Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information for

Molecular dynamics study on aggregation behaviours of different positional isomers of sodium dodecyl benzenesulphonate

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Table S1 Detailed shape of micelles

	1Φ12	2Φ12	3Φ12	4Φ12	5Φ12	6Φ12
R11/R22	1.04	1.04	1.04	1.06	1.04	1.08
R22/R33	1.12	1.07	1.08	1.13	1.34	1.32

R11, R22, and R33 are the square roots of the principal moments of inertia with three axes, where R11 > R22 > R33.

Table S2 The hydration numbers of different sections for SDBS molecules

	1Φ12	2Φ12	3Φ12	4Φ12	5Φ12	6Φ12
sulphonate group	1.89	1.93	1.93	1.94	1.94	1.94
benzene ring	1.03	1.01	0.92	0.91	0.87	0.87
long chain	0.10	0.06	0.06	0.06	0.06	0.10
short chain	-	0.37	0.30	0.25	0.22	0.16

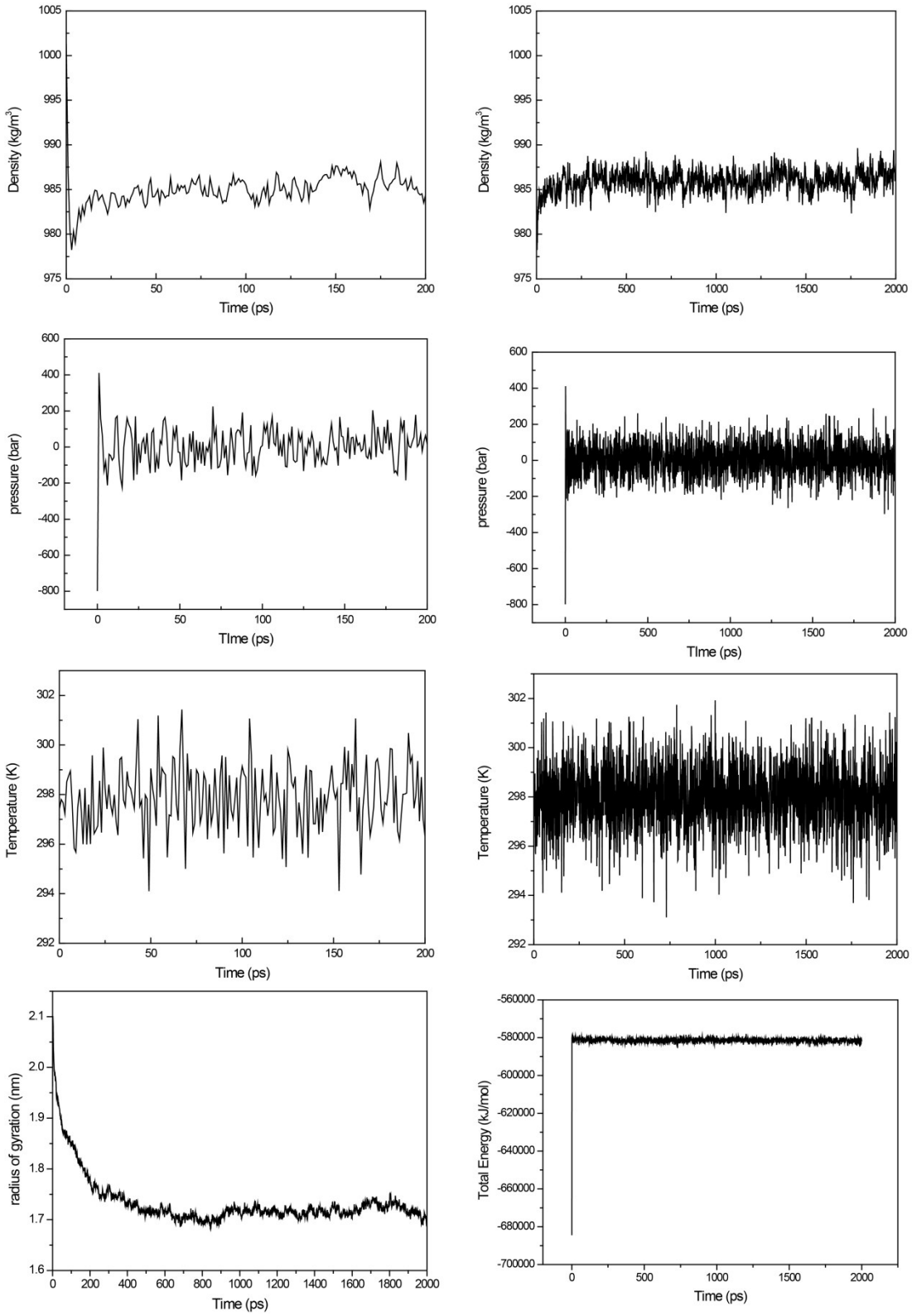


Fig. S1 Different criterion for the equilibrium justification of 1Φ12 with different time evolution

