

Abstract Submitted
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Investigating bile salt aggregation using coarse-grained molecular dynamics simulations ANA VILA VERDE, AMOLF Institute, Amsterdam, Netherlands and Department of Physics, University of Minho, Portugal, DAAN FRENKEL, Department of Chemistry, University of Cambridge, Cambridge, UK — Bile salts are necessary for fat digestion due to their unusual surfactant properties: they assemble into small, polydisperse micelles and easily form mixed micelles with poorly soluble amphiphiles. Understanding these properties requires molecular scale information about bile salt micelles, something challenging to obtain experimentally but amenable to computational modeling. To address this issue we build a coarse-grained model of bile salts. We investigate their aggregation behavior through molecular dynamics simulations in a grand-canonical parallel tempering scheme. We validate our model against available solubility and light scattering data. Our results indicate that at physiological bile salt and counter ion concentrations, bile salts pack in many different orientations in pure bile micelles, contrary to standard surfactants. This feature may be physiologically relevant, allowing bile salts to solubilize the heterogeneous blends of fats typical of digestion.

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