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

ORGANIZING & SCIENTIFIC COMMITTEE
Editorial Board of Journal of Research in Pharmacy
https://www.jrespharm.com/

JRP

Journal of Research in Pharmacy
An international open-access journal of pharmacy and pharmaceutical sciences
Formerly published as Marmara Pharmaceutical Journal

ONLINE SYMPOSIUM

CURRENT RESEARCH TOPICS IN PHARMACY:
Pharmacology Debates

April 19th, 2023 10.00 AM ISTANBUL

FOR REGISTRATION:

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

Chair
Prof. Hatice Kübra ELÇİOĞLU

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

ORGANIZING & SCIENTIFIC COMMITTEE
Editorial Board of Journal of Research in Pharmacy
https://www.jrespharm.com/

JRP

Journal of Research in Pharmacy
An international open-access journal of pharmacy and pharmaceutical sciences
Formerly published as Marmara Pharmaceutical Journal

ONLINE SYMPOSIUM

CURRENT RESEARCH TOPICS IN PHARMACY:
Pharmacology Debates

April 19th, 2023 10.00 AM ISTANBUL

ORGANIZING & SCIENTIFIC COMMITTEE
Editorial Board of Journal of Research in Pharmacy
https://www.jrespharm.com/

Esra Tatar
(Vice Chair of Organizing Committee)
Marmara University, Istanbul, Türkiye

Levent Kabasakal
(Vice Chair of Organizing Committee)
Marmara University, Istanbul, Türkiye

Ayşe Nur Hazar Yavuz
(Secretary)
Marmara University, Istanbul, Türkiye

Abdikarim Mohammed Abdi
Yeditepe University, Istanbul, Türkiye

Afife Büşra Uğur Kaplan
Atatürk University, Erzurum, Türkiye

Ahmet Emir
Ege University, Izmir, Türkiye

Ali Demir Sezer
Marmara University, Istanbul, Türkiye

Ammad Ahmad Farooqi
Institute of Biomedical and Genetic Engineering (IBGE), Islamabad, Pakistan

Ana V. Pejčić
University of Kragujevac, Kragujevac, Serbia

Anil Kumar Dwivedi
Central Drug Research Institute, Lucknow, India

Anisa Elhamili
University of Tripoli, Tripoli, Libya

Annalisa Chiavaroli
G. d'Annunzio University of Chieti-Pescara, Chieti, Italy

Antoaneta Trendafilova
Bulgarian Academy of Sciences, Sofia, Bulgaria

Ayça Toprak Semiz
Giresun University, Giresun, Türkiye

Ayfer Beceren
Marmara University, Istanbul, Türkiye

Ayşe Esra Karadağ
Istanbul Medipol University, Istanbul, Türkiye

Ayşenur Günaydın Akyıldız
Bezmialem Vakıf University, Istanbul, Türkiye

Bahadır Bülbül
Düzce University, Düzce, Türkiye

Betül Okuyan
Marmara University, Istanbul, Türkiye

Beyza Ecem Öz Bedir
Ankara Yıldırım Bayezıt University, Ankara, Türkiye

Burcu Üner
The University of Health Science and Pharmacy in St. Louis, USA

Büşra Ertaş
Marmara University, Istanbul, Türkiye

Ceren Emir
Ege University, Izmir, Türkiye

Ceyda Ekentok Atıcı
Marmara University, Istanbul, Türkiye

Claudio Ferrante
G. d'Annunzio University of Chieti-Pescara, Chieti, Italy

Debora Dummer Meira
Federal University of Espírito Santo, Vitória- Espírito Santo, Brazil

