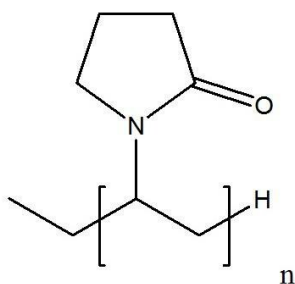
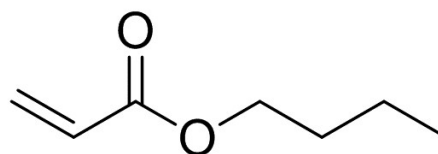


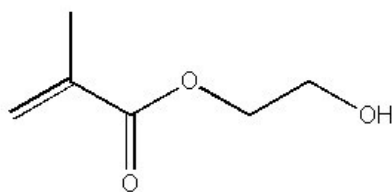
Supporting information 1: molecular formula



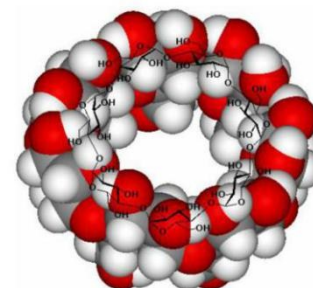
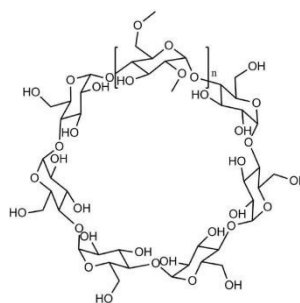
PVP



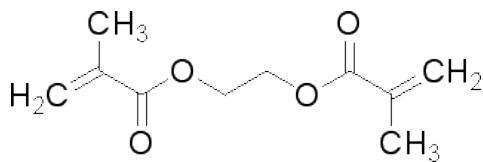
BA



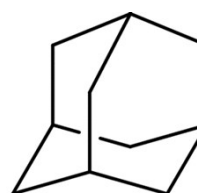
HEMA



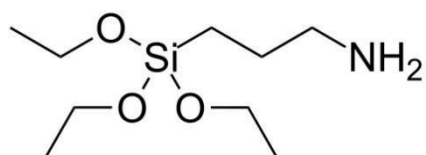
β -CD



EGDMA



Ad



APTES

Supporting information 2:

1. *Synthesis of guest molecule and host molecule*

1.1 Synthesis of guest molecule HEMA-Ad

2.3 g of Ad-COOH is dissolved in 50 mL of SOCl_2 and stirred at 90°C for 5 h to obtain 1-adamantanecarboxyl chloride. Then the 1-adamantanecarboxyl chloride is dissolved in 30 mL of CH_2Cl_2 . The reaction solution is prepared by dissolving 1 mL of HEMA and 1.6 mL of triethylamine in 100 mL of CH_2Cl_2 at 0°C , and 1-adamantanecarboxyl chloride is slowly dropped into the reaction solution. After washing with 1 mol/L hydrochloric acid solution, sodium bicarbonate and deionized water, respectively, anhydrous sodium sulfate is added. Lastly, HEMA-Ad is obtained after filtering and evaporating excess solvent.

1.2 Synthesis of host molecule CD- Al_2O_3 NPs

a) 50 g of β -CD is dispersed in 1200 mL deionized water. Then 13 g of TOS-Cl is added slowly under vigorous stirring. After that, 20 g NaOH is added. Then the solution is filtered to remove excess TOS-Cl. Ammonium chloride is added to the solution to pH 8. Lastly, the solution is placed at 4°C for 12 h and filtered to obtain TOS-CD.

b) 0.5 g $\text{NH}_2\text{-Al}_2\text{O}_3$ NPs are dispersed in 25 mL of DMSO solution. After stirring vigorously for 30 min, 8 g of TOS-CD is added. When the TOS-CD is completely dissolved, the solution should be adjusted to pH 7-8. Then the solution is placed to 65°C for 12 h under inert gas protection. After removing excess DMSO, the product is washed with ethanol to obtain CD- Al_2O_3 NPs.

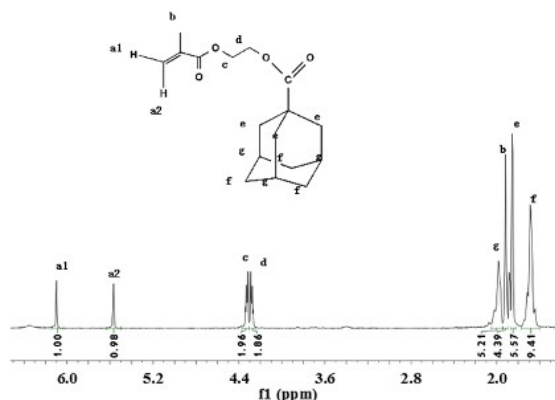
2. Characterization of guest molecule and host molecule

