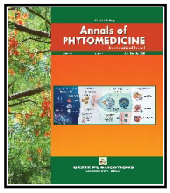
Annals of Phytomedicine 14(2): 409-419, 2025

DOI: http://dx.doi.org/10.54085/ap.2025.14.2.39

Annals of Phytomedicine: An International Journal
http://www.ukaazpublications.com/publications/index.php

Print ISSN : 2278-9839 Online ISSN : 2393-9885



Original Article : Open Access

Phytochemical profiling, nutritional composition, and *in silico* ADMET-antioxidant analysis of *Asparagus racemosus* (Willd.) root

K. Preethi*, R. Yogeswari*◆, T. Ramasamy, A. Raja*** and S. Ramesh***

**Department of Veterinary Pharmacology and Toxicology, Madras Veterinary College, Chennai-600007, Tamil Nadu, India*
*** Department of Veterinary Clinical Complex, Veterinary College and Research Institute, Salem-636112, Tamil Nadu, India*
**** Department of Animal Biotechnology, Madras Veterinary College, Chennai-600007, Tamil Nadu, India*

Article Info

Article history
Received 7 November 2025
Revised 9 December 2025
Accepted 10 December 2025
Published Online 30 December 2025

Keywords
Asparagus racemosus (Willd.)
Phytochemical profiling
Antioxidant
Molecular docking
ADME

Abstract

This study explored the phytochemical composition, proximate parameters, and *in silico* antioxidant potential of *Asparagus racemosus* (Willd.) root. Proximate analysis revealed a rich nutritional profile, notably high in dietary fiber (37.2%). Phytochemical screening confirmed the presence of glycosides, saponins, tannins, flavonoids, and steroids, while HPTLC detected inulin (0.05%) and GC-MS identified five major bioactive constituents. Molecular docking of major phytocompounds (asparanin B, asparagamine A, shatavarin I, β-sitosterol, and sarsasapogenin) with antioxidant enzymes like catalase, glutathione peroxidase, superoxide dismutase, and lipoxygenase, showed strong binding affinities (−8.04 to −10.98 kcal/mol), particularly for asparanin B, asparagamine A, and sarsasapogenin. Among the compounds that showed strong binding affinities, sarsasapogenin possess favorable pharmacokinetic and safety properties, predicted by ADMET lab 3.0. Collectively, these findings highlight *A. racemosus* as a nutritionally rich and pharmacologically promising plant with potent prebiotic and antioxidant potential.

1. Introduction

The genus *Asparagus* comprises nearly 300 species worldwide and is recognized for its medicinal importance due to the presence of steroidal saponins and sapogenins in various plant parts. Among the 22 *Asparagus* species identified in India, *A. racemosus* is most widely utilized in traditional medicine (Thakur *et al.,* 2012). *Asparagus racemosus* (Willd.) (family Liliaceae), commonly referred to as Shatavari, is a perennial shrub characterized by its tuberous root system, recurved spiny stems, and clusters of slender, linear leaves. The plant produces small, white, fragrant flowers that typically bloom during October (Goyal *et al.,* 2003). *A. racemosus* is often regarded as the "queen of herbs" because of its broad range of therapeutic properties (Anubhav *et al.,* 2023).

Asparagus is also a widely consumed perennial vegetable valued for its high nutritional content and low caloric value. Its spears are rich in polyphenols, flavonoids, ascorbic acid, and amino acids, while the roots are traditionally employed in medicine owing to their abundance of saponins and fructans. The plant develops from an underground rhizome with fleshy storage roots that persist for several years, primarily accumulating fructans as reserve carbohydrates (Witzel and Matros, 2020). In humans, the intake of inulin-type fructans provides several health benefits, including the promotion of regular bowel movements, reduction of serum cholesterol and triglycerides, enhancement of mineral absorption (such as calcium and magnesium), maintenance of colonic microflora balance, and regulation of appetite (Alonso-Allende, 2024).

Traditionally, *A. racemosus* has been used as a tonic, diuretic, galactagogue, and antiulcer agent. Its roots are reported to be beneficial in treating nervous disorders, inflammation, and certain infections due to their mucosal-protective and immunomodulatory effects (Alok *et al.,* 2013). In Ayurvedic medicine, *A. racemosus* is renowned for its immunomodulatory, adaptogenic, and rejuvenating properties, enhancing immune responses, stimulating corticosteroid secretion, and promoting cellular regeneration. Its roots have long been employed in the management of infertility, gastric ulcers, and respiratory ailments (Hossain *et al.,* 2012). Owing to its phytoestrogenic constituents and adaptogenic activity, the plant has also been reported to possess antioxidant, antidiarrheal, immunostimulant, antitussive, and digestive-supporting effects (Visavadiya *et al.,* 2009).

Oxidative stress arises from an imbalance between free radical generation and the body's antioxidant defence mechanisms, resulting in cellular and molecular damage. Dietary antioxidants help to mitigate this damage by neutralizing reactive oxygen species. Regular consumption of plant-based antioxidants is essential for maintaining physiological balance and preventing oxidative stress-related disorders, as plants are rich sources of bioactive antioxidant compounds (Karuna *et al.,* 2018). Given the increasing scientific interest in elucidating the antioxidant potential of *A. racemosus* through *in silico* methodologies, this study aims to comprehensively evaluate its phytochemical composition, proximate nutritional profile, and *in silico* ADME, toxicity and antioxidant properties. The findings are expected to contribute to the growing body of evidence supporting the therapeutic and nutraceutical applications of *A. racemosus*, while also identifying promising lead compounds for future drug development.

Corresponding author: Dr. R. Yogeswari
Associate Professor, Department of Veterinary Pharmacology and Toxicology, Madras Veterinary College, Chennai-600007, Tamil Nadu, India
E-mail: dryogavet@gmail.com
Tel.: +91-9080805060

2. Materials and Methods

2.1 Plant material

The dried roots of *Asparagus racemosus* (Willd.) were procured from the Siddha Medicinal Plants Garden, Mettur Dam, Salem, Tamil Nadu, along with an authentication certificate. The Voucher Specimen Number is A19022521R. The roots were pulverized using a commercial mixer grinder and stored in an airtight container until further analysis.

2.2 Proximate analysis

The proximate composition, including moisture, crude protein, crude fibre, crude fat, ash, and total carbohydrate contents, was determined following the procedure described by Rajni *et al.* (2023) in accordance with the AOAC (2010) guidelines.The dietary soluble and insoluble fibre contents were quantified using the method of Rajni *et al.* (2023) and Prosky (1990).Total carbohydrate content was calculated by the difference method (AOAC, 2016) using the formula:

Total carbohydrate (%) = 100 – [Moisture (%) + Ash (%) + Crude fat (%) + Crude fiber (%) + Crude protein (%)]

2.3 Preparation of aqueous root extract

The aqueous extract of *A. racemosus* roots was prepared following the method of Hamdi *et al.* (2022) and the final extract was collected and stored at 20°C for further analyses.

2.4 Qualitative phytochemical screening

Qualitative phytochemical screening of *A. racemosus* root extract was performed following the procedure described by Birader (2016). The presence or absence of major phytochemical groups including glycosides, saponins, tannins, carbohydrates, alkaloids, steroids, flavonoids, terpenoids, quinones, proteins, reducing sugars, phlobotannins, and oils and lipidswas evaluated using standard colorimetric and precipitation tests.

2.5 Estimation of inulin by HPTLC

The inulin content in the aqueous extract was determined using high-performance thin-layer chromatography (HPTLC), following the method of Petkova and Denev (2013). Inulin standard (Loba Chemie Pvt. Ltd.) and sample solutions were spotted to the plates using a CamagLinomat 5 applicator andthe developed chromatograms were scanned using a Camag TLC Scanner 3 at 441 nm with deuterium and tungsten light sources.