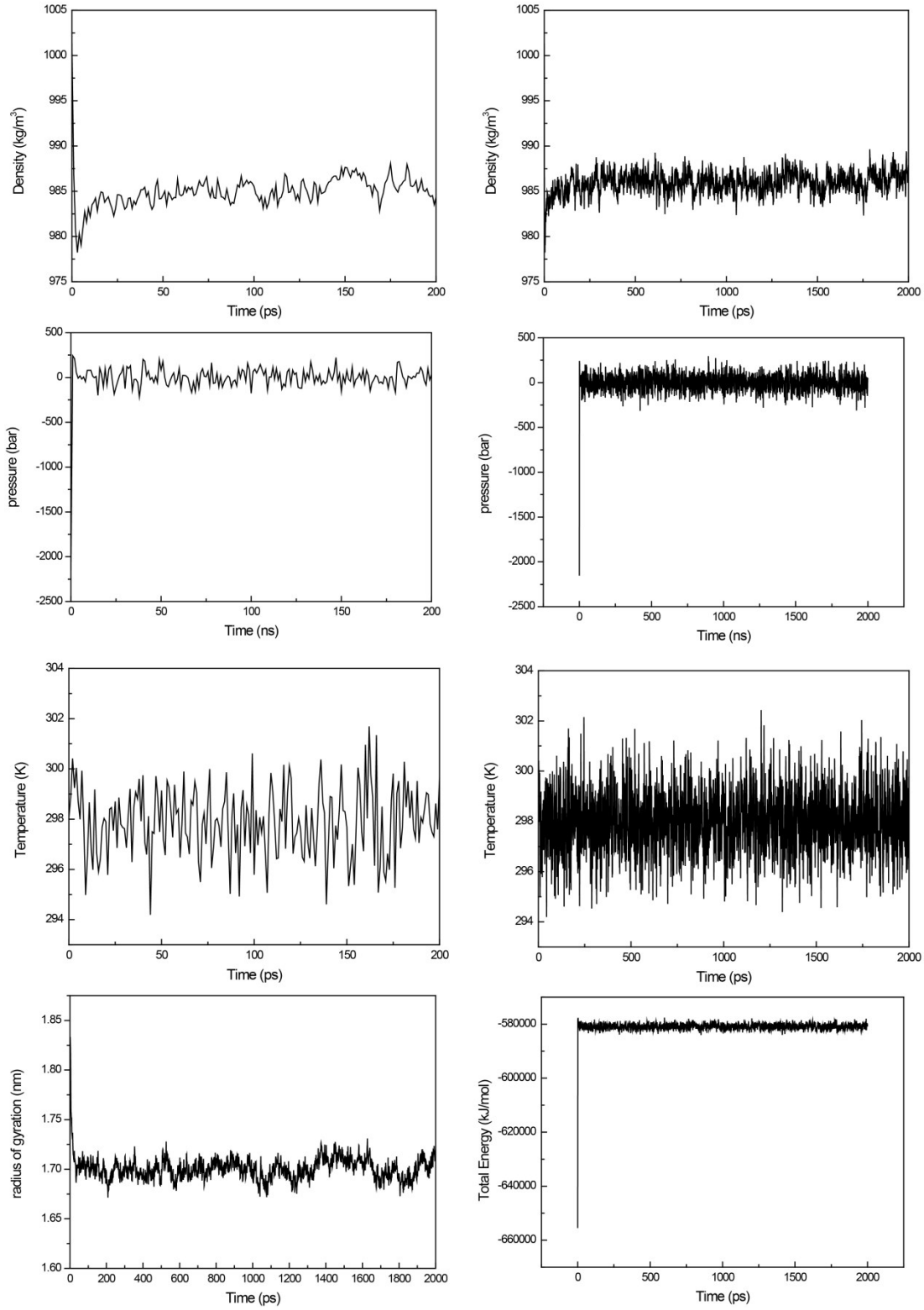


Fig. S2 Different criterion for the equilibrium justification of 6Φ12 with different time evolution

As shown in Fig. S1 and Fig. S2, the short time (200 ps) is adequate to reach the appropriate temperature, pressure, and density (or volume). Especially, the average density for 1Φ12 and 6Φ12 between 100ps and 200ps are 985.50±1.25 kg/m^3 and 985.24±1.11 kg/m^3, respectively, which are consistent with the density of ca. 0.99 g/cm^3 for SPC water model.[5] And the density is

smooth among the long lasting ca. 2 ns trajectory. Above all, the appropriate and stable density is important for the next NVT simulation.

