Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic supporting information

Dithiafulvene derivatized donor-acceptor norbornadienes with redshifted absorption

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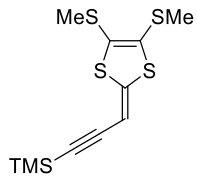
Contents

NMR spectra

Compound 5



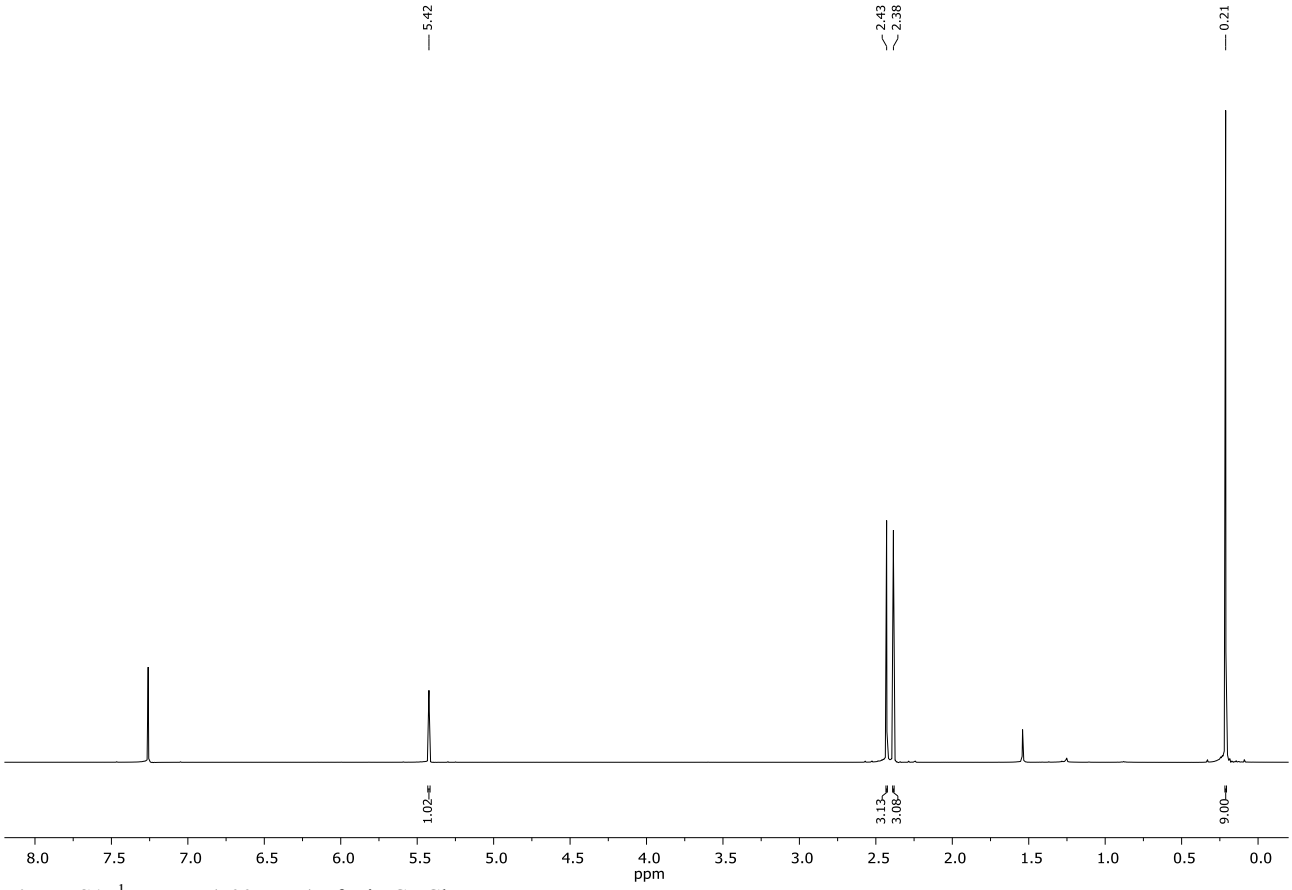


Figure S1: ^{1}H NMR (500 MHz) of **5** in $CDCl_3$.

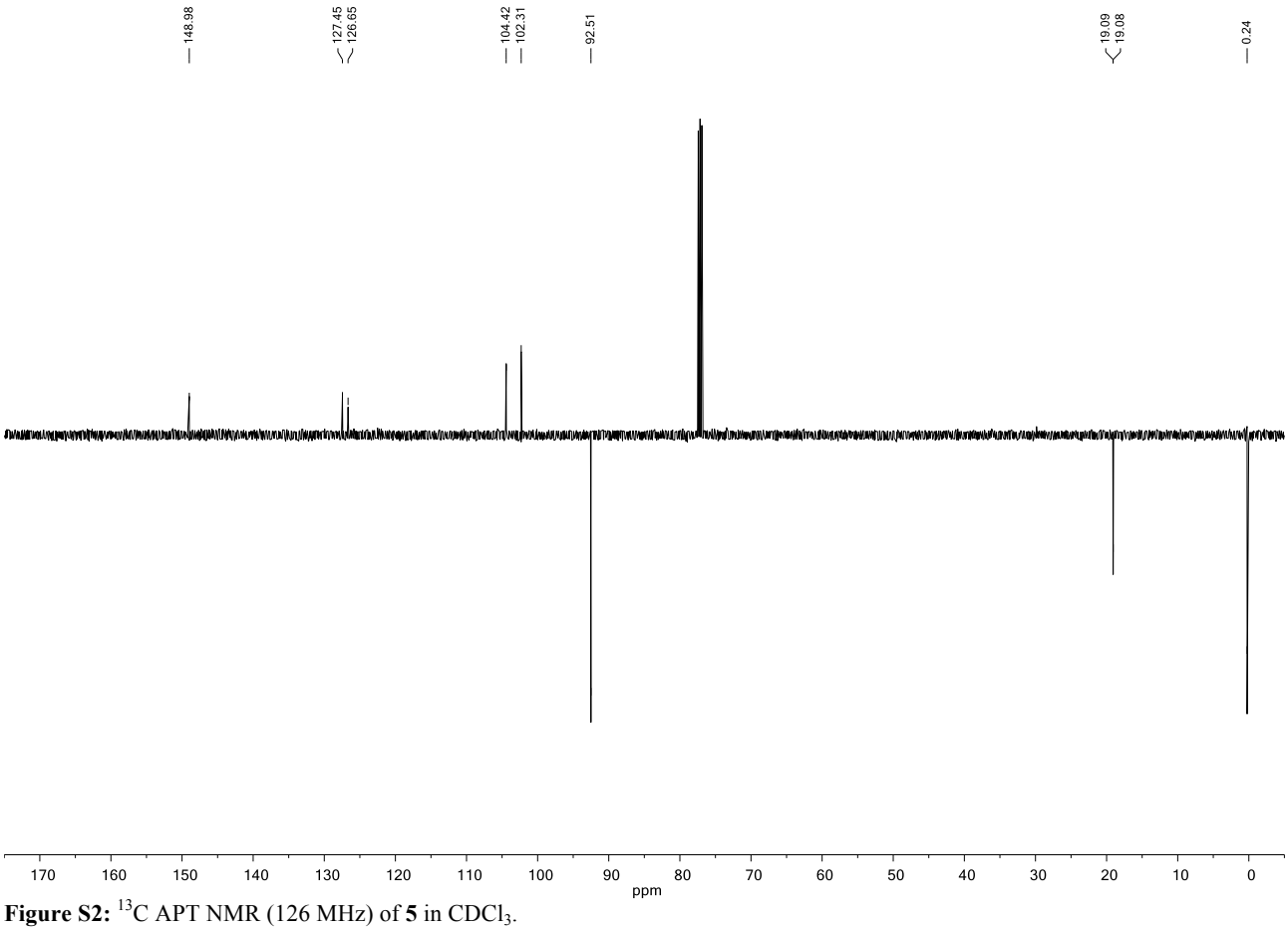


Figure S2: ^{13}C APT NMR (126 MHz) of **5** in $CDCl_3$.

