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 – Assistant Prof. Sneha Agrawal
  Bharati Vidyapeeth’s College of Pharmacy, Maharashtra, India
- Pharmacokinetics evaluation with SimCYP program – Assoc.Prof. Enkelejda Goci
  Aldent University, Tirana, Albania
- A new approach in drug discovery: Network pharmacology – Dr. Yajmur Diker
  Hacettepe University, Ankara, Turkey

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

- Computational identification of novel targets for drug candidate compounds – Assoc.Prof. Ceren Sucularli
  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

Chair
Prof. Halice Kübra ELÇIĞİL

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

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

ONLINE SYMPOSIUM
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Hepatitis C Virus (HCV) is a blood-borne RNA virus that causes inflammation of the liver that can lead to liver cirrhosis and hepatocellular carcinoma [1]. Non-structural protein 5B (NS5B) is an essential component of HCV for viral transcription and genome replication [2]. As there is no close mammalian analog for this enzyme, it has been the focus of many drug discovery projects [3]. In the present work, a combination of different computer-aided drug design approaches such as ensemble docking, binding free energy calculations, and quantitative structure-activity relationship (QSAR) model generation was applied to identify novel inhibitors of NS5B.

In the first step, all available protein structures in Protein Data Bank in a complex with thumb site 2 inhibitors were collected. Then, an automated KNIME [4] workflow was generated to select a few representative structures of the conformational changes in the binding pocket upon ligand binding. In total eight NS5B-inhibitor complexes were selected for further in silico work. Next, a virtual combinatorial library was obtained using the privileged substructures of known NS5B inhibitors. Different congeneric series of compounds including phenylalanine derivatives, thiophene-2-carboxylic acid derivatives, and anthranilic acid derivatives were used for the database formation. Upon ligand preparation, over 182,000 molecules were built. Consequently, known thumb site 2 inhibitors were docked with GLIDE-SP [5-7] and rescored with Prime MM-GBSA [8,9] protocol implemented in Schrödinger software to estimate the docking and binding free energy scores that will be used as a threshold for filtering the newly produced combinatorial library. In addition, categorical and numerical QSAR models were generated based on the known thumb site 2 inhibitors and used in the post-filtering step. Compounds that were predicted as actives will be visually analyzed and selected further for synthesis and biological evaluation.
Keywords: HCV, NS5B, ensemble docking, MM-GBSA, QSAR
REFERENCES