2.6 Gas chromatography-mass spectrometry (GC-MS) analysis

The aqueous extract subjected to GC-MS analysis was reconstituted in methanol at a concentration of 1 mg/ml prior to analysis (Kumar *et al.,* 2021). GC-MS analysis of the aqueous extract was carried out using a Shimadzu QP2020 spectrometer equipped with an Rtx-5MS column (30 m × 0.53 mm, 0.25 µm). Helium was used as the carrier gas (1 ml/min). The oven temperature was programmed from 50°C to 300°C at 10°C/min. The injector operated in split mode (1:10) with a 1 µl injection volume, and spectra were recorded in EI mode (70 eV) across m/z 40-600. Compounds were identified by comparing their mass spectra and retention indices with NIST library data.

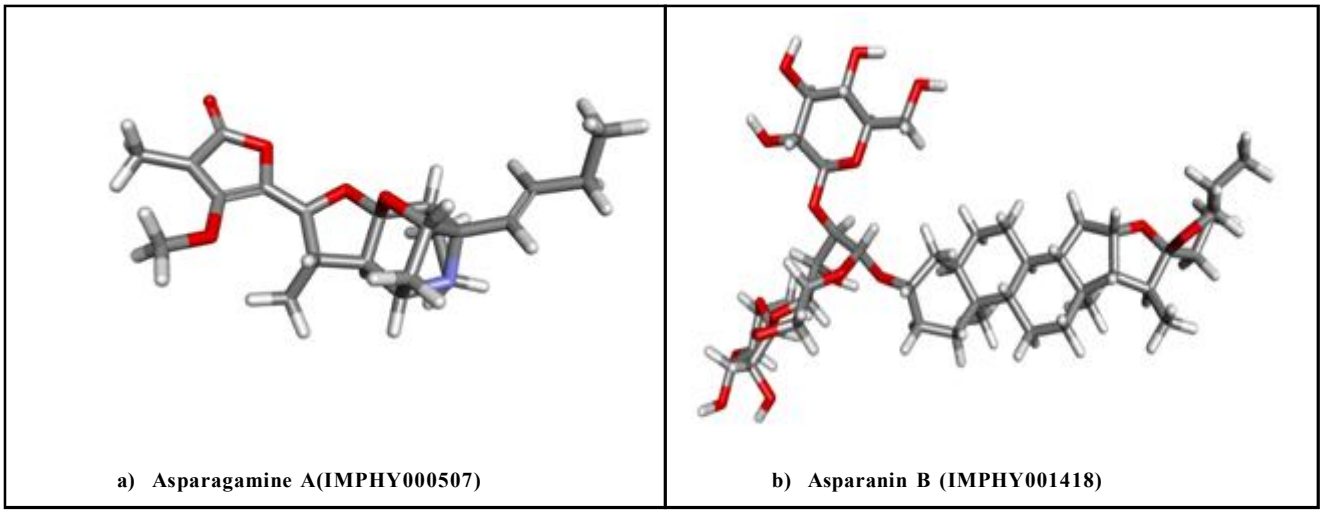
2.7 *In silico* analysis

2.7.1 Molecular docking

Molecular docking was performed to predict the antioxidant potential of *A. racemosus* root constituents by evaluating their interactions with key enzymes involved in oxidative stress regulation: catalase, glutathione peroxidase, lipoxygenase, and superoxide dismutase (SOD). Docking simulations were conducted using AutoDockTools (MGL Tools version 1.5.7), with vitamin C serving as the reference antioxidant compound.

2.7.1.1 Ligand preparation

The five major phytochemicals identified from *Asparagus racemosus* roots, asparagamine A, asparanin B, β-sitosterol, sarsasapogenin, and shatavarin I were retrieved in SDF format from the IMPPAT database, while vitamin C was obtained from PubChem. The 3D structures of all ligands are presented in Figure 1. Ligand structures were converted to PDB format using Molegro Molecular Viewer, followed by the addition of hydrogen atoms, assignment of Kollman charges, and definition of rotatable bonds to ensure torsional flexibility. The optimized ligand files were saved in PDBQT format for use in Auto Dock Tools (Kumar and Mamidala, 2025).



a) Asparagamine A(IMPHY000507)

b) Asparanin B (IMPHY001418)

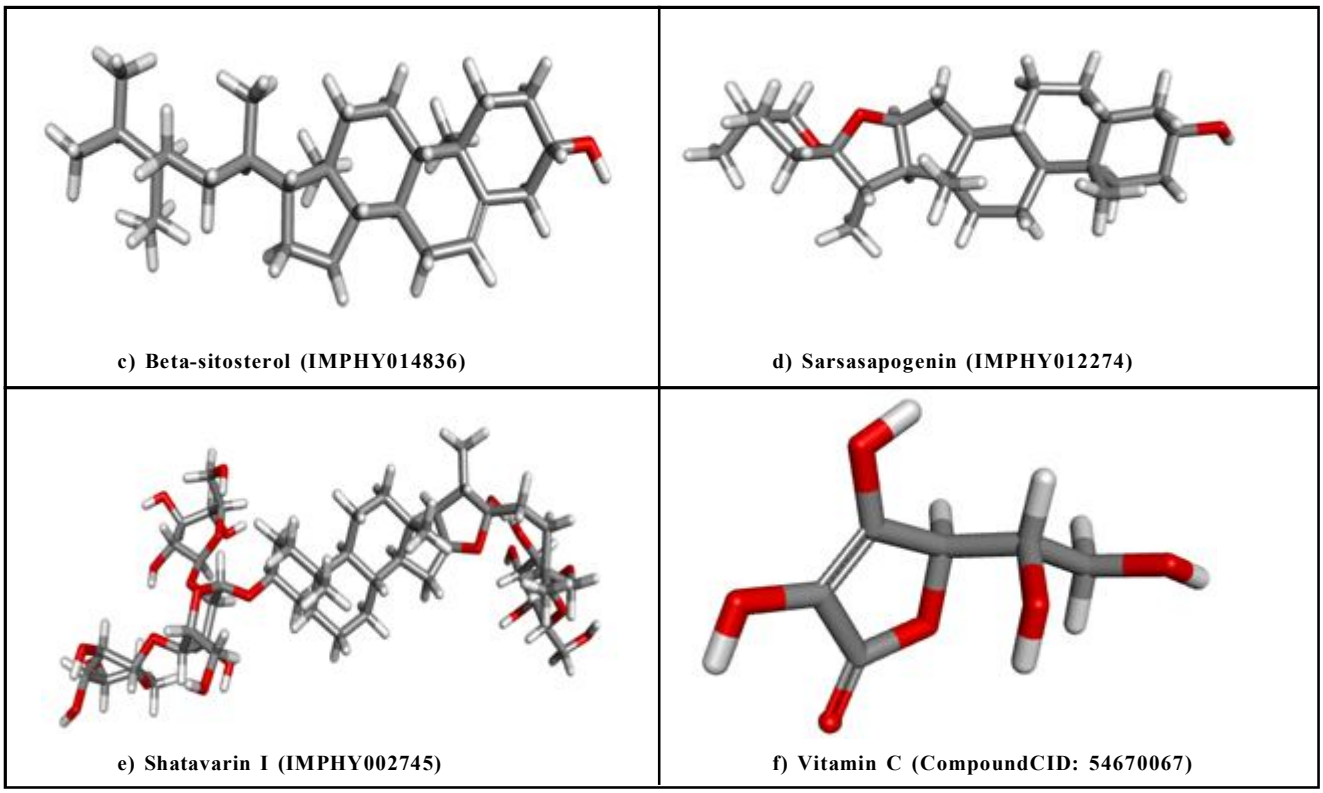


Figure 1: Three-dimensional structure of various phytochemicals present in roots of *A. racemosus* with ID.

