Electronic Supplementary Material (ESI) for Dalton Transactions.

A lipophilic copper(II) complex as an optical probe for intracellular detection of NO

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Supplementary information

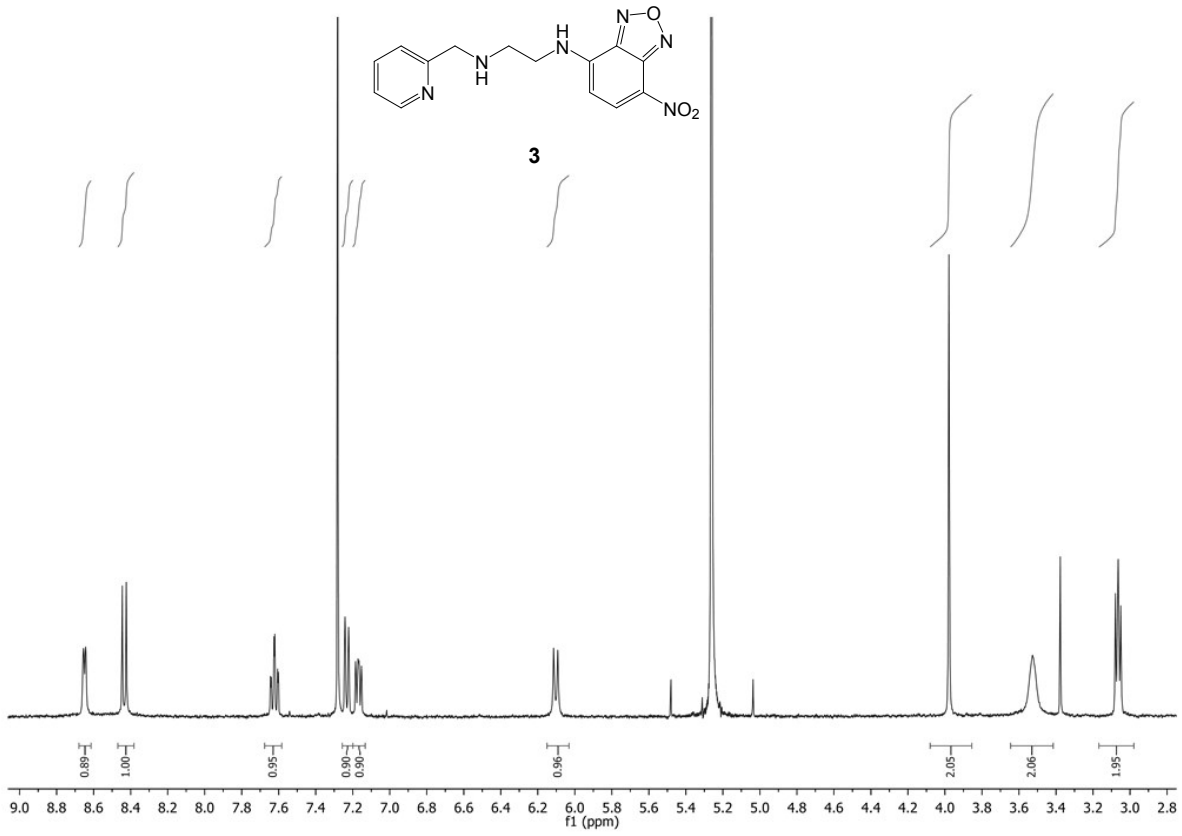

Figure S1. ^{1}H NMR spectrum of ligand **3** in a mixture of $CDCl_3$ and CD_2Cl_2 (peaks at 7.2 and 5.2 ppm correspond to residual solvents)

