Journal of Ayurveda & Holistic Medicine

https://jahm.co.in eISSN-2321-1563

ORA-Analytical Study

Network Pharmacology Based Anti-inflammatory Activity of *Datura* (*Datura metel* L.): An In-Silico Study

[1]Sreeja Kaimal V, [2*]Rajeshwari V. Kamat, [3]Sunil S. Jalalpure, [4]Amal S. Chandran

ABSTRACT:

Background: Rheumatoid arthritis (RA), is a chronic autoimmune disease, which is having the symptoms joint pain, swelling, and gradual joint destruction by refractory joint inflammation. Even though the current available treatments are effective in managing and reducing the progression of the disease but these interventions are associated with severe complications. *Datura metel* L., is a shrub which is known for its therapeutic potential in Ayurveda for the treatment of a variety of inflammatory conditions like arthritis. **Objective:** A network pharmacology-based study was planned to validate Ayurveda knowledge and to understand the mechanism of action of *Datura* in inflammation. **Materials and Methods**: The databases like Dr. Dukes, PubChem, Gene Cards and IMPPAT were utilised to identify the potential targets and related pathways. The open-source databases revealed 14 phytocompounds in Datura and the Swiss target Prediction Server predicted 79 target protein molecules. The STRING 10.5, KEGG Pathway database and Cytoscape 3.7.2 were utilised in the network pharmacology study for identifying protein targets, potential interactions, pathway analysis and for the construction of the network. **Results:** 14 phytocompounds identified in Datura which were expected to be targeting 79 inflammatory proteins. The gene enrichment analysis identified 27 targets among which The MAPK signaling pathway acts as the key hub. The majority of compounds fulfilled acceptable standards in drug-likeness screening. The phytocompounds Atropine (1.39) and Hyoscyamine (1.29) shows high score according to drug-likeness screening which predicts the suitability of the compounds as a drug in the disease. **Conclusion:** The study concludes that the phytocompounds like hyoscyamine, deoxywithastramonolide, fastusic acid, scopolamine, and tigloidine have major action on TNF, IL6, COX, APK14, and other proteins through P38 MAPK signalling pathway and the Rheumatoid arthritis pathway. The network pharmacology study validates the anti-inflammatory potential of *Datura metel.*

KEYWORDS: Anti-inflammatory activity, Ayurveda, *Datura*, Rheumatoid arthritis; Cytokine modulation; In silico analysis; Systems pharmacology

RECEIVED ON:
16-12-2025
REVISED ON:
25-12-2025
ACCEPTED ON:
29-12-2025

Access This Article Online:

Quick Response Code:

Website Link:

https://jahm.co.in

DOI Link:

https://doi.org/10.70066/jahm.v13i12.2482

Corresponding Author Email:

drrajeshwarikamat@gmail.com

CITE THIS ARTICLE AS

Sreeja Kaimal V, Rajeshwari V. Kamat, Sunil S. Jalalpure, Amal S. Chandran. Network Pharmacology Based Anti-inflammatory Activity of *Datura* (*Datura metel* L.): An In-Silico Study. *Journal of Ayurveda and Holistic Medicine (JAHM).*2025;13(12):40-49.

1. INTRODUCTION

Rheumatoid arthritis (RA) is a chronic autoimmune disease with a prevalence of around 0.5- 1% globally is characterized by inflammation, gradual destruction of joint, degradation of cartilage causing disability and affecting the quality of life. The cytokines, immune cells and signalling pathways plays an important role in the pathogenesis of RA. The key molecular targets involved in the disease are IL-6, TNF, NF-κB, IL-1β, JAK/STAT (STAT3, JAK1, JAK3), MAPKs (MAPK14, MAPK14), PI3K-Akt signalling proteins. [1] The currently available treatment methodologies include corticosteroids, NSAIDs and antirheumatic drugs such as methotrexate have been effective in managing and reducing the progression of the disease. However, these interventions are associated with severe complications like bleeding of the gastrointestinal tract, cardiovascular diseases and hepatotoxicity. Therefore, a safer and effective alternative natural drug without complication is the need of the hour.