2.7.1.2 Protein preparation

The key antioxidant enzymes - catalase (CAT), glutathione peroxidase (GP), lipoxygenase (LPO), and superoxide dismutase (SOD) - were selected as target proteins, with their 3D crystal structures obtained from the RCSB Protein Data Bank (PDB). The corresponding PDB IDs and structures are shown in Figure 2. Protein models were refined by removing co-crystallized ligands and water molecules, retaining only the relevant protein chains. Polar hydrogens were added, and Gasteiger charges were assigned using AutoDockTools. The prepared protein structures were saved in PDBQT format for molecular docking. Blind docking was employed, allowing ligands to explore the entire protein surface and identify both known and potential novel binding sites (Kumar and Mamidala, 2025).

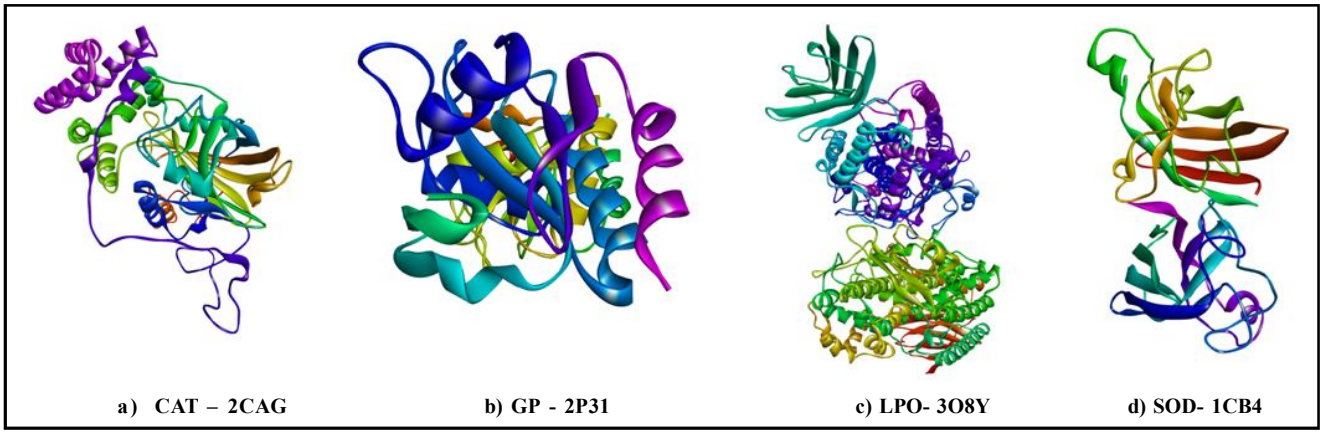


Figure 2: Three-dimensional structure of the proteins with PDB ID.

2.7.1.3 Molecular docking method

Molecular docking was performed using AutoDock to analyze receptor-ligand interactions. Receptor and ligand structures were prepared in PDBQT format after removing water molecules and co-crystallized ligands, followed by the addition of polar hydrogens and partial charges. A grid box covering the entire protein structure was generated to perform blind docking, enabling the exploration of all potential ligand-binding sites. Docking was executed with default parameters, generating up to 20 conformations per ligand at a grid spacing of 1.0 Å. The best binding poses were selected based on binding energy (ΔG) and key molecular interactions (Kumar and Mamidala, 2025).

2.7.1.4 Post-docking analysis

Post-docking analyses were performed using BIOVIA Discovery Studio and AutoDockTools to visualize key non-covalent interactions such as hydrogen bonding, hydrophobic contacts, and π-π stacking. These interactions revealed ligand binding orientation, stability, and affinity within the active site, with compounds showing strong binding and favourable profiles identified as potential antioxidants comparable to vitamin C.

2.7.2 ADMET predictions

The pharmacokinetic (ADME) properties, including absorption, distribution, metabolism, and excretion, along with the toxicity profiles of the phytochemicals exhibiting higher binding affinities in molecular docking, were predicted using the ADMETlab 3.0 web server as per Xiong *et al.* (2021). The SMILES notations of the selected compounds were retrieved from the Indian Medicinal plants, phytochemistry, and therapeutics (IMPPAT) database and subsequently submitted to ADMET lab 3.0 for *in silico* prediction of their pharmacokinetic and toxicity characteristics.

3. Results

3.1 Proximate composition

The proximate composition of *A. racemosus* root contained 9.90 ± 0.085% moisture, 9.28 ± 0.133% crude protein, 11.53 ± 0.06% crude fibre, 0.81 ± 0.044% crude fat, 7.90 ± 0.028% ash, and 60.58 ± 0.079% total carbohydrates. The total dietary fibre content was 37.20 ± 0.12%, comprising 10.10 ± 0.05% soluble fibre and 27.10 ± 0.07% insoluble fibre.

3.2 Qualitative phytochemical analysis

The results of the qualitative phytochemical analysis of the aqueous extract of *A. racemosus* root are presented in Table 1. The aqueous extract of *A. racemosus* root tested positive for carbohydrates, glycosides, steroids, flavonoids, tannins, saponins, proteins, and reducing sugars.

Table 1: Qualitative phytochemical screening of *A. racemosus* root aqueous extract

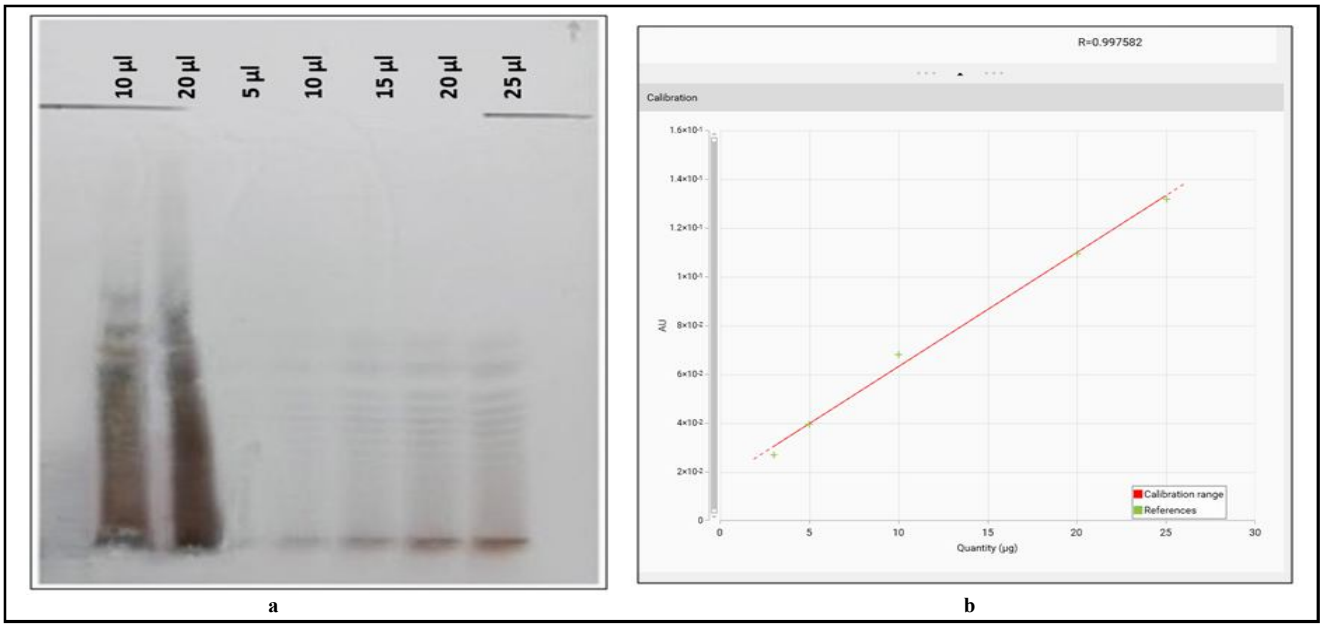
Phytochemical	Indications
Alkaloids	Absent
Carbohydrates	Present
Flavanoids	Present
Glycosides	Present
Oils and lipids	Absent
Phlobotannin	Absent
Proteins	Present
Quinone	Absent
Reducing sugars	Present
Saponin	Present
Steroids	Present
Tannin	Present
Terpenoids	Absent

3.3 Estimation of inulin

The HPTLC analysis of the aqueous extract confirmed the presence of a high-molecular-weight fraction corresponding to inulin (Figure 3a). Based on the linearity curve (Figure 3b), the inulin content in the *A. racemosus* aqueous extract was quantified as 0.05%. The chromatographic profiles, including the peak areas of the inulin standard and the sample, are presented in Figures 3c and 3d, respectively.

