

Structural characterisation of the photoisomers of reactive sulfonated azo dyes by NMR spectroscopy and *ab initio* calculations

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Supporting Information

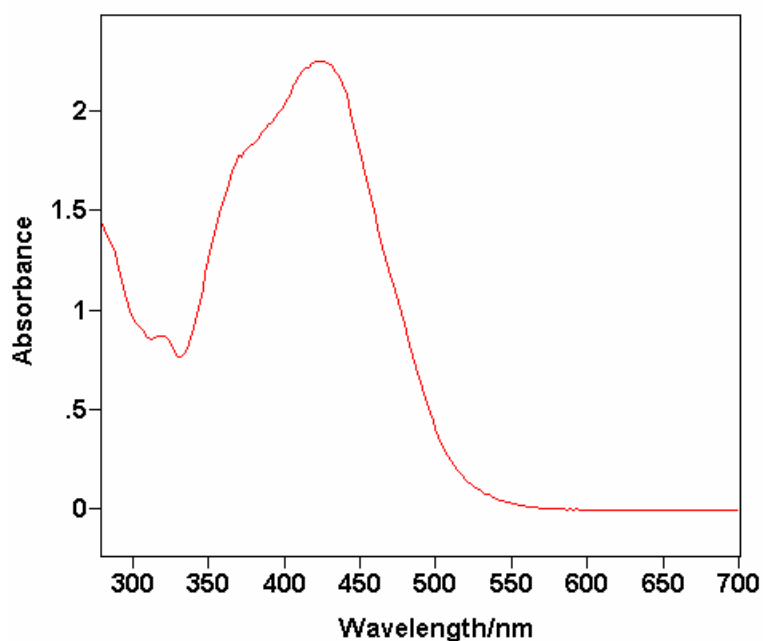


Figure S1 UV-Vis absorption spectrum of **1** in DMSO. Sample concentration = 1×10^{-4} M.

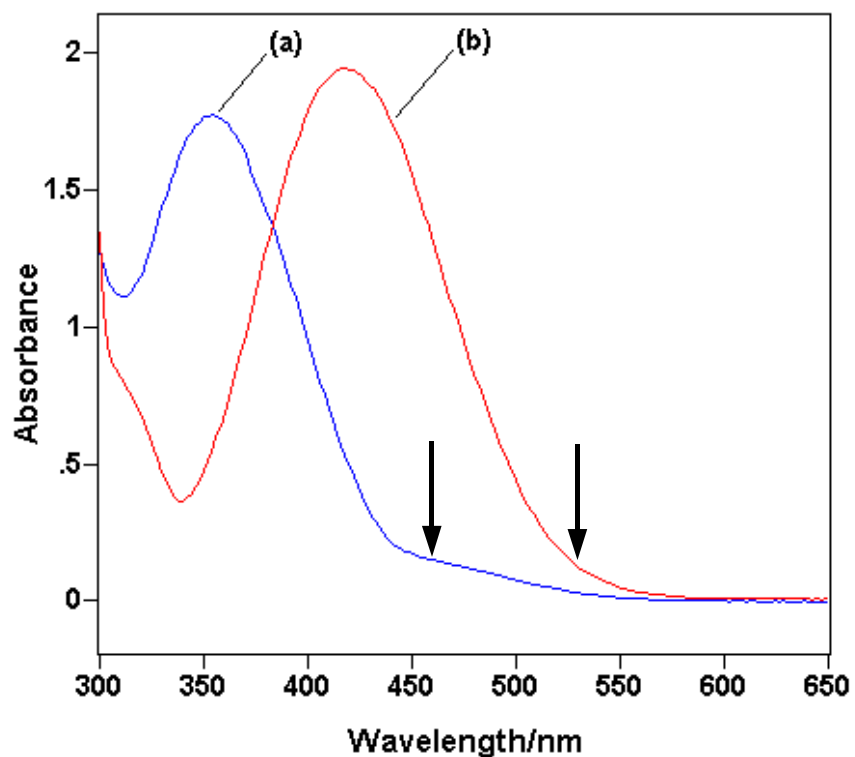


Figure S2 UV-Visible spectra of (a) **2** and (b) **2a** (the dyebase of **2**) in DMSO. Sample concentration = 1×10^{-4} M. Irradiation wavelengths of 457 and 530 nm, respectively, are shown by arrows.

