

## Supplementary Information:

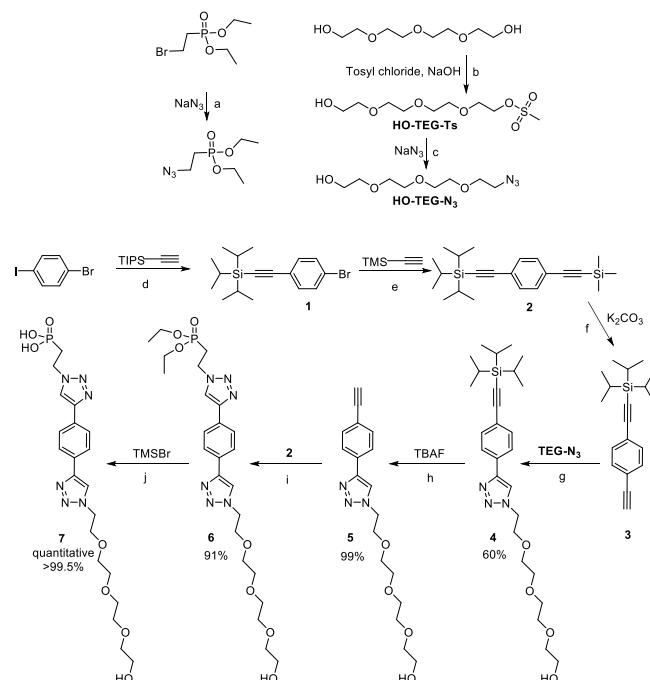
### Magnetic Resonance Imaging/Fluorescence Dual Modality Protocol Using Designed Phosphonate Ligands Coupled to Superparamagnetic Iron Oxide Nanoparticles

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Scheme 1. Synthesis of the Linear Linker. Reaction Conditions: a) EtOH, Ar atmosphere, reflux overnight; b) THF, Ar atmosphere, 0°C 2 hrs c) EtOH, Ar atmosphere, 77°C overnight; d) Pd(TPP)<sub>2</sub>Cl<sub>2</sub>, CuI, DEA, Ar atmosphere, r.t. overnight; e) Pd(TPP)<sub>2</sub>Cl<sub>2</sub>, CuI, TGA, Benzene, Ar atmosphere, reflux overnight; f) acetone:water:THF(1:1:1), r.t overnight; g) CuSO<sub>4</sub>·5H<sub>2</sub>O, Na Ascorbate, water:THF (0.5:1), Ar atmosphere, r.t. overnight; h) dry ice/acetone bath, Ar atmosphere overnight; i) CuSO<sub>4</sub>·5H<sub>2</sub>O, Na Ascorbate, water:THF (0.5:1), Ar atmosphere, r.t. overnight; j) Dry chloroform, Ar atmosphere, r.t. 48 hrs

**Scheme S1 Design and Synthesis of Phosphonate-TEG-OH.** Synthesis was adapted from T. Lam, P.K. Avti, P. Pouliot, F. Maafi, J-C. Tardif, E. Rheaume, F. Lesage and A. Kakkar, *Langmuir*, 2016, submitted for publication.