Compound 6

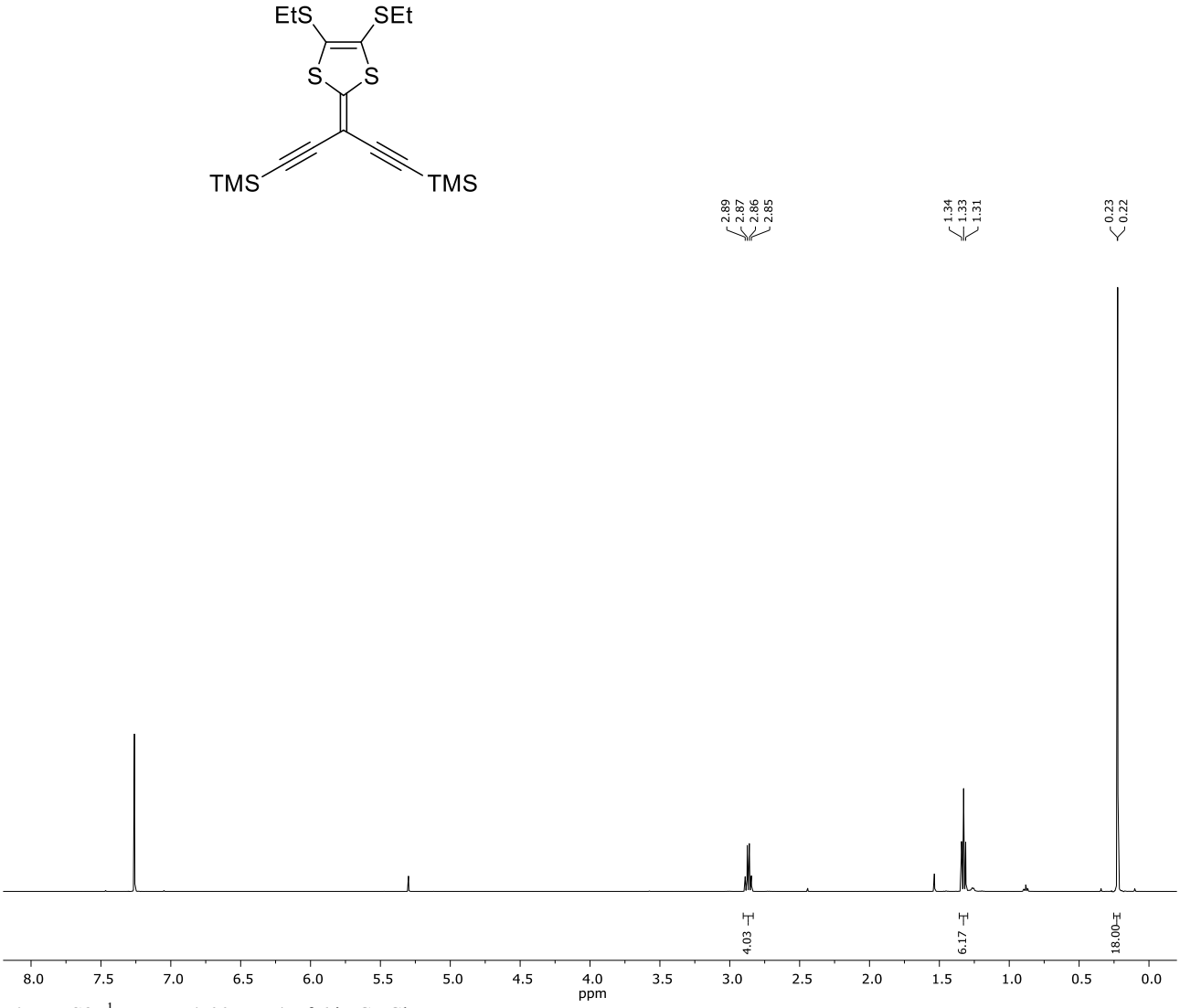


Figure S3: ^{1}H NMR (500 MHz) of **6** in $CDCl_3$.

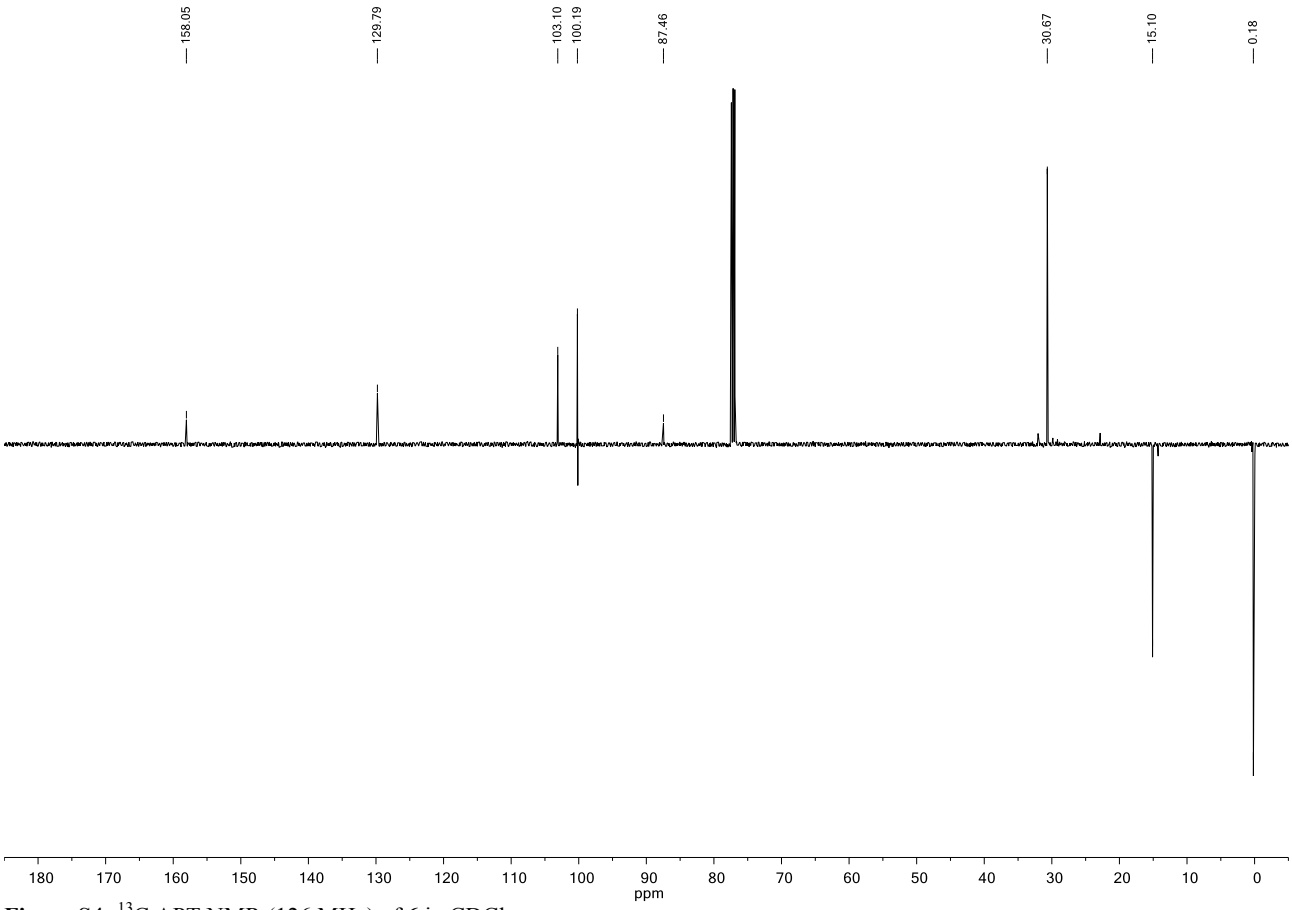
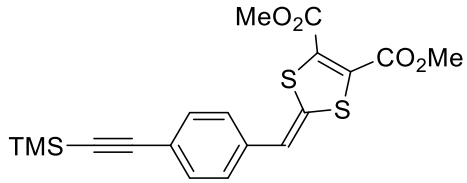


Figure S4: ^{13}C APT NMR (126 MHz) of **6** in $CDCl_3$.

Compound 9



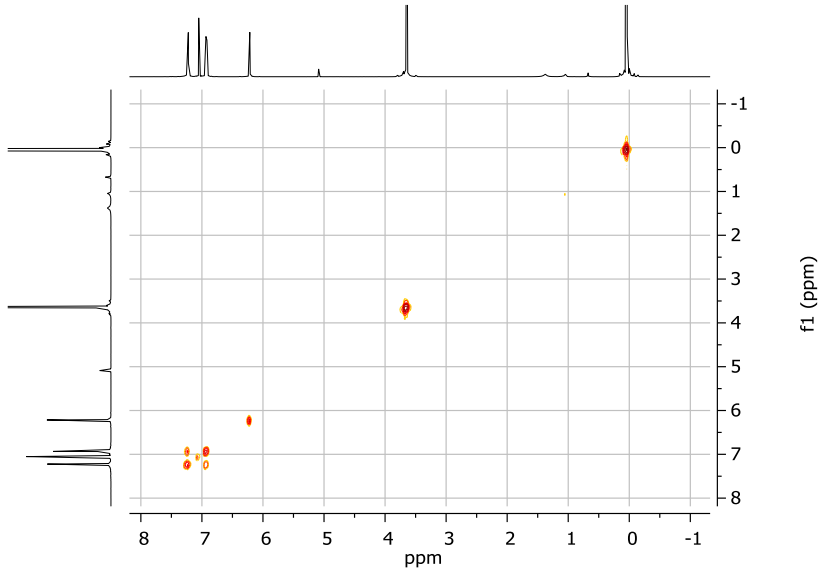


Figure S5: COSY NMR (500 MHz) of **9** in $CDCl_3$.

