Conformational Transition of a Non-Associative Fluorinated Amphiphile in Aqueous Solution. II. Conformational Transition vs. Supramolecular Assembly†

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Supporting information

Table S1. $R_2(^1H_2O)$ and C(solute) for three amphiphiles[a]

^{19}FIT-27		α-CD		NaC_8	
C, mM	$R_2(^1H_2O)$, s^{-1}	C, mM	$R_2(^1H_2O)$, s^{-1}	C, mM	$R_2(^1H_2O)$, s^{-1}
0.19	0.389	0.2	0.353	9.0	0.319
0.22	0.384	0.5	0.360	14.0	0.320
0.28	0.379	1.0	0.375	19.0	0.323
0.38	0.390	2.1	0.401	38.0	0.365
0.5	0.378	3.3	0.437	75.0	0.382
0.75	0.390	4.6	0.477	150.0	0.421
1.0	0.395	6.0	0.500	300.0	0.451
1.88	0.398	7.5	0.536	600.0	0.466
3.75	0.407	9.5	0.592	900.0	0.485
5.0	0.415	13.0	0.690	1200.0	0.524
7.5	0.427	20.0	0.856	1500.0	0.571
10.0	0.430	30.0	1.082	1800.0	0.637
18.8	0.448	40.0	1.299	2000.0	0.724
37.5	0.569	60.0	1.745	2200.0	0.808
50.0	0.709	105.0	2.710	2400.0	0.900
75.0	0.881	—	—	—	—
100.0	1.087	—	—	—	—

[a] Green entries highlight the approximate transition points for ^{19}FIT-27 (~10 mM, from this work) and NaC_8 (300–400 mM for 1st transition point, and 900–1,200 mM for 2nd transition point [1]). α-CD has no transition point.

Table S2. Normalized $R_2(^1H_2O)$ and C(solute) for three amphiphiles[a,b]

^{19}FIT-27		α-CD		NaC_8	
C, mM	$R_2(^1H_2O)$, s^{-1}	C, mM	$R_2(^1H_2O)$, s^{-1}	C, mM	$R_2(^1H_2O)$, s^{-1}
0.000	0.000	0.000	0.000	0.000	0.000
0.000	-0.007	0.003	0.003	0.002	0.002
0.001	-0.014	0.008	0.009	0.004	0.007
0.002	0.001	0.018	0.020	0.012	0.079
0.003	-0.016	0.030	0.036	0.028	0.108
0.006	0.001	0.042	0.053	0.059	0.176
0.008	0.009	0.055	0.062	0.122	0.227
0.017	0.013	0.070	0.078	0.247	0.253
0.036	0.026	0.089	0.101	0.373	0.286
0.048	0.037	0.122	0.143	0.498	0.353
0.073	0.054	0.189	0.213	0.624	0.434
0.098	0.059	0.284	0.309	0.749	0.547
0.186	0.085	0.380	0.401	0.833	0.697
0.374	0.258	0.571	0.591	0.916	0.842
0.499	0.458	1.000	1.000	1.000	1.000
0.750	0.705	—	—	—	—
1.000	1.000	—	—	—	—

[a] Normalized data are calculated from the experimental values listed in Table S1 using the following equation:

$$X_{\text{normalized}} = \frac{X_i - X_{\text{min}}}{X_{\text{max}} - X_{\text{min}}},$$

where X_i is the experimental value of $R_2(^1H_2O)$ or C(solute), respectively; X_{min} is the minimum value of $R_2(^1H_2O)$ or C(solute), respectively; and X_{max} is the maximum values of $R_2(^1H_2O)$ or C(solute), respectively.

[b] Green entries highlight the approximate transition points on the normalized concentration scale for ^{19}FIT-27 (~0.10) and NaC_8 (~0.12 for 1st transition point, and ~0.50 for 2nd transition point). α-CD has no transition point.

