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(I) Learning from Life: Understanding and Design of Complex Biophysical Systems through Multiscale Modeling and Machine Learning

Monday 6 June 2022 16:00 (30 minutes)

In recent years, the drug discovery industry has seen a steady decline in productivity due partially to the difficulty in rationally designing and exploring novel search spaces. At the same time, cutting-edge deep learning techniques offer the possibility of rapidly enhancing design of novel biomolecules, but suffer from a lack of interpretability. By employing physics-based techniques, including multi-scale molecular dynamics and manifold theory, my lab group hopes to engage with these problems to perform physics-based design of novel search spaces for therapeutics. In this talk, I will discuss our initial attempts to design an interpretable search space for (i) small molecule antibiotics, and (ii) short peptides. We focus on assessing search space quality and on the characterization through molecular dynamics of potential initial design points. I will also discuss our future work in creating an integrated and transferable platform for search space design.

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