In *Ayurveda, Datura metel* L. is used in diseases like Shotha (inflammation), *Kandu* (itching), *Bahya Krimi* (external worms), *Udara Krimi* (intestinal worms), and *Jwara* (fever). As a drug mentioned in E1 drug of D&C Act 1940, Ayurveda follows proper purification and dosage of Datura during its administration to avoid toxicity in clinical practice. Datura is a potent drug by its *Vyavayi* (fast spreading) and *Vikasi* (dispersing) qualities. The drug possesses therapeutic activity as well as some adverse effect due to the presence of potent alkaloids. [2] The drug is useful in muscle spasm, Pain and inflammation. [3, 4]

Network pharmacology is a recently emerging branch that helps us to understand about the mechanism of action of various drugs in diseases. [5] Even though *Datura* is widely used in Ayurveda as an anti-inflammatory drug, there is dearth of information related to the mechanism of its action. So, a network pharmacology-based Molecular docking study was planned to validate and understand the anti-inflammatory activity of *Datura metel.* We hypothesized that certain phytochemical compounds are having anti-inflammatory activity which works in Rheumatoid activity. The hypothesis will be tested by using a network pharmacology approach along with molecular docking. It may demonstrate the activity of important inflammatory mediators and signaling pathways, including the signaling cascades of MAPK, TNF, NF-κB, and IL-17.

2. MATERIAL AND METHODS

In silico approaches in the drug discovery:

Drug likeness characters of active biomolecules from Datura metel were predicted using Molsoft online server.

Lipinski made set of rules for drugs likely to penetrate CNS if:

- Molecular weight $\leq$500 g/mol
- Log p $\leq$5
- Hydrogen bond donor $\leq$5
- Hydrogen bond acceptor $\leq$10

Retrieval of phytocompounds and their intended targets

The databases like Dr. Duke's, IMPPAT database v2.0 (accessed June 2025) and literature research were utilized to obtain the information related to phytocompounds of *Datura metel.* The structural information of these phytocompounds were obtained from PubChem and other open – source libraries. [6]

Phytocompounds probable protein targets

The targets with a similarity of more than 0.1% were identified using Swiss Target Prediction database by using canonical SMILES of each compound. The Therapeutic Target Database (TTD) was used to analyse the presence of proteins linked to RA in the current identified targets. [7]

Disease targets retrieval

The TTD and Gene Card Database (accessed June 2025) provided information about the genes related to RA. The Venny 2.0 was utilized to analyze the common targets between disease and phytocompound targets.[8]

Pathway enrichment and network building

STRING database v10.5 was used to perform Protein–protein interaction (PPI) analysis. The minimum required interaction confidence score was 0.7 (high confidence). Active interaction sources included curated databases, experiments, co-expression, and text mining. Isolated nodes were hidden to enhance network robustness. The pathway analysis was performed by using the KEGG pathway database. The key signalling pathways related to the pathophysiology of RA was identified through literature search. [9,10]

Network analysis

Cytoscape version 3.7.2 was utilized to construct a network of phytocompounds of *Datura metel*, associated signaling pathways and predicted Protein targets. The topological parameter "edge count" (degree centrality) was used during the construction of network to examine the number of connections or interactions associated with each node. The customization of the size, shape and colour of nodes and edges were done to differentiate between phytocompounds, target proteins, and signaling pathways. Based on the degree of connectivity phytocompounds, protein targets and signalling pathways were given distinct shape and size. The edges were styled to improve clarity and to reflect interaction types.

Docking methodology:

The targets from top 10 hub genes and the chemicals that had the highest degree layout were made to dock. By downloading the 3D structures of the ligand and the targets from PubChem and RCS PDB respectively, the targets were taken further into Autodock tool 1.5.7 for adding the hydrogen bond and kollmann charges and removing the hetero atoms and water molecules. Later the targets that are uploaded into PyRx software where it is made to dock with the 3d structures of the phytochemicals. [11] Later the docking is visualized with the Discovery Biovia studio for 2D and 3D structures and the binding affinity of each target towards ligand is tabulated and the highest binding affinity between the ligand – target is also noted.

3. RESULTS

In silico pharmacology

Mining of phytoconstituents and their target prediction

A thorough literature review and data mining from open-source phytochemical databases identified 14 phytocompounds in *Datura metel.* The Swiss Target Prediction program was used to anticipate the targets of these phytochemicals. The result explained that 79 possible protein targets may act with the phytochemicals present in *Datura metel*. This screening acts as the foundation for network studies to prove *Datura metel*'s potential in the treatment of RA.

