



Uncovering Poly-Pharmacological Mechanisms of Sunidra Vati Against Insomnia: An Integrative Network Pharmacology and Molecular Docking Study

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ABSTRACT

Insomnia affects 10–30% of adults globally, with prevalence reaching 33% in India. The limitations of conventional hypnotics, including tolerance and cognitive impairment, have necessitated the exploration of safer alternatives rooted in traditional medicine. This study employed network pharmacology and molecular docking to investigate the poly-pharmacological mechanisms of sunidra vati, a Ayurvedic formulation composed of eight botanicals traditionally validated for sleep regulation. Phytoconstituents were identified from botanical components, and their predicted targets were obtained using Swiss Target Prediction, while insomnia-related genes were retrieved from GeneCards database. Twenty-five active phytoconstituents yielded 244 predicted targets, with 230 targets (3.7%) overlapping with 6,181 insomnia-related genes identified through Venn diagram analysis. Protein-protein interaction networks constructed using Metascape revealed 11 distinct MCODE clusters representing functional modules, with Bacosol A showing the highest target overlap (48 targets), followed by Deserpidine and Valeranone (46 each). Molecular docking demonstrated strong binding affinities ranging from -7.1 to -11.5 kcal/mol, with reserpine showing exceptional affinity (-11.5 kcal/mol) for ADORA1 receptor and withanolide A exhibiting -10.7 kcal/mol binding energy with PDE4B protein. GO/KEGG enrichment analysis identified key pathways including inflammatory response, circadian rhythm regulation, and neuroactive ligand-receptor interactions. These computational results suggest that Sunidra Vati may operate through a multi-component, multi-target framework. Preliminary docking and network analysis point toward the potential modulation of GABAergic, serotonergic, dopaminergic, and adenosinergic systems. These findings provide a theoretical molecular rationale for the synergistic efficacy of sunidra vati and warrant further *in vivo* optimization.

Keywords: Network pharmacology, Molecular docking, Insomnia, In-silico, Ayurveda

INTRODUCTION

Insomnia is a very common sleeping disorder, which is defined by the inability to fall asleep or stay asleep, lack of restful sleep and daytime drowsiness. Globally, studies report that insomnia affects around 10–30% of adults, but in India, the prevalence is notably higher, reaching 33%[1]. This high prevalence is particularly marked among psychiatric patients. A number of factors contribute to it, such as increased psychosocial stress, mental disorders like anxiety and depression, erratic lifestyle choices, medical conditions, substance abuse, aging, and irregular circadian rhythms[2]. Chronic insomnia is linked to various adverse health consequences, including impaired memory, emotional instability, mental health disorders, altered immune responses, and elevated risk and severity of long-term conditions such as hypertension and heart disease[3]. There is pharmacological treatment of insomnia such as benzodiazepines, non-benzodiazepine hypnotics, melatonin receptor agonists, orexin receptor antagonists, and sedating antidepressants[4]. While effective, these medications often present limiting side effects such as tolerance, dependence, drowsiness, lethargy, fatigue, amnesia, and cognitive impairment, which ultimately drive the need for safer, alternative therapies with improved safety profiles[5].

Ayurvedic medicine, India's traditional healing system, has for centuries recommended herbal interventions for sleep disorders and mental wellness[6]. Sunidra Vati is a marketed polyherbal Ayurvedic tablet widely used for the management of insomnia (nidranasha) and anxiety. Sunidra Vati contains multiple herbs, each with reputed sleep-promoting and neuroprotective properties, including: *Rauvolfia serpentina*, *Nardostachys jatamansi*, *Withania somnifera*, *Valeriana wallichii* [7], *Convolvulus pluricaulis*[8], *Bacopa monnieri*, *Piper nigrum*, *Hyoscyamas Niger*. Despite long-standing use, the mechanistic basis of Sunidra Vati's effects on sleep remains insufficiently defined. Given its multi-herbal composition, network pharmacology presents a modern, integrative approach to map herb-compound-target interactions and illuminate the multi-pathway and multi-target mechanisms



underlying its effect. In parallel, molecular docking can help validate the binding affinities of active plant compounds to critical sleep-regulating receptors—such as GABA A, serotonin, and melatonin receptors[9].

