Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Electronic supporting information

Heteroaryl-linked norbornadiene dimers with redshifted absorptions

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Contents

NMR spectra

Compound 1

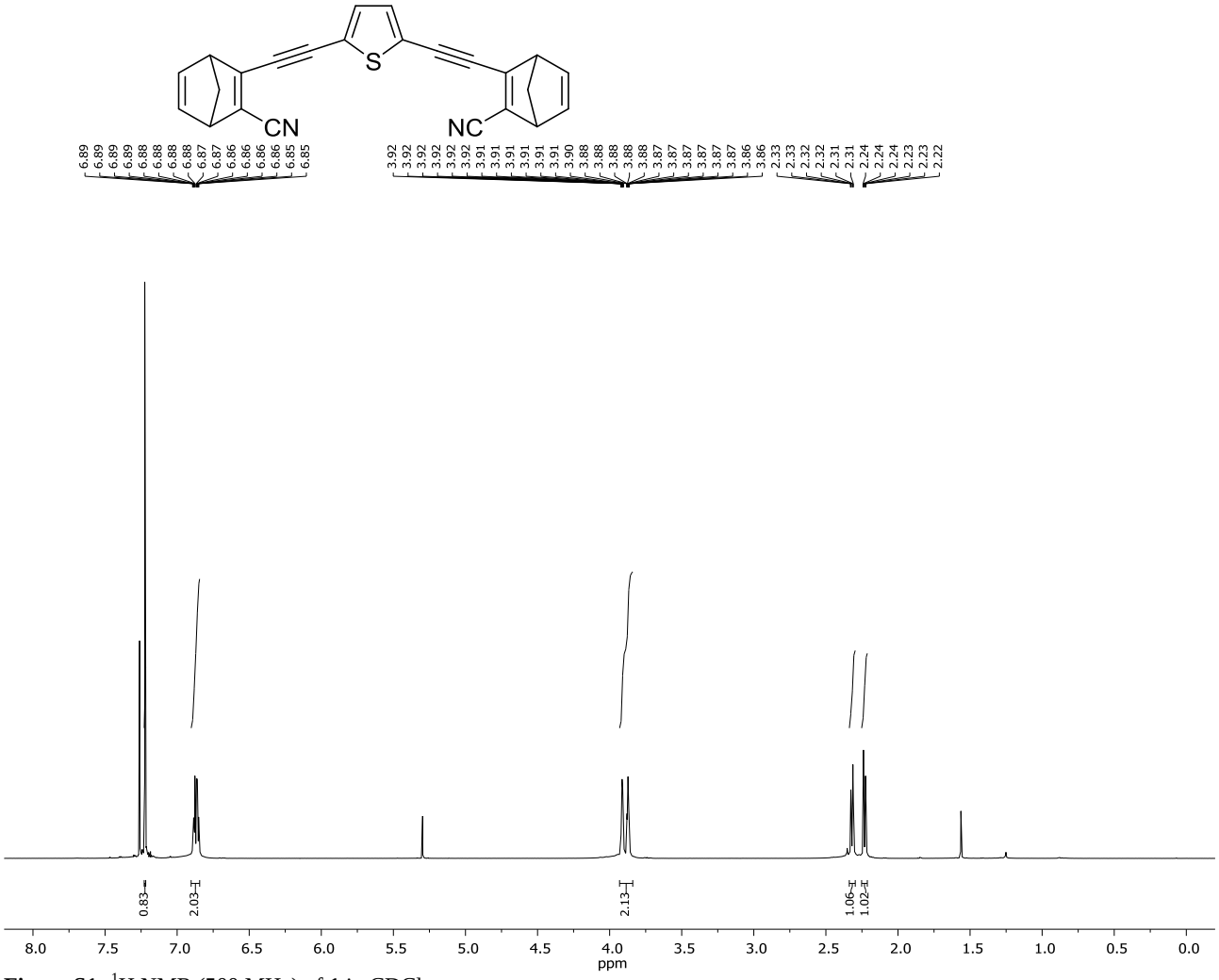


Figure S1: ^{1}H NMR (500 MHz) of **1** in $CDCl_3$.

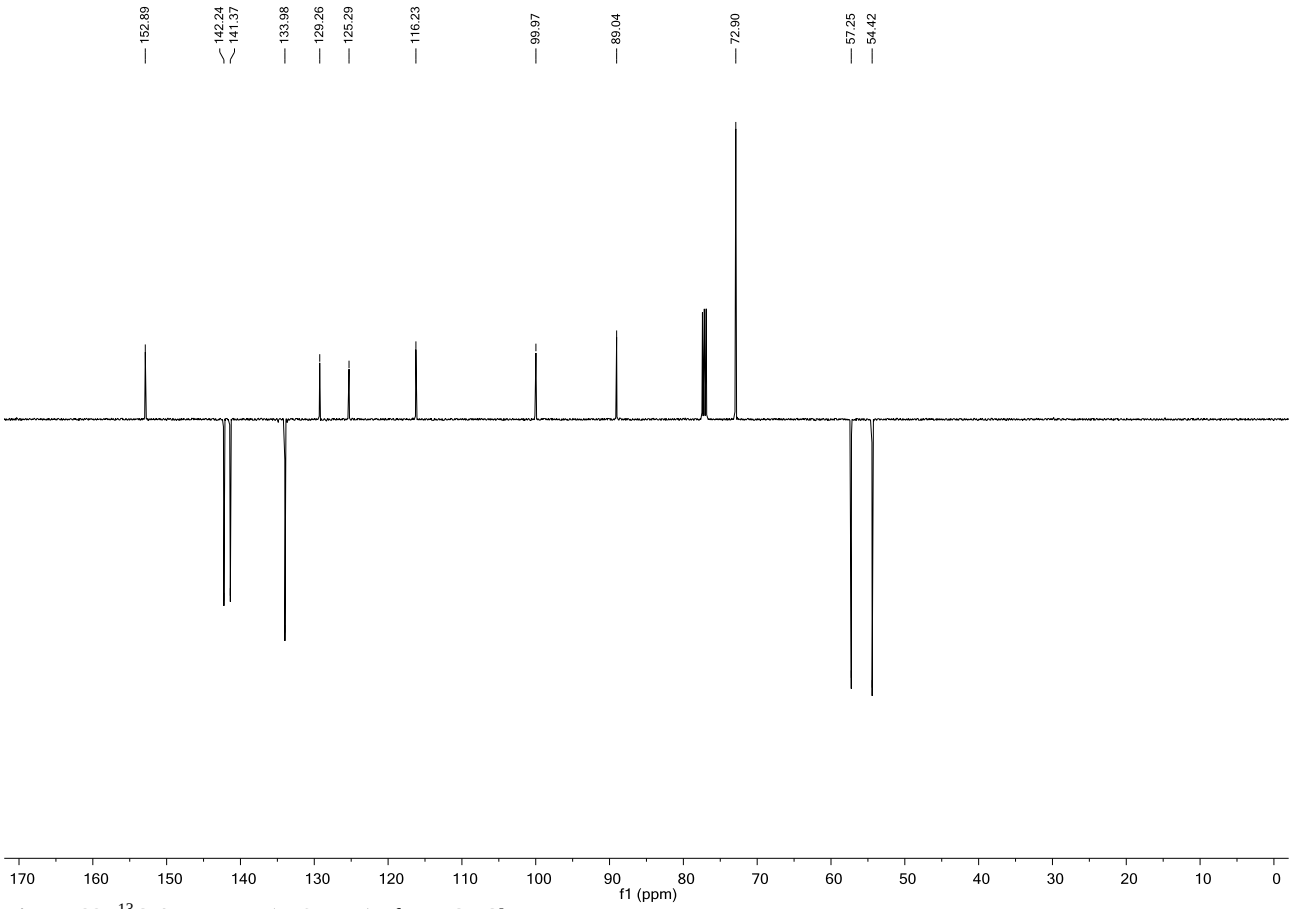


Figure S2: ^{13}C APT NMR (126 MHz) of **1** in $CDCl_3$.

Compound 2

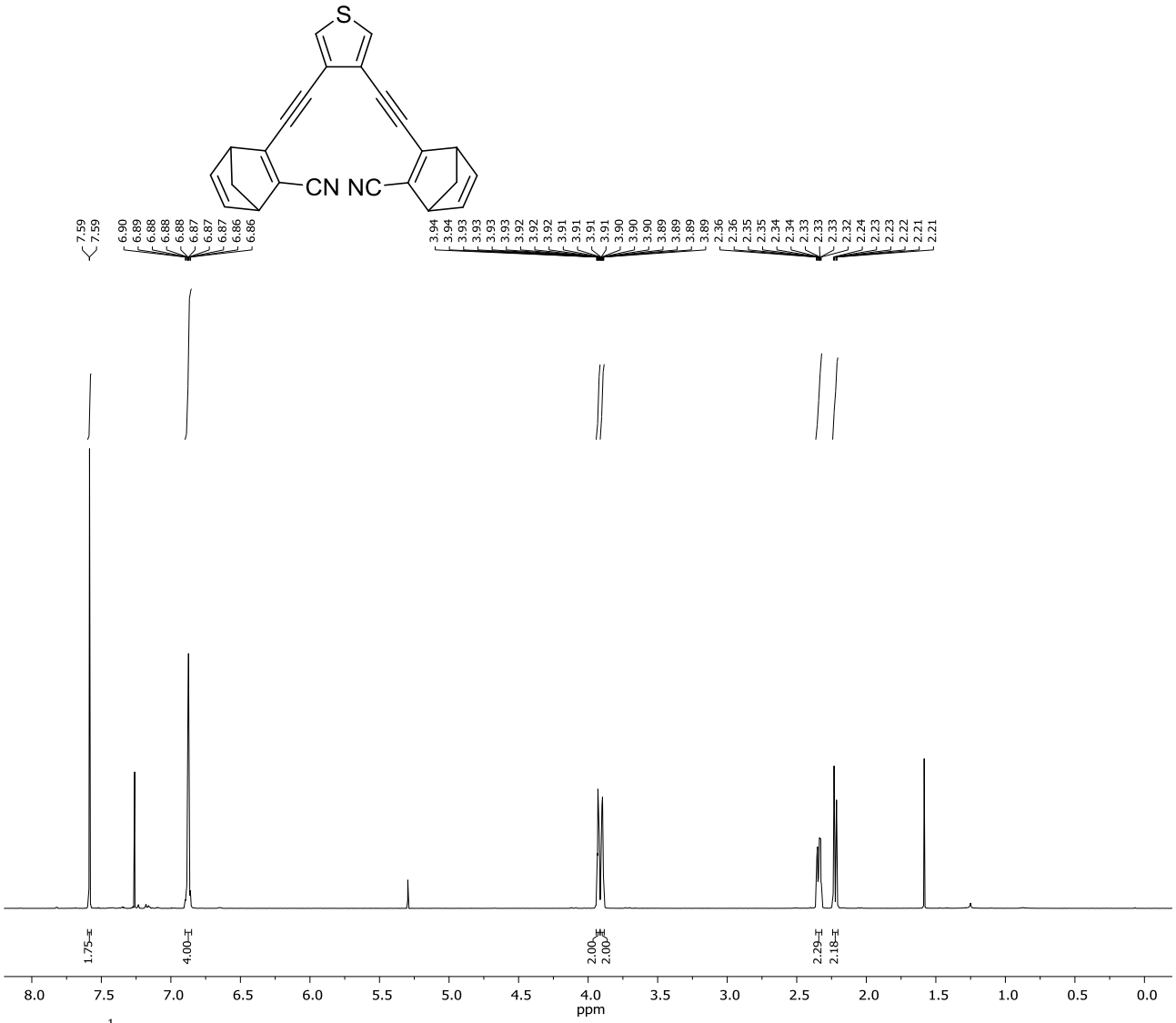


Figure S3: ^{1}H NMR (400 MHz) of **2** in $CDCl_3$.

