# Electronic Supplementary Information

## Tetrahydro[5]helicene-based full-color emission dyes in both solution and solid state: synthesis, structures, photophysical properties and optical waveguide application

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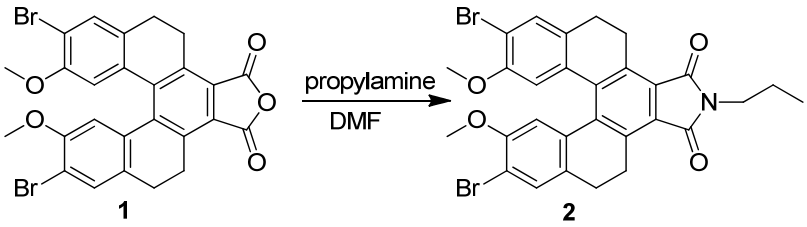
## Contents

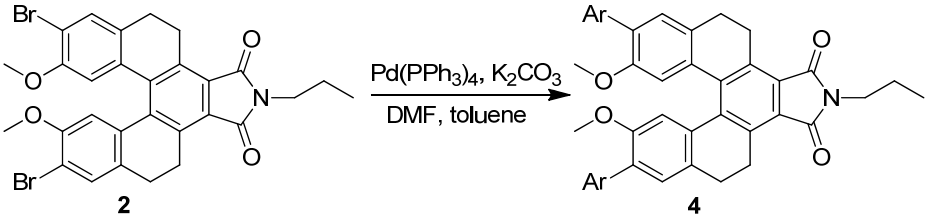
## 1. General information

All reactants were commercial and used without further purification excepted as noted. Melting points are uncorrected. $^{1}H$ NMR and $^{13}C$ NMR spectra were recorded with a DMX300 NMR spectrometer. MALDI-TOF mass spectra were recoreded with a BIFLEXIII mass spectrometer. HRMS mass spectra were measured in the ESI mode. All calculations were performed using the SHELXL97 and crystal structure crystallographic software packages. The UV-Vis absorption spectra were recorded on a JASCO V-550 spectrophotometer. Fluorescence spectra were measured on a Hitachi F-7000 fluorometer equipped with a Xenon lamp excitation source. Photographs of emissions were recorded with a Cannon digital camera. Absolute fluorescence quantum yield, measured by Hamamatsu Absolute PL Quantum Yield Spectrometer C11347. Fluorescence lifetimes were measured by Quantaurus Tau C11367-11. PL images were recorded with Olympus research inverted system microscope (FV1000-IX81) equipped with a charge couple device camera (CCD, Olympus DP71).

## 2. Synthesis and characterization of new compounds



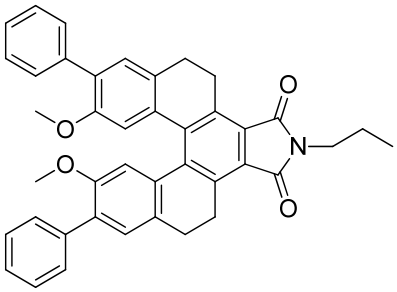

**Compound 2.** A mixture of **1** (11.4 g, 20 mmol) and *n*-propylamine (11.8 g, 0.1 mol) in DMF (100 mL) was heated at 70 °C for 24 hours. The reaction mixture was cooled to room temperature, and then added ethyl acetate (200 mL). The organic phase was washed with saturated brine (3×100 mL), dried over anhydrous $MgSO_4$. The solvent was removed in *vacuo*, and the residue was purified by column chromatography (ethyl acetate : petroleum ether 1:3, v/v, $R_f$ = 0.45) to give **2** (8.5 g, 70%) as yellow solid. m. p.: 271-272 °C. $^1$H NMR (300 MHz, $CDCl_3$): δ 7.52 (s, 2H), 6.66 (s, 2H), 4.18–4.07 (m, 2H), 3.71–3.60 (m, 2H), 3.38 (s, 6H), 2.90–2.75 (m, 4H), 2.55–2.43 (m, 2H), 1.78–1.65 (m, 2H), 0.97 (t, *J* = 7.4 Hz, 3H). $^{13}$C NMR (75 MHz, $CDCl_3$): δ 168.9, 153.8, 138.5, 137.9, 133.2, 133.1, 132.6, 126.6, 114.5, 112.1, 56.1, 39.6, 27.5, 24.3, 22.0, 11.5. MALDI-TOF MS: *m/z* 610.1 $[M+H]^+$. HRMS (ESI): *m/z* calcd for $C_{29}H_{26}Br_2NO_4$ $[M + H]^+$ 610.0223, found 610.0215.



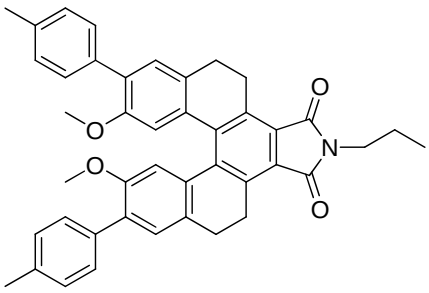

**General procedure for the synthesis of 4 by Suzuki-Miyaura cross coupling:**

To a mixture of compound **2** (600 mg, 0.99 mmol), $K_2CO_3$ (1.36 g, 9.9 mmol), and arylboronic acid (2.97 mmol) in DMF (30 mL) and toluene (20 mL) under argon atmosphere was added catalytic amount of $Pd(PPh_3)_4$ (5% mol). The resulting mixture was stirred for 12 hours at 90°C under argon atmosphere, cooled to room temperature and then poured into ethyl acetate (100 mL). The organic layer was washed with saturated brine (3×100 mL), dried over anhydrous $MgSO_4$, and then concentrated in *vacuo*. The

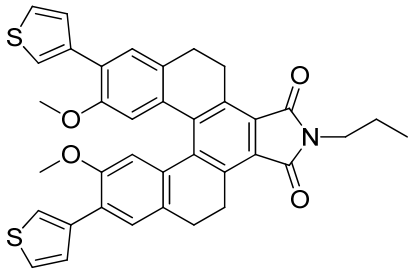
residue was purified by column chromatography with ethyl acetate and petroleum ether (1:5, v/v) as eluent to give the pure product.



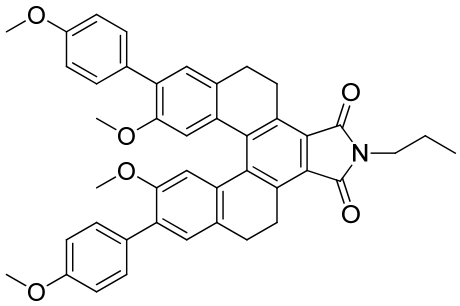
**Compound 4a.** According to the general method, **4a** (473 mg, 79%) was obtained as yellow powder. m. p.: 267-268 °C. $^{1}$H NMR (300 MHz, $CDCl_3$): δ 7.54–7.51 (m, 4H), 7.44–7.39 (m, 4H), 7.37–7.27 (m, 4H), 6.87 (s, 2H), 4.19–4.14 (m, 2H), 3.70–3.64 (m, 2H), 3.33 (s, 6H), 2.95–2.83 (m, 4H), 2.64–2.52 (m, 2H), 1.80–1.68 (m, 2H), 0.99 (t, $J$ = 7.4 Hz, 3H). $^{13}$C NMR (75 MHz, $CDCl_3$): δ 169.2, 154.3, 138.7, 138.5, 138.0, 133.2, 132.1, 131.0, 130.1, 129.4, 128.3, 127.4, 126.2, 114.1, 55.3, 39.5, 27.7, 24.5, 22.1, 11.6. MALDI-TOF MS: *m/z* 605.4 $[M]^+$. HRMS (ESI): *m/z* calcd for $C_{41}H_{36}NO_4$ $[M + H]^+$ 606.2639, found 606.2631.



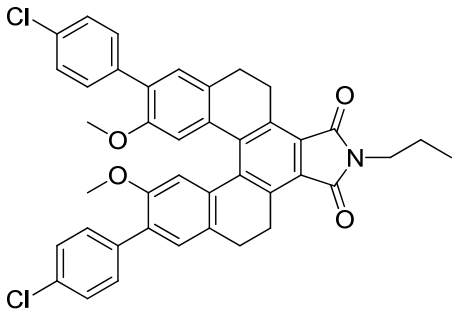
**Compound 4b.** According to the general method, **4b** (445 mg, 71%) was obtained as yellow powder. m. p.: 251-253 °C. $^{1}$H NMR (300 MHz, $CDCl_3$): δ 7.43–7.41 (m, 4H), 7.27 (s, 2H), 7.23–7.21 (m, 4H), 6.85 (s, 2H), 4.18–4.13 (m, 2H), 3.73–3.59 (m, 2H), 3.31 (s, 6H), 2.97–2.80 (m, 4H), 2.65–2.49 (m, 2H), 2.39 (s, 6H), 1.79–1.67 (m, 2H), 0.98 (t, $J$ = 7.4 Hz, 3H). $^{13}$C NMR (75 MHz, $CDCl_3$): δ 169.2, 154.3, 138.7, 138.5, 137.2, 135.0, 132.9, 132.0, 130.9, 129.9, 129.3, 129.0, 126.2, 114.0, 55.2, 39.5, 27.7, 24.5, 22.1, 21.4, 11.6. MALDI-TOF MS: *m/z* 633.4 $[M]^+$. HRMS (ESI): *m/z* calcd for $C_{43}H_{40}NO_4$: $[M + H]^+$ 634.2952, found 634.2944.



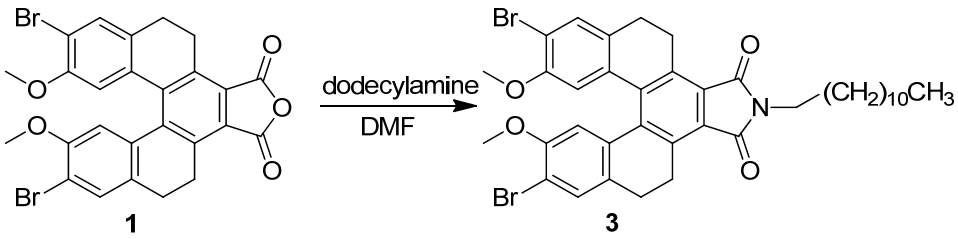
**Compound 4c.** According to the general method, **4c** (495 mg, 81%) was obtained as yellow powder. m. p.: 279-281 °C. $^{1}$H NMR (300 MHz, $CDCl_3$): δ 7.67–7.65 (m, 2H), 7.54–7.41 (m, 4H), 7.37–7.34 (m, 2H), 6.86 (s, 2H), 4.18–4.13 (m, 2H), 3.69–3.63 (m, 2H), 3.35 (s, 6H), 2.99–2.80 (m, 4H), 2.64–2.47 (m, 2H), 1.79–1.67 (m, 2H), 0.98 (t, $J$ = 7.4 Hz, 3H). $^{13}$C NMR (75 MHz, $CDCl_3$): δ 169.1, 154.3, 138.7, 138.3, 137.7, 132.8, 132.0, 128.8, 128.3, 126.2, 125.1, 124.8, 123.7, 114.1, 55.3, 39.5, 27.8, 24.5, 22.1, 11.5. MALDI-TOF MS: *m/z* 617.2 $[M]^+$. HRMS (ESI): *m/z* calcd for $C_{37}H_{32}S_2NO_4$ $[M + H]^+$ 618.1767, found 618.1761.



**Compound 4d.** According to the general method, **4d** (494 mg, 75%) was obtained as yellow powder. m. p.: 256-257 °C. $^{1}$H NMR (300 MHz, $CDCl_3$): δ 7.49–7.46 (m, 4H), 7.26 (s, 2H), 6.96–6.93 (m, 4H), 6.85 (s, 2H), 4.18–4.13 (m, 2H), 3.85 (s, 6H), 3.68–3.64 (m, 2H), 3.32 (s, 6H), 3.00–2.78 (m, 4H), 2.65–2.48 (m, 2H), 1.81–1.67 (m, 2H), 0.98 (t, $J$ = 7.4 Hz, 3H). $^{13}$C NMR (75 MHz, $CDCl_3$): δ 169.2, 159.1, 154.2, 138.7, 138.5, 132.7, 132.1, 130.5, 130.3, 129.8, 126.1, 114.0, 113.8, 55.5, 55.3, 39.5, 29.9, 27.7, 24.5, 22.1, 11.6. MALDI-TOF MS: *m/z* 665.4 $[M]^+$. HRMS (ESI): *m/z* calcd for $C_{43}H_{40}NO_6$ $[M + H]^+$ 666.2850, found 666.2836.

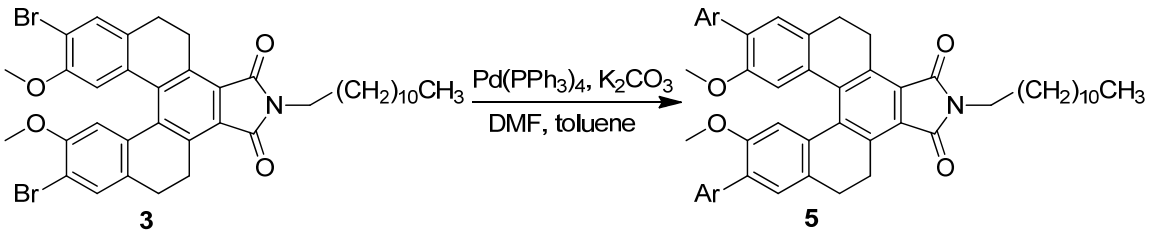


**Compound 4e.** According to the general method, **4e** (467 mg, 70%) was obtained as yellow powder. m. p.: 288-289 °C. $^1$H NMR (300 MHz, $CDCl_3$): δ 7.53–7.42 (m, 4H), 7.42–7.32 (m, 4H), 6.84 (s, 2H), 4.22–4.11 (m, 2H), 3.69–3.64 (m, 2H), 3.31 (s, 6H), 2.97–2.81 (m, 4H), 2.62–2.50 (m, 2H), 1.80–1.67 (m, 2H), 0.98 (t, $J$ = 7.4 Hz, 3H). $^{13}$C NMR (75 MHz, $CDCl_3$): δ 169.1, 154.1, 138.7, 138.3, 136.3, 133.5, 133.4, 132.2, 130.7, 129.9, 129.6, 128.4, 126.4, 114.1, 55.3, 39.6, 27.7, 24.4, 22.1, 11.6. MALDI-TOF MS: *m/z* 673.3 $[M]^+$. HRMS (ESI): *m/z* calcd for $C_{41}H_{34}Cl_2NO_4$ $[M + H]^+$ 674.1859, found 674.1845.




**1** **3**

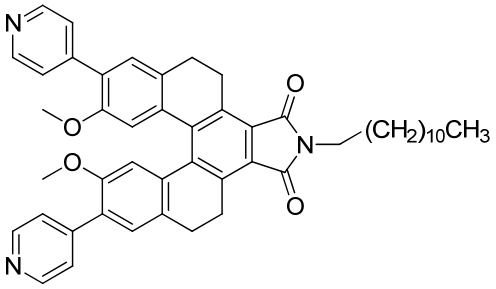
**Compound 3.** A mixtrue of **1** (11.4 g, 20 mmol) and *n*-dodecyl amine (9.25 g, 50 mmol) in DMF (100 mL) was heated at 100 °C for 24 hours. The reaction mixture was cooled to room temperature, and then added ethyl acetate (200 mL). The organic phase was washed with saturated brine (3×100 mL), and then dried over anhydrous $MgSO_4$. The solvent was removed in *vacuo*, and the residue was purified by column chromatography (ethyl acetate : petroleum ether 1:5, v/v, $R_f$ = 0.67) to give **3** (11.37 g, 77%) as yellow solid. m. p.: 75-76 °C. $^1$H NMR (300 MHz, $CDCl_3$): δ 7.52 (s, 2H), 6.66 (s, 2H), 4.14–4.09 (m, 2H), 3.69–3.64 (m, 2H), 3.38 (s, 6H), 2.90–2.73 (m, 4H), 2.55–2.43 (m, 2H), 1.74–1.60 (m, 2H), 1.38–1.21 (m, 18H), 0.87 (t, $J$ = 6.6 Hz, 3H). $^{13}$C NMR (75 MHz, $CDCl_3$): δ 168.8, 153.8, 138.4, 137.9, 133.2, 133.1, 132.6, 126.6, 114.5, 112.0, 56.0, 38.0, 32.0, 29.74, 29.71, 29.6, 29.5, 29.4, 28.7, 27.4, 27.0, 24.2, 22.8, 14.3. MALDI-TOF MS: *m/z* 738.2 $[M]^+$. HRMS (ESI): *m/z* calcd for $C_{38}H_{44}Br_2NO_4$ $[M + H]^+$ 736.1632, found 736.1623.



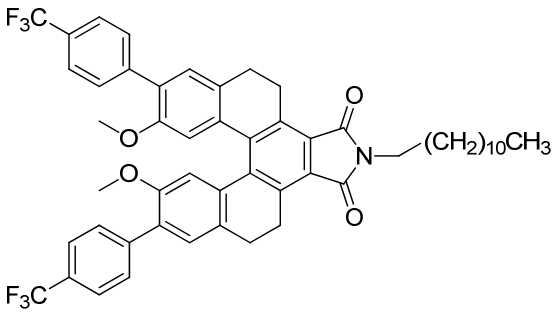

**3** **5**

**General procedure for the synthesis of 5 by Suzuki-Miyaura cross coupling:**

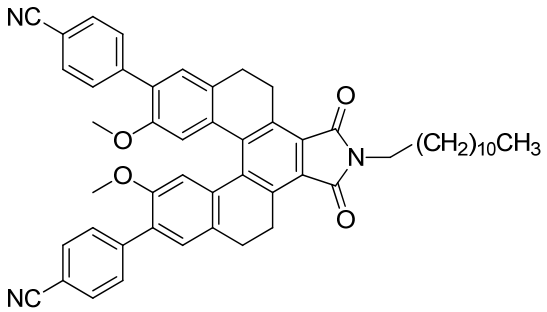
To a mixture of compound **3** (700 mg, 0.95 mmol), $K_2CO_3$ (1.31 g, 9.9 mmol), and arylboronic acid (2.85 mmol) in DMF (30 mL) and toluene (20 mL) under argon atmosphere was added catalytic amount of $Pd(PPh_3)_4$ (5% mol). The resulting mixture was stirred for 12 hours at 90°C under argon atmosphere, cooled to room temperature, and then poured into ethyl acetate (100 mL). The organic layer was washed with saturated brine (3×100 mL), dried over anhydrous $MgSO_4$, and then concentrated in *vacuo*. The residue was purified by column chromatography with ethyl acetate and petroleum ether (1:5, v/v) as eluent to give the pure product.



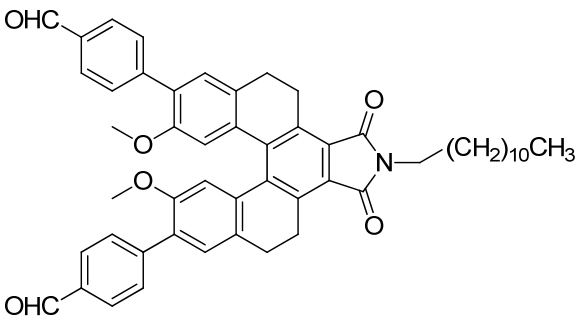

**Compound 5a.** According to the general method, **5a** (425 mg, 61%) was obtained as yellow powder. $R_f$ = 0.11. m. p.: 196-198 °C. $^1$H NMR (300 MHz, $CDCl_3$): δ 8.64–8.62 (m, 4H), 7.47–7.45 (m, 4H), 7.34 (s, 2H), 6.86 (s, 2H), 4.22–4.16 (m, 2H), 3.75–3.64 (m, 2H), 3.34 (s, 6H), 3.02–2.83 (m, 4H), 2.63–2.51 (m, 2H), 1.73–1.66 (m, 2H), 1.34–1.25 (m, 18H), 0.87 (t, *J* = 6.6 Hz, 3H). $^{13}$C NMR (75 MHz, $CDCl_3$): δ 169.0, 154.4, 149.8, 145.6, 138.8, 138.3, 134.6, 132.4, 129.9, 127.9, 126.7, 124.1, 114.3, 55.3, 38.1, 32.1, 29.8, 29.74, 29.65, 29.5, 29.4, 28.8, 27.7, 27.1, 24.4, 22.8, 14.3. MALDI-TOF MS: *m/z* 734.5 $[M+H]^+$. HRMS (ESI): *m/z* calcd for $C_{48}H_{52}N_3O_4$ $[M + H]^+$ 734.3952, found 734.3942.



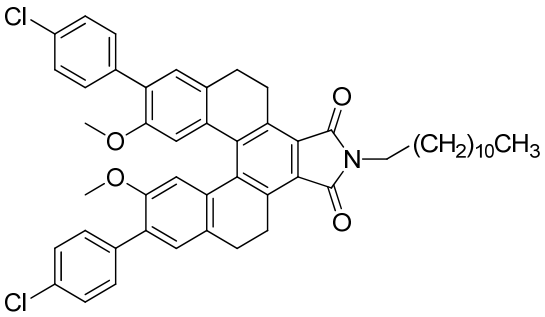

**Compound 5b.** According to the general method, **5b** (577 mg, 70%) was obtained as yellow powder. $R_f$ = 0.61. m. p.: 160-161 °C. $^1$H NMR (300 MHz, $CDCl_3$): δ 7.69–7.61 (m, 8H), 7.30 (s, 2H), 6.86 (s, 2H), 4.21–4.16 (m, 2H), 3.72–3.66 (m, 2H), 3.33 (s, 6H), 2.98–2.83 (m, 4H), 2.64–2.52 (m, 2H), 1.76–1.63 (m, 2H), 1.34–1.26 (m, 18H), 0.88 (t, *J* = 6.7 Hz, 3H). $^{13}$C NMR (75 MHz, $CDCl_3$): δ 169.0, 154.2, 141.5, 138.7, 138.3, 134.0, 132.3, 130.1, 129.7, 129.4, 129.2, 126.5, 125.2, 125.1, 125.1, 114.1, 55.3, 38.1, 32.1, 29.8, 29.74, 29.66, 29.5, 29.4, 28.8, 27.7, 27.1, 24.4, 22.8, 14.3. MALDI-TOF MS: *m/z* 867.2 $[M]^+$. HRMS (ESI): *m/z* calcd for $C_{52}H_{52}NO_4F_6$ $[M + H]^+$ 868.3795, found 868.3786.



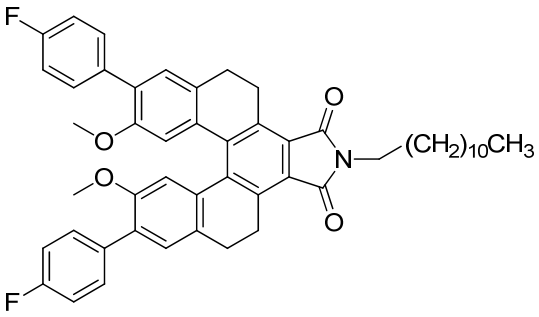

**Compound 5c.** According to the general method, **5c** (467 mg, 63%) was obtained as yellow powder. $R_f$ = 0.22. m. p.: 178-179 °C. $^1$H NMR (300 MHz, $CDCl_3$): δ 7.71–7.63 (m, 8H), 7.30 (s, 2H), 6.85 (s, 2H), 4.22–4.16 (m, 2H), 3.71–3.67 (m, 2H), 3.33 (s, 6H), 3.00–2.83 (m, 4H), 2.63–2.51 (m, 2H), 1.75–1.64 (m, 2H), 1.34–1.25 (m 18H), 0.87 (t, *J* = 6.5 Hz, 3H). $^{13}$C NMR (75 MHz, $CDCl_3$): δ 168.9, 154.1, 142.6, 138.7, 138.2, 134.4, 132.4, 132.0, 130.1, 130.0, 128.8, 126.7, 119.1, 114.1, 110.9, 55.3, 38.1, 32.1, 29.76, 29.76, 29.73, 29.6, 29.5, 29.4, 28. 8, 27.7, 27.1, 24.3, 22.8, 14.3. MALDI-TOF MS: *m/z* 781.0 $[M]^+$. HRMS (ESI): *m/z* calcd for $C_{52}H_{52}N_3O_4$ $[M + H]^+$ 782.3952, found 782.3944.



