## **Supplementary Material (ESI)**

**Figure S1.** Nitrogen adsorption-desorption isotherms of (a) A647@MSN, (b) A647@MSN-PEG, and (c) A647@MSN-RGD



**Figure S2.** X-Ray diffraction (XRD) patterns of (a) A647@MSN,and (b) A647@MSN-RGD-PdTPP.



**Figure S3.** Thermogravimetric analyses (TGA) profiles of (a) A647@MSN, (b) A647@MSN-PEG, and (c) A647@MSN-RGD



## Quantification of immobilized functional groups on MSNs

To determine the amounts of functional groups on the surface of A647@MSN, such as NHS-PEG<sub>24</sub>-maleimide (MW 1394) and RGDyK molecule, the thermogravimetric analyses (TGA) was performed as shown in Figure S3. The PEG-maleimide was conjugated to MSNs via amide bond, therefore the maleimide groups were directly correlated to the weigh loss of PEG by heating above 280 °C. The weight loss of A647@MSN-PEG and A647@MSN-RGD were 19% (equal to 238.3  $\mu$ mole/g of MSN) and 24% respectively as indicated in Figure S2-(b) and (c). The 5% difference in weight loss was contributed by RGD molecules (equal to 112.8  $\mu$ mole/g of MSN). Given that, the proportion of RGD peptide/maleimide groups could be calculated as 0.474.

The amounts of Atto-647N and PdTPP incorporated in frameworks and nanochannels of MSN were quantified by UV-Vis spectroscopy. All quantitative amounts of immobilized functional groups on MSNs were summarized in Table S1.

Table S1				
Samples	Atto647	PEG	RGDyK	PdTPP
A647-MSN-PEG	2.58	238.3		
A647-MSN-RGD	2.58	238.3	112.8	
A647-MSN-RGD-PdTPP	2.58	238.3	112.8	49.2

(unit: µmole/g of MSN)