CURRENT RESEARCH TOPICS IN PHARMACY:

In silico Approaches for Drug Design and Discovery

January 25th, 2023 13.00 PM
ISTANBUL

FOR REGISTRATION:

First Session- *Moderator: Esra TATAR 13.00-14.30 PM*

Welcome- Prof. Mesut SANCAR

***In silico* pharmakokinetics prediction of major coumarins present in *Aegle marmelos* L – Assist. Prof. Sneha Agrawal**
Bharati Vidyapeeth's College of Pharmacy, Maharashtra, India

Pharmakokinetics evaluation with SimCYP program - Assoc.Prof.Enkelejda Goci
Aldent University, Tirana, Albania

A new approach in drug discovery: Network pharmacology - Dr. Yağmur Diker
Hacettepe University, Ankara, Turkey

Second Session- *Moderator: Esra TATAR 15.00-16.30 PM*

Computational identificaion of novel targets for drug candidate compounds - Assoc.Prof.Ceren Sucularlı
Hacettepe University, Ankara, Turkey

Designing novel mitochondrial fission inhibitors targeting Drp1-GTPase interaction using computational methods - Dr.Sefer Baday
Istanbul Technical University, Istanbul, Turkey

Artificial Intelligence: A member of drug discovery team – Assoc.Prof.Somaieh Soltani
Tabriz University of Medical Sciences, Tabriz, Iran

Discovery of novel Hepatitis C NS5B polymerase Inhibitors by in silico approaches - Dr. Berin Karaman Mayack
University of California Davis, Davis, USA

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Vice Chairs
Prof. Levent KABASAKAL & Assoc. Prof. Esra TATAR

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ONLINE SYMPOSIUM

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A NEW APPROACH IN DRUG DISCOVERY: NETWORK PHARMACOLOGY

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The main aim of traditional drug discovery is to find specific ligands. The theory of "one gene, one drug, one disease" contains the hypothesis that the main drug action is only on a single target—the stronger drug selectivity, the more specific mechanism of action, and the higher degree of correlation with the target phenotype. Therefore, discovering specific ligands plays a vital role in drug design [1]. This approach has led researchers working on natural products to the isolation and structure determination of bioactive natural compounds from plants.

Some diseases are caused by a variety of factors with very complex pathologies, and the use of a single drug cannot solve these problems. Many effective compounds act via the modulation of multiple proteins rather than a single protein [2]. A new perspective, the concept of network pharmacology was first proposed by Andrew L. Hopkins in 2007 who combined network biology with polypharmacology. Network pharmacology focuses on understanding the internal mechanism and drug action of complex diseases and syndromes [3-4]. The therapeutic efficacy of plant extract is rooted in their complexity of chemical composition and molecular mechanism. Consequently, network pharmacology studies are mostly applied to TCM formulas [5].

Methodologies of network pharmacology are based on two essential sections; network construction and network analysis. The networks are composed of nodes and edges. The nodes are investigated subjects or entries. The edges are node connections and node connections can be based on different data sources such as knowledge-based, experiment-based, and computation-based. Network analysis lets us identify novel biomarkers and discriminate effective pathways. Topological metrics analysis focused on the topological characteristics of a network or its components. The network module is expressed enrichment analysis such as the detection of pathways or gene ontology [6].

Predominantly, databases are widely used in network pharmacology studies as data sources. Traditional Chinese Medicine databases (SymMap, BATMAN-TCM, TCMID,

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etc.) contain much information such as the plants in the mixtures, the compounds in the plants, and the bioavailability information of the compounds. Biological databases (OMIM, DisGeNET, MalaCards, etc.) contain clinical and basic research results and it is also described as disease phenotype and genotype association database. Gene targets databases (TTD, PDB, KEGG, GeneCards, etc.) included comprehensive information about genes, proteins, or compounds. Protein interaction databases (BioGRID, DIP, IntAct, STITCH, etc.) are included information on gene-protein or chemical-protein interaction [7]. Online or offline softwares are used in this method. Cytoscape is a well-known and commonly used visualization software. This is an open-source platform suitable for visualizing molecular interaction networks and biological pathways [8].

Various issues can be often researched in network pharmacology studies. In target discovery studies, complex diseases occur with the change of multi-targets in biological systems. The content of plant extract shows a similar effect when it gets into the body. These affected targets are used for the discovery of new targets. In the bioactive compounds screening studies, network pharmacology provides an easy method for seeking potential bioactive compounds by mapping chemical compounds into the disease-gene network and mechanism research. In toxicity evaluation, network pharmacology can break the limitations of traditional methods to find toxic compounds and mechanisms of toxicity rapidly [5,9]. Network pharmacology gives a general aspect of view and provides the prediction of the key metabolic pathways.

Keywords; Network Pharmacology, Drug Discovery, Herbal Medicine

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REFERENCES

[1] Li S, Ding Q, Wang X. "Network Target" Theory and Network Pharmacology. In: Li, S. (Eds). Network Pharmacology. Springer, Singapore, 2021, pp. 1-34.

[2] Gertsch J. Botanical drugs, synergy, and network pharmacology: Forth and back to intelligent mixtures. Planta Med. 2011; 77: 1086-1098. [CrossRef]

[3] Hopkins AL. Network pharmacology. Nat Biotechnol. 2007; 25(10):1110-1111. [CrossRef]

[4] Hopkins, AL. Network pharmacology: The next paradigm in drug discovery. Nat Chem Biol. 2008; 4(11):682-690. [CrossRef]

[5] Wang X, Wang ZY, Zheng JH, Li S. TCM network pharmacology: A new trend towards combining computational, experimental and clinical approaches. Chin J Nat Med. 2021; 19(1): 1-11. [CrossRef]

[6] Xu H, Zang Y, Gou F. Common Network Pharmacology Databases. In: Li, S. (Eds). Network Pharmacology. Springer, Singapore, 2021, pp. 75-126.

[7] Liu YF, Ai N, Keys A, Fan WH, Chen MJ. Network pharmacology for traditional Chinese medicine research: Methodologies and applications. Chin Herb Med. 2015; 7(1): 18-26. [CrossRef]

[8] Shannon P, Markiel A, Ozier O, Baliga NS, Wang JT, Ramage D, Amin N, Schwikowski B, Ideker T. Cytoscape: a software environment for integrated models of biomolecular interaction networks. Genome Res. 2003; 13(11): 2498-2504. [CrossRef]

[9] Sun X, Xiaoyan x, Wang M. Drug-Based Network Pharmacology Practice Process. In: Li, S. (Eds). Network Pharmacology. Springer, Singapore, 2021, pp. 321-394.

http://dx.doi.org/10.29228/jrp.454