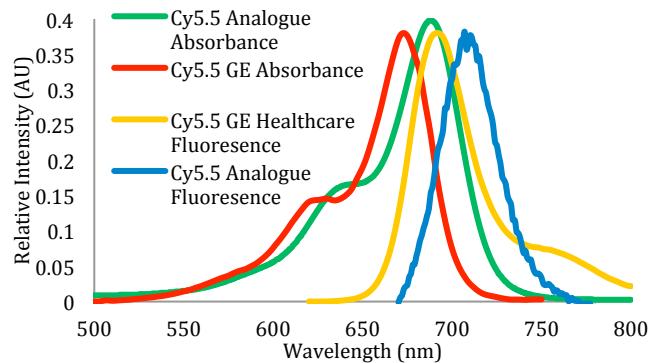
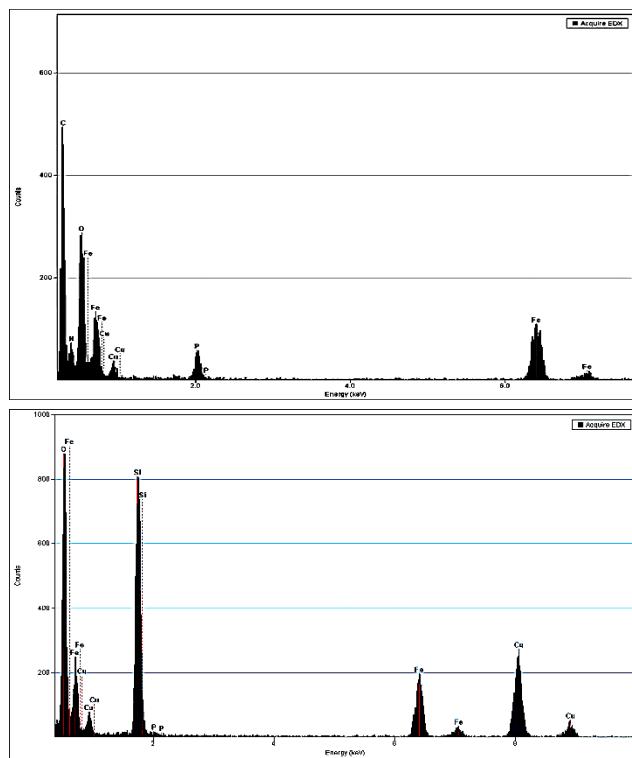


Figure S2: Relative absorbance and emission spectral overlay for Cy5.5 (GE Healthcare) and Cy5.5 analogue (Cy5.5A) in DMSO.



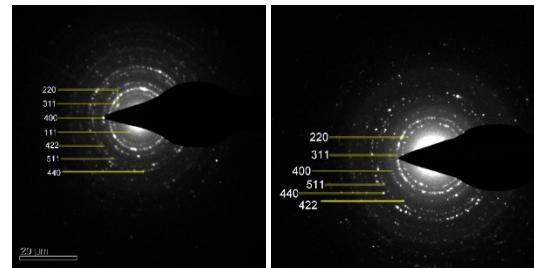


Figure S4: SAED images for SPIONs-TEG-OH (Left) and SPIONs-PEG-OH (Right).

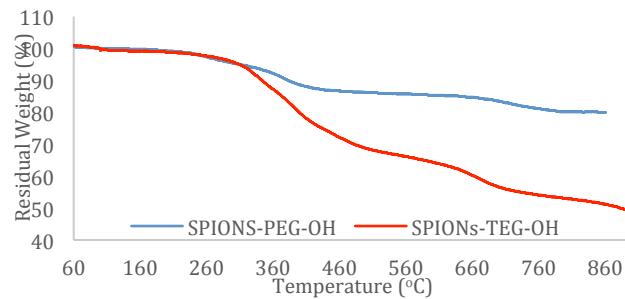


Figure S5: TGA spectral overlay of weight loss at increasing temperatures for PSIONs-TEG-OH and SPIONs-PEG-OH.

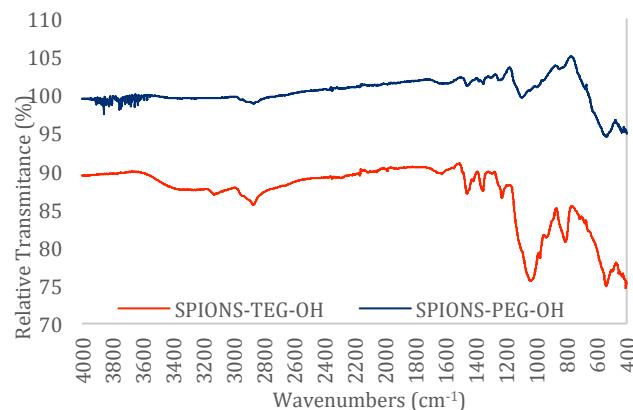


Figure S6: FTIR spectral overlay for SPIONs-TEG-OH and SPIONs-PEG-OH.