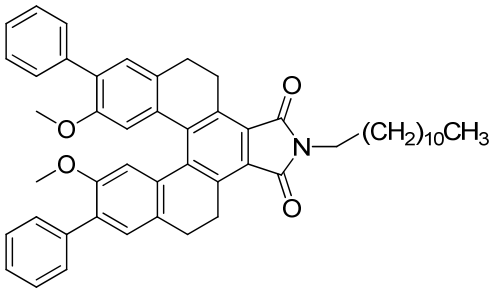

**Compound 5d.** According to the general method, **5d** (613 mg, 82%) was obtained as yellow powder. $R_f$ = 0.14. m. p.: 89-91 °C. $^1$H NMR (300 MHz, $CDCl_3$): δ 10.05 (s, 2H), 7.92 (d, *J* = 8.2 Hz, 4H), 7.71 (d, *J* = 8.1 Hz, 4H), 7.34 (s, 2H), 6.88 (s, 2H), 4.12–4.17 (m, 2H), 3.71–3.67 (m, 2H), 3.35 (s, 6H), 3.02–2.83 (m, 4H), 2.64–2.52 (m, 2H), 1.75–1.64 (m, 2H), 1.34–1.26 (m, 18H), 0.88 (t, *J* = 6.6 Hz, 3H). $^{13}$C NMR (75 MHz, $CDCl_3$): δ 192.1, 169.0, 154.3, 144.3, 138.7, 138.3, 135.2, 134.2, 132.3, 130.1, 129.7, 129.5, 126.6, 114.2, 100.1, 55.3, 32.1, 29.77, 29.76, 29.73, 29.65, 29.5, 29.4, 28.8, 27.68, 27.65, 2718, 24.4, 22.8, 14.3. MALDI-TOF MS: *m/z* 787.5 $[M]^+$. HRMS (ESI): *m/z* calcd for $C_{52}H_{54}NO_6$ $[M + H]^+$ 788.3946, found 788.3933.



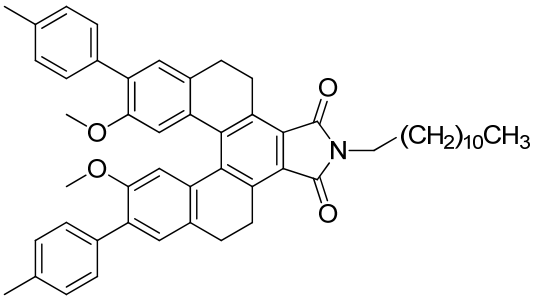

**Compound 5e.** According to the general method, **5e** (622 mg, 82%) was obtained as yellow powder. $R_f$ = 0.67. m. p.: 147-148 °C. $^1$H NMR (300 MHz, $CDCl_3$): δ 7.47–7.45 (m, 4H), 7.38–7.36 (m, 4H), 6.84 (s, 2H), 4.19–4.14 (m, 2H), 3.70–3.66 (m, 2H), 3.31 (s, 6H), 2.92–2.82 (m, 4H), 2.62–2.50 (m, 2H), 1.71–1.64 (m, 2H), 1.34–1.25 (m, 18H), 0.87 (t, *J* = 5.9 Hz, 3H). $^{13}$C NMR (75 MHz, $CDCl_3$): δ 169.1, 154.1, 138.7, 138.3, 136.3, 133.5, 133.4, 132.2, 130.7, 129.9, 129.6, 128.5, 126.4, 114.1, 55.3, 38.0, 32.1, 29.82, 29.78, 29.75, 29.66, 29.5, 29.4, 28.8, 27.7, 27.1, 24.4, 22.8, 14.3. MALDI-TOF MS: *m/z* 800.4 $[M + H]^+$. HRMS (ESI): *m/z* calcd for $C_{50}H_{52}NO_4Cl_2$ $[M + H]^+$ 800.3268, found 800.3260.



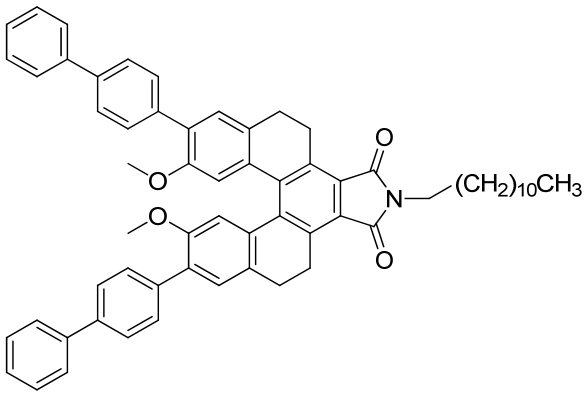

**Compound 5f.** According to the general method, **5f** (626 mg, 86%) was obtained as yellow powder. $R_f$ = 0.64. m. p.: 108-109 °C. $^1$H NMR (300 MHz, $CDCl_3$): δ 7.51–7.47 (m, 4H), 7.26 (s, 2H), 7.12–7.06 (m, 4H), 6.85 (s, 2H), 4.19–4.14 (m, 2H), 3.70–3.66 (m, 2H), 3.32 (s, 6H), 2.98–2.81 (m, 4H), 2.60–2.50 (m, 2H), 1.75–1.63 (m, 2H), 1.34–1.26 (m, 18H), 0.87 (t, *J* = 6.5 Hz, 3H). $^{13}$C NMR (75 MHz, $CDCl_3$): δ 169.1, 163.9, 160.7, 154.1, 138.7, 138.4, 133.9, 133.8, 133.3, 132.2, 131.1, 131.0, 130.0, 129.9, 126.4, 115.3, 115.0, 114.1, 55.3, 38.0, 32.1, 29.78, 29.77, 29.74, 29.65, 29.5, 29.4, 28.8, 27.7, 27.1, 24.5, 22.8, 14.3. MALDI-TOF MS: *m/z* 767.6 $[M]^+$. HRMS (ESI): *m/z* calcd for $C_{50}H_{52}NO_4F_2$ $[M + H]^+$ 768.3859, found 768.3850.



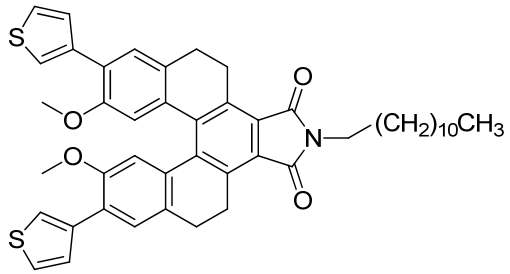

**Compound 5g.** According to the general method, **5g** (639 mg, 92%) was obtained as yellow powder. $R_f$ = 0.71. m. p.: 120-121 °C. $^1$H NMR (300 MHz, $CDCl_3$): δ 7.56–7.49 (m, 4H), 7.44–7.38 (m, 4H), 7.37–7.27 (m, 4H), 6.86 (s, 2H), 4.19–4.14 (m, 2H), 3.74–3.63 (m, 2H), 3.33 (s, 6H), 2.97–2.82 (m, 4H), 2.64–2.51 (m, 2H), 1.75–1.64 (m, 2H), 1.34–1.26 (m, 18H), 0.88 (t, *J* = 6.7 Hz, 3H). $^{13}$C NMR (75 MHz, $CDCl_3$): δ 169.2, 154.2, 138.7, 138.4, 138.0, 133.2, 132.0, 130.9, 130.1, 129.4, 128.3, 127.4, 126.3, 114.1, 55.3, 38.0, 32.1, 29.77, 29.75, 29.66, 29.5, 29.4, 28.8, 27.7, 27.1, 24.5, 22.8, 14.3. MALDI-TOF MS: *m/z* 731.4 $[M]^+$. HRMS (ESI): *m/z* calcd for $C_{50}H_{54}NO_4$ $[M + H]^+$ 732.4047, found 732.4038.



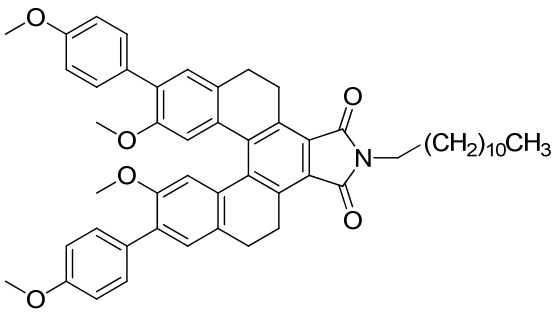
**Compound 5h.** According to the general method, **5h** (613 mg, 85%) was obtained as yellow powder. $R_f$ = 0.72. m. p.: 175-178 °C. $^1$H NMR (300 MHz, $CDCl_3$): δ 7.43–7.41 (m, 4H), 7.27 (s, 2H), 7.24–7.21 (m, 4H), 6.84 (s, 2H), 4.18–4.13 (m, 2H), 3.74–3.62 (m, 2H), 3.31 (s, 6H), 2.96–2.80 (m, 4H), 2.63–2.50 (m, 2H), 2.39 (s, 6H), 1.74–1.64 (m, 2H), 1.34–1.25 (m, 18H), 0.87 (t, *J* = 6.6 Hz, 3H). $^{13}$C NMR (75 MHz, $CDCl_3$): δ 169.2, 154.2, 138.7, 138.4, 137.2, 135.0, 132.9, 132.0, 130.9, 129.9, 129.3, 129.0, 126.2, 114.0, 55.3, 38.0, 32.1, 29.8, 29.7, 29.5, 29.4, 28.8, 27.7, 27.1, 24.5, 22.8, 21.4, 14.3. MALDI-TOF MS: *m/z* 759.5 $[M]^+$. HRMS (ESI): *m/z* calcd for $C_{52}H_{58}NO_4$ $[M + H]^+$ 760.4360, found 760.4353.



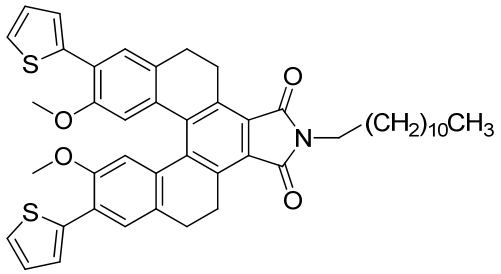
**Compound 5i.** According to the general method, **5i** (671 mg, 80%) was obtained as yellow powder. $R_f$ = 0.55. m. p.: 147-149 °C. $^1$H NMR (300 MHz, $CDCl_3$): δ 7.68–7.60 (m, 12H), 7.48–7.43 (m, 4H), 7.39–7.33 (m, 4H), 6.90 (s, 2H), 4.21–4.16 (m, 2H), 3.76–3.63 (m, 2H), 3.38 (s, 6H), 2.95–2.86 (m, 4H), 2.66–2.54 (m, 2H), 1.74–1.66 (m, 2H), 1.35–1.26 (m, 18H), 0.88 (t, *J* = 6.6 Hz, 3H). $^{13}$C NMR (75 MHz, $CDCl_3$): δ 169.1, 154.3, 141.0, 140.2, 138.7, 138.4, 136.9, 133.3, 132.1, 130.4, 129.98, 129.79, 128.9, 127.4, 127.2, 127.0, 126.3, 114.0, 55.3, 38.0, 32.1, 29.77, 29.75, 29.65, 29.5, 29.4, 28.8, 27.7, 27.1, 24.5, 22.8, 14.3. MALDI-TOF MS: *m/z* 883.7 $[M]^+$. HRMS (ESI): *m/z* calcd for $C_{62}H_{62}NO_4$ $[M + H]^+$ 884.4673, found 884.4659.



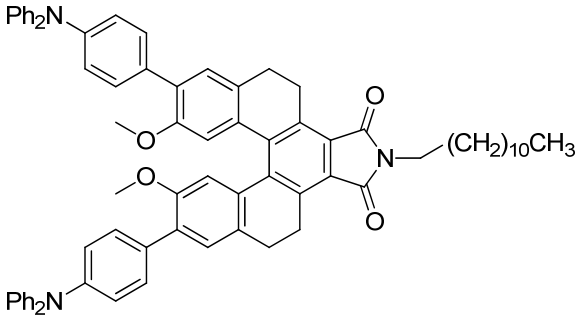
**Compound 5j.** According to the general method, **5j** (600 mg, 85%) was obtained as yellow powder. $R_f$ = 0.60. m. p.: 148-149 °C. $^1$H NMR (300 MHz, $CDCl_3$): δ 7.67–7.66 (m, 2H), 7.47–7.46 (m, 4H), 7.36–7.33 (m, 2H), 6.86 (s, 2H), 4.19–4.13 (m, 2H), 3.70–3.66 (m, 2H), 3.35 (s, 6H), 2.92–2.83 (m, 4H), 2.61–2.49 (m, 2H), 1.75–1.63 (m, 2H), 1.34–1.26 (m, 18H), 0.88 (t, $J$ = 6.5 Hz, 3H). $^{13}$C NMR (75 MHz, $CDCl_3$): δ 169.1, 154.3, 138.7, 138.4, 137.8, 132.9, 132.0, 128.8, 128.3, 126.2, 125.2, 124.9, 123.7, 114.1, 55.3, 38.0, 32.1, 29.78, 29.77, 29.74, 29.65, 29.5, 29.4, 28.8, 27.8, 27.1, 24.5, 22.8, 14.3. MALDI-TOF MS: *m/z* 743.4 $[M]^+$. HRMS (ESI): *m/z* calcd for $C_{46}H_{50}NO_4S_2$ $[M + H]^+$ 744.3176, found 744.3170.



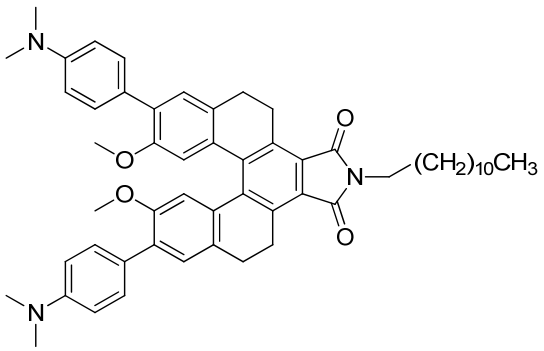
**Compound 5k.** According to the general method, **5k** (676 mg, 90%) was obtained as yellow powder. $R_f$ = 0.43. m. p.: 97-99 °C. $^1$H NMR (300 MHz, $CDCl_3$): δ 7.49–7.46 (m, 4H), 7.26 (s, 2H), 6.96–6.93 (m, 4H), 6.85 (s, 2H), 4.18–4.13 (m, 2H), 3.85 (s, 6H), 3.70–3.66 (m, 2H), 3.32 (s, 6H), 2.97–2.81 (m, 4H), 2.64–2.48 (m, 2H), 1.76–1.62 (m, 2H), 1.34–1.26 (m, 18H), 0.87 (t, $J$ = 6.6 Hz, 3H). $^{13}$C NMR (75 MHz, $CDCl_3$): δ 169.2, 159.1, 154.2, 138.7, 138.4, 132.8, 132.1, 130.6, 130.5, 130.3, 129.8, 126.2, 114.0, 113.8, 55.5, 55.3, 38.0, 32.1, 29.78, 29.77, 29.75, 29.66, 29.5, 29.4, 28.8, 27.7, 27.1, 24.5, 22.8, 14.3. MALDI-TOF MS: *m/z* 791.5 $[M]^+$. HRMS (ESI): *m/z* calcd for $C_{52}H_{58}NO_6$ $[M + H]^+$ 792.4259, found 792.4253.



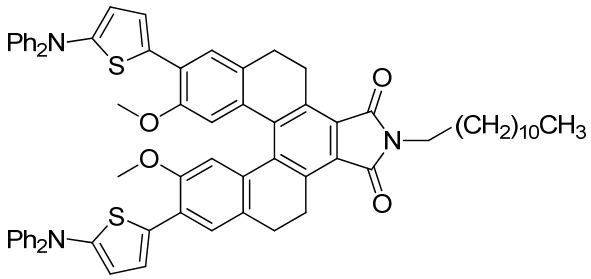
**Compound 5l.** According to the general method, **5l** (586 mg, 83%) was obtained as yellow powder. $R_f$ = 0.67. m. p.: 147-148 °C. $^1$H NMR (300 MHz, $CDCl_3$): δ 7.61 (s, 2H), 7.56–7.55 (m, 2H), 7.35–7.33 (m, 2H), 7.11–7.08 (m, 2H), 6.86 (s, 2H), 4.19–4.13 (m, 2H), 3.70–3.65 (m, 2H), 3.40 (s, 6H), 3.00–2.81 (m, 4H), 2.61–2.49 (m, 2H), 1.74–1.63 (m, 2H), 1.33–1.26 (m, 18H), 0.87 (t, *J* = 6.6 Hz, 3H). $^{13}$C NMR (75 MHz, $CDCl_3$): δ 169.1, 153.5, 139.0, 138.7, 138.2, 132.9, 132.1, 127.4, 127.1, 126.3, 126.0, 125.9, 123.6, 114.3, 55.4, 38.0, 32.1, 29.77, 29.76, 29.74, 29.65, 29.5, 29.4, 28.79, 27.81, 27.1, 24.5, 22.8, 14.3. MALDI-TOF MS: *m/z*743.3 $[M]^+$. HRMS (ESI): *m/z* calcd for $C_{46}H_{50}NO_4S_2$ $[M + H]^+$ 744.3176, found 744.3168.



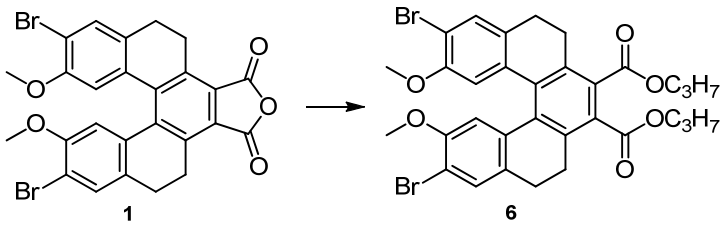
**Compound 5m.** According to the general method, **5m** (791 mg, 78%) was obtained as yellow powder. $R_f$ = 0.56. m. p.: 120-122°C. $^1$H NMR (300 MHz, $CDCl_3$): δ 7.43 (d, *J* = 8.6 Hz, 4H), 7.31–7.22 (m, 10H), 7.17–6.99 (m, 16H), 6.86 (s, 2H), 4.15 (d, *J* = 15.9 Hz, 2H), 3.70–3.65 (m, 2H), 3.33 (s, 6H), 3.02–2.76 (m, 4H), 2.67–2.46 (m, 2H), 1.77–1.62 (m, 2H), 1.34–1.26 (m, 18H), 0.87 (t, *J* = 6.5 Hz, 3H). $^{13}$C NMR (75 MHz, $CDCl_3$): δ 169.2, 154.3, 147.8, 147.1, 138.7, 138.5, 132.9, 132.1, 131.8, 130.4, 130.2, 129.8, 129.4, 126.2, 124.7, 123.2, 123.1, 114.1, 55.3, 38.0, 32.1, 29.8, 29.74, 29.65, 29.5, 29.4, 28.8, 27.8, 27.1, 24.5, 22.8, 14.2. MALDI-TOF MS: *m/z* 1066.7 $[M+H]^+$. HRMS (ESI): *m/z* calcd for $C_{74}H_{72}N_3O_4$ $[M + H]^+$ 1066.5517, found 1066.5509.



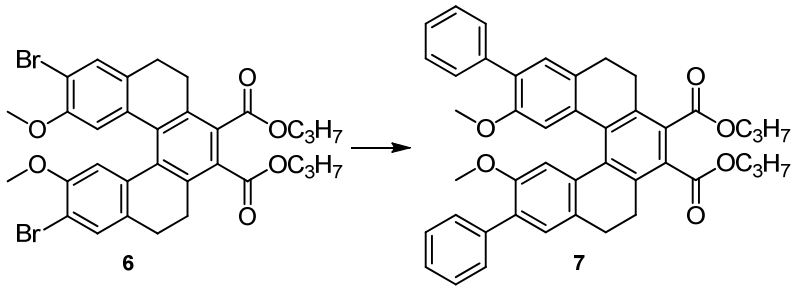
**Compound 5n.** According to the general method, **5n** (675 mg, 87%) was obtained as orange-red powder. $R_f$ = 0.27. m. p.: 196-197 °C. $^1$H NMR (300 MHz, $CDCl_3$): δ 7.47–7.44 (m, 4H), 7.25 (s, 2H), 6.84 (s, 2H), 6.79–6.76 (m, 4H), 4.17–4.11 (m, 2H), 3.69–3.65 (m, 2H), 3.31 (s, 6H), 2.99 (s, 12H), 2.93–2.79 (m, 4H), 2.62–2.50 (m, 2H), 1.76–1.62 (m, 2H), 1.34–1.26 (m, 18H), 0.87 (t, *J* = 6.5 Hz, 3H). $^{13}$C NMR (75 MHz, $CDCl_3$): δ 169.3, 154.3, 149.9, 138.6, 138.5, 132.1, 132.0, 131.1, 130.1, 129.4, 126.0, 125.9, 114.0, 112.3, 55.3, 40.7, 38.0, 32.1, 29.78, 29.77, 29.74, 29.65, 29.5, 29.4, 28.8, 27.8, 27.1, 24.5, 22.8, 14.3. MALDI-TOF MS: *m/z* 817.1 $[M]^+$. HRMS (ESI): *m/z* calcd for $C_{54}H_{64}N_3O_4$ $[M + H]^+$ 818.4891, found 818.4879.



**Compound 5o**. According to the general method, **5o** (828 mg, 81%) was obtained as red powder. m. p.: 117-118 °C. $^1$H NMR (300 MHz, $CDCl_3$): δ 7.49 (s, 2H), 7.36 (d, *J* = 4.0 Hz, 2H), 7.29–7.24 (m, 8H), 7.20–7.17 (m, 8H), 7.03 (t, *J* = 7.1 Hz, 4H), 6.82 (s, 2H), 6.65 (d, *J* = 4.0 Hz, 2H), 4.13 (d, *J* = 16.1 Hz, 2H), 3.71–3.62 (m, 2H), 3.38 (s, 6H), 2.93–2.77 (m, 4H), 2.59–2.44 (m, 2H), 1.72–1.65 (m, 2H), 1.32–1.25 (m, 18H), 0.87 (t, *J* = 6.6 Hz, 3H). $^{13}$C NMR (75 MHz, $CDCl_3$): δ 169.1, 153.4, 152.0, 149.0, 138.7, 138.2, 132.7, 132.4, 132.1, 129.3, 126.6, 126.2, 125.0, 123.7, 123.2, 123.0, 120.8, 114.1, 55.5, 38.0, 32.1, 29.8, 29.74, 29.65, 29.5, 29.4, 28.8, 27.8, 27.1, 24.5, 22.8, 14.3. MALDI-TOF MS: *m/z* 1078.5 $[M + H]^+$. HRMS (ESI): *m/z* calcd for $C_{70}H_{68}N_3O_4S_2$ $[M + H]^+$ 1078.46458, found 1078.46460.

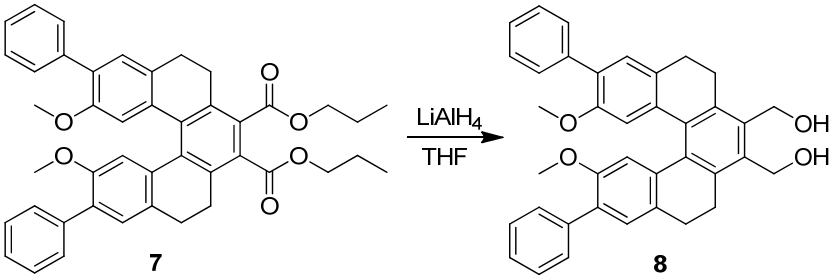



**Compound 6.** A mixture of **1** (1.71 g, 3 mmol), 1-bromopropane (10 g), 1-propanol (10 g) and DBU (8 g) in acetonitrile (40 mL) was refluxed overnight, and then cooled to room temperature. To the reaction mixture was added ethyl acetate (100 mL). The organic phase was washed with saturated brine (3×100 mL), dried over anhydrous $MgSO_4$, and then concentrated in *vacuo*. The residue was submitted to column chromatography with ethyl acetate and petroleum ether (1:5, v/v) as eluent to give **6** (1.47 g, 73%) as white solid. m. p.: 84-85 °C. $^1$H NMR (300 MHz, $CDCl_3$): δ 7.47 (s, 2H), 6.57 (s, 2H), 4.34–4.18 (m, 4H), 3.36 (s, 6H), 3.09–2.98 (m, 2H), 2.85–2.73 (m, 4H), 2.70–2.56 (m, 2H), 1.82–1.70 (m, 4H), 1.01 (t, $J$ = 7.4 Hz, 6H). $^{13}$C NMR (75 MHz, $CDCl_3$): δ 168.1, 153.8, 137.7, 134.8, 133.7, 132.8, 132.1, 130.5, 114.8, 111.4, 67.5, 56.1, 28.0, 27.7, 22.1, 10.7. MALDI-TOF MS: *m/z* 672.3 $[M]^+$. HRMS (ESI) *m/z* calcd for $C_{32}H_{33}Br_2O_6$ $[M + H]^+$ 671.0638, found 671.0644.




