

Supplementary Information

Bioreductive molecular probe: fluorescence signalling upon reduction of an azo group

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¶ Equal contribution to this research.

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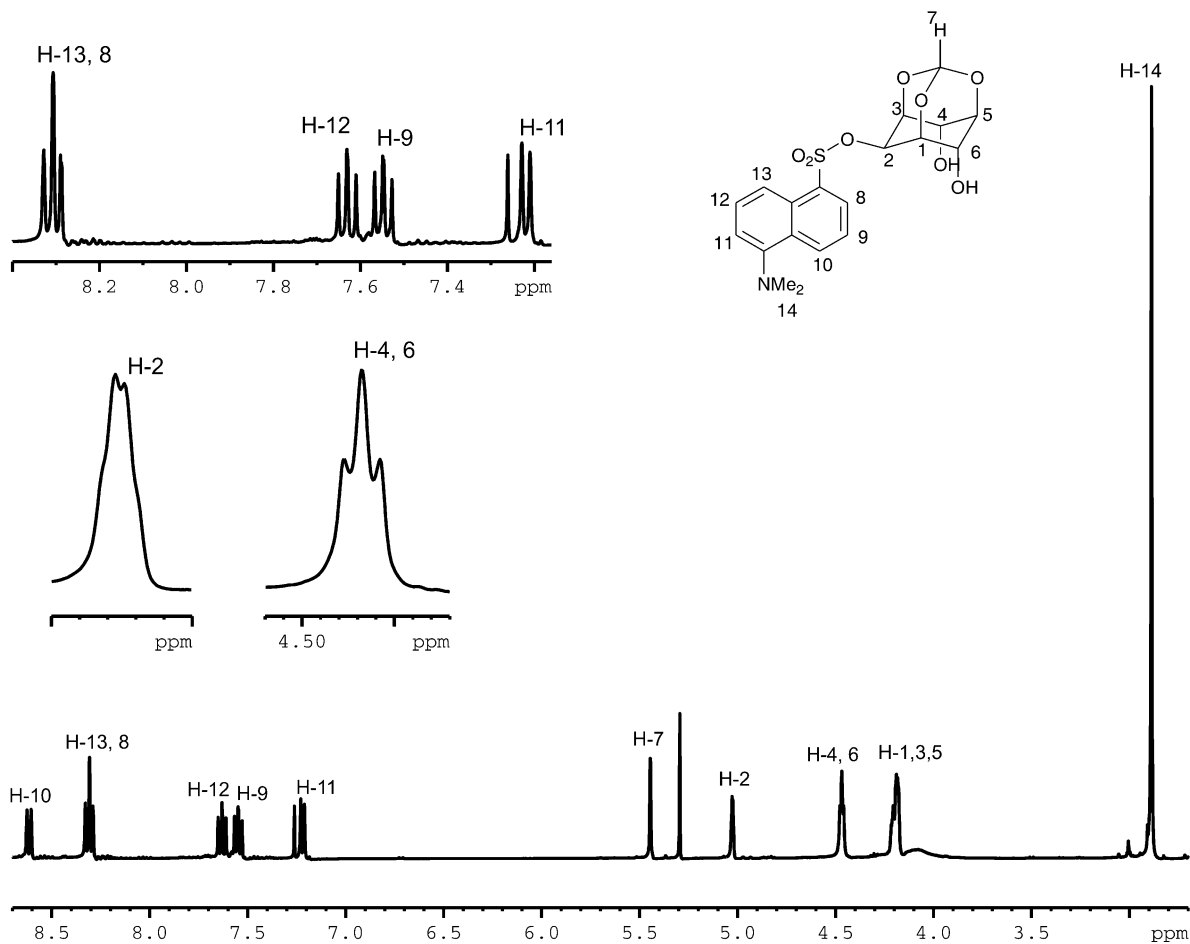


Figure SI 1: ¹H NMR spectrum (400 MHz) of 2-O-dansyl-myoinositol-1,3,5-orthoformate (**6**) in CDCl₃. The peak at ~5.3 ppm is DCM, the solvent used for recrystallisation. The chemical shift data and coupling constant are reported in the experimental.