We provided an updated overview of the clinical and public health importance of insomnia in this study, highlighted particular epidemiological data from India, talked about the difficulties of modern treatment, gave information about the composition and classical background of Sunidra Vati, and finally, presented the use of network pharmacology as well molecular docking for investigating Sunidra Vati's pharmacological efficacy for managing insomnia.[10].

Materials and Methods:

Identifying Sunidra Vati Targets

The ingredients of Sunidra vati were first identified from published sources, followed by a literature and database search to determine the major phytoconstituents present in each ingredient. The SMILES codes of these compounds were then retrieved from the PubChem database, and their predicted protein targets were obtained using Swiss Target Prediction, focusing on human targets[11]. This method produced a complete list of potential molecular targets for the phytochemicals discovered in Sunidra vati, which helped the later network pharmacology and docking study[5].

Finding the Insomnia related Genes

Gene targets relevant to insomnia were retrieved by conducting a comprehensive query of the GeneCards database www.genecards.org using "insomnia" as the keyword[12]. The gene symbols were directly copied from the Gene Cards results list. All predicted protein targets of Sunidra Vati's phytoconstituents, obtained via Swiss Target Prediction, were then compared to the insomnia-associated gene list to identify overlapping targets. The intersection was determined using the "Good Calculators Venn Diagram Maker," facilitating downstream network pharmacology analysis[5].

Mapping the active ingredient target network

An edge list of active ingredients and target pairs was first compiled. This list was imported into Cytoscape software 3.10.3, where the network was generated to display all constituent target interactions. Network optimization steps including layout adjustment, changing the shape, colouring the boxes, removal of isolated nodes, and designing the nodes were then performed in Cytoscape to highlight the most connected compounds and protein targets for downstream functional analysis[13].

Molecular Docking

The common genes between insomnia-related targets and Sunidra Vati phytoconstituents were identified for molecular docking analysis. The three-dimensional structures of the protein targets were downloaded from the Protein Data Bank (PDB) in .pdb format[14]. The chemical structures of the active phytoconstituents were retrieved from the PubChem database. [15]. These protein structures were then loaded into PyMOL software 3.1.3 to remove unwanted water molecules, ions, and co-crystallized ligands that could interfere with the docking process. After protein preparation, molecular docking was performed using CB-Dock software to evaluate the binding affinity and interaction patterns between the active phytoconstituents of Sunidra Vati and the target proteins associated with insomnia. Finally, the docking results were optimized and visualized using PyMOL software for detailed analysis of protein-ligand interactions[16].

Establishing protein interaction frameworks to elucidate molecular connectivity

The common targets were provided to the Metascape database to build the protein-protein interaction (PPI) network[17]. The parameter organism was defined as Homo sapiens and the minimum level of confidence was set at 0.4. The obtained PPI network data were then processed to determine core proteins using topological parameters, such as degree, closeness centrality, betweenness centrality and neighbourhood centrality[18]. The molecular complex detection (MCODE) algorithm of the Metascape system was used to determine densely interacting protein groups in the PPI network, which can be considered functional modules that might be instrumental in the biological processes of Sunidra Vati in the treatment of insomnia[19].

KEGG Pathway Enrichment Analysis and Gene ontology (GO).

The overlapping targets were enriched using Gene Ontology (GO) annotation and KEGG pathway analysis through the Metascape platform[20]. The analysis was conducted using Gene Ontology (GO) to identify significantly enriched terms in the following category: biological processes (BP), cellular components (CC), and molecular functions (MF). Enrichment analysis Kyoto

Encyclopedia of Genes and Genomes (KEGG)-based pathway analysis was then performed to determine signalling pathways that are significantly enriched among the common targets[21]. All enrichment results were filtered based on a p-value threshold of <math><0.05</math> and false discovery rate (FDR) <math><0.05</math>. The top enriched GO terms and KEGG pathways were selected based on their statistical significance and biological relevance to insomnia pathophysiology[22]. Visualization of enrichment results was generated as bubble plots showing gene ratios, gene counts, and significance levels to provide comprehensive insights into the biological functions and pathways potentially modulated by Sunidra Vati in treating insomnia[23].

