Investigation of the aggregation behavior of Sodium Caprate by Coarse-Grained MD simulations and Small-angle Scattering

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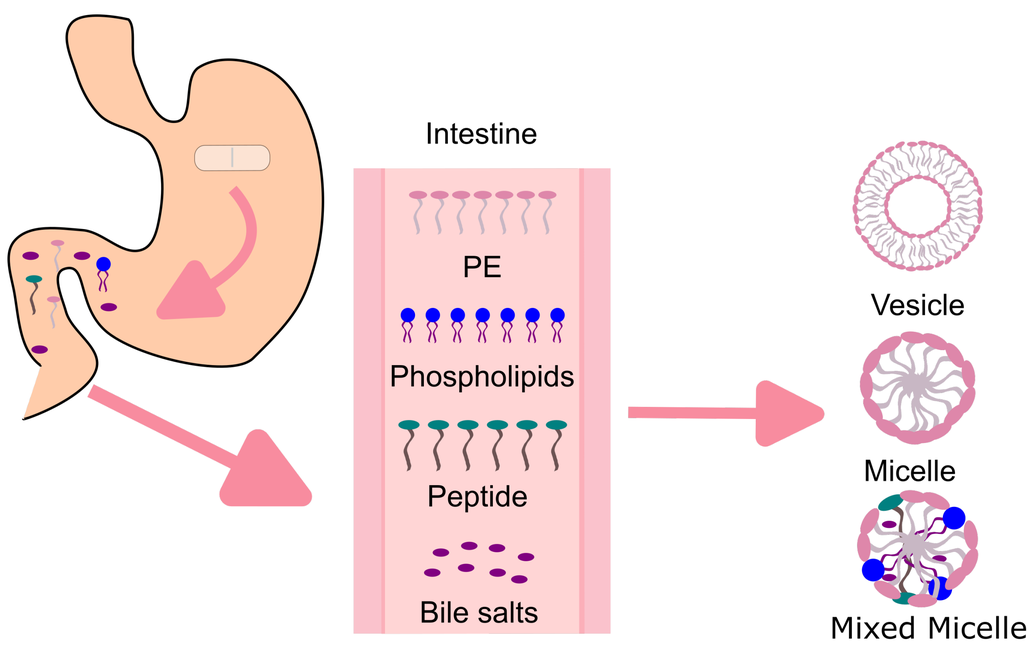
Objective

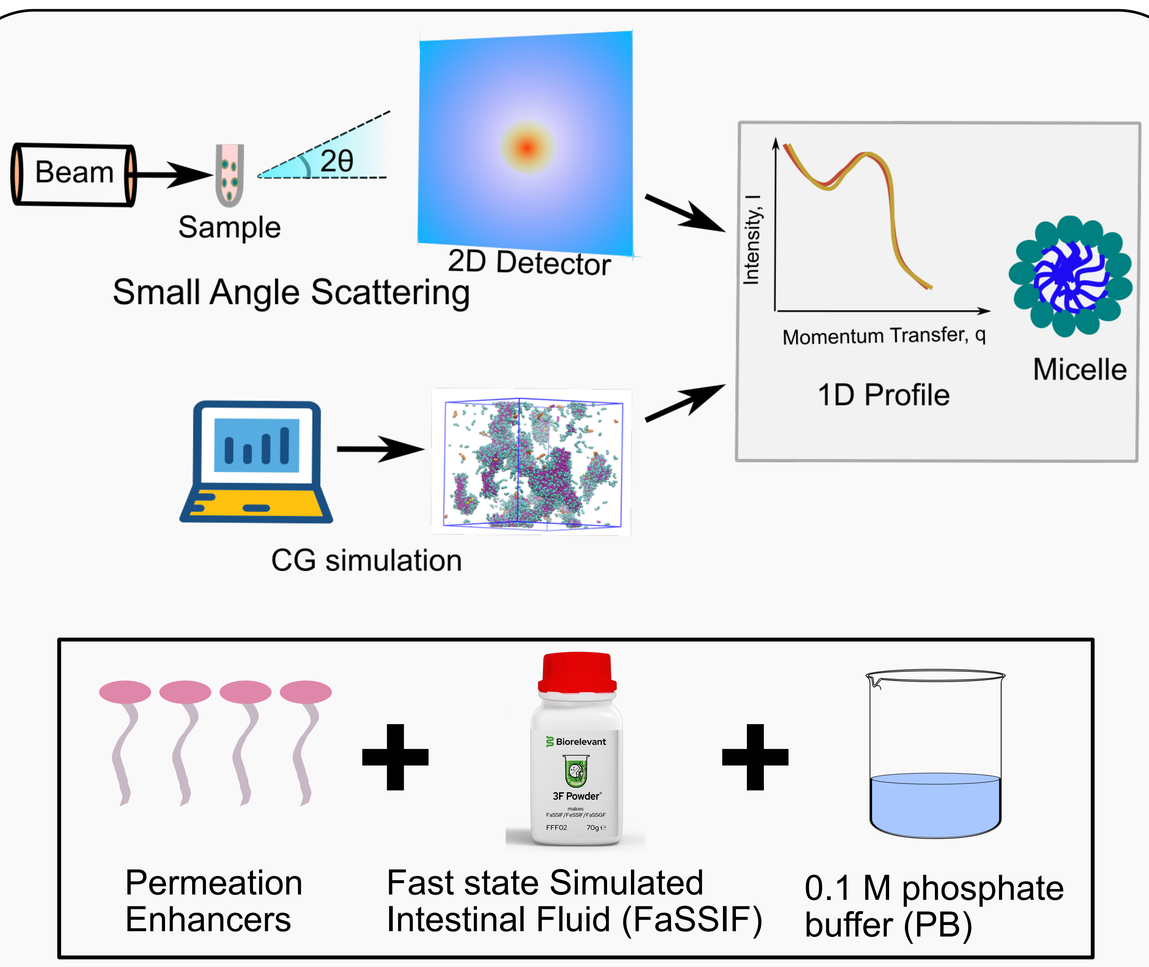
The aim of the study is to investigate the aggregation characteristics of Sodium Caprate using coarse-grained molecular dynamics (CG-MD) simulations (Martini 3 and Martini 2 force fields) in combination with the small-angle scattering technique.