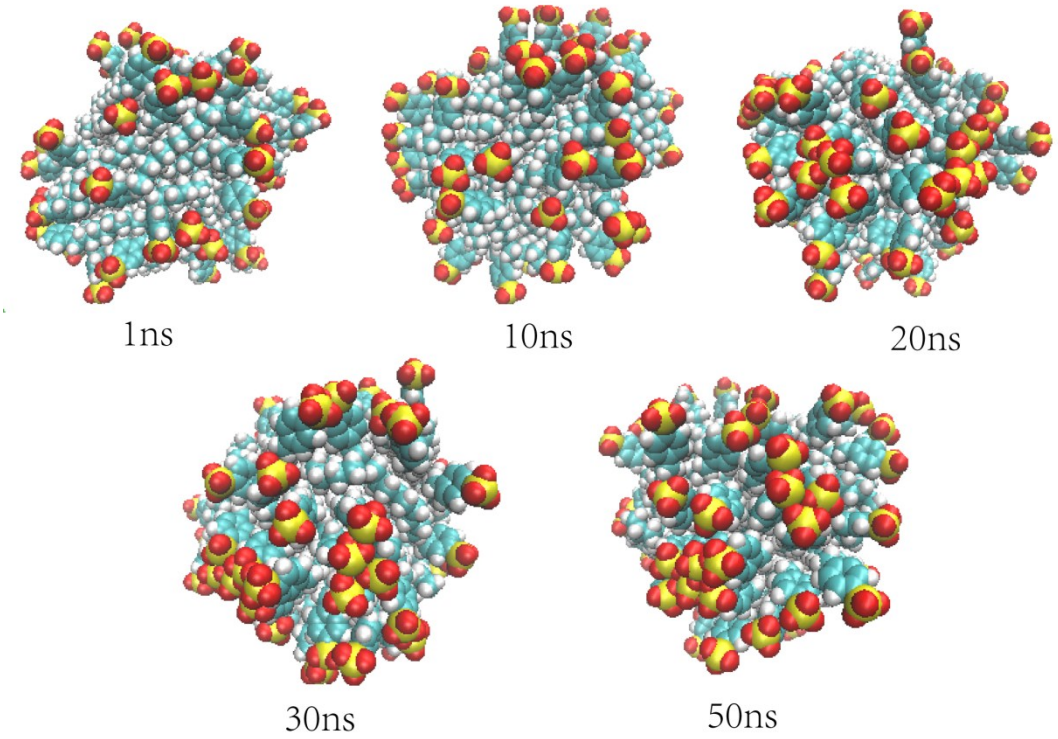


Fig. S3 Snapshots at different time points of 1Φ12 micelle. For clarity, water molecules and sodium ions are removed. Red: O atom; Yellow: S atoms; Turquoise: C atoms; Light gray: H atoms.

