

Learning Antibody-Specific Epitopes with Domain-Specialized Language Model Embeddings

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Accurate epitope prediction requires modeling antibody specificity in addition to antigen context. Existing protein language model-based approaches largely treat epitopes as antigen-only properties, limiting antibody awareness. This work introduces a graph-based, residue-level framework that conditions predictions on paired antibody–antigen inputs by fusing domain-specialized and general-purpose embeddings. Antibody sequences are encoded with Ablang2, trained on clustered antibody repertoires, while antigens are encoded with ESM-2. The resulting representations are lifted to graphs and integrated via cross-attention to capture interaction-aware features. Training data are derived from SAbDab with contact-based residue labels under leakage-controlled, antigen-cluster splits. The evaluation design comprises ablations of the antibody encoder and attention modules and comparisons to antigen-only baselines under identical graph heads, targeting robust, antibody-aware epitope scoring.