Norbornadiene-Dihydroazulene Conjugates

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ELECTRONIC SUPPORTING INFORMATION

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NMR spectra

Compound 3a$_{NBD\text{-}DHA}$

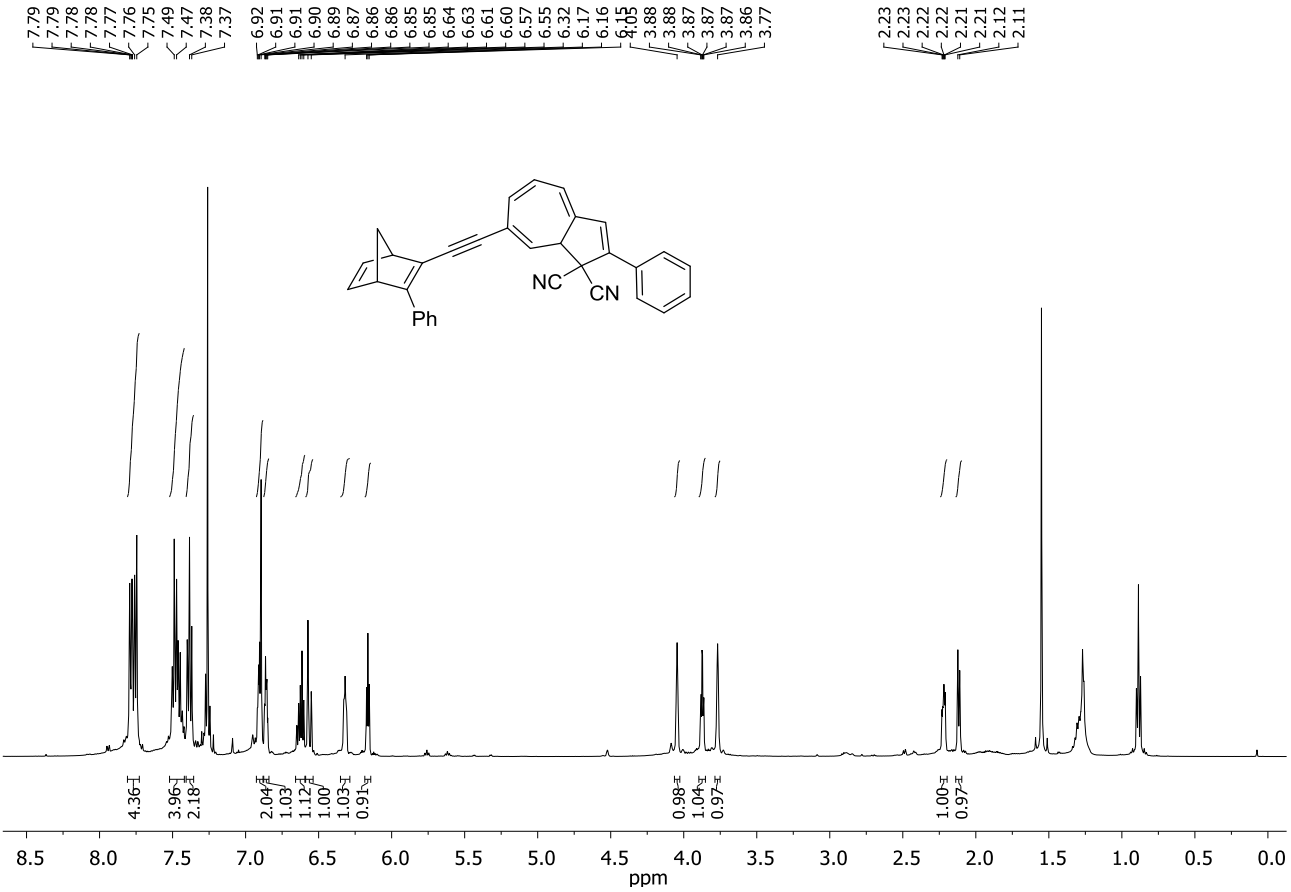

Figure S1: ^{1}H-NMR spectrum of **3a$_{NBD\text{-}DHA}$** in $CDCl_3$ (500 MHz).

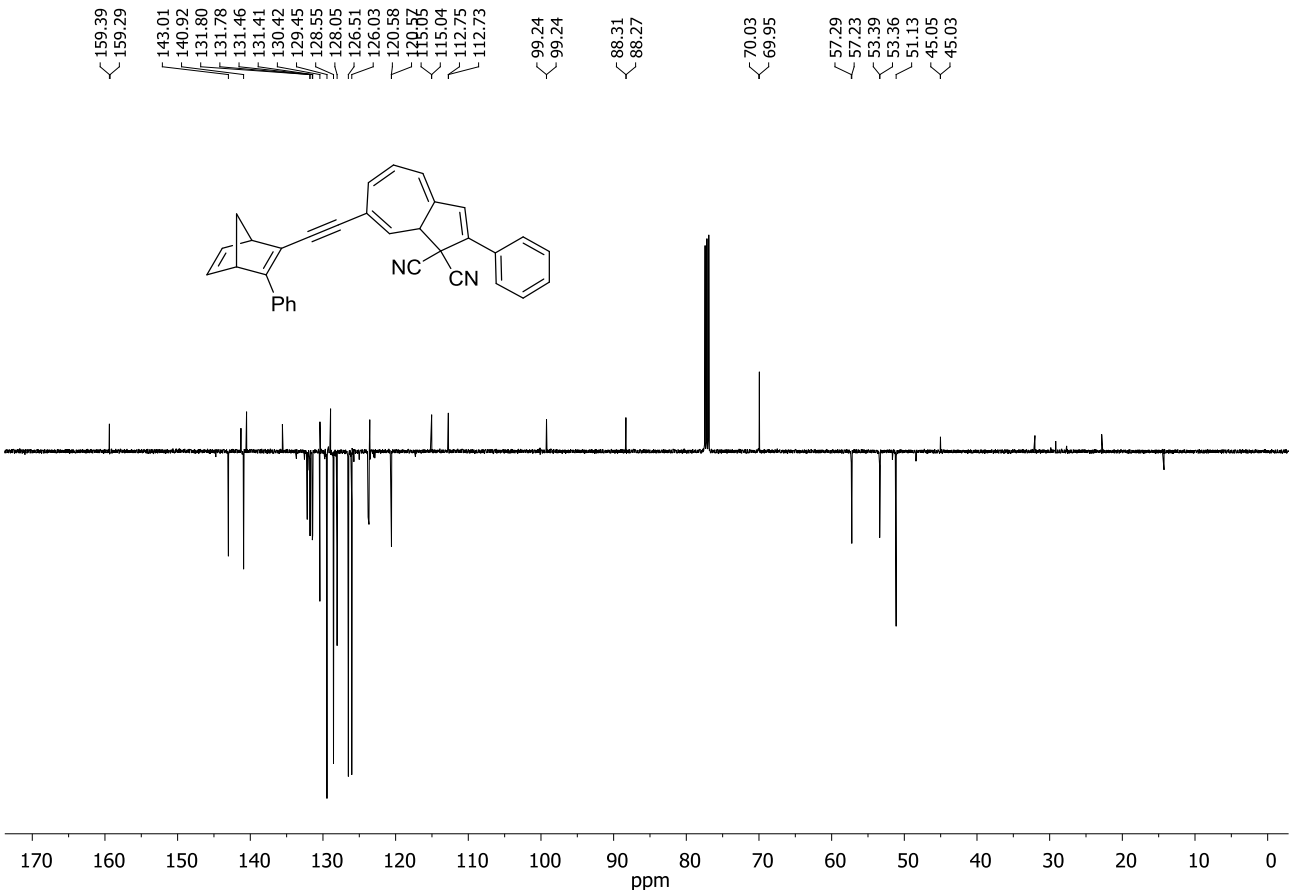

Figure S2: ^{13}C-APT spectrum of **3a$_{NBD-DHA}$** in $CDCl_3$ (126 MHz).

Compound $3b_{NBD\text{-}DHA}$

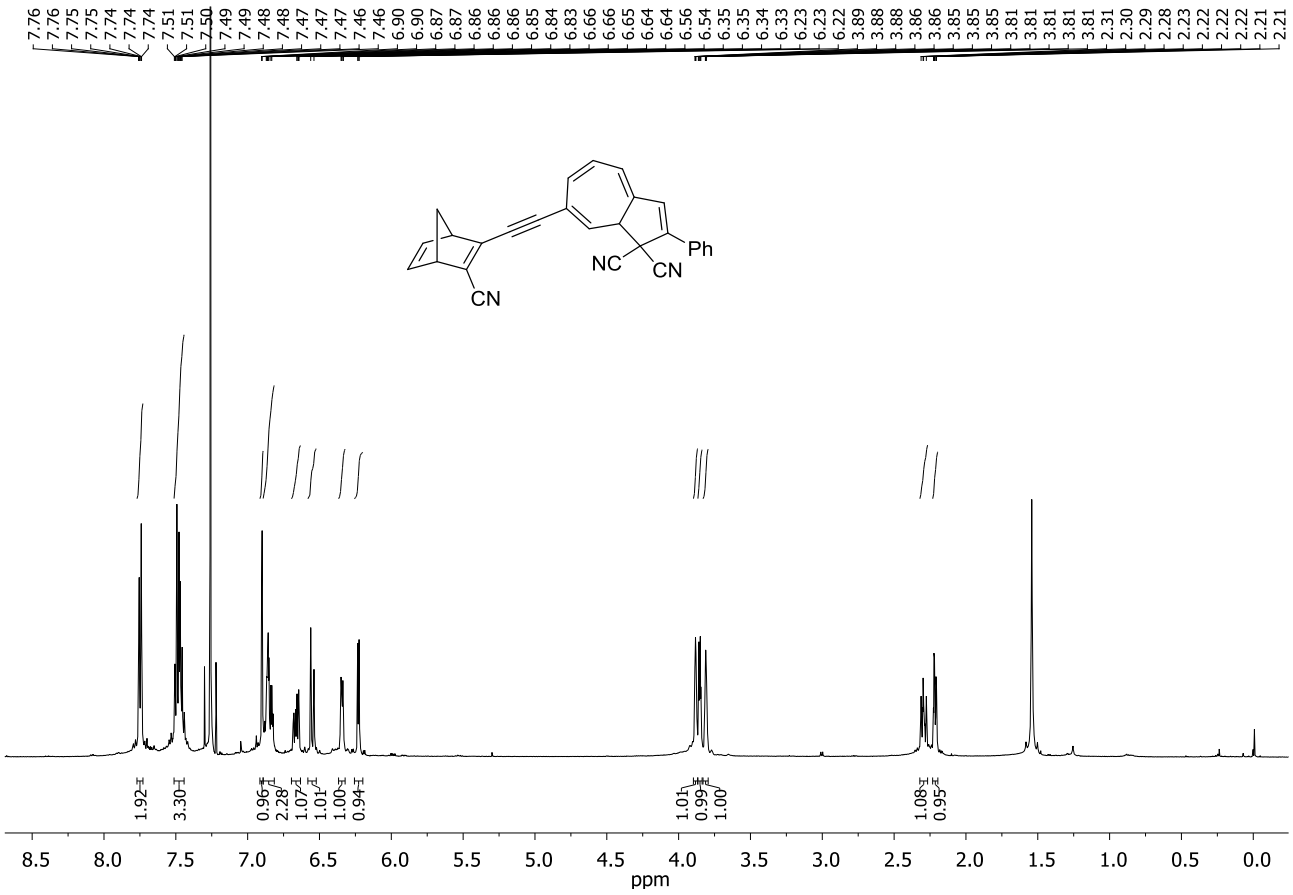

Figure S3: ^{1}H-NMR spectrum of **$3b_{NBD\text{-}DHA}$** in $CDCl_3$ (500 MHz).

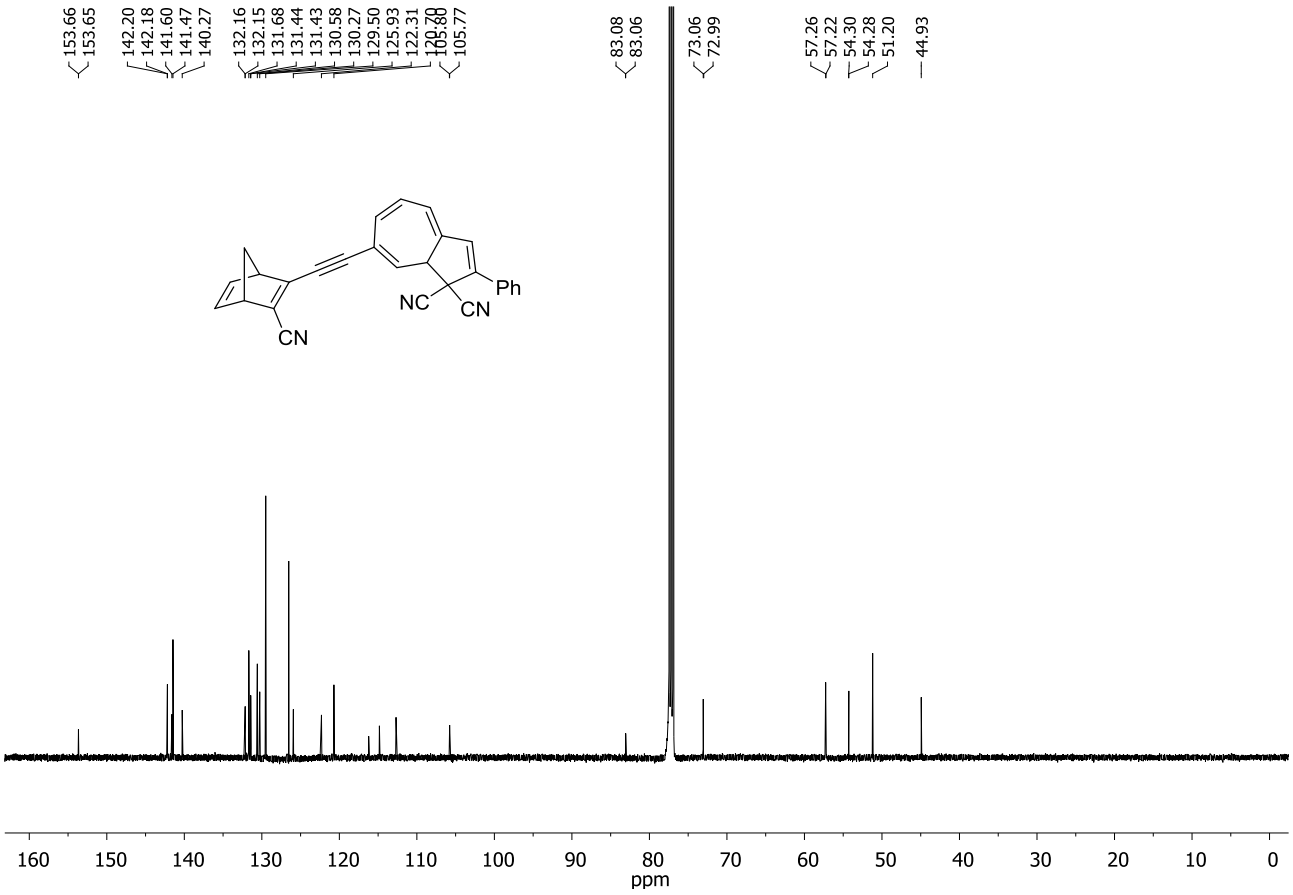

Figure S4: ^{13}C spectrum of **3b$_{NBD-DHA}$** in $CDCl_3$ (126 MHz).

Compound 4a$_{NBD-DHA}$

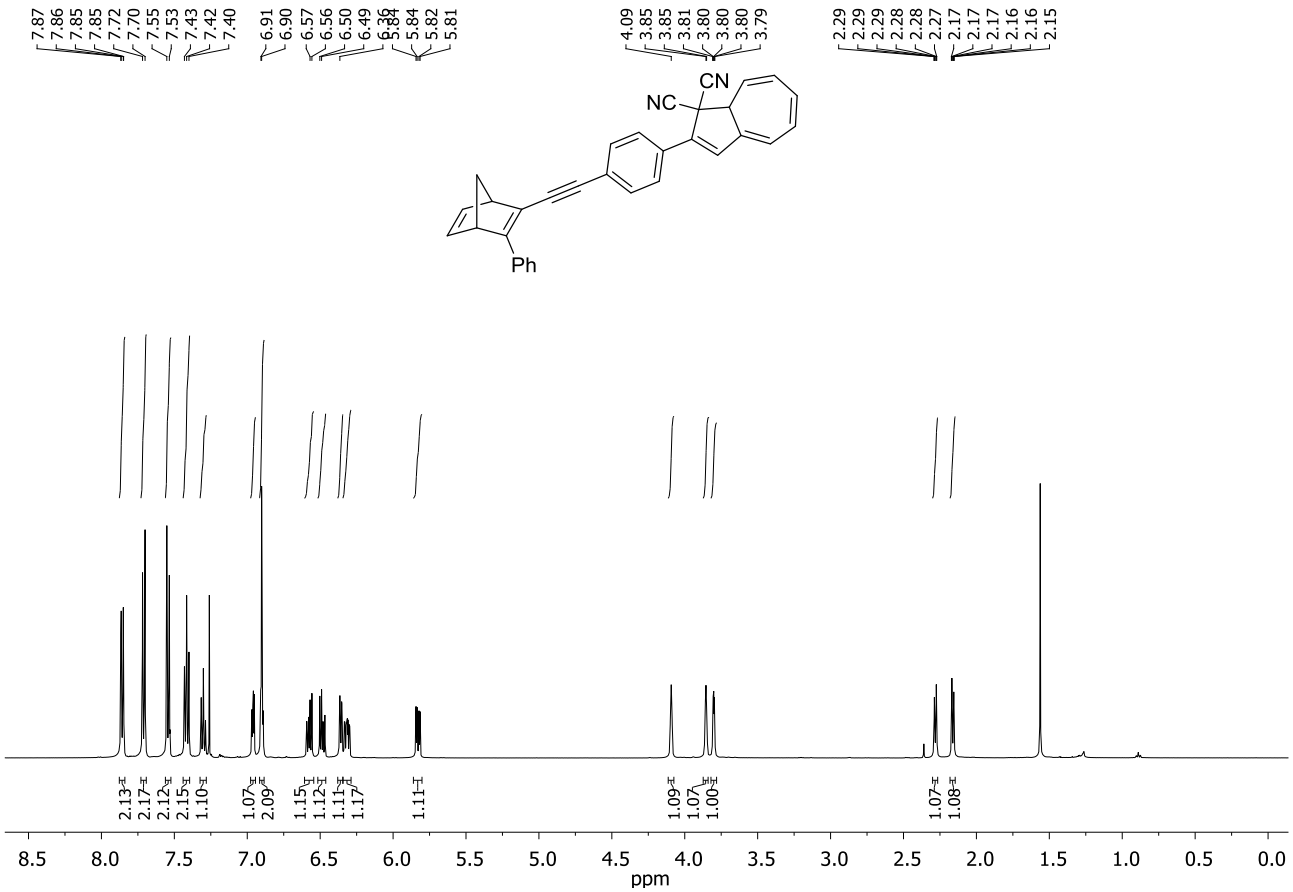

Figure S5: ^{1}H-NMR spectrum of **4a$_{NBD-DHA}$** in $CDCl_3$ (500 MHz).

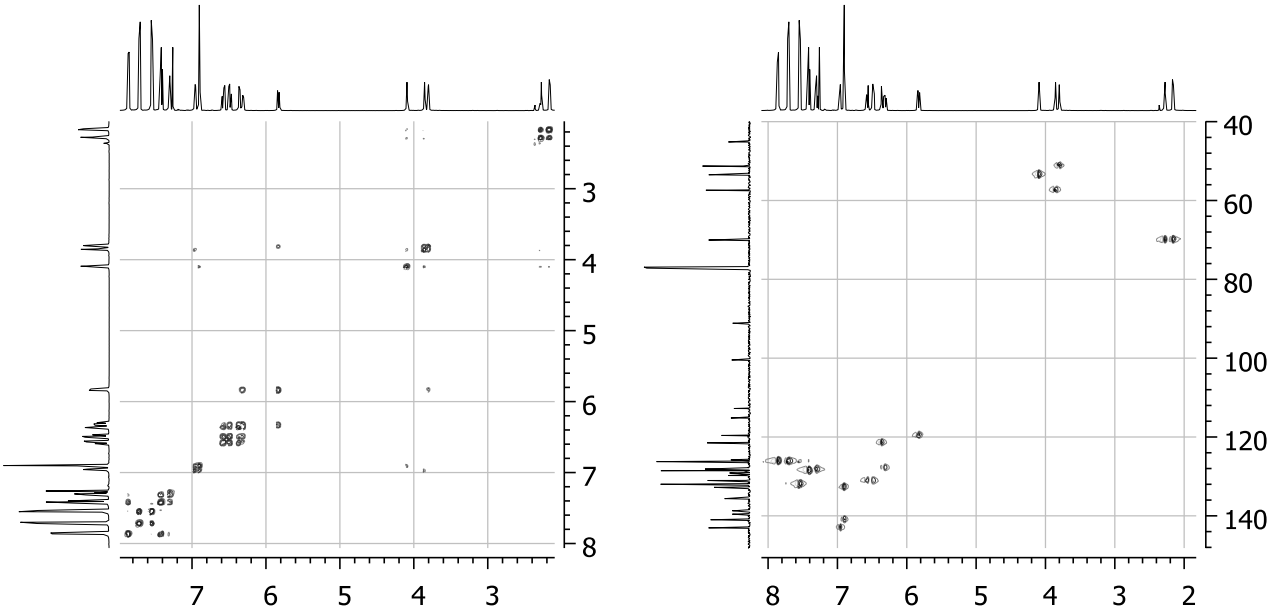

Figure S6: COSY (left) and (right) ^{1}H / ^{13}C HSQC spectra of **4a$_{NBD-DHA}$** in $CDCl_3$ (500 / 126 MHz).

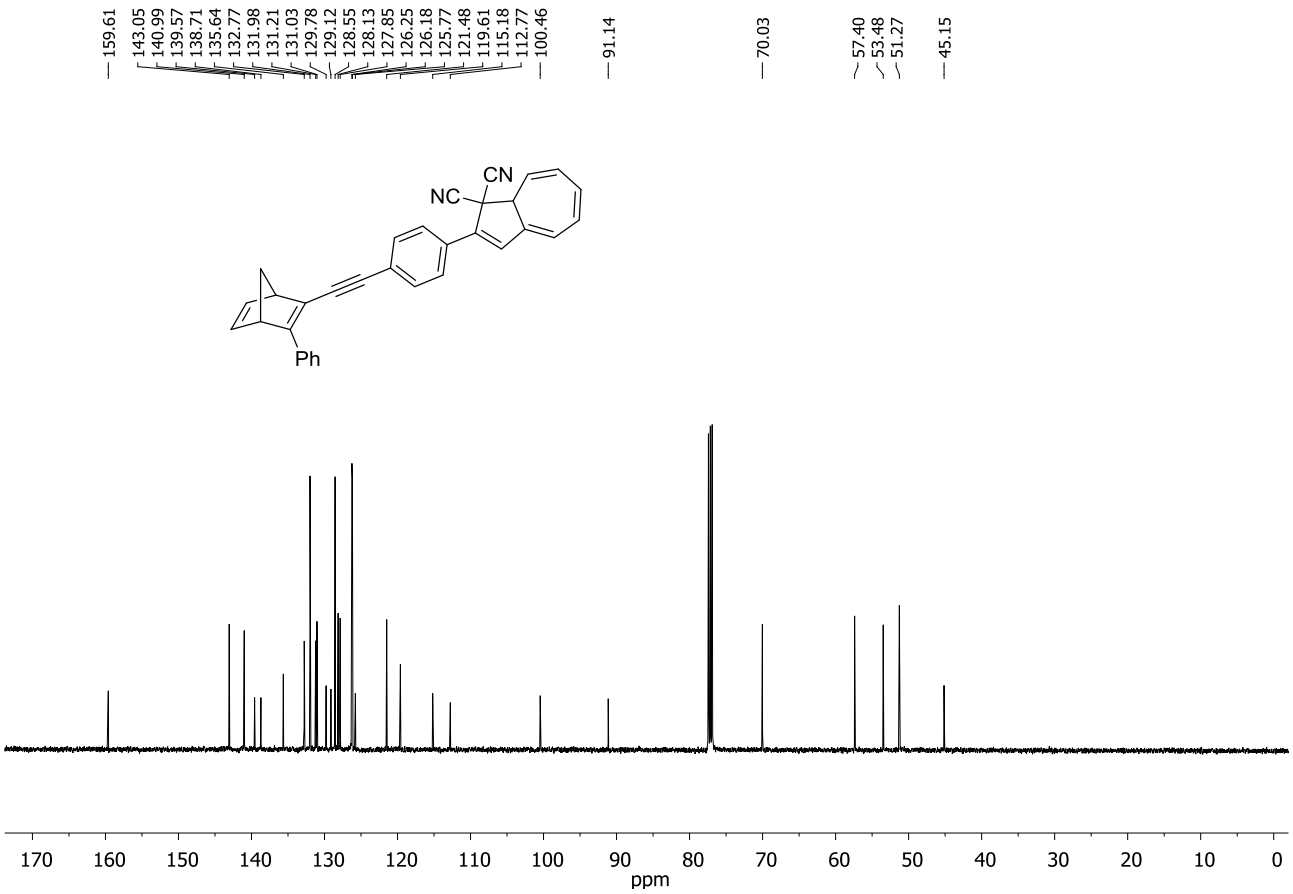

Figure S7: ^{13}C spectrum of **4a$_{NBD\text{-}DHA}$** in $CDCl_3$ (126 MHz).

Compound 4b$_{NBD-DHA}$

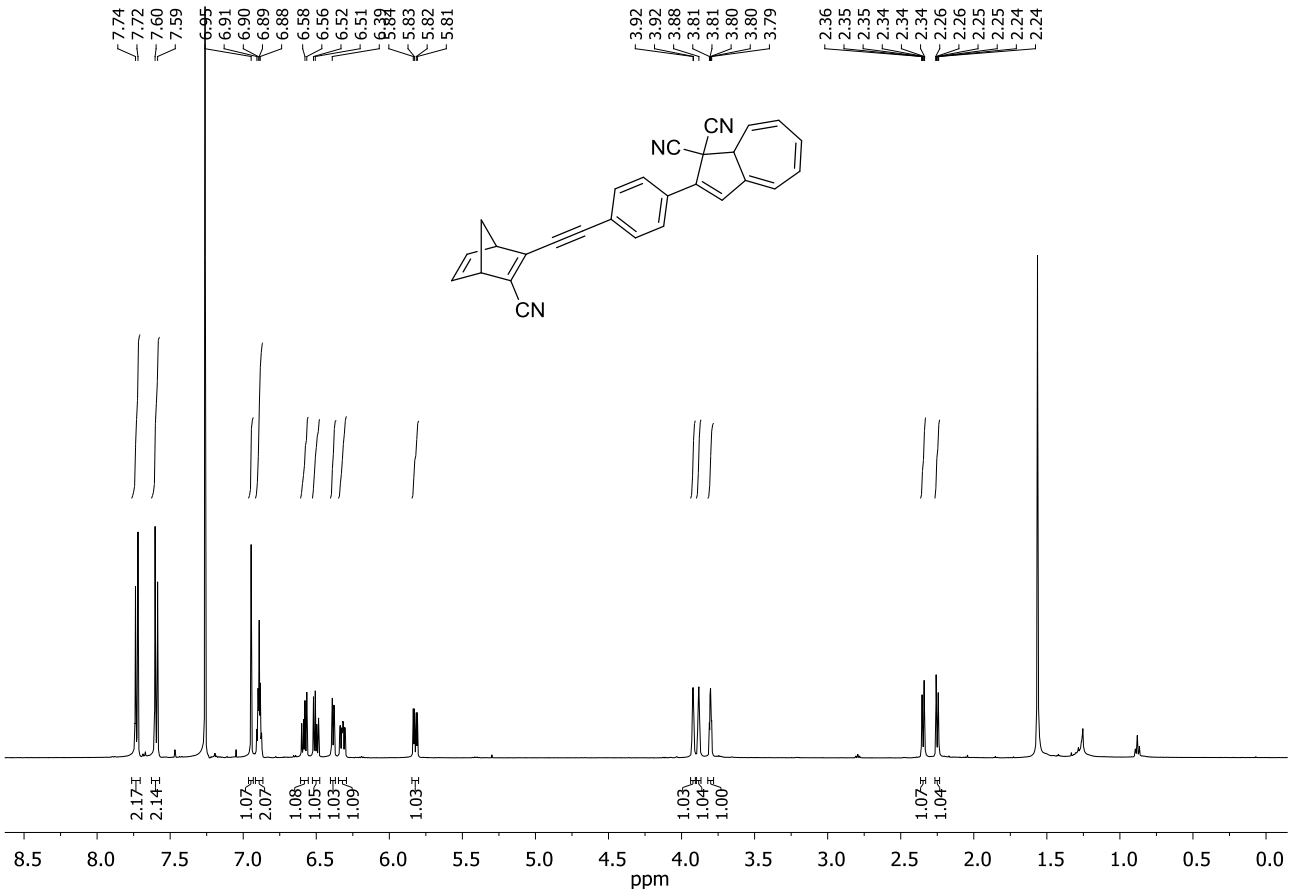

Figure S8: ^{1}H-NMR spectrum of **4b$_{NBD-DHA}$** in $CDCl_3$ (500 MHz).

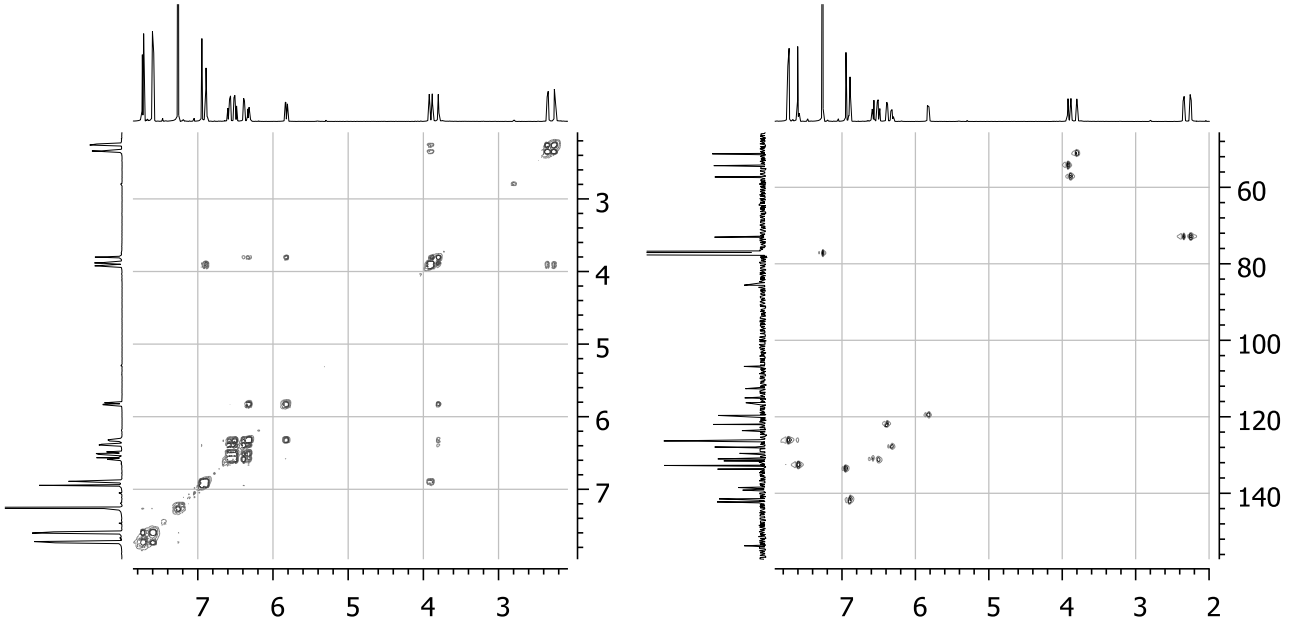

Figure S9: COSY (left) and (right) ^{1}H / ^{13}C HSQC spectra of **4b$_{NBD-DHA}$** in $CDCl_3$ (500 / 126 MHz).

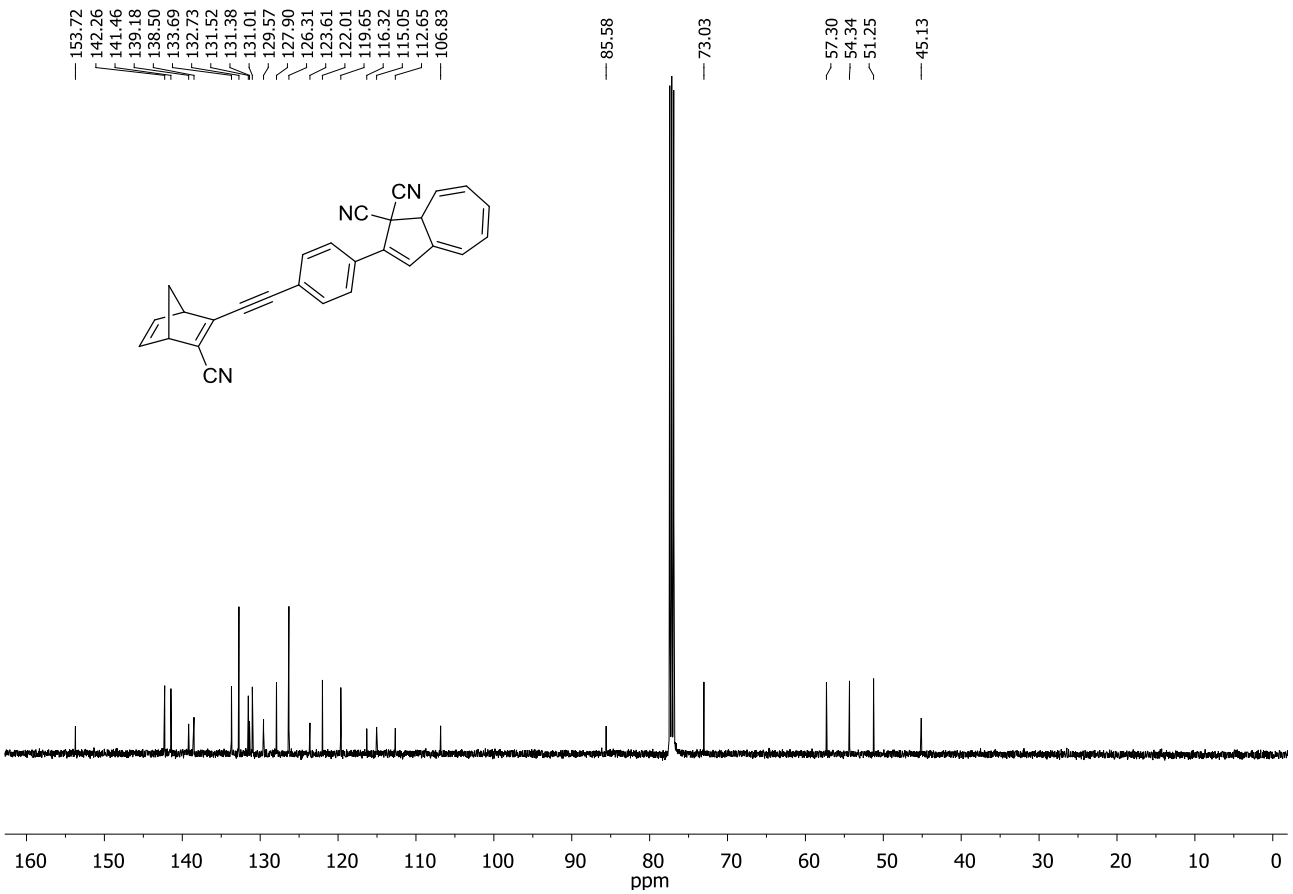

Figure S10: ^{13}C spectrum of **4b$_{NBD-DHA}$** in $CDCl_3$ (126 MHz).

Compound 5a$_{NBD-DHA}$

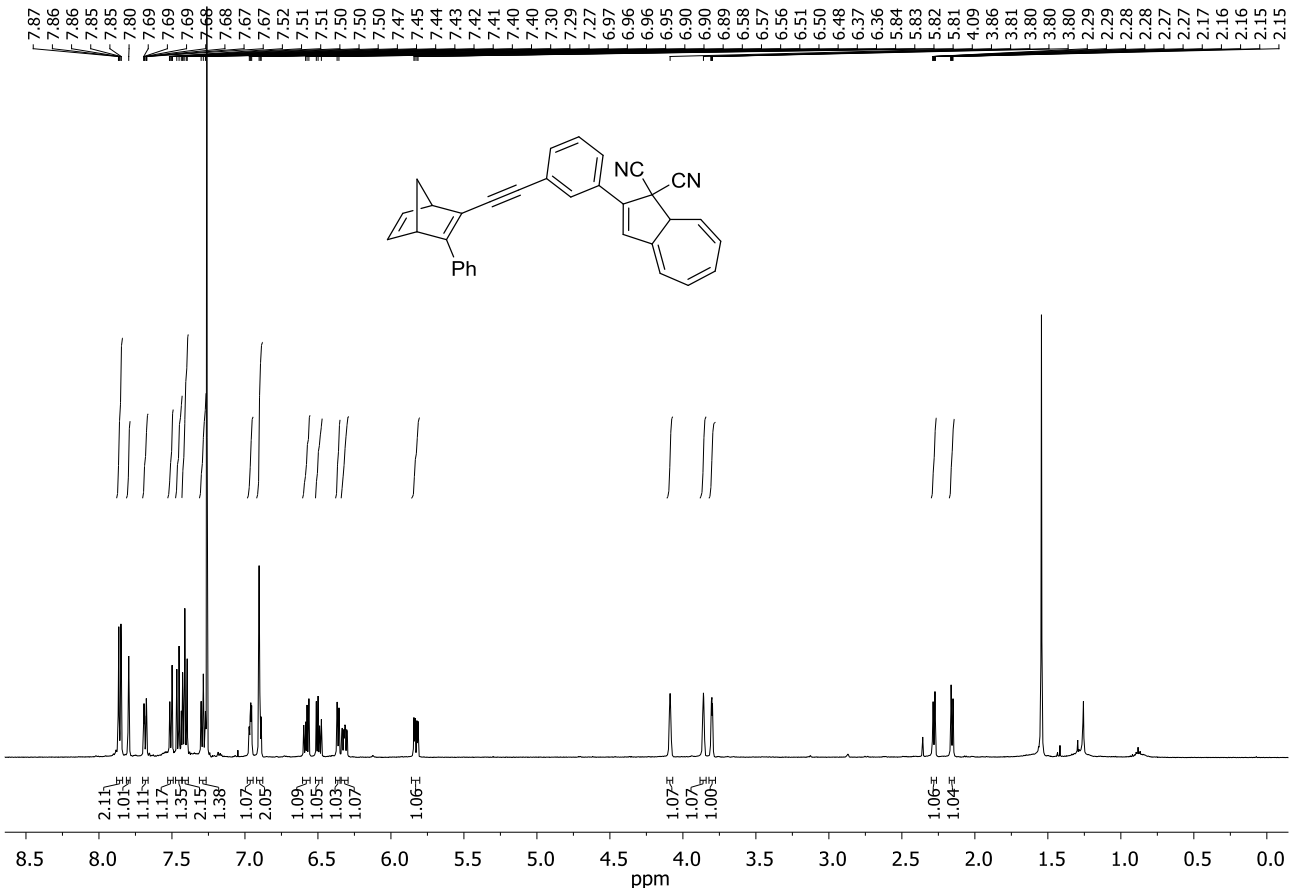

Figure S11: ^{1}H-NMR spectrum of **5a$_{NBD-DHA}$** in $CDCl_3$ (500 MHz).

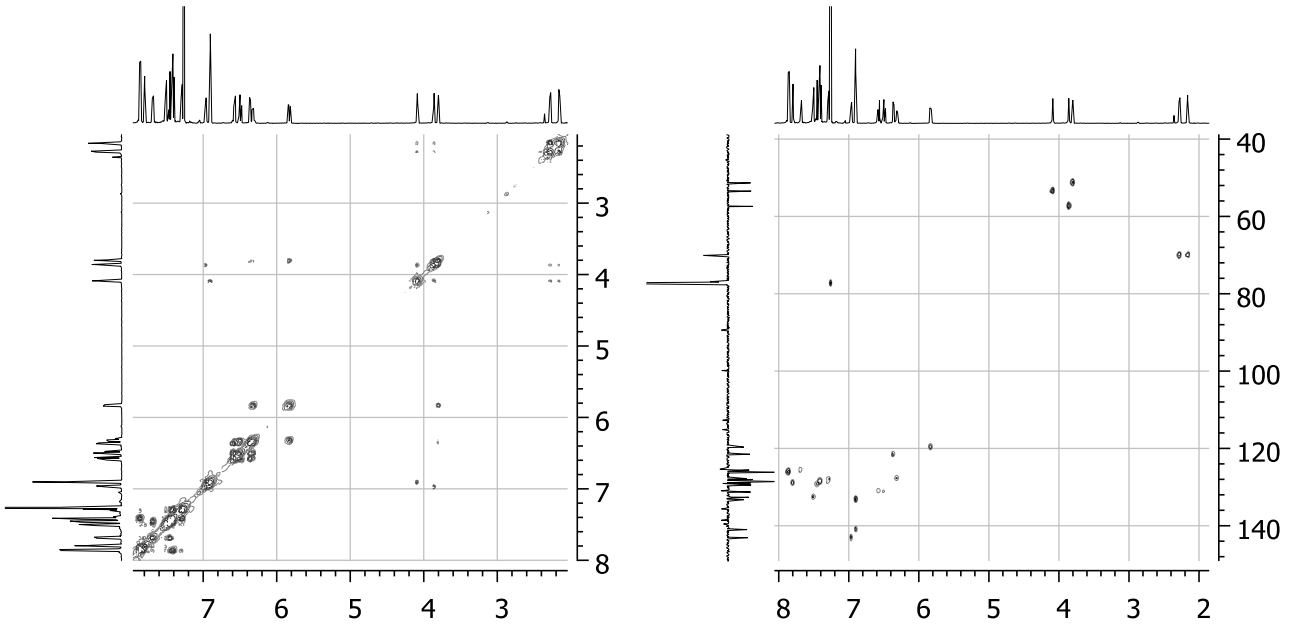

Figure S12: COSY (left) and (right) ^{1}H / ^{13}C-APT HSQC spectra of **5a$_{NBD-DHA}$** in $CDCl_3$ (500 / 126 MHz).

