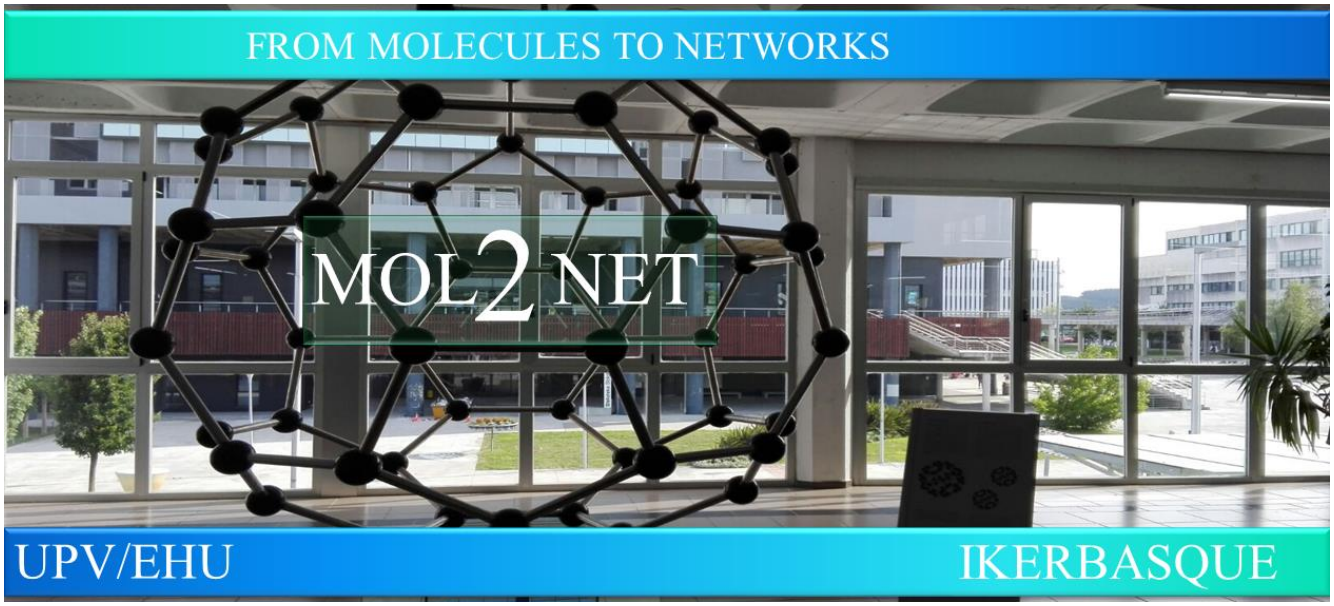
MDPI sciforum

MOL2NET'21, Conference on Molecular, Biomedical & Computational Sciences and Engineering, 7th ed.



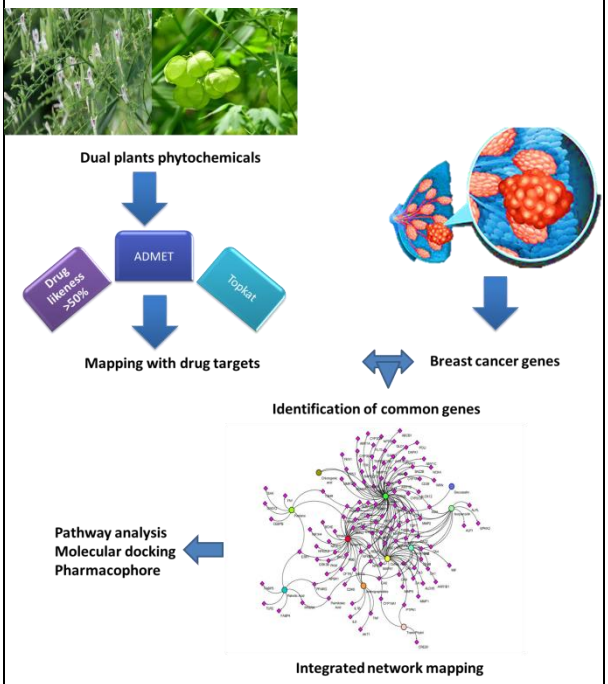
Integrated bimolecular network pharmacology approach on *Andrographis paniculata* and *Cardiospermum halicacabum* synergistic therapeutic effects in targeting breast cancer

