Supporting information for

Mesoporous silica nanoparticles functionalized with Fluorescent and MRI reporters for the visualization of murine tumors overexpressing $\alpha_v\beta_3$ receptors

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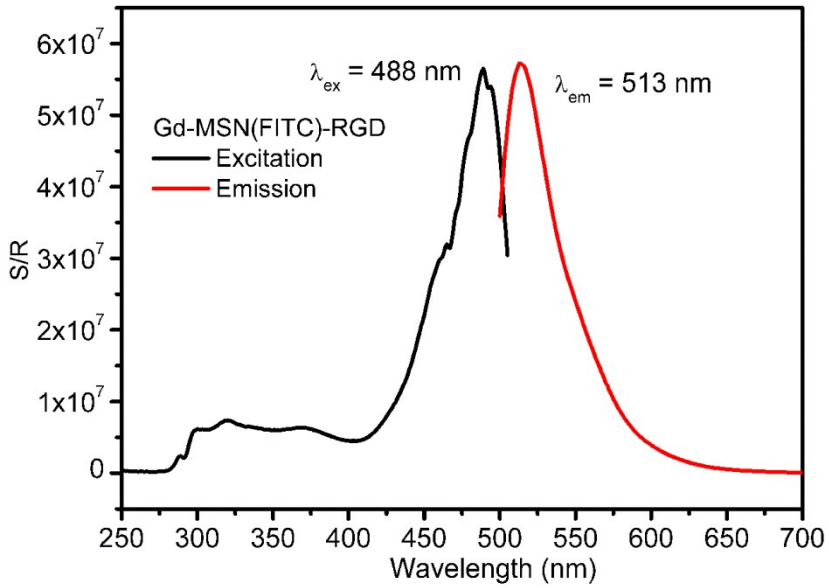


Figure S1. The room-temperature (R.T.) absorption and emission spectra of Gd-MSNs-RGD in aqueous solution with concentration of 50 μg/mL.

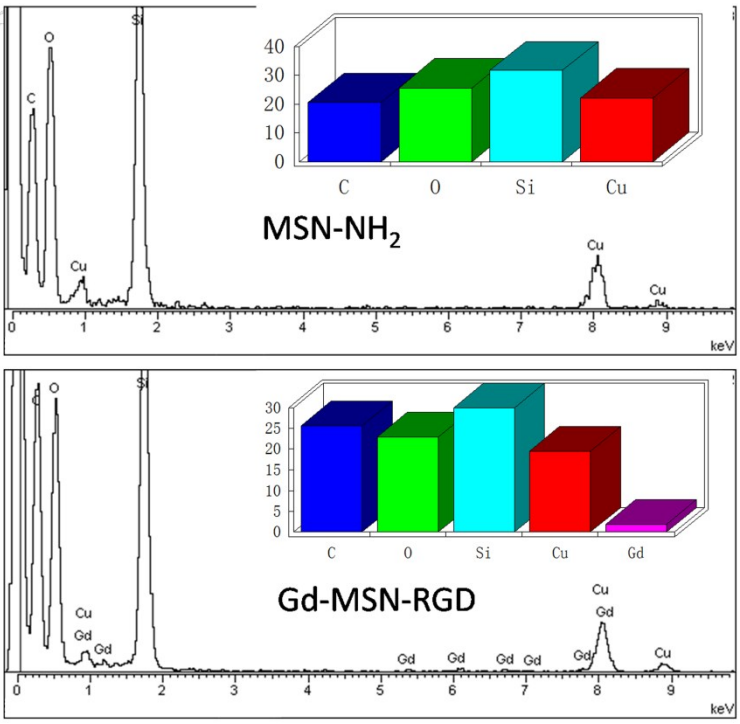


Figure S2. The Energy dispersive x-ray analysis (EDXA) spectrum of original MSNs-NH_2 and final nanoprobe Gd-MSNs-RGD obtained during TEM observation.

