Pharmacogn. Res., 2024; 16(4):887-896.
https://www.phcogres.com

Original Article

# Melezitose a Potential of Bioactive Compound from Aqueous Extract of Indian Satavari: An Web Based *in silico* Study Utilizing GC-MS Analysis

**Sandip Sen[1,*], Kalepu Swathi[2], Dubbasi Vishwanath[3], Bairam Ravindar[4], Mitta Chaitanya[2], Srinivas Cherukupally[5], Shapuram Tejasree[6], Hema Varaha Santhoshi Allu[7]**

[1]Department of Pharmaceutical Chemistry, School of Pharmacy, Guru Nanak Institutions Technical Campus, Ibrahimpattnam, Telangana, INDIA.
[2]Department of Pharmaceutical Chemistry, Bojjam Narasimhulu Pharmacy College for Women, Saidabad, Hyderabad, Telangana, INDIA.
[3]Department of Pharmaceutics, Sree Dattha Institute of Pharmacy, Nagarjuna Sagar Road, Sheriguda, Ibrahimpatnam. Telangana, INDIA.
[4]Department of Pharmaceutical Chemistry, Srikrupa Institute of Pharmaceutical Sciences, Velikatta, Telangana, INDIA.
[5]Department of Pharmacology, Nalla Narsimha Reddy College of Pharmacy, Chowdariguda, Narapally, Korremula X Road, Hyderabad, Telangana, INDIA.
[6]Department of Pharmacology, Vijaya College of Pharmacy, Hayathnagar, Thorrur, Hyderabad, Telangana, INDIA.
[7]Department of Pharmacy, Avanthi Institute of Pharmaceutical Sciences, Cherukupally, Vizianagaram, Andhra Pradesh, INDIA.

## ABSTRACT

**Background:** Historical records indicate that medicinal plants and their components have been utilized for treating diverse conditions since antiquity. *Asparagus racemosus*, in particular, demonstrates a broad spectrum of therapeutic possibilities. **Aim:** This study aimed to pinpoint potential bioactive compounds found within the aqueous extract of *Asparagus racemosus*. **Materials and Methods:** Gas Chromatography employed to identify the presence of various molecules, while Mass Spectrometry and FTIR analysis validated their molecular structures. The molecule was subjected to thorough scrutiny for its potential as a drug candidate, its biological activity, and its predicted targets using *in silico* techniques. **Results:** The aqueous extract stands out as the richest reservoir of carbohydrates and steroidal alkaloids. The molecule Melezitose was found in the highest concentration (37.86%). The identified molecule is a carbohydrate in nature. The computational analysis revealed promising drug-like properties and therapeutic potential for the investigated molecule. **Conclusion:** It could serve as a viable therapeutic option for addressing multiple disorders.

**Keywords:** *Asparagus racemosus*, Aqueous extract, Chromatography, Mass Spectroscopy, *In silico* study, Target analysis.

**Correspondence:**
**Dr. Sandip Sen**
Professor, Department of Pharmaceutical Chemistry, School of Pharmacy, Guru Nanak Institutions Technical Campus, Ibrahimpattnam, RR District-501506, Telangana, INDIA.
Email: sandipsen2010@gmail.com

**Received:** 20-06-2024;
**Revised:** 22-07-2024;
**Accepted:** 04-09-2024.

## INTRODUCTION

Many individuals exhibit reluctance towards the abundant synthetic and chemical medications available today, primarily due to their perceived adverse effects.[1] The traditional herbs gain popularity due minimal toxicity.[2] Although there are many effective modern synthetic medications available, individuals are choosing plant-based natural remedies.[3] This inclination arises from the diverse phytoconstituents present in various plant parts, which can treat and cure diseases.[4,5] The practice of using plants as medicine is deeply rooted in the Indian medical tradition, with evidence indicating its prevalence since ancient times.[6]

Medicinal plants provide more than a quarter of the active ingredients present in modern prescription medications.[7] Bioactive chemicals isolated from these plants have been associated with a range of pharmacological actions, including antioxidant, anti-cancer, anti-fungal, anti-bacterial, and anti-inflammatory properties.[8] Therefore, it's crucial to evaluate the potential of these bioactive compounds to comprehend their viability in treating different ailments.[9]

The basis of many highly efficient medications originates from the bioactive compounds extracted and identified from medicinal plants.[10] Understanding the chemical and pharmacological actions of these herbs relies heavily on chromatographic and spectrophotometric techniques.[11,12] The utilization of the hypernated techniques is a advanced tool for tracing biomolecule in herbal extracts.[13] This is why we have employed the same method in the analysis of *Asparagus racemosus*, commonly known as Shatavari, a therapeutic herb.

**DOI:** 10.5530/pres.16.4.101

*Asparagus racemosus* (Liliaceae family) is a lower attitude plant from Asian origin. The dried roots of this plant are utilized in medicine.[14] These roots are attributed with ulcer-healing properties, likely achieved by enhancing mucosal resistance or providing cytoprotection.[15] Additionally, recent studies indicate its effectiveness in reducing AIDS symptoms, as well as its historical use by Ayurvedic practitioners for treating neurological issues. It has been utilized for diverse applications, there is a scarcity of scientific evidence substantiating these assertions. Nonetheless, some research suggests the beneficial effects of *A. racemosus* root extracts, including galactagogue properties, antihepatotoxic effects, immunomodulatory effects, immunoadjuvant effects, antilithiatic effects, and teratogenicity.[16]

In recent times, the development of new drugs has increasingly leaned on computer-aided technologies. Identifying active molecules from phytochemicals in medicinal plants has become more streamlined.[17] In recent times, the development of new drugs has increasingly leaned on computer-aided technologies.[18] *In silico* study along with target prediction is a valuable tool for prediction of target and diseases identification techniques.[19]

The aquous extract derived from *Asparagus racemosus* underwent GC-MS analysis to identify its bioactive constituents. Following this, potential bioactive compounds were further examined utilizing computer-aided molecular analysis and *in silico* methodologies.

## MATERIALS AND METHODS

### Procurement of Plant Material

Fresh stems of Shatavari (*Asparagus racemosus*) were collaected from the Lingmpally village Ibrahimpatnam, Telangana. Authentication of the plant materials was carried out by the Department of Botany at Hyderabad University in Hyderabad.