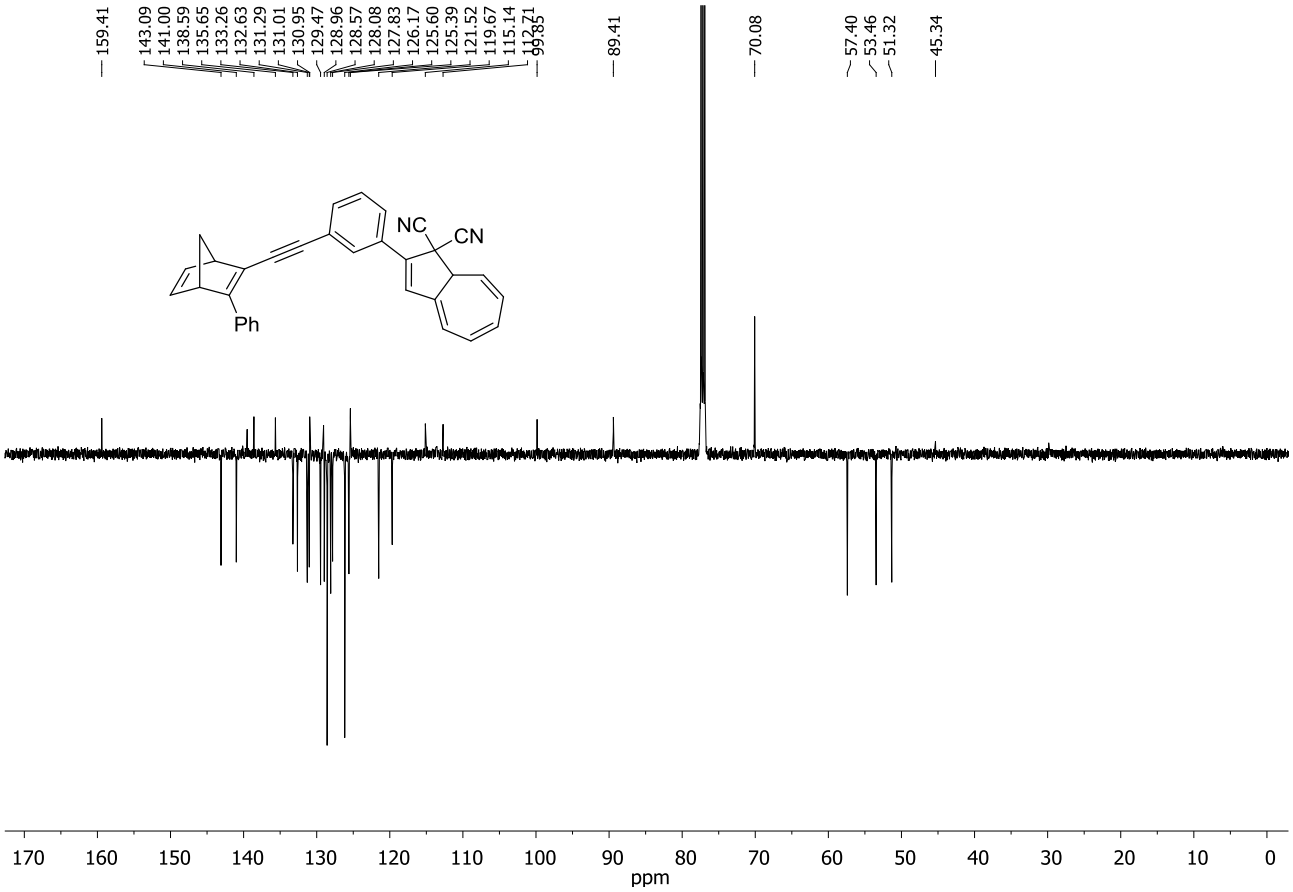

Figure S13: ^{13}C-APT spectrum of **5a$_{NBD\text{-}DHA}$** in $CDCl_3$ (126 MHz).

Compound $\mathbf{5b_{NBD\text{-}DHA}}$

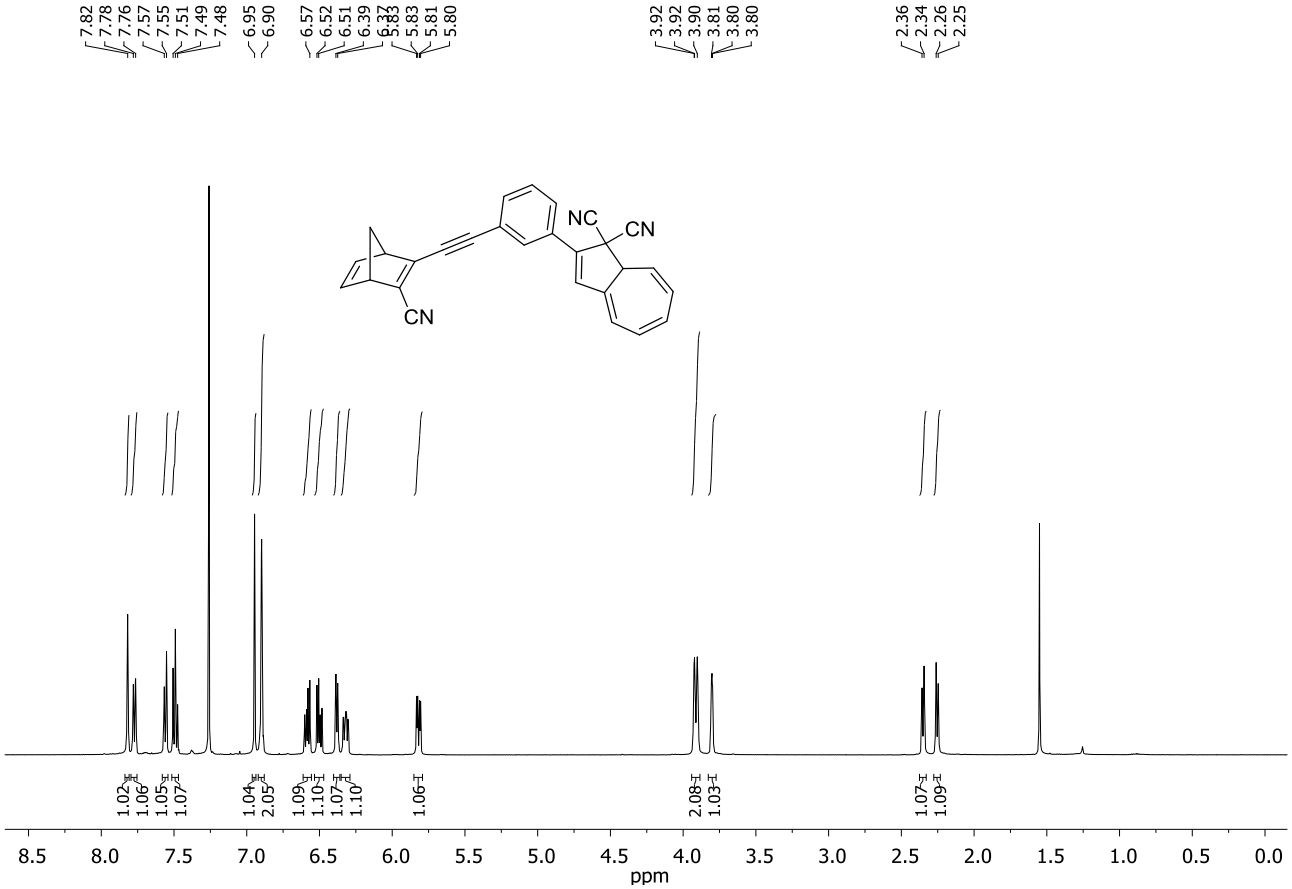

Figure S14: ^{1}H-NMR spectrum of $\mathbf{5b_{NBD\text{-}DHA}}$ in $CDCl_3$ (500 MHz).

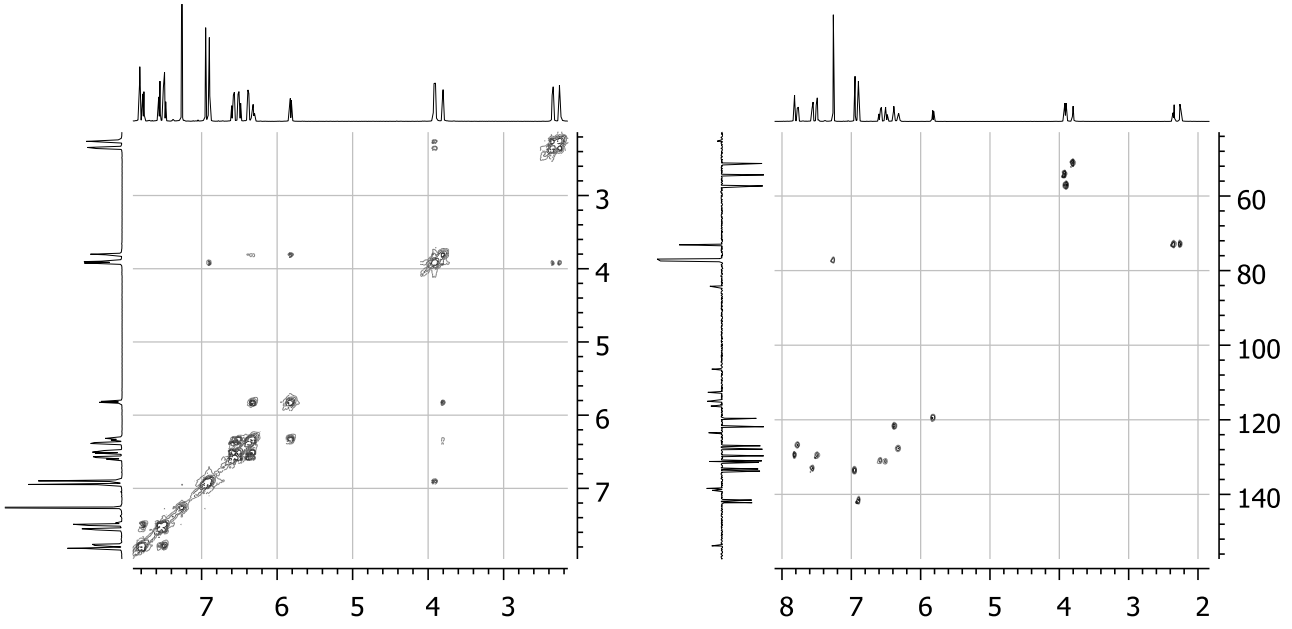

Figure S15: COSY (left) and (right) ^{1}H / ^{13}C-APT HSQC spectra of $\mathbf{5b_{NBD\text{-}DHA}}$ in $CDCl_3$ (500 / 126 MHz).

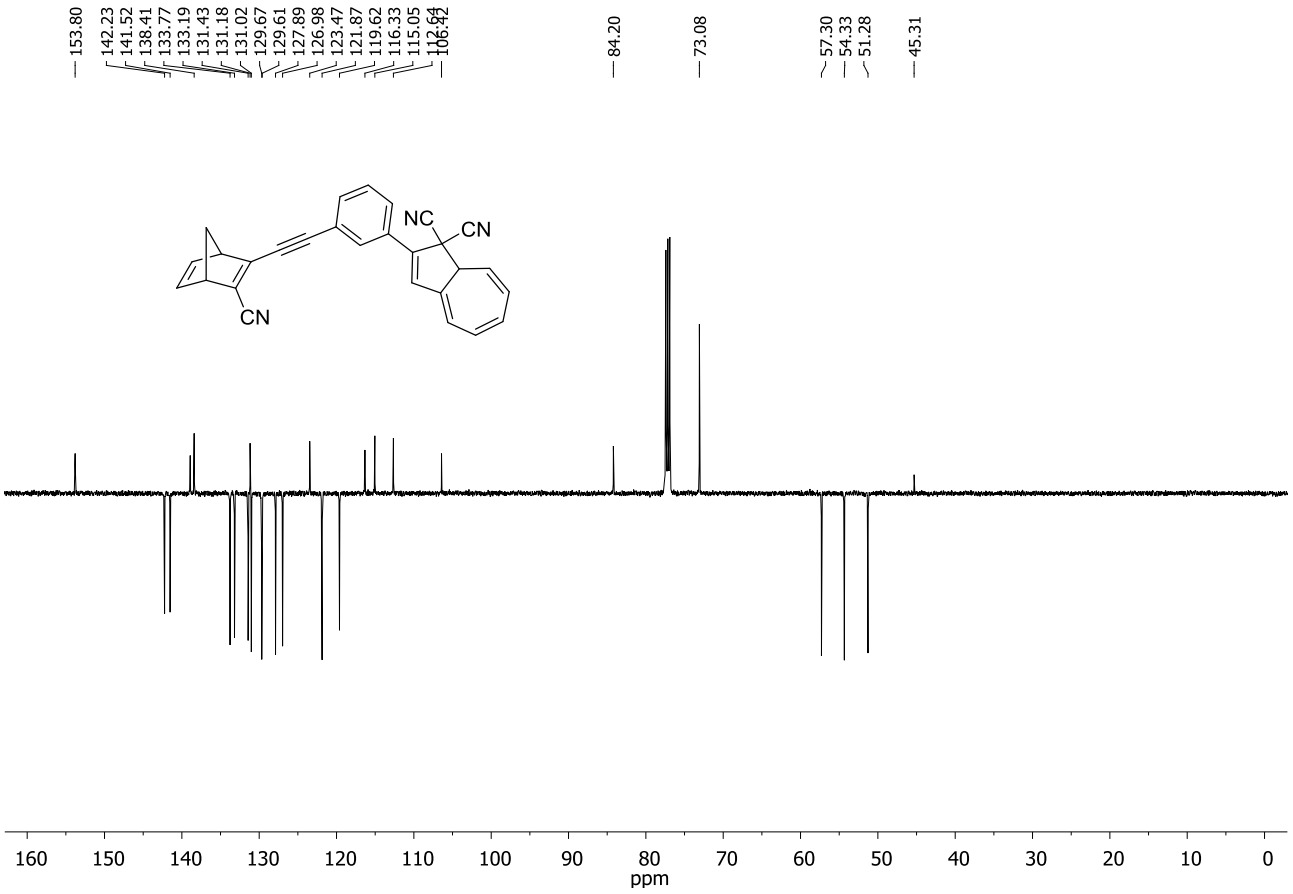

Figure S16: ^{13}C-APT spectrum of **5b$_{NBD-DHA}$** in $CDCl_3$ (126 MHz).

Compound 6

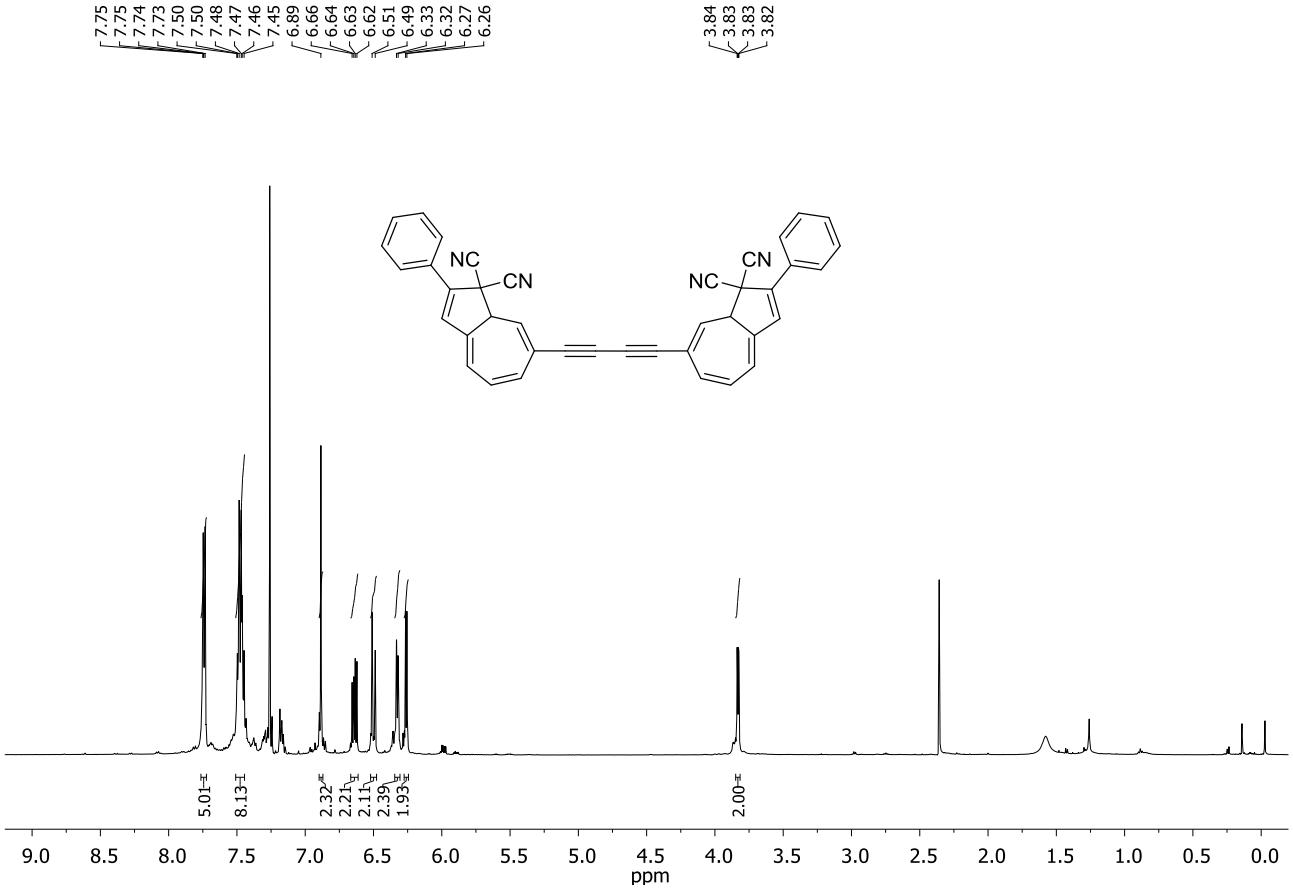

Figure S17: ^{1}H NMR spectrum of **6** in $CDCl_3$.

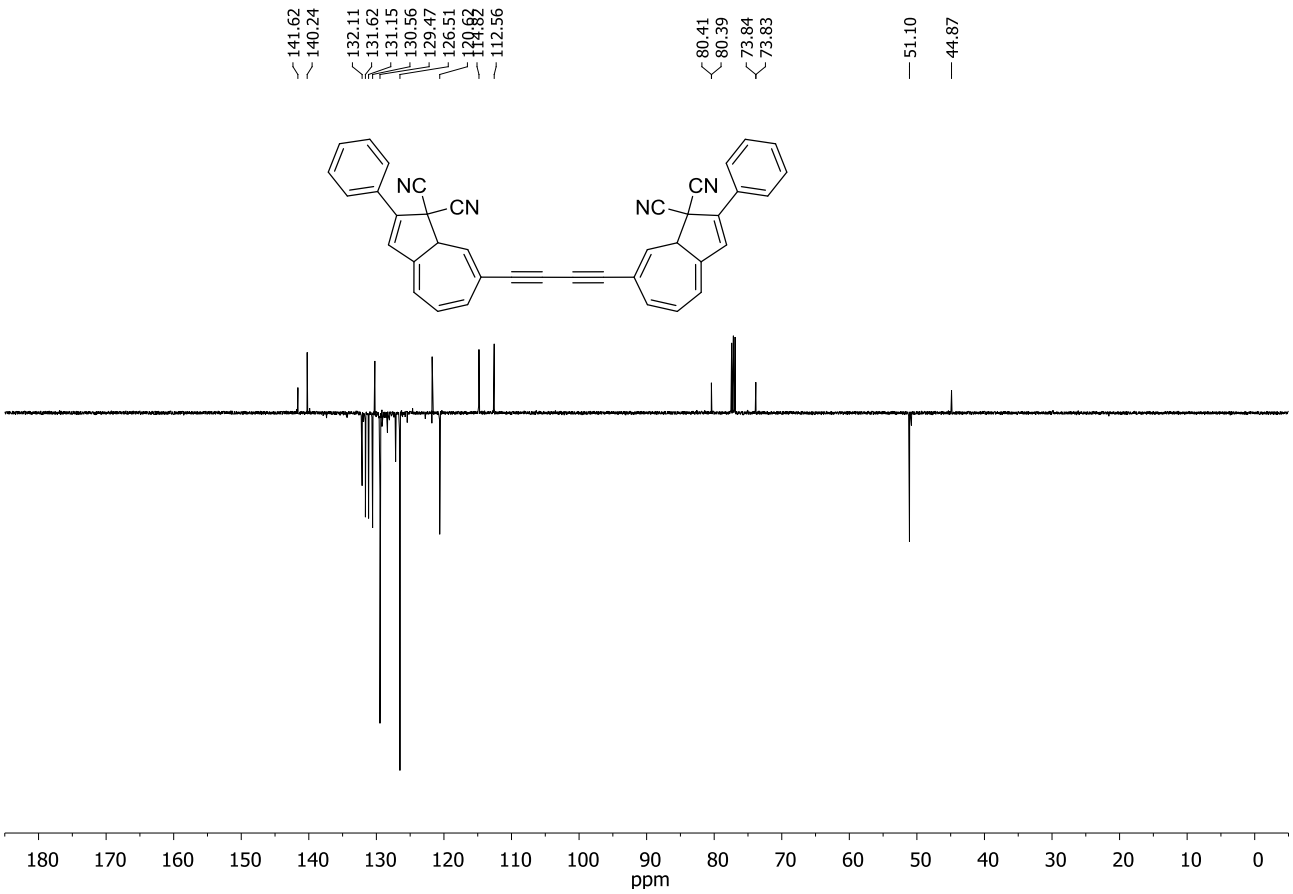

Figure S18: ^{13}C-APT NMR spectrum of **6** in $CDCl_3$.

Compound 7

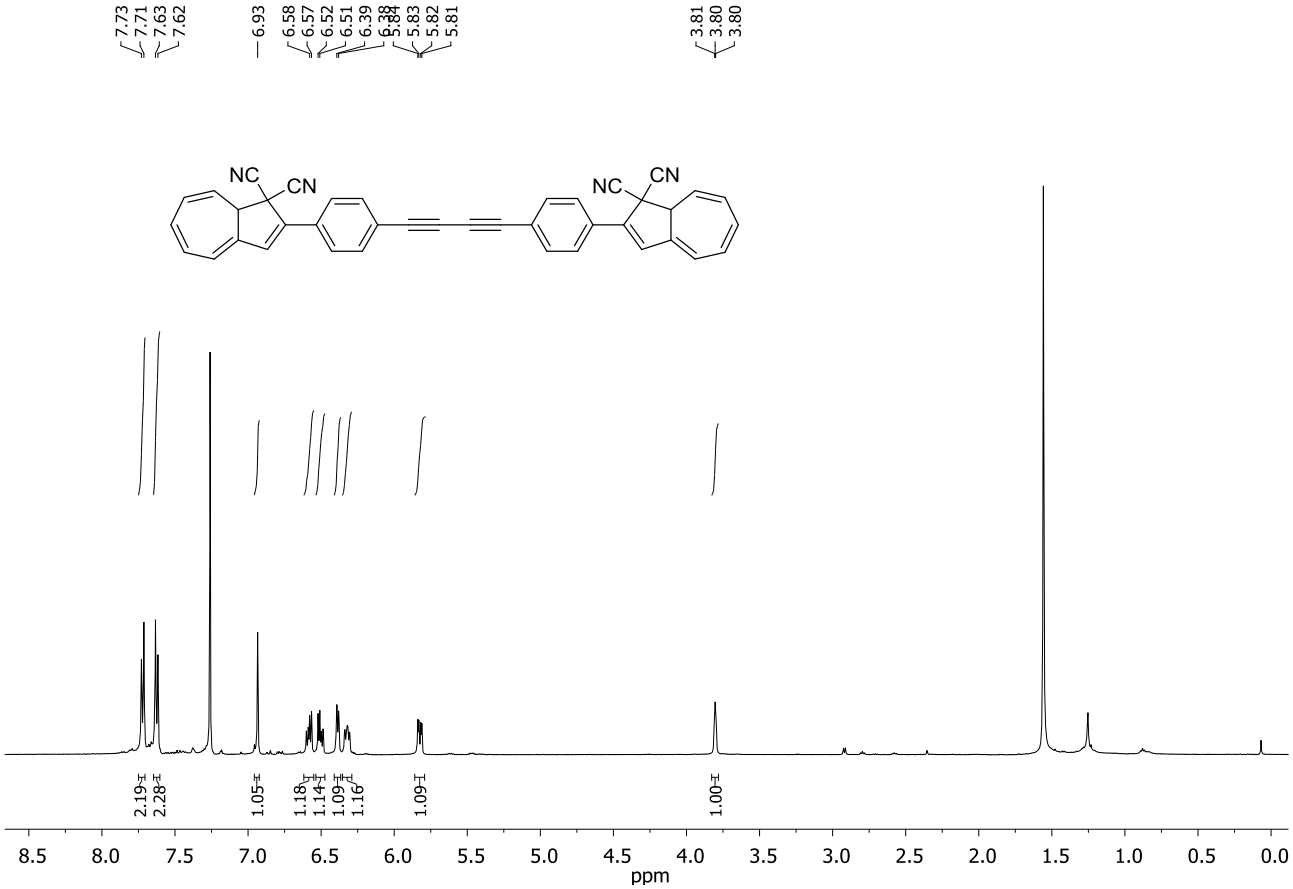

Figure S19: ^{1}H NMR spectrum of **7** in $CDCl_3$ (500 MHz).

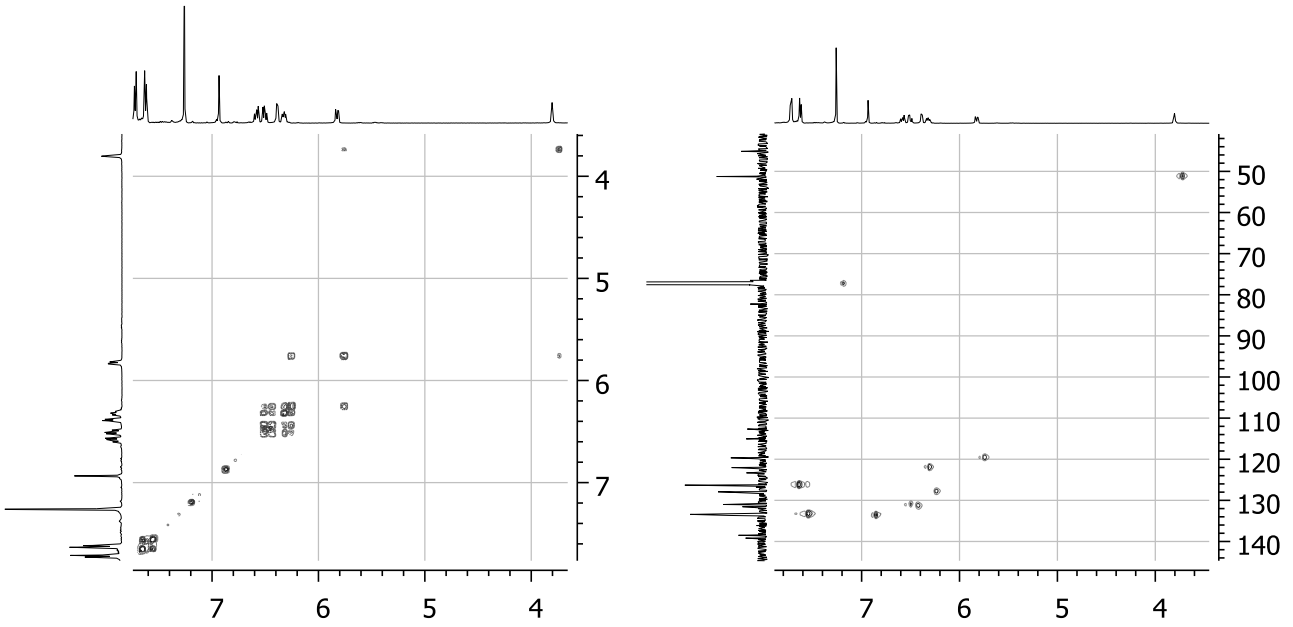

Figure S20: COSY (left) and (right) ^{1}H / ^{13}C HSQC spectra of **7** in $CDCl_3$ (500 / 126 MHz).

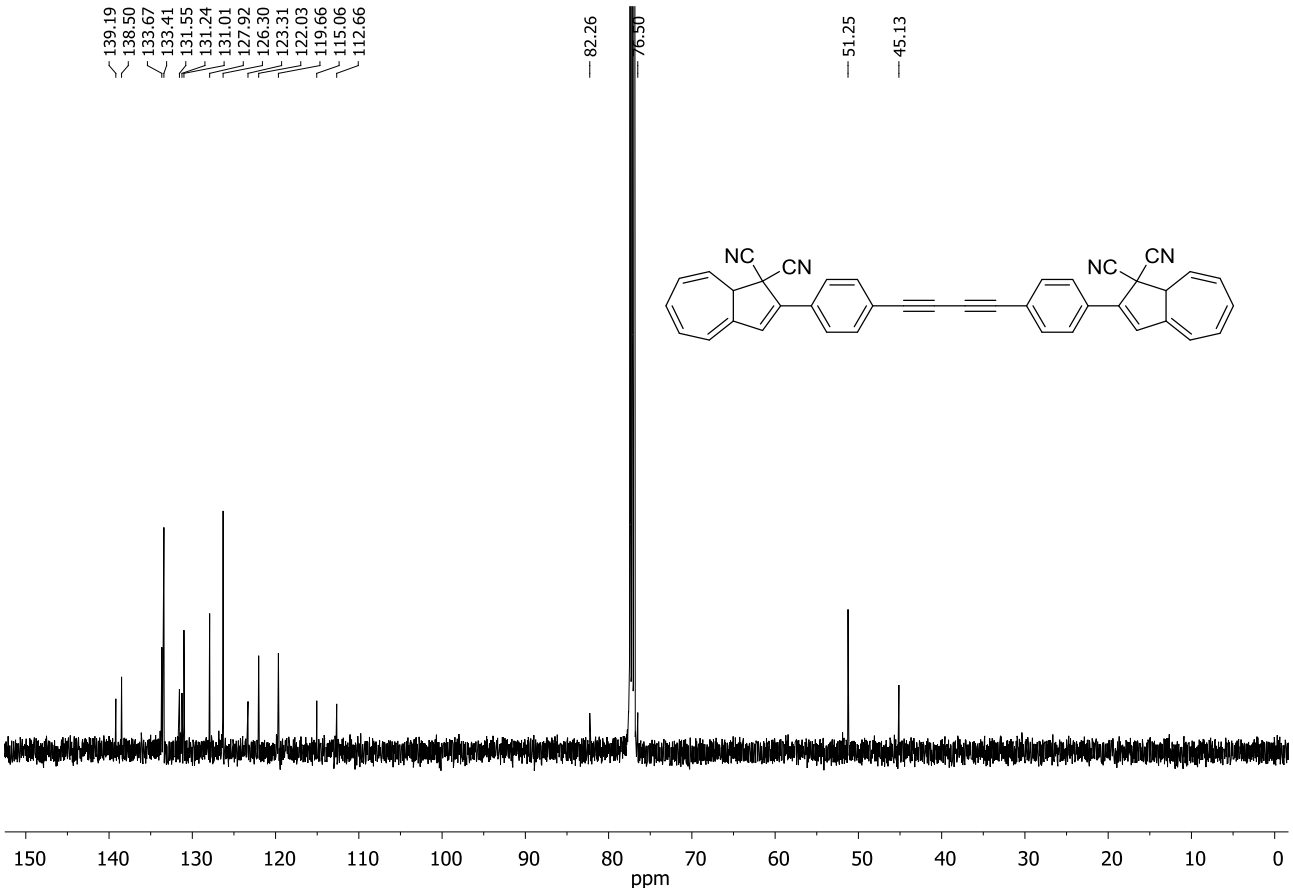

Figure S21: ^{13}C spectrum of **7** in $CDCl_3$ (126 MHz).

Compound 8

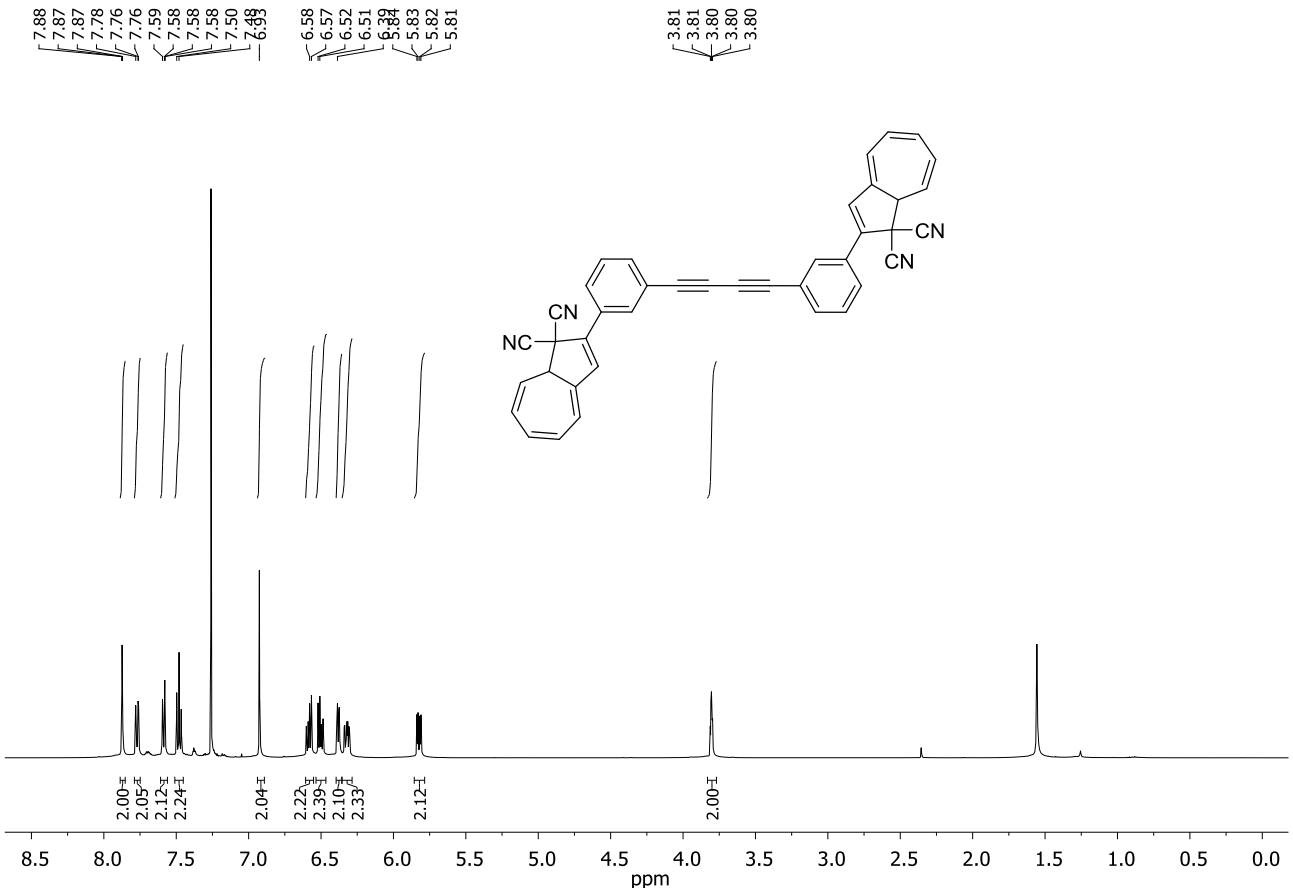

Figure S22: ^{1}H NMR spectrum of **8** in $CDCl_3$ (500 MHz).

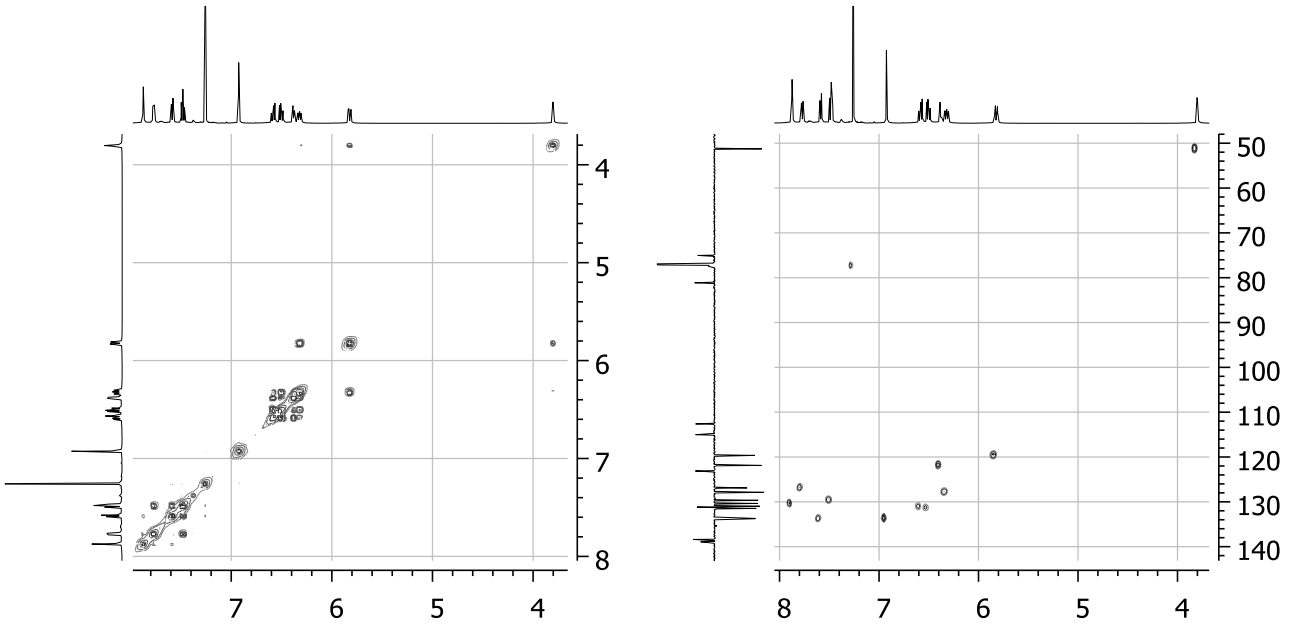

Figure S23: COSY (left) and (right) ^{1}H / ^{13}C-APT HSQC spectra of **8** in $CDCl_3$ (500 / 126 MHz).

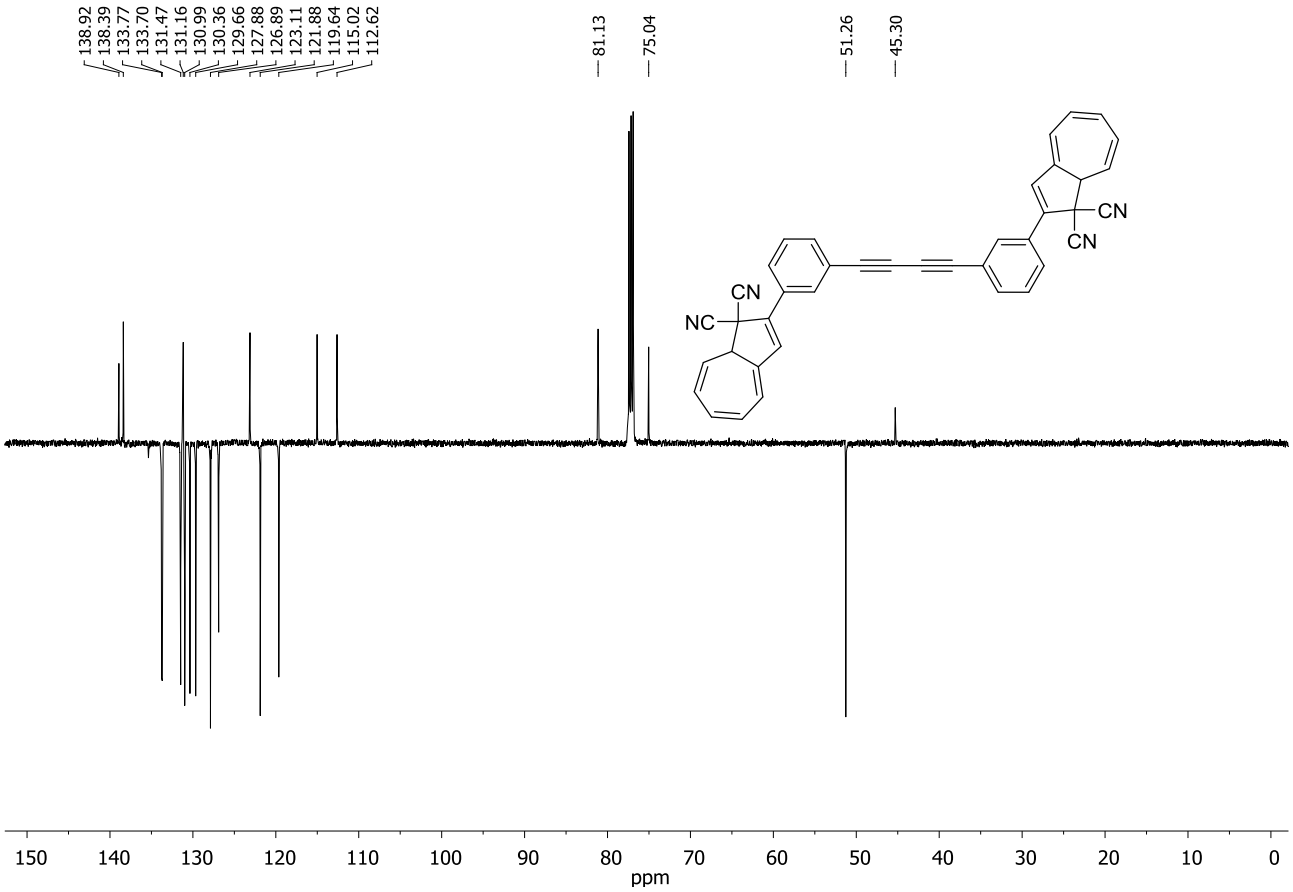

Figure S24: ^{13}C-APT spectrum of **8** in $CDCl_3$ (126 MHz).

