RESEARCH PAPER

Network Pharmacology-Based Investigation into the Multi-Target Mechanisms of Nardostachys jatamansi in the Treatment of Adhd

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ABSTRACT

Background: Attention Deficit Hyperactivity Disorder (ADHD) is a common neurodevelopmental disorder characterized by inattention, hyperactivity, and impulsivity. Current treatments may have limitations and side effects. Nardostachys jatamansi is traditionally used for neurological conditions.

Objective: To explore the multi-target mechanism of N. jatamansi in ADHD using a network pharmacology approach.

Methods: Phytochemicals were screened using SwissADME. Target proteins were predicted using SwissTargetPrediction. ADHD-related genes were obtained from GeneCards. Overlapping targets were analyzed using STRING database. Functional enrichment was performed using Metascape.

Results: Thirty overlapping targets were identified. Key hub genes included BDNF, DRD2, DRD4, SLC6A4, COMT, MAOA, TNF, and NFKB1. Enrichment analysis showed involvement in neurotransmitter signaling, synaptic transmission, and cAMP pathways. Cluster analysis identified core functional modules. Regulatory and disease enrichment analyses further supported neuronal and psychiatric relevance.

Conclusion: N. jatamansi acts through multiple targets related to neurotransmission, neurodevelopment, and inflammation, suggesting its potential role in ADHD management.

Keywords: ADHD, Nardostachys jatamansi, Network pharmacology, Multi-target mechanism, Neurotransmission.

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Introduction

ADHD is a neurodevelopmental disorder affecting both children and adults and is characterized by inattention, hyperactivity, and impulsivity [1]. The disorder is strongly associated with dysregulation of neurotransmitters such as dopamine, serotonin, and norepinephrine [2].

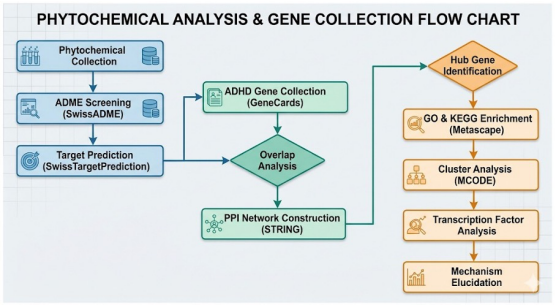
Current pharmacological treatments, although effective, may produce adverse effects and are not suitable for all patients [3]. Therefore, alternative and complementary therapeutic approaches are being explored.

Nardostachys jatamansi is a traditional medicinal plant known for its neuroprotective, anxiolytic, and cognitive-enhancing properties [4]. However, its molecular mechanism in ADHD remains unclear.

Network pharmacology provides a systematic approach to study multi- component and multi-target interactions and has become an important tool in drug discovery [5]. This study aims to investigate the mechanism of *N. jatamansi* in ADHD using this approach.

METHODOLOGY

Figure 1: Workflow of the network pharmacology approach used to investigate the therapeutic mechanisms of *Nardostachys jatamansi* in ADHD.



1. Phytochemical Screening

Phytochemicals were collected and evaluated for pharmacokinetic properties using SwissADME [6]. Compounds with favorable ADME profiles were selected (Table 1).

Table 1: ADME properties and drug-likeness evaluation of selected phytochemicals from Nardostachys jatamansi

Compound	GI Absorption	BBB Permeant	P-gp Substrate	CYP Inhibition	Lipinski Rule	Bioavailability Score	PAINS Alert	Lead-likeness	Synthetic Accessibility
Patchouli Alcohol	High	Yes	No	CYP2C9	Yes (0 violation)	0.55	0	No	3.38
Angelicin	High	Yes	No	CYP2C19, CYP2C9	Yes (0 violation)	0.55	0	No	3.71
Valerianone	High	Yes	No	CYP2C9	Yes (0 violation)	0.55	0	No	3.06
Nardosinone	High	Yes	No	None	Yes (0 violation)	0.55	0	Yes	4.82
Jatamol A	High	Yes	No	CYP2C19, CYP2C9	Yes (0 violation)	0.55	0	No	3.71
Pinoresinol	High	Yes	Yes	CYP2D6, CYP3A4	Yes (0 violation)	0.55	0	No	3.99
Cubebol	High	Yes	No	CYP2C19, CYP2C9	Yes (0 violation)	0.55	0	No	4.13
Beta-Eudesmol	High	Yes	No	CYP2C9	Yes (0 violation)	0.55	0	No	3.38
Jatamansin	High	Yes	No	CYP2C19, CYP2C9, CYP3A4	Yes (0 violation)	0.55	0	No	4.08
Seychellene	Low	No	No	CYP1A2, CYP2C19,	Yes (1	0.55	0	No	4.01

