BOTANY

Won Excelsior Award

Dr. R. Beema Shafreen

Unraveling the bioactive potential of pitaya against *Candida albicans* biofilm and human disease network using a Network pharmacology based approach

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Abstract

The identification of drug-target interaction and systematic screening is an important step in drug discovery research. It is experimentally difficult and cost-effective to screen all the possible interactions. Hence, computational-based approaches are used as an alternative strategy to study molecular interaction and their associated pathways. Therefore, Network-based approaches have been used as an important tool in drug discovery. A protein-protein (PPI) network has enabled the understanding of multi-protein at target level and immunomodulatory effects information and in the key signaling pathways. Network pharmacology has a major impact on studying the drug response in the context of the cellular or phenotypic network. It is always crucial to study the mechanism of action of compounds involved in different molecular pathways. The network-based approach is envisaged to provide supporting evidence for designing and performing the experiments. In the present study, bioactive molecules obtained from pitaya have antibiofilm activity against *Candida albicans* biofilm. The extract subjected to GC-MS has revealed 18 molecules. Among the compounds, N-methylfuran-2-carboxamide was present as the major peak area. Thus, molecular interaction and target prediction reveal effective role ligands that have shown interaction 92 genes. Specifically, the top hit was observed as muscarinic acetylcholine receptors (mAChRs) which mediate acetylcholine-induced neurotransmission. Apart from the functional analysis, it was observed that proteins were involved in two disease pathways Diabetes mellitus, type 2, susceptibility, and Schizophrenia. Therefore, it is envisaged that the consumption of pitaya will have the potential biological activity to prevent and overcome diseases such as type 2 diabetes and neurodegenerative disorders.

Keywords: PPI network, pitaya, network pharmacology, schizophrenia, neurodegenerative disease

Won Second Prize

Prisho Mariam Paul

Insilico docking analysis of FDA approved drugs against Human AKR1 protein binding site of SARS CoV-2 membrane protein

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Abstract

Severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) is responsible for an ongoing COVID-19 pandemic that has devastated mankind. The SARS-CoV-2 membrane protein plays a decisive role in the viral life cycle. In infected people, membrane protein impedes the conversion of testosterone from active form to its inactive form via its interaction with human Aldo-keto reductase family 1 member C2 protein. This leads to the high availability of active testosterone which in turn promotes the SARS-CoV-2 entry into the host cell. From the literature study find out the interaction site between membrane protein and Aldo-keto reductase family 1 member C2 protein. So targeting this conserved binding site with small drug-like molecules would inhibit the interaction which leads to inhibition of SARS-CoV-2 entry into the host cell. In this study we used several potential ligands which were FDA approved pharmaceuticals such as Hydroxychloroquine, Chloroquine, Favipiravir, Colchicine, Remdesivir, Nitazoxanide, Toremfene, Umifenovir were surveyed using PubChem database and its docking studies were done in order to get the best ligand. The docking simulations revealed that Chloroquine and Toremfene have high binding energy with SARS CoV 2 wild type and mutant E protein of SARS CoV 2 Omicron variant. This *insilico* data gives insights to test these high binding compounds in *invitro* studies to prove its efficacy and these pharmaceutical compounds are a potential alternative in the future for a novel drug development to treat several emerging variants of SARS CoV 2. **Keywords:Hydroxychloroquine, SARS CoV 2, Aldo-keto reductase**

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