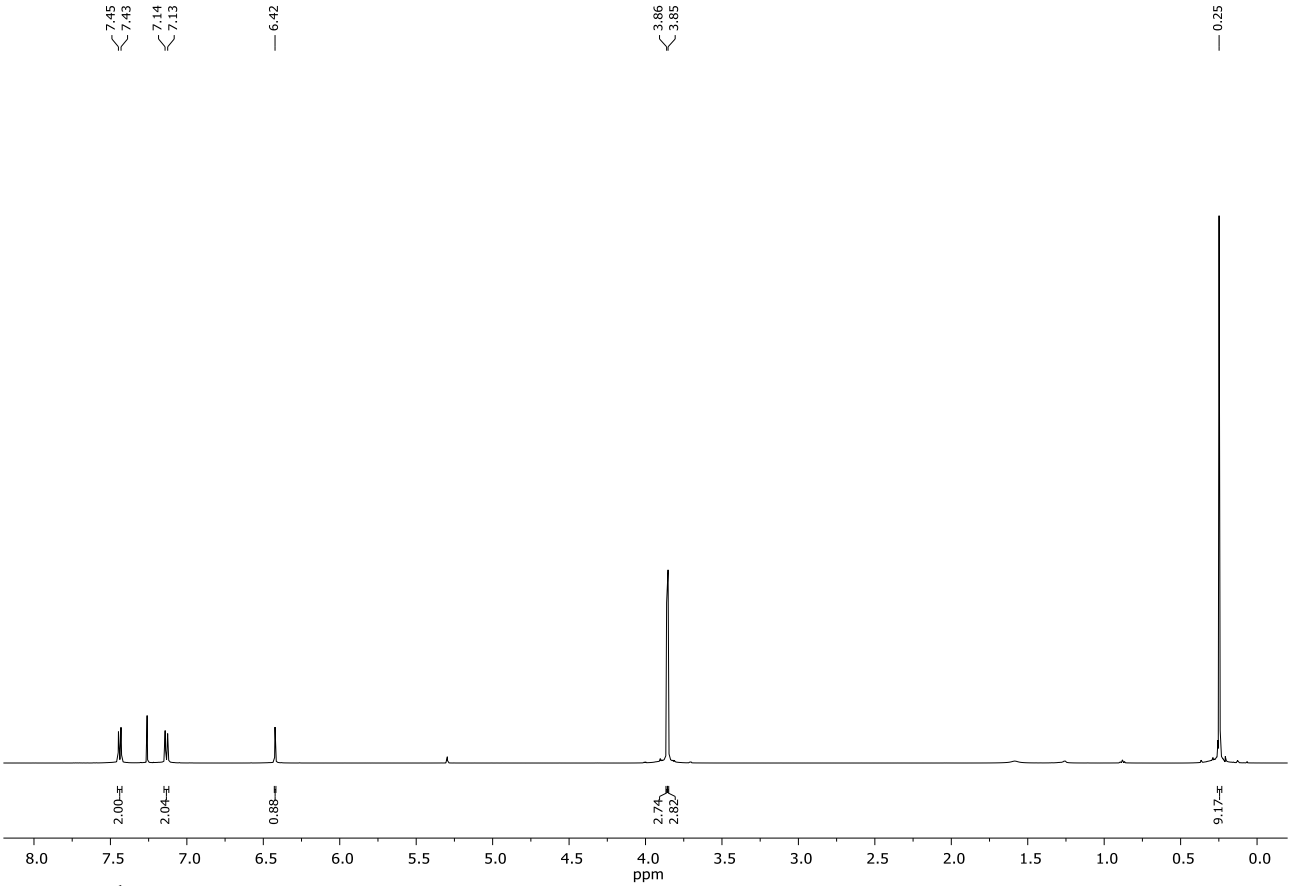


Figure S6: ^1H NMR (500 MHz) of **9** in $CDCl_3$.

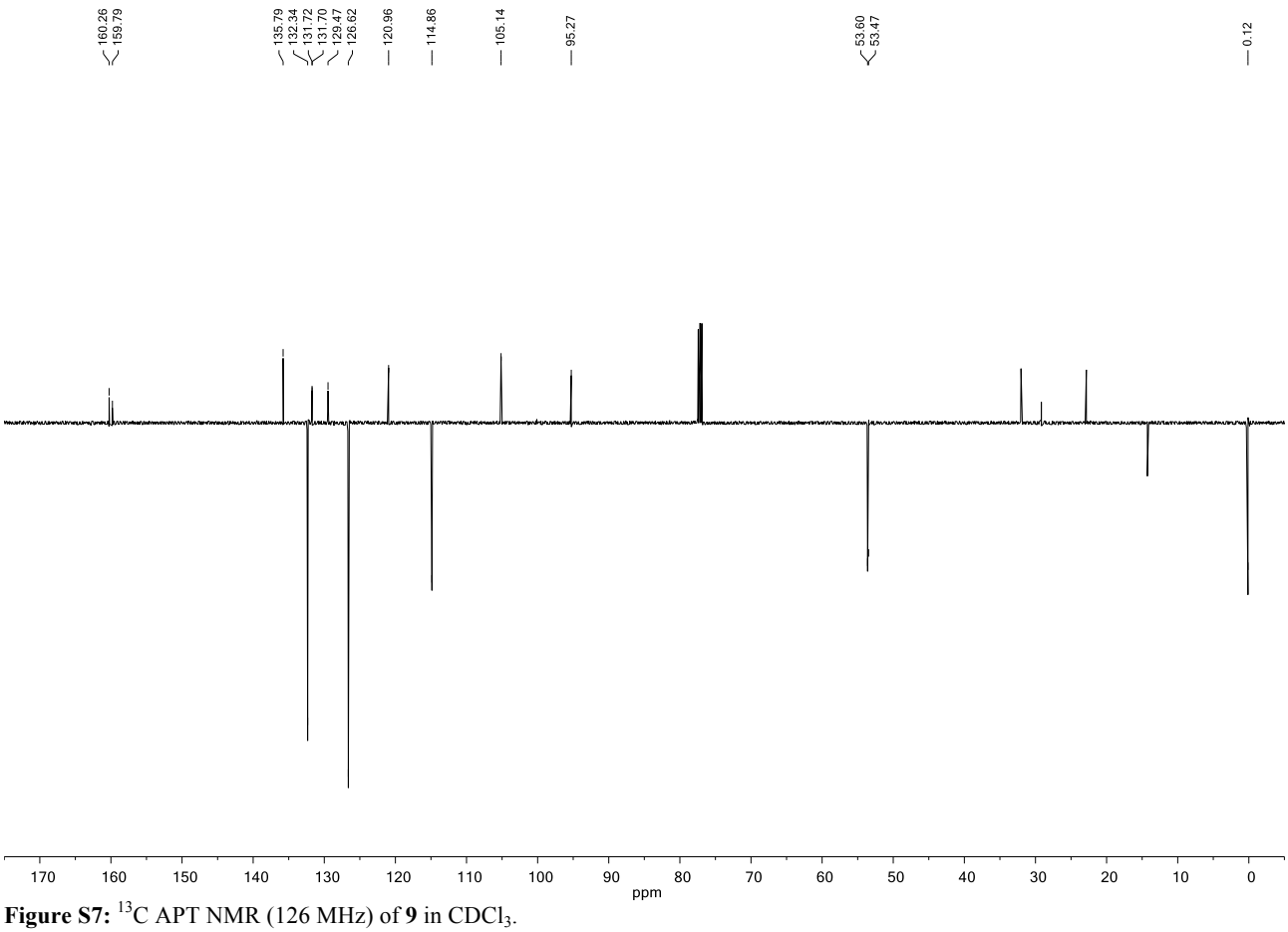
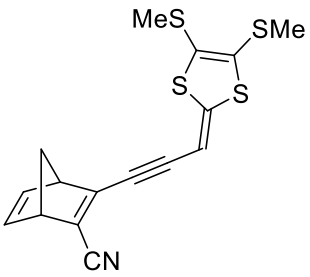


Figure S7: ^{13}C APT NMR (126 MHz) of **9** in $CDCl_3$.

Compound 10



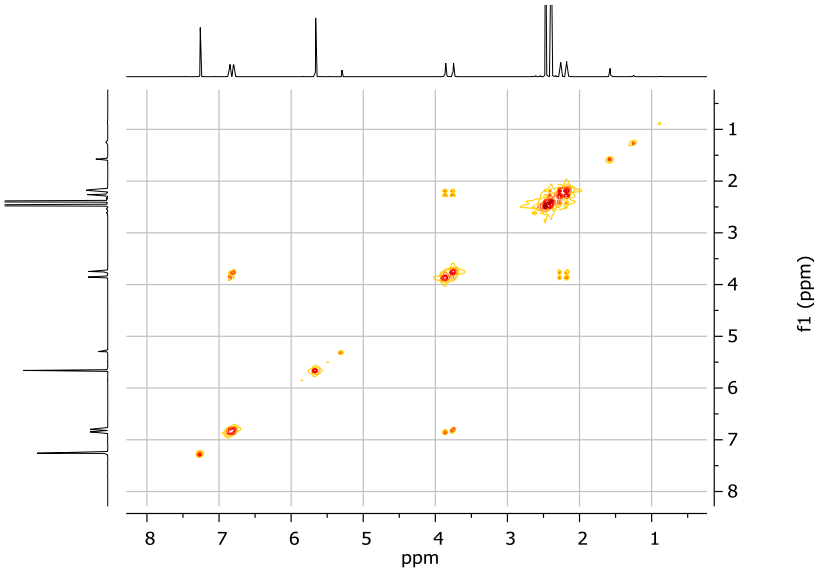


Figure S8: COSY NMR (500 MHz) of **10** in $CDCl_3$.