Drug-Likeness and Druggability Assessment

Lipinski's Rule of Five was used to examine the drug-likeness features like molecular weight, hydrogen bond acceptors (HBA), hydrogen bond donors (HBD), and lipophilicity (log P). It is used to determine the pharmacokinetic fitness of the phytocompounds present in *Datura metel*. [12] The majority of compounds present within acceptable limits for oral bioavailability and druggability. They showed a drug-likeness scores ranging from -1.18 to 1.39 (Table 1). Datura can be chosen for development of a new drug due to the good drug-likeness scores of Atropine and Hyoscyamine present in it.

Gene enrichment and network analysis

The GSEA (gene set enrichment analysis) revealed that a total of 27 out of 110 protein targets (Figure 1) were linked directly to 12 biochemical processes involved in the pathophysiology of RA.

Table no.1: Rule of five Drug likeness score of phytocompounds & Druggability.

Compounds		Lipinski Rule of Five				
		Molecular weight (g/mol)	HBA	HBD	Log P	Drug likeness score
S. No	Acceptable Values	< 500	< 5	< 5	< 10	0 to 2
1	5α-pregnane3β	288.5	3	1	2.68	0.29
2	Apohyoscine	2.68	3	1	2.68	0.29
3	Atropine	289.4	4	1	1.38	1.39
4	Cuscohygrine	224.34	3	0	0.52	-1.18
5	Daturadiol	442.38	2	2	7.18	-0.04
6	Deoxywithastramonolide	470.6	6	2	3.95	0.12
8	Hyoscyamine	289.4	4	1	1.38	1.29
9	Scopalamine	303.35	5	1	1.15	0.68
10	Tigloidine	223.16	3	0	1.88	-0.18
11	Tigloyloxytropane	223.16	3	0	2.13	-0.61
12	Tri-terpene	172.15	2	2	1.47	-0.60
13	Tropine	141.12	2	1	0.83	-1.07
14	Withanolides	504.27	8	5	1.25	0.55

The study showed that most of the phytoconstituents interacted with the targets were alkaloids which might be responsible for the anti- inflammatory activity of the drug. Among the various pathways, the MAPK pathway with its five genes (PTGS2, TNF, IRAK4, MAPK12, MAPK14) plays a vital role in mediating inflammatory responses in RA.

The TRP channels pathway, IL-17 signaling pathway, NF-kappa B signaling pathway, Th17 cell differentiation, PI3K-Akt signaling pathway and TNF signaling pathway (Table 2; Figure 2) were the notable pathways related to RA pathogenesis. The above said pathways are responsible for the inflammation and joint destruction in RA which might be influenced by the phytocompounds present in *Datura.*

Table no.2: Pathways modulated by proteins of Rheumatoid Arthritis.

KEGG ID	Pathway name	Gene count	FDR	Genes set within the pathway
hsa04659	Th17 cell differentiation	12	1.66E-18	MAPK12, MAPK14, IL27RA, STAT3, STAT6, IFNGR1, IL6R, IL6ST, IL6, TYK2, JAK3, JAK1
hsa04630	JAK-STAT signaling pathway	12	1.66E-16	IL27RA, PIK3CA, STAT3,CSF2,STAT6,IFNGR1,IL6R,IL6ST,IL6 ,TYK2, JAK3,JAK1
hsa04060	Cytokine-cytokine receptor interaction	8	3.45E-08	IL37,IL27RA,CSF2,IFNGR1,IL6R,IL6ST,IL6,TNF
hsa04657	IL-17 signaling pathway	6	3.46E-08	MAPK12, MAPK14, CSF2, PTGS2, IL6, TNF
hsa04066	HIF-1 signaling pathway	6	5.92E-08	PIK3CA, STAT3, NOS2, IFNGR1, IL6R, IL6
hsa04064	NF-kappa B signaling pathway	4	6.33E-05	PTGS2, SYK, TNF, IRAK4
hsa04010	MAPK signaling pathway	2	0.0072	PIK3CA, TNF
hsa04668	TNF signaling pathway	7	2.88E-09	MAPK12, MAPK14, PIK3CA, CSF2, PTGS2, IL6, TNF

Larger nodes and higher number of edges show that phytocompounds, proteins, and pathways are closely coupled, reflecting considerable network modulation and centrality. Smaller nodes and fewer edges, on the other hand, depict components that interact and modulate less.