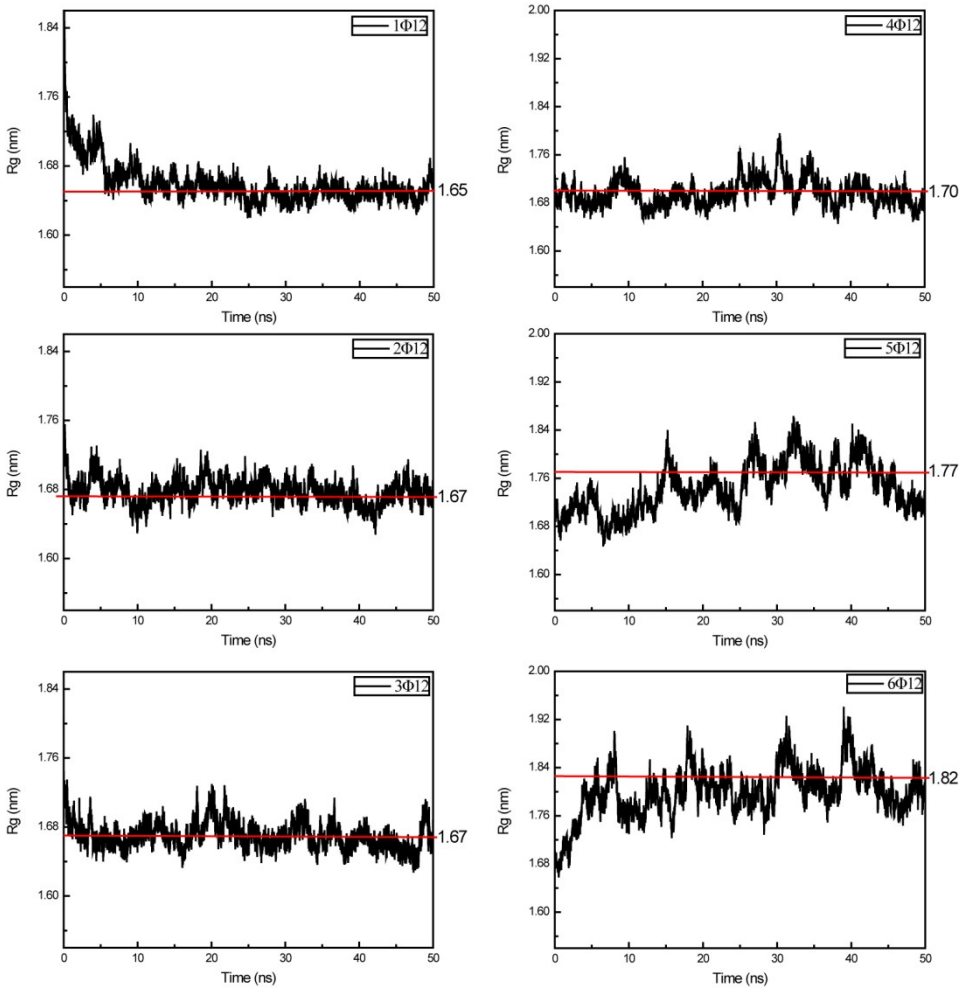


Fig. S4 Radius of gyration for the micelle during the 50 ns NVT simulation in all six systems.

As shown in the figure, the former four micelles converge well after about 30 ns NVT simulation while the latter two micelles behave not as well as the four micelles. However, it is reasonable to use the last 20 ns data to do analyses considering slight fluctuations of the curves.

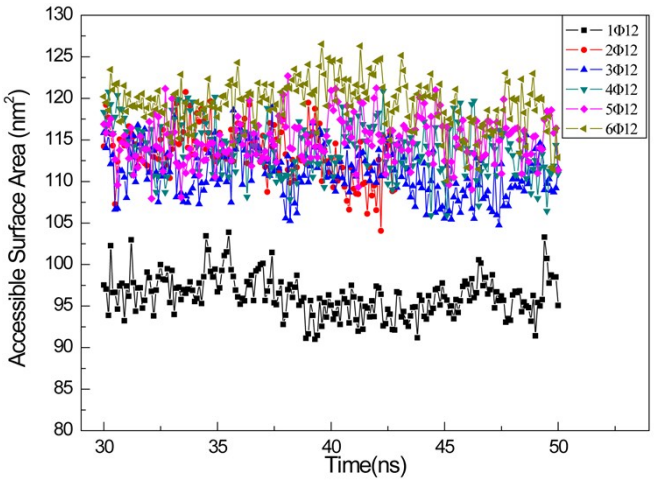


Fig. S5. Accessible surface areas

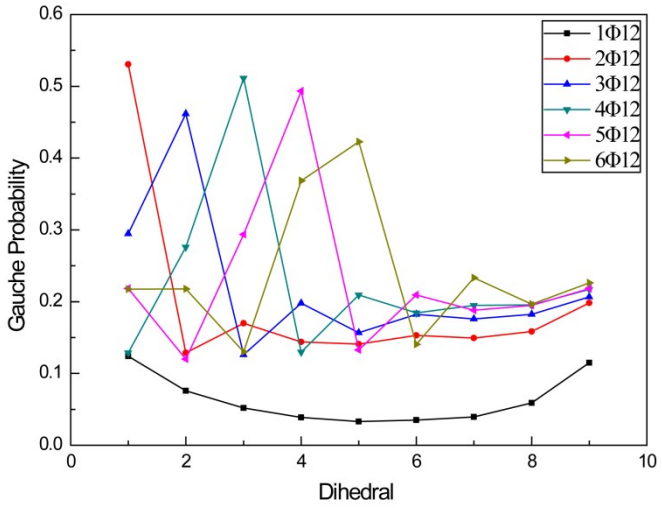


Fig. S6 Probability of gauche defects in the hydrophobic chain. Dihedral 1 represents the dihedral nearest to the benzene ring in 1Φ12 micelle and the dihedral from the terminal C atom of short chain in other five micelles.