### Preparation of Extracts

The stems were air-dried under shaded conditions at a temperature of 38±5°C. The dried material was ground into a coarse powder using electric grinder made of a Crompton TRET500 India. The powdered material was then moistened with aqueous and subjected to extraction using a Soxhlet apparatus. About 200 g of stem powder was placed inside a muslin cloth bag with a mesh size of 100. The stem powder was defatted with petroleum ether. The extraction process utilized 1 L of methanol and proceeded until a colorless liquid was achieved. The was recycled by a rotary flash evaporator under reduced pressure conditions at 75°C and 55 rpm (Aditya Scientific RE-3A rotary evaporator, Hyderabad, India). The dried residue kept in desiccator, and the percentage yield was calculated.[20]

### Phyto-chemical examination

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

### GC-MS analysis

The chromatographic study was performed using the Agilent 7890A GC System coupled with the AccuTOF GCv/JMS-T100GCv from JEOL. 100 mg of extract was weighed and dissolved in 100 mL of HPLC grade methanol. The resulting mixture was further diluted to a concentration of 30 µg/mL. The total runtime for the scanning was 60 min. The sample was injected into column (HP5 column: 30 m x 0.25 mm x 0.25 µm, helium carrier gas at 1 mL/min, oven at 280°C). The compounds isolated during the analysis were identified by comparing their mass spectra with NIST library database.[21]

### *In silico* Study

The molecular and physicochemical properties, along with the toxicity profile, was calculated using the Osiris Data Warrior software and the Swiss ADME tool available at http://www.swissadme.ch/index.php. Additionally, the absorption percentage (% Abs) was estimated using the method described by Zhao *et al.* (2002).

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

### Drug likeliness and Pharmacokinetic Potential

The drug likeliness and pharmacokinetic profile toxicity profile predicted using Swiss ADME (http://www.swissadme.ch/index.php). The Bioavailability Score was determined using Molinspiration software version 2011.06 (www.molinspiration.com). A bioactivity radar and boiled egg diagram of molecules was confirmed using Swiss ADME tool.[22]

### Target Prediction

The therapeutic effectiveness of the identified molecules was predicted using Swiss target prediction (http://www.swisstargetprediction.ch/).Top of Form The obtained results included target, target class, and probability, which were used to interpret the findings. The target with the highest probability was regarded as significant for the molecule under scrutiny. This procedure provided valuable insights into the identification of particular proteins and the therapeutic possibilities of the drug.[23]

## RESULTS

The aim of this research was to pinpoint various nonpolar biomolecules present in the aqueous extract derived from *Asparagus racemosus*. Chromatographic analysis was used to identify the various types of molecules present in extract. Spectral analysis confirms the structures of the identified compounds. *In silico* study and target prediction confirmed the drug-likeliness behavior of the different compounds in extract. The chosen plant has been associated with numerous medicinal applications. This study focused on assessing the target potential of the plant extract,

aiming to discern its molecular identity for desired therapeutic potential.

## Yield proportion and Plant compound examination

The aqueous extract exhibited a yield of 28.1%. Subsequent analysis unveiled the existence of alkaloids, flavonoids, steroids, phenolic compounds, terpenoids, and aliphatic compounds within the extract.

## GC-MS analysis

The maximum percentage peak areas 37.86% were traced for compound 1. The retention time was found to be 4.81 min respectively (Figure 1 and Table 1). The structure of the compounds was confirmed by mass spectroscopy (Figure 2). Ten compounds were identified in the aqueous extract (Figure 3).

## FTIR analysis

Functional groups within various molecules were confirmed using FTIR analysis. FTIR peaks at ($Cm^{-1}$): 3295 (OH, str); 3174 (OH, str), 2685 (C=O, str, -COOH); 1627.70 (C=O, str); and indicated presence of molecule-9 (Figure 4).

## Molecular Property

Factors such as molecular shape, flexibility, and complexity significantly impact the effectiveness of drug action and receptor binding. Generally, molecules with a spherical shape are thought to demonstrate improved absorption.[24] Additionally, increased flexibility and reduced molecular complexity are typically advantageous for efficient receptor binding.[25,26] These findings are summarized in Table 2. Specifically, compounds 1 and 10 exhibit spherical shapes remaining molecules demonstrate linear shapes, and compounds 5, 6, 7, 8 and 10 display low flexibility. Additionally, all molecules exhibit increased molecular complexity.

## Physicochemical properties

The physicochemical properties of molecules significantly influence their drug likeliness.[27,28] These findings are summarized in Table 3 and Figures 5 & 6. Molecules 2, 3, 5, 8 and 10 exhibit cLog *p* values of 0.06 - 3.28. Except for molecules 2, 3, 5, 7, 8 and 9 all molecules possess more than 5 hydrogen acceptor sites. Additionally, all molecules have fewer than 10 hydrogen donor sites except 1. The molecules have a molar refractive index ranging from 40 to 130 except 4, 5, 7, 8 and 9. Similarly, Total Polar Surface Area (TPSA) values fall out of the range of 90-140 for all molecules except molecule-4 and 6.

