EpiGraph: Recommender-Style Graph Neural Networks for Highly Accurate Prediction of Conformational B-Cell Epitopes

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Abstract

The accurate identification of B-cell epitopes is crucial to the development of antibodies and biologics, but traditional experimental methods for epitope identification are time-consuming and resource-intensive. While robust methods exist for the prediction of T-cell epitopes in silico using machine learning, reliable in silico

approaches have yet to be developed for the prediction of B-cell epitopes, due largely to their conformational complexity and the sparsity of publicly available structural data. In this work, we demonstrate both in silico and via in vitro lab assays that recommender-style graph neural networks trained on all publicly available structures of antibody-antigen complexes achieve state-of-the-art predictive performance for conformational epitopes on both known and novel antigens. Our method EpiGraph is broadly applicable to any B-cell epitope prediction task, and to the best of our knowledge, is the first to be experimentally validated on antibody-antigen complexes for which no experimental structures are publicly available.