Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Supramolecular control of unidirectional rotary motion in a sterically overcrowded photoswitchable receptor

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Experimental section

General methods and materials: Toluene, THF and CH_2Cl_2 were dried by using an MBraun solvent purification system. Solvents were degassed by purging with N_2 for 30 min. All other chemicals were commercial products and were used as received. Flash chromatography (FC) was performed using silica gel (SiO_2) purchased from Merck (type 9385, 230-400 mesh) and thin-layer chromatography (TLC) was carried out on aluminum sheets coated with silica 60F254 obtained from Merck; compounds were visualized with a UV lamp (254 nm) or by staining with phosphomolybdic acid (PMA). Melting points (m.p.) were determined using a Büchi-B545 capillary melting point apparatus. ^1H, and ^{13}C spectra were recorded on Varian VXR-300S, Varian Mercury Plus-400 and Varian Inova-500 spectrometers at 298 K. Chemical shifts (δ) are denoted in parts per million (ppm) relative to residual protiated solvent ($CDCl_3$: for ^1H detection δ = 7.26 ppm, for ^{13}C detection δ = 77.16 ppm; CD_2Cl_2: for ^1H detection δ = 5.32 ppm, for ^{13}C detection δ = 53.50 ppm; DMSO-d_6: for ^1H detection δ = 2.50 ppm, for ^{13}C detection δ = 39.52 ppm). For ^1H NMR spectroscopy, the splitting pattern of peaks is designated as follows: s (singlet), d (doublet), t (triplet), (multiplet), br (broad), or dd (doublet of doublets). High resolution mass spectrometry (HRMS) was performed on an LTQ Orbitrap XL spectrometer with ESI or APCI ionization. UV-vis spectra were recorded on a Hewlett-Packard HP 8543 diode array in a 1 cm quartz cuvette. Irradiation experiments were carried out using a Spectroline model ENB-280C/FE lamp positioned at a distance of 3 cm from the sample.

Ethyl 3-(4-bromo-2,5-dimethylphenyl)propanoate (4): A solution of *n*-BuLi (24.1 mL, 38.6 mmol, 1.6 M in hexane) was added to a solution of 1,4-dibromo-2,5-dimethylbenzene (10.0 g, 37.9 mmol) in THF (200 mL) at -78 °C. Subsequently, copper(I)-iodide (3.60 g, 18.9 mmol) and sodium iodide (11.4 g, 75.8 mmol) were added. The resulting mixture was stirred at 0 °C for 30 min and cooled to −78 °C. Trimethylsilyl chloride (21 mL, 167 mmol) was added and

stirring was continued for 20 min. Then, ethyl acrylate (18.6 mL, 171 mmol) was added, the mixture was allowed to warm up to 0 °C, and was stirred for 48 h at this temperature. A saturated aqueous NH_4Cl solution (100 mL) was added and the aqueous phase was extracted with CH_2Cl_2 (2 x 200 mL). The combined organic layers were washed with brine, dried over Na_2SO_4 and concentrated in vacuo. The product was purified by column chromatography (SiO_2, pentane/EtOAc 19:1) to afford compound **4** (5.17 g, 48%) as a light-yellow oil. ^1H NMR (400 MHz, $CDCl_3$) δ 7.29 (s, 1H; ArH), 6.99 (s, 1H; ArH), 4.13 (q, J = 7.1 Hz, 2H; CH_2), 2.85 (t, J = 7.9 Hz, 2H; CH_2), 2.56 - 2.50 (m, 2H; CH_2), 2.31 (s, 3H; CH_3), 2.25 (s, 3H; CH_3), 1.24 (t, J = 7.1 Hz, 3H; CH_3); ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.4, 140.5, 137.9, 137.8, 136.3, 133.7, 124.9, 63.1, 37.2, 30.4, 24.9, 21.1, 16.9; HRMS (ESI) *m/z*: 285.0318 ($[M + H]^+$, calcd for $C_{13}H_{17}BrO2^+$: 285.0308).

6-Bromo-4,7-dimethyl-2,3-dihydro-1H-inden-1-one (5): Concentrated H_2SO_4 (30 mL, 95%) was added to compound **4** (2.84 g, 10 mmol) and the mixture was stirred for 24 h at rt. The reaction mixture was poured onto ice and extracted with Et_2O (2 x 20 mL). The organic layer was washed with saturated aqueous $NaHCO_3$ (50 mL), dried over Na_2SO_4 and concentrated in vacuo. The product was purified by column chromatography (SiO_2, pentane/EtOAc 5:1) to afford compound **5** (1.86 g, 7.8 mmol, 78% yield) as an off-white solid. M.p. 130.5°C; ^1H NMR (400 MHz, $CDCl_3$) δ 7.52 (s, 1H; ArH), 2.90 - 2.84 (m, 2H; CH_2), 2.69 (m, 2H; CH_2), 2.67 (s, 3H; CH_3), 2.27 (s, 3H; CH_3); ^{13}C NMR (101 MHz, $CDCl_3$) δ 209.7, 156.8, 140.4, 138.2, 138.0, 137.1, 127.6, 39.4, 26.3, 19.8, 19.2; HRMS (ESI) *m/z*: 239.0066 ($[M + H]^+$, calcd for $C_{11}H_{12}BrO^+$: 239.0072).

(*E/Z*)-6,6'-dibromo-4,4',7,7'-tetramethyl-2,2',3,3'-tetrahydro-1,1'-biindenylidene [(*E*/*Z*)-6]: zinc powder (1.61 g, 4.2 equiv.) was suspended in THF (0.2 M) and $TiCl_4$ (1.4 mL, 2.1

equiv.) was added slowly whilst stirring the suspension vigorously. The mixture was heated at reflux for 2 h and then the reaction was cooled to rt. Ketone **5** (6.3 mmol, 1.5 g) was added in portions and the mixture was stirred at reflux for 24 h. After cooling to rt, the reaction mixture was treated with saturated aqueous NH_4Cl, and the aqueous phase was extracted with CH_2Cl_2, (3 x 50 mL). The volume of the combined organic layers was reduced to 15 mL and the precipitate was filtered off and air-dried to afford (*E*)-**6** (1.01g, 76%) as a white solid. M.p. >350°C (dec.); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (s, 2H; ArH), 2.69 (m, 8H; CH_2), 2.35 (s, 6H; CH_3), 2.22 (s, 6H; CH_3); ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.1, 143.9, 138.1, 132.5, 132.2, 130.1, 124.4, 37.3, 30.7, 22.3, 18.2; HRMS (APCI) *m/z*: 445.0169 ($[M + H]^+$, calcd for $C_{22}H_{23}Br_2^+$: 445.0167).

The filtrate was concentrated and purification by column chromatography (SiO_2, pentane to pentane/Et_2O 1:1) afforded (*Z*)-**6** (93 mg, 7%) as white solid. M.p. >350°C (dec.); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 (s, 2H; ArH), 2.94 (t, *J* = 6.2 Hz, 4H; CH_2), 2.83 (q, *J* = 6.1, 5.3 Hz, 4H; CH_2), 2.25 (s, 6H; CH_3), 1.57 (s, 6H; CH_3); ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.5, 143.8, 137.0, 132.1, 131.9, 131.7, 123.7, 37.9, 30.3, 21.6, 18.3; HRMS (APCI) *m/z*: 445.0174 ($[M + H]^+$, calcd for $C_{22}H_{23}Br_2^+$: 445.0167).

(*E*)-4,4',7,7'-tetramethyl-2,2',3,3'-tetrahydro-[1,1'-biindenylidene]-6,6'-diamine [(*E*)-7]: Compound (*E*)-**6** (1.01 g, 2.27 mmol), palladium(II) acetate (44 mg, 0.20 mmol), DPPF (136 mg, 0.25 mmol) and sodium tert-butoxide (473 mg, 4.92 mmol) were brought under a N_2 atmosphere in a Schlenk tube via three vacuum/N_2 cycles. Then, degassed toluene (12 mL) was added, followed by benzophenone imine (1.03 mL, 6.15 mmol). The mixture was stirred at 110 °C for 20 h, cooled to rt and diluted with water (10 mL). The mixture was extracted with $CHCl_3$ (3 x 25 mL) and the combined organic phases were dried over Na_2SO_4 and concentrated. Purification by column chromatography (SiO_2, 0.1% NEt_3 in CH_2Cl_2) afforded the imine

intermediate as a yellow solid, which was redissolved in THF (100 mL). Subsequently, a 2M aqueous HCl solution (50 mL) was added and after 1.5h of stirring, the solution was basified by addition of a saturated aqueous $KHCO_3$ solution (pH ~ 10). The mixture was extracted with EtOAc (3× 50 mL) and the combined organic phases were dried over Na_2SO_4 and concentrated. The product was precipitated in Et_2O, filtered off and air-dried to afford (*E*)-**7** (503 mg, 78%) as a light-brown solid. M.p. 290°C (dec.); ^{1}H NMR (400 MHz, DMSO-d_6) δ 6.41 (s, 2H; ArH), 4.58 (s, 4H; NH), 2.68 (d, J = 9.6 Hz, 8H; CH_2), 2.06 (s, 6H; CH_3), 1.99 (s, 6H; CH_3); ^{13}C NMR (101 MHz, DMSO- d_6) δ 145.7, 142.2, 136.6, 132.0, 129.8, 114.6, 114.1, 36.9, 29.5, 18.2, 16.4; HRMS (ESI) *m/z*: 319.2166 ([M + H]$^+$, calcd for $C_{22}H_{27}N_2^+$: 319.2174).

(*Z*)-4,4',7,7'-tetramethyl-2,2',3,3'-tetrahydro-[1,1'-biindenylidene]-6,6'-diamine [(*Z*)-7]: The procedure used to prepare the imine intermediate toward (*Z*)-**7** was the same as that used for (*E*)-**7**, except for the use of less starting material [*i.e.* 93 mg, 0.21 mmol of (*Z*)-**6**]. The imine intermediate was dissolved in THF (10 mL) and subsequently, a 2M aqueous HCl solution (5 mL) was added. After stirring for 1 h, the mixture was extracted with Et_2O. Then, the water layer was basified with $NaHCO_3$ and extracted with CH_2Cl_2. The organic layer (CH_2Cl_2) was concentrated and the product was precipitated in Et_2O, filtered off and air-dried to afford (*Z*)-**7** (40 mg, 60%) as a light-brown solid. M.p. 205 °C (dec.); ^{1}H NMR (400 MHz, DMSO-d_6) δ 6.34 (s, 2H; ArH), 4.40 (s, 4H; NH), 2.82 – 2.64 (m, 8H; CH_2), 2.10 (s, 6H; CH_3), 1.25 (s, 6H; CH_3); ^{13}C NMR (101 MHz, DMSO- d_6) δ 144.6, 142.4, 135.7, 133.8, 129.1, 116.0, 114.3, 37.5, 29.2, 18.3, 15.4; HRMS (ESI) m/z: 319.2167 ([M + H]$^+$, calcd. for $C_{22}H_{27}N_2^+$: 319.2174).