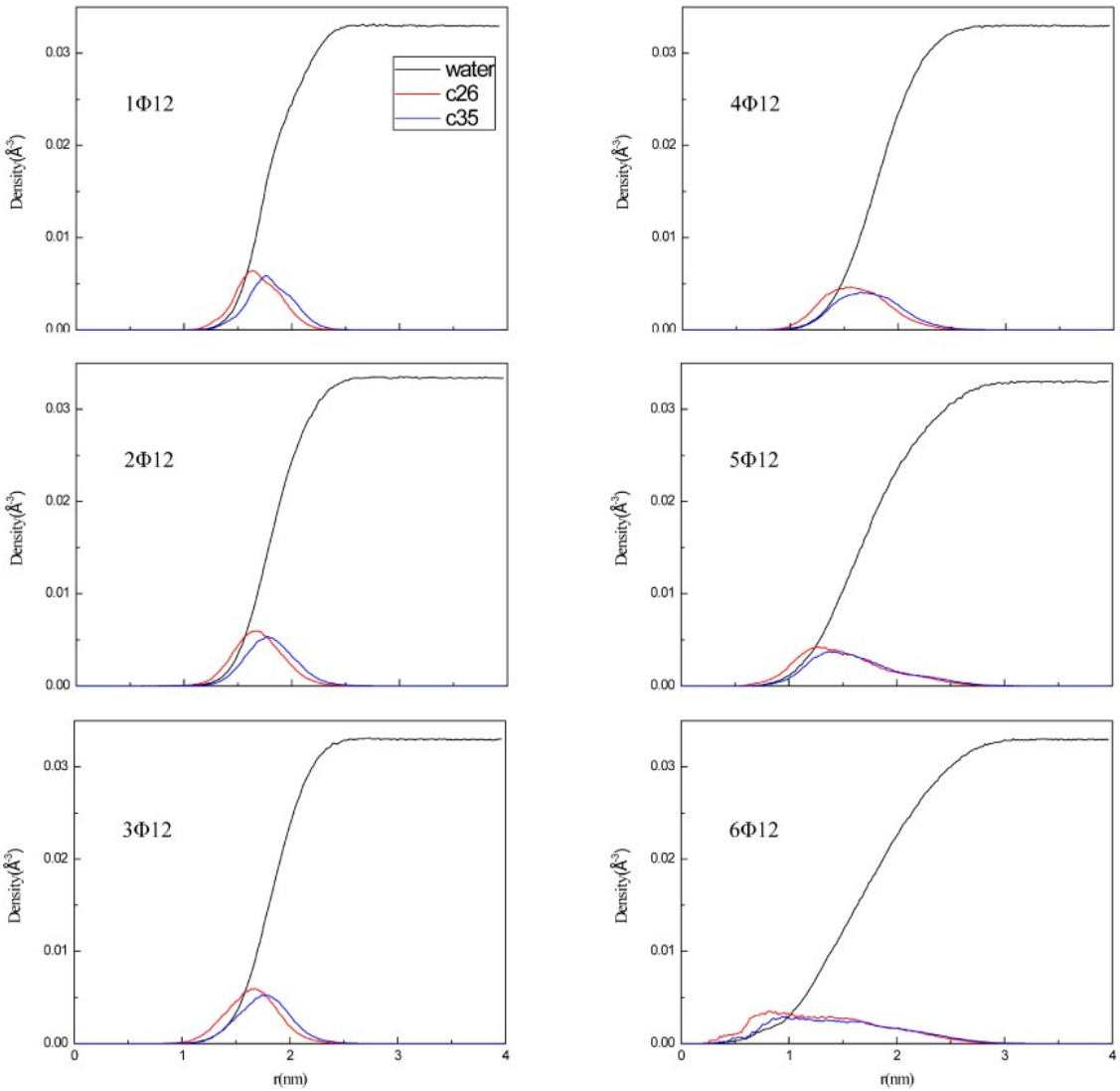


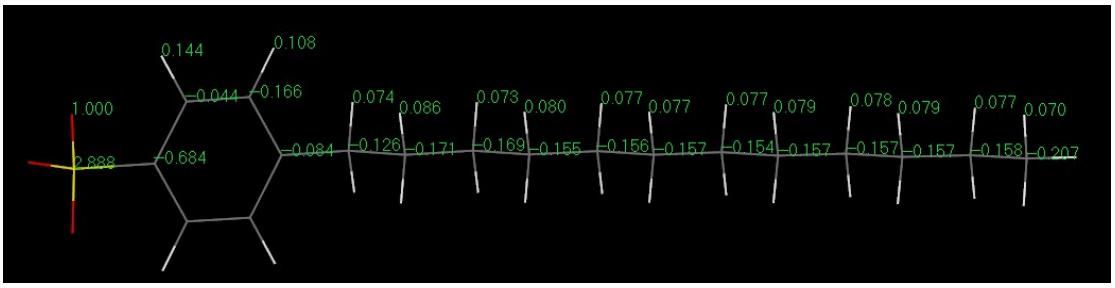
Fig. S7 The density distribution of the selected atoms to micelle center of mass distance. The c26 represents two carbon atoms meta to the sulphonate group, and the c35 represents two carbon atoms ortho to the sulphonate group on the benzene ring.

The curve of water for 1Φ12 micelle is consistent with previous study.