

Molecular salts of urocanic acid and L-histidine

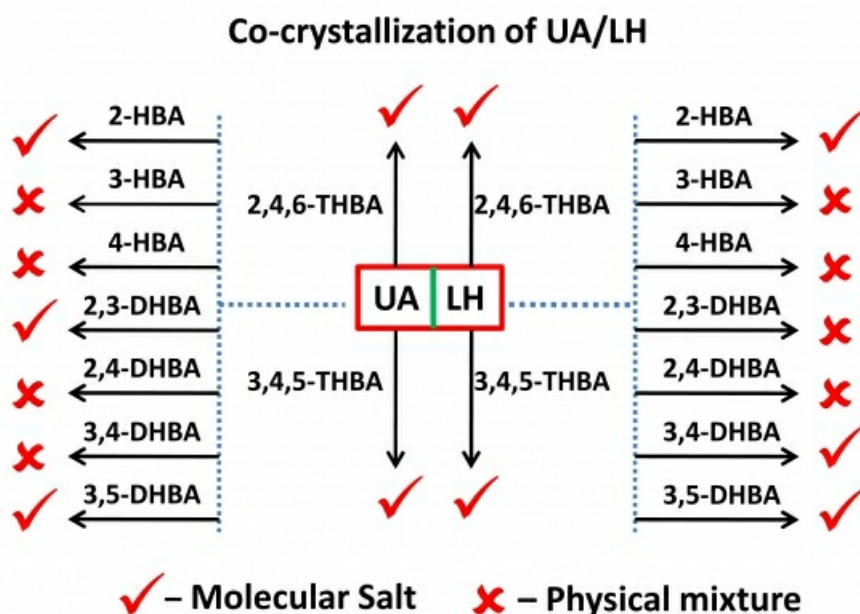
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Urocanic acid (UA), an intermediate of L-Histidine (LH) catabolism, is a natural sunscreen and photoprotectant against UV-B induced DNA damage. UA exists as a hydrated zwitterion in the crystalline state, unlike its precursor L-Histidine which is an anhydrate, and interestingly, no multi-component crystal forms of UA are reported. In our endeavour to understand the subtle factors that govern the co-crystallization behavior of structurally related molecules, UA and LH have been selected for extensive co-crystallization studies with hydroxybenzoic acids. It is noteworthy that UA prefers to form anhydrous molecular salts while LH results in salts which are hydrated! Based on the single crystal structural analysis it has been clearly illustrated that the presence of an additional amine group in LH which anticipates an auxiliary hydrogen bond for a stable supramolecular assembly, a moiety like water which hydrates the compound would be preferred. In this context, the role of ortho-hydroxy group and symmetrically substituted hydroxy groups in the formation and/or non-formation (in certain cases) of UA and LH molecular salts is analysed. In addition, we also report the first ever guest-free (anhydrous form) structure of native UA and studied its hydration/dehydration property. The formation of anhydrous salts in hydrated UA and hydrated salts in anhydrous LH have been explored.

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