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Unveiling the Aggregation Patterns of Curcumin and Piperine Mixtures in different Polar Media: A Molecular Dynamics Investigation

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Curcumin, a natural yellow pigment derived from the rhizome of turmeric (Curcuma longa L.), possesses significant biological properties. Nonetheless, its therapeutic potential is hindered by its limited bioavailability.[1] To address this challenge, and thus enhance the bioavailability and pharmacological efficacy of curcumin, one proposed strategy is the co-administration of curcumin with piperine, a bioactive compound of black pepper (Piper nigrum L.).[2] Regardless of the extensive scientific research that has been conducted on the curcumin and piperine systems, it is still clear the lack of knowledge at the molecular level of these compounds behavior in solution.[3] In this study, by employing molecular dynamics (MD) simulations, we intend to contribute to a better understanding of the aggregation patterns of curcumin (both enol and keto tautomers) and piperine in water, ethanol, and water-ethanol mixture. In particular, we investigated the influence of piperine on the self-aggregation of curcumin, while analyzing the structural characteristics of the resulting aggregates. For the characterization of the formed aggregates, a range of properties were calculated, such as: radial distribution functions; distances between molecules or atoms; interaction energies and the number of hydrogen bonds; clustering analysis. In the MD simulations involving two solute molecules a rapid formation of curcumin dimers in water was observed, as a result of its low solubility, while piperine formed less stable dimers. In contrast, both curcumin and piperine showed limited ability to form dimers in the presence of ethanol. Larger and more complex aggregates were obtained when additional solute molecules were introduced in water solutions, characterized by stacked or cage-like structures.

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