[1] It's noted that the density of water between c26 and c35 is too small to be recognized in the figure for 6Φ12. However, we have checked the data to verify that the water penetration is between the c26 and c35 in agreement with other isomers and previous experimental study.[2]

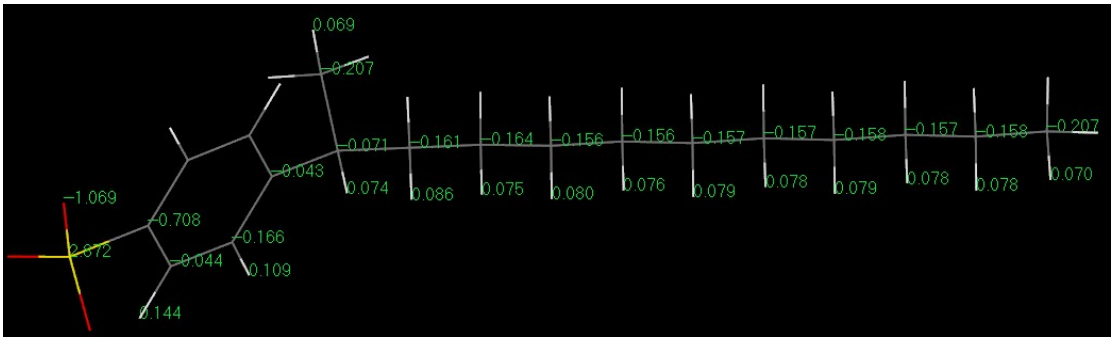
The detailed force field parameters for all the studied systems are as follows:

Partial atomic charges of six isomers:

