Electronic Supplementary Information for Dalton Transactions

Designing Zn(II) and Cu(II) derivatives as probes for *in vitro* fluorescence imaging

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SUPPLEMENTARY MATERIALS

Figure S1. ^{1}H NMR spectrum of Complex **1** in d^{6}-DMSO (300 MHz, 18 ^{o}C). No significant changes were observed in NMR spectra recorded after 3 weeks.

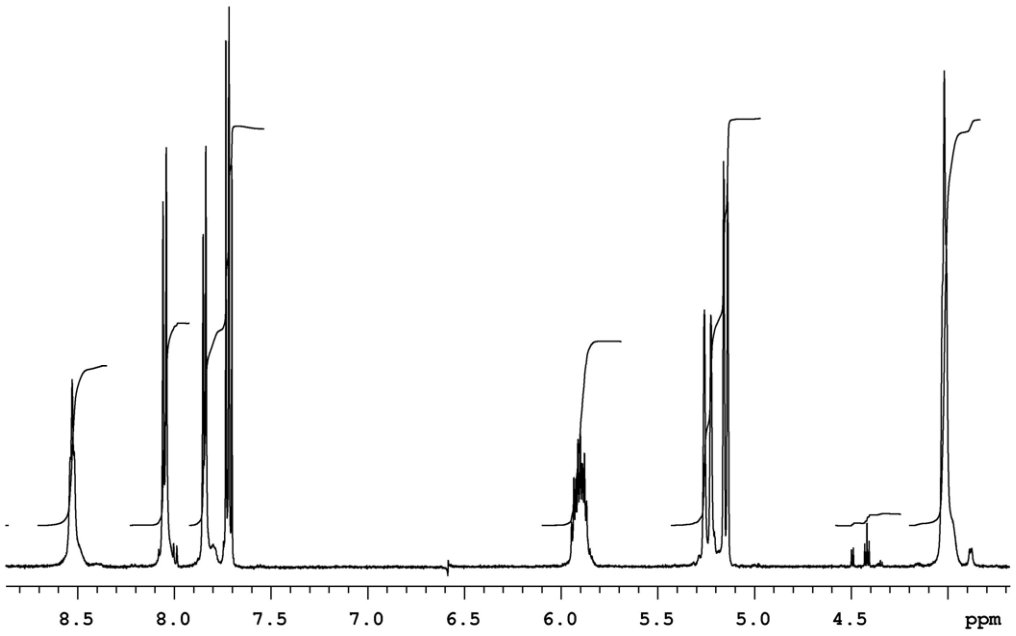
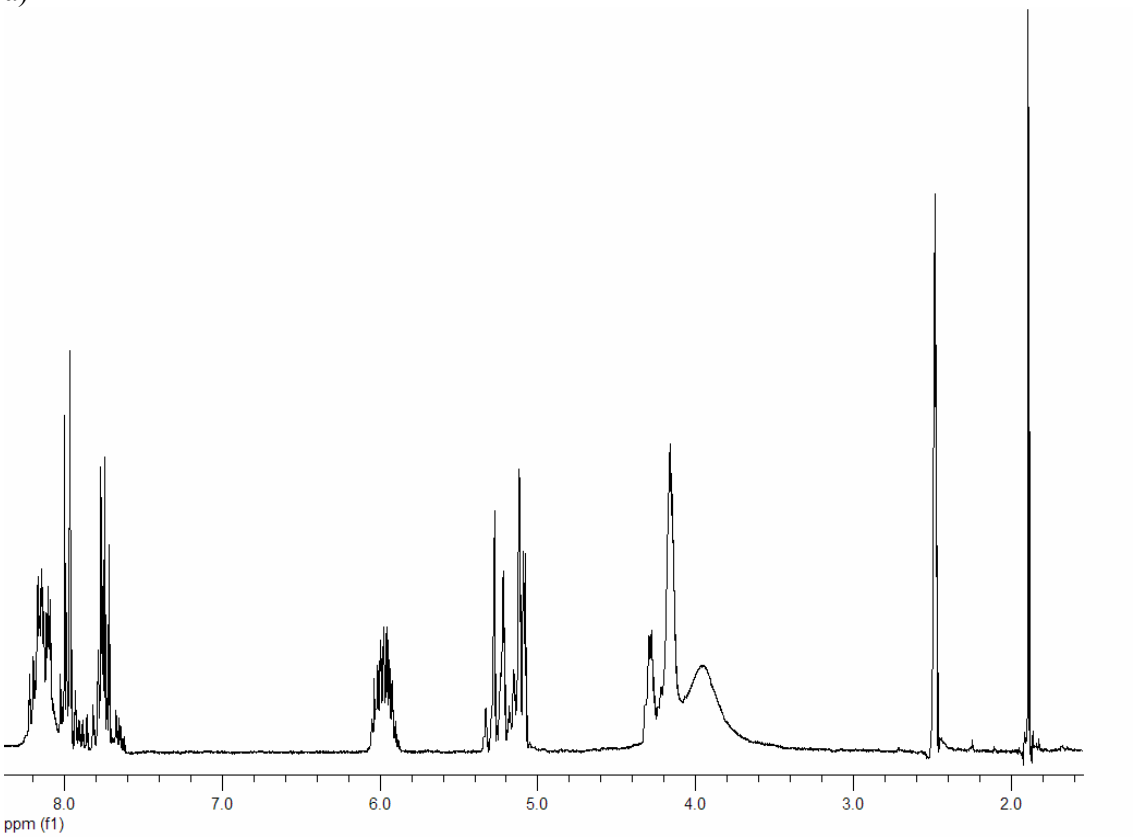


