Pharmacogn. Res., 2024; 16(1):161-171.
https://www.phcogres.com

Original Article

In silico Based Virtual Screening of Non-polar Phytochemicals obtained From Petroleum Ether Extract of *Asparagus racemosus* by GC-MS Analysis

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ABSTRACT

Background: Evidence shows that people have used medicinal plants and plant components to treat various conditions since ancient times. *Asparagus racemosus* have a wide range of therapeutic potential Antioxidant, anti-cancer, anti-fungal, anti-bacterial, and anti-inflammatory. **Aim and Objectives:** The current study sought to identify potential bioactive molecules present in the petroleum ether extract of *Asparagus racemosus*. **Materials and Methods:** The presence of different molecules was identified by Gas Chromatography. Mass spectroscopy and FTIR analysis confirmed the molecular structure. The identified molecule was analyzed for drug likeliness, bioactivity, and target prediction analysis by *in silico* approaches using Swiss ADME, Swiss target prediction, Oasis datawarior, and mole inspiration software. Results: The petroleum ether extract is the highest source of alkaloids and steroids. The molecule (5.beta.) Pregnane-3,20, beta.-diol, 14.alpha.,1, 8. alpha.-[4-methyl-3-oxo-(1-oxa-4-azabutane-1,4-diyl)]-diacetate was found in the highest concentration (37.33%). The identified molecule is steroidal. The *in silico* study exhibited good drug likeliness and therapeutic potential for the reported molecule. The molecule can be considered a potential therapeutic agent for the treatment of cancer and analgesic anti-inflammatory agents. **Conclusion:** The molecule (5.beta.) Pregnane-3, 20. beta.-diol, 14.alpha.,1, 8. alpha.- [4-methyl-3-oxo-(1-oxa-4-azabutane-1,4-diyl)]-,diacetate can be considered as poteintial therapeutic agent.

Keywords: *Asparagus racemosus*, Petroleum ether, Gas Chromatography, Mass Spectroscopy, *in silico* study, Drug likeliness, Target prediction.

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Received: 13-07-2023;
Revised: 31-08-2023;
Accepted: 12-09-2023.

INTRODUCTION

Various people are hesitant to use the many synthetic and chemical medications available today because of the apparent adverse effects linked with them.[1] Traditional herbal remedies are gaining popularity due to their purported lack of harmful side effects and low environmental impact.[2] Reasons, despite the accessibility of several effective contemporary synthetic medications, a growing percentage of individuals are opting for plant-based natural treatments instead is because of this.[3] Diseases may be treated and cured thanks to the diverse phytoconstituents in different plant sections.[3-5] Using plants as medication is not new to the Indian medical tradition. Evidence shows that people have used medicinal plants and plant components to treat various conditions since ancient times. There are many different medical traditions in India, yet they all have a common practice of using over 80,000 plants to heal sickness.[6]

Medicinal plants are the source of more than 25% of the active components in today's prescription medications.[7] Antioxidant, anti-cancer, anti-fungal, anti-bacterial, anti-inflammatory, and many other pharmacological actions have all been attributed to bioactive chemicals isolated from medicinal plants.[8] For this reason, it is crucial to evaluate these bioactive chemicals' potential to comprehend their practicability in the therapy of diverse diseases.[9]

Bioactive chemicals extracted and characterized from medicinal plants are the basis for several very effective medications.[10] Vital to understanding the chemical and pharmacological actions of herbaceous are chromatographic and spectrophotometric techniques. Interns aid in identifying physiologically active plant species for research.[11,12] Chemicals that may be used to utilize the GC-MS approach, regarded as a proper procedure, allow the detection of amino acids, organic acids, steroids, esters, and steroid esters, alkaloids, alcohols, and long-chain hydrocarbons.[13] This is why we are using the same method in

DOI: 10.5530/pres.16.1.21

the. *Asparagus racemosus* Shatavari, a therapeutic herb, has been analyzed for its phytochemical content.

Plants of the genus *Asparagus racemosus* also known as Salwar, Satamuli, and Satavari, grow naturally at low elevations in India and are members of the Liliaceae family. Medicine is made from the plant's dried roots.[14] The medicine has an ulcer-healing effect, most likely by bolstering the mucosal resistance or providing cytoprotection, and the roots are believed to have tonic, diuretic, and galactagogue properties.[15] Moreover, it is now shown to be an effective medication for reducing AIDS symptoms. The ayurvedic doctors used to treat neurological problems, inflammation, and infections. *A. racemosus* root extract has been used for various purposes.[16] However, no scientific evidence to support these claims. Some studies have shown that *A. racemosus* root extracts have beneficial effects as galactagogue, antihepatotoxic, immunomodulatory, immunoadjuvant, antilithiatic effect, and teratogenicity.

New drug research has been more reliant on computer-aided technologies in recent years. Screening the active molecules from phytochemicals in medicinal plants is a breeze.[17] Foreseeing the drug's binding orientation to the target protein requires knowledge of the receptor-drug interaction; in this regard, the molecular docking approach is the most efficient to emerge and the most cost-efficient way.[18] Methods using non-covalent ligand binding are helpful in systems biology because they allow for specific ligand binding to the active sites of object macromolecules.[19]

This petroleum ether extract of *Asparagus racemosus* was processed by a GC-MS analysis to determine which bioactive chemicals it contained. The possible bioactive chemicals were then analyzed using computer-aided molecular analysis and *in silico* approaches.

