Computational Pipeline and Method for Predicting Clinical Intervention Strategies for Complex Diseases

Identification of ideal drug candidates and understanding potential interactions of a therapeutic molecule with non-target entities is essential when developing an efficient therapeutic intervention strategy for various diseases. This is especially applicable in the case of complex diseases which cannot be attributed to a single, specific underlying reason but as a result from a combination of multiple environmental, genetic and lifestyle factors. Owing to this complex etiology, diagnosis and treatment of diseases such as Gulf War Illness (GWI) and Myalgic Encephalomyelitis (Chronic Fatigue Syndrome) is even more difficult. Considering these challenges, a computational pipeline that implements machine learning to identify drug target candidates can substantially enhance the efforts to develop an efficient therapy for complex diseases.

Technology

The proposed technology invented by Dr. Travis Craddock and Dr. Gordon Broderick involves a technique that applies computational science, applied mathematics and machine learning for more accurate prediction of clinical intervention strategies for complex diseases such as GWI. The invention allows for combining methods of understanding the interactions within and between cells, and across bodily systems, into a single integrative platform. Unlike more conventional drug target selection/ screening technologies, this AI-based method can identify potential interactions with non-target entities and thus reduce the chances of negative side effects resulting from non-specific influences of the therapeutic molecule. The ability of this computational platform to identify drug targets by cross-referencing with known pharmacogenomics databases makes it the ideal tool for selecting drug candidates for a multi-drug, multi-target-based therapy.

Application

- For predicting the appropriate clinical intervention strategy for complex diseases such as GWI and Chronic Fatigue Syndrome.
- For refining identified drug candidates by determining potential interactions with non-target entities so that side effects of the medication are minimized.

Advantages/Benefits

- This computational system will allow researchers to identify therapeutic molecules faster and more accurately than traditional methods of screening.
- Application of this machine learning can be utilized to construct models of regulatory networks based on known protein-protein interactions, resulting in more efficient prediction of treatment strategies for complex diseases such as GWI.

Status of Development

- Virtual docking was used to evaluate interaction of 43 FDA-approved therapeutic molecules with multiple structures of GCR, AR, IL-2 and TNF-alpha.
- This computational method has been applied to identify possible interactions between drugs used for GWI and those used for treating comorbidities such as hypertension or hyperlipidemia.

Patent Status – Provisional Patent Application filed on 29 May 2019.

Information on Inventors

Dr. Travis Craddock – Dr. Craddock, is an Associate Professor in the Department of Psychology & Neuroscience, Computer Science, and Clinical Immunology at NSU. Dr. Craddock also serves as the Director of the Clinical Systems Biology Group at Institute for Neuro-Immune Medicine.

Dr. Gordon Broderick – Dr. Broderick is the Director of the Center for Clinical Systems Biology at Rochester General Hospital Research Institute.

Contact

Gary Margules, Sc.D., Vice President of Research and Technology Transfer
margules@nova.edu

Arunodoy Sur, Ph.D., Technology Licensing Officer
asur@nova.edu • (954) 262-1022