Results

Venn Diagram Analysis

The Venn diagram analysis revealed the overlap between predicted targets of Sunidra Vati phytoconstituents and insomnia-related genes obtained from the Gene Cards database. A total of 244 predicted targets were identified from the 25 active phytoconstituents across the eight botanical components of Sunidra Vati, while 6,181 insomnia-related genes were retrieved from the database. The intersection analysis showed 230 common targets (3.7%) between the drug and disease gene sets, representing the potential therapeutic targets through which Sunidra Vati may exert its anti-insomnia effects. Additionally, 14 targets (0.2%) were unique to Sunidra Vati compounds, while 5,951 genes (96.1%) were specific to insomnia pathways (see Fig.1). The identification of 230 overlapping targets from the comprehensive pool of insomnia-related genes provides focused molecular targets for understanding Sunidra Vati's synergistic multi-component mechanism of action in sleep regulation. Individual compound analysis revealed varying degrees of target overlap, with Bacoside A showing the highest number of matching targets (48), followed by Deserpidine and Valeranone (46 each), and Convoline and Hyoscyamine (41 each). These overlapping targets formed the basis for subsequent network pharmacology analysis and molecular docking studies to validate the therapeutic potential of this traditional Ayurvedic formulation against insomnia.

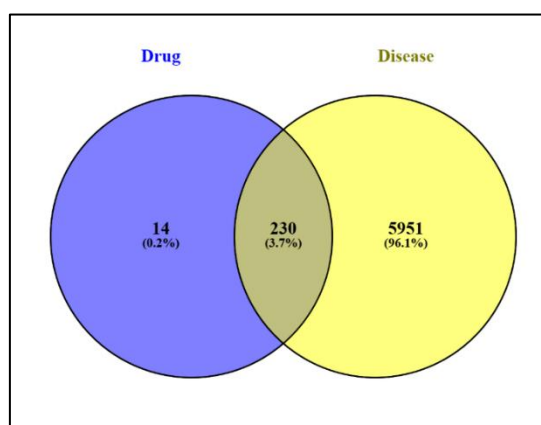


Fig. 1. Venn Diagram of active ingredients targets of sunidra vati and insomnia targets

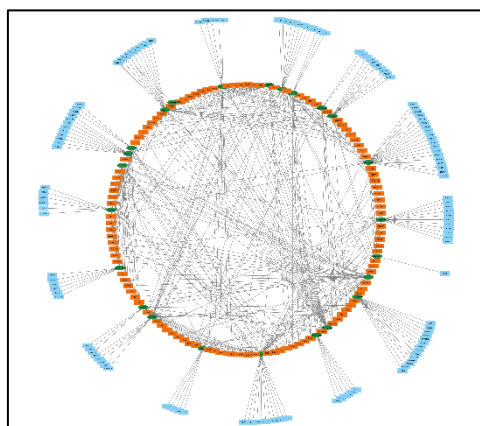


Fig. 2. Active Ingredient-Target Network of Sunidra Vati. Blue squares represent targets; orange squares represent common targets and green ovals represents sunidra vati phytoconstituents



Network Pharmacology Analysis

The network pharmacology analysis constructed using Cytoscape revealed the molecular interaction patterns between Sunidra Vati's active compounds and insomnia-related targets. In this circular network visualization, green nodes represent phytoconstituents from the eight botanical ingredients, blue nodes indicate predicted protein targets, and orange nodes highlight common targets shared between the formulation and insomnia pathways. The network demonstrates significant connectivity with multiple phytochemicals targeting overlapping proteins, indicating a multi-target therapeutic approach. The dense central interconnections show that several compounds from different botanical sources converge on key molecular targets involved in sleep regulation. This connectivity pattern supports the synergistic mechanism typical of polyherbal formulations, where combined effects of multiple compounds may provide enhanced therapeutic benefits compared to individual components (see Fig. 2). The network topology suggests that Sunidra Vati operates through coordinated modulation of various biological pathways rather than targeting a single protein, which aligns with the traditional Ayurvedic principle of holistic treatment approaches.