(*E*)-1,1'-(4,4',7,7'-tetramethyl-2,2',3,3'-tetrahydro-[1,1'-biindenylidene]-6,6'-diyl)bis(3-phenylthiourea) [(*E*)-1]: Phenyl isothiocyanate (250 µL, 2.1 mmol) was added to **(*E*)-7** (0.31 g, 1.0 mmol) in THF (10 mL) under a N_2 atmosphere. The mixture was stirred for 16 h, after

which the white precipitate was filtered off, washed with THF, and dried in vacuo to afford (*E*)-**1** (447 mg, 76%) as a white solid. M.p. 185.6 °C (dec.); ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.60 (s, 2H; NH), 9.40 (s, 2H; NH), 7.50 (d, J = 7.9 Hz, 4H; ArH), 7.33 (t, J = 7.7 Hz, 4H; ArH), 7.13 (t, J = 7.4 Hz, 2H; ArH), 6.95 (s, 2H; ArH), 2.70 (d, J = 25.1 Hz, 8H; CH_2), 2.19 (s, 12H; CH_3); ^{13}C NMR (101 MHz, DMSO-d_6) δ 180.5, 142.7, 142.6, 139.7, 136.9, 136.9, 130.2, 128.3, 127.9, 127.8, 124.2, 123.6, 36.5, 30.0, 17.9, 17.2; HRMS (ESI) *m/z*: 611.2265 ([M + Na]$_+$, calcd for $C_{36}H_{46}N_4S_2Na^+$: 611.2279), 589.2436 ([M + H]$^+$, calcd for $C_{36}H_{37}N_4S_2^+$: 589.2460).

(*Z*)-1,1'-(4,4',7,7'-tetramethyl-2,2',3,3'-tetrahydro-[1,1'-biindenylidene]-6,6'-diyl)bis(3-phenylthiourea) [(Z)-1]: Phenyl isothiocyanate (25 μL, 0.21 mmol) was added to (*Z*)-**7** (31 mg, 0.10 mmol) in CH_2Cl_2 (1 mL) under a N_2 atmosphere. The mixture was stirred for 24 h, after which the white precipitate was filtered off, washed with THF and dried in vacuo to afford (*Z*)-**1** (44 mg, 75%) as a white solid. M.p. 167.5 °C (dec.); ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.60 (s, 2H; NH), 9.40 (s, 2H; NH), 7.50 (d, J = 7.9 Hz, 4H; ArH), 7.33 (t, J = 7.7 Hz, 4H; ArH), 7.13 (t, J = 7.4 Hz, 2H; ArH), 6.95 (s, 2H; ArH), 2.70 (d, J = 25.1 Hz, 8H; CH_2), 2.19 (s, 12H; CH_3); ^{13}C NMR (101 MHz, DMSO-d_6) δ 180.5, 142.7, 142.6, 139.7, 136.9, 136.9, 130.2, 128.3, 127.9, 127.8, 124.2, 123.6, 36.5, 30.0, 17.9, 17.2; HRMS (ESI) *m/z*: 589.2443 ([M + H]$^+$, calcd for $C_{36}H_{37}N_4S_2^+$: 589.2460).

^{1}H NMR titrations

For the titration experiments, 5.0 mM receptor solutions were prepared in 1 mL DMSO-d_6/0.5%H_2O (v/v). The tetrabutylammonium salt of the corresponding anion was dissolved in 0.5 mL of this solution to reach a concentration of 5.0×10^{-2} M. Then, the anion solution was added stepwise to 0.5 mL of the receptor solution and a ^{1}H NMR spectrum (500 MHz) was recorded at 298 K after each addition.

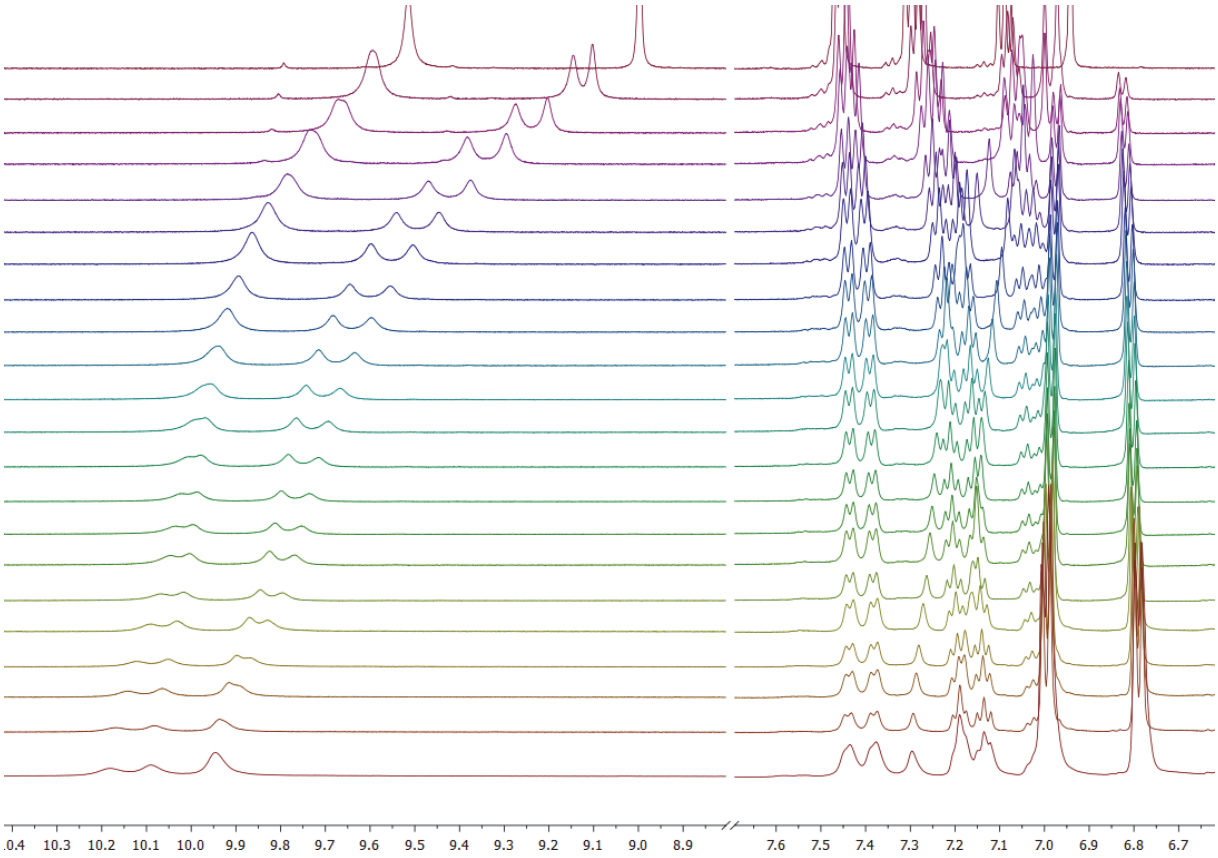


Figure S1. ^{1}H NMR spectral changes (500 MHz, 298 K) in the aromatic region of (*Z*)-**1** (5.0 mM in DMSO-d_6/0.5%H_2O) upon the stepwise addition of $[Bu_4N]^+[(S)\text{-}\mathbf{2})]^-$ (from top to bottom: 0.00, 0.19, 0.37, 0.55, 0.71, 0.88, 1.03, 1.18, 1.33, 1.47, 1.61, 1.74, 1.87, 1.99, 2.11, 2.22, 2.44, 2.75, 3.21, 3.61, 4.27 and 4.76 equivalents).

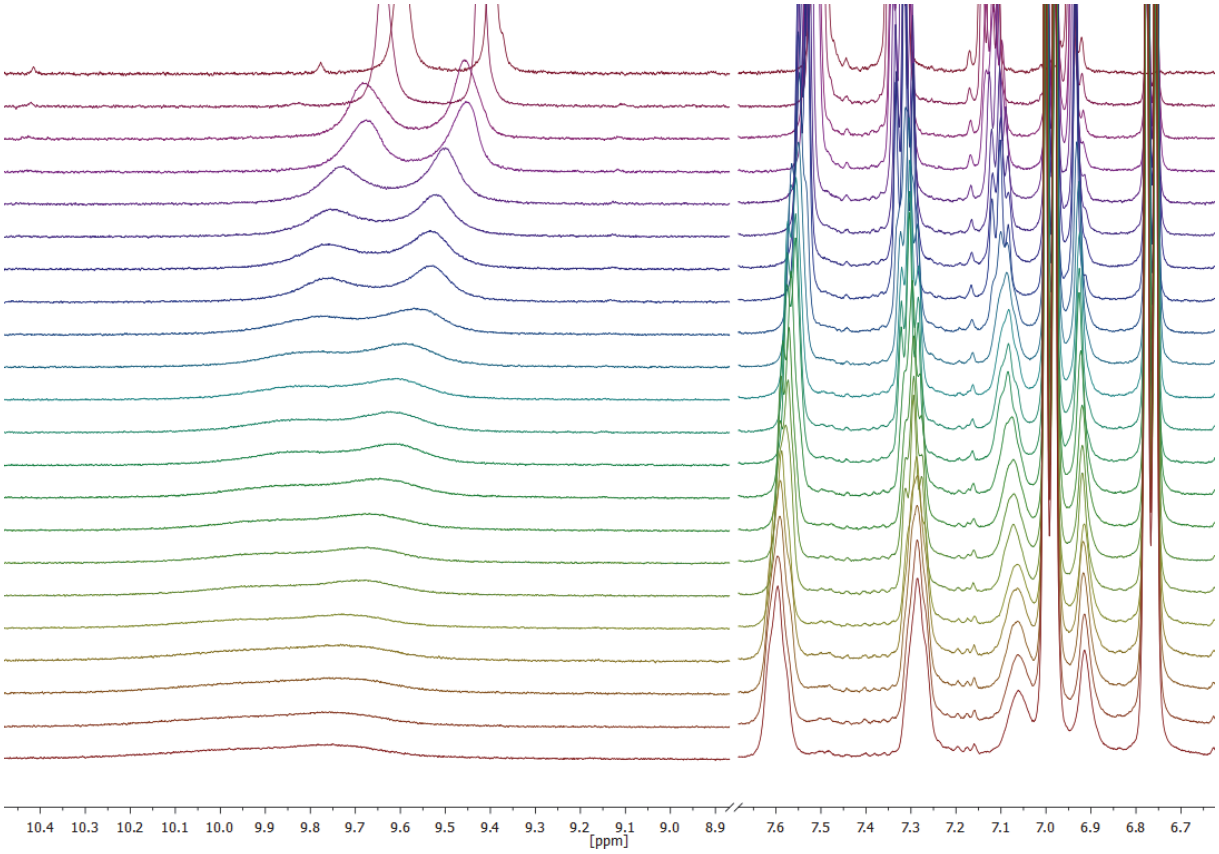
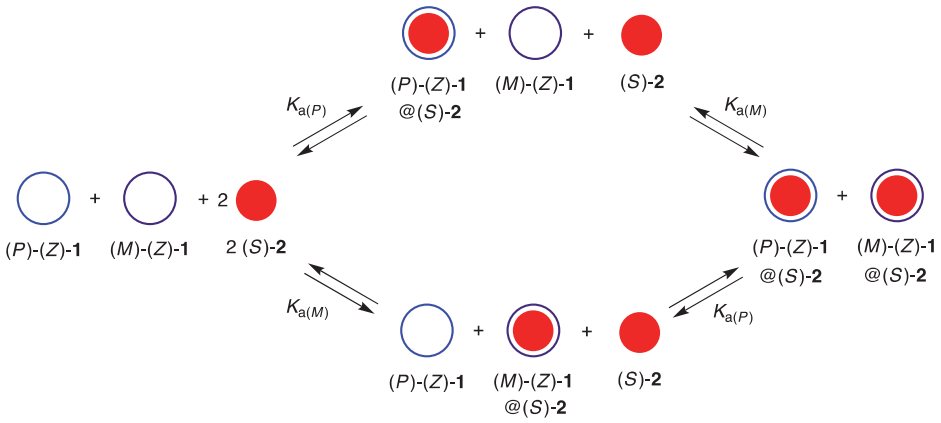


Figure S2. ^{1}H NMR spectral changes (500 MHz, 298 K) in the aromatic region of (*E*)-**1** (5.0 mM in DMSO-d_6/0.5%H_2O) upon the stepwise addition of $[Bu_4N]^+[(S)\text{-}\mathbf{2})]^-$ (from top to bottom: 0.00, 0.19, 0.37, 0.55, 0.72, 0.88, 1.04, 1.19, 1.34, 1.48, 1.62, 1.75, 1.88, 2.00, 2.12, 2.24, 2.46, 2.77, 3.26, 3.64, 4.31 and 4.85 equivalents).