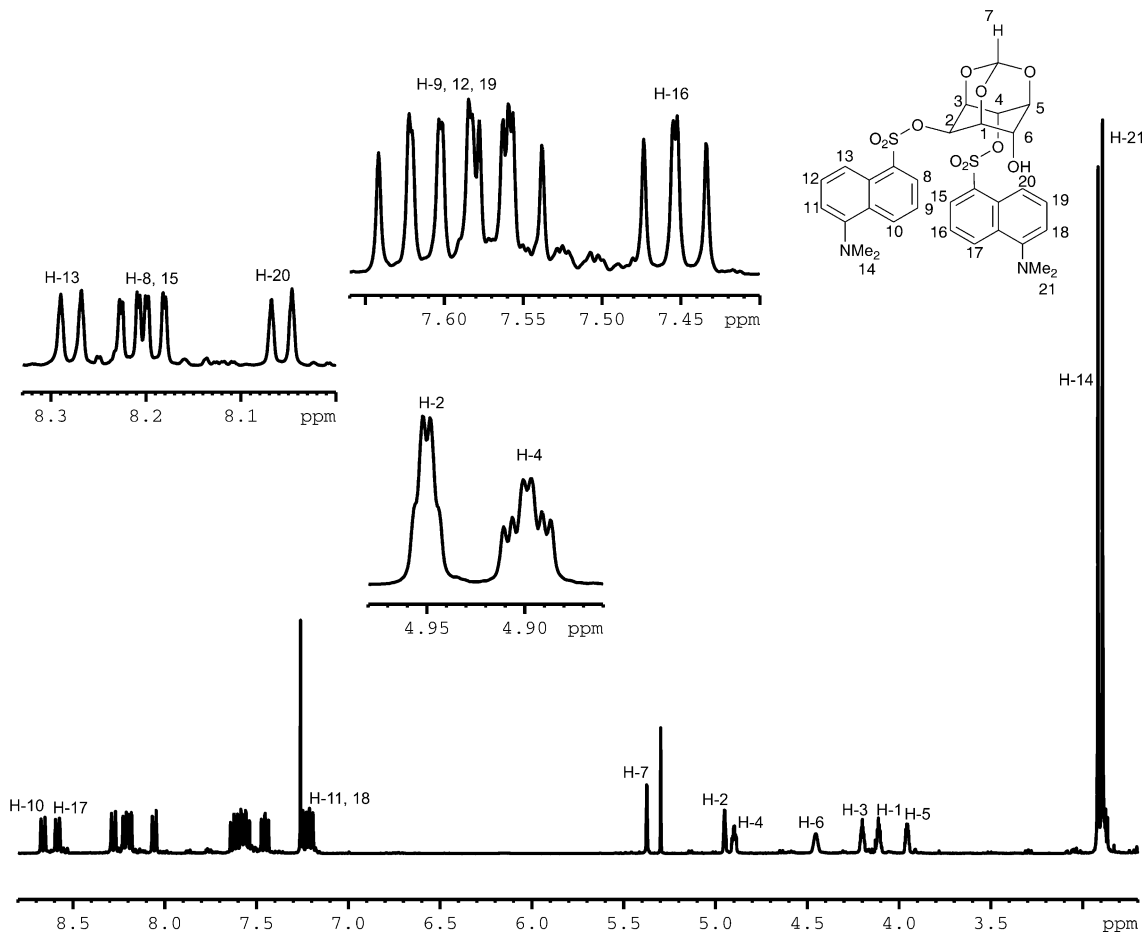


Figure SI 2: ^1H NMR spectrum (400 MHz) of 2,4-O-bisdansyl-myoinositol-1,3,5-orthoformate (**8**) in CDCl_3 . The peak at ~ 5.3 ppm is DCM, the solvent used for column chromatography. The chemical shift data and coupling constant are reported in the experimental.