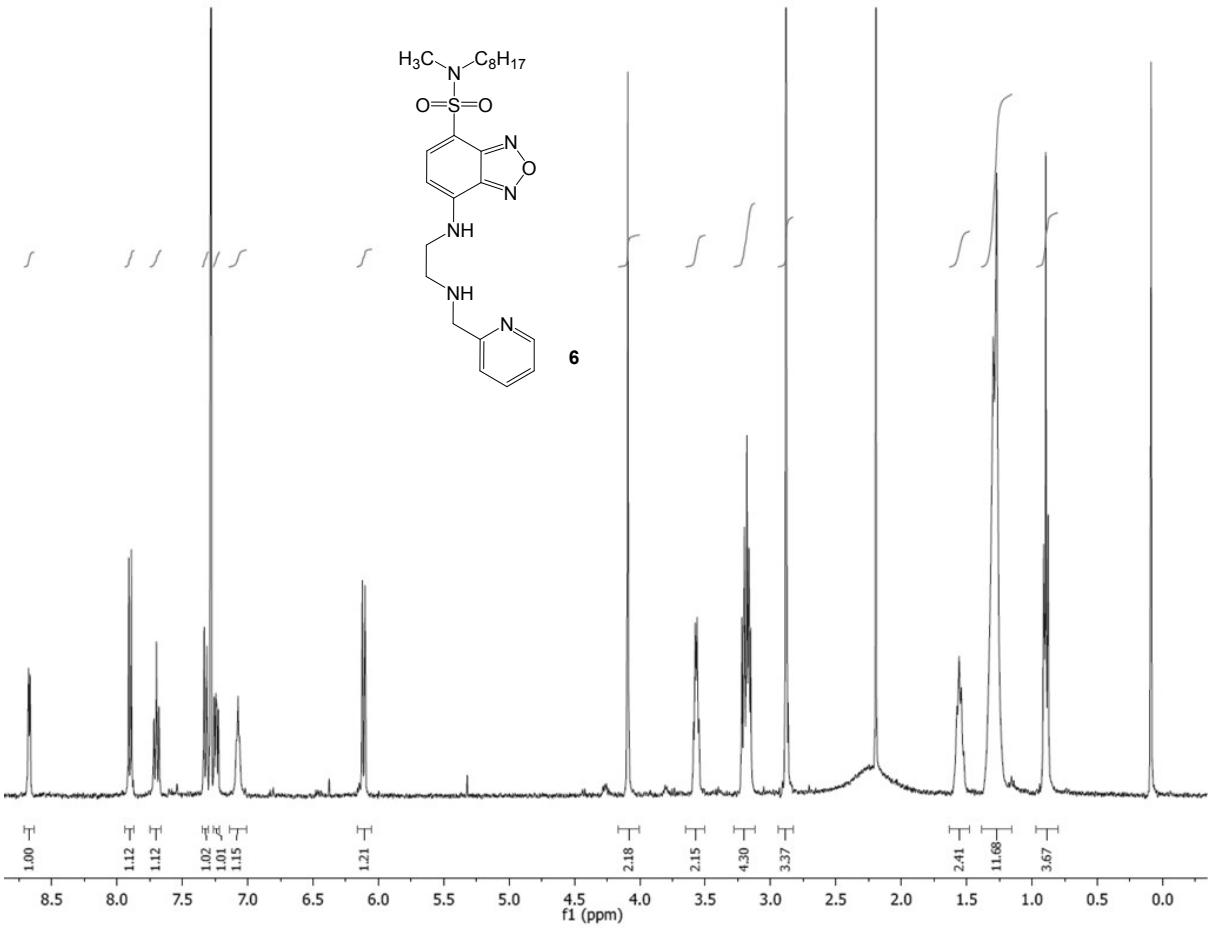

Figure S2. ^{1}H NMR spectrum of ligand **6** in $CDCl_3$

