Electronic Supplementary Information (ESI)

Manganese-52: applications in cell radiolabelling and liposomal nanomedicine PET imaging using oxine (8-hydroxyquinoline) as an ionophore.

Peter Gawne,^a Francis Man,^a Jesper Fonslet,^b Riya Radia,^a Jayanta Bordoloi,^a Matthew Cleveland,^c Pilar Jimenez-Royo,^c Alberto Gabizon,^d Philip J. Blower,^a Nicholas Long^e and Rafael T. M. de Rosales^{*a}

 ^a School of Biomedical Engineering & Imaging Sciences, King's College London, St. Thomas' Hospital, London, SE1 7EH, U.K.
^b The Hevesy Lab, Technical University of Denmark, 4000 Roskilde, Denmark.
^c GSK Medicines Research Centre, Gunnels Wood Road, Stevenage, Hertfordshire, SG1 2NY, U.K.
^d Oncology Institute, Shaare Zedek Medical Center and Hebrew University–School of Medicine, Jerusalem 9103102, Israel.
^e Department of Chemistry, Imperial College London, South Kensington Campus, London SW7 2AZ, U.K.

E-mail: rafael.torres@kcl.ac.uk

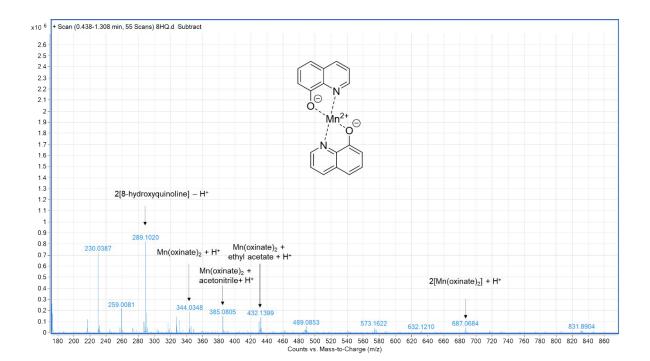


Figure S1: Mass spectrum (ESI, +ve mode) of $Mn(oxinate)_2$. Mass peak at 343.0348 corresponds to the bis-oxine manganese(II) complex $[M + H]^+$.

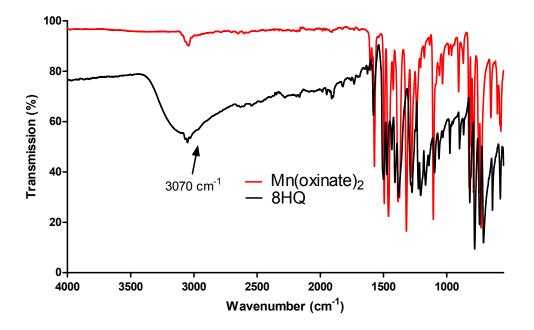


Figure S2: Infra-red spectrum of 8-hydroxyquinoline (black line) and $Mn(oxinate)_2$ (red line). After reaction with $MnCl_2$, a reduction of the broad O-H stretch band at 2700-3400 cm⁻¹ occurs - relating to the formation of the Mn-O bond.

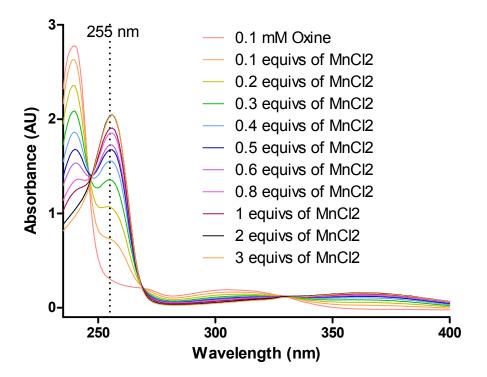


Figure S3: Representative UV-vis titration of MnCl₂ into a 0.1 mM solution of oxine at pH 9.

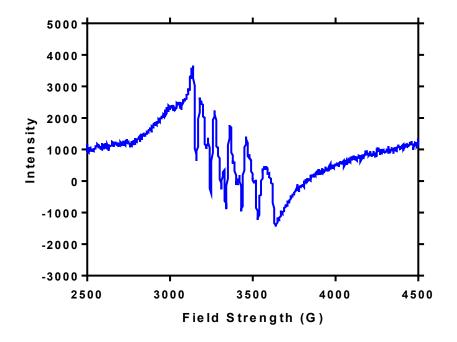


Figure S4: EPR spectrum of a 1 mM oxine solution (in 1 mM ammonium acetate buffer, pH 9) after addition of 0.5 equivalents of $MnCl_2$ at 100 K. Formation of a Mn^{2+} species is clearly evident.

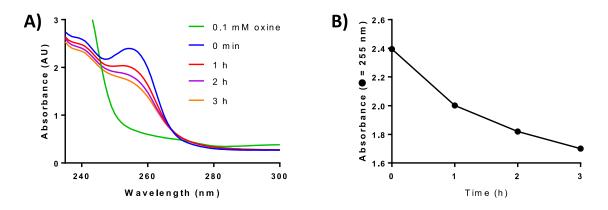


Figure S5: **A)** Overlaid UV-vis spectra of a 0.1 mM oxine solution (in 1 mM ammonium acetate buffer, pH 9, green line) and at different time points after addition of 0.5 equivalents of $MnCl_{2}$; **B)** plot of absorbance at λ = 255 nm versus hours after addition of $MnCl_{2}$.

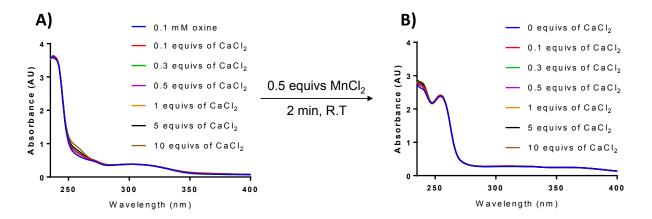


Figure S6: A) Overlaid UV-vis spectra of a 0.1 mM oxine solution in 1 mM ammonium acetate buffer (pH 9) in the absence and presence of various equivalents of CaCl₂; **B)** Overlaid UV-vis spectra after addition of 0.5 equivalents of $MnCl_2$ to each of these solutions. The presence of calcium chloride appeared to have no inhibitory effect on the $Mn(oxinate)_2$ complex being formed *in situ*.

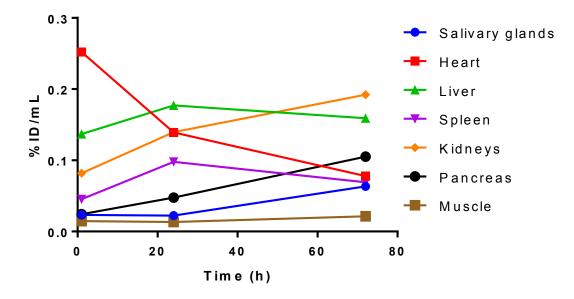


Figure S7: Time-activity curve based on the imaging study shown in Figure 6 (n = 1). A gradual clear increase in activity in the pancreas, salivary glands and kidneys is consistent with the release of ⁵²Mn from the [⁵²Mn]Mn-DOXIL complex.