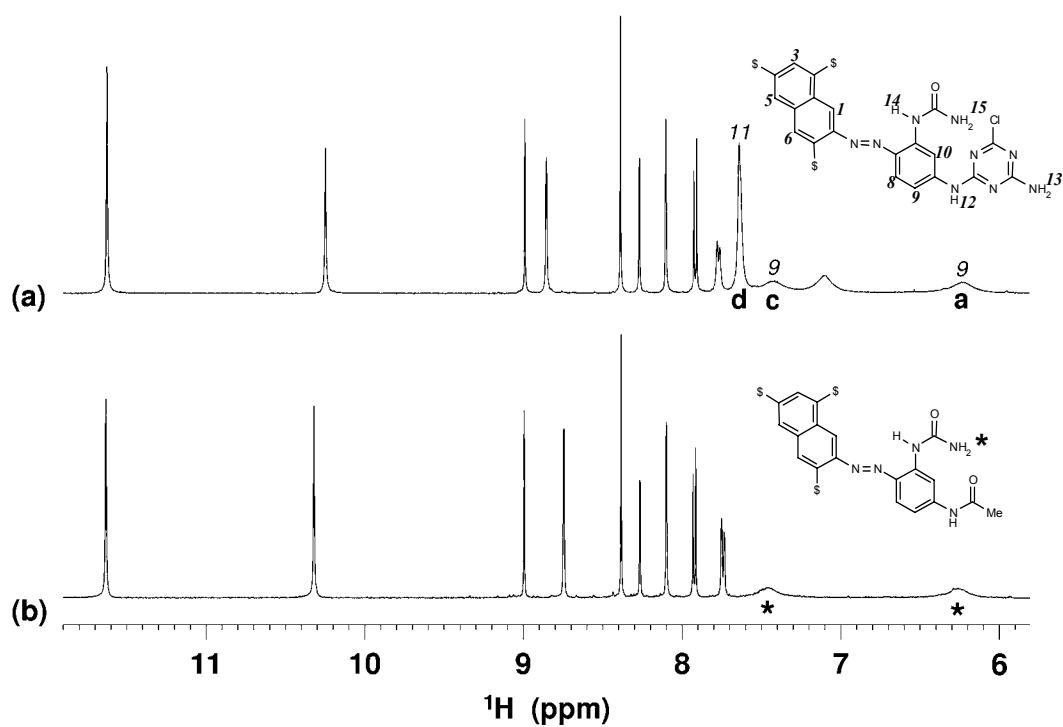


Figure S3 500 MHz 1D ¹H NMR spectra of (a) **1** (1.77 mM in *d*₆-DMSO) and (b) the closely related molecule designated **6** (1.28 mM in *d*₆-DMSO) recorded in darkness. In (b) asterisks indicate the broadened resonances associated with unique magnetic environments of the two individual NH protons associated with the only NH₂ group of **6**.

