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Computational screening of phytocompounds found in Ayurvedic Herb *Jatāmāṃsī* for drug likeness properties and therapeutic activity used for Mental Health Management

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Abstract : Mental health disorders such as anxiety, depression, insomnia, phobias, addiction, Parkinson's disease, memory and sleep related issues have become major global concerns, prompting the need for safer and more effective alternative treatments. Jatāmāṃsī that is *Nardostachys jatamansi* (D. Don) DC., a perennial herb native to the Himalayas which has been an integral part of Ayurvedic, Unani and Chinese medicine for centuries due to its wide range of therapeutic benefits. This study with the help of in-silico approach delves into its pharmacological potential in highlighting its role in the mental health management using the rhizome part of the plant. Key bioactive compounds of flower were identified in the IMPPAT database and further were analyzed for *in*-silico pharmacokinetics, blood-brain barrier permeability, and drug-likeness using SwissADME online tools. The pharmacological analysis has been done using Swiss ADME (Absorption-Distribution-Metabolism-Excretion) online platform for phytocompounds found in rhizome part of the plant. With 36 phytocompounds in rhizome part of the plant, 60 therapeutic activities were found. Among these it has mental health properties like anticonvulsants, antidepressive agents, antihypertensive agents, Epilepsy, hypertension, hypotension, anti-stress, nervous system diseases, neurotic disorders, mental disorders, hysteria, parasympatholytic, sleep initiation and maintenance disorders, anti-stress and tardive dyskinesia. By bridging traditional wisdom with modern pharmacological insights, this research underscores the importance of further in-vitro, in-vivo and clinical investigations to confirm the herb's efficacy and safety. With its diverse therapeutic benefits of *N. jatamansi* emerges as a promising natural remedy for promoting mental and physical well-being.

Keywards- *Jatāmāṃsī, in-silico approach, mental health management, database IMPPAT, SwissADME, phytocompounds,* blood-brain barrier permeability, and drug-likeness

I. INTRODUCTION

Ayurveda, the traditional Indian medical system, has been practiced since the Vedic period (4500-1600 BC) and continues to play an important role in modern healthcare [8]. Medicinal herbs have been used for therapeutic purposes since antiquity, serving as a natural alternative to manufactured pharmaceuticals. Anxiety, depression, sleeplessness, alcohol dependency syndrome and nicotine addiction have all emerged as serious global challenges, demanding the quest for safer and more effective treatments. While traditional drugs like benzodiazepines and selective serotonin reuptake inhibitors (SSRIs) are commonly utilized, they are frequently accompanied with negative side effects and addiction risks [5].

Nardostachys jatamansi, commonly known as Indian spikenard, is a perennial herb indigenous to the Himalayan regions, traditionally utilized in various medicinal systems, including Ayurveda, Unani and traditional Chinese medicine. The rhizomes and roots of *N. jatamansi* are rich in bioactive compounds, contributing to a wide array of therapeutic properties [3]. *Nardostachys jatamansi* (D. Don) DC., commonly known as *Jatamansi*, is a small, perennial, rhizomatous herb that thrives on steep, moist and rocky slopes in the alpine Himalayas [20]. It is primarily found at elevations between 3000 and 5200 meters in regions of Uttarakhand, Himachal Pradesh, Arunachal Pradesh and Sikkim in India, as well as parts of Nepal, Tibet, China and Bhutan [2]. The name "*Jatāmāṃsi*" is derived from the Sanskrit word "*Jatā*," meaning matted or uncombed hair, resembling its rhizome structure. This plant has been valued in Ayurveda, ethnomedicine and alternative healing systems since the Vedic period (1000–800 B.C.), where it was traditionally used for treating neurological and psychological disorders [2].

Common names of *Nardostachys jatamansi* found in Ayurvedic pharmacopoeia of India are, Sanskrit: *Māṁsī, Jaā, Jailā*, Assamese: Jatamansi, Jatamangshi, Bengali: Jatamamsi, English: Nardus root, Gujrati: Baalchad, Kalichad, Hindi: Balchara, Kannada: Bhootajata, Ganagila maste, Kashmiri: Bhutijata, Malayalam: Manchi, Jatamanchi, Marathi: Jatamansi, Oriya: Jatamansi, Punjabi: Billilotan, Balchhar, Chharguddi, Tamil: Jatamanji, Telugu: Jatamams, Urdu: Sumbul-ut-teeb [21].

Phytochemical investigations have revealed that *N. jatamansi* contains esters, phenolic compounds and terpenic ketones, which contribute to its broad pharmacological properties, including antidepressant, anti-stress, antioxidant, anticonvulsant, hypotensive, anti-asthmatic, cardioprotective, neuroprotective, antidiabetic, antifungal, antibacterial, and anticancer effects [2]. Due to its ability to balance all three *Śarīra Doṣa* (body humors) and *Mānasa Doṣa* (psychic humor), it is widely used in Ayurvedic

psychiatric treatments. Recent studies suggest that *N. jatamansi* is effective in managing test anxiety in children when combined with Yoga therapy [1].

The methanolic extract of *N. jatamansi* has demonstrated significant antidepressant activity in both normal and sleep-deprived mice, comparable to the standard drug imipramine. Additionally, it improves locomotor activity in sleep-deprived conditions, indicating its potential for treating depression associated with sleep disturbances. Moreover, the hydro-ethanolic extract has shown strong anti-stress effects, likely due to its potent antioxidant properties, as it effectively reduces lipid peroxidation and nitric oxide levels while restoring catalase activity in the brain [5].

In today's fast-paced society, insomnia is becoming a bigger problem. Recent research by that *Nardostachys jatamansi* may be a natural solution for sleep-related problems. According to their research, this therapeutic herb is essential for fostering calm and lowering anxiety, two factors that are major causes of sleep disorders. The results show that by lengthening sleep duration and decreasing the time it takes to fall asleep, *Nardostachys jatamansi* contributes to better sleep quality [6]. Its impact on neurotransmitters like GABA, which are in charge of promoting relaxation and controlling sleep cycles, is probably what causes this effect. The herb may also be useful in treating insomnia because of its neuroprotective and stress-relieving qualities. Beyond its neuroprotective effects, *N. jatamansi* has also exhibited anticancer potential. Oral administration of its root extract at doses of 50, 100, and 200 mg/kg for seven days significantly improved learning and memory in young mice and reversed diazepam- and scopolamine-induced amnesia. Oral administration of its root extract at doses of 50, 100, and 200 mg/kg for seven days significantly improved learning and memory in young mice and reversed diazepam- and scopolamine-induced amnesia [6]. Additionally, its crude extract and isolated bioactive compounds, including nardal, jatamansic acid and nardin contribute to hair regeneration following chemotherapy-induced hair loss [5].

Building on this, a recent study reviewed the evolving role of traditional medicinal herbs, including *Nardostachys jatamansi*, in the management of Alzheimer's disease. Their review highlighted the plant's antioxidant and neuroprotective properties, emphasizing its potential in slowing neurodegenerative processes and supporting cognitive function [17]. Another research conducted additional experiments to demonstrate its efficacy in an Alzheimer's disease model. *Nardostachys jatamansi* was reported to help prevent cognitive decline and memory damage in sleep-deprived rats, implying that it has the potential to be a neuroprotective agent [10].

