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Electronic Supporting Information

Core vs surface labelling of mesoporous silica nanoparticles: advancing the understanding of nanoparticle fate and design of labelling strategies.

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Characterization of MSNs

ESI Figure 1 (A) Dynamic light scattering of MSNs at 0.2 mg mL^{-1} in saline of MSNs functionalized with APTES prior to the PEGylation reaction and (B) thermogravimetric analysis of MSNs-NH_2 and MSNs-PEG_{5000}

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^{89}Zr Labelling

Radiochemical incorporation is enhanced when the MSNs are incubated with zirconium before the PEGylation step at temperatures of 25, 40, 70 and 90 °C degrees after 1 hour of incubation. The incubation time was evaluated at 10, 30, 60 and 90 min at 70 °C. The optimal incubation time was 60 min with no significant increase in radiochemical incorporation observed for longer incubation periods. The incorporation of zirconium was performed at concentrations between 2 and 10 mg mL^{-1} in HEPES buffer at pH 7.4 with similar results.

ESI Figure 2 (A) Scheme of the radiolabelling optimization integration procedure for incorporating of ^{89}Zr on MSNs, before and after PEGylation with PEG 5000 Da. (B) % radiochemical incorporation (RCI) for different MSNs at different temperatures after 1 hour of incubation at different temperatures and (C) % RCI for MSNs-NH_2 incubated with ^{89}Zr at 70 °C for different incubation times.

In vitro p32 expression

ESI Figure 3 Confocal images of B16F10 melanoma cells. Nucleus is stained with blue DAPI, p32 protein overexpressed on the membrane of the cells (green channel) and incubated with MSNs-(RhB)-PEG_{5000}-TT1 (center) and MSNs-(RhB)-PEG_{5000} (right) both in red channel.

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^{131}I labelling

The study of the radiochemical stability of iodine shows that activity is retained in the peptide and the PEG-^{131}I-TT1 is lost from the MSNs when is incubated below the solubility limit for silica.

ESI Figure 4 Radio-stability of ^{131}I of labelled peptide ^{131}I-TT1 (left) and MSNs-PEG$_{5000}$-^{131}I-TT1 at 0.1mg mL^{-1} (right) incubated at 37 °C in simulated body fluid (SBF) and SBF-EDTA

HPLC-MS of TT1 degradation in serum.

The evaluation of the integrity of the peptide in serum was evaluated by HPLC-MS by the incubation of the peptide TT1 in freshly purified mouse serum at 37 °C. At each time point a fraction of serum containing 1 mg mL^{-1} of TT1 was collected. The fraction was ice-cooled and immediately mixed with 4 volumes of acetonitrile (1% TFA) to precipitate the protein fractions. The organic mixture was centrifuged, and supernatant analyzed in a HPLC Waters Acquity coupled with a Mass spectrometer. The fraction control of TT1 at 1 mg mL^{-1} in PBS and in serum was evaluated in parallel to determine degradation of the peptide. The control maintains the initial concentration during the experiment.

ESI Figure 5 Relative intensities of mass spectrometer signal of peptide TT1 after incubation with serum and PBS at 37 °C, under agitation.

The graph expresses the ratio between the intensity of the signal of the TT1 incubated in serum and the TT1 incubated in PBS at the same time. The loss of signal indicated a degradation of the peptide in some of their fraction. In the incubation conditions, the half-live of the peptide in serum was approximate 20 minutes.

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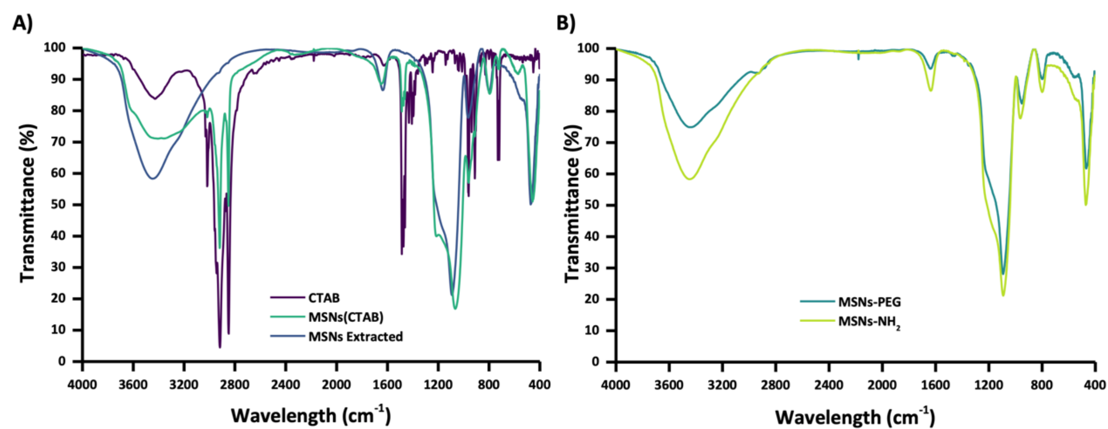
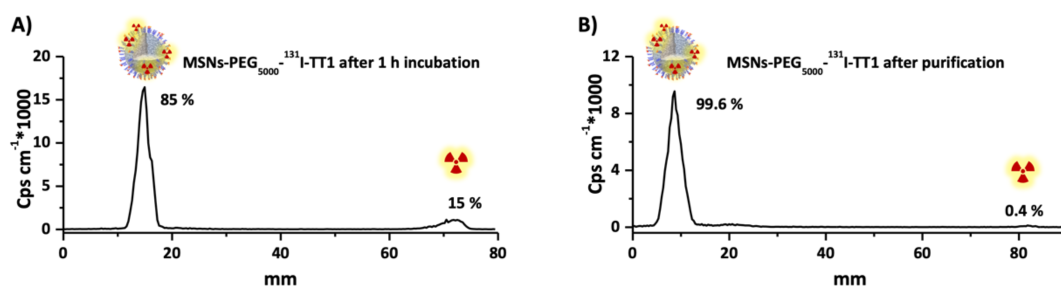


ESI Figure 6 FT-IR spectra of (A) sequential synthesis and surfactant extraction of MSNs and (B) functionalization of MSNs with APTES and PEG_{5000}



ESI Figure7 radio-TLC of (A) MSNs-PEG_{5000}-^{131}I-TT1 after 60 minutes of incubation at room temperature and (B) after purification

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