

Supplementary Information

Aggregation behavior of sodium caprate under different pH, concentration, and intestinal fluid conditions: a coarse-grained molecular dynamics study comparing Martini 2 and Martini 3

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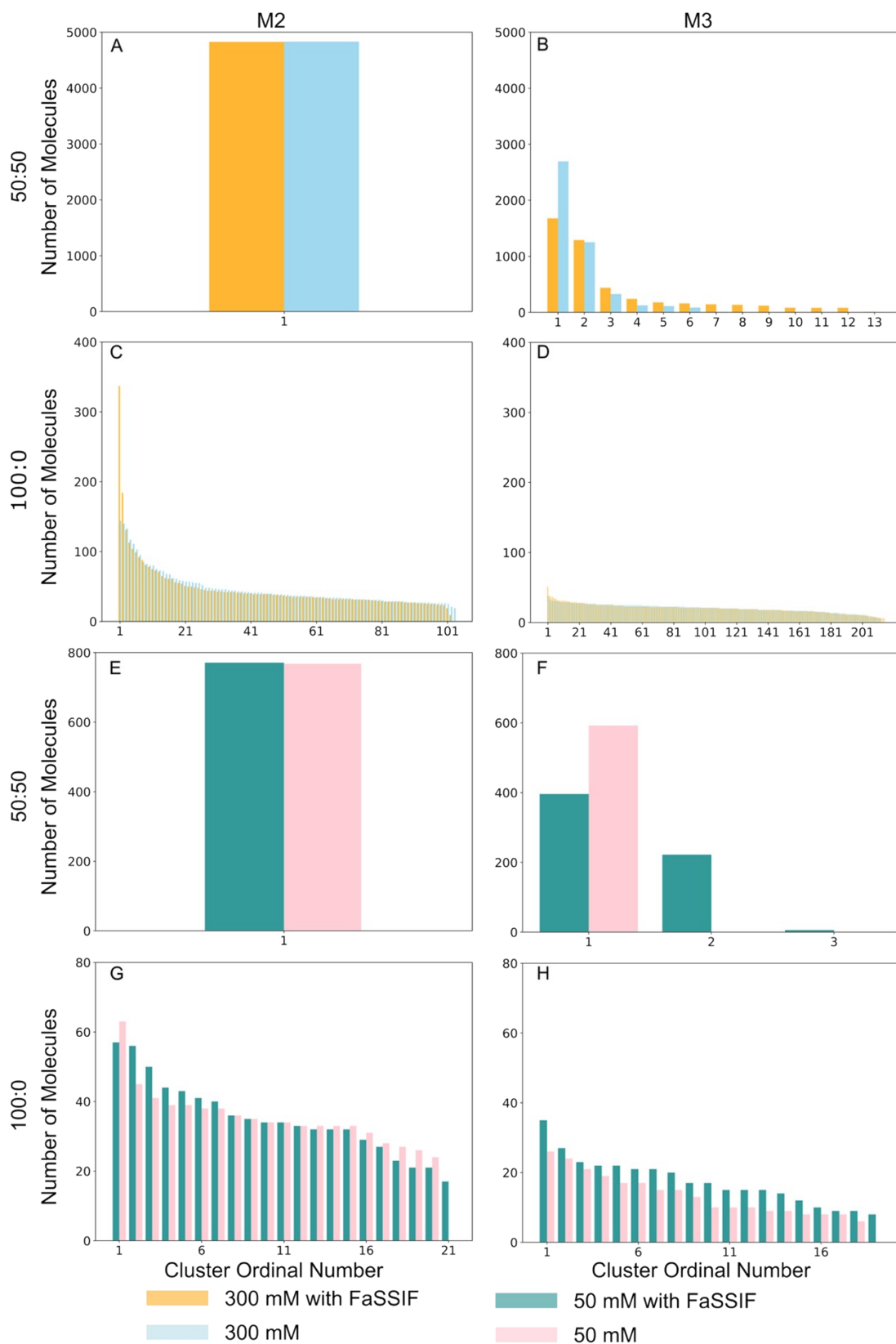
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Supplementary Figure 1: The number of molecules in each cluster across all systems. (A) and (B) depict 300 mM C10 with charged-uncharged ratios of 50:50 for Martini 2 and Martini 3, respectively. (C) and (D) present 300 mM C10 with charged-uncharged ratios of 100:0 for

Martini 2 and Martini 3. Similarly, (E) and (F) show 50 mM C10 with 50:50 charged-uncharged ratios for Martini 2 and Martini 3, respectively, while (G) and (H) display 50 mM C10 with 100:0 charged-uncharged ratios for Martini 2 and Martini 3, respectively.