Beyond cognitive performance, investigated the psychosocial impact of *Nardostachys jatamansi* on clinical patients suffering from stress. Their findings showed that the root extract helped to reduce stress-related symptoms, promote relaxation and improve general mental health [19]. These investigations demonstrate *Nardostachys jatamansi's* therapeutic potential in cognitive enhancement, neuroprotection and stress management making it a suitable option for future research in neuropsychology and integrative medicine. *Nardostachys jatamansi* is known to contain multiple bioactive compounds that contribute to its pharmacological effects. These include jatamansone, nardosinone, calarene, aristolen-9beta-ol, patchouli alcohol and other sesquiterpenoids. These compounds were selected based on their reported anxiolytic, neuroprotective and anti-inflammatory properties, which are crucial for psychological well-being. Jatamansone, in particular, has demonstrated significant neuroprotective and cognitive-enhancing effects, making it a primary candidate for further computational analysis.

Given its diverse pharmacological properties, *N. jatamansi* holds immense potential as a natural therapeutic agent for managing stress, depression, anxiety, cognitive impairment and chemotherapy-induced hair loss. The increasing reliance on plant-based therapeutics underscores the need for extensive scientific validation to explore its mechanisms of action and clinical applications. In recent research conducted had reported that *N. jatamansi* has a good properties of antioxidant agents [15]. Numerous studies have explored the cognitive and psychological benefits of *Nardostachys jatamansi*, a medicinal herb known for its neuroprotective properties. This research aims to bridge the gap between traditional knowledge and modern pharmacological investigations, offering insights into the potential of *N. jatamansi* in holistic mental and physical health management.

II. RESEARCH METHODOLOGY

The purpose of this study is to determine the potential of *Nardostachys jatamansi* in the management of psychological symptoms by exploring its bioactive compounds and their pharmacokinetic properties using computational tools such as IMPPAT and SwissADME. The methodology involves several key steps, including the identification of bioactive compounds, in silico screening for chemical and pharmacological properties and an assessment of their pharmacokinetic profiles with a focus on their CNS-targeting potential and BBB permeability

Computational Screening and Data Collection

1. IMPPAT Database Analysis

The Indian Medicinal Plants, Phytochemistry and Therapeutics (IMPPAT) database was used to evaluate the therapeutic significance of *Nardostachys jatamansi* bioactive compounds concerning psychological symptom management. IMPPAT provides comprehensive information on medicinal plants, emphasizing their phytochemistry and traditional uses. Each bioactive compound was analyzed for its ethnopharmacological applications, historical therapeutic significance and reported toxicity. This step ensured the relevance of the selected compounds in the context of psychological health and clinical applications [9,14].

2. SwissADME Analysis

SwissADME was employed to estimate the pharmacokinetic properties of *Nardostachys jatamansi* bioactive compounds. This online tool evaluates key pharmacokinetic attributes, including:

- **Absorption**: Assessing the compounds' gastrointestinal absorption, essential for oral administration.
- **Bioavailability**: Evaluating the proportion of compounds that enter systemic circulation and their potential therapeutic effects.
- **Blood-Brain Barrier (BBB) Permeability**: Determining whether the compounds can cross the BBB, which is crucial for CNS-targeting effects.
- **Lipophilicity and Solubility**: Factors influencing absorption, distribution and bioavailability.

- **Pharmacokinetics**: Analyzing key parameters such as GI absorption, BBB permeability, P-glycoprotein (Pgp) substrate status and inhibition of cytochrome P450 enzymes (CYP1A2, CYP2C19, CYP2C9, CYP2D6 and CYP3A4), which affect drug metabolism.
- **Drug-likeness**: Evaluating compliance with Lipinski's Rule of Five and other filters (Ghose, Veber, Egan, Muegge) along with bioavailability scores.

Each bioactive compound was assessed using SwissADME and their pharmacokinetic profiles were compared to identify the most promising candidates for psychological well-being. These computational analyses provided critical insights into the pharmacological viability of *Nardostachys jatamansi* as a natural remedy for psychological symptom management. This methodology integrates traditional ethnopharmacological knowledge with modern computational tools to investigate the role of *Nardostachys jatamansi* in managing psychological symptoms. By utilizing IMPPAT and SwissADME, this study provides a deeper understanding of the plant's bioactive compounds and their suitability as CNS-targeting agents for psychological disorder management [11,12,13].

III. RESULTS AND DISCUSSION

Retrieving data from IMPPAT Database:

The IMPPAT data base was able to provide insight into the Phytochemicals available in *Nardostachys jatamansi* which have been enlisted and categorized in the following tables.

Table 1: Phytocompounds of *Nardostachys jatamansi* rhizome parts as per IMPPAT database

Sr No	Plant Part	IMPPAT Phytochemical Identifier	Phytochemical Name	SMILE
1	rhizome	IMPHY000061	Patchouli alcohol	C[C@H]1CC[C@@]2([C@@]3([C@H]1C[C@H](C2(C)C)CC3)C)O
2	rhizome	IMPHY000104	Nardostachysin	C[C@@H]1CC[C@H]2[C@@H]1CC(=CC=C2C(=O)OC[C@]1(O)[C@@H](O)C[C@@H]2[C@H]1C(=O)OCC2=C)C(C)C
3	rhizome	IMPHY000575	Angelicin	O=c1ccc2c(o1)c1ccoc1cc2
4	rhizome	IMPHY001109	Isovaleric acid	CC(CC(=O)O)C
5	rhizome	IMPHY002234	Nardol	CC([C@@H]1CCC(=C)[C@H]2[C@@H](C1)[C@](C)(O)CC2)C
6	rhizome	IMPHY002360	Jatamol A	O[C@H]1CC(=C)[C@H]2[C@@](C1)(C)CC[C@H](C2)C(=C)C
7	rhizome	IMPHY002479	Jatamol B	O=C(CC(O)(C)C)O[C@H]1CC(=C)[C@H]2[C@@](C1)(C)CC[C@H](C2)C(=C)C
8	rhizome	IMPHY002513	(1S,5S,9R)-9-Isopropyl-1-methyl-6-methylenespiro[4.5]decan-1-ol	CC(C1CCC(=C)C2(C1)CCCC2(C)O)C
9	rhizome	IMPHY002800	8-(2-Hydroxypropan-2-yl)furo[2,3-h]chromen-2-one	O=c1ccc2c(o1)c1cc(oc1cc2)C(O)(C)C
10	rhizome	IMPHY003631	Valeranone	CC([C@H]1CC[C@@]2([C@@](C1)(C)C(=O)CCC2)C)C
11	rhizome	IMPHY003638	(-)-Valeranone	CC([C@@H]1CC[C@]2([C@](C1)(C)C(=O)CCC2)C)C
12	rhizome	IMPHY003715	Pinoresinol	COc1cc(ccc1O)[C@H]1OC[C@H]2[C@@H]1CO[C@@H]2c1ccc(c(c1)OC)O
13	rhizome	IMPHY003822	Cubebol	CC([C@@H]1CC[C@H]([C@]23[C@H]1[C@H]2[C@@](C)(O)CC3)C)C
14	rhizome	IMPHY004022	Tricyclo(6.3.1.02,5)dodecan-1-ol, 4,4,8-trimethyl-, (1R,2S,5R,8S)-	C[C@]12CCC[C@](C2)(O)[C@@H]2[C@@H](CC1)C(C2)(C)C
15	rhizome	IMPHY004168	Jatamansin	C/C=C(C(=O)O[C@@H]1Cc2c(OC1(C)C)ccc1c2oc(=O)cc1)/C
16	rhizome	IMPHY004521	alpha-Patchoulene	CC1CCC23C1CC(C3(C)C)CC=C2C
17	rhizome	IMPHY004670	Seychellene	CC1CCC2(C3(C1CC(C2=C)CC3)C)C
18	rhizome	IMPHY005078	Nardosinone	O=C1C[C@H]2OOC([C@H]2[C@@]2(C1=CCC[C@H]2C)C)(C)C
19	rhizome	IMPHY006153	8,8-dimethyl-2H,8H-pyrano[2,3-f]chromene-2,9(10H)-dione	O=c1ccc2c(o1)c1CC(=O)C(Oc1cc2)(C)C
20	rhizome	IMPHY006189	Virolin	C/C=C/c1ccc(c(c1)OC)O[C@H]([C@H](c1ccc(c(c1)OC)OC)O)C
21	rhizome	IMPHY006317	Norseychellanon	CC1CCC2(C3(C1CC(C2=O)CC3)C)C