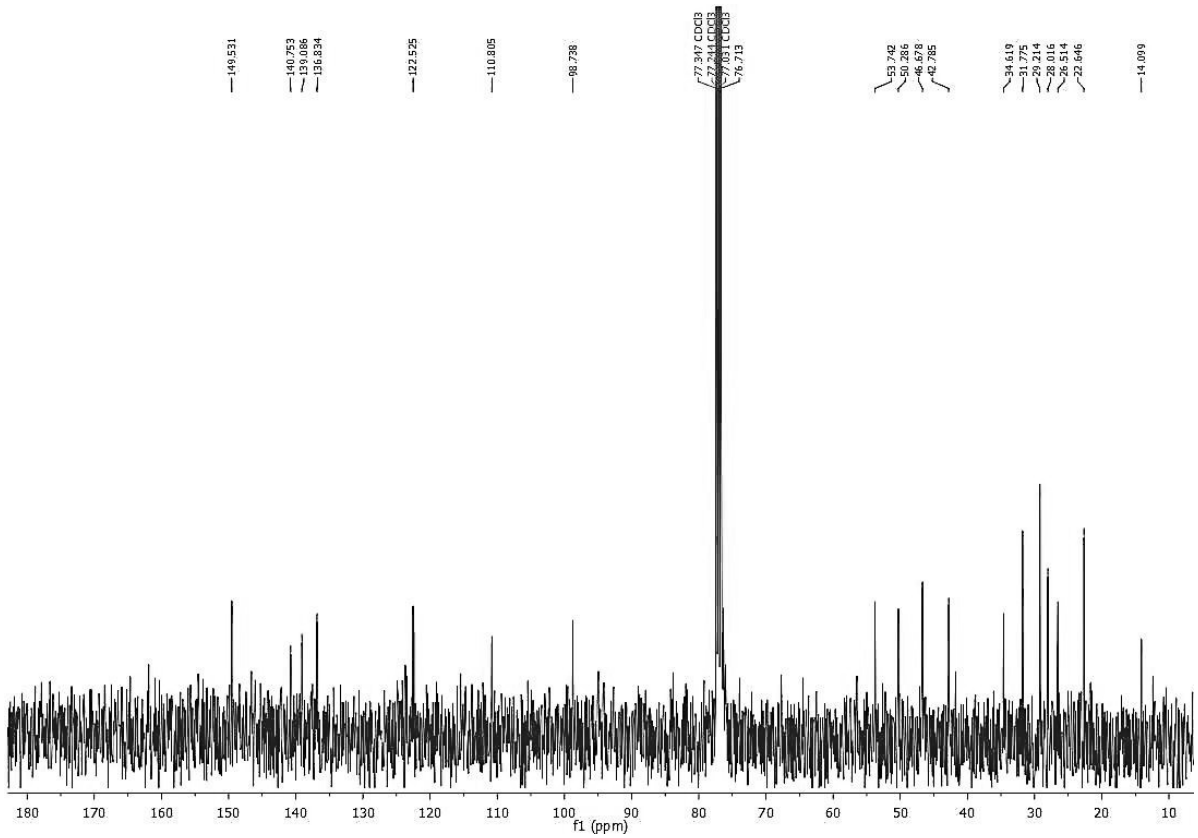

Figure S3. ^{13}C NMR spectrum of ligand **6** in $CDCl_3$.