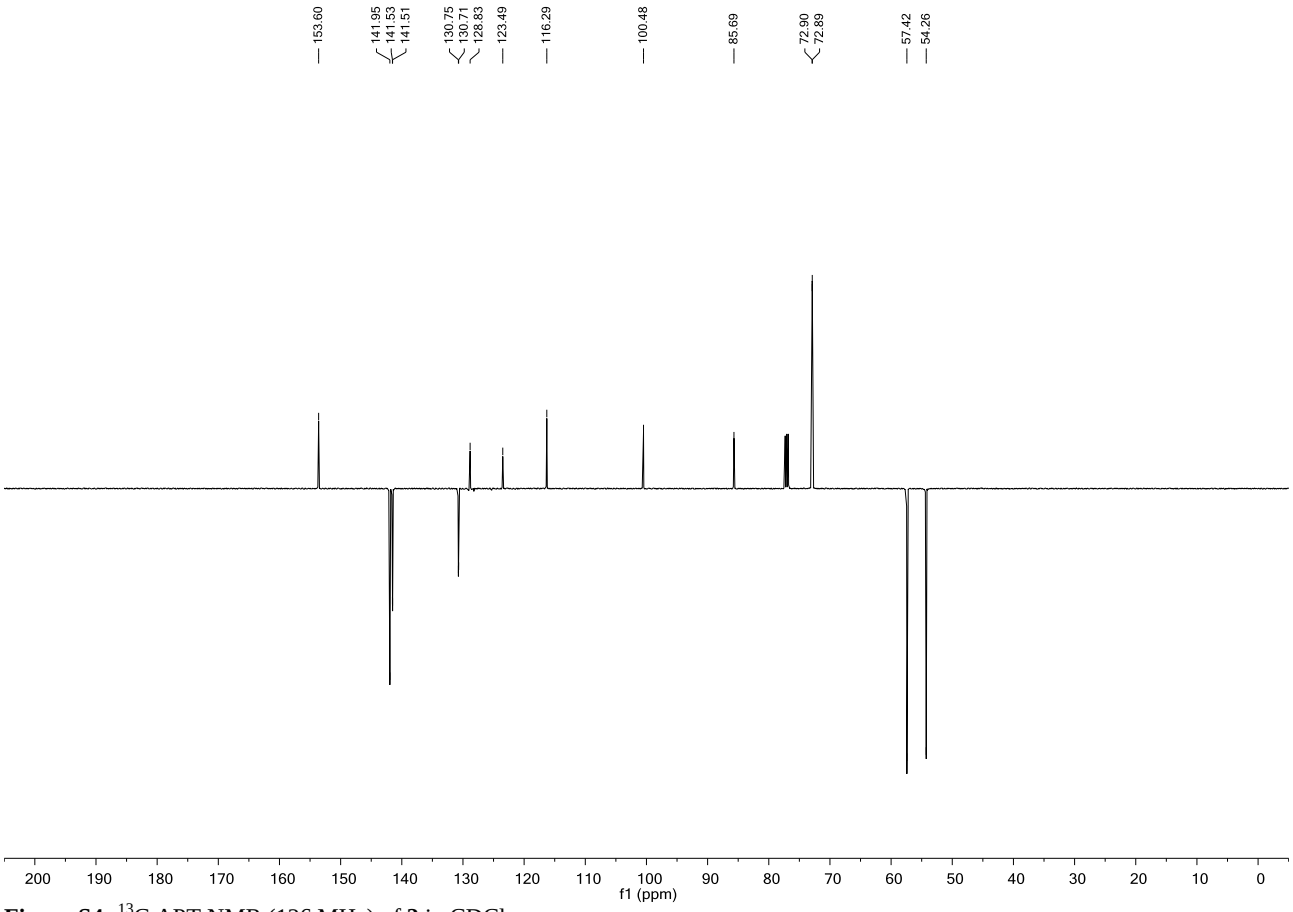
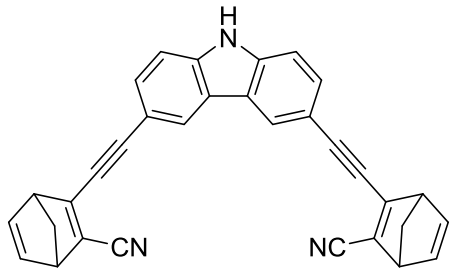


Figure S4: ^{13}C APT NMR (126 MHz) of **2** in $CDCl_3$.

Compound 3



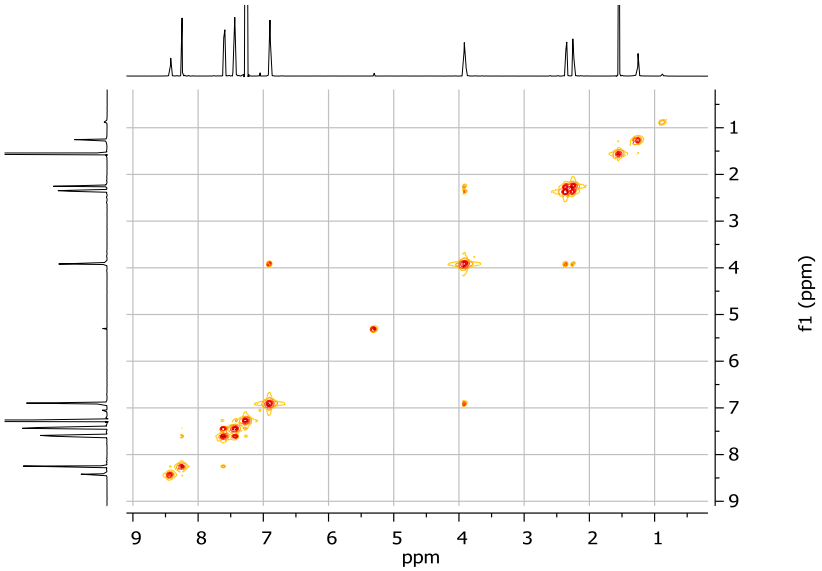


Figure S5: COSY NMR (400 MHz) of 3 in $CDCl_3$.

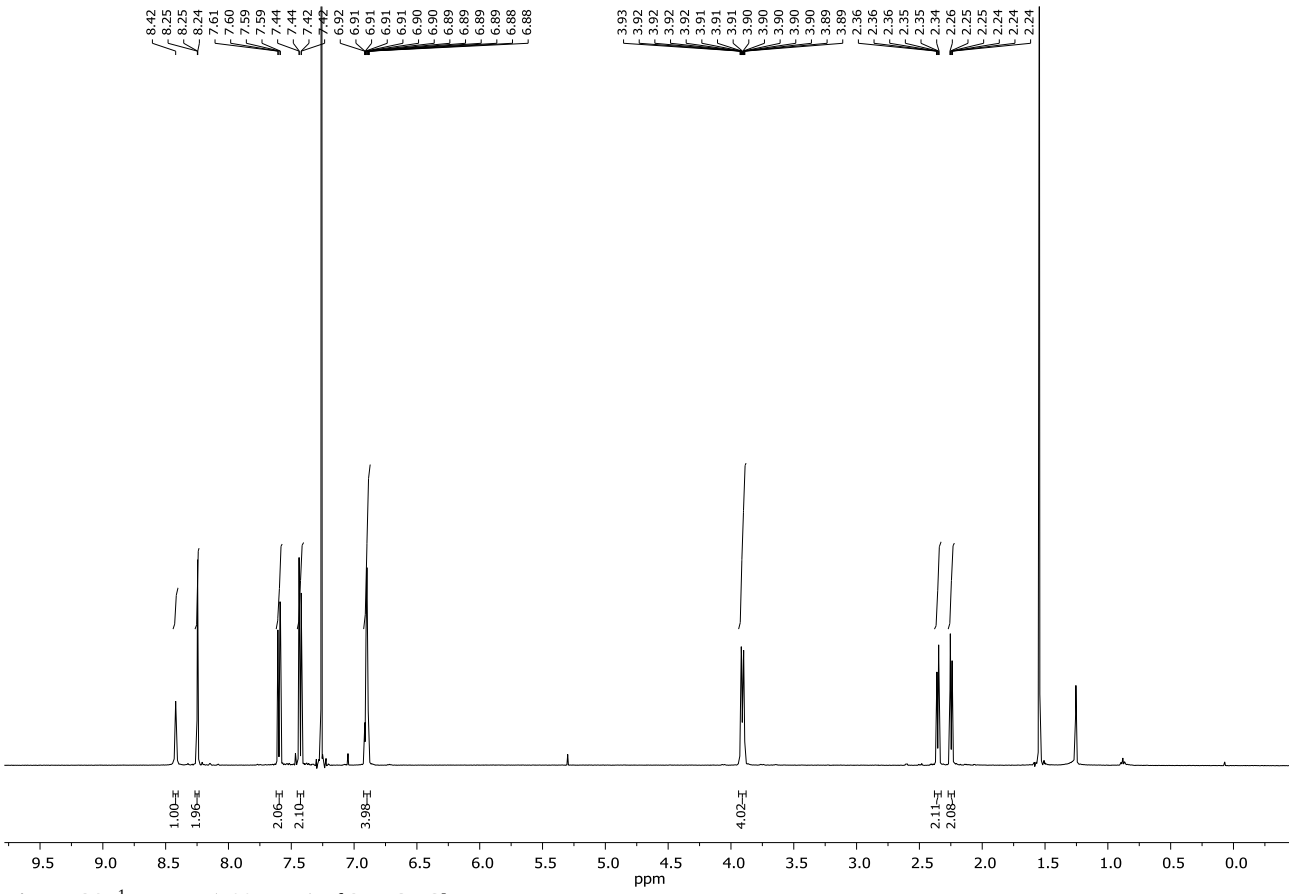


Figure S6: ^{1}H NMR (400 MHz) of **3** in $CDCl_3$.

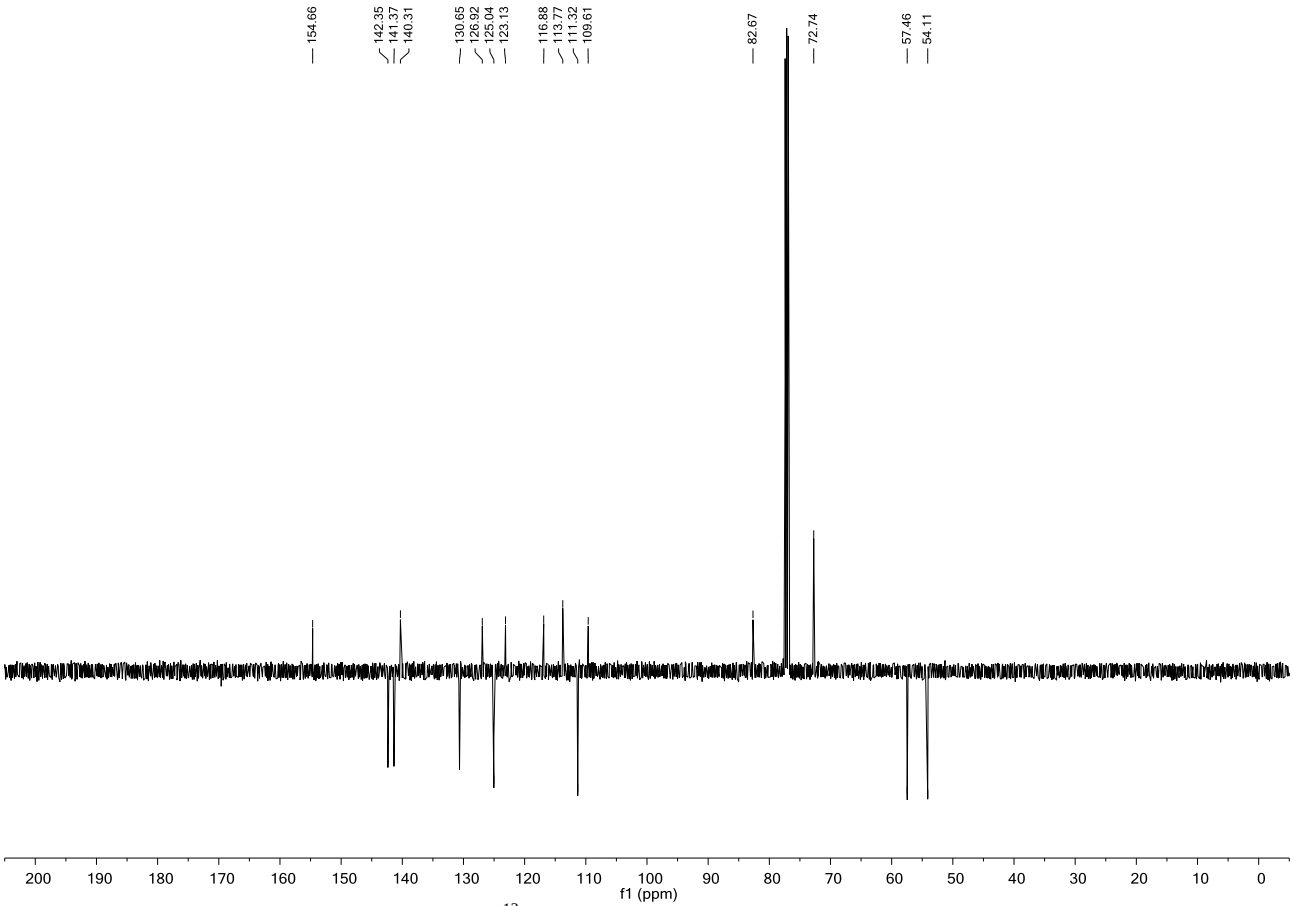
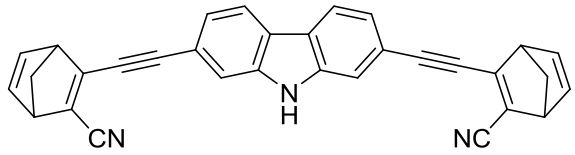


Figure S7: ^{13}C APT NMR (126 MHz) of **3** in $CDCl_3$.

