ChemE MIT Chemical Engineering

Seminar Series
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Accelerating Protein Engineering with Artificial Intelligence

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66-110

Proteins are central to health, sustainability, and chemical synthesis, yet engineering them for specific functions is challenging due to the vastness of the sequence design space. Directed evolution, inspired by natural evolution, has enabled remarkable advances but is slow and limited to local optimization. In this talk, I present my research on integrating machine learning with experimental workflows to overcome key bottlenecks of directed evolution. First, I introduce Active Learning-Assisted Directed Evolution (ALDE), which leverages Bayesian optimization to enable efficient and rapid protein fitness optimization. Next, I discuss Contrastive Reaction-Enzyme Pretraining (CREEP), a retrieval model for discovering enzymes with new-to-nature functions. Finally, I present emerging generative approaches to unify these two perspectives, to enable holistic data-driven protein engineering. Together, these innovations point toward a future where AI-driven strategies can automate biomolecular engineering: unlocking sustainable synthesis, novel therapeutics, and programmable biology at the molecular scale.

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