Center for Traditional Knowledge and Informatics The University of Transdisciplinary Health Sciences and Technology (TDU) Bangalore

COURSE TITLE: NETWORK PHARMACOLOGY FOR DRUG DISCOVERY BASED ON AYURVEDA DRAVYAGUNA

Focus Area/Subject Area: Network Pharmacology for Drug Discovery based on Ayurveda Dravyaguna

Credits: 2

Eligibility: Under Graduation (UG) Degree

Prerequisite: Having Science Background with knowledge of Botany and Ayurveda

Details of Instructors:

- 1. Dr. Venugopalan Nair, Professor, TDU
- 2. Dr. Tabassum, Assistant Professor, TDU
- 3. Dr. CN. Vishnuprasad, Associate Professor, TDU
- 4. Dr. Subrahmanya Kumar K, Associate Professor, TDU

Course Objectives:

- 1. Explore the principles and applications of Network Pharmacology (NP).
- 2. *Dravyaguna* Profile mapping and networking
- 3. Study the relationships of *Dravyaguna* profile (*Rasapanchakas*) of *Ayurvedic* plants and its recommended indications or formulations using NP methods in relation with bioactives and its targets and disease pathways.
- 4. Suggest a list of shortlisted medicines or plants for a given clinical conditions or disease using the outcome of the study.
- 5. Gain proficiency in **Gene Ontology** (**GO**) and pathway analysis for identifying drug targets and mechanisms.
- 6. Acquire hands-on experience with tools such as *Cytoscape* and *ClueGO*.
- 7. Discuss the relevance of network pharmacology in drug discovery, with a focus on traditional medicineand *Ayurvedic* formulations.

Learning Outcome:

By the end of this course, the participants will be equipped to explore the molecular basis of plant drugs, especially of those used in Indian Traditional Medicine; also explore the new avenues in drug discovery and contribute to the advancement of healthcare through evidence-based approaches in herbal medicine.

SYLLABUS

Module 1: Introduction to Network Pharmacology and Rasapanchaka

- Challenges in traditional drug discovery approaches
- Principles of Network Pharmacology
- Significance of multi-component and multi-target interactions
- Concept of *Rasapanchaka*

Module 2: Network Pharmacology for Ayurvedic Rasapanchaka

- Gather data on the relationship between *"Rasapanchaka"* and *Ayurvedic* plants, and establishconnections.
- Extract phytochemicals and disease pathways through data mining, and identify disease targets from open-source databases.

Module 3: Target Retrieval and Network Construction

- Methods for target retrieval from biological databases
- Techniques for Network Construction and Visualization

Module 4: GO and Pathway Analysis

- Understanding Gene Ontology (GO) and pathway databases
- Practical application of GO and pathway analysis in drug target identification

References/ Learning Resources:

- Mohanraj K., Karthikeyan B.S., Vivek-Ananth R.P., Chand BharathR.P., Aparna S.R., Mangalapandi P., and Samal A., 2018. IMPPAT: A curated database of Indian Medicinal Plants, Phytochemistry and Therapeutics, Nature, Science Reports, 8:4329 , DOI:10.1038/s41598
- 2. Sastry K (ed.) *Charaka Samhita-Hindi translation*, part-1&2, Chowkhamba Orientalia Varanasi.
- 3. Sharma PV. History of medicine in India, Chowkhamba Orientalia Varanasi.
- 4. K.R. Srikantha Murthy. Astanga Hrdayam, Chowkhambakrishnadas Academy, Varanasi; 2018.
- Chandran Uma, Mehendale Neelay, Tillu Girish and Patwardhan Bhushan, 2015. Network Pharmacology of Ayurveda Formulation Triphala with Special Reference to Anti-Cancer Property, Combinatorial Chemistry & High Throughput Screening; 18(9). Link
- 6. Chandran, Uma et al., 2017. "Network Pharmacology." Innovative Approaches in Drug Discovery. 127–164. doi:10.1016/B978-0-12-801814-9.00005-2

- 7. Liu AL, Du GH. 2010. *Network pharmacology: new guidelines for drug discovery, Yao Xue Xue Bao.* Dec;45(12) 1472-1477. PMID: 21351485.
- Li S, Shao Y, Chen H, Wang J., 2022. Using Network Pharmacology to Systematically Decipher the Potential Mechanisms of Jisuikang in the Treatment of Spinal Cord Injury. Evidence-based Complementary and Alternative Medicine: Ecam.;2022:4932153. DOI: 10.1155/2022/4932153. PMID: 35265147; PMCID: PMC8898796.
- Mukherjee P.K., Shiv Bahadur, Ranjit K.Harwash, Sayan Biswas, Subhsdip Banerjee, 2017. Paradigm shift in natural product research: traditional medicine inspired approaches, Springer, Phytochem Rev 16: 803-826, DOI 10.1007/s11101-016-9489-6
- 10. Nair SNV, 2018. *Network Pharmacology as an Appropriate Bioinformatics Tool for Drug Discovery*, Bioinformatics and Proteomics Open Access Journal, Vol 2, Issue 1
- 11. Sakle, N.S., More, S.A. & Mokale, S.N. 2020. A network pharmacology-based approach to explore potential targets of *Caesalpinia pulcherima*: an updated prototype in drug discovery. *SciRep* **10**, 17217. Link