^{1}H-NMR spectroscopy and switching studies in toluene-d_8

DHA 1a + NBD 9 to VHF 1a + NBD 9

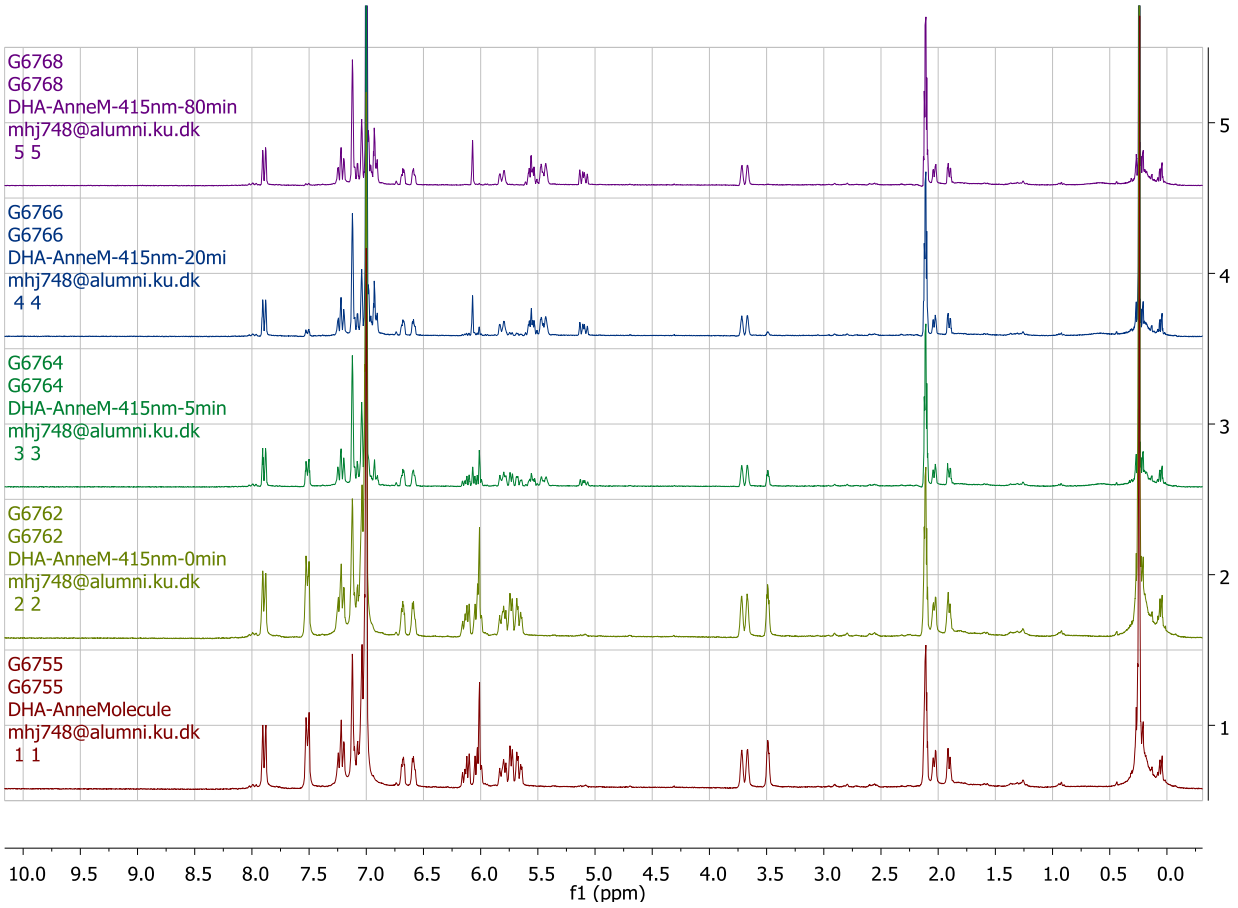

Figure S25: Stacked spectra of the gradual light irradiation (415 nm) of a mixture of DHA **1a** and NBD **9** in *d*-toluene. Bottom spectrum 1): 0 min irradiation DHA **1a** + NBD **9**. Top spectrum 5): 80 min irradiation (415) resulting in VHF **1a** + NBD **9**. The signal at 3.49 ppm is assigned to DHA H*8a*.

VHF 1a + NBD 9 to VHF 1a + QC 9

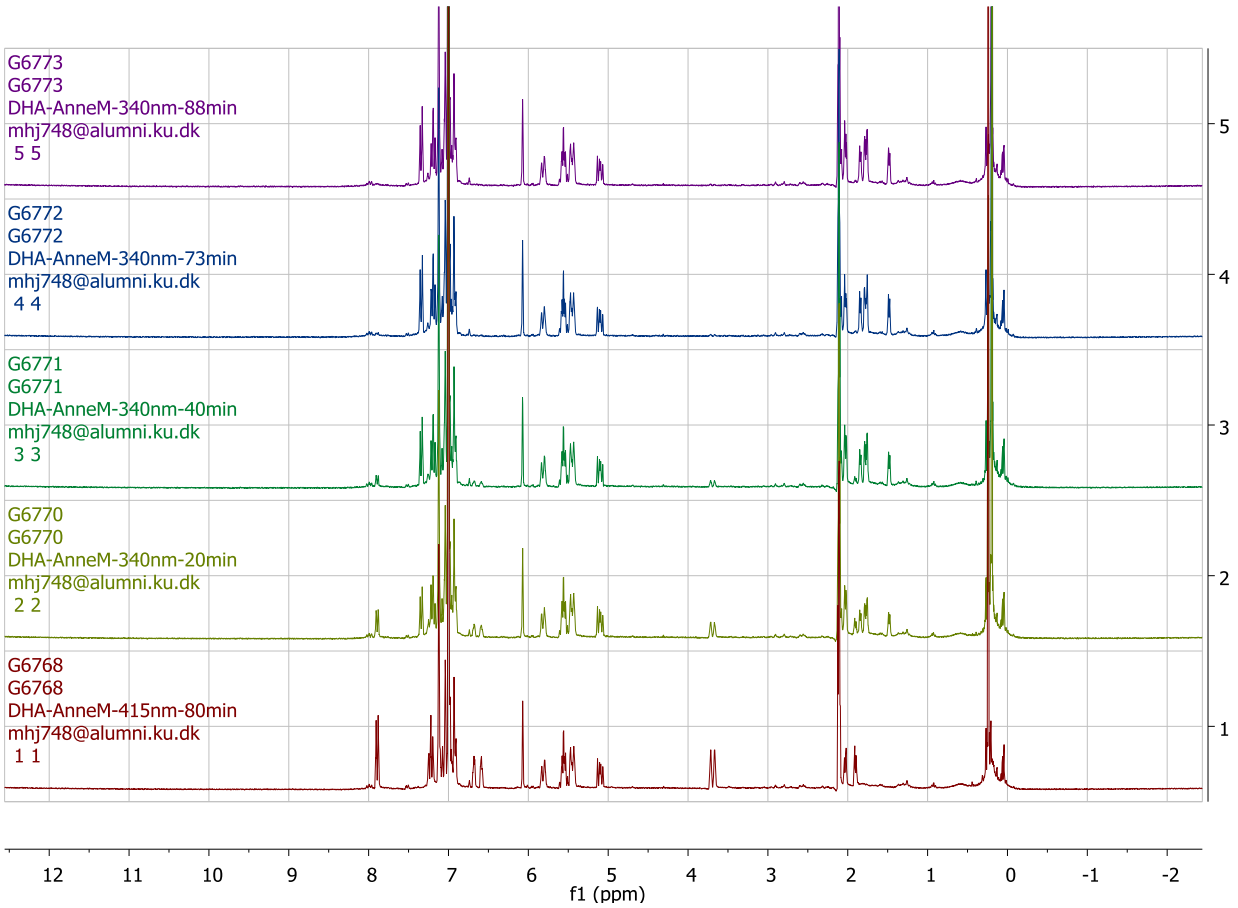

Figure S26: Stacked spectra of the gradual light irradiation (340 nm) of a mixture of VHF **1a** and NBD **9** in *d*-toluene. Bottom spectrum 1): 0 min irradiation VHF **1a** + NBD **9**. Top spectrum 5): 88 min irradiation (340) resulting in VHF **1a** + QC **9**.

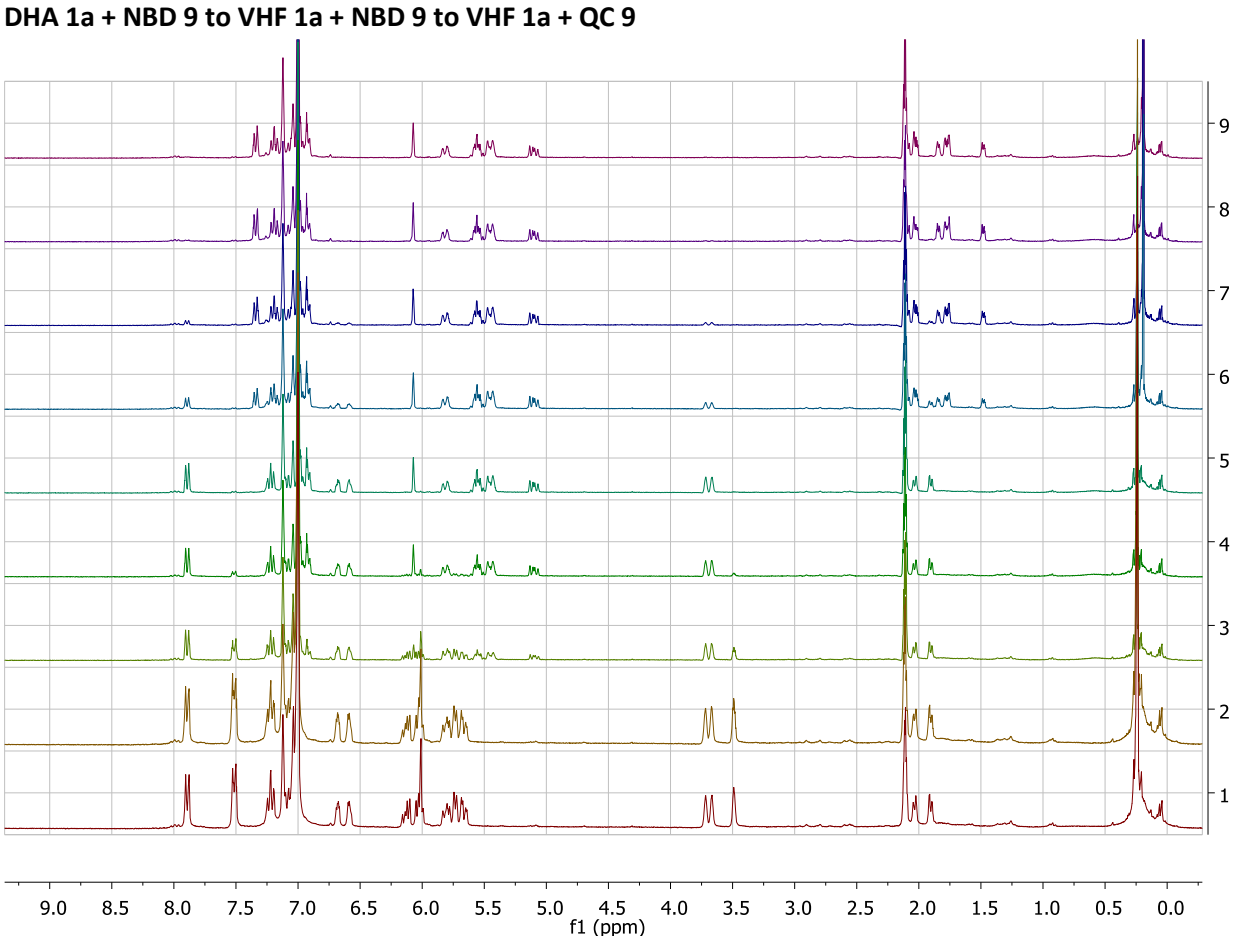

Figure S27: Stacked spectra of the gradual light irradiation (415 nm) of a mixture of DHA **1a** and NBD **9** in *d*-toluene followed by light irradiation (340 nm) of a mixture of VHF **1a** and NBD **9**.

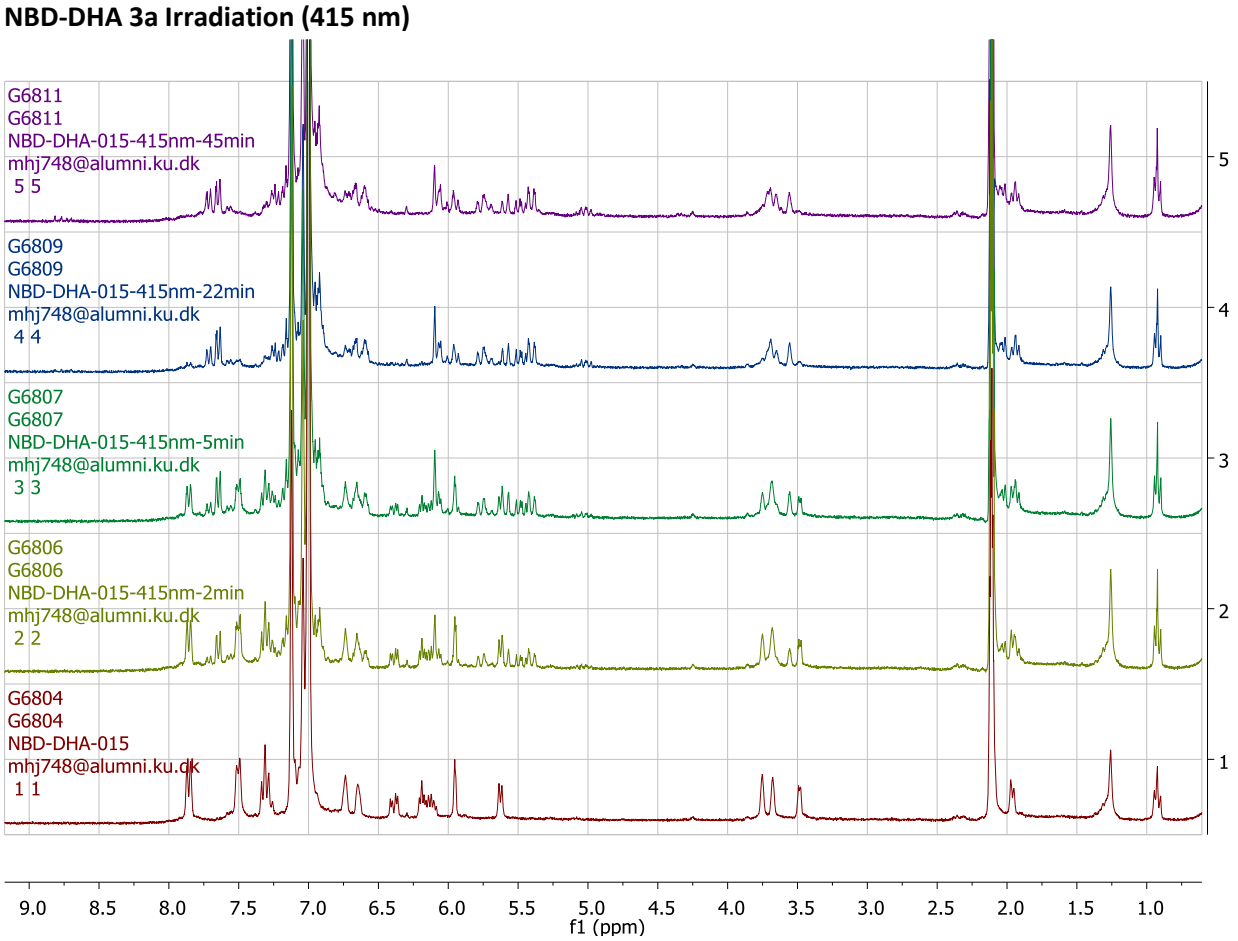

Figure S28: Stacked ^{1}H-NMR spectra of the gradual light irradiation (415 nm) of NBD-DHA **3a**. Bottom spectrum 1): 0 min irradiation of NBD-DHA **3a**. Top spectrum 5): 45min min irradiation (415 nm) resulting in NBD-VHF **3a**. The signal at 3.49 ppm is assigned to DHA H*8a*.

NBD-VHF 3a Irradiation (340 nm)

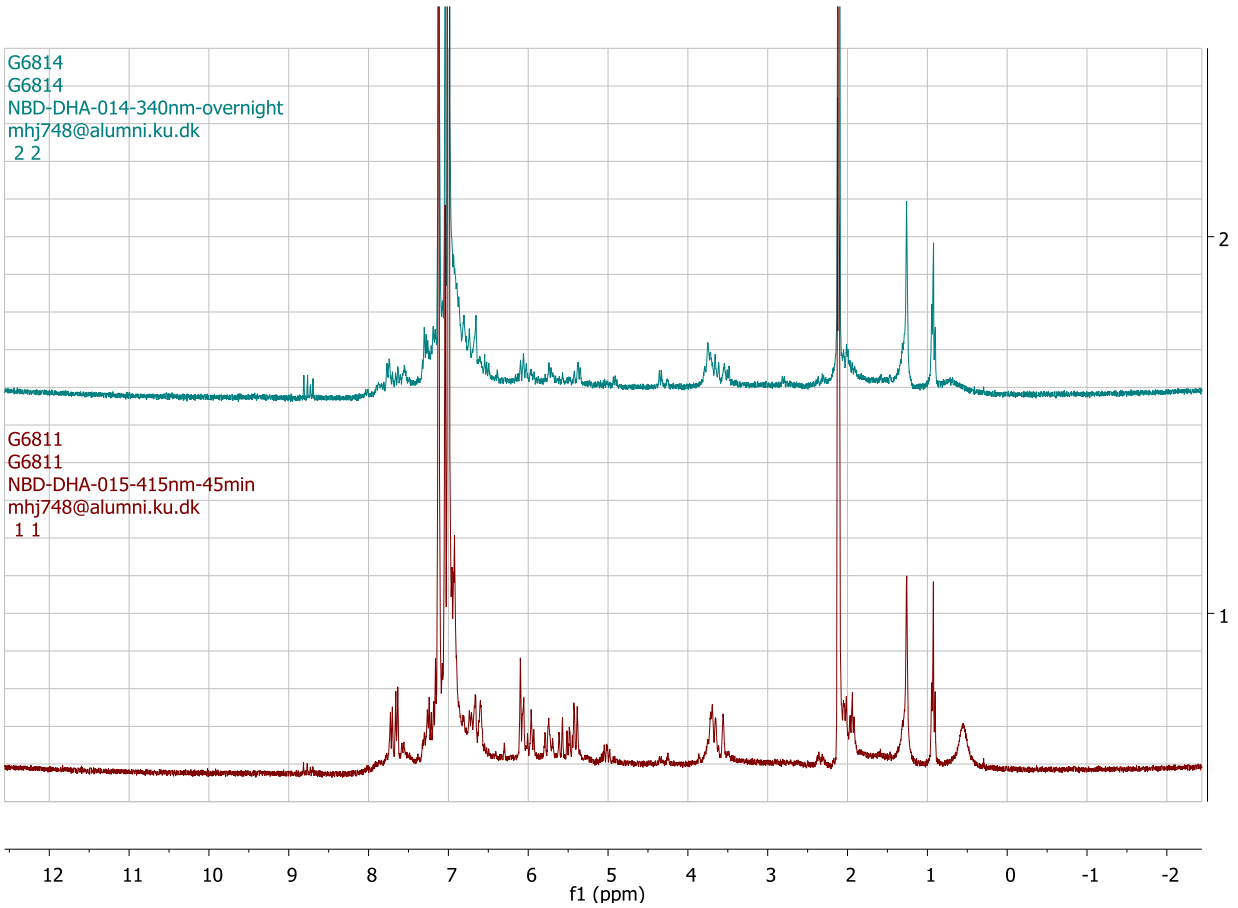

Figure S29: Stacked ^{1}H-NMR spectra of the light irradiation (340 nm) of NBD-VHF **3a** resulting in photochemical degradation. Bottom spectrum 1): 0 min irradiation of NBD-VHF **3a**. Top spectrum 5): Overnight irradiation (340 nm) of NBD-VHF **3a**.

NBD-DHA 3b Irradiation (415 nm)

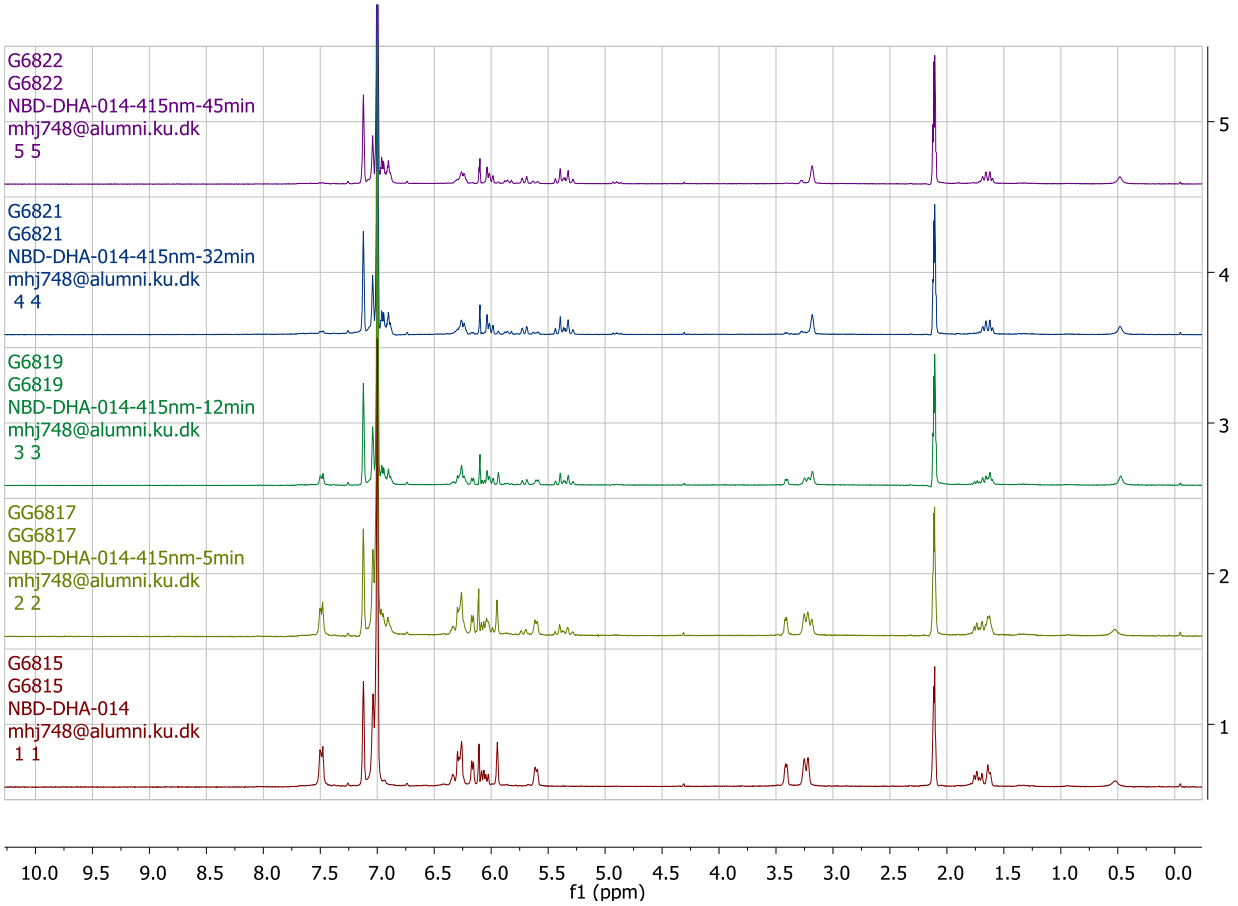

Figure S30: Stacked ^{1}H-NMR spectra of the gradual light irradiation (415 nm) of NBD-DHA **3b**. Bottom spectrum 1): 0 min irradiation of NBD-DHA **3b**. Top spectrum 5): 45min min irradiation (415 nm) resulting in NBD-VHF **3b**. The signal at 3.41 ppm is assigned to DHA H*8a*.

NBD-VHF 3b Irradiation (340 nm)

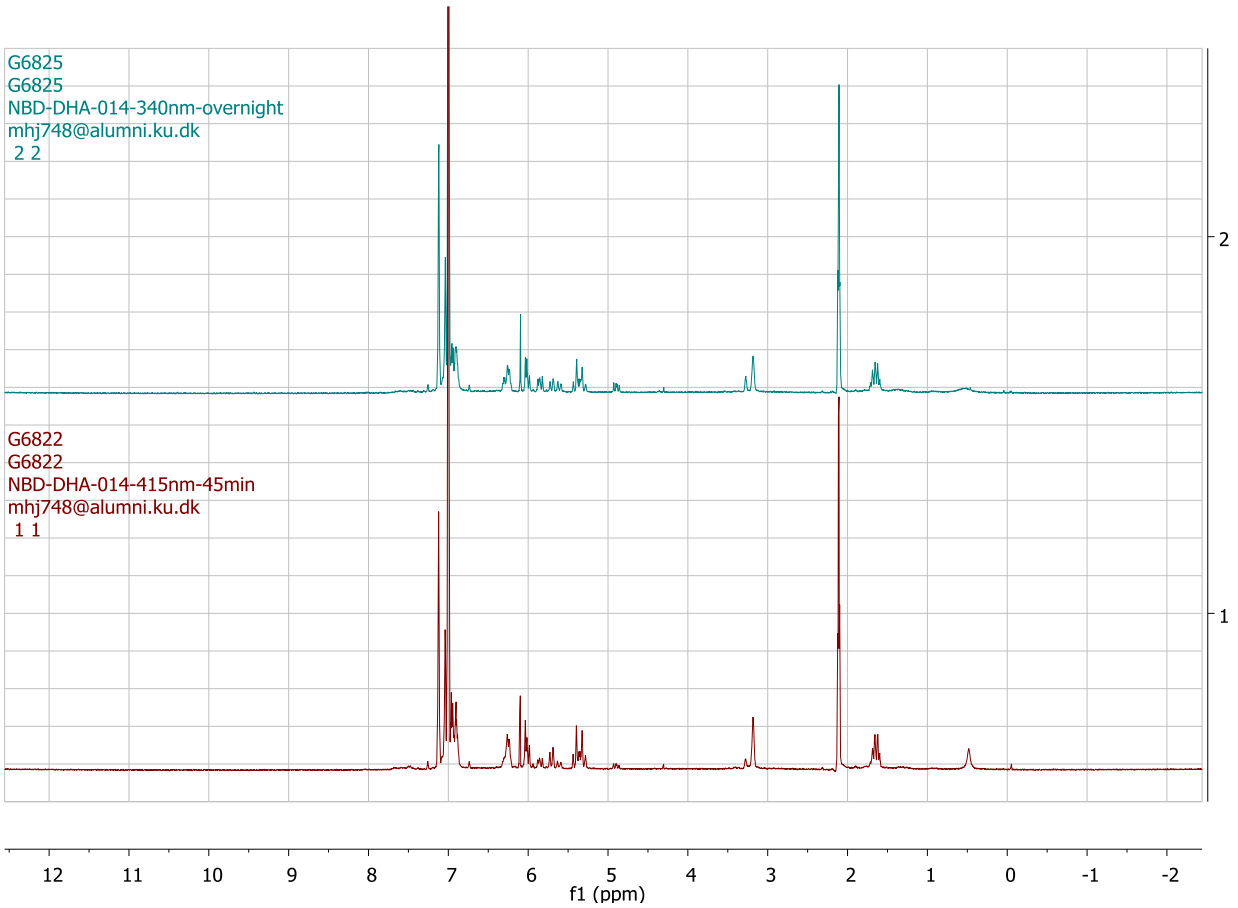

Figure S31: Stacked ^{1}H-NMR spectra of the light irradiation (340 nm) of NBD-VHF **3a** resulting in no photochemical conversion. Bottom spectrum 1): 0 min irradiation of NBD-VHF **3a**. Top spectrum 5): Overnight irradiation (340 nm).

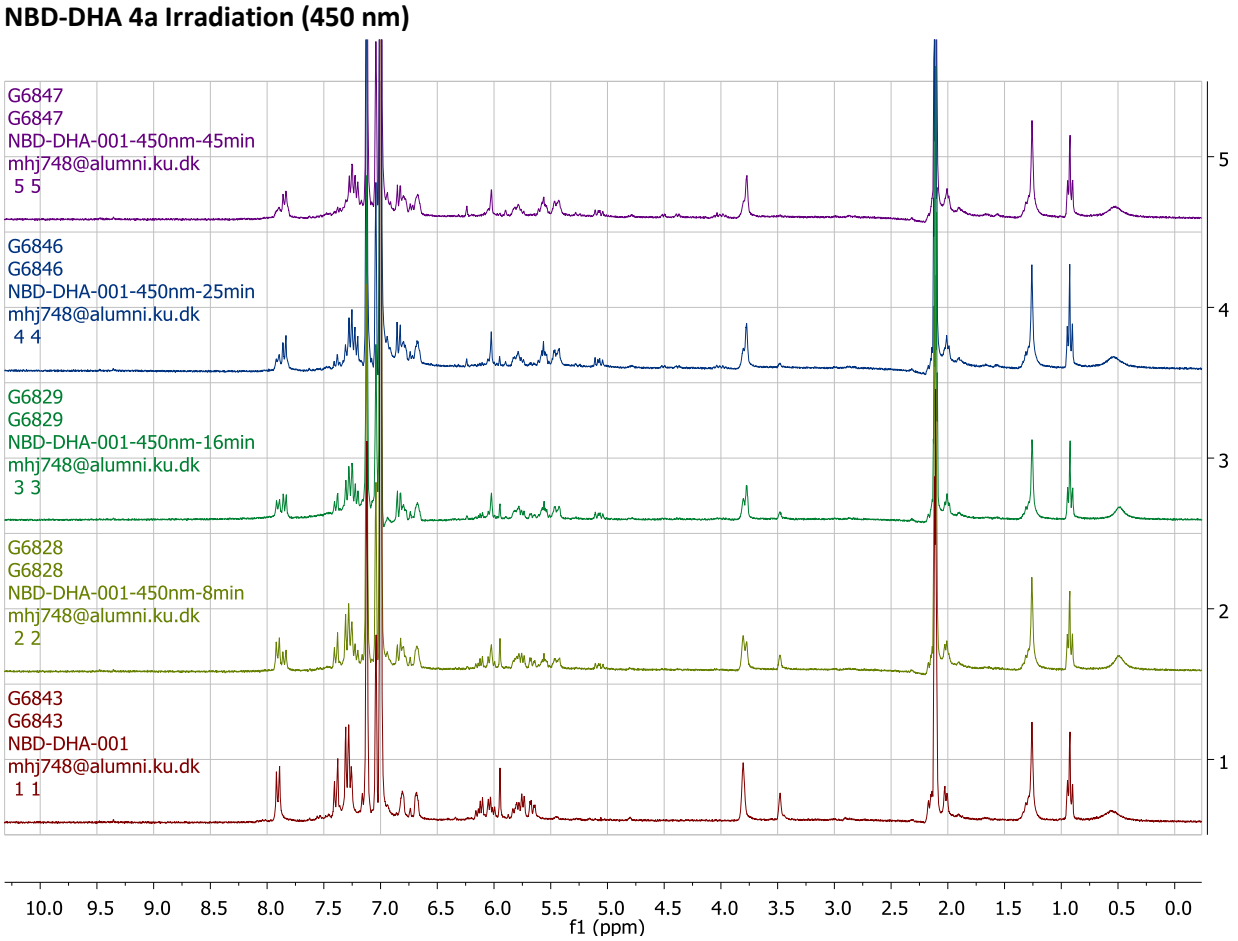

Figure S32: Stacked ^{1}H-NMR spectra of the gradual light irradiation (450 nm) of NBD-DHA **4a**. Bottom spectrum 1): 0 min irradiation of NBD-DHA **4a**. Top spectrum 5): 45min min irradiation (450 nm) resulting in NBD-VHF **4a**. The signal at 3.48 ppm is assigned to DHA H*8a*.

NBD-DHA 4a Irradiation (340 nm)

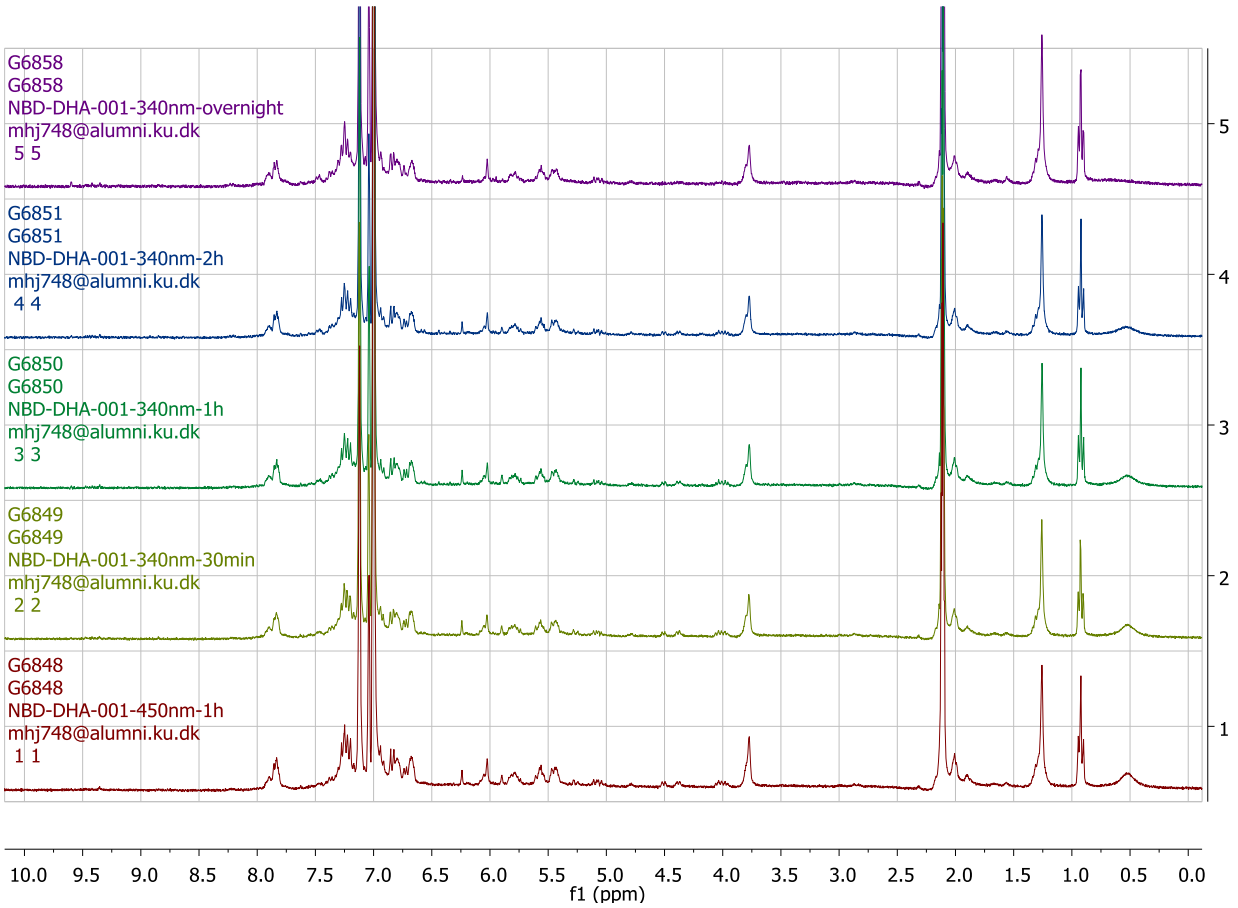

Figure S33: Stacked ^{1}H-NMR spectra of the light irradiation (340 nm) of NBD-VHF **4a** resulting in no photochemical conversion. Bottom spectrum 1): 0 min irradiation of NBD-VHF **4a**. Top spectrum 5): Overnight irradiation (340 nm).

NBD-DHA 4b Irradiation (450 nm)

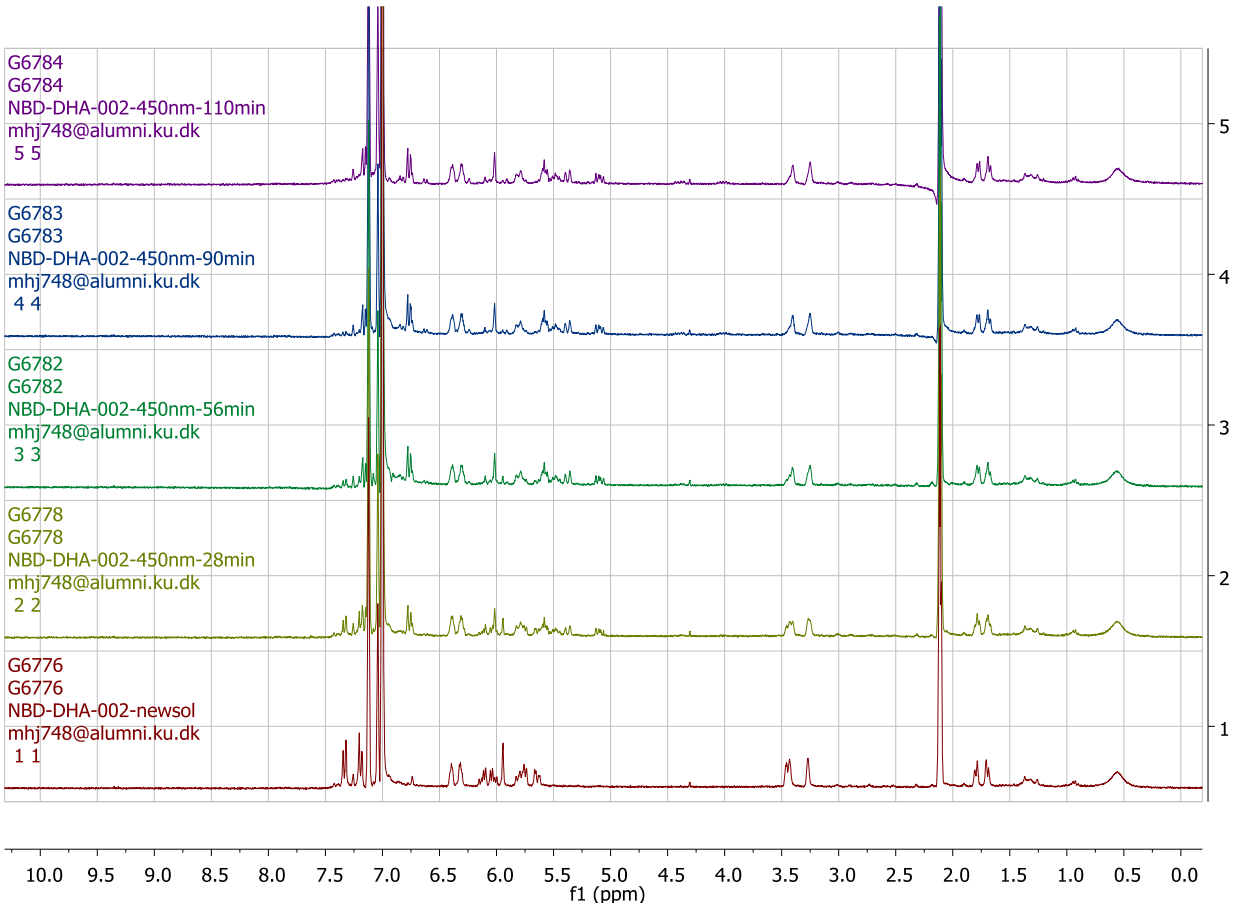

Figure S34: Stacked ^{1}H-NMR spectra of the gradual light irradiation (450 nm) of NBD-DHA **4b**. Bottom spectrum 1): 0 min irradiation of NBD-DHA **4b**. Top spectrum 5): 110 min irradiation (450 nm) resulting in NBD-VHF **4b**. The signal at 3.27 ppm is assigned to DHA H*8a*.

NBD-VHF 4b Irradiation (340 nm)

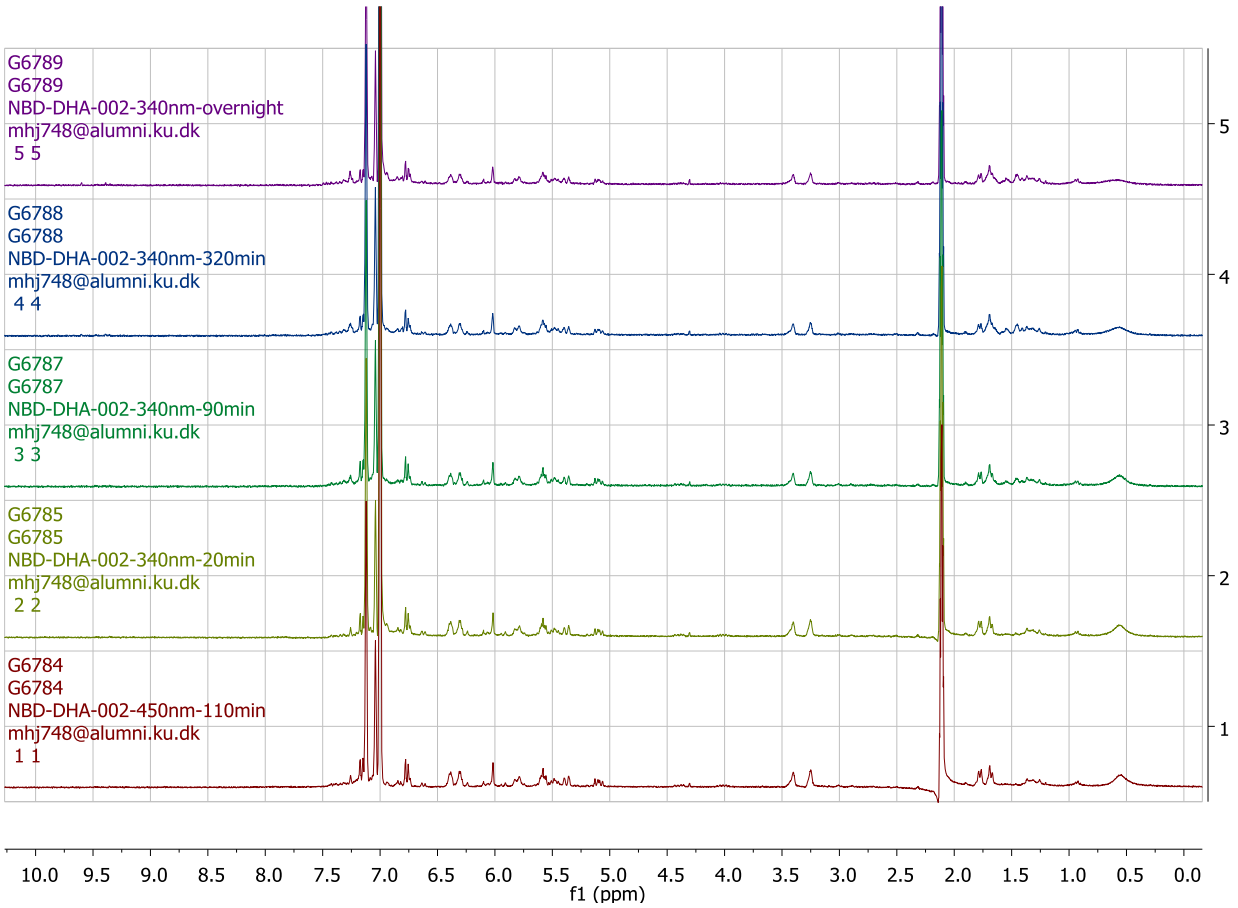

Figure S35: Stacked ^{1}H-NMR spectra of the gradual light irradiation (340 nm) of NBD-VHF **4b** resulting in no photochemical conversion. Bottom spectrum 1): 0 min irradiation of NBD-VHF **4b**. Top spectrum 5): Overnight irradiation (340 nm).