Compound 4



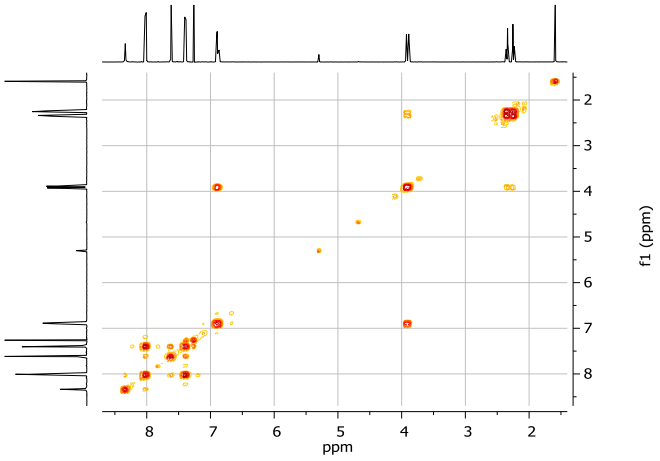


Figure S8: COSY NMR (400 MHz) of **4** in $CDCl_3$.

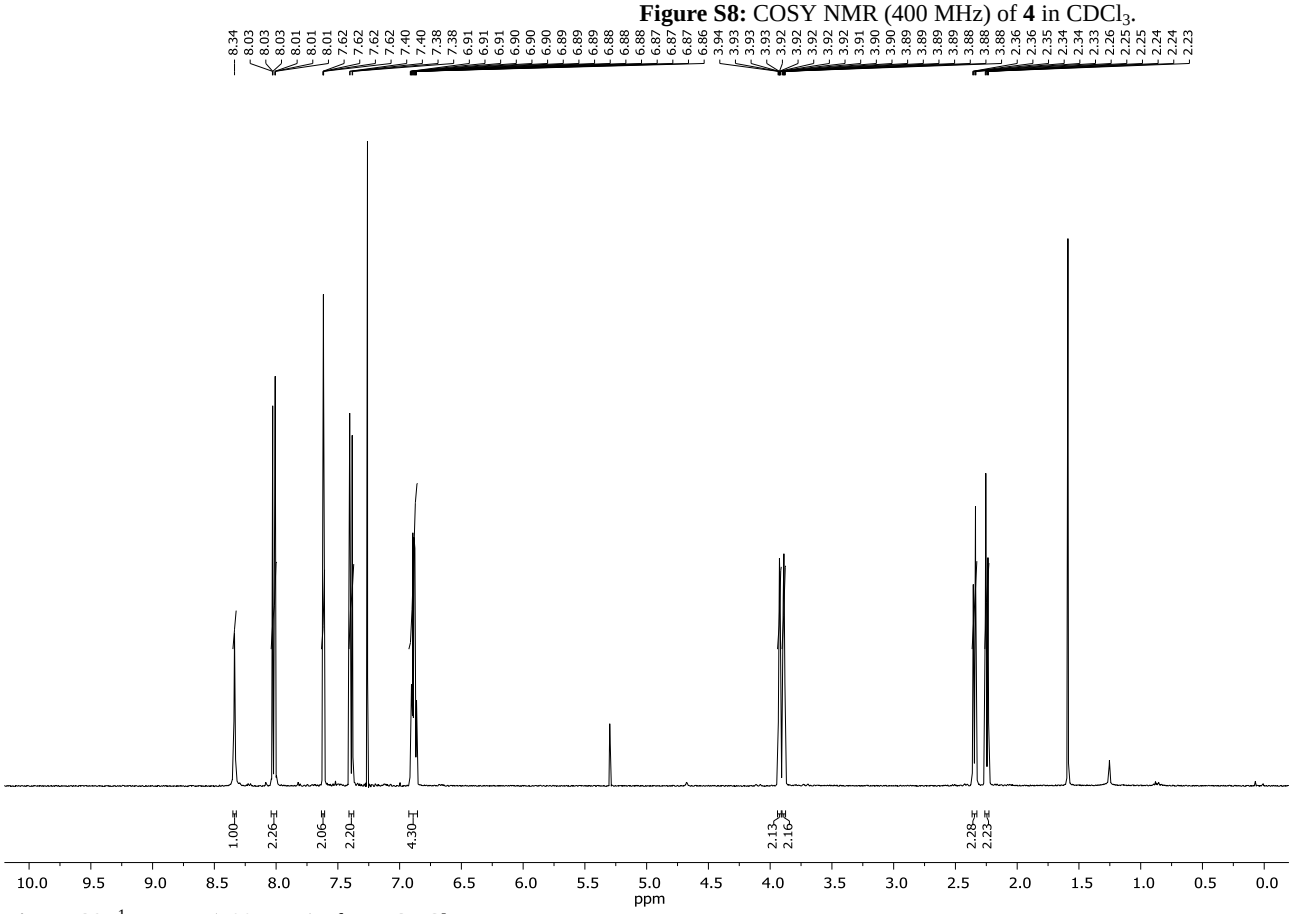


Figure S9: ^1H NMR (400 MHz) of **4** in $CDCl_3$

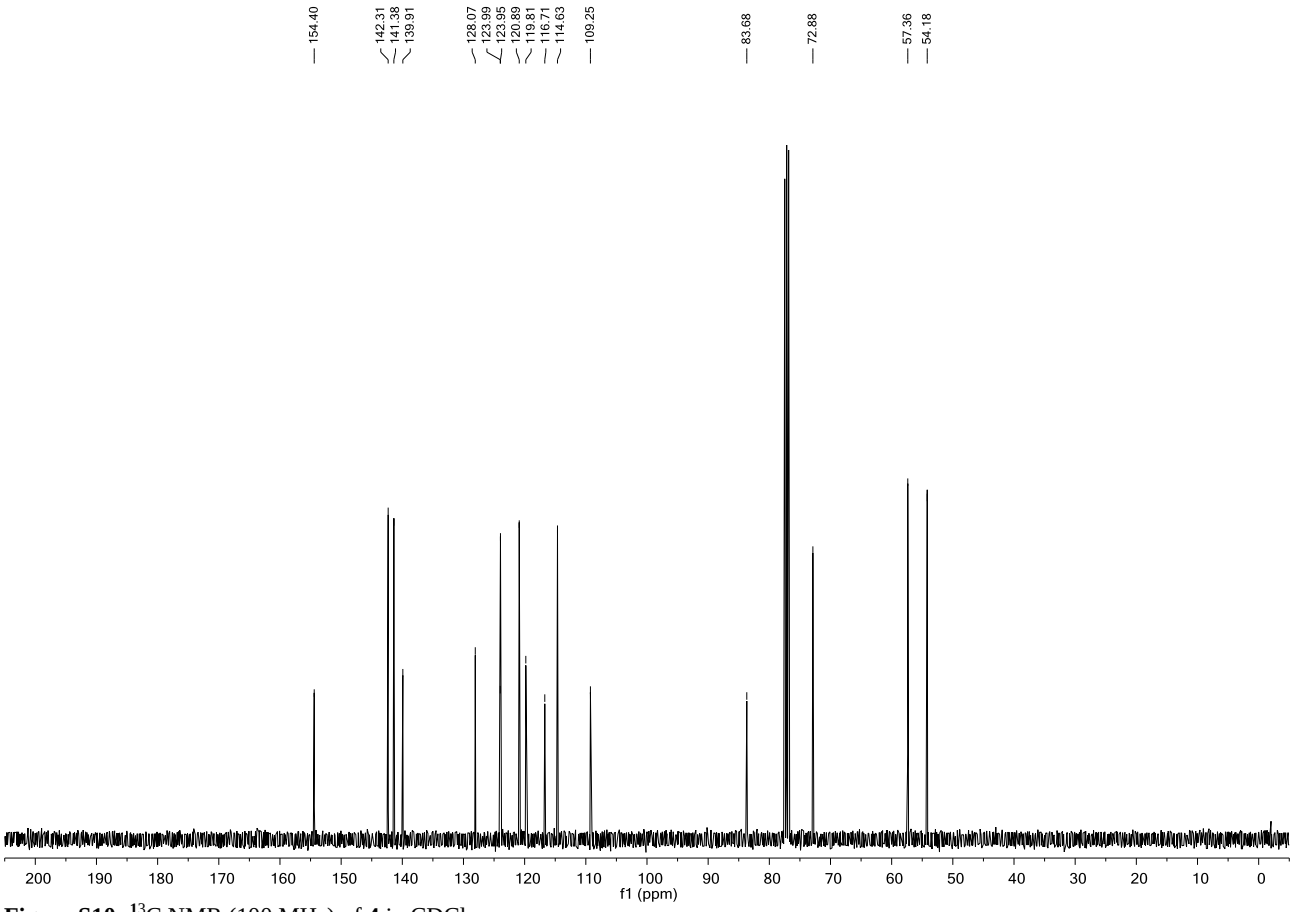
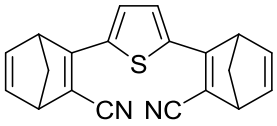


Figure S10: ^{13}C NMR (100 MHz) of **4** in $CDCl_3$.

Compound 5



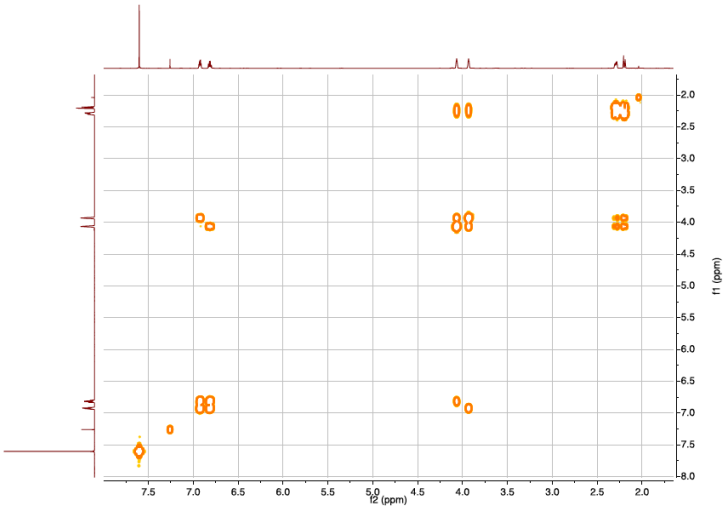


Figure S11: COSY NMR (400 MHz) of **5** in $CDCl_3$.