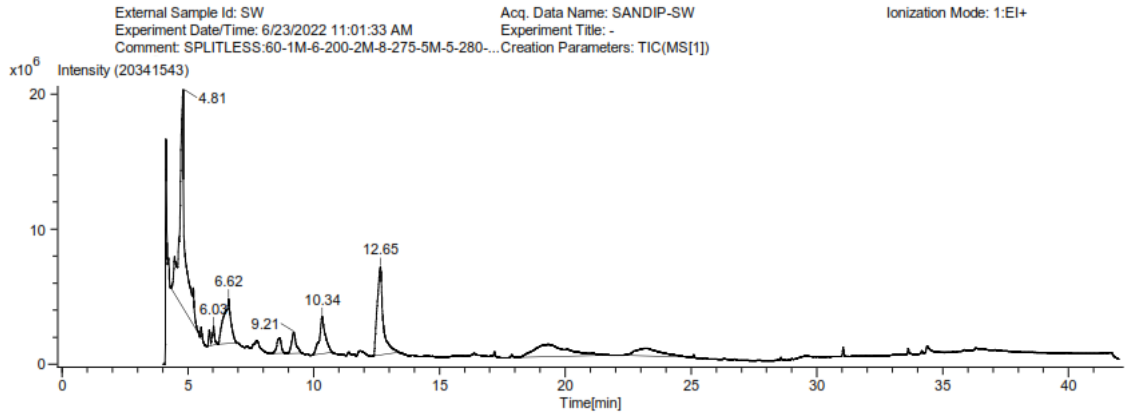



**Figure 1:** Chromatographic profile of the aqueous extract from *Asparagus racemosus* obtained via GC.

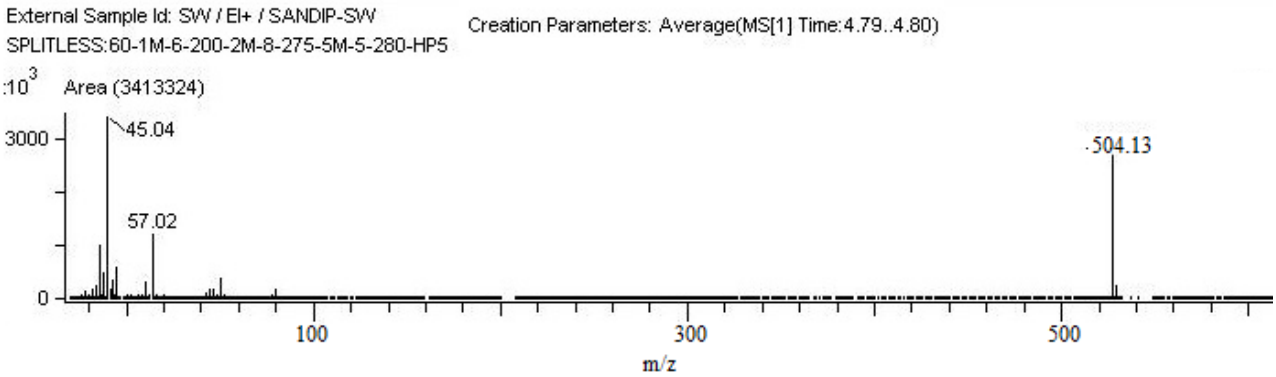



**Figure 2:** Mass spectrum of molecule-1 identified in the Aqueous extract *Asparagus racemosus*.

## Druglikeliness

Identified molecules followed the Lipinski rule except for molecules 9. Only molecules 2, 3 and 10 followed the Ghose rule. Similarly, except the molecules 6 and 9 other molecules followed Veber and Egan rules. Similarly, no molecules except 10 followed the Muegge rules. From the detailed analysis, it was found that only molecules 3, 6 and 10 follow drug-likeliness behavior positive drug-likeness values respectively.[29] The bioavailability score was determined to be 0.55 to 0.85 for all molecules except 9 (0.17). These findings indicate that molecule-8 possesses favorable drug-like properties (Table 4).

**Table 1: Gas Chromatography Analysis of Aqueous Extract from *Asparagus racemosus* (Shatavari).**

| Peak Number | Time [min] | Peak Width (FWH [min] | Area [Intens. * sec] | Percentage peak area | Height | MW | MF |
|---|---|---|---|---|---|---|---|
| 1 | 4.81 | 0.13 | 236444458.3 | 37.86 | 16155316 | 504 | C18H32O16 |
| 2 | 5.85 | 0.07 | 4860734.64 | 0.78 | 1168255 | 174 | C8H14O4 |
| 3 | 6.03 | 0.1 | 8450585.11 | 1.35 | 1373473 | 169 | C10H19N0 |
| 4 | 6.62 | 0.34 | 65258722.36 | 10.45 | 3336508 | 119 | C3H5NO4 |
| 5 | 8.64 | 0.18 | 14170009.89 | 2.27 | 1146730 | 128 | C6H8O3 |
| 6 | 9.21 | 0.17 | 19267075.25 | 3.09 | 1527256 | 296 | C11H12N4O6 |
| 7 | 10.34 | 0.21 | 45640162.8 | 7.31 | 2733839 | 144 | C6H8O4 |
| 8 | 12.65 | 0.22 | 107264684.6 | 17.18 | 6512426 | 126 | C6H6O3 |
| 9 | 19.33 | 1.46 | 83794531.95 | 13.42 | 926581 | 90 | C4H10O2 |
| 10 | 23.23 | 1.06 | 39314310.17 | 6.30 | 564698 | 489 | C28H43NO6 |

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

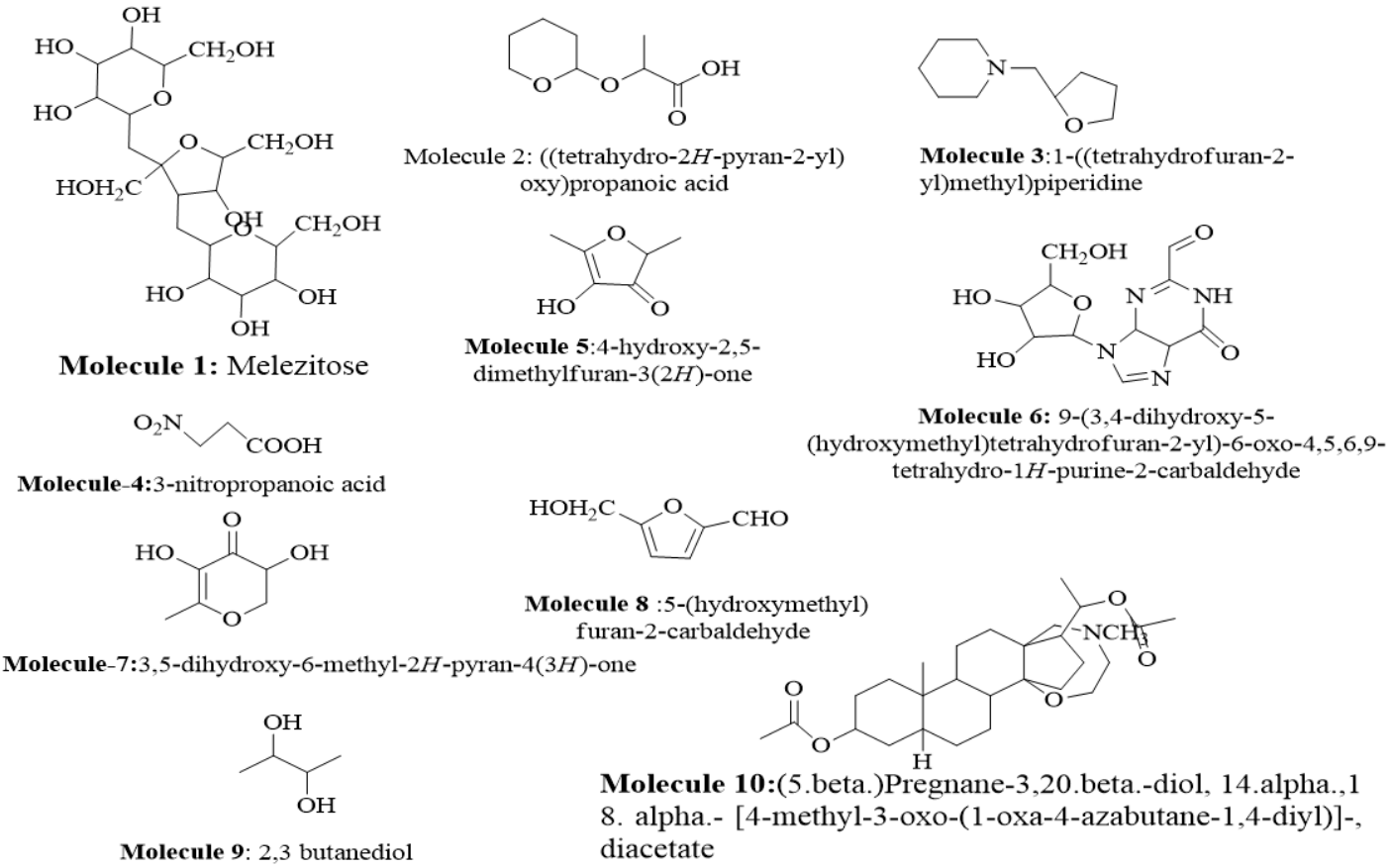



**Figure 3:** Molecular Structures Identified in the Aqueous extract of *Asparagus racemosus.*

## Bioactivity score and Toxicity profiles

The hierarchy of bioactivity for molecules with target receptors is as follows: EI> IC> GL> PI>NR>KI, as depicted in Table 5. Molecule 9 exhibited bioactivity scores greater than zero with various receptors and displayed a notable binding affinity for G-protein coupled receptors.[30] Molecules exhibited no toxic properties except molecule 8 (Table 6).