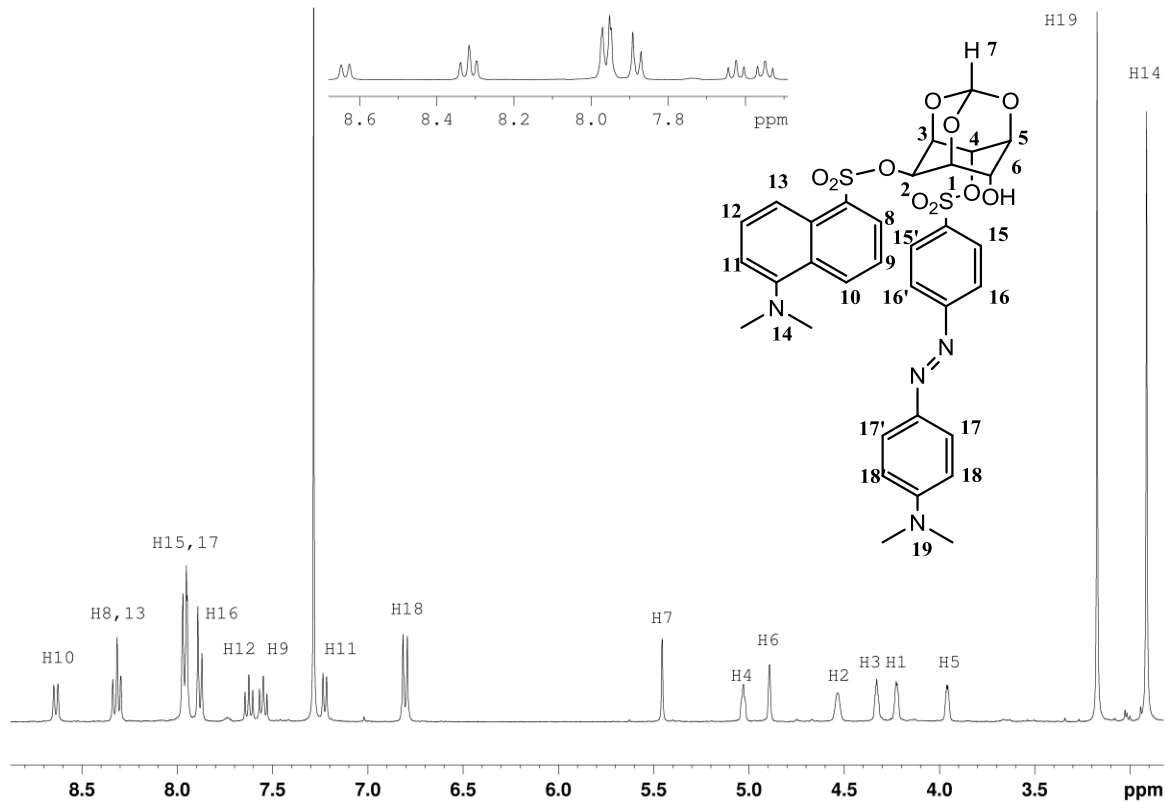


Figure SI 3: ¹H NMR (400 MHz) spectrum of 4-*O*-dabsyl-2-*O*-dansyl-*myo*-inositol-1,3,5-orthoformate (**4**) in CDCl₃. The chemical shift data and coupling constant are reported in the experimental.

