

## Chain Length Dependent Alkanes/ $\beta$ -Cyclodextrin

### Nonamphiphilic Supramolecular Building Blocks

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### Supporting Information

#### 1. <sup>1</sup>H NMR spectra of alkane/ $\beta$ -CD precipitates.

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

a) pentane/ $\beta$ -CD (H1/7:H<sub>pentane</sub>/12=1.00/7:(1.13+0.33)/12=1.1:1),

b) hexane/ $\beta$ -CD (H1/7:H<sub>hexane</sub>/14=2.86/7:(4.15+0.98)/14=1.1:1),

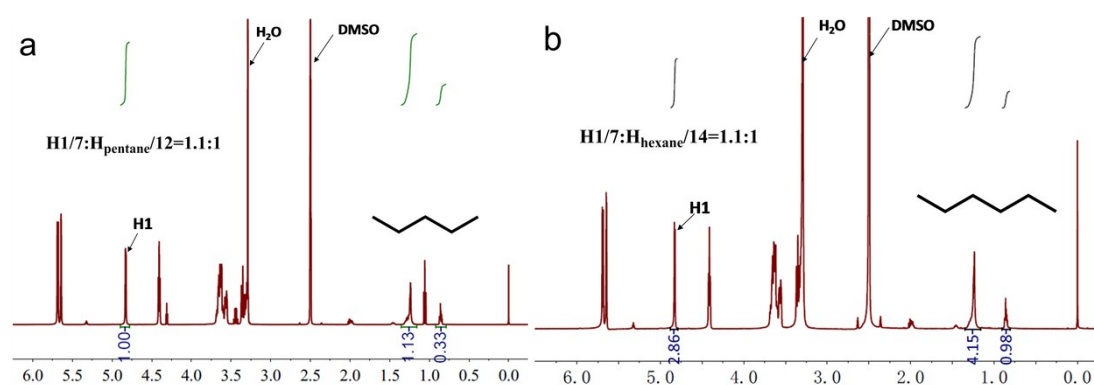
c) octane/ $\beta$ -CD (H1/7:H<sub>octane</sub>/18=1.00/7:(1.72+0.51)/18=1.1:1),

