Experimental and theoretical insights into a novel lightfast thiophene azo dye

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Supplementary Materials

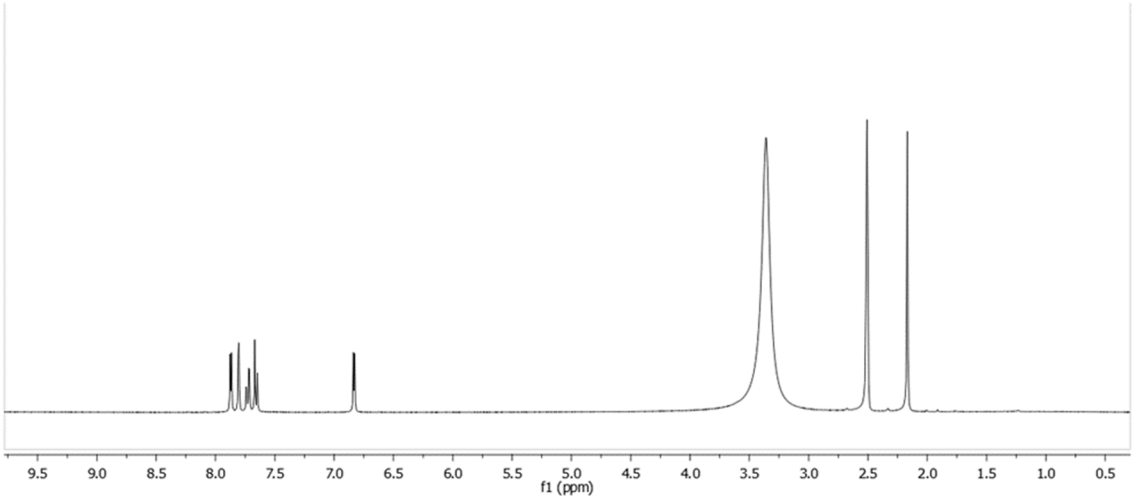

Figure S1. ^{1}H NMR of TA-OH (DMSO-d_6; 400 MHz)

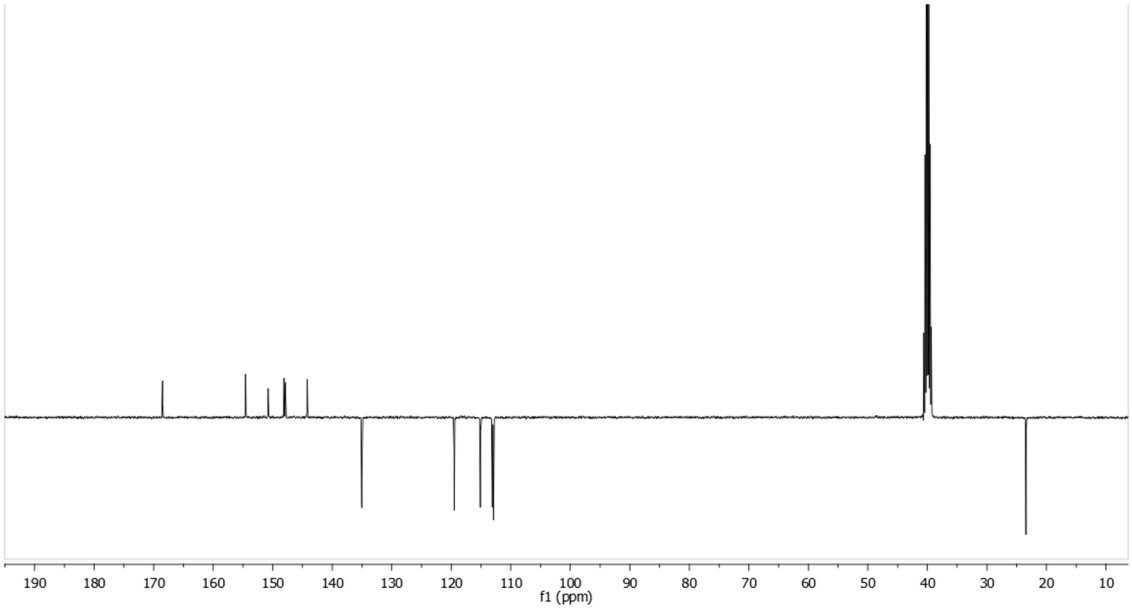

Figure S2. ^{13}C NMR of TA-OH (DMSO-d_6; 400 MHz). DEPTQ polarization transfer with decoupling during acquisition, shaped pulse for 180-degree pulse on f1 channel.