Docking results:

In molecular docking study, the selected phytochemicals were Scopolamine, Hyoscyamine and Tigloidine and targets were STAT3, TNF and IL-6. The result of molecular docking study showed that Scopolamine had highest docking score with -7.6 kcal/mol binding affinity towards STAT3. The lowest docking score was of -5.3 kcal/mol for tigloidine towards TNF. All the phytochemicals had highest docking score towards STAT3. The docking between the top 3 phytochemicals and the targets that are done based on the degree layout in the topological analysis (Table 3). The action of STAT3 target towards scopolamine and IL6 towards Hyoscyamine are visualized in the study (Figure 3).

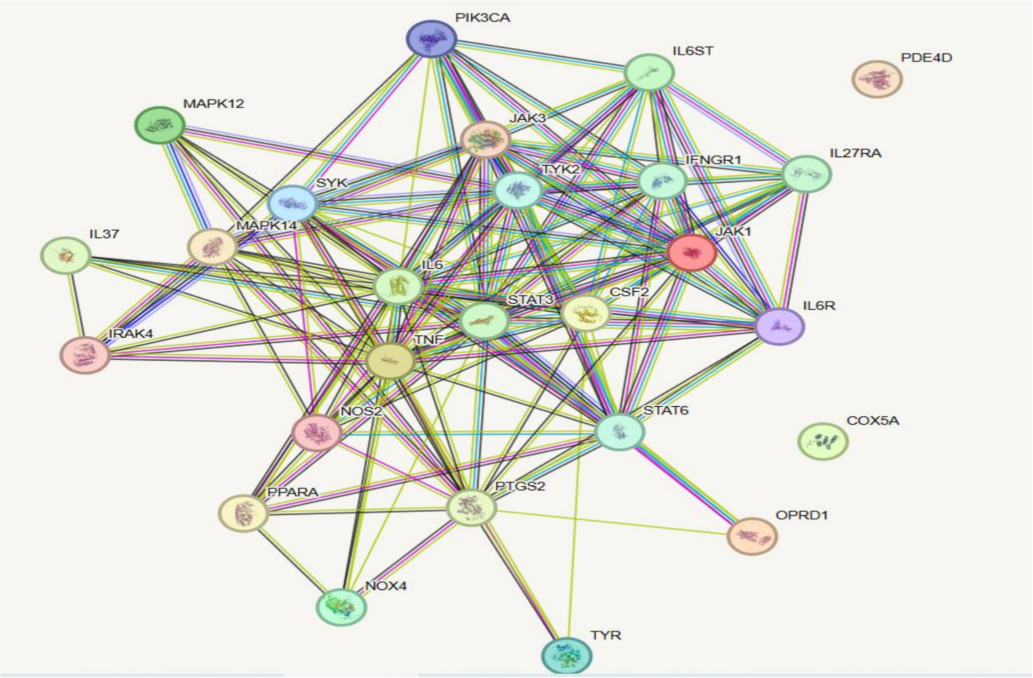

Figure no: 01: Protein-Protein interaction of Rheumatoid arthritis.