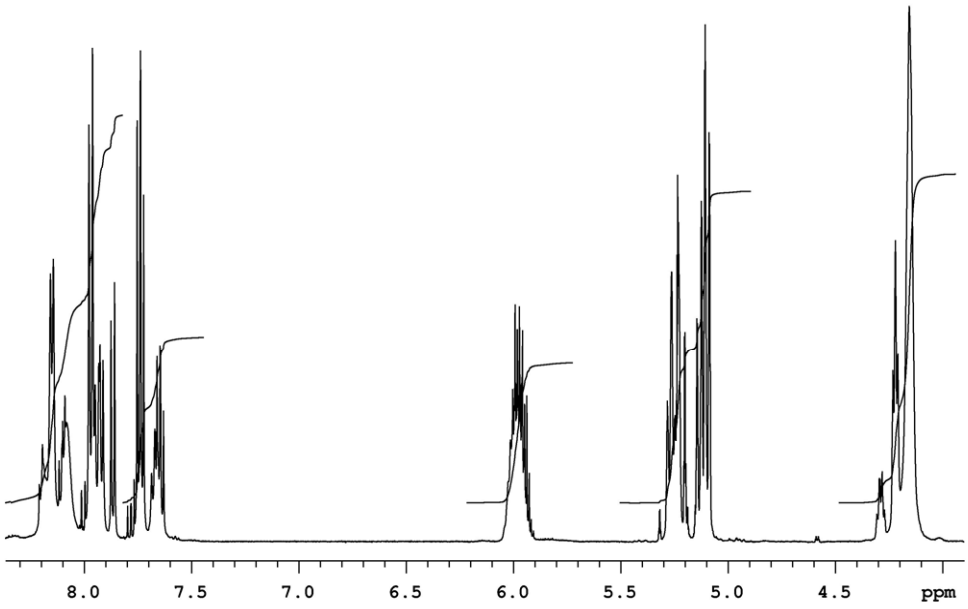
Figure S2. ^{1}H NMR spectra of Complex **2** in d^{6}-DMSO (300 MHz, 18 ^{o}C)

a) Fresh sample (5 min in DMSO)
b) 20 min in DMSO
c) 48 h in DMSO

a)



b)



c)