MATERIALS AND METHODS

Collection of Plant Material

The fresh stems of Shatavari (*Asparagus racemosus*) were collected from the Manchal Road, Ibrahimpatnam, Rangareddy District, Telangana at an altitude of 373 m (1,224 ft) at 16.5811°N 77.7489°E. The plant materials were authenticated by Osmania University's Department of Botany in Hyderabad.

Preparation of Extracts

The fresh plant materials were air-dried in shades at a temperature of 40 ± 5°C. The dried plant material was ground to coarse powder with a mixer and grinder made up of Crompton TRET500, Made in India. Moist the powder with petroleum ether 60. The extraction was carried out with soxhlet apparatus. Approximately 200 g of stem powder was taken and put in a bag of muslin cloth of 100 mash size. The extraction was continued with 1 lit of petroleum ether and continued till colorless liquid was obtained. The petroleum ether layer was recollected by a rotary flash evaporator under reduced pressure setting 55°C and 50 rpm (Aditya Scientific RE-2A rotary evaporator, Hyderabad, India). Collect the residue for complete dryness in the desiccator and calculated the percentage yield.[20]

Phyto-chemical analysis

The petroleum ether extract was subjected to phytochemical testing by literature procedure.[21]

GC-MS analysis

Agilent 7890A GC System assembled Mass Spectrometer The AccuTOFGCv/JMS-T100GCv made of JEOL was used for GC-MS analysis. Weigh 25 mg of petroleum ether extract accurately and dissolve in 100 mL of HPLC-grade solvent methanol. The final mixture was thinned to 30 g/mL and used for analysis. The total run time was 50 min. The sample was eluted out using an HP5 Column having a dimension of 30 m X 0.25 mm X 0.25 micro. The carrier gas helium was supplied at a flow rate of 1 mL/min. During analysis oven temperature was maintained at 280°C. The isolated compounds were recognized by comparing their mass spectra in the NIST library database.[21]

Preparation of Structure

The SMILES notation of the compounds was obtained using ACD labs Chemsketch version 12.0, Bangalore, India.

Calculation of molecular and physicochemical properties and toxicity potential of compounds

Osiris data warrior software and Swiss ADME online tool (http://www.swissadme.ch/index.php) was used to determine the molecular and physicochemical properties, as well as the toxicity potential. The reported method of Zhao *et al.* (2002) was also used to calculate the absorption percentage (% Abs).

$$\%Abs = 109 - (0.345 \times TPSA)$$

Calculation of drug likeliness, bioactivity score and Pharmacokinetic Potential

The prediction of drug likeliness and toxicity potential was determined by Swiss ADME (http://www.swissadme.ch/index.php). Bioavailability Score was determined against different types of receptors by Molinspiration software version 2011.06 (www.molin spiration.com). Bioactivity rader of molecules was prepared using the Swiss ADME tool.[22]

Calculation of Pharmacokinetic Potential

The pharmacokinetic properties toward absorption, permeation, excretion, metabolism CYP1A2 inhibitor, CYP2C19 inhibitor, CYP2C9 inhibitor, CYP2D6 inhibitor, CYP3A4 inhibitor, Log Kp (skin permeation) were calculated using Swiss ADME (http://www.swissadme.ch/index.php). The Swiss ADME tool generated the boiled egg diagram.[22]

Target Prediction

The preliminary therapeutic efficacy of the identified molecule was determined by Swiss target prediction (http://www.swissta rgetprediction.ch/). The SMILES notation of the molecule was entered into an online tool to predict the target. The following information was used to interpret the results target, target class, and probability. The target which has the maximum probability was considered significant for the molecule under investigation. It provided valuable information to identify specific proteins and the therapeutic efficacy of the drug.[23]

RESULTS AND DISCUSSION

The current study sought to identify various nonpolar biomolecules present in *Asparagus racemosus* petroleum ether extract. GC-MS analysis was used to identify the various types of biomolecules. FTIR studies confirmed the structures of the identified compounds. For the extract's noted compounds, *in silico* analyses such as molecular properties, physicochemical properties, bioactivity score, toxicity potential, pharmacokinetic properties, and target prediction were performed.

The selected plant has been linked to a variety of medicinal uses. The current study concentrated on determining the target potential of the plant extract. The study's goal was to determine the molecular selectivity for appropriate therapeutic effects.

Percentage yield and Phytochemical analysis

The percentage yield of petroleum ether extract was calculated. It was observed to be 12.8%. The extract contained Alkaloids, flavonoids, steroids, phenolic compounds, terpenoids, and aliphatic compounds were found.

GC-MS analysis

A full scan GC-MS chromatogram is depicted in Figure 1 and Table 1. A total of 7 nos of compounds were identified in petroleum ether extract. The maximum percentage peak area 21.30 and 37.33% were traced for molecule 1 and molecule 6. The retention time was found to be 5.89 and 19.02 min respectively for both compounds. The structure of the compounds was confirmed by mass spectroscopy (Suppl. image-1).

FTIR analysis

The presence of functional groups in different molecules was confirmed by FTIR (Suppl. image-2). The FTIR peaks at 3371 (-NH-, str); 3295 (OH, str); 3174 (OH, str, -COOH); 2810 (C=N, str); 2685 (C=O, str, -COOH); 1627.70 (C=O, str) and 1414.61(N-CH_3, str) Cm^{-1} exhibited the presence of different functional groups in identified molecules. The structure of the compounds depicted in Figure 2.

Molecular Property

Drug action and receptor binding are all influenced by the molecular shape, flexibility, and complexity. In general, spherical shape molecules are thought to have better absorption.[24] High flexibility and low molecular complexity are considered for receptor binding.[25,26] The results are shown in Table 2. Molecules-1, 2, 4, 5, and 7 have linear shapes, whereas molecules-3 and 6 have spherical shapes. Molecules 3 and 7 have high flexibility, whereas molecules 1, 2, 4, 5, and 6 have low flexibility. Similarly, all of the molecules have increased molecular complexity.