**Compound 7.** To a mixture of compound **6** (60 mg, 0.09 mmol), $K_2CO_3$ (124 mg, 0.9 mmol), and phenylboronic acid (33 mg, 0.27 mmol) in DMF (15 mL) and toluene (10 mL) under argon atmosphere was added catalytic amount of $Pd(PPh_3)_4$ (5% mol). The resulting mixture was stirred for 12 hours at 90°C under argon atmosphere, cooled to room temperature, and then added ethyl acetate (100 mL). The organic layer was washed with saturated brine (3×100 mL), dried over anhydrous $MgSO_4$, and then concentrated in *vacuo*. The residue was purified by column chromatography with ethyl acetate and petroleum ether (1:5, v/v) as eluent to give **7** (53 mg, 88%) as white solid. m. p.: 147-149 °C. $^1$H NMR (300 MHz, $CDCl_3$): δ 7.55–7.48 (m, 4H), 7.42–7.37 (m, 4H), 7.34–7.29 (m, 2H), 7.25 (s, 2H), 6.77 (s,

2H), 4.36–4.20 (m, 4H), 3.30 (s, 6H), 3.11–3.06 (m, 2H), 2.93–2.80 (m, 4H), 2.78–2.65 (m, 2H), 1.84–1.72 (m, 4H), 1.02 (t, $J$ = 7.4 Hz, 6H). $^{13}$C NMR (75 MHz, $CDCl_3$): δ 168.5, 154.2, 138.2, 137.7, 135.4, 133.8, 131.6, 130.3, 130.1, 129.6, 129.4, 128.2, 127.2, 114.3, 67.4, 55.3, 28.3, 28.0, 22.1, 10.8. MALDI-TOF MS: *m/z* 666.3 $[M]^+$. HRMS (ESI) *m/z* calcd for $C_{44}H_{43}O_6$ $[M + H]^+$ 667.3054, found 667.3060.




**7** **8**

**Compound 8.** To a stirred solution of **7** (80 mg, 0.12 mmol) in THF (20 mL) and ether (20 mL) at 0 °C $LiAlH_4$ (23 mg, 0.60 mmol) was added in portions during a period of 30 min. The resulting reaction mixture was stirred at room temperature for 1 hours, and then refluxed gently for 2 hours. The reaction mixtrue was cooled to room temperature, quenched with water (5 mL) and an excess of concentrated hydrochloric acid, and then extracted with ethyl acetate (50 mL). The combined organic phase was washed with saturated $NaHCO_3$ (3×50 mL), dried over anhydrous $MgSO_4$, and then concentrated in *vacuo*. The residue was purified by column chromatography with methanol and $CH_2Cl_2$ (1:20, v/v, $R_f$ = 0.32) to give **8** (53 mg, 80%) as white solid. $^1$H NMR (300 MHz, $CDCl_3$): δ 7.53–7.51 (m, 4H), 7.42–7.37 (m, 4H), 7.33–7.28 (m, 2H), 7.25 (s, 2H), 6.77 (s, 2H), 4.97 (d, J = 4.6 Hz, 4H), 3.38–3.33 (m, 2H), 3.30 (s, 6H), 2.97–2.82 (m, 4H), 2.65–2.54 (m, 2H), 2.44 (t, J = 4.5 Hz, 2H). $^{13}$C NMR (75 MHz, $CDCl_3$): δ 154.1, 138.6, 138.4, 135.9, 134.9, 133.7, 131.2, 129.5, 129.43, 129.35, 128.2, 127.1, 114.6, 59.5, 55.3, 28.6, 26.4. MALDI-TOF MS: *m/z* 577.5 $[M+Na]^+$. HRMS (ESI): *m/z* calcd for $C_{38}H_{34}NaO_4$: $[M + Na]^+$ 577.2349, found 577.2339.

## 3. X-ray crystallographic data of 4c-e

**Table S1**. X-ray crystallographic data of **4c**

| Name | **4c** (CCDC 915889) |
|---|---|
| Empirical formula | $C_{37}H_{31}NO_4S_2$ |
| Formula weight | 617.75 |
| Temperature | 173(2) K |
| Wavelength | 0.71073 A |
| Crystal system | Triclinic |
| Space group | P-1 |
| a, Å | 9.848(2) |
| b, Å | 12.546(3) |
| c, Å | 12.957(3) |
| alpha, deg | 85.32(3) |
| beta, deg | 80.81(3) |
| gamma, deg | 69.90(3) |
| Volume, $Å^3$ | 1483.4(5) |
| Z | 2 |
| Calculated density, $Mg/m^3$ | 1.383 |
| Absorption coefficient, $mm^{-1}$ | 0.224 |
| F(000) | 648 |
| Crystal size, mm | 0.30 x 0.21 x 0.09 |
| Theta range for data collection, deg | 1.73 to 27.48 |
| Limiting indices | -12<=h<=12, -16<=k<=16, -16<=l<=16 |
| Reflections collected / unique | 13363 / 6727 [R(int) = 0.0349] |
| Completeness to theta = 27.48 | 99.0 % |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 1.0000 and 0.8228 |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 6727 / 30 / 419 |
| Goodness-of-fit on $F^2$ | 1.064 |
| Final R indices [I>2sigma(I)] | $R_1$ = 0.0602, $wR_2$ = 0.1498 |
| R indices (all data) | $R_1$ = 0.0674, $wR_2$ = 0.1555 |
| Largest diff. peak and hole, $e.A^{-3}$ | 0.694 and -0.701 |

**Table S2**. X-ray crystallographic data of **4d**

| Name | **4d** (CCDC 915891) |
|---|---|
| Empirical formula | $C_{43}H_{39}NO_6$ |
| Formula weight | 665.75 |
| Temperature | 173(2) K |
| Wavelength | 0.71073 A |
| Crystal system | Monoclinic |
| Space group | P2(1)/c |
| a, Å | 13.701(5) |
| b, Å | 14.227(5) |
| c, Å | 18.390(7) |
| alpha, deg | 90 |
| beta, deg | 109.695(8) |
| gamma, deg | 90 |
| Volume, $Å^3$ | 3375(2) |
| Z | 4 |
| Calculated density, $Mg/m^3$ | 1.310 |
| Absorption coefficient, $mm^{-1}$ | 0.087 |
| F(000) | 1408 |
| Crystal size, mm | 0.27 x 0.24 x 0.05 |
| Theta range for data collection, deg | 2.16 to 25.00 |
| Limiting indices | -16<=h<=12, -14<=k<=16, -21<=l<=21 |
| Reflections collected / unique | 12274 / 5930 [R(int) = 0.0650] |
| Completeness to theta = 27.48 | 99.6 % |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 1.0000 and 0.4763 |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 5930 / 64 / 476 |
| Goodness-of-fit on $F^2$ | 1.214 |
| Final R indices [I>2sigma(I)] | $R_1$ = 0.1245, $wR_2$ = 0.2267 |
| R indices (all data) | $R_1$ = 0.1600, $wR_2$ = 0.2475 |
| Largest diff. peak and hole, $e.A^{-3}$ | 0.258 and -0.234 |

**Table S3**. X-ray crystallographic data of **4e**

| Name | **4e** (CCDC 915888) |
|---|---|
| Empirical formula | $C_{41}H_{33}Cl_2NO_4$ |
| Formula weight | 674.58 |
| Temperature | 173(2) K |
| Wavelength | 0.71073 A |
| Crystal system | Orthorhombic |
| Space group | P2(1)2(1)2(1) |
| a, Å | 10.076(2) |
| b, Å | 10.201(2) |
| c, Å | 30.956(6) |
| alpha, deg | 90 |
| beta, deg | 90 |
| gamma, deg | 90 |
| Volume, $Å^3$ | 3181.8(11) |
| Z | 4 |
| Calculated density, $Mg/m^3$ | 1.408 |
| Absorption coefficient, $mm^{-1}$ | 0.251 |
| F(000) | 1408 |
| Crystal size, mm | 0.24 x 0.18 x 0.17 |
| Theta range for data collection, deg | 2.10 to 27.50 |
| Limiting indices | -13<=h<=9, -12<=k<=13, -25<=l<=39 |
| Reflections collected / unique | 13001 / 7143 [R(int) = 0.0468] |
| Completeness to theta = 27.48 | 98.5 % |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 1.0000 and 0.7444 |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 7143 / 0 / 436 |
| Goodness-of-fit on $F^2$ | 1.086 |
| Final R indices [I>2sigma(I)] | $R_1$ = 0.0614, $wR_2$ = 0.1211 |
| R indices (all data) | $R_1$ = 0.0690, $wR_2$ = 0.1269 |
| Largest diff. peak and hole, $e.A^{-3}$ | 0.237 and -0.253 |

**Table S4**. Torsion angles and dihedral angles of **4c-e**

| compound | torsion angle | dihedral angle |
|---|---|---|
| **4c** | 50.27 | 28.14 |
| **4d** | 43.64 | 56.51 |
| **4e** | 41.89 | 38.27 |

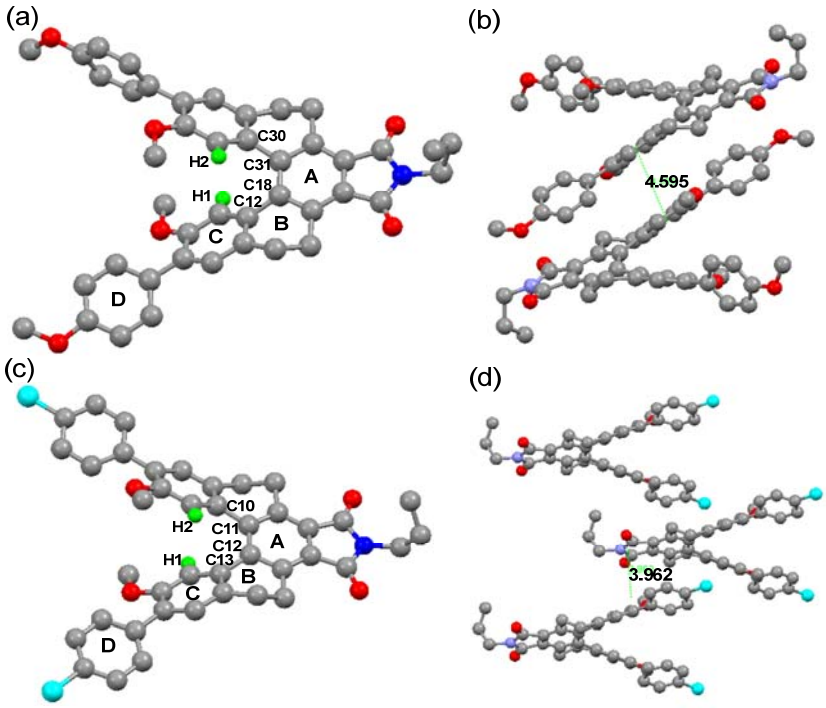



**Fig. S1** Crystal structures and intermolecular distances of **4d** (a and b); **4e** (c and d). Hydrogen atoms were omitted for clarity.

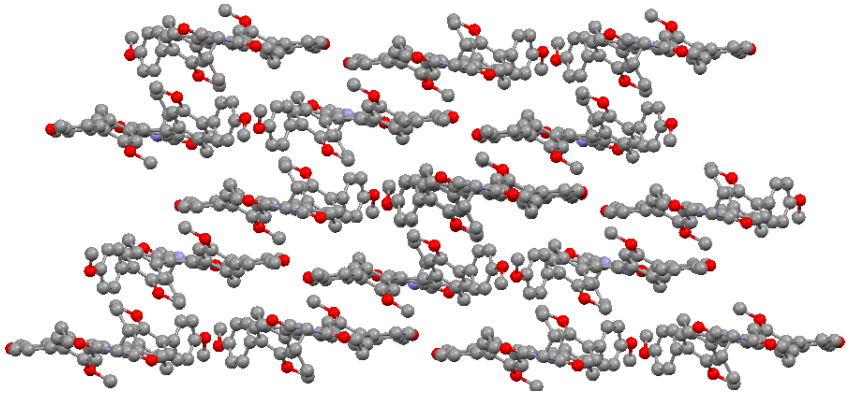


**Fig. S2** Packing mode of **4d**. Hydrogen atoms were omitted for clarity.

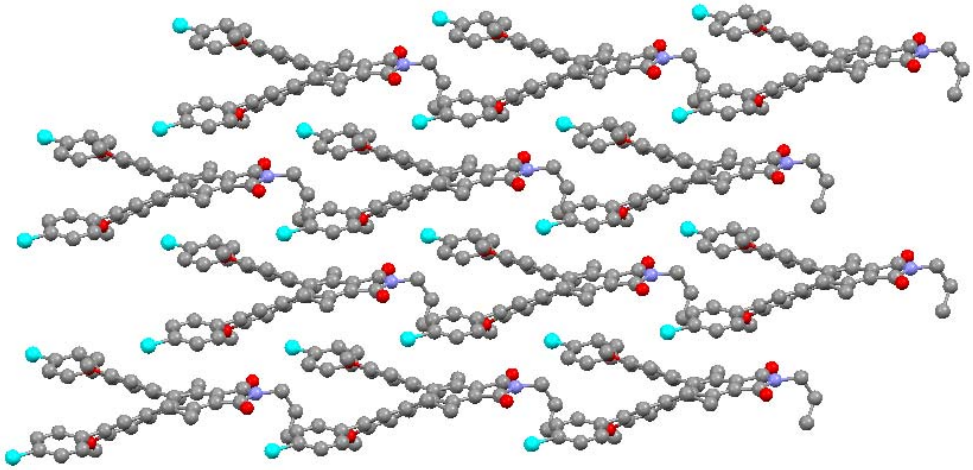


**Fig. S3** Packing mode of **4e**. Hydrogen atoms were omitted for clarity.

## 4. Photophysical properties of 5a-o

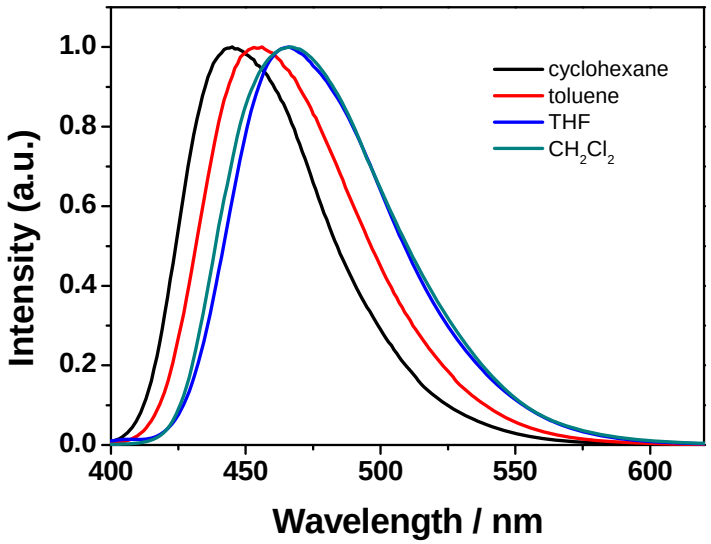



**Fig. S4** Fluorescence spectra of **5a** in various solvents ($c$ = 1.0 × $10^{-5}$ M).

**Table S5**. Photophysical data of **5a** in various solvents ($c$ = 1.0 × $10^{-5}$ M) and in film

| | $\lambda_{abs}$/nm | $\lambda_{em}$/nm | $\Phi_f{}^b$/% |
|---|---|---|---|
| Cyclohexane | 378 | 445 | 31.0 |
| Toluene | 383 | 459 | 38.3 |
| Dichoromethane | 383 | 472 | 37.3 |
| THF | 381 | 466 | 34.8 |
| Film | 388 | 498 | 16.7 |

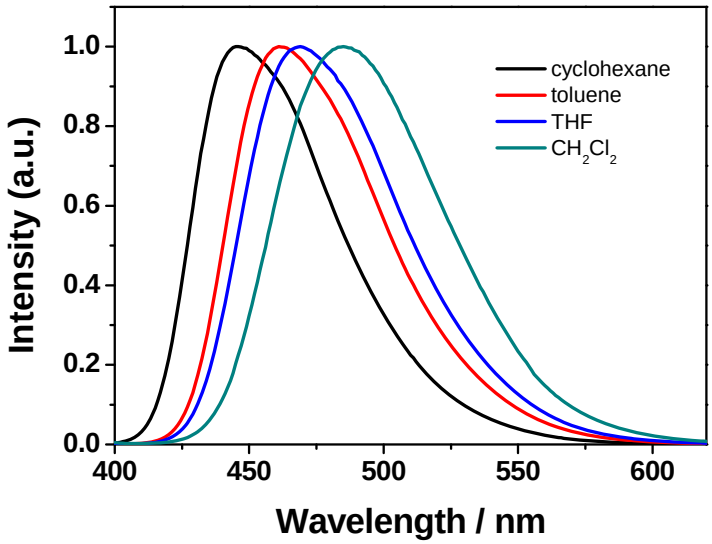



**Fig. S5** Fluorescence spectra of **5b** in various solvents ($c$ = 1.0 × $10^{-5}$ M).

**Table S6**. Photophysical data of **5b** in various solvents ($c$ = 1.0 × $10^{-5}$ M) and in film

| | $\lambda_{abs}$/nm | $\lambda_{em}$/nm | $\Phi_f{}^b$/% |
|---|---|---|---|
| Cyclohexane | 376 | 446 | 39.3 |
| Toluene | 385 | 470 | 43.9 |
| Dichoromethane | 384 | 485 | 46.3 |
| THF | 381 | 469 | 60.8 |
| Film | 387 | 493 | 56.6 |

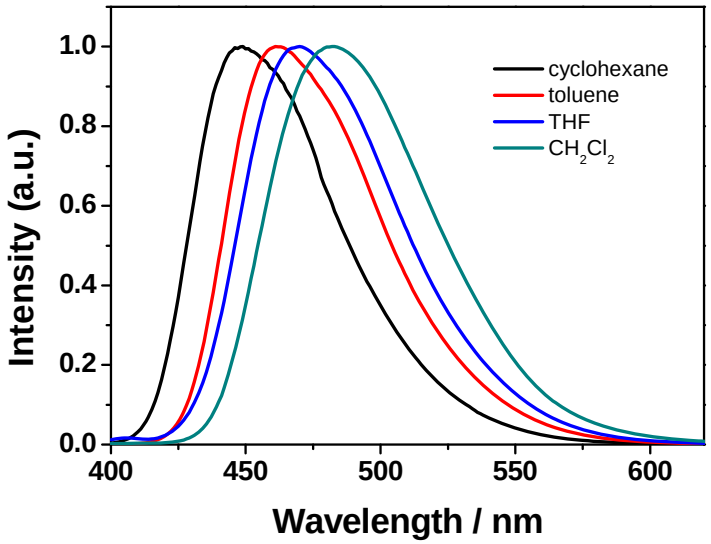



**Fig. S6** Fluorescence spectra of **5c** in various solvents ($c$ = 1.0 × $10^{-5}$ M).

**Table S7**. Photophysical data of **5c** in various solvents ($c$ = 1.0 × $10^{-5}$ M) and in film

| | $\lambda_{abs}$/nm | $\lambda_{em}$/nm | $\Phi_f{}^b$/% |
|---|---|---|---|
| Cyclohexane | 378 | 450 | 43.4 |
| Toluene | 390 | 460 | 52.3 |
| Dichoromethane | 384 | 483 | 43.8 |
| THF | 382 | 470 | 41.6 |
| Film | 391 | 501 | 45.0 |

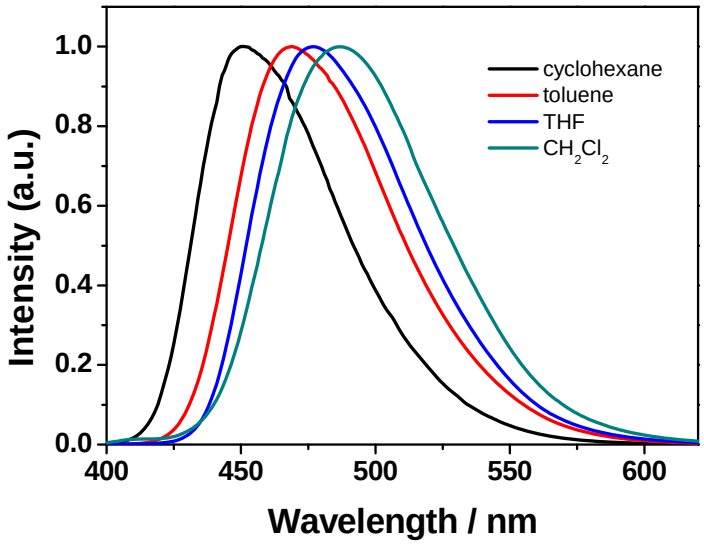



**Fig. S7** Fluorescence spectra of **5d** in various solvents ($c$ = 1.0 × $10^{-5}$ M).

**Table S8**. Photophysical data of **5d** in various solvents ($c$ = 1.0 × $10^{-5}$ M) and in film

| | $\lambda_{abs}$/nm | $\lambda_{em}$/nm | $\Phi_f^b$/% |
|---|---|---|---|
| Cyclohexane | 380 | 451 | 46.1 |
| Toluene | 388 | 467 | 54.1 |
| Dichoromethane | 386 | 487 | 50.1 |
| THF | 384 | 477 | 48.0 |
| Film | 387 | 502 | 21.4 |

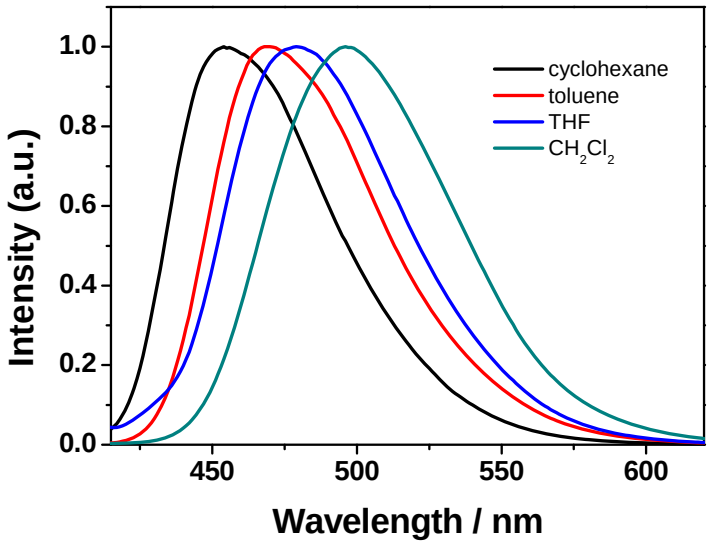



**Fig. S8** Fluorescence spectra of **5e** in various solvents ($c$ = 1.0 × $10^{-5}$ M).

**Table S9**. Photophysical data of **5e** in various solvents ($c$ = 1.0 × $10^{-5}$ M) and in film

| | $\lambda_{abs}$/nm | $\lambda_{em}$/nm | $\Phi_f{}^b$/% |
|---|---|---|---|
| Cyclohexane | 380 | 453 | 44.3 |
| Toluene | 385 | 471 | 52.1 |
| Dichoromethane | 384 | 496 | 65.1 |
| THF | 382 | 479 | 52.4 |
| Film | 389 | 500 | 41.8 |

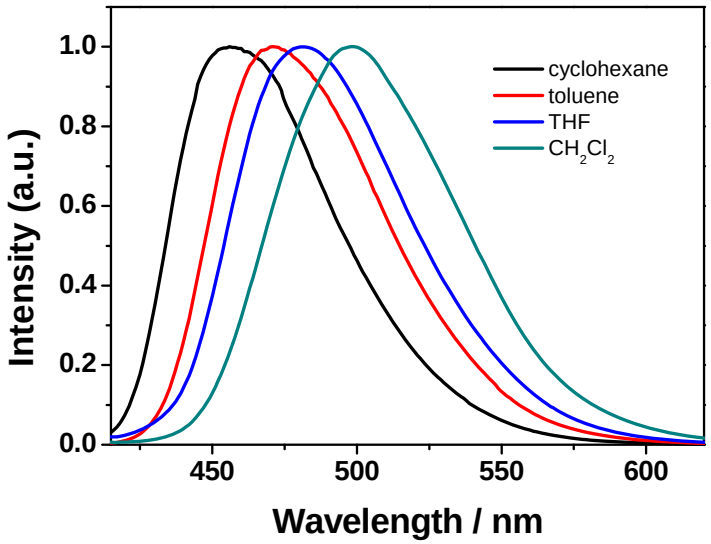



**Fig. S9** Fluorescence spectra of **5f** in various solvents ($c$ = 1.0 × $10^{-5}$ M).

**Table S10**. Photophysical data of **5f** in various solvents ($c$ = 1.0 × $10^{-5}$ M) and in film

| | $\lambda_{abs}$/nm | $\lambda_{em}$/nm | $\Phi_f^b$/% |
|---|---|---|---|
| Cyclohexane | 380 | 456 | 40.1 |
| Toluene | 385 | 472 | 50.6 |
| Dichoromethane | 384 | 499 | 68.5 |
| THF | 384 | 481 | 54.0 |
| Film | 388 | 499 | 34.4 |

