data for further investigation of the anti-hypertensive potential of *C. zeylanica*.

Keywords: *Capparis zeylanica* L, Ethyl Acetate Extract, Phytochemicals, GC-MS, Angiotensin-Converting Enzyme, Molecular Docking, Anti-Hypertensive.

How to Cite: J. Priyadharshini; Abdul Rahim S.; Jayasridhar P.; Ramlega R.; Selvaganapathi S.; Thirisha G. (2026) In Silico Molecular Docking Studies on the Phytochemicals of *Capparis zeylanica* Linn. for Anti-Hypertensive Activity. *International Journal of Innovative Science and Research Technology*, 11(9), 2660-2666. <https://doi.org/10.38124/ijisrt/26sep1371>

I. INTRODUCTION

Hypertension is a common cardiovascular disorder characterised by persistently elevated arterial blood pressure and is an important risk factor for cardiovascular morbidity and mortality [1]. Blood pressure is determined by the interaction between cardiac output and total peripheral resistance, with multiple renal, neuronal, hormonal and vascular mechanisms contributing to its regulation [3,4]. The renin–angiotensin–aldosterone system is an important physiological pathway involved in blood-pressure regulation. Angiotensin-converting enzyme (ACE) converts angiotensin I to angiotensin II, which promotes vasoconstriction and stimulates aldosterone secretion, thereby contributing to an increase in blood pressure [5,7,8].

Anti-hypertensive drugs act through different mechanisms, including reduction of cardiac output, reduction of blood volume and relaxation of vascular smooth muscle.

Captopril is an ACE inhibitor that suppresses the pressor action of angiotensin II by inhibiting ACE and also potentiates the action of bradykinin [5]. Although conventional pharmacotherapy is effective, medicinal plants remain an important source of structurally diverse phytochemicals that are investigated for cardiovascular and other pharmacological activities [25,27,28]. Several reports have described traditional and pharmacological uses of *Capparis zeylanica* Linn., including antioxidant, anti-inflammatory, antimicrobial and other biological activities [12,15,25].

Molecular docking is a structure-based in silico method used to predict the orientation of a ligand within a receptor binding site and to estimate the strength of ligand–target interactions [10,11,51,52]. The approach is useful for preliminary screening of phytochemicals and for identifying compounds that may interact with a selected therapeutic target [47–54].

Therefore, the present study focused on the phytochemical profile of *C. zeylanica* leaf extracts and the in silico docking of selected constituents against ACE (PDB ID: 1J37), using captopril as the reference ligand.

➤ Plant Profile



Fig 1 *Capparis zeylanica* Linn. Leaf and Flower

Capparis zeylanica Linn. is a medicinal plant traditionally used in different regions. The thesis records its traditional use in conditions including dysentery, cough and cold, diabetes, boils, swelling, rheumatism and other ailments. The plant material used in the present investigation consisted of leaves collected from Pudukkottai, Tamil Nadu, India and authenticated by Dr. Radha, Research Officer (Botany), Siddha Medicinal Plants Garden, Ministry of Ayush, Government of India, Mettur, Tamil Nadu.

II. MATERIALS AND METHODS

➤ Collection and Authentication of Plant Material

The leaves of *Capparis zeylanica* Linn. were collected from Pudukkottai, Tamil Nadu, India. The plant was authenticated by Dr. Radha, Research Officer (Botany), Siddha Medicinal Plants Garden, Ministry of Ayush, Government of India, Mettur, Tamil Nadu.

➤ Preparation of Plant Extracts

The leaves were dried in the shade for 20 days, powdered to obtain a coarse powder and passed through mesh No. 36. The powdered leaves were subjected to successive Soxhlet extraction using chloroform, ethyl acetate, ethanol and distilled water. The concentrated extracts were filtered through Whatman No. 1 filter paper and stored at 4°C until further use [41]. For each solvent, 150 g of coarse powder was extracted for up to 8 h; the extracts were subsequently concentrated under reduced pressure and kept in a desiccator.

➤ Preliminary Phytochemical Screening

The different extracts were subjected to qualitative phytochemical screening for alkaloids, carbohydrates, steroids, proteins, tannins, phenolic compounds, flavonoids, gums and mucilage, glycosides, saponins and triterpenoids using standard chemical tests [55–57].

