Supporting Information

Cytotoxicity of PEG-Coated Gold and Gold-Iron Alloy Nanoparticles: ROS or Ferroptosis?

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1. XRD of PEG-Au, PEG-Au-Fe n1 and TEOS-PEG-Au-Fe b NPs

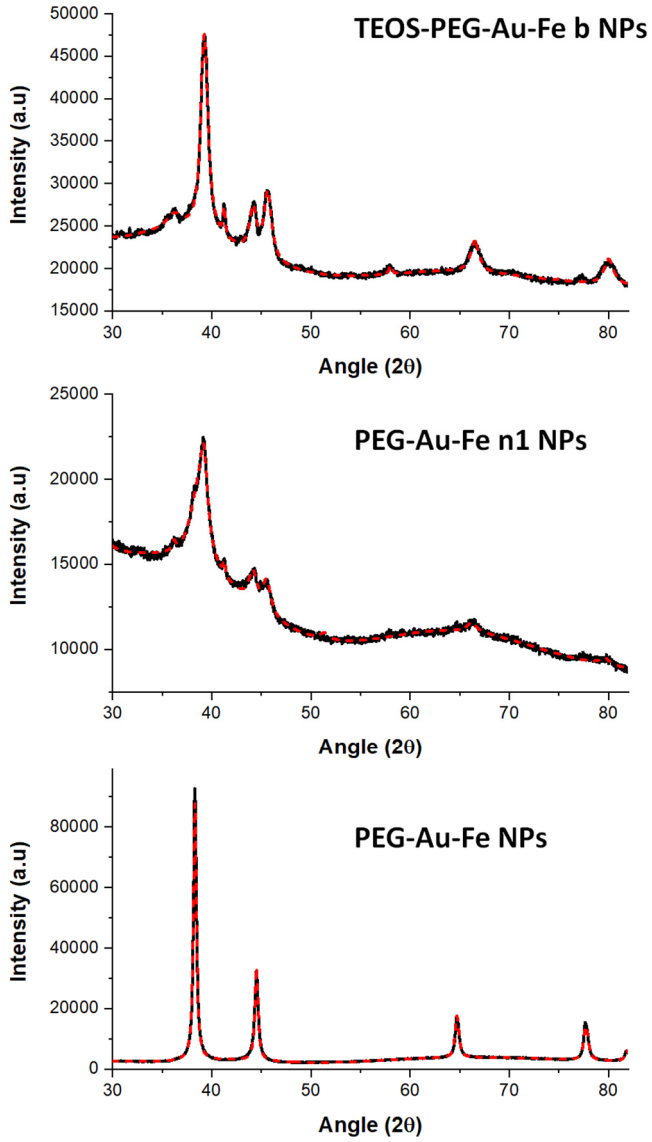

Figure S1. XRD pattern (continuous lines) and Rietveld refinement (dashed lines) of the PEG-Au, PEG-Au-Fe n1 and TEOS-PEG-Au-Fe b NPs samples. The Au NPs have the typical face centered cubic (FCC) lattice with a cell parameter in agreement with that of bulk gold (4.0775 ± 0.0001 Å). The Au-Fe NPs have the well-known disordered structure (large peaks) due to the metastability of the alloy, and two FCC components can be identified, one ascribable to an Au-rich alloy (cell parameter of 4.0011 ± 0.0022 Å for PEG-Au-Fe n1 and 3.9783 ± 0.0006 Å for TEOS-PEG-Au-Fe b) and another to iron-rich alloy (cell parameter 3.5703 ± 0.0020 Å for PEG-Au-Fe n1 and 3.5558 ± 0.0007 Å for TEOS-PEG-Au-Fe b). Therefore, the same phases are observed in the PEG-Au-Fe n1 and TEOS-PEG-Au-Fe b NPs samples.