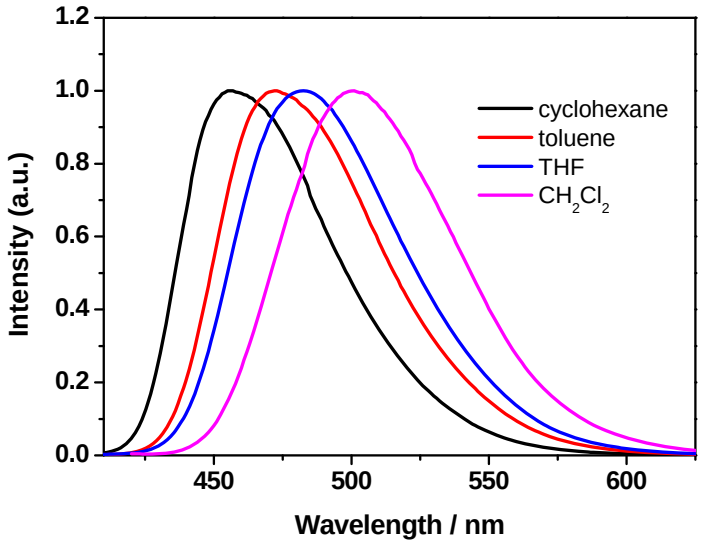



**Fig. S10** Fluorescence spectra of **5g** in various solvents ($c$ = 1.0 × $10^{-5}$ M).

**Table S11**. Photophysical data of **5g** in various solvents ($c$ = 1.0 × $10^{-5}$ M) and in film

| | $\lambda_{abs}$/nm | $\lambda_{em}$/nm | $\Phi_f{}^b$/% |
|---|---|---|---|
| Cyclohexane | 380 | 456 | 43.5 |
| Toluene | 385 | 474 | 52.9 |
| Dichoromethane | 385 | 502 | 74.3 |
| THF | 382 | 483 | 51.0 |
| Film | 390 | 502 | 51.0 |

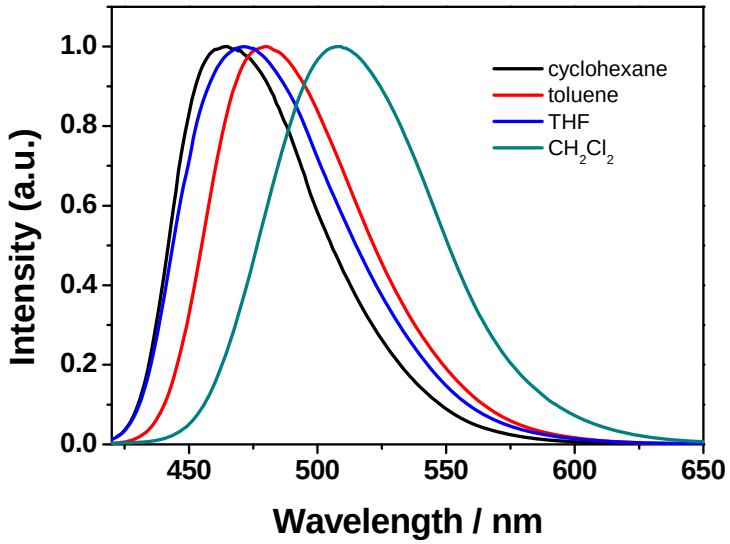



**Fig. S11** Fluorescence spectra of **5h** in various solvents ($c$ = 1.0 × $10^{-5}$ M).

**Table S12**. Photophysical data of **5h** in various solvents ($c$ = 1.0 × $10^{-5}$ M) and in film

| | $\lambda_{abs}$/nm | $\lambda_{em}$/nm | $\Phi_f^b$/% |
|---|---|---|---|
| Cyclohexane | 382 | 463 | 48.7 |
| Toluene | 390 | 480 | 60.8 |
| Dichoromethane | 387 | 509 | 80.3 |
| THF | 385 | 490 | 60.1 |
| Film | 391 | 503 | 53.7 |

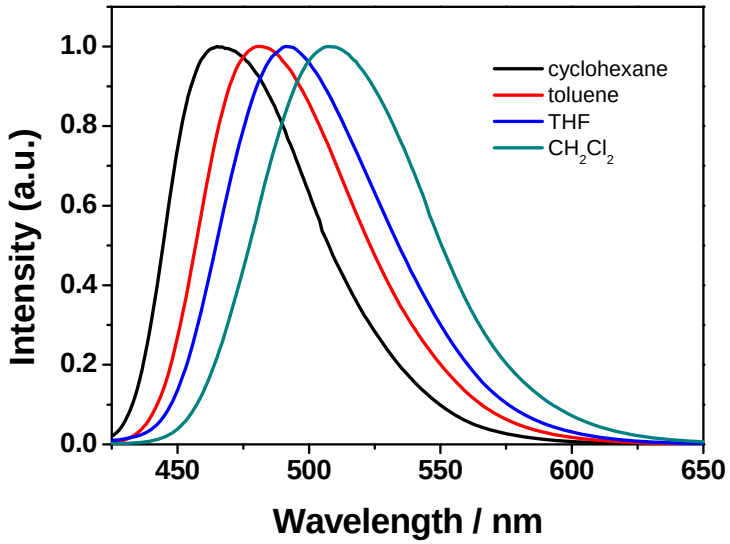



**Fig. S12** Fluorescence spectra of **5i** in various solvents ($c$ = 1.0 × $10^{-5}$ M).

**Table S13**. Photophysical data of **5i** in various solvents ($c$ = 1.0 × $10^{-5}$ M) and in film

| | $\lambda_{abs}$/nm | $\lambda_{em}$/nm | $\Phi_f{}^b$/% |
|---|---|---|---|
| Cyclohexane | 384 | 470 | 55.9 |
| Toluene | 395 | 490 | 64.5 |
| Dichoromethane | 388 | 507 | 77.5 |
| THF | 386 | 491 | 64.3 |
| Film | 394 | 508 | 28.9 |

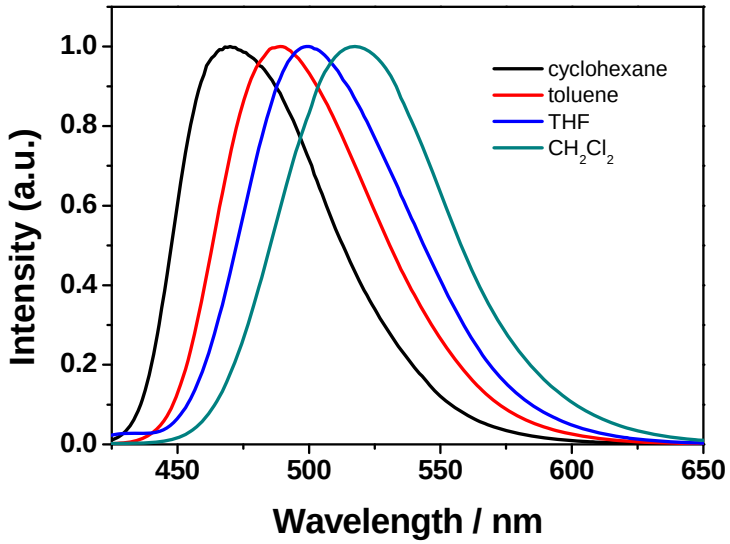



**Fig. S13** Fluorescence spectra of **5j** in various solvents ($c$ = 1.0 × $10^{-5}$ M).

**Table S14**. Photophysical data of **5j** in various solvents ($c$ = 1.0 × $10^{-5}$ M) and in film

| | $\lambda_{abs}$/nm | $\lambda_{em}$/nm | $\Phi_f^b$/% |
|---|---|---|---|
| Cyclohexane | 386 | 474 | 40.1 |
| Toluene | 400 | 490 | 50.0 |
| Dichoromethane | 391 | 518 | 75.6 |
| THF | 389 | 500 | 50.0 |
| Film | 397 | 517 | 45.5 |

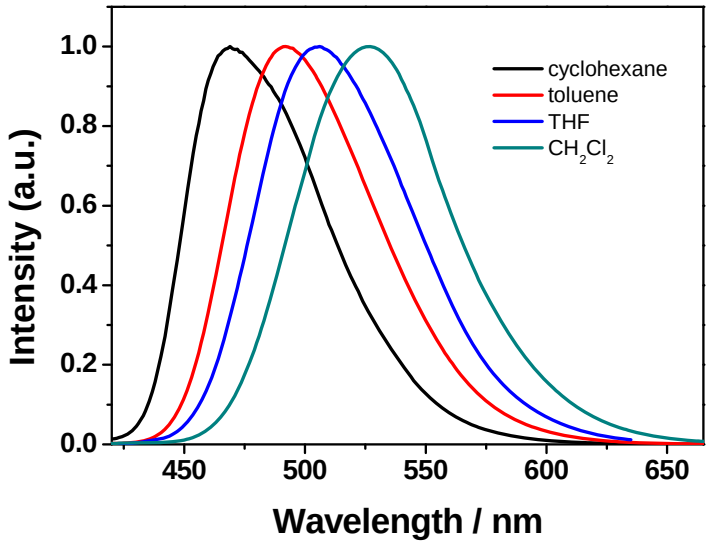



**Fig. S14** Fluorescence spectra of **5k** in various solvents ($c$ = 1.0 × $10^{-5}$ M).

**Table S15**. Photophysical data of **5k** in various solvents ($c$ = 1.0 × $10^{-5}$ M) and in film

| | $\lambda_{abs}$/nm | $\lambda_{em}$/nm | $\Phi_f{}^b$/% |
|---|---|---|---|
| Cyclohexane | 385 | 469 | 63.7 |
| Toluene | 391 | 491 | 76.0 |
| Dichoromethane | 390 | 526 | 85.3 |
| THF | 388 | 506 | 90.3 |
| Film | 395 | 518 | 61.8 |

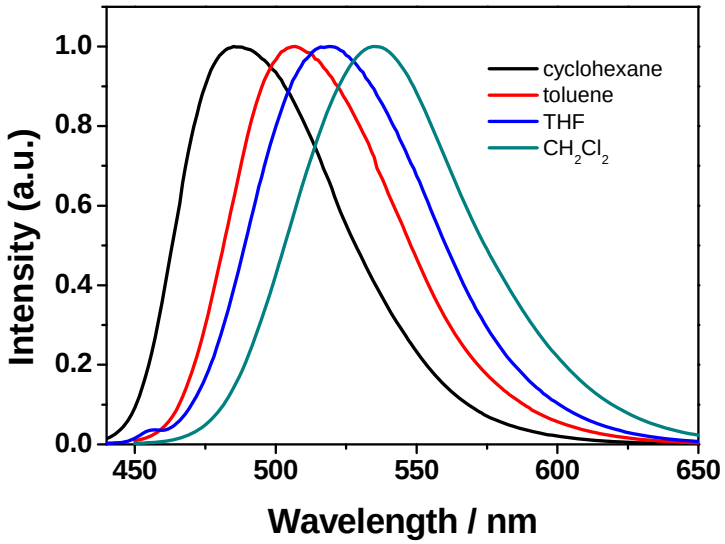



**Fig. S15** Fluorescence spectra of **5l** in various solvents ($c$ = 1.0 × $10^{-5}$ M).

**Table S16**. Photophysical data of **5l** in various solvents ($c$ = 1.0 × $10^{-5}$ M) and in film

| | $\lambda_{abs}$/nm | $\lambda_{em}$/nm | $\Phi_f^b$/% |
|---|---|---|---|
| Cyclohexane | 396 | 486 | 52.7 |
| Toluene | 402 | 507 | 64.2 |
| Dichoromethane | 400 | 535 | 71.5 |
| THF | 399 | 519 | 52.1 |
| Film | 407 | 535 | 32.1 |

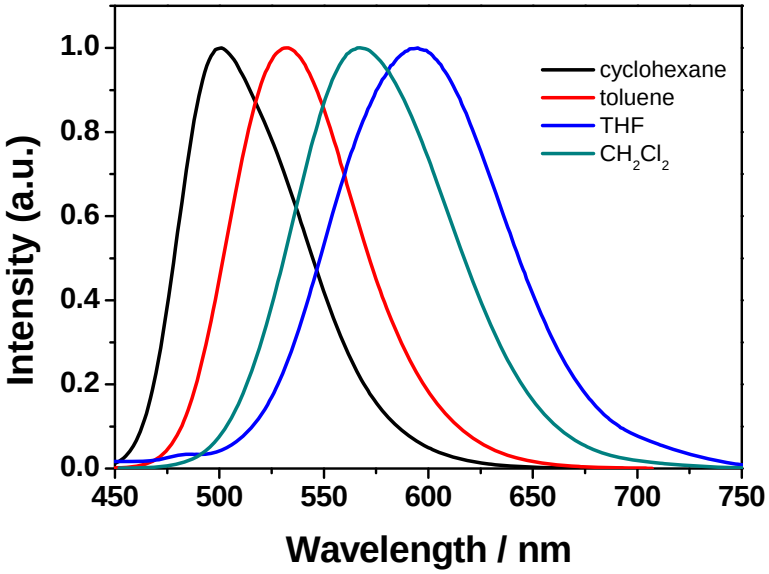



**Fig. S16** Fluorescence spectra of **5m** in various solvents ($c$ = 1.0 × $10^{-5}$ M).

**Table S17**. Photophysical data of **5m** in various solvents ($c$ = 1.0 × $10^{-5}$ M) and in film

| | $\lambda_{abs}$/nm | $\lambda_{em}$/nm | $\Phi_f{}^b$/% |
|---|---|---|---|
| Cyclohexane | 405 | 501 | 76.6 |
| Toluene | 411 | 533 | 68.5 |
| Dichoromethane | 407 | 595 | 7.1 |
| THF | 404 | 568 | 30.3 |
| Film | 440 | 556 | 67.3 |

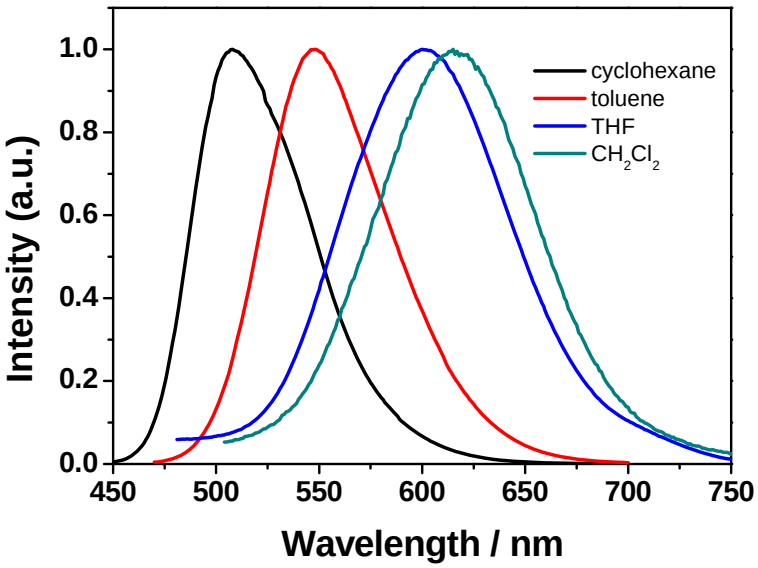



**Fig. S17** Fluorescence spectra of **5n** in various solvents ($c$ = 1.0 × $10^{-5}$ M).

**Table S18**. Photophysical data of **5n** in various solvents ($c$ = 1.0 × $10^{-5}$ M) and in film

| | $\lambda_{abs}$/nm | $\lambda_{em}$/nm | $\Phi_f{}^b$/% |
|---|---|---|---|
| Cyclohexane | 404 | 508 | 76.4 |
| Toluene | 414 | 549 | 72.4 |
| Dichoromethane | 411 | 615 | 2.6 |
| THF | 411 | 600 | 2.8 |
| Film | 416 | 586 | 11.6 |

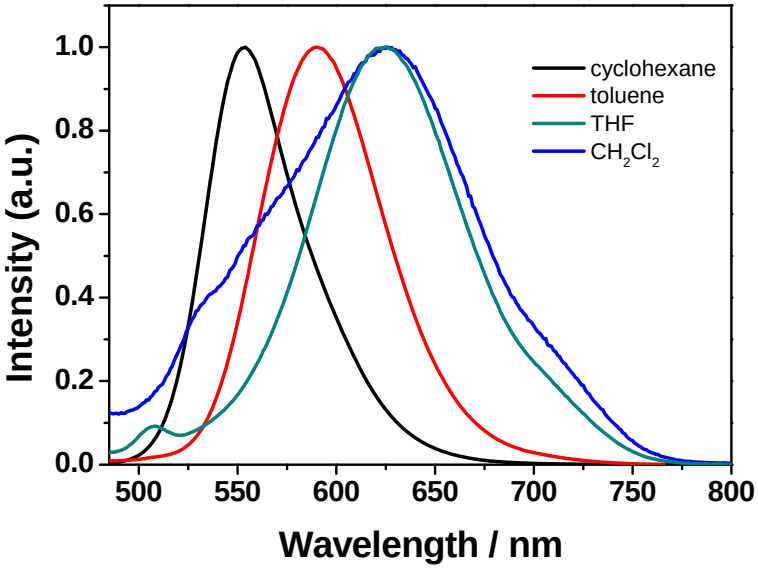



**Fig. S18** Fluorescence spectra of **5o** in various solvents ($c$ = 1.0 × $10^{-5}$ M).

**Table S19**. Photophysical data of **5o** in various solvents ($c$ = 1.0 × $10^{-5}$ M) and in film

| | $\lambda_{abs}$/nm | $\lambda_{em}$/nm | $\Phi_f{}^b$/% |
|---|---|---|---|
| Cyclohexane | 430 | 554 | 49.1 |
| Toluene | 440 | 590 | 46.2 |
| Dichoromethane | 436 | 626 | 1.9 |
| THF | 431 | 625 | 7.9 |
| Film | 462 | 625 | 27.1 |

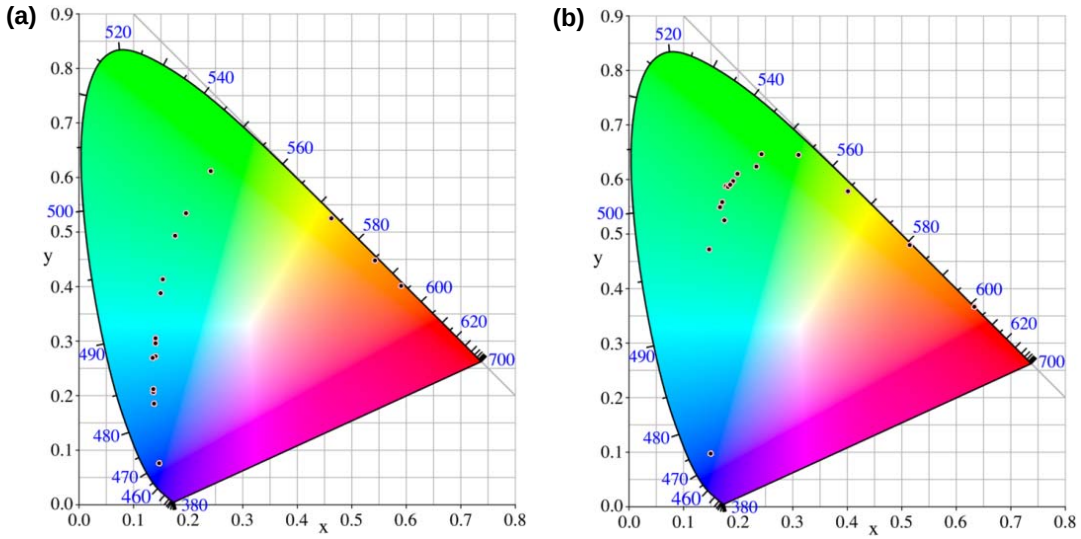



**Fig. S19** The 1931CIE coordinate diagram marked with **5a-o** and **7** in THF (a) and solid state (b).

**Table S20**. The 1931CIE coordinate values of **5a-o** and **7** in THF and in solid state.

| compounds | THF (x, y) | Solid (x, y) |
|---|---|---|
| **7** | 0.1469, 0.0755 | 0.1496, 0.0967 |
| **5a** | 0.1374, 0.1854 | 0.1747, 0.5255 |
| **5b** | 0.136, 0.2072 | 0.1473, 0.4719 |
| **5c** | 0.1357, 0.2114 | 0.1771, 0.588 |
| **5d** | 0.135, 0.2687 | 0.1909, 0.5969 |
| **5e** | 0.1396, 0.2716 | 0.1706, 0.558 |
| **5f** | 0.1403, 0.2962 | 0.1669, 0.5488 |
| **5g** | 0.1396, 0.3058 | 0.1812, 0.5867 |
| **5h** | 0.1491, 0.3878 | 0.1851, 0.591 |
| **5i** | 0.1538, 0.4132 | 0.1986, 0.6111 |
| **5j** | 0.1764, 0.4938 | 0.2425, 0.6466 |
| **5k** | 0.1963, 0.5351 | 0.2334, 0.6243 |
| **5l** | 0.2411, 0.612 | 0.3111, 0.6452 |
| **5m** | 0.4623, 0.5258 | 0.402, 0.5785 |
| **5n** | 0.5428, 0.4479 | 0.5144, 0.4797 |
| **5o** | 0.5913, 0.4008 | 0.6332, 0.3661 |

## 5. DFT calculations of 5a-o and 7

Calculations were performed with the DFT method at the B3LYP/6-31G(d) level with Gaussian 09 program.[S1]