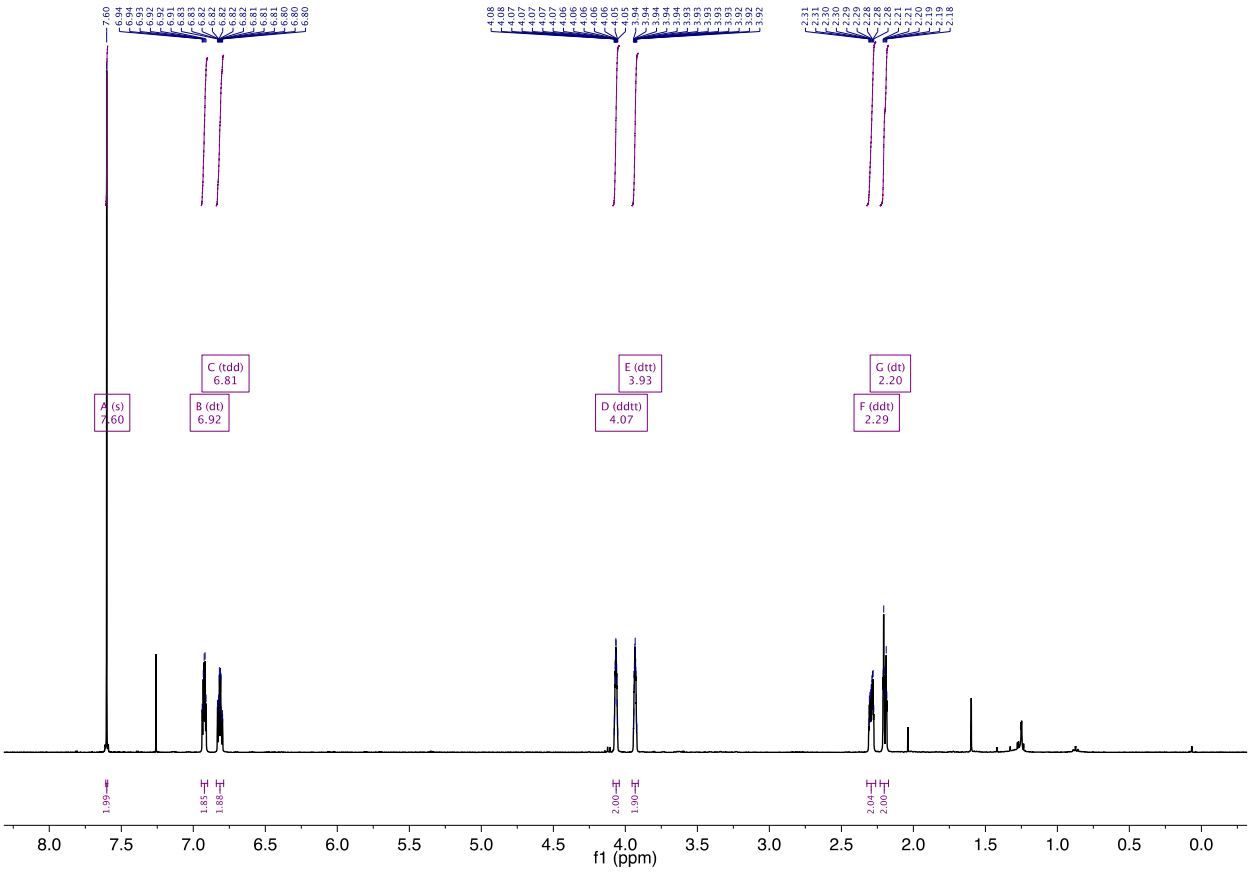


Figure S11: ^{1}H NMR (400 MHz) of **5** in $CDCl_3$.

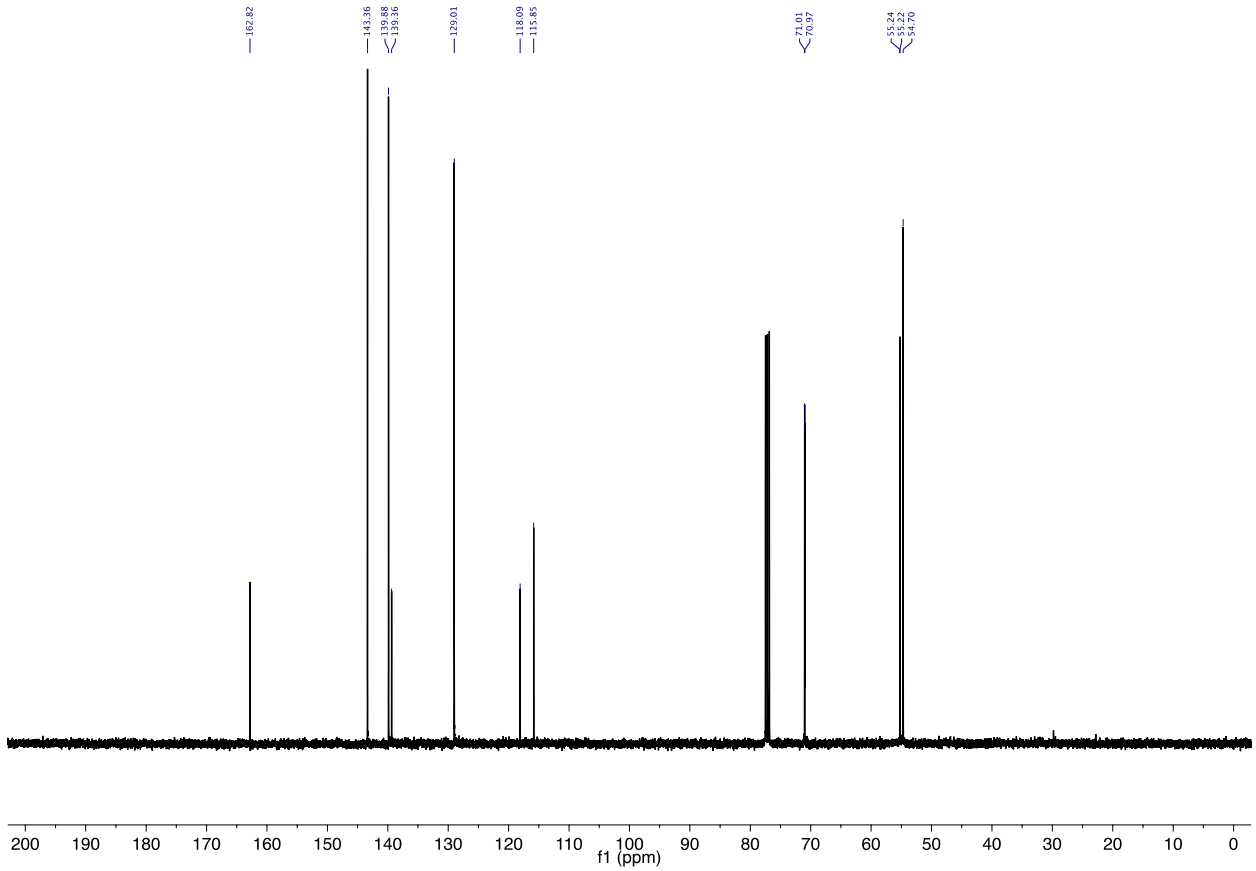


Figure S12: ^{13}C NMR (100 MHz) of **5** in $CDCl_3$.

Compound 12

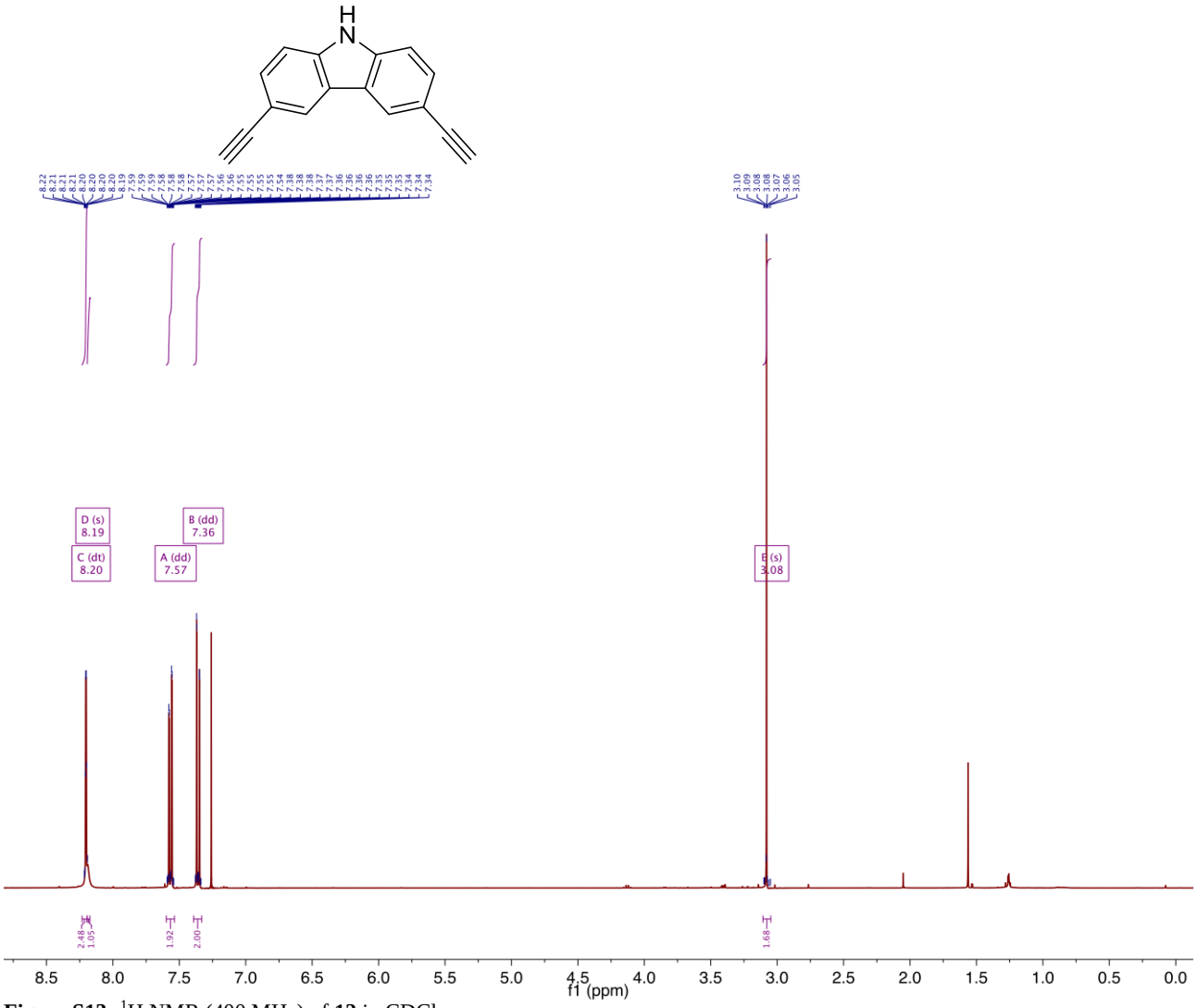


Figure S13: ^{1}H NMR (400 MHz) of **12** in $CDCl_3$.

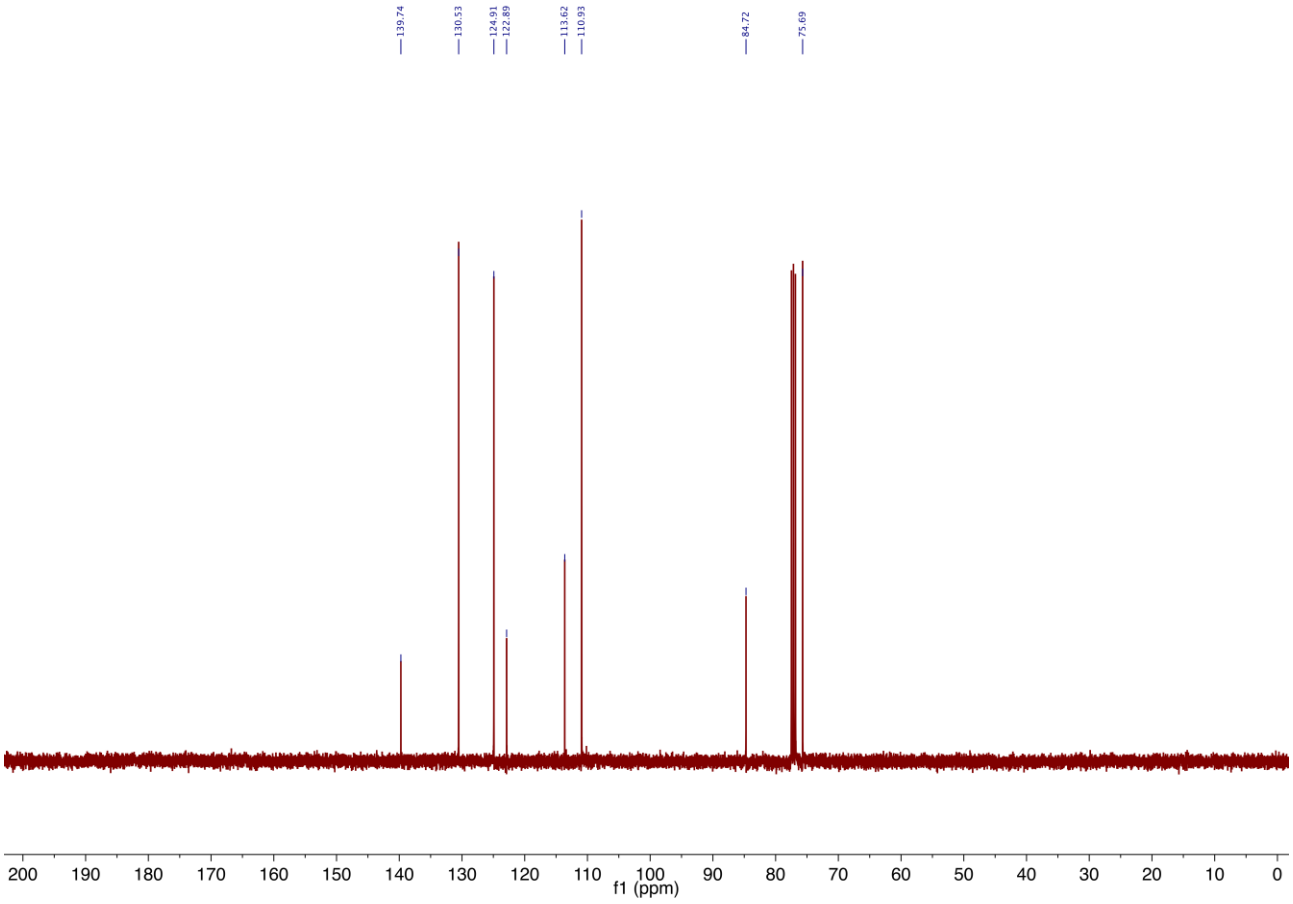


Figure S14: ^{13}C NMR (100 MHz) of **12** in $CDCl_3$.

