Supplementary Information

Temperature and concentration effects on decyltrimethylammonium micelles in water

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Table S1: Lennard-Jones and Coulomb parameters used for the reference potentials

Atom Label	Atom Type	ε / kJmol^{-1}	σ / Å	q / e	Mass /amu
Br	Br	0.566	4.465	-1.0000	80
MH	H	0.200	2.580	0.0000	2
M	H	0.200	2.580	0.0000	2
CH	C	0.200	3.700	0.0000	12
C1-9	C	0.200	3.960	0.0000	12
CT	C	0.200	3.960	0.0000	12
N	N	0.200	3.200	+1.0000	14
OW	O	0.650	3.166	-0.8476	16
HW	H	0.000	0.000	+0.4238	2

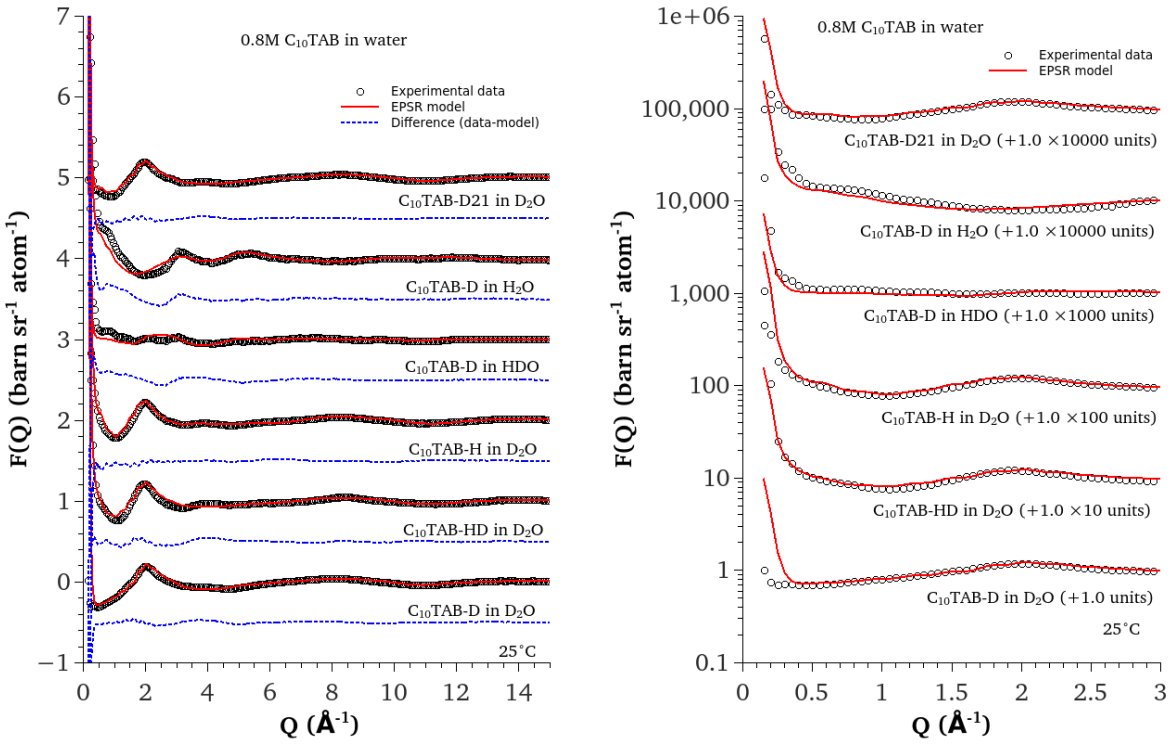

Figure S1: EPSR model fits for 0.8M C_{10}TAB at 25 °C (solid red lines) and fit residuals (dashed blue lines offset by 1.0 down the ordinate axis) to the diffraction data (black circles) of the five isotopic samples. The right hand graph expands the low Q region to highlight the fits to the data in this region. For clarity, each data set is offset up the ordinate, and each residual from its data set.