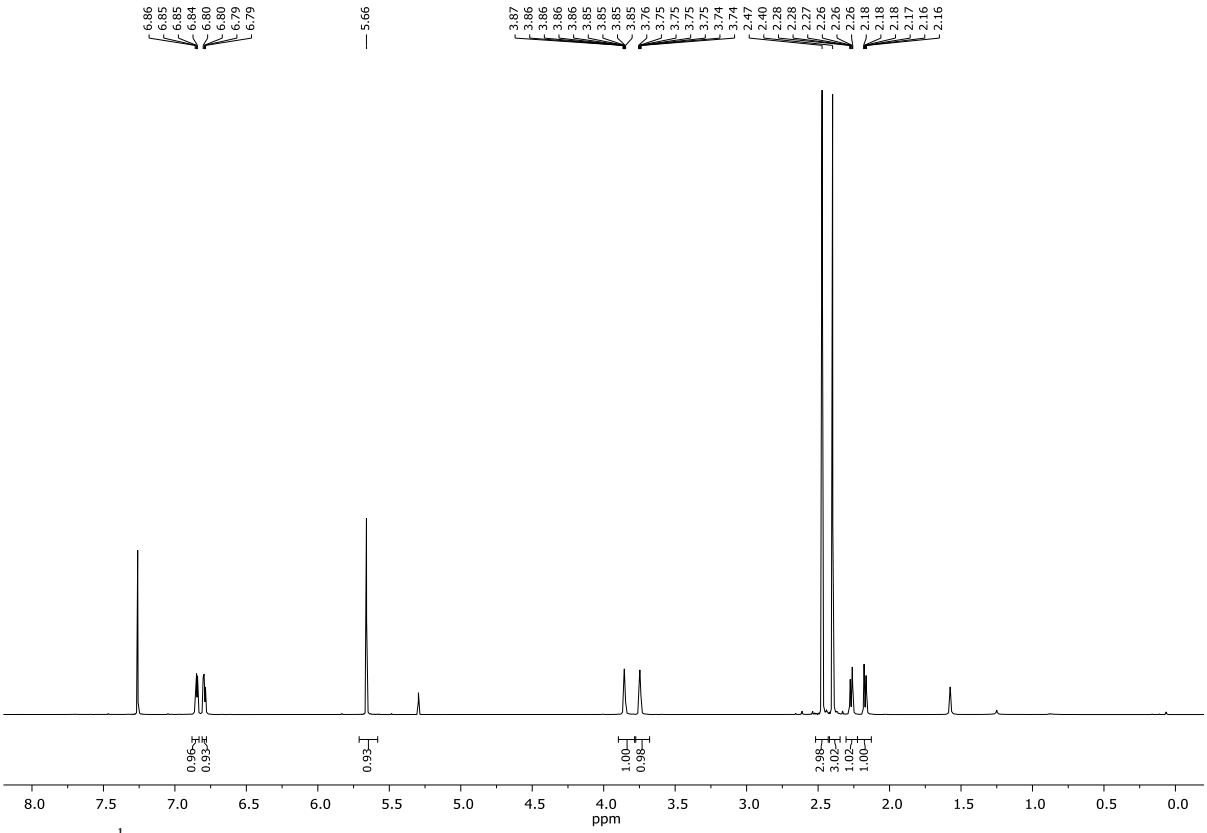


Figure S9: ^1H NMR (500 MHz) of **10** in $CDCl_3$.

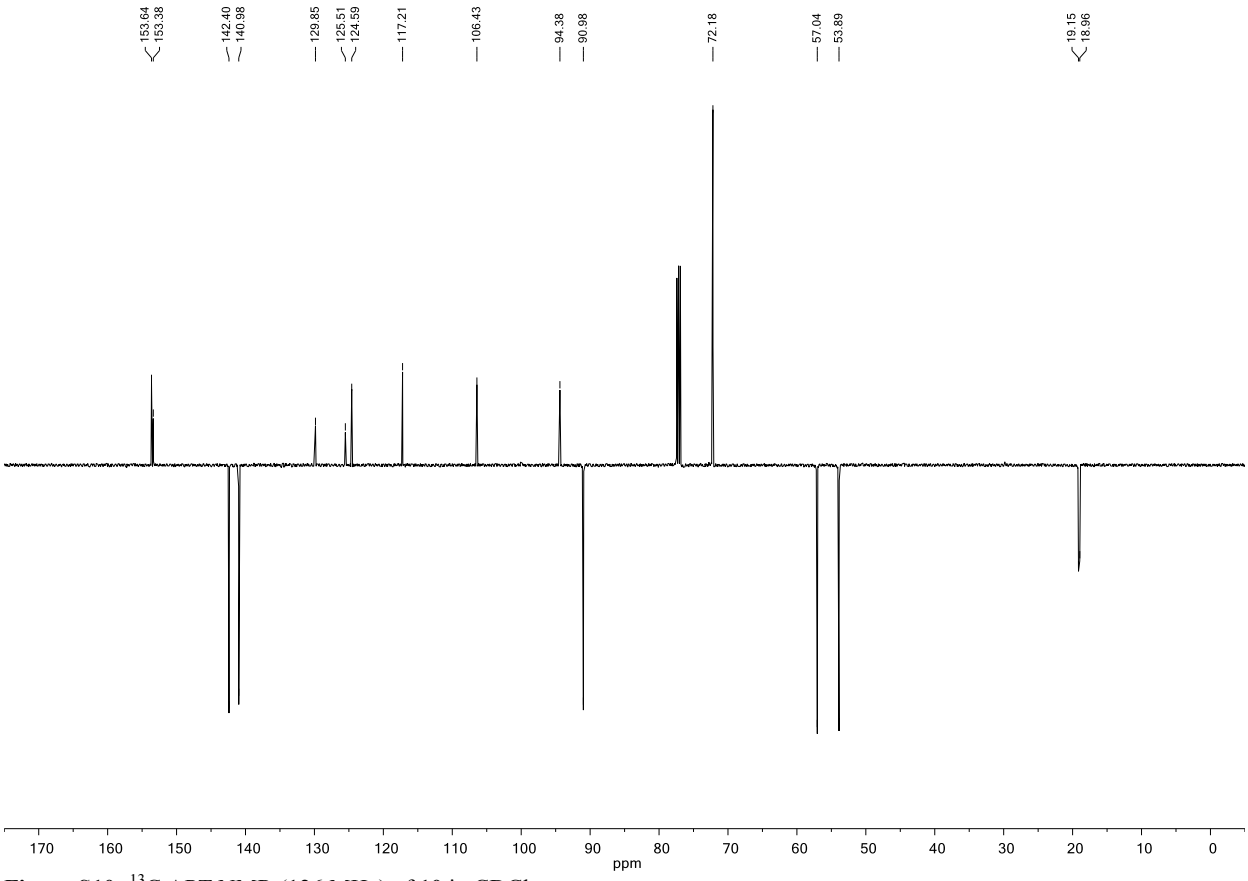


Figure S10: ^{13}C APT NMR (126 MHz) of **10** in $CDCl_3$.