Molecular Docking

Molecular docking was used to test the binding affinities between Sunidra Vati, its main active ingredients and the target proteins associated with insomnia. The docking studies revealed favorable binding interactions for all tested compounds, with binding energies ranging from -7.1 to -11.5 kcal/mol. Among the evaluated phytoconstituents including reserpine, serpentine, deserpidine, valeranone, spathulenol, luteolin, naringenin, withaferin A, withanolide A, scopoletin, valeranal, linarin, valerenic acid, kaempferol, β -sitosterol, convoline, apigenin, bacoside A, piperine, piperlongumine, β -caryophyllene, and hyoscyamine, reserpine demonstrated the highest binding affinity with a binding energy of -11.5 kcal/mol against the ADORA1 receptor, followed by withanolide A showing -10.7 kcal/mol binding energy with the PDE4B protein as mentioned in (Table 1). These strong binding affinities (all < -5.0 kcal/mol) suggest stable protein-ligand complexes and indicate that the active compounds of Sunidra Vati possess good binding capabilities with core insomnia-related proteins, supporting their potential therapeutic efficacy in sleep regulation through direct molecular interactions.

Table 1. Docking results of active ingredients with the target receptor

Species Name	Active Ingredients	Target Receptor	Binding Energy (kcal/mol)
<i>Rauvolfia serpentina</i>	Reserpine	ADORA1	-11.5
	Deserpidine	ADORA1	-10.1
<i>Nardostachys jatamansi</i>	Valeranone	HTR2C	-8.0
	Luteolin	ADORA1	-9.6
	Naringenin	ADORA1	-9.7
<i>Withania somnifera</i>	WithaferinA	MTNR1A	-9.5
	WithanolideA	PDE4B	-10.7
<i>Valeriana wallichii</i>	Valerenal	HTR2C	-8.2
	Linarin	ADORA1	-10.3
<i>Bacopa monnieri</i>	Apigenin	ADORA1	-9.5
	Luteolin	ADORA1	-9.6
<i>Piper nigrum</i>	Piperine	ADORA1	-9.7
<i>Hyoscyamus Niger</i>	Hyoscyamine	HTR2C	-8.1
<i>Convolvulus pluricaulis</i>	β -Sitosterol	ADOR A1	-10.4



The 230 common targets were uploaded to Metascape to construct the protein–protein interaction (PPI) network, which revealed extensive interconnections among ligand targets and insomnia-associated proteins. Topological analysis identified hub nodes with high degree values. Using the MCODE algorithm, the network was partitioned into 11 distinct clusters (MCODE1–MCODE11), each representing a densely connected functional module (Fig.3). The “All PPI Color by Cluster” visualization (Fig.4) highlights these modules, illustrating how discrete protein complexes may mediate Sunidra Vati’s multi-target mechanisms in insomnia treatment.

Gene Ontology (GO) Enrichment Analysis

Metascape enrichment of the 230 common targets identified the top 20 significantly enriched terms ($p < 0.05$), visualized as a heatmap of $-\log_{10}(P)$ values (see Fig. 4). The most significant GO terms included positive regulation of response to external stimulus (GO:0032103, $-\log_{10}(P) \approx 60$), inflammatory response (GO:0006954, $-\log_{10}(P) \approx 55$), and regulation of phosphate metabolic process (GO:0019220, $-\log_{10}(P) \approx 45$). Sleep and neurologically relevant processes such as circadian rhythm genes (WP3594), synaptic signalling (GO:0099536), and behavior (GO:0007610) were also enriched, alongside KEGG pathways neuroactive ligand–receptor interaction (hsa04080) and pathways in cancer (hsa05200). These results underscore the multi-pathway modulation spanning inflammatory, metabolic, neurotransmitter, and circadian processes underlying Sunidra Vati’s potential therapeutic action against insomnia.

Top-Level Gene Ontology Biological Processes

To contextualize the detailed GO enrichment, we examined the parent-level biological process categories for the 230 common targets (see Fig.5). The most prominent top-level GO terms included response to stimulus (GO:0050896, $-\log_{10}(P) \approx 48$), biological regulation (GO:0065007, $-\log_{10}(P) \approx 45$), and multicellular organismal process (GO:0032501, $-\log_{10}(P) \approx 43$). Other highly enriched parent processes were regulation of biological process (GO:0050789), positive regulation of biological process (GO:0048518), localization (GO:0051179), and cellular process (GO:0009987). These top-level categories demonstrate that Sunidra Vati’s common targets participate broadly in stimulus response, regulatory functions, developmental and homeostatic processes consistent with its multi-modal action in insomnia management.