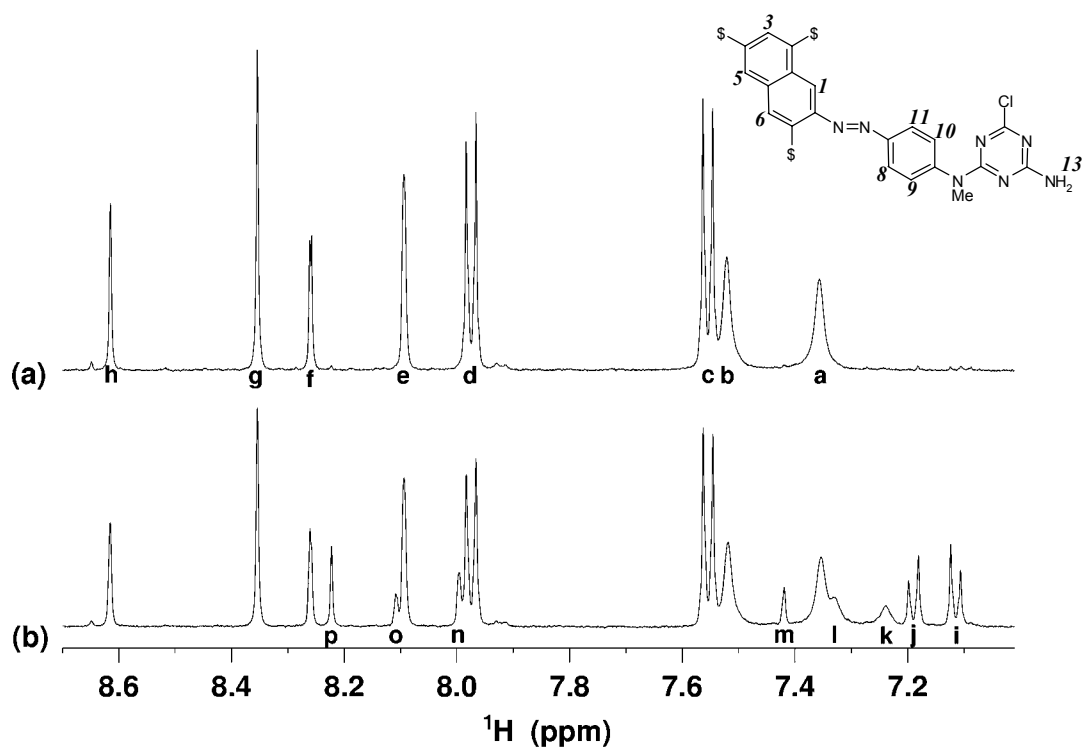


Figure S4: 500 MHz 1D ¹H NMR spectra of **2** (0.75 mM in *d*₆-DMSO) (a) prior to irradiation and (b) after irradiation to the 457 nm PSS. Atom labeling is indicated in the molecular diagram.

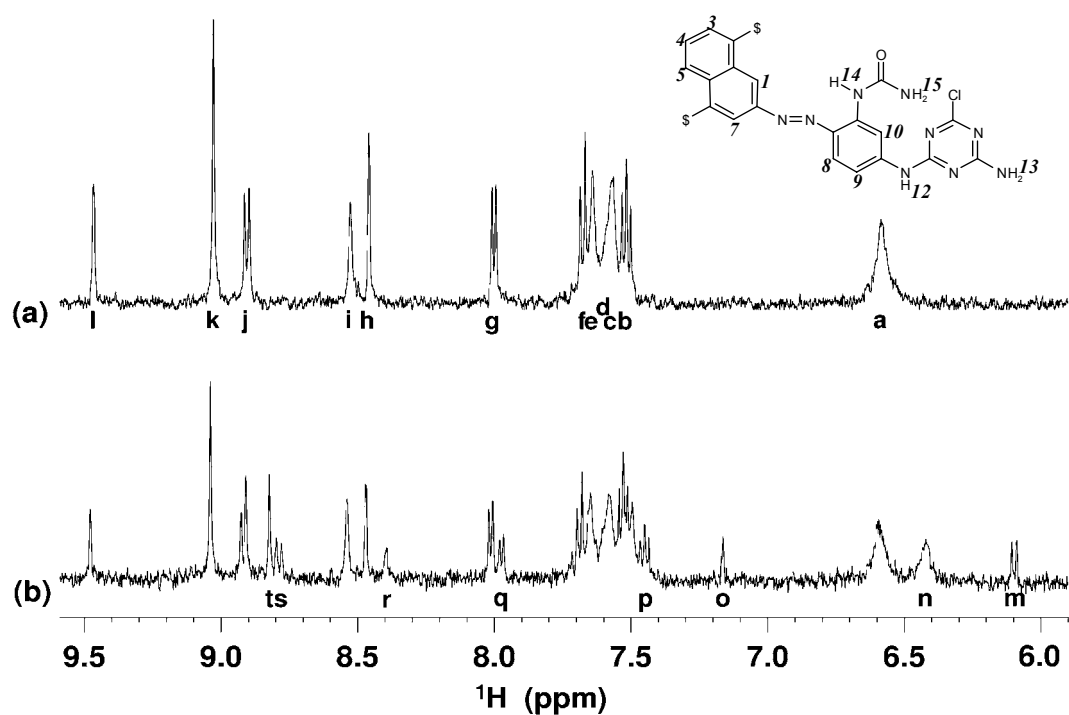


Figure S5 500 MHz 1D ^1H NMR spectra of **3** (0.38 mM in d_6 -DMSO) (a) prior to irradiation and (b) after irradiation to the 514 nm PSS.

