Supporting Information

Surface Protected and Modified Iron Based Core-Shell Nanoparticles for Biological Applications

Kanchana Somaskandan, Teodor Veres, Mereck Niewczas, and Benoit Simard

Preparation of Dopamine-PEG:

Dopamine-PEG molecule was synthesized using the literature procedure\(^1\). In order to PEGylate dopamine, PEG-COOH was used in the preparation. PEG-COOH was made in the laboratory using the following preparation method.

Synthesis of PEG-COOH

In a 100 mL round-bottomed flask under a nitrogen atmosphere, triethylene glycol monomethyl ether (5g, 30 mmol) was dissolved in 11 mL of dry THF. Sodium metal (10 mg, 0.4 mmol) was then added and the mixture was stirred until the sodium dissolved. Following sodium dissolution, \(t\)-butyl acrylate (3.9g, 30 mmol) was added and mixed for ~60 hours. The THF was then removed through rotary evaporation and, the crude product was redissolved in 30 mL ethyl acetate and washed with brine solution three times. The \(t\)-butyl ester protected PEG-COOH product was purified via column chromatography (5% methanol in dichloromethane, \(R_f=0.3\)).

\(^1\)H-NMR: CDCl\(_3\), \(\delta\) 3.55-3.80 (broad multiplet, 14H), 3.66 (singlet, 3H), 2.51 (triplet, 2H), 1.43 (singlet, 9H).

Following purification, the \(t\)-butyl ester was removed by stirring in 50:50 dichloromethane:trifluoroacetic acid for three hours, generating the free carboxylic acid group. Again the product was purified via column chromatography with 5% methanol in dichloromethane.

\(^1\)H-NMR: CDCl\(_3\), \(\delta\) 10.64 (broad singlet, 1H), 3.55-3.80 (broad multiplet, 14H), 3.66 (singlet, 3H), 2.58 (triplet, 2H).
Figures for Supporting Information:

**Fig. S1.** TEM images of Fe@Fe$_x$O$_y$ nanoparticles (a) soon after the synthesis and, (b) after 18 h in air

**Fig. S2.** a) TEM image of Fe@Fe$_x$O$_y$@Fe$_x$O$_y$ nanoparticles exchanged with dopamine hydrochloride and b) particle solubility in water before and after exchange.
**Fig. S3.** Fe@Fe₃O₅@Fe₃O₅ nanoparticles exchanged with dopamine and dopamine PEG in a) pH 6 buffer (A and B) and b) pH 7.6 buffer with 0.3 M salt (C and D).

**Fig. S4.** UV/Vis spectra of Fe@Fe₃O₅@Fe₃O₅ nanoparticles surface exchanged with dopamine and dopamine-PEG molecules taken soon after the exchange (a and b) and after a month of exchange (c and d).
Fig. S5. TEM image of silica coated Fe@FexOy nanoparticles showing clear core shell morphology of Fe@FexOy within the silica beads. (Note: the iron oxide coated iron nanoparticles used here were kept under ambient conditions and were coated after a year)