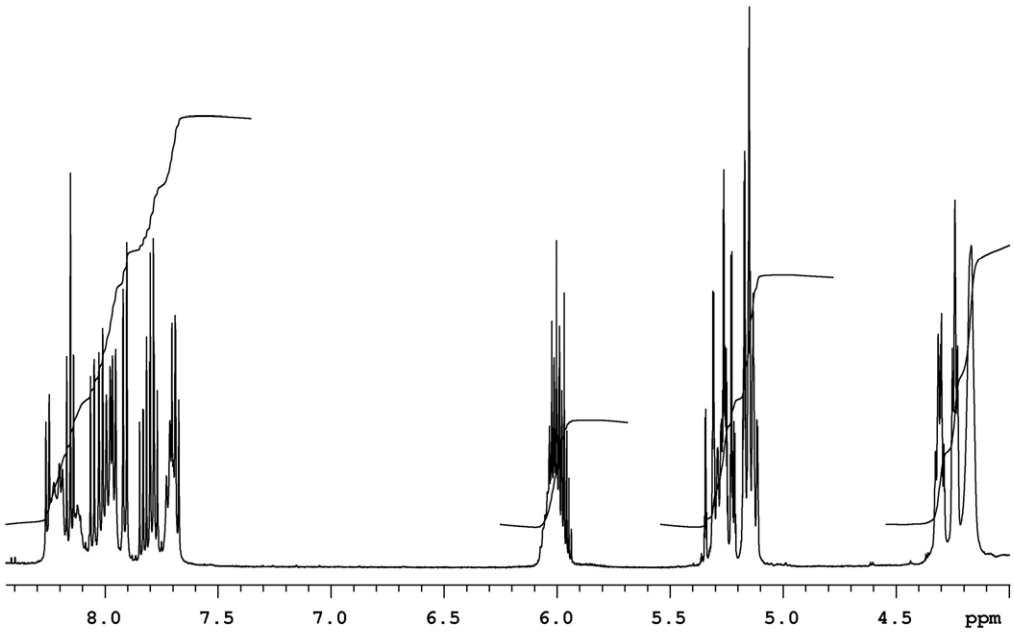


Figure S3. ^{1}H NMR spectrum of Complex 2 in d^{8}-THF (500 MHz, 15 ^{o}C)