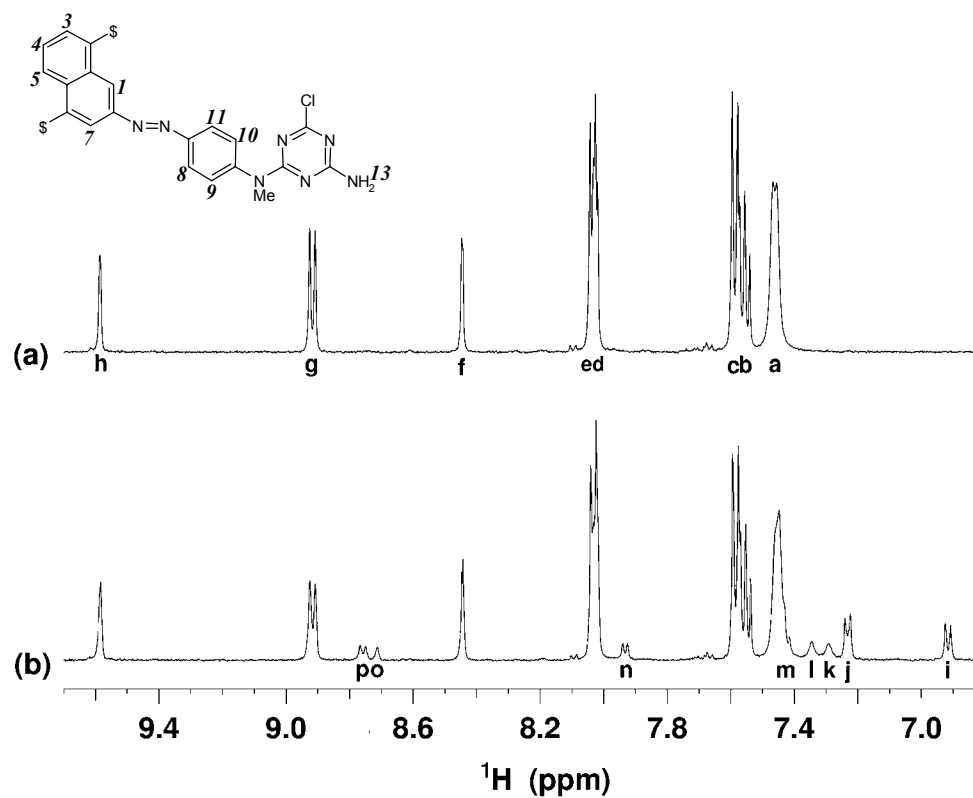


Figure S6 500 MHz 1D ¹H NMR spectra of 4 (1.23 mM in *d*₆-DMSO) (a) prior to irradiation and (b) after irradiation to the 488 nm PSS.