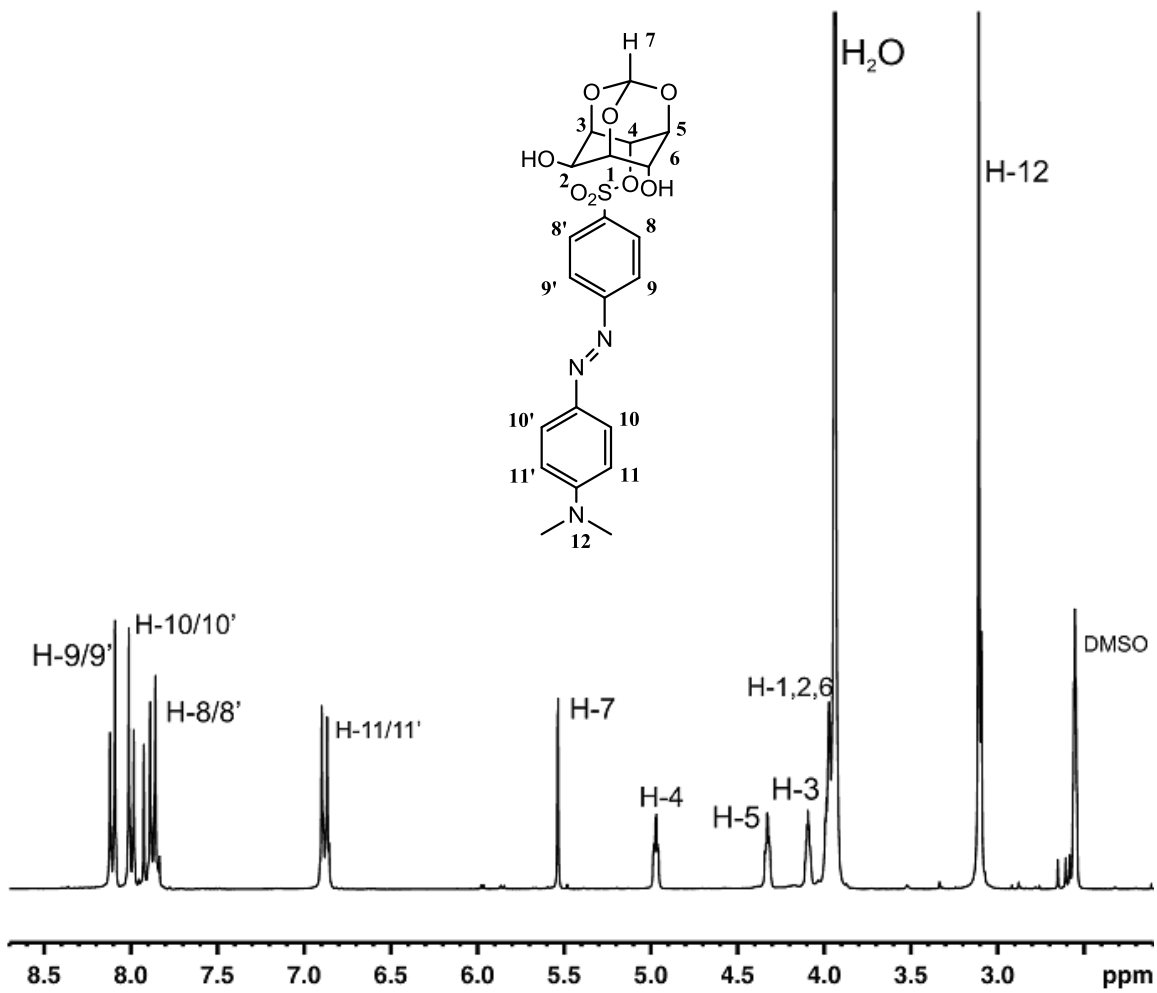


Figure SI 4: ¹H NMR (500 MHz) spectrum of 4-*O*-dabsyl-*myo*-inositol-1,3,5-orthoformate (**9**) in DMSO-d₆/D₂O.