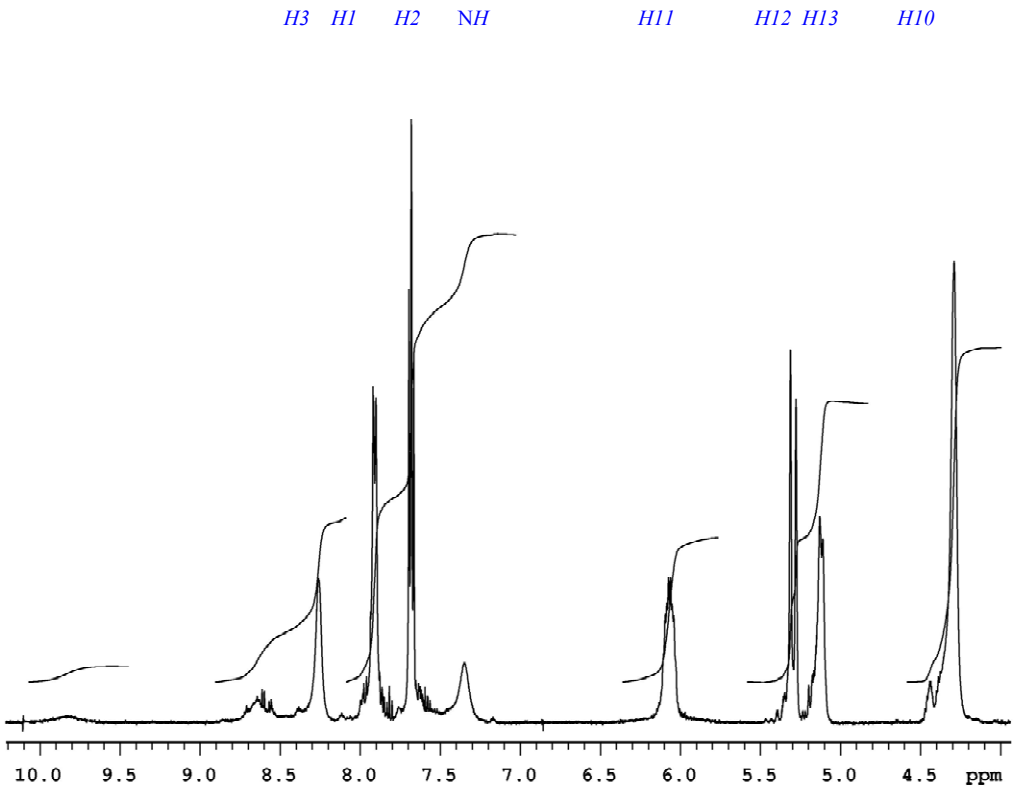


Figure S4. VT ^{1}H NMR spectra of Complex 2:DABCO mixtures (1:1) in d8-THF (500 MHz, +15 – 90 ^{o}C)

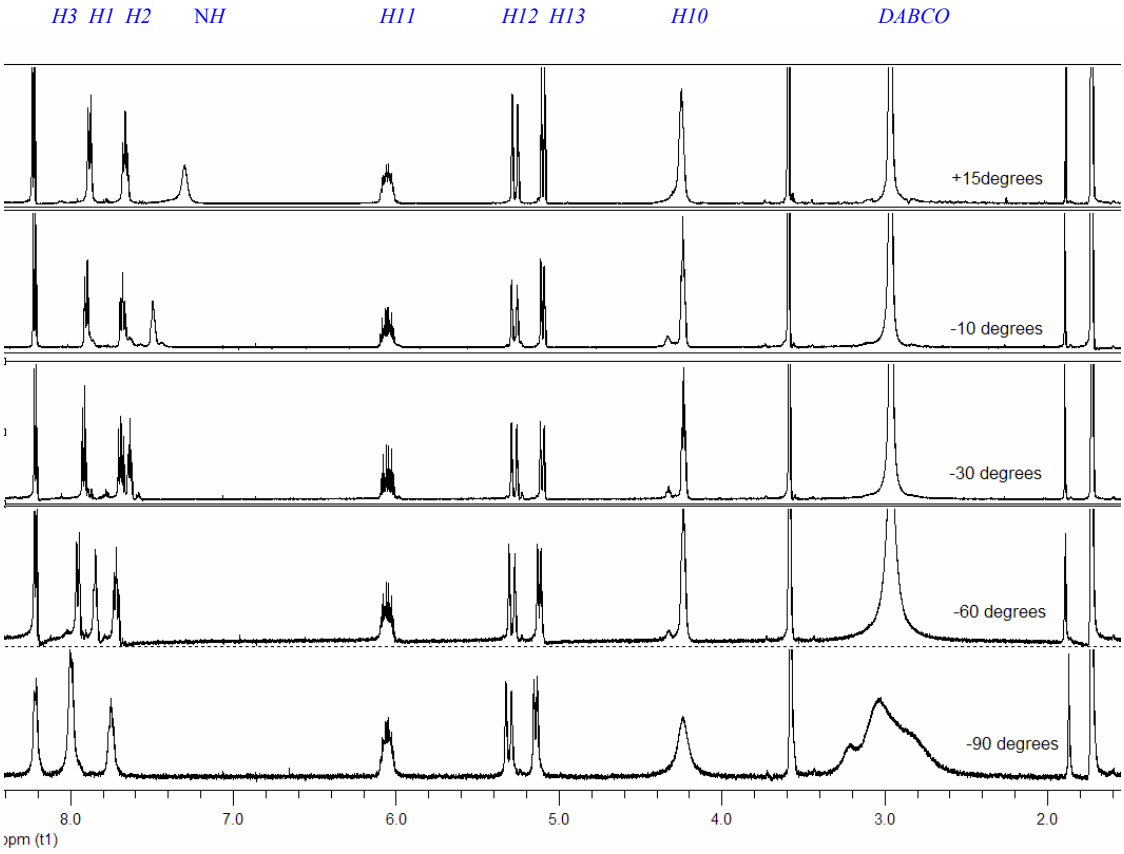
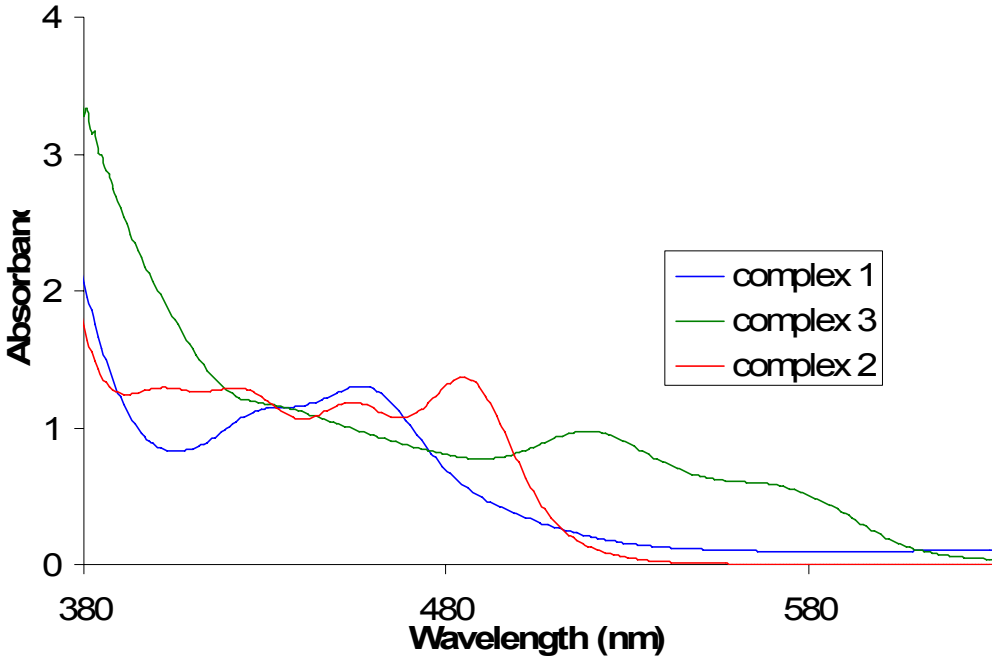


