Structural Characterization of Functionalized β-Cyclodestrins

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β-Cyclodextrins (β-CD) have received considerable attention for their suitability to serve as relatively low molecular weight models for drug delivery and for artificial enzymes. In fact, β-CD shows remarkable ability to form inclusion complexes with various natural and synthetic molecules that fit inside the β-CD cavity. The inclusion process is influenced by the interaction between the guest molecules and the cavity, and also by the shape and size of the guest. This process can change the chemical and physical properties of the guest. In particular, pharmacological properties, such as stability, solubility, and toxicity, can be improved. Then, the rational design of functionalized β-CDs with bioactive moieties can represent an important step for the development of new drugs.

In this work, we report a detailed conformational analysis at atomic resolution by x-ray diffraction data and computational techniques on several functionalized β-CDs to understand the structural requirement to modulate the binding properties and basic phenomena governing the inclusion process for β-CDs.

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