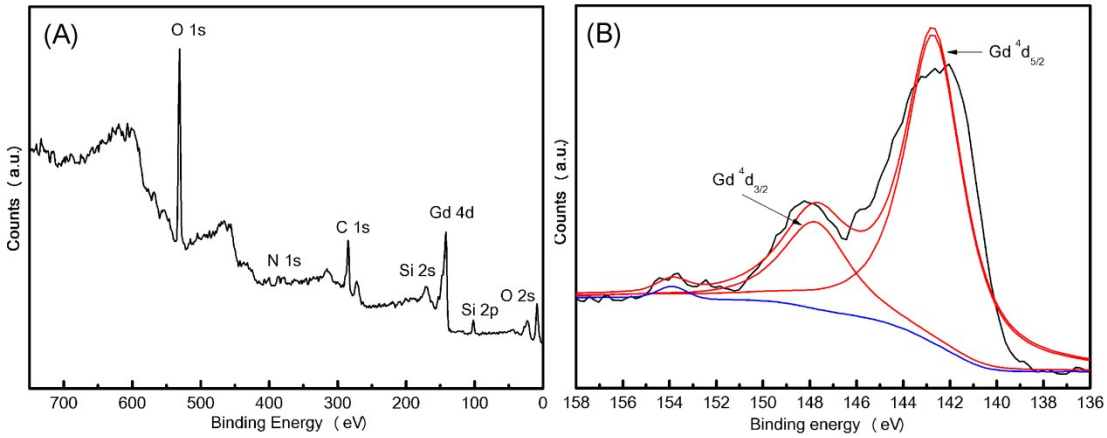


Figure S3. The XPS wide-scan and high-resolution spectra of Gd-MSNs-RGD nanoprobe.

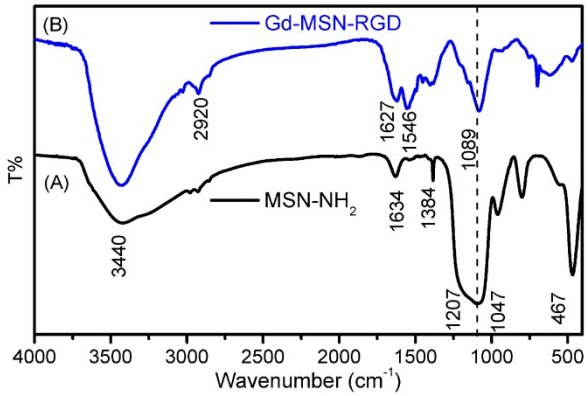


Figure S4. The FTIR of MSNs-NH_2 and Gd-MSNs-RGD.

The strong and broad band in the range of 1207 ~1047 $cm^{-1}$and a relative weak peak at 460 cm^{-1}, corresponding to the Si-O-Si asymmetric (ν_{as}) stretching vibration from the SiO_2 matrix. The characteristic absorption peak at 1634 cm^{-1} can be assigned to N-H deformation vibrations. The characteristic bond of amino groups should be at 3200 cm^{-1} that may be covered by the strong absorption of H-O and Si-O vibration. After further reaction with Mal-PEG27-NSH, the new peaks at ν =1546 and 1627 cm^{-1} attributed to the vibration of imide-bond appear in Figure S3B, and the sharp peak at 1089 cm^{-1} belongs to the C-O-C stretching vibration from the PEG chains, thus corroborating successful synthesis of the Gd-MSNs-RGD by this strategy.

