Structural characterisation of the photoisomers of reactive sulfonated azo dyes by NMR spectroscopy and \textit{ab initio} calculations

Katrina M. Tait\textsuperscript{a}, John A. Parkinson\textsuperscript{b}, David I. Gibson\textsuperscript{a}, Patricia R. Richardson\textsuperscript{a} Warren J. Ebenezer\textsuperscript{c}, Michael G. Hutchings\textsuperscript{c} and Anita C. Jones\textsuperscript{*a}

Supporting Information

![Graph](image)

**Figure S1** UV-Vis absorption spectrum of 1 in DMSO. Sample concentration = $1\times10^{-4}$ M.
Figure S2  UV-Visible spectra of (a) 2 and (b) 2a (the dyebase of 2) in DMSO. Sample concentration = 1x10^{-4} M. Irradiation wavelengths of 457 and 530 nm, respectively, are shown by arrows.
Figure S3  500 MHz 1D $^1$H 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 NH$_2$ group of 6.
Figure S4: 500 MHz 1D $^1$H 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 $^1$H 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 $^1$H 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 $^1$H 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 $^1$H 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 $^1$H NMR spectra of 3a (1.28 mM in d$_6$-DMSO) (a) prior to irradiation and (b) after irradiation to the 530 nm PSS.
Figure S10  500 MHz 1D $^1$H NMR spectra of 4a (0.80 mM in d$_6$-DMSO) (a) prior to irradiation and (b) after irradiation to the 514 nm PSS.
Figure S11 500 MHz 1D $^1$H NMR spectra of 5a (0.19 mM in d$_6$-DMSO) (a) prior to irradiation and (b) after irradiation to the 530 nm PSS.