Sr No	Plant Part	IMPPAT Phytochemical Identifier	Phytochemical Name	SMILE
22	rhizome	IMPHY006485	beta-Ionone	CC(=O)/C=C/C1=C(C)CCCC1(C)C
23	rhizome	IMPHY007122	Actinidine	C[C@H]1CCc2c1cncc2C
24	rhizome	IMPHY007273	1-Hexacosanol	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCO
25	rhizome	IMPHY008730	Jatamansic acid	CC(C1=CC=C([C@@H]2[C@H](C1)[C@H](C)CC2)C(=O)O)C
26	rhizome	IMPHY008832	Nardostachone	O=C1C=C(C)C2(C(=C1)C=C[C@H](C2)C(C)C)C
27	rhizome	IMPHY009359	Hexacosane	CCCCCCCCCCCCCCCCCCCCCCCCCCCC
28	rhizome	IMPHY010605	Lomatin	O=c1ccc2c(o1)c1CC(O)C(Oc1cc2)(C)C
29	rhizome	IMPHY011392	3-Carene	CC1=CCC2C(C1)C2(C)C
30	rhizome	IMPHY011542	beta-Eudesmol	C=C1CCC[C@]2([C@H]1C[C@@H](CC2)C(O)(C)C)C
31	rhizome	IMPHY011581	alpha-Selinene	CC1=CCC[C@]2([C@H]1C[C@@H](CC2)C(=C)C)C
32	rhizome	IMPHY011609	alpha-Carotene	C/C(=CC=CC=C(C=CC=C(C=CC1=C(C)CCCC1(C)C)/C)/C)/C=C/C=C(/C=C/[C@H]1C(=CCCC1(C)C)C)C
33	rhizome	IMPHY011667	alpha-Gurjunene	C[C@@H]1CC[C@@H]2[C@H](C3=C(CC[C@H]13)C)C2(C)C
34	rhizome	IMPHY011761	Humulene	C/C/1=CCC(C)(C)/C=C/C/C(=C/CC1)/C
35	rhizome	IMPHY011890	Elemol	C=C[C@]1(C)CC[C@H](C[C@H]1C(=C)C)C(O)(C)C
36	rhizome	IMPHY014836	beta-Sitosterol	CC[C@@H](C(C)C)CC[C@H]([C@H]1CC[C@@H]2[C@]1(C)CC[C@H]1[C@H]2CC=C2[C@]1(C)CC[C@@H](C2)O)C

There is total 36 phytocompounds we found in the IMPPAT database for the rhizome part of the plant.

Table 2: Therapeutic Activity of *Nardostachys jatamansi* rhizome found in IMPPAT database:

Sr No	Plant Part	Therapeutic use	Therapeutic use identifiers
1	rhizome	Hair loss	MESH:D000505, UMLS:C0002170, DOID:987, ICD-11:ED70
2	rhizome	Analgesics	MESH:D000700, UMLS:C0002771, ICD-11:XM49F7
3	rhizome	Anthelmintics	MESH:D000871, UMLS:C0003158, ICD-11:XM4EC0
4	rhizome	Anti-arrhythmia agents	MESH:D000889, UMLS:C0003195, ICD-11:BC9Z
5	rhizome	Anticonvulsants	MESH:D000927, UMLS:C0003286, ICD-11:XM07T3
6	rhizome	Antidepressive agents	MESH:D000928, UMLS:C0003289, ICD-11:6A7Z
7	rhizome	Antihypertensive agents	MESH:D000959, UMLS:C0003364, ICD-11:XM2PT6
8	rhizome	Anti-infective agents	MESH:D000890, UMLS:C0003204, ICD-11:XM4TV0
9	rhizome	Anti-infective agents, local	MESH:D000891, UMLS:C0003205, ICD-11:XM4VG4
10	rhizome	Anti-inflammatory agents	MESH:D000893, UMLS:C0003209, ICD-11:XM7XD1
11	rhizome	Antiprotozoal agents	MESH:D000981, UMLS:C0003416, ICD-11:XM4393
12	rhizome	Antipyretics	MESH:D058633, UMLS:C0003419, ICD-11:XM1RS7
13	rhizome	Antirheumatic agents	MESH:D018501, UMLS:C0003191, ICD-11:XM95N2
14	rhizome	Antitussive agents	MESH:D000996, UMLS:C0003449
15	rhizome	Appetite stimulants	MESH:D019167, UMLS:C0376447
16	rhizome	Asthma	MESH:D001249, UMLS:C0004096, DOID:2841, ICD-11:CA23
17	rhizome	Bronchial diseases	MESH:D001982, UMLS:C0006261, DOID:1176, ICD-11:CB40.Y
18	rhizome	Cardiotonic agents	MESH:D002316, UMLS:C0007209, ICD-11:XM91S1
19	rhizome	Cardiovascular diseases	MESH:D002318, UMLS:C0007222, DOID:1287, ICD-11:BE2Z
20	rhizome	Chemoprevention	MESH:D018890, UMLS:C0282515
21	rhizome	Cholinesterase inhibitors	MESH:D002800, UMLS:C0008425
22	rhizome	Colic	MESH:D003085, UMLS:C0232488, ICD-11:MD81.4
23	rhizome	Common cold	MESH:D003139, UMLS:C0009443, DOID:10459, ICD-11:CA00
24	rhizome	Diarrhea	MESH:D003967, UMLS:C0011991, DOID:13250, ICD-11:ME05.1
25	rhizome	Digestive system diseases	MESH:D004066, UMLS:C0012242, ICD-11:DE2Z
26	rhizome	Diuretics	MESH:D004232, UMLS:C0012798, ICD-11:XM4D06