Table 1 Preliminary Phytochemical Screening of *Capparis zeylanica* L. Leaf Extracts

Chemical test	Chloroform	Ethyl acetate	Ethanol	Distilled water
Alkaloids – Mayer's	+	+	+	+
Alkaloids – Dragendorff's	+	+	+	+
Alkaloids – Hager's	+	+	+	+
Carbohydrates – Molisch's	+	–	–	–
Reducing sugar – Fehling's	+	–	–	–
Steroids – Liebermann–Burchard	–	–	–	–
Proteins – Biuret	–	–	–	–
Proteins – Millon's	–	–	–	–
Tannins	–	–	–	–
Phenolic compounds – FeCl ₃	–	+	–	–
Phenolic compounds – 10% NaCl	–	+	–	–
Flavonoids – Shinoda	–	+	–	–

Glycosides – Keller–Kiliani	+	+	–	–
Saponins – Foam test	–	+	–	–
Triterpenoids	–	+	–	–

Phytochemicals Present (+); Phytochemicals Absent (–).

➤ GC-MS Analysis

Gas chromatography–mass spectrometry (GC-MS) was used for the identification of phytochemical constituents in the ethyl acetate extract. The technique separates volatile or

thermally stable compounds by gas chromatography and identifies the resulting components using their mass spectra [9]. The identified compounds and their reported chemical nature in the thesis are presented in Table 2.

Table 2 Phytochemical Constituents Identified by GC-MS in the Ethyl Acetate Extract

S. No.	Compound	Nature
1	Ethyl benzene	Aromatic hydrocarbon
2	Pinolenic acid	Polyunsaturated fatty acid
3	2,4-Dihydroxybenzaldehyde	Polyphenol
4	Salicylic acid	Phenolic compound
5	2,4-Diamino-5-butyl-8-hydroxy-5H-chromeno[2,3-b]pyridine-3-carbonitrile	Chromeno pyridine
6	Penigequinolone	Quinoline alkaloid
7	Tetracosanoic acid	Saturated fatty acid
8	Valeric acid	Alkyl carboxylic acid
9	Cinnamic acid	Unsaturated carboxylic acid
10	Benzamide	Phenolic amide

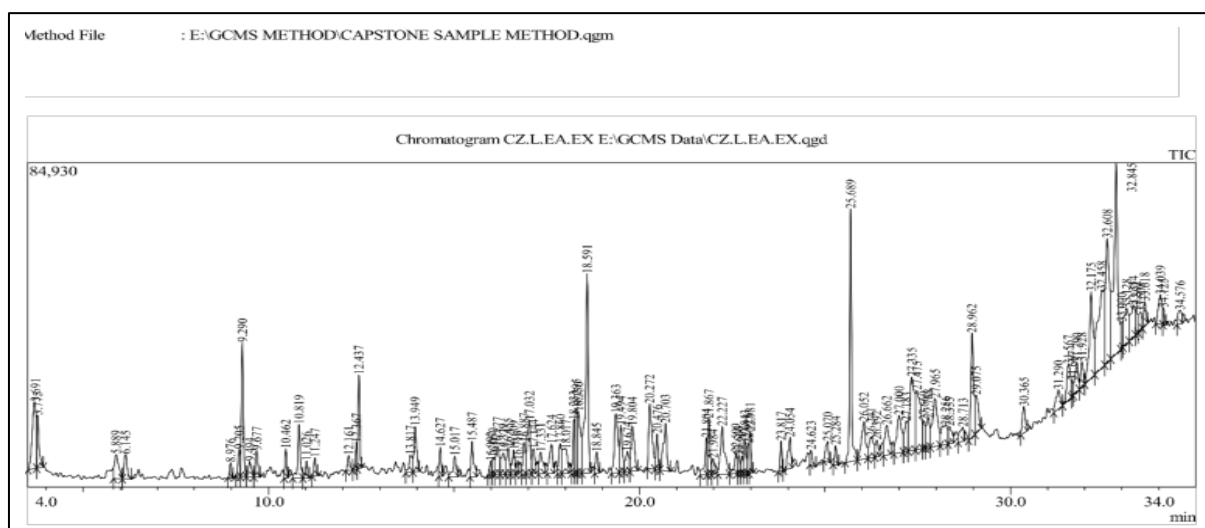


Fig 2 GC-MS Chromatogram of the Ethyl Acetate Extract of *Capparis zeylanica* Linn.

