

Supporting Information for:

**Construction of a pH-sensitive self-assembly in aqueous solutions
based on a dansyl-modified β -cyclodextrin**

Bing Jiang, Yu Liu, Linlin Zhao, Li Zhao,* Ce Wang, Changyao Liu, Baocai Xu

School of Light Industry, Beijing Technology and Business University, Beijing 100048,
China. E-mail: zhaol@btbu.edu.cn.

Synthesis of β CD-C₆-Dns

β CD-C₆-Dns was synthesized by the following procedure. β CD-C₆ was synthesized according to literature. [1] β CD-C₆ (0.123 g, 0.1mmol) and triethylamine (0.06 mL, 0.4 mmol) were dissolved into DMF (20 mL), and the mixture was cooled at -10°C. A dansyl (0.03 g, 0.1 mmol) solution in DMF (10 mL) was added dropwise into above solution. After the addition, the mixture was stirred for 2 h at -10°C and then for 5 h at room temperature. Acetone was added into the reaction mixture, and a light brown solid was precipitated. β CD-C₆-Dns was obtained after filtration. The product was characterized by HR-MS (Fig. S1) and ¹HNMR (Fig. S2).

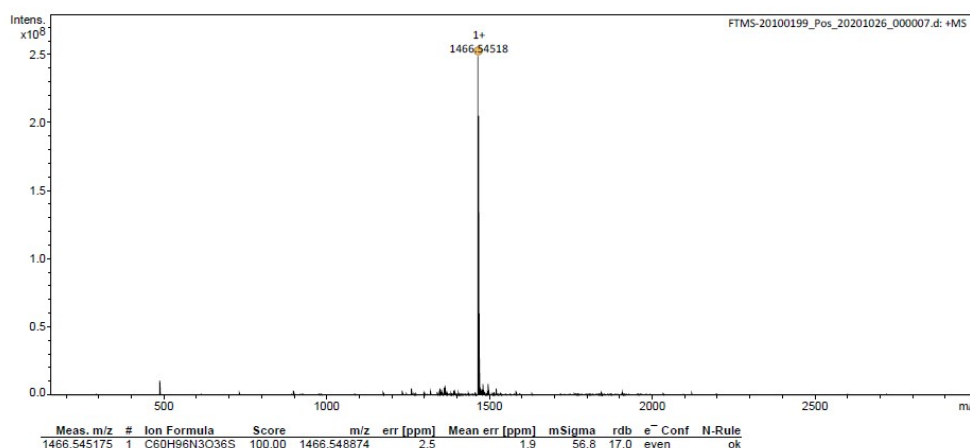


Fig. S1. FTMS result of β CD-C₆-Dns.

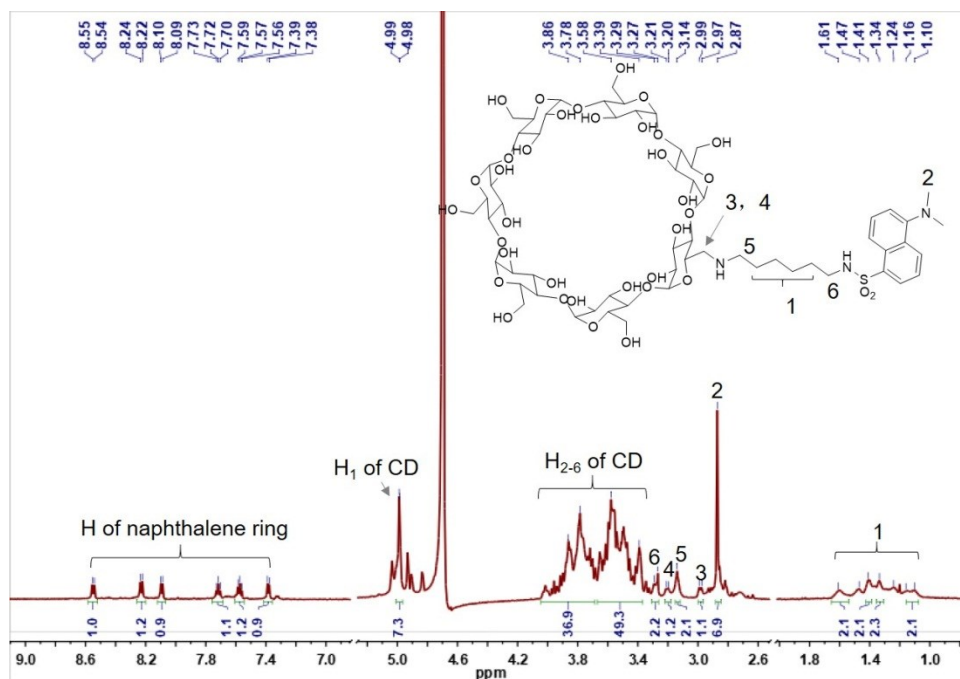


Fig.S2. ^1H NMR spectrum of $\beta\text{CD-C}_6\text{-Dns}$.