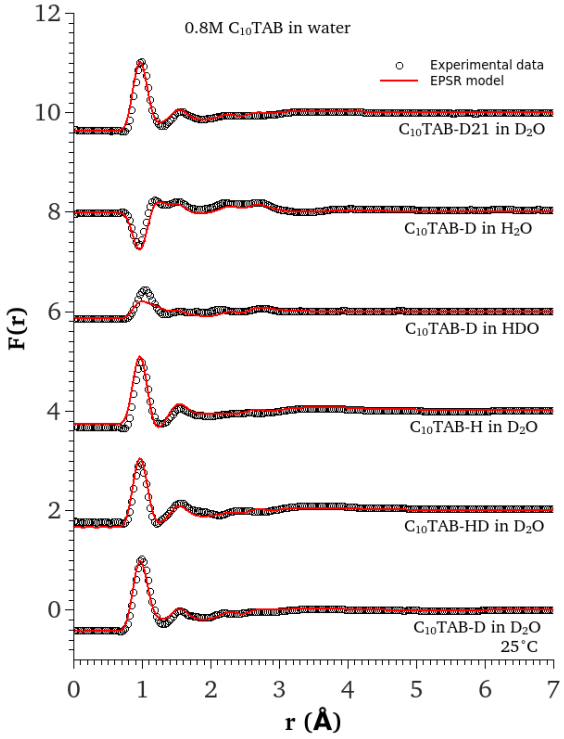

Figure S2: Comparison of the unnormalized pair distribution functions calculated from the EPSR model of the 0.8M C_{10}TAB at 25 °C data.

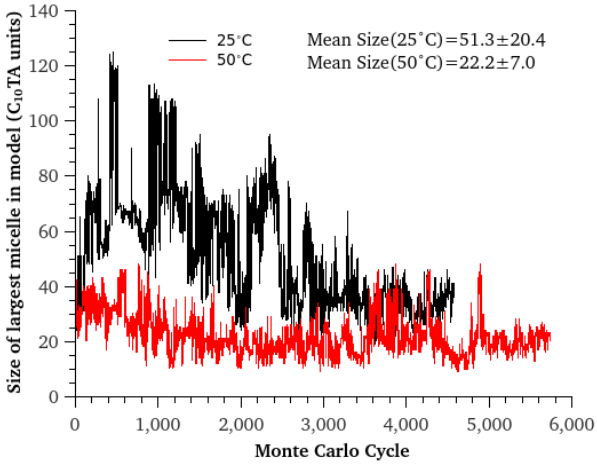

Figure S3: Tracking the number of C_{10}TA monomers that make up the largest micelle in the EPSR refined model box as the ensemble averages are calculated, shows that larger micelles are formed in the 25 °C solution than in the 50 °C solution.

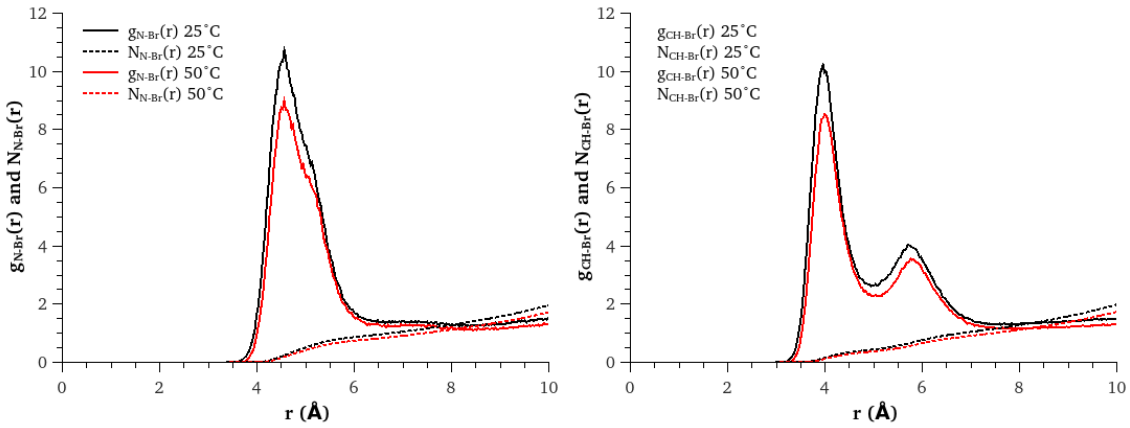

Figure S4: Partial distribution functions at 25 °C and 50 °C which show the relatively close association of the bromide anions with the cationic surfactant head group nitrogen sites (left) and methyl carbon sites (right).