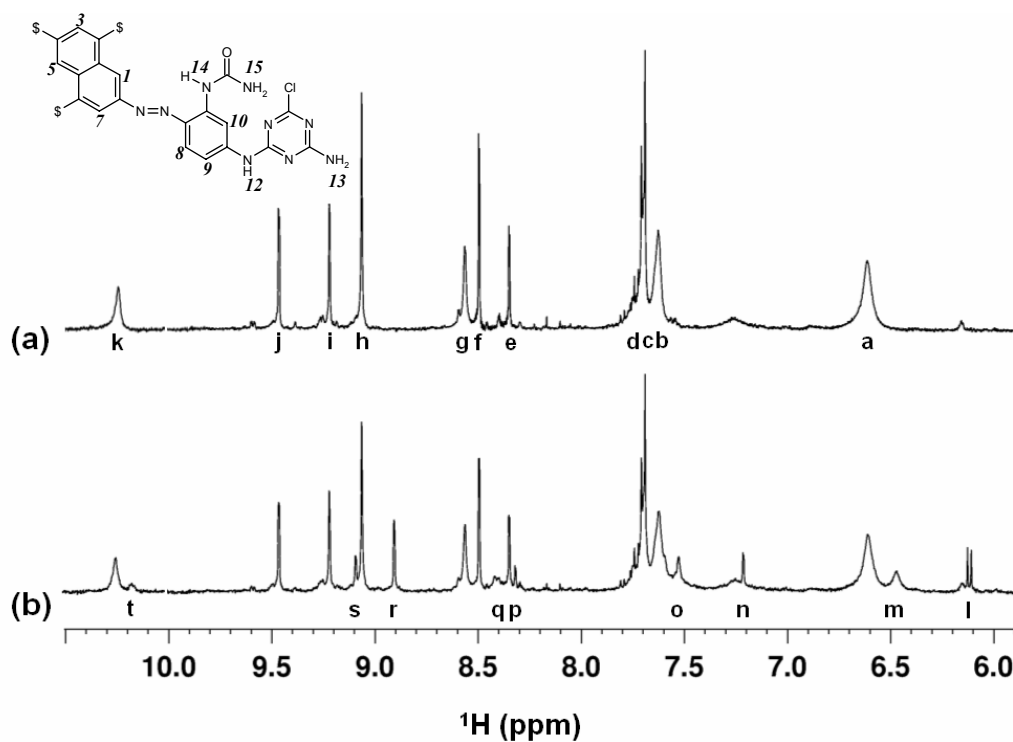


Figure S7 500 MHz 1D ^1H NMR spectrum of **5** (0.35 mM in d_6 -DMSO) (a) prior to irradiation and (b) after irradiation to the 530 nm PSS.

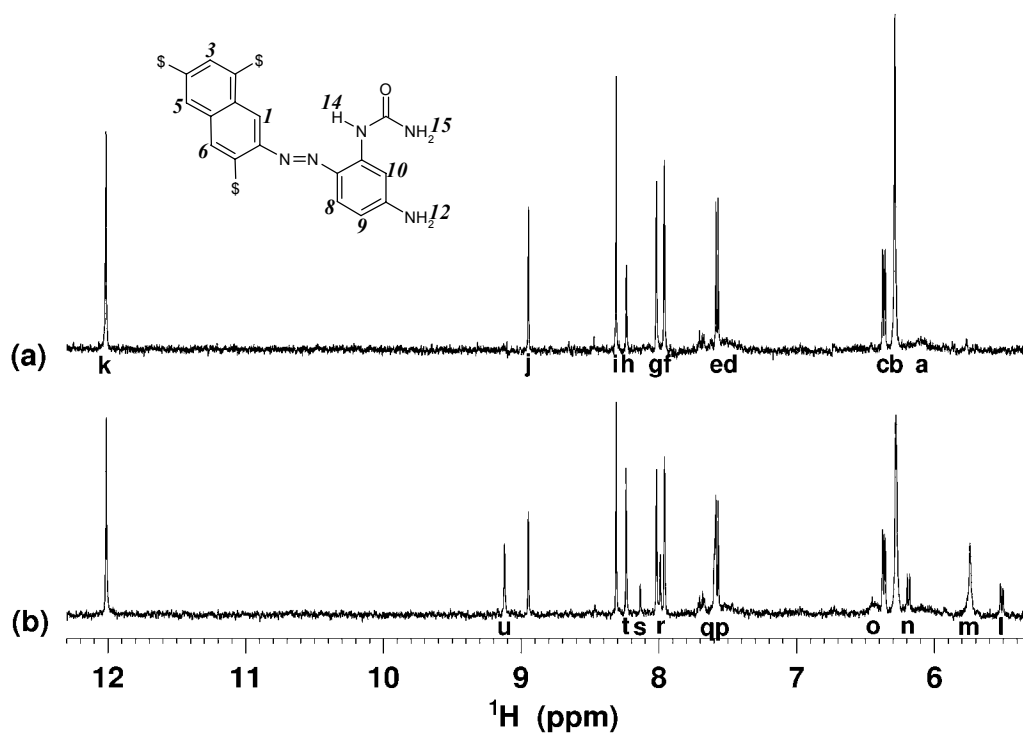


Figure S8 500 MHz 1D ^1H NMR spectrum of **1a** (0.45 mM in d_6 -DMSO) (a) prior to irradiation and (b) after irradiation to the 530 nm PSS.