3.4 GC-MS analysis

GC-MS analysis was performed to identify the bioactive compounds present in the roots of *A. racemosus*. The chromatogram (Figure 4) illustrates the various phytochemical constituents detected in the extract. The identified compounds, along with their corresponding peak areas (%) and molecular formulas, are summarized in Table 2. The analysis revealed five distinct compounds eluting at different retention times, each represented by separate peaks. Compound identification was achieved through comparison with the NIST library database, which provided five major hits for each observed peak.



a b

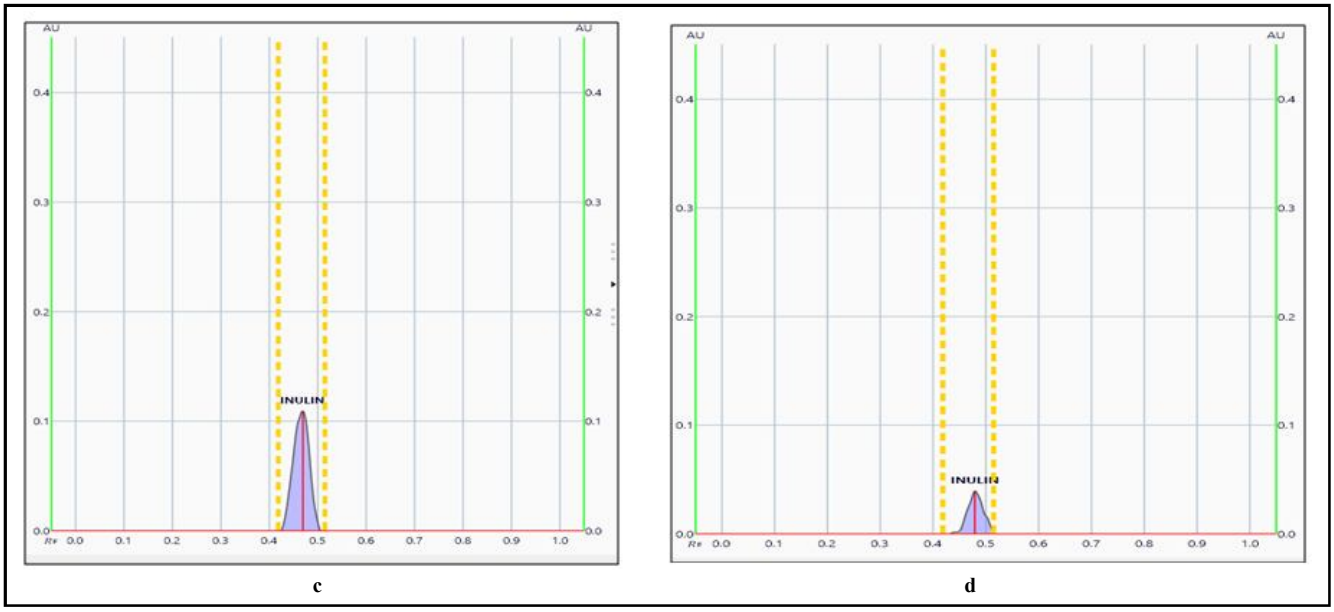


Figure 3: HPTLC analysis of inulin in the aqueous extract of *Asparagus racemosus* (Willd.): (a) Silica gel plate showing developed spots of standards and sample, (b) linearity curve of inulin standards, (c) chromatographic peak area of the inulin standard, and (d) chromatographic peak area of the sample.

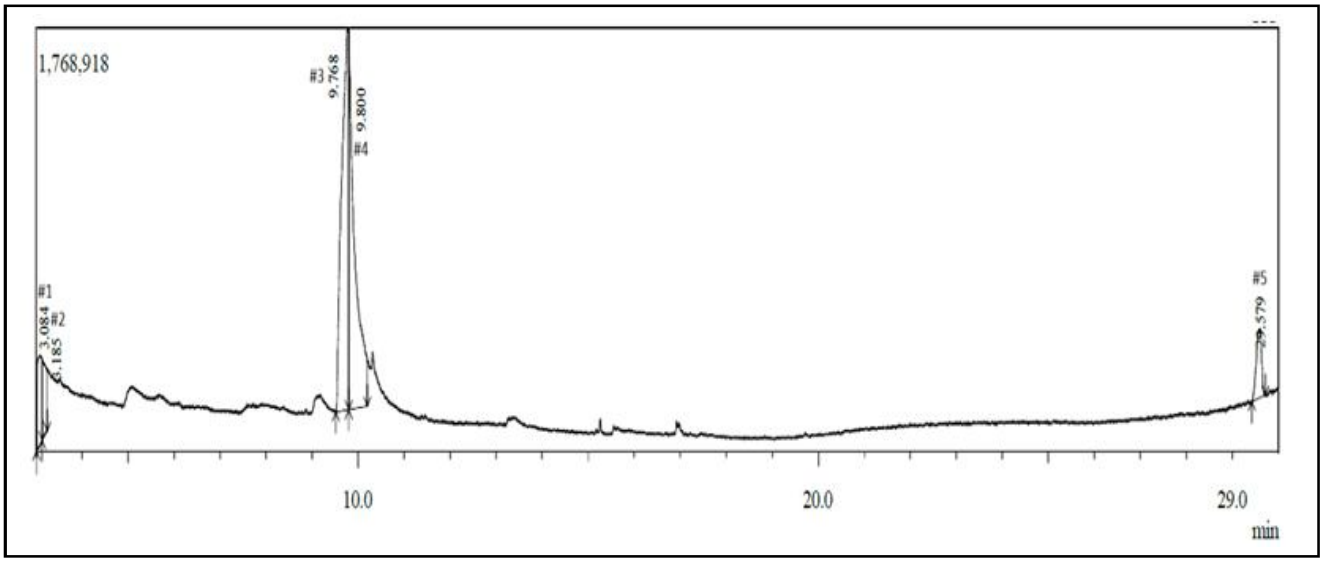


Figure 4: Chromatogram of the aqueous extract of *A. racemosus* root obtained by GC-MS analysis (Five compounds as listed in the table is mentioned near the peaks as #1, #2, #3, #4 and #5).