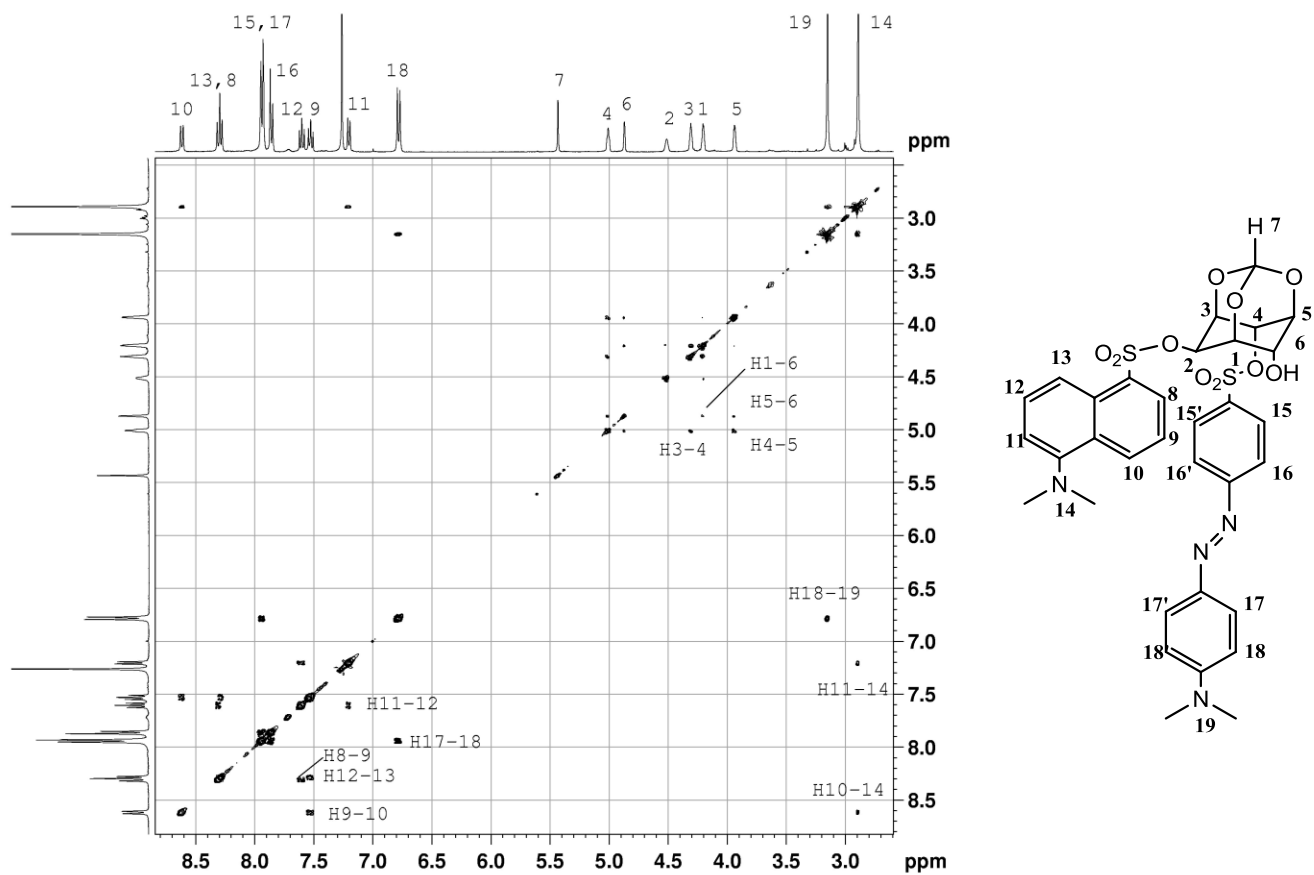


Figure S15 ^1H - ^1H NOESY (400 MHz) spectrum of 2-dansyl-4-*O*-dabsyl-*myo*-inositol-1,3,5-orthoformate (**4**) in CDCl_3 .

