

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 $532.7 \mathrm{eV}(\mathrm{C}-\mathrm{O}-\mathrm{C})$. 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 $870-906 \mathrm{~cm}^{-1}\left(\mathrm{CH}_{2} \mathrm{CH}_{3}\right), 1,064 \mathrm{~cm}^{-1}(\mathrm{C}-\mathrm{N}), 1,469 \mathrm{~cm}^{-1}(\mathrm{~N}-\mathrm{H}), 1,563 \mathrm{~cm}^{-1}(\mathrm{C}=\mathrm{O})$, and $2,797 \mathrm{~cm}^{-1}(\mathrm{C}-\mathrm{H})$.


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 $50 \mu \mathrm{~g}$ ATP@SPIONs (A) or GA $(0.05 \mu \mathrm{~mol}[\mathrm{~B}], 0.25 \mu \mathrm{~mol}$ [C], and $1.26 \mu \mathrm{~mol}$ [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 $1.26 \mu \mathrm{~mol}$ GAATP@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 ${ }^{125} \mathrm{I}-\mathrm{cMBP}$-conjugated GAATP@SPION. In the blocking study, cMBP significantly reduced the cellular binding of ${ }^{125} \mathrm{I}$ -cMBP-conjugated GA-ATP@SPION $(* P<0.001)$. The data represent the mean $\pm$ SD $(n=4)$.


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


Supplemental Figure 9. In vivo $\mathrm{T}_{2}$-weighted MR images of the mice with U87MG tumors before (A) and at 3 h after (B) the injection of GA-ATP@SPIONs.