Sr No	Plant Part	Therapeutic use	Therapeutic use identifiers
27	rhizome	Dysmenorrhea	MESH:D004412, UMLS:C0013390, ICD-11:GA34.3
28	rhizome	Dyspepsia	MESH:D004415, UMLS:C0013395, ICD-11:DD90.3
29	rhizome	Epilepsy	MESH:D004827, UMLS:C0014544, DOID:1826, ICD-11:8A6Z
30	rhizome	Erysipelas	MESH:D004886, UMLS:C0014733, DOID:11330, ICD-11:1B70.0
31	rhizome	Estrogen receptor modulators	MESH:D020847, UMLS:C0752229
32	rhizome	Flatulence	MESH:D005414, UMLS:C0016204, ICD-11:ME08
33	rhizome	Headache	MESH:D006261, UMLS:C0018681, ICD-11:8A81.Z
34	rhizome	Heart diseases	MESH:D006331, UMLS:C0018799, DOID:114, ICD-11:BC4Z
35	rhizome	Hematologic diseases	MESH:D006402, UMLS:C0018939, DOID:74, ICD-11:3C0Z
36	rhizome	Hypertension	MESH:D006973, UMLS:C0020538, DOID:10763, ICD-11:BA00.Z
37	rhizome	Hypotension	MESH:D007022, UMLS:C0020649, ICD-11:BA2Z
38	rhizome	Hysteria	MESH:D007046, UMLS:C0020701
39	rhizome	Jaundice	MESH:D007565, UMLS:C0022346, ICD-11:ME10.1
40	rhizome	Laxatives	MESH:D054368, UMLS:C0282090, ICD-11:XM62T3
41	rhizome	Liver diseases	MESH:D008107, UMLS:C0023895, DOID:409, ICD-11:SA0Z
42	rhizome	Lung diseases	MESH:D008171, UMLS:C0024115, DOID:850, ICD-11:CB40.Y
43	rhizome	Menstrual cycle	MESH:D008597, UMLS:C0025329
44	rhizome	Menstruation disturbances	MESH:D008599, UMLS:C0025345, ICD-11:GA20.30
45	rhizome	Menstruation-inducing agents	MESH:D008600, UMLS:C0025346
46	rhizome	Mental disorders	MESH:D001523, UMLS:C0004936, ICD-11:6E8Z
47	rhizome	Nervous system diseases	MESH:D009422, UMLS:C0027765, DOID:863, ICD-11:8E7Z
48	rhizome	Neurotic disorders	MESH:D009497, UMLS:C0027932, DOID:4964
49	rhizome	Pain	MESH:D010146, UMLS:C0030193, ICD-11:MG3Z
50	rhizome	Parasympatholytics	MESH:D010276, UMLS:C0030511, ICD-11:XM3A77
51	rhizome	Radiation-protective agents	MESH:D011837, UMLS:C0034540
52	rhizome	General tonic for rejuvenation	MESH:D012060, UMLS:C0035016
53	rhizome	Scorpion stings	MESH:D065008, UMLS:C0238417, ICD-11:NE61
54	rhizome	Skin diseases	MESH:D012871, UMLS:C0037274, DOID:37, ICD-11:EM0Z
55	rhizome	Sleep initiation and maintenance disorders	MESH:D007319, UMLS:C0021603
56	rhizome	Snake bites	MESH:D012909, UMLS:C0037379
57	rhizome	Stress, physiological	MESH:D013312, UMLS:C0449430, ICD-11:6E40.4
58	rhizome	Ulcer	MESH:D014456, UMLS:C0041582
59	rhizome	Urination disorders	MESH:D014555, UMLS:C0042035, ICD-11:GB0Y
60	rhizome	Tardive dyskinesia	MESH:D000071057, UMLS:C0686347, ICD-11:8A02.10

Nardostachys jatamansi showed 60 therapeutic activities in the rhizome part of the plant as per IMPPAT database. Among these it has mental health properties like anticonvulsants, antidepressive agents, antihypertensive agents. It can also manage the symptoms of epilepsy, hypertenstion, hypotension, nervous system diseases, neurotic disorders, hysteria, parasympatholytics, sleep initiation and maintainance disorders, stress and tardive dyskinesia.

Table 3: Physicochemical Properties Of Selected Phytochemicals of *Nardostachys jatamansi:*

Sr No	Phytochemical Name	Formula	MW	#Heavy atoms	#Aromatic heavy atoms	Fraction Csp3	#Rotatable bonds	#H-bond acceptors	#H-bond donors	MR	TPSA
1	Patchouli alcohol	C15H26O	222.37	16	0	1	0	1	1	68.56	20.23
2	Nardostachysin	C25H34O6	430.53	31	0	0.68	5	6	2	117.34	93.06
3	Angelicin	C11H6O3	186.16	14	13	0	0	3	0	52.26	43.35
4	Isovaleric acid	C5H10O2	102.13	7	0	0.8	2	2	1	27.92	37.3
5	Nardol	C15H26O	222.37	16	0	0.87	1	1	1	70.72	20.23
6	Jatamol A	C15H24O	220.35	16	0	0.73	1	1	1	69.94	20.23
7	Jatamol B	C20H32O3	320.47	23	0	0.75	5	3	1	95.3	46.53
8	(1S,5S,9R)-9-Isopropyl-1-	C15H26O	222.37	16	0	0.87	1	1	1	70.46	20.23

Sr No	Phytochemical Name	Formula	MW	#Heavy atoms	#Aromatic heavy atoms	Fraction Csp3	#Rotatable bonds	#H-bond acceptors	#H-bond donors	MR	TPSA
	methyl-6-methylenespiro[4.5]decan-1-ol										
9	8-(2-Hydroxypropan-2-yl)furo[2,3-h]chromen-2-one	C14H12O4	244.24	18	13	0.21	1	4	1	67.88	63.58
10	Valeranone	C15H26O	222.37	16	0	0.93	1	1	0	69.67	17.07
11	(-)-Valeranone	C15H26O	222.37	16	0	0.93	1	1	0	69.67	17.07
12	Pinoresinol	C20H22O6	358.39	26	12	0.4	4	6	2	94.9	77.38
13	Cubebol	C15H26O	222.37	16	0	1	1	1	1	68.82	20.23
14	Tricyclo(6.3.1.02,5)dodecan-1-ol, 4,4,8-trimethyl-, (1R,2S,5R,8S)-	C15H26O	222.37	16	0	1	0	1	1	68.56	20.23
15	Jatamansin	C19H20O5	328.36	24	10	0.37	3	5	0	91.13	65.74
16	alpha-Patchoulene	C15H24	204.35	15	0	0.87	0	0	0	66.88	0
17	Seychellene	C15H24	204.35	15	0	0.87	0	0	0	66.88	0
18	Nardosinone	C15H22O3	250.33	18	0	0.8	0	3	0	69.55	35.53
19	8,8-dimethyl-2H,8H-pyrano[2,3-f]chromene-2,9(10H)-dione	C14H12O4	244.24	18	10	0.29	0	4	0	66.49	56.51
20	Virolin	C21H26O5	358.43	26	12	0.33	8	5	1	102.57	57.15
21	Norseychellanon	C14H22O	206.32	15	0	0.93	0	1	0	62.75	17.07
22	beta-Ionone	C13H20O	192.3	14	0	0.62	2	1	0	61.48	17.07
23	Actinidine	C10H13N	147.22	11	6	0.5	0	1	0	46.64	12.89
24	1-Hexacosanol	C26H54O	382.71	27	0	1	24	1	1	128.26	20.23
25	Jatamansic acid	C15H22O2	234.33	17	0	0.67	2	2	1	70.81	37.3
26	Nardostachone	C15H20O	216.32	16	0	0.53	1	1	0	68.51	17.07
27	Hexacosane	C26H54	366.71	26	0	1	23	0	0	127.1	0
28	Lomatin	C14H14O4	246.26	18	10	0.36	0	4	1	67.45	59.67
29	3-Carene	C10H16	136.23	10	0	0.8	0	0	0	45.22	0
30	beta-Eudesmol	C15H26O	222.37	16	0	0.87	1	1	1	70.46	20.23
31	alpha-Selinene	C15H24	204.35	15	0	0.73	1	0	0	68.78	0
32	alpha-Carotene	C40H56	536.87	40	0	0.45	10	0	0	184.43	0
33	alpha-Gurjunene	C15H24	204.35	15	0	0.87	0	0	0	67.14	0
34	Humulene	C15H24	204.35	15	0	0.6	0	0	0	70.42	0
35	Elemol	C15H26O	222.37	16	0	0.73	3	1	1	72.1	20.23
36	beta-Sitosterol	C29H50O	414.71	30	0	0.93	6	1	1	133.23	20.23