				CYP 2C9	viola tion)				

ADME properties were predicted using SwissADME. GI: gastrointestinal; BBB: blood–brain barrier; P-gp: P-glycoprotein; CYP: cytochrome P450 enzymes.

2. Target Prediction

Target proteins were predicted using SwissTargetPrediction [7].

3. ADHD Gene Collection

ADHD-related genes were retrieved from GeneCards [8].

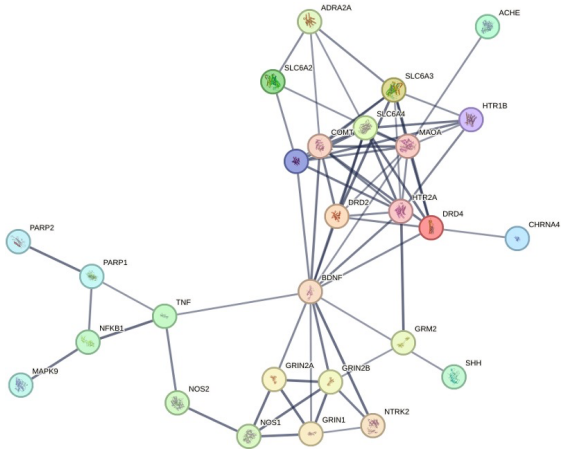
4. Overlap Analysis

Common targets between phytochemicals and ADHD-associated genes were identified.

5. PPI Network Construction

Protein–protein interaction (PPI) network was constructed using STRING database [9] (Figure 2).

Figure 2: Protein–protein interaction (PPI) network of overlapping targets constructed using the STRING database.



6. Functional Enrichment Analysis

Gene Ontology (GO) and pathway enrichment analyses were performed using Metascape [10] (Figure 3 and Figure 4).

Figure 3: Gene Ontology (GO) and pathway enrichment analysis showing significant biological processes and pathways associated with the overlapping targets.

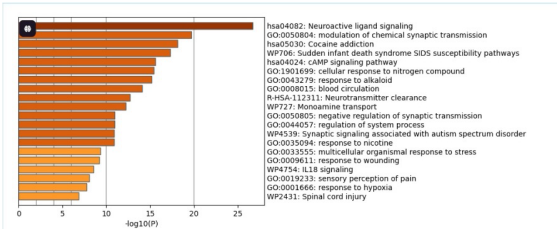
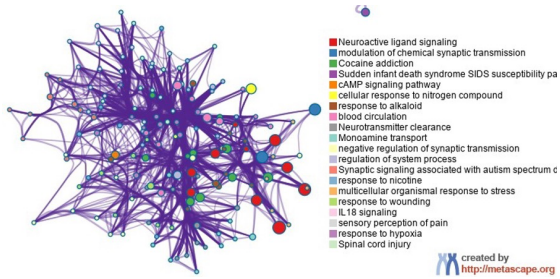


Figure 4: Network visualization of enriched biological pathways generated using Metascape.



7. Disease Enrichment Analysis

Disease association analysis was performed using DisGeNET [11] (Figure 7).

RESULTS

1. ADME Screening

Selected phytochemicals showed good pharmacokinetic and drug- likeness properties (Table 1).

2. Target Identification

Predicted targets of selected compounds are listed in Table 2.

Table 2: Active phytochemicals of Nardostachys jatamansi and their predicted target genes

Compound	Targets
Patchouli Alcohol	DRD2, DRD4, SLC6A3, SLC6A4, MAOA, COMT
Angelicin	ACHE, HTR2A, TNF, NFKB1
Valeranone	CA1, CA2, AR, HSD11B1
Nardosinone	CHRM1, CHRM2, DRD4, MAOB
Jatamol A	UGT2B7, PTGS1, CYP19A1, ESR1
Pinoresinol	SHBG, PIK3CA, MAPK9
Cubebol	UGT2B7, CDC25A, TRPM8
Beta-Eudesmol	UGT2B7, AR, ESR1
Jatamansin	PDE4D, NOS1, CDK2
Seychellene	CYP1A2, CYP2C19, CYP2C9

Targets were predicted using SwissTargetPrediction and validated through database cross- referencing.

