INSTITUTE for COMPUTATIONAL MEDICINE

Distinguished Seminar Series Fall 2024

Artificial Intelligence Tools for Antibody Engineering and Protein Docking

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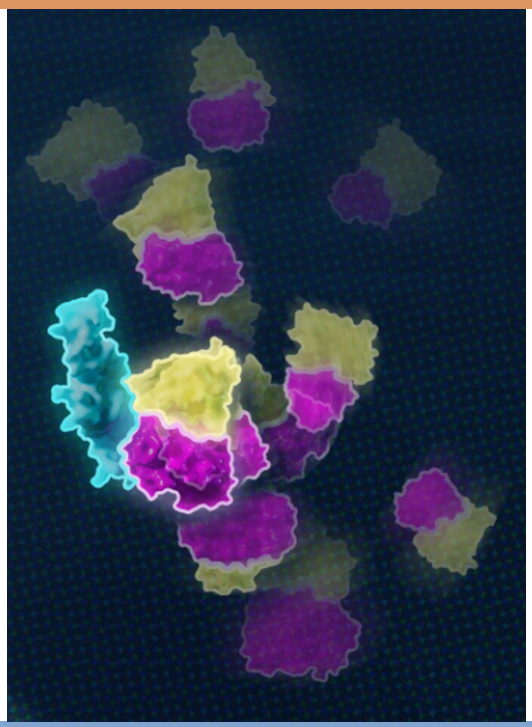

In a blind prediction challenge in 2020, AlphaFold2 calculated highly accurate three-dimensional structures of hundreds of proteins from their sequences, thus "solving…one of the biggest problems in biology".1 This achievement and others based on artificial intelligence (AI) algorithms have unlocked incredible possibilities for biomolecular engineering. In this talk, I will share advances from my lab in antibody engineering and protein-protein docking based on AI. Our neural network models (CNNs and multi-track transformer networks) outperform physical models for antibody structure prediction. Generative language models offer multiple promising routes for design of antibody therapeutics, and they produce repertoire distributions different than those produced with heuristic, gene-recombination and somatic-mutation models. Docking methods reveal biological mechanisms and allow for screening of potential therapeutics. I will use the docking case to show how AI methods differ from physics-based approaches, suggesting ways to benefit from their combination.

Tuesday, October 1, 2024 @ 4:00PM ET in Clark 110

Live Webcast: https://wse.zoom.us/j/92636200923

Faculty Host: Dr. Joel Bader

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