Subject: FW: Dissertation Defense - Sarah Altalhi , PHD Bioinformatics & Computational Biology
Date: Friday, July 5, 2024 at 1:23:09 PM Eastern Daylight Time
From: SSB Faculty List on behalf of Diane St. Germain
To: SSB-FACULTY-LIST-L@LISTSERV.GMU.EDU

Dissertation Defense Announcement
To: The George Mason University community
Candidate: Sarah Altalhi
Program: PhD Bioinformatics & Computational Biology

Date: Monday, July 22, 2024

Time: 10:00 AM Eastern Time (US and Canada)

Location: Via Zoom
All are invited to attend the defense.

Join Zoom Meeting
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Committee Chair: Dr. M. Saleet Jafri
Committee Members: Dr. Iosif Vaisman and Dr. Dmitri Klimov

Title: "Computational Analysis of T-Lymphocyte Activation by Peptide Antigen"

Abstract:
The major histocompatibility complex (MHC) molecules are critical to the immune response because they recognize and differentiate between foreign antigens and host proteins. MHC Class I, found on the surface of most human cells and MHC Class II are found on antigen presenting cells which are a type of phagocyte MHC Class I, is restricted to macrophages and lymphocytes. MHC molecules play an important role in the demonstration of foreign antigens and play an important role the activation of T cells and are therefore a significant mechanism of adaptive immunity. Antigen Present Cells (APCs) do not present all likely epitopes to T cells but instead focus on only a range of the foremost antigenic or immunodominant epitopes. The idea behind this research work is to calculate physiochemical and structural properties of antigenic epitopes and to simulate receptor of MHC-II and antigenic peptides to understand the binding mechanism and their biological response in developing the vaccine. Replica exchange molecular dynamics (REMD) simulations produced conformational ensembles of protein structure of the epitope in immunogenic and non-immunogenic response. Obtained simulations output were inspected by machine learning approach based in MDPPM methods. Machine learning empowers a set of rules to examine further bundles of information by rapidly outcome key ingredients that distinct each variable for molecular dynamics as of the absolute volume of data produced during apiece simulation. Finally, using VMD dihedral angles of the protein backbone are to be retrieved for the different conformational change with the trajectories is analyzed different dynamics in the prediction model. The complete mean structural discoveries by taking raw torsional angles values and their trajectories have been classified with regards to antigenicity using MDPPM. This approach is advantageous for enumerating minor changes in the protein with respect to other methods and may have error. From the cluster we learn how global structural changes and the phi-psi backbone and other simulation data within the protein on the principal component data to evaluate immunogenic/ non-immunogenic response and accuracy.

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