Supporting Information

for

Simulating pH titration of a single surfactant in ionic and nonionic micelles

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Figure S1: Cumulative unprotonated fraction of lauric acid in the SDS, DTA, and DE3 micelles from the explicit-solvent titration simulations. For each micelle S values are shown at 2 pK unit intervals as indicated.
Figure S2: Titration data for lauric acid in the DTA micelle, fit to a linear combination of modified Hill equations.

The titration data for lauric acid in DTA can be fit to a linear combination of two modified Hill equations (Eqn 9 in Ref. (1)):

\[
S = x \left( \frac{s_{A^-} + s_{HA}10^n(pK_{a,1}-pH)}{1 + 10^n(pK_{a,1}-pH)} \right) + (1-x) \left( \frac{s_{A^-} + s_{HA}10^n(pK_{a,2}-pH)}{1 + 10^n(pK_{a,2}-pH)} \right)
\]  

(1)

where \(s_{A^-}\) and \(s_{HA}\) are fitting parameters, which represent the \(S\) values at extreme pH conditions, \(pK_{a,1}\) and \(pK_{a,2}\) represent the \(pK_a\) of lauric acid in two distinct conformational states, and \(x\) denotes the relative population of the two states. When we fit the titration data to Eqn. 1 with \(n = 1\), we obtain the fit shown in Fig. S2, with \(pK_{a,1} = 7.4\), \(pK_{a,2} = 6.2\), and \(x = 0.33\). This indicates that the lauric acid molecule experiences two distinct conformational states due to fluctuations of the DTA micelle, with the lower-\(pK_a\) state dominating, and the exchange between these states is slow relative to the simulation time. When the titration data is fit to a single Hill equation, the result is a \(pK_a\) of 6.5, with a Hill coefficient of 0.5.
References