SUPPORTING INFORMATION

Activatable magnetic resonance imaging agents for myeloperoxidase sensing: mechanism of activation, stability and toxicity

Elisenda Rodríguez¹, Mark Nilges², Ralph Weissleder^{1,3} and John W Chen^{1,3,}*

SI1a

SI1b

SI1c

SI1d

Figure SI1. ^1H NMR spectra (400 MHz, D_2O) of the chelates synthesized in this work: (a) mono-5HT-DTPA; (b) bis-5HT-DTPA; (c) bis-*o*-diansidine-DTPA; (d) bis-4-aminophenol-DTPA.

SI2

Figure SI2. MS spectra of the chelates synthesized in this work: (a) mono-5HT-DTPA; (b) bis-5HT-DTPA; (c) bis-*o*-diansidine-DTPA; (d) bis-4-aminophenol-DTPA.

SI3

Figure SI3. Analytical RP-HPLC spectra of the imaging agents synthesized in this work using a reverse-phase C18 column (15 x 0.46 cm, 5 μ m), demonstrating > 96% purity of the products. The integrated peak area percentages are shown when the product peak was < 99%. Gradient elution was performed at 25 $^{\circ}$ C with a flow rate of 1mL/min by starting with 90% of eluent A (water) and 10% of eluent B (acetonitrile) for 2 min, then applying a linear gradient from 10 to 100% acetonitrile in 14 min. UV detection was at 280 nm. (a) mono-5HT-DTPA-Gd; (b) bis-5HT-DTPA-Gd; (c) bis-*o*-diansidine-DTPA-Gd; (d) bis-4-aminophenol-DTPA-Gd.

SI4

Figure SI4. MS spectra of the imaging agents synthesized in this work: (a) mono-5HT-DTPA-Gd; (b) bis-5HT-DTPA-Gd; (c) bis-*o*-diansidine-DTPA-Gd; (d) bis-4-aminophenol-DTPA-Gd.

SI5

Figure SI5. (a) EPR spectrum of the control solution with MPO and H_2O_2 using the 2-methyl-2-nitrosopropane (MNP) as a spin trap. (b) EPR spectrum of MNP.

SI6a

SI6b

SI6c

Figure SI6. MALDI-TOF spectra for the imaging agents after MPO activation. (a) mono-5HT-DTPA-Gd, (b) bis-5HT-DTPA-Gd and (c) bis-*o*-dianisidine-DTPA-Gd.

SI7

Figure SI7. Transmetallation kinetic stability of the imaging agents in the presence of equimolar Zn^{2+} . Decrease of the T_1 relaxation time with time has been expressed as the percentage of R_1 compared to the initial value: $R_1(t) / R_1(0)$.