Compound 13

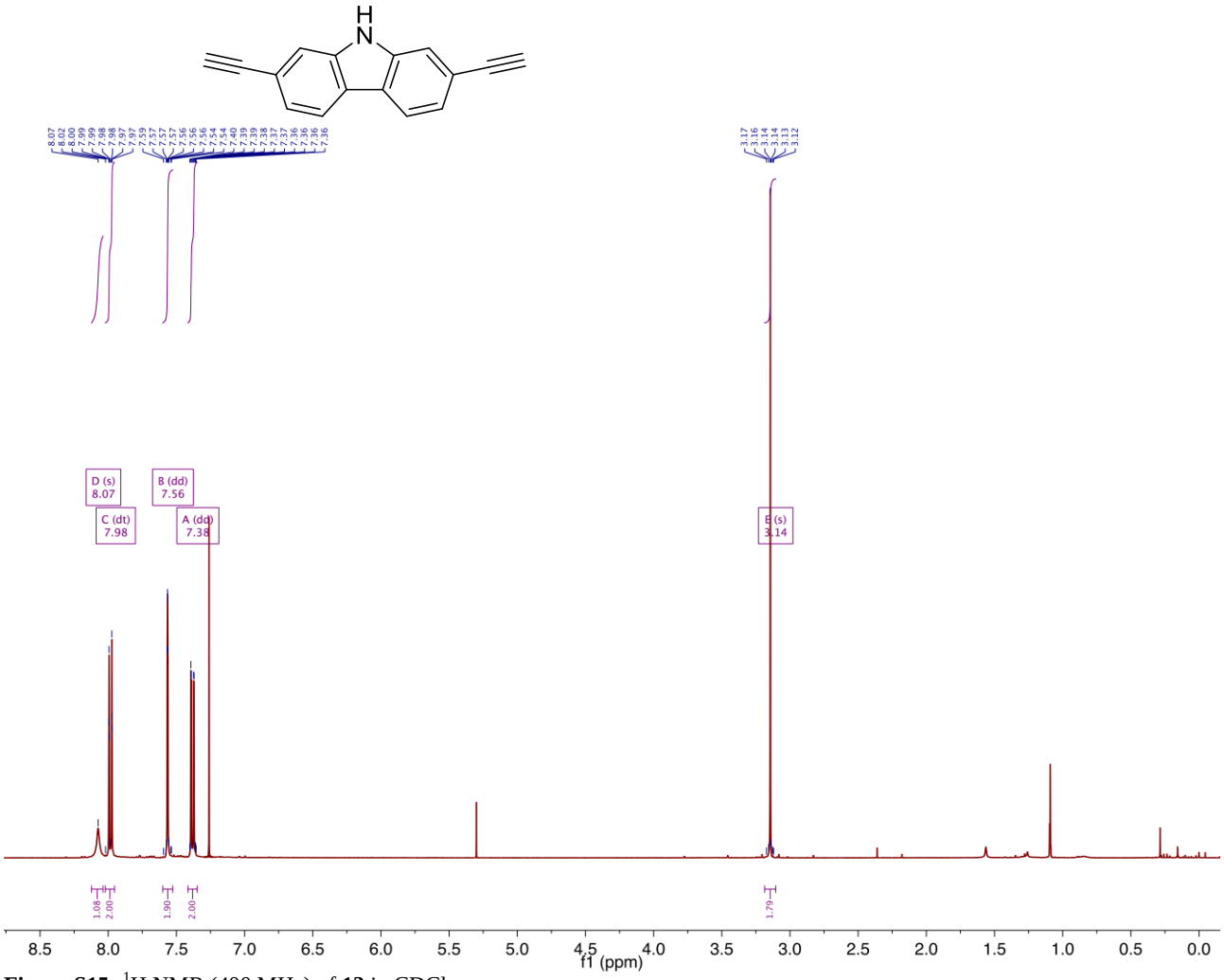


Figure S15: ^{1}H NMR (400 MHz) of **13** in $CDCl_3$.

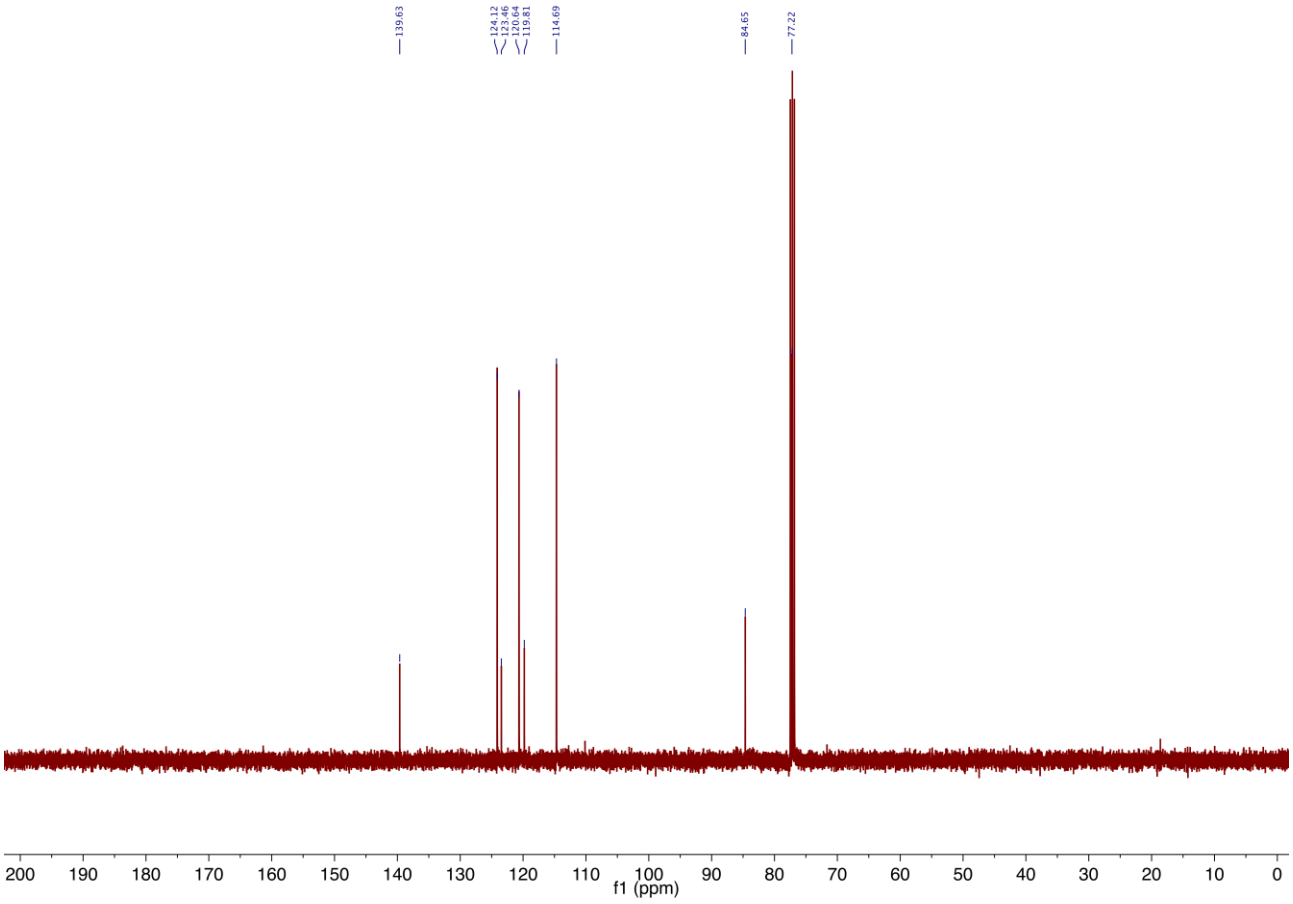
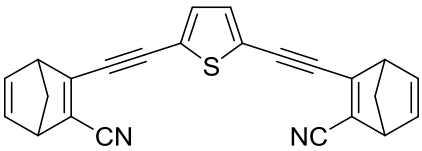


Figure S16: ^{13}C NMR (100 MHz) of **13** in $CDCl_3$.

UV-absorption and switching studies

Compound 1



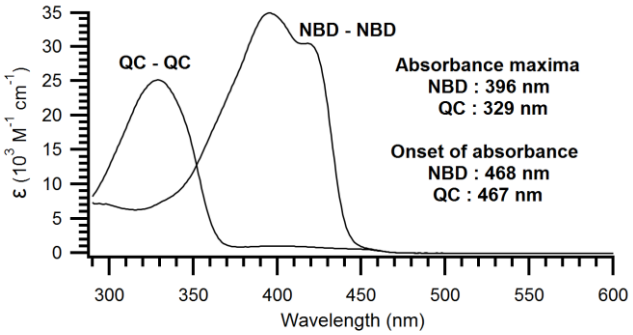


Figure S17: UV-Vis absorption spectrum of **1** and $\mathbf{1}_{\mathbf{OC\text{-}OC}}$.

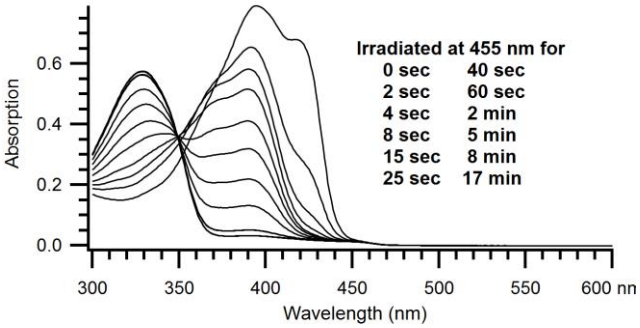


Figure S18: UV-Vis absorption spectra after varying irradiation times with a 455 nm diode.

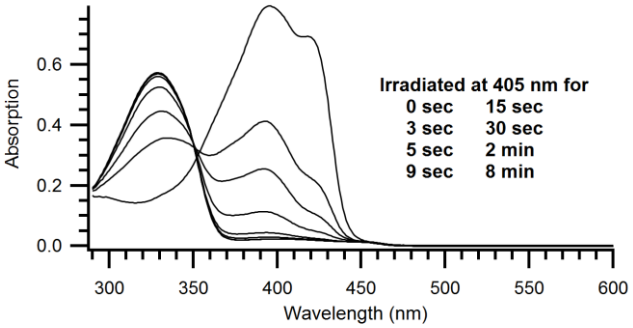


Figure S19: UV-Vis absorption spectra after varying irradiation times with a 405 nm diode.

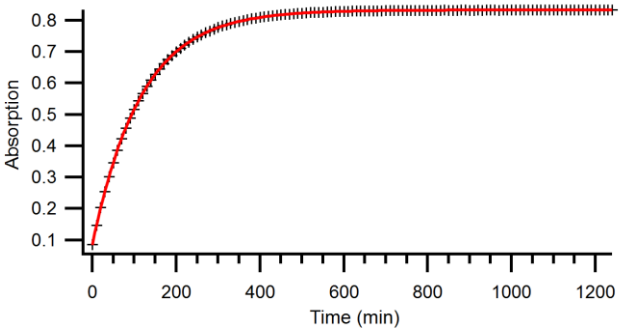


Figure S20: Increase at absorbance maximum of NBD (396 nm) at 24.9 °C.