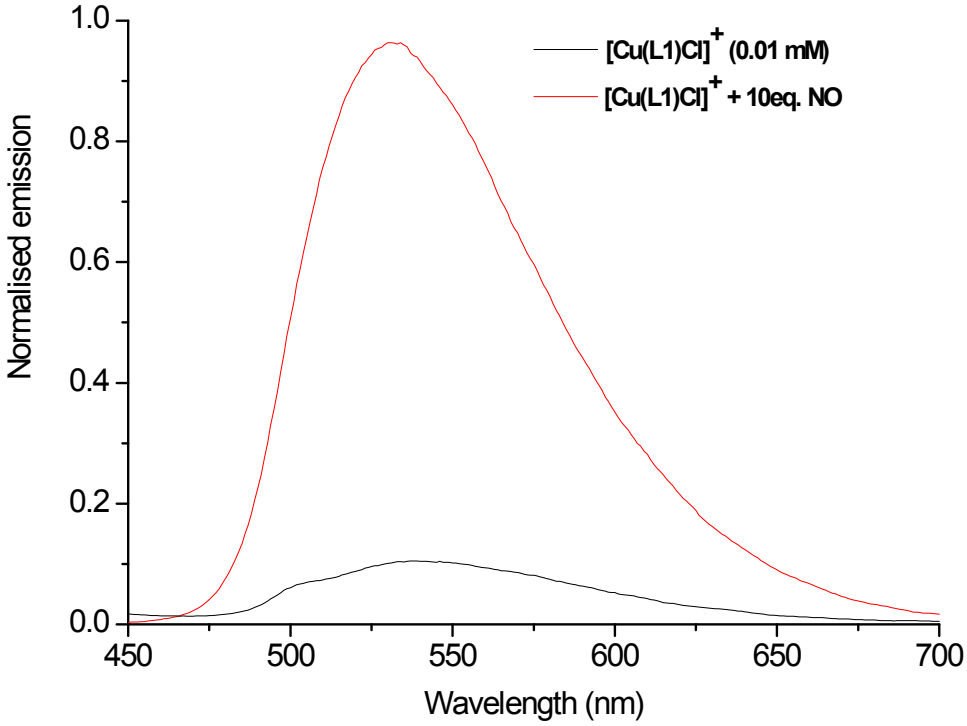

Figure S4. Fluorescent enhancement of complex **4** (0.01 mM) in presence of 10 eq. of NO (red trace) generated from DEA-NO (50 mM PIPES, pH 7.0, 100 mM KCl).

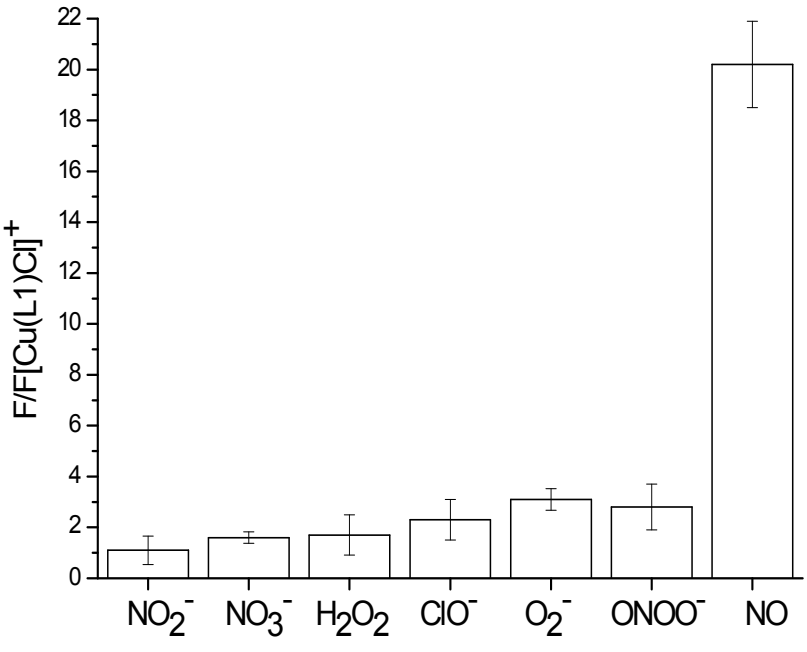

Figure S5. The fluorescent response of complex **4** (540 nm) after addition of 100 eq. of NO_2^-, NO_3^-, H_2O_2, ClO^-, $O_2^{\cdot-}$ and NO for 1 hour in buffered PBS (pH 7). All data (emission intensity, F) are normalised with respect to the emission of a 10 μM solution of **4** (50 mM PIPES, pH 7.0, 100 mM KCl).