➤ Drug-Likeness and ADME Screening

Drug-likeness and ADME screening of selected phytoconstituents was performed using the SwissADME web tool as described in the thesis. The reported screening criteria included molecular weight below 500 g/mol, fewer than 5

hydrogen-bond donors, fewer than 10 hydrogen-bond acceptors and fewer than 10 rotatable bonds. The selected compounds showed zero Lipinski violations and high gastrointestinal absorption in the reported analysis.

Table 3 Drug-Likeness Prediction of Selected Phytoconstituents

Compound	Molecular weight (g/mol)	Lipinski violations	GI absorption	H-bond acceptors	H-bond donors	Rotatable bonds
Pinolenic acid	278.43	0	High	2	1	13
Salicylic acid	138.12	0	High	3	2	1
2,4-Dihydroxybenzaldehyde	138.12	0	High	3	2	1
2,4-Diamino-5-butyl-8-hydroxy-5H-chromeno[2,3-b]pyridine-3-carbonitrile	310.35	0	High	4	3	3

• Note: The rotatable-bond value for pinolenic acid is reproduced from the thesis table.

➤ Molecular Docking Analysis

Molecular docking was performed to evaluate the binding mode of the selected phytochemicals with angiotensin-converting enzyme (ACE; PDB ID: 1J37). Captopril was used as the standard drug. AutoDock Vina version 1.17.3 through the Chimera platform was used for docking, while ChimeraX version 1.10.1 was used to analyse ligand–receptor interactions. All ligand bonds were set as rotatable, and the best pose was considered for the reported binding affinity. Hydrogen bonds and other contacts were analysed for the docked complexes.

extract, 5.28 g of ethanol extract and 10.68 g of distilled-water extract from the respective 150 g portions of powdered material. The preliminary phytochemical investigation demonstrated alkaloids in all four extracts. The ethyl acetate extract additionally showed phenolic compounds, flavonoids, cardiac glycosides, saponins and triterpenoids, while the chloroform extract showed carbohydrates and reducing sugars together with alkaloids and cardiac glycosides. These observations were consistent with the qualitative screening recorded in the thesis and supported selection of the ethyl acetate extract for further GC-MS profiling.

III. RESULTS AND DISCUSSION

➤ Extraction Yield and Preliminary Phytochemical Screening

Successive Soxhlet extraction of *C. zeylanica* leaves produced 2.62 g of chloroform extract, 0.39 g of ethyl acetate

Table 4 Extract Yields Obtained from *Capparis zeylanica* L. Leaves

Plant material	Extraction method	Chloroform	Ethyl acetate	Ethanol	Distilled water
<i>C. zeylanica</i> leaves (150 g each)	Soxhlet	2.62 g	0.39 g	5.28 g	10.68 g

➤ GC-MS Identified Phytoconstituents

GC-MS analysis of the ethyl acetate extract identified ten compounds according to the thesis data. Among these, pinolenic acid, salicylic acid, 2,4-dihydroxybenzaldehyde and 2,4-diamino-5-butyl-8-hydroxy-5H-chromeno[2,3-b]pyridine-3-carbonitrile were selected for the molecular docking study. The identified chemical classes included aromatic and unsaturated compounds, fatty acids, phenolic compounds, an alkaloid and other oxygen-containing constituents.

score of –6.7 kcal/mol and formed hydrogen-bond contacts with PRO226 and GLU594, together with hydrophobic contacts involving residues including GLU594, ARG39, VAL42, ILE65 and GLU68. Salicylic acid showed a docking score of –6.4 kcal/mol, with hydrophobic contacts involving PRO226 and LEU227 and hydrogen bonds with GLU587 and ARG590. 2,4-Dihydroxybenzaldehyde showed a score of –6.0 kcal/mol and the same reported PRO226/LEU227 hydrophobic contacts and GLU587/ARG590 hydrogen-bond contacts. The highest docking score in the reported set was observed for 2,4-diamino-5-butyl-8-hydroxy-5H-chromeno[2,3-b]pyridine-3-carbonitrile at –8.8 kcal/mol, with hydrophobic contacts involving PRO226 and GLU594 and a weak hydrogen bond involving GLU594.

