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Biological Systems: Open Access

Editor Note

Editorial Note on Immune System Modeling Combines Cellular Function with Structural Plasticity to Model Mhc I And Antigen Selection

Alekhya Thirunahari*

Department of Biotechnology, Osmania University, Telangana, India

EDITORIAL

The control of the immune system plays a key role in both healthy and diseased states and the presentation of peptides at the surface of most nucleated cells by major histocompatibility complex class I molecules (MHC I) is crucial for eliciting or evading an immune response.

Understanding the selection process is critical for the production of therapies such as vaccines that rely on the selection of particular peptides, as the pool of surface presented peptides only represents a limited sample of all available peptides. The peptide selection process is mediated primarily by a weakly interacting multi-protein peptide loading complex..

which regulates MHC class I conformation (PLC). To gain a better understanding of the mechanisms of peptide selection by MHC I, we created computational systems models encoding different mechanistic hypotheses of PLC action. We were able to infer that the system is under kinetic control and that a conformational intermediate of MHC I is essential for peptide selection using in vivo biochemical data.

We use a combination of X-ray, NMR, and biophysical techniques, as well as molecular dynamics simulations, to investigate the molecular determinants of peptide selection. We show that peptide selector function correlates with protein plasticity rather than structure using this method.
This was then tested in vivo in an experimental setting and applied to the PLC resident chaperone tapasin. We discovered a previously undetected link between protein plasticity and MHC I's in vivo peptide selector feature using a combination of computational systems models, in-cell biochemical evidence, and structural methods, with implications for host protection and immunotheraphy.

***Correspondence to:** Alekhya Thirunahari, MSc, Department of Biotechnology, Osmania University, Telangana, India, E-mail: thirunaharialekhya151315@gmail.com

Received date: 5 March, 2020; **Accepted:** 15 March, 2021; **Published:** 31 March, 2021

Citation: Thirunahari, A (2021) Editorial Note on Effect of Shapes, Binders and Densities of Faecal Matter. J Biol Syst Open Access 10: 193.