Physico-chemical properties

The physico-chemical properties of molecules have a large impact on their biological activity and drug likeliness.[27,28] The result is shown in Table 3. Molecules 5 and 6 have cLogP values of 0.24 and 3.28 respectively. Except for molecules 2, 4, and 5, all the molecules have an H-acceptor site more than 5. All the molecules have an H-doner site of less than 10. All the molecules other than 6 and 7 have a molar refractive index between 40-130. Similarly, TPSA values reside in the range of 90-140 for all the molecules

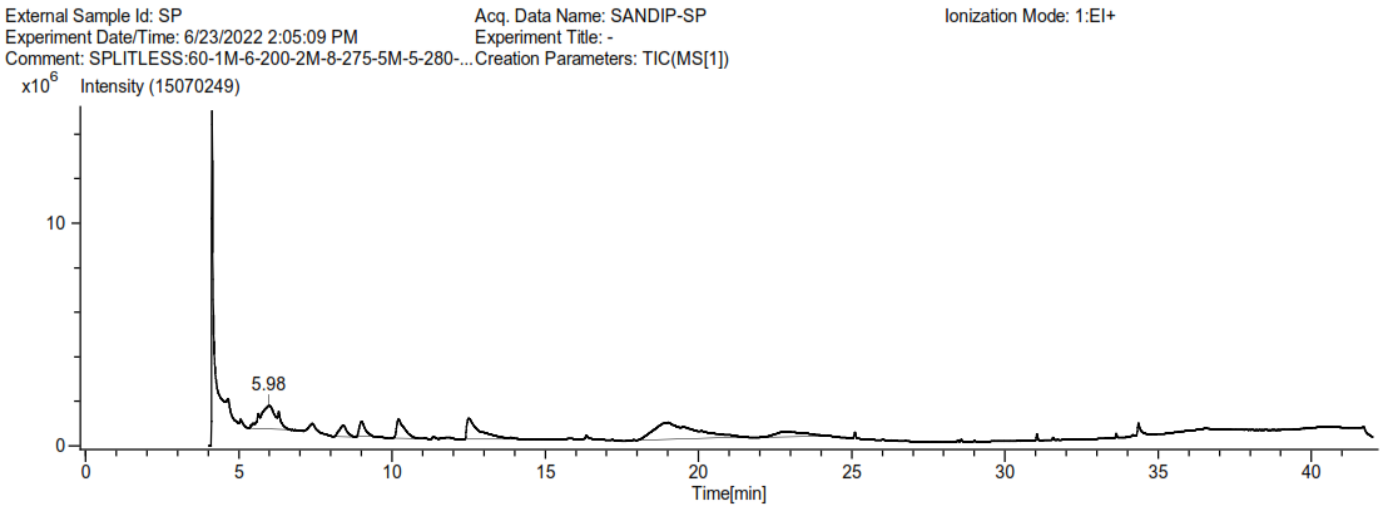


Figure 1: GC-MS Chromatogram of Petroleum ether extract of *Asparagus racemosus*.

except molecule-1. Figure 3 depicts a bioactivity reader based on molecular and physicochemical properties.

Druglikeness

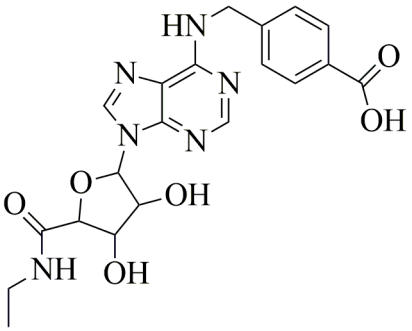
Table 4 represents the drug-likeliness behavior of identified molecules. Except for 1, 3, and 7, all of the molecules followed Lipinski, Veber, and Egan's rule of drug likeliness.[29] Except for molecules 1, 2, 4, 5, and 7, all of the molecules followed the Muegge rules. The bioavailability score was found to be 0.55 for molecules 2, 3, 5, and 6, and 0.85 for molecule 4. Molecules 1, 2, and 6 had positive drug-likeliness values of 2.74, 1.82, and 2.82, respectively. The results showed that molecule-6 has good drug-like properties.

Bioactivity score

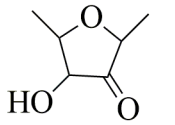
A bioactivity score greater than 0 is considered good, -0.50 to 0 is considered moderate, and less than -0.5 is considered inactive.[30] The bioactivity order for the molecules with target receptors is Enzyme inhibitor > Protease inhibitor > GCPR ligand > Nuclear receptor > Ion channel modulator > Kinase inhibitor, as shown in Table 5. Molecules 1, 6, and 3 showed bioactivity scores greater than zero with different receptors. Molecule 1 demonstrated a potential binding affinity for various receptors.

