Chain Length Dependent Alkanes/β-Cyclodextrin

Nonamphiphilic Supramolecular Building Blocks

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Supporting Information

1. 1H NMR spectra of alkane/β-CD precipitates.

The actual host-guest ratio of β-CD to alkane is calculated based on the integrations of β-CD (H1 protons) and the total integration of alkane protons.

a) pentane/β-CD (H1/7:H_{pentane}/12=1.00/7:(1.13+0.33)/12=1.1:1),
b) hexane/β-CD (H1/7:H_{hexane}/14=2.86/7:(4.15+0.98)/14=1.1:1),
c) octane/β-CD (H1/7:H_{octane}/18=1.00/7:(1.72+0.51)/18=1.1:1),
d) decane/β-CD (H1/7:H_{decane}/22=1.00/7:(1.90+0.54)/22=1.2:1),
e) tetradecane/β-CD (H1/7:H_{tetradecane}/30=1.00/7:(2.06+0.49)/30=1.7:1),
f) hexadecane/β-CD (H1/7:H_{hexadecane}/34=1.00/7:(3.04+0.60)/34=1.3:1),
g) octadecane/β-CD (H1/7:H_{octadecane}/38=3.01/7:(11.68+2.72)/38=1.1:1).
Figure S1  a)-g) $^1$H NMR spectra with assignments and integration of alkane/β-CD precipitates dissolved in DMSO-d6 (alkane: pentane, hexane, octane, decane, tetradecane, hexadecane and octadecane, respectively).

2. ESI-MS spectra of alkane/β-CD sample.

ESI-MS measurement of hexane/β-CD vesicle sample showed the presence of $[2\text{hexane}@2\beta-CD\cdot5\text{H}_2\text{O}\cdot3\text{H}]^{3+}$ (m/z = 784.89421, the theoretical value m/z = 784.97754) (Figure S2a). In Figure S2b, octadecane/β-CD vesicle showed the presence of $[2\text{octadecane}@2\beta-CD\cdot9\text{H}_2\text{O}\cdot2\text{Na}]^{2+}$ (m/z = 2747.26566, the theoretical value m/z = 2747.29566, error: -10 ppm). The larger error in our case may be attributed to that the large molecular mass for 2alkane@2β-CD exceeds the upper...
limit of 2000 for the HR-ESI-MS.

Figure S2 ESI-MS results of a) hexane/β-CD sample and b) octadecane/β-CD sample in positive mode.

3. Addition of urea into the hexane/β-CD sample.

Figure S3 a) The macrographs of hexane/β-CD sample (C_β-CD=16 mM) and b) normalized intensity correlation function of hexane/β-CD vesicles sample with the macrographs of the scattering intensity (inset) before and after the addition of 5 M urea.