Supplementary Material (ESI) for Photochemical & Photobiological Sciences

Coumaric amide rotaxanes: effects of hydrogen bonding and mechanical interlocking on the photochemistry and photophysics

Albert M. Brouwer,*[a] Sandro M. Fazio,[a] Natalia Haraszkiewicz,[a] David A. Leigh,*[b] and Claire M. Lennon (neé Keaveney)[b]

[a] Van 't Hoff Institute for Molecular Sciences, University of Amsterdam, Nieuwe Achtergracht 129, 1018 WS Amsterdam, The Netherlands. Fax: +31 205 255 680; Tel: +31 205 255 491; E-mail: a.m.brouwer@uva.nl

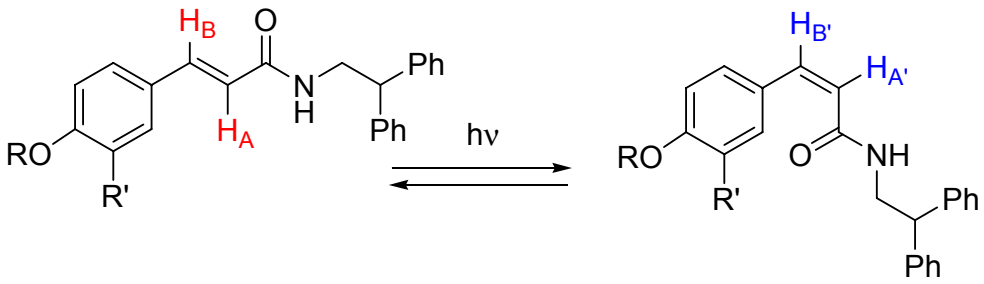
[b] School of Chemistry, University of Edinburgh, The King's Buildings, West Mains Road, Edinburgh EH9 3JJ, United Kingdom. Fax: +44 131 667 9085; Tel: +44 131 650 4730; E-mail: David.Leigh@ed.ac.uk

TABLE S1. ^{1}H NMR chemical shifts of olefinic protons H_A and H_B in *E* and *Z* isomers of threads **1**, **3** and **5**, and rotaxanes **2**, **4** and **6**.

Compound(s)	*E*-isomer		*Z*-isomer	
	$\delta(H_A)$	$\delta(H_B)$	$\delta(H_A)$	$\delta(H_B)$
1	6.09	7.52	5.75	6.59
2	4.88	6.46	[a]	5.85
3	5.97	7.44	5.71	6.53
4	4.77	6.40	[b]	[b]
5	5.97	7.43	5.75	6.53
6	4.77	6.42	[b]	[b]

[a] not determined, signal hidden by others. [b] not determined.

The ^{1}H-NMR spectra (400 MHz, $CDCl_3$) of thread *E*-**1** and rotaxane *E*-**2** and the photostationary mixtures produced are shown in the paper, figure 1. The corresponding data for **3** can be found in the ESI of ref. 1. In Figure S1, the same set of spectra is shown for thread **5**. The two isomers are readily characterized by the signals of the olefinic protons, labelled as H_B and H_A for the *E* isomer and $H_{B'}$ and $H_{A'}$ for the *Z* isomer. Rotaxanes **4** and **6** do not show noticeable conversion under the same conditions of irradiation.