Toxicity profiles

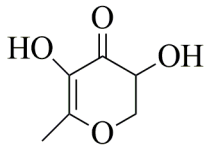
The toxicity potential of the molecules for mutagenic, tumorigenic, reproductive effects, and irritant properties was determined and



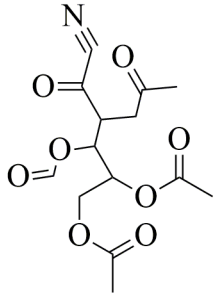
Molecule 1: 4-(((9-(5-(ethylcarbamoyl)-3,4-dihydroxy tetrahydrofuran-2-yl)-9*H*-purin-6-yl)amino) methyl) benzoic acid



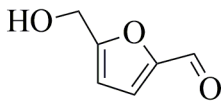
Molecule 2: 4-hydroxy-2,5-dimethyldihydrofuran-3(2*H*)-one



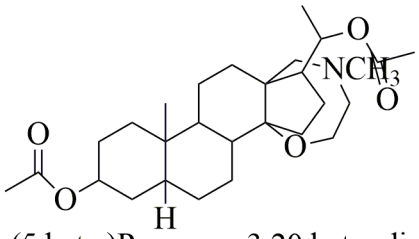
Molecule 4: 3,5-dihydroxy-6-methyl-2*H*-pyran-4(3*H*)-one



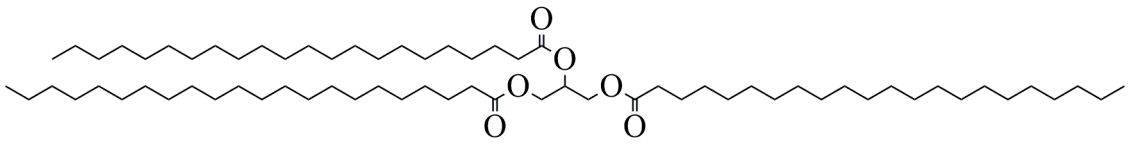
Molecule 3: (2*S*,3*R*)-4-(cyanocarbonyl)-3-(formyloxy) -6-oxoheptane-1,2-diyl diacetate



Molecule 5: 5-(hydroxymethyl)furan-2-carbaldehyde



Molecule 6:(5.beta.)Pregnane-3,20.beta.-diol, 14.alpha.,18. alpha.- [4-methyl-3-oxo-(1-oxa-4-azabutane-1,4-diyl)]-, diacetate



Molecule 7: Docosanoic acid, 1,2,3-propanetriyl ester

Figure 2: Structure of molecules identified in Petroleum ether extract of Asparagus racemosus.

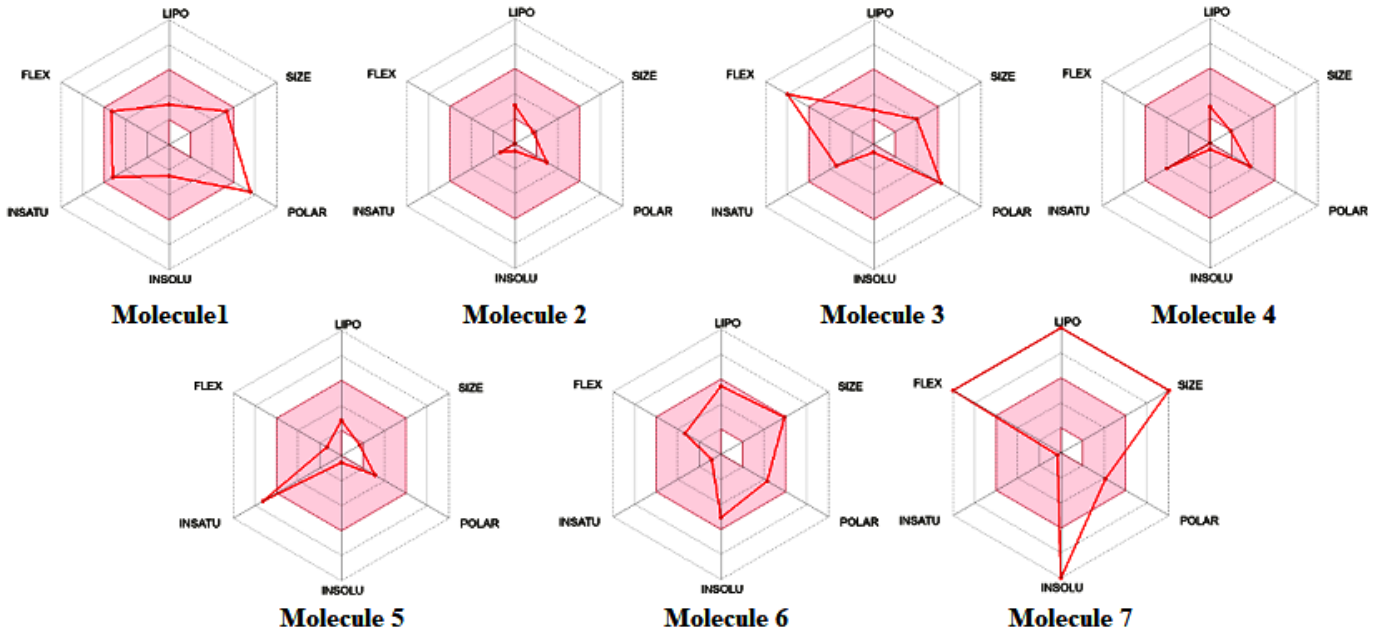


Figure 3: Bioactivity rader of molecules identified in Petroleum ether extract of *Asparagus racemosus*.

Table 1: GC-MS analysis for Petroleum ether extract of *Asparagus racemosus* (Shatavari).

Peak No	Time [min]	Type	Peak Width (FWH) [min]	Area [Intens.*sec]	Peak area (%)	Height	MW[a]	MF[b]
1	5.98	BB	0.52	39703396.34	21.30	1040990	442	$C_{20}H_{22}N_6O_6$
2	8.40	BB	0.26	8750742.49	4.69	514313	128	$C_6H_8O_3$
3	9.01	BB	0.21	9104676.06	4.88	674113	343	$C_{14}H_{17}NO_9$
4	10.21	BB	0.27	15269044.35	8.19	851027	144	$C_6H_8O_4$
5	12.50	BB	0.32	27354049.28	14.67	929857	126	$C_6H_6O_3$
6	19.02	BB	1.44	69568976.71	37.33	765209	489	$C_{28}H_{43}NO_6$
7	22.74	BB	1.28	16609944.17	8.91	241126	1058	$C_{69}H_{134}O_6$

[a] Molecular weight, [b]Molecular formula.