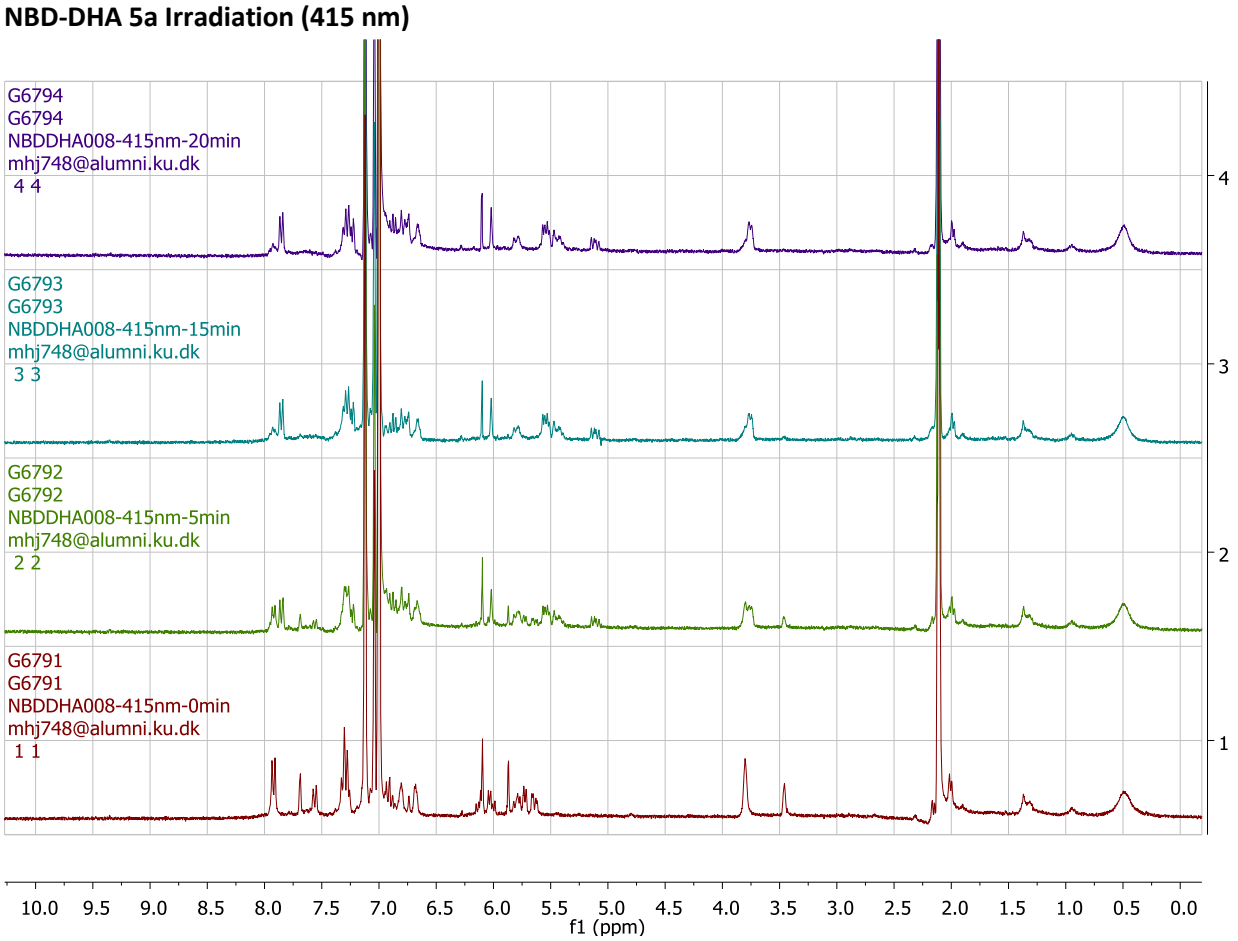

Figure S36: Stacked ^{1}H-NMR spectra of the gradual light irradiation (415 nm) of NBD-DHA **5a**. Bottom spectrum 1): 0 min irradiation of NBD-DHA **5a**. Top spectrum 5): 20 min irradiation (415 nm) resulting in NBD-VHF **5a**. The signal at 3.46 ppm is assigned to DHA H*8a*.

NBD-VHF 5a Irradiation (340 nm)

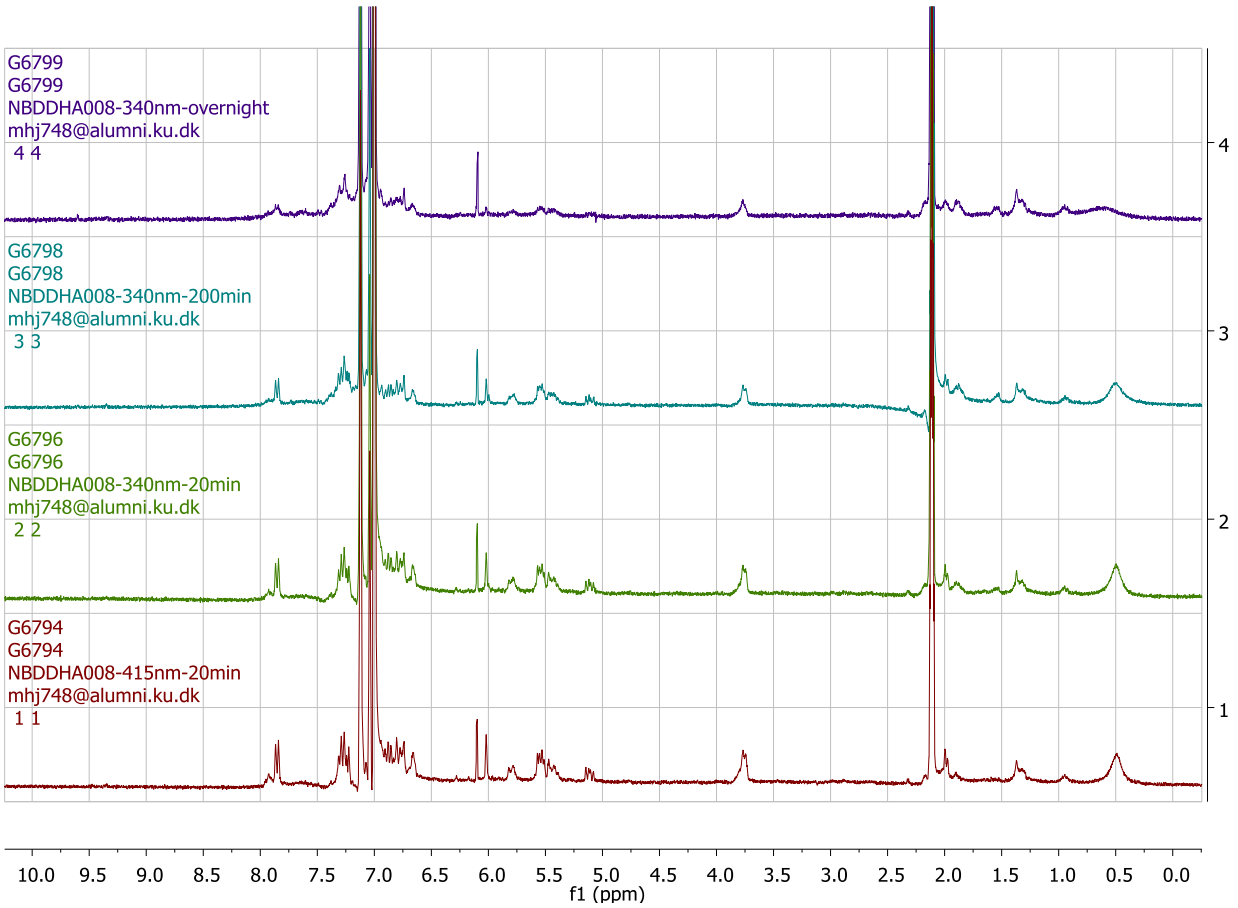

Figure S37: Stacked ^{1}H-NMR spectra of the gradual light irradiation (340 nm) of NBD-VHF **5a** resulting in photochemical degradation. Bottom spectrum 1): 0 min irradiation of NBD-VHF **5a**. Top spectrum 5): Overnight irradiation (340 nm).

NBD-VHF 5b Irradiation (415 nm)

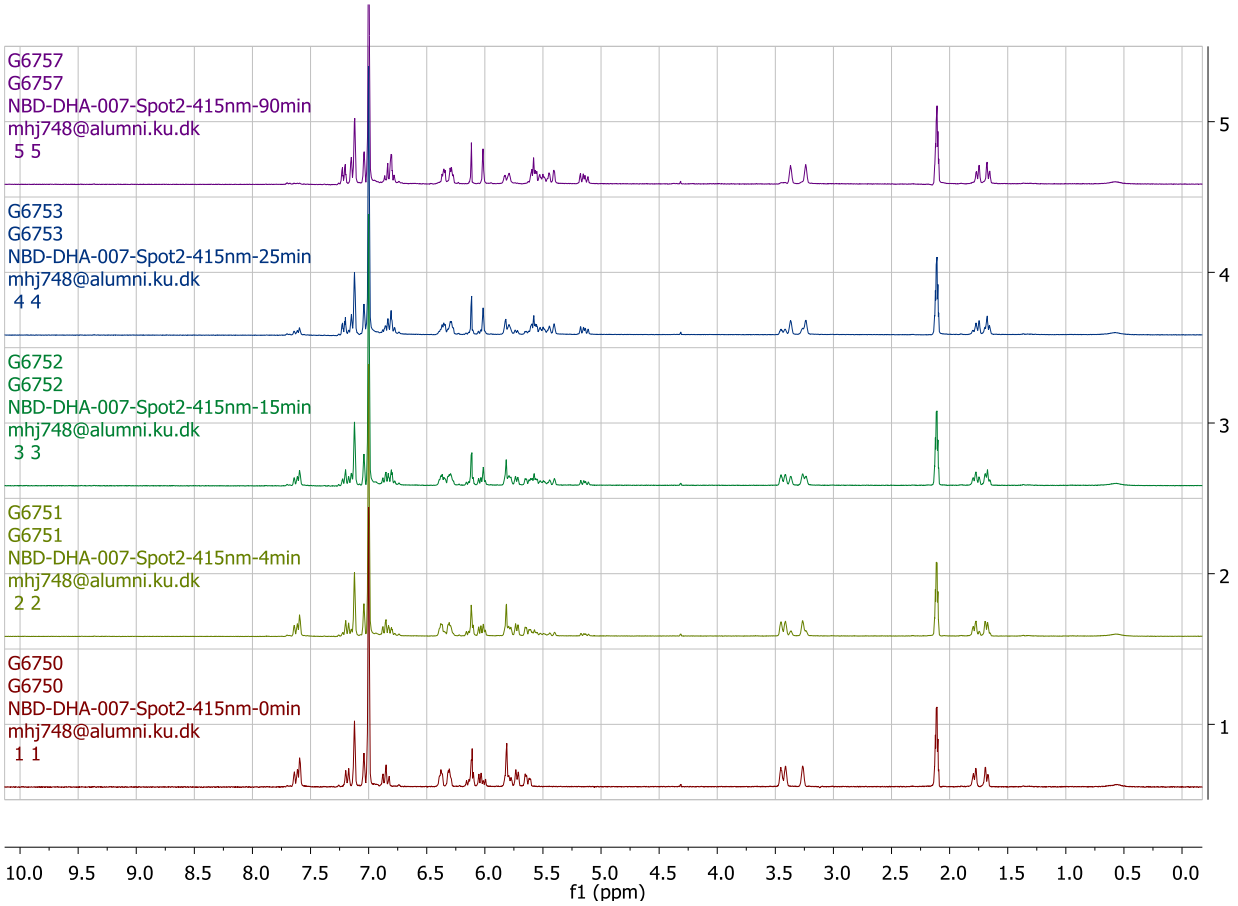

Figure S38: Stacked ^{1}H-NMR spectra of the gradual light irradiation (415 nm) of NBD-DHA **5b**. Bottom spectrum 1): 0 min irradiation of NBD-DHA **5b**. Top spectrum 5): 90 min irradiation (415 nm) resulting in NBD-VHF **5b**. The signal at 3.26 ppm is assigned to DHA H*8a*.

NBD-VHF 5b Irradiation (340 nm)

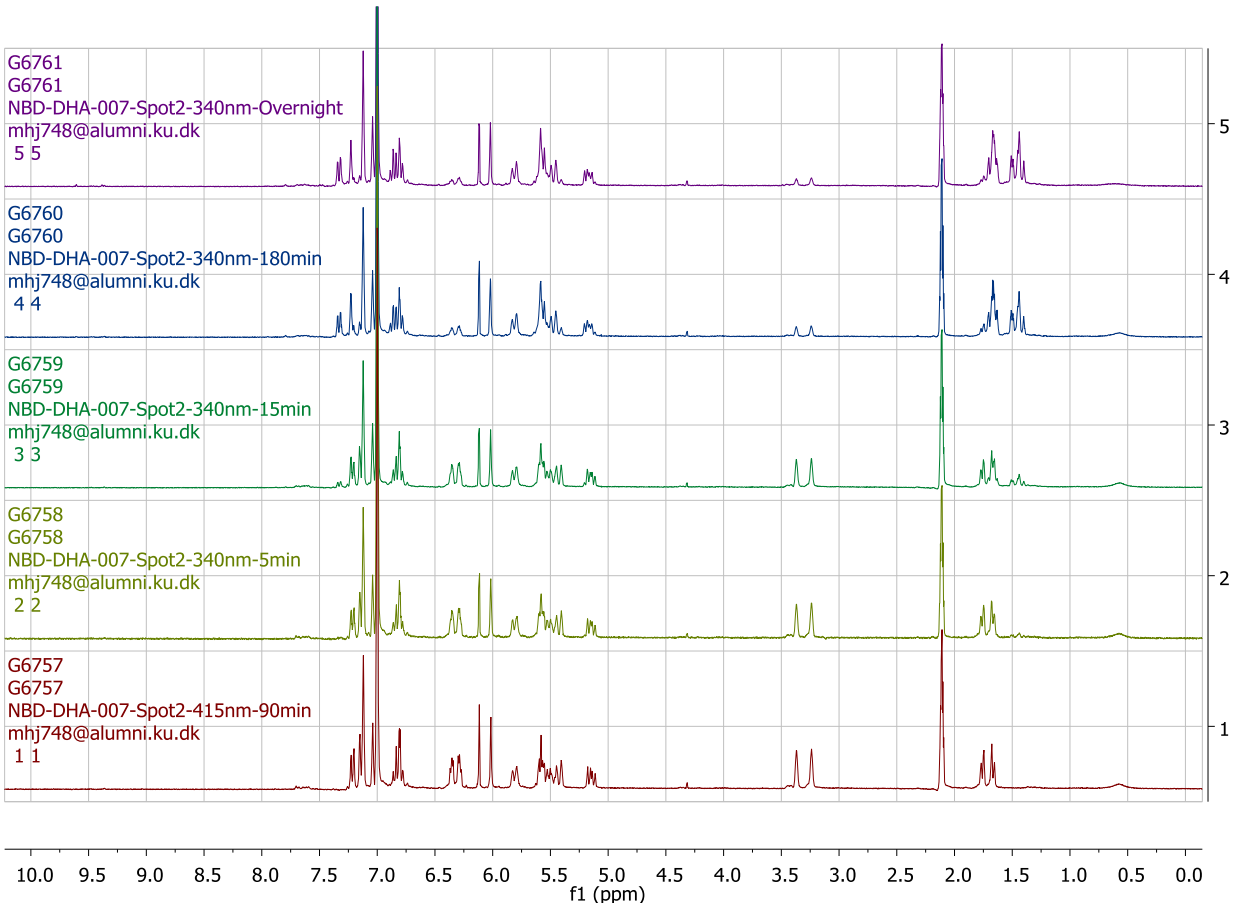

Figure S39: Stacked ^{1}H-NMR spectra of the gradual light irradiation (340 nm) of NBD-VHF **5b** resulting in around 70% photochemical conversion to QC-VHF **5b**. Bottom spectrum 1): 0 min irradiation of NBD-VHF **5b**. Top spectrum 5): Overnight irradiation (340 nm).

UV-Vis absorption spectroscopy and switching studies in toluene

Compound 3a

$3a_{NBD\text{-}DHA}$/$3a_{NBD\text{-}VHF}$ and photodegradation of $3a_{NBD\text{-}VHF}$

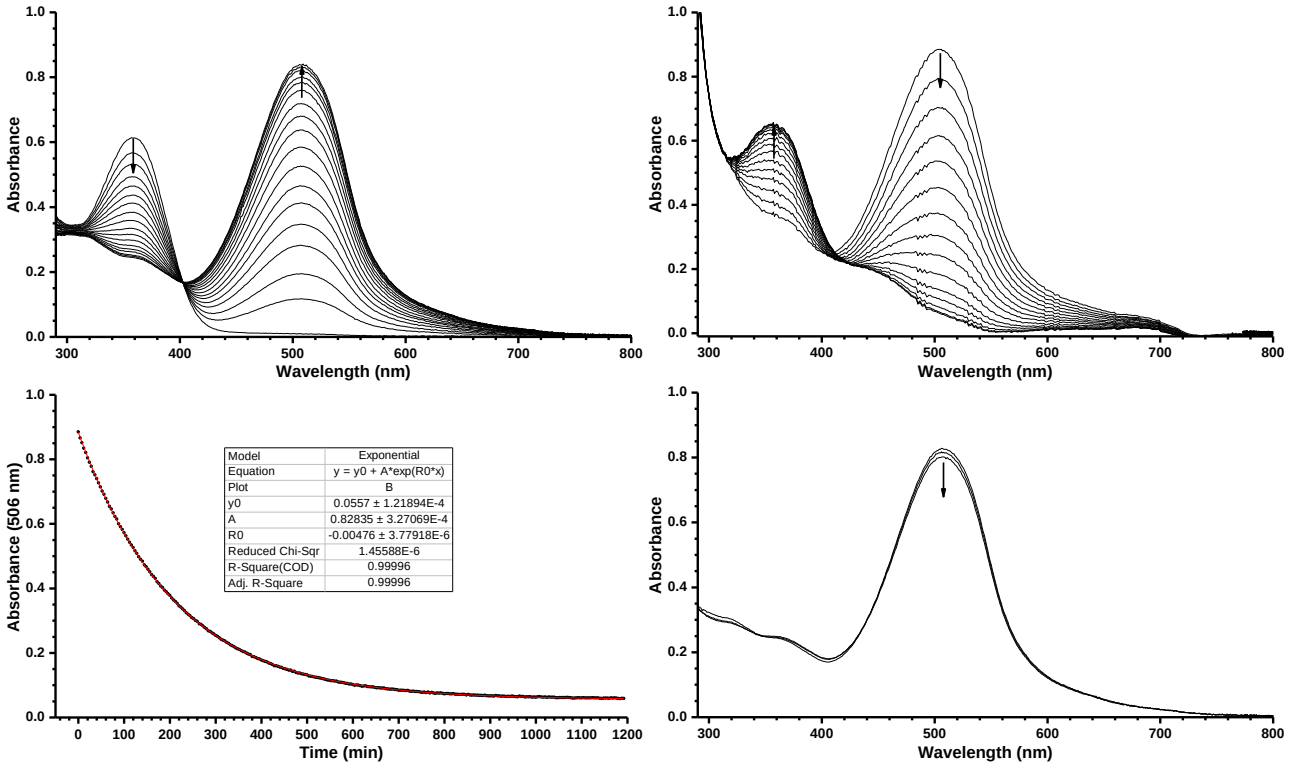

Figure S40: Top left: Light irradiation (400 nm) of **$3a_{NBD\text{-}DHA}$** in toluene. Top right: Thermal back-reaction of **$3a_{NBD\text{-}VHF}$** in toluene at 50 °C. Bottom left: Exponential decay at 506 nm of **$3a_{NBD\text{-}VHF}$** to **$3a_{NBD\text{-}DHA}$** in toluene at 50 °C. Bottom right: Light irradiation (360 nm) of **$3a_{NBD\text{-}VHF}$** in toluene at 25 °C.

Compound 3b

$3b_{NBD-DHA}$/$3b_{NBD-VHF}$ and photodegradation of $3b_{NBD-VHF}$

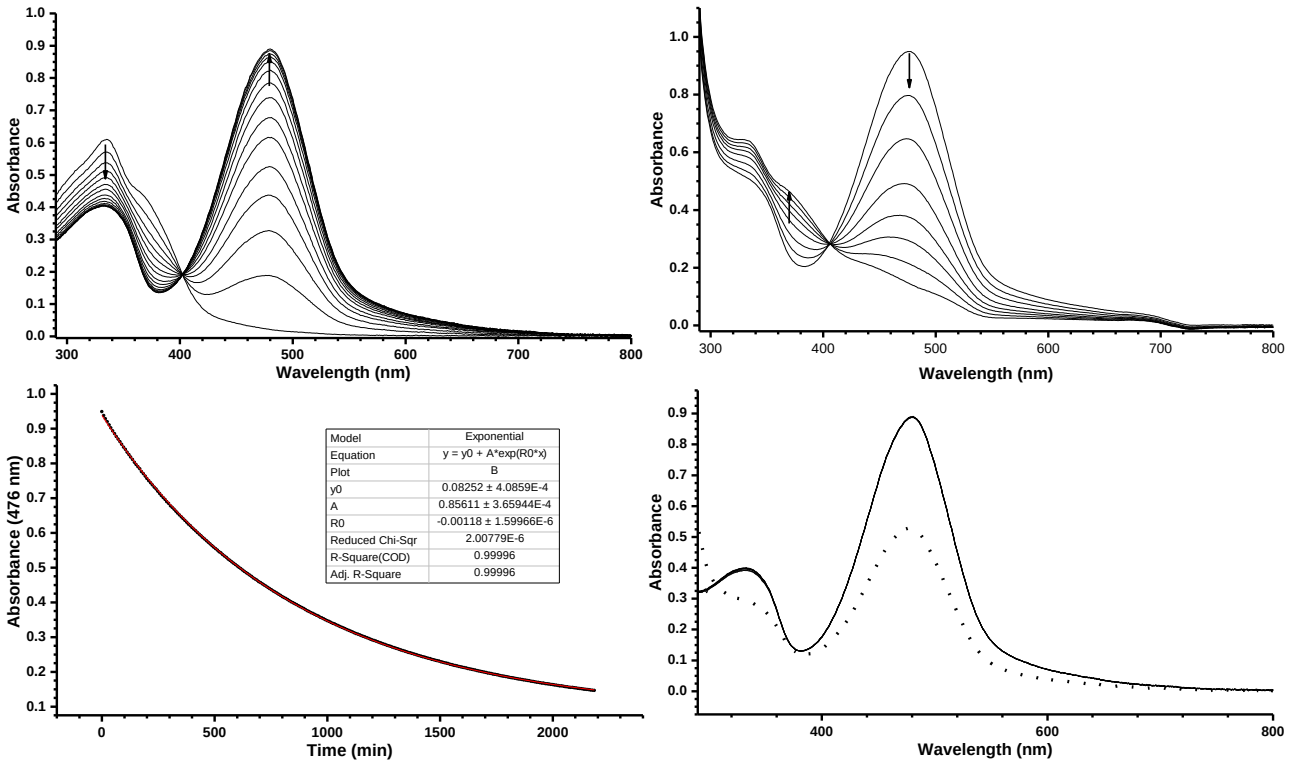

Figure S41: Top left: Light irradiation (400 nm) of **$3b_{NBD-DHA}$** in toluene. Top right: Thermal back-reaction of **$3b_{NBD-VHF}$** in toluene at 50 °C. Bottom left: Exponential decay at 476 nm of **$3b_{NBD-VHF}$** to **$3b_{NBD-DHA}$** in toluene at 50 °C. Bottom right: Light irradiation (360 nm) of **$3b_{NBD-VHF}$** in toluene at 25 °C (dotted line represents light irradiation at 360 nm after 23 h).

$3b_{NBD-DHA}$/$3b_{NBD-VHF}$ photo/thermal cycles

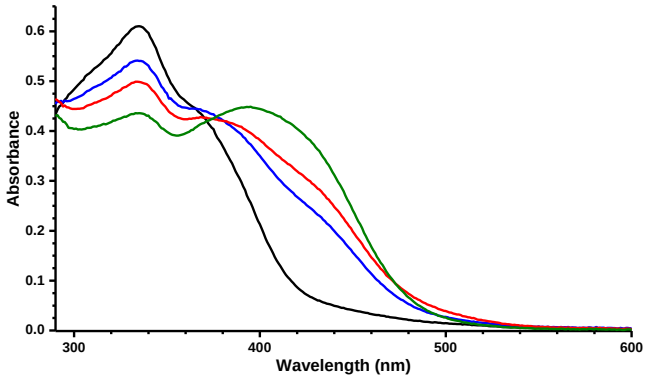

Figure S42: UV-Vis absorption spectra of **$3b_{NBD-DHA}$** showing isomerization from 7-substitution to 6-substitution in the seven membered ring over three photo/thermal cycles. Black: **$3b_{NBD-DHA}$**, blue: **$3b_{NBD-DHA}$** after one photo/thermal cycle, red: **$3b_{NBD-DHA}$** after two photo/thermal cycles, green: **$3b_{NBD-DHA}$** after three photo/thermal cycles.

Compound 4a

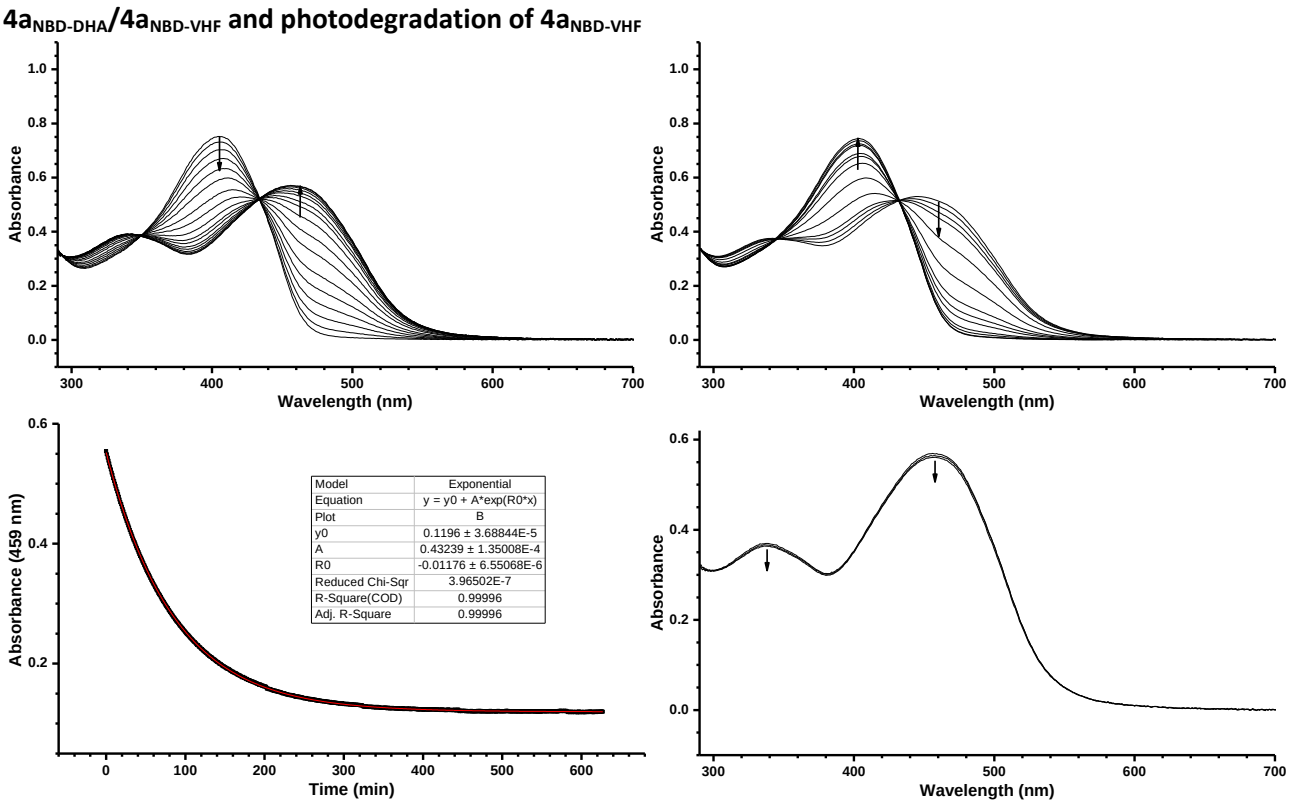

Figure S43: Top left: Light irradiation (404 nm) of **4a$_{NBD-DHA}$** in toluene at 25 °C. Top right: Thermal back-reaction of **4a$_{NBD-VHF}$** in toluene at 50 °C. Bottom left: Exponential decay at 459 nm from **4a$_{NBD-VHF}$** to **4a$_{NBD-DHA}$** in toluene at 50 °C. Bottom right: Light irradiation (338 nm) of **4a$_{NBD-VHF}$** in toluene at 25 °C.

Compound 4b

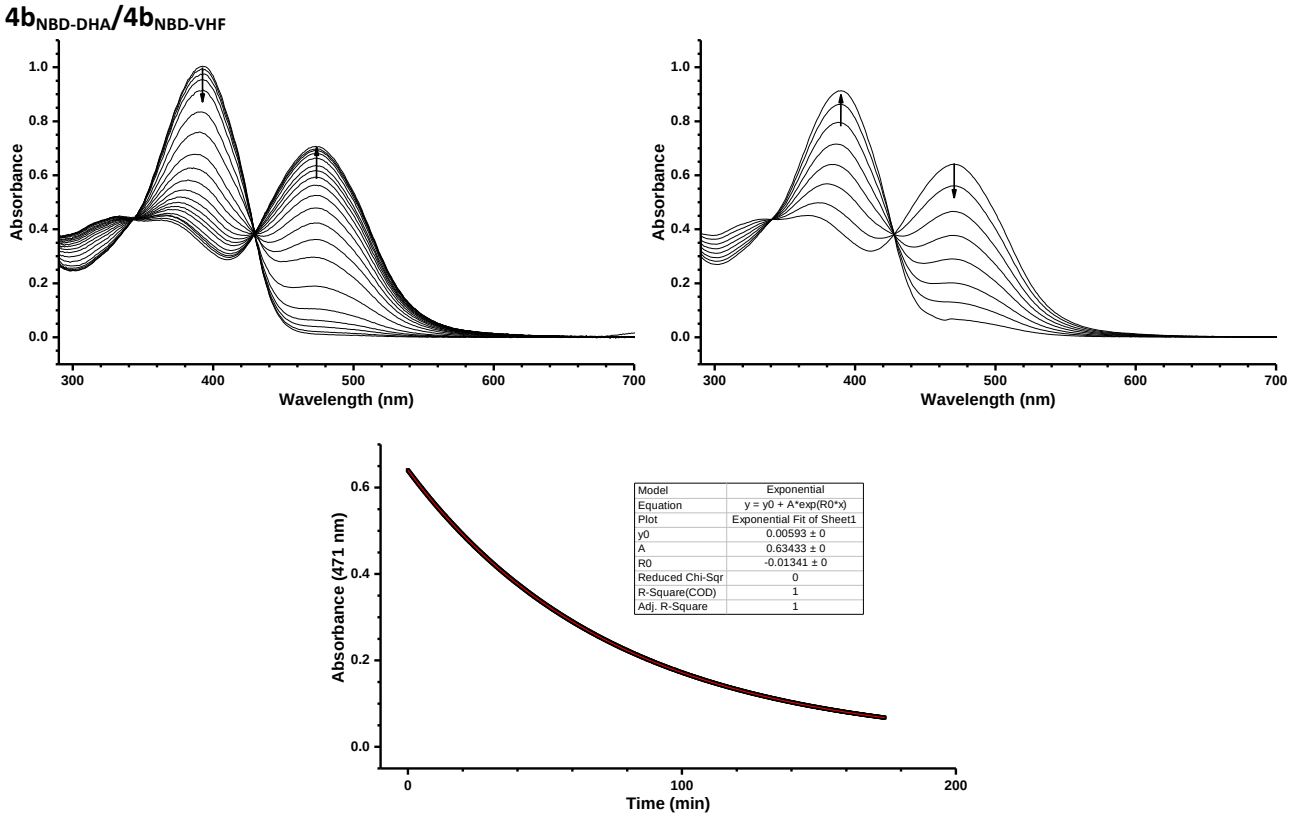

Figure S44: Top left: Light irradiation (392 nm) of **4b$_{NBD-DHA}$** in toluene at 25 °C. Top right: Thermal back-reaction of **4b$_{NBD-VHF}$** in toluene at 50 °C. Bottom: Exponential decay at 471 nm from **4b$_{NBD-VHF}$** to **4b$_{NBD-DHA}$** in toluene at 50 °C.

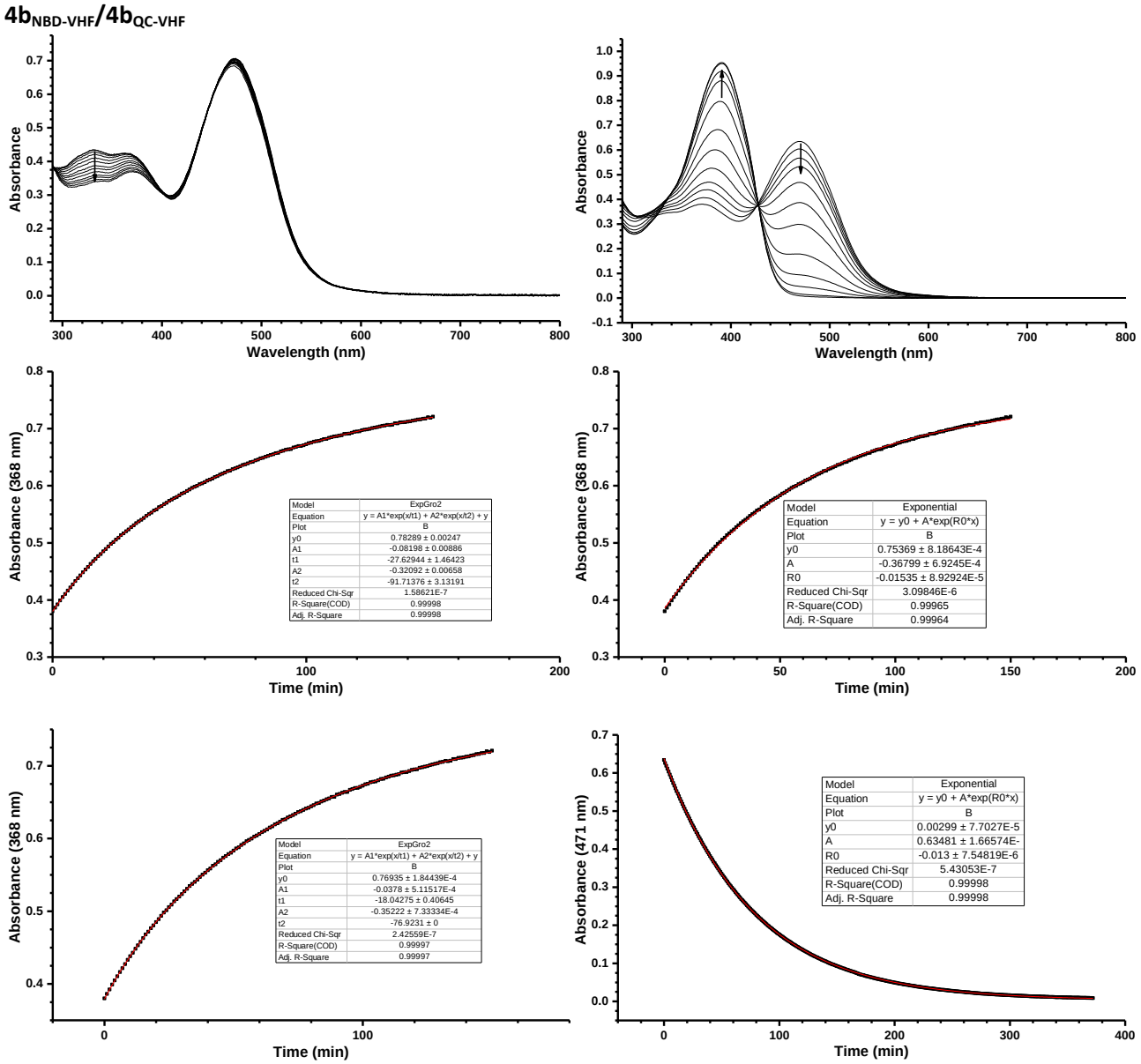

Figure S45: Top left: Light irradiation (320 nm) of **4b$_{NBD-VHF}$** in toluene at 25 °C. Top right: Thermal back-reaction of **4b$_{QC-VHF}$** in toluene at 50 °C. Middle left: Growth of absorbance at 368 nm fitted with a single exponential fit of **4b$_{QC-VHF}$** to **4b$_{NBD-DHA}$** in toluene at 50 °C. Middle right: Growth of absorbance at 368 nm fitted with a double exponential fit of **4b$_{QC-VHF}$** to **4b$_{NBD-DHA}$** in toluene at 50 °C. Bottom left: Growth of absorbance at 368 nm fitted with a double exponential fit, locking the k_1 value obtained from figure Bottom right, of **4b$_{QC-VHF}$** to **4b$_{NBD-DHA}$** in toluene at 50 °C. Bottom right: Exponential decay at 471 nm from **4b$_{QC-VHF}$** to **4b$_{NBD-DHA}$** in toluene at 50 °C.

Compound 5a

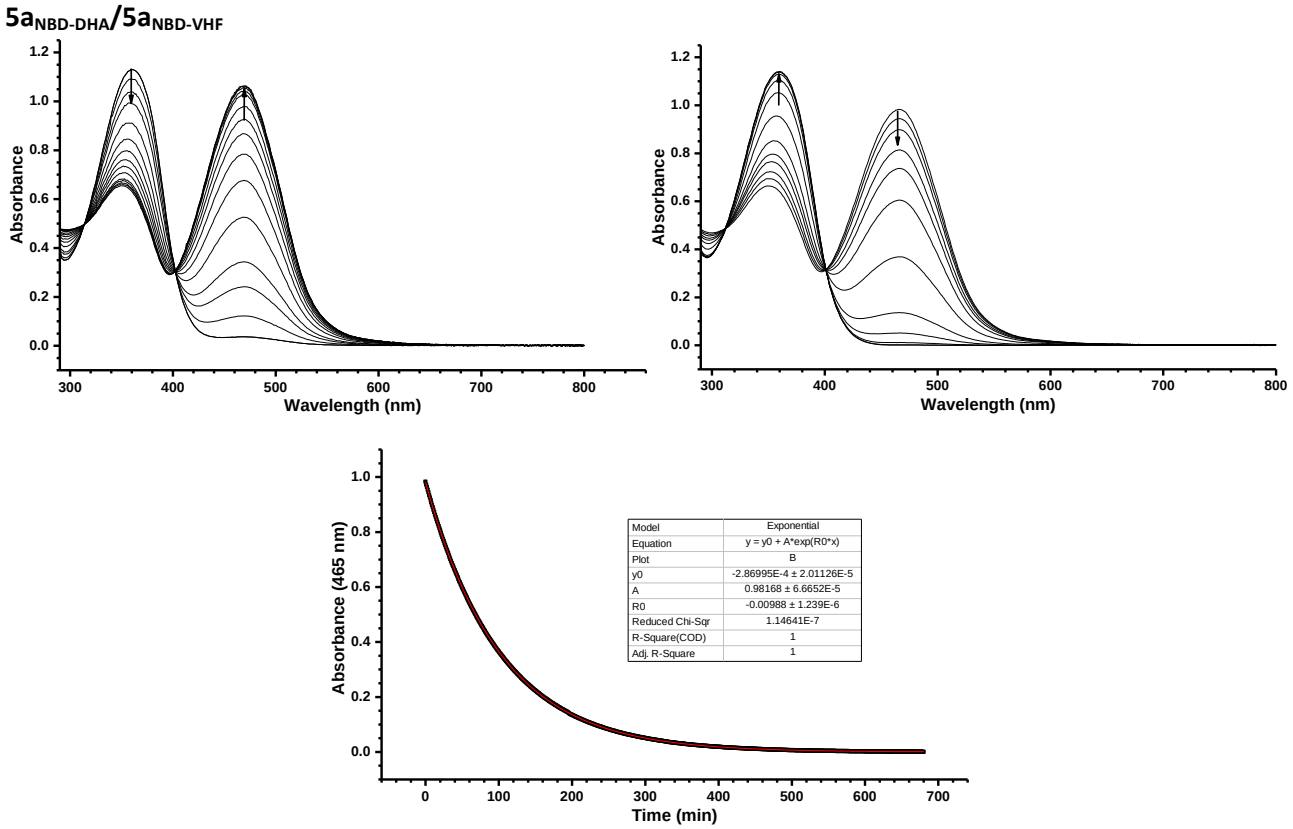

Figure S46: Top left: Light irradiation (400 nm) of **5a$_{NBD-DHA}$** in toluene at 25 °C. Top right: Thermal back-reaction of **5a$_{NBD-VHF}$** in toluene at 50 °C. Bottom: Exponential decay at 465 nm from **5a$_{NBD-VHF}$** to **5a$_{NBD-DHA}$** in toluene at 50 °C.