Titration data analysis

As the spectral changes for the titration of $[Bu_4N]^+[(S)\text{-}\mathbf{2})]^-$ to (*E*)-**1** were minor, revealing very weak binding, and significant broadening of the NH signals was observed, the data was not analyzed further. For the titration to (*Z*)-**1**, the binding model depicted in Scheme S1 was used: (*S*)-**2** can bind to either the *P* or *M* helical isomer of sterically overcrowded (*Z*)-**1**, of which interconversion is slow and insignificant on the timescale the ^{1}H NMR titration was carried out. The resulting complexes are diastereomeric and have different stability constants [$K_{a(P)} \neq K_{a(M)}$].



Scheme S1. Overview of species and equilibria involved in the titration of (*S*)-**2** to (*Z*)-**1**.

Throughout the ^{1}H NMR titration (Figure S5), four NH signals could be distinguished of which two must belong to each possible diastereomeric complex. First, the changes in chemical shift ($\Delta\delta$) were normalized and plotted (Figure S6, left). From the shape of the titration curves and inflection points it can be deduced that NH(a) and NH(d) belong to one diastereomeric complex and NH(b) and NH(c) to the other. The titration data was fitted with HypNMR[1] using the binding model described above considering three species [(*P*)-(*Z*)-**1**, (*M*)-(*Z*)-**1**, (*S*)-**2**] and two equilibrium constants [$K_{a(P)}$, $K_{a(M)}$]. The two sets of chemical shift data (*i.e.* NH(a), NH(d) and NH(b), NH(c)] were arbitrarily assigned to different hosts. Fitting of the data (Figure S6, right)

afforded two equilibrium constants (3.1 x 10^2 M^{-1} and 4.6 x 10^2 M^{-1} of which the highest was assigned to (*P*)-(*Z*)-**1**@⊃(*S*)-**2** since it is the lower energy complex according to the DFT calculations. Hence, $K_{a(P)}$ = 4.6 x 10^2 M^{-1} and $K_{a(M)}$ = 3.1 x 10^2 M^{-1}, NH(b) and NH(c) belong to (*P*)-(*Z*)-**1**@⊃(*S*)-**2** and NH(a) and NH(d) to (*M*)-(*Z*)-**1**@⊃(*S*)-**2**.

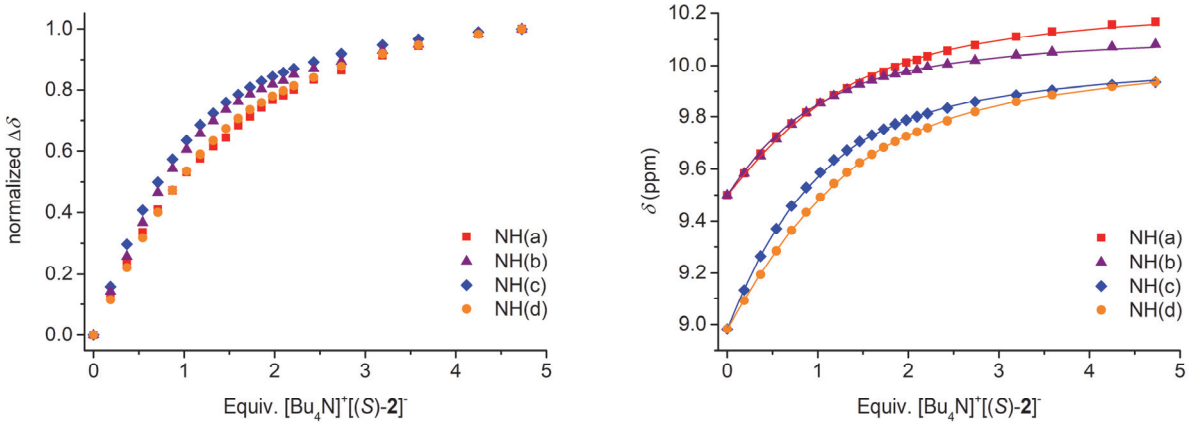


Figure S3. (left) Plot of normalized NH chemical shift changes for the addition of $[Bu_4N]^+[(S)$-**2**$)]^-$ to (*Z*)-**1** and (right) titration curves and data fitting obtained by simultaneous analysis of the NH signals using HypNMR and the binding model in Scheme S1.

^{1}H NMR studies of diastereomeric complex interconversion

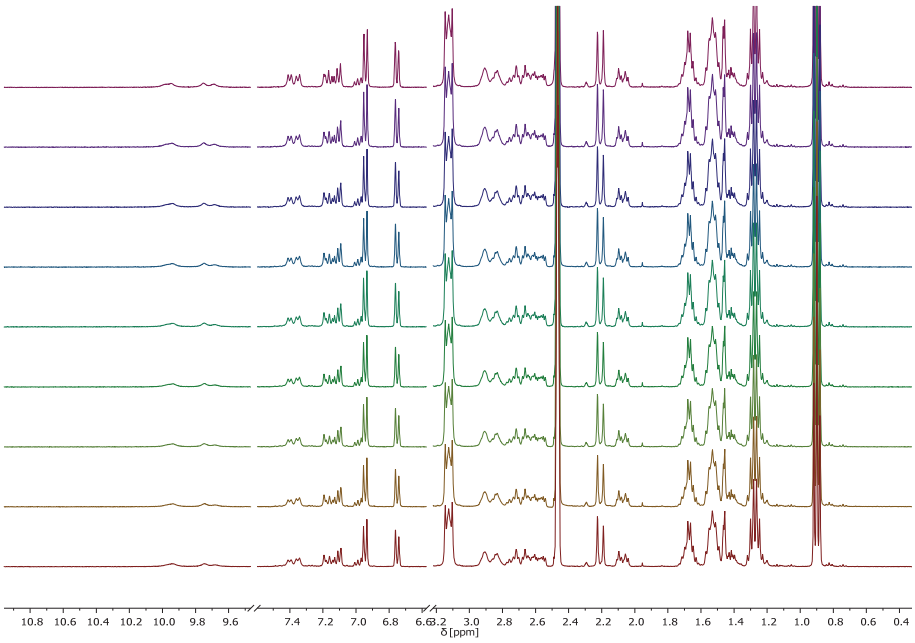


Figure S4. ^{1}H NMR spectra measured over time starting with a freshly prepared solution of (*Z*)-**1** (5.0 mM) with 2 equiv. $[Bu_4N]^+[(S)\text{-}\mathbf{2})]^-$ (10.0 mM) in degassed DMSO-d_6/0.5%H_2O. The ratio changed from (1:1) to (1:1.27) as was determined by integration of the Ar-H signals. (from top to bottom: 0, 6, 12, 26, 36, 48, 60, 69 and 84 h).

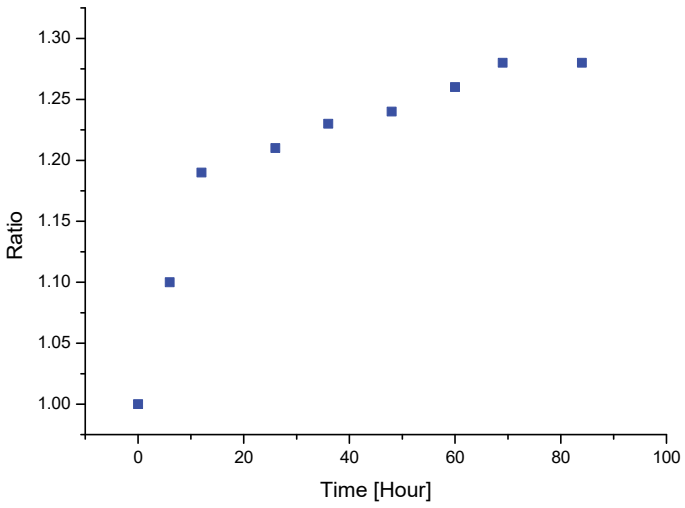


Figure S5. Corresponding plot of the diastereomeric ratio as a function of time as determined by ^{1}H NMR starting with a freshly prepared solution of (*Z*)-**1** (5.0 mM) with 2 equiv. $[Bu_4N]^+[(S)\text{-}\mathbf{2})]^-$ (10.0 mM) in degassed DMSO-d_6/0.5%H_2O.

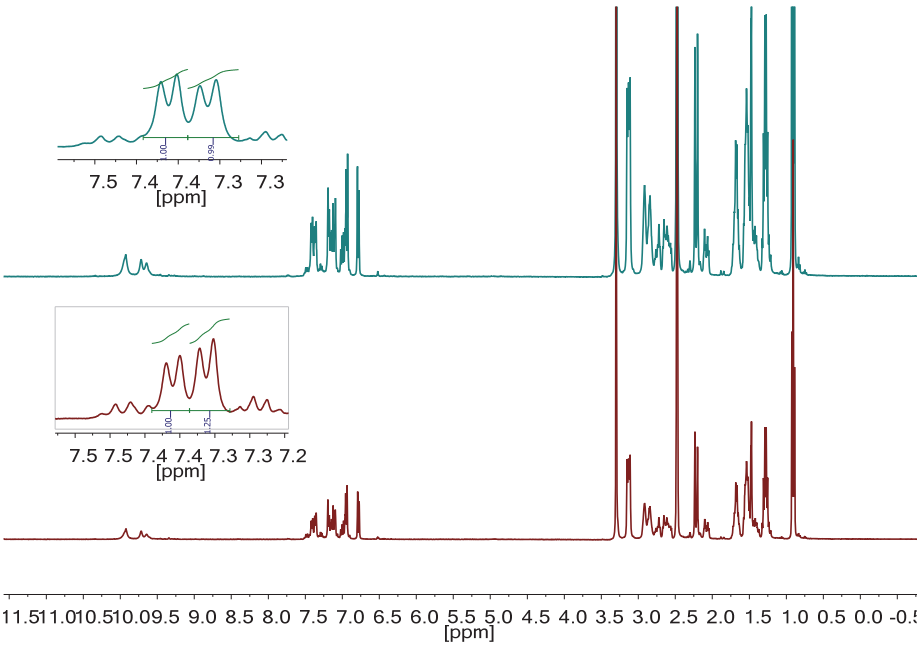


Figure S6. ^{1}H NMR spectrum of (*Z*)-**1** with $[Bu_4N]^+[(R)\text{-}\mathbf{2})]^-$ freshly prepared (green) and after 3 days (red) in degassed DMSO-d_6/0.5%H_2O. The ratio changed from (1:1) to (1:1.25) as was determined by integration of the Ar-H signals.