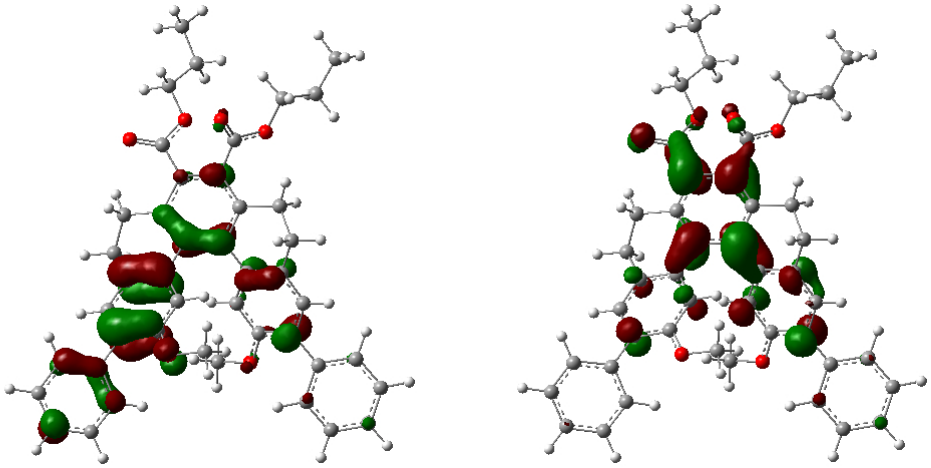


**Fig. S20** The HOMO and LUMO of **7**.

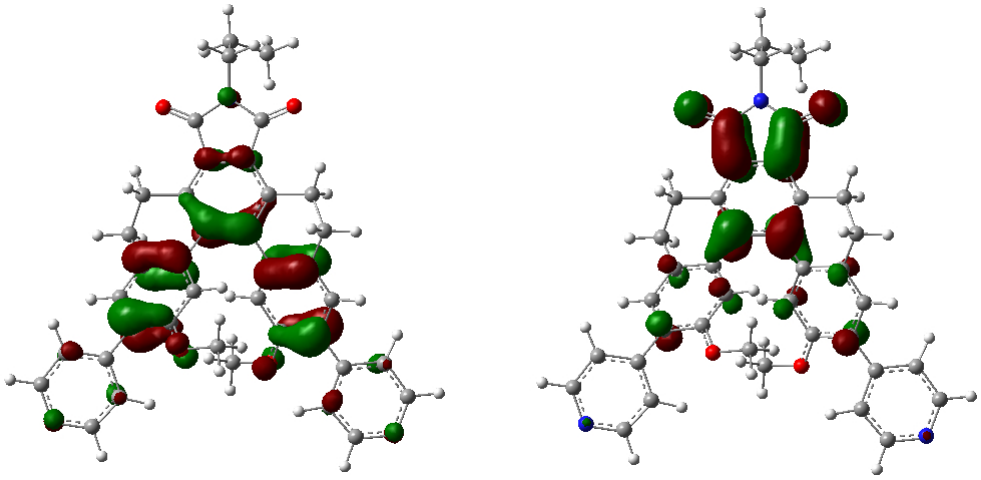


**Fig. S21** The HOMO and LUMO of **5a**.

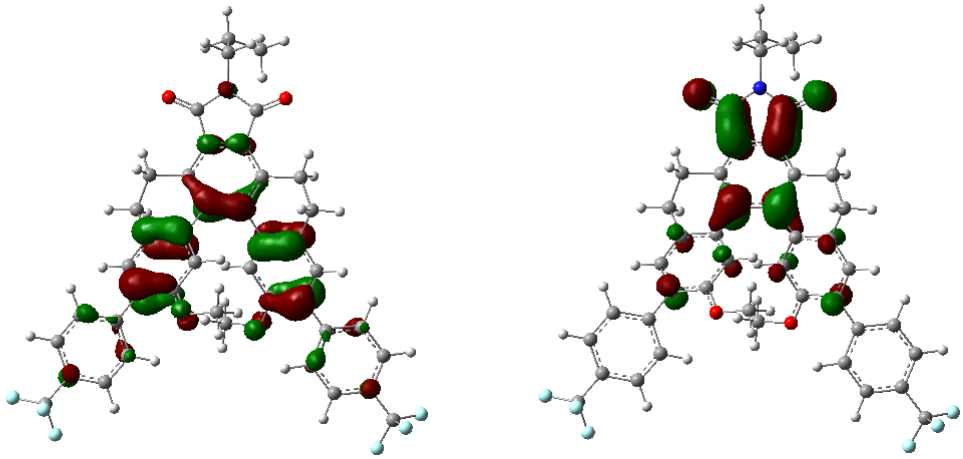


**Fig. S22** The HOMO and LUMO of **5b**.

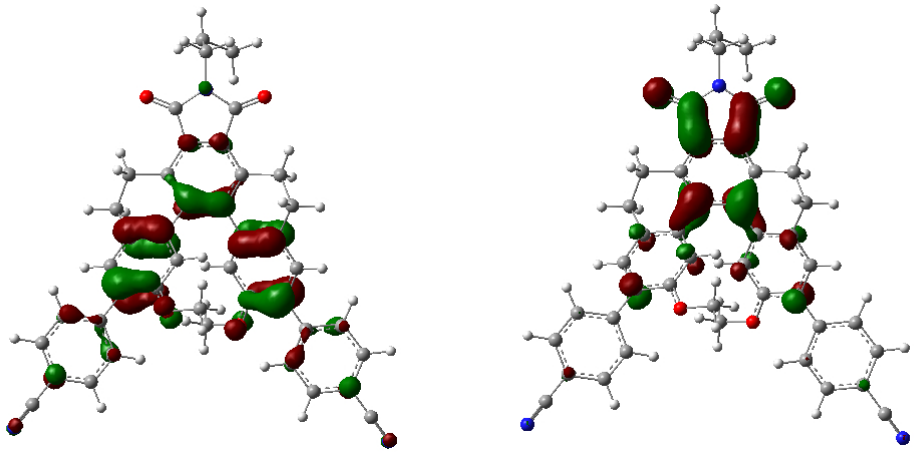


**Fig. S23** The HOMO and LUMO of **5c**.

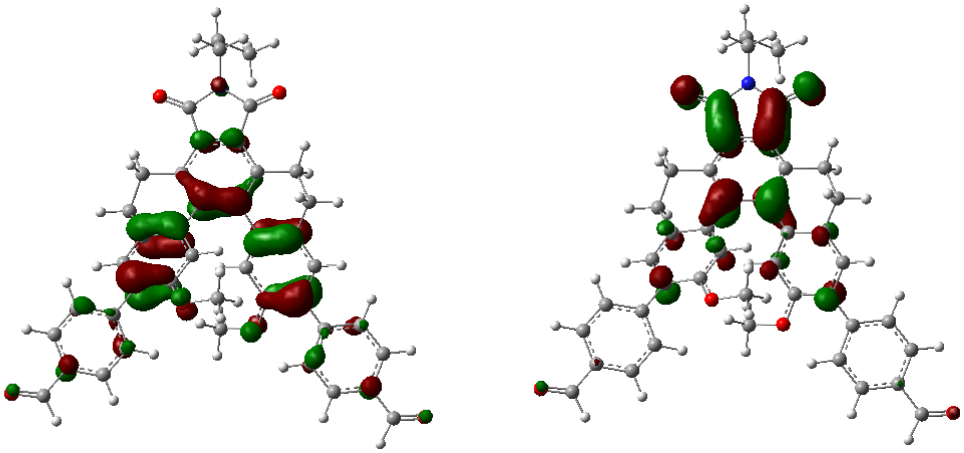


**Fig. S24** The HOMO and LUMO of **5d**.

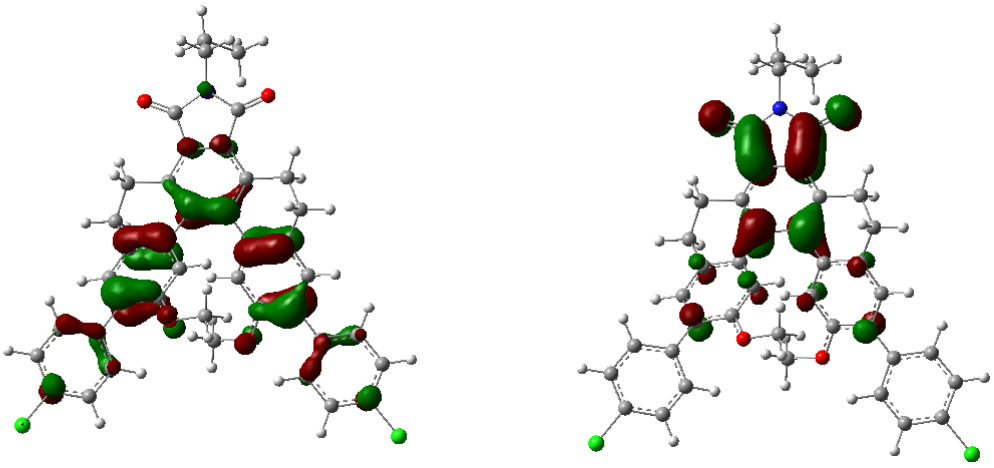


**Fig. S25** The HOMO and LUMO of **5e**.

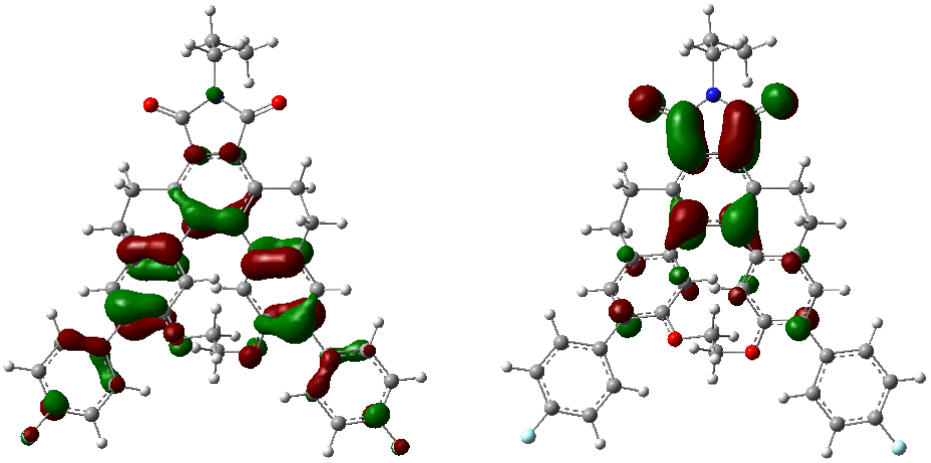


**Fig. S26** The HOMO and LUMO of **5f**.

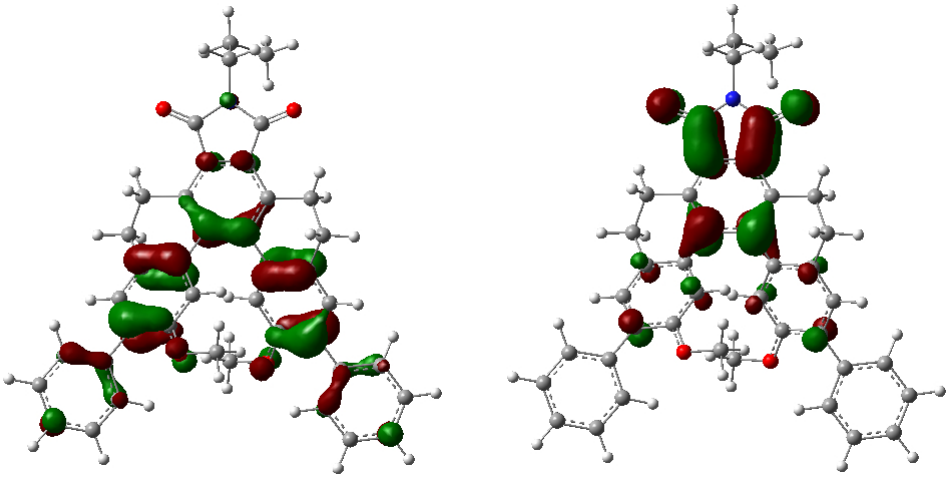


**Fig. S27** The HOMO and LUMO of **5g**.

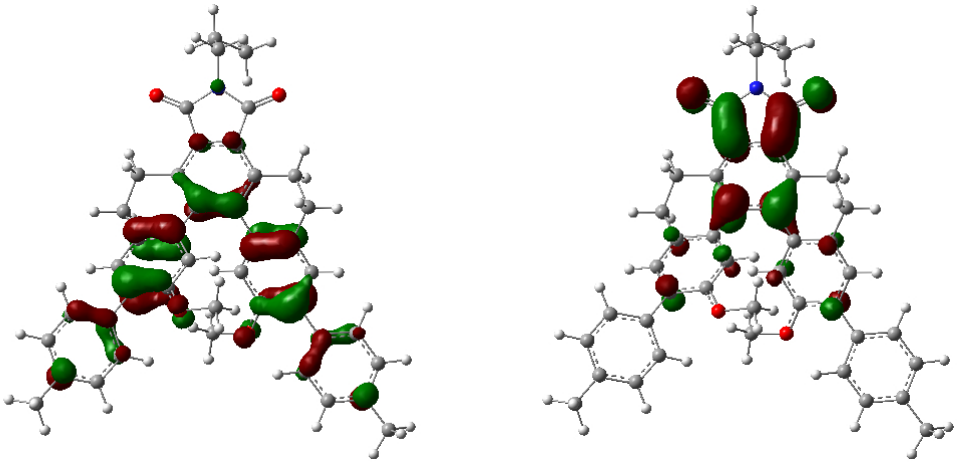


**Fig. S28** The HOMO and LUMO of **5h**.

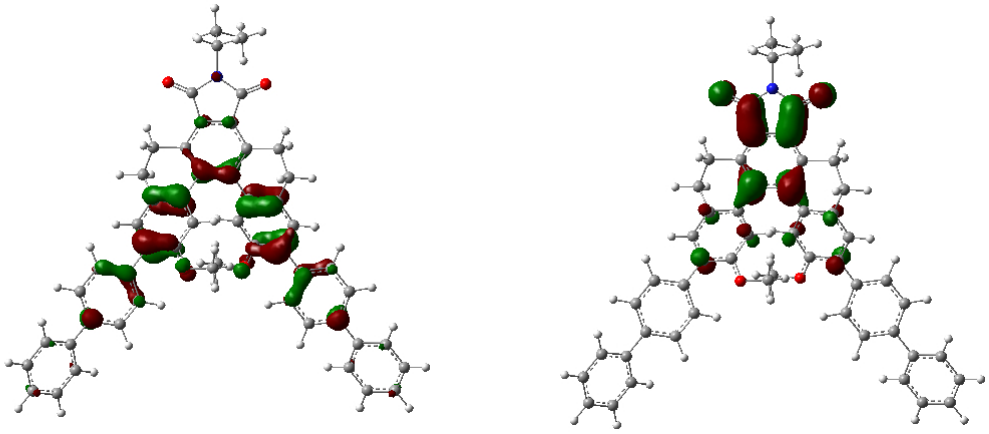


**Fig. S29** The HOMO and LUMO of **5i**.

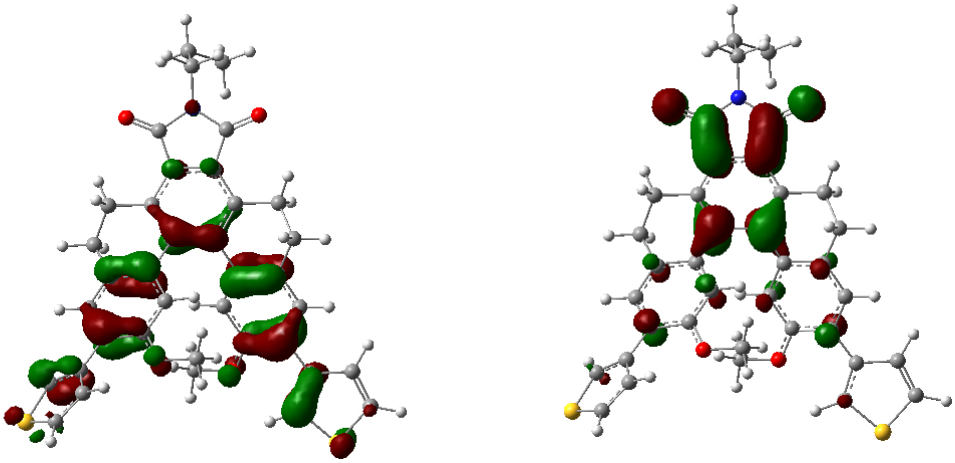


**Fig. S30** The HOMO and LUMO of **5j**.

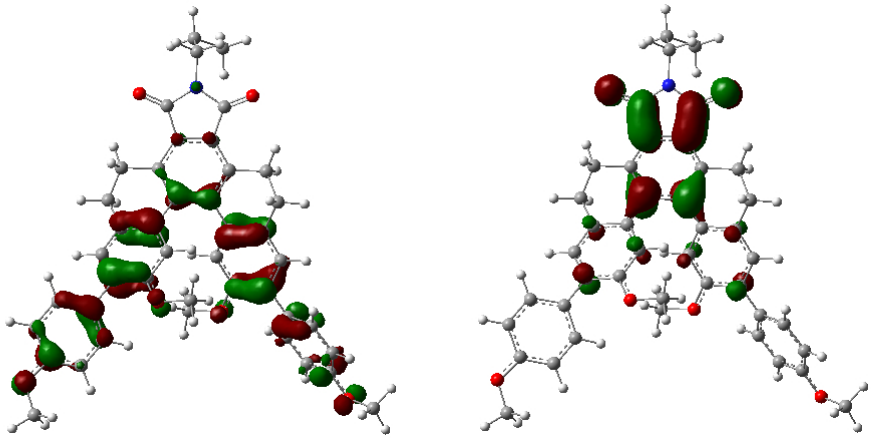


**Fig. S31** The HOMO and LUMO of **5k**.

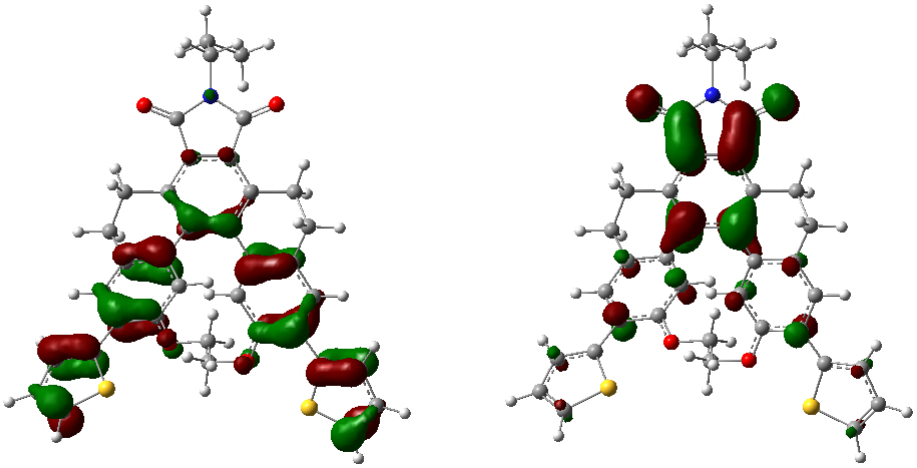


**Fig. S32** The HOMO and LUMO of **5l**.

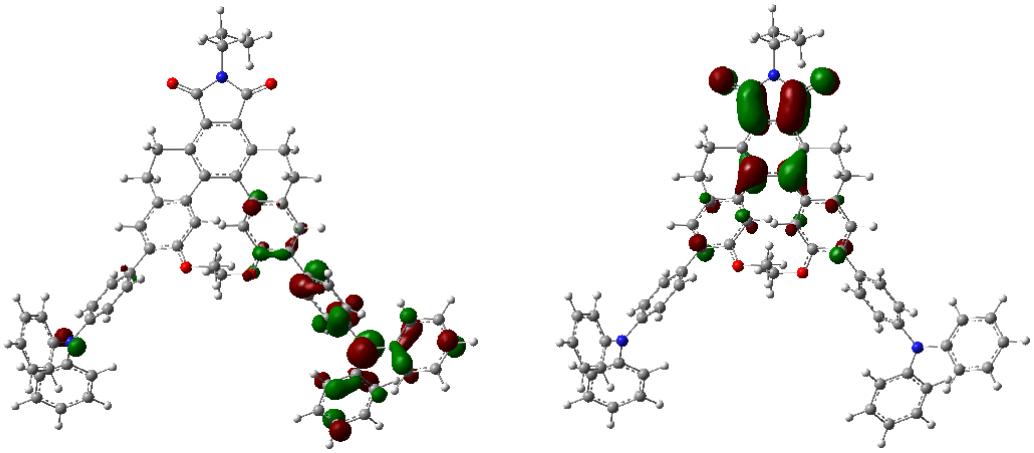


**Fig. S33** The HOMO and LUMO of **5m**.

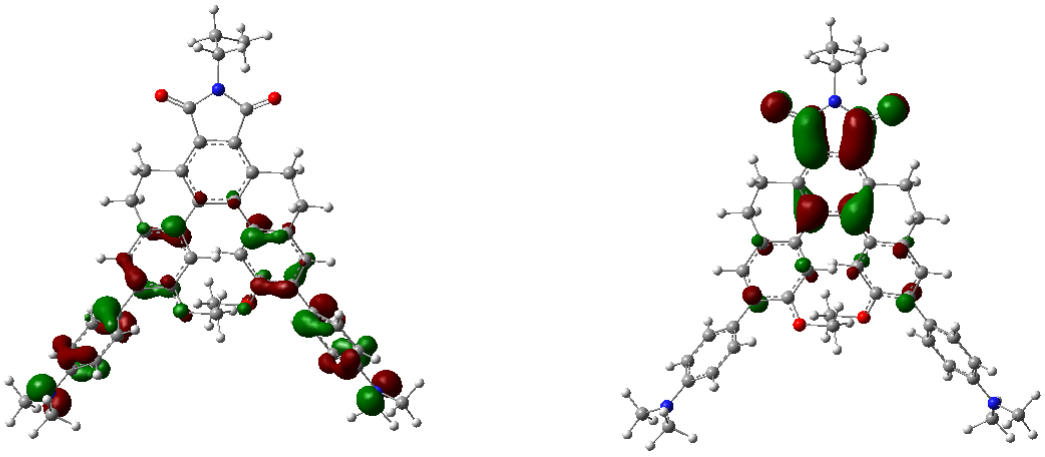


**Fig. S34** The HOMO and LUMO of **5n**.

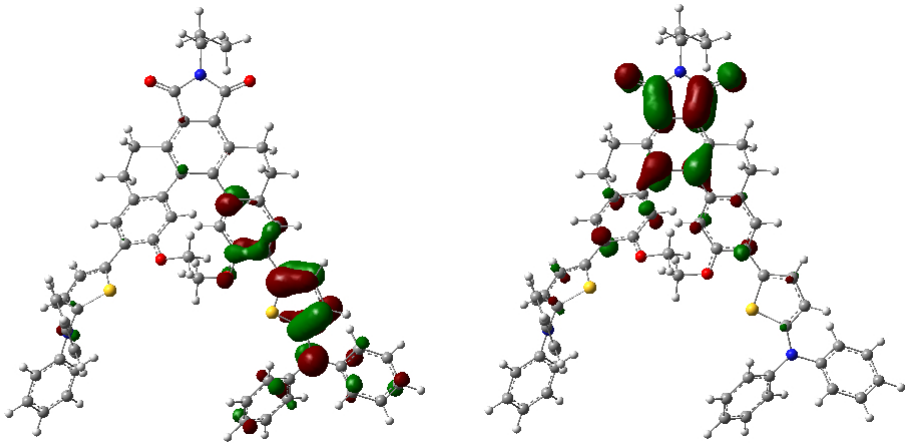


**Fig. S35** The HOMO and LUMO of **5o**.

**Table S21**. Thermal data of **5a-o** and **7**

| Compound | Ar | HOMO (eV) | LUMO (eV) | $E_g$ (eV) |
|---|---|---|---|---|
| **7** | $C_6H_5$ | -5.15 | -2.11 | 3.03 |
| **5a** | 4-pyridine | -5.72 | -2.84 | 2.88 |
| **5b** | 4-$CF_3C_6H_4$ | -5.66 | -2.82 | 2.84 |
| **5c** | 4-$CNC_6H_4$ | -5.83 | -2.85 | 2.99 |
| **5d** | 4-$OHCC_6H_4$ | -5.70 | -2.89 | 2.81 |
| **5e** | 4-$ClC_6H_4$ | -5.51 | -2.73 | 2.78 |
| **5f** | 4-$FC_6H_4$ | -5.41 | -2.64 | 2.76 |
| **5g** | $C_6H_5$ | -5.35 | -2.57 | 2.78 |
| **5h** | 4-$MeC_6H_4$ | -5.25 | -2.50 | 2.75 |
| **5i** | 4-$C_6H_5$-$C_6H_4$ | -5.26 | -2.59 | 2.67 |
| **5j** | 3-thiophene | -5.27 | -2.58 | 2.70 |
| **5k** | 4-$CH_3OC_6H_4$ | -5.07 | -2.45 | 2.62 |
| **5l** | 2-thiophene | -5.10 | -2.58 | 2.53 |
| **5m** | 4-$Ph_2NC_6H_4$ | -4.81 | -2.51 | 2.29 |
| **5n** | 4-$Me_2NC_6H_4$ | -4.63 | -2.28 | 2.35 |
| **5o** | 5-$Ph_2N$-2-thienyl | -4.53 | -2.44 | 2.08 |

Cartesian Coordinates (Å) and Energies at 298.15 K/1 atm for the Optimized Structures of **7**.

B3LYP/6-31G* SCF energy: -2153.365976 a.u.

**Table 22**. Cartesian coordinates (Å) of **7**

| | x | y | z |
|---|---|---|---|
| O | -3.26367600 | 2.15486300 | 2.09706800 |
| O | -4.06219800 | -1.22235300 | -1.80826300 |
| C | -7.19742200 | -4.97335800 | -0.51907000 |
| C | -7.15574400 | -3.57638800 | -0.56079600 |
| H | -8.07925900 | -3.00719700 | -0.62221800 |
| C | -5.93996400 | -2.90428000 | -0.51793100 |

| | | | |
|---|---|---|---|
| H | -5.92404200 | -1.82250200 | -0.53902700 |
| C | -4.71965400 | -3.61500000 | -0.41655100 |
| C | -4.78586700 | -5.02879200 | -0.36924200 |
| H | -3.86614100 | -5.60348800 | -0.32845600 |
| C | -6.00312100 | -5.69546400 | -0.42722500 |
| H | -6.02266900 | -6.78157000 | -0.40830600 |
| C | -3.42033500 | -2.94463400 | -0.31429200 |
| C | -3.10011200 | -1.71912000 | -0.99263300 |
| C | -1.85765800 | -1.11673700 | -0.84037100 |
| H | -1.62596500 | -0.21551200 | -1.38717800 |
| C | -0.85929500 | -1.67432700 | -0.01300200 |
| C | 0.46948300 | -1.08669600 | 0.12750400 |
| C | 0.71647700 | 0.31875100 | -0.17941000 |
| C | -0.26827500 | 1.35648100 | 0.03880300 |
| C | -1.31598500 | 1.23607800 | 0.99142800 |
| H | -1.32979700 | 0.36463100 | 1.63180700 |
| C | -2.26951800 | 2.23268700 | 1.15753200 |
| C | -2.23254100 | 3.42378200 | 0.37625300 |
| C | -1.15845900 | 3.54039900 | -0.53963100 |
| H | -1.11259200 | 4.43011700 | -1.16230500 |
| C | -0.19675800 | 2.56345000 | -0.71637100 |
| C | 0.91451600 | 2.67122400 | -1.72506400 |
| H | 0.65984300 | 2.09698900 | -2.63036400 |
| C | 2.01935000 | 0.69210800 | -0.60901400 |
| C | 2.86976800 | -1.52504700 | 0.08069500 |
| C | 1.55730200 | -1.96686800 | 0.34311300 |
| C | 1.27153200 | -3.38361800 | 0.80658700 |
| H | 2.06992700 | -3.73161400 | 1.46223400 |
| H | 1.29469700 | -4.06431600 | -0.05565900 |
| C | -0.08290500 | -3.48530000 | 1.51881900 |
| H | -0.30450000 | -4.52231000 | 1.79312800 |
| H | -0.02869500 | -2.90677200 | 2.45512500 |

| | | | |
|---|---|---|---|
| C | -1.15928500 | -2.91687600 | 0.64897400 |
| C | -2.39347300 | -3.50841300 | 0.48113700 |
| H | -2.60762600 | -4.42188300 | 1.02762400 |
| C | -3.81861900 | -0.00702100 | -2.51637700 |
| H | -2.98482200 | -0.12234100 | -3.21831300 |
| H | -3.60874100 | 0.81928200 | -1.82794300 |
| H | -4.73650000 | 0.19492800 | -3.06986200 |
| C | -3.29287900 | 1.03786700 | 2.96923700 |
| H | -3.43333300 | 0.09698500 | 2.42040800 |
| H | -2.37535000 | 0.96987800 | 3.56806800 |
| C | -3.20830900 | 4.52235700 | 0.50779400 |
| H | 1.05624400 | 3.71149700 | -2.03939600 |
| C | 2.21306100 | 2.10660100 | -1.13501000 |
| C | 3.06799100 | -0.21638000 | -0.49258600 |
| C | 4.02357500 | -2.38592300 | 0.40136000 |
| H | -4.14531500 | 1.20108400 | 3.63172000 |
| C | -4.58227600 | 4.29847000 | 0.74428600 |
| C | -2.78728900 | 5.86133300 | 0.35147300 |
| H | 3.00248400 | 2.12992600 | -1.89003900 |
| H | 2.55333200 | 2.75459700 | -0.31520400 |
| C | 4.40316300 | 0.09550300 | -1.09789800 |
| O | 4.03614600 | -3.60993000 | 0.41143400 |
| H | -4.94030900 | 3.28359700 | 0.86607600 |
| C | -5.48259700 | 5.35800700 | 0.81070900 |
| C | -3.68931900 | 6.91916500 | 0.42200400 |
| H | -1.73218300 | 6.07222600 | 0.20411200 |
| O | 4.93773100 | -0.58256800 | -1.95298800 |
| H | -6.53613100 | 5.15287000 | 0.98499100 |
| C | -5.04558600 | 6.67555100 | 0.65007900 |
| H | -3.32969400 | 7.93885100 | 0.30845300 |
| H | -5.75104500 | 7.50024800 | 0.70627500 |
| H | -8.14992200 | -5.49426100 | -0.55930000 |

| | | | |
|---|---|---|---|
| O | 4.94252600 | 1.24251000 | -0.62121800 |
| O | 5.12418400 | -1.65540500 | 0.74693000 |
| C | 6.33490000 | -2.40544000 | 0.94528000 |
| H | 6.14156500 | -3.22238300 | 1.64849700 |
| H | 6.63543000 | -2.85469400 | -0.00896200 |
| C | 7.39633000 | -1.45252700 | 1.47544900 |
| H | 7.53918200 | -0.63752300 | 0.75496100 |
| H | 7.02866400 | -0.99194800 | 2.40099000 |
| C | 8.72812400 | -2.16577900 | 1.73173800 |
| H | 9.48164400 | -1.46686500 | 2.11044800 |
| H | 8.61585100 | -2.96717300 | 2.47200600 |
| H | 9.12332100 | -2.61606700 | 0.81311000 |
| C | 6.20011800 | 1.63361200 | -1.20972700 |
| H | 6.06090000 | 1.79118800 | -2.28593600 |
| H | 6.91774600 | 0.81454600 | -1.09121200 |
| C | 6.66799800 | 2.90053500 | -0.50940300 |
| H | 6.75582000 | 2.69902800 | 0.56535400 |
| H | 5.89917300 | 3.67539500 | -0.62105100 |
| C | 8.00539400 | 3.40045700 | -1.06562400 |
| H | 8.32742200 | 4.31128000 | -0.55002400 |
| H | 8.79581400 | 2.65042400 | -0.94116900 |
| H | 7.93283000 | 3.63133400 | -2.13534600 |

Cartesian Coordinates (Å) and Energies at 298.15 K/1 atm for the Optimized Structures of **5a**.