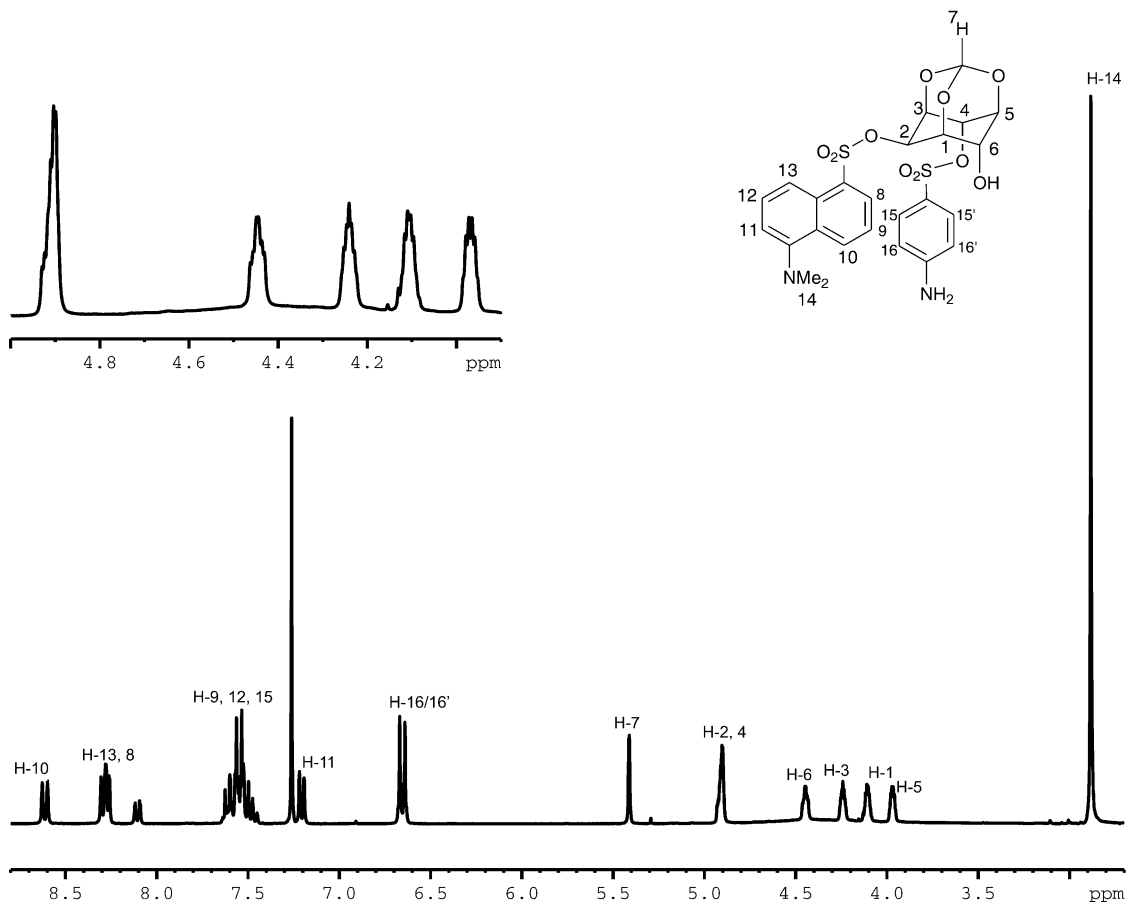


Figure SI 6: ¹H NMR (400 MHz) spectrum of 4-*O*-(4-aminobenzene)-sulfonyl-2-*O*-dansyl-*myo*-inositol-1,3,5-orthoformate (**5**) in CDCl₃. The impurity at $\sim\delta_{\text{H}}$ 8.09 (J 8.5 Hz) is attributed to the decomposition product, 4-aminobenzenesulfonic acid. The chemical shift data and coupling constant are reported in the experimental.