Background

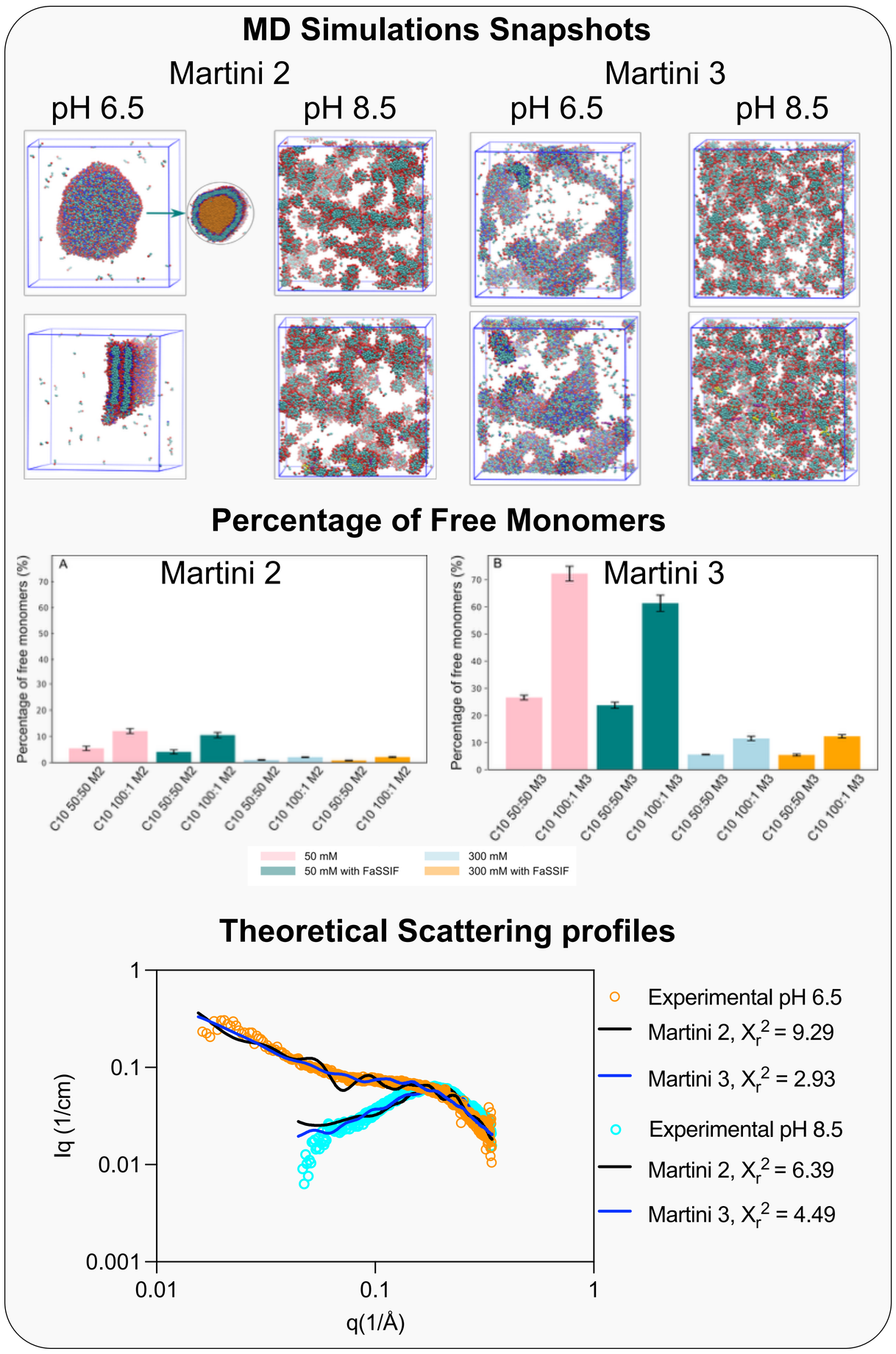


Sodium caprate (C10), a fatty acid-based permeation enhancer, can temporarily increase peptide permeability for oral delivery. The size and shape of the resulting colloidal structures in the GI tract depend on intestinal fluid composition, peptide properties, and permeation enhancer's concentration. The study examined the aggregation behavior of sodium caprate (C10) under different pH conditions. The amphiphilic nature of C10 causes it to self-associate in aqueous solutions, with its apparent pKa changing depending on its concentration. The aggregation behavior of C10 is determined by the ratio of ionized to unionized species.

Experimental Overview



Results



Highlights

- A variety of large and small aggregate structures coexist at low pH conditions.
- At high pH, the system predominantly forms smaller spherical micelles.
- Simulations using the Martini 3 coarse-grained model closely align with experimental observations.
- FaSSIF affects aggregation behavior, as captured by Martini 3 simulations.

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