IECAN 2025 Conference
The 2nd International Electronic Conference on Antioxidants
07–09 April 2025 | Online
MDPI

Clarifying the Antioxidant and Antiproliferative Potential of *Nyctanthes arbor-tristis* Extracts by Combining Network Pharmacology and Molecular Docking Approach

Kalpesh Rajendra Yeole*[1], Raju Ratan Wadekar[2]

[1] Department of Pharmacognosy, Shri Vile Parle Kelavani Mandal's Institute of Pharmacy, Dhule-424001, Maharashtra, India

INTRODUCTION & AIM

Nyctanthes arbor-tristis, commonly known as Parijat, is a medicinal plant recognized for its potent antioxidant and therapeutic properties. Oxidative stress is a major contributor to various pathological conditions, including cancer, neurodegenerative disorders, and inflammatory diseases. Recent advancements in network pharmacology have facilitated the identification of bioactive phytoconstituents and their interactions with key antioxidant enzymes by integrating computational approaches such as molecular docking.

This study aims to explore the plant's potential in modulating oxidative stress-related pathways and its role in disease mitigation.

METHODOLOGY

1 **Phytochemical Identification:**
The Screening of *NAT* phytoconstituents was done from the IMPPAT database, and bioactive compounds were selected based on pharmacological relevance.

2 **Target Identification & Network Analysis:**
We identified the therapeutic targets related to oxidative stress and antiproliferative agents from databases like Gene Cards and STRING.

3 **ADMET & Drug-Likeness Analysis:**
The Evaluation of pharmacokinetics and drug-likeness properties were carried out using SwissADME and pkCSM tool and top candidates were identified based on the Lipinski's Rule of Five.

4 **Molecular Docking & MMGBSA Analysis:**
The Molecular docking of selected compounds with key antioxidant (SOD1, CAT, GPx1, Nrf2) and antiproliferative (CASP3, NFKB1, NOTCH1, GSK3B, HF1A, SRC, AKT1, MMP9) targets was carried out using Auto Dock software.

5 **Data Interpretation & Conclusion:**
The Top candidates ranked based on docking scores and MMGBSA energy with greater Biological significance related to oxidative stress and cancer prevention potential, were analyzed.

DOCKING ANALYSIS

Table 1. Top 10 network ranked by Degree method

Rank	Phytochemical	Degree score	Docking score
1	β-Sitosterol	222	-9.1
2	Naringetol	202	-8.4
3	Curlone	195	-7.6
4	Ar- turmerone	188	-6.4
5	Melanin	182	-4.1

