TRANSITION METAL COMPLEXES AS OPTICAL PROBES FOR DETECTING STRUCTURAL CHANGES IN PEPTIDES AND PROTEINS: SPECTRAL CHARACTERIZATION AND THEIR SUPRAMOLECULAR INTERACTIONS

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Proteins are inherently dynamic, flexible molecules that execute precise conformational changes to perform their functions. However, current techniques for directly measuring relevant structural changes in solution remain limited. Here, we demonstrate the use of transition metals, such as Fe(II) or Cu(II), and their complexes as optical probes for the peptide and protein structural changes due to their ability to exhibit a wide range of spectral properties upon coordination with biomolecules. In recent studies, inherently CD-silent Fe(II) clathrochelates have been shown to give a strong CD output (induced CD (ICD) signals) in the presence of globular proteins, suggesting their potential as ICD-reporter properties for probing the spatial structure of macromolecules of a wide range of globular proteins and their structural alterations [1-2]. In addition, the CD analysis of the metalloproteinase domain's structure has revealed that the substitution of Zn(II) with Cu(II) in the metal-binding domain can lead to the formation of an unusual left-handed polyproline II (PPII) structure. The PPII helix is a relatively rare conformation in proteins and plays a crucial role in conformational changes leading to the formation of amyloid fibrils by the prion protein or amyloidogenic lysozyme. It is noteworthy that only the substitution of a metal ion from Zn(II) to Cu(II) in the metal-binding domain led to the adoption of the PPII structure [3]. Taken together, those findings highlight the importance of transition metals in detecting structural changes in peptides and proteins. The spectral properties of transition metal complexes, such as Cu(II)-PPII structures and Fe(II)-clathrochelate-biomolecules, provide valuable information on the supramolecular interactions of biomolecules and can help identify potential drug targets.

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