8th liquid matter conference

Wien, Austria
September 6 - 10, 2011

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Schönbrunn Castle: Star Pool

LMC8 is jointly organized by

European Physical Society — Liquids Section of the Condensed Matter Division

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Structure and mechanism of formation of bile salt micelles from molecular dynamics simulations

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Bile salts (BS) play a key role in the absorption of fats and fat soluble nutrients by intestinal cells: they form dietary mixed micelles (DMMs) into which these nutrients are solubilized, transported near the intestinal cell wall and then released. The molecular scale mechanisms associated with these processes are still unclear, and to study them we require coarse-grained (CG) models of each of the components of DMMs. Bile salts are among the least studied DMM components and have atypical structure for surfactants (concave steroid ring group with hydrophilic and hydrophobic faces, attached to which is a short and flexible tail), so we focus on them. Here report our simulation study of the structure and mechanism of formation of micelles of pure di- or trihydroxy (2OH; 3OH) BSs at physiological bile salt and NaCl concentration, using a CG model of these molecules. Grand-canonical parallel tempering simulations ensure adequate sampling of equilibrium static properties. Our results agree with reported experiments and point to the origin and biological significance of the bile salts' unusual surfactant properties. The micelle size distribution shows the typical qualitative surfactant behavior, but dimers and trimers are abundant even far from the critical micellar concentration (CMC), the peak of the distribution is broad and a shallow minimum separates micelles from monomers. These observations indicate that BSs are poorly cooperative micelle formers and that the free energy barrier to disassembly is low. The bile salts' high CMC and low micelle stability mean DMMs may rapidly aggregate and then easily release nutrients near the intestinal wall. The interior of bile micelles is rich in hydrophilic groups, and molecules may pack in many different orientations in the micelle. These features may reduce the incidence of undesired smectic phases in the intestine and may facilitate formation of micelles with nutrients with diverse shapes, sizes and hydrophilicity.