Table 2: List of bioactive compounds identified in the aqueous extract of *A. racemosus* root through GC-MS analysis, along with their retention time, peak area (%), molecular formula, and molecular weight

S.No.	Compound name	Peak area (%)	Retention time	Molecular formula	Molecular weight
1	N-Ethyl-N' nitroguanidine	6.76	3.084	$C_3H_8N_4O_2$	132
2	(S)-(+)-1-Cyclohexylethylamine, N-acetyl-	5.24	3.185	$C_{10}H_{19}NO$	169
3	1,3-Propanediol,2-ethyl-2(hydroxymethyl)-	44.10	9.678	$C_6H_{14}O_3$	134
4	4-Piperidinecarboxamide	37.66	9.800	$C_6H_{12}N_2O$	128
5	2-tert-Butyl-4,6-bis(3,5-di-tert-butyl-4-hydroxybenzyl)phenol	6.24	29.579	$C_{40}H_{58}O_3$	586

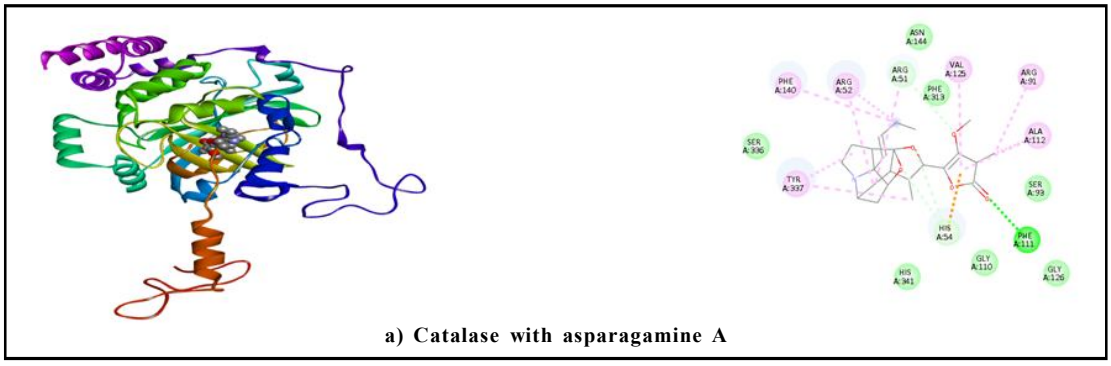
3.5 *In silico* predictions

3.5.1 Molecular docking

The docking results, including binding energies, hydrogen bond interactions, and hydrophobic contacts, were analyzed and compared across all compounds. Among the tested phytochemicals, asparanin B, asparagamine A, and sarsasapogenin exhibited the strongest binding affinities toward all target enzymes, with binding energies ranging from –8.04 to –10.98 kcal/mol. The detailed binding affinities and interaction profiles of each ligand - enzyme complex are presented in Table 4. The three-dimensional and two dimensional docking conformations of the best-scoring ligand for each protein are illustrated in Figure 5.

Table 4: Comparative binding affinities and interaction profiles of *A. racemosus* root phytochemicals and vitamin C with antioxidant enzymes

S.No.	Protein	Compound	Binding energy (kcal/mole)	No. of hydrogen bonds	Inhibition constant
1	Catalase	Asparagamine A	**-10.57**	-	17.81 nM
		Asparanin B	**-9.87**	1 (Glu414)	57.96 nM
		Beta-setosterol	-6.45	-	18.86 µM
		Sarsasapogenin	**-9.01**	-	249.17 nM
		Shatavarin I	-1.37	1 (Glu404)	98.29 mM
		Vit C	-4.75	-	328.08 µM
2	Glutathione peroxidase	Asparagamine A	**-8.3**	1 (Val165)	827.33 nM
		Asparanin B	**-9.25**	-	164.49 nM
		Beta-setosterol	-7.61	1 (Ala119)	2.65 µM
		Sarsasapogenin	**-8.91**	2 (Arg34, Asn80)	293.52 nM
		Shatavarin I	-3.62	2 (Lys29, Lys117)	2.22 mM
		Vit C	-6.98	2 (Glu99, Glu99)	7.61 µM
3	Lipoxygenase	Asparagamine A	**-8.99**	1 (Gln329)	255.75 nM
		Asparanin B	**-10.98**	1 (Glu146)	8.95 nM
		Beta-setosterol	-7.4	1 (Gln227)	3.75 µM
		Sarsasapogenin	**-10.51**	2 (Leu288, Arg370)	19.81 nM
		Shatavarin I	-1.01	-	183.25 mM
		Vit C	-6.9	5 (Asp166, Asp170, Trp102, Asp166, Asp166)	8.8 µM
4	Superoxide dismutase	Asparagamine A	**-8.1**	-	1.15 µM
		Asparanin B	**-8.04**	1 (Asn63)	1.28 µM
		Beta-setosterol	-6.51	-	16.85 µM
		Sarsasapogenin	**-8.85**	-	323.55 nM
		Shatavarin I	-2.87	2 (Lys151, Arg113)	7.85 mM
		Vit C	-5.18	1 (Val146)	159.99 µM



a) Catalase with asparagamine A

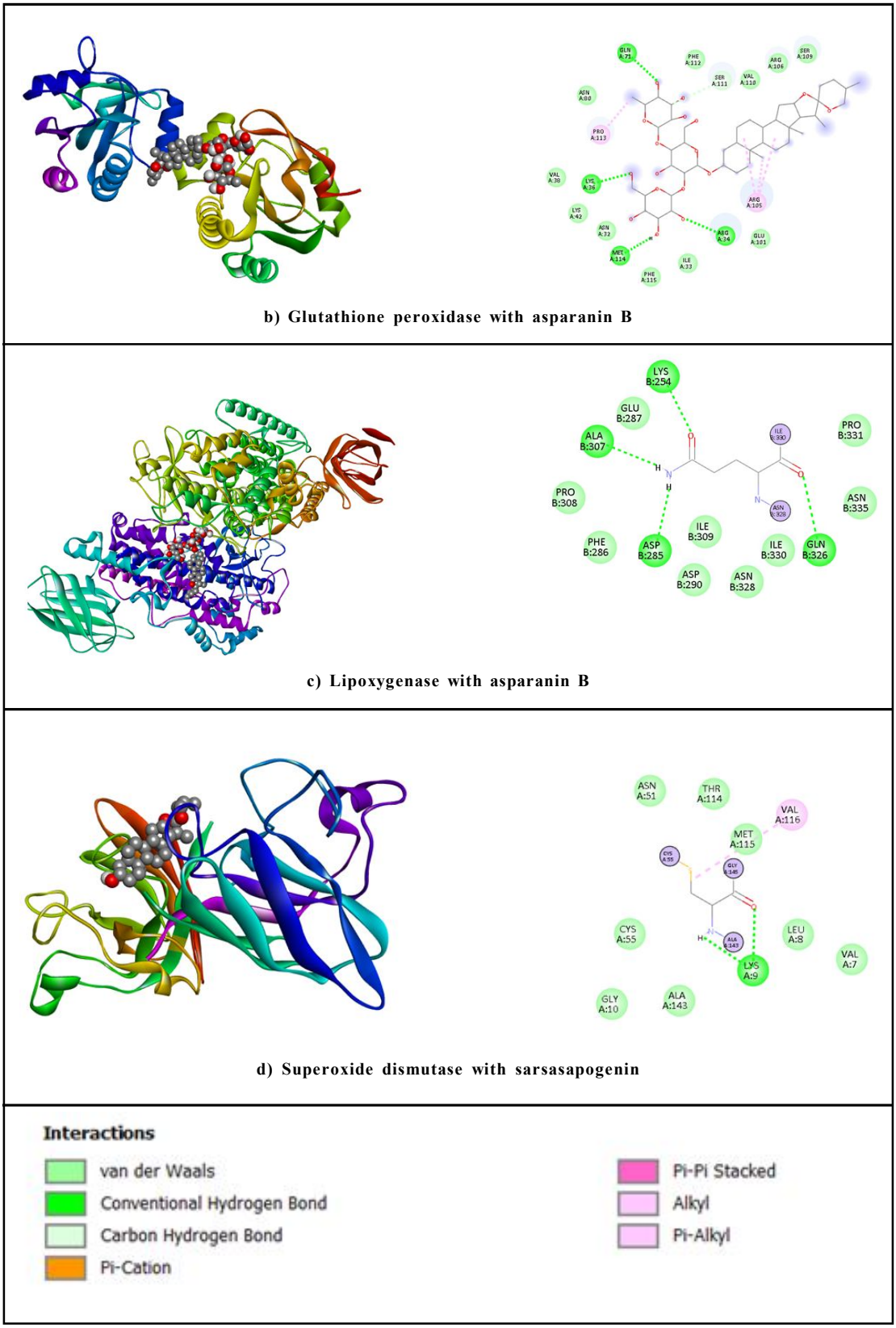


Figure 5: Three-dimensional and two-dimensional interaction views of antioxidant enzymes docked with *A. racemosus* phytochemicals showing the highest binding affinities.

