

## Electronic supplementary information (ESI)

### **Plastic antibody for DNA damages: Fluorescent imaging of BPDE-dG adducts in genomic DNA**

**Junfa Yin, Zhixin Wang, Maoyong Song, Chao Zhao and Hailin Wang\***

*State Key Laboratory of Environmental Chemistry and Ecotoxicology, Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences, Beijing, 100085, China. Fax: +86 10 62849600; Tel: +86 10 62849611; E-mail: hlwang@rcees.ac.cn*

## 1. Rebinding assay

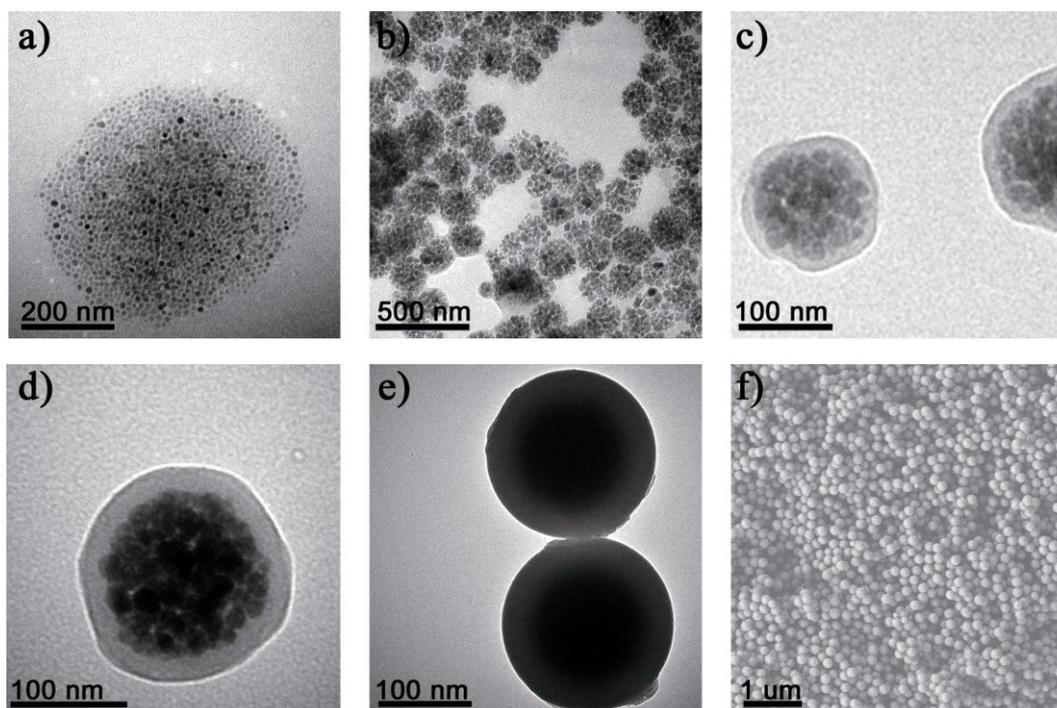
Rebinding experiment was carried out for investigation of binding properties of nanoMIP. The synthetic nanoMIP (10 mg) was immersed into 1.0 mL of a series of known concentration of BPDE-DNA adduct solutions in polypropylene vials. These vials were continuously shaken at 25°C for 6 h, and then centrifuged at 3000 × g for 10 min. The concentration of free BPDE-DNA adduct in the supernatant was determined by HPLC-FL detection ( $\lambda_{\text{ex}} = 343 \text{ nm}$ ,  $\lambda_{\text{em}} = 400 \text{ nm}$ ). The amount of BPDE-ssDNA adducts bound to nanoMIP,  $Q$ , was calculated from multiplying the concentration difference by solution volume. Binding isotherms were measured for BPDE-16merG16 (probe **6**) in the concentration range of 0.05 - 2.5  $\mu\text{M}$ , and for BPDE-16merG9 (probe **7**) in the concentration range of 0.1 - 2.5  $\mu\text{M}$ .

