Advances in drug discovery on the biofunctionalities of bioactive peptides: The role that molecular docking plays in targeted therapy development

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Abstract:

Biofunctionalities of bioactive peptides (BAPs) are sequences of 3 to 40 amino acid residues in length. These proteins, which have similar properties to those of endogenous peptide hormones, are derived from parental polypeptide sequences through controlled and specific proteolytic cleavages. In the first half of the 20th century, BAPs fundamental to medicine were discovered, such as insulin, regarded as one of the largest scientific achievements in drug discovery for its impact on the treatment of diabetes. Novel tools are expeditiously being used to screen and target BAPs chain-based drug candidates. Molecular docking has drawn attention since its fundamental theoretical simulation capabilities in computational chemistry. It is a core method in drug research for testing how BAPs and target proteins can interact with small molecules. The algorithms simulate binding affinities to identify potential candidates, optimizing their specificity, which is essential for therapeutic safety and efficacy. Better scoring methods and their integration with structural biology not only streamline the process, but also progress the comprehension of protein-peptide relationships and aid in the discovery of more targeted and effective drugs. The review seeks assess the scope of this field and underline the crucial role that proteins play in the drug's discovery and development.

Keywords: Proteins; Peptides; Biofunctionalities; Molecular docking; Drug discovery; Drug development.