## Pharmacokinetics profiles

The absorption of the active molecule occurs primarily through a diffusion process. When considering bimolecular substances, GI absorptivity and Human Intestinal Absorption (HIA) are crucial parameters.[31,32] The small intestine offers a greater area for drug absorption than the stomach does. Furthermore, the blood-brain barrier controls the passage of drug molecules into the central nervous system, thus averting cytotoxic effects.[33]

P-Glycoprotein (PGP) is pivotal in the process of drug excretion and distribution.[34] It acts as a deterrent to drug absorption in both oral bioavailability and the blood-brain barrier, curtailing drug buildup in the brain. Inhibiting PGP can result in drug interactions and heightened drug accumulation in the brain.[35] Cytochrome P450 (CYP) enzymes are vital for drug metabolism. If certain drugs inhibit these enzymes, it can decrease drug metabolism and other metabolic activities. Skin Permeability (KSP) is a critical factor for drugs intended for topical use.[36]

GI absorptivity is low for 6 and 9. BBB penetrability was observed for 3, 5 and 8. Higher Human Intestinal Absorption (HIA)

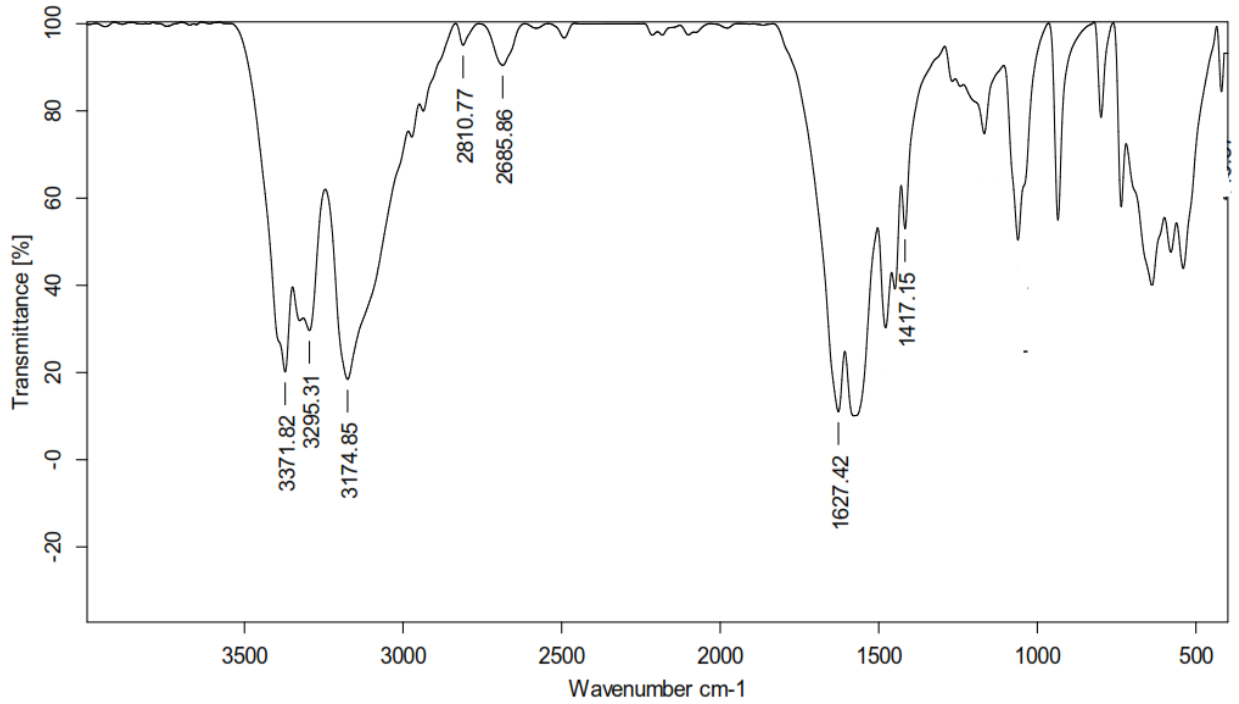



**Figure 4:** FTIR of molecule-1 identified in the Aqueous extract *Asparagus racemosus.*

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

| Molecule | Shape Index | Molecular Flexibility | Molecular Complexity |
|---|---|---|---|
| 1 | 0.41 | 0.59 | 0.93 |
| 2 | 0.66 | 0.59 | 0.59 |
| 3 | 0.66 | 0.51 | 0.54 |
| 4 | 0.75 | 0.85 | 0.64 |
| 5 | 0.55 | 0 | 0.84 |
| 6 | 0.52 | 0.41 | 0.89 |
| 7 | 0.6 | 0.30 | 0.75 |
| 8 | 0.77 | 0.49 | 0.74 |
| 9 | 0.66 | 0.75 | 0.80 |
| 10 | 0.45 | 0.39 | 0.96 |

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

capacity was traced for 1, 2, 4, 6, 7, 9 and 10. No molecules exhibited the PGP efflux effect, whereas none of them showed any CYP inhibitory effect. Additionally, the findings indicate that the skin permeability of the molecules is within an acceptable range (Table 7 and Figure 4).

### Prediction and analysis of molecular targets

Based on the bioactivity score, target prediction analysis was conducted for all the molecules with the results presented in Table 8 and correlated with the results obtained during GCMS and *in silico* studies. The analysis revealed that molecule 1 targets the Protein kinase C gamma receptor, suggesting its potential use as a diverse biological processes, many involving cell-survival pathways. Thus molecule 1 can be a significant biomolecule from satavari for the retention of cellular activity.[37]

## DISCUSSION

The compound 1 was traced as Melazitose. The reported compound is a carbohydrate in nature. The structure of the compound was confirmed by characteristic FTIR peaks and Mass spectrum ($m/z$=504.13). The molecular properties of the compound showed spherical nature with low molecular flexibility and high molecular complexity. The molecular properties demonstrated good adsorption property but energy minimization required