From the table 3, Physicochemical properties of selected phytochemicals of *Nardostachys jatamansi*, 13 compounds have no rotatable bonds; In rhizome - Patchouli alcohol; Angelicin; Tricyclo(6.3.1.02,5)dodecan-1-ol, 4,4,8-trimethyl-, (1R,2S,5R,8S)-; alpha-Patchoulene; Seychellene; Nardosinone; 8,8-dimethyl-2H,8H-pyrano[2,3-f]chromene-2,9(10H)-dione; Norseychellanon; Actinidine; Lomatin; 3-Carene; alpha-Gurjunene and Humulene. Among 36 phytocompounds in rhizome part of *Nardostachys jatamansi* only Angelicin, 8-(2-Hydroxypropan-2-yl)furo[2,3-h]chromen-2-one have thirteen #Aromatic heavy atoms. Jatamansin compound have the highest value of 65.74 TPSA value.

Table 4: Lipophilicity of Selected Phytochemicals Of *Nardostachys jatamansi*

Sr No	Phytochemical Name	iLOGP	XLOGP3	WLOGP	MLOGP	Silicos-IT Log P	Consensus Log P
1	Patchouli alcohol	2.91	4.05	3.61	3.81	3.4	3.56

Sr No	Phytochemical Name	iLOGP	XLOGP3	WLOGP	MLOGP	Silicos-IT Log P	Consensus Log P
2	Nardostachysin	3.35	2.78	2.95	2.88	3.21	3.03
3	Angelicin	2.03	2.08	2.54	1.48	2.91	2.21
4	Isovaleric acid	1.35	1.16	1.12	0.89	0.35	0.98
5	Nardol	3	3.58	3.78	3.67	3.51	3.51
6	Jatamol A	3	4.09	3.7	3.56	3.51	3.57
7	Jatamol B	3.33	4.54	4.41	3.66	4.24	4.04
8	(1S,5S,9R)-9-Isopropyl-1-methyl-6-methylenespiro[4.5]decan-1-ol	3.12	3.69	3.92	3.67	3.9	3.66
9	8-(2-Hydroxypropan-2-yl)furo[2,3-h]chromen-2-one	2.32	1.89	2.66	1.44	3.11	2.28
10	Valeranone	2.92	4.43	4.21	3.67	4.22	3.89
11	(-)-Valeranone	2.92	4.43	4.21	3.67	4.22	3.89
12	Pinoresinol	2.67	2.28	2.54	1.17	2.66	2.26
13	Cubebol	3.1	3.92	3.47	3.81	3.22	3.5
14	Tricyclo(6.3.1.02,5)dodecan-1-ol, 4,4,8-trimethyl-, (1R,2S,5R,8S)-	3.01	4.16	3.75	3.81	3.57	3.66
15	Jatamansin	3.32	3.69	3.38	2.64	4.06	3.42
16	alpha-Patchoulene	3.19	4.77	4.42	5.65	3.91	4.39
17	Seychellene	3.11	5.08	4.42	5.65	4.19	4.49
18	Nardosinone	2.61	2.87	3.05	2.56	2.83	2.78
19	8,8-dimethyl-2H,8H-pyrano[2,3-f]chromene-2,9(10H)-dione	2.33	1.99	2.08	1.52	3.4	2.26
20	Virolin	3.94	4.09	3.81	2.51	4.46	3.76
21	Norseychellanon	2.62	3.51	3.43	3.41	3.51	3.3
22	beta-Ionone	2.77	2.91	3.66	2.94	3.81	3.22
23	Actinidine	2.13	2.38	2.44	2.1	3.1	2.43
24	1-Hexacosanol	6.68	12.53	9.36	6.67	10.07	9.06
25	Jatamansic acid	2.6	3.79	3.65	3.35	2.63	3.2
26	Nardostachone	2.84	3.39	3.68	3.37	3.39	3.34
27	Hexacosane	7.08	13.7	10.39	8.66	10.64	10.09
28	Lomatin	2.46	1.91	1.87	1.6	2.81	2.13
29	3-Carene	2.63	4.38	3	4.29	2.79	3.42
30	beta-Eudesmol	3.06	3.74	3.92	3.67	3.64	3.6
31	alpha-Selinene	3.31	5.2	4.73	4.63	4.14	4.4
32	alpha-Carotene	7.96	13.65	12.46	8.96	12.25	11.06
33	alpha-Gurjunene	3.29	4.1	4.42	5.65	3.91	4.27
34	Humulene	3.29	4.55	5.04	4.53	3.91	4.26
35	Elemol	3.2	4.41	3.94	3.56	3.74	3.77
36	beta-Sitosterol	5.05	9.34	8.02	6.73	7.04	7.24

The lipophilicity investigation of the phytocompounds in Table No. 4 revealed that isovaleric acid had the lowest value of 1.16 in XLOGP3 and alpha-carotene had the highest value of 13.65.