B3LYP/6-31G* SCF energy: -1971.231157 a.u.

**Table 23**. Cartesian coordinates (Å) of **5a**

| | x | y | z |
|---|---|---|---|
| O | -3.24952100 | -1.66765700 | -1.75684500 |
| C | -4.87618700 | -3.46216000 | -0.25338000 |

| | | | |
|---|---|---|---|
| H | -5.02690500 | -2.39352200 | -0.33636000 |
| C | -5.97472500 | -4.31605800 | -0.20565300 |
| H | -6.98155800 | -3.90414100 | -0.25537900 |
| C | -4.65695800 | -6.16444000 | -0.03139700 |
| H | -4.59479500 | -7.24876900 | 0.04595500 |
| C | -3.49217700 | -5.40316000 | -0.06120800 |
| H | -2.52725500 | -5.89903000 | -0.02888600 |
| C | -3.57726700 | -4.00138300 | -0.17542600 |
| C | -2.35785500 | -3.17361300 | -0.16302100 |
| C | -2.20693600 | -1.98716300 | -0.94422800 |
| C | -1.03471300 | -1.24299900 | -0.88597000 |
| C | 0.04113200 | -1.61694700 | -0.04818900 |
| C | -0.07816800 | -2.83594700 | 0.69543900 |
| C | -1.25341200 | -3.56264500 | 0.62478500 |
| H | -1.34405600 | -4.46058600 | 1.22910800 |
| C | 1.09448400 | -3.26308800 | 1.53530300 |
| H | 1.00003300 | -4.31571200 | 1.82259600 |
| H | 1.11982700 | -2.67744000 | 2.46795300 |
| C | -3.14585700 | -0.52429200 | -2.59862100 |
| H | -2.32008500 | -0.63043200 | -3.31240700 |
| H | -3.00672600 | 0.39259300 | -2.01245100 |
| H | -0.92015200 | -0.37183800 | -1.51486500 |
| C | 1.27963800 | -0.85190700 | 0.03309700 |
| C | 2.39317500 | -3.01468900 | 0.76003500 |
| H | -4.09093900 | -0.47316500 | -3.14101800 |
| C | 2.46584700 | -1.57721800 | 0.29433500 |
| C | 1.35926500 | 0.57066400 | -0.33127200 |
| H | 3.27615600 | -3.24678900 | 1.35941700 |
| H | 2.43624700 | -3.68497300 | -0.11167300 |
| C | 3.68215900 | -0.96036300 | 0.01824700 |
| C | 2.60298600 | 1.13174600 | -0.70505300 |
| C | 0.24768800 | 1.49499500 | -0.14166200 |

| | | | |
|---|---|---|---|
| C | 5.04943800 | -1.47864000 | 0.13233600 |
| C | 3.74587400 | 0.35613600 | -0.53581800 |
| C | 2.68061000 | 2.56807200 | -1.17335600 |
| C | 0.22481200 | 2.72218500 | -0.88079200 |
| C | -0.78485100 | 1.26544700 | 0.79670600 |
| O | 5.46647700 | -2.56327500 | 0.54624800 |
| N | 5.87412900 | -0.44802700 | -0.35712300 |
| C | 5.15335000 | 0.68546600 | -0.78523300 |
| H | 3.52854000 | 2.68258900 | -1.85194200 |
| H | 2.89090900 | 3.22217500 | -0.31369500 |
| C | 1.36129400 | 2.99138300 | -1.82876500 |
| C | -0.82996600 | 3.60053500 | -0.70614000 |
| H | -0.72841600 | 0.38343900 | 1.41840700 |
| C | -1.83563600 | 2.16042700 | 0.95846700 |
| C | 7.32114800 | -0.56510500 | -0.44632400 |
| O | 5.66643000 | 1.70042800 | -1.26149400 |
| H | 1.38277700 | 4.04829900 | -2.11497600 |
| H | 1.22212700 | 2.41132800 | -2.75481900 |
| C | -1.89771800 | 3.35948500 | 0.18455300 |
| H | -0.85539700 | 4.50585500 | -1.30584900 |
| O | -2.83058100 | 1.98254400 | 1.86834300 |
| H | 7.64582600 | 0.18085200 | -1.17767700 |
| H | 7.54633900 | -1.56570200 | -0.82947200 |
| C | -2.98862100 | 4.34345500 | 0.30386200 |
| C | -2.79793600 | 0.83873900 | 2.71511400 |
| C | -2.72573900 | 5.72219000 | 0.18323500 |
| C | -4.33629100 | 3.98159500 | 0.49467200 |
| H | -2.84439600 | -0.09085900 | 2.13435500 |
| H | -3.68152900 | 0.91887600 | 3.34981400 |
| H | -1.89742600 | 0.83399900 | 3.34094600 |
| H | -1.70908700 | 6.08394700 | 0.06698400 |
| C | -3.77593800 | 6.63281400 | 0.25542900 |

| | | | |
|---|---|---|---|
| C | -5.31031500 | 4.97518800 | 0.54232700 |
| H | -4.62081500 | 2.94160200 | 0.59052900 |
| H | -3.57569900 | 7.69996700 | 0.17363200 |
| H | -6.35537200 | 4.70122800 | 0.67887100 |
| C | 8.03972200 | -0.35670800 | 0.89668200 |
| H | 9.10830000 | -0.54679800 | 0.72591400 |
| H | 7.69304300 | -1.12485200 | 1.59781100 |
| C | 7.85108200 | 1.03937000 | 1.49648300 |
| H | 8.19078300 | 1.81982800 | 0.80615200 |
| H | 6.79751300 | 1.23801500 | 1.72115400 |
| H | 8.41540800 | 1.14077700 | 2.43065500 |
| N | -5.89188500 | -5.64907500 | -0.09734900 |
| N | -5.05856600 | 6.28634700 | 0.42784400 |

Cartesian Coordinates (Å) and Energies at 298.15 K/1 atm for the Optimized Structures of **5b**.

B3LYP/6-31G* SCF energy: -2613.233159 a.u.

**Table 24**. Cartesian coordinates (Å) of **5b**

| | x | y | z |
|---|---|---|---|
| O | 1.54539500 | 2.05607800 | -1.79423900 |
| O | 2.18900100 | -1.64052400 | 1.75837100 |
| C | 5.08863700 | -5.38252300 | 0.03401200 |
| C | 5.11937800 | -3.98997100 | 0.16094900 |
| H | 6.07327600 | -3.47470500 | 0.20903900 |
| C | 3.93649000 | -3.26399000 | 0.21092500 |
| H | 3.97742800 | -2.18620900 | 0.30160400 |
| C | 2.68277900 | -3.90782800 | 0.12356300 |
| C | 2.67640900 | -5.31337800 | -0.00821800 |
| H | 1.72976600 | -5.84259900 | -0.04790200 |
| C | 3.85897100 | -6.04193400 | -0.04700600 |

| | | | |
|---|---|---|---|
| H | 3.82900200 | -7.12254000 | -0.13915800 |
| C | 1.41201200 | -3.16268000 | 0.11822800 |
| C | 1.17643200 | -2.00836500 | 0.92614600 |
| C | -0.04225900 | -1.34302900 | 0.87657800 |
| H | -0.21943000 | -0.49961300 | 1.52817800 |
| C | -1.08620800 | -1.76633200 | 0.02155700 |
| C | -2.37293000 | -1.08396500 | -0.04803300 |
| C | -2.54872300 | 0.31928400 | 0.35135000 |
| C | -1.50056800 | 1.32003500 | 0.19094200 |
| C | -0.45086800 | 1.18288200 | -0.74668300 |
| H | -0.44505900 | 0.31458200 | -1.38953400 |
| C | 0.53796900 | 2.14944700 | -0.88354600 |
| C | 0.51666300 | 3.33357500 | -0.08482900 |
| C | -0.56967000 | 3.47937100 | 0.80653900 |
| H | -0.60707400 | 4.36857800 | 1.42934800 |
| C | -1.56240000 | 2.52831400 | 0.95729700 |
| C | -2.71617100 | 2.69614000 | 1.90841900 |
| H | -2.53903300 | 2.10337600 | 2.81977100 |
| C | -3.82843800 | 0.78668700 | 0.73226100 |
| C | -4.76264300 | -1.35334100 | -0.04981400 |
| C | -3.50666400 | -1.88048500 | -0.33396100 |
| C | -3.33518500 | -3.29731200 | -0.83576300 |
| H | -4.19779800 | -3.57263000 | -1.44643800 |
| H | -3.33707400 | -3.99103200 | 0.01855100 |
| C | -2.01880000 | -3.43828900 | -1.60845400 |
| H | -1.85297300 | -4.47477900 | -1.92114800 |
| H | -2.07874900 | -2.83237400 | -2.52638500 |
| C | -0.88135400 | -2.95535600 | -0.74964800 |
| C | 0.33861700 | -3.60406100 | -0.68711900 |
| H | 0.49202900 | -4.47756800 | -1.31429900 |
| C | 1.99444300 | -0.53975600 | 2.63966100 |
| H | 1.16804100 | -0.72930900 | 3.33519400 |

| | | | |
|---|---|---|---|
| H | 1.80049300 | 0.38753600 | 2.08632900 |
| H | 2.92599700 | -0.44431000 | 3.19938800 |
| C | 1.59001500 | 0.92874600 | -2.66223200 |
| H | 1.69279900 | -0.00693800 | -2.09868100 |
| H | 0.69483200 | 0.87794700 | -3.29369000 |
| C | 1.53575600 | 4.39318300 | -0.17756800 |
| H | -2.80974900 | 3.74155900 | 2.22123500 |
| C | -4.00349300 | 2.20128300 | 1.23935400 |
| C | -4.91639200 | -0.05858700 | 0.53636200 |
| C | -6.09212300 | -1.95795700 | -0.18596900 |
| H | 2.46968700 | 1.07708500 | -3.29021200 |
| C | 2.90592100 | 4.11220500 | -0.36797200 |
| C | 1.15867100 | 5.74634900 | -0.03198100 |
| H | -4.85656800 | 2.23862300 | 1.92018800 |
| H | -4.25982300 | 2.86301300 | 0.39819900 |
| C | -6.34389600 | 0.16978700 | 0.78511900 |
| O | -6.43421500 | -3.05656900 | -0.63078900 |
| N | -6.98578400 | -0.99766800 | 0.32430600 |
| H | 3.22910000 | 3.08559400 | -0.48225500 |
| C | 3.84975100 | 5.13159700 | -0.39499300 |
| C | 2.09974400 | 6.76706100 | -0.07021700 |
| H | 0.10902100 | 6.00007300 | 0.07583600 |
| O | -6.92610000 | 1.13579900 | 1.28333100 |
| C | -8.42246700 | -1.21195700 | 0.39995000 |
| H | 4.89927100 | 4.89425000 | -0.53432000 |
| C | 3.45333000 | 6.46406500 | -0.24734600 |
| H | 1.78433400 | 7.80122300 | 0.02224500 |
| H | -8.79935500 | -0.51120300 | 1.15079100 |
| H | -8.58321300 | -2.23612100 | 0.75201900 |
| C | -9.14644900 | -1.01123500 | -0.94131900 |
| H | -10.20119900 | -1.27584100 | -0.78409100 |
| H | -8.74627300 | -1.73380600 | -1.66217000 |

| | | | |
|---|---|---|---|
| C | -9.04651600 | 0.41121100 | -1.49890400 |
| H | -9.44092400 | 1.14710900 | -0.78901800 |
| H | -9.61045700 | 0.50289500 | -2.43434800 |
| H | -8.00686000 | 0.68475200 | -1.70893500 |
| C | 6.37315400 | -6.16465200 | 0.04756400 |
| C | 4.47977300 | 7.56299900 | -0.21969800 |
| F | 6.77306000 | -6.44536500 | 1.31015600 |
| F | 7.38141800 | -5.47993900 | -0.53795000 |
| F | 6.25262200 | -7.34509500 | -0.59823300 |
| F | 4.88019500 | 7.83701800 | 1.04480100 |
| F | 3.99580900 | 8.71511900 | -0.73422300 |
| F | 5.58802800 | 7.23663500 | -0.92031400 |

Cartesian Coordinates (Å) and Energies at 298.15 K/1 atm for the Optimized Structures of **5c**.

B3LYP/6-31G* SCF energy: -2123.648101 a.u.

**Table 25**. Cartesian coordinates (Å) of **5c**

| | x | y | z |
|---|---|---|---|
| O | -2.34780700 | 1.91734000 | 1.84553200 |
| O | -2.73398400 | -1.67762200 | -1.79071400 |
| C | -5.40210100 | -5.59781300 | -0.01904200 |
| C | -5.50289500 | -4.19660000 | -0.17302400 |
| H | -6.48451600 | -3.73625400 | -0.22336300 |
| C | -4.36491100 | -3.41415900 | -0.25432400 |
| H | -4.46972800 | -2.34259700 | -0.36443700 |
| C | -3.06903500 | -3.98578700 | -0.16951400 |
| C | -2.98626900 | -5.39417300 | -0.01241900 |
| H | -2.01269200 | -5.87349900 | 0.01542500 |
| C | -4.11879300 | -6.18485000 | 0.05336700 |
| H | -4.02886900 | -7.26177700 | 0.15336500 |

| | | | |
|---|---|---|---|
| C | -1.84578400 | -3.17754700 | -0.18340800 |
| C | -1.69129300 | -1.98673200 | -0.97847600 |
| C | -0.51991300 | -1.24692200 | -0.93124900 |
| H | -0.41869500 | -0.36671000 | -1.55059700 |
| C | 0.56444900 | -1.62702400 | -0.11114500 |
| C | 1.81981900 | -0.86800000 | -0.05049000 |
| C | 1.89633100 | 0.55526600 | -0.28843100 |
| C | 0.75232500 | 1.46139800 | -0.12608800 |
| C | -0.29125900 | 1.21612100 | 0.79247300 |
| H | -0.24003100 | 0.32976700 | 1.40934900 |
| C | -1.35461800 | 2.09379900 | 0.93671100 |
| C | -1.43543500 | 3.29283600 | 0.14299600 |
| C | -0.34543600 | 3.54739000 | -0.71625200 |
| H | -0.36772900 | 4.44845700 | -1.32116300 |
| C | 0.73787100 | 2.69086200 | -0.85073600 |
| C | 1.91526300 | 3.01581200 | -1.73152300 |
| H | 1.84869500 | 2.46735000 | -2.68329700 |
| C | 3.14812600 | 1.15705100 | -0.60327600 |
| C | 4.22371700 | -0.97357900 | -0.05249700 |
| C | 3.01213200 | -1.61794800 | 0.16191100 |
| C | 2.92899500 | -3.07352800 | 0.55850300 |
| H | 3.83454700 | -3.35538800 | 1.09928900 |
| H | 2.90260800 | -3.70193100 | -0.34457500 |
| C | 1.66393000 | -3.32860400 | 1.38823500 |
| H | 1.56441600 | -4.39088200 | 1.63366200 |
| H | 1.74246700 | -2.78784100 | 2.34356700 |
| C | 0.46411200 | -2.85433800 | 0.61186400 |
| C | -0.72259100 | -3.57205100 | 0.57389600 |
| H | -0.80008000 | -4.47064400 | 1.17784200 |
| C | -2.64079900 | -0.53565600 | -2.63578700 |
| H | -1.81427800 | -0.63772300 | -3.34949100 |
| H | -2.50861700 | 0.38291600 | -2.05051200 |

| | | | |
|---|---|---|---|
| H | -3.58645000 | -0.49351400 | -3.17733200 |
| C | -2.30799000 | 0.78438800 | 2.70615500 |
| H | -2.34916700 | -0.15185400 | 2.13550500 |
| H | -1.40653800 | 0.79330900 | 3.33089000 |
| C | -2.54873600 | 4.24303600 | 0.22798100 |
| H | 1.92343800 | 4.08185800 | -1.98048100 |
| C | 3.20599100 | 2.61232500 | -1.00619700 |
| C | 4.28741300 | 0.37232700 | -0.47985500 |
| C | 5.61054600 | -1.49514800 | 0.04265100 |
| H | -3.19148300 | 0.86647100 | 3.34026200 |
| C | -3.89124100 | 3.83127400 | 0.43267500 |
| C | -2.31244000 | 5.63127200 | 0.04824300 |
| H | 4.09063700 | 2.78365600 | -1.62251400 |
| H | 3.32879600 | 3.23973400 | -0.11047600 |
| C | 5.71455300 | 0.72789800 | -0.68644500 |
| O | 6.01116200 | -2.60945400 | 0.37607800 |
| N | 6.43366200 | -0.42824000 | -0.34501900 |
| H | -4.11285600 | 2.78009100 | 0.56433400 |
| C | -4.93026400 | 4.74433100 | 0.44198300 |
| C | -3.34364300 | 6.55205300 | 0.07259500 |
| H | -1.29470800 | 5.98993600 | -0.06971100 |
| O | 6.21072500 | 1.78435800 | -1.07264400 |
| C | 7.88714500 | -0.52655000 | -0.40936900 |
| H | -5.95157600 | 4.40520500 | 0.58329400 |
| C | -4.67694100 | 6.12352200 | 0.26342900 |
| H | -3.13479000 | 7.61032000 | -0.04713600 |
| H | 8.21950400 | 0.27842600 | -1.07096100 |
| H | 8.12853800 | -1.48990000 | -0.86933600 |
| C | 8.57039400 | -0.42079500 | 0.96304600 |
| H | 9.64456600 | -0.58280200 | 0.80100600 |
| H | 8.22112200 | -1.24861500 | 1.59128900 |
| C | 8.34896200 | 0.91887300 | 1.67032400 |

| | | | |
|---|---|---|---|
| H | 8.68800000 | 1.75781800 | 1.05215600 |
| H | 8.89629600 | 0.95161900 | 2.61900200 |
| H | 7.28910200 | 1.08338300 | 1.89402600 |
| C | -6.57383300 | -6.40497800 | 0.05941400 |
| N | -7.53345000 | -7.06529400 | 0.12445100 |
| C | -5.74591900 | 7.06525900 | 0.27812200 |
| N | -6.62168100 | 7.83621700 | 0.28955800 |

Cartesian Coordinates (Å) and Energies at 298.15 K/1 atm for the Optimized Structures of **5d**.

B3LYP/6-31G* SCF energy: -2165.807656 a.u.

**Table 26**. Cartesian coordinates (Å) of **5d**

| | x | y | z |
|---|---|---|---|
| O | 2.22523400 | 2.06099600 | -1.83502400 |
| O | 2.76180500 | -1.63102600 | 1.77785200 |
| C | 5.52917800 | -5.51332900 | 0.09575800 |
| C | 5.60642600 | -4.12103900 | 0.24446000 |
| H | 6.58173400 | -3.64484500 | 0.32341300 |
| C | 4.45611700 | -3.34528400 | 0.28660300 |
| H | 4.53604700 | -2.27158700 | 0.39553100 |
| C | 3.17842800 | -3.93970000 | 0.16801900 |
| C | 3.11754100 | -5.34804500 | 0.01596900 |
| H | 2.14937800 | -5.83553800 | -0.04001300 |
| C | 4.26642100 | -6.11955000 | -0.01424500 |
| H | 4.21556400 | -7.19950100 | -0.11369700 |
| C | 1.93901700 | -3.14968900 | 0.15382000 |
| C | 1.74152700 | -1.97458700 | 0.94518000 |
| C | 0.54793000 | -1.26758000 | 0.88319500 |
| H | 0.39988700 | -0.40946400 | 1.52271600 |
| C | -0.51153300 | -1.66685600 | 0.03457000 |

| | | | |
|---|---|---|---|
| C | -1.77412400 | -0.94448300 | -0.04076200 |
| C | -1.90541500 | 0.46690600 | 0.34339000 |
| C | -0.82858800 | 1.43269200 | 0.17379500 |
| C | 0.21513800 | 1.25546400 | -0.76491300 |
| H | 0.19194500 | 0.38127300 | -1.39949600 |
| C | 1.22987400 | 2.19144000 | -0.91608100 |
| C | 1.24872600 | 3.38454000 | -0.12697900 |
| C | 0.16770500 | 3.56857700 | 0.76680100 |
| H | 0.15828700 | 4.46207700 | 1.38395300 |
| C | -0.85170400 | 2.64954100 | 0.92881500 |
| C | -1.99669400 | 2.86059900 | 1.88206800 |
| H | -1.83604200 | 2.27046800 | 2.79804200 |
| C | -3.17132200 | 0.97786500 | 0.72305100 |
| C | -4.17097300 | -1.13763400 | -0.03874900 |
| C | -2.93497400 | -1.70765100 | -0.31997500 |
| C | -2.80964400 | -3.13324000 | -0.81017700 |
| H | -3.67941000 | -3.38516000 | -1.42081800 |
| H | -2.83666300 | -3.81904900 | 0.05000600 |
| C | -1.49717300 | -3.32533900 | -1.57831100 |
| H | -1.36592200 | -4.36982900 | -1.88030900 |
| H | -1.53488500 | -2.72691600 | -2.50221600 |
| C | -0.34638300 | -2.87239000 | -0.72106100 |
| C | 0.84887700 | -3.56237600 | -0.64746100 |
| H | 0.97148000 | -4.44744700 | -1.26459100 |
| C | 2.60149300 | -0.51292100 | 2.64413100 |
| H | 1.76678400 | -0.66551500 | 3.33882500 |
| H | 2.44101200 | 0.41302800 | 2.07811300 |
| H | 3.53377300 | -0.44182700 | 3.20626800 |
| C | 2.22469400 | 0.93054300 | -2.69995800 |
| H | 2.30608800 | -0.00634900 | -2.13507600 |
| H | 1.32064800 | 0.90571100 | -3.32018900 |
| C | 2.29616600 | 4.41060800 | -0.22939000 |

| | | | |
|---|---|---|---|
| H | -2.05761000 | 3.91093000 | 2.18607000 |
| C | -3.30035900 | 2.40100900 | 1.21942800 |
| C | -4.28322500 | 0.16554200 | 0.53396100 |
| C | -5.52174400 | -1.70128200 | -0.16782800 |
| H | 3.10065600 | 1.05031900 | -3.33913200 |
| C | 3.65360000 | 4.08891200 | -0.46148900 |
| C | 1.96355200 | 5.77701800 | -0.04883600 |
| H | -4.15067400 | 2.47147500 | 1.90106600 |
| H | -3.53623700 | 3.06329500 | 0.37283000 |
| C | -5.70543400 | 0.44052900 | 0.78142500 |
| O | -5.89670000 | -2.79163500 | -0.60093500 |
| N | -6.38502100 | -0.70918600 | 0.33232600 |
| H | 3.94032400 | 3.05406700 | -0.59505600 |
| C | 4.62214200 | 5.08254700 | -0.49898600 |
| C | 2.93058500 | 6.76621300 | -0.09771500 |
| H | 0.92463300 | 6.05707800 | 0.09332300 |
| O | -6.25386100 | 1.42784300 | 1.27132800 |
| C | -7.82831600 | -0.87808800 | 0.41167100 |
| H | 5.66388000 | 4.81505200 | -0.66456200 |
| C | 4.27657000 | 6.42978000 | -0.31999000 |
| H | 2.67032000 | 7.81310200 | 0.02499800 |
| H | -8.18207300 | -0.15662100 | 1.15401000 |
| H | -8.01997100 | -1.89190400 | 0.77775000 |
| C | -8.54727700 | -0.67204800 | -0.93116900 |
| H | -9.60932800 | -0.90196000 | -0.76917400 |
| H | -8.17127200 | -1.41566600 | -1.64357600 |
| C | -8.40474000 | 0.73956000 | -1.50687900 |
| H | -8.77562000 | 1.49611200 | -0.80606700 |
| H | -8.96729000 | 0.83645300 | -2.44253000 |
| H | -7.35771500 | 0.97887200 | -1.72240400 |
| C | 6.75979700 | -6.32968300 | 0.05962200 |
| O | 6.78280200 | -7.54062700 | -0.06488100 |

| | | | |
|---|---|---|---|
| H | 7.70465200 | -5.74985500 | 0.15643800 |
| C | 5.31484500 | 7.47945600 | -0.36810400 |
| O | 5.10223800 | 8.66951000 | -0.22323400 |
| H | 6.34625600 | 7.10422800 | -0.55162600 |

Cartesian Coordinates (Å) and Energies at 298.15 K/1 atm for the Optimized Structures of **5e**.