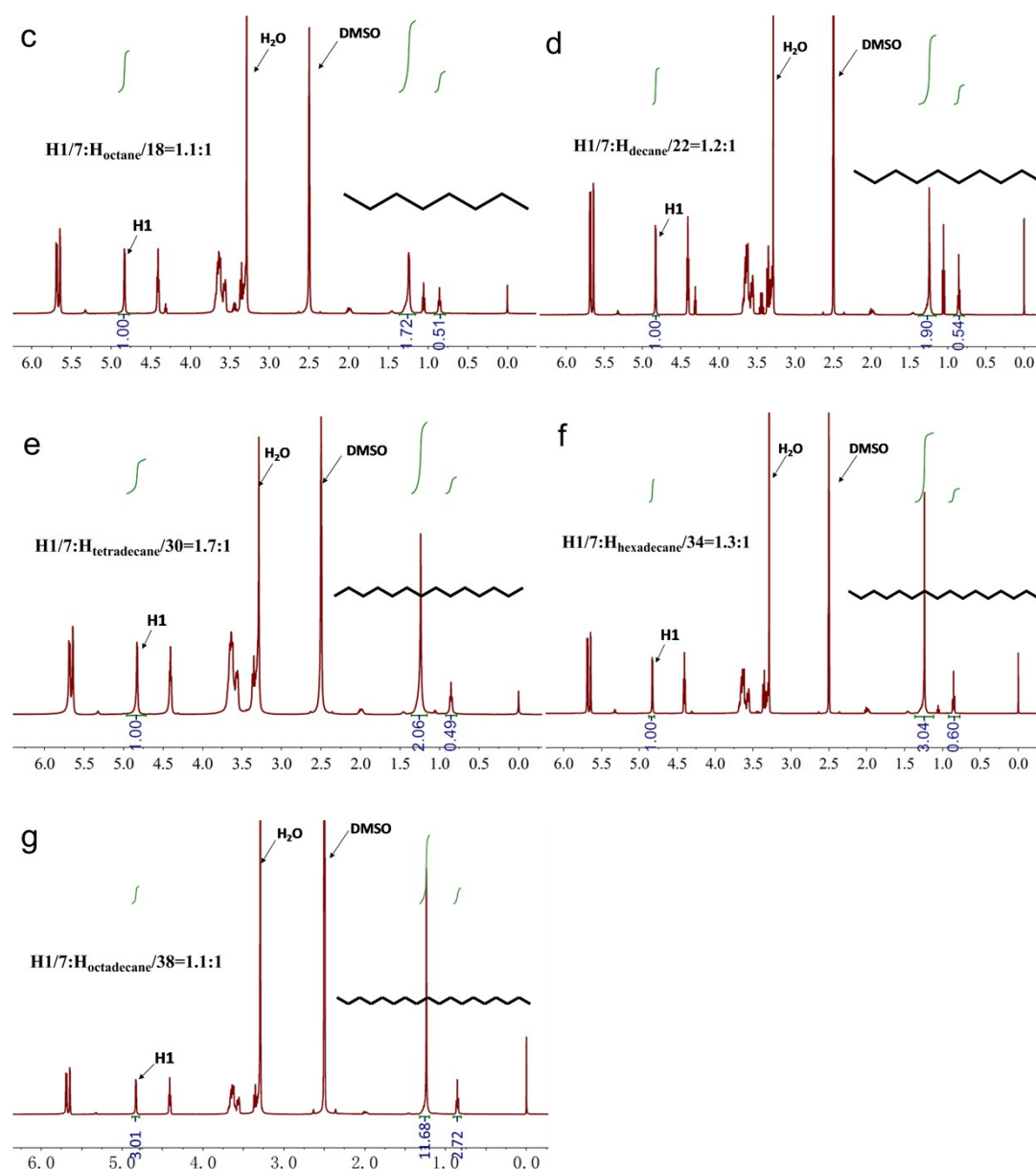
d) decane/ $\beta$ -CD (H1/7:H<sub>decane</sub>/22=1.00/7:(1.90+0.54)/22=1.2:1),

e) tetradecane/ $\beta$ -CD (H1/7:H<sub>tetradecane</sub>/30=1.00/7:(2.06+0.49)/30=1.7:1),

f) hexadecane/ $\beta$ -CD (H1/7:H<sub>hexadecane</sub>/34=1.00/7:(3.04+0.60)/34=1.3:1),

g) octadecane/ $\beta$ -CD (H1/7:H<sub>octadecane</sub>/38=3.01/7:(11.68+2.72)/38=1.1:1).