Table 3: Predicted ADMET and toxicity profiles of major phytochemicals from *A. racemosus* root, as obtained using ADMETlab 3.0

	Asparagamine A	Asparanin B	Sarsasapogenin
ADME			
Caco-2 permeability	-4.782	-6.23	-5.132
logP	2.573	1.899	5.491
Lipinski	Accepted	Rejected	Accepted
PPB %	95.1%	59.7	94
VDss	0.026	-0.381	0.49
BBB	—	—	—
CYP1A2	++	—	—
CYP2D6	—	—	—
CYP3A4	-	+++	—
CL_{plasma}	7.499	0.148	17.351
T1/2	1.122	3.291	1.583
Toxicity			
hERG blockers	0.087	0.019	0.133
AMES toxicity	0.674	0.841	0.171
Rat oral acute toxicity	0.739	0.004	0.183
Skin sensitization	**0.987**	**1**	**0.988**
Eye irritation	0.024	0.001	0.901
Respiratory	0.717	0.0	0.292
Hepatotoxicity	0.67	0.545	0.597
Nephrotoxicity	0.542	0.726	0.353
Neurotoxicity	0.402	0.0	0.034
Genotoxicity	0.951	0.0	0.001
LC_{50} FM	5.122	4.015	4.588

3.5.2 ADMET predictions

The ADMETlab 3.0 predictions for the compounds with higher binding affinity, asparagamine A, asparanin B, and sarsasapogenin from *A. racemosus* root are summarized in Table 3.

3.5.2.1 Distribution

The log P values (2.573, 1.899, and 5.491 for asparagamine A, asparanin B, and sarsasapogenin, respectively) fall within the acceptable range (0–5) for good lipophilicity and membrane permeability. However, sarsasapogenin is at the upper limit, indicating higher lipophilicity. Lipinski's rule of five was accepted for asparagamine A and sarsasapogenin, while asparanin B was rejected, indicating possible deviation from ideal drug-likeness criteria.The plasma protein binding (PPB%) was high for asparagamine A (95.1%) and sarsasapogenin (94%), suggesting strong plasma binding and lower free drug availability, whereas asparanin B show edmoderate binding (59.7%). The volume of distribution (VDss) values (0.026, –0.381, and 0.49, respectively) indicated that sarsasapogenin exhibits higher tissue distribution, while asparanin B is more confined to plasma. None of the compounds were predicted to cross the blood–brain barrier (BBB), suggesting limited CNS penetration.

3.5.2.2 Metabolism

Cytochrome P450 (CYP) enzyme inhibition prediction indicated that asparagamine A inhibits CYP1A2, while asparanin B strongly inhibits CYP3A4 (+++), suggesting potential drug-drug interaction risks. All three compounds were non-inhibitors for CYP2D6.

3.5.2.3 Excretion

The plasma clearance (CL plasma) values (7.499, 0.148, and 17.351 ml/min/kg for asparagamine A, asparanin B, and sarsasapogenin, respectively) suggest that sarsasapogenin and asparagamine A have high clearance rates and are eliminated rapidly, whereas asparanin B is cleared slowly. Correspondingly, the half-life ($T_{1/2}$) values (1.122, 3.291, and 1.583 h) indicate that asparanin B has the longest retention in the body.

3.5.2.4 Toxicity

Toxicity parameters included hERG inhibition (cardiotoxicity), AMES test (mutagenicity), and organ-specific toxicity probabilities (hepatic, renal, neural, genotoxic, and others) ranging from 0 (low) to 1 (high).

- **hERG blockers:** All compounds showed low hERG inhibition probabilities (0.087, 0.019, and 0.133), indicating no cardiotoxic risk.
- **AMES toxicity:** Asparanin B (0.841) was predicted to be mutagenic, while asparagamine A (0.674) and sarsasapogenin (0.171) were likely non-mutagenic.
- **Rat acute oral toxicity:** Asparanin B (0.004) had very low acute oral toxicity, indicating safety, while asparagamine A (0.739) and sarsasapogenin (0.183) showed mild toxicity.
- **Skin sensitization:** All three compounds were predicted to be skin sensitizers (0.987-1.000).
- **Eye irritation:** Sarsasapogenin (0.901) exhibited a higher probability for eye irritation, while asparanin B (0.001) was least irritant.
- **Respiratory toxicity:** Asparagamine A (0.717) showed moderate risk, while asparanin B (0.000) and sarsasapogenin (0.292) were safer.
- **Hepatotoxicity:** All compounds had moderate hepatic toxicity risk (0.545-0.67).
- **Nephrotoxicity:** Asparanin B (0.726) showed slightly higher renal toxicity, whereas sarsasapogenin (0.353) was lowest.
- **Neurotoxicity:** Asparagamine A (0.402) showed mild neurotoxic potential, while asparanin B (0.000) and sarsasapogenin (0.034) were safer.
- **Genotoxicity:** Asparagamine A (0.951) was predicted to be highly genotoxic, while asparanin B (0.000) and sarsasapogenin (0.001) were non-genotoxic.
- **Aquatic toxicity (LC_{50} FM):** The values (5.122, 4.015, and 4.588) indicates low aquatic toxicity for all compounds, with asparagamine A being the least toxic to aquatic organisms.

4. Discussion

This study highlights the antioxidant potential of *A. racemosus* and underscores its possible use as a prebiotic and natural antioxidant source. The findings of the qualitative phytochemical analysis in the present study are consistent with those reported by Agarwal *et al.* (2008). Similarly, Tripathi *et al.* (2021) observed that the petroleum ether extract contained only saponins, while the ethyl acetate extract lacked steroids, terpenoids, glycosides, and proteins. Furthermore, the methanolic extract exhibited a comparable phytochemical profile to that of the current study, with the exception of the absence of proteins.

Saini *et al.* (2016) reported a comparable proximate composition, though with higher levels of protein (21.8 ± 0.56%) and fat (3.76 ± 0.11%), along with a total dietary fibre content of 25.72 ± 0.74%, comprising 6.93 ± 0.15% soluble and 18.65 ± 0.42% insoluble fractions. The presence of 10.1 ± 0.05% soluble dietary fibre in the present study suggests its potential as a valuable source of prebiotics in the human diet (Slavin, 2013).

HPTLC analysis confirmed the presence of inulin, a fructan, at 0.05% concentration, lower than the 12.22 ± 1.51% reported by Mudannayake *et al.* (2025). Yaneva *et al.* (2025) similarly reported 24 g/100 g total fructans, including 21.22 g/100 g inulin and smaller amounts of 1-kestose, sucrose, glucose, and fructose, identifying inulin as the predominant polysaccharide in *A. racemosus* roots (~88% of total fructans). Viera-Alcaide *et al.* (2022) observed fructan content in *Asparagus* species ranging from 3–12% (fresh weight) or 8–33% (dry weight), influenced by factors such as harvest season, fertilizer use, altitude, and shade intensity (Majumdar *et al.,* 2021). These environmental and agronomic variations likely affect fructan polymerization and molecular weight among *Asparagus* accessions.

The considerable soluble fibre content (~10%), together with earlier reports of inulin-type fructans (~11.8%), supports the potential of *A. racemosus* root as a natural and sustainable prebiotic source with beneficial effects on gut microbiota (Hamdi *et al.,* 2022). The gut microbiota plays a pivotal role in the gut-brain axis through the production of short-chain fatty acids (SCFAs), which serve as key signalling molecules mediating bidirectional communication between the gut and the central nervous system (Ansari *et al.,* 2023).