2. FTIR of PEG-Au, PEG-Au-Fe n1 and TEOS-PEG-Au-Fe b NPs

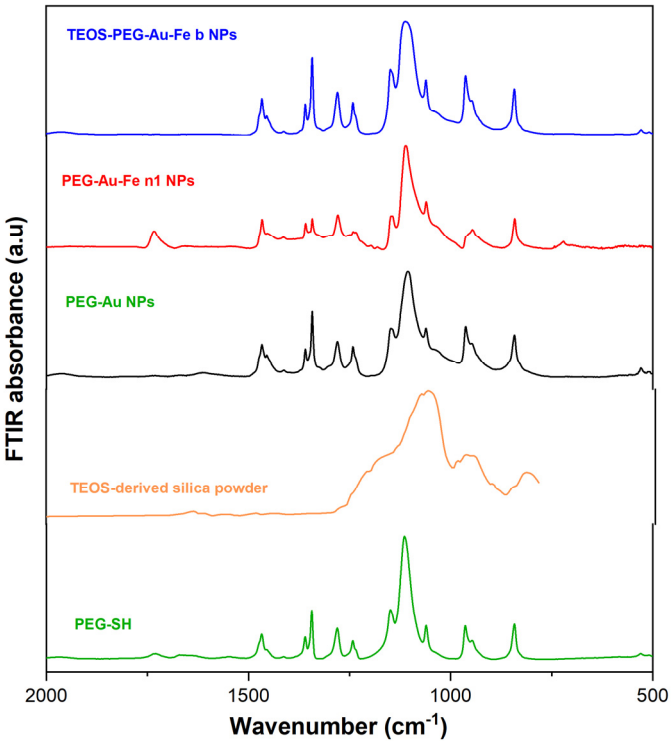

Figure S2. FTIR spectra of PEG-Au, PEG-Au-Fe n1 and TEOS-PEG-Au-Fe b NPs samples. In all cases, the peaks characteristic of PEG are well evident, indicating a comparable polymeric coating. The peaks of the TEOS-derived silica shell are difficult to identify below the intense PEG signals in the TEOS-PEG-Au-Fe b NPs sample.

3. Z-potential and DLS of PEG-Au, PEG-Au-Fe n1 and TEOS-PEG-Au-Fe b NPs

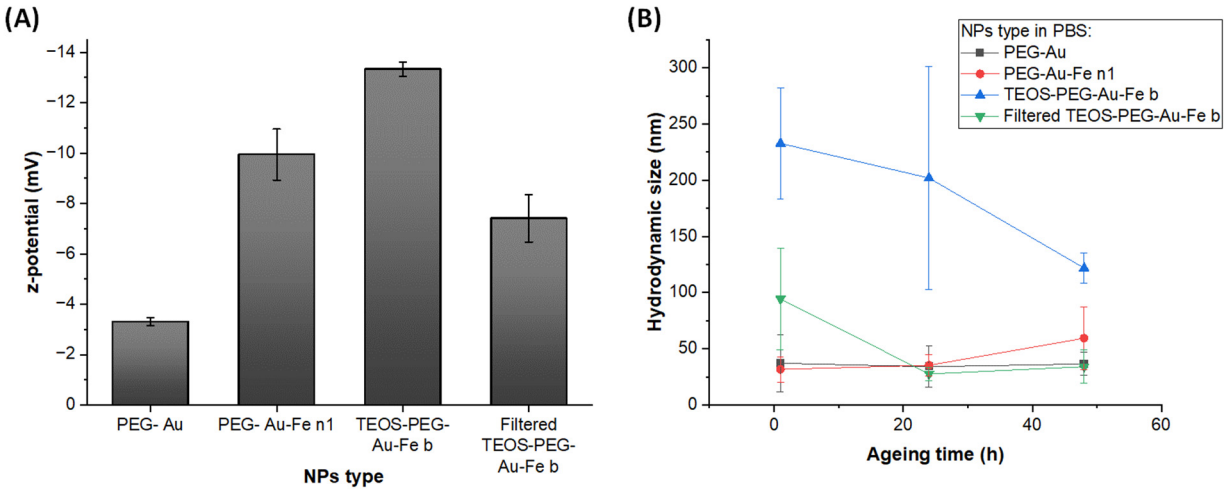

Figure S3. Z-potential (A) and DLS measured hydrodynamic size (B) of PEG-Au, PEG-Au-Fe n1 and TEOS-PEG-Au-Fe b NPs in phosphate buffered saline solution after ageing for 1, 24 and 48 h at 37 °C. The results for the TEOS-PEG-Au-Fe b NPs after filtration with a with a 200 nm pore size filter are also shown, indicating the size reduction to values similar to PEG-Au and PEG-Au-Fe n1 NPs. This is accompanied by a reduced cytotoxicity to values equivalent to the PEG-Au-Fe n1 NPs. Note the relatively low z-potential, suggesting the prevalence of a steric repulsion mechanism for the stability of the NPs.