Table 5: Water Solubility of Selected Phytochemicals of *Nardostachys Jatamansi*

Sr No	Phytochemical Name	ESOL Log S	ESOL Solubility (mg/ml)	ESOL Solubility (mol/l)	ESOL Class	Ali Log S	Ali Solubility (mg/ml)	Ali Solubility (mol/l)	Ali Class	Silicos-IT Log Sw	Silicos-IT Solubility (mg/ml)	Silicos-IT Solubility (mol/l)	Silicos-IT class
1	Patchouli alcohol	-3.77	3.77E-02	1.70E-04	Soluble	-4.18	1.47E-02	6.63E-05	Moderately soluble	-3.18	1.46E-01	6.55E-04	Soluble
2	Nardostachysin	-3.93	5.05E-02	1.17E-04	Soluble	-4.39	1.75E-02	4.07E-05	Moderately	-3.05	3.87E-01	8.99E-04	Soluble

Sr No	Phytochemical Name	ESOL Log S	ESOL Solubility (mg/ml)	ESOL Solubility (mol/l)	ESOL Class	Ali Log S	Ali Solubility (mg/ml)	Ali Solubility (mol/l)	Ali Class	Silicos-IT Log Sw	Silicos-IT Solubility (mg/ml)	Silicos-IT Solubility (mol/l)	Silicos-IT class
									soluble				
3	Angelicin	-2.99	1.90E-01	1.02E-03	Soluble	-2.62	4.47E-01	2.40E-03	Soluble	-4.5	5.87E-03	3.16E-05	Moderately soluble
4	Isovaleric acid	-1.07	8.65E+00	8.47E-02	Very soluble	-1.54	2.96E+00	2.90E-02	Very soluble	-0.41	4.01E+01	3.93E-01	Soluble
5	Nardol	-3.41	8.69E-02	3.91E-04	Soluble	-3.69	4.53E-02	2.04E-04	Soluble	-2.98	2.32E-01	1.04E-03	Soluble
6	Jatamol A	-3.72	4.23E-02	1.92E-04	Soluble	-4.22	1.33E-02	6.02E-05	Moderately soluble	-2.99	2.24E-01	1.02E-03	Soluble
7	Jatamol B	-4.36	1.41E-02	4.39E-05	Moderately soluble	-5.24	1.85E-03	5.76E-06	Moderately soluble	-3.88	4.21E-02	1.32E-04	Soluble
8	(1S,5S,9R)-9-Isopropyl-1-methyl-6-methylenespiro[4.5]decan-1-ol	-3.48	7.41E-02	3.33E-04	Soluble	-3.81	3.48E-02	1.57E-04	Soluble	-3.43	8.22E-02	3.70E-04	Soluble
9	8-(2-Hydroxypropan-2-yl)furo[2,3-h]chromen-2-one	-3.01	2.37E-01	9.70E-04	Soluble	-2.85	3.47E-01	1.42E-03	Soluble	-4.75	4.29E-03	1.76E-05	Moderately soluble
10	Valeranone	-3.94	2.53E-02	1.14E-04	Soluble	-4.51	6.92E-03	3.11E-05	Moderately soluble	-3.9	2.83E-02	1.27E-04	Soluble
11	(-)-Valeranone	-3.94	2.53E-02	1.14E-04	Soluble	-4.51	6.92E-03	3.11E-05	Moderately soluble	-3.9	2.83E-02	1.27E-04	Soluble
12	Pinoresinol	-3.58	9.52E-02	2.66E-04	Soluble	-3.54	1.03E-01	2.87E-04	Soluble	-4.19	2.29E-02	6.40E-05	Moderately soluble
13	Cubebol	-3.62	5.31E-02	2.39E-04	Soluble	-4.04	2.01E-02	9.04E-05	Moderately soluble	-2.73	4.10E-01	1.85E-03	Soluble
14	Tricyclo(6.3.1.02,5)dodecan-1-ol, 4,4,8-trimethyl-, (1R,2S,5R,8S)-	-3.84	3.22E-02	1.45E-04	Soluble	-4.29	1.13E-02	5.09E-05	Moderately soluble	-3.31	1.10E-01	4.94E-04	Soluble
15	Jatamansin	-4.31	1.61E-02	4.89E-05	Moderately	-4.76	5.70E-03	1.73E-05	Moderately	-5.24	1.88E-03	5.73E-06	Moderately

Sr No	Phytochemical Name	ESOL Log S	ESOL Solubility (mg/ml)	ESOL Solubility (mol/l)	ESOL Class	Ali Log S	Ali Solubility (mg/ml)	Ali Solubility (mol/l)	Ali Class	Silicos-IT Log Sw	Silicos-IT Solubility (mg/ml)	Silicos-IT Solubility (mol/l)	Silicos-IT class
					soluble				soluble				soluble
16	alpha-Patchoulene	-4.11	1.58E-02	7.73E-05	Moderately soluble	-4.5	6.45E-03	3.15E-05	Moderately soluble	-3.52	6.19E-02	3.03E-04	Soluble
17	Seychellene	-4.31	1.01E-02	4.93E-05	Moderately soluble	-4.82	3.07E-03	1.50E-05	Moderately soluble	-3.77	3.49E-02	1.71E-04	Soluble
18	Nardosinone	-3.2	1.58E-01	6.31E-04	Soluble	-3.28	1.33E-01	5.30E-04	Soluble	-2.89	3.23E-01	1.29E-03	Soluble
19	8,8-dimethyl-2H,8H-pyrano[2,3-f]chromene-2,9(10H)-dione	-3.02	2.34E-01	9.57E-04	Soluble	-2.8	3.84E-01	1.57E-03	Soluble	-4.84	3.53E-03	1.45E-05	Moderately soluble
20	Virolin	-4.45	1.26E-02	3.53E-05	Moderately soluble	-5	3.62E-03	1.01E-05	Moderately soluble	-5.38	1.50E-03	4.18E-06	Moderately soluble
21	Norseychellanon	-3.33	9.64E-02	4.67E-04	Soluble	-3.55	5.79E-02	2.81E-04	Soluble	-3.27	1.11E-01	5.37E-04	Soluble
22	beta-Ionone	-2.73	3.55E-01	1.85E-03	Soluble	-2.93	2.26E-01	1.18E-03	Soluble	-3.1	1.54E-01	8.02E-04	Soluble
23	Actinidine	-2.66	3.25E-01	2.21E-03	Soluble	-2.29	7.52E-01	5.11E-03	Soluble	-3.38	6.18E-02	4.20E-04	Soluble
24	1-Hexacosanol	-8.52	1.15E-06	3.00E-09	Poorly soluble	-12.98	4.02E-11	1.05E-13	Insoluble	-9.75	6.84E-08	1.79E-10	Poorly soluble
25	Jatamansic acid	-3.55	6.63E-02	2.83E-04	Soluble	-4.27	1.27E-02	5.40E-05	Moderately soluble	-2.06	2.05E+00	8.75E-03	Soluble
26	Nardostachone	-3.25	1.21E-01	5.61E-04	Soluble	-3.43	8.08E-02	3.74E-04	Soluble	-2.94	2.47E-01	1.14E-03	Soluble
27	Hexacosane	-9.23	2.18E-07	5.93E-10	Poorly soluble	-13.77	6.26E-12	1.71E-14	Insoluble	-10.32	1.77E-08	4.82E-11	Insoluble
28	Lomatin	-2.98	2.57E-01	1.04E-03	Soluble	-2.79	4.03E-01	1.64E-03	Soluble	-4.14	1.76E-02	7.16E-05	Moderately soluble
29	3-Carene	-3.44	4.90E-02	3.60E-04	Soluble	-4.1	1.09E-02	8.01E-05	Moderately soluble	-2.23	8.06E-01	5.92E-03	Soluble
30	beta-Eudesmol	-3.5	6.89E-02	3.10E-04	Soluble	-3.	3.09E-02	1.39E-04	Soluble	-3.21	1.36E-01	6.12E-04	Soluble