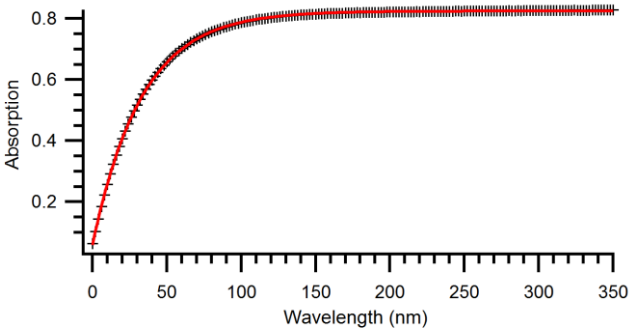


Figure S21: Increase at absorbance maximum of NBD (396 nm) at 34.9 °C

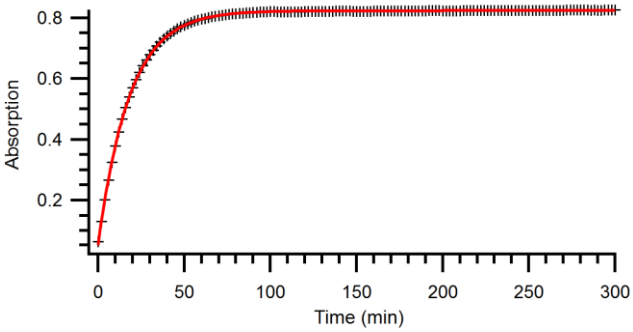


Figure S22: Increase at absorbance maximum of NBD (396 nm) at 39.7 °C

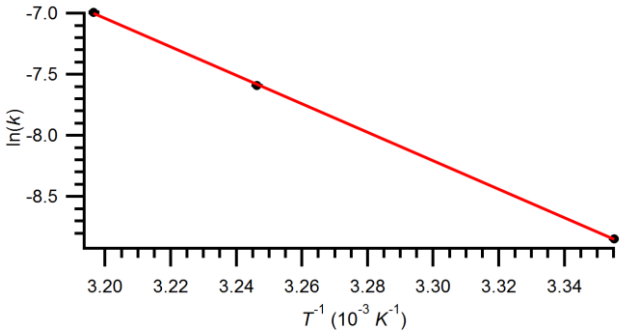


Figure S23: Arrhenius plot giving the values E_a = 96972 J/mol and A = 1.42 x 10^{13}.

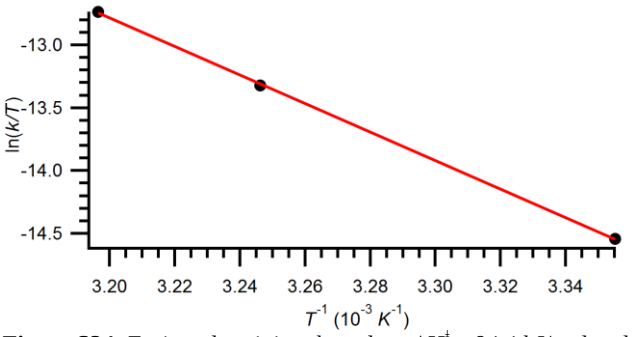
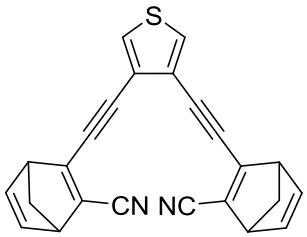


Figure S24: Eyring plot giving the values $\Delta H^{\ddagger}$ = 94.4 kJ/mol and $\Delta S^{\ddagger}$ = -1.65 J mol^{-1} K^{-1}

Compound 2



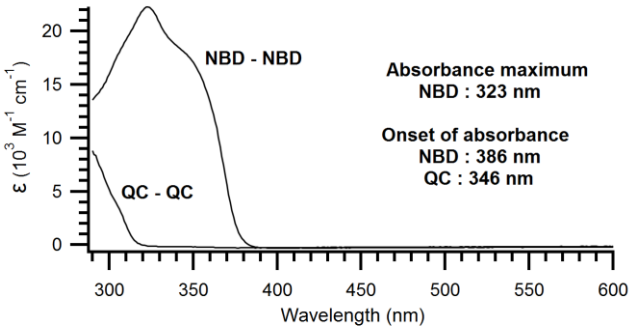


Figure S25: UV-Vis absorbance spectrum of **2** and $\mathbf{2_{QC\text{-}QC}}$.

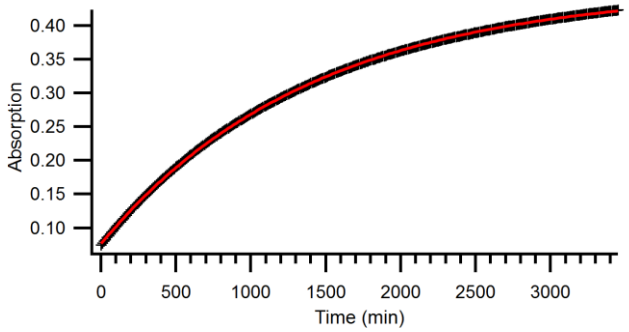


Figure S26: Increase at absorbance maximum of NBD (323 nm) at 24.9 °C.

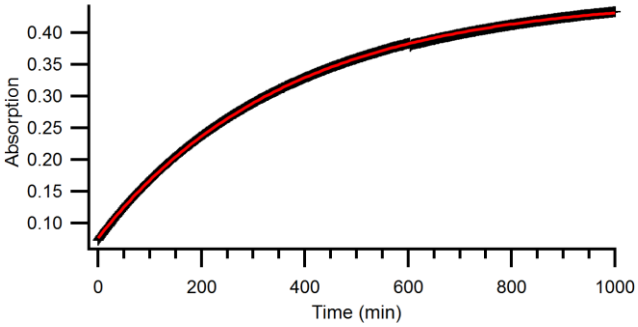


Figure S27: Increase at absorbance maximum of NBD (323 nm) at 34.9 °C.

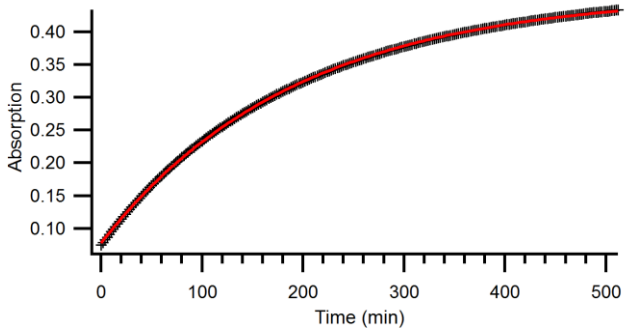


Figure S28: Increase at absorbance maximum of NBD (323 nm) at 39.7 °C

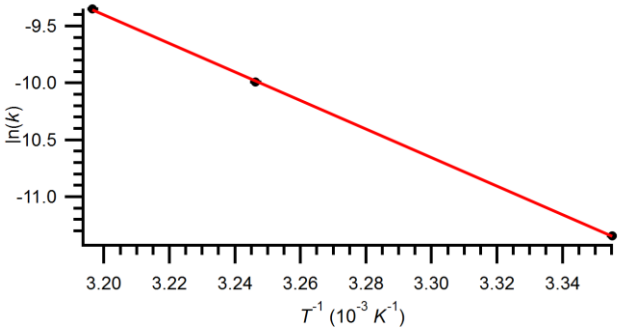


Figure S29: Arrhenius plot giving the values E_a = 104213 J/mol and A = 2.17 x 10^{13}.

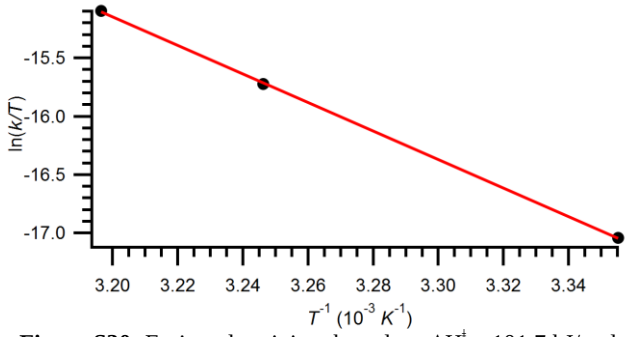
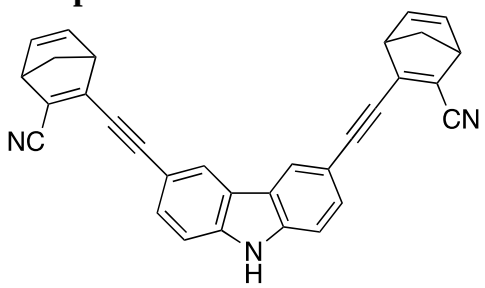


Figure S30: Eyring plot giving the values $\Delta H^{\ddagger}$ = 101.7 kJ/mol and $\Delta S^{\ddagger}$ = 1.89 J mol^{-1} K^{-1}

Compound 3



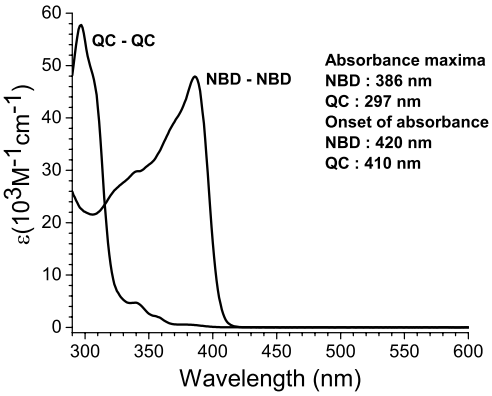


Figure S31: UV-Vis absorption spectrum of **3** and $\mathbf{3}_{\mathbf{QC\text{-}QC}}$.

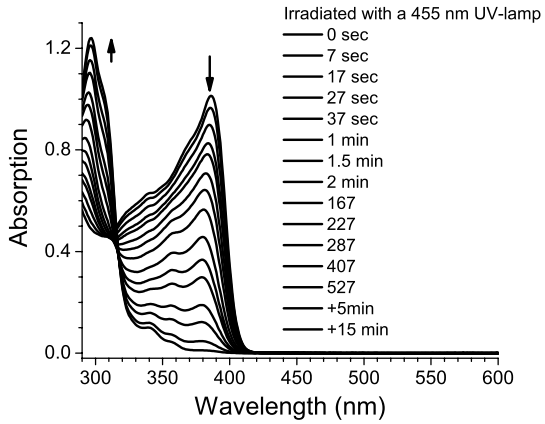


Figure S32: UV-Vis absorption spectra after varying irradiation times with a 455 nm diode.

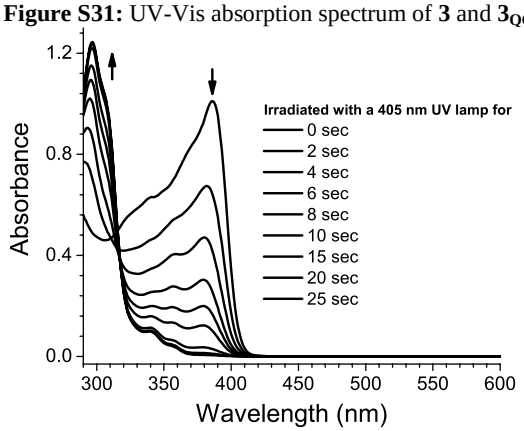


Figure S33: UV-Vis absorption spectra after varying irradiation times with a 405 nm diode.

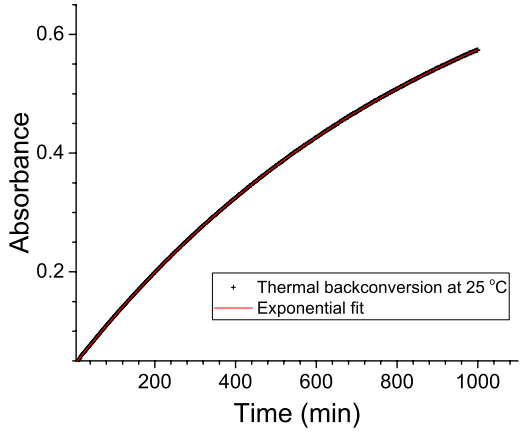


Figure S34: Increase at absorbance maxima of NBD at 25 °C.

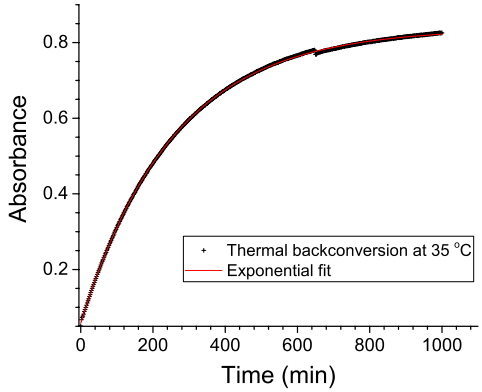


Figure S35: Increase at absorbance maxima of NBD at 35 °C.

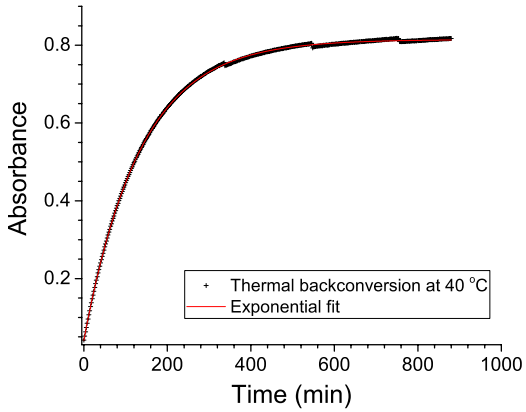


Figure S36: Increase at absorbance maxima of NBD at 40 °C.