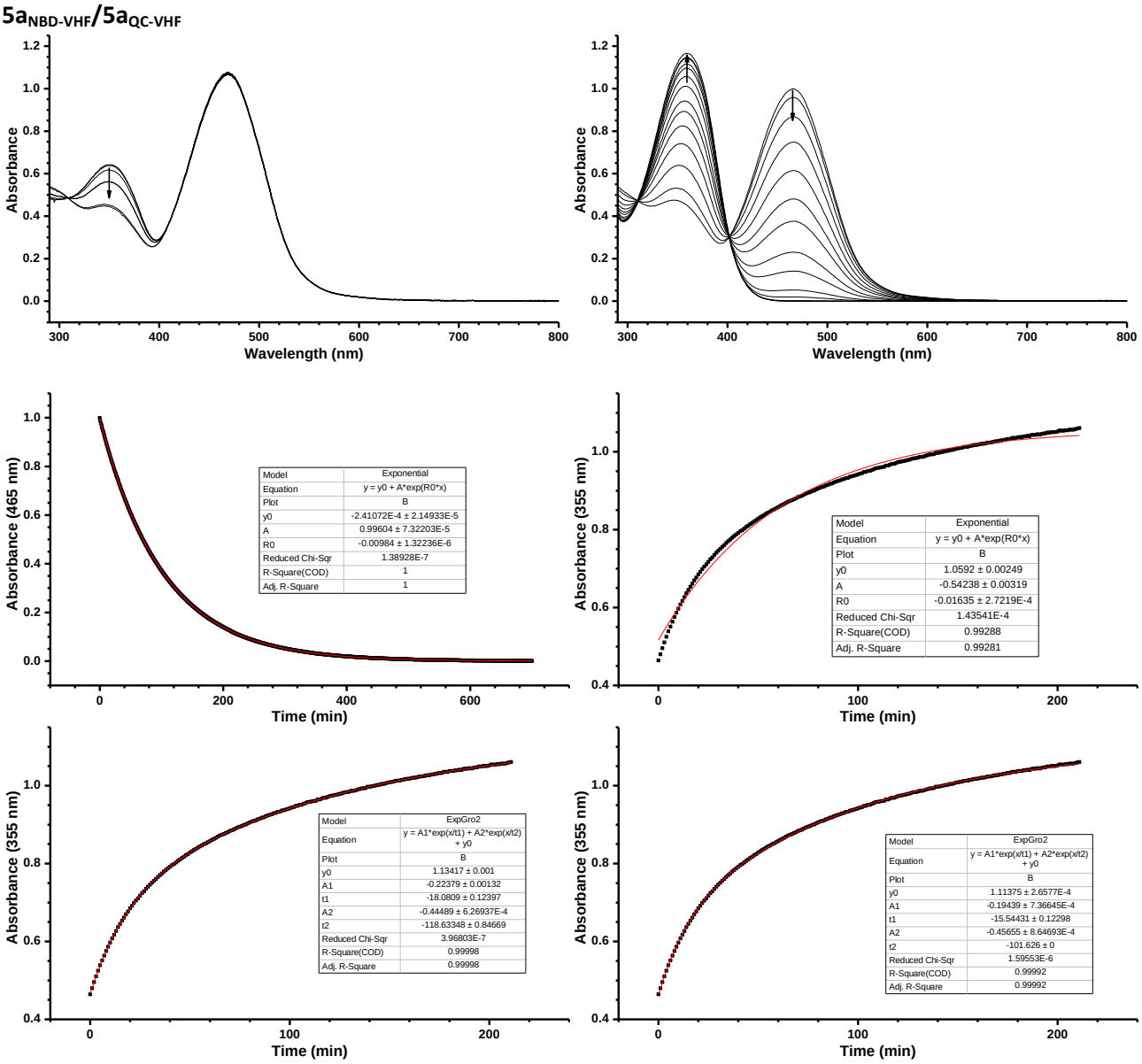

Figure S47: Top left: Light irradiation (350 nm) of **5a$_{NBD-DHA}$** in toluene at 25 °C. Top right: Thermal back-reaction of **5a$_{QC-VHF}$** in toluene at 50 °C. Middle left: Exponential decay at 465 nm from **5a$_{QC-VHF}$** to **5a$_{NBD-DHA}$** in toluene at 50 °C. Middle right: Growth of absorbance at 355 nm fitted with a single exponential fit of **5a$_{QC-VHF}$** to **5a$_{NBD-DHA}$** in toluene at 50 °C. Bottom left: Growth of absorbance at 355 nm fitted with a double exponential fit of **5a$_{QC-VHF}$** to **5a$_{NBD-DHA}$** in toluene at 50 °C. Bottom right: Growth of absorbance at 355 nm fitted with a double exponential fit, locking the k_1 value obtained from the exponential decay (Middle left), of **5a$_{QC-VHF}$** to **5a$_{NBD-DHA}$** in toluene at 50 °C.

Compound 5b

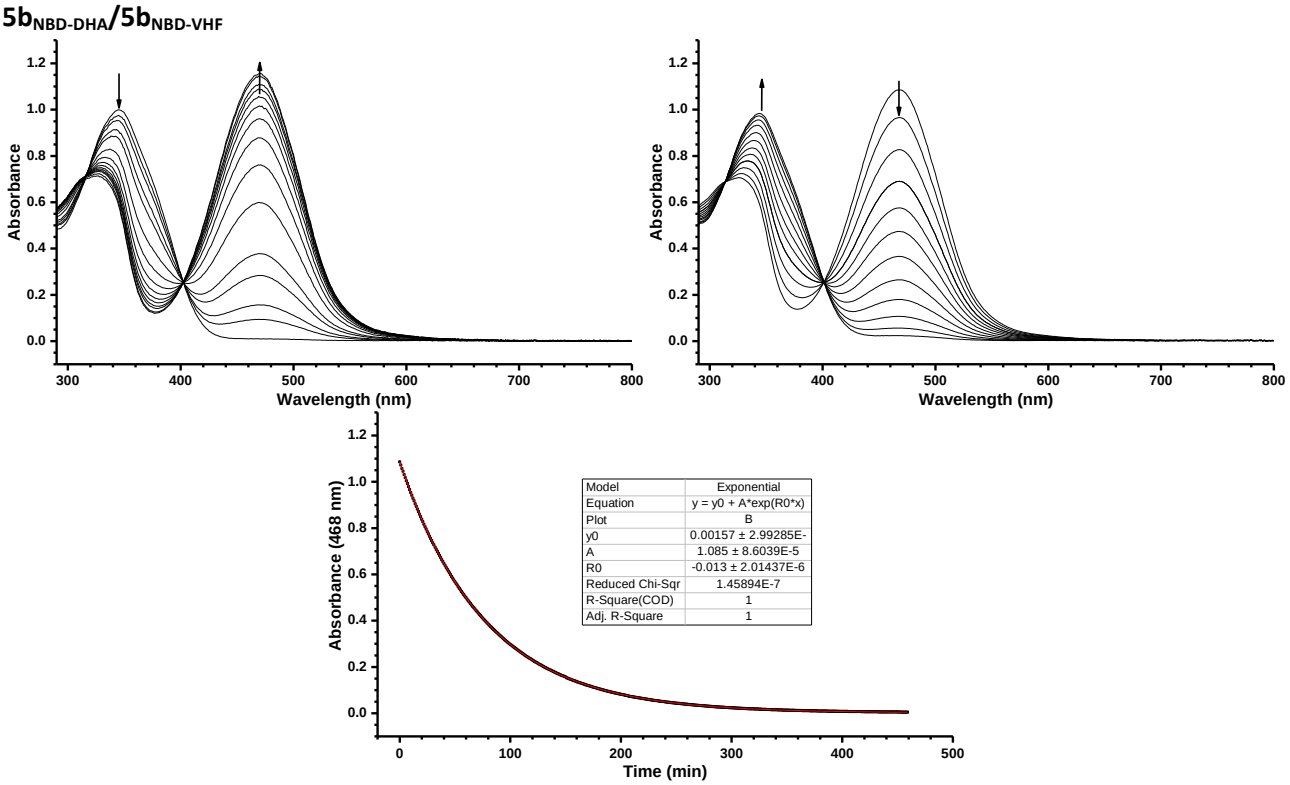

Figure S48: Top left: Light irradiation (400 nm) of **5b$_{NBD-DHA}$** in toluene at 25 °C. Top right: Thermal back-reaction of **5b$_{NBD-VHF}$** in toluene at 50 °C. Bottom: Exponential decay at 468 nm from **5b$_{NBD-VHF}$** to **5b$_{NBD-DHA}$** in toluene at 50 °C.

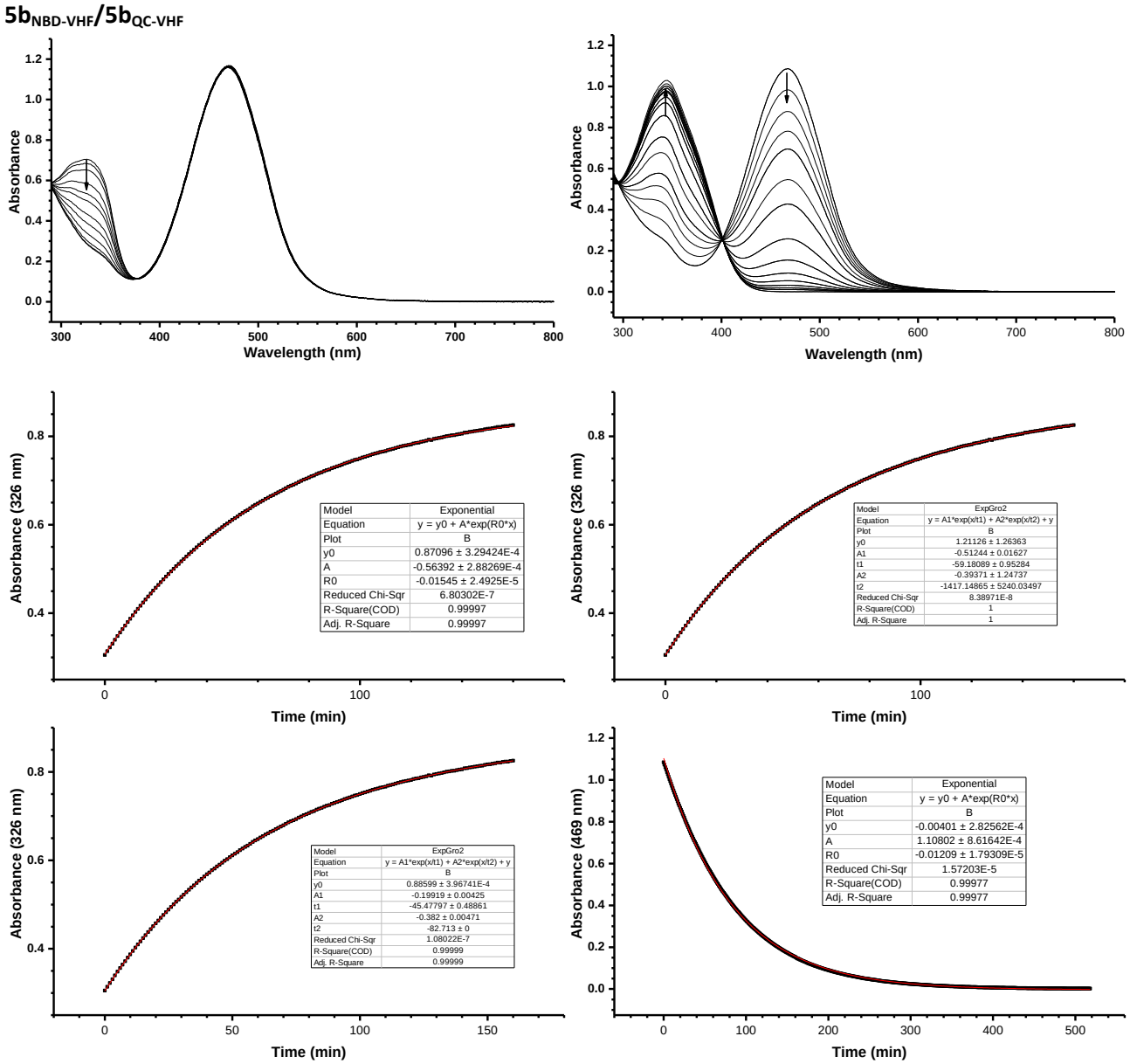

Figure S49: Top left: Light irradiation (330 nm) of **5b$_{NBD-VHF}$** in toluene at 25 °C. Top right: Thermal back-reaction of **5b$_{QC-VHF}$** in toluene at 50 °C. Middle left: Growth of absorbance at 326 nm fitted with a single exponential fit of **5b$_{QC-VHF}$** to **5b$_{NBD-DHA}$** in toluene at 50 °C. Middle right: Growth of absorbance at 326 nm fitted with a double exponential fit of **5b$_{QC-VHF}$** to **5b$_{NBD-DHA}$** in toluene at 50 °C. Bottom left: Growth of absorbance at 326 nm fitted with a double exponential fit, locking the k_1 value obtained from figure Bottom right, of **5b$_{QC-VHF}$** to **5b$_{NBD-DHA}$** in toluene at 50 °C. Bottom right: Exponential decay at 469 nm from **5b$_{QC-VHF}$** to **5b$_{NBD-DHA}$** in toluene at 50 °C.

UV-Vis absorption spectroscopy and switching studies in CH_2Cl_2

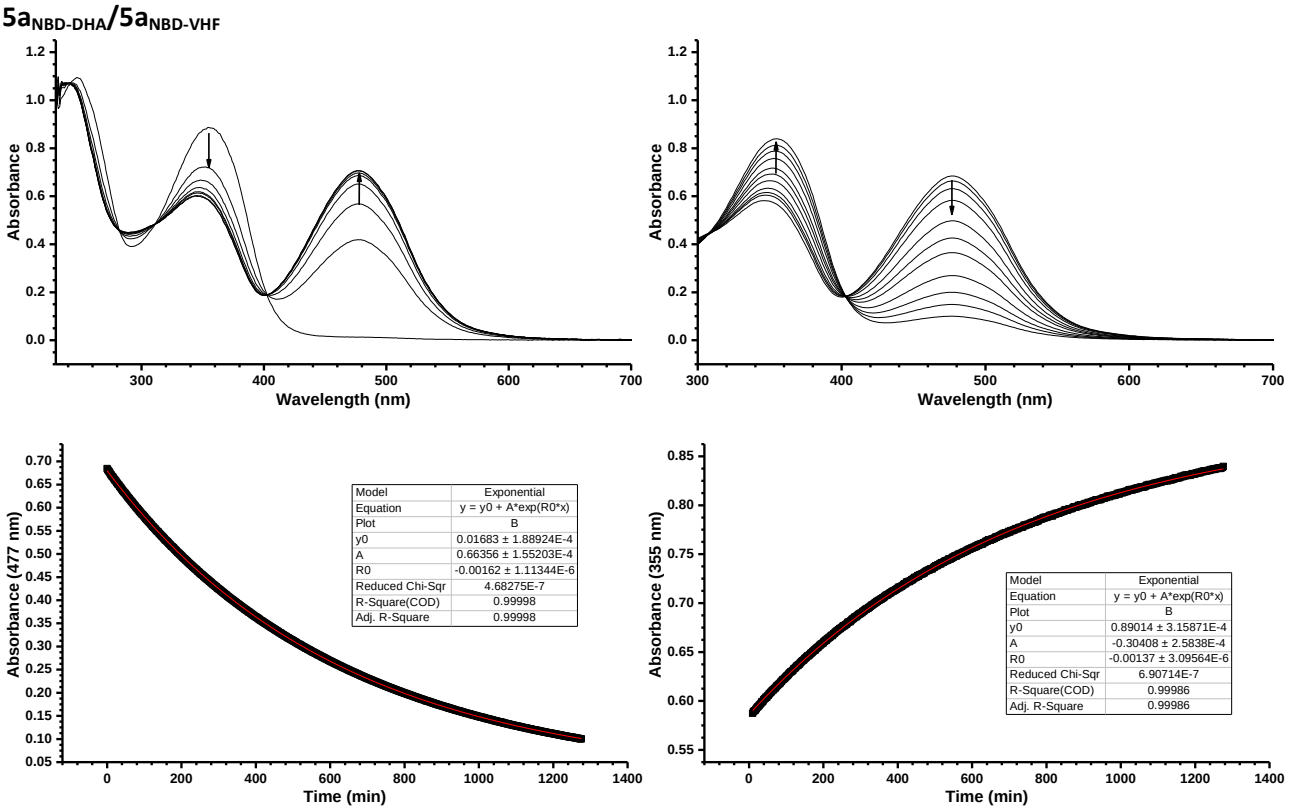

Figure S50: Top left: Light irradiation (400 nm) of **5a$_{NBD-DHA}$** in CH_2Cl_2. Top right: Thermal back-reaction of **5a$_{NBD-VHF}$** in CH_2Cl_2 at 25 °C. Bottom left: Exponential decay at 477 nm of **5a$_{NBD-VHF}$** to **5a$_{NBD-DHA}$** in CH_2Cl_2 at 25 °C. Bottom right: Exponential growth at 355 nm from **5a$_{NBD-VHF}$** to **5a$_{NBD-DHA}$** in CH_2Cl_2 at 25 °C.

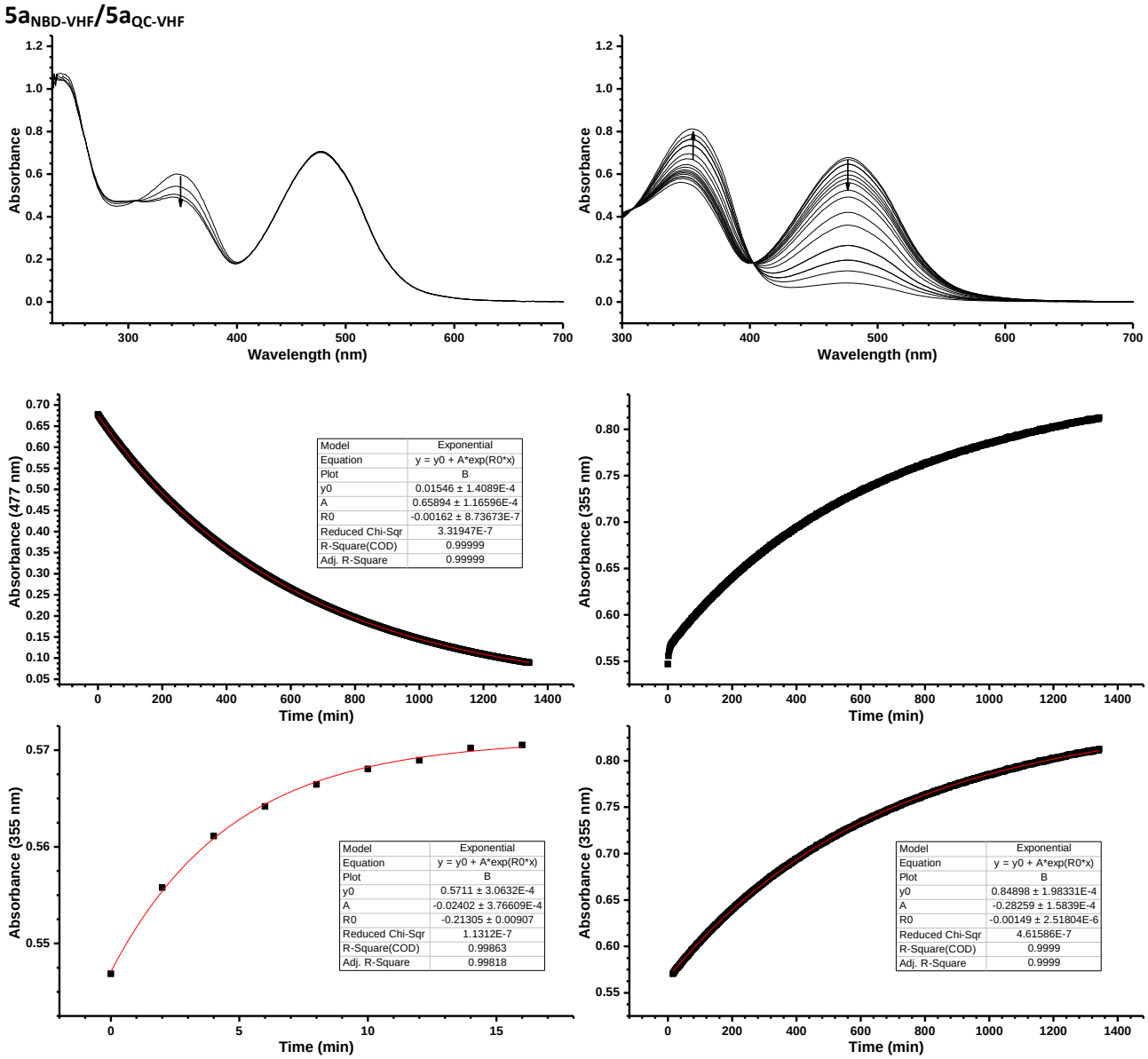

Figure S51: Top left: Light irradiation (347 nm) of **5a$_{NBD-VHF}$** in CH_2Cl_2. Top right: Thermal back-reaction of **5a$_{QC-VHF}$** in CH_2Cl_2 at 25 °C. Middle left: Exponential decay at 477 nm of **5a$_{QC-VHF}$** to **5a$_{NBD-DHA}$** in CH_2Cl_2 at 25 °C. Middle right: Growth at 355 nm from **5a$_{QC-VHF}$** to **5a$_{NBD-DHA}$** in CH_2Cl_2 at 25 °C. Bottom left: Exponential growth at 355 nm from **5a$_{QC-VHF}$** to **5a$_{NBD-VHF}$** in CH_2Cl_2 at 25 °C (data originates from the first 16 minutes from the growth in Middle right figure). Bottom right: Exponential growth at 355 nm from **5a$_{NBD-VHF}$** to **5a$_{NBD-DHA}$** in CH_2Cl_2 at 25 °C (data originates from 16th minute from the growth in Middle right figure).

$5a_{NBD\text{-}DHA}$/$5a_{NBD\text{-}VHF}$ and the $Cu(MeCN)_4BF_4$ promoted back-reaction

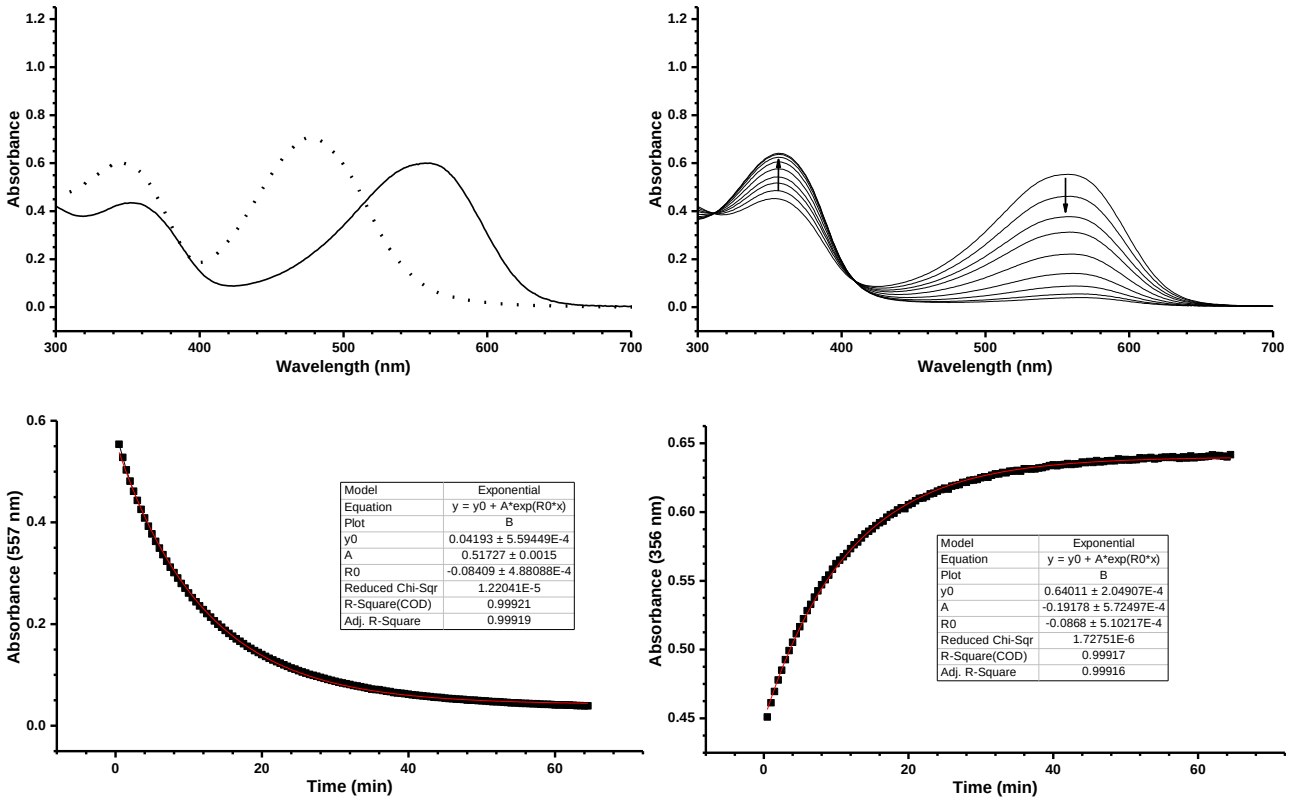

Figure S52: Top left: **$5a_{NBD\text{-}VHF}$** (dashed) and **$5a_{NBD\text{-}VHF}$** after addition of 8 equiv. of $Cu(MeCN)_4BF_4$ (solid). Top right: Thermal backreaction of **$5a_{NBD\text{-}VHF}$** after addition of 8 equiv. of $Cu(MeCN)_4BF_4$ in CH_2Cl_2 at 25 °C. Bottom left: Exponential decay at 557 nm of the cupper complexed Cu@**$5a_{NBD\text{-}VHF}$** to Cu@**$5a_{NBD\text{-}DHA}$** in CH_2Cl_2 at 25 °C. Bottom right: Exponential growth at 356 nm from the cupper complexed Cu@**$5a_{NBD\text{-}VHF}$** to Cu@**$5a_{NBD\text{-}DHA}$** in CH_2Cl_2 at 25 °C.

$5a_{QC\text{-}VHF}$ and the $Cu(MeCN)_4BF_4$ promoted back-reaction

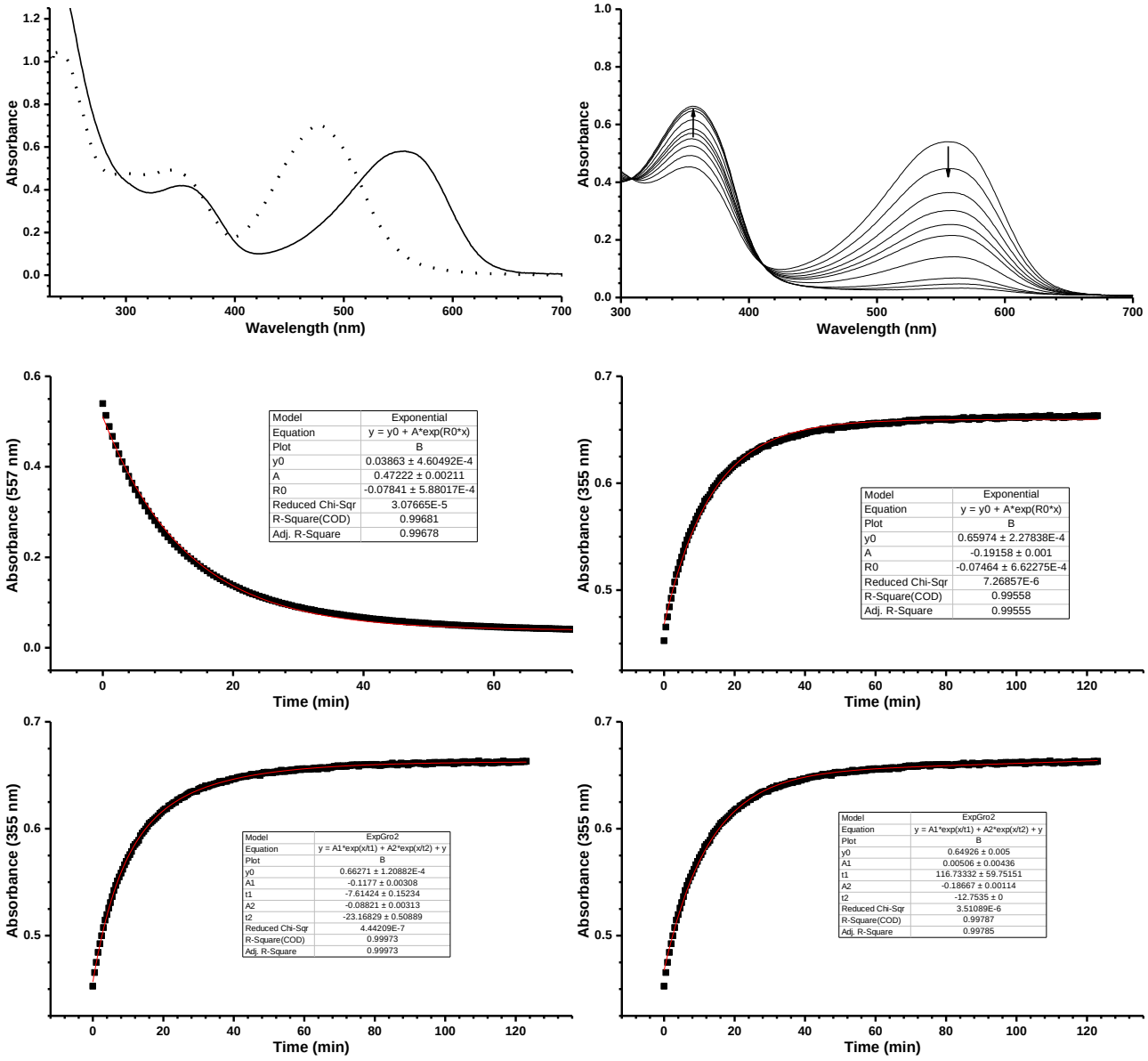

Figure S53: Top left: **$5a_{QC\text{-}VHF}$** (dashed) and **$5a_{QC\text{-}VHF}$** after addition of 8 equiv. of $Cu(MeCN)_4BF_4$ (solid). Top right: Thermal back-reaction of **$5a_{QC\text{-}VHF}$** after addition of 8 equiv. of $Cu(MeCN)_4BF_4$ in CH_2Cl_2 at 25 °C. Middle left: Decay of absorbance at 557 nm fitted with a single exponential fit of the cupper complexed Cu@**$5a_{QC\text{-}VHF}$** to Cu@**$5a_{NBD\text{-}DHA}$** in CH_2Cl_2 at 25 °C. Middle right: Growth of absorbance at 355 nm fitted with a single exponential fit from the cupper complexed Cu@**$5a_{QC\text{-}VHF}$** to Cu@**$5a_{NBD\text{-}DHA}$** in CH_2Cl_2 at 25 °C. Bottom left: Growth of absorbance at 355 nm fitted with a double exponential fit from the cupper complexed Cu@**$5a_{QC\text{-}VHF}$** to Cu@**$5a_{NBD\text{-}DHA}$** in CH_2Cl_2 at 25 °C. Bottom right: Growth of absorbance at 355 nm fitted with a double exponential fit, locking the k_1 value obtained from figure Middle left, from the cupper complexed Cu@**$5a_{QC\text{-}VHF}$** to Cu@**$5a_{NBD\text{-}DHA}$** in CH_2Cl_2 at 25 °C.

Gibbs free energies of the lowest energy conformers

The following tables hold the results of the Gibbs free energies of the lowest-energy conformers. The results were calculated at the CAM-B3LYP/6-311+G(d) level of theory with the IEF-PCM solvation model to mimic the polarization effects of toluene. Note that the units are in kJ/mol and that the relative energies are taken with respect to the lowest-energy isomer.

State	NBD – DHA	NBD – s-*cis*-VHF	NBD – s-*trans*-VHF	QC – DHA	QC – s-*cis*-VHF	QC – s-*trans*-VHF
Energy [kJ/mol]	-3621075,286	-3621060,591	-3621067,611	-3620972,63	-3620959,023	-3620969,623
Rel. Energy [kJ/mol]	0	14,6949235	7,6743365	102,6544245	116,262391	105,6632475

Table S1: The Gibbs free energies of the **3a** system.

State	NBD – DHA	NBD – s-*cis*-VHF	NBD – s-*trans*-VHF	QC – DHA	QC – s-*cis*-VHF	QC – s-*trans*-VHF
Energy [kJ/mol]	-3257017,556	-3256999,645	-3257007,312	-3256918,88	-3256903,673	-3256911,113
Rel. Energy [kJ/mol]	0	17,911161	10,244701	98,6794175	113,883688	106,443021

Table S2: The Gibbs free energies of the **3b** system.

State	NBD – DHA	NBD – s-*cis*-VHF	NBD – s-*trans*-VHF	QC – DHA	QC – s-*cis*-VHF	QC – s-*trans*-VHF
Energy [kJ/mol]	-3621079,116	-3621061,652	-3621070,216	-3620978,32	-3620964,461	-3620969,528
Rel. Energy [kJ/mol]	0	17,464826	8,900445	100,792945	114,655585	109,58837

Table S3: The Gibbs free energies of the **4a** system.

State	NBD – DHA	NBD – s-*cis*-VHF	NBD – s-*trans*-VHF	QC – DHA	QC – s-*cis*-VHF	QC – s-*trans*-VHF
Energy [kJ/mol]	-3257021,342	-3257002,355	-3257011,499	-3256922,95	-3256906,201	-3256914,658
Rel. Energy [kJ/mol]	0	18,987616	9,8429995	98,393238	115,1413025	106,684567

Table S4: The Gibbs free energies of the **4b** system.

State	NBD – DHA	NBD – s-*cis*-VHF	NBD – s-*trans*-VHF	QC – DHA	QC – s-*cis*-VHF	QC – s-*trans*-VHF
Energy [kJ/mol]	-3621077,391	-3621061,405	-3621069,806	-3620977,49	-3620958,364	-3620969,539
Rel. Energy [kJ/mol]	0	15,9866695	7,5850695	99,8976495	119,0270425	107,8529145

Table S5: The Gibbs free energies of the **5a** system.

State	NBD – DHA	NBD – s-*cis*-VHF	NBD – s-*trans*-VHF	QC – DHA	QC – s-*cis*-VHF	QC – s-*trans*-VHF
Energy [kJ/mol]	-3257020,31	-3257002,037	-3257010,937	-3256922,5	-3256906,012	-3256914,049
Rel. Energy [kJ/mol]	0	18,27348	9,373035	97,810377	114,298517	106,2618615

Table S6: The Gibbs free energies of the **5b** system.

Simulating the UV-Vis spectra

Here we present the expression needed in order to simulate the UV-Vis spectra. The expression is derived from the assumption of Gaussian band shapes by applying Gaussian functions to convolute the calculated oscillator strengths. Thus, the UV-Vis spectra can be plotted as the extinction coefficient, ϵ, vs. the wavelength, λ, using the following equation[1]

$$\epsilon(\lambda) = \sum_{i=1}^{n} \epsilon_i(\lambda) = \sum_{i=1}^{n} k \cdot \frac{f_i}{\sigma} \cdot \exp\left[-4 \cdot \ln(2) \cdot \left(\frac{\frac{1}{\lambda} - \frac{1}{\lambda_i}}{\sigma \cdot 10^{-7}}\right)^2\right]$$

where f_i is the calculated oscillator strength, λ_i is the corresponding wavelength in nm, λ is an independent variable defining the simulated spectrum, and σ is the standard deviation also known as the full width at half maximum of the Gaussian band (in these simulations $\sigma = 0.4$ eV $= 0.4 \cdot 8065.54\ \mathrm{cm}^{-1} = 3226.22\ \mathrm{cm}^{-1}$). Furthermore, the constant k is given by

$$k = \frac{N_A \cdot e^2}{2 \cdot m_e \cdot c^2 \cdot \epsilon_0 \cdot \ln(10)} \cdot \sqrt{\frac{\ln(2)}{\pi}} = 2.1751 \cdot 10^8 \ \frac{L}{mol \cdot cm^2}$$

where N_A is Avogadro's constant, c is the speed of light, e is the elementary charge, m_e is the mass of an electron, and ϵ_0 is the vacuum permittivity.

[1] Serr, A.; O'Boyle, N. M. Convoluting UV-Vis spectra using oscillator strengths. http: //gausssum.sourceforge.net/GaussSum_UVVis_Convolution.pdf, 2009.

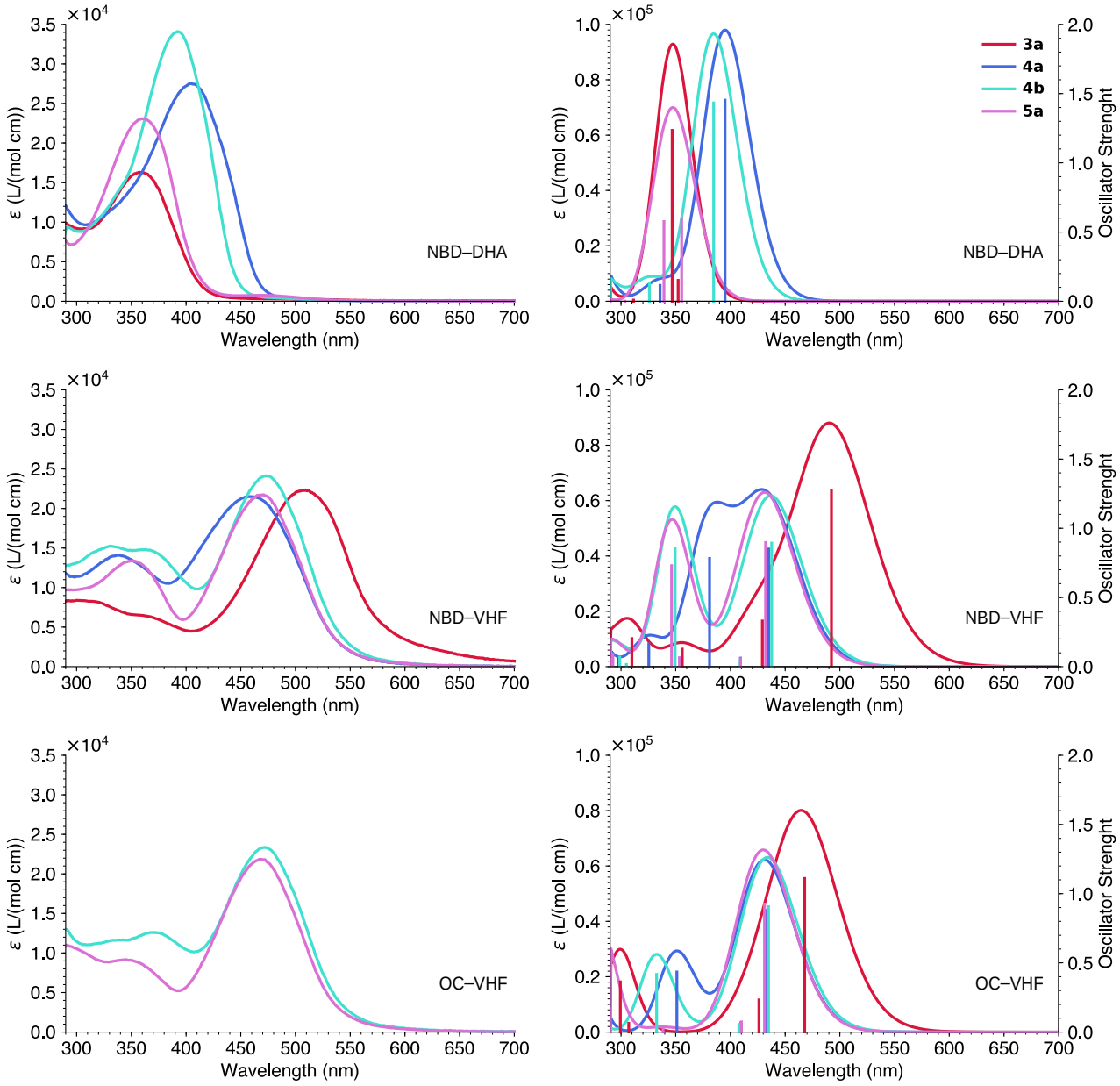

Figure S54: A comparison of the experimental and calculated UV-Vis spectra. Right-hand side figures show the experimental UV-Vis spectra and left-hand side figures show the calculated UV-Vis spectra. Note that only the s-*trans*-VHF structures are shown in calculated UV-Vis spectra.

The following figures depict the calculated UV-Vis spectra of all the investigated isomers.