**Table 3: Physical and chemical traits of the molecules detected via GC analysis.**

| Molecule | cLogP | cLogS | H-Acceptors | H-Donors | Total Surface Area | Relative PSA | MR | Polar Surface Area | % abs | Solubility |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | -5.88 | 0.20 | 14 | 11 | 328.32 | 0.53 | 107.98 | 250.22 | 22.67 | Highly soluble |
| 2 | 0.45 | -1.36 | 4 | 1 | 136.4 | 0.34 | 42.4 | 55.76 | 89.76 | Very soluble |
| 3 | 1.30 | -1.45 | 2 | 0 | 143.14 | 0.09 | 53.85 | 12.47 | 104.70 | Very soluble |
| 4 | -1.38 | -0.65 | 5 | 1 | 88.79 | 0.64 | 26.41 | 83.12 | 80.32 | Very soluble |
| 5 | 0.06 | -1.43 | 3 | 1 | 94.04 | 0.38 | 31.22 | 46.53 | 92.95 | Very soluble |
| 6 | -4.38 | -0.22 | 10 | 4 | 197.59 | 0.57 | 81.17 | 144.05 | 59.30 | Highly soluble |
| 7 | -0.77 | -0.93 | 4 | 2 | 101.89 | 0.48 | 32.39 | 66.76 | 85.97 | Very soluble |
| 8 | 0.24 | -1.53 | 3 | 1 | 102.6 | 0.39 | 30.22 | 50.44 | 91.60 | Very soluble |
| 9 | -0.16 | -0.73 | 2 | 2 | 75.72 | 0.35 | 23.67 | 40.46 | 95.04 | Highly soluble |
| 10 | 3.28 | -4.45 | 7 | 0 | 358.44 | 0.20 | 136.32 | 82.14 | 80.66 | Moderately soluble |

Partition coefficient (P=[n-Octanol]/[Water]) (cLogP); b: Solubility in water (S=moles/liter at pH=7.5, 25°C) (cLogS); c: Relative polar surface area (Relative PSA); d: Molar refractive index; e: Topological polar surface area (TPSA); f: Absorption percentage (%Abs).

**Table 4: Drug likliness of the molecules identified by GC-MS analysis.**

| Molecule | Drug likeness | Lipinski | Ghose | Veber | Egan | Muegge | Bioavailability Score |
|---|---|---|---|---|---|---|---|
| 1 | -2.70 | 0 | GR3 | 0 | 0 | MR2 | 0.55 |
| 2 | -6.03 | 0 | 0 | 0 | 0 | MR1 | 0.85 |
| 3 | 0.67 | 0 | 0 | 0 | 0 | MR1 | 0.55 |
| 4 | -6.75 | 0 | GR3 | 0 | 0 | MR2 | 0.56 |
| 5 | -0.89 | 0 | GR3 | 0 | 0 | MR1 | 0.85 |
| 6 | 0.39 | 0 | GR1 | VR1 | ER1 | MR1 | 0.55 |
| 7 | -1.38 | 0 | GR3 | 0 | 0 | MR1 | 0.85 |
| 8 | -2.03 | 0 | GR3 | 0 | 0 | MR1 | 0.55 |
| 9 | -6.16 | LR3 | GR2 | VR1 | ER1 | MR4 | 0.17 |
| 10 | 2.82 | 0 | GR3 | 0 | 0 | 0 | 0.55 |

LR2: violations: MW>500, MLOGP>4.15, LR3: violations: MW>500, NorO>10, NHorOH>5, GR2: violations: MW>480, WLOGP<-0.4, GR3: violations: MW>480, MR>130, #atoms>70, GR4: violations: MW>480, WLOGP>5.6, MR>130, #atoms>70, VR1: violation: Rotors>10 and TPSA>140, ER1: violation: TPSA>131.6 and violation: WLOGP>5.88, MR1: violation: Heteroatoms<2, MR2: violations: XLOGP3>5, Rotors>15, MR3: No; 3 violations: MW>600, XLOGP3>5, Rotors>15, MR4: violations: XLOGP3<-2, TPSA>150, H-acc>10, H-don>5,

**Table 5:** **The bioactivity scores for the molecules pinpointed via GC-MS analysis.**

| Molecule | GL | IC | KI | NR | PI | EI |
|---|---|---|---|---|---|---|
| 1 | -3.67 | -3.63 | -3.69 | -3.61 | -3.63 | -3.49 |
| 2 | -0.34 | -0.23 | -1.01 | -0.61 | -0.54 | 0.3 |
| 3 | -0.86 | -0.61 | -1.22 | -1.65 | -1.13 | -0.69 |
| 4 | -0.86 | -0.61 | -1.22 | -1.65 | -1.13 | -0.69 |
| 5 | -1.9 | -1.43 | -2.1 | -1.7 | -1.9 | -0.99 |
| 6 | 0.03 | 0.28 | -0.49 | -0.82 | -0.54 | 0.2 |
| 7 | 0.22 | 0.16 | 0.1 | 0.12 | 0.22 | 0.41 |
| 8 | 0.1 | 0.1 | -0.38 | 0.35 | 0.09 | 0.23 |
| 9 | 0.01 | 0.04 | -0.54 | 0.38 | -0.15 | 0.53 |
| 10 | -3.72 | -3.81 | -3.8 | -3.81 | -3.65 | -3.75 |
| 11 | 0.1 | -0.25 | -0.07 | -0.04 | 0.08 | 0.08 |

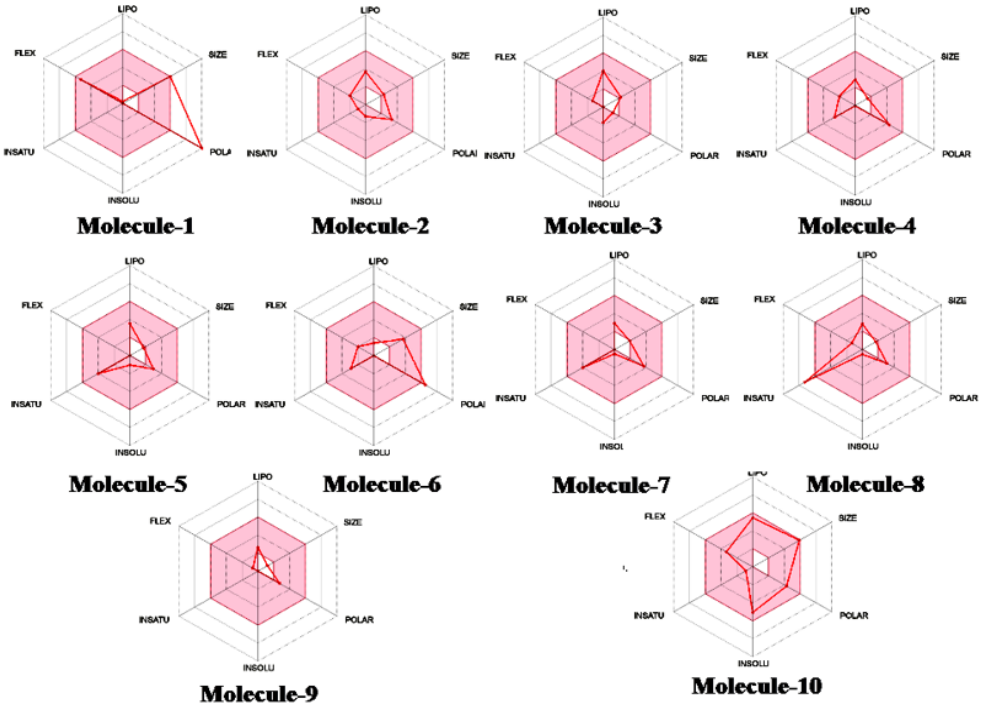
≥0: Good, 0-0.5: Moderate, ≤0.5: Poor, GL: GPCR ligand, IC: Ion channel modulator, KI: Kinase inhibitor, NR: Nuclear receptor ligand, PI: Protease inhibitor, EI: Enzyme inhibitor.