B3LYP/6-31G* SCF energy: -2858.349915 a.u.

**Table 27**. Cartesian coordinates (Å) of **5e**

| | x | y | z |
|---|---|---|---|
| O | -2.17974500 | 2.02749000 | 1.81091900 |
| O | -2.65397500 | -1.68422300 | -1.76288000 |
| C | -5.34332900 | -5.59808500 | -0.08020300 |
| C | -5.46278500 | -4.21490200 | -0.22875400 |
| H | -6.44506100 | -3.76086900 | -0.30679500 |
| C | -4.31754400 | -3.42879300 | -0.26957300 |
| H | -4.41978300 | -2.35702100 | -0.37975800 |
| C | -3.02947300 | -3.99686500 | -0.15150500 |
| C | -2.95001700 | -5.39941600 | -0.00118000 |
| H | -1.97744000 | -5.87753800 | 0.05662100 |
| C | -4.08724700 | -6.19726300 | 0.03033600 |
| H | -4.00434700 | -7.27431100 | 0.12982000 |
| C | -1.80224500 | -3.18507300 | -0.13750800 |
| C | -1.62427800 | -2.01235400 | -0.93301800 |
| C | -0.43971200 | -1.28777700 | -0.87729300 |
| H | -0.30554200 | -0.42952600 | -1.51979000 |
| C | 0.62452900 | -1.66512100 | -0.02699600 |
| C | 1.87989500 | -0.92208300 | 0.04317400 |
| C | 1.98925300 | 0.48875100 | -0.34522200 |
| C | 0.89269600 | 1.43943100 | -0.18379000 |

| | | | |
|---|---|---|---|
| C | -0.14763800 | 1.25210200 | 0.75465400 |
| H | -0.11165400 | 0.38169800 | 1.39395100 |
| C | -1.18016000 | 2.17154300 | 0.89613100 |
| C | -1.21640500 | 3.35732400 | 0.10086100 |
| C | -0.13817200 | 3.55315600 | -0.79233900 |
| H | -0.14183900 | 4.44333600 | -1.41493600 |
| C | 0.89737100 | 2.64988100 | -0.94611700 |
| C | 2.04630300 | 2.87675700 | -1.89163900 |
| H | 1.90623300 | 2.27691800 | -2.80465100 |
| C | 3.24538200 | 1.02026700 | -0.71790500 |
| C | 4.28086800 | -1.08026700 | 0.04050500 |
| C | 3.04949500 | -1.66755200 | 0.31821400 |
| C | 2.94520300 | -3.09538500 | 0.80794000 |
| H | 3.82291100 | -3.33647500 | 1.41157400 |
| H | 2.97331400 | -3.78150200 | -0.05214900 |
| C | 1.64098200 | -3.30181100 | 1.58656500 |
| H | 1.52488600 | -4.34669700 | 1.89415000 |
| H | 1.67783700 | -2.69829800 | 2.50720200 |
| C | 0.47879500 | -2.86759200 | 0.73434600 |
| C | -0.70649300 | -3.57620500 | 0.66544700 |
| H | -0.81478200 | -4.46046200 | 1.28697000 |
| C | -2.51356900 | -0.56237000 | -2.62709800 |
| H | -1.68126800 | -0.70171900 | -3.32754100 |
| H | -2.36129800 | 0.36438900 | -2.05997300 |
| H | -3.45010300 | -0.50173700 | -3.18361900 |
| C | -2.16252100 | 0.90151900 | 2.68078100 |
| H | -2.22331500 | -0.03966800 | 2.12027800 |
| H | -1.26146600 | 0.89573500 | 3.30592500 |
| Cl | -6.78540000 | -6.59337700 | -0.03666500 |
| C | -2.28042800 | 4.36902800 | 0.19977500 |
| H | 2.08935700 | 3.92629000 | -2.20216700 |
| C | 3.35185000 | 2.44603200 | -1.21311500 |

| | | | |
|---|---|---|---|
| C | 4.37361100 | 0.22618800 | -0.53097500 |
| C | 5.63637800 | -1.62340800 | 0.17057500 |
| H | -3.04387500 | 1.00746000 | 3.31520500 |
| C | -3.63339000 | 4.03135700 | 0.42579700 |
| C | -1.97338800 | 5.73674800 | 0.02435500 |
| H | 4.20883900 | 2.53282300 | -1.88443800 |
| H | 3.56323100 | 3.11443200 | -0.36467400 |
| C | 5.78804500 | 0.52382900 | -0.77790500 |
| O | 6.03083200 | -2.71031200 | 0.60315300 |
| N | 6.48415700 | -0.61683200 | -0.32896700 |
| H | -3.90883600 | 2.99324700 | 0.55885400 |
| C | -4.62633300 | 5.00292300 | 0.46288800 |
| C | -2.95576600 | 6.71850700 | 0.06976100 |
| H | -0.94075900 | 6.04001900 | -0.11502700 |
| O | 6.32481400 | 1.52145800 | -1.26693900 |
| C | 7.92858000 | -0.76415200 | -0.40952500 |
| H | -5.66260700 | 4.72498100 | 0.62342000 |
| C | -4.28332200 | 6.34469000 | 0.28578200 |
| H | -2.69738500 | 7.76502200 | -0.05121600 |
| H | 8.27183900 | -0.03326500 | -1.14770700 |
| H | 8.13628700 | -1.77320000 | -0.78044900 |
| C | 8.64516300 | -0.55503300 | 0.93418100 |
| Cl | -5.53217100 | 7.57355900 | 0.33984200 |
| H | 9.71082400 | -0.76826800 | 0.77187000 |
| H | 8.27915900 | -1.30773200 | 1.64221900 |
| C | 8.48121900 | 0.85128400 | 1.51717000 |
| H | 8.84105200 | 1.61679500 | 0.82025600 |
| H | 9.04111800 | 0.95230700 | 2.45416800 |
| H | 7.43027700 | 1.07340500 | 1.73166500 |

Cartesian Coordinates (Å) and Energies at 298.15 K/1 atm for the Optimized Structures of **5f**.

B3LYP/6-31G* SCF energy: -2137.624319 a.u.

**Table 28**. Cartesian coordinates (Å) of **5f**

| | x | y | z |
|---|---|---|---|
| O | -2.51587600 | 2.00282200 | 1.83400700 |
| O | -2.94997300 | -1.68017400 | -1.75332300 |
| C | -5.57441400 | -5.62887100 | -0.08939500 |
| C | -5.72260600 | -4.25102100 | -0.21996900 |
| H | -6.71808700 | -3.82399800 | -0.28413000 |
| C | -4.58637900 | -3.45184200 | -0.25896700 |
| H | -4.69840900 | -2.37978300 | -0.35536300 |
| C | -3.29104500 | -4.00881900 | -0.15767100 |
| C | -3.19244000 | -5.41269900 | -0.02503300 |
| H | -2.21280800 | -5.87731900 | 0.02011900 |
| C | -4.32006900 | -6.22430800 | 0.00564100 |
| H | -4.24216800 | -7.30311400 | 0.09056500 |
| C | -2.07277900 | -3.18256100 | -0.14284900 |
| C | -1.91176200 | -2.00307300 | -0.93116900 |
| C | -0.73491200 | -1.26534800 | -0.87646300 |
| H | -0.61407500 | -0.40045500 | -1.51277700 |
| C | 0.33660400 | -1.63515900 | -0.03306500 |
| C | 1.58472300 | -0.87682500 | 0.03740100 |
| C | 1.67491300 | 0.53839300 | -0.33598800 |
| C | 0.56401600 | 1.47342600 | -0.16596400 |
| C | -0.47174600 | 1.26491700 | 0.77223100 |
| H | -0.42279300 | 0.39016000 | 1.40480500 |
| C | -1.51797600 | 2.16812600 | 0.92009500 |
| C | -1.57226200 | 3.35823400 | 0.13324700 |
| C | -0.49737600 | 3.57633400 | -0.75812200 |
| H | -0.51381600 | 4.47167100 | -1.37326200 |
| C | 0.55148500 | 2.68905200 | -0.91848500 |

| | | | |
|---|---|---|---|
| C | 1.69893200 | 2.94132800 | -1.85962500 |
| H | 1.57012200 | 2.34779400 | -2.77839900 |
| C | 2.92267700 | 1.09075500 | -0.70308000 |
| C | 3.98793400 | -1.00533600 | 0.02586800 |
| C | 2.76351300 | -1.61081800 | 0.29903800 |
| C | 2.67798500 | -3.04510400 | 0.77362500 |
| H | 3.56289300 | -3.28332100 | 1.36781100 |
| H | 2.70610100 | -3.72199500 | -0.09379900 |
| C | 1.38198900 | -3.27281300 | 1.56014300 |
| H | 1.27941800 | -4.32157100 | 1.85947800 |
| H | 1.41917600 | -2.67671800 | 2.48557900 |
| C | 0.20899700 | -2.84429600 | 0.71967200 |
| C | -0.96879600 | -3.56605500 | 0.65193800 |
| H | -1.06363700 | -4.45621200 | 1.26734700 |
| C | -2.82780800 | -0.54772200 | -2.60598100 |
| H | -1.99854200 | -0.66958600 | -3.31333000 |
| H | -2.68218500 | 0.37462700 | -2.02984300 |
| H | -3.76851200 | -0.49157000 | -3.15602600 |
| C | -2.48102500 | 0.87134000 | 2.69565200 |
| H | -2.52787800 | -0.06696500 | 2.12885500 |
| H | -1.57956000 | 0.87440800 | 3.32032200 |
| C | -2.65174000 | 4.35358800 | 0.24111800 |
| H | 1.72693300 | 3.99428600 | -2.16039100 |
| C | 3.00897800 | 2.52368400 | -1.18151700 |
| C | 4.06263800 | 0.30914800 | -0.52961000 |
| C | 5.34965700 | -1.53287200 | 0.14633500 |
| H | -3.36342300 | 0.95928900 | 3.33149400 |
| C | -4.00138400 | 3.98979100 | 0.45097700 |
| C | -2.36146900 | 5.72856400 | 0.09066300 |
| H | 3.86686500 | 2.63125500 | -1.84867300 |
| H | 3.20656600 | 3.18587300 | -0.32484500 |
| C | 5.47166700 | 0.62771800 | -0.77719700 |

| | | | |
|---|---|---|---|
| O | 5.75984900 | -2.62049100 | 0.56474700 |
| N | 6.18305500 | -0.50952700 | -0.34360500 |
| H | -4.25892700 | 2.94481100 | 0.56445900 |
| C | -5.00933300 | 4.94540500 | 0.49751600 |
| C | -3.35840700 | 6.69537600 | 0.14489400 |
| H | -1.33159100 | 6.04585600 | -0.03656200 |
| O | 5.99529800 | 1.63834300 | -1.25589800 |
| C | 7.62863900 | -0.63797600 | -0.43032600 |
| H | -6.04770200 | 4.66705400 | 0.64499300 |
| C | -4.67393200 | 6.28766500 | 0.34496000 |
| H | -3.13224900 | 7.75185900 | 0.04585200 |
| H | 7.96050600 | 0.10422600 | -1.16245500 |
| H | 7.84779600 | -1.64082800 | -0.81139200 |
| C | 8.34717700 | -0.43291400 | 0.91294300 |
| H | 9.41499100 | -0.63130900 | 0.74555700 |
| H | 7.99259100 | -1.19684900 | 1.61477300 |
| C | 8.16753700 | 0.96557600 | 1.50998500 |
| H | 8.51526600 | 1.74215300 | 0.81918700 |
| H | 8.72911800 | 1.06478900 | 2.44623400 |
| H | 7.11451200 | 1.17224100 | 1.72949400 |
| F | -6.67250900 | -6.40590500 | -0.05753900 |
| F | -5.64689800 | 7.21590700 | 0.39559400 |

Cartesian Coordinates (Å) and Energies at 298.15 K/1 atm for the Optimized Structures of **5g**.

B3LYP/6-31G* SCF energy: -1939.157401 a.u.

**Table 29**. Cartesian coordinates (Å) of **5g**

| | x | y | z |
|---|---|---|---|
| O | -2.83909100 | 1.96613800 | 1.86334600 |
| O | -3.24776000 | -1.66086800 | -1.75232600 |

| | | | |
|---|---|---|---|
| C | -5.87408100 | -5.64175600 | -0.08977900 |
| C | -5.99887000 | -4.25323500 | -0.18632000 |
| H | -6.98485600 | -3.79754700 | -0.22230800 |
| C | -4.86839700 | -3.44375500 | -0.23273900 |
| H | -4.98095600 | -2.36905700 | -0.30138600 |
| C | -3.57275700 | -4.00261200 | -0.17123600 |
| C | -3.46809300 | -5.40770700 | -0.07134500 |
| H | -2.48538500 | -5.86899300 | -0.05696800 |
| C | -4.60055100 | -6.21454200 | -0.03610000 |
| H | -4.48970300 | -7.29371900 | 0.02549800 |
| C | -2.35464100 | -3.17383400 | -0.16157400 |
| C | -2.20370500 | -1.98584200 | -0.94003400 |
| C | -1.02986300 | -1.24300000 | -0.88535700 |
| H | -0.91765900 | -0.37002000 | -1.51223000 |
| C | 0.04719900 | -1.61551300 | -0.05114100 |
| C | 1.28990500 | -0.84836700 | 0.02556900 |
| C | 1.36713000 | 0.57368800 | -0.32447800 |
| C | 0.24746200 | 1.49598900 | -0.13905800 |
| C | -0.78556200 | 1.26370100 | 0.79586100 |
| H | -0.72796000 | 0.38064000 | 1.41606900 |
| C | -1.84242400 | 2.15301700 | 0.95367000 |
| C | -1.90926200 | 3.35285600 | 0.18192600 |
| C | -0.83531200 | 3.59690000 | -0.70237900 |
| H | -0.86089800 | 4.50230700 | -1.30217000 |
| C | 0.22338500 | 2.72278800 | -0.87382500 |
| C | 1.36896400 | 3.00118200 | -1.80950400 |
| H | 1.24586700 | 2.42199100 | -2.73826200 |
| C | 2.60933200 | 1.14268500 | -0.68414000 |
| C | 3.69422100 | -0.95624700 | 0.00736500 |
| C | 2.47521900 | -1.57642000 | 0.27265600 |
| C | 2.40234100 | -3.01879100 | 0.72431900 |
| H | 3.29223200 | -3.26038400 | 1.30959500 |

| | | | |
|---|---|---|---|
| H | 2.42970300 | -3.68146300 | -0.15404600 |
| C | 1.11234200 | -3.26780200 | 1.51427600 |
| H | 1.01857500 | -4.32164100 | 1.79821700 |
| H | 1.15045600 | -2.68557000 | 2.44853100 |
| C | -0.06849000 | -2.83513500 | 0.68732400 |
| C | -1.24346600 | -3.56225200 | 0.61933000 |
| H | -1.33040400 | -4.46103900 | 1.22314000 |
| C | -3.14287300 | -0.51116300 | -2.58359600 |
| H | -2.31897200 | -0.61175200 | -3.30061700 |
| H | -2.99989600 | 0.40094500 | -1.99062400 |
| H | -4.08894000 | -0.45257800 | -3.12405800 |
| C | -2.79997100 | 0.81884400 | 2.70329100 |
| H | -2.83847600 | -0.10884800 | 2.11856500 |
| H | -1.90089300 | 0.81573000 | 3.33152500 |
| C | -3.00348900 | 4.33290100 | 0.29809700 |
| H | 1.38702600 | 4.05923300 | -2.09262600 |
| C | 2.68253100 | 2.58431700 | -1.13795200 |
| C | 3.75653900 | 0.36797700 | -0.52649500 |
| C | 5.06043100 | -1.47386600 | 0.11706700 |
| H | -3.68534600 | 0.88899100 | 3.33716500 |
| C | -4.35033700 | 3.94516700 | 0.47054000 |
| C | -2.72565100 | 5.71338900 | 0.19152100 |
| H | 3.53972100 | 2.71138600 | -1.80255900 |
| H | 2.87320200 | 3.23359000 | -0.26986300 |
| C | 5.16198300 | 0.70283600 | -0.77144900 |
| O | 5.48138000 | -2.56460500 | 0.51719000 |
| N | 5.88383100 | -0.43525600 | -0.35760200 |
| H | -4.59447300 | 2.89305100 | 0.54786200 |
| C | -5.36606400 | 4.89444500 | 0.52221200 |
| C | -3.74258900 | 6.66038900 | 0.25532500 |
| H | -1.69594500 | 6.04303800 | 0.09279600 |
| O | 5.67653900 | 1.72568300 | -1.23462300 |

| | | | |
|---|---|---|---|
| C | 7.33019400 | -0.54935000 | -0.44833500 |
| H | -6.39627900 | 4.56979900 | 0.64215900 |
| C | -5.07042100 | 6.25627700 | 0.41732600 |
| H | -3.49827100 | 7.71689600 | 0.18595600 |
| H | 7.65419000 | 0.20507700 | -1.17146600 |
| H | 7.55778200 | -1.54535000 | -0.84218800 |
| C | 8.04921100 | -0.35455000 | 0.89629600 |
| H | 9.11855300 | -0.54101800 | 0.72479500 |
| H | 7.70276800 | -1.13044700 | 1.58904200 |
| C | 7.85767100 | 1.03466300 | 1.51102100 |
| H | 8.19607900 | 1.82297000 | 0.82895000 |
| H | 8.42058300 | 1.12772700 | 2.44713200 |
| H | 6.80324700 | 1.22841500 | 1.73540900 |
| H | -5.86581200 | 6.99493300 | 0.46440900 |
| H | -6.75936000 | -6.27092400 | -0.05986200 |

Cartesian Coordinates (Å) and Energies at 298.15 K/1 atm for the Optimized Structures of **5h**.

B3LYP/6-31G* SCF energy: -2017.793797 a.u.

**Table 30**. Cartesian coordinates (Å) of **5h**

| | x | y | z |
|---|---|---|---|
| O | -2.50573300 | 1.97936100 | 1.83591900 |
| O | -2.92845400 | -1.67304800 | -1.75531600 |
| C | -5.60039500 | -5.64792600 | -0.07372200 |
| C | -5.69618600 | -4.25418800 | -0.20433400 |
| H | -6.67898900 | -3.79152800 | -0.26280100 |
| C | -4.56505500 | -3.44916400 | -0.25453300 |
| H | -4.67840100 | -2.37656500 | -0.34825200 |
| C | -3.26969600 | -4.00468600 | -0.15944300 |
| C | -3.17989600 | -5.40777000 | -0.02074700 |

| | | | |
|---|---|---|---|
| H | -2.20263300 | -5.87841300 | 0.02539800 |
| C | -4.31606100 | -6.20570100 | 0.01691200 |
| H | -4.20684600 | -7.28371500 | 0.11139300 |
| C | -2.04961600 | -3.18233200 | -0.15108900 |
| C | -1.88929800 | -2.00010400 | -0.93625600 |
| C | -0.71126600 | -1.26375100 | -0.88297600 |
| H | -0.59239000 | -0.39568300 | -1.51536800 |
| C | 0.36135300 | -1.63581700 | -0.04325900 |
| C | 1.60973900 | -0.87543900 | 0.02906100 |
| C | 1.69691300 | 0.54230100 | -0.33027200 |
| C | 0.58147200 | 1.47361600 | -0.15751400 |
| C | -0.45484500 | 1.25700700 | 0.77718100 |
| H | -0.40397700 | 0.37908800 | 1.40523000 |
| C | -1.50692500 | 2.15380000 | 0.92482300 |
| C | -1.56558900 | 3.34689600 | 0.14222800 |
| C | -0.48673500 | 3.57488600 | -0.74195600 |
| H | -0.50471100 | 4.47410300 | -1.35126900 |
| C | 0.56670400 | 2.69297900 | -0.90287200 |
| C | 1.71824100 | 2.95649200 | -1.83621000 |
| H | 1.59730300 | 2.36906200 | -2.75999300 |
| C | 2.94362300 | 1.10148100 | -0.68902000 |
| C | 4.01378500 | -0.99961600 | 0.01690100 |
| C | 2.78954300 | -1.60990100 | 0.28235700 |
| C | 2.70589300 | -3.04867600 | 0.74395400 |
| H | 3.59388600 | -3.29276400 | 1.33110500 |
| H | 2.72828300 | -3.71774300 | -0.12975600 |
| C | 1.41378400 | -3.28253600 | 1.53521800 |
| H | 1.31281900 | -4.33352200 | 1.82741900 |
| H | 1.45552600 | -2.69305000 | 2.46470500 |
| C | 0.23660300 | -2.84864800 | 0.70307600 |
| C | -0.94149200 | -3.57012100 | 0.63610100 |
| H | -1.03416200 | -4.46357500 | 1.24687400 |

| | | | |
|---|---|---|---|
| C | -2.81229800 | -0.52883400 | -2.59230500 |
| H | -1.98640000 | -0.63877800 | -3.30570100 |
| H | -2.66530300 | 0.38572000 | -2.00411700 |
| H | -3.75583900 | -0.46659000 | -3.13694400 |
| C | -2.47260900 | 0.83879400 | 2.68480800 |
| H | -2.51450600 | -0.09352800 | 2.10773200 |
| H | -1.57442000 | 0.83641200 | 3.31438400 |
| C | -2.65229100 | 4.33396300 | 0.24437800 |
| H | 1.74342800 | 4.01181600 | -2.12906500 |
| C | 3.02617800 | 2.53930600 | -1.15362900 |
| C | 4.08604700 | 0.32093200 | -0.52371200 |
| C | 5.37618800 | -1.52526900 | 0.13354300 |
| H | -3.35843700 | 0.91775500 | 3.31717600 |
| C | -4.00039200 | 3.96653400 | 0.44859700 |
| C | -2.37534100 | 5.71132800 | 0.09625300 |
| H | 3.88788000 | 2.65713000 | -1.81410200 |
| H | 3.21431500 | 3.19480800 | -0.28963200 |
| C | 5.49419200 | 0.64529300 | -0.76699800 |
| O | 5.78956800 | -2.61642500 | 0.54122600 |
| N | 6.20774500 | -0.49482200 | -0.34464600 |
| H | -4.25514800 | 2.92057500 | 0.56360800 |
| C | -5.00652000 | 4.92419100 | 0.48869900 |
| C | -3.38592000 | 6.66242400 | 0.14998200 |
| H | -1.34706800 | 6.03880700 | -0.02238100 |
| O | 6.01697800 | 1.66207100 | -1.23500300 |
| C | 7.65337900 | -0.61900300 | -0.43135800 |
| H | -6.03604200 | 4.60573500 | 0.63682700 |
| C | -4.72576900 | 6.29049700 | 0.34018200 |
| H | -3.13203100 | 7.71550000 | 0.05212500 |
| H | 7.98418700 | 0.13033000 | -1.15674900 |
| H | 7.87563600 | -1.61799400 | -0.82076900 |
| C | 8.37056100 | -0.42362000 | 0.91406700 |

| | | | |
|---|---|---|---|
| H | 9.43915700 | -0.61795400 | 0.74634400 |
| H | 8.01693800 | -1.19420000 | 1.60911600 |
| C | 8.18671400 | 0.96936500 | 1.52261800 |
| H | 8.53275200 | 1.75253100 | 0.83842200 |
| H | 8.74709500 | 1.06251500 | 2.46028500 |
| H | 7.13286400 | 1.17118200 | 1.74244000 |
| C | -6.83196300 | -6.51825000 | -0.06088500 |
| H | -7.10491300 | -6.83196100 | -1.07797600 |
| H | -6.67458500 | -7.42894300 | 0.52662000 |
| H | -7.69451300 | -5.98742600 | 0.35574000 |
| C | -5.82538600 | 7.32254800 | 0.36197900 |
| H | -5.48387800 | 8.26382600 | 0.80604100 |
| H | -6.17238600 | 7.55284400 | -0.65485500 |
| H | -6.69379300 | 6.97261000 | 0.92967800 |

Cartesian Coordinates (Å) and Energies at 298.15 K/1 atm for the Optimized Structures of **5i**.