Figure S5 Overlay of selected regions in the UV-Vis spectra of **1-3**. (r.t., DMSO solutions 100 µM conc.)



Cytotoxicity studies for 2 and 3

MCF-7 cells; an adherent cell line, were cultured at 37^0C in a humidified atmosphere of 5% CO_2 in air. The cells were cultured in DMEM (Sigma) with added 10% Foetal Calf serum, 2mM glutamine and antibiotics (100 units/ml penicillin and 100μg/ml streptomycin). Cells were diluted when they reached a density of about $1x10^6$/ml. Cells were seeded in 6-well plates at a suspended cell concentration of approximately $2x10^5$ cells/ml in DMEM (4 mL per well). The cells were left to adhere for 6 hours. The supernatant was then discarded and replaced with 4 ml fresh medium containing a solution of the compound of interest (100, 50, 25 and 12.5 μM) in DMSO to give a final overall DMSO concentration of 1%. After 48 hours, the supernatant was collected and the adhered cells washed carefully with 2x1ml PBS and trypsinised with 100μL of trypsin/EDTA solution for 5 minutes at room temperature.
The cell suspension was then made up to 1 ml with fresh medium and cell counts performed using a trypan blue stain and haemocytometer grid to count a sample of the cells (The trypan blue stain is taken up by dead cells but cannot permeate the cell membrane of live cells). Repeat counts of live and dead cells for each experiment were made on four separate wells. The average number of viable cells is recorded with error bars indicating the range in counts made.