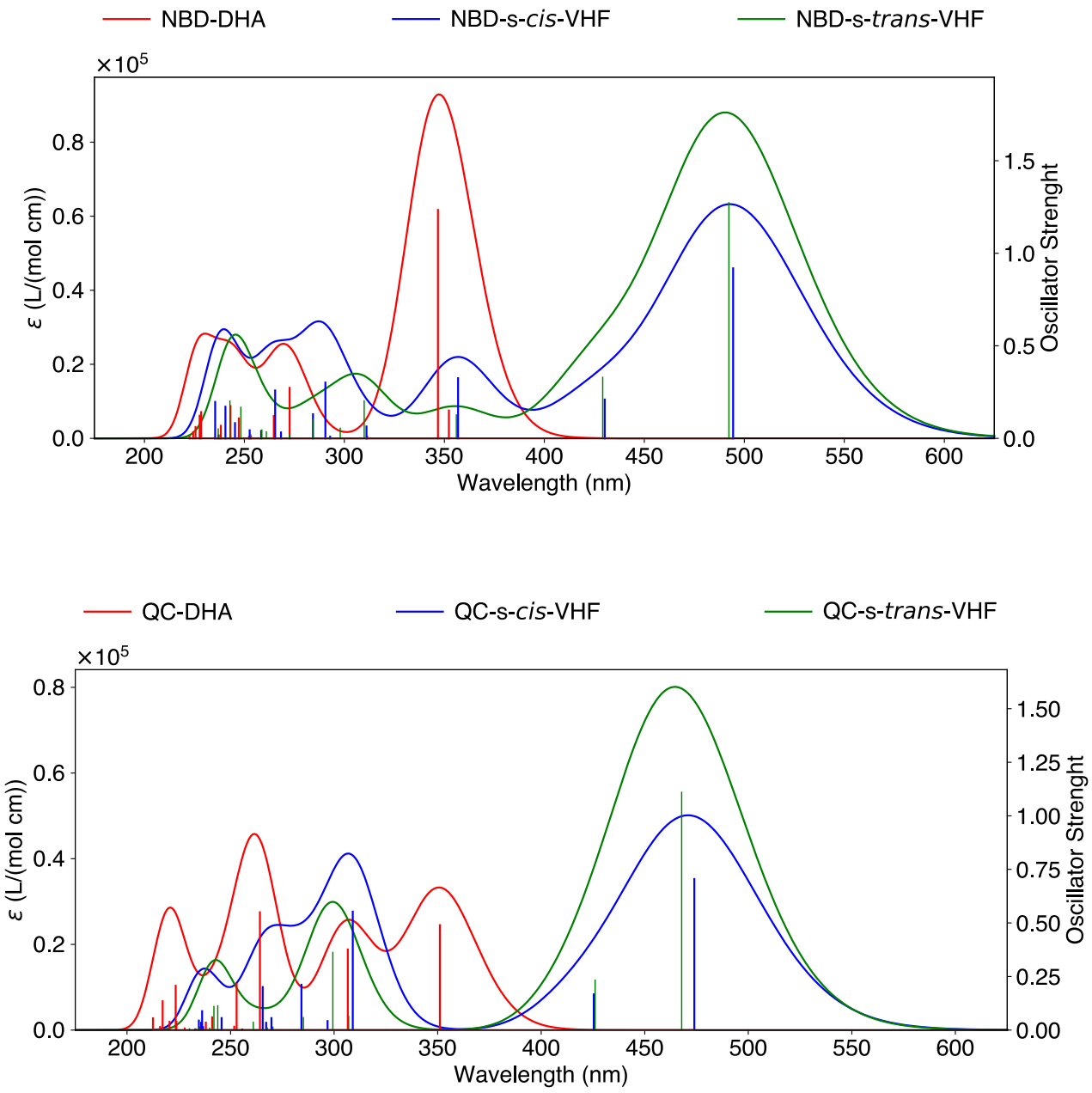

Figure S55: The calculated UV-Vis spectra of the **3a** system.

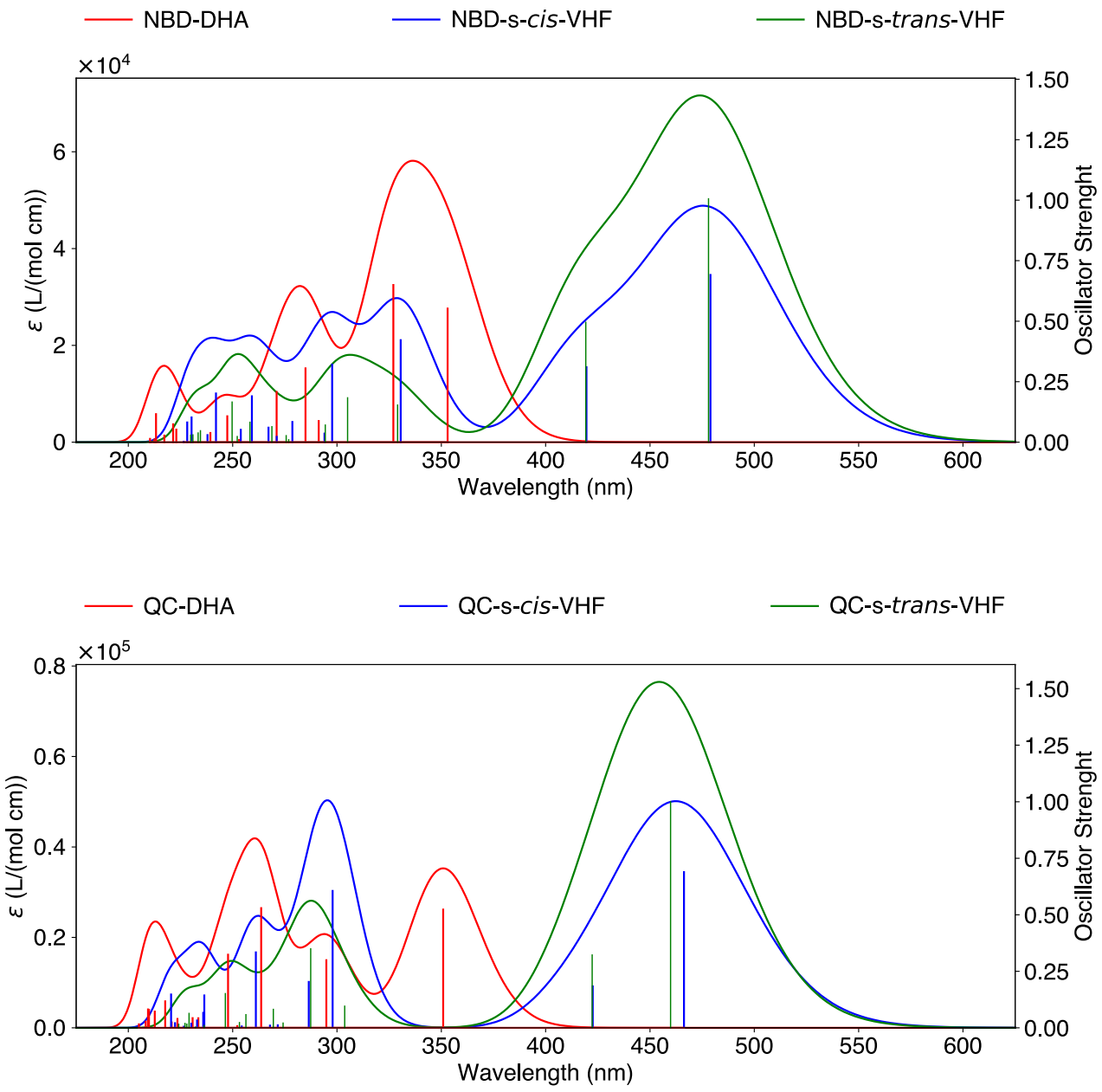

Figure S56: The calculated UV-Vis spectra of the **3b** system.

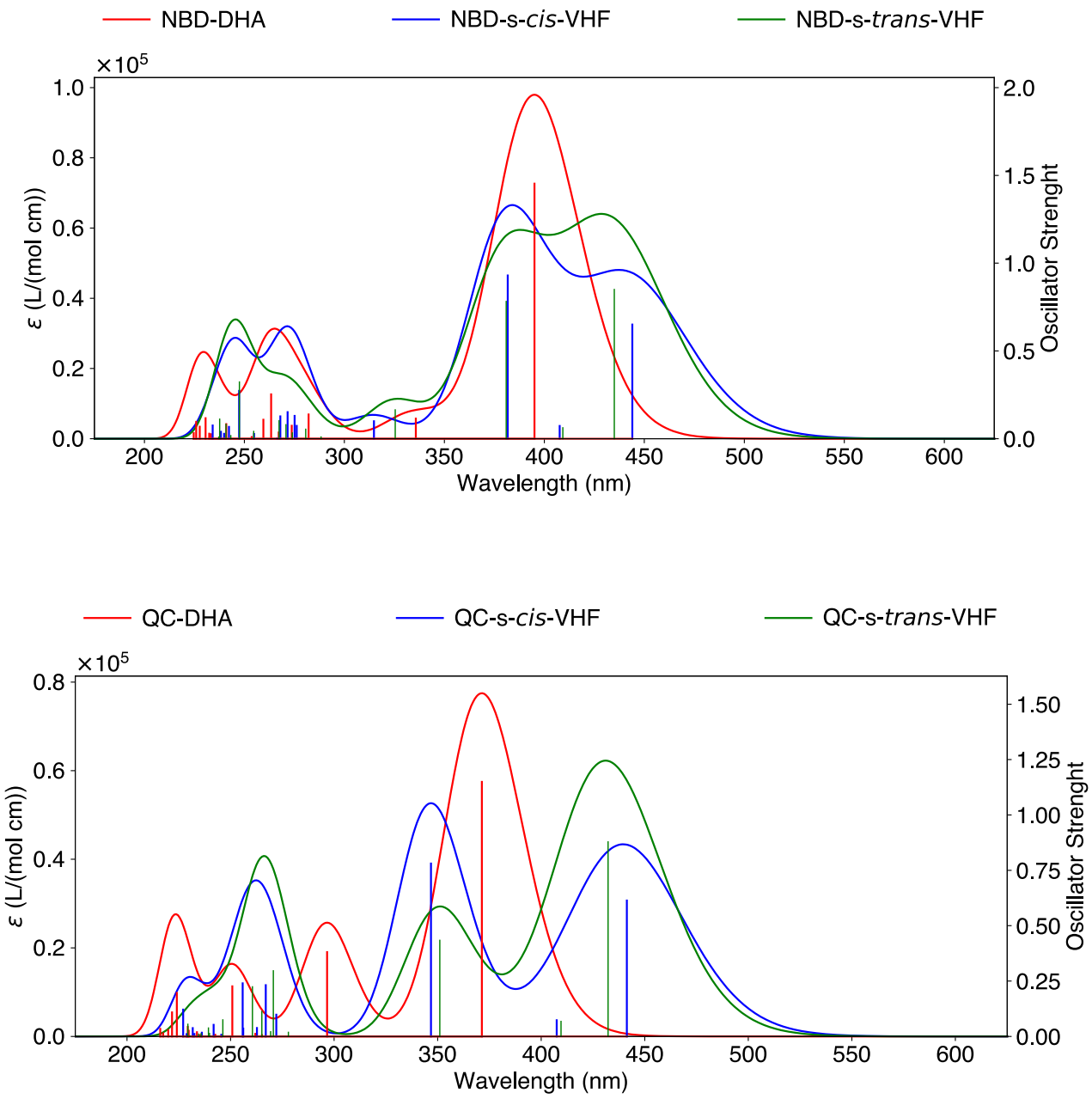

Figure S57: The calculated UV-Vis spectra of the **4a** system.

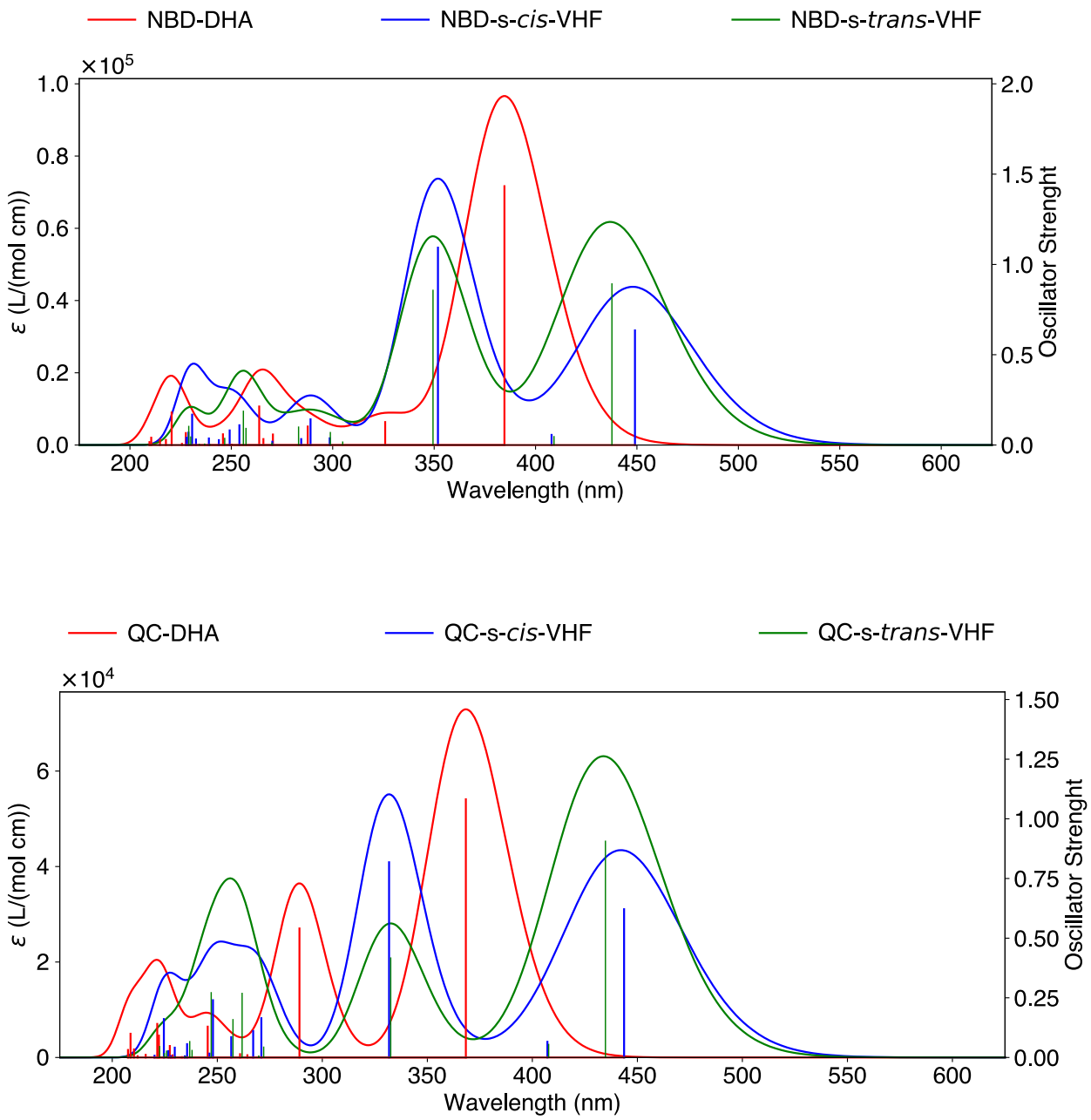

Figure S58: The calculated UV-Vis spectra of the **4b** system.

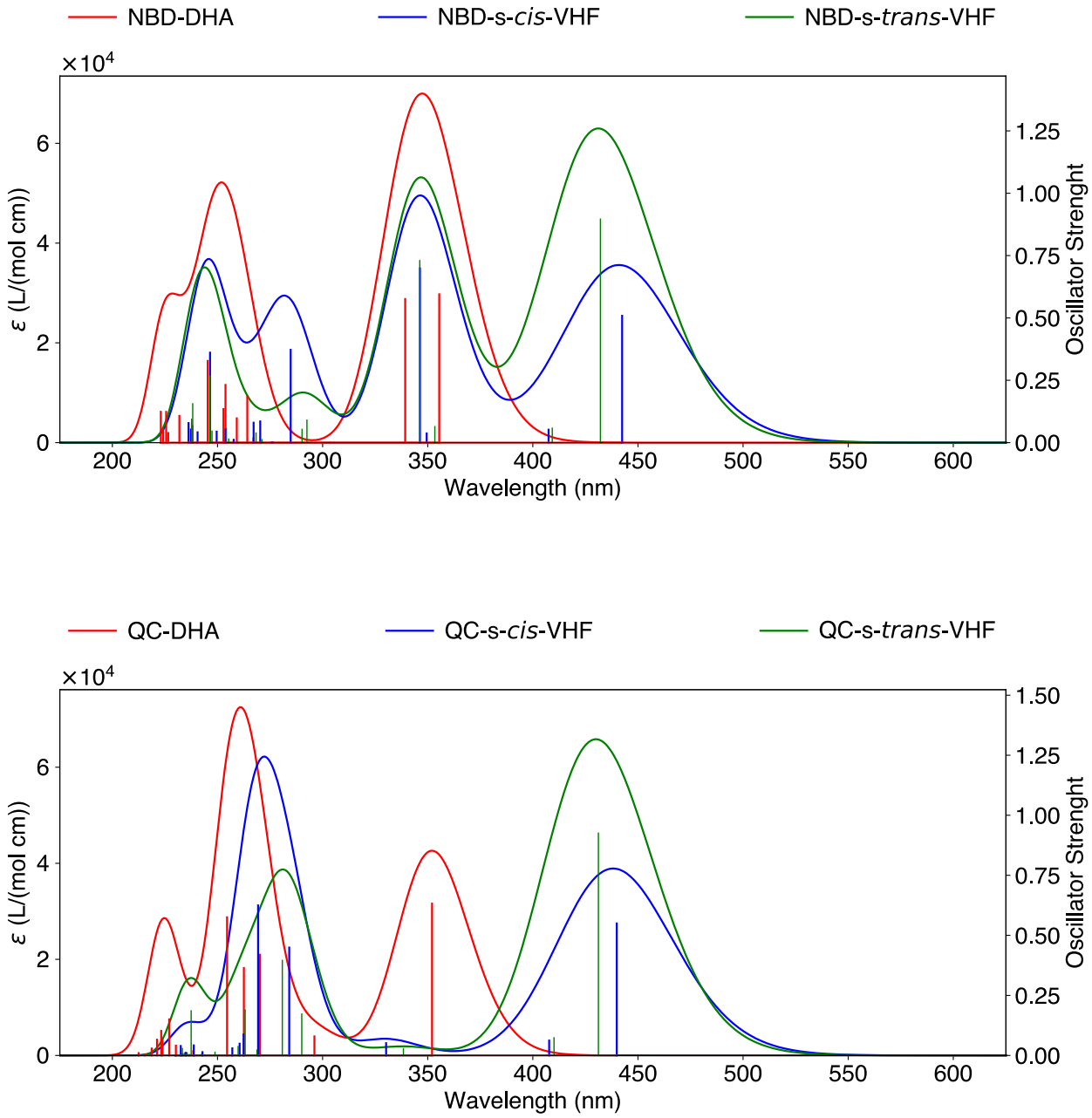

Figure S59: The calculated UV-Vis spectra of the **5a** system.

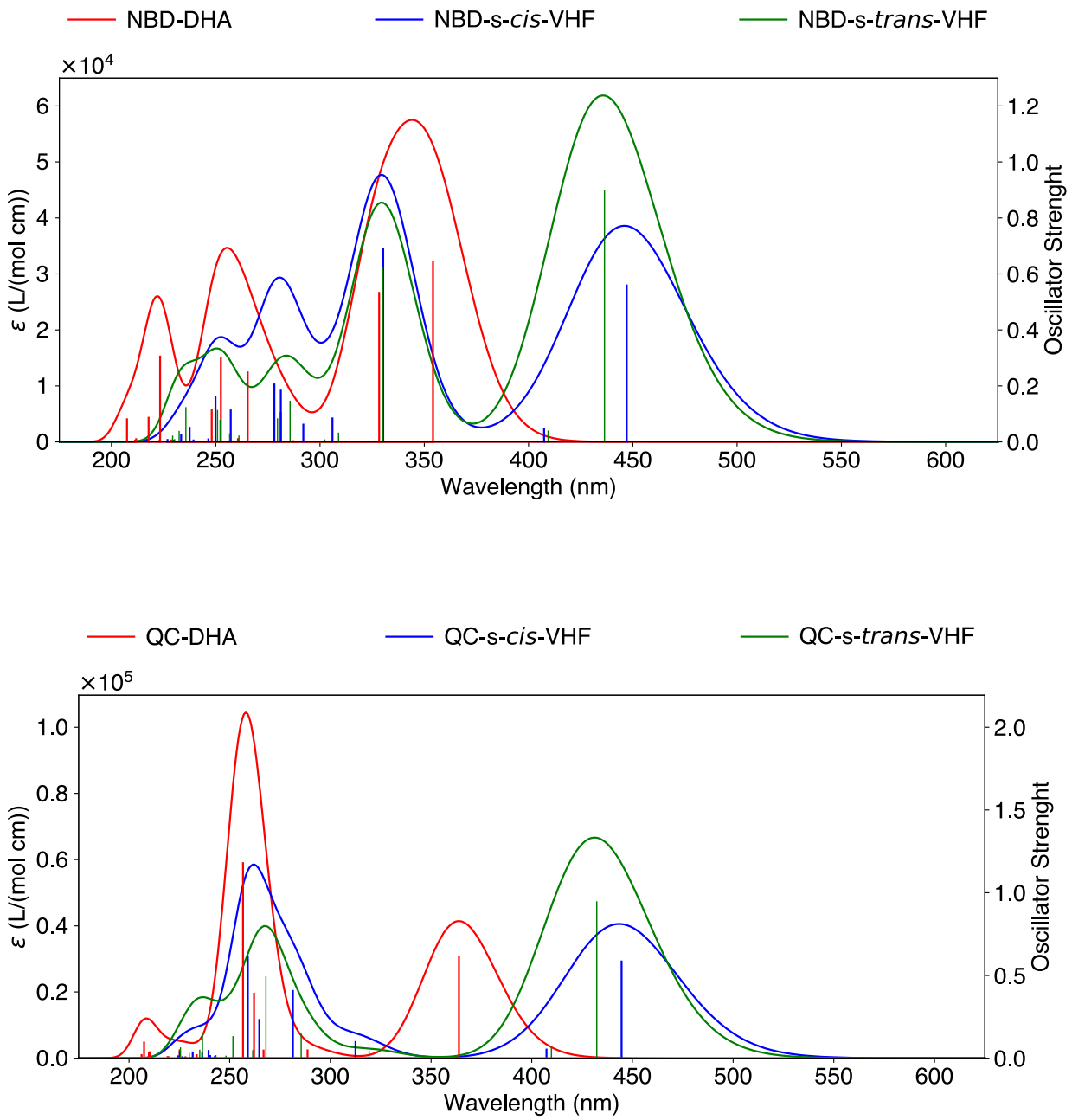

Figure S60: The calculated UV-Vis spectra of the **5b** system.

Natural transition orbitals (NTOs)

In the following, we present enlarged figures of the NTOs shown in Fig. 2 of the article. The depicted molecules are the lowest-energy conformers calculated at the CAM-B3LYP/6-311+G(d) level of theory with the IEF-PCM solvation model to mimic the polarization effects of toluene. The Roman numbers corresponds to the strong transitions shown in the UV-Vis spectra from Fig. 2 of the article.

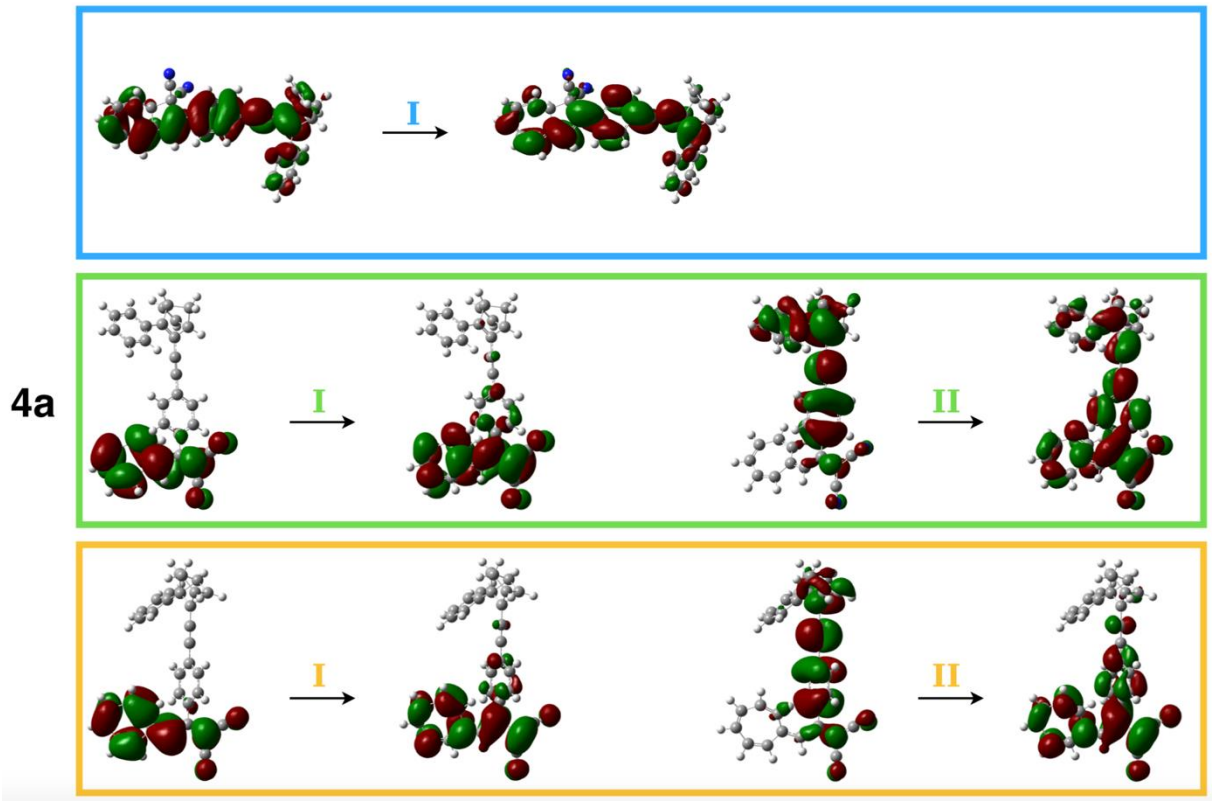

Figure S61: The NTOs of the **4a** system.

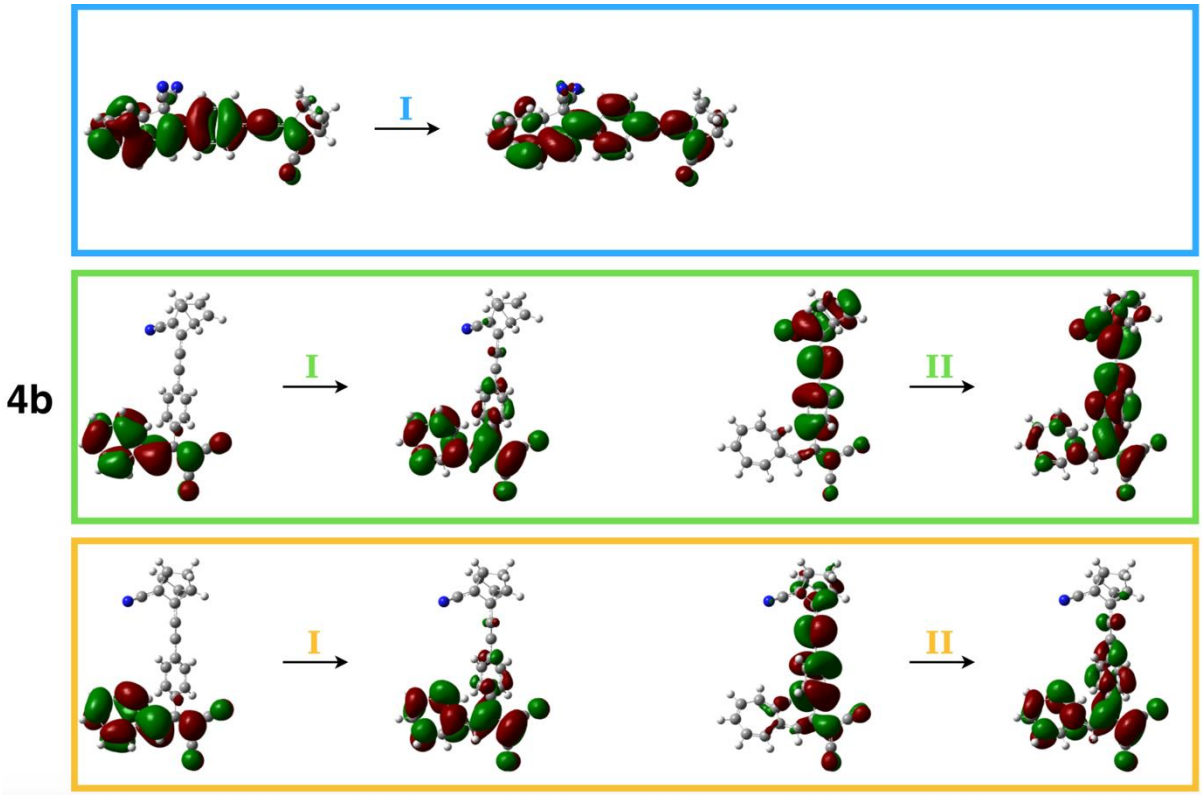

Figure S62: The NTOs of the **4b** system.

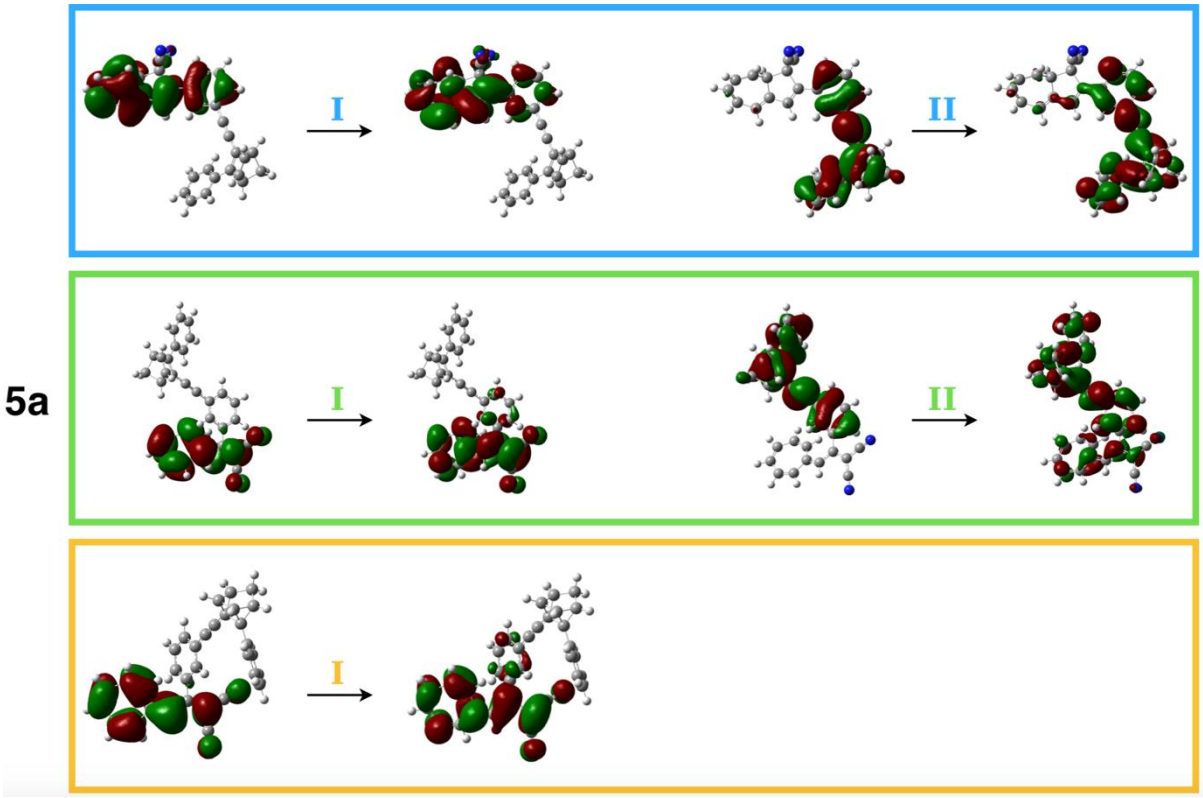

Figure S63: The NTOs of the **5a** system.

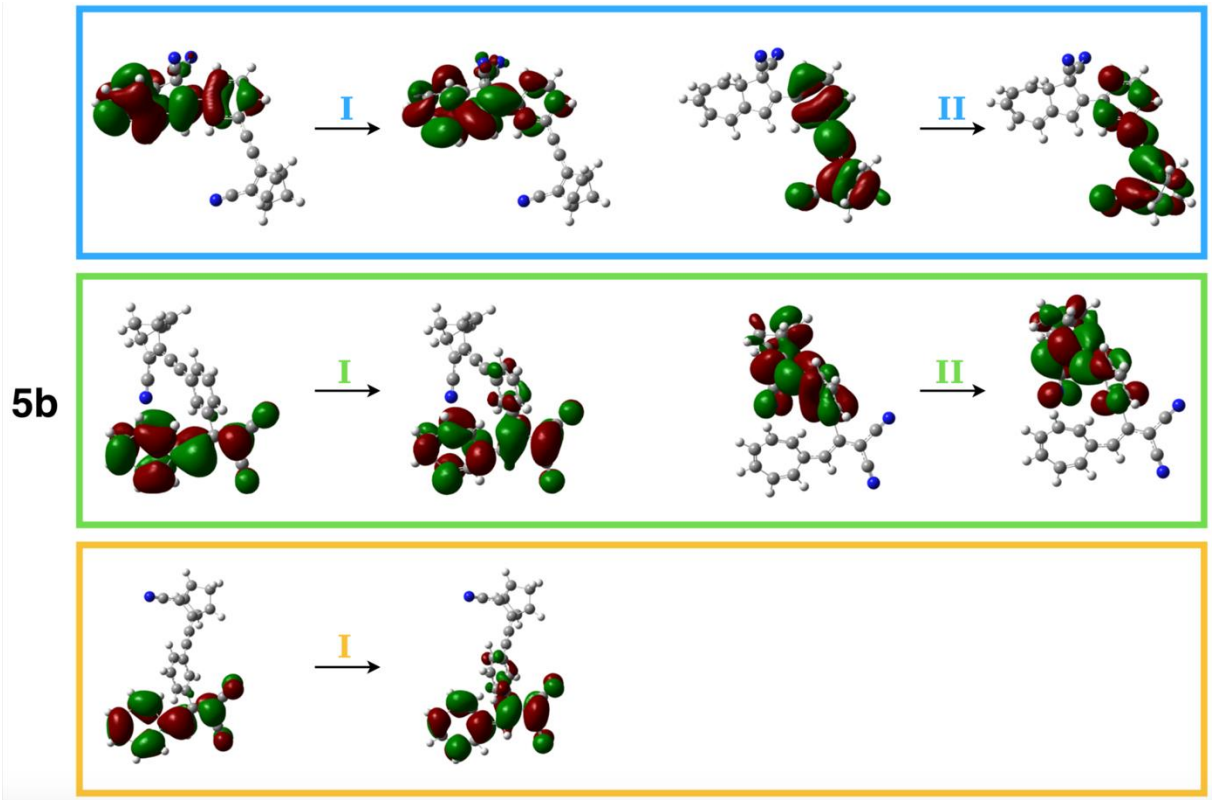

Figure S64: The NTOs of the **5b** system.

Molecular geometries

Here we present the geometries and energies of the lowest-energy conformers calculated at the CAM-B3LYP/6-311+G(d) level of theory with the IEF-PCM solvation model to mimic the polarization effects of toluene. Furthermore, we present the geometries and energies of the unsubstituted NBD/QC photothermal switch at the same level of theory. Energies are reported in units of Hartree and coordinates in units of Ångstrøm for the X-, Y-, and Z-axis, respectively, in the columns.

$3a_{NBD\text{-}DHA}$
Electronic energy: -1379.58282769
Gibbs free energy: -1379.194548

Atom	X	Y	Z
C	0.44954	-2.21238	0.68538
C	-0.40458	-3.18471	0.30087
C	-1.68767	-2.99491	-0.33444
C	0.26331	-0.77519	0.48472
C	-2.48328	-1.93521	-0.11540
C	-0.93347	-0.15460	0.52243
C	-2.17386	-0.89091	0.93074
H	-0.05835	-4.21020	0.39020
H	-2.01810	-3.76425	-1.02622
H	-0.98995	0.89812	0.27284
C	-3.74286	-1.60892	-0.74292
H	-4.15186	-2.18398	-1.56389
C	-4.34480	-0.54441	-0.19447
C	-3.50445	-0.04089	1.00296
H	-1.99938	-1.37050	1.89804
C	-4.18472	-0.34281	2.27491
C	-3.27691	1.40923	0.93155
N	-4.69664	-0.61603	3.26344
N	-3.08914	2.53717	0.85740
C	-5.60080	0.08790	-0.61588
C	-6.05463	-0.08345	-1.92959
C	-6.37078	0.86516	0.25326
C	-7.24568	0.48230	-2.34993
H	-5.45710	-0.64654	-2.63665
C	-7.56368	1.43309	-0.17034
H	-6.05999	1.02562	1.27796
H	-7.57508	0.34013	-3.37291
H	-8.14648	2.02784	0.52339
C	-8.00782	1.24237	-1.47029
H	-8.93805	1.69019	-1.80058
H	1.42273	-2.51148	1.06051
C	1.44752	-0.02395	0.21031
C	2.47526	0.56651	-0.01180
C	3.63629	1.32194	-0.26307
C	3.62936	2.86689	-0.28813
C	4.91933	0.92842	-0.40397
C	4.37519	3.33113	0.96946
C	4.75204	3.07807	-1.32868
H	2.65778	3.31912	-0.47314
C	5.75096	2.22213	-0.51319
C	5.64022	2.94885	0.83507
H	3.91114	3.82008	1.81557
H	5.06167	4.11980	-1.42302
H	4.51970	2.65803	-2.30873
H	6.75334	2.09977	-0.91706
H	6.44843	3.05410	1.54681
C	5.50474	-0.41067	-0.37919
C	6.83184	-0.59062	0.02684
C	4.77246	-1.54198	-0.76021
C	7.40092	-1.85488	0.07029
H	7.42335	0.26657	0.32713
C	5.34520	-2.80331	-0.72484
H	3.75110	-1.42673	-1.09996
C	6.66055	-2.96742	-0.30616
H	8.42833	-1.97024	0.39759
H	4.76257	-3.66485	-1.03250
H	7.10638	-3.95540	-0.27897

3a$_{NBD\text{-}s\text{-}cis\text{-}VHF}$
Electronic energy: -1379.57510627
Gibbs free energy: -1379.188951

Atom	X	Y	Z
C	2.57601	1.13196	0.14829
C	3.94022	1.14945	-0.05512
H	4.42742	2.11055	0.07198
C	4.84601	0.07715	-0.33930
C	4.54776	-1.00901	-1.13779
C	3.39389	-1.05435	-1.96788
C	5.39580	-2.15144	-1.23962
N	2.47357	-1.09761	-2.65784
N	6.03621	-3.10272	-1.33534
C	6.21068	0.22031	0.22751
C	7.34802	0.02862	-0.55798
C	6.36546	0.59185	1.56468
C	8.61248	0.19630	-0.01443
H	7.24483	-0.23208	-1.60437
C	7.63051	0.74250	2.11124
H	5.48670	0.74551	2.18063
C	8.75660	0.54665	1.32157
H	9.48759	0.05337	-0.63770
H	7.73776	1.01418	3.15515
H	9.74625	0.67045	1.74664
C	1.93318	2.41293	0.32911
H	2.61909	3.25355	0.37444
C	0.61820	2.73089	0.39837
H	0.40697	3.79206	0.48797
C	-0.54464	1.91059	0.33522
H	-1.48926	2.44243	0.31291
C	-0.61370	0.54762	0.33423
C	0.52013	-0.34618	0.42270
H	0.24874	-1.38665	0.56536
C	1.84353	-0.10332	0.33342
H	2.46847	-0.98258	0.43714
C	-1.89338	-0.07148	0.28476
C	-2.98065	-0.59288	0.22975
C	-4.22470	-1.24345	0.18706
C	-4.39694	-2.74318	0.51604
C	-5.46063	-0.73597	-0.01182
C	-5.12635	-2.81558	1.86329
C	-5.58810	-3.04120	-0.42264
H	-3.49537	-3.34294	0.41573
C	-6.43967	-1.90704	0.19815
C	-6.34364	-2.31851	1.67434
H	-4.68059	-3.15599	2.78836
H	-6.02103	-4.03044	-0.26891
H	-5.35816	-2.88441	-1.47774
H	-7.44033	-1.75390	-0.19914
H	-7.12116	-2.15891	2.40968
C	-5.88325	0.63347	-0.29396
C	-5.05894	1.53047	-0.98436
C	-7.14384	1.07804	0.12036
C	-5.47775	2.82708	-1.23702
H	-4.09223	1.19982	-1.34241
C	-7.55720	2.37897	-0.12441
H	-7.80328	0.40318	0.65395
C	-6.72601	3.25927	-0.80448
H	-4.82926	3.50296	-1.78364
H	-8.53425	2.70501	0.21453
H	-7.05183	4.27396	-1.00390

3a$_{\text{NBD-s-}\textit{trans}\text{-VHF}}$

Electronic energy: -1379.57801983

Gibbs free energy: -1379.191625

Atom	X	Y	Z
C	-2.77073	1.44841	-0.45303
C	-4.13624	1.52244	-0.27271
H	-4.55123	2.52429	-0.29687
C	-5.09844	0.48693	-0.06474
C	-6.44117	0.75552	-0.23908
C	-6.88811	2.00722	-0.75104
C	-7.46989	-0.16448	0.11077
N	-7.24121	3.02105	-1.16589
N	-8.33013	-0.87775	0.38595
C	-4.70963	-0.85955	0.42859
C	-5.05914	-2.01057	-0.27502
C	-3.99489	-0.97740	1.62080
C	-4.68507	-3.26020	0.19855
H	-5.61289	-1.92845	-1.20313
C	-3.63859	-2.22762	2.10101
H	-3.72573	-0.08501	2.17411
C	-3.97717	-3.37129	1.38756
H	-4.95502	-4.14865	-0.36051
H	-3.09472	-2.30987	3.03507
H	-3.69346	-4.34851	1.76149
C	-2.07199	2.71222	-0.51853
H	-2.72438	3.57918	-0.55693
C	-0.74534	2.98712	-0.49364
H	-0.49589	4.04354	-0.51249
C	0.38435	2.12409	-0.40638
H	1.34248	2.61917	-0.29422
C	0.40761	0.76191	-0.48539
C	-0.74820	-0.07981	-0.70697
H	-0.50067	-1.11683	-0.90840
C	-2.06750	0.20183	-0.69331
H	-2.70495	-0.64446	-0.90809
C	1.65969	0.09260	-0.39556
C	2.72379	-0.47074	-0.30727
C	3.94070	-1.16780	-0.23043
C	4.08203	-2.65154	-0.63760
C	5.17909	-0.71851	0.06913
C	4.88820	-2.67372	-1.94221
C	5.20380	-3.04703	0.34917
H	3.15632	-3.22230	-0.62630
C	6.12871	-1.91148	-0.15252
C	6.10782	-2.23372	-1.65359
H	4.48755	-2.94326	-2.91025
H	5.61190	-4.04108	0.16224
H	4.91674	-2.94254	1.39682
H	7.10818	-1.81894	0.31063
H	6.93299	-2.06098	-2.33174
C	5.63099	0.61605	0.45404
C	6.93173	1.03157	0.14762
C	4.79521	1.50774	1.13761
C	7.37429	2.30042	0.49016
H	7.60082	0.36062	-0.37876
C	5.24244	2.77161	1.48804
H	3.79480	1.19794	1.41183
C	6.53175	3.17600	1.16217
H	8.38285	2.60504	0.23379
H	4.58341	3.44355	2.02686
H	6.87973	4.16525	1.43732