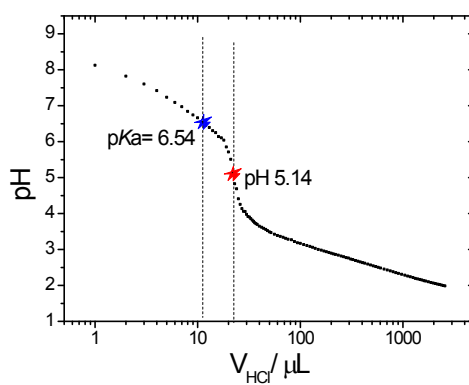


Fig. S3 The acid-base titration curve of $\beta\text{CD-C}_6\text{-Dns}$ solution (0.1 mM).

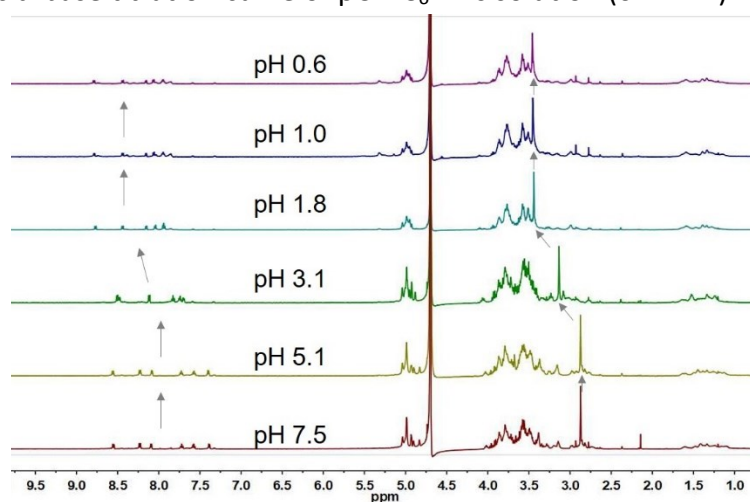


Fig. S4 ^1H NMR spectra of $\beta\text{CD-C}_6\text{-Dns}$ solution under various pH values.

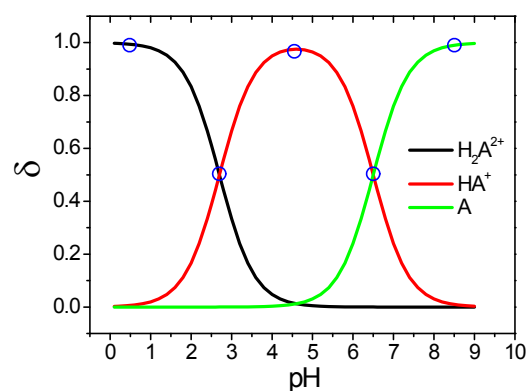


Fig. S5 Species distribution resulting from β CD- C_6 -Dns solution.

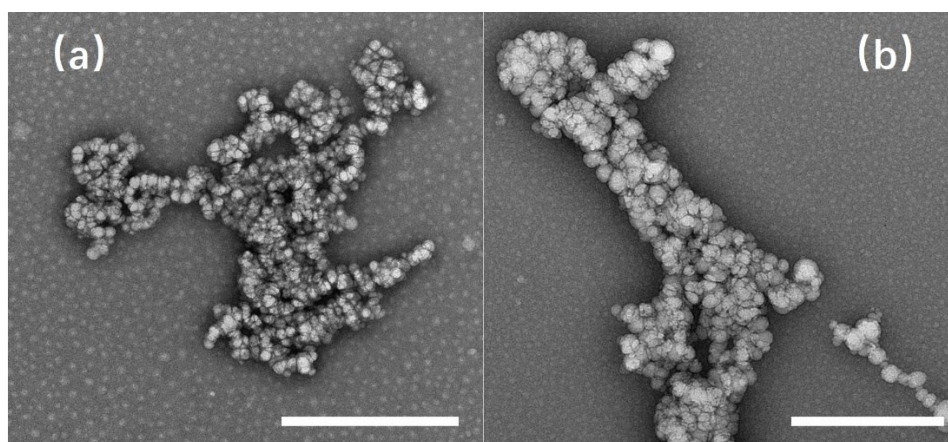


Fig. S6 TEM images of 1mM β CD- C_6 -Dns solution (pH 8.5) after aging for 5d (a) and 14d (b), respectively. The bar= 500 nm.

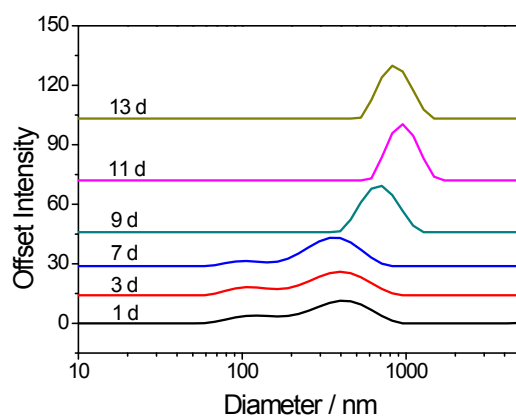


Fig. S7 Time-dependent size distribution of β CD- C_6 -Dns aggregates in 1 mM solution (pH 8.5).