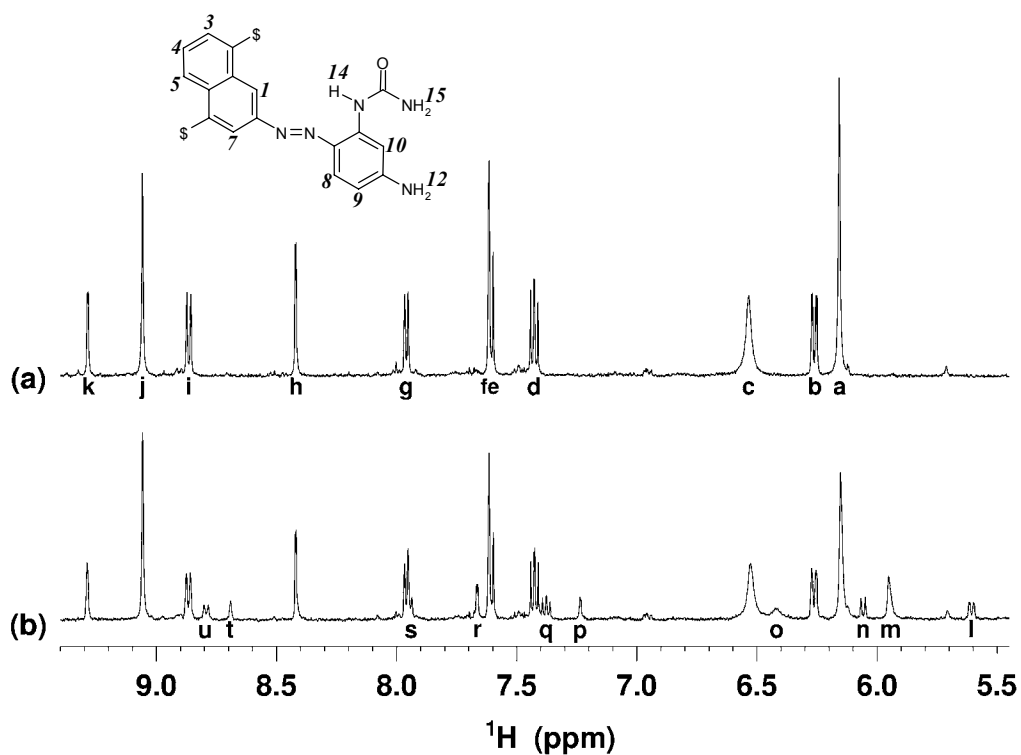


Figure S9 500 MHz 1D ¹H NMR spectra of **3a** (1.28 mM in d₆-DMSO) (a) prior to irradiation and (b) after irradiation to the 530 nm PSS.