Sr No	Phytochemical Name	ESOL Log S	ESOL Solubility (mg/ml)	ESOL Solubility (mol/l)	ESOL Class	Ali Log S	Ali Solubility (mg/ml)	Ali Solubility (mol/l)	Ali Class	Silicos-IT Log Sw	Silicos-IT Solubility (mg/ml)	Silicos-IT Solubility (mol/l)	Silicos-IT class
		1				86							
31	alpha-Selinene	-4.32	9.85E-03	4.82E-05	Moderately soluble	-4.95	2.31E-03	1.13E-05	Moderately soluble	-3.55	5.79E-02	2.83E-04	Soluble
32	alpha-Carotene	-11.11	4.19E-09	7.80E-12	Insoluble	-13.72	1.03E-11	1.92E-14	Insoluble	-7.14	3.87E-05	7.21E-08	Poorly soluble
33	alpha-Gurjunene	-3.69	4.17E-02	2.04E-04	Soluble	-3.81	3.20E-02	1.56E-04	Soluble	-3.52	6.19E-02	3.03E-04	Soluble
34	Humulene	-3.97	2.17E-02	1.06E-04	Soluble	-4.27	1.09E-02	5.34E-05	Moderately soluble	-3.52	6.19E-02	3.03E-04	Soluble
35	Elemol	-3.8	3.53E-02	1.59E-04	Soluble	-4.55	6.23E-03	2.80E-05	Moderately soluble	-3	2.24E-01	1.01E-03	Soluble
36	beta-Sitosterol	-7.9	5.23E-06	1.26E-08	Poorly soluble	-9.67	8.90E-08	2.15E-10	Poorly soluble	-6.19	2.69E-04	6.49E-07	Poorly soluble

From the table 5, among 36 phytocompunds in rhizome part of *Nardostachys jatamansi* only Nardol, (1S,5S,9R)-9-Isopropyl-1-methyl-6-methylenespiro[4.5]decan-1-ol, Nardosinone, Norseychellanon, beta-Ionone, Actinidine, Nardostachone, beta-Eudesmol, alpha-Gurjunene are soluble in all three classes such as ESOL Class, Ali Class and Silicos-IT class. Isovaleric acid is the one which is very soluble in ESOL Class and Ali Class but in Silicos-IT class of solubility criteria we didn't find any compound which is very soluble like this.

Table 6: Pharmacokinetic Properties Of the selected phytochemicals of *Nardostachys Jatamansi*

Sr No	Phytochemical Name	GI absorption	BBB permeant	Pgp substrate	CYP1A2 inhibitor	CYP2C19 inhibitor	CYP2C9 inhibitor	CYP2D6 inhibitor	CYP3A4 inhibitor	log Kp(cm/s)
1	Patchouli alcohol	High	Yes	No	No	No	Yes	No	No	-4.78
2	Nardostachysin	High	No	Yes	No	No	No	No	Yes	-6.95
3	Angelicin	High	Yes	No	Yes	No	No	No	No	-5.96
4	Isovaleric acid	High	Yes	No	No	No	No	No	No	-6.1
5	Nardol	High	Yes	No	No	Yes	No	No	No	-5.11
6	Jatamol A	High	Yes	No	No	Yes	Yes	No	No	-4.74
7	Jatamol B	High	Yes	No	No	Yes	Yes	Yes	No	-5.03
8	(1S,5S,9R)-9-Isopropyl-1-methyl-6-methylenespiro[4.5]decan-1-ol	High	Yes	No	No	No	Yes	No	No	-5.04
9	8-(2-Hydroxypropan-2-yl)furo[2,3-h]chromen-2-one	High	Yes	No	Yes	No	No	No	No	-6.45
10	Valeranone	High	Yes	No	No	No	Yes	No	No	-4.51
11	(-)-Valeranone	High	Yes	No	No	No	Yes	No	No	-4.51
12	Pinoresinol	High	Yes	Yes	No	No	No	Yes	Yes	-6.87
13	Cubebol	High	Yes	No	No	Yes	Yes	No	No	-4.87
14	Tricyclo(6.3.1.02,5)dodecan-1-ol, 4,4,8-trimethyl-, (1R,2S,5R,8S)-	High	Yes	No	No	No	Yes	No	No	-4.7

Sr No	Phytochemical Name	GI absorption	BBB permeant	Pgp substrate	CYP1A2 inhibitor	CYP2C19 inhibitor	CYP2C9 inhibitor	CYP2D6 inhibitor	CYP3A4 inhibitor	log Kp(cm/s)
15	Jatamansin	High	Yes	No	No	Yes	Yes	No	Yes	-5.68
16	alpha-Patchoulene	Low	No	No	No	Yes	Yes	No	No	-4.16
17	Seychellene	Low	No	No	Yes	Yes	Yes	No	No	-3.94
18	Nardosinone	High	Yes	No	No	No	No	No	No	-5.79
19	8,8-dimethyl-2H,8H-pyrano[2,3-f]chromene-2,9(10H)-dione	High	Yes	No	Yes	Yes	No	No	No	-6.38
20	Virolin	High	Yes	Yes	Yes	No	No	Yes	Yes	-5.58
21	Norseychellanon	High	Yes	No	No	No	No	No	No	-5.07
22	beta-Ionone	High	Yes	No	No	No	No	No	No	-5.41
23	Actinidine	High	Yes	No	Yes	No	No	No	No	-5.51
24	1-Hexacosanol	Low	No	No	No	No	No	No	No	0.26
25	Jatamansic acid	High	Yes	No	No	No	Yes	No	No	-5.04
26	Nardostachone	High	Yes	No	No	Yes	Yes	No	No	-5.21
27	Hexacosane	Low	No	Yes	No	No	No	No	No	1.19
28	Lomatin	High	Yes	No	Yes	No	No	No	No	-6.45
29	3-Carene	Low	Yes	No	No	No	Yes	No	No	-4.02
30	beta-Eudesmol	High	Yes	No	No	No	Yes	No	No	-5
31	alpha-Selinene	Low	No	No	No	Yes	Yes	No	No	-3.85
32	alpha-Carotene	Low	No	Yes	No	No	No	No	No	0.12
33	alpha-Gurjunene	Low	No	No	No	Yes	Yes	No	No	-4.64
34	Humulene	Low	No	No	No	No	Yes	No	No	-4.32
35	Elemol	High	Yes	No	No	No	Yes	No	No	-4.53
36	beta-Sitosterol	Low	No	No	No	No	No	No	No	-2.2

From the table 6, among 36 phytocompounds in rhizome part of *Nardostachys jatamansi* 10 compounds shows low GI absorption and 26 phytocompounds have high GI absorption and for 10 compounds GI absorption is low. Also 11 phytocompounds displays no BBB permeability and 25 phytocompounds appears to have BBB permeability.