Derya Özsavcı
Marmara University, Istanbul, Türkiye

Dhanashree P. Sanap
Bharati Vidyapeeth's College of Pharmacy,Navi Mumbai, India

Dinesh Kumar
Indian Institute of Technology (BHU), Varanasi, India

Ebru Altuntaş
Istanbul University, Istanbul, Türkiye

Efe Doğukan Dincel
Istanbul University, Istanbul, Türkiye

Ela Hoti
University of Medicine, Tirana, Albania

Emine Terzi
Ankara Yıldırım Bayezıt University, Ankara , Türkiye

Emirhan Nemutlu
Hacettepe University, Anakara, Türkiye

Emre Kara
Hacettepe University, Anakara, Türkiye

Emrah Özakar
Atatürk University, Erzurum, Türkiye

Enkelejda Goci
Aldent University, Tirana, Albania

Entela Haloci
University of Medicine, Tirana, Albania

Erkan Rayaman
Marmara University, Istanbul, Türkiye

Fatiha Missoun
University of Mostaganem, Mostaganem, Algeria

Gizem Tatar Yılmaz
Karadeniz Technical University, Trabzon, Türkiye

Gülberk Uçar
Hacettepe University, Ankara, Türkiye

Gülgün Tınaz
Marmara University, Istanbul, Türkiye

Gülşah Gedik
Trakya University, Edirne, Türkiye

Haidar A. Abdulamir
Al-Maaql University, Basra, Iraq

Hamide Sena Özbay
Hacettepe University, Ankara, Türkiye

Hasan Erdinç Sellitepe
Karadeniz Technical University, Trabzon, Türkiye

İ. İrem Tatlı Çankaya
Hacettepe University, Ankara, Türkiye

Kerem Buran
University of Health Sciences, Istanbul, Türkiye

Kleva Shpati
Albanian University, Tirana, Albania

Klodiola Dhamo
Aldent University, Tirana, Albania

Laleh Khodaie
Tabriz University of Medical Sciences, Tabriz, Iran

Lejla Klepo
University of Sarajevo, Sarajevo, Bosnia and Herzegovina

Lokman Ayaz
Trakya University, Edirne, Türkiye

Lorena Memushaj
Aldent University, Tirana, Albania

Maja Ortner Hadžiabdić
University of Zagreb, Zagreb, Croatia

Mehmet Gümüştaş
Ankara University, Ankara, Türkiye

Merve Kabasakal
University of Health Sciences, Istanbul, Türkiye

Mesut Sancar
Marmara University, Istanbul, Türkiye

Mirela Miraçi
University of Medicine, Tirana, Albania

Mirjana Marčetić
University of Belgrade, Belgrade, Serbia

Mohd Younis Rather
Government Medical College Srinagar, Srinagar, India

Murat Doğan
Cumhuriyet University, Sivas, Türkiye

Nasir Idkaidek
Petra Universty, Amman, Jordan

Nurdan Tekin
University of Health Sciences, Istanbul, Türkiye

Nurettin Yaylı
Karadeniz Technical University, Trabzon, Türkiye

Ongun Mehmet Saka
Ankara University, Ankara, Türkiye

Oya Kerimoğlu
Marmara University, Istanbul, Türkiye

Pablo Miralles Ibarra
University of Valencia, Burjassot, Spain

Pankaj Dwivedi
The University of Health Science and Pharmacy in St. Louis, USA

Patricia Rijo
Lusofona University, Lisbon, Portugal

Pınar Talay Pınar
Yüzüncü Yıl University, Van, Türkiye

Renuka Khatik
Washington University in St. Louis, USA

Rezarta Shkreli
Aldent University, Tirana, Albania

Rukiye Sevinç Özakar
Atatürk University, Erzurum, Türkiye

Rümeysa Keleş Kaya
Sakarya University, Sakarya, Türkiye

Saeideh Soltani
Isfahan University of Medical Sciences, Isfahan, Iran

Sakine Tuncay Tanrıverdi
Ege University, Izmir, Türkiye

Simone Carradori
G. d'Annunzio° University of Chieti-Pescara, Chieti, Italy

Sinan Sermet
Istanbul Arel University, Istanbul, Türkiye

Sneha Agrawal
Bharati Vidyapeeth's College of Pharmacy, Navi Mumbai, Maharashtra, India

Somaieh Soltani
Tabriz University of Medical Sciences, Tabriz, Iran

Tarık Catić
Sarajevo School of Science and Technology, Sarajevo, Bosnia and Herzegovina