3. Overlapping Targets

A total of 30 common targets were identified between phytochemicals and ADHD-related genes.

4. PPI Network

The PPI network demonstrated strong interactions among targets, with key hub genes such as BDNF, DRD2, DRD4, and SLC6A4 (Figure 2).

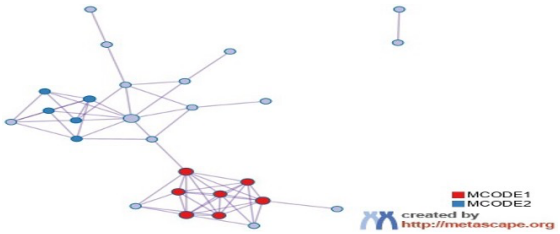
5. Enrichment Analysis

Enrichment analysis revealed significant involvement in neurotransmitter signaling, synaptic transmission, and cAMP signaling pathways (Figure 3 and Figure 4).

6. Cluster Analysis

Cluster analysis identified highly interconnected modules associated with neurotransmitter systems (Figure 5).

Figure 5: Cluster analysis of the PPI network showing highly interconnected modules identified using MCODE.



7. Transcription Factor Analysis

Key transcription factors such as NFKB1, SP1, and NR3C1 were identified, indicating regulatory roles in gene expression (Figure 6).

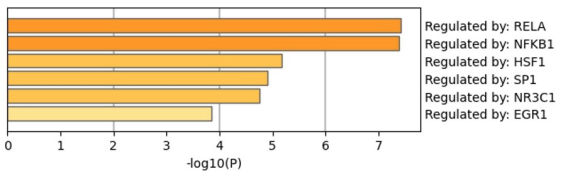


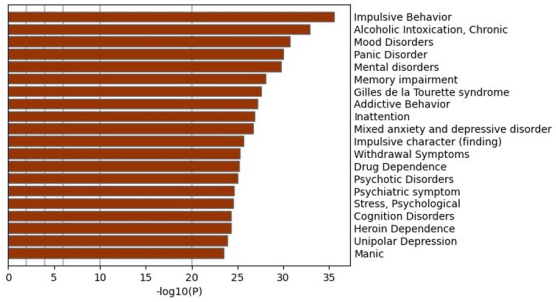
Figure 6: Transcription factor enrichment analysis highlighting key regulatory elements involved in gene expression.

8. Disease and Cell-Type Enrichment

Disease enrichment analysis showed associations with impulsivity, inattention, and mood disorders (Figure 7).

Cell-type enrichment indicated predominant expression in neuronal populations, especially midbrain neurons (Figure 8).

Figure 7: Disease association analysis of overlapping targets showing relevance to neurological and psychiatric disorders.



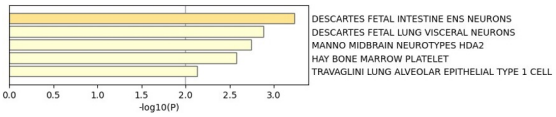


Figure 8: Cell-type enrichment analysis indicating predominant expression in neuronal cell populations.

DISCUSSION

The present study demonstrates that *N. jatamansi* exerts its effects through multiple targets and pathways associated with ADHD. Dopamine-related genes such as DRD2 and DRD4 suggest its role in improving attention and behavioral control.

Serotonergic and noradrenergic pathways further support its role in mood regulation. The involvement of BDNF indicates a role in neurodevelopment and synaptic plasticity.

Additionally, inflammatory markers such as TNF and NFKB1 suggest anti-inflammatory effects, which may contribute to its neuroprotective action.

Overall, the findings support a multi-target mechanism involving neurotransmission, neurodevelopment, and inflammation.

CONCLUSION

Nardostachys jatamansi acts through multiple biological pathways relevant to ADHD. Its effects on neurotransmitter systems, neurodevelopment, and inflammation support its potential as a complementary therapeutic option.

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