Table 7: Druglikeness properties of the selected phytochemicals of *Nardostachys Jatamansi*

Sr No	Phytochemical Name	Lipinski #violations	Ghose #violations	Veber #violations	Egan #violations	Muegge #violations	Bioavailability Score
1	Patchouli alcohol	0	0	0	0	1	0.55
2	Nardostachysin	0	0	0	0	0	0.55
3	Angelicin	0	0	0	0	1	0.55
4	Isovaleric acid	0	3	0	0	1	0.85
5	Nardol	0	0	0	0	1	0.55
6	Jatamol A	0	0	0	0	1	0.55
7	Jatamol B	0	0	0	0	0	0.55
8	(1S,5S,9R)-9-Isopropyl-1-methyl-6-methylenespiro[4.5]decan-1-ol	0	0	0	0	1	0.55
9	8-(2-Hydroxypropan-2-yl)furo[2,3-h]chromen-2-one	0	0	0	0	0	0.55
10	Valeranone	0	0	0	0	1	0.55
11	(-)-Valeranone	0	0	0	0	1	0.55
12	Pinoresinol	0	0	0	0	0	0.55
13	Cubebol	0	0	0	0	1	0.55
14	Tricyclo(6.3.1.02,5)dodecan-1-ol, 4,4,8-trimethyl-, (1R,2S,5R,8S)-	0	0	0	0	1	0.55
15	Jatamansin	0	0	0	0	0	0.55
16	alpha-Patchoulene	1	0	0	0	1	0.55

17	Seychellene	1	0	0	0	2	0.55
18	Nardosinone	0	0	0	0	0	0.55
19	8,8-dimethyl-2H,8H-pyrano[2,3-f]chromene-2,9(10H)-dione	0	0	0	0	0	0.55
20	Virolin	0	0	0	0	0	0.55
21	Norseychellanon	0	0	0	0	1	0.55
22	beta-Ionone	0	0	0	0	2	0.55
23	Actinidine	0	1	0	0	2	0.55
24	1-Hexacosanol	1	2	1	1	3	0.55
25	Jatamansic acid	0	0	0	0	0	0.85
26	Nardostachone	0	0	0	0	1	0.55
27	Hexacosane	1	2	1	1	3	0.55
28	Lomatin	0	0	0	0	0	0.55
29	3-Carene	1	1	0	0	2	0.55
30	beta-Eudesmol	0	0	0	0	1	0.55
31	alpha-Selinene	1	0	0	0	2	0.55
32	alpha-Carotene	2	4	0	1	2	0.17
33	alpha-Gurjunene	1	0	0	0	1	0.55
34	Humulene	1	0	0	0	1	0.55
35	Elemol	0	0	0	0	1	0.55
36	beta-Sitosterol	1	3	0	1	2	0.55

Total of 26 compounds are following the Lipinski rule without violating any criteria set for the drug likeness and only 2 phytocompounds Isovaleric acid and Jatamansic acid has high Bioavailability Score which is 0.85. Alpha-Carotene has 0.17 Bioavailability score but this score is the lowest here and rest of the compound has same Bioavailability score of 0.55.

Table 8 : Medicinal Chemistry Of Selected Phytochemicals of *Nardostachys Jatamansi*

Sr No	Phytochemical Name	PAINS #alerts	Brenk #alerts	Leadlikeness #violations	Synthetic Accessibility
1	Patchouli alcohol	0	0	2	3.73
2	Nardostachysin	0	2	1	5.93
3	Angelicin	0	1	1	3.07
4	Isovaleric acid	0	0	1	1
5	Nardol	0	1	2	3.68
6	Jatamol A	0	1	2	3.71
7	Jatamol B	0	1	1	4.48
8	(1S,5S,9R)-9-Isopropyl-1-methyl-6-methylenespiro[4.5]decan-1-ol	0	1	2	3.97
9	8-(2-Hydroxypropan-2-yl)furo[2,3-h]chromen-2-one	0	1	1	3.01
10	Valeranone	0	0	2	3.06
11	(-)-Valeranone	0	0	2	3.06
12	Pinoresinol	0	0	1	3.99
13	Cubebol	0	0	2	4.13
14	Tricyclo(6.3.1.02,5)dodecan-1-ol,4,4,8-trimethyl-, (1R,2S,5R,8S)-	0	0	2	4.03
15	Jatamansin	0	2	1	4.08
16	alpha-Patchoulene	0	1	2	5.53
17	Seychellene	0	1	2	4.01
18	Nardosinone	0	1	0	4.82
19	8,8-dimethyl-2H,8H-pyrano[2,3-f]chromene-	0	1	1	2.99

	2,9(10H)-dione				
20	Virolin	0	0	3	3.91
21	Norseychellanon	0	0	2	3.6
22	beta-Ionone	0	1	1	3.38
23	Actinidine	0	0	1	2.28
24	1-Hexacosanol	0	0	3	3.47
25	Jatamansic acid	0	0	2	4.28
26	Nardostachone	0	0	1	4.39
27	Hexacosane	0	0	3	3.44
28	Lomatin	0	1	1	3.55
29	3-Carene	0	1	2	3.84
30	beta-Eudesmol	0	1	2	3.38
31	alpha-Selinene	0	1	2	4.22
32	alpha-Carotene	0	2	3	6.62
33	alpha-Gurjunene	0	1	2	4.57
34	Humulene	0	1	2	3.66
35	Elemol	0	1	2	3.54
36	beta-Sitosterol	0	1	2	6.3

In the above table, all the 36 compounds do not have any PAINS alert. Since the synthetic accessibility is in between 1 (very easy) to 10 (very difficult), compound named isovaleric acid has synthetic accessibility 1 and alpha-Carotene has 6.62 synthetic accessibility.

IV. CONCLUSION:

This study highlights the therapeutic potential of Nardostachys jatamansi as a natural remedy by using IMPPAT and SWISS ADME data analysis, for managing various psychological and neurological disorders. In-silico ADME analysis, combined with IMPPAT-based screening it provides a robust computational framework for evaluating the pharmacokinetic and therapeutic potential of rhizome part of the plant *Nardostachys jatamansi* in managing psychological and neurological disorders. By predicting crucial parameters such as absorption, distribution, metabolism, excretion and toxicity, these methods facilitate the identification of bioactive compounds with neuroprotective, antidepressant, antioxidant, anticonvulsant, antihypertensive and cognitive-enhancing properties. IMPPAT has a curated database of Indian medicinal plants which enhances this process by offering comprehensive phytochemical and pharmacological insights. The ability of *N. jatamansi* to balance *Śarīra Doṣa* and *Mānasa Doṣa* further supports its traditional use in Ayurvedic psychiatry. Computational and experimental studies validate its efficacy in neuropharmacology, indicating its potential in treating test anxiety and sleep-deprivation-induced depression. The integration of ethnomedicinal knowledge with modern pharmacological research underscores the scientific relevance of *N. jatamansi* in plant-based neurotherapeutics. However, while preliminary findings are promising, further in-vitro, in-vivo, and clinical studies are required to confirm its safety, efficacy, and precise mechanisms of action. This research serves as a foundation for future investigations into natural alternatives for mental and neurological health management.

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