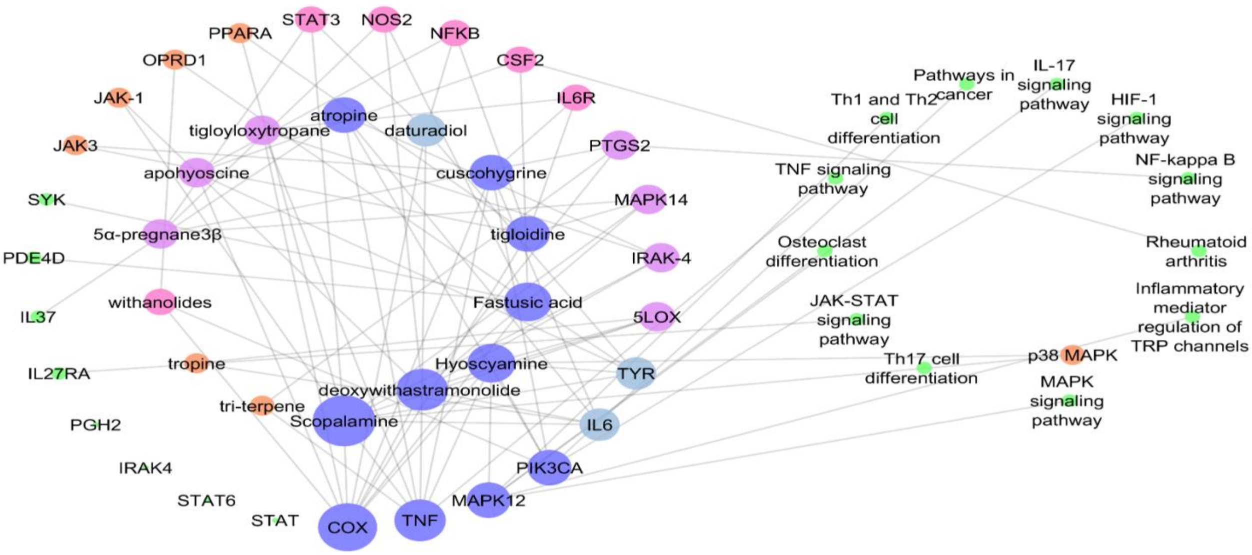

Figure no: 02: Network analysis of interaction between Phytocompounds, proteins and pathways.

Table no.3: Binding affinity of Phytochemicals and targets in Molecular docking

Phytochemicals	Binding Affinity (kcal/mol)		
	TNF	STAT3	IL6
Scopolamine	-5.9	-7.6	-6.2
Hyoscyamine	-6.2	-7.5	-6.4
Tigloidine	-5.3	-7.2	-5.7

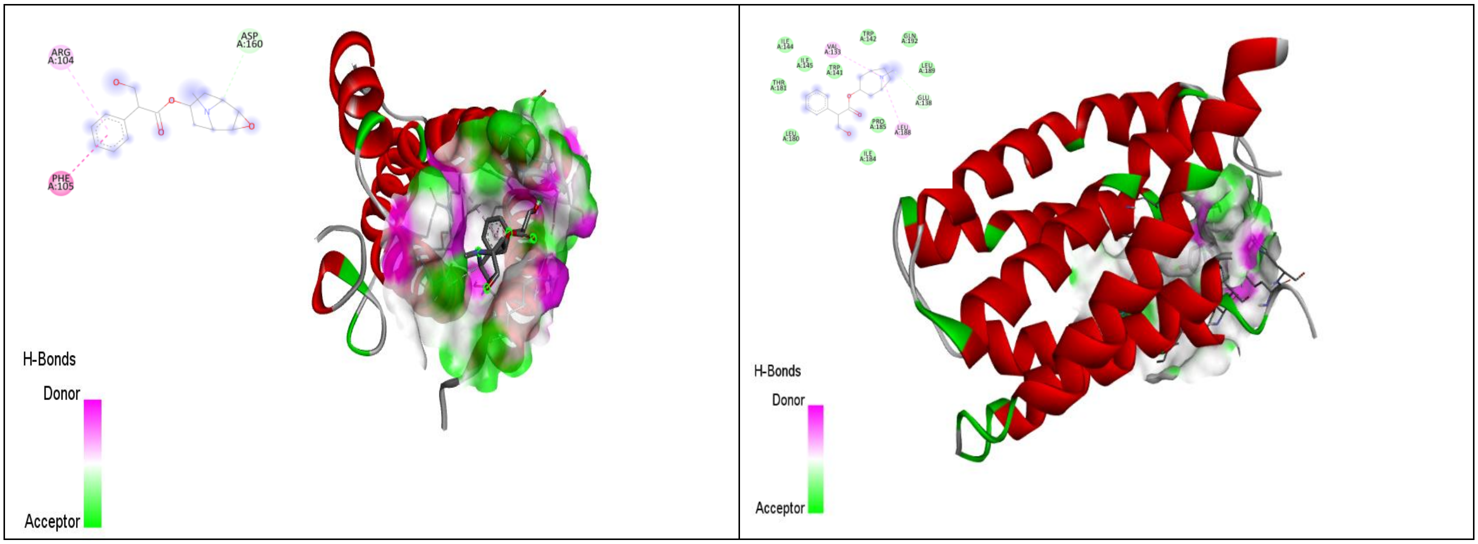

Figure no: 03: Visualization of STAT3 target towards scopolamine and IL6 towards Hyoscyamine

