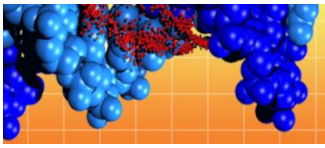

CENTER FOR BIOINFORMATICS & COMPUTATIONAL BIOLOGY

BIOINFORMATICS 2016 FALL SEMINAR SERIES

Hosted by: Department of Computer and Information Sciences,
Department of Electrical and Computer Engineering &
Center for Bioinformatics and Computational Biology
http://bioinformatics.udel.edu/Seminars/Current

MONDAY, November 28, 2016
3:30pm
DBI Room 102

A Network Visualization of Dinaciclib and its Interactions with Different Proteins and Target Kinases

Juan Paolo Sicat

PhD Student-Bioinformatics & Systems Biology

ABSTRACT: Presented is a network analysis of the effects of the experimental drug Dinaciclib primarily incorporating information found in the text mining result of the tool called DiMex. DiMex uses natural language process modules that processes abstracts and apply analysis to extract mutation-disease association. Different resources are then used to support the found associations and identify other interactions in the hopes to identify key biological effects of the drug. Cytoscape then provides the visual component of the analysis of the information. Aside from the analysis of Dinaciclib and its important biological relations the goal also is to compare the network created by the NLP tool and a human-curated network to understand how far NLP tools have come.

The Evolution of Biological Electron Transfer: Conservation of Sequence Determinants of the Reduction Potential in Bacterial Ferredoxins

Mike Fajardo

PhD Student-Bioinformatics & Systems Biology

ABSTRACT: The diminutive electron maintains a role of endless importance for all life on earth. Chemical and radiant energy sources allow organisms to acquire much needed energy, converting harnessed energy to work utilizing schemes dependent on the transfer of electrons through electron transport chains. These electron transport chains employ oxidation-reduction (redox) proteins to mediate the transfer of electrons with high efficiency. Often a metallic cofactor plays a central role in this transfer. The aqueous environment of the cofactor, the overall protein fold, and the amino acid composition of the surrounding protein all affect the electrostatic interactions and potentially the efficiency of electron transfer. Here, we examine the evolution of electron transfer through an analysis of the 2[4Fe-4S] bacterial ferredoxin; a common non-membrane bound electron transfer protein. An analysis of over 700 ferredoxin sequences from green & purple bacteria and cyanobacteria revealed seven possible ferredoxin clades. Each clade is unique in the identity and position of charged and polar residues that may play a role in the transfer of electrons. Additionally, using x-ray crystal structures of four distinct ferredoxin proteins, we were able to identify a simple method for a first pass prediction of possible sequence determinants of the reduction potential