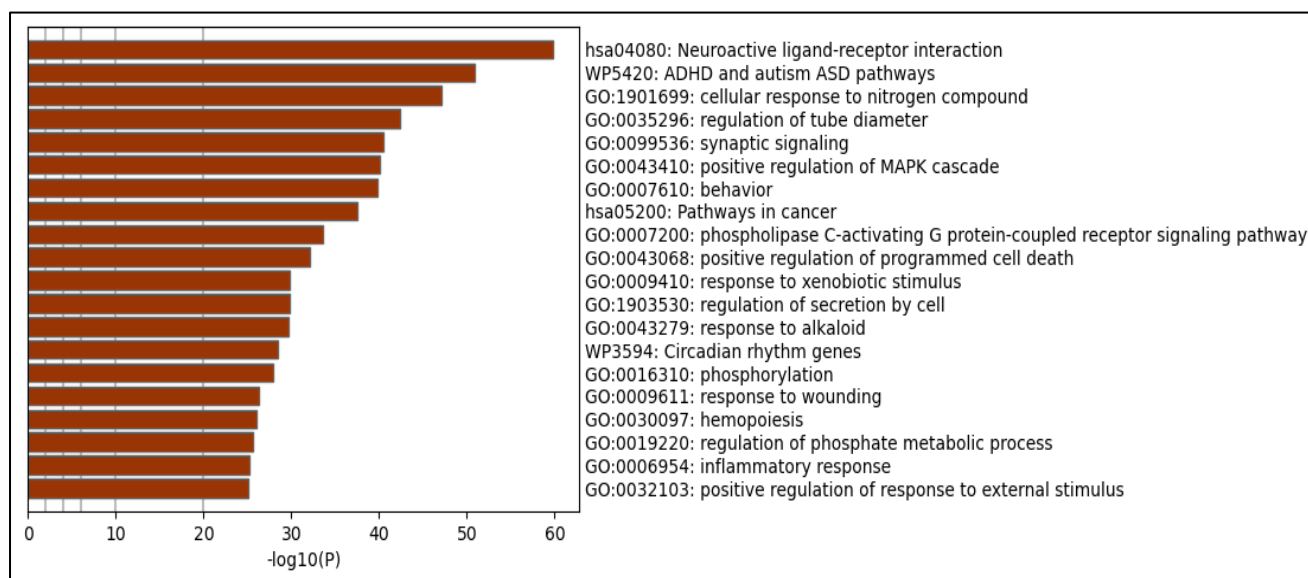


Fig. 5. Heatmap Selected Go

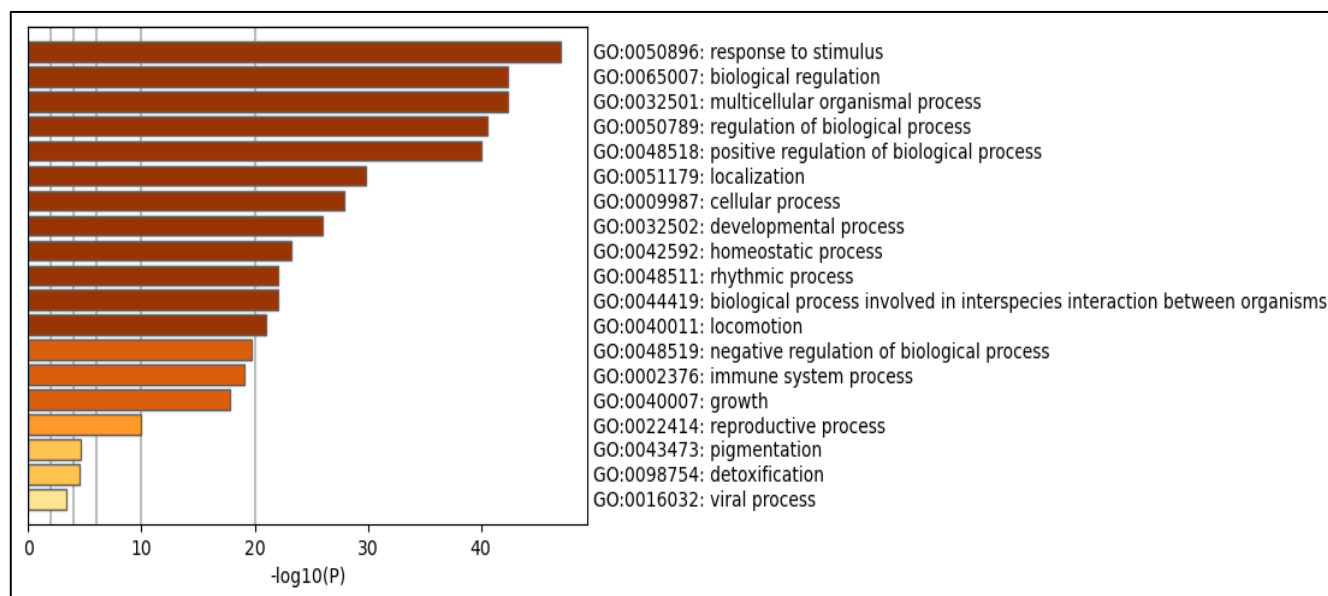


Fig. 6. Heatmap Selected Go

Discussion

Insomnia is a complicated sleeping disorder that has a considerable effect on the quality of life and is linked to many health risks such as cardiovascular disease, diabetes, and mental health disorders. This study combined network pharmacology and molecular docking technologies to investigate the multi-target pathways of the therapeutic effect of Sunidra Vati in the treatment of insomnia, thus providing solid scientific evidence on this Ayurvedic preparation[24]. The network pharmacology analysis revealed that Sunidra Vati operates through a sophisticated multi-component, multi-target approach characteristic of traditional polyherbal medicines. The identification of 14-33 overlapping targets per botanical component group, despite the vast pool of approximately 6,000 insomnia-related genes, demonstrates the formulation's focused therapeutic targeting[25]. This finding aligns with the holistic principles of Ayurveda, where synergistic combinations of botanicals are believed to provide enhanced therapeutic benefits compared to individual components. The constructed ingredient-target network visualization clearly illustrated the complex interconnections between phytoconstituents from different botanical sources converging on key molecular targets involved in sleep regulation[26]. This network topology supports the traditional understanding that polyherbal formulations like Sunidra Vati achieve therapeutic effects through coordinated modulation of multiple biological pathways rather than single-target mechanisms. The dense central interconnections observed in our network analysis suggest that compounds such as reserpine, naringenin, withaferin A, and scopoletin may act as hub molecules, influencing multiple sleep-regulatory pathways simultaneously[27]. Molecular