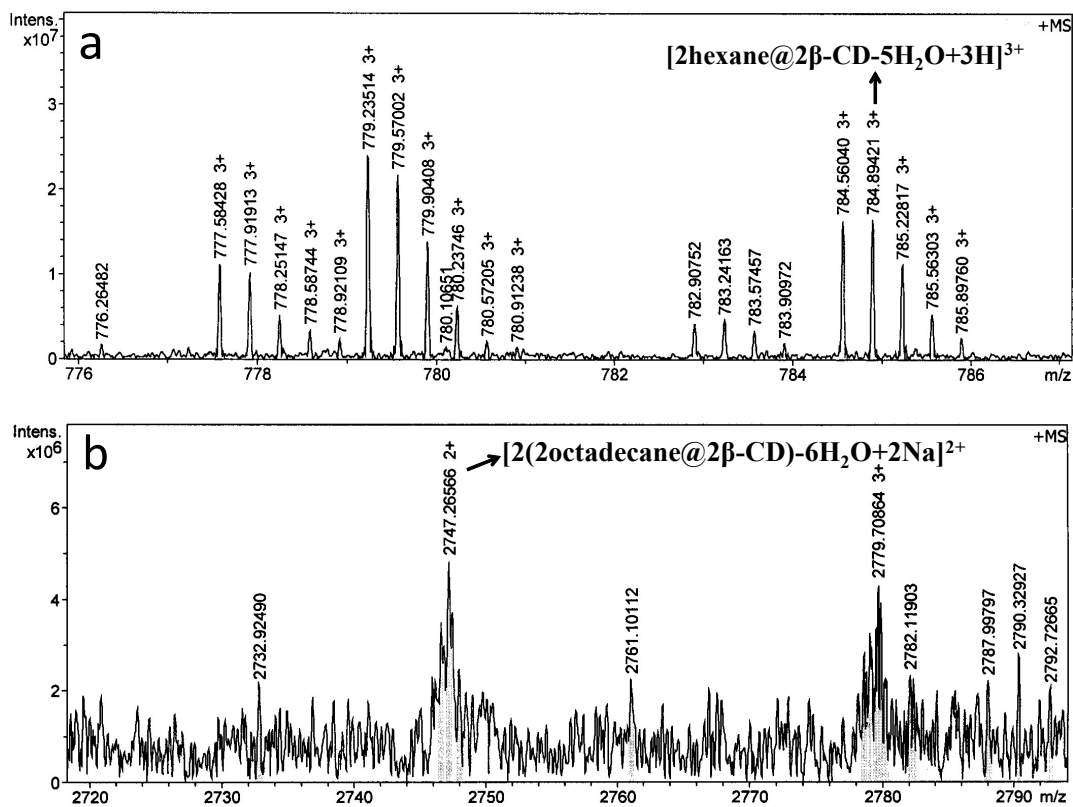


**Figure S1** a)-g) <sup>1</sup>H NMR spectra with assignments and integration of alkane/β-CD precipitates dissolved in DMSO-d<sub>6</sub> (alkane: pentane, hexane, octane, decane, tetradecane, hexadecane and octadecane, respectively).

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

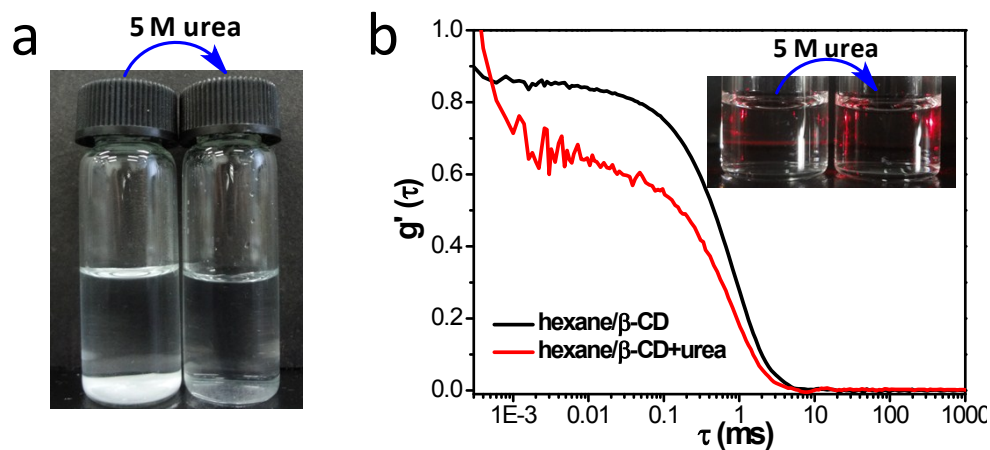
ESI-MS measurement of hexane/β-CD vesicle sample showed the presence of  $[2\text{hexane}@2\beta\text{-CD}-5\text{H}_2\text{O}+3\text{H}]^{3+}$  ( $m/z = 784.89421$ , the theoretical value  $m/z=784.97754$ ) (Figure S2a). In Figure S2b, octadecane/β-CD vesicle showed the presence of  $[2(2\text{octadecane}@2\beta\text{-CD})-6\text{H}_2\text{O}+2\text{Na}]^{2+}$  ( $m/z = 2747.26566$ , 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  $2\text{alkane}@2\beta\text{-CD}$  exceeds the upper

limit of 2000 for the HR-ESI-MS.



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

### 3. Addition of urea into the hexane/ $\beta$ -CD sample.



**Figure S3** a) The macrographs of hexane/ $\beta$ -CD sample ( $C_{\beta\text{-CD}}=16$  mM) and b) normalized intensity correlation function of hexane/ $\beta$ -CD vesicles sample with the macrographs of the scattering intensity (inset) before and after the addition of 5 M urea.