B3LYP/6-31G* SCF energy: -2401.272907 a.u.

**Table 31**. Cartesian coordinates (Å) of **5i**

| | x | y | z |
|---|---|---|---|
| O | 1.03332300 | 2.07419600 | -1.73429100 |
| O | 1.88684400 | -1.56855900 | 1.81587400 |
| C | 5.08423400 | -5.12516800 | 0.08908900 |
| C | 4.99041600 | -3.73066600 | 0.26495600 |
| H | 5.89788100 | -3.14729900 | 0.39131300 |
| C | 3.76433100 | -3.08473000 | 0.31476200 |
| H | 3.73489300 | -2.01237600 | 0.45839500 |
| C | 2.55216400 | -3.79857100 | 0.17268300 |
| C | 2.65075700 | -5.19749100 | -0.00785100 |
| H | 1.74486900 | -5.78901800 | -0.09498700 |

| | | | |
|---|---|---|---|
| C | 3.87816100 | -5.84134700 | -0.04111000 |
| H | 3.90723700 | -6.91640300 | -0.19262200 |
| C | 1.23773700 | -3.14235500 | 0.16270200 |
| C | 0.91324400 | -2.00888300 | 0.96844100 |
| C | -0.34956900 | -1.43130500 | 0.90853500 |
| H | -0.58990500 | -0.60165400 | 1.55772500 |
| C | -1.35284400 | -1.92022100 | 0.04247500 |
| C | -2.68789200 | -1.32712900 | -0.03413400 |
| C | -2.96471500 | 0.05815000 | 0.35142800 |
| C | -1.98102800 | 1.13181800 | 0.21138100 |
| C | -0.91167700 | 1.07061000 | -0.70938300 |
| H | -0.83348900 | 0.20383000 | -1.34938200 |
| C | 0.00990100 | 2.10354400 | -0.83358300 |
| C | -0.10446900 | 3.28536500 | -0.03978700 |
| C | -1.21540000 | 3.35028700 | 0.83397900 |
| H | -1.32686800 | 4.23306700 | 1.45695500 |
| C | -2.13868100 | 2.33082300 | 0.97239900 |
| C | -3.32239200 | 2.41922300 | 1.89868400 |
| H | -3.12994800 | 1.83470900 | 2.81209300 |
| C | -4.28004200 | 0.44128700 | 0.70070400 |
| C | -5.05492800 | -1.76376500 | -0.06831900 |
| C | -3.75860700 | -2.20362900 | -0.32388300 |
| C | -3.48057400 | -3.60734500 | -0.81601200 |
| H | -4.32089200 | -3.95127800 | -1.42303200 |
| H | -3.42633400 | -4.29395700 | 0.04251700 |
| C | -2.15784500 | -3.65055800 | -1.59003200 |
| H | -1.91678400 | -4.67192200 | -1.90444500 |
| H | -2.26329600 | -3.04832300 | -2.50606900 |
| C | -1.05978100 | -3.08799500 | -0.72660100 |
| C | 0.20005100 | -3.65265700 | -0.65224900 |
| H | 0.41652000 | -4.51137400 | -1.28132000 |
| C | 1.60082800 | -0.48299700 | 2.68948600 |

| | | | |
|---|---|---|---|
| H | 0.78231700 | -0.72960300 | 3.37674300 |
| H | 1.34513500 | 0.42630900 | 2.13128300 |
| H | 2.51602100 | -0.31673400 | 3.26013600 |
| C | 1.16661700 | 0.94523100 | -2.58952900 |
| H | 1.32415300 | 0.02292300 | -2.01649600 |
| H | 0.28677500 | 0.82693400 | -3.23370700 |
| C | 0.83443800 | 4.41191000 | -0.11656400 |
| H | -3.49204700 | 3.45539300 | 2.21133100 |
| C | -4.55779200 | 1.84404300 | 1.19639200 |
| C | -5.30719300 | -0.47680000 | 0.49672100 |
| C | -6.33705500 | -2.45690800 | -0.22670700 |
| H | 2.04345600 | 1.14700500 | -3.20705200 |
| C | 2.21956900 | 4.24408700 | -0.34795400 |
| C | 0.37662700 | 5.73498500 | 0.08613700 |
| H | -5.43013000 | 1.82952400 | 1.85338400 |
| H | -4.83076600 | 2.48745200 | 0.34608200 |
| C | -6.75076400 | -0.34225900 | 0.71479500 |
| O | -6.59791100 | -3.58063200 | -0.66782900 |
| N | -7.30406600 | -1.55390800 | 0.25333200 |
| H | 2.61701900 | 3.24738700 | -0.48936800 |
| C | 3.08377600 | 5.32808800 | -0.36442000 |
| C | 1.24278800 | 6.81667800 | 0.05952900 |
| H | -0.68517400 | 5.91671600 | 0.21901700 |
| O | -7.40917300 | 0.58709700 | 1.19082800 |
| C | -8.72486100 | -1.85903500 | 0.29418000 |
| H | 4.14664500 | 5.15045000 | -0.50052700 |
| C | 2.62336400 | 6.64462800 | -0.16383700 |
| H | 0.83990400 | 7.81872400 | 0.17335900 |
| H | -9.16514800 | -1.17800600 | 1.02867600 |
| H | -8.83103100 | -2.88863900 | 0.65138000 |
| C | -9.42456600 | -1.71411400 | -1.06689000 |
| H | -10.46571400 | -2.04084900 | -0.93637900 |

| | | | |
|---|---|---|---|
| H | -8.96105900 | -2.41640200 | -1.76972600 |
| C | -9.39427200 | -0.29276000 | -1.63527300 |
| H | -9.85004500 | 0.42403100 | -0.94273100 |
| H | -9.93645200 | -0.24130500 | -2.58674100 |
| H | -8.36683600 | 0.03943100 | -1.81847100 |
| C | 6.39419800 | -5.80948800 | 0.04513200 |
| C | 6.55228500 | -7.10772500 | 0.56608600 |
| C | 7.52075800 | -5.18195500 | -0.51968200 |
| C | 7.78678700 | -7.75124800 | 0.52495100 |
| H | 5.70662800 | -7.60222600 | 1.03505000 |
| C | 8.75424400 | -5.82716100 | -0.56341300 |
| H | 7.41912900 | -4.19237800 | -0.95575500 |
| C | 8.89392800 | -7.11484400 | -0.04076400 |
| H | 7.88680900 | -8.74915500 | 0.94338400 |
| H | 9.60702200 | -5.32672500 | -1.01433700 |
| H | 9.85647700 | -7.61766600 | -0.07386200 |
| C | 3.54885600 | 7.79694900 | -0.18938800 |
| C | 3.32658400 | 8.92348800 | 0.62519500 |
| C | 4.67916600 | 7.80080600 | -1.02864800 |
| C | 4.19976900 | 10.00820900 | 0.60269300 |
| H | 2.47862300 | 8.93419300 | 1.30382300 |
| C | 5.55066500 | 8.88689400 | -1.05269200 |
| H | 4.85665800 | 6.95769000 | -1.68989600 |
| C | 5.31599200 | 9.99596200 | -0.23677300 |
| H | 4.01286200 | 10.86213300 | 1.24828500 |
| H | 6.41059200 | 8.87136600 | -1.71696900 |
| H | 5.99636300 | 10.84282900 | -0.25525700 |

Cartesian Coordinates (Å) and Energies at 298.15 K/1 atm for the Optimized Structures of **5j**.

B3LYP/6-31G* SCF energy: -2580.669532 a.u.

**Table 32**. Cartesian coordinates (Å) of **5j**

| | x | y | z |
|---|---|---|---|
| O | 5.52296400 | -2.60979800 | 0.51985600 |
| C | -2.13620600 | -1.96496600 | -1.02606100 |
| C | -2.30884900 | -3.14873000 | -0.25044600 |
| C | -1.21509100 | -3.54227600 | 0.55578100 |
| H | -1.29344700 | -4.47613800 | 1.10531400 |
| C | -0.03501600 | -2.82749000 | 0.64026300 |
| C | 0.10194200 | -1.61109100 | -0.09671400 |
| C | -0.95722200 | -1.23086400 | -0.95015300 |
| H | -0.83245700 | -0.35232400 | -1.56667100 |
| C | 1.14029800 | -3.28556800 | 1.46352500 |
| H | 1.03329000 | -4.34223200 | 1.73213100 |
| H | 1.18154300 | -2.71727400 | 2.40615000 |
| C | 2.43679900 | -3.04189500 | 0.68312300 |
| H | 3.32108800 | -3.30016200 | 1.26973900 |
| H | 2.46075300 | -3.69438000 | -0.20291700 |
| C | 2.52776100 | -1.59542300 | 0.24806900 |
| C | 1.35136800 | -0.85521400 | -0.00469900 |
| C | 1.44396600 | 0.56674600 | -0.34316500 |
| C | 2.69419300 | 1.13060700 | -0.68112900 |
| C | 3.83447200 | 0.34613600 | -0.51666400 |
| C | 3.75455900 | -0.98241100 | 0.00245500 |
| C | 5.11611700 | -1.51208400 | 0.12421300 |
| C | 2.78363300 | 2.57575900 | -1.12074600 |
| H | 2.96930600 | 3.21614500 | -0.24497600 |
| C | 1.48108300 | 3.00806100 | -1.80400600 |
| H | 1.51091100 | 4.06808500 | -2.07888800 |
| H | 1.36403900 | 2.43619800 | -2.73790600 |

| | | | |
|---|---|---|---|
| C | 0.32268400 | 2.73119600 | -0.88276500 |
| C | 0.32960200 | 1.49814600 | -0.16050000 |
| C | -0.71336300 | 1.26849800 | 0.76302000 |
| H | -0.67510500 | 0.37401500 | 1.36775200 |
| O | -3.18520400 | -1.59877300 | -1.81679900 |
| C | 5.24476000 | 0.67197500 | -0.74098900 |
| N | 5.95304100 | -0.47600500 | -0.32926800 |
| H | 3.64953000 | 2.70194900 | -1.77418200 |
| C | -0.72501900 | 3.61473900 | -0.70873200 |
| C | -1.76124800 | 2.16743200 | 0.92537900 |
| C | -3.09859000 | -0.38750900 | -2.55814800 |
| O | 5.77354100 | 1.69502700 | -1.18801300 |
| C | 7.39967300 | -0.59994100 | -0.40164400 |
| C | -1.80785400 | 3.38196000 | 0.17355900 |
| H | -0.72474400 | 4.52511400 | -1.29953700 |
| O | -2.77403600 | 1.96318400 | 1.81375900 |
| H | -4.05963800 | -0.28319100 | -3.06447400 |
| H | -2.29607100 | -0.42995500 | -3.30489500 |
| H | -2.93566400 | 0.47280500 | -1.89750000 |
| H | 7.73887000 | 0.15918100 | -1.11280200 |
| H | 7.62562700 | -1.59353600 | -0.80246900 |
| C | 8.10174000 | -0.42351200 | 0.95434000 |
| C | -2.87555900 | 4.37373400 | 0.29224500 |
| C | -2.75484500 | 0.79648900 | 2.62926300 |
| H | 7.74034800 | -1.20349000 | 1.63477200 |
| H | 9.17203900 | -0.61595300 | 0.79575300 |
| C | 7.91159100 | 0.96105900 | 1.57991300 |
| C | -4.15227000 | 4.15327700 | 0.79379700 |
| C | -2.73612400 | 5.74642900 | -0.14464200 |
| H | -2.79341600 | -0.11656500 | 2.02278100 |
| H | -3.64821700 | 0.85941400 | 3.25269700 |
| H | -1.86478200 | 0.77376700 | 3.26929600 |

| | | | |
|---|---|---|---|
| H | 6.85567900 | 1.15968000 | 1.79274400 |
| H | 8.26370200 | 1.75343900 | 0.90959300 |
| H | 8.46314900 | 1.04158000 | 2.52393500 |
| S | -5.14935300 | 5.55397400 | 0.72296400 |
| H | -4.54863900 | 3.22973600 | 1.18229200 |
| C | -3.85972800 | 6.49288100 | 0.02549000 |
| H | -1.81641900 | 6.16383400 | -0.53547900 |
| H | -4.00720100 | 7.54047800 | -0.19909100 |
| C | -3.53446500 | -3.95131700 | -0.26041500 |
| C | -3.92293100 | -4.73639500 | 0.81626500 |
| C | -4.47540600 | -4.07718800 | -1.34892700 |
| S | -5.38295100 | -5.59969900 | 0.52216000 |
| H | -3.44016800 | -4.81536100 | 1.78023400 |
| C | -5.50355000 | -4.92733500 | -1.07926400 |
| H | -4.36048300 | -3.56101000 | -2.29093700 |
| H | -6.32340100 | -5.21080200 | -1.72535200 |

Cartesian Coordinates (Å) and Energies at 298.15 K/1 atm for the Optimized Structures of **5k**.

B3LYP/6-31G* SCF energy: -2168.203753 a.u.

**Table 33**. Cartesian coordinates (Å) of **5k**

| | x | y | z |
|---|---|---|---|
| O | -5.42050200 | 7.14188000 | 0.64510500 |
| O | -2.22911400 | 1.86925200 | 1.86612100 |
| O | 6.29632300 | 1.71566700 | -1.23258400 |
| N | 6.52237700 | -0.44963000 | -0.37132300 |
| C | -4.43457500 | 6.22707700 | 0.46617400 |
| C | -3.80901000 | 5.95166300 | -0.75919900 |
| H | -4.10266300 | 6.46816400 | -1.66579800 |
| C | -2.80438900 | 4.99195500 | -0.81585800 |

| | | | |
|---|---|---|---|
| H | -2.35152200 | 4.77574200 | -1.77842300 |
| C | -2.38818300 | 4.26680200 | 0.32173000 |
| C | -3.04403900 | 4.56142700 | 1.54326300 |
| C | -1.29370200 | 3.29157700 | 0.21081800 |
| C | -1.21158500 | 2.09602000 | 0.98506500 |
| C | -0.15258800 | 1.20946700 | 0.81656900 |
| C | 0.86556800 | 1.43788500 | -0.13286200 |
| C | 0.82576200 | 2.65539600 | -0.87563400 |
| C | -0.23662300 | 3.52365300 | -0.69995300 |
| H | -0.23567300 | 4.45667800 | -1.25657900 |
| C | 1.97920000 | 2.95141100 | -1.79830600 |
| H | 1.98661300 | 4.01074600 | -2.07807700 |
| H | 1.87384900 | 2.37303600 | -2.72973900 |
| C | 3.29114200 | 2.54971900 | -1.11473200 |
| H | 4.15390200 | 2.69220300 | -1.76896500 |
| H | 3.46209100 | 3.19723600 | -0.24110300 |
| C | 3.23234500 | 1.10414500 | -0.67026400 |
| C | 1.99645800 | 0.52127200 | -0.31583000 |
| C | 4.38869800 | 0.33860100 | -0.52438900 |
| C | 5.78969300 | 0.68580000 | -0.77346000 |
| C | 5.70815800 | -1.49806500 | 0.09715800 |
| C | 4.33817200 | -0.98992100 | -0.00390200 |
| C | 1.93143900 | -0.89834600 | 0.02774200 |
| C | -5.85417600 | 7.90589500 | -0.47342500 |
| C | -2.24334600 | 0.65324800 | 2.60364100 |
| C | 7.96835300 | -0.55313900 | -0.47188500 |
| C | -4.03742300 | 5.52053300 | 1.61565800 |
| H | -2.74875300 | 4.03830100 | 2.44293000 |
| H | -0.09293100 | 0.32106700 | 1.42866300 |
| O | 6.14032400 | -2.58931400 | 0.48671800 |
| C | 3.12276600 | -1.61962100 | 0.26078300 |
| C | 0.69094000 | -1.67856700 | -0.03899000 |

| | | | |
|---|---|---|---|
| H | -6.27896600 | 7.26427000 | -1.25570500 |
| H | -5.03280000 | 8.49882600 | -0.89465500 |
| H | -6.62778600 | 8.57498700 | -0.09400500 |
| H | -1.37947500 | 0.57961200 | 3.27573500 |
| H | -2.25904200 | -0.21760800 | 1.93673000 |
| H | -3.16056100 | 0.67896000 | 3.19463200 |
| H | 8.28285800 | 0.20868700 | -1.19161000 |
| H | 8.20134200 | -1.54449700 | -0.87445700 |
| H | -4.52313000 | 5.75421800 | 2.55788900 |
| C | 3.06198100 | -3.06469400 | 0.70699600 |
| C | 0.59066000 | -2.89653400 | 0.69699900 |
| C | -0.39308900 | -1.31717800 | -0.86695800 |
| H | 3.96080900 | -3.30495000 | 1.27908800 |
| H | 3.07934000 | -3.72404300 | -0.17430400 |
| C | 1.78333100 | -3.32142500 | 1.51294300 |
| C | -0.57644800 | -3.63636100 | 0.63237900 |
| H | -0.29324500 | -0.44042700 | -1.49087100 |
| C | -1.56096500 | -2.07105400 | -0.91836800 |
| H | 1.69988600 | -4.37610600 | 1.79788400 |
| H | 1.82963000 | -2.73847800 | 2.44624300 |
| C | -1.69738800 | -3.26150100 | -0.14368600 |
| H | -0.64840300 | -4.53567200 | 1.23764200 |
| O | -2.61107600 | -1.75024300 | -1.72979200 |
| C | -2.90075300 | -4.10553700 | -0.15189000 |
| C | -2.51113300 | -0.60153500 | -2.56164900 |
| C | -2.78789400 | -5.51031600 | -0.00241300 |
| C | -4.20594500 | -3.57922000 | -0.26233400 |
| H | -2.37238700 | 0.31250400 | -1.97071100 |
| H | -3.45761900 | -0.54722900 | -3.10248500 |
| H | -1.68704500 | -0.69866000 | -3.27913300 |
| H | -1.80303700 | -5.96307700 | 0.05073700 |
| C | -3.89941600 | -6.33150800 | 0.03289400 |

| | | | |
|---|---|---|---|
| C | -5.33319200 | -4.39242900 | -0.21826500 |
| H | -4.33836200 | -2.51045100 | -0.36996600 |
| H | -3.80193100 | -7.40822400 | 0.12873100 |
| C | -5.18927300 | -5.78052700 | -0.07206500 |
| H | -6.31520600 | -3.93923200 | -0.29216700 |
| O | -6.21543000 | -6.66679500 | -0.02490500 |
| C | -7.54611300 | -6.17795200 | -0.13962400 |
| H | -7.79295100 | -5.49373700 | 0.68190600 |
| H | -8.19067200 | -7.05644900 | -0.08580100 |
| H | -7.70287900 | -5.66774600 | -1.09819300 |
| C | 8.69495000 | -0.36272800 | 0.86909200 |
| H | 9.76484000 | -0.54044800 | 0.69075900 |
| H | 8.35755100 | -1.14546600 | 1.55866700 |
| C | 8.49692400 | 1.02088700 | 1.49436500 |
| H | 8.82664100 | 1.81605300 | 0.81593200 |
| H | 7.44200100 | 1.20548000 | 1.72369000 |
| H | 9.06307700 | 1.11193000 | 2.42886400 |

Cartesian Coordinates (Å) and Energies at 298.15 K/1 atm for the Optimized Structures of **5l**.

B3LYP/6-31G* SCF energy: -2580.672978 a.u.

**Table 34**. Cartesian coordinates (Å) of **5l**

| | x | y | z |
|---|---|---|---|
| O | 5.56134500 | -2.51735400 | 0.52408000 |
| C | -2.13155500 | -2.02753000 | -0.89890200 |
| C | -2.27719100 | -3.20085100 | -0.10171500 |
| C | -1.15331500 | -3.56273800 | 0.68761700 |
| H | -1.20183700 | -4.47074700 | 1.27917700 |
| C | 0.01060600 | -2.82387400 | 0.73536600 |
| C | 0.11440400 | -1.61688400 | -0.02269300 |

| | | | |
|---|---|---|---|
| C | -0.96665700 | -1.27080800 | -0.86163100 |
| H | -0.87076700 | -0.40477500 | -1.50081200 |
| C | 1.20653500 | -3.24229000 | 1.55127100 |
| H | 1.12287500 | -4.29422100 | 1.84571700 |
| H | 1.25335600 | -2.65117000 | 2.47915300 |
| C | 2.48502800 | -2.99509100 | 0.74294200 |
| H | 3.38333000 | -3.22833200 | 1.31867000 |
| H | 2.50332000 | -3.66479400 | -0.13033500 |
| C | 2.54584500 | -1.55619200 | 0.27865000 |
| C | 1.35342100 | -0.83813800 | 0.03253100 |
| C | 1.41739400 | 0.57518000 | -0.33403600 |
| C | 2.65531800 | 1.15421500 | -0.69559100 |
| C | 3.80955300 | 0.39200800 | -0.53144200 |
| C | 3.75908800 | -0.92813700 | 0.00654400 |
| C | 5.13172300 | -1.43309000 | 0.11833000 |
| C | 2.71274300 | 2.59146900 | -1.16527700 |
| H | 2.88121900 | 3.25395200 | -0.30262600 |
| C | 1.40139300 | 2.97878400 | -1.85816100 |
| H | 1.40890800 | 4.03288800 | -2.15651600 |
| H | 1.29757000 | 2.38400100 | -2.77895700 |
| C | 0.24692500 | 2.69892000 | -0.93084500 |
| C | 0.28610400 | 1.49012300 | -0.17005900 |
| C | -0.73898300 | 1.27242800 | 0.77576000 |
| H | -0.67784500 | 0.40277400 | 1.41443600 |
| O | -3.19423700 | -1.71534600 | -1.68818700 |
| C | 5.21385500 | 0.73736600 | -0.77986700 |
| N | 5.94667800 | -0.39073300 | -0.36070900 |
| H | 3.57621300 | 2.72411500 | -1.82056700 |
| C | -0.81653700 | 3.56504300 | -0.78232300 |
| C | -1.80090600 | 2.15776900 | 0.91575100 |
| C | -3.14999100 | -0.54589300 | -2.49847300 |
| O | 5.71774800 | 1.76105800 | -1.25037100 |

| | | | |
|---|---|---|---|
| C | 7.39425300 | -0.49341700 | -0.45316800 |
| C | -1.89176000 | 3.33519600 | 0.11655500 |
| H | -0.81789900 | 4.47340000 | -1.37538600 |
| O | -2.80756000 | 1.97500800 | 1.81203900 |
| H | -4.11769000 | -0.49985600 | -2.99972700 |
| H | -2.35186700 | -0.61334800 | -3.24729300 |
| H | -3.00628900 | 0.35343200 | -1.88774700 |
| H | 7.71091400 | 0.26206700 | -1.17847100 |
| H | 7.62980600 | -1.48780400 | -0.84644200 |
| C | 8.11367100 | -0.29018500 | 0.88951200 |
| C | -2.98688800 | 4.28248500 | 0.19517500 |
| C | -2.80885600 | 0.82042900 | 2.64419800 |
| H | 7.77444900 | -1.06715000 | 1.58467600 |
| H | 9.18433100 | -0.46846200 | 0.71732900 |
| C | 7.91195500 | 1.09878700 | 1.50168100 |
| C | -3.17387200 | 5.40609100 | -0.61093600 |
| H | -2.83677000 | -0.09855400 | 2.04661700 |
| H | -3.71507100 | 0.89460700 | 3.24680600 |
| H | -1.93143400 | 0.80518100 | 3.30159400 |
| H | 6.85609900 | 1.28524300 | 1.72562000 |
| H | 8.24471200 | 1.88825000 | 0.81810200 |
| H | 8.47403700 | 1.19804000 | 2.43765300 |
| H | -2.49787400 | 5.67631300 | -1.41263300 |
| C | -5.04148400 | 5.62074100 | 0.74324700 |
| H | -5.95976200 | 5.99125400 | 1.18035100 |
| C | -3.47432800 | -4.01851700 | -0.07988600 |
| C | -3.69514600 | -5.15003100 | 0.70678400 |
| C | -4.95847000 | -5.74981900 | 0.52023100 |
| H | -2.96378600 | -5.53485900 | 1.40648900 |
| H | -5.28980100 | -6.63457400 | 1.05258400 |
| S | -4.90634900 | -3.71709800 | -1.07107000 |
| C | -5.72392700 | -