SUPPORTING INFORMATION

for

Noncovalent functionalization of mesoporous silica nanoparticles with amphiphilic peptides

Melis Sardan,^{$\ddagger a,b$} Adem Yildirim,^{$\ddagger a,b$} Didem Mumcuoglu,^{a,b} Ayse B. Tekinay,^{$\ast a,b$} and Mustafa O. Guler^{$\ast a,b$}



Fig. S1 Fluorescence spectra of MSNs showing the successful FITC conjugation to the silica network.



Fig. S2 (a) Liquid chromatogram of Lauryl-PPPPGE-OH; (b) Mass spectrum of corresponding peptide amphiphile molecule. Mass data $[M-H]^-$ (calculated) = 773.45, $[M-H]^-$ (observed) = 773.41 (observed $[M-2H]^{-2}$ m/z = 386.20)



Fig. S3 (a) Liquid chromatogram of Lauryl-PPPPGK-Am; (b) Mass spectrum of corresponding peptide amphiphile molecule. Mass data $[M+H]^+$ (calculated) = 773.52, $[M+H]^+$ (observed) = 773.53 (observed $[M+2H]^{+2} m/z = 387.27, [2M+H]^+ = 1546.04)$



Fig. S4 TEM image of the K-PA coated OMSNs.



Fig. S5 DLS spectra of MSN, E-OMSN and K-OMSN

S1. Calculation of grafting density

We calculated the peptide grafting density on OMSN as^{1,2};

We assumed that OMSNs are spherical in shape and their average diameter is 100 nm based on the TEM images.

Volume of single OMSN = $\frac{4}{3}\pi r^3$ = 5.23x10⁻¹⁶ cm³/ # of OMSN

Density of amorphous silicon is 2.65 g/cm³ and pore volume of OMSNs is 1 cm³/g according to our previous work.³ Thus, number density of OMSN per gram (x) can be calculated by:

$$x = \frac{\left[\frac{1}{2.65} \left(\frac{cm^3}{g}\right) + 1\left(\frac{cm^3}{g}\right)\right]}{5.23x10^{-16} \left(\frac{cm^3}{\# of \ OMSN}\right)} = 2.63x10^{15} \left(\frac{\# of \ OMSN}{g}\right)$$

By using the TGA results, we calculated amount of peptide amphiphile (PA) per gram of OMSN for both E-PA and K-PA coated particles. For MSN, OMSN, E-OMSN and K-OMSN, weight losses (wt %) at 800 °C are 7.8%, 11.9%, 19.6% and 32.5%, respectively.

Gram of peptide per OMSN can be calculated by using the following equation;

$$\frac{(W_{peptide \,OMSN} - W_{OMSN})}{100 - W_{MSN}} x \frac{100}{(100 - W_{MSN}) - (W_{peptide \,OMSN} - W_{OMSN})} = x \left(\frac{g \, of \, peptide}{g \, of \, OMSN}\right)$$

,where W is the weight loss in percentage of corresponding particle.

Accordingly, for E-OMSN and K-OMSN gram of peptides per gram of OMSN values were calculated as 0.099 and 0.312, respectively. Molecular weights of E-PA and K-PA are 774 g/mol and 772 g/mol, respectively. Using the following formula, number of peptides per OMSN can be calculated:

 $\frac{g \ of \ peptide \ perg \ of \ OMSN}{Mw_{peptide}} x \ Avogadro \ number}{2.63 x 10^{15}}$

Numbers of peptides per OMSN were found as 29360 and 92770 for E-OMSN and K-OMSN, respectively.

Surface area (SA) of single OMSN was calculated with the assumption of smooth particle surface which follows as:

$$SA_{OMSN} = 4\pi (50 \text{ nm})^2 = 3.14 \text{x} 10^4 \text{ nm}^2$$

Finally, grafting densities (# of peptides/nm²) were calculated as 0.94 and 2.95 for E-OMSN and K-OMSN, respectively.

Supporting References:

1. M. Kar, P. S. Vijayakumar, B. L. V. Prasad, and S. S. Gupta, *Langmuir*, 2010, **26**(8), 5772–5781.

2. D. Kim, S. Finkenstaedt-Quinn, K. R. Hurley, J. T. Buchman and C. L. Haynes, *Analyst*, 2014, DOI: 10.1039/c3an01679j

3. A. Yildirim, G. B. Demirel, R. Erdem, B. Senturk, T. Tekinay and M. Bayindir, *Chem. Commun.*, 2013, **49**, 9782-9784