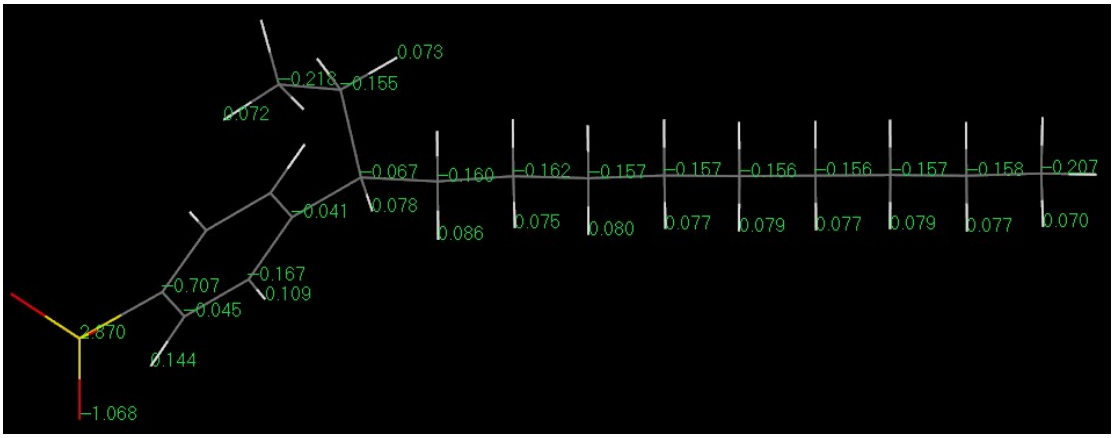
1Φ12



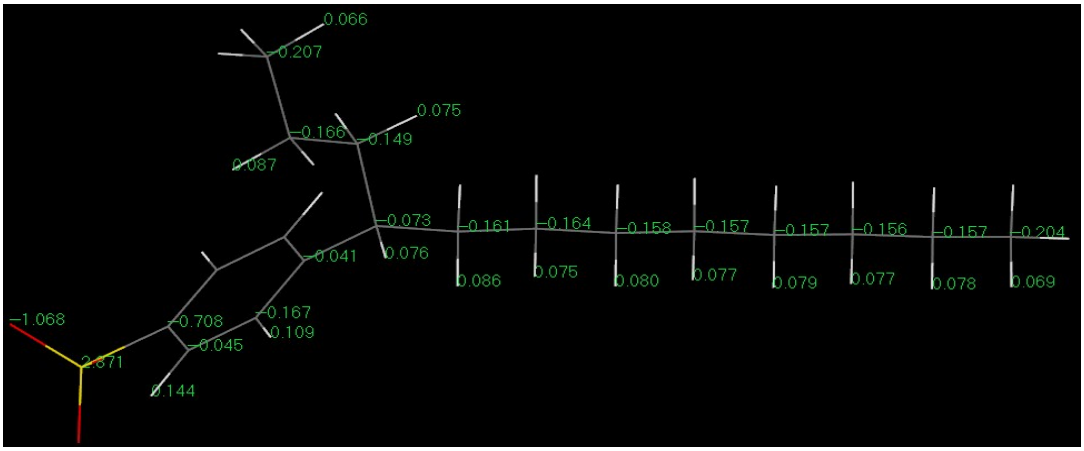
2Φ12



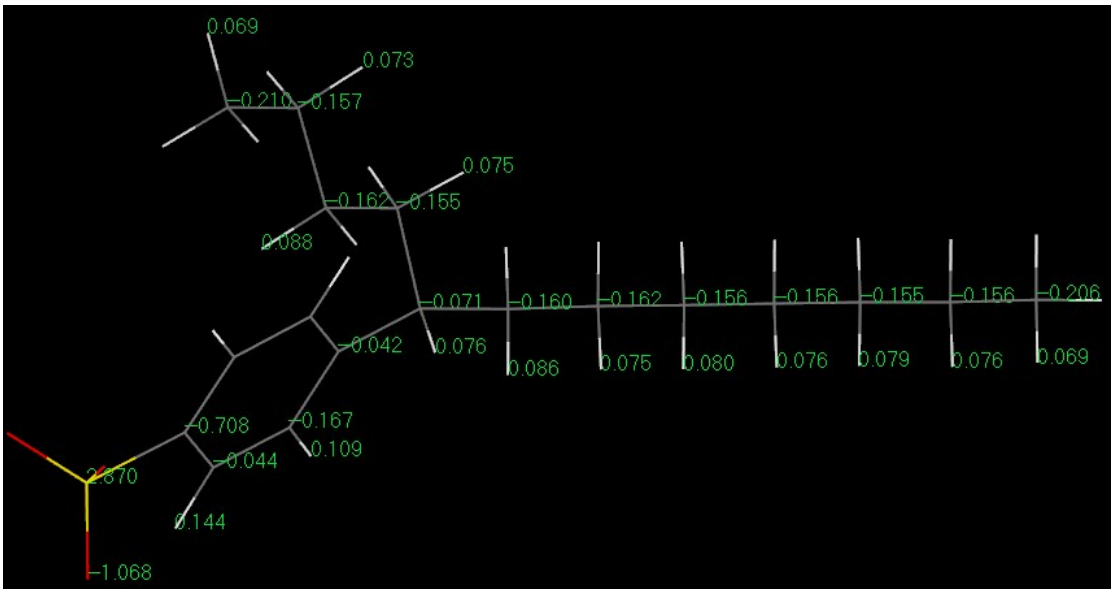
3Φ12



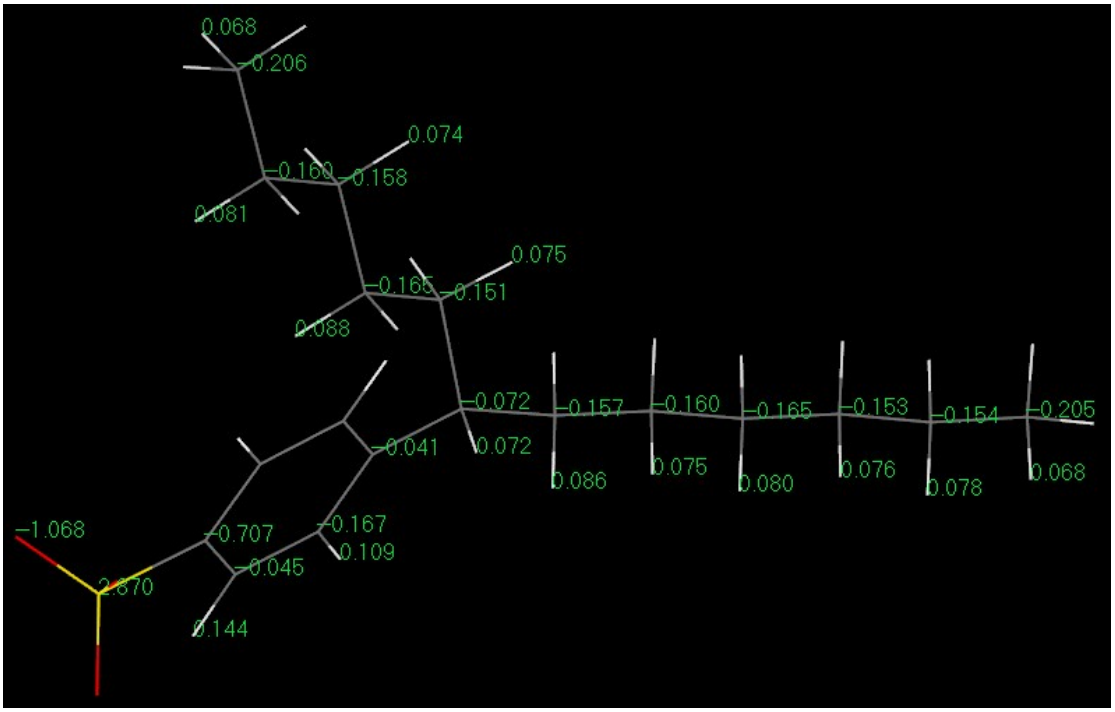
4Φ12



5Φ12


0.069
0.073
-0.210
-0.157
0.075
-0.162
-0.155
0.088
-0.071
-0.160
-0.162
-0.156
-0.156
-0.155
-0.156
-0.206
-0.042
0.076
0.086
0.075
0.080
0.076
0.079
0.076
0.069
-0.708
-0.167
0.109
-0.044
2.870
0.144
-1.068

6Φ12


0.068
-0.206
0.074
-0.160
-0.158
0.081
0.075
-0.165
-0.151
0.088
-0.072
-0.157
-0.160
-0.165
-0.153
-0.154
-0.205
-0.041
0.072
0.086
0.075
0.080
0.076
0.078
0.068
-1.068
-0.707
-0.167
0.109
-0.045
2.870
0.144

Non bonded and bonded parameters:

Normal van der Waals Parameters

Atom type	$[C6(I,I)]^{1/2}$ $[(kJmol^{-1}nm^{6})^{1/2}]$	$[C12(I,I)]^{1/2}$ $[10^{-3}(kJmol^{-1}nm^{12})^{1/2}]$
OM	0.04756	0.8611
HC	0.009200	0.1230
SDmso	0.10277	4.6366
C	0.04838	2.222

Bond-Stretching Parameters

	Force constant K_b ($10^6 kJmol^{-1}nm^{-4}$)	Ideal bond length b_0(nm)
C-C	5.43	0.152
C-C (benzene)	8.66	0.139
C-H	12.1	0.110
C-S	5.94	0.178