Compound 11

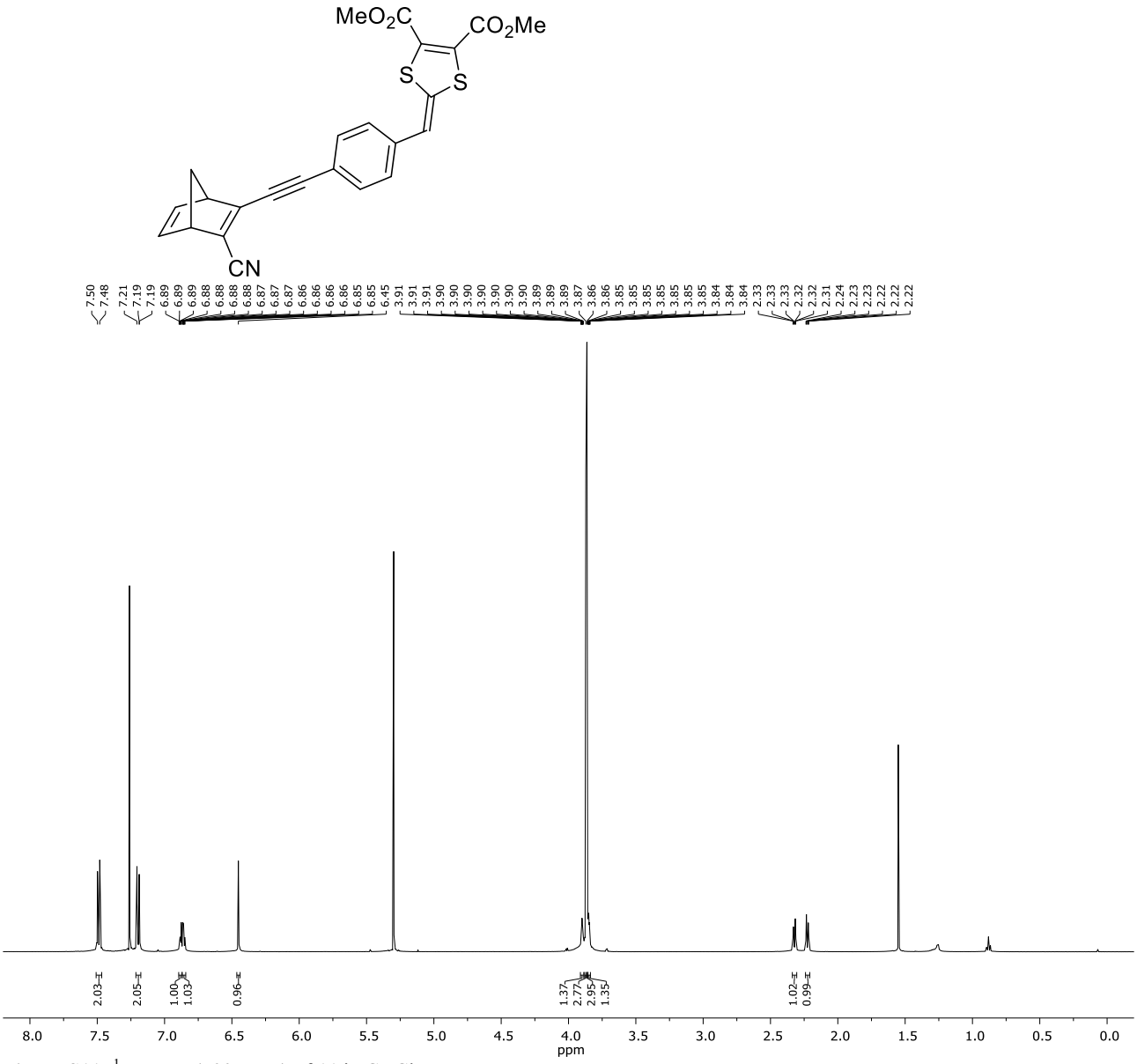


Figure S11: ^{1}H NMR (500 MHz) of **11** in $CDCl_3$.

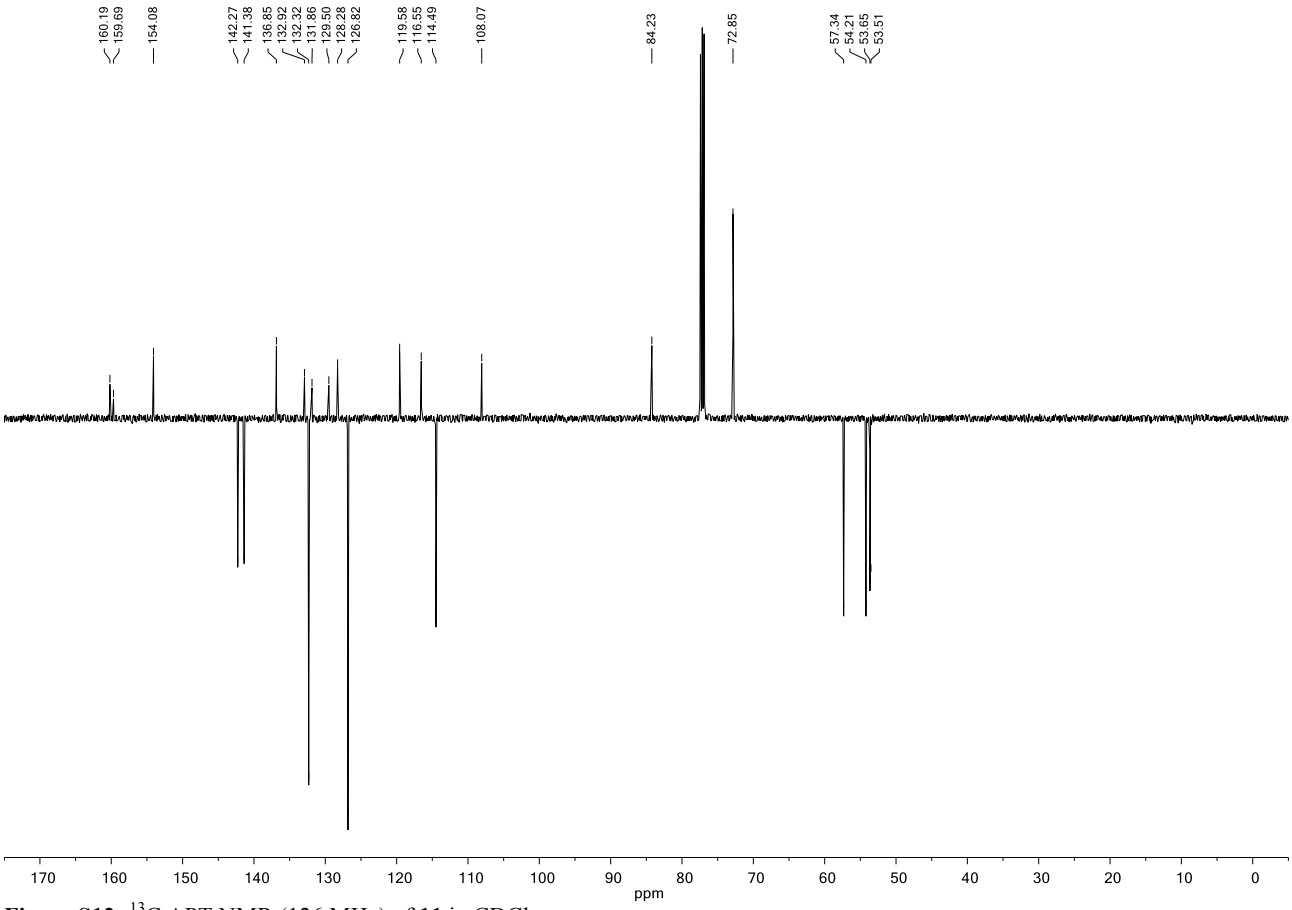
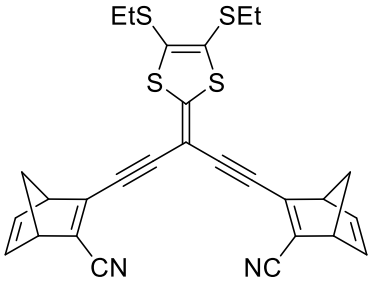


Figure S12: ^{13}C APT NMR (126 MHz) of **11** in $CDCl_3$.

Compound 12



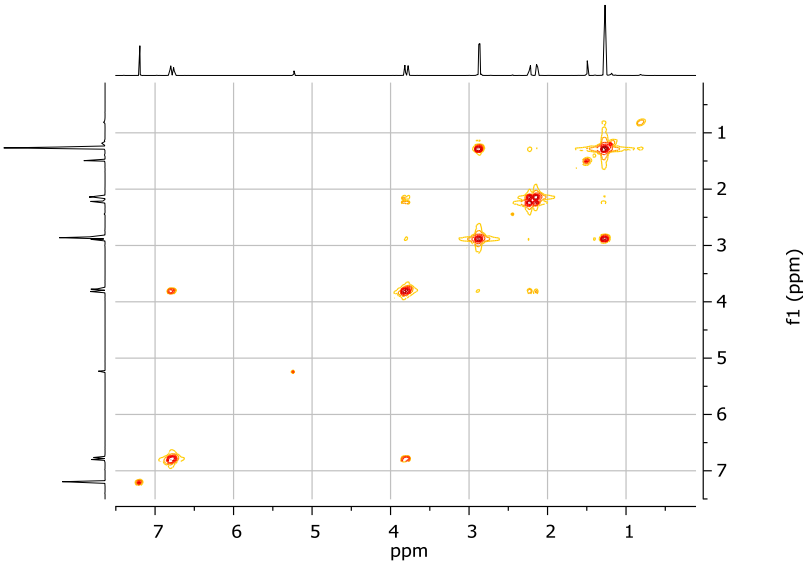


Figure S13: COSY NMR (500 MHz) of **12** in $CDCl_3$.

