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High Accuracy Antibody-Antigen Complex Structure Prediction with Epitope Information

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The accurate prediction of antigen-antibody complexes is crucial for the design of de novo antibodies and the analysis of antibody functions. However, traditional deep learning-based methods often struggle to predict high-quality antigen-antibody complex structures due to the lack of co-evolutionary data between antigens and antibodies, as well as the complexities introduced by loop-mediated interactions. In this study, we present RF-AbAg, a novel unbound docking tool for antigen-antibody interactions that incorporates epitope information to improve the prediction of antigen-antibody complexes. RF-AbAg is a fine-tuned version of RoseTTAFold, enriched with loop-mediated protein-protein interaction (PPI) data and antigen-antibody complex structures. This enables RF-AbAg to predict antigen-antibody complex structures using the individual structures of antigens and antibodies. RF-AbAg outperforms traditional docking methods and other deep learning-based models. By incorporating an additional epitope scanning algorithm, RF-AbAg is capable of predicting antigen-antibody complexes without relying on experimental epitope data, further demonstrating its utility in antibody research and development.

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