➤ Molecular Docking Study

The standard drug captopril showed a docking score of –6.0 kcal/mol against ACE (1J37). Pinolenic acid showed a

Table 5 Docking Scores of Selected Phytochemicals and Captopril against ACE (PDB ID: 1J37)

S. No.	Ligand	PDB/Chem ID	Docking score (kcal/mol)
1	Captopril (standard)	44093	–6.0
2	Pinolenic acid	5312495	–6.7
3	Salicylic acid	338	–6.4
4	2,4-Dihydroxybenzaldehyde	7213	–6.0
5	2,4-Diamino-5-butyl-8-hydroxy-5H-chromeno[2,3-b]pyridine-3-carbonitrile	110875302	–8.8

Table 6 Reported Interaction Residues of Ligands with ACE (PDB ID: 1J37)

Ligand	Hydrogen-bond interactions reported in thesis	Hydrophobic/other contacts reported
Captopril	ASP223, GLU587, ARG590	ILE224, LEU227, ALA583
Pinolenic acid	PRO226, GLU594	GLU594, ARG39, VAL42, ILE65, GLU68
Salicylic acid	GLU587, ARG590	PRO226, LEU227
2,4-Dihydroxybenzaldehyde	GLU587, ARG590	PRO226, LEU227
2,4-Diamino-5-butyl-8-hydroxy-5H-chromeno[2,3-b]pyridine-3-carbonitrile	GLU594 (weak H-bond)	PRO226, GLU594