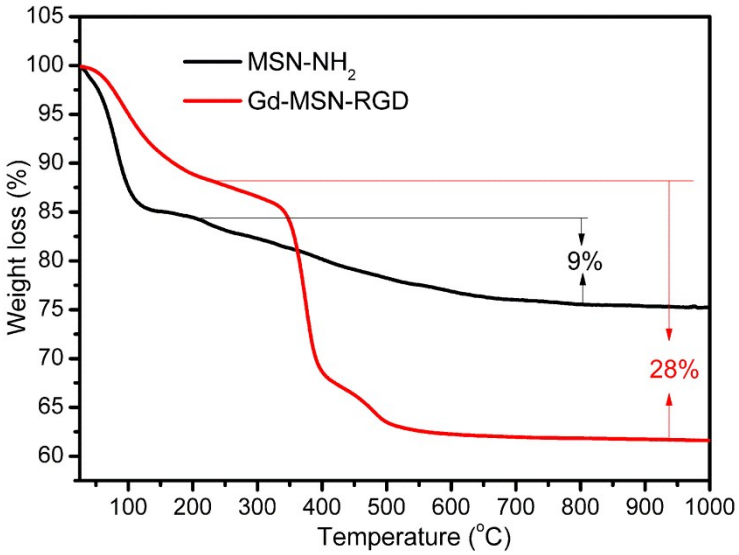


Figure S5. Thermal gravimetric analysis (TGA) of MSNs-NH_2 and Gd-MSNs-RGD.

The early weight loss at temperatures below 150 °C is seen from TGA curve due to loosely bound water, followed by a steady weight loss from about 300 to 550 °C were mainly due to the decompositions of organics (aminopropyl groups and PEG chains). The organics content of MSNs-NH_2 and Gd-MSNs-RGD is 9 % and 28 % respectively. The conjugated Gd^{3+}-DOTAGA, PEG and RGD was about 19 % according to the TGA data.

