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Modeling of immune recognition and protein complexes with deep learning and physics-based docking

Friday, 16 February 2024 11:00 (30 minutes)

The Pierce group has utilized a combination of AlphaFold and traditional docking methods, including Rosetta and ZDOCK, to model protein complexes in recent CAPRI and CASP/CAPRI rounds. This has led to success for several challenging targets, as well as useful lessons learned for prospective modeling efforts. Our group has been particularly focused on the utilization and adaptation of AlphaFold and other deep learning methods for accurate modeling of immune recognition, including antibodies and T cell receptors. We recently reported a comprehensive benchmarking of AlphaFold for its performance on a large set of antibody-protein antigen complexes, and have also been testing its performance for antibody-peptide complexes. Additionally, we adapted AlphaFold to predict T cell receptor complexes with peptide-MHC targets, which is available to the public as the TCRmodel2 web server.

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