GC-MS analysis identified five major bioactive compounds in *A. racemosus* root extract, including 1,3-propanediol, 2-ethyl-2-(hydroxymethyl)-, and 4-piperidine carboxamide as the predominant constituents. The presence of phenolic antioxidants corroborates the observed radical-scavenging and enzyme-interaction activities, suggesting that the phytochemical profile of *A. racemosus* contributes significantly to its functional and therapeutic potential (Eden and Kumar, 2025). Nitrogen-containing compounds such as 4-piperidine carboxamide and other amine derivatives may further enhance anti-inflammatory and antimicrobial effects. The synergistic action between phenolic, flavonoid, and other secondary metabolites likely underpins the strong antioxidant efficacy of the extract (Meher *et al.,* 2024).

The major *A. racemosus* phytoconstituents such as asparanin B, asparagamine A and sarsasapogenin exhibited strong and specific interactions with key antioxidant enzymes, implying their potential in modulating oxidative stress. When compared with the reference antioxidant vitamin C, which showed relatively lower binding affinities (−4.75 to −6.98 kcal/mol across all targets), the phytochemicals demonstrated superior interaction energies and more stable complexes. While vitamin C is a well-established direct radical scavenger also acts through non-enzymatic mechanisms (Liu *et al.,* 2020). The presence of hydrogen bonds, C–H, π–alkyl, and π–σ interactions indicates strong binding affinity of sarsasapogenin with their target receptors, supporting their potential for clinical drug development (Rana *et al.,* 2024). Benavente-García *et al.* (1997) reported that flavonoids play a crucial role in plant antioxidant systems, acting through multiple mechanisms including free radical neutralization, metal ion chelation, and inhibition of oxidative enzymes. The abundance of phenolic and flavonoid compounds in *A. racemosus* extracts likely contributes to its strong antioxidant potential (Samant, 2022). Sekine *et al*. (1994) reported that asparagamine A exhibited antitumor activity in experimental models in a dose-dependent manner. ADMET lab 3.0 predictions revealed that sarsasapogenin exhibited favourable ADMET characteristics likebetter absorption, optimal plasma protein binding and efficient tissue distribution and less drug interaction. Rana *et al*. (2024) reported that this compound is non-cardiotoxic, with sarsasapogenin showing the best drug-like behavior and high bioavailability. Sarsasapogenin, a natural steroidal sapogenin, is a potent compound known for its anti-inflammatory, anticancer, antidiabetic, anti-

osteoclastogenic, and neuroprotective properties (Mustafa *et al.,* 2022). Furthermore, Choudhary *et al*. (2025) reported that *A. racemosus* was found to be safe in both acute and sub-acute toxicity studies in mice.

Collectively, these findings reinforce the potential of sarsasapogenin as a potent natural antioxidant and prebiotic lead compound. Its favorable ADMET profile, and strong molecular interactions with key antioxidant enzymes underscore its promise as a candidate for pharmacological applications aimed at mitigating oxidative stressrelated disorders and the root of the plant as a whole with high dietary fibre and inulin content can be used to modulating the gut-brain axis.

5. Conclusion

The present study establishes *A. racemosus* as a nutritionally rich and phytochemically diverse plant with remarkable prebiotic and antioxidant potential. The identification of inulin-type fructans and key bioactive compounds through GC-MS analysis reinforces its relevance in promoting gut health and maintaining gut-brain homeostasis. Furthermore, strong molecular interactions exhibited by asparagamine A, asparanin B, and sarsasapogenin and the favourable ADMET properties by sarsasapogenin suggest their therapeutic promise against oxidative stress related disorders. Collectively, these findings position *A. racemosus* as a valuable candidate for the development of nutraceutical and pharmacological formulations, warranting further *in vivo* and clinical investigations of the lead compounds to validate its efficacy and elucidate the underlying molecular signalling pathways.

Acknowledgements

The authors would like to thank Tamil Nadu Veterinary and Animal Sciences University in Chennai, India, for helping to provide the tools and facilities needed to carry out this research.

Conflict of interest

The author declares no conflicts of interest relevant to this article.

References

Agrawal, A.; Sharma, M.; Rai, S. K.; Singh, B.; Tiwari, M. and Chandra, R. (2008). The effect of the aqueous extract of the roots of *Asparagus racemosus* on hepatocarcinogenesis initiated by diethylnitrosamine. Phytotherapy Research, **22**(9):1175-1182.

Alok, S.; Jain, S. K.; Verma, A.; Kumar, M., Mahor, A. and Sabharwal, M. (2013). Plant profile, phytochemistry and pharmacology of *Asparagus racemosus* (Shatavari): A review. Asian Pacific Journal of Tropical Disease, **3**(3):242-251.

Alonso-Allende, J.; Milagro, F.I. and Aranaz, P. (2024). Health effects and mechanisms of inulin action in human metabolism. Nutrients, **16**(17):2935.

Ansari, F.; Neshat, M.; Pourjafar, H.; Jafari, S. M.; Samakkhah, S. A. and Mirzakhani, E. (2023). The role of probiotics and prebiotics in modulating the gut-brain axis. Frontiers in Nutrition, **10**:1173660.

Anubhav, D.; Mrinmoy, B.; Biplab, D. and Niladry, G. (2023). Queen of all herbs (*Asparagus racemosus*): An assessment of its botany, conventional utilization, phytochemistry and pharmacology. Research Journal of Biotechnology, **18**(6):1-9.

AOAC (2010). Official Methods of Analysis (19thEdn). Association of Official Analytical Chemists: Washington, D.C., U.S.A.

AOAC (2016). Official Methods of Analysis (20thEdn). Association of Official Analytical Chemists: Washington, D.C., U.S.A.

Benavente-Garcia, O.; Castillo, J.; Marin, F. R.; Ortuno, A. and Del-Rio, J. A. (1997). Uses and properties of citrus flavonoids. Journal of Agricultural and Food Chemistry, **45**(12):4505-4515.

Biradar, V. (2016). Extraction of phytochemicals from local selected plants and their antibacterial role. International Journal of Current Microbiology and Applied Sciences, **5**:707-720.

Chikhale, R. V.; Sinha, S. K.; Patil, R. B.; Prasad, S. K.; Shakya, A.; Gurav, N.; Prasad, R.; Dhaswadikar, S. R.; Wanjari, M. and Gurav, S. S. (2021). *In silico* investigation of phytochemicals from *Asparagus racemosus* as plausible antiviral agents in COVID-19. Journal of Biomolecular Structure and Dynamics, **39**(14):5033-5047. doi:10.1080/07391102.2020.1784289.

Choudhary, D.; Naik, S. N.; Tyagi, V.; Pal, A. and Hariprasad, P. (2025). Toxicological evaluation of *Asparagus racemosus* - based low-alcohol nutraceutical beverage: acute and subacute safety assessment in mice. Sustainable Food Technology, **3**(5):1439-1449.

Eden, A. H. and Kumar, V. S. (2025). GC-MS profiling of bioactive compounds in *Asparagus racemosus*: Implications for pharmacological properties. International Journal of Pharmaceutical Sciences and Research, **16**(3):791-809. doi:10.13040/IJPSR.0975-8232.16(3).791-09.

Goyal, R. K.; Singh, J. and Lal, H. (2003). *Asparagus racemosus* - An update. Indian Journal of Medical Sciences, **57**:408-414.

Hamdi, A.; Viera-Alcaide, I.; Guillén-Bejarano, R.; Rodríguez-Arcos, R.; Muñoz, M. J.; Monje-Moreno, J. M. and Jiménez-Araujo, A. (2022). *Asparagus* fructans as emerging prebiotics. Foods, **12**(1):81.