**Table 6:** **Assessment of the toxicity potential linked to the molecules identified through GC-MS analysis.**

| Molecule | Mutagenic | Tumorigenic | Reproductive Effective | Irritant |
|---|---|---|---|---|
| 1 | - | - | - | - |
| 2 | - | - | - | - |
| 3 | - | - | - | - |
| 4 | - | - | - | - |
| 5 | - | - | - | - |
| 6 | - | - | - | - |
| 7 | - | - | - | - |
| 8 | ++ | ++ | - | ++ |
| 9 | - | - | - | - |
| 10 | - | - | - | - |

**Table 7:** **Pharmacokinetic capabilities of the molecules pinpointed through GC-MS analysis.**

| Molecule | GI absorption | BBB permeant | Pgp substrate | CYP1A2 inhibitor | CYP2C19 inhibitor | CYP2C9 inhibitor | CYP2D6 inhibitor | CYP3A4 inhibitor | log Kp (cm/s) |
|---|---|---|---|---|---|---|---|---|---|
| 1 | ++ | - | - | - | - | - | - | - | -7.5 |
| 2 | ++ | - | - | - | - | - | - | - | -6.7 |
| 3 | ++ | ++ | - | - | - | - | - | - | -6.25 |
| 4 | ++ | - | - | - | - | - | - | - | -7.37 |
| 5 | ++ | ++ | - | - | - | - | - | - | -6.6 |
| 6 | + | - | - | - | - | - | - | - | -10.28 |
| 7 | ++ | - | - | - | - | - | - | - | -7.44 |
| 8 | ++ | ++ | - | - | - | - | - | - | -7.48 |
| 9 | + | - | + | - | - | - | - | - | -12.99 |
| 10 | ++ | - | - | - | - | - | - | - | -6.43 |




**The colored zone is suitable physicochemical space for oral bioavailability. LIPO (Liphophilicity): 0.7≤XLOGP3 ≤+5.0; SIZE: 150 g/mole ≤ MV; POLAR (Polarity): 20 Å$^2$≤ TPSA ≤ 130 Å$^2$; INSOLU (Insolubility): 0 ≤LOGS (ESOL)≤ 5.0; INSATU (Insaturation): 0.25 ≤Fraction Csp$^3$≤1; FLEX (Flexibility): 0 ≤Number of rotatable bond < 9**

**Figure 5:** Bioactivity rader for molecules in aqueous extract of *Asparagus racemosus.*

**Table 8: Predicting targets for the molecules, detailing their therapeutic action.**

| Molecule | Target | Target Class | Probability* | Activity |
|---|---|---|---|---|
| 1 | Protein kinase C gamma (by homology) | Kinase | 0.26 | Diverse biological processes, many involving cell-survival pathways. |
| 2 | Serine/threonine protein phosphatase PP1-gamma catalytic subunit | Phosphatase | 0.14 | Regulates neuronal insulin signaling and aggravates insulin resistance leading to AD-like phenotypes. |
| 3 | Sigma opioid receptor | Membrane receptor | 0.18 | Involved in higher-ordered brain functions including memory and drug dependence. |
| 4 | Sigma opioid receptor | Membrane receptor | 0.18 | Involved in higher-ordered brain functions including memory and drug dependence. |
| 5 | Gamma-butyrobetaine dioxygenase | Enzyme | 0.02 | Carnitine is essential for the transport of activated fatty acids across the mitochondrial membrane during mitochondrial beta oxidation. |
| 6 | Glutamate carboxypeptidase II | Enzyme | 0.18 | Neuroprotective by reducing excitotoxic glutamate and increasing levels of NAAG. |
| 7 | Beta-glucocerebrosidase | Enzyme | 0.13 | Break down a large molecule called glucocerebroside into a sugar (glucose) and a simpler fat molecule (ceramide). |
| 8 | Kappa Opioid receptor | Family A G protein-coupled receptor | 0.11 | Provide analgesia, diuresis, and dysphoria. |
| 9 | Alpha-L-fucosidase I | Enzyme | 0.02 | Involved in many biological processes like inflammation, growth regulation, receptor interactions, and antigenicity. |
| 10 | Protein kinase C theta | Kinase | 0.69 | A critical factor for type 2 innate lymphoid cells activation that contributes to TH2 cell differentiation. |

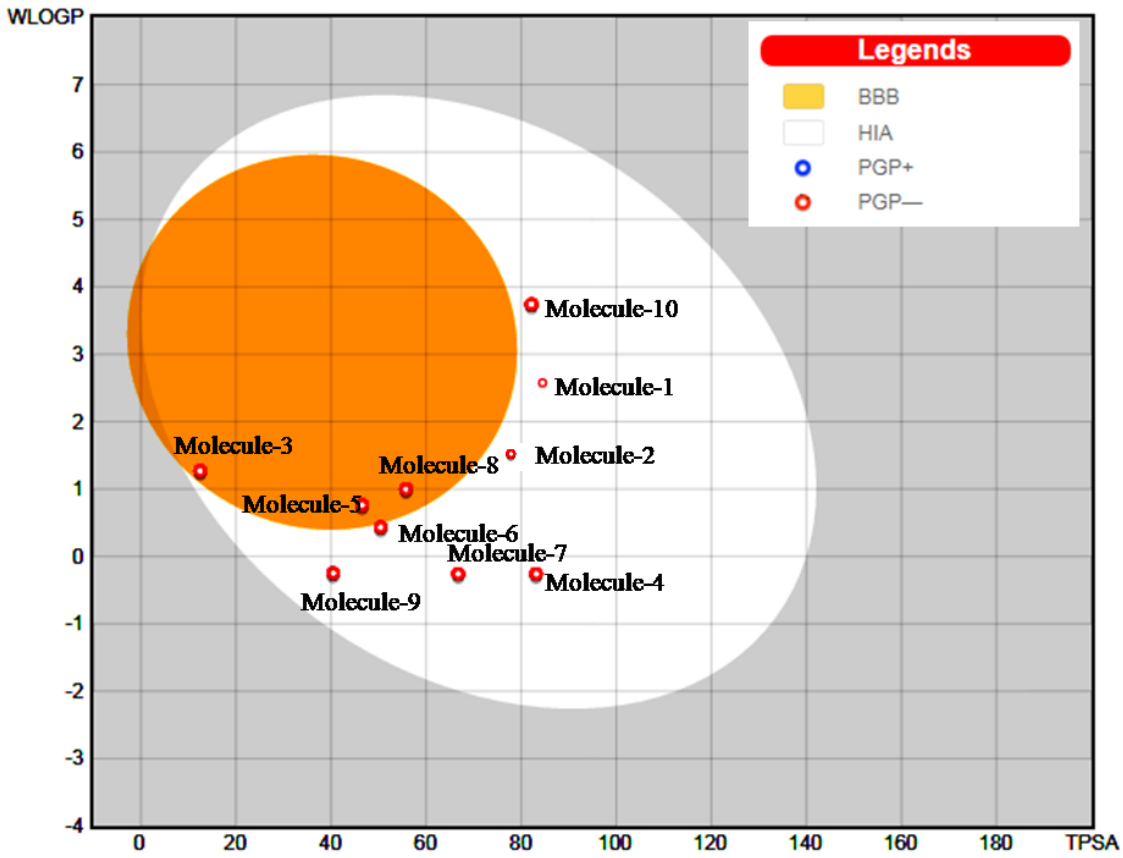



**Figure 6:** Schematic representation of molecules identified in the aqueous extract of *Asparagus racemosus*, akin to a boiled egg diagram.