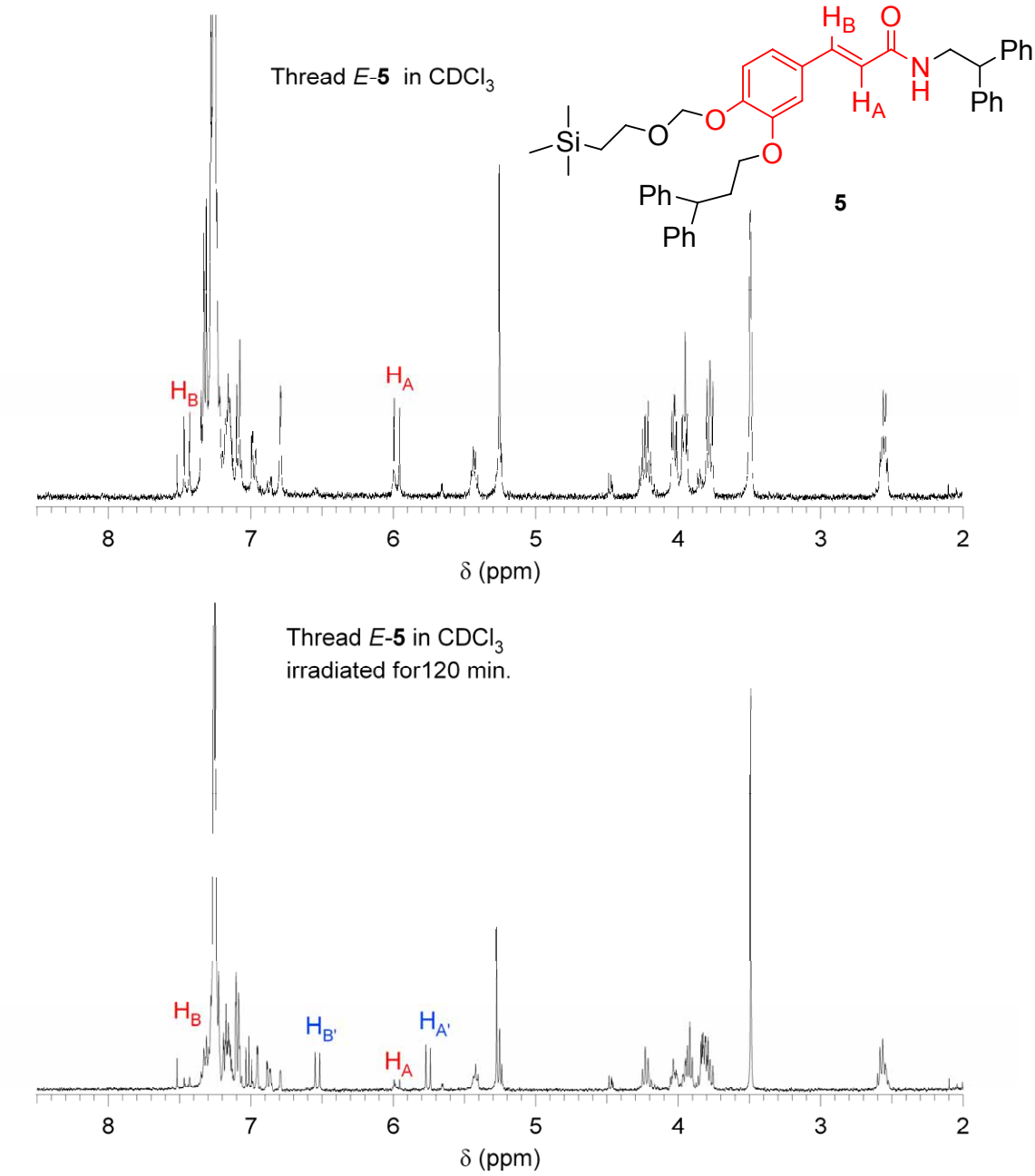


Figure S1. ^{1}H NMR spectra of **5**, and the photostationary mixture produced upon irradiation at 313 nm.

Table S2. Absorption spectral data (solvent dichloromethane).

compound	λ_{max}/nm (ε/dm^3 mol^{-1} cm^{-1})
1	293 (23700), 308 (23000)
2	300 (19600), 313 (21300)
3	292 (14700), 317 (16600)
4	294 (13200), 322 (16700)
5	292 (17900), 317 (17500)
6	286 (14300), 295 (14500), 322 (16700)

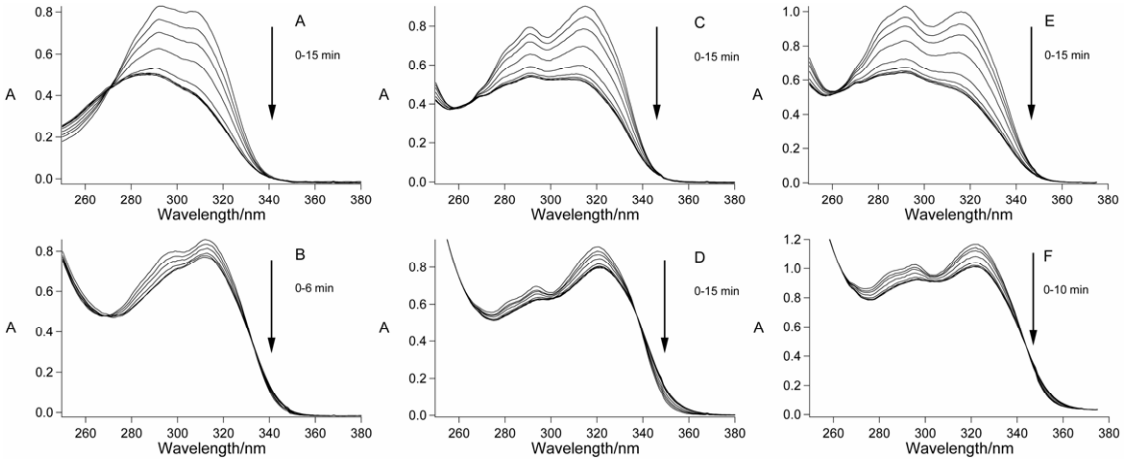


Figure S2. Monitoring photoinduced conversion (313 nm) of **1 - 6** (in dichloromethane) with UV absorption spectra

Reference

1. Berná, J., Brouwer, A.M., Fazio, S.M., Haraszkiewicz, N., Leigh, D.A., and Lennon, C.M. A rotaxane mimic of the photoactive yellow protein chromophore environment: Effects of hydrogen bonding and mechanical interlocking on a coumaric amide derivative. *Chem. Commun.*, 2007, **submitted**.