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Perspective

# Structural Basis of Flexible Peptide Sequence by an Antibody

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## DESCRIPTION

Antibodies have a high specificity and affinity for recognizing various types of antigens, and peptide is one of their primary targets. Understanding the molecular recognition mechanism of an antibody for peptide is critical for developing clones with higher specificity and affinity. Such intra molecular hydrogen bonds limit peptide fluctuation and reduce conformational entropy, resulting in destabilization of the unbound state and increased binding affinity *via* free energy change. Antibodies have a high specificity and affinity for a wide range of antigens, including proteins, peptides, sugar chains, nucleic acids, and small molecules. This property makes antibodies appealing as a therapeutic and diagnostic agent.

To target different antigens, antibodies use six loops known as Complementarity Determining Regions (CDRs) that form a surface structure that is complementary to the target antigen's structure. Several non-covalent bonds are formed between an antibody and its antigen in this manner, stabilizing the complex structure. Hydrogen bonds, interactions, electrostatic interactions, and a hydrophobic effect are examples of non-covalent interactions.

Peptides are one of the most commonly recognized targets by antibodies. Despite its popularity, a complete understanding of the binding mechanism between antibodies and flexible peptide antigens remains elusive. Peptides, in general, are less structured in solution due to the lack of intense intra molecular interactions, and this flexibility makes structural evaluation difficult.

From a thermodynamic standpoint, the formation of the antibody-peptide complex fixes the peptide conformation results in an unfavourable contribution of conformational entropic change, inducing the formation of several non-covalent bonds between the antibody. Furthermore; hydration has a significant impact on enthalpic and entropic contributions. As a result, determining the source of the favourable free energy change is extremely difficult. A thorough understanding of the binding mechanism of anti-peptide antibodies will be useful in future antibody design. Currently, despite numerous design efforts, it is extremely difficult to create an antibody for specific target antigens.

One reason for the difficulty comes from the dynamic and flexible nature of CDR rings and their target structure. For this reason, the accumulation of experimental information is crucial for a successful design. Similarities can be found in the importance of preformed and retained conformation for stability in the protein folding domain. For example, structural stress by backbone cycling is a popular technique for stabilizing proteins. The backbone cycle limits the fluctuations of the polypeptide in the unopened state, which corresponds to the unbound state in the peptide-antibody reaction, and reduces its structural entropy (destabilization of the state) and folded (stability of the folded structure by the instability of the unfolded structure). These comprehensive analyses of complex formation between the flexible peptide and the antibody fragment reveal the important role of preformed intra molecular hydrogen bonding in molecular recognition. Recently, it has become clear that all or part of many eukaryotic proteins have a long unstructured polypeptide region known as Intrinsically Disordered Protein (IDP). It has been suggested that some IDPs are structured after binding to their target. Understanding the molecular mechanism of the antibody's flexible peptide recognition process could provide important insights into how IDPs can be recognized and transformed into a given conformation.

## CONCLUSION

There is a great interest in neuro protective molecules that inhibit signaling, conduction and amplification of inflammatory and oxidative pathways to reverse or prevent brain cell damage and neuro degeneration. Peptides derived from dietary protein represent a potential natural source for this action. Although several food sources and amino acid sequences have shown promising effects, the mechanism of action on brain cells is not fully understood. Dietary peptides must resist digestion and be absorbed across the digestive and brain barriers. The intact form or its metabolites must reach the brain tissue to be effective at the cellular level.

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