for drug-receptor binding. The physicochemical properties and drug-likeliness studies exhibited good drug-likeliness behavior of melazitose. The molecule exhibited high aqueous solubility but exhibited less percentage of absorption due to high TPSA value. The compound exhibited good drug-likeliness behavior as per Lipinski, Veber and Egan rules. The moderate oral bioavailability was observed with a value of 0.55. The moderate bioactivity score against different receptors s without any toxicity potential suggest molecular modification is required for getting more binding affinity. The pharmacokinetic study exhibited high GI absorptivity and Higher Human Intestinal Absorption (HIA) capacity with no BBB was traced for 1. The molecule exhibited the PGP efflux effect, whereas not showed any CYP inhibitory effect. The skin permeability of the molecules is -7.5 cm/s suggests good skin permeability. The target prediction analysis revealed that molecule 1 targets the Protein kinase C gamma receptor, suggesting its potential use as a diverse biological process, many involving cell-survival pathways.

## CONCLUSION

The study identified eleven molecules through Gas chromatographic analysis, with their structures confirmed by spectral analysis. The highest concentration was observed for Melezitose. It exhibits good drug likeliness behaviour without any toxicity and higher Human Intestinal Absorption (HIA) capacity. Target prediction analysis confirmed therapeutic potential as a diverse biological process, many involving cell-survival pathways. These findings highlight the success of the molecule Melezitose as potential therapeutic agent for the treatment of multiple disorders

## ACKNOWLEDGEMENT

We express our sincere appreciation to SAIF, IIT Bombay for their assistance with GC-MS and FTIR analysis. Additionally, we extend our heartfelt thanks to the School of Pharmacy, Guru Nanak Institutions Technical Campus for generously providing the necessary facilities for this study.

## CONFLICT OF INTEREST

The authors declare that there is no conflict of interest.

## ABBREVIATIONS

**GC-MS:** Gas Chromatography-Mass Spectrometry; **FTIR:** Fourier Transform Infrared Spectroscopy; **TPSA:** Total Polar Surface Area; **cLogP:** Partition Coefficient; **cLogS:** Solubility; **HIA:** Human Intestinal Absorption; **BBB:** Blood-Brain Barrier; **PGP:** P-Glycoprotein; **CYP:** Cytochrome P450; **KSP:** Skin Permeability; **GPCR:** G-Protein Coupled Receptor; **IC:** Ion

Channel; **KI:** Kinase Inhibitor; **NR:** Nuclear Receptor; **PI:** Protease Inhibitor; **EI:** Enzyme Inhibitor; **AD:** Alzheimer's Disease; **NAAG:** N-Acetylaspartylglutamate; **TH2:** T Helper 2.

## SUMMARY

Malazitose can be a potential bioactive molecule with good drugliness behavior obtained from the aquous extract of *A. recemosus*. Futher molecular development can improve the therapeutic profile for the treatment of multiple disorder.