Turgut Taşkın
Marmara University, Istanbul, Türkiye

Uğur Karagöz
Trakya University, Edirne, Türkiye

Ünzile Yaman
Katip Çelebi University, İzmir, Türkiye

Viktorija Maksimova
Goce Delcev University, Stip, Republic of N. Macedonia

Vildan Çeliksoy
Cardiff University, Cardiff, UK

Vilma Toska Papajanı
University of Medicine, Tirana, Albania

Yeliz Şahin
Ağrı İbrahim Çeçen University, Ağrı, Türkiye

Zahraa Amer Hashim
Mosul University, Mosul, Iraq

Zarife Nigar Özdemir Kumral
Marmara University, Istanbul, Türkiye

Zeina Althanoon
Mosul University, Mosul, Iraq

Zoran Zeković
University of Novi Sad, Novi Sad, Serbia

JRP
Journal of Research in Pharmacy
An international open-access journal of pharmacy and pharmaceutical sciences
Formerly published as Marmara Pharmaceutical Journal

ONLINE SYMPOSIUM

APPLICATIONS OF MACHINE LEARNING FROM CONSTRUCTING THE DATABASE TO THE LEAD DISCOVERY: PRACTICAL APPROACHES ON CANCER-RELATED PROTEINS

Said MOSHAWIH[1*], Long Chaiu MING[1,2], Nurolaini KIFLI[1], Hui Poh GOH[1]

[1]PAP Rashidah Sa'adatul Bolkiah Institute of Health Sciences, Universiti Brunei Darussalam, Gadong, Brunei Darussalam
[2]School of Medical and Life Sciences, Sunway University, Sunway City 47500, Malaysia

saeedmomo@hotmail.com

*Presenting and corresponding author

Drug discovery using advanced computational tools such as machine learning has succeeded in reducing about 40% and 60% of the time and costs required by conventional drug discovery pipelines respectively. In this study we aim at building a combinatorial library of anthraquinone and chalcone derivative and producing a workflow of different screening and scoring methodologies to find hits against cancer-related proteins, and examine them using molecular dynamic and mechanics simulations. A combinatorial library, consisting of virtual compounds, was synthesized using 20 anthraquinone and 24 chalcone core structures via R-group enumeration methodology. The resulting compounds were optimized to the near drug-likeness properties and the physicochemical descriptors were calculated for all datasets and compared with commercially available databases such as FDA, Non-FDA, and natural products (NPs) datasets from ZINC 15. A workflow of a novel virtual screening and scoring methods was optimized based on the nature of the protein target. As a result; the optimized enumeration resulted in 1,610,268 compounds with NP-Likeness, and synthetic feasibility mean scores close to FDA, Non-FDA, and NPs datasets. The cheminformatic analysis illustrated an overlap between the chemical space of the generated library was more prominent with NPs with the lowest molecular diversity compared with other natural and synthetic drugs databases. Moreover, the consensus scoring methodology that we produced was based on quantitative structure-activity relationship, pharmacophore fitness, shape similarity, and docking scores. The optimized virtual screening for the protein targets was found to be beneficial in the retrospective enrichment studies, as it prioritized true positives in high percentage (ROC curve > 0.9). Compared to all other conventional screening methods individually, consensus scoring outperformed them. It was also found that this method of multistage virtual screening overcome challenges in the training set such as limited number of data

points and limited diversity of activity. In molecular mechanic simulations, the range of activity of the experimental datasets plays a crucial role in the nature of the correlation between experimental activity values and binding free energy obtained by MM/GBSA calculations. In conclusion, consensus scoring using z-score fusion method is a beneficial way of virtual screening especially when the training dataset is imbalanced.

REFERENCES

[1] Moshawih S, Goh HP, Kifli N, Idris AC, Yassin H, Kotra V, Goh KW, Liew KB, Ming LC. Synergy between machine learning and natural products cheminformatics: Application to the lead discovery of anthraquinone derivatives. Chem Biol Drug Des. 2022;100(2):185-217. [CrossRef]

[2] Moshawih S, Lim AF, Ardianto C, Goh KW, Kifli N, Goh HP, Jarrar Q, Ming LC. Target-Based Small Molecule Drug Discovery for Colorectal Cancer: A Review of Molecular Pathways and In Silico Studies. Biomolecules. 2022;12(7):878. [CrossRef]

[3] Moshawih S, Hadikhani P, Fatima A, Goh HP, Kifli N, Kotra V, Goh KW, Ming LC. Comparative analysis of an anthraquinone and chalcone derivatives-based virtual combinatorial library. A cheminformatics "proof-of-concept" study. J Mol Graph Model. 2022;117:108307. [CrossRef]