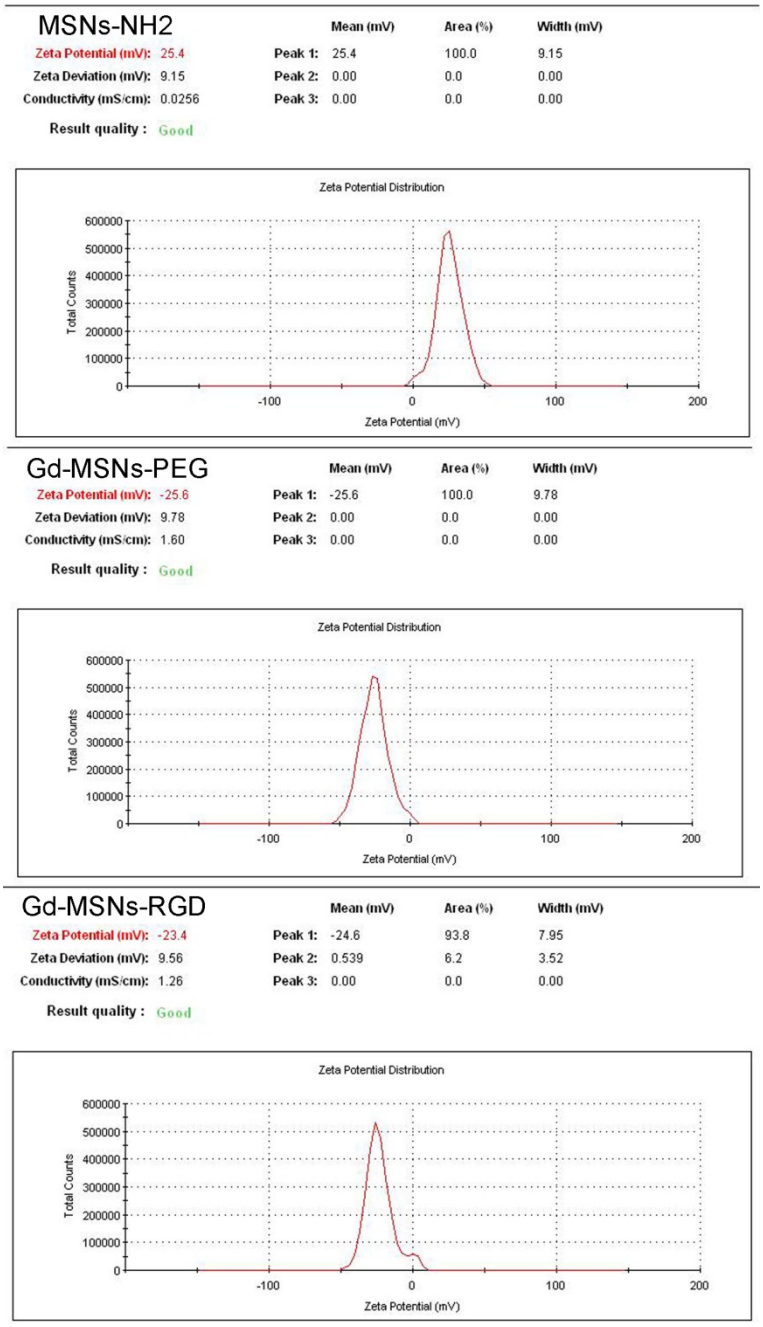


Figure S6. The zeta-potential of MSNs-NH_2, Gd-MSNs-PEG and Gd-MSNs-RGD in PBS buffer at neutral pH monitored after each functional process.

Calculation of the graft density of -NH_2 and final RGD on the surface of MSNs-NH_2 and Gd-MSNs-RGD:

The density of grafted -NH_2 is expressed as d_{NH2}. It was determined as follows:

$$d_{NH2} = \frac{amount\ of\ NH_2\ (mol\ g^{-1}) \times m_{MSN} \times N_A}{S_{MSN}}$$, (equation 1)

Where the N_A is the Avogadro constant, m_{MSN} is the mass of each MSN:

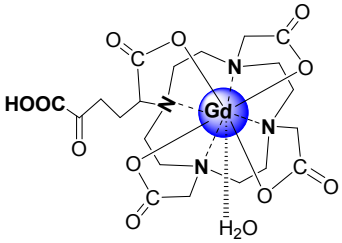
$$m_{MSN} = \rho_{SiO_2} \times \frac{4\pi r^3}{3}, \text{ (equation 2)}$$

The ρ_{SiO_2} is density of silica, and r is the radius of MSNs as obtained from the TEM image,

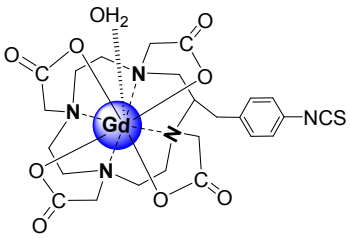
The S_{MSN} is the surface area of each MSN $(4\pi r^2)$ (equation 3)

By substituting Eq.2 and Eq.3 into Eq.1, one obtains:

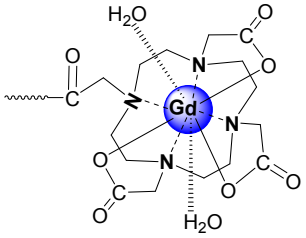
$$d_{NH2} == \frac{amount\ of\ NH_2\ (mol\ g^{-1}) \times \rho_{SiO_2} \times r \times N_A}{3}$$



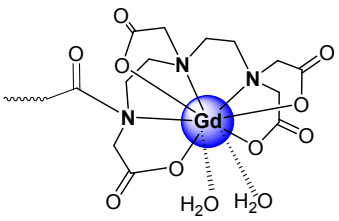
Gd-DOTAGA in this work



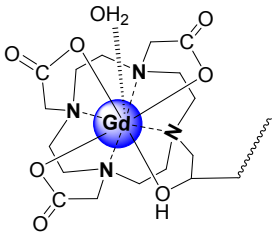
Gd-DOTA Ref. 5



Gd-DOTA Ref. 3, 6, 7,8



Gd-DTPA Ref. 9,11,28



Gd-HPDO3A Ref.29

Figure S7.The molecular structures of the Gd-complexes cited in the manuscript.