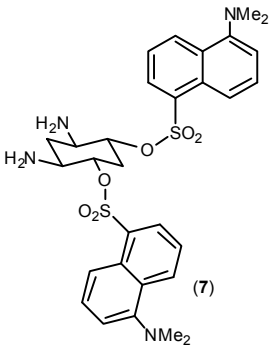
Electronic Supporting Information for CC-COM-06-2011-013902

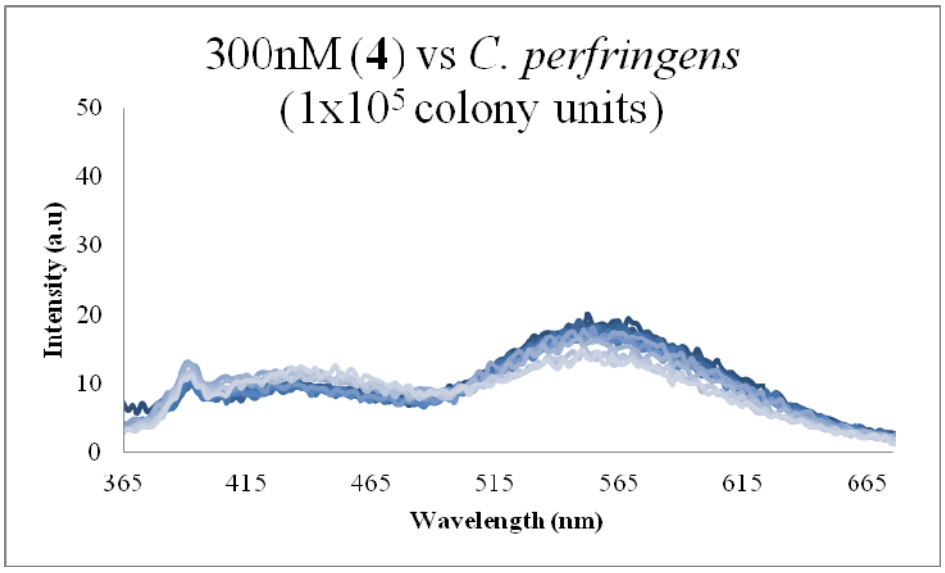
'Fluorescent probe for detection of bacteria: conformational trigger upon bacterial reduction of an azo bridge'



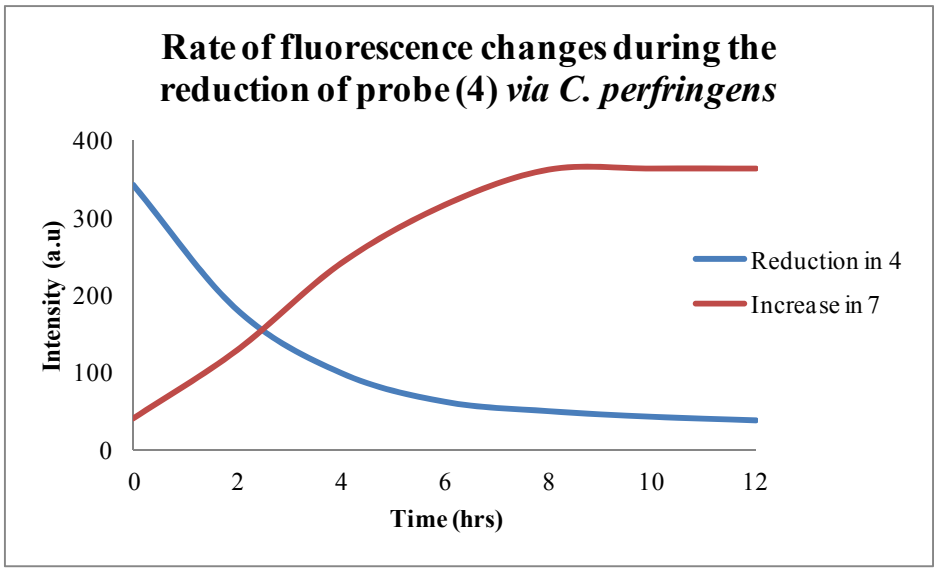
(**7**)

^{1}H-NMR for reduced probe **7** (400MHz, D_6-DMSO) δ_H 8.65 (2H, d, $^{3}J_{1'\text{-}2'}$ 8.2Hz, H-1'), 8.04 (2H, d, $^{3}J_{6'\text{-}5'}$ 7.9Hz, H-6'), 7.86 (2H, d, $^{3}J_{3'\text{-}2'}$ 8.0Hz, H-3'), 7.70 (2H, t, $^{3}J_{2'\text{-}1'/3'}$, H-2'), 7.59 (2H, t, $^{3}J_{5'\text{-}4'/6'}$, H-5'), 7.33 (2H, d, $^{3}J_{4'\text{-}5'}$ 8.0Hz, H-4'), 4.51 (2H, dt, H-2/4), 3.89 (2H, dt, H-1/5), 2.80 (12H, s, H-7'), 2.31 (1H, d, $^{2}J_{3ax\text{-}3eq}$ 14.2Hz, H-3_{ax}), 2.14 (1H, m, H-8_{ax}), 1.66 (1H, m, H-8_{eq}), 1.54 (1H, m, H-3_{eq})

ESI 1: NMR data from reduced probe **7**.



ESI 2: Fluorescence spectra of 300nM (**4**) upon exposure to cell supernatant from $1x10^5$ *C. perfringens* colony forming units containing azo-reductase enzymes. The Limit of Detection for this probe system against azoreductase expression by *C.perfringens* is thus deemed 300nM of (**4**) vs. $1x10^5$ colony forming units/ml over a 15hr time period.



ESI 3: *Fluorescent time course kinetic graph of the reduction of 2,4-O-bisdansyl-6,7-diazabicyclooct-6-ene (**4**) to generate its reduced form (**7**). At 10μM concentration, the probe was treated with C. perfringens cellular extract known to contain azoreductive enzymes Excitation at 335nm initially showed a dimer type emission at ca. 552nm (blue line). Subsequent tracking of fluorescence over a 12h period (showed the appearance of a monomer band at ca. 451nm (red line).*