Dhivya Shanmugarajan[a], *Arpana Parihar* [b],*Charles David* [a], *Bhavana Boppanaa* [a]

[a] *Department of Biotechnology, Vignan's Foundation for Science, Technology & Research (Deemed to be University), Vadlamudi, Andhra Pradesh, India- 522 213.*

[b] *CSIR-Advanced Materials & Processes Research Institute (AMPRI), Hoshangabad Road, Bhopal, Madhya Pradesh (462026), India*

Graphical Abstract



Abstract.

Medicinal plants are a rich source of bioactive compounds, combination therapy of two plants treatment is gaining more prominence because of synergistic therapeutic effects. But, characterizing the molecular synergism activity of two medicinal herbal sources against specific drug targets in cancer is still considered a painstaking task that requires more meticulous screening, human intervention and high experimental resources. To understand the rationale, an integrated network pharmacology approach was introduced to understand the interaction network between compounds and drug targets. The interaction was constructed for compounds possessing >50% drug-likeness, non-mutagen non-carcinogen. Also, these compounds were compared in the activity landscape in a database of collective molecular activities of useful plants, only compounds <100µm were considered for bimolecular interaction with human drug target proteins. Further, a Venn diagram was constructed between genes of breast cancer and the gene that are mapped with *Andrographis paniculata* and *Cardiospermum halicacabum*. The STRING database was used to construct a protein-protein interaction network and relationships of each gene were analyzed. Consequently, GO biological function analysis and KEGG enrichment analysis for crucial targets were performed. Finally, docking of phytochemicals with drug target protein was carried out and its active site pharmacophore was reported. Thus, active ingredients owning pharmacophores of phenols and flavonoids exhibiting strong molecular interaction can be served as drug candidates for treating breast cancer. Moreover, herbal-based compounds potentially have fewer side effects and are safe for treatment.

Keywords: Medicinal plants; Combination therapy; network pharmacology; *Andrographis paniculata* ;*Cardiospermum halicacabum*; Protein-protein interaction; Pharmacophores

References

1. Laigen Zhang, Xiaoqing Shi, Zhengquan Huang, Jun Mao, Wei Mei, Liang Ding, Li Zhang, Runlin Xing and
   Peimin Wang. Network Pharmacology Approach to Uncover the Mechanism Governing the Effect of Radix Achyranthis Bidentatae on Osteoarthritis, BMC Complementary Medicine and Therapies (2020), 20:121.
2. Niannian Wang, Feifei Zhu, Mingxiang Shen, Lipeng Qiu, Min Tang, Hengchuan Xia,Liang Chen, Yi Yuaa, Shangshang Ma, Keping Chen.Network pharmacology-based analysis on bioactive anti-diabetic compounds in Potentilla discolor bunge,Journal of Ethnopharmacology (2019), 241:111905.
3. Kushwaha S and Shakya M. Protein interaction network analysis–approach for potential drug target identification in Mycobacterium tuberculosis, J. Theor. Biol. (2010),262:284–294.
4. Mohan Rao, Rishi Gupta, Michael J.Liguori , Mufeng Hu, Xin Huang,Srinivasa R. Mantena, Scott W. Mittelstadt, Eric Blomme, Terry R.Van Vleet.Novel Computational Approach to Predict Off-Target Interactions for Small Molecules, Front. Big Data.(2019), 2:25.
5. Hai Zhang, Shifan Ma, Zhiwei Feng, Dongyao Wang, Chengjian Li, Yan Cao,Xiaofei Chen, Aijun Liu, Zhenyu Zhu, Junping Zhang, Guoqing Zhang, Yifeng Chai,Lirong Wang, Xiang-Qun Xie.Cardiovascular Disease Chemogenomics Knowledgebaseguided Target Identification and Drug Synergy Mechanism Study of an Herbal Formula, Scientific Reports.(2016),6:33963.
6. https://www.genecards.org/Search/Keyword?queryString=breast%20cancer
7. https://www.nhp.gov.in/introduction-and-importance-of-medicinal-plants-and-herbs_mtl