IntelliBind: A Novel Deep-Learning Framework for High-Affinity Antibody Design

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The development of therapeutic antibodies with high binding affinities is essential for various in vivo applications, including passive immunization, antigen-presence diagnostics, and cancer treatment. However, conventional techniques for designing high-affinity antibodies require time-consuming and expensive procedures, along with specialized equipment and extensive experimentation. To address these challenges, I introduce IntelliBind, a deep-learning workflow for generating affinity-optimized antibody amino acid (AA) sequences from low-affinity antibodies. IntelliBind uses an encoder-decoder framework with gated recurrent units (GRU) and an attention mechanism to analyze 3D protein structures and fine-tune specific amino acids in the initial antibody AA sequences. The model is trained on a diverse range of antibodies—as opposed to a single type—utilizing UniProt and PDB protein data. Systematic evaluation shows that IntelliBind successfully generates antibody sequences with binding affinities up to 10-fold or 1000% stronger than their low-affinity counterparts, as indicated by the equilibrium dissociation constant (KD). The highly specific AA sequences produced by IntelliBind can bind with robust affinity to their target antigens, giving them the potential to reduce antibody production costs and enhance their use in clinical settings for therapeutics against infectious diseases.