Table 2: Molecular properties of the molecules identified by GC-MS analysis.

Molecules	Shape Index	Molecular Flexibility	Molecular Complexity
1	0.59375	0.43775	0.926
2	0.55556	0.1239	0.805
3	0.43478	0.75009	0.779
4	0.6	0.30611	0.752
5	0.77778	0.49258	0.749
6	0.45714	0.39479	0.966
7	0.65333	0.5676	0.656

a: Molecular shape index (Spherical ≤ 0.5 ≤ Linear); b: Molecular Flexibility (Low ≤ 0.5 ≤ High); c:Molecular Complexity (Low ≤ 0.5 ≤ High).

Table 3: Physico-chemical properties of the molecules identified by GC-MS analysis.

Molecules	cLogP[a]	cLogS[b]	H-Acceptors	H-Donors	Total Surface Area	Relative PSA[c]	MR[d]	TPSA[e]	%abs[f]	Solubility
1	-0.6721	-3.919	12	5	316.85	0.43	110.48	171.72	49.75	Soluble
2	-0.3651	-1	3	1	96.12	0.37	31.29	46.53	92.94	Very soluble
3	-0.8258	-2.31	9	0	257.55	0.42	73.81	136.83	61.79	Very soluble
4	-0.7707	-0.925	4	2	101.89	0.48	32.39	66.76	85.96	Very soluble
5	0.2383	-1.53	3	1	102.60	0.39	30.22	50.44	91.59	Very soluble
6	3.2816	-4.453	7	0	358.44	0.20	136.32	82.14	80.66	Moderately soluble
7	27.274	-17.27	6	0	999.15	0.07	337.65	78.9	81.77	Insoluble

a:P=[n-Octanol]/[Water]; (cLogP); b: S=Water solubility in moles/ liter at PH=7.5 (25°C) (cLogS); c: Relative polar surface area (Relative PSA); d: Molar refractive index; e: Toplogical polar surface area (TPSA); f: Percentage of absorption (%Abs).

Table 4: Druglikeness of the molecules identified by GC-MS analysis.

Molecules	Druglikeness	Lipinski	Ghose	Veber	Egan	Muegge	Bioavailability Score
1	2.7402	Yes; 1 violation: NorO>10	No; 1 violation: WLOGP<-0.4	No; 1 violation: TPSA>140	No; 1 violation: TPSA>131.6	No; 1 violation: TPSA>150	0.11
2	1.8273	Yes; 0 violation	No; 3 violations: MW<160, MR<40, #atoms<20	Yes	Yes	No; 1 violation: MW<200	0.55
3	-4.1628	Yes; 0 violation	Yes	No; 1 violation: Rotors>10	No; 1 violation: TPSA>131.6	Yes	0.55
4	-1.3848	Yes; 0 violation	No; 3 violations: MW<160, MR<40, #atoms<20	Yes	Yes	No; 1 violation: MW<200	0.85
5	-2.0338	Yes; 0 violation	No; 3 violations: MW<160, MR<40, #atoms<20	Yes	Yes	No; 1 violation: MW<200	0.55
6	2.8223	Yes; 0 violation	No; 3 violations: MW>480, MR>130, #atoms>70	Yes	Yes	Yes	0.55
7	-26.013	No; 2 violations: MW>500, MLOGP>4.15	No; 4 violations: MW>480, WLOGP>5.6, MR>130, #atoms>70	No; 1 violation: Rotors>10	No; 1 violation: WLOGP>5.88	No; 3 violations: MW>600, XLOGP3>5, Rotors>15	0.17

Table 5: Bioactivity scores of the molecules identified by GC-MS analysis.

Molecules	GPCR ligand	Ion channel modulator	Kinase inhibitor	Nuclear receptor ligand	Protease inhibitor	Enzyme inhibitor
1	0.79	0.12	0.49	-0.84	0.17	0.66
2	-1.76	-1.66	-2.55	-2.22	-1.8	-1.03
3	-0.16	-0.04	-0.56	0.04	0.17	0.44
4	-1.59	-0.96	-2.25	-1.6	-1.53	-0.65
5	-2.71	-2.19	-2.92	-2.73	-3.21	-2.24
6	0.1	0.1	-0.38	0.35	0.09	0.23
7	-3.72	-3.81	-3.8	-3.81	-3.65	-3.75

Table 6: Toxicity potential of the molecules identified by GC-MS analysis.

Molecules	Mutagenic	Tumorigenic	Reproductive Effective	Irritant
1	None	None	None	None
2	None	None	None	None
3	None	None	None	High
4	None	None	None	None
5	High	High	None	High
6	None	None	None	None
7	None	None	None	None

Table 7: Pharmacokinetic potential of the molecules identified by GC-MS analysis.