4. DISCUSSION

The main characteristic feature of Rheumatoid arthritis is cartilage deterioration, Chronic synovitis and bone loss. The pathophysiology of RA has the following steps; stimulation of inflammatory kinase, dysregulated cytokine signaling, and transcription factors that activate systemic immune stimulation and synovial inflammation. This study examined all the phytoconstituents present in *Datura metel* by using network pharmacology techniques. It studies about the interaction of the phytoconstituents with the protein targets of Rheumatoid arthritis

12 significant pathways are found by the Gene enrichment analysis in which MAPK signaling pathway is considered as the main hub. A thorough study on the compound – target – pathway network reveled five related genes i.e.; MAPK12, MAPK14, TNF, IRAK4 and PTGS2. The serine/threonine protein kinases also known as p38 MAPKs, which include MAPK14 (p38α) and MAPK12 is activated by Inflammatory cytokines and environmental stressors. The synovial membranes of RA patients are having a high concentration of these kinases. It is supposed to mediate the transcription of pro-inflammatory genes. In chronic inflammation, these kinases represent attractive molecular targets for small-molecule inhibitors. [13, 14] The effective strategy to reduce immune cell infiltration and synovial hyperplasia is to block MAPK14 as it is essential for stress response, cell differentiation, and apoptosis. The phytocompounds of *Datura metel* may inhibit important pro-inflammatory pathways that are essential to RA pathogenesis by their ability to interact with MAPKs. The network analysis identified that the phytochemical components of *Datura metel* are having an action on TNF, IL-6, and STAT3 which are considered as the key targets. A major inflammatory cytokine TNF, causes synovial inflammation, cartilage degradation, and Treg cell dysfunction by dephosphorylating FOXP3 and increasing the phosphatase activity. This process reduces immunological tolerance, which aggravates the condition. The Atropine and Hyoscyamine acts as TNF-modulating agents is supported by their interaction with

TNF. IL-6 has a role in acute-phase protein synthesis, B-cell differentiation and Th17 cell growth. The overexpression of IL-6 causes the Systemic symptoms and joint inflammation. The cytokines like IL -6 also stimulates STAT3, a transcription factor, which regulates a multitude of immune-related genes and facilitates the activation and survival of pathogenic T cells. Based on the analysis of network done on IL-6/STAT3 axis*, Datura* may decrease the inflammation in RA by suppressing these key nodes.

In this network study IL-37 is also targeted which is an anti-inflammatory cytokine that blocks innate immune responses. IL 37 is working with SMAD3 to reduce the level of IL-1β, IL-6, IL-23A and chemokines such as CXCL13 while keeping anti-inflammatory cytokine levels stable. Due to this dual regulatory effect of IL-37, the substances which alter its activity may help to restore immunological homeostasis. The targets of *Datura metel* phytochemicals, such as PTGS2 (COX-2), IRAK4 (a kinase downstream of IL-1R and TLRs), and PIK3CA (a catalytic component of PI3K), emphasize their polypharmacological reach. These proteins are having an important role in RA-related joint inflammation and injury because they regulate inflammatory mediators, production of prostaglandins, and cell survival.

PPARA (Peroxisome Proliferator-Activated Receptor Alpha), a transcription factor was one of the anticipated targets which controls inflammation and lipid metabolism. The anti-inflammatory activity and metabolic balancing effects of *Datura metel* phytochemical components may get enhanced by the activation of PPARA, particularly in RA patients with metabolic comorbidities, by inflammatory cytokine production and modifying genes implicated in fatty acid oxidation

According to a drug-likeness evaluation using Lipinski's Rule of Five (Table 1), the phytocompounds present in *Datura metel* like Atropine, hyoscyamine, and scopolamine are having favourable physicochemical properties (molecular weight, log P, and hydrogen bonding potential) that support good oral bioavailability and pharmacokinetic behaviour. In order to improve bioavailability, compounds like cuscohygrine and withanolides may need to be structurally optimized or have their delivery methods targeted.

These findings were visually reinforced in the network constructed using Cytoscape (Figure 2), where high-degree nodes—phytochemicals such as atropine—were directly linked to multiple key RA-associated proteins and pathways. A multi-target mechanism is a need in RA, that may offer a better therapeutic effect due to its synergistic or additive nature.