➤ Docking Pose of Captopril with 1j37

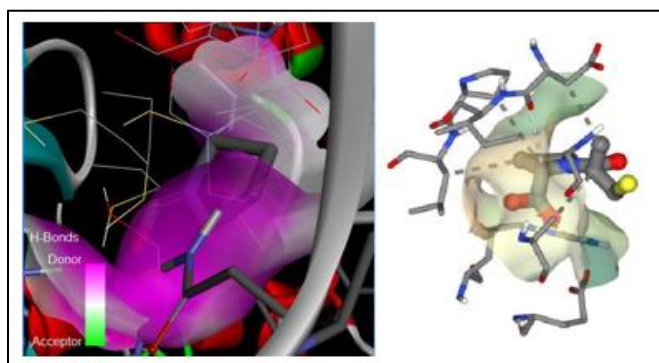


Fig 3 Docking Pose of Captopril with 1j37

➤ Docking Pose of Pinolenic Acid with 1j37

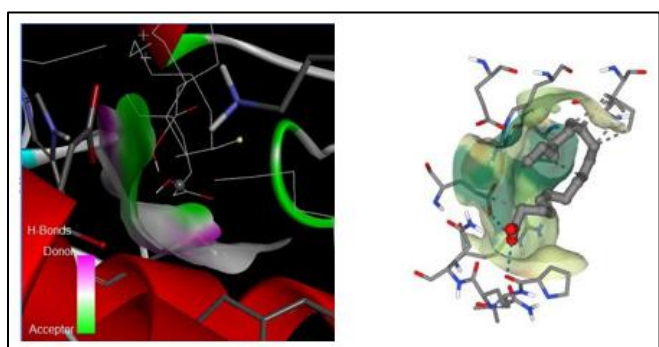


Fig 4 Docking Pose of Pinolenic Acid with 1j37

➤ Docking Pose of Salicylic Acid with 1j37

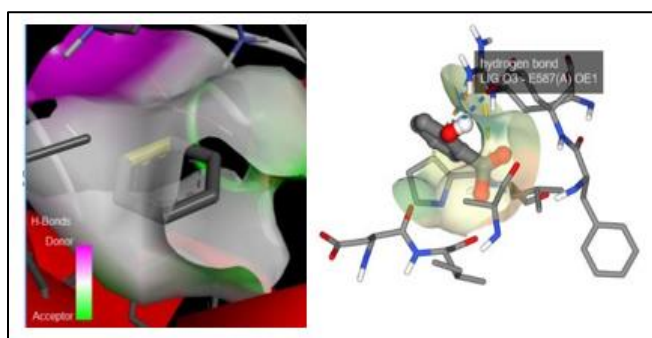


Fig 5 Docking Pose of Salicylic Acid with 1j37

➤ Docking Pose of 2,4-Dihydroxybenzaldehyde with 1j37

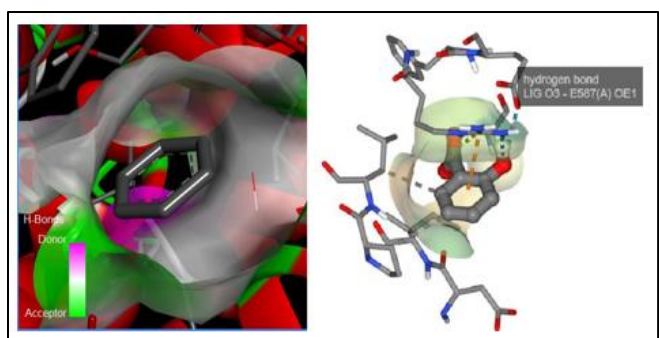


Fig 6 Docking Pose of 2,4-Dihydroxybenzaldehyde with 1j37

➤ Docking Pose of 2,4-Diamino-5-Butyl-8-Hydroxy-5h-Chromeno[2,3-B]Pyridine-3-Carbonitrile with 1j37

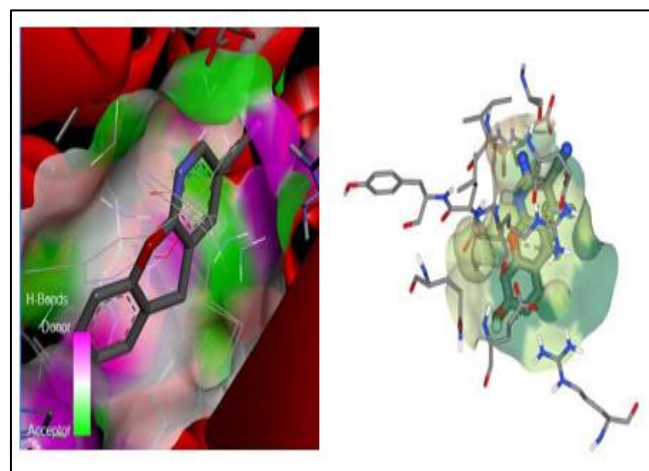


Fig 7 Docking Pose of 2,4-Diamino-5-Butyl-8-Hydroxy-5h-Chromeno[2,3-B]Pyridine-3-Carbonitrile with 1j37

The docking results provide a *in silico* comparison of the selected phytochemicals with captopril at the ACE target. The more negative binding score observed for 2,4-diamino-5-butyl-8-hydroxy-5H-chromeno[2,3-b]pyridine-3-carbonitrile indicates a stronger predicted binding affinity within the scoring framework used in the study. Pinolenic acid and salicylic acid also produced docking scores within the range observed for the reference drug. These *in silico* findings support further experimental investigation; however, docking scores alone do not establish pharmacological efficacy or clinical anti-hypertensive activity.

IV. CONCLUSION

The present study investigated the phytochemical profile of *Capparis zeylanica* Linn. leaves and evaluated selected GC-MS-identified constituents by molecular docking against ACE (PDB ID: 1J37). The ethyl acetate extract showed a broader qualitative phytochemical profile than the other tested extracts, and GC-MS analysis identified ten constituents. Among the compounds evaluated by docking, 2,4-diamino-5-butyl-8-hydroxy-5H-chromeno[2,3-b]pyridine-3-carbonitrile showed the most negative docking score (−8.8 kcal/mol), followed by pinolenic acid (−6.7 kcal/mol), salicylic acid (−6.4 kcal/mol) and 2,4-dihydroxybenzaldehyde (−6.0 kcal/mol), while captopril showed −6.0 kcal/mol. The results provide a molecular-level basis for further investigation of the selected *C. zeylanica* phytochemicals as potential anti-hypertensive leads. Further *in vitro*, *in vivo* and toxicological studies are required to establish their pharmacological activity and safety.

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