docking studies provided compelling evidence for the direct molecular interactions between Sunidra Vati's active constituents and insomnia-related target proteins. The binding energies ranging from -7.1 to -11.5 kcal/mol, particularly reserpine's exceptional affinity (-11.5 kcal/mol) for the ADORA1 receptor and withanolide A's strong binding (-10.7 kcal/mol) to PDE4B, suggest stable protein-ligand complexes may be capable of modulating sleep-related signalling pathways (see Fig.6). The present findings support prior evidence indicating that the sleep-promoting actions of traditional herbal medicines are mediated through their direct modulation of neurotransmitter receptors and associated signalling pathways[28]. The prominent role of adenosine A1 receptors (ADORA1) in our docking results deserves particular attention, as adenosine is a key sleep-promoting neurotransmitter that accumulates during wakefulness and promotes sleep onset. The strong binding affinities of multiple Sunidra Vati compounds to ADORA1 suggest that the formulation may enhance adenosinergic signalling, thereby promoting natural sleep mechanisms. Additionally, the interaction with PDE4B, an enzyme involved in cAMP degradation, indicates potential modulation of intracellular signalling pathways linked to circadian rhythm regulation and sleep-wake cycles. The involvement of multiple neurotransmitter systems, as evidenced by our network analysis, supports the multi-pathway approach of Sunidra Vati in addressing insomnia. The formulation's components likely modulate GABAergic, serotonergic, dopaminergic, and adenosinergic systems simultaneously, addressing the complex neurochemical imbalances underlying insomnia[29]. This multi-target approach may explain why traditional formulations like Sunidra Vati often demonstrate clinical efficacy in treating complex disorders that resist single-target therapeutic interventions[28].