Molecules	GI absorption	BBB permeant	Pgp substrate	CYP1A2 inhibitor	CYP2C19 inhibitor	CYP2C9 inhibitor	CYP2D6 inhibitor	CYP3A4 inhibitor	log Kp (cm/s)
1	Low	No	Yes	No	No	No	No	No	-8.89
2	High	No	No	No	No	No	No	No	-7.16
3	High	No	No	No	No	No	No	No	-8.79
4	High	No	No	No	No	No	No	No	-7.44
5	High	No	No	No	No	No	No	No	-7.48
6	High	No	No	No	No	No	No	No	-6.43
7	Low	No	Yes	No	No	No	No	No	9.74

shown in Table 6. Molecule 5 has high mutagenic, tumorigenic, and irritant properties. Molecule 3 is an irritant in nature

Pharmacokinetics profiles

The active molecule absorbed by diffusion process. The GI-absorptivity and HIA of bimolecular substances is an important parameter to consider. The permeability of its membrane, the small intestine is largest area for drug absorption compared to stomach.[31,32] The blood-brain barrier regulates drug molecule entry into the central nervous system and produce cytotoxicity.[33]

The PGP has critical role in the drug excretion and disposition process.[34] It is also an important factor in the oral bioavailability absorption barrier and the blood-brain barrier, which limits drug accumulation in the brain. PGP inhibition causes drug interactions and increases drug accumulation in the brain.[35]

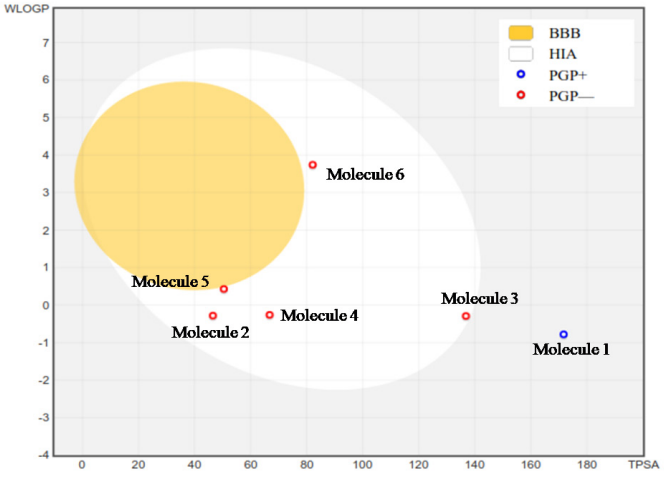


Figure 4: Boiled egg diagram of molecules identified in Petroleum ether extract of *Asparagus racemosus*.

Table 8: Target prediction of the molecules along with biological role and therapeutic application.

Molecule	Target	Target Class	Probability	Pharmacological Action
1	Adenosine A1 receptor	Family G protein-coupled receptor	0.44	Bone remodelling.
	Adenosine A2a receptor		0.32	Cardioprotective, Miocardial infraction, Ischimic heart diseases.
	Adenosine A3 receptor		0.30	Anticancer, Bone remodeling.
2	Alpha-L-fucosidase I	Enzyme	0.02	Immunemodulator.
3	Protein kinase C delta (by homology)	Kinase	0.10	Neoplastic agent.
	Leukocyte elastase	Protease	0.10	Pulmonary emphysema, Rheumatoid arthritis, infections and Inflammation.
	Urokinase-type plasminogen activator		0.10	Thrombolytic agent and Antineoplastic agent.
	Protein kinase C eta (by homology)	Kinase	0.10	Renal cell carcinoma, Glioblastoma, Breast cancer, Non-small cell lung cancer, and Acute myeloid leukemia.
	Protein kinase C theta		0.10	Treatment of allergies and autoimmune disorder.
	PI3-kinase p110-delta subunit	Enzyme	0.10	Neoplastic agent.
	PI3-kinase p110-beta subunit		0.10	Chemotherapeutic agent in MDR cancer.
	PI3-kinase p110-alpha subunit		0.10	Chemotherapeutic agent in MDR cancer.
	Carbonic anhydrase XII	Lyase	0.10	Antinociceptive and Anticancer.
4	Tyrosinase	Oxidoreductase	0.02	Melanin synthesis.
	D-amino-acid oxidase	Enzyme	0.02	Neurological and psychiatric diseases.
5	Alpha-L-fucosidase I	Enzyme	0.03	Immunemodulator.
6	Kappa Opioid receptor	Family A G protein-coupled receptor	0.11	Narcotic analgesic, Antiepileptic, Diuretics.
	Glycine transporter 1,2	Electrochemical transporter	0.11	Neural development, embryogenesis.
	Glycine transporter 2	Electrochemical transporter	0.11	Inhibitory phenotype in the physiology and pathology of inhibitory circuits.
	Thymidine kinase, mitochondrial	Enzyme	0.11	Neoplastic agent.
	Epoxide hydratase	Protease	0.11	Neoplastic agent.
	p53-binding protein Mdm-2	Other nuclear protein	0.11	Neoplastic agent.
	Glycogen synthase kinase-3 beta	Kinase	0.11	Neoplastic agent.
	Calcitonin gene-related peptide type 1 receptor	Family B G protein-coupled receptor	0.11	Vasodilator.