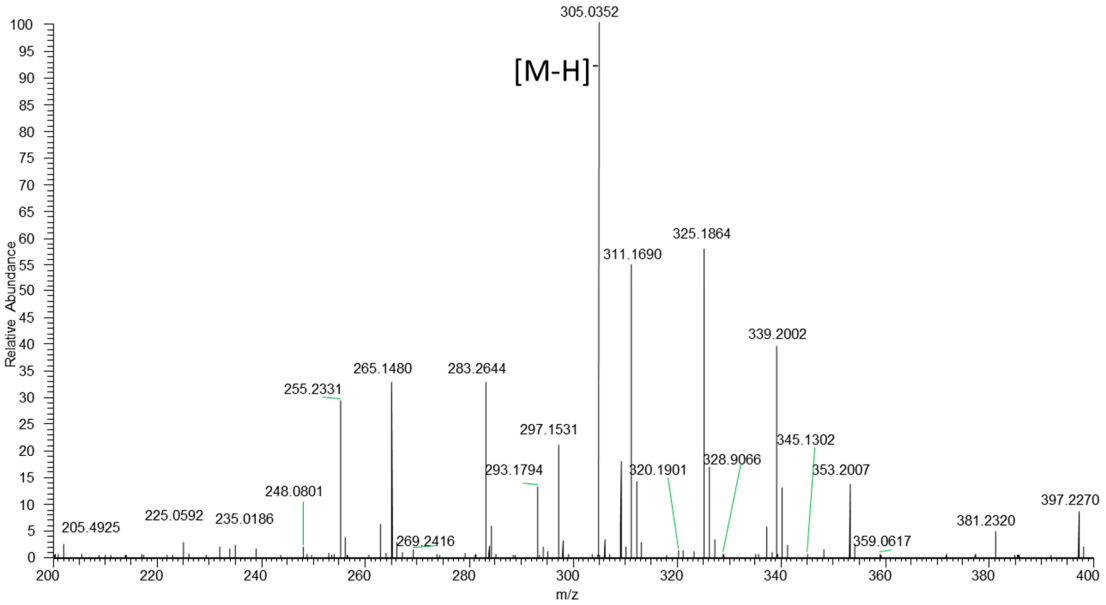

Figure S3. Mass spectrum of TA-OH. Formula $[M-H]^-$ $C_{12}H_9O_4N_4S$. Found m/z: 305.03.

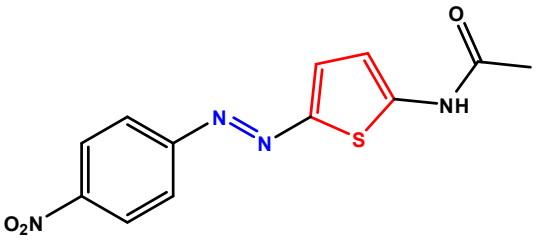

Figure S4. Chemical structure of the model molecule TA. The model TA is entirely analogous to TA-OH, but without the hydroxyl group on the phenyl ring.