Binding kinetic profiles were investigated according to our previous work (*Chem. Commun.*, 2010, 46, 7688). The prepared nanoMIP (10 mg) was suspended in 1.0 mL DNA solutions containing either BPDE-16merG16 adduct or the unmodified 16merG16 oligonucleotides (initial concentration, 1.0  $\mu\text{M}$ ). Aliquots of 10  $\mu\text{L}$  of DNA solutions were taken out and subjected to HPLC analysis at different intervals (0 - 240 min), then the binding amounts could be calculated. Plotting the binding amount of BPDE-16merG16 adduct (or 16merG16) versus the binding time, the binding kinetic profiles could be obtained.

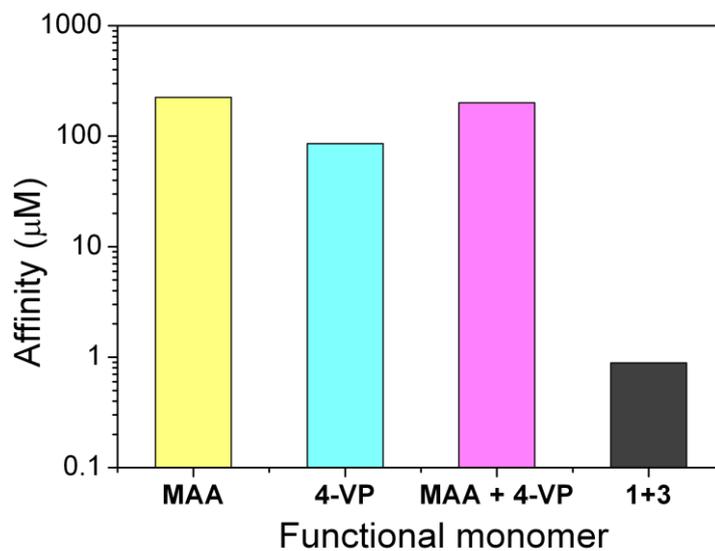
## 2. MALDI-TOF/MS analysis

The captured BPDE-16merDNA was desorbed from the  $\text{Fe}_3\text{O}_4\text{@MIP}$  nanocomposites with PBS buffer (containing 5% methanol), and then identified by MALDI-TOF/MS. DNA samples (1.0  $\mu\text{L}$ ) were mixed with 2.0  $\mu\text{L}$  of AA/NA/DHC (anthranilic acid/nicotinic acid/diammonium hydrogen citrate) matrix solution, and then deposited onto a 384-well AnchorChip MALDI plate (Bruker Daltonics, Billerica, MA, USA) immediately, which was allowed to stand for 15 min to dry and crystallize naturally. AA/NA/DHC matrix consists of 3.0 mg (20  $\mu\text{mol}$ ) AA, 1.5 mg (10  $\mu\text{mol}$ ) NA and 6  $\mu\text{L}$  DHC (10 mM) in 80 mL

acetonitrile/water (50:30, v/v), with the final molar ratio of AA/NA/DHC = 2:1:0.003. Mass spectra were acquired on a Bruker Autoflex III Smartbeam MALDI-TOF MS (Bruker Daltonics, Germany) equipped with a nitrogen laser operating at 337 nm. Linear positive-ion mode was employed. The total acceleration voltage was 20 kV. In the range of  $m/z$  100-6000, the mass spectra were obtained with 70%-80% laser energy, 70%-90% laser attenuation,  $2 \times 10^{-6}$  mbar vacuum and 200 Hz trigger frequency. Spectra were accumulated from 200 laser shots, and 200 ns extraction delay time was used for data acquisition.



**Figure S1.** TEM images for a) magnetic Fe<sub>3</sub>O<sub>4</sub> nanoparticles (10 nm) in Span 80 miniemulsion, b) nFe<sub>3</sub>O<sub>4</sub>@SiO<sub>2</sub> nanocomposites, and nanoMIP with a shell thickness of c)10 nm, d) 20 nm and e) 40 nm, and f) SEM image for the fabricated nanoMIP (the diameter is ca.160 nm).



**Figure S2.** Different functional monomers produce different affinities of the fabricated nanoMIP towards BPDE-16merG16 adduct. Abbreviations for these functional monomers are: MAA, methacrylic acid; 4-VP, 4-vinylpyridine; **1**, the allylated guanine (G-); **3**, the allylated *p-tert*-butylcalix[6]arene (calix[6]arene-).