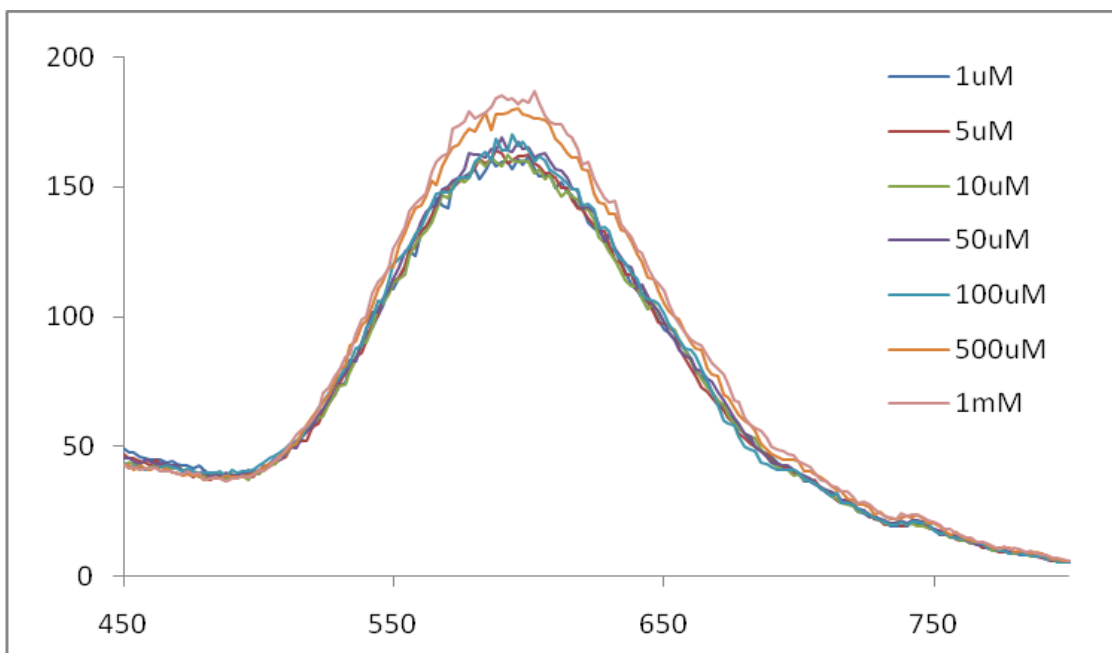


Fig SI 7: Emission spectra of 10 μM 2-*O*-dansyl-*myo*-inositol-1,3,5-orthoformate (**6**) titrated against varying concentrations of 4-aminobenzene sulfonic acid.

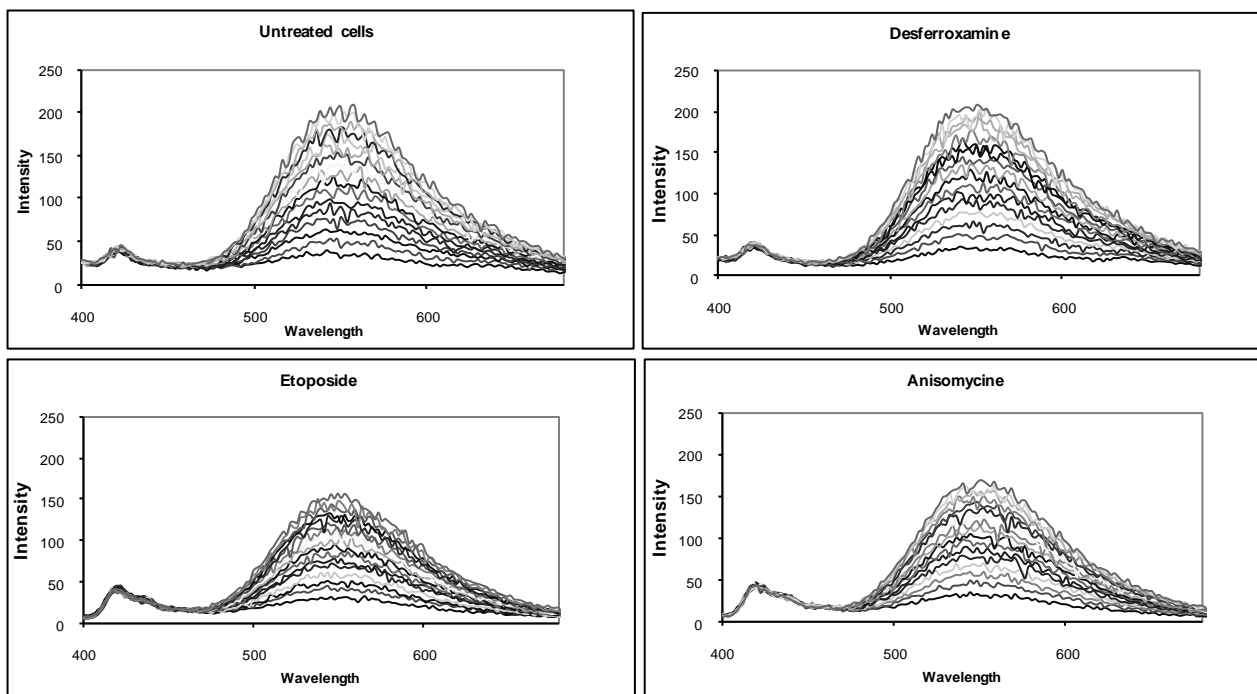


Figure SI 8: Fluorescence study of azo probe (**4**) incubated with Human U2OS osteosarcoma cells. An increase in fluorescence is noted with each line representing a fluorescence scan taken every hour over a 16-hour period, summarized as a time course in **Fig. 5**.