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Complex Formation in the ATP - Curcumin System in the Presence of Mg^{2+} and Ca^{2+} Ions

Interactions between nucleotides, biologically active polyphenols, and metal ions play an important role in biochemical processes and molecular recognition in living systems. Adenosine triphosphate (ATP) is a key molecule involved in cellular energy metabolism, while curcumin, a natural polyphenolic compound derived from *Curcuma longa*, exhibits pronounced antioxidant, anti-inflammatory, and anticancer activity. Divalent metal ions such as Mg^{2+} and Ca^{2+} are essential cofactors in many enzymatic reactions and may significantly affect intermolecular interactions in aqueous solutions.

In this work, the mechanisms of heteroassociation between ATP, curcumin, and metal ions were investigated using fluorescence spectroscopy. Fluorescence emission and excitation spectra of aqueous ATP solutions were recorded at different temperatures (293–313 K) in the absence and presence of curcumin as well as Mg^{2+} and Ca^{2+} ions. The addition of curcumin to ATP solutions resulted in pronounced quenching of ATP fluorescence, indicating the formation of ATP–curcumin complexes.

Analysis of Stern–Volmer plots showed large quenching constants ($K_q \approx 10^{12} \text{ M}^{-1} \text{ s}^{-1}$), which exceed the diffusion-controlled limit and therefore indicate a static quenching mechanism associated with complex formation. Binding parameters obtained from Hill analysis suggest the presence of approximately one binding site in the ATP–curcumin system.

The presence of Mg^{2+} and Ca^{2+} ions noticeably modifies the interaction between ATP and curcumin. Both ions promote the formation of heteroassociates, which is reflected in changes of Stern–Volmer constants, binding parameters, and thermodynamic characteristics. Thermodynamic analysis revealed negative Gibbs free energy values, confirming the spontaneous nature of the complexation process.

Overall, the results demonstrate that ATP, curcumin, and divalent metal ions form stable heteroassociates in aqueous solution. The formation of these complexes is governed by a combination of electrostatic interactions, coordination effects of metal ions, and molecular association processes. These findings provide new insight into nucleotide–polyphenol interactions in the presence of biologically relevant metal ions and may be important for understanding their behavior in biochemical systems.

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