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## Thio[2-(benzoylamino)ethylamino]-b-CD Fragment Modified Gold Nanoparticles as Recycling Extractors for [60]Fullerene

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## Experimental.

## Measurements.

UV-Vis spectra were obtained on a Shimadzu UV-2401PC spectrophotometer equipped with a PTC-348WI temperature controller to keep the temperature at 25°C. Fluorescence spectra were measured in a conventional quartz cell ( $10 \times 10 \times 45$  mm) at 25°C on a JASCO FP-750 spectrometer equipped with a constant-temperature water bath, with the excitation and emission slits of 10 nm width for all measurement. FT-IR spectra were recorded on Bio-Rad FTS 135 instrument. TEM measurements were performed in a top-entry Philips EM300 microscope, operated at an accelerating voltage of 80 or 200 keV. The size distribution of the bis( $\beta$ -CD)-modified gold nanoparticles was determined from individual diameter measurements on at least 200 particles.

1: To a solution of DMF (100 mL) containing 4,4'-dithiobis(benzoic acid) (0.3 g) and dicyclohexyl-carbodiimide (DCC) (0.33 g) was added 3.0 g of mono[6-(2-aminoethylene amino)-6-deoxy]- $\beta$ -CD and 25 mL of dry pyridine in the presence of molecular sieves 4Å.

The resultant mixture was stirred for 12 h in an ice bath and another 18h at room temperature and then allowed to stand for 3 days until no more precipitation deposited. The precipitate was removed by filtration, and the filtrate was evaporated to dryness under reduced pressure. The residue was dissolved in a minimum amount of hot water and then poured into 300 mL of acetone. The precipitate formed was collected by filtration to obtain a brown powder, which was purified on a column of Sephadex G-25 to give 1.0 g (35 % yield) of **1** as a light brown solid. <sup>1</sup>H NMR (D<sub>2</sub>O, TMS, ppm):  $\delta$  2.69-2.88 (m, 8H); 3.24-3.72 (m, 84H); 4.86 (s, 14H); 6.85-7.97 (m, Ar 8H). <sup>13</sup>C NMR (D<sub>2</sub>O, ppm):  $\delta$  177.3, 130.4, 130.0, 127.3, 102.1, 83.3, 81.1, 73.2, 72.2, 71.9, 70.4, 60.2, 48.8, 46.0, 38.6. Anal. Calcd. for C<sub>102</sub>H<sub>158</sub>O<sub>70</sub>N<sub>4</sub>S<sub>2</sub>•16H<sub>2</sub>O: C, 42.06; H, 6.58; N, 1.92; S, 2.20. Found: C, 41.95; H, 6.78; N, 2.01; S, 2.16. IR (KBr): v<sub>max</sub>/cm<sup>-1</sup>: 3342, 2927, 1651, 1592, 1544, 1427, 1367, 1206, 1155, 1079, 1030, 945, 844, 778, 756, 707, 607, 579, 528.

2: A mixture of NaBH<sub>4</sub> (38 mg) and 1 (35.9 mg) in DMF (10 mL) was quickly added to a solution of HAuCl<sub>4</sub> (25 mg) in DMF (10 mL). The resultant deep brown mixture was stirred for 24h under N<sub>2</sub> atmosphere. Then the precipitate was collected by centrifugation and washed with DMF (4 × 30 mL). TLC experiment verified the complete removal of free bis( $\beta$ -CD) from this solid. The solid was further washed (4 × 30 mL) with ethanol/water (9:1, v/v), collected by centrifugation, and dried under vacuum for 24h at 50°C to give 48 mg of **2**.

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Figure S1. FT-IR spectra of (a)  $bis(\beta$ -CD) 1, (b) 1-modified gold nanoparticles 2. All spectra were recorded on KBr pellets.



Figure S2. Size distribution histogram of  $bis(\beta$ -CD)-modified gold nanoparticles 2.

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Figure S3. UV-vis spectra of (a) 2 (0.1 mg/mL) and (b)  $C_{60}/2$  assembly (0.1 mg/mL) (c) the

toluene extract of  $C_{60}/2$  assembly in aqueous solution.



Figure S4. Fluorescence spectra of (a) bis( $\beta$ -CD)-modified gold nanoparticles 2 (0.1mg/mL) and (b)

 $C_{60}/2$  assembly in aqueous solutions. Excitation wavelength: 299nm.

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Scheme S1