Breaking Barriers in Drug Discovery: The Fusion of Atomistic Simulation and Machine Learning in Computational Biophysics

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Abstract

In recent years, the field of drug design has undergone a remarkable transformation due to advancements in computer hardware and algorithms. This talk will explore how computational biophysics tools are driving this revolution, ultimately accelerating therapeutic discovery. The presentation will commence with an introduction to various computational biophysics tools utilized in drug design, providing attendees with a comprehensive understanding of the technological landscape shaping the field. Following this, specific examples will be presented to illustrate the profound impact of techniques such as molecular dynamics and enhanced sampling coupled with machine learning in drug design. These examples will highlight the unprecedented insights and efficiencies gained through the integration of computational methods into the drug discovery process. Drawing from my research group experiences, the talk will delve into the entire drug design pipeline, spanning from target identification to lead optimization and clinical trials. Research findings will be shared, elucidating key insights and successes achieved through the application of computational techniques. Lastly, the presentation will conclude with a discussion on the broader societal implications of employing these innovative approaches. By leveraging computational biophysics tools, we have the potential to address pressing societal challenges and advance the development of novel therapeutics, ultimately improving human health and well-being.