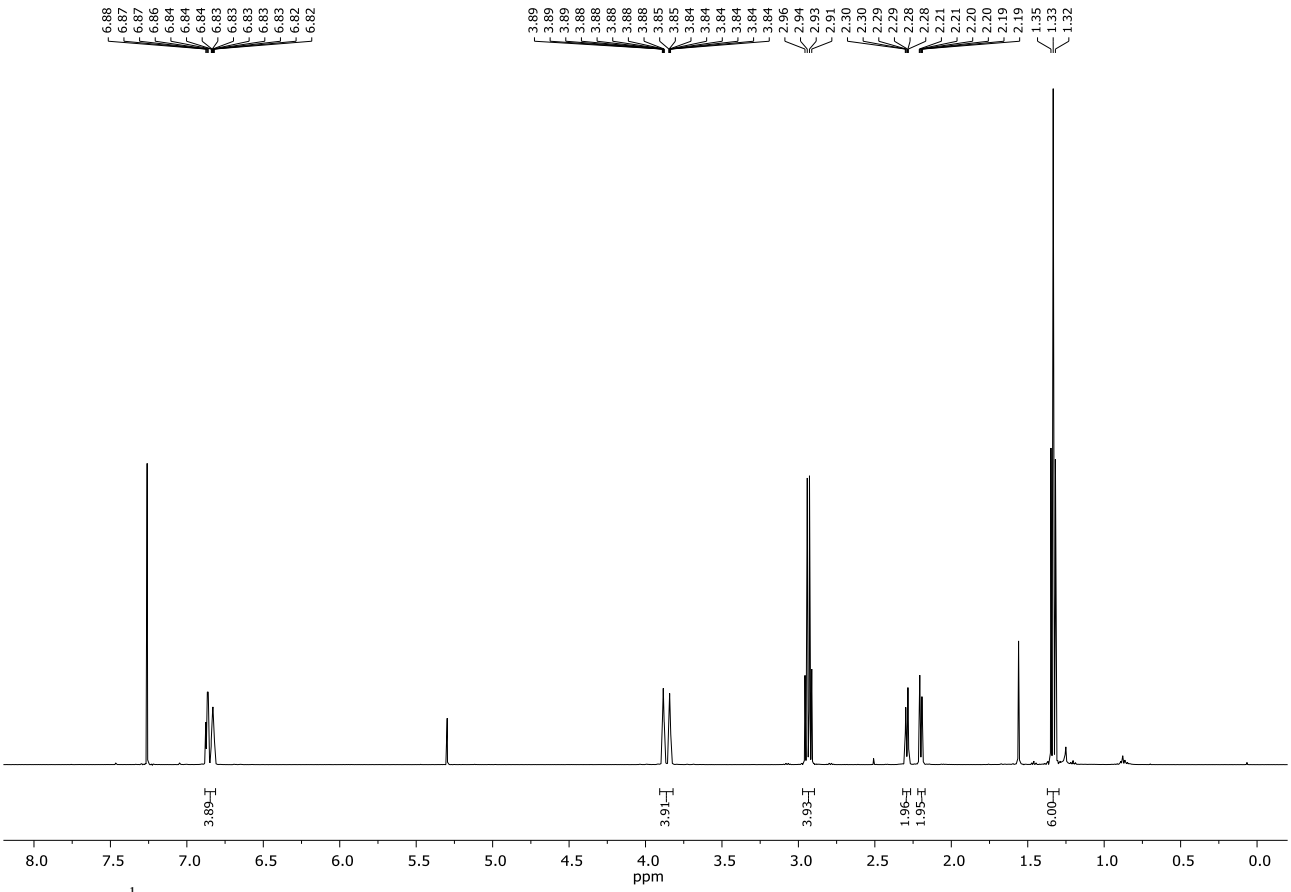


Figure S14: ^1H NMR (500 MHz) of **12** in $CDCl_3$.

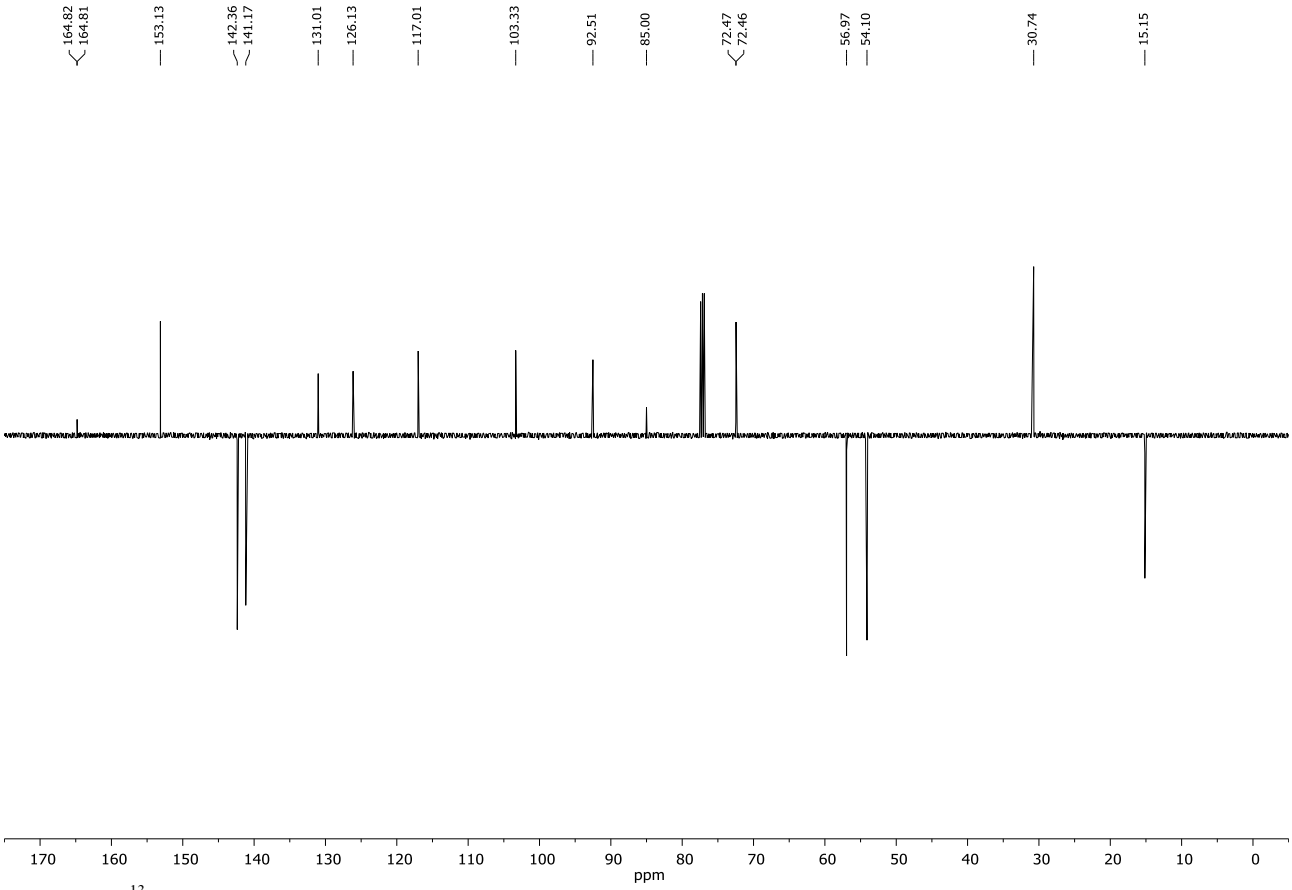


Figure S15: ^{13}C APT NMR (126 MHz) of **12** in $CDCl_3$.

Compound 13

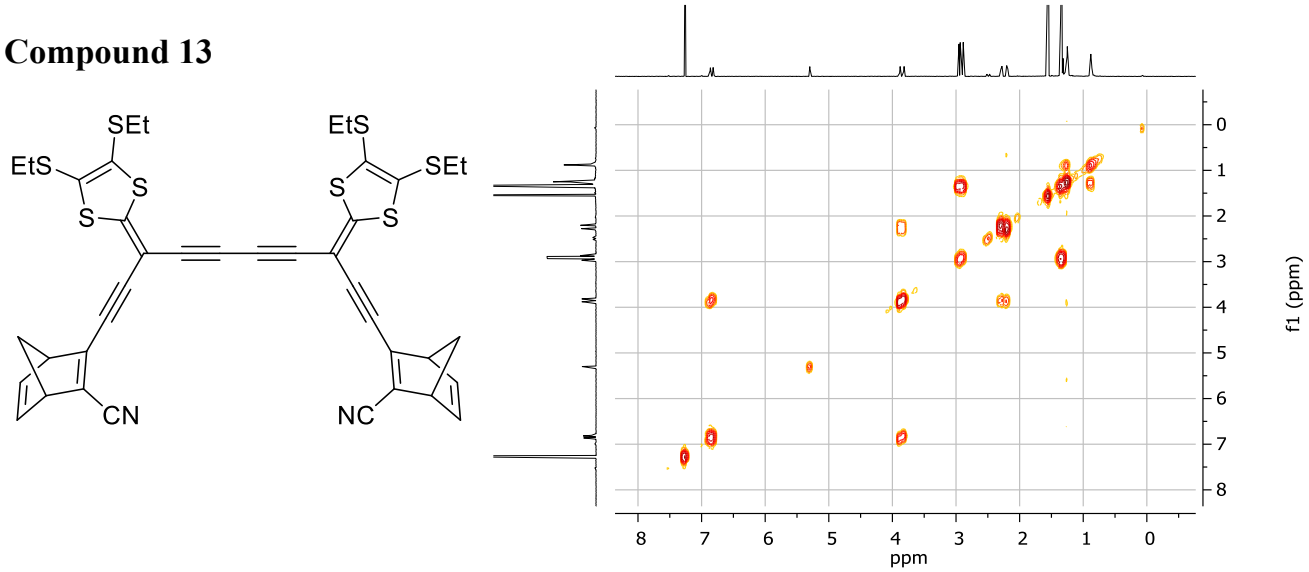


Figure S16: COSY NMR (500 MHz) of **13** in $CDCl_3$.