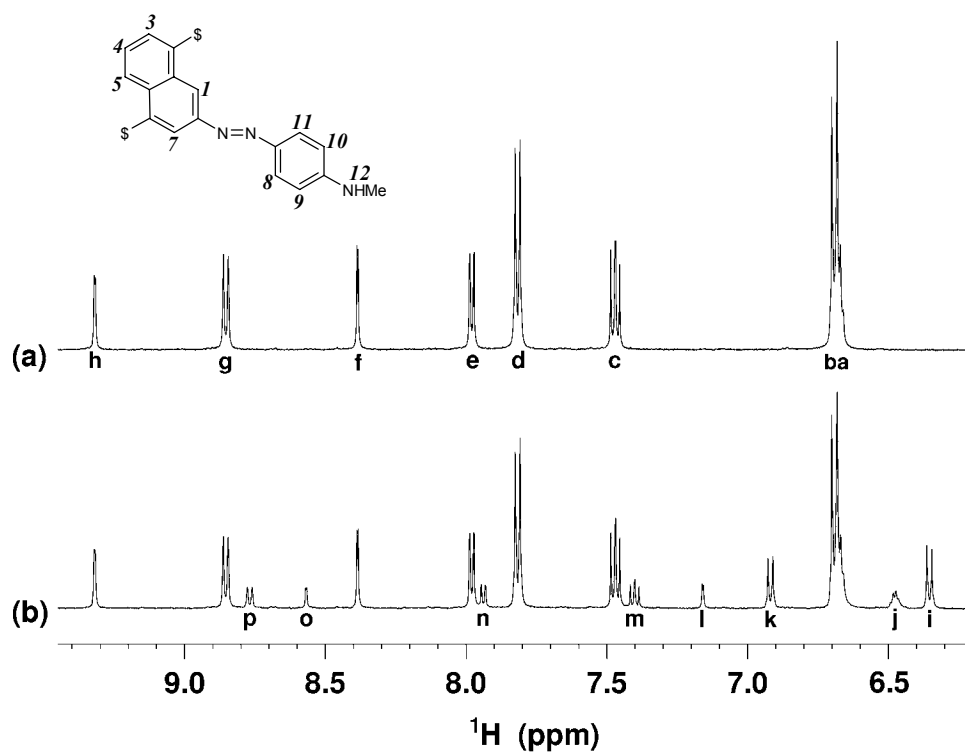


Figure S10 500 MHz 1D ¹H NMR spectra of 4a (0.80 mM in d₆-DMSO) (a) prior to irradiation and (b) after irradiation to the 514 nm PSS.

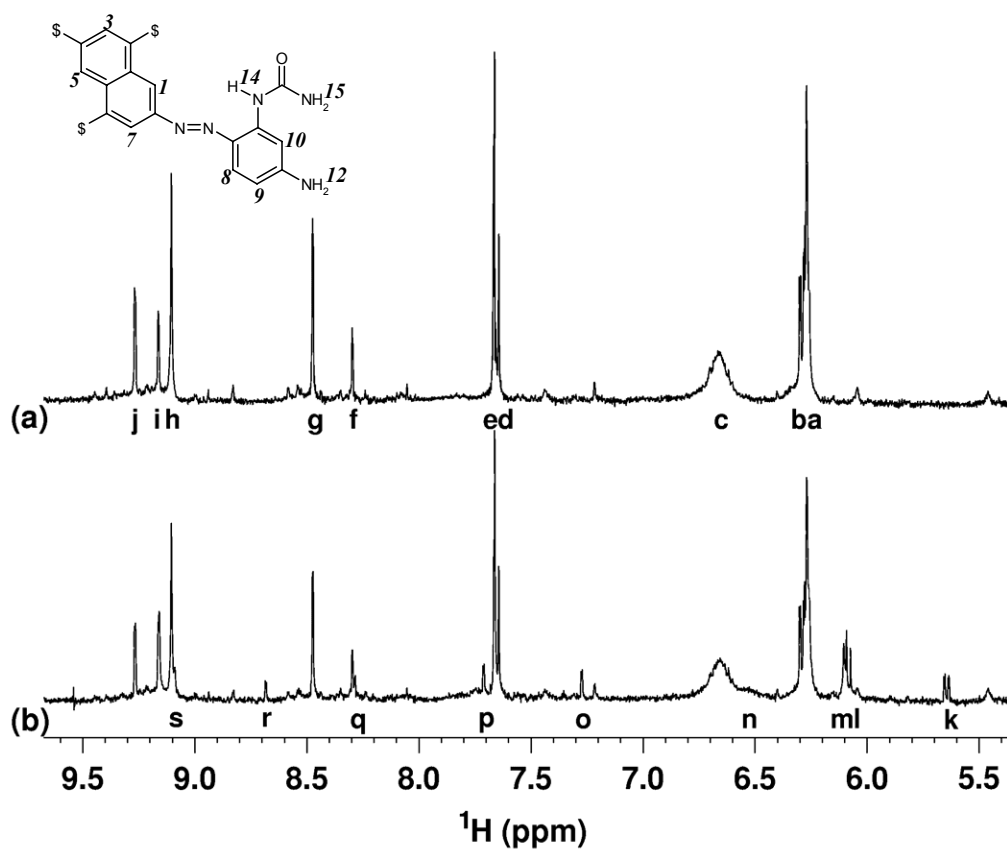


Figure S11 500 MHz 1D ^1H NMR spectra of **5a** (0.19 mM in d_6 -DMSO) (a) prior to irradiation and (b) after irradiation to the 530 nm PSS.