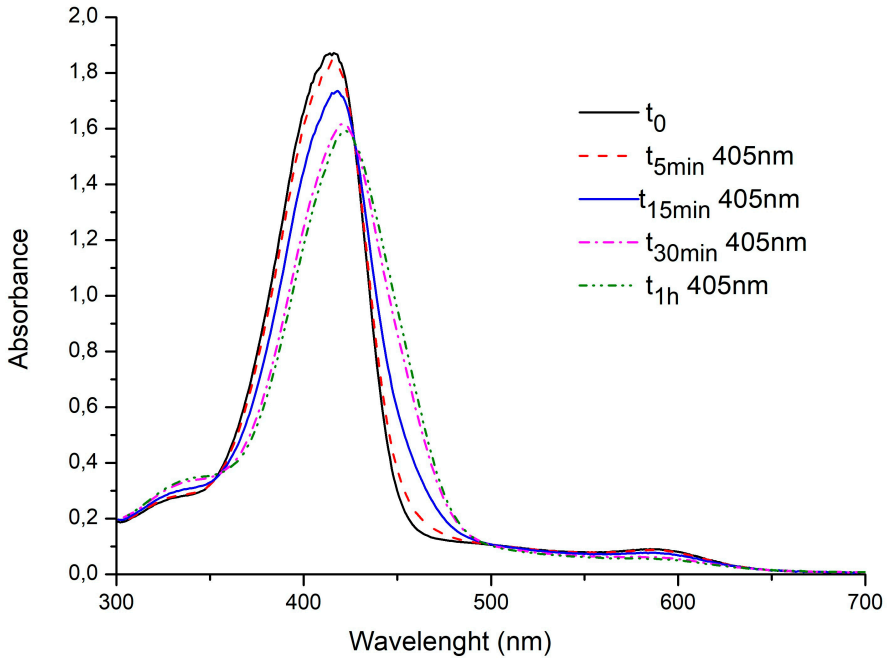

Figure S5. UV-Vis photoisomerization of model TA. The experimental UV-vis spectra under excitation at 405 nm show the possibility of photoswitching from the *trans* to the *cis* form.

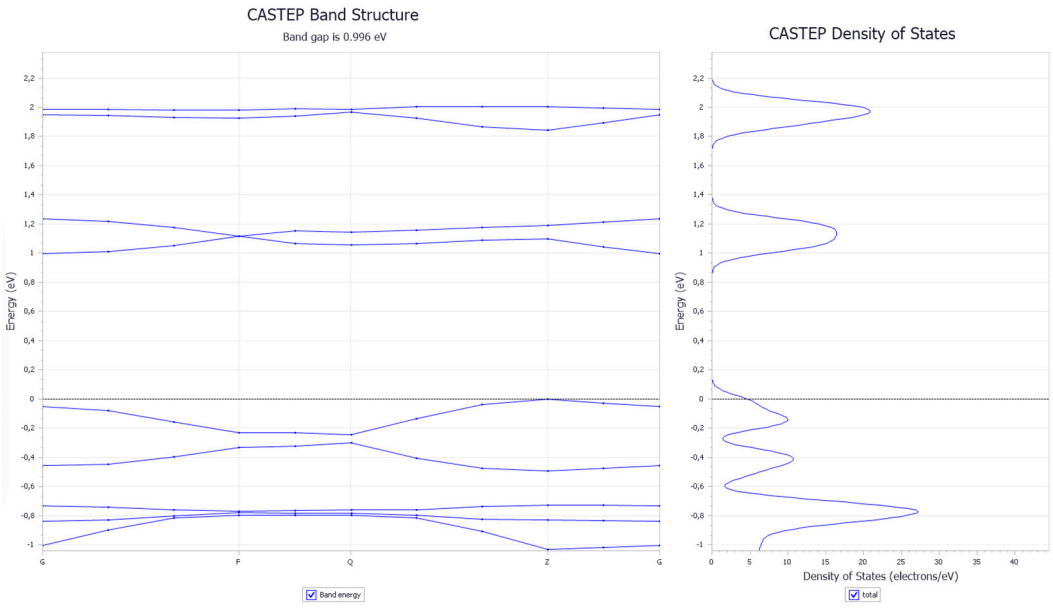

Figure S6. Band structure and density of states of the TA-OH crystal.

Table S1. Vertical transition energies of protonated TA-OH and deprotonated TA-OH.

System	Orbital type	Energy (E_h)	Energy (eV)
TA-OH protonated	HOMO-2	-0.252760	-6.8779
	HOMO-1	-0.249303	-6.7839
	HOMO	-0.211623	-5.7586
	LUMO	-0.113521	-3.0891
	LUMO+1	-0.074052	-2.0151
	LUMO+2	-0.017551	-0.4776
	LUMO+3	-0.015075	-0.4102
TA-OH deprotonated	HOMO-3	-0.232040	-6.3141
	HOMO-2	-0.207225	-5.6389
	HOMO-1	-0.173592	-4.7237
	HOMO	-0.168527	-4.5859
	LUMO	-0.086070	-2.3421
	LUMO+1	-0.051329	-1.3967