

Supplemental Figure 1. High-resolution x-ray photoelectron spectroscopy spectra of ATP@SPION. The peaks for the iron in ATP@SPIONs were observed at binding energy 715 eV (2p3) and 727 eV (2p1). A single N peak for the adenine rings and P 2p peak for the phosphate groups in ATP@SPIONs were obtained at 398.3 eV and 132.7 eV, respectively. The O 1s peaks were observed at binding energy 529.5, 530.7, 531.5, and 532.7 eV (C–O–C). These peaks match the main peaks of ATP and iron particles, which would allow us to assign ATP@SPIONs.



Supplemental Figure 2. Photographs of ATP@SPION and Feridex in various pH solutions.



Supplemental Figure 3. Fourier transform-infrared spectroscopy spectra of bare SPION (black line), ATP@SPION (blue line), and GA-ATP@SPION (red line). After GA conjugation, the specific peaks were observed at 870–906 cm⁻¹ (CH₂CH₃), 1,064 cm⁻¹ (C–N), 1,469 cm⁻¹ (N–H), 1,563 cm⁻¹ (C=O), and 2,797 cm⁻¹ (C–H).



Supplemental Figure 4. Cytotoxicity of GA-ATP@SPIONs on CHO cells and MDA-MB231 cells.

The results are represented as mean values (n = 4).



Supplemental Figure 5. Microscopic images of RAW cells stained after incubation for 1 h in the presence of 50 µg ATP@SPIONs (A) or GA (0.05 µmol [B], 0.25 µmol [C], and 1.26 µmol [D])-ATP@SPIONs. The blue-stained dots indicate the presence of iron. The percent of iron-positive cells to all cells was 73%, 36%, 34%, and 10% for ATP@SPIONs and 0.05, 0.25, and 1.26 µmol GA-ATP@SPIONs, respectively.



Supplemental Figure 6. Microscopic images of organs, such as liver, lung, spleen, and kidney, of mice stained at 1 h after injection of ATP@SPION or GA-ATP@SPION. The blue-stained dots indicate the presence of iron.



Supplemental Figure 7. In vitro U87MG cellular binding of ¹²⁵I-cMBP-conjugated GA-ATP@SPION. In the blocking study, cMBP significantly reduced the cellular binding of ¹²⁵I-cMBP-conjugated GA-ATP@SPION (*P < 0.001). The data represent the mean \pm SD (n = 4).



Supplemental Figure 8. Biodistribution of ¹²⁵I-cMBP–conjugated GA-ATP@SPION in U87MG cell– bearing mice at 3 h after injection. The data represent the mean \pm SD (n = 4).



Supplemental Figure 9. In vivo T_2 -weighted MR images of the mice with U87MG tumors before (A) and at 3 h after (B) the injection of GA-ATP@SPIONs.