Baicalin/sulfobutylether-β-cyclodextrin inclusion complexes for advanced drug delivery applications: a physico-chemical characterization through spectroscopic and computational methods

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Supramolecular compounds based on modified cyclodextrins represent an attractive strategy for the engineering of bio-compatible host-guest inclusion complexes capable to improve the chemical/physical properties of pharmaceutical agents both in solution and in solid state. In this context, investigation aimed at assessing the nature of the intermolecular interactions existing between a specific carrier and pharmacologically active compounds provide useful notions including the binding affinity, structure, kinetics, and thermodynamics of the resulting supramolecular assembly, furnishing insights for the definition of optimized procedures capable to provide safe high-performance drug-delivery systems with enhanced therapeutic outcomes. Here, the physico-chemical characterization of a novel type of inclusion complex based on sulfobutylether β-cyclodextrins (SBE-β-CD), used as hosting agent, and baicalin (BA), a pharmacologically active agents of great interest for its antimicrobial activity, is presented. In particular, a combined approach involving μ-Raman spectroscopy, Fourier-transform infrared spectroscopy in attenuated total reflectance geometry (FTIR-ATR) and X-Ray Diffraction (XRD), was employed to shed light into the nature of the intermolecular interactions existing between investigated components, starting from the analysis of the spectral changes induced by the complexation process on characteristic vibrational bands/diffraction peaks of both BA and macrocycle. Moreover, to deeply explore the inclusion geometry, experimental data were accompanied by *molecular docking* simulations, which evidenced how BA can be included within the SBE-β-CD cavity in all energetically favourable orientations. It is worth noting that the proposed approach not only provides useful insights for the development of next-generation drug-carriers but also furnishes a detailed scenario of the structural/dynamical behaviour exhibited by supramolecular materials of particular therapeutic interest.