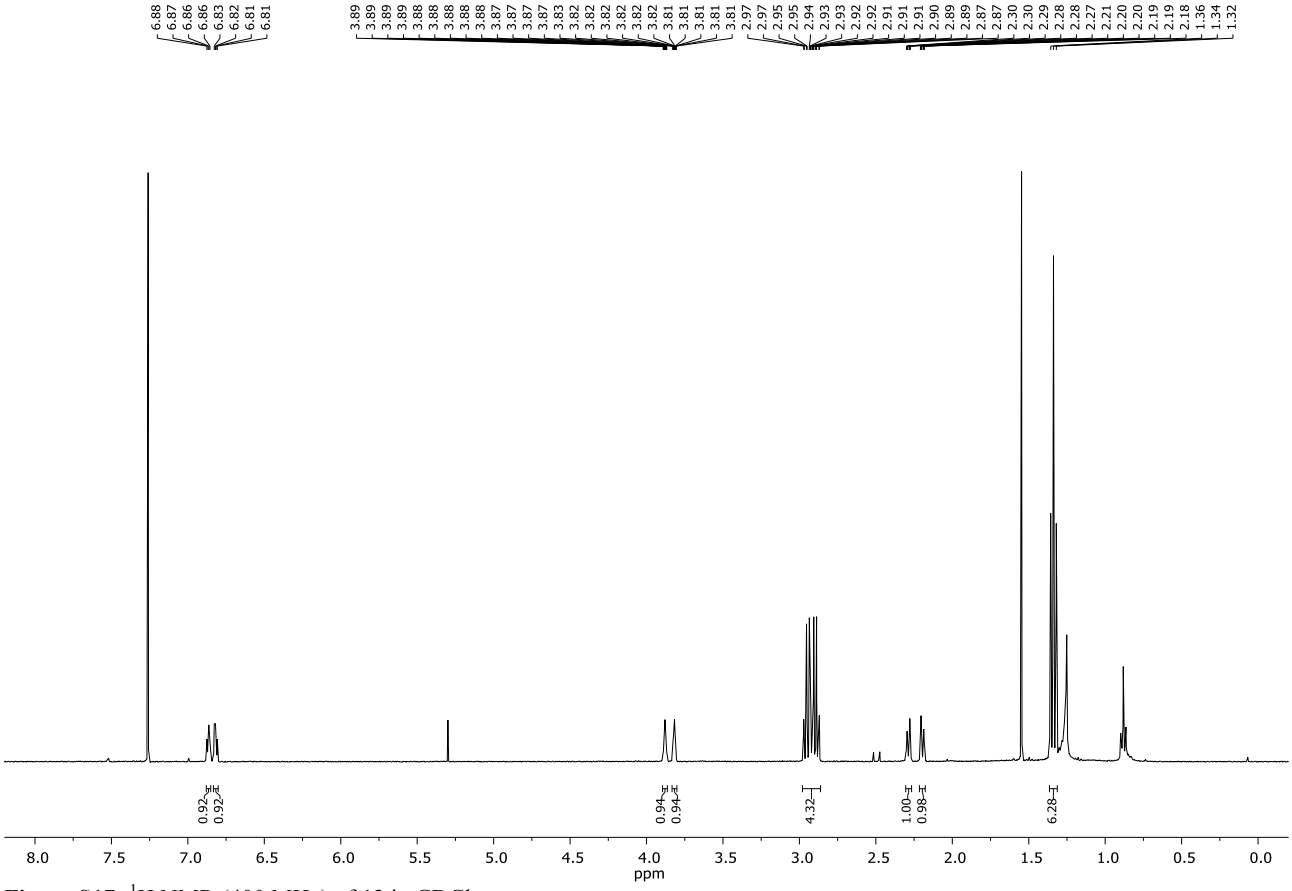


Figure S17: ^1H NMR (400 MHz) of **13** in $CDCl_3$.

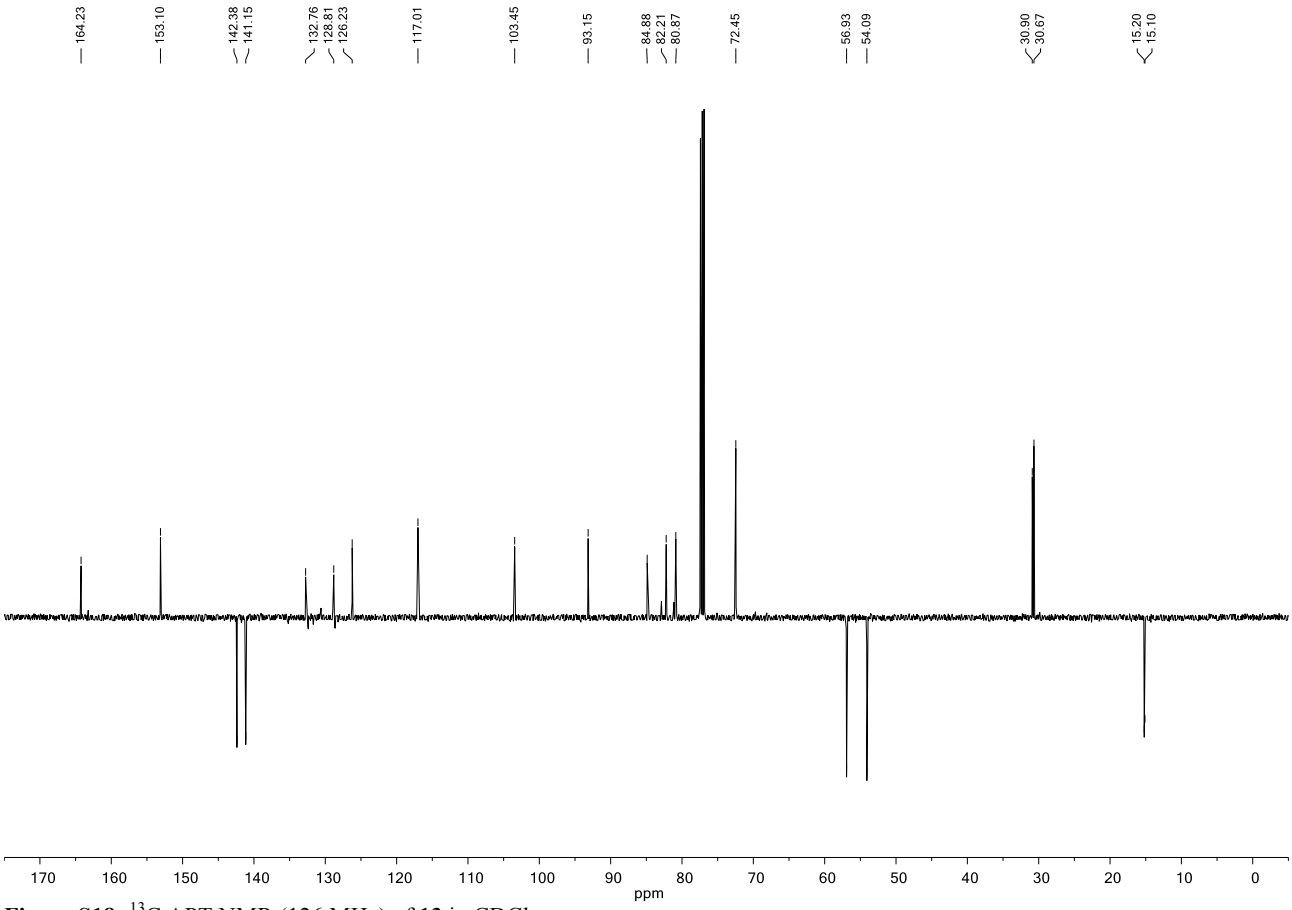


Figure S18: ^{13}C APT NMR (126 MHz) of **13** in $CDCl_3$.

