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Antipasti: Interpretable Prediction of Antibody Binding Affinity Exploiting Normal Modes and Deep Learning

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The high binding affinity of antibodies toward their cognate targets is key to eliciting effective immune responses, as well as to the use of antibodies as research and therapeutic tools. Here, we propose ANTIPASTI, a convolutional neural network model that achieves state-of-the-art performance in the prediction of antibody binding affinity using as input a representation of antibody-antigen structures in terms of normal mode correlation maps derived from elastic network models. This representations are interpretable: they reveal similarities of binding patterns among antibodies targeting the same antigen type, and can be used to quantify the importance of antibody regions contributing to binding affinity. Our results show the importance of the antigen imprint in the normal mode landscape, and the dominance of cooperative effects and long-range correlations between antibody regions to determine binding affinity.