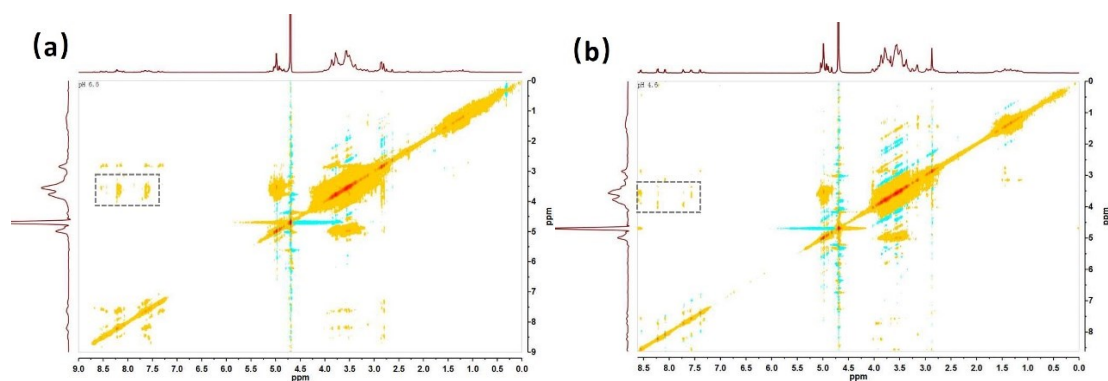
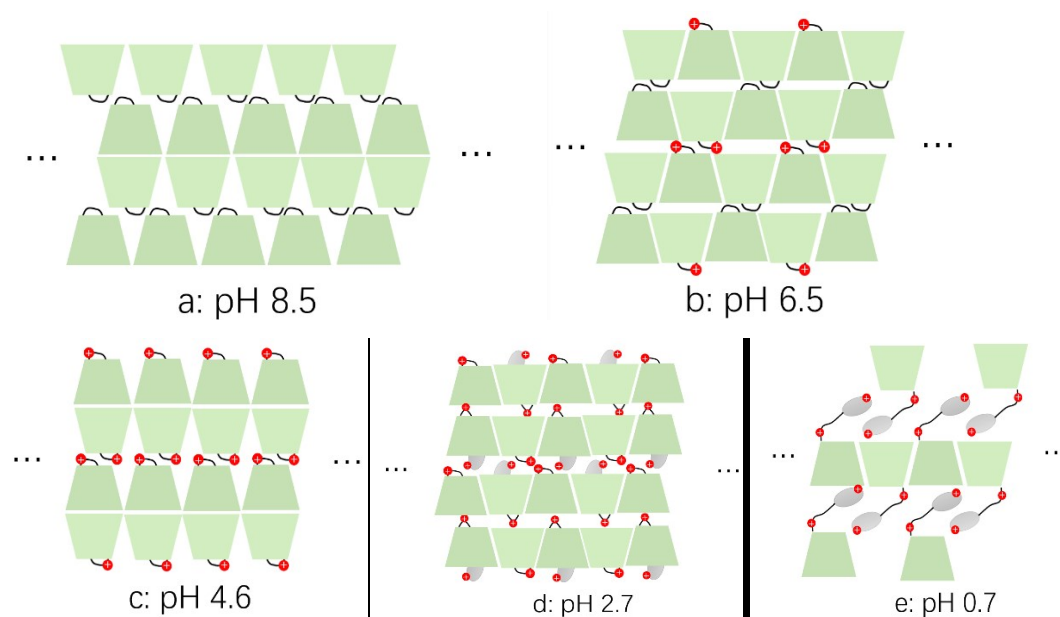


Fig. S8 NOESY spectra of β CD- C_6 -Dns solution at pH 6.5 (a) and pH 4.6 (b).

Table S1. The fluorescence lifetime of β CD- C_6 -Dns solution.

pH	τ_1/ns	A1/%	τ_2/ns	A2/%	χ^2
8.5	16.8	83.9	5.0	16.1	1.174
6.5	16.8	84.7	4.9	15.3	1.058
4.6	16.7	84.1	5.0	15.9	1.111
2.7	15.6	83.7	5.1	16.3	1.156



Scheme S1. Proposed schematic representation of the packing manner of β CD- C_6 -Dns vesicles.

Reference:

- [1] T. Sun, H. Zhang, L. Kong, H. Qiao, Y. Li, F. Kin, A. Hao, Controlled transformation from nanorods to vesicles induced by cyclomaltoheptaoses (beta-cyclodextrins), Carbohydrate Research, 346 (2011) 285-293.