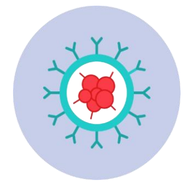
RESULTS & DISCUSSION

NAT

SIB

Swiss Target Prediction

Targets of NAT

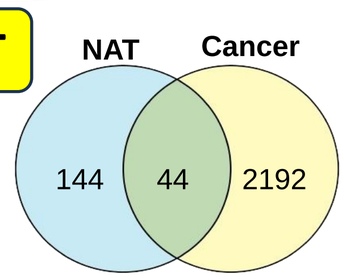


Cancer

DisGeNET

GeneCards HUMAN GENE DATABASE

Targets of Cancer



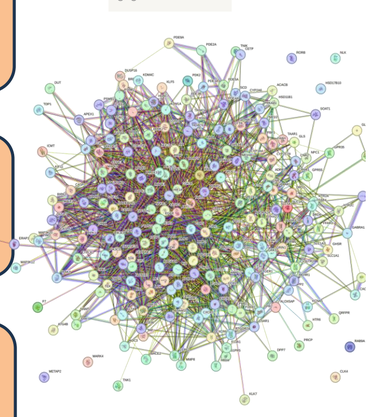
Intersection of Targets

PPI Network

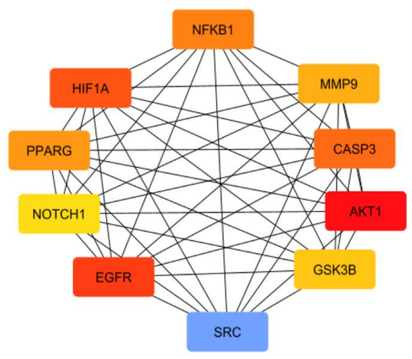
Cytoscape

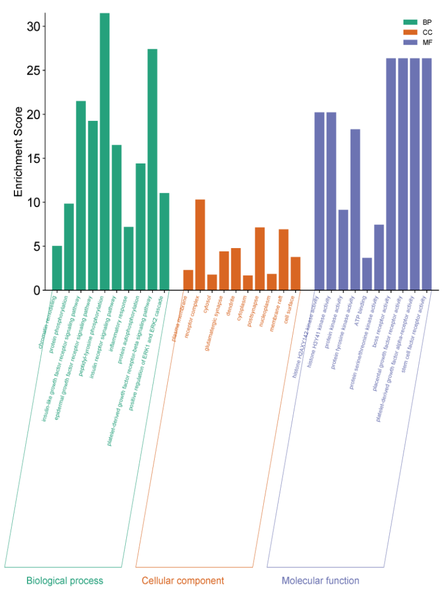
Enrichment Analysis

STRING

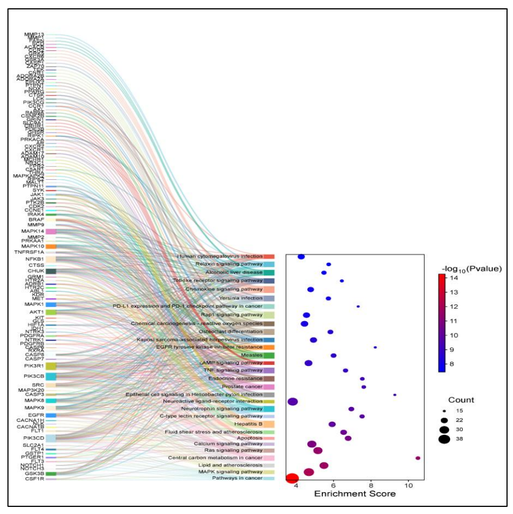


Cytoscape

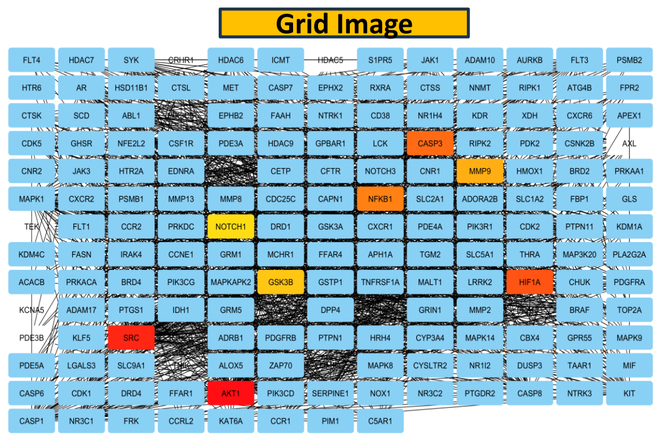




Shankey and Dot analysis



Grid Image



CONCLUSION

This study highlights *Nyctanthes arbor-tristis* as a promising source of antioxidant and antiproliferative agents, with β-sitosterol emerging as the most potent candidate based on molecular docking and MMGBSA analysis. The identified phytoconstituents exhibit strong interactions with key oxidative stress-related targets (CASP3, NFKB1, NOTCH1, GSK3B, HF1A, SRC, AKT1, MMP9), suggesting their potential for therapeutic applications against oxidative stress-associated diseases.

REFERENCES

1] Ahmad V, Khan MI, Jamal QMS, Alzahrani FA, Albiheyri R. Computational molecular docking and simulation-based assessment of anti-inflammatory properties of *Nyctanthes arbor-tristis* Linn phytochemicals. Pharmaceuticals. 2024;17(1):18. doi: 10.3390/ph17010018.