S-O	2.66	0.141

Bond-Angle Bending Parameters

	Force constant K_θ ($kJmol^{-1}$)	Ideal bond angle ϑ_0 (degree)
C-C-H	285	109.5
C(benzene) -C(benzene) -H	505	120.0
C-C-C	530	111.0
H-C-H	1440	107.0
H(methyl)-C-H(methyl)	443	108.5
C-S-O	503	106.8
S-C-C	750	125.0
H-C-C (benzene)	505	120.0

Dihedral-angle parameters

	Force constant K_ζ ($kJmol^{-1}degree^{-2}$)	Ideal dihedral angle ζ_0 (degree)
C-C-C-H	5.92	0.0
C(benzene)-C(benzene)-S-O	1.00	0.0
C-C-C-C	5.92	0.0

Improper (harmonic) dihedral-angle parameters

	Force constant K_ζ ($kJmol^{-1}degree^{-2}$)	Ideal improper dihedral angle ζ_0(degree)
C-C-C-H (benzene)	167.36	0.0
C-C-C-C (benzene)	167.36	0.0

Notes and References

1. Palazzesi, F.; Calvaresi, M.; Zerbetto, F., A molecular dynamics investigation of structure and dynamics of SDS and SDBS micelles. *Soft Matter* **2011,** 7, (19), 9148.

2. Das, S.; Bhirud, R. G.; Nayyar, N.; Narayan, K. S.; Kumar, V. V., Chemical shift changes on micellization of linear alkyl benzenesulphonate and oleate. *J. Phys. Chem.* **1992,** 96, (18), 7454-7457.