## **Supporting Information**

## A Catch-Release Catalysis System Based on Supramolecular Host-Guest Interactions

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**Figure S1**. (Top) <sup>1</sup>H NMR spectrum of carboxyl- $\beta$ -CD ( $\beta$ -CD-COOH) in D<sub>2</sub>O (300 MHz, 25 °C); (bottom) <sup>13</sup>C NMR spectrum of  $\beta$ -CD-COOH in DMSO-*d*<sub>6</sub> (75.5 MHz, 25 °C).



**Figure S2**. (Top) Representative histogram showing the size distribution of  $\beta$ -CD coated Fe<sub>3</sub>O<sub>4</sub> magnetic nanoparticles ( $\beta$ -CD-MNP) by DLS at room temperature in water (0.1 mg/mL, pH 6.0, at least 3 individual measurements); (bottom) Zeta potential measurement for  $\beta$ -CD-MNP by DLS at room temperature in water (0.1 mg/mL, pH 6.0, at least 3 individual measurements).



**Figure S3**. Characterization by pXRD (in solid) and DLS (in water, room temperature) for bare MNP (top) and succinate MNP (bottom). Conditions for DLS: 0.1 mg/mL, pH 6.0, at least 3 individual measurements.



**Figure S4.** Calibration curve of absorbance versus concentration of catalyst (Ad-L-PdCl<sub>2</sub>) in  $H_2O$ -CH<sub>3</sub>OH (2/1, v/v) (Cuvette: quartz; slit width: 1.0 nm; wavelength range: 200 nm – 800 nm; absorption peak: 209 nm; room temperature).



**Figure S5.** SEM-EDS analysis of separated  $\beta$ -CD-MNP from the mixture of catalyst and  $\beta$ -CD-MNP in H<sub>2</sub>O-CH<sub>3</sub>OH (2/1, v/v). Amount of catalyst (before catch): 0.35 mg in H<sub>2</sub>O-CH<sub>3</sub>OH (2/1, v/v), 1.5 mL;  $\beta$ -CD/Ad molar ratio: 0.70; room temperature.



**Figure S6.** Calibration curve of absorbance versus concentration of catalyst (Ad-L-PdCl<sub>2</sub>) in methanol (Cuvette: quartz; slit width: 1.0 nm; wavelength range: 200 nm - 800 nm; absorption peak: 209 nm; room temperature).



**Figure S7.** SEM-EDS analysis of separated  $\beta$ -CD-MNP from the mixture of a Suzuki-Miyaura coupling reaction filtrate and  $\beta$ -CD-MNP in H<sub>2</sub>O-CH<sub>3</sub>OH (2/1, v/v). Initial catalyst loading: 0.35 mg in H<sub>2</sub>O-CH<sub>3</sub>OH (2/1, v/v), 1.5 mL;  $\beta$ -CD/Ad molar ratio: 2.0; room temperature.