CURRENT RESEARCH TOPICS IN PHARMACY:

Pharmacology Debates

April 19th, 2023 10.00 AM ISTANBUL

FOR REGISTRATION:

First Session- *Moderator: Esra TATAR 10.00-11.30 AM*

Welcome- Prof. Hatice Kübra Elçioğlu
Marmara University, Istanbul, Türkiye

The roles of cheminformatics in natural product-based drug discovery-Prof.Long Chiau Ming
School of Medical and Life Sciences, Sunway University, Kuala Lumpur, Malaysia

Applications of machine learning to the lead discovery: Practical approaches – Dr.Said Moshawih
Universiti Brunei Darussalam, Gadong, Brunei Darussalam

Second Session – Moderator: Ayşe Nur HAZAR YAVUZ 12:00-13.30 PM

Can Vitamin C supplements prevent premature rupture of membranes and preterm birth- Assist. Prof. Ana V. Pejcic
University of Kragujevac, Kragujevac, Serbia

Drugs affecting newborn weight, length and head circumference at birth -Assist.Prof. Milos N. Milosavljevic
University of Kragujevac, Kragujevac, Serbia

From traditional medicine to brain tumor theraphy using Plectranthus diterpenes-Assoc.Prof.Patricia Rijo
Lusofona University, Lisbon, Portugal

Chair
Prof. Hatice Kübra ELÇİOĞLU

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

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Third Session- *Moderator: Mehmet GÜMÜŞTAŞ 14.00-15.30 PM*

Side effects of COVID 19 vaccines and the contribution of graphenes- Assoc.Prof.Beril Anılanmert
Institute of Forensic Sciences and Legal Medicine, Istanbul University-Cerrahpaşa, Istanbul, Türkiye

Knowledge and behaviour of medical university students about drug store and use-Assist.Prof.Klodiola Dhamo
Aldent University, Tirana, Albania

The advancement of herbal-based treatments for hair loss- Dr.Oğuzhan Aydemir
Istinye University, Istanbul, Türkiye

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INSIGHT INTO APPLICATION OF MACHINE LEARNING IN NATURAL PRODUCTS CHEMINFORMATICS

Said MOSHAWIH [1,*], Hui Poh GOH [1], Nurolaini KIFLI [1*], Vijay KOTRA [2], Long Chiau MING [1,3]**

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Cheminformatics utilizing machine learning (ML) techniques have opened up a new horizon in drug discovery. This is owing to vast chemical space expansion with rocketing numbers of expected hits and lead compounds that match druggable macromolecular targets, in particular from natural compounds. Due to the natural products' (NP) structural complexity, uniqueness, and diversity, they could occupy a bigger space in pharmaceuticals, allowing the industry to pursue more selective leads in the nanomolar range of binding affinity. ML is an essential part of each step of the drug design pipeline, such as target prediction, compound library preparation, and lead optimization. Notably, molecular mechanic and dynamic simulations, induced docking, and free energy perturbations are essential in predicting best binding poses, binding free energy values, and molecular mechanics force fields. Those applications have leveraged from artificial intelligence (AI), which decreases the computational costs required for such costly simulations. This seminar aimed to describe chemical space and compound libraries related to NPs. High-throughput virtual screening and their strategies in leveraging NPs libraries can be optimized to match the specificity of the chemical space that is occupied by such kind of complex compounds. Particular emphasis was given to AI approaches, ML tools, algorithms, and techniques, especially in drug discovery of macrocyclic compounds and approaches in computer-aided and ML-based drug discovery. The various functionalities and stereochemical complexities of macrocycles give them more selectivity and affinity to protein targets. Natural products were discussed as having the most distinct features differentiating them from synthetic compounds by the number of aromatic atoms, chiral centers, nitrogen, and oxygen atoms. Aromaticity is eminent among the synthetic compounds, while the chiral centers are more prevalent in NP compounds. Furthermore, the oxygen atoms are more prevalent in NPs, while nitrogen atoms are less. Those features make NPs as source

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of new lead compounds that can be developed using ML tools for diverse medicinal uses specifically in cancer, infectious diseases, and metabolic disorders.

Keywords: Medicinal plant; artificial intelligence; high throughput screening; herbal medicine.

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