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Insights: Publications

The role of the asymmetric bolaamphiphilic character of VECAR on the kinetic and structural aspects of its self-assembly: A molecular dynamics simulation study

Colloids and Surfaces A: Physicochemical and Engineer Aspects 523, 9-18

June 20, 2017

VECAR are novel bolaamphiphilic molecules consisting of two hydrophilic molecular groups, a carnosine derivative and a chromanol group, covalently linked by a hydrophobic alkyl spacer of varying length. Despite the potential for application in various biomedical applications VECAR properties, including their bulk properties, are still largely unknown. The early stage of the self-assembly process of VECAR molecules in water is studied using molecular dynamics simulations. The study reveals that the length of the hydrophobic spacer in VECAR affects the aggregation kinetics as well as the size, shape, density, and atomistic structure of the self-assembled aggregates. A mechanism based on cooperative interactions between water, the hydrophilic hydroxyl group, and the hydrophobic benzene ring of the chromanol head is proposed to explain the ordered packings of chromanols in the self-assembled aggregate structures at the aggregate-water interface.