Cytotoxicity studies using MTT assay.

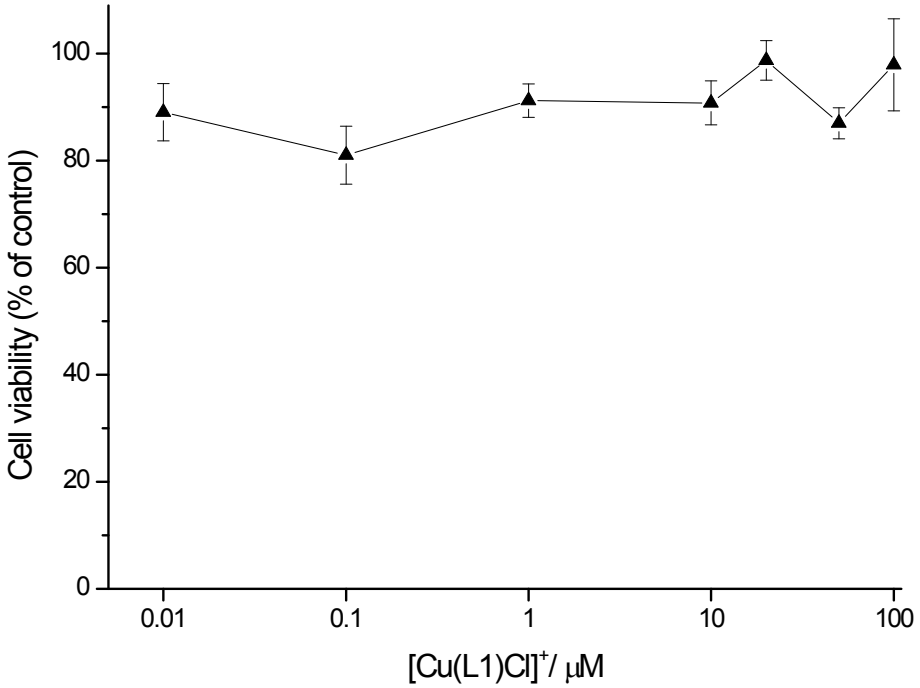

Figure S6. MTT cytotoxicity assay of **4** against NIH 3T3 mouse fibroblasts cells. NIH 3T3 cells were transferred to a 96 well plate in 90 μl of phenol red free media and 10 μl of **4** (0.01 – 100 mM) was added and incubated for 1 hour (37^{o}C). To each well was then added 20 μL of 5 mg/ml of thiazolyl blue tetrazolium bromide (yellow) and incubated for 3.5 hours (37^{o}C). The media was removed carefully and the precipitated formazon (purple) was dissolved in 150 μL of MTT solvent (4 mM HCl, 0.1% Nondet P-40). The plate was analysed by UV-vis spectroscopy at 590 nm and compared against the control to determine cell viability in the presence of **4**.