Molecule	Target	Target Class	Probability	Pharmacological Action
	Protein-tyrosine phosphatase 1B	Phosphatase	0.11	Neoplastic agent.
	Thymidine kinase, cytosolic	Transferase	0.11	Neoplastic agent.
	Sodium/glucose cotransporter 1	Electrochemical transporter	0.11	Diabetis.
	Muscarinic acetylcholine receptor M1, M3, M4	Family A G protein-coupled receptor	0.11	Muscarinic action.
	C-C chemokine receptor type 1	Family A G protein-coupled receptor	0.11	Antiinflammatory.
	6-phosphofructo-2-kinase/ fructose-2,6-bisphosphatase 3	Enzyme	0.11	Carbohydrate metabolism and Hyperglycemic agent.
	Proteinase-activated receptor 1,4	Family A G protein-coupled receptor	0.11	Thrombolutic agent, Antineoplastic agent, Anti-inflammatory.
	C5a anaphylatoxin chemotactic receptor	Family A G protein-coupled receptor	0.11	Anti-inflammatory, Anticancer, Antiobesity.
	Vanilloid receptor	Voltage-gated ion channel	0.11	Anipyratic and antiinflammatory.
	Heat shock protein HSP 90-alpha	Other cytosolic protein	0.11	Antiviral.
	Cyclooxygenase-2	Oxidoreductase	0.11	Analgesic and anti-inflammatory.
	Platelet activating factor receptor	Family A G protein-coupled receptor	0.11	Platelet aggregation and dilation of blood vessels.
7	Protein kinase C gamma (by homology)	Kinase	0.26	Neoplastic agent.
	Protein kinase C alpha		0.26	Neoplastic agent.
	Protein kinase C epsilon		0.26	Cardiac ischemia and Alzheimer's disease, Neoplastic agent.
	Protein kinase C eta (by homology)		0.26	Neoplastic agent.
	Protein kinase C theta		0.26	T-cell activation, proliferation, and differentiation, Aids.

Cytochrome P450 is a type of enzyme that is required for drug metabolism. A drug that inhibits Cytochrome P450 (CYP) enzymes may reduce drug metabolism and other metabolic processes. For tropical application skin permeability (K_{SP}) of drug substances is important criterion.[36]

The results are shown in Table 7 and Figure 4. The molecules 2, 3, 4, 5, and 6 have GI absorption capacity, but they do not penetrate the blood-brain barrier. Human Intestinal Absorption (HIA) capacity is higher for molecules 2, 3, 4, and 6. The PGP initiator effect was observed in molecules 1 and 7. None of the molecules demonstrated a PGP inhibitory effect. The results also showed that the molecules' skin permeability was within an acceptable range.

Target Prediction and Analysis

Based on the bioactivity score target prediction analysis was carried out for molecule-1, 3 and 6. The result was depicted in Table 8. From the study, it was found that molecule 1 is targeted at G-Protein coupled Adenosine A receptor. The molecule can be used as a cardiovascular agent along with bone remodeling and anticancer agents. Molecule 3 is a multi-targeted agent. It acts on different types of Protase, kinase, and ligase receptors. It is a suitable muti-therapeutic agent for the treatment of inflammation,

and arterial and venous thrombosis and a chemotherapeutic agent for the treatment of different types of cancer. Similarly, molecule-6 binds with different receptors like G protein-coupled receptor, Electrochemical transporter, Protease, Kinase, and Voltage-gated ion channel. Due to multi-receptor binding affinity, it can be considered a therapeutic agent as a narcotic analgesic, antiepileptic, diuretic, neoplastic agent, vasodilator, diabetes, antiinflammatory, antiobesity, antipyretic and antiinflammatory, platelet aggregation and dilation of blood vessels.[37]

CONCLUSION

The current finding showed seven identified molecules by Gas chromatographic analysis. The structure of the compounds was confirmed by mass spectroscopy and FTIR study. The highest concentration was found for (5.beta.) Pregnane-3, 20. beta.-diol, 14.alpha.,1, 8. alpha.- [4-methyl-3-oxo-(1-oxa-4-azabutane-1,4-diyl)]-,diacetate. Molecule-6 have spherical shapes and good to moderate molecular flexibility. The molecule-6 showed good drug-likeliness character without any toxicity. Human Intestinal Absorption (HIA) capacity is higher for molecules 6. The target prediction analysis exhibited molecule 6 as a potential target molecule as the analgesic anti-inflammatory, Anti-epileptic, Diuretics, and Neoplastic agent. It can also be used as a vasodilator, anti-diabetic, and antiobesity agent. So the present investigation can be considered a successful goal for the further development of petroleum ether extract as a potential therapeutic agent for the treatment of different types of diseases.

ACKNOWLEDGEMENT

We like to acknowledge our sincere thanks to SAIF, IIT Bombay for GC-MS and FTIR study. We also give our sincere gratitude to the School of Pharmacy, Guru Nanak Institutions Technical Campus for providing all the facilities for the study.

CONFLICT OF INTEREST

All the authors declare no conflict of interest.

ABBREVIATIONS

GC-MS: Gas chromatography Mass spectroscopy; **HPLC:** High Performance Liquid Chromatography; **SMILES:** Simplified Molecular Input Line Entry System; **ADME:** Absorption Distribution Metabolism Excretion; **CYP:** Human Cytochrome P-450 enzyme; **FTIR:** Fourier Transform Infrared Spectroscpy,

SUMMARY

The current study sought to identify potential bioactive molecules present in the petroleum ether extract of *Asparagus racemosus*. The presence of different molecules was identified by GCMS. The identified molecule was analyzed for *in silico* based screening. The molecule (5.beta.) Pregnane-3,20, beta.-diol, 14.alpha.,1, 8. alpha. -[4-methyl-3-oxo-(1-oxa-4-azabutane-1,4-diyl)]diacetate was found in the highest concentration. The identified is a potential therapeutic agent for the treatment of cancer and analgesic anti-inflammatory agents.