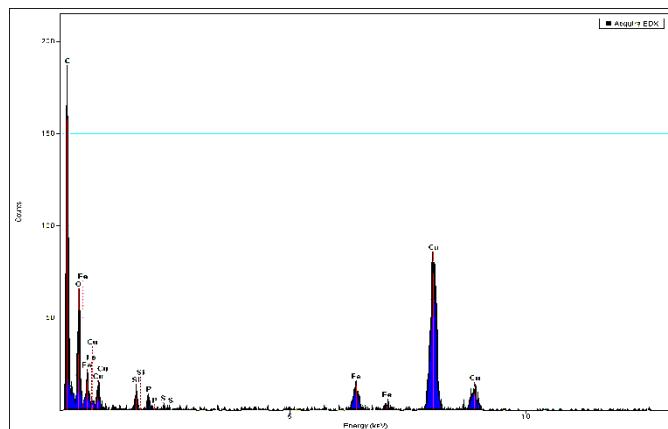


Figure S7: EDX for SPIONs-PEG-O-Cy5.5A.

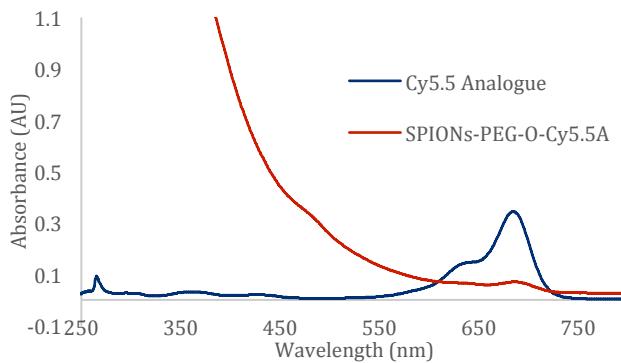


Figure S8: UV-Vis spectral overlay of Cy5.5A and SPIONs-PEG-O-Cy5.5A in DMF.

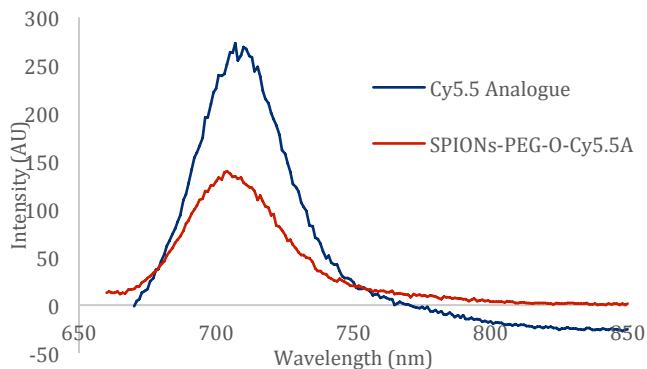
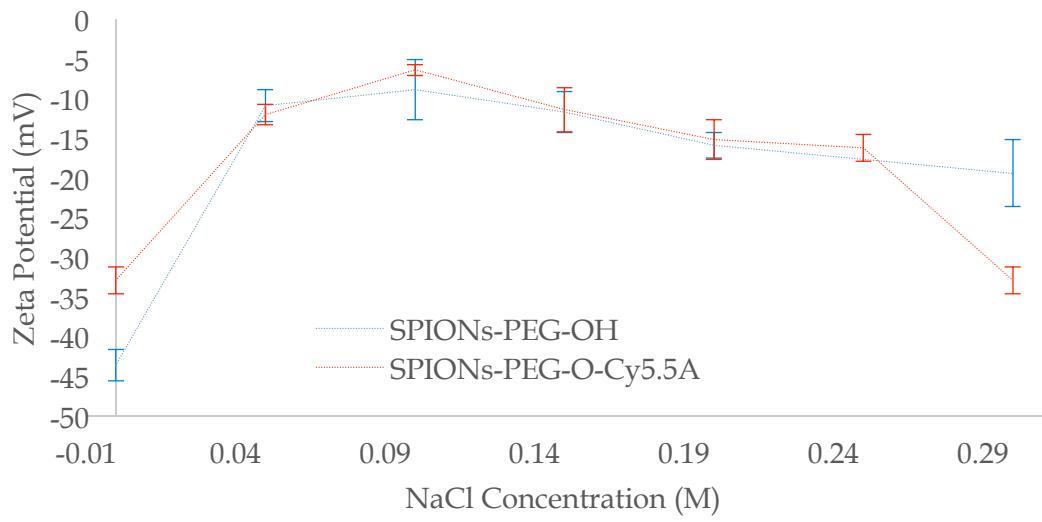


Figure S9: Fluorescence spectral overlay of Cy5.5A and SPIONs-PEG-O-Cy5.5A in DMF.



**Figure S10:** Zeta Potential values for SPIONs species at varying NaCl concentrations in water.