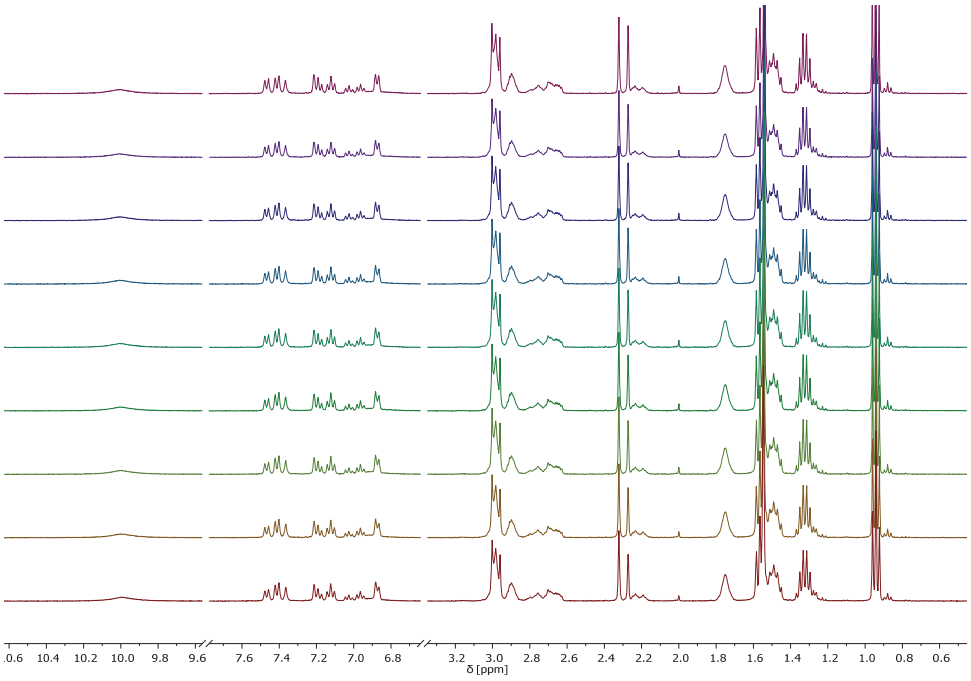


Figure S7. ^{1}H NMR spectra measured over time starting with a freshly prepared solution of (*Z*)-**1** (2.0 mM) with 1 equiv. $[Bu_4N]^+[(R)\text{-}\mathbf{2})]^-$ (2.0 mM) in degassed CD_2Cl_2. The ratio changed from (1:1) to (1:1.46) as was determined by integration of the Ar-H signals (from top to bottom time intervals: 0, 2, 3.5, 5, 6.5, 8.5, 11, 14 and 18 h).

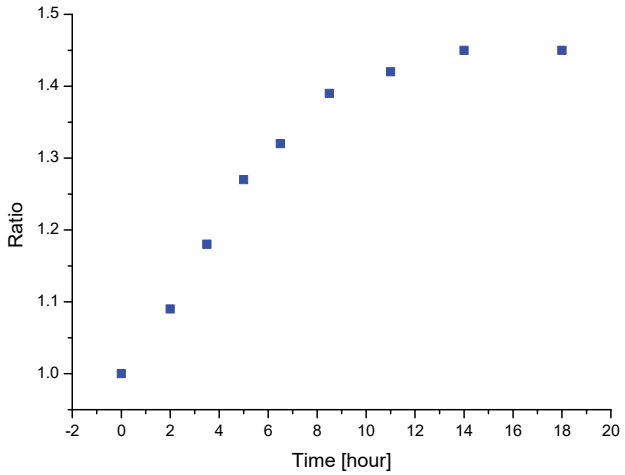


Figure S8. Corresponding plot of the diastereomeric ratio as a function of time as determined by ^{1}H NMR starting with a freshly prepared solution of (*Z*)-1 (2.0 mM) with 1 equiv. $[Bu_4N]^+[(R)\text{-}2)]^-$ (2.0 mM) in degassed CD_2Cl_2. The ratio changed from (1:1) to (1:1.46) as was determined by integration of the Ar-H signals.

CD studies of diastereomeric complex interconversion

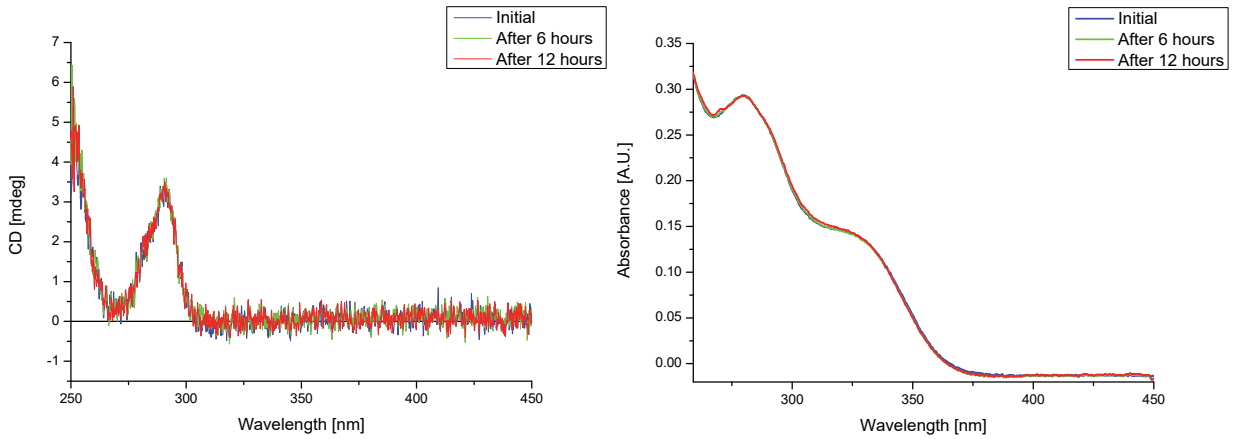


Figure S9. CD (left) and corresponding UV-Vis (right) spectra of a 1:1 mixture of (*Z*)-**1** with $[Bu_4N]^+[(R)\text{-}\mathbf{2})]^-$ (0.050 mM) in degassed DMSO/0.5%H_2O, freshly prepared and after 6 and 12 h. CD spectral changes are absent as there is insignificant complex formation at this concentration in this solvent mixture. The CD absorption below 300 nm stems from (*R*)-**2**.

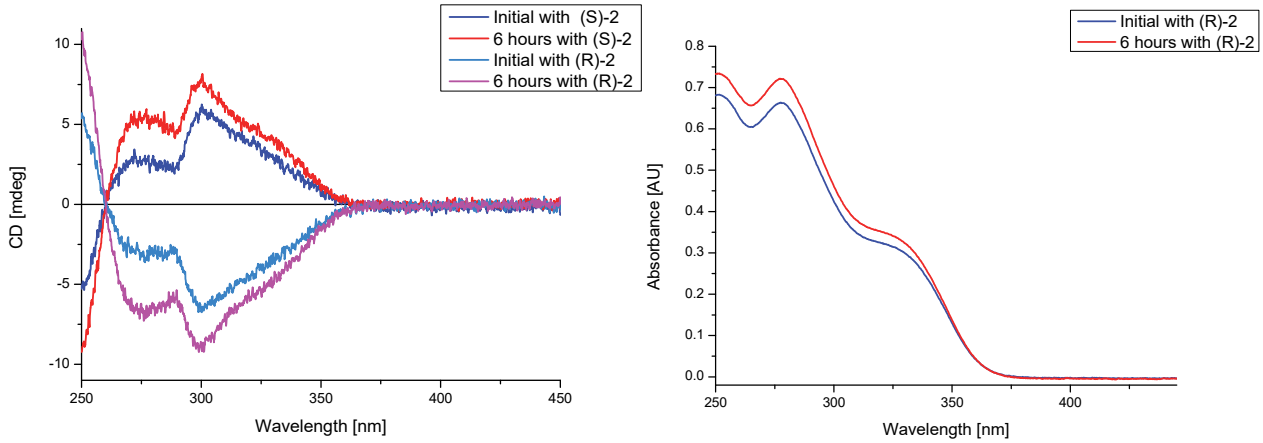


Figure S10. CD (left) and UV-Vis (right) spectra of (*Z*)-**1** with either $[Bu_4N]^+[(S)\text{-}\mathbf{2})]^-$ or $[Bu_4N]^+[(R)\text{-}\mathbf{2})]^-$ (0.1 mM) in degassed CH_2Cl_2, freshly prepared and after 6 h. The slight increase in absorbance is ascribed to some solvent evaporation. Please note that the CD absorbance increase is significantly larger.

Irradiation experiments

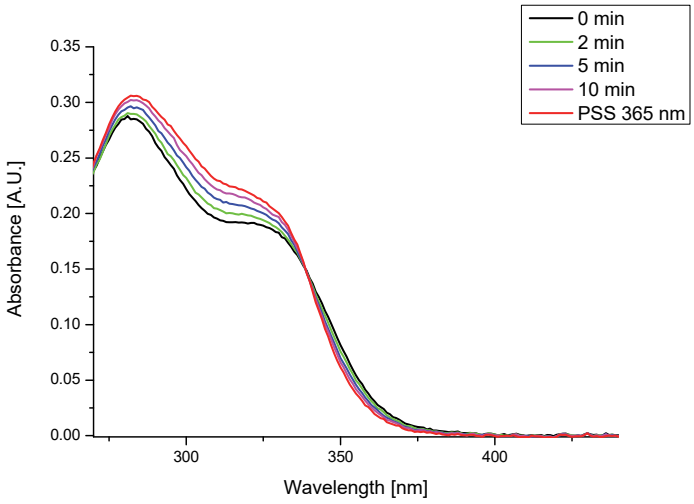


Figure S11. UV-vis spectral changes of (*Z*)-**1** (1 x 10^{-5} M in degassed DMSO) upon 365 nm irradiation for a total of 15 min (PSS 365).