$3a_{QC\text{-}DHA}$
Electronic energy: -1379.54297663
Gibbs free energy: -1379.155449

Atom	X	Y	Z
C	-0.54110	2.02120	0.89050
C	0.25471	3.02836	0.47091
C	1.51596	2.89249	-0.21899
C	-0.30572	0.59324	0.67984
C	2.36271	1.86557	-0.03828
C	0.91534	0.02267	0.66007
C	2.14178	0.80871	1.01703
H	-0.13125	4.03821	0.57456
H	1.78427	3.67555	-0.92227
H	1.00430	-1.02652	0.40513
C	3.60489	1.59063	-0.72252
H	3.95362	2.18206	-1.55950
C	4.27261	0.55029	-0.20473
C	3.50775	0.01324	1.02825
H	1.99159	1.27926	1.99276
C	4.23160	0.34306	2.26879
C	3.33672	-1.44511	0.96612
N	4.77607	0.63678	3.23381
N	3.19322	-2.58007	0.90050
C	5.53217	-0.03135	-0.68454
C	5.91619	0.15423	-2.01842
C	6.37346	-0.77382	0.14809
C	7.10818	-0.36406	-2.49387
H	5.26353	0.69044	-2.69717
C	7.56721	-1.29419	-0.33064
H	6.11800	-0.94291	1.18657
H	7.38279	-0.21193	-3.53150
H	8.20596	-1.86240	0.33559
C	7.94133	-1.08985	-1.65042
H	8.87234	-1.50063	-2.02383
H	-1.51042	2.28063	1.30294
C	-1.47441	-0.20481	0.46707
C	-2.47956	-0.84707	0.30577
C	-3.66633	-1.60093	0.12079
C	-3.72197	-3.05248	-0.33603
C	-5.10444	-1.05417	-0.13939
C	-4.26196	-2.68341	1.01527
C	-4.84726	-3.23693	-1.32584
H	-2.79015	-3.59848	-0.40597
C	-5.82820	-2.24178	-0.75247
C	-5.67408	-2.13841	0.74441
H	-3.86667	-3.03365	1.95774
H	-5.23836	-4.25825	-1.31591
H	-4.54783	-2.98704	-2.34692
H	-6.79962	-2.06483	-1.19701
H	-6.49168	-2.08794	1.44984
C	-5.48976	0.36024	-0.31459
C	-6.60108	0.89348	0.33650
C	-4.75181	1.18927	-1.16175
C	-6.97780	2.21485	0.13409
H	-7.17452	0.27013	1.01413
C	-5.12165	2.51215	-1.35703
H	-3.87907	0.79412	-1.66958
C	-6.23887	3.02996	-0.71277
H	-7.84711	2.61063	0.64802
H	-4.53574	3.14149	-2.01821
H	-6.52874	4.06341	-0.86698

3a$_{\text{QC-s-}cis\text{-VHF}}$
Electronic energy: -1379.53553917
Gibbs free energy: -1379.150266

Atom	X	Y	Z
C	-2.38379	1.74531	-0.05401
C	-3.70608	1.38154	-0.21679
H	-4.42902	2.18927	-0.16950
C	-4.29629	0.08767	-0.36835
C	-3.71906	-0.96576	-1.05193
C	-2.59037	-0.80191	-1.90057
C	-4.23854	-2.29314	-1.00815
N	-1.68775	-0.68204	-2.60502
N	-4.60804	-3.38284	-0.98430
C	-5.65710	-0.07012	0.20478
C	-6.69752	-0.62980	-0.53783
C	-5.91680	0.38368	1.49953
C	-7.96790	-0.74037	0.00662
H	-6.51888	-0.96170	-1.55348
C	-7.18337	0.25705	2.04878
H	-5.11417	0.82157	2.08202
C	-8.21195	-0.30371	1.30209
H	-8.76941	-1.16855	-0.58411
H	-7.36821	0.59732	3.06128
H	-9.20425	-0.39736	1.72872
C	-2.10128	3.16061	-0.02327
H	-2.98403	3.79263	-0.04415
C	-0.91563	3.81661	-0.02584
H	-0.99162	4.89937	-0.05241
C	0.42217	3.32843	-0.04272
H	1.19200	4.08356	-0.15560
C	0.84725	2.03983	0.09407
C	-0.01038	0.89564	0.30840
H	0.52619	-0.01580	0.54972
C	-1.35176	0.77287	0.23408
H	-1.72212	-0.22319	0.44643
C	2.24364	1.76021	0.07101
C	3.41415	1.47573	0.04963
C	4.78005	1.11003	0.03093
C	5.93521	1.66532	0.86284
C	5.90521	1.90944	-0.61615
C	5.36773	-0.32316	0.20888
C	6.50498	0.24629	1.02339
H	5.87184	2.43326	1.62010
C	6.84966	0.97131	-1.32918
H	5.67490	2.89877	-0.98962
C	6.75738	-0.21032	-0.39261
H	6.98924	-0.15743	1.90141
H	6.51125	0.73042	-2.33995
H	7.86324	1.37790	-1.38645
H	7.30961	-1.12620	-0.56101
C	4.59002	-1.57046	0.35382
C	4.87582	-2.48977	1.36123
C	3.55378	-1.85604	-0.53761
C	4.15659	-3.67349	1.46732
H	5.66476	-2.27488	2.07394
C	2.82758	-3.03283	-0.42600
H	3.31351	-1.15013	-1.32512
C	3.12879	-3.94839	0.57558
H	4.39503	-4.37857	2.25624
H	2.02521	-3.23707	-1.12645
H	2.56234	-4.86895	0.66143

3a$_{\text{QC-s-}\textit{trans}\text{-VHF}}$
Electronic energy: -1379.53822156
Gibbs free energy: -1379.154303

Atom	X	Y	Z
C	-2.69568	1.87925	0.22060
C	-4.02857	1.53375	0.12111
H	-4.72126	2.36837	0.11296
C	-4.64688	0.25012	0.03465
C	-6.00160	0.12425	0.27282
C	-6.77987	1.22416	0.73362
C	-6.72266	-1.08119	0.04206
N	-7.40172	2.11820	1.10629
N	-7.34167	-2.03502	-0.13620
C	-3.89695	-0.95746	-0.39875
C	-3.23638	-0.95473	-1.62735
C	-3.85511	-2.10073	0.39691
C	-2.54809	-2.07991	-2.05288
H	-3.27124	-0.06946	-2.25190
C	-3.14960	-3.21947	-0.02303
H	-4.36443	-2.11094	1.35363
C	-2.49773	-3.21227	-1.24868
H	-2.04995	-2.07322	-3.01565
H	-3.11685	-4.10077	0.60704
H	-1.95595	-4.09069	-1.58070
C	-2.40301	3.29321	0.16732
H	-3.28181	3.93044	0.18700
C	-1.21962	3.94340	0.05187
H	-1.29638	5.02459	-0.01036
C	0.11271	3.44904	-0.04337
H	0.87385	4.19514	-0.24261
C	0.54318	2.16544	0.11912
C	-0.30109	1.03821	0.44924
H	0.25111	0.13747	0.69669
C	-1.64466	0.91658	0.49012
H	-1.99208	-0.06328	0.78643
C	1.93486	1.87983	0.01234
C	3.10439	1.60223	-0.07104
C	4.47347	1.25796	-0.15706
C	5.53383	2.02900	-0.93579
C	5.10746	-0.14577	0.08577
C	5.66718	1.89704	0.55136
C	6.45241	1.05909	-1.64003
H	5.25526	2.98300	-1.36420
C	6.45148	-0.05058	-0.61513
C	6.28138	0.50583	0.77699
H	5.63452	2.71798	1.25284
H	7.44958	1.48038	-1.79486
H	6.05504	0.73653	-2.60564
H	7.01463	-0.96503	-0.75225
H	6.83284	0.17947	1.64739
C	4.37426	-1.39506	0.37380
C	4.74188	-2.22472	1.43120
C	3.29783	-1.77506	-0.43046
C	4.06343	-3.41294	1.67103
H	5.56325	-1.93571	2.07785
C	2.61280	-2.95615	-0.18536
H	2.99542	-1.13884	-1.25523
C	2.99539	-3.78221	0.86499
H	4.36569	-4.04712	2.49727
H	1.77835	-3.23525	-0.81961
H	2.46141	-4.70646	1.05545

$3b_{NBD-DHA}$
Electronic energy: -1240.84206537
Gibbs free energy: -1240.532301

Atom	X	Y	Z
C	-1.01949	2.70801	0.18134
C	-0.04762	3.49888	-0.32110
C	1.21502	3.06241	-0.86860
C	-0.99632	1.24706	0.21977
C	1.87624	1.96731	-0.45870
C	0.11513	0.50316	0.39353
C	1.42899	1.14213	0.72499
H	-0.27184	4.55736	-0.41258
H	1.64884	3.66988	-1.65749
H	0.04602	-0.57498	0.31178
C	3.10251	1.40927	-0.97917
H	3.59219	1.80176	-1.86115
C	3.56637	0.38300	-0.25254
C	2.64545	0.16315	0.97115
H	1.29784	1.78392	1.60087
C	3.32659	0.56474	2.21454
C	2.24422	-1.24529	1.09532
N	3.84261	0.91646	3.17564
N	1.91732	-2.34092	1.17109
C	4.75036	-0.44129	-0.52348
C	5.26016	-0.51252	-1.82595
C	5.39653	-1.16818	0.47973
C	6.38714	-1.26432	-2.10823
H	4.75602	0.00825	-2.63128
C	6.52527	-1.92293	0.19459
H	5.03940	-1.14366	1.50151
H	6.76155	-1.30811	-3.12461
H	7.01261	-2.47414	0.99037
C	7.02698	-1.97229	-1.09735
H	7.90679	-2.56536	-1.31898
H	-1.95864	3.17244	0.46202
C	-2.25245	0.59277	0.03266
C	-3.33210	0.07968	-0.11618
C	-4.57310	-0.55406	-0.29054
C	-4.77682	-2.08117	-0.35292
C	-5.80083	-0.00649	-0.37682
C	-5.53616	-2.47020	0.92285
C	-5.95619	-2.11449	-1.35700
H	-3.88093	-2.65172	-0.58264
C	-6.81242	-1.16197	-0.48530
C	-6.13447	1.36247	-0.30194
C	-6.74521	-1.92722	0.84365
H	-5.10773	-3.03507	1.73933
H	-6.39461	-3.10678	-1.46117
H	-5.70798	-1.70079	-2.33559
H	-7.80044	-0.88250	-0.84148
N	-6.43213	2.47377	-0.24809
H	-7.53626	-1.94537	1.58083

$3b_{NBD\text{-}s\text{-}cis\text{-}VHF}$
Electronic energy: -1240.83316675
Gibbs free energy: -1240.525479

Atom	X	Y	Z
C	1.83654	-1.22674	-0.33947
C	3.18324	-1.02380	-0.52838
H	3.76430	-1.89580	-0.80975
C	3.97498	0.15982	-0.33425
C	3.55157	1.43465	-0.63931
C	2.37403	1.69040	-1.39673
C	4.27798	2.60453	-0.26385
N	1.43348	1.91551	-2.02020
N	4.81483	3.57633	0.03739
C	5.35355	-0.06439	0.16615
C	6.45519	0.54285	-0.43832
C	5.56228	-0.93202	1.24055
C	7.73662	0.29478	0.02923
H	6.31376	1.19471	-1.29183
C	6.84259	-1.16541	1.71760
H	4.71220	-1.41087	1.71309
C	7.93243	-0.55337	1.11116
H	8.58453	0.76509	-0.45496
H	6.99035	-1.82729	2.56320
H	8.93473	-0.74078	1.47937
C	1.32519	-2.53619	-0.68931
H	2.09297	-3.25508	-0.95949
C	0.05231	-2.98358	-0.78065
H	-0.05510	-4.00915	-1.11927
C	-1.18656	-2.31425	-0.54506
H	-2.07610	-2.87350	-0.81224
C	-1.38195	-1.08058	-0.00216
C	-0.34277	-0.19200	0.47204
H	-0.71299	0.66789	1.01977
C	0.99478	-0.24978	0.32276
H	1.53592	0.56533	0.78899
C	-2.72078	-0.62210	0.16098
C	-3.85379	-0.23410	0.29550
C	-5.16798	0.23213	0.45230
C	-5.55297	1.64885	0.92241
C	-6.32540	-0.40368	0.18381
C	-6.18528	2.34974	-0.28771
C	-6.84540	1.28932	1.69769
H	-4.76575	2.18686	1.44367
C	-7.46922	0.58656	0.46568
C	-6.48410	-1.70769	-0.33156
C	-7.32319	1.72138	-0.55777
H	-5.72527	3.16469	-0.82937
H	-7.40604	2.16801	2.01558
H	-6.67612	0.61760	2.54068
H	-8.45499	0.14065	0.56766
N	-6.63808	-2.77098	-0.74618
H	-8.01122	1.90343	-1.37193

3b$_{\text{NBD-s-}\textit{trans}\text{-VHF}}$
Electronic energy: -1240.83573282
Gibbs free energy: -1240.528399

Atom	X	Y	Z
C	-2.10549	1.56388	-0.13575
C	-3.46887	1.45624	0.00962
H	-3.99450	2.39140	0.16955
C	-4.31114	0.29734	-0.02392
C	-5.66781	0.44785	-0.20963
C	-6.24209	1.71928	-0.50102
C	-6.59405	-0.62786	-0.08921
N	-6.69836	2.74893	-0.73652
N	-7.37411	-1.46823	0.00517
C	-3.77729	-1.06517	0.22901
C	-3.98392	-2.09808	-0.68363
C	-3.06814	-1.32088	1.40299
C	-3.47556	-3.36460	-0.43257
H	-4.53083	-1.90783	-1.59985
C	-2.57813	-2.59139	1.65993
H	-2.90956	-0.52198	2.11821
C	-2.77518	-3.61423	0.73979
H	-3.63509	-4.15907	-1.15230
H	-2.04081	-2.78405	2.58141
H	-2.38704	-4.60654	0.93957
C	-1.55040	2.88800	0.06065
H	-2.29549	3.67413	0.13690
C	-0.26741	3.29001	0.21149
H	-0.13343	4.35098	0.39648
C	0.94589	2.53865	0.21194
H	1.83714	3.09110	0.48757
C	1.11835	1.23043	-0.12657
C	0.07810	0.33440	-0.58442
H	0.44959	-0.60591	-0.97809
C	-1.26295	0.47029	-0.58884
H	-1.79705	-0.37162	-1.00713
C	2.43695	0.69295	-0.08294
C	3.55420	0.24272	-0.04072
C	4.85150	-0.29017	0.00837
C	5.24041	-1.71651	-0.42858
C	5.99657	0.31591	0.37921
C	6.10329	-1.56476	-1.68864
C	6.36487	-1.97344	0.60616
H	4.41334	-2.41944	-0.48256
C	7.13717	-0.69830	0.18354
C	6.15730	1.65352	0.79929
C	7.22931	-0.96218	-1.32582
H	5.78997	-1.85567	-2.68186
H	6.91875	-2.89108	0.40975
H	6.01982	-1.94843	1.64090
H	8.06417	-0.45982	0.69797
N	6.31063	2.74013	1.14827
H	8.05114	-0.64550	-1.95325

$3b_{QC\text{-}DHA}$
Electronic energy: -1240.80432961
Gibbs free energy: -1240.494716

Atom	X	Y	Z
C	-1.10327	2.57075	0.28807
C	-0.19010	3.37436	-0.29831
C	1.05743	2.96060	-0.89557
C	-1.02768	1.11421	0.38368
C	1.77848	1.90738	-0.47690
C	0.11841	0.41983	0.52626
C	1.42277	1.12066	0.76185
H	-0.45978	4.41903	-0.42129
H	1.42505	3.54745	-1.73233
H	0.08833	-0.66256	0.49103
C	2.99332	1.36676	-1.04098
H	3.42096	1.73470	-1.96489
C	3.53074	0.38923	-0.29804
C	2.68644	0.19697	0.98415
H	1.31470	1.79519	1.61592
C	3.42019	0.68274	2.16605
C	2.34628	-1.21666	1.19911
N	3.97580	1.09903	3.07813
N	2.06906	-2.31843	1.34850
C	4.72666	-0.40722	-0.59873
C	5.45625	-1.05991	0.39829
C	5.16309	-0.52661	-1.92407
C	6.59432	-1.78853	0.08364
H	5.15743	-0.99604	1.43697
C	6.29954	-1.25217	-2.23598
H	4.59383	-0.06530	-2.72226
H	7.14685	-2.28170	0.87495
H	6.61614	-1.33425	-3.26953
C	7.02272	-1.88552	-1.23182
H	7.91006	-2.45809	-1.47628
H	-2.04320	3.01481	0.59804
C	-2.27454	0.41667	0.29320
C	-3.33663	-0.14333	0.22504
C	-4.59459	-0.79190	0.13977
C	-4.82787	-2.28728	-0.00764
C	-5.92283	-0.16315	-0.36568
C	-5.37950	-1.56896	1.19063
C	-5.91550	-2.54963	-1.02254
H	-3.97544	-2.94248	0.11184
C	-6.79326	-1.35195	-0.74648
C	-6.11466	1.16963	-0.80970
C	-6.69248	-0.94134	0.69192
H	-5.09744	-1.75259	2.21655
H	-6.43991	-3.48868	-0.82890
H	-5.53707	-2.56144	-2.04672
H	-7.70674	-1.15933	-1.29359
N	-6.26834	2.25325	-1.16372
H	-7.51198	-0.57941	1.29469

3b$_{\text{QC-s-}cis\text{-VHF}}$
Electronic energy: -1240.79604367
Gibbs free energy: -1240.488925

Atom	X	Y	Z
C	1.79300	1.16239	-0.38968
C	3.15365	0.99968	-0.54493
H	3.70803	1.88637	-0.83422
C	3.98009	-0.14668	-0.31209
C	3.60163	-1.45071	-0.56269
C	2.44128	-1.78120	-1.31548
C	4.36826	-2.57488	-0.13433
N	1.51459	-2.06536	-1.93633
N	4.94029	-3.51173	0.21104
C	5.35582	0.13921	0.16725
C	5.54683	1.04427	1.21338
C	6.47068	-0.44910	-0.43128
C	6.82374	1.33437	1.66843
H	4.68596	1.50796	1.68151
C	7.74815	-0.14486	0.01358
H	6.34125	-1.13143	-1.26269
C	7.92708	0.74130	1.06765
H	6.95810	2.02542	2.49272
H	8.60614	-0.60140	-0.46613
H	8.92642	0.97252	1.41870
C	1.24347	2.43693	-0.79278
H	1.98845	3.17060	-1.08569
C	-0.04473	2.83668	-0.91045
H	-0.18094	3.84504	-1.28889
C	-1.26378	2.14068	-0.66093
H	-2.16728	2.66489	-0.95137
C	-1.42677	0.91982	-0.07867
C	-0.36293	0.08421	0.43019
H	-0.70808	-0.77091	1.00136
C	0.97491	0.18054	0.29030
H	1.53545	-0.60280	0.78691
C	-2.74984	0.41559	0.09415
C	-3.85927	-0.02843	0.23582
C	-5.17811	-0.51839	0.39155
C	-5.83863	-1.21840	1.57534
C	-5.61750	-1.97327	0.29772
C	-6.48884	0.27763	0.14839
C	-7.13391	-0.42358	1.33535
H	-5.38999	-1.45323	2.52895
C	-6.90057	-2.07769	-0.49225
H	-4.84405	-2.72805	0.25169
C	-7.55526	-0.78809	-0.05655
C	-6.58958	1.63316	-0.25496
H	-7.77235	0.02200	2.08343
H	-6.72589	-2.11361	-1.56931
H	-7.49099	-2.94978	-0.20070
H	-8.52500	-0.47444	-0.41973
N	-6.66321	2.73478	-0.57740

3b$_{\text{QC-s-}\textit{trans}\text{-VHF}}$
Electronic energy: -1240.79864711
Gibbs free energy: -1240.491759

Atom	X	Y	Z
C	2.08514	1.69749	0.02263
C	3.44016	1.46340	-0.07162
H	4.05068	2.34483	-0.23554
C	4.17615	0.24080	0.02131
C	5.53833	0.27886	0.23703
C	6.21505	1.50419	0.50137
C	6.36852	-0.87639	0.17456
N	6.75459	2.49817	0.71457
N	7.07448	-1.78395	0.12736
C	3.53335	-1.08015	-0.19771
C	3.61592	-2.08630	0.76303
C	2.84160	-1.32263	-1.38471
C	2.99987	-3.31086	0.54732
H	4.14881	-1.90549	1.68939
C	2.24349	-2.55305	-1.60538
H	2.77921	-0.54445	-2.13676
C	2.31480	-3.54706	-0.63669
H	3.05998	-4.08290	1.30557
H	1.71691	-2.73626	-2.53494
H	1.83789	-4.50563	-0.80611
C	1.65909	3.05659	-0.23254
H	2.47486	3.76627	-0.33065
C	0.41988	3.57137	-0.41198
H	0.39182	4.63313	-0.63658
C	-0.86161	2.94584	-0.39498
H	-1.69260	3.57907	-0.68530
C	-1.16348	1.66975	-0.02747
C	-0.21474	0.68726	0.44972
H	-0.67602	-0.21112	0.84629
C	1.13412	0.69704	0.47170
H	1.57700	-0.18810	0.90637
C	-2.52572	1.24668	-0.05581
C	-3.66627	0.86284	-0.06961
C	-4.99807	0.38309	-0.08612
C	-6.26163	1.20627	0.12381
C	-5.45223	-1.07056	0.21665
C	-6.06610	0.47571	-1.17206
C	-7.22371	0.46124	1.01881
H	-6.16127	2.28307	0.14826
C	-6.92802	-0.94902	0.56593
C	-6.50930	-0.96688	-0.87348
C	-4.61285	-2.16288	0.55254
H	-5.97069	0.93610	-2.14400
H	-8.26255	0.73892	0.82435
H	-7.01050	0.61201	2.07888
H	-7.42385	-1.81328	0.98759
H	-6.77787	-1.72718	-1.59149
N	-3.92508	-3.04492	0.82051

4a$_{NBD-DHA}$
Electronic energy: -1379.58497453
Gibbs free energy: -1379.196007

Atom	X	Y	Z
C	8.53686	1.20729	0.53482
C	7.94081	2.03654	-0.35298
C	6.51965	2.19901	-0.53851
C	7.85914	0.35022	1.48584
C	5.60563	1.23506	-0.32793
C	6.67262	-0.24385	1.30939
C	5.97343	-0.19622	-0.02106
H	9.61572	1.27776	0.63643
H	8.57882	2.72292	-0.90177
H	6.17402	3.17550	-0.86590
H	6.22212	-0.79117	2.12943
C	4.16829	1.34191	-0.40820
H	3.66495	2.28547	-0.57652
C	3.54067	0.16447	-0.27105
C	4.59232	-0.96055	-0.12588
H	6.65178	-0.58107	-0.78743
C	4.61435	-1.80892	-1.33039
C	4.30971	-1.81374	1.03731
N	4.65830	-2.44187	-2.28507
N	4.09264	-2.46251	1.95661
H	8.36476	0.19746	2.43518
C	2.09637	-0.08177	-0.25546
C	1.55062	-1.34325	-0.51155
C	1.21155	0.96861	0.02409
C	0.18223	-1.54447	-0.51121
H	2.18752	-2.19017	-0.73246
C	-0.15407	0.77389	0.02477
H	1.59866	1.95050	0.26831
H	-0.81803	1.59885	0.25339
C	-0.69568	-0.48953	-0.24762
H	-0.21580	-2.53012	-0.71901
C	-2.10389	-0.69296	-0.24636
C	-3.30070	-0.84523	-0.24720
C	-4.68595	-1.09021	-0.24333
C	-5.27484	-2.51884	-0.22314
C	-5.72347	-0.23247	-0.14410
C	-5.88589	-2.72298	1.16885
C	-6.56948	-2.23807	-1.01881
H	-4.60446	-3.29722	-0.58022
C	-6.99021	-1.10620	-0.05065
C	-6.90941	-1.88246	1.27163
H	-5.49080	-3.38977	1.92357
H	-7.26544	-3.07811	-1.02001
H	-6.38607	-1.89212	-2.03742
H	-7.92672	-0.59256	-0.25535
H	-7.54352	-1.70514	2.13029
C	-5.73773	1.22574	-0.05092
C	-4.72421	2.01002	-0.61544
C	-6.78545	1.87728	0.60962
C	-4.75473	3.39150	-0.51106
H	-3.91633	1.53069	-1.15348
C	-6.80979	3.25957	0.72122
H	-7.58427	1.29564	1.05517
C	-5.79468	4.02339	0.16085
H	-3.96457	3.98061	-0.96374
H	-7.62702	3.74166	1.24629
H	-5.81638	5.10443	0.24126

4a$_{NBD\text{-}s\text{-}cis\text{-}VHF}$
Electronic energy: -1379.57577808
Gibbs free energy: -1379.189355

Atom	X	Y	Z
C	5.29723	0.83440	0.66962
C	4.13824	0.10879	0.85604
H	3.55023	0.36951	1.72974
C	3.53630	-0.89947	0.03625
C	4.23876	-1.84280	-0.68899
C	5.62858	-2.07361	-0.49853
C	3.62320	-2.69541	-1.65224
N	6.75016	-2.28177	-0.34418
N	3.17296	-3.38680	-2.45451
C	2.05422	-0.93996	0.05245
C	1.35578	-2.13614	0.22786
C	1.32844	0.24750	-0.06982
C	-0.02580	-2.14808	0.27085
H	1.89693	-3.06561	0.35539
C	-0.05335	0.23981	-0.04476
H	1.85674	1.18459	-0.20243
C	-0.75296	-0.96093	0.12697
H	-0.60468	1.16597	-0.15314
C	5.67594	1.72510	1.74810
H	4.93999	1.78945	2.54420
C	6.80607	2.44074	1.94529
H	6.84661	2.99289	2.87933
C	7.97645	2.56027	1.12933
C	8.15293	2.08790	-0.12406
C	7.20760	1.36600	-0.92081
H	7.51172	1.20977	-1.95115
C	6.01077	0.83143	-0.58833
H	5.49296	0.33076	-1.39797
H	9.10160	2.30125	-0.60543
H	8.79640	3.11904	1.56844
H	-0.55427	-3.08199	0.41791
C	-2.17602	-0.96932	0.16040
C	-3.38203	-0.95261	0.17814
C	-4.78754	-0.98978	0.22559
C	-5.57031	-2.21479	0.74936
C	-5.69233	-0.02244	-0.03384
C	-6.17836	-1.80514	2.09665
C	-6.82736	-2.07246	-0.13838
H	-5.02281	-3.15420	0.72672
C	-7.06714	-0.61689	0.33052
C	-7.07149	-0.85388	1.84753
H	-5.86796	-2.19453	3.05708
H	-7.63431	-2.74950	0.14522
H	-6.61598	-2.15550	-1.20572
H	-7.92573	-0.09126	-0.08099
H	-7.65887	-0.28751	2.55819
C	-5.49970	1.35348	-0.48667
C	-6.42739	2.34273	-0.14153
C	-4.40258	1.72251	-1.27466
C	-6.25480	3.65702	-0.54961
H	-7.28723	2.08467	0.46605
C	-4.23657	3.03428	-1.68951
H	-3.68573	0.96977	-1.57703
C	-5.15869	4.00883	-1.32604
H	-6.98182	4.40856	-0.26221
H	-3.38526	3.29690	-2.30803
H	-5.02696	5.03442	-1.65231

4a$_{\text{NBD-s-}\textit{trans}\text{-VHF}}$
Electronic energy: -1379.57851858
Gibbs free energy: -1379.192617

Atom	X	Y	Z
C	4.68150	1.30962	0.35791
C	4.95426	0.11765	-0.28095
H	5.91326	0.07123	-0.78534
C	4.17672	-1.07801	-0.37422
C	4.78229	-2.26035	-0.75125
C	6.19402	-2.34997	-0.91611
C	4.05573	-3.44926	-1.04309
N	7.33572	-2.41439	-1.04679
N	3.50312	-4.42770	-1.29172
C	2.70702	-1.07348	-0.16875
C	2.10155	-1.94018	0.74015
C	1.90678	-0.19574	-0.90178
C	0.73079	-1.92013	0.92680
H	2.70857	-2.62541	1.32004
C	0.53565	-0.18488	-0.73223
H	2.36592	0.47905	-1.61476
C	-0.07425	-1.04378	0.19123
H	0.27258	-2.59138	1.64276
C	5.64942	2.36978	0.15116
H	6.54843	2.04798	-0.36590
C	5.59869	3.68711	0.45284
H	6.46189	4.26623	0.13929
C	4.56886	4.44765	1.09398
C	3.45732	3.97227	1.69687
C	3.06647	2.60160	1.83744
H	2.21521	2.44244	2.49253
C	3.57778	1.47885	1.28245
H	3.08846	0.56219	1.58119
H	2.80009	4.69565	2.16817
H	4.72684	5.52089	1.11887
H	-0.07741	0.49433	-1.31218
C	-1.48604	-1.02455	0.37437
C	-2.68420	-0.99604	0.51079
C	-4.07504	-0.99874	0.72256
C	-4.73681	-1.76785	1.88802
C	-5.05182	-0.30723	0.09852
C	-5.23760	-0.71371	2.88340
C	-6.07742	-2.10742	1.19812
H	-4.14323	-2.58215	2.29711
C	-6.35167	-0.62071	0.86560
C	-6.20091	-0.03057	2.27507
H	-4.81865	-0.54556	3.86658
H	-6.81582	-2.53493	1.87779
H	-5.96272	-2.73613	0.31367
H	-7.27264	-0.38554	0.33712
H	-6.75007	0.82427	2.64728
C	-4.97834	0.62983	-1.02043
C	-5.92132	1.65698	-1.13918
C	-3.98310	0.53000	-2.00035
C	-5.86006	2.56501	-2.18581
H	-6.70453	1.75646	-0.39637
C	-3.92884	1.43242	-3.05068
H	-3.25903	-0.27291	-1.94540
C	-4.86357	2.45675	-3.14670
H	-6.59636	3.35836	-2.25239
H	-3.15628	1.33079	-3.80504
H	-4.81962	3.16108	-3.96987

$4a_{QC\text{-}DHA}$
Electronic energy: -1379.54497155
Gibbs free energy: -1379.157617

Atom	X	Y	Z
C	8.43294	1.33133	0.37380
C	7.78760	2.10877	-0.52637
C	6.35754	2.22117	-0.67816
C	7.80778	0.48989	1.37355
C	5.48021	1.23822	-0.40783
C	6.63617	-0.14593	1.25126
C	5.90165	-0.16883	-0.06068
H	9.51140	1.43817	0.44288
H	8.38906	2.79344	-1.11707
H	5.97293	3.17426	-1.03025
H	6.22430	-0.67558	2.10264
C	4.03834	1.29743	-0.45039
H	3.50010	2.21801	-0.63695
C	3.45268	0.10702	-0.25341
C	4.54366	-0.97894	-0.10085
H	6.57224	-0.55996	-0.83073
C	4.55953	-1.86585	-1.27730
C	4.32129	-1.80157	1.09687
N	4.59763	-2.52888	-2.21162
N	4.15172	-2.42620	2.04251
H	8.34269	0.38808	2.31365
C	2.01809	-0.18362	-0.18665
C	1.10826	0.84805	0.08095
C	1.50536	-1.46906	-0.38256
C	-0.25015	0.61159	0.12890
H	1.47049	1.84981	0.27847
C	0.14389	-1.71162	-0.33681
H	2.16196	-2.30378	-0.59251
H	-0.22784	-2.71583	-0.50000
C	-0.75875	-0.67626	-0.08338
H	-0.93380	1.42369	0.34521
C	-2.16186	-0.92065	-0.03138
C	-3.34849	-1.11913	0.01563
C	-4.74777	-1.33607	0.08020
C	-5.46762	-2.59827	-0.37491
C	-5.86758	-0.25201	0.15327
C	-5.53852	-2.18897	1.06784
C	-6.74330	-2.23083	-1.09438
H	-4.86569	-3.45228	-0.65721
C	-7.11039	-0.99740	-0.30346
C	-6.63746	-1.11498	1.12426
H	-5.13835	-2.75778	1.89456
H	-7.50015	-3.01618	-1.01358
H	-6.57599	-2.01380	-2.15248
H	-7.99659	-0.41392	-0.51951
H	-7.21130	-0.82485	1.99324
C	-5.67857	1.21090	0.08734
C	-4.88079	1.77019	-0.91290
C	-6.30078	2.06321	0.99768
C	-4.71797	3.14494	-1.00304
H	-4.38286	1.12133	-1.62502
C	-6.14629	3.44032	0.90250
H	-6.90759	1.64467	1.79335
C	-5.35327	3.98653	-0.09750
H	-4.09471	3.56189	-1.78678
H	-6.64069	4.08751	1.61882
H	-5.22759	5.06116	-0.16944

4a$_{\text{QC-s-}cis\text{-VHF}}$

Electronic energy: -1379.53517658

Gibbs free energy: -1379.152337

Atom	X	Y	Z
C	-5.15968	0.92852	-0.38974
C	-4.01819	0.24318	-0.75005
H	-3.42407	0.69037	-1.54008
C	-3.43918	-0.94441	-0.19472
C	-4.16772	-2.01794	0.28051
C	-5.56061	-2.16388	0.03505
C	-3.58129	-3.09088	1.01444
N	-6.68497	-2.30383	-0.16826
N	-3.15738	-3.96580	1.63025
C	-1.95905	-1.00932	-0.21643
C	-1.28053	-2.14818	-0.65440
C	-1.21122	0.10493	0.17294
C	0.10109	-2.17729	-0.69377
H	-1.83670	-3.01444	-0.99102
C	0.17050	0.07588	0.15194
H	-1.72238	0.99763	0.51469
C	0.84903	-1.06825	-0.28394
H	0.73822	0.94019	0.47462
C	-5.51926	2.05892	-1.22287
H	-4.78260	2.29492	-1.98523
C	-6.63299	2.82507	-1.23707
H	-6.66181	3.58489	-2.01222
C	-7.80016	2.77210	-0.40885
C	-7.98644	2.01871	0.69670
C	-7.05704	1.10677	1.29284
H	-7.36413	0.71574	2.25788
C	-5.87307	0.64086	0.83559
H	-5.36651	-0.05022	1.49908
H	-8.92986	2.13154	1.22066
H	-8.60777	3.43683	-0.69748
H	0.61269	-3.06465	-1.04607
C	2.27367	-1.09792	-0.31234
C	3.47738	-1.12241	-0.32561
C	4.89387	-1.12550	-0.34106
C	5.77650	-2.33633	-0.06394
C	5.83630	0.10047	-0.10747
C	5.85643	-1.65541	-1.39889
C	6.93837	-1.93507	0.81329
H	5.29620	-3.30321	0.01326
C	7.14475	-0.52945	0.29777
C	6.77319	-0.44388	-1.16662
H	5.60124	-2.11346	-2.34370
H	7.81298	-2.57065	0.64975
H	6.68184	-1.95810	1.87548
H	7.93640	0.10830	0.67084
H	7.33228	0.10221	-1.91324
C	5.39485	1.48546	0.17117
C	5.76968	2.14065	1.34229
C	4.57189	2.15779	-0.73460
C	5.34363	3.43779	1.60043
H	6.40049	1.62750	2.05998
C	4.14116	3.45082	-0.47777
H	4.27103	1.66119	-1.65087
C	4.52762	4.09647	0.69134
H	5.64826	3.93272	2.51617
H	3.50545	3.95947	-1.19442
H	4.19427	5.10891	0.89095

4a$_{\text{QC-s-}\textit{trans}\text{-VHF}}$
Electronic energy: -1379.53837136
Gibbs free energy: -1379.154267

Atom	X	Y	Z
C	-4.57668	1.27845	0.30115
C	-4.85139	0.08914	-0.34013
H	-5.79340	0.05799	-0.87673
C	-4.09505	-1.12360	-0.39643
C	-4.71659	-2.29856	-0.76930
C	-6.12617	-2.36132	-0.96350
C	-4.01002	-3.50747	-1.02668
N	-7.26586	-2.40415	-1.11836
N	-3.47528	-4.50222	-1.24802
C	-2.63130	-1.14277	-0.15621
C	-2.06072	-2.01396	0.77053
C	-1.79886	-0.28399	-0.87583
C	-0.69406	-2.01572	0.98818
H	-2.69175	-2.68492	1.34151
C	-0.43127	-0.29828	-0.67836
H	-2.22924	0.39296	-1.60460
C	0.14253	-1.16039	0.26430
H	-0.26460	-2.68930	1.71971
C	-5.51555	2.35717	0.05702
H	-6.40132	2.05133	-0.49163
C	-5.45040	3.67374	0.35805
H	-6.29026	4.26868	0.01241
C	-4.43045	4.41596	1.03628
C	-3.35093	3.92090	1.67963
C	-2.99008	2.54312	1.83450
H	-2.16584	2.36929	2.51977
C	-3.50163	1.42931	1.26266
H	-3.03988	0.50405	1.57847
H	-2.69836	4.63264	2.17465
H	-4.56945	5.49198	1.05475
H	0.20766	0.35917	-1.25545
C	1.55255	-1.16603	0.47563
C	2.74464	-1.16986	0.64399
C	4.15070	-1.17075	0.82133
C	4.88894	-1.73404	2.02872
C	5.18948	-0.23471	0.12925
C	5.12957	-2.33180	0.67315
C	6.02283	-0.81332	2.41193
H	4.31646	-2.28834	2.76111
C	6.40689	-0.32949	1.03349
C	6.14599	-1.39577	-0.00131
H	4.88872	-3.34628	0.39051
H	6.83775	-1.35060	2.90517
H	5.69552	0.00057	3.06404
H	7.21105	0.37731	0.87162
H	6.81258	-1.64724	-0.81424
C	4.88810	0.88776	-0.78158
C	5.55909	1.03769	-1.99373
C	3.92824	1.83830	-0.42816
C	5.29256	2.11807	-2.82508
H	6.29304	0.29768	-2.29383
C	3.65428	2.91249	-1.26212
H	3.39148	1.73293	0.50835
C	4.33824	3.05895	-2.46320
H	5.82656	2.21850	-3.76374
H	2.90533	3.64148	-0.97180
H	4.12514	3.89933	-3.11444

$4b_{NBD-DHA}$
Electronic energy: -1240.84417787
Gibbs free energy: -1240.533743

Atom	X	Y	Z
C	-7.87092	-0.80469	0.46327
C	-7.35873	-1.65742	-0.45401
C	-5.96056	-1.95799	-0.64202
C	-7.11417	-0.05709	1.44656
C	-4.95455	-1.10024	-0.39510
C	-5.87263	0.41926	1.29378
C	-5.17536	0.34925	-0.03676
H	-8.95180	-0.76786	0.56088
H	-8.06057	-2.25430	-1.02875
H	-5.71497	-2.95292	-1.00259
H	-5.37309	0.88784	2.13400
C	-3.53532	-1.35166	-0.47444
H	-3.13027	-2.33515	-0.67587
C	-2.79165	-0.25058	-0.29193
C	-3.72250	0.97098	-0.11060
H	-5.80632	0.82983	-0.78942
C	-3.64837	1.85792	-1.28495
C	-3.36157	1.75080	1.08207
N	-3.61756	2.52465	-2.21686
N	-3.08275	2.34267	2.02284
H	-7.60657	0.11130	2.40014
C	-1.32906	-0.15756	-0.26390
C	-0.56238	-1.30592	-0.02271
C	-0.65439	1.04960	-0.47021
C	0.81577	-1.25642	-0.01087
H	-1.05185	-2.25041	0.18048
C	0.72749	1.10641	-0.45760
H	-1.19828	1.96582	-0.66024
H	1.22851	2.05184	-0.62545
C	1.48427	-0.04551	-0.23138
H	1.38980	-2.15454	0.18160
C	2.90578	0.00551	-0.21510
C	4.11061	0.02566	-0.19859
C	5.51332	0.07122	-0.18480
C	6.35377	1.35287	-0.35376
C	6.39137	-0.92976	0.02261
C	7.02630	1.61309	1.00088
C	7.55910	0.73893	-1.10926
H	5.82606	2.18768	-0.80718
C	7.80258	-0.31517	-0.00023
C	6.09803	-2.28335	0.29141
C	7.88786	0.62472	1.21023
H	6.77262	2.43098	1.66120
H	8.38766	1.43779	-1.22250
H	7.29305	0.30102	-2.07249
H	8.61599	-1.02422	-0.12966
N	5.88495	-3.39429	0.50810
H	8.50298	0.44696	2.08175

4b$_{NBD\text{-}s\text{-}cis\text{-}VHF}$
Electronic energy: -1240.83468805
Gibbs free energy: -1240.526511