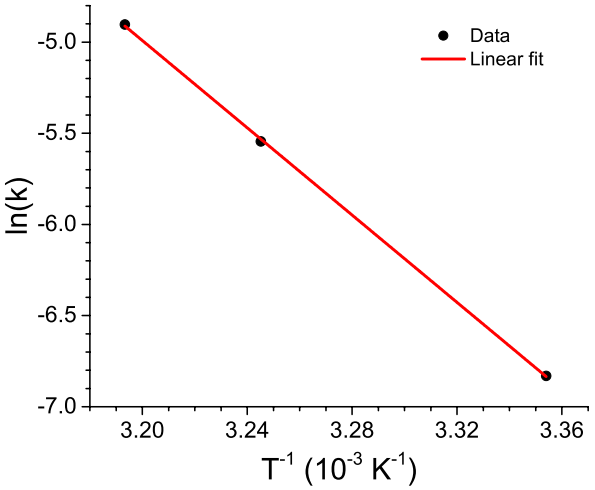


Figure S37: Arrhenius plot giving the values: A = 2.9 x 10^{14} s^{-1} and E_a = 99508 J/mol

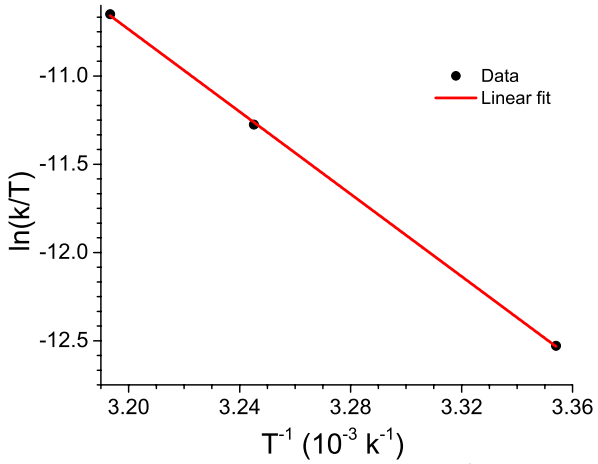
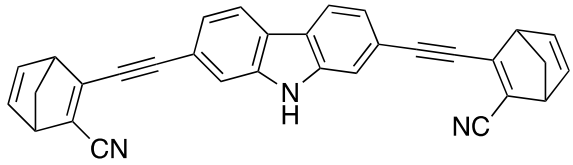


Figure S38: Eyring plot giving the values: $\Delta H^{\ddagger}$ = 96971 J/mol and $\Delta S^{\ddagger}$ = 23.28 J mol^{-1} K^{-1}

Compound 4



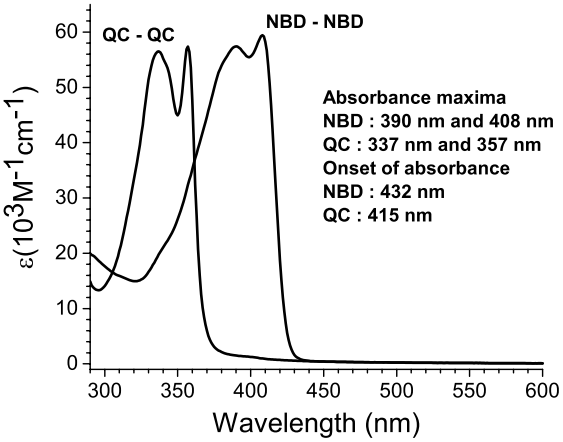


Figure S39: UV-Vis absorption spectra of **4** and $\mathbf{4}_{\mathbf{QC\text{-}QC}}$.

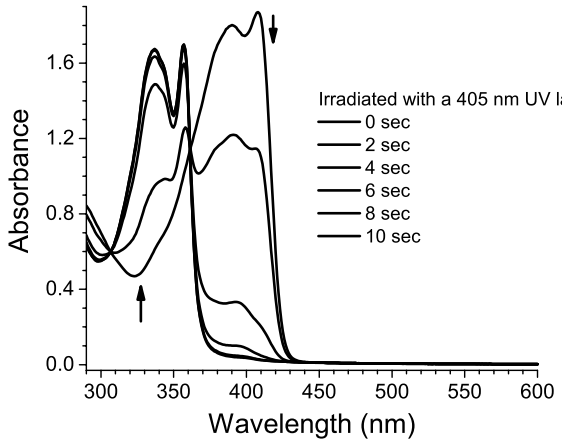


Figure S40: UV-Vis spectra after varying irradiation times of **4** with a 405 nm diode.

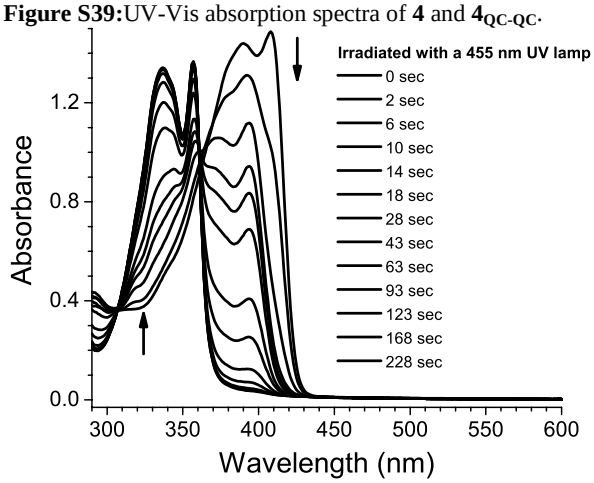


Figure S41: UV-Vis spectra after varying irradiation times of **4** with a 455 nm diode.

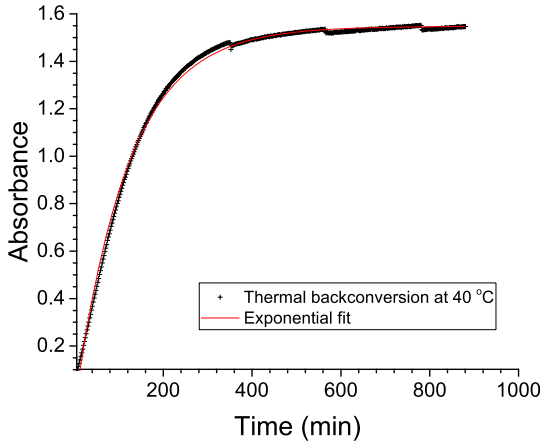


Figure S42: Increase at absorbance maxima of NBD at 40 °C.

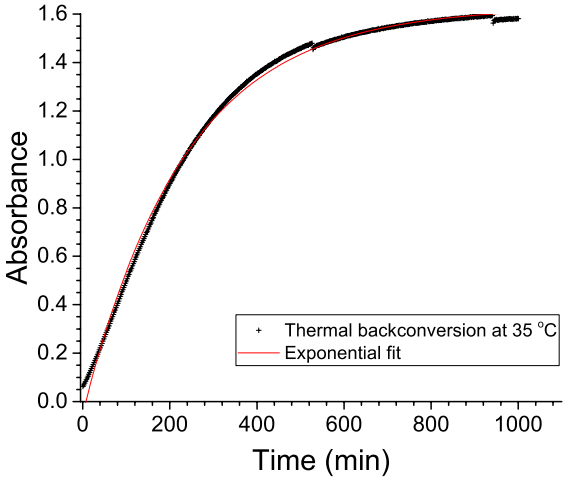


Figure S43: Increase at absorbance maxima of NBD at 35 °C.

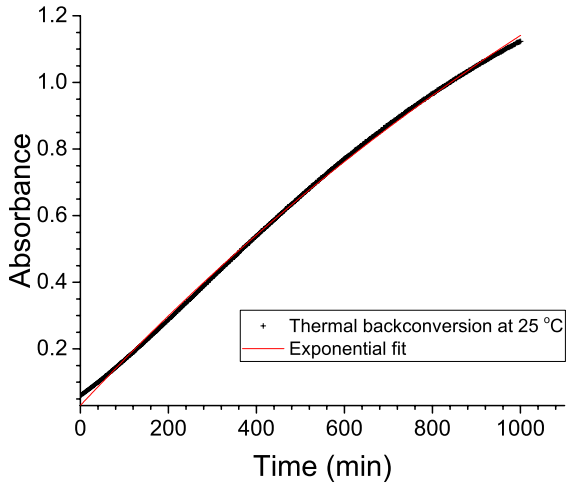


Figure S44: Increase at absorbance maxima of NBD at 25 °C.

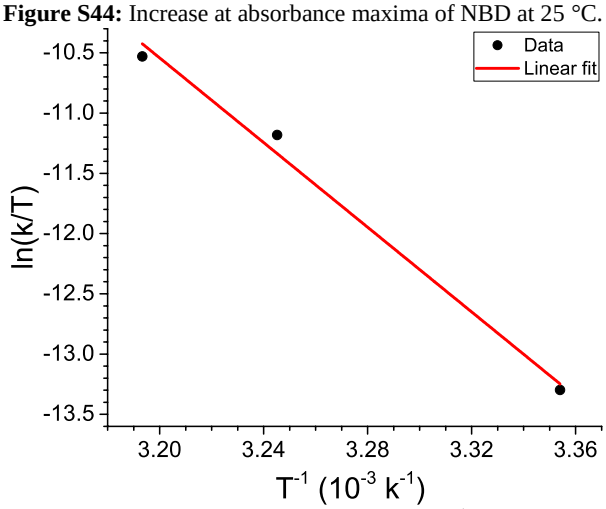


Figure S46: Eyring plot giving the values: $\Delta H^{\ddagger}$ = 146063 J/mol and $\Delta S^{\ddagger}$ = 182.9 J mol^{-1} K^{-1}.

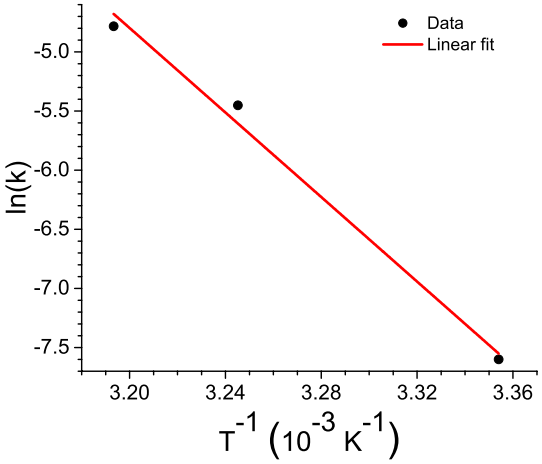
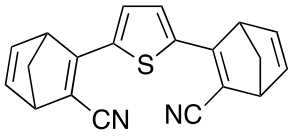


Figure S45: Arrhenius plot giving the values: A = 5.7x10^{22} s^{-1} and E_a = 148600 J/mol

Compound 5



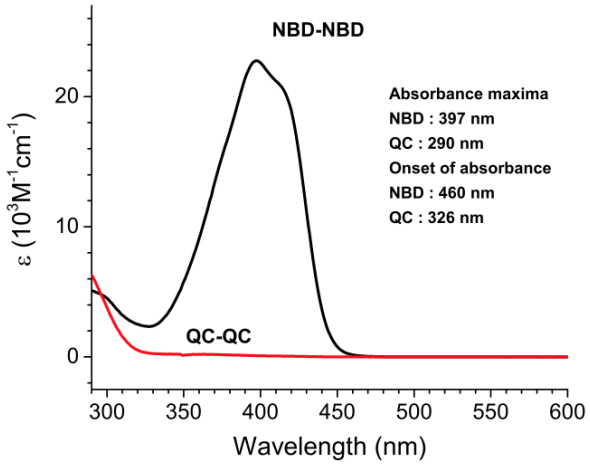


Figure S47: UV-Vis absorption spectra of **5** and $\mathbf{5}_{\mathbf{QC\text{-}QC}}$.

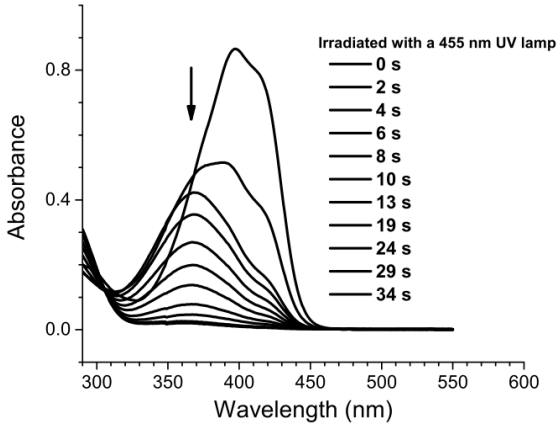


Figure S48: UV-Vis spectra after varying irradiation times of **5**.