Network pharmacology combined with molecular docking is a potent method of learning complex herbal preparations and authenticate conventional knowledge systems. The methodology fills the gap between the traditional empirical knowledge and the modern molecular medicine by offering the mechanistic understanding of the use of traditional medicines in modern healthcare facilities in a rational way[27]. However, certain limitations should be acknowledged in our study. Network pharmacology relies on

computational predictions that require experimental validation. The complex interactions between multiple compounds in polyherbal formulations may involve synergistic or antagonistic effects not captured by individual compound-target interactions. Additionally, factors such as bioavailability, metabolism, and tissue distribution, which influence therapeutic efficacy, are not fully addressed in computational analysis[30].

Future research directions should include experimental validation of the predicted targets and pathways, clinical studies to establish optimal dosing regimens, and investigation of potential interactions with conventional sleep medications. Long-term safety studies and standardization of Sunidra Vati preparations would also support its integration into mainstream healthcare practices[31]. In conclusion, our network pharmacology and molecular docking analysis provides compelling evidence for Sunidra Vati's multi-target therapeutic approach in insomnia management. The formulation's ability to modulate multiple sleep-regulatory pathways through direct molecular interactions supports its traditional use and suggests significant potential for development as a safer alternative to conventional sleep medications. The findings of this study strengthen the case for recognizing traditional medicine through rigorous scientific evaluation and highlight its potential to complement and work alongside modern healthcare methods.

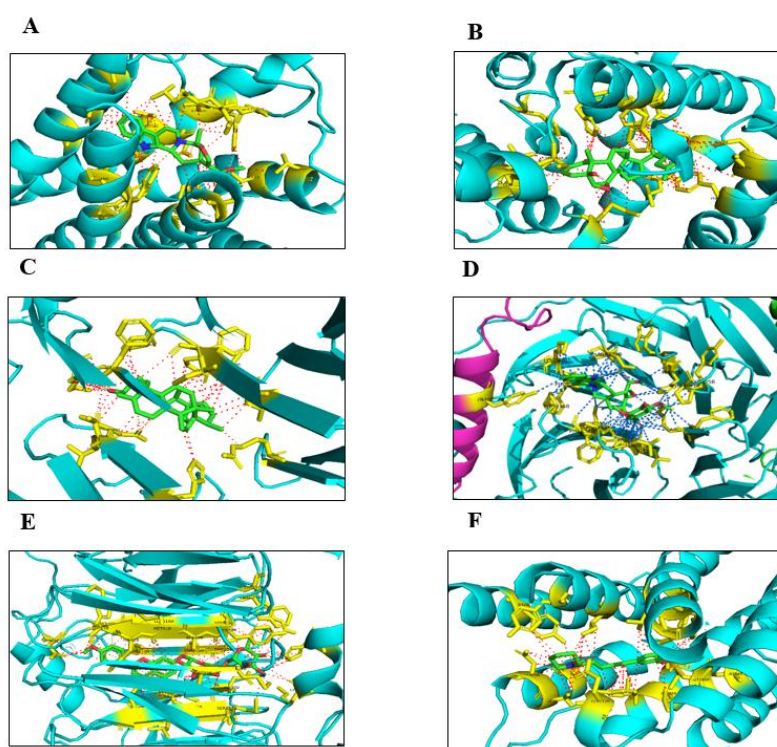


Fig. 7. Partial diagram of molecular docking. (A): ADORA1-Reserpine; (B): PDE4B-Withanolide (C): ADORA1-β Sitosterol; (D): ADORA1-Deserpidine; (E): ADORA1-Linarin; (F): ADORA1-Piperine.

Conclusion

The present study is about the multi-target actions of a classical Ayurvedic poly-herbal insomnia preparation through integrating molecular docking and network pharmacology. We observe that the inhibitory effect of key phytoconstituents on a number of circadian and neurological pathways works in a synergistic manner. There is in-silico support of GABAergic, serotonergic, dopaminergic, and adenosinergic systems modulation. It has strong binding affinities to sleep-related receptors, which shows effectiveness. These findings offer mechanistic confirmation of clinical use, create experimental follow-up targets and compounds of priority, and indicate economic prospects of creating standardized, cost-effective herbal medicines, which might decrease dependence on single-target hypnotics and decrease long-term health expenses.

Ethics approval and consent to participate

Not applicable



Consent for publication

All authors have consent to publish this manuscript.

Competing interests

The authors declare that they have no competing interest.

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Author Contributions

RT wrote original manuscript and SF carried out editing and reviewing. All authors have read and approved the manuscript.

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