Atom	X	Y	Z
C	-4.66988	-0.93619	0.34048
C	-3.42836	-0.43435	0.68232
H	-2.84472	-1.03931	1.36827
C	-2.74703	0.73484	0.22145
C	-3.36011	1.93167	-0.09864
C	-4.71195	2.21138	0.23967
C	-2.67604	3.00235	-0.74588
N	-5.80092	2.45479	0.52257
N	-2.16767	3.88221	-1.28608
C	-1.26654	0.63494	0.16496
C	-0.44747	1.62444	0.71106
C	-0.67209	-0.48927	-0.41234
C	0.92886	1.50029	0.67327
H	-0.88873	2.49034	1.18882
C	0.70350	-0.61329	-0.46643
H	-1.29739	-1.26555	-0.83752
C	1.52211	0.38241	0.07792
H	1.15558	-1.48143	-0.93010
C	-5.11580	-2.09944	1.07819
H	-4.37138	-2.50157	1.75904
C	-6.31354	-2.72808	1.09428
H	-6.39007	-3.55879	1.78917
C	-7.51065	-2.45055	0.36163
C	-7.66822	-1.56256	-0.64511
C	-6.67199	-0.70400	-1.20802
H	-6.98509	-0.17439	-2.10233
C	-5.41373	-0.43254	-0.79143
H	-4.86686	0.26422	-1.41557
H	-8.64708	-1.50843	-1.10988
H	-8.37482	-3.04637	0.63652
H	1.55441	2.27011	1.10807
C	2.93903	0.25191	0.02845
C	4.13558	0.12195	-0.02470
C	5.53231	-0.00844	-0.08241
C	6.53754	1.03935	0.43607
C	6.26679	-1.04479	-0.53152
C	7.23054	0.41228	1.65330
C	7.65450	0.82481	-0.61625
H	6.12940	2.03822	0.56484
C	7.74765	-0.69035	-0.30626
C	5.79256	-2.27101	-1.04393
C	7.95055	-0.61285	1.21317
H	7.08578	0.73926	2.67383
H	8.56987	1.36586	-0.37744
H	7.33806	1.03967	-1.63799
H	8.45935	-1.29069	-0.86672
N	5.43049	-3.27865	-1.46809
H	8.53162	-1.31904	1.79038

4b$_{\text{NBD-s-}\textit{trans}\text{-VHF}}$
Electronic energy: -1240.83729015
Gibbs free energy: -1240.529994

Atom	X	Y	Z
C	-4.19433	-1.13405	-0.10599
C	-4.33779	0.19543	0.23679
H	-5.30596	0.46718	0.64299
C	-3.41285	1.27849	0.13641
C	-3.86620	2.58016	0.21874
C	-5.25812	2.87748	0.26537
C	-2.99590	3.70343	0.30394
N	-6.38502	3.10845	0.30110
N	-2.32256	4.63389	0.37715
C	-1.94758	1.05167	0.04427
C	-1.30595	0.27784	1.01220
C	-1.19486	1.61181	-0.98659
C	0.05826	0.06711	0.95235
H	-1.88237	-0.15563	1.82086
C	0.16917	1.39178	-1.06005
H	-1.68060	2.21280	-1.74609
C	0.81303	0.61728	-0.09047
H	0.55185	-0.52504	1.71313
C	-5.30101	-1.99858	0.25349
H	-6.17351	-1.46537	0.61890
C	-5.40799	-3.34704	0.25257
H	-6.35264	-3.73567	0.62034
C	-4.45697	-4.34726	-0.12626
C	-3.26523	-4.15405	-0.73308
C	-2.69327	-2.90653	-1.14059
H	-1.79835	-3.00015	-1.74853
C	-3.08021	-1.63533	-0.88521
H	-2.46285	-0.87376	-1.34113
H	-2.68622	-5.03702	-0.98270
H	-4.75188	-5.37222	0.07307
H	0.74494	1.82443	-1.86895
C	2.21740	0.39076	-0.15660
C	3.40390	0.18566	-0.19574
C	4.78928	-0.03572	-0.25412
C	5.76290	0.71395	-1.18539
C	5.54504	-0.86492	0.49173
C	6.63927	1.59089	-0.28070
C	6.76345	-0.43944	-1.44831
H	5.29562	1.20220	-2.03642
C	7.00986	-0.65997	0.06531
C	5.11043	-1.71839	1.52803
C	7.38108	0.77612	0.46002
H	6.58741	2.67024	-0.24168
H	7.65549	-0.11211	-1.98192
H	6.31517	-1.30155	-1.94466
H	7.69636	-1.44583	0.36891
N	4.77912	-2.42785	2.37256
H	8.07792	1.03461	1.24554

$4b_{QC\text{-}DHA}$
Electronic energy: -1240.80626440
Gibbs free energy: -1240.496267

Atom	X	Y	Z
C	-7.82111	-0.96063	0.31815
C	-7.25936	-1.75856	-0.61927
C	-5.84819	-2.00768	-0.78468
C	-7.11220	-0.23149	1.34976
C	-4.87591	-1.13042	-0.47816
C	-5.88279	0.28806	1.24770
C	-5.15259	0.29520	-0.06684
H	-8.90469	-0.96137	0.38950
H	-7.92777	-2.35258	-1.23552
H	-5.56280	-2.97861	-1.17983
H	-5.41766	0.73497	2.11889
C	-3.44742	-1.33241	-0.53293
H	-3.00491	-2.29310	-0.76347
C	-2.74467	-0.21681	-0.28770
C	-3.71988	0.96561	-0.08023
H	-5.78170	0.78573	-0.81460
C	-3.64878	1.90142	-1.21615
C	-3.41310	1.70812	1.15083
N	-3.62079	2.60647	-2.11955
N	-3.17839	2.27070	2.12118
H	-7.63199	-0.11838	2.29700
C	-1.28744	-0.07637	-0.21708
C	-0.64806	1.15871	-0.35548
C	-0.48705	-1.20653	-0.00341
C	0.73098	1.26045	-0.30394
H	-1.21713	2.06417	-0.52298
C	0.88828	-1.11139	0.04917
H	-0.94804	-2.17518	0.14685
H	1.48630	-1.99815	0.22083
C	1.52209	0.12775	-0.10319
H	1.20229	2.22865	-0.42102
C	2.94325	0.22591	-0.04379
C	4.14275	0.30037	0.00744
C	5.55751	0.35597	0.07694
C	6.44763	1.47288	-0.44512
C	6.51793	-0.86138	0.17609
C	6.47036	1.13400	1.01818
C	7.65410	0.89524	-1.14700
H	5.96844	2.38611	-0.77157
C	7.86567	-0.32939	-0.28860
C	6.14743	-2.22905	0.22499
C	7.41686	-0.07443	1.11898
H	6.17459	1.79401	1.81985
H	8.51343	1.56934	-1.10868
H	7.44979	0.64282	-2.18950
H	8.65743	-1.04296	-0.47505
N	5.84174	-3.33708	0.26915
H	7.90869	-0.44480	2.00601

4b$_{\text{QC-s-}cis\text{-VHF}}$
Electronic energy: -1240.79708076
Gibbs free energy: -1240.489888

Atom	X	Y	Z
C	4.60527	0.95893	-0.32357
C	3.38871	0.42652	-0.70067
H	2.81233	1.01266	-1.40872
C	2.71862	-0.75569	-0.25040
C	3.35284	-1.93711	0.08447
C	4.71742	-2.18604	-0.22667
C	2.68366	-3.02201	0.72372
N	5.81706	-2.40674	-0.48597
N	2.18999	-3.91304	1.25928
C	1.23753	-0.68439	-0.22310
C	0.44546	-1.69928	-0.76247
C	0.60895	0.43889	0.31941
C	-0.93363	-1.60000	-0.75295
H	0.90992	-2.56593	-1.21649
C	-0.76970	0.53579	0.34880
H	1.21023	1.23641	0.74024
C	-1.56103	-0.48451	-0.18967
H	-1.24523	1.40374	0.78903
C	5.04344	2.13443	-1.04845
H	4.30637	2.52223	-1.74544
C	6.22690	2.78852	-1.03461
H	6.30226	3.62270	-1.72550
C	7.41259	2.53436	-0.27388
C	7.56369	1.65044	0.73677
C	6.57064	0.77289	1.27769
H	6.87195	0.25254	2.18149
C	5.32975	0.47454	0.83035
H	4.78109	-0.23199	1.44198
H	8.53226	1.61534	1.22443
H	8.27106	3.14694	-0.52917
H	-1.53513	-2.38983	-1.18602
C	-2.98346	-0.38186	-0.16690
C	-4.18243	-0.28946	-0.14221
C	-5.59241	-0.15400	-0.09287
C	-6.60715	-0.92330	-0.92438
C	-6.37636	1.10548	0.36855
C	-6.64434	-1.03445	0.57297
C	-7.68991	0.00676	-1.41890
H	-6.24708	-1.75834	-1.51024
C	-7.76428	0.93844	-0.23237
C	-5.82060	2.32763	0.82415
C	-7.41578	0.21429	1.03322
H	-6.47710	-1.93816	1.13959
H	-8.63591	-0.51519	-1.58306
H	-7.40832	0.52461	-2.33803
H	-8.43978	1.78290	-0.19469
N	-5.36523	3.31588	1.19715
H	-7.88813	0.37195	1.99127

4b$_{\text{QC-s-}\textit{trans}\text{-VHF}}$
Electronic energy: -1240.79979533
Gibbs free energy: -1240.493109

Atom	X	Y	Z
C	4.04559	1.24589	0.06736
C	4.28486	-0.07666	-0.24595
H	5.27235	-0.28771	-0.64179
C	3.43731	-1.22013	-0.12469
C	3.98474	-2.48734	-0.16903
C	5.39484	-2.68468	-0.19331
C	3.19978	-3.67294	-0.23588
N	6.53570	-2.83582	-0.21193
N	2.59948	-4.65320	-0.29429
C	1.96038	-1.09345	-0.04659
C	1.27354	-0.37444	-1.02562
C	1.23797	-1.68863	0.98603
C	-0.10220	-0.25379	-0.97548
H	1.82427	0.08758	-1.83656
C	-0.13786	-1.55322	1.05201
H	1.75615	-2.24717	1.75658
C	-0.82723	-0.83564	0.07066
H	-0.62745	0.29631	-1.74665
C	5.09169	2.17909	-0.30284
H	6.00475	1.70127	-0.64490
C	5.10044	3.53119	-0.33688
H	6.01888	3.97803	-0.70513
C	4.07377	4.46846	0.00446
C	2.89427	4.20434	0.60824
C	2.41352	2.92986	1.04971
H	1.51071	2.97429	1.65147
C	2.89385	1.68419	0.83046
H	2.33150	0.89101	1.30341
H	2.24836	5.04829	0.82681
H	4.29323	5.50636	-0.22346
H	-0.68731	-2.00914	1.86653
C	-2.24617	-0.69612	0.13096
C	-3.44210	-0.57680	0.17491
C	-4.84903	-0.40609	0.21625
C	-5.89492	-1.51127	0.23226
C	-5.63639	0.83454	-0.28932
C	-5.82818	-0.53884	1.37526
C	-7.03340	-1.16707	-0.69875
H	-5.54994	-2.52625	0.37679
C	-7.05573	0.33070	-0.50528
C	-5.08582	2.01095	-0.85754
C	-6.60362	0.69338	0.87743
H	-5.60179	-0.79105	2.40047
H	-7.97312	-1.62930	-0.38642
H	-6.82747	-1.45049	-1.73288
H	-7.75109	0.97626	-1.02539
N	-4.63370	2.96591	-1.31234
H	-7.01574	1.49062	1.47785

$5a_{NBD-DHA}$
Electronic energy: -1379.58405742
Gibbs free energy: -1379.195350

Atom	X	Y	Z
C	-6.25893	-3.07882	0.88341
C	-5.43193	-3.42551	-0.12988
C	-4.19717	-2.76542	-0.47804
C	-6.04413	-1.99911	1.82505
C	-3.95048	-1.45754	-0.28713
C	-5.42095	-0.84189	1.57156
C	-5.00379	-0.47937	0.17307
H	-7.09400	-3.74029	1.09414
H	-5.65276	-4.34552	-0.66298
H	-3.41612	-3.38066	-0.91592
H	-5.23838	-0.14426	2.38093
C	-2.71769	-0.74128	-0.51949
H	-1.80086	-1.23893	-0.80893
C	-2.83599	0.58288	-0.35088
C	-4.30636	0.92719	-0.01818
H	-5.87925	-0.53481	-0.47957
C	-4.94486	1.61786	-1.15253
C	-4.40541	1.79287	1.16557
N	-5.44994	2.11822	-2.05172
N	-4.47505	2.45321	2.09951
H	-6.41315	-2.16474	2.83331
C	-1.77681	1.59531	-0.45260
C	-0.44268	1.20861	-0.30502
C	-2.05578	2.94358	-0.69050
C	0.59717	2.13127	-0.41311
H	-0.19730	0.17929	-0.07598
C	-1.02689	3.86922	-0.79386
H	-3.07434	3.28899	-0.81232
H	-1.26248	4.91007	-0.98204
C	0.29211	3.47529	-0.66041
H	1.09382	4.19940	-0.73926
C	1.94992	1.70635	-0.25967
C	3.08625	1.32234	-0.13629
C	4.42717	0.92764	0.03273
C	5.53285	1.90900	0.48229
C	4.98611	-0.29869	-0.02714
C	5.90492	1.52338	1.91967
C	6.72321	1.26004	-0.25959
H	5.31756	2.95934	0.29981
C	6.45772	-0.11721	0.39510
C	6.45787	0.31668	1.86808
H	5.68470	2.12027	2.79462
H	7.68837	1.68522	0.01915
H	6.60694	1.25431	-1.34465
H	7.12297	-0.93595	0.13048
H	6.79426	-0.29876	2.69204
C	4.38545	-1.59494	-0.33585
C	3.27535	-1.70833	-1.18181
C	4.92262	-2.76674	0.20857
C	2.71972	-2.94687	-1.46098
H	2.85846	-0.81845	-1.63618
C	4.35919	-4.00460	-0.06377
H	5.78324	-2.70906	0.86513
C	3.25538	-4.10067	-0.90062
H	1.86777	-3.01366	-2.12898
H	4.78693	-4.89816	0.37732
H	2.81972	-5.06877	-1.12113

5a$_{\text{NBD-s-}cis\text{-VHF}}$
Electronic energy: -1379.57540028
Gibbs free energy: -1379.189261

Atom	X	Y	Z
C	3.51556	-1.08991	-0.78331
C	2.99710	0.16729	-1.02220
H	2.39615	0.27051	-1.91958
C	3.05752	1.35628	-0.22885
C	4.14281	1.73968	0.53466
C	5.41730	1.12092	0.41546
C	4.09180	2.81784	1.46687
N	6.45804	0.63892	0.31762
N	4.09023	3.66445	2.24631
C	1.87144	2.24718	-0.31572
C	0.59752	1.69465	-0.21244
C	2.00408	3.61814	-0.53941
C	-0.54316	2.49559	-0.30429
H	0.48481	0.62985	-0.04766
C	0.87640	4.41831	-0.64764
H	2.98767	4.05731	-0.65092
C	-0.38888	3.86878	-0.52570
H	0.98700	5.48068	-0.83036
H	-1.26831	4.49655	-0.60464
C	3.34873	-2.06373	-1.84268
H	2.73895	-1.71364	-2.67024
C	3.86474	-3.30520	-1.98812
H	3.61187	-3.80471	-2.91837
C	4.72162	-4.05521	-1.12089
C	5.09211	-3.73854	0.13940
C	4.70621	-2.58443	0.89286
H	5.00520	-2.60549	1.93624
C	4.05024	-1.46666	0.50612
H	3.88485	-0.73892	1.29184
H	5.72612	-4.44665	0.66269
H	5.08509	-4.99529	-1.52286
C	-1.83884	1.91478	-0.17880
C	-2.92220	1.39718	-0.06602
C	-5.49085	1.64002	-0.29174
C	-4.59282	-0.42280	0.31823
C	-6.04737	1.05297	-1.59513
C	-6.44848	0.95740	0.71094
H	-5.38218	2.72141	-0.25135
C	-6.12547	-0.44982	0.15324
C	-6.42730	-0.19206	-1.33011
H	-6.05487	1.56487	-2.54818
H	-7.49244	1.24156	0.57154
H	-6.15197	1.08992	1.75272
H	-6.62870	-1.29882	0.61020
H	-6.81729	-0.93124	-2.01742
C	-4.21093	0.84195	0.04333
C	-3.79053	-1.60437	0.62860
C	-4.26504	-2.88073	0.30590
C	-2.54208	-1.50316	1.25481
C	-3.51142	-4.01299	0.57796
H	-5.22925	-2.98965	-0.17723
C	-1.79405	-2.63591	1.53370
H	-2.16561	-0.52875	1.53890
C	-2.27230	-3.89596	1.19341
H	-3.89610	-4.99105	0.31063
H	-0.83401	-2.53577	2.02827
H	-1.68572	-4.78089	1.41355

5a$_{\text{NBD-s-}\textit{trans}\text{-VHF}}$

Electronic energy: -1379.57787228

Gibbs free energy: -1379.192461

Atom	X	Y	Z
C	3.96045	1.55533	0.31858
C	4.40153	0.45522	-0.38830
H	5.17511	0.65614	-1.12144
C	4.00344	-0.91389	-0.30807
C	4.79516	-1.89387	-0.87184
C	6.07391	-1.58959	-1.42012
C	4.38837	-3.25361	-0.98382
N	7.10653	-1.33485	-1.85986
N	4.09337	-4.36034	-1.09579
C	2.70289	-1.31989	0.28706
C	2.64595	-2.25096	1.32229
C	1.52556	-0.76561	-0.20465
C	1.42031	-2.60875	1.86686
H	3.55933	-2.68588	1.71044
C	0.28787	-1.13155	0.32811
H	1.56515	-0.04431	-1.01182
C	0.24814	-2.05850	1.37716
H	1.38119	-3.32930	2.67534
H	-0.70910	-2.34753	1.79411
C	4.49492	2.83323	-0.11016
H	5.29508	2.75156	-0.83972
C	4.13385	4.09672	0.21021
H	4.68543	4.87885	-0.30239
C	3.11282	4.56739	1.09630
C	2.37254	3.83141	1.95395
C	2.45200	2.41882	2.17443
H	1.87458	2.06354	3.02268
C	3.11951	1.45785	1.49527
H	3.01317	0.46058	1.89877
H	1.66558	4.36310	2.58229
H	2.94741	5.63976	1.09162
C	-0.91568	-0.56621	-0.18537
C	-1.94621	-0.09627	-0.59943
C	-3.14225	1.15505	-2.52391
C	-4.38980	0.43165	-0.69206
C	-3.91973	0.22612	-3.46502
C	-4.25021	2.19302	-2.23618
H	-2.17707	1.51013	-2.87784
C	-5.24565	1.09541	-1.78957
C	-5.17395	0.19167	-3.02889
H	-3.48105	-0.33125	-4.28181
H	-4.57977	2.72995	-3.12673
H	-3.99191	2.89420	-1.44073
H	-6.23776	1.41437	-1.47856
H	-5.99622	-0.40041	-3.40843
C	-3.11767	0.46516	-1.14134
C	-4.94802	-0.16302	0.52071
C	-4.18680	-0.31041	1.68686
C	-6.27739	-0.59975	0.54178
C	-4.73354	-0.88329	2.82398
H	-3.16291	0.04074	1.70295
C	-6.82068	-1.18097	1.67797
H	-6.89091	-0.49863	-0.34600
C	-6.05147	-1.32513	2.82477
H	-4.12865	-0.98101	3.71892
H	-7.85029	-1.52111	1.66709
H	-6.47691	-1.77390	3.71536

$5a_{QC\text{-}DHA}$
Electronic energy: -1379.54392236
Gibbs free energy: -1379.157301

Atom	X	Y	Z
C	8.25772	-0.63731	-0.02832
C	7.99685	0.30183	-0.96687
C	6.81710	1.12991	-1.03118
C	7.41472	-0.96637	1.10291
C	5.60134	0.76271	-0.58952
C	6.07764	-0.91034	1.13480
C	5.28591	-0.63443	-0.11341
H	9.23953	-1.10101	-0.04592
H	8.78779	0.53578	-1.67332
H	6.93367	2.12059	-1.46160
H	5.55670	-1.09385	2.06756
C	4.39685	1.55847	-0.53237
H	4.38258	2.61248	-0.77949
C	3.31746	0.85769	-0.15853
C	3.71073	-0.62583	0.03131
H	5.56978	-1.36413	-0.87662
C	3.13751	-1.45743	-1.04171
C	3.24120	-1.14719	1.32285
N	2.72746	-2.09662	-1.90036
N	2.89053	-1.54087	2.34028
H	7.93011	-1.26928	2.01003
C	1.95605	1.36444	0.05781
C	0.84091	0.53035	-0.00335
C	1.75951	2.72274	0.33538
C	-0.44989	1.02978	0.19045
H	0.94459	-0.52502	-0.21864
C	0.48385	3.22585	0.52310
H	2.61167	3.38476	0.42901
H	0.34874	4.27884	0.74199
C	-0.62089	2.39103	0.45230
H	-1.61854	2.78296	0.60875
C	-1.57695	0.15654	0.12060
C	-2.52873	-0.57770	0.06432
C	-3.65808	-1.43327	0.00883
C	-3.65739	-2.85956	-0.52358
C	-5.16078	-1.01396	0.00286
C	-4.01106	-2.60896	0.91408
C	-4.90273	-3.10276	-1.34209
H	-2.70392	-3.31014	-0.76684
C	-5.86512	-2.23410	-0.56699
C	-5.49009	-2.18838	0.89341
H	-3.44460	-2.96319	1.76307
H	-5.19753	-4.15596	-1.33672
H	-4.78842	-2.77688	-2.37910
H	-6.90544	-2.12906	-0.84855
H	-6.18951	-2.25037	1.71541
C	-5.68748	0.36496	-0.02680
C	-6.71491	0.76652	0.82519
C	-5.17216	1.29285	-0.93410
C	-7.22816	2.05560	0.76217
H	-7.11331	0.06509	1.55033
C	-5.67745	2.58364	-0.99118
H	-4.36709	1.00028	-1.59906
C	-6.71054	2.96980	-0.14541
H	-8.02932	2.34847	1.43213
H	-5.26467	3.29109	-1.70230
H	-7.10646	3.97825	-0.19144

5a$_{\text{QC-s-}cis\text{-VHF}}$
Electronic energy: -1379.53518730
Gibbs free energy: -1379.150015

Atom	X	Y	Z
C	-3.39299	-1.07290	-0.63529
C	-2.89026	0.17254	-0.95213
H	-2.32564	0.23657	-1.87640
C	-2.92658	1.39862	-0.21469
C	-3.98457	1.81747	0.56705
C	-5.25888	1.18771	0.53040
C	-3.90523	2.94710	1.43441
N	-6.29968	0.69710	0.49831
N	-3.88011	3.83746	2.16297
C	-1.74874	2.28753	-0.38839
C	-0.46932	1.74986	-0.27352
C	-1.89767	3.63930	-0.69923
C	0.66304	2.54901	-0.44314
H	-0.34590	0.70095	-0.03194
C	-0.77789	4.43584	-0.88527
H	-2.88706	4.06404	-0.81620
C	0.49379	3.90212	-0.75470
H	-0.89896	5.48323	-1.13579
H	1.36645	4.52867	-0.89537
C	-3.26638	-2.09417	-1.65542
H	-2.69293	-1.78073	-2.52287
C	-3.78554	-3.34073	-1.72395
H	-3.57116	-3.88150	-2.64082
C	-4.60514	-4.05096	-0.78918
C	-4.92382	-3.67773	0.46953
C	-4.50985	-2.49051	1.15432
H	-4.76475	-2.46544	2.20922
C	-3.87351	-1.39103	0.69110
H	-3.67683	-0.62852	1.43552
H	-5.53463	-4.36148	1.04977
H	-4.98400	-5.00776	-1.13326
C	1.96681	1.98491	-0.30063
C	3.05921	1.49640	-0.17191
C	4.33491	0.89984	-0.00490
C	5.65346	1.46923	-0.50967
C	4.63781	-0.60689	0.26580
C	5.44891	1.27683	0.96570
C	6.50872	0.36109	-1.07611
H	5.65065	2.47017	-0.92141
C	6.09311	-0.75373	-0.14544
C	5.74132	-0.21161	1.21776
H	5.42750	2.07101	1.69781
H	7.57600	0.58791	-1.00124
H	6.26986	0.14391	-2.12041
H	6.49515	-1.75582	-0.22721
H	6.03035	-0.66144	2.15726
C	3.64984	-1.70296	0.31863
C	3.65395	-2.63363	1.35601
C	2.69610	-1.83541	-0.69268
C	2.74044	-3.67982	1.37653
H	4.37500	-2.53509	2.16026
C	1.77687	-2.87410	-0.66786
H	2.67453	-1.11617	-1.50405
C	1.79689	-3.80300	0.36580
H	2.76064	-4.39508	2.19161
H	1.04257	-2.96138	-1.46151
H	1.07877	-4.61523	0.38458

5a$_{\text{QC-s-}\textit{trans}\text{-VHF}}$
Electronic energy: -1379.53822362
Gibbs free energy: -1379.154271

Atom	X	Y	Z
C	4.59254	-0.04800	0.62384
C	4.06034	1.03741	-0.04065
H	4.68171	1.92631	-0.04848
C	2.80772	1.18341	-0.71254
C	2.32709	2.44460	-1.00013
C	2.98814	3.61475	-0.52821
C	1.17545	2.67698	-1.80458
N	3.52813	4.55558	-0.14372
N	0.25202	2.90942	-2.45091
C	2.04122	0.00843	-1.20361
C	2.65795	-0.91200	-2.05152
C	0.71368	-0.17707	-0.83705
C	1.94424	-2.00136	-2.52553
H	3.69164	-0.76689	-2.34242
C	-0.00793	-1.28138	-1.30060
H	0.22740	0.52912	-0.17503
C	0.62258	-2.19260	-2.15231
H	2.42164	-2.70798	-3.19455
H	0.06754	-3.04585	-2.52339
C	5.95490	0.10981	1.09563
H	6.34086	1.11936	0.99026
C	6.82879	-0.79164	1.59822
H	7.81328	-0.39916	1.83370
C	6.67038	-2.19378	1.84116
C	5.52923	-2.91258	1.76409
C	4.22215	-2.43107	1.43074
H	3.42561	-3.15379	1.58065
C	3.82093	-1.22998	0.95496
H	2.75430	-1.13436	0.80699
H	5.58726	-3.96503	2.02179
H	7.56784	-2.71878	2.15158
C	-1.37037	-1.45030	-0.91186
C	-2.52279	-1.54914	-0.57973
C	-3.88011	-1.60702	-0.17494
C	-4.94792	-2.51638	-0.76539
C	-4.68103	-0.48081	0.54968
C	-4.59254	-2.64230	0.68863
C	-6.23874	-1.75074	-0.93282
H	-4.63373	-3.28554	-1.45905
C	-6.12936	-0.84292	0.26955
C	-5.38129	-1.52336	1.38932
H	-4.15416	-3.51749	1.14611
H	-7.11347	-2.40527	-0.88095
H	-6.27269	-1.19470	-1.87311
H	-6.88761	-0.10853	0.51072
H	-5.66035	-1.48764	2.43315
C	-4.18098	0.86779	0.88503
C	-4.41209	1.43480	2.13738
C	-3.47363	1.60946	-0.06333
C	-3.96310	2.71604	2.43071
H	-4.94287	0.86603	2.89348
C	-3.01317	2.88446	0.23278
H	-3.27649	1.18373	-1.04066
C	-3.25967	3.44455	1.48064
H	-4.15478	3.14164	3.40988
H	-2.45874	3.44001	-0.51561
H	-2.90105	4.44142	1.71180

$5b_{NBD-DHA}$
Electronic energy: -1240.84363443
Gibbs free energy: -1240.533350

Atom	X	Y	Z
C	-6.10104	-2.95172	0.32869
C	-5.31305	-3.21468	-0.73921
C	-4.01368	-2.64168	-0.99374
C	-5.77510	-2.06867	1.42994
C	-3.62855	-1.41611	-0.59723
C	-5.03053	-0.95862	1.35972
C	-4.56964	-0.41881	0.03401
H	-7.00273	-3.54624	0.44162
H	-5.62898	-4.00712	-1.41108
H	-3.30224	-3.25673	-1.53757
H	-4.77863	-0.42582	2.26952
C	-2.32567	-0.80781	-0.73446
H	-1.47005	-1.34659	-1.12141
C	-2.29919	0.47540	-0.34939
C	-3.72096	0.91583	0.06822
H	-5.44285	-0.26890	-0.60683
C	-4.28197	1.85741	-0.91670
C	-3.71643	1.57206	1.38364
N	-4.72890	2.55940	-1.70504
N	-3.70309	2.06907	2.41610
H	-6.16383	-2.35616	2.40278
C	-1.13550	1.37094	-0.30842
C	0.14888	0.82509	-0.26381
C	-1.26371	2.76267	-0.31094
C	1.27984	1.63987	-0.24664
H	0.28463	-0.24801	-0.22106
C	-0.14180	3.57942	-0.28848
H	-2.23908	3.23064	-0.34534
H	-0.26509	4.65582	-0.29506
C	1.12726	3.03098	-0.25964
H	2.00353	3.66728	-0.24035
C	2.57623	1.04912	-0.20551
C	3.66020	0.52441	-0.17712
C	4.92905	-0.07599	-0.14386
C	6.26135	0.68261	0.01824
C	5.24430	-1.38520	-0.18750
C	6.81179	0.30289	1.39966
C	7.15409	-0.23153	-0.85820
H	6.21431	1.74283	-0.21573
C	6.77319	-1.49478	-0.04608
C	4.35218	-2.47521	-0.26960
C	7.11792	-0.98852	1.36135
H	6.86727	0.97926	2.24154
H	8.21264	0.01773	-0.78733
H	6.84028	-0.27654	-1.90216
H	7.20029	-2.44898	-0.34301
N	3.64214	-3.37920	-0.34179
H	7.48273	-1.61349	2.16497

5b$_{NBD\text{-}s\text{-}cis\text{-}VHF}$
Electronic energy: -1240.83461398
Gibbs free energy: -1240.526390

Atom	X	Y	Z
C	3.33544	1.19514	-0.50595
C	2.65912	0.05465	-0.90057
H	2.08420	0.13941	-1.81667
C	2.52980	-1.21130	-0.25395
C	3.51369	-1.82300	0.50090
C	4.86281	-1.37671	0.50213
C	3.26949	-2.98261	1.29360
N	5.96183	-1.03403	0.49690
N	3.10953	-3.90597	1.96177
C	1.24794	-1.92644	-0.49290
C	0.04711	-1.23586	-0.35878
C	1.22261	-3.26556	-0.88480
C	-1.17338	-1.87503	-0.58745
H	0.05349	-0.19495	-0.05913
C	0.01460	-3.90266	-1.12680
H	2.15075	-3.80709	-1.01978
C	-1.17983	-3.21929	-0.97414
H	0.00677	-4.94048	-1.43782
H	-2.12425	-3.71752	-1.15700
C	3.34937	2.28928	-1.45264
H	2.73886	2.11724	-2.33404
C	4.03036	3.45853	-1.44009
H	3.88904	4.08478	-2.31558
C	4.93399	3.98816	-0.46673
C	5.20195	3.48841	0.76066
C	4.63735	2.32122	1.36328
H	4.88870	2.18701	2.41073
C	3.85856	1.35065	0.83106
H	3.56409	0.57111	1.52356
H	5.89513	4.04545	1.38220
H	5.43196	4.91102	-0.74540
C	-2.39374	-1.15626	-0.43095
C	-3.41296	-0.52799	-0.29755
C	-6.02036	-0.43888	-0.17516
C	-4.78802	1.49805	0.11162
C	-6.57791	-0.32575	1.25024
C	-6.78169	0.74213	-0.82795
H	-6.07460	-1.41682	-0.64602
C	-6.30164	1.73832	0.25711
C	-3.78728	2.47634	0.29113
C	-6.74733	0.96599	1.50642
H	-6.73294	-1.16575	1.91332
H	-7.86222	0.60010	-0.82831
H	-6.42758	0.98900	-1.82999
H	-6.61674	2.77573	0.18278
N	-2.98868	3.29368	0.43513
H	-7.07409	1.42784	2.42806
C	-4.61158	0.18685	-0.14300

5b$_{\text{NBD-s-}\textit{trans}\text{-VHF}}$
Electronic energy: -1240.83698460
Gibbs free energy: -1240.529780

Atom	X	Y	Z
C	-2.90402	1.71836	-0.02578
C	-3.37477	0.59714	-0.68050
H	-3.96085	0.79319	-1.57165
C	-3.20854	-0.78613	-0.37464
C	-4.02409	-1.72711	-0.97219
C	-5.12780	-1.34097	-1.78478
C	-3.80686	-3.12924	-0.85954
N	-6.01953	-1.02063	-2.43809
N	-3.65964	-4.26876	-0.79219
C	-2.10681	-1.27059	0.49917
C	-2.36601	-2.07826	1.60509
C	-0.79397	-0.92408	0.19728
C	-1.32288	-2.52494	2.40443
H	-3.38649	-2.34900	1.84859
C	0.26016	-1.38169	0.98967
H	-0.58256	-0.29890	-0.66152
C	-0.01569	-2.18536	2.10170
H	-1.53368	-3.14796	3.26546
H	0.80060	-2.53940	2.71961
C	-3.13588	2.98136	-0.69682
H	-3.78417	2.90504	-1.56452
C	-2.64189	4.21703	-0.45297
H	-2.95028	4.98455	-1.15607
C	-1.74465	4.66593	0.56698
C	-1.30846	3.96653	1.63785
C	-1.65396	2.62427	1.99389
H	-1.31126	2.31826	2.97783
C	-2.32685	1.67549	1.30224
H	-2.46036	0.74013	1.82794
H	-0.65587	4.48152	2.33505
H	-1.40848	5.69335	0.47497
C	1.60165	-1.02501	0.66688
C	2.72894	-0.70829	0.38417
C	5.30566	-1.05621	0.63044
C	4.49645	0.57569	-0.79597
C	5.95263	-1.79987	-0.54591
C	6.24725	0.17271	0.68801
H	5.13994	-1.62828	1.53947
C	6.03350	0.49032	-0.81326
C	3.72073	1.43721	-1.60045
C	6.38687	-0.88248	-1.40185
H	5.97538	-2.87599	-0.64927
H	7.27701	-0.09404	0.92485
H	5.89378	0.96255	1.35266
H	6.54192	1.35216	-1.23734
N	3.11113	2.15695	-2.26132
H	6.84834	-1.03431	-2.36798
C	4.05154	-0.35777	0.06736

$5b_{QC\text{-}DHA}$
Electronic energy: -1240.80478856
Gibbs free energy: -1240.496096

Atom	X	Y	Z
C	-7.32108	-1.27710	-0.08115
C	-7.29876	0.06416	0.06951
C	-6.18142	0.94481	-0.16975
C	-6.23576	-2.10662	-0.56356
C	-4.88018	0.61262	-0.10077
C	-4.92461	-1.86992	-0.45081
C	-4.35398	-0.73134	0.35070
H	-8.27267	-1.77879	0.06652
H	-8.23509	0.55150	0.32446
H	-6.42317	1.98082	-0.39057
H	-4.23625	-2.55916	-0.92574
C	-3.76412	1.51176	-0.26367
H	-3.89781	2.54831	-0.54522
C	-2.57708	0.94737	0.00186
C	-2.78126	-0.55954	0.26612
H	-4.60808	-0.87114	1.40722
C	-2.15864	-1.00121	1.52337
C	-2.19424	-1.33291	-0.84365
N	-1.70871	-1.33966	2.52163
N	-1.74297	-1.92107	-1.71781
H	-6.53258	-3.01348	-1.08308
C	-1.26134	1.60002	0.02269
C	-0.07422	0.87007	-0.00488
C	-1.17948	2.99744	0.08419
C	1.16952	1.50703	0.00845
H	-0.08238	-0.21055	-0.04920
C	0.04834	3.63430	0.09556
H	-2.08228	3.59267	0.14180
H	0.09158	4.71608	0.14553
C	1.22455	2.90055	0.05527
H	2.18613	3.39885	0.06729
C	2.37001	0.73473	-0.02641
C	3.38100	0.08469	-0.05482
C	4.58504	-0.66283	-0.09558
C	4.78756	-2.07854	0.42142
C	6.02516	-0.08198	-0.14629
C	5.01885	-1.78316	-1.03327
C	6.09992	-2.18197	1.16206
H	3.90855	-2.63520	0.71739
C	6.91687	-1.21695	0.33577
C	6.38516	1.28907	-0.17319
C	6.44292	-1.20361	-1.08657
H	4.45847	-2.20274	-1.85527
H	6.51229	-3.19349	1.12772
H	6.01633	-1.87009	2.20512
H	7.95242	-0.99224	0.55487
N	6.67342	2.40237	-0.19957
H	7.08004	-1.11850	-1.95419

5b$_{\text{QC-s-}cis\text{-VHF}}$
Electronic energy: -1240.79674613
Gibbs free energy: -1240.489816

Atom	X	Y	Z
C	3.18166	-1.25058	-0.45229
C	2.54176	-0.09855	-0.86996
H	1.93125	-0.19391	-1.76159
C	2.48632	1.19669	-0.27015
C	3.52142	1.79371	0.42547
C	4.85078	1.29215	0.39644
C	3.35504	2.99028	1.18287
N	5.93476	0.90548	0.36713
N	3.26116	3.94131	1.82429
C	1.22715	1.95422	-0.49446
C	0.00486	1.31559	-0.30125
C	1.24330	3.27879	-0.93233
C	-1.19760	1.99002	-0.51882
H	-0.01721	0.28594	0.03462
C	0.05250	3.95079	-1.16249
H	2.18669	3.77888	-1.11327
C	-1.16213	3.31827	-0.95407
H	0.07271	4.97675	-1.51070
H	-2.09130	3.84651	-1.13152
C	3.10927	-2.38339	-1.35067
H	2.46737	-2.22252	-2.21160
C	3.74201	-3.57857	-1.31583
H	3.53678	-4.23470	-2.15609
C	4.66610	-4.10445	-0.35900
C	5.00478	-3.56739	0.83437
C	4.51034	-2.35543	1.41099
H	4.80878	-2.19082	2.44168
C	3.74981	-1.37570	0.87012
H	3.51400	-0.55789	1.54065
H	5.70219	-4.12622	1.44957
H	5.11630	-5.05675	-0.61943
C	-2.44224	1.32283	-0.30451
C	-3.48538	0.75298	-0.12269
C	-4.69918	0.04880	0.08348
C	-5.91990	0.54605	0.84229
C	-4.86832	-1.49592	0.09155
C	-6.04934	0.17945	-0.60920
C	-6.47160	-0.55016	1.72294
H	-5.94125	1.58826	1.13120
C	-6.16988	-1.73892	0.84131
C	-3.84932	-2.45865	-0.12010
C	-6.21329	-1.35032	-0.60606
H	-6.31553	0.85773	-1.40605
H	-7.54471	-0.43716	1.89614
H	-5.96260	-0.60701	2.68727
H	-6.40983	-2.75431	1.12810
N	-3.01987	-3.23568	-0.29746
H	-6.59962	-1.96609	-1.40448

5b$_{\text{QC-s-}\textit{trans}\text{-VHF}}$
Electronic energy: -1240.79939229
Gibbs free energy: -1240.492877

Atom	X	Y	Z
C	4.16695	-0.58125	-0.49604
C	3.93254	0.76512	-0.29937
H	4.77682	1.41564	-0.50029
C	2.74969	1.44438	0.12137
C	2.63666	2.80800	-0.06149
C	3.62061	3.54411	-0.78132
C	1.56713	3.57786	0.47716
N	4.42007	4.13103	-1.36531
N	0.72082	4.23381	0.89911
C	1.65700	0.74221	0.84494
C	1.93998	0.05888	2.02717
C	0.35485	0.76555	0.35950
C	0.92494	-0.59082	2.71183
H	2.95388	0.04342	2.40932
C	-0.66897	0.09788	1.03612
H	0.12762	1.29046	-0.56043
C	-0.37154	-0.58026	2.22144
H	1.14560	-1.11126	3.63649
H	-1.16298	-1.09421	2.75331
C	5.53588	-0.94010	-0.81110
H	6.18167	-0.08679	-0.99509
C	6.14541	-2.14629	-0.86948
H	7.20799	-2.11625	-1.09029
C	5.61633	-3.45862	-0.65419
C	4.31892	-3.80019	-0.49369
C	3.18460	-2.92686	-0.51221
H	2.22564	-3.43632	-0.51641
C	3.11287	-1.57558	-0.51713
H	2.10890	-1.17630	-0.54915
H	4.09403	-4.85544	-0.37896
H	6.34507	-4.26256	-0.65350
C	-2.00131	0.11232	0.52273
C	-3.12550	0.12862	0.09666
C	-4.45415	0.12635	-0.39889
C	-5.31883	1.34882	-0.66855
C	-5.48585	-1.02680	-0.25547
C	-4.98792	0.41282	-1.79609
C	-6.72586	1.11381	-0.17239
H	-4.84232	2.31893	-0.62553
C	-6.83913	-0.36347	-0.46586
C	-5.27342	-2.27842	0.37562
C	-6.00527	-0.73300	-1.65576
H	-4.41837	0.66932	-2.67684
H	-7.46158	1.69520	-0.73366
H	-6.83635	1.33721	0.89064
H	-7.72787	-0.93737	-0.23873
N	-5.09455	-3.29466	0.88409
H	-6.28188	-1.45524	-2.40931

NBD
Electronic energy: -271.375738916
Gibbs free energy: -271.273985

Atom	X	Y	Z
C	-0.23038	0.14716	1.11842
C	-0.23038	-1.32116	0.66422
C	-0.23038	-1.32116	-0.66422
C	-0.23038	0.14716	-1.11842
C	1.10489	0.76075	-0.66403
C	1.10489	0.76075	0.66403
C	-1.13620	0.72901	0.00000
H	-0.51516	0.33086	2.15266
H	-0.17992	-2.17254	1.33027
H	-0.17992	-2.17254	-1.33027
H	-0.51516	0.33086	-2.15266
H	1.89848	1.06931	-1.33183
H	1.89848	1.06931	1.33183
H	-1.17506	1.81957	0.00000
H	-2.14392	0.31020	-0.00000

QC

Electronic energy: -271.342221875

Gibbs free energy: -271.240647

Atom	X	Y	Z
C	1.14736	0.54887	-0.00006
C	0.77243	-0.70498	0.75512
C	-0.77141	-0.70604	0.75514
C	-1.14818	0.54722	-0.00008
C	-0.77147	-0.70617	-0.75501
C	0.77249	-0.70509	-0.75501
C	-0.00105	1.53176	-0.00008
H	2.18080	0.87321	0.00007
H	1.42432	-1.22758	1.44110
H	-1.42268	-1.22954	1.44101
H	-2.18196	0.87050	0.00003
H	-1.42229	-1.23023	-1.44089
H	1.42394	-1.22819	-1.44104
H	-0.00157	2.16899	-0.88908
H	-0.00156	2.16942	0.88862