In molecular docking study, the stability and strength of ligand-protein interactions are explained by larger negative binding affinity values which indicates the stronger binding potential. Among the three targets, STAT3 is more susceptible to being modulated by the Phytochemicals. STAT3 showed the strongest interaction with all of the phytochemicals that were tested. This suggests that the phytochemicals of *Datura metel* may be strongly interfered with STAT3-mediated signaling pathways, that are involved in immune dysregulation and chronic inflammation. Hyoscyamine had the best binding affinity for TNF (−6.2 kcal/mol), followed by

Scopolamine (−5.9 kcal/mol) and Tigloidine (−5.3 kcal/mol). Scopolamine had specific affinity for STAT3, while Hyoscyamine showed consistent binding of all targets, suggesting a wide range of anti-inflammatory potential. The result explains the activity of phytochemicals of Datura metel in the multi-target therapeutic potential.

The *Datura metel*'s anti-inflammatory potential in RA could be viewed at the systemic level by combining network and gene set enrichment analysis along with molecular docking approach. Concurrent modulation of metabolic regulation (PPARA), inflammatory signalling (MAPK, TNF, NF-κB), and cytokine regulation (IL-6, IL-37, STAT3) points to a complex mechanism that is in line with modern therapeutic strategies that target many pathogenic pathways.

Strengths and Limitations

The main strength of this study is a thorough network pharmacology approach with molecular docking that integrates phytochemical profiling, target prediction, PPI analysis, and pathway enrichment. This study provides the scientific validation of anti-inflammatory property of Datura metel.

Limitations include dependence on *in silico* predictions and potential database bias. ADMET predictions were limited to drug-likeness parameters and do not fully represent *in vivo* pharmacokinetics or toxicity.

5. CONCLUSION

The study describes the anti-inflammatory activity of Datura in inflammation. The key phytocompounds present in *Datura* such as hyoscyamine, fastusic acid, scopolamine, deoxywithastramonolide and tigloidine are having an effect on TNF, IL6, COX, MAPK14 through Rheumatoid arthritis and P38 MAPK signalling pathway. The molecular docking shows the action of Scopolamine, Hyoscyamine and Tigloidine towards STAT3, TNF and IL6. The current study validates the potential of *Datura metel* as a *Shophahara* (anti-inflammatory and swelling-reducing action) drug through a network pharmacology and molecular docking approach.

Authors Details:

[1]Ph.D. Scholar, Department of Rasashastra and Bhaishajya Kalpana, KAHER's Shri BMK Ayurveda Mahavidyalaya, Shahapur, Belagavi, Karnataka, India

[2*]Professor, Department of Rasashastra and Bhaishajya Kalpana, KAHER's Shri BMK Ayurveda Mahavidyalaya, Shahapur, Belagavi, Karnataka, India.

[3]Principal and Professor, Department of Pharmacognosy, KLE College of Pharmacy, Belagavi, Karnataka, India

[4]Ph.D. Scholar, Department of Swasthavritta, KAHER's Shri BMK Ayurveda Mahavidyalaya, Belagavi, Karnataka, India

Authors Contribution:

Conceptualization and clinical management: SKV, RVK

Data collection and literature search: SKV, ASC

Writing original draft: SKV, ASC

Reviewing & editing: All authors

Approval of final manuscript: All authors

Declaration of Generative AI

The authors declare this manuscript was written without the use of generative artificial intelligence tools. All the content, including text generation, data analysis and references was developed and reviewed by the author without assistance from AI technologies.

Conflict of Interest – The authors declare no conflicts of interest.

Source of Support – The authors declare no source of support.

Publisher's Note:

REFERENCES:

1. Zhu M, Ding Q, Lin Z, Fu R, Zhang F, Li Z, et al. New Targets and Strategies for Rheumatoid Arthritis: From Signal Transduction to Epigenetic Aspect. Biomolecules [Internet]. 2023 Apr 28 [cited 2023 Nov 6];13(5):766–6. Available from: https://pubmed.ncbi.nlm.nih.gov/37238636/
2. Namewar PD, Patil AB. Toxic Plant Dhattura (*Datura metel* Linn)–A Medicine in Ayurved Literature And Its Pharmacological Activities-A Review. The Journal of Oriental Research Madras. 2024 Jan; Vol. XCV-I available from: https://www.researchgate.net/publication/382091445_Toxic_Plant_Dhattura_Datura_Metel_Linn_A_Medicine_In_Ayurved_Literature_And_Its_Pharmacological_Activities_-A_Review
3. Islam T, Ara I, Islam T, Sah PK, de Almeida RS, Matias EF, Ramalho CL, Coutinho HD, Islam MT. Ethnobotanical uses and phytochemical, biological, and toxicological profiles of *Datura metel* L.: A review. Current Research in Toxicology. 2023 Jan 1; 4:100106-6. Available from: https://www.sciencedirect.com/science/article/pii/S2666027X2300004X
4. Prasathkumar M, Anisha S, Khusro A, Mohamed Essa M, Babu Chidambaram S, Walid Qoronfleh M, et al. Anti-pathogenic, anti-diabetic, anti-inflammatory, antioxidant, and wound healing efficacy of *Datura metel* L. leaves. Arabian Journal of Chemistry [Internet]. 2022 Sep 1;15(9):104112. Available from: https://www.sciencedirect.com/science/article/pii/S1878535222004282
5. 1.Joshi CP, Baldi A, Kumar N, Pradhan J. Harnessing network pharmacology in drug discovery: an integrated approach. Naunyn-Schmiedeberg's Archives of Pharmacology. 2024 Dec 2;398(5):4689–703. Available from: https://link.springer.com/article/10.1007/s00210-024-03625-3
6. Ugare SR, Khatib NA, Patil VS, Patil D, Dodakallanavar J. Computational and experimental pharmacology reveals hepatoprotective effect of Cucurbita pepo in isoniazid-induced liver cirrhosis. Journal of Applied Pharmaceutical Science. 2024 Jan 4;14(1):177-88. doi:10.7324/JAPS.2024.148502 available from: https://japsonline.com/admin/php/uploads/4112_pdf.pdf
7. Chen IJ, Foloppe N. Drug-like bioactive structures and conformational coverage with the LigPrep/ConfGen suite: comparison to programs MOE and catalyst. Journal of chemical information and modeling. 2010 Apr 27;50(5):822-39. DOI:10.1021/ci100026x available from: https://pubs.acs.org/doi/full/10.1021/ci100026x
8. Szklarczyk D, Gable AL, Nastou KC, Lyon D, Kirsch R, Pyysalo S et al. The STRING database in 2021: customizable protein–protein networks, and functional characterization of user-uploaded gene/measurement sets. Nucleic acids research. 2020 Nov 25;49(D1):D605–12. https://doi.org/10.1093/nar/gkaa1074
9. Khanal P, Patil VS, Bhandare VV, Dwivedi PS, Shastry CS, Patil BM,et al. Computational investigation of benzalacetophenone derivatives against SARS-CoV-2 as potential multi-target bioactive compounds. Computers in Biology and Medicine. 2022 Jul 1;146:105668. DOI: 10.1016/j.compbiomed.2022.105668
10. Patil AA, Suryawanshi SS. Computer-Assisted Prediction of Drug-Like Properties of Selected Phytochemicals from Terminalia chebula. International Journal of Pharmaceutical Investigation. 2025 Feb 12;15(2):614–30. DOI: https://jpionline.org/10.5530/ijpi.20250067
11. Morris GM, Huey R, Lindstrom W, Sanner MF, Belew RK, Goodsell DS, Olson AJ. AutoDock4 and AutoDockTools4: Automated docking with selective receptor flexibility. Journal of computational chemistry. 2009 Dec;30(16):2785-91. DOI: https://doi.org/10.1002/jcc.21256
12. Raudvere U, Kolberg L, Kuzmin I, Arak T, Adler P, Peterson H et al. g: Profiler: a web server for functional enrichment analysis and conversions of gene lists (2019 update). Nucleic acids research. 2019 Jul 2;47(W1):W191-8. https://doi.org/10.1093/nar/gkz369
13. Raman K. Construction and analysis of protein–protein interaction networks. Automated experimentation. 2010 Dec;2(1)2 available from: https://link.springer.com/content/pdf/10.1186/1759-4499-2-2.pdf
14. Schett G, Tohidast-Akrad M, Smolen JS, Schmid BJ, Steiner CW, Bitzan P, et al. Activation, differential localization, and regulation of the stress-activated protein kinases, extracellular signal-regulated kinase, c-Jun N-terminal kinase, and p38 mitogen-activated protein kinase, in synovial tissue and cells in rheumatoid arthritis. Arthritis & Rheumatism. 2000 Nov;43(11):2501–12 DOI: https://doi.org/10.1002/1529-0131(200011)43:11%3C2501::aid-anr18%3E3.0.co;2-k