In Silico Modeling of PICK1 Protein Dynamics and Interactions: Pathway to Peptide-based Therapies for Substance Use Disorders

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Substance use disorder, a persistent societal problem not only in New Mexico but also on a wider global scale, may find a hopeful resolution in the novel scaffolding protein known as Protein Interacting with CKinase-1 (PICK1). PICK1 plays a significant role in the realm of drug addiction, as suggested by experimental evidence that interference with PICK1-DAT (Dopamine Transporter) interactions can attenuate the behavioral effects of cocaine in animal models. While we have made considerable progress in understanding PICK1's role in addiction, developing a drug that can effectively inhibit PICK1 remains adaunting task. This is primarily due to the protein's dynamic nature and complex structural characteristics. Our research team employs a diverse array of computational tools to delve deeper into the key residues and physical interactions that govern PICK1's structural, dynamic, and mechanical properties, all of which are highly relevant to its biological function. Acquiring such comprehensive information will enable us to design synthetic peptides that specifically target PICK1. These peptides, in turn, hold the potential to form the foundation of innovative treatments for substance use disorders.

Bell Hall 143

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(Also available remotely: https://utep-edu.zoom.us/j/84398694840)