UV-absorption and switching studies

Compound 11

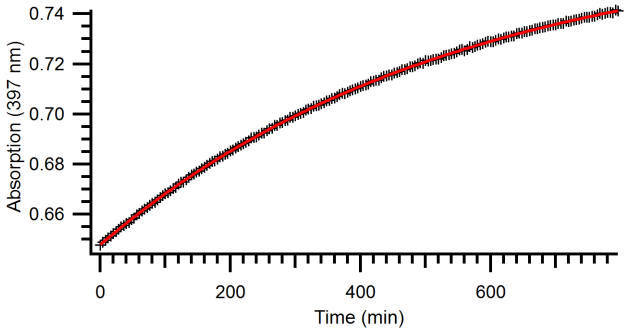


Figure S19: Exponential growth of **11** at 25 °C, after irradiation at 397 nm for 8 h.

^{1}H NMR switching studies

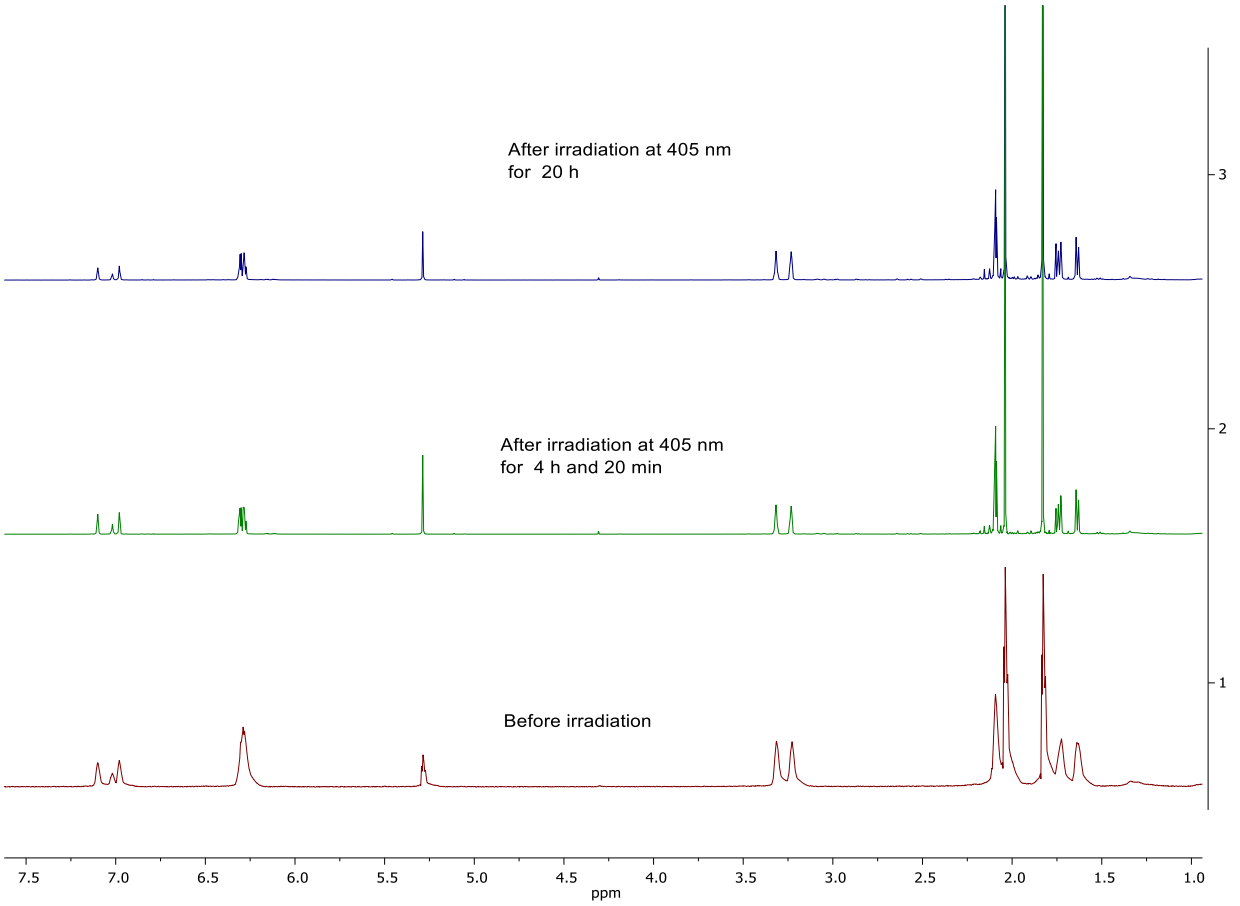


Figure S20: ^{1}H NMR (400 MHz) spectra of compound **10** after irradiation with a 405 nm diode.

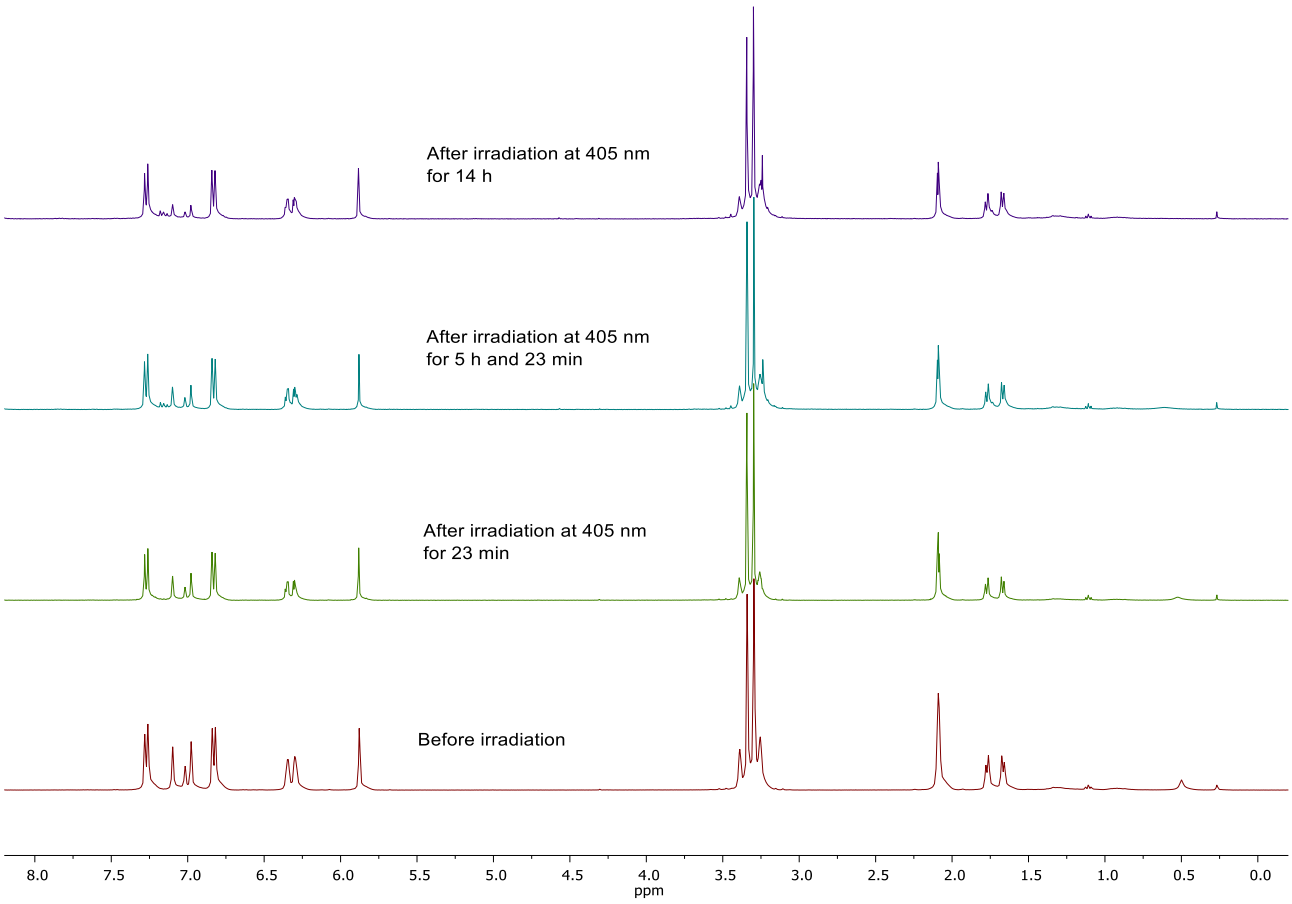


Figure S21: ^{1}H NMR (400 MHz) spectra of compound **11** after irradiation with a 405 nm diode.

Calculations

Table S1: Calculated absorption energies using either B3LYP or CAM-B3LYP.

Compound	Type	*ΔH* to Q	λ_{max} (nm)	
		(eV, B3LYP)	B3LYP	CAM-B3LYP
11	N	-1.30	413	374
11	Q	0.00	371	332
12	N	-1.25	467	375
12	Q	0.00	460	363
13	NN	-2.39	470	381
13	NQ	-1.25	429	382
13	QQ	0.00	367	330
14	NN	-2.60	539	419
14	NQ	-1.30	513	414
14	QQ	0.00	460	398