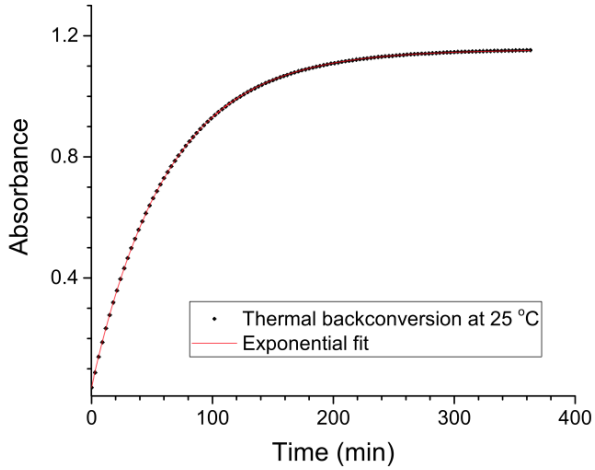


Figure S49: Increase at absorbance maxima of NBD at 25 °C.

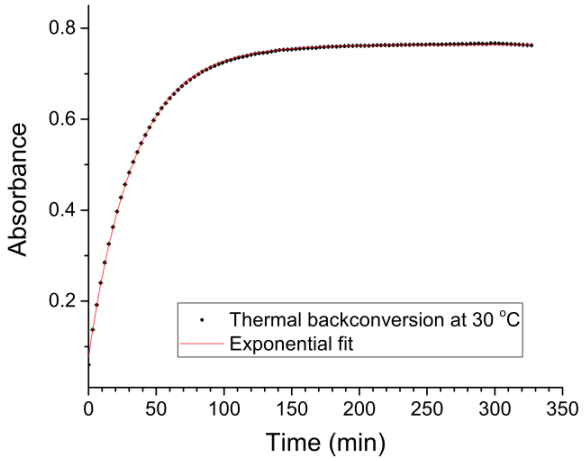


Figure S50: Increase at absorbance maxima of NBD at 30 °C.

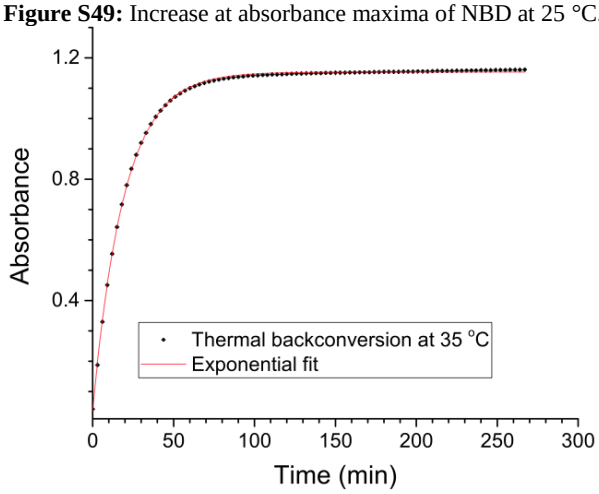


Figure S51: Increase at absorbance maxima of NBD at 35 °C.

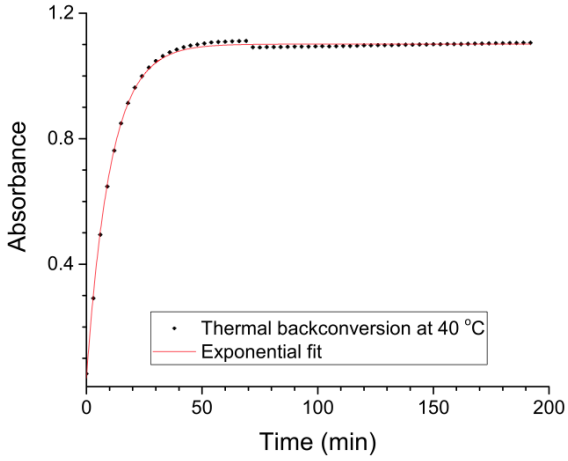


Figure S52: Increase at absorbance maxima of NBD at 40 °C.

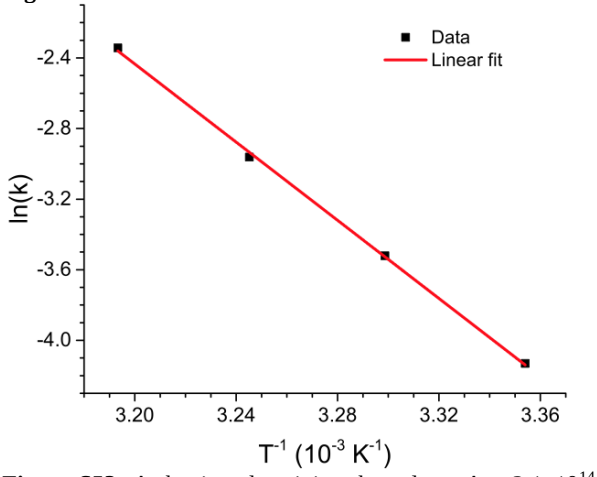


Figure S53: Arrhenius plot giving the values: A = 2.1×10^{14} s^{-1} and Ea = 92051 J/mol

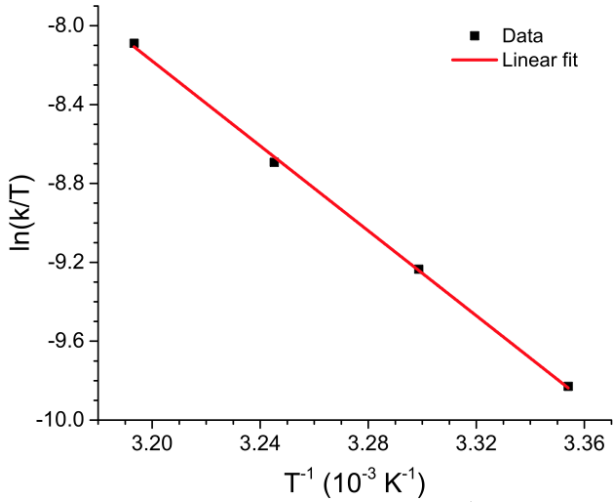


Figure S54: Eyring plot giving the values: $\Delta H^{\ddagger}$ = 89514 J/mol and $\Delta S^{\ddagger}$ = 155.2 J mol^{-1} K^{-1}.

Photoisomerization quantum yields

Photonflux

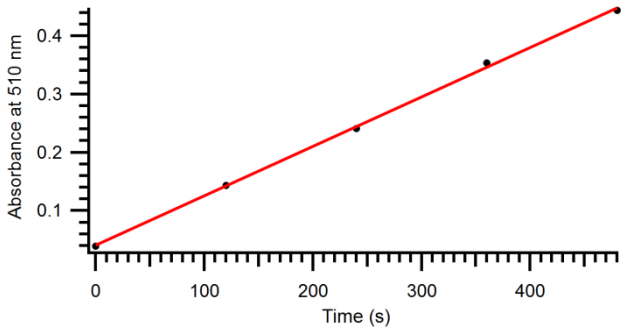


Figure S55: Photon flux for lamp at 340 nm is 9.32652 x 10^{-9} mol s^{-1}. Used for 2.

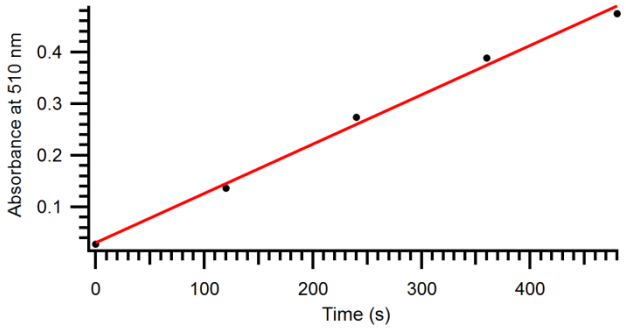


Figure S56: Photon flux for lamp at 405 nm is 1.31811 x 10^{-7} mol s^{-1}. Used for **1**, **3, 4** and **5**.

Compound 1

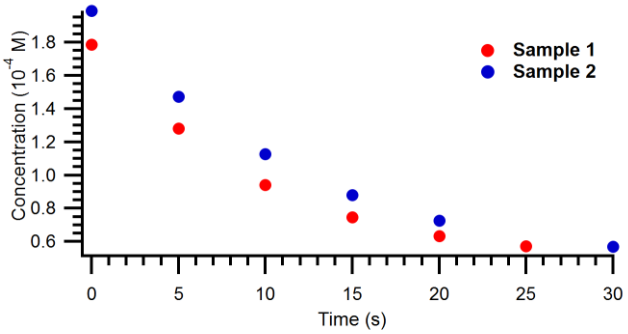


Figure S57: Plot of the quantum yield measurements for compound **1** at 405 nm. The quantum yield could not be calculated as the data deviated from linearity.

Compound 2

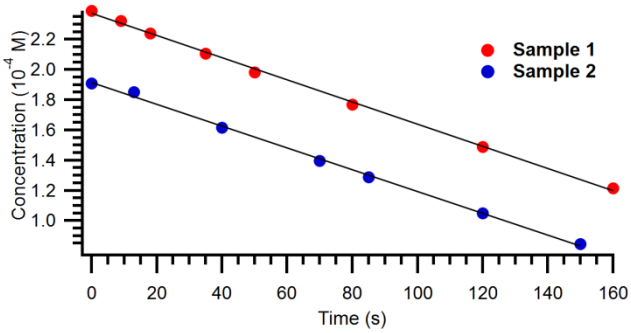


Figure S58: Plot of the quantum yield measurements for compound **2** at 340 nm. $\Phi_{sample\ 1}$ = 50%. $\Phi_{sample\ 2}$ = 50%.

Compound 3

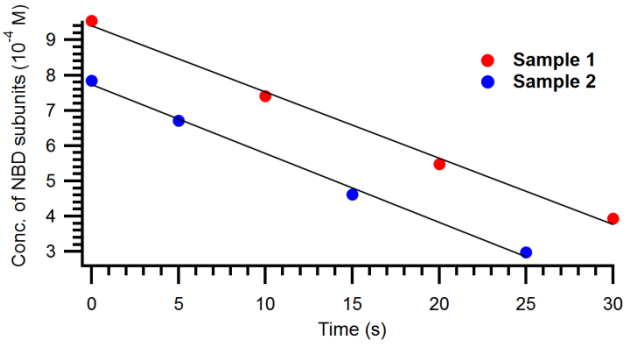


Figure S59: Plot of the quantum yield measurements for compound **3** at 405 nm. $\Phi_{sample\ 1}$ = 46%. $\Phi_{sample\ 2}$ = 42%.

Compound 4

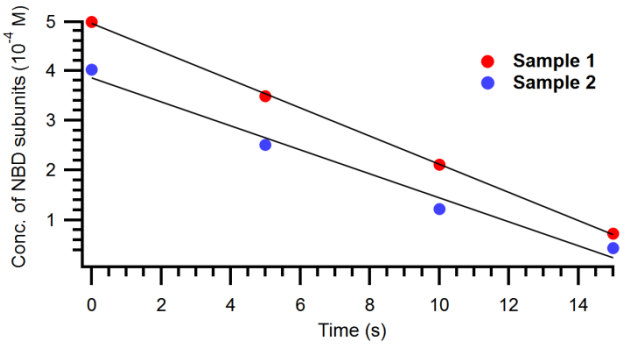


Figure S60: Plot of the quantum yield measurements for compound **4** at 405 nm. $\Phi_{sample\ 1}$ = 70%. $\Phi_{sample\ 2}$ = 70%.

Compound 5

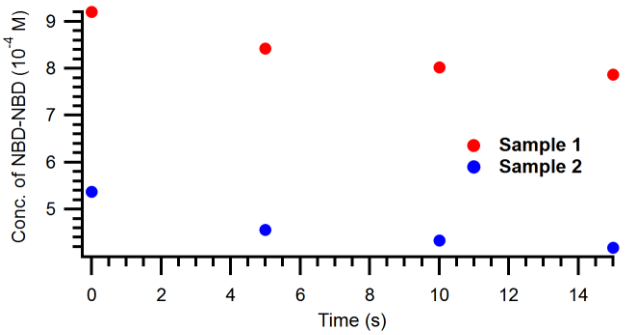


Figure S61: Plot of the quantum yield measurements for compound **5** at 405 nm. The quantum yield could not be calculated as the data deviated from linearity.