Hossain, M. I.; Sharmin, F. A.; Akhter, S.; Bhuiyan, M. A. and Shahriar, M. (2012). Investigation of cytotoxicity and *invitro* antioxidant activity of *Asparagus racemosus* root extract. International Current Pharmaceutical Journal, **1**(9):250-257.

Karuna, D. S.; Dey, P.; Das, S.; Kundu, A. and Bhakta, T. (2018).*In vitro* antioxidant activities of root extract of *Asparagus racemosus* Linn. Journal of Traditional and Complementary Medicine, **8**(1):60-65.

Kumar, A. S. and Mamidala, E. (2025).*In silico* screening of CCR5 inhibitors using pharmacophore modeling and molecular docking techniques. Proceedings of the Two-Day National Seminar on Recent Trends in Animal Biotechnology (RTAB-2024), pp:172-183.

Kumar, A.;Mahanty, B.; Goswami, R.C.D.; Barooah, P.K. and Choudhury, B.(2021).*In vitro* antidiabetic, antioxidant activities and GC-MS analysis of *Rhynchostylis retusa* and *Euphorbia neriifolia* leaf extracts. Biotech, **11**(7):315. doi: 10.1007/s13205-021-02869-7.

Liu, Y.; Liu, C. and Li, J. (2020). Comparison of vitamin C and its derivative antioxidant activity: Evaluated by using density functional theory. ACS Omega, **5**(39):25467-25475. doi:10.1021/acsomega.0c04318.

Majumdar, S.; Gupta, S.; Prajapati, S. K. and Krishnamurthy, S. (2021). Neuro-nutraceutical potential of *Asparagus racemosus*: A review. Neurochemistry International, 145:105013.https://doi.org/10.1016/j.neuint.2021.105013

Meher, D.; Singh, M. and Meher, B. (2024). An update on phytoconstituents and pharmacological importance of *Asparagus racemosus*. Journal of Applied Pharmaceutical Research, **12**(4):11-20. https://doi.org/10.69857/joapr.v12i4.588

Mudannayake, D. C.; Meegahawaththa, W. K.; Illippangama, A. U.; Pitawala, H. M.; Wimalasiri, K. M. and Silva, K. F. (2025). Extraction, purification and structural characterization of inulin-type fructans from different selected *Asparagus* species. Bioactive Carbohydrates and Dietary Fibre, 100486.

Mustafa, N. H.; Sekar, M.; Fuloria, S.; Begum, M. Y.; Gan, S. H.; Rani, N. N. I. M.; Ravi, S.; Chidambaram, K.; Subramaniyan, V.; Sathasivam, K. V.; Jeyabalan, S.; Uthirapathy, S.; Ponnusankar, S.; Lum, P. T.; Bhalla, V. and Fuloria, N. K. (2022). Chemistry, biosynthesis and pharmacology of sarsasapogenin: A potential natural steroid molecule for new drug design, development and therapy. Molecules, **27**(6):2032.

Palanisamy, N. and Manian, S. (2012). Protective effects of *Asparagus racemosus* on oxidative damage in isoniazid-induced hepatotoxic rats: an *in vivo* study. Toxicology and Industrial Health, **28**(3):238-244.

Prosky, L. (1990). Collaborative study of a method for soluble and insoluble dietary fiber. In New Developments in Dietary Fiber: Physiological, Physicochemical, and Analytical Aspects (pp:193-203). Boston, MA: Springer US.

Rajni; Rani, V.; Sindhu, S. C. and Neha (2023). Nutritional analysis of *Asparagus racemosus* (Willd.) root powder and its efficacy in increasing prolactin level in lactating women. Annals of Phytomedicine, **12**(2):912-917. DOI: http://dx.doi.org/10.54085/ap.2023.12.2.108

Rana, M.; Lakhera, S. and Devlal, K. (2024). Detailed quantum chemical, ADMET, reactivity, and molecular docking interaction analysis of potential phytochemicals from *Asparagus racemosus* targeting HIV enzyme/DNA receptors. Life in Silico, **2**(1):1-16.

Saini, P.; Singh, P. and Dubey, S. (2016). Optimization and characterization of *Asparagus racemosus* Willd. (Shatavari) root powder. International Journal of Natural Products Research, **6**(2):36-44.

Samant, L. (2022). Evaluation of phytochemicals profile and antioxidant activities of *Asparagus racemosus* using *in vitro* and *in silico* approach. Der Pharma Chemica, **14**(8):1-9. DOI: 10.4172/0975-413X.14.8.01-10.

Sekine, T.; Fukasawa, N.; Kashiwagi, Y.; Ruangrungsi, N. and Murakoshi, I. (1994). Structure of asparagamine A, a novel polycyclic alkaloid from *Asparagus racemosus*. Chemical and Pharmaceutical Bulletin, **42**(6):1360-1362.

Siddiqui, A. J.; Elkahoui, S.; Alshammari, A. M.; Patel, M.; Ghoniem, A. E. M.; Abdalla, R. A. H.; Dwivedi-Agnihotri, H.; Badraoui, R. and Adnan, M. (2025). Mechanistic insights into the anticancer potential of *Asparagus racemosus* Willd. against triple-negative breast cancer: A network pharmacology and experimental validation study. Pharmaceuticals (Basel), **18**(3):433. DOI: 10.3390/ph18030433.

Slavin, J. (2013). Fiber and prebiotics: Mechanisms and health benefits. Nutrients, **5**(4):1417–1435.

Thakur, M.; Connellan, P.; Deseo, M. A.; Morris, C.; Praznik, W.; Loeppert, R. and Dixit, V. K. (2012). Characterization and *in vitro* immunomodulatory screening of fructo-oligosaccharides of *Asparagus racemosus* Willd. International Journal of Biological Macromolecules, **50**(1):77-81.

Tripathi, R.; Baghel, S. B. S.; Hingwasiya, S. and Upadhyay, R. (2021). Qualitative analysis of *Asparagus racemosus* Willd. (Shatavari) root of family Asparagaceae. International Journal for Research in Applied Science and Engineering Technology, **9**(11):1221–1225.

Viera-Alcaide, I.; Hamdi, A.; Guillén-Bejarano, R.; Rodríguez-Arcos, R.; Espejo-Calvo, J. A. and Jiménez-Araujo, A. (2022). *Asparagus* roots: From an agricultural by-product to a valuable source of fructans. Foods, **11**(5):652.

Visavadiya, N. P.; Soni, B.; Soni, B. and Madamwar, D. (2009). Suppression of reactive oxygen species and nitric oxide by *Asparagus racemosus* root extract using *in vitro* studies. Cellular and Molecular Biology, **55**:1083-1095. PMID: 19267991.

Witzel, K. and Matros, A. (2020). Fructans are differentially distributed in root tissues of asparagus. Cells,**9**(9):1943.

Xiong, G.; Wu, Z.; Yi, J.; Fu, L.; Yang, Z.; Hsieh, C. and Cao, D. (2021). ADMETlab 2.0: An integrated online platform for accurate and comprehensive predictions of ADMET properties. Nucleic Acids Research, **49**(W1): W5-W14.

Yaneva, D.; Hambarlyiska, I.; Petkova, N.; Ivanov, I. and Vassilev, D. (2025). Microwave-assisted isolation of inulin from shatavari roots – chemical characterization and functional properties. Bulgarian Chemical Communications, **57**(A):63-67.

Citation **K. Preethi, R. Yogeswari, T. Ramasamy, A. Raja and S. Ramesh (2025). Phytochemical profiling, nutritional composition, and *in silico* ADMET-antioxidant analysis of *Asparagus racemosus* (Willd.) root. Ann. Phytomed., 14(2):409-419. http://dx.doi.org/10.54085/ap.2025.14.2.39.**