## REFERENCES


1. Galeano D, Li S, Gerstein M, Paccanaro A. Predicting the frequencies of drug side effects. Nat Commun. 2020;11(1):4575. doi: 10.1038/s41467-020-18305-y, PMID 32917868.
2. Sahoo N, Manchikanti P. J. Herbal Drug regulation and commercialization: an Indian industry perspective. J Altern Complement Med. 2013;19(12):957-63. doi: 10.1089/acm.2012.0275, PMID 23829812.
3. Yuan H, Ma Q, Ye L, Piao G. The traditional medicine and modern medicine from natural products. Molecules. 2016; 21(5): 559-73: 21050559. doi: 10.3390/molecules, PMID 27136524.
4. Anand U, Jacobo-Herrera N, Altemimi A, Lakhssassi N. A comprehensive review on medicinal plants as antimicrobial therapeutics: potential avenues of biocompatible drug discovery. Metabolites. 2019; 9(11) 0258: 258-71. doi: 10.3390/metabo.
5. Semwal DK, Chauhan A, Kumar A, Aswal S, Semwal RB, Kumar A. Status of Indian medicinal plants in the International Union for Conservation of Nature and the future of Ayurvedic drugs: shouldn't think about Ayurvedic fundamentals? J Integr Med. 2019;17(4):238-43. doi: 10.1016/j.joim.2019.04.008, PMID 31076374.
6. Pandey MM, Rastogi S, Rawat AK. Indian traditional ayurvedic system of medicine and nutritional supplementation. Evid Based Complement Alternat Med. 2013; 2013:376327. doi: 10.1155/2013/376327, PMID 23864888.
7. Malongane F, McGaw LJ, Mudau FN. The synergistic potential of various teas, herbs and therapeutic drugs in health improvement: a review. J Sci Food Agric. 2017;97(14):4679-89. doi: 10.1002/jsfa.8472, PMID 28585285.
8. Yadav R, Khare RK, Singhal A. Qualitative phytochemical screening of some selected medicinal plants of Shivpuri District. Int. J Life SciSci.Res. 2017;3(1):844-7.
9. Juszczak AM, Zovko-Končić M, Tomczyk M. Recent trends in the application of chromatographic techniques in the analysis of luteolin and its derivatives. Biomolecules. 2019;9(11):731-41. doi: 10.3390/biom9110731, PMID 31726801.
10. Satapute P, Paidi MK, Kurjogi M, Jogaiah S. Physiological adaptation and spectral annotation of arsenic and cadmium heavy metal-resistant and susceptible strain *Pseudomonas taiwanensis*. Environ Pollut. 2019;251:555-63. doi: 10.1016/j.envpol.2019.05.054, PMID 31108288.
11. Fan S, Chang J, Zong Y, Hu G, Jia J. GC-MS analysis of the composition of the essential oil from *Dendranthema indicum* Var. Aromaticum using three extraction methods and two columns. Molecules. 2018;23(3):576-86. doi: 10.3390/molecules23030576, PMID 29510531.
12. Razack S, Kumar KH, Nallamuthu I, Naika M, Khanum F. Antioxidant, biomolecule Oxidation Protective Activities of *Nardostachys jatamansi* DC and Its Phytochemical Analysis by RP-HPLC and GC-MS. Antioxidants (Basel). 2015;4(1):185-203. doi: 10.3390/antiox4010185, PMID 26785345.
13. Krishnaveni M, Mirunalini S. Therapeutic potential of *Phyllanthus emblica* (amla): the ayurvedic wonder. J Basic Clin Physiol Pharmacol. 2010;21(1):93-105. doi: 10.1515/jbcpp.2010.21.1.93, PMID 20506691.
14. Vishwakarma R, Goswami PK. A review through Charaka Uttara-Tantra. Ayu. 2013;34(1):17-20. doi: 10.4103/0974-8520.115438, PMID 24049400.
15. Kamat JP, Boloor KK, Devasagayam TP, Venkatachalam SR. Antioxidant properties of *Asparagus racemosus* against damage induced by gamma-radiation in rat liver mitochondria. J Ethnopharmacol. 2000;71(3):425-35. doi: 10.1016/s0378-8741(00)00176-8, PMID 10940579.
16. Sliwoski G, Kothiwale S, Meiler J, Lowe EW Jr. Computational methods in drug discovery. Pharmacol Rev. 2014;66(1):334-95. doi: 10.1124/pr.112.007336, PMID 24381236.
17. Lee K, Kim D. *In silico* Molecular Binding Prediction for Human Drug Targets Using Deep Neural Multi-Task Learning. Genes (Basel). 2019;10(11):906-21. doi: 10.3390/genes10110906, PMID 31703452.
18. Lamers I, Feys P. Assessing upper limb function in multiple sclerosis. Mult Scler. 2014;20(7):775-84. doi: 10.1177/1352458514525677, PMID 24664300.
19. Senthil kumar D, Karthikeyan D, Roy B. *In silico*, ADMET and Docking Analysis for the compounds of chloroform Extract of *Tinospora cardifolia* (Wild.) Identified by GC-MS and Spectral Analysis for antidiabetic and anti-inflammatory Activity. Asian J Chem. 2022;34(2):342-54: 2022.23521. doi: 10.14233/ajchem.
20. Morris GM, Lim-Wilby M. Molecular docking. Methods Mol Biol. 2008;443:365-82. doi: 10.1007/978-1-59745-177-2_19, PMID 18446297.
21. Kokate CK. Pharmacognosy. 17th ed. Pune: Nirali Prakashan; 2001. p. 106.
22. Sen S, Ravindar B, Jala S, Dharabonia L. *In silico* design and docking study of some 4-(10-Acetyl-10h-Phenothiazines-3-Yl)-1-Phenylazeti Din-2-One derivatives. Int J Pharm Sci Res. 2022;13(8):3163-73. doi: 10.13040/IJPSR.0975-8232.13(8).3163-73.
23. Senthil kumar D, Karthikeyan D, Roy B. Identification of antidiabetic and anti-inflammatory potential compounds of ethyl acetate Extract of *Tinospora cardifolia* (Wild) Identified by GC-MS and Spectral Analysis: A Computational Approach. Asian J Chem. 2022;34(6):1401-12. doi: 10.14233/ajchem.2022.23624.
24. Nicholls A, McGaughey GB, Sheridan RP, Good AC, Warren G, Mathieu M, *et al*. Brown, J. Andrew Grant. James A. Haigh, Neysa Nevins∞, Ajay N. Jain, Brian Kelley. Molecular Shape and Medicinal Chemistry: A Perspective, J. Med. Chem. 2010,53(10),3862-86. https://doi.org/10.1021/jm900818s.
25. Rohs R, Bloch I, Sklenar H, Shakked Z. Molecular flexibility in ab initio drug docking to DNA: binding-site and binding-mode transitions in all-atom Monte Carlo simulations. Nucleic Acids Res. 2005;33(22):7048-57. doi: 10.1093/nar/gki1008, PMID 16352865.
26. Méndez-Lucio OM, Medina-Franco JL. The many roles of molecular complexity in drug discovery. Drug Discov Today. 2017;22(1):120-6. doi: 10.1016/j.drudis.2016.08.009, PMID 27575998.
27. Benet LZ, Hosey CM, Ursu O, Oprea TI. BDDCS, the Rule of 5 and Drugability. Adv Drug Deliv Rev. 2016;101:89-98. doi: 10.1016/j.addr.2016.05.007, PMID 27182629.
28. Prasanna S, Doerksen RJ. Topological polar surface area: A useful descriptor in 2D-QSAR. Curr Med Chem. 2009;16(1):21-41. doi: 10.2174/092986709787002817, PMID 19149561.
29. Ji D, Xu M, Udenigwe CC, Agyei D. Physicochemical characterisation, molecular docking, and drug-likeness evaluation of hypotensive peptides encrypted in flaxseed proteome. Curr Res Food Sci. 2020;3:41-50. doi: 10.1016/j.crfs.2020.03.001, PMID 32914119.
30. Husain A, Ahmad A, Khan SA, Asif M, Bhutani R, Al-Abbasi FA. Synthesis, molecular properties, toxicity and biological evaluation of some new substituted imidazolidine derivatives in search of potent anti-inflammatory agents. Saudi Pharm J. 2016;24(1):104-14. doi: 10.1016/j.jsps.2015.02.008, PMID 26903774.
31. Prescott LF. Gastrointestinal absorption of drugs. Med Clin North Am. 1974;58(5):907-16. doi: 10.1016/s0025-7125(16)32088-0, PMID 4609045.
32. Wessel MD, Jurs PC, Tolan JW, Muskal SM. Prediction of human intestinal absorption of drug compounds from molecular structure. J Chem Inf Comput Sci. 1998;38(4):726-35. doi: 10.1021/ci980029a, PMID 9691477.
33. Pardridge WM. Drug transport across the blood-+brain barrier. J Cereb Blood Flow Metab. 2012;32(11):1959-72. doi: 10.1038/jcbfm.2012.126, PMID 22929442.
34. Tanigawara Y. Role of P-glycoprotein in drug disposition. Ther Drug Monit. 2000;22(1):137-40. doi: 10.1097/00007691-200002000-00029, PMID 10688277.
35. Lin JH, Lu AY. Inhibition and induction of cytochrome P450 and the clinical implications. Clin Pharmacokinet. 1998;35(5):361-90. doi: 10.2165/00003088-199835050-00003, PMID 9839089.
36. Potts RO, Guy RH. Predicting skin permeability. Pharm Res. 1992;9(5):663-9. doi: 10.1023/a:1015810312465, PMID 1608900.
37. Gfeller D, Grosdidier A, Wirth M, Daina, Michielin O, Zoete V. SwissTargetPrediction. SwissTargetPrediction: a web server for target prediction of bioactive small molecules. Nucleic Acids Res. 2014; 42(Web Server issue);Web Server Issue:W32-8. doi: 10.1093/nar/gku293, PMID 24792161.


**Cite this article:** Sen S, Swathi K, Vishwanath D, Ravindar B, Chaitanya M, Cherukupally S, *et al*. Melezitose a Potential of Bioactive Compound from Aqueous Extract of Indian Satavari: An Web Based *in silico* Study Utilizing GC-MS Analysis. Pharmacog Res. 2024;16(4):887-96.