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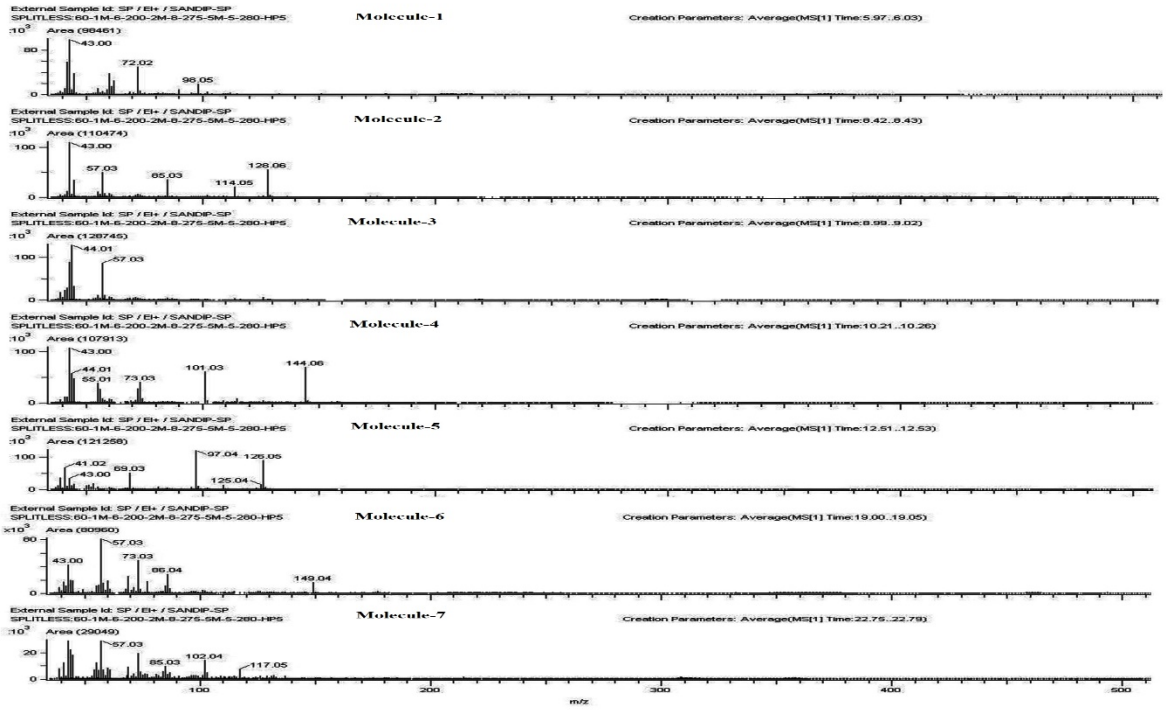
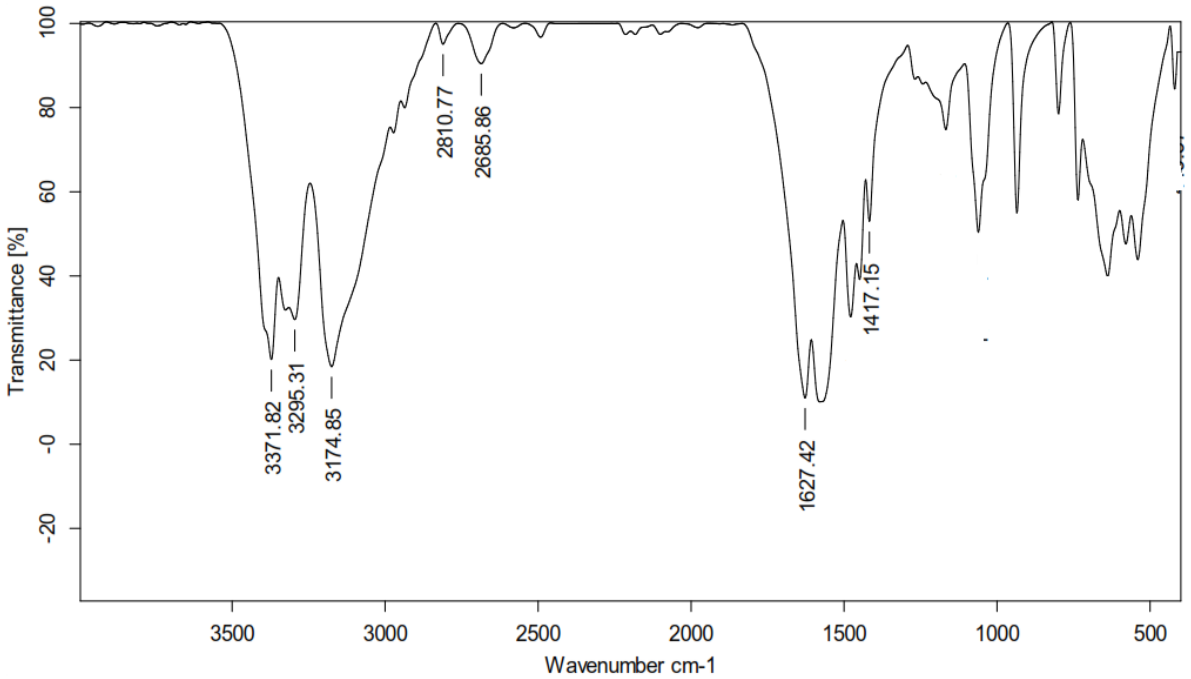
Cite this article: Rasheed SH, Vakkalagadda RK, Mustak S, Sen S. *In silico* Based Virtual Screening of Non-polar Phytochemicals obtained From Petroleum Ether Extract of *Asparagus racemosus* by GC-MS Analysis. Pharmacog Res. 2024;16(1):161-71.

Supplementary Images



Suppl Figure 1 : Mass spectrum of Petroleum ether extract of *Asparagus racemosus.*



Suppl Figure 2 : FTIR spectra of Petroleum ether extract of *Asparagus racemosus.*