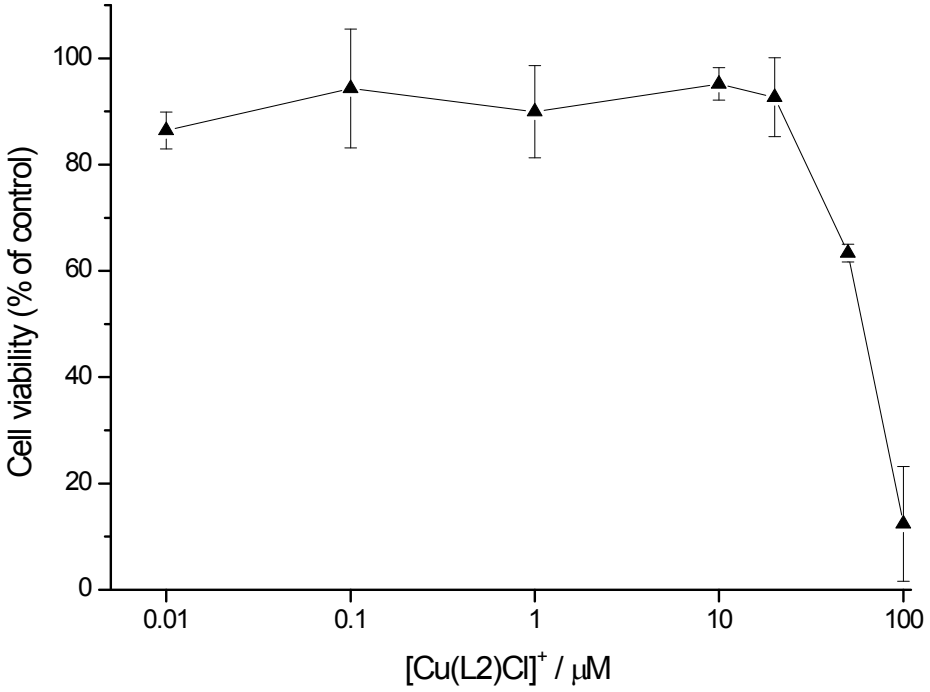

Figure S7. MTT cytotoxicity assay of **7** against NIH 3T3 mouse fibroblasts cells. NIH 3T3 cells were transferred to a 96 well plate in 90 μl of phenol red free media and 10 μL of **7** (0.01 – 100 mM) was added and incubated for 1 hour (37°C). To each well was then added 20 μL of 5 mg/ml of thiazolyl blue tetrazolium bromide (yellow) and incubated for 3.5 hours (37°C). The media was removed carefully and the precipitated formazon (purple) was dissolved in 150 μL of MTT solvent (4 mM HCl, 0.1% Nondet P-40). The plate was analysed by UV-Vis spectroscopy at 590 nm and compared against the control to determine cell viability in the presence of **7**.

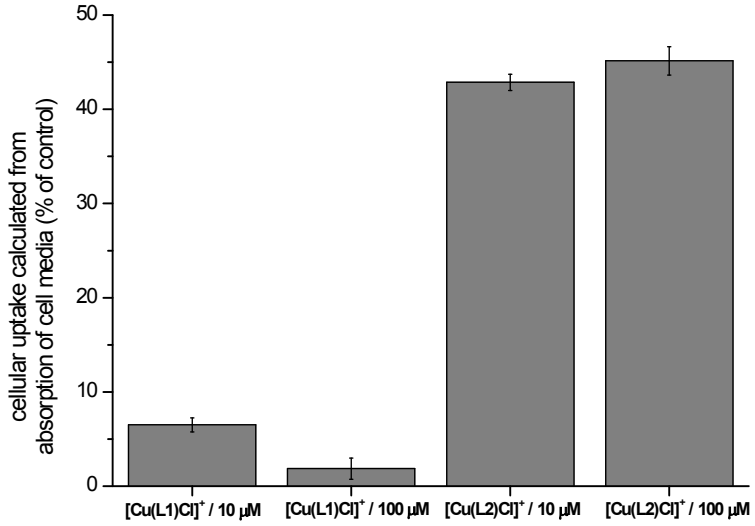

Figure S8. Uptake determination in cell media of **4** (i.e. [Cu(**L1**)Cl]Cl) vs. **7** (i.e. [Cu(**L2**)Cl]Cl) by NIH 3T3 mouse fibroblast cells measured via UV/Vis spectroscopy. NIH 3T3 cells were incubated for 1 hour at 37°C with 500 µL of 10 and 100 µM solutions of **4** or **7** in phenol red free media. After this time, the cells were spun down and 200 µl aliquots of cell free media were transferred to a 96 well plate and the absorbance was measured at 480 nm for **4** and 440 nm for **7.** The values were compared with the controls (known concentration of compound in cell free, phenol red free media) in order to determine the percentage of cellular uptake (triplicate +/- SD) of each compound.