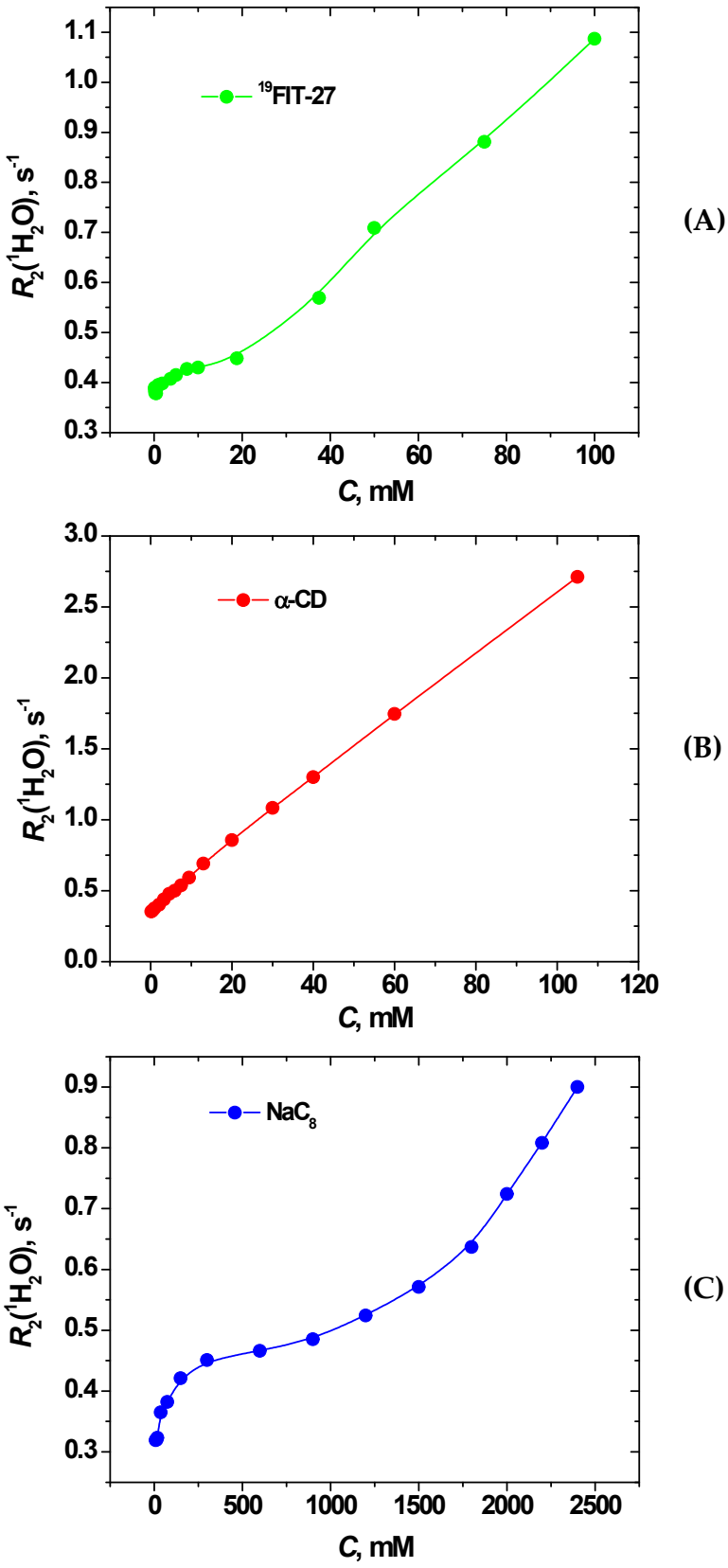

Figure S1. Concentration-dependent changes of water proton transverse relaxation rates $R_2(^1H_2O)$ for three amphiphiles: (A) ^{19}FIT-27; (B) α-CD; (C) NaC_8 (this plot was previously reported by us in [2]. It is shown here again for side-by-side comparison).

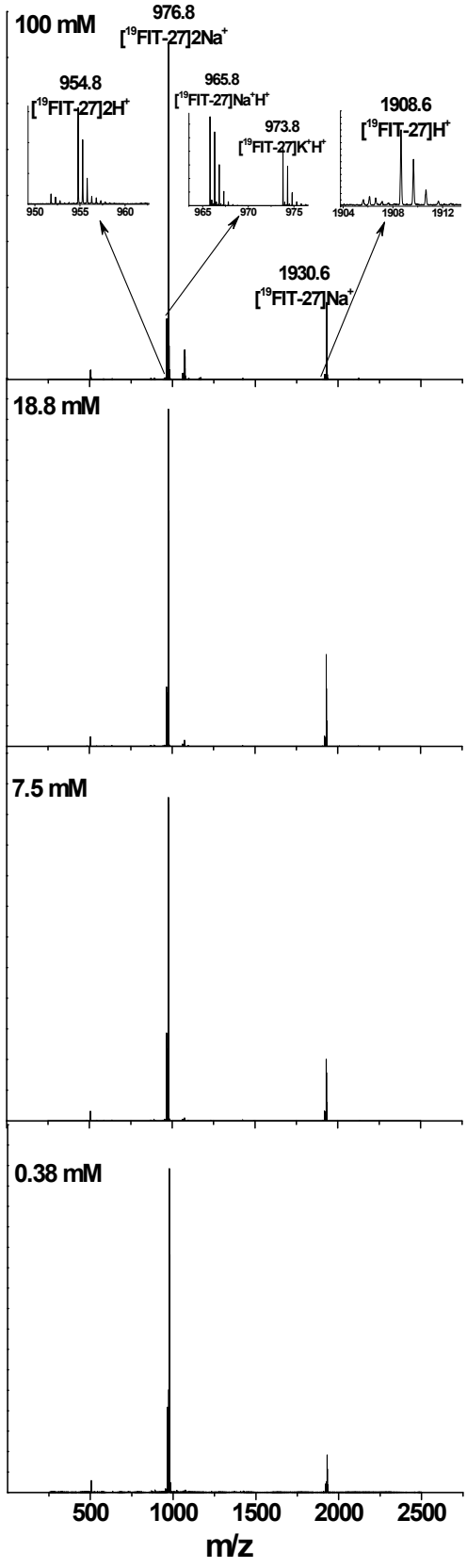

Figure S2. ESI-MS spectra of ^{19}FIT-27 at different concentrations.

References

1. (*a*) J. B. Hayter and T. Zemb, *Chem. Phys. Lett*., 1982, **93**, 91-94; (*b*) B. O. Persson, T. Drakenberg and B. Lindman, *J. Phys. Chem.*, 1979, **83**, 3011-3015; (*c*) T. Zemb, M. Drifford, M. Hayoun and A. Jehanno, *J. Phys. Chem.*, 1983, **87**, 4524-4528; (*d*) D. K. Chokappa and S. Das, *Indian J. Chem.*, 1994, **33A**, 795-800.

2. Y. Feng, M. B. Taraban and Y. B. Yu, *Chem. Commun.*, 2015, **51**, 6804-6807.