2.1 Characterization of adamantane grafted with HEMA

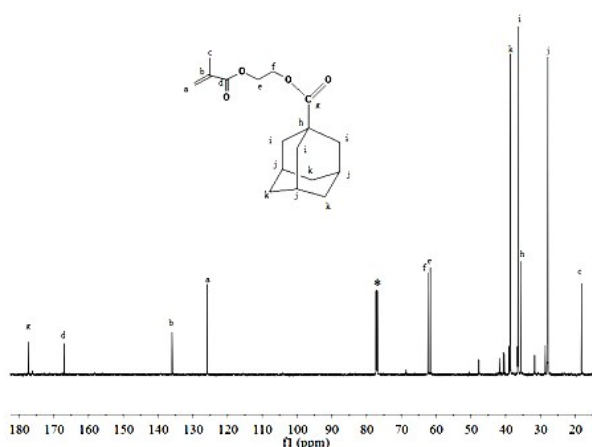
In order to test the effect of adamantane grafted with HEMA, the ^1H NMR and ^{13}C NMR spectra of the guest molecule HEMA-Ad were analyzed (shown in S 1a-b).

It can be found in **S 1a** that there are signal peaks at δ 6.09 (s, 1H), 5.55 (s, 1H), 4.31 (t, 2H), 4.26 (t, 2H), 1.68-1.92 (m, 15H). The peaks at 6.09 ppm and 5.55 ppm correspond to the hydrogen atoms of olefinic bond of 2-hydroxyethyl-methacrylate, and the ratio of their peak area is 1:1. The peaks at 4.31 ppm and 4.26 ppm (c and d) correspond to the methylene hydrogens that adjacent to ester bond, and the ratio of their peak area is also 1:1, indicating that the formation of ester bonds. The peak at 1.77 ppm corresponds to the hydrogen atom at the methylene (position "e") on adamantane, and the ratio of peak area of position "e" and "a" is 6:1, which is in accordance with the hydrogen number ratio of HEMA-Ad, indicating that the HEMA-Ad product is successfully prepared.

As shown in **S 1b**, two peaks at 177.40 ppm and 167.30 ppm correspond to the two carbonyl carbons, respectively, and 136.01 ppm and 125.90 ppm correspond to the two carbons on the double bond. The peaks at 62.40 ppm and 61.71 ppm correspond to the two carbon atoms on - $\text{OCH}_2\text{CH}_2\text{O}$ -. The four peaks from 38.59 ppm to 27.88 ppm correspond to the four types of carbon atoms on the adamantane. The peak at the 18.17 ppm corresponds to the methyl at position "c", which also demonstrates the successful preparation of the HEMA-Ad product.



S 1a ¹H NMR spectrum of HEMA-Ad



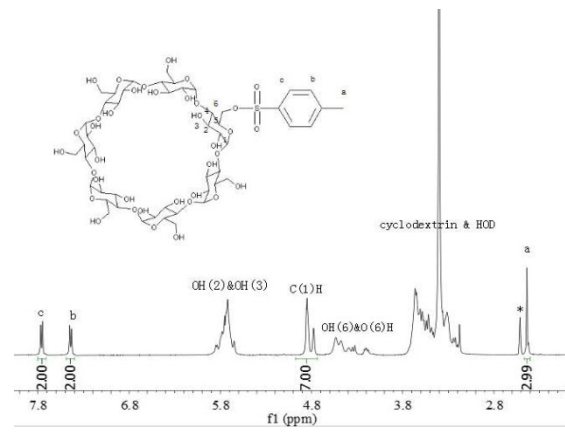
S 1b ¹³C NMR spectrum of HEMA-Ad

2.2 Characterization of CD grafted with TOS

To study the grafting effect of p-toluenesulfonyl chloride on cyclodextrin, ¹H NMR and ¹³C NMR spectra of TOS-CD were used. The results were shown in S 2a-b.

As **S 2a** shown, the peak at 2.39 ppm attributed to the methyl group that adjacent to the benzene ring. The peak at 4.30-4.55 ppm is the resonant peak of hydroxyl hydrogen that adjacent to C6 in the cyclodextrin. The peak at 4.75-4.96 ppm is the resonant peak of hydrogen bonded to C1 in the cyclodextrin. The peak at 5.61-5.80 ppm are the hydroxy hydrogen peak of C2 and C3. The two peaks at 7.41-7.7 ppm correspond to the absorption peak of the benzene ring in p-toluenesulfonyl chloride, which shift to the lower field because of adjacency of cyclodextrin. The ratio of the peak area of hydrogen atom, bonded to C(1) in the cyclodextrin (peak at 4.75-4.96 ppm), to the peak area of benzene ring proton in p-toluenesulfonyl chloride (peak at 7.71 mmp) is 7:2, which is in agreement with the theoretical ratio of hydrogen number, confirming the successful synthesis of TOS-CD.

The ¹³C NMR spectrum in **S 2b** shows that the four peaks at 144.83-1127.60 ppm ascribe to 4 carbon atoms in different chemical environment in the benzene ring of p-toluenesulfonyl chloride. The peak at 21.21 ppm is attributed to the carbon atom on the methyl group that bonded to the benzene ring. 101.96-59.94 ppm are the peaks of the cyclodextrin. It also proves that the product is successfully synthesized.



S 2a ^1H NMR spectrum of TOS-CD

S 2b ^{13}C NMR spectrum of TOS-CD