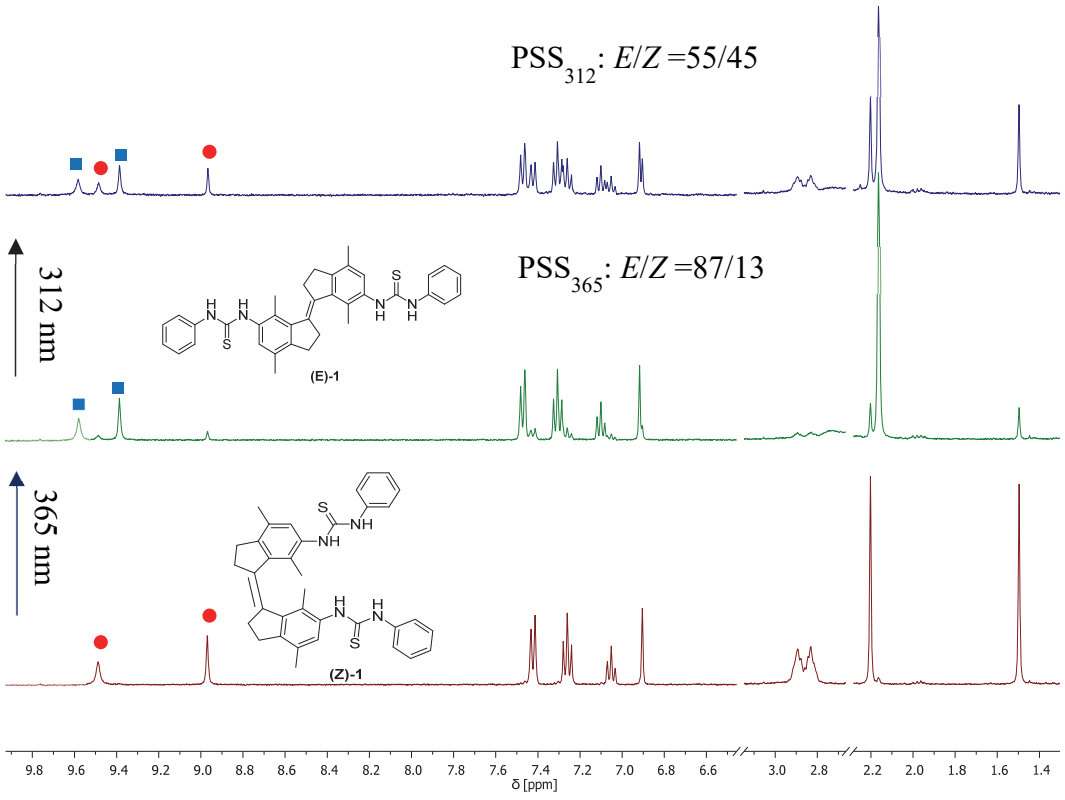
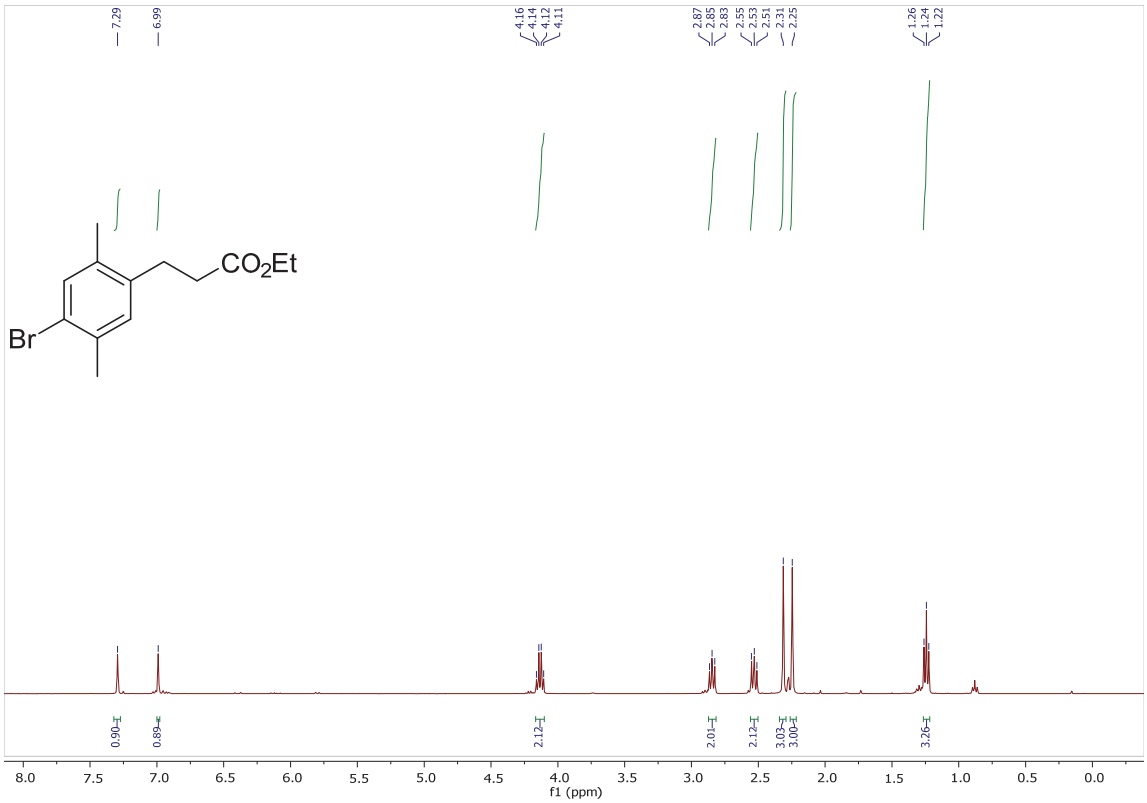
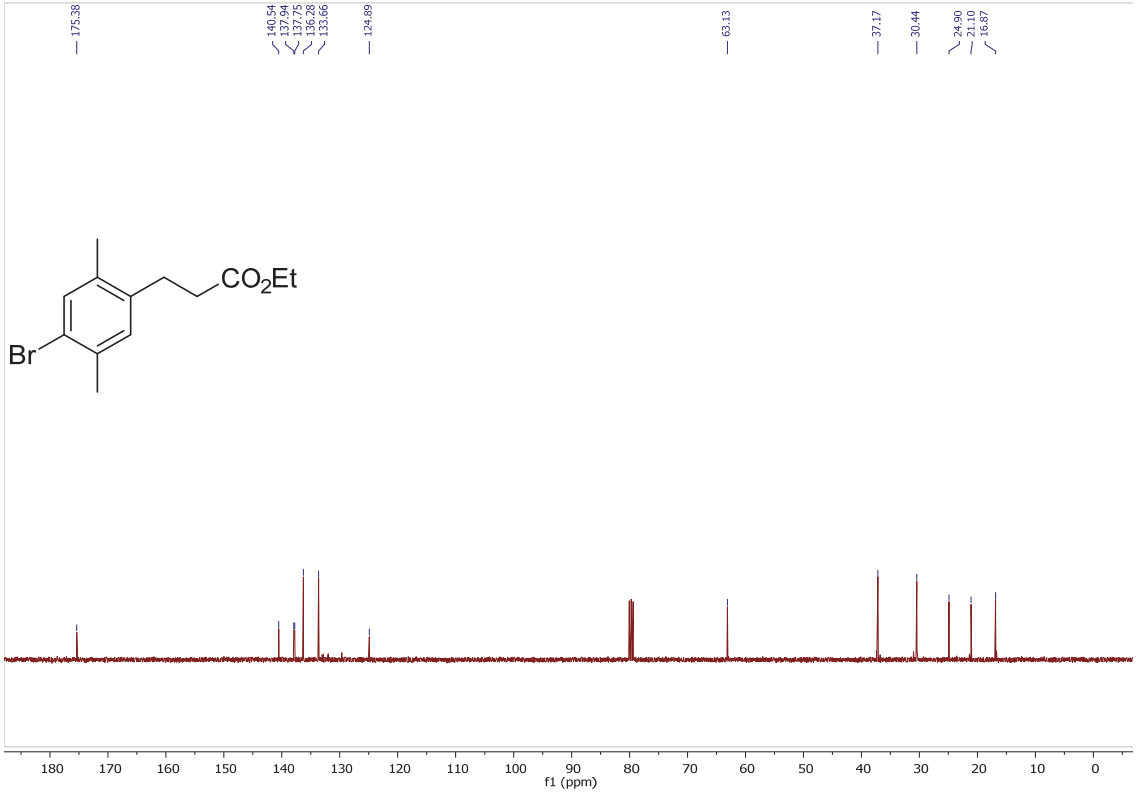


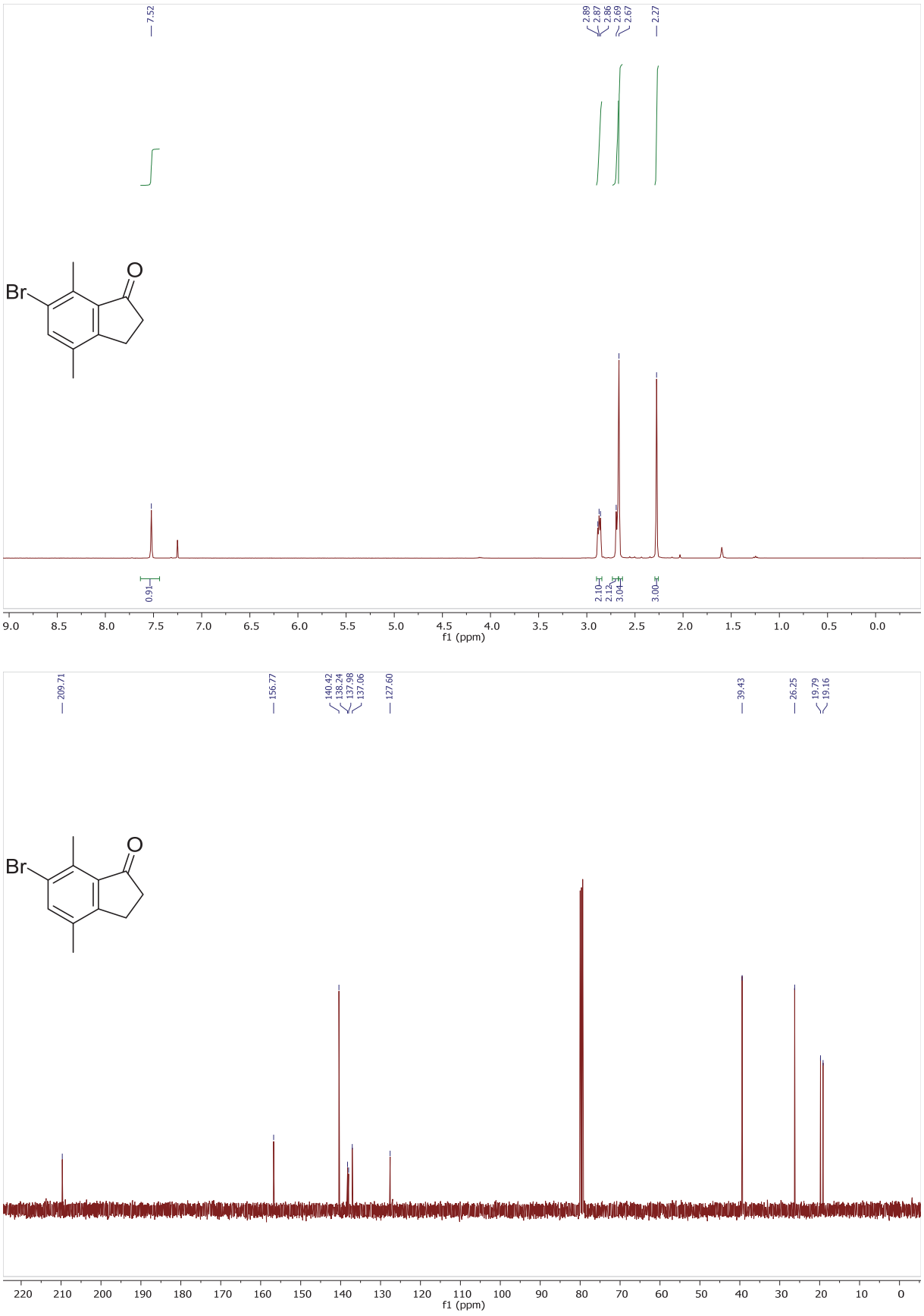
Figure S12. ^{1}H NMR spectral changes after irradiation of (bottom) (*Z*)-**1** (1 x 10^{-3} M in degassed DMSO-d_6/0.5%H_2O) with (middle) 365 nm light for 1 h followed by irradiation with (top) 312 nm light for 1 h.

^{1}H and ^{13}C NMR spectra

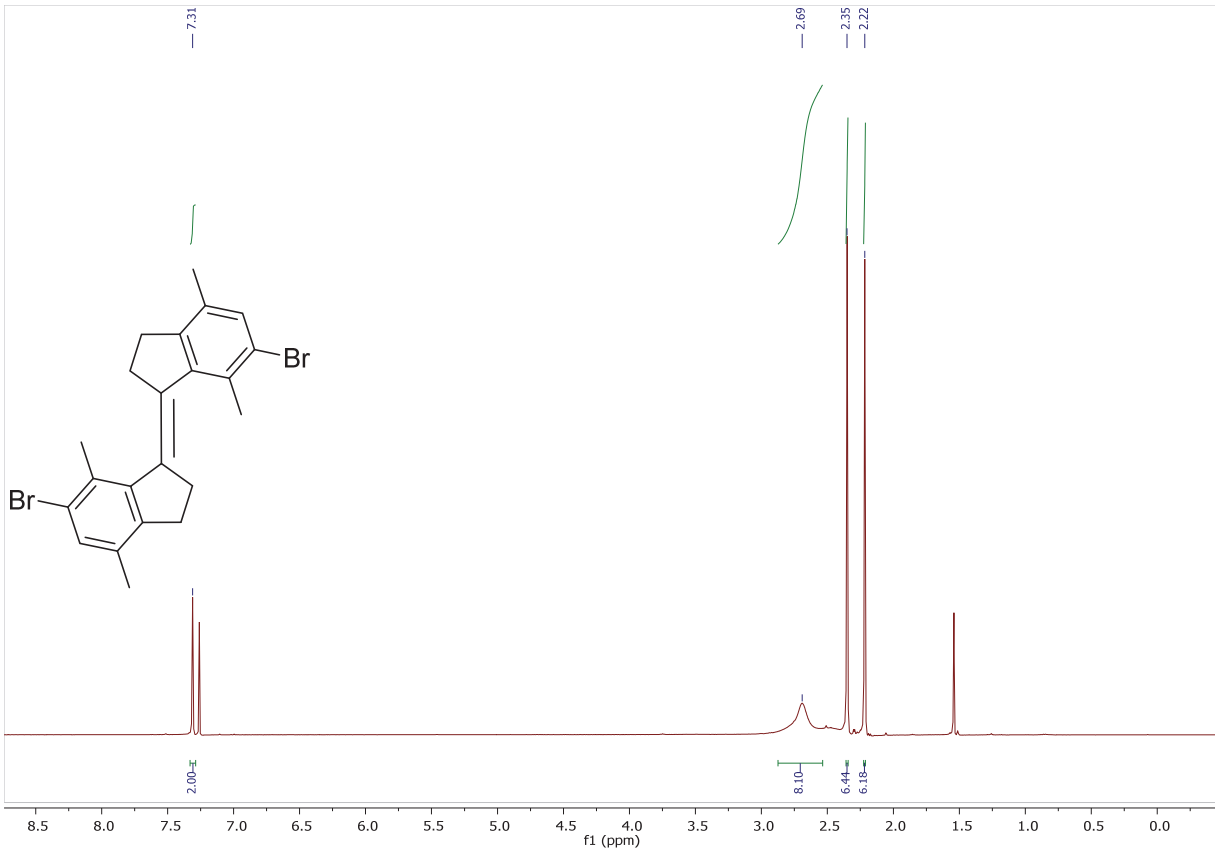




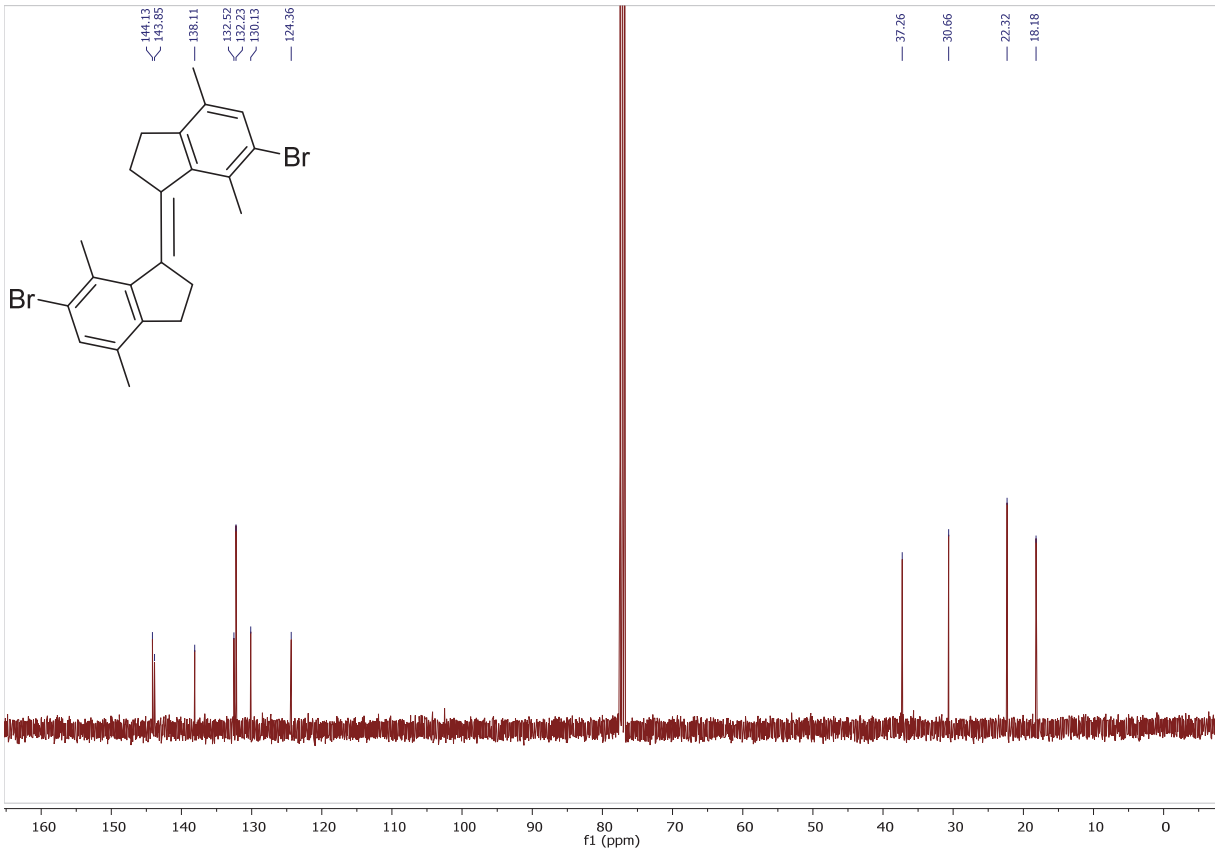
400 MHz ^{1}H NMR (top) and 100 MHz ^{13}C NMR (bottom) spectra of **4** measured at 298 K in $CDCl_3$.



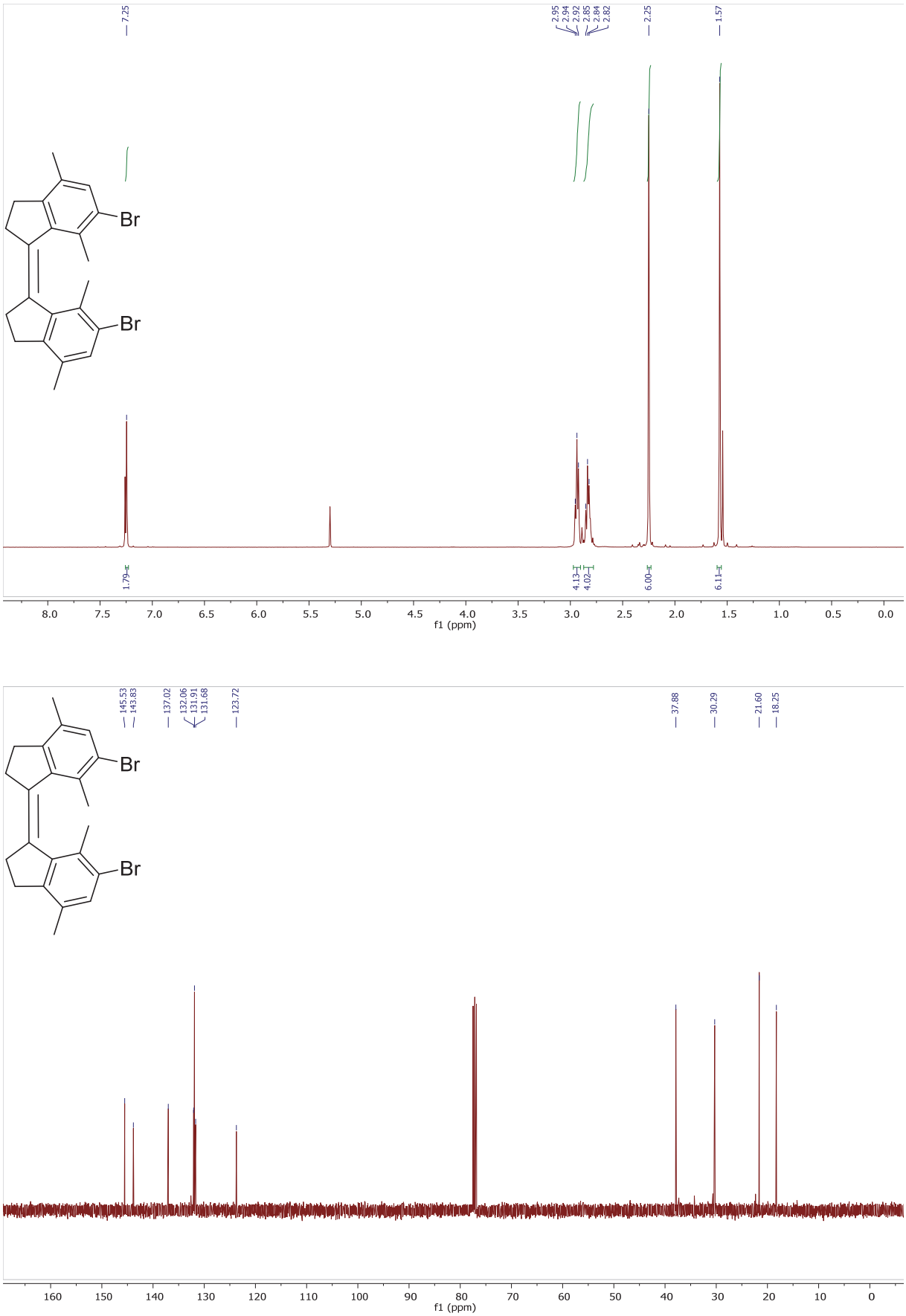
400 MHz ^{1}H NMR (top) and 100 MHz ^{13}C NMR (bottom) spectra of **5** measured at 298 K in $CDCl_3$.



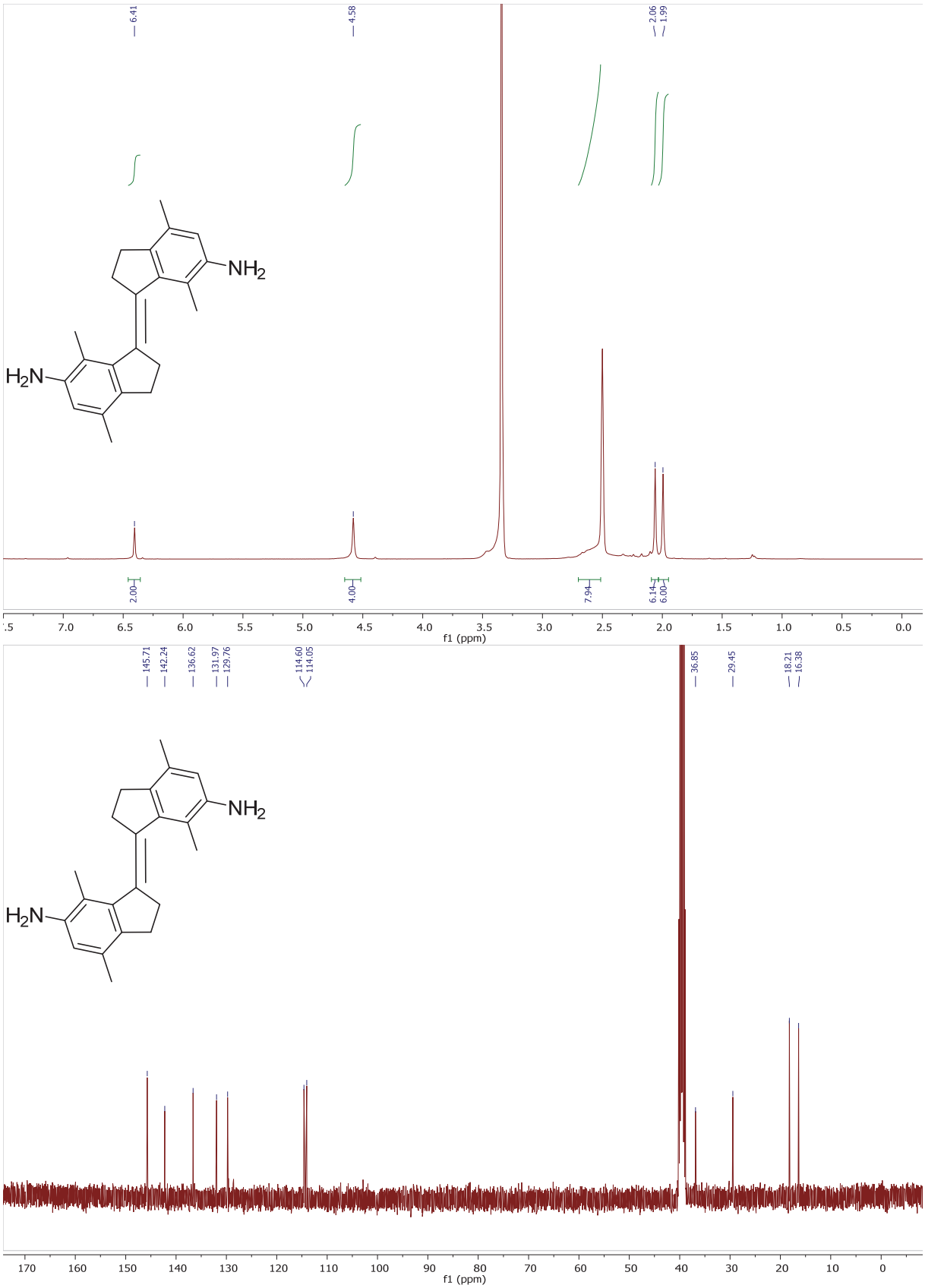
ii



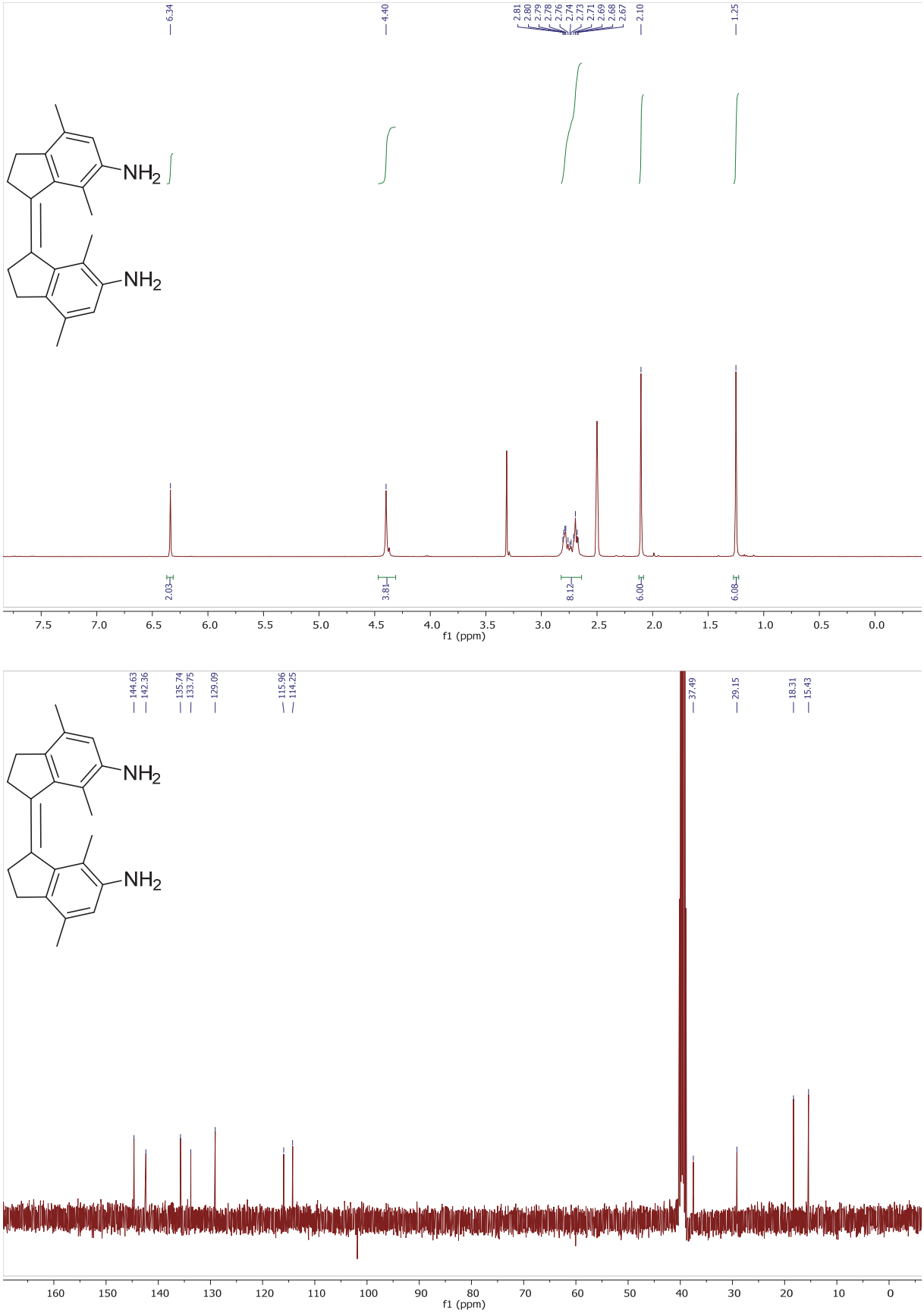
400 MHz ^{1}H NMR (top) and 100 MHz ^{13}C NMR (bottom) spectra of (*E*)-**6** measured at 298 K in $CDCl_3$.



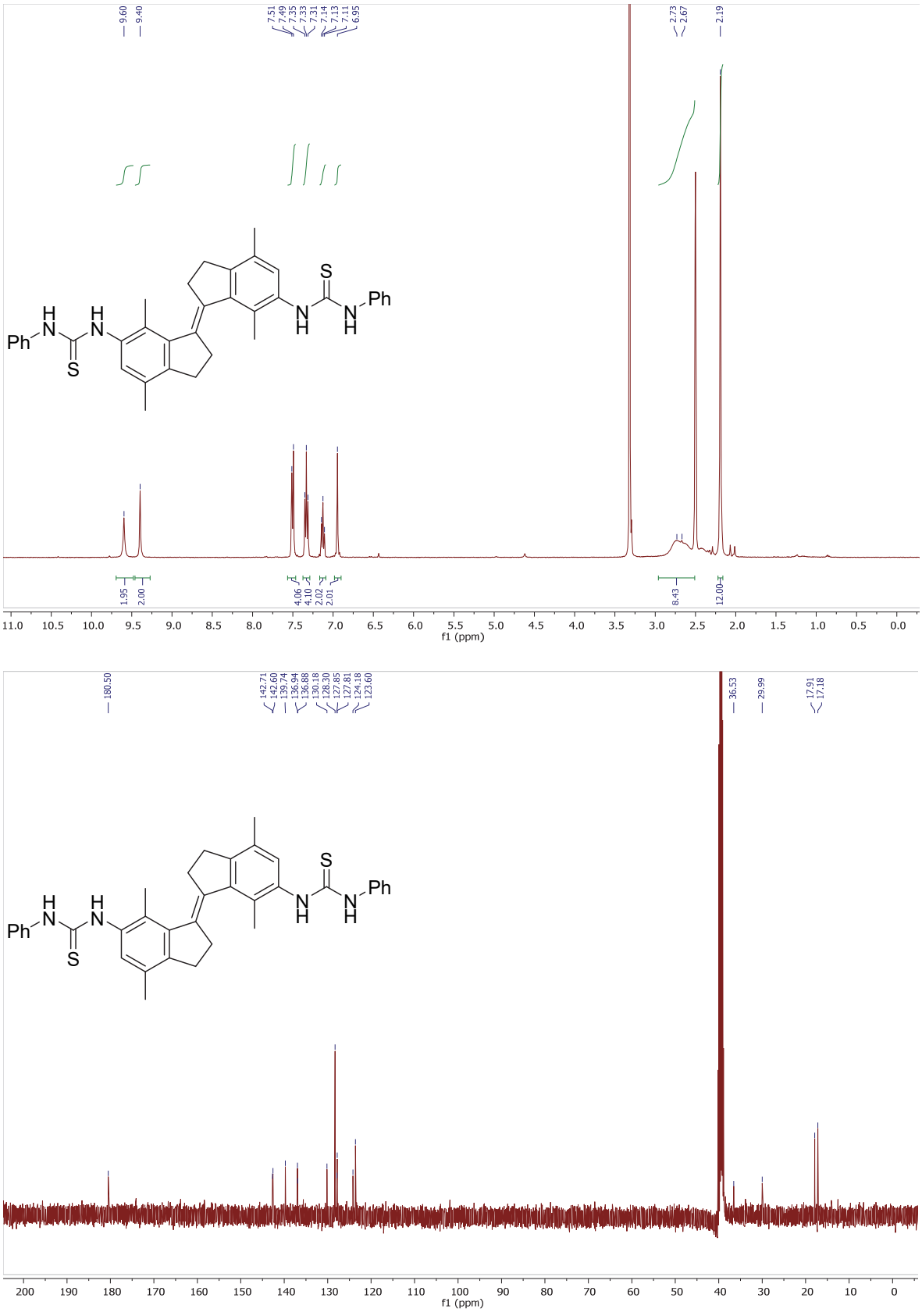
400 MHz ^{1}H NMR (top) and 100 MHz ^{13}C NMR (bottom) spectra of (*Z*)-**6** measured at 298 K in $CDCl_3$.



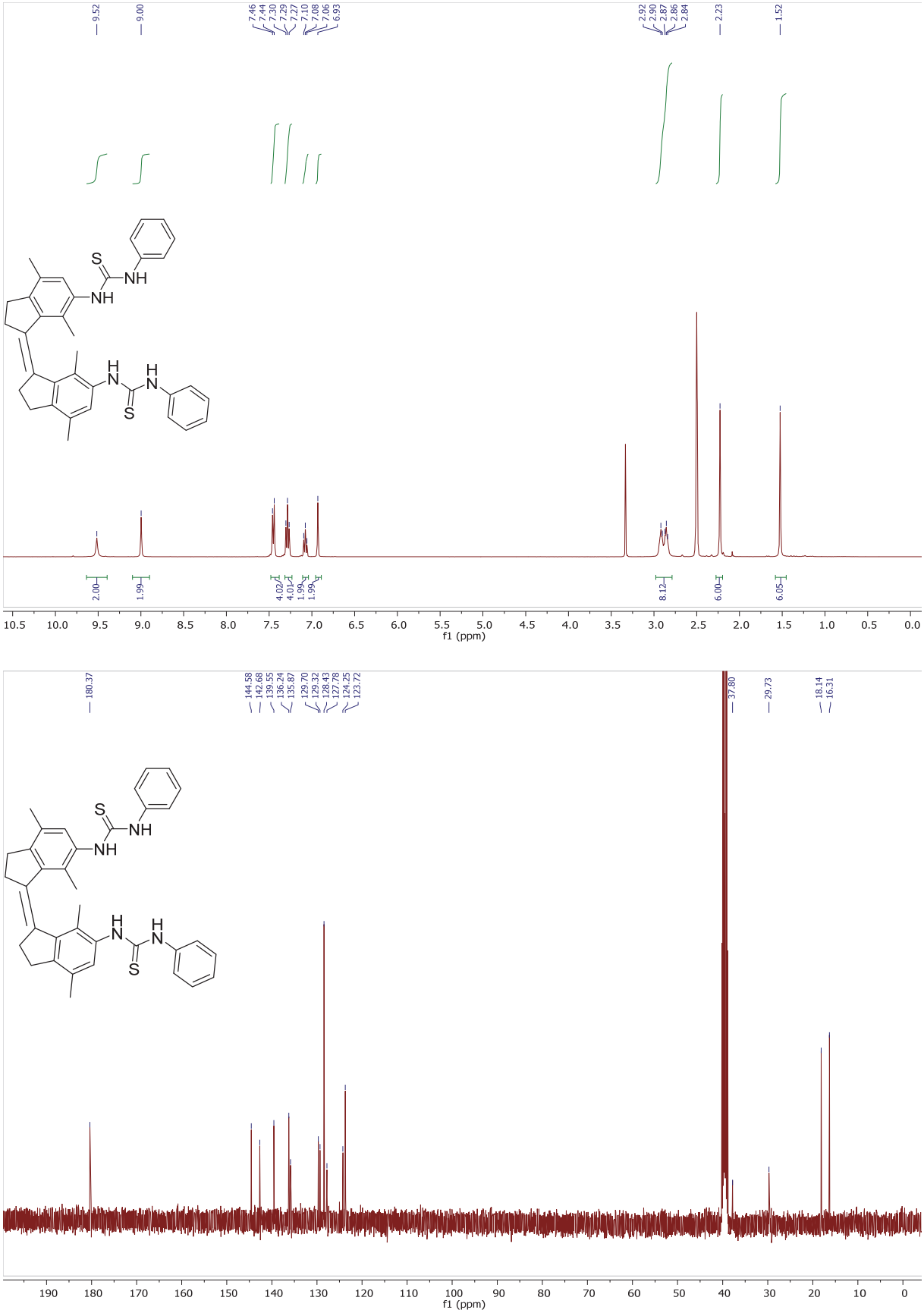
400 MHz ^{1}H NMR (top) and 100 MHz ^{13}C NMR (bottom) spectra of (*E*)-**7** measured at 298 K in DMSO-d_6.



400 MHz ^{1}H NMR (top) and 100 MHz ^{13}C NMR (bottom) spectra of (*Z*)-**7** measured at 298 K in DMSO-*d*6.



400 MHz ^{1}H NMR (top) and 100 MHz ^{13}C NMR (bottom) spectra of (*E*)-**1** measured at 298 K in DMSO-*d*6.

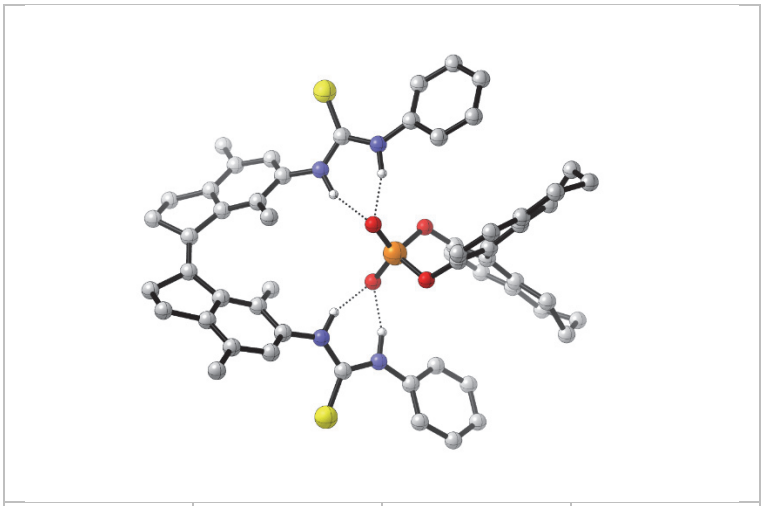


400 MHz ^{1}H NMR (top) and 100 MHz ^{13}C NMR (bottom) spectra of (*Z*)-**1** measured at 298 K in DMSO-*d*6.

Computational details

All the calculations were carried out using the Gaussian 16 Rev. B.01[2] at the at the SMD(DMSO)-ωB97X-D/def2-SVP(def2-TZVP) or at the SMD(DMSO)-ωB97X-D/def2-TZVPP//SMD(DMSO)-ωB97X-D/def2-SVP level of theory. All the optimizations were confirmed to be stationary points by the number of imaginary frequencies found (0 for the minima,1 for the transition state). The solvent contribution was treated implicitly applying the SMD method (DMSO as solvent).

(*M*)-(*Z*)-1⊃(*S*)-2



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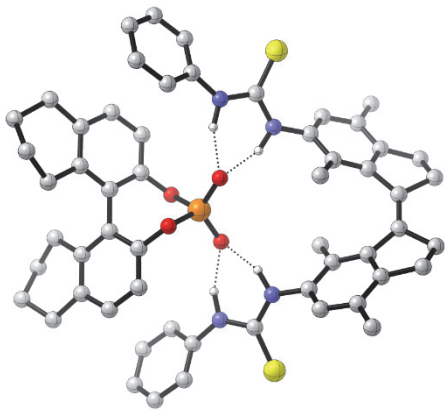
(*P*)-(*Z*)-1⊃(*S*)-2



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Thermal correction to Gibbs Free Energy= 0.921684
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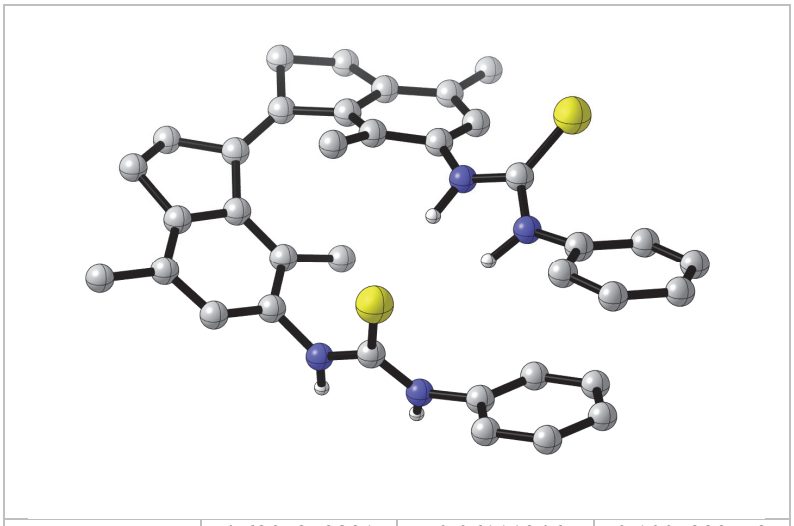
(*Z*)-1



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H	1.0712696332	0.0050835681	-1.4876191726
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Zero-point correction= 0.647198 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.575768
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Sum of electronic and thermal Energies= -2406.703218
Sum of electronic and thermal Enthalpies= -2406.702274
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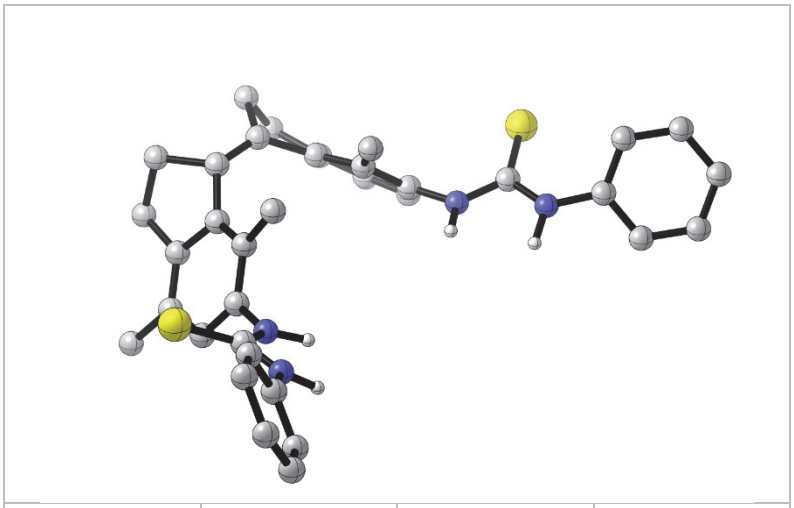

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C	5.7739910025	4.2889557283	-0.7679466503
C	5.8808921248	3.3055992751	1.4395677828
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H	7.2287548042	4.2501416966	2.8222477957
H	7.982935705	5.9849315622	1.1976017411
C	-5.209057025	3.5445714424	-0.0665900186
C	-6.0135484816	3.5887130858	1.0785339237
C	-5.3177712613	4.560521681	-1.0247229688
C	-6.9295529767	4.626376803	1.2406340979
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H	-4.6827357136	4.5285228453	-1.9139643135
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H	-7.7626330357	6.4461175046	0.4199607911
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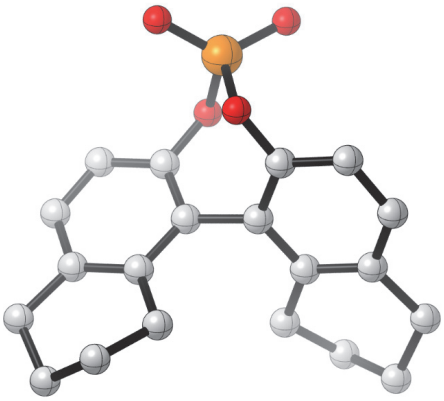
S	5.4459824893	0.1348699434	0.7262918157

Energy= -2407.3450333
Zero-point correction= 0.646747 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.572041
Sum of electronic and zero-point Energies= -2406.698287
Sum of electronic and thermal Energies= -2406.660576
Sum of electronic and thermal Enthalpies= -2406.659632
Sum of electronic and thermal Free Energies= -2406.772992
Energy (ωB97X-D/def2-TZVPP)= -2409.0384966

(*S*)-2



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C	5.2344889578	0.0589599285	0.4926354099
C	4.1161735151	-0.170770063	2.6305060111
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C	4.2485902552	-1.1396764681	-1.5376539265
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C	6.3147544897	-2.5926331295	-1.2410990734
C	6.9693191429	-3.8107276639	-1.8844579169
C	6.2322433902	-3.127523188	-4.1684449981
C	5.208031727	-2.2351296897	-3.4926532241
C	7.4042237864	1.56969019	1.6951309462
C	4.1541765591	-1.7271660412	-4.2635585981
C	6.1933846574	1.2321851126	2.5577029748
C	7.4342106496	-3.4634265797	-3.2929400692
C	6.9540160915	1.916363146	0.2817334432
O	0.3355932468	-1.9420145753	-1.7132319176
P	1.0170908531	-0.9510109911	-0.8333147246
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H	2.2696112534	-0.6523211603	-4.2756608481

Energy= -1415.4894868
Zero-point correction= 0.367399 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.319262
Sum of electronic and zero-point Energies= -1415.122088
Sum of electronic and thermal Energies= -1415.102208
Sum of electronic and thermal Enthalpies= -1415.101264
Sum of electronic and thermal Free Energies= -1415.170225
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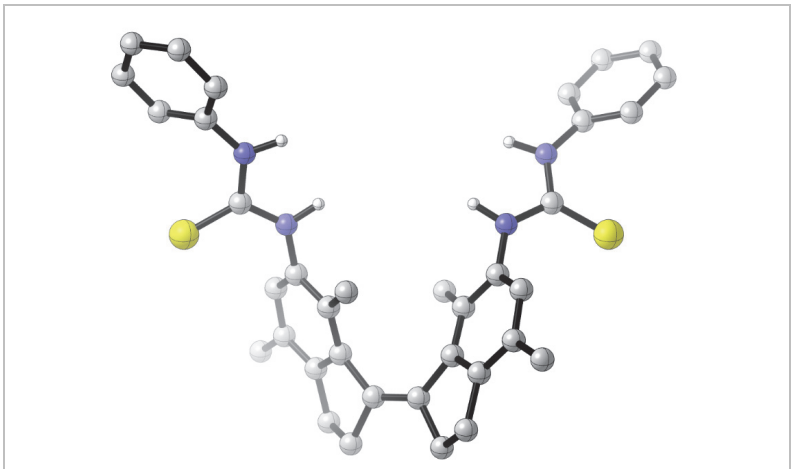

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Energy= -2407.1019306
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Thermal correction to Gibbs Free Energy= 0.572234
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Sum of electronic and thermal Energies= -2406.416201
Sum of electronic and thermal Enthalpies= -2406.415257
Sum of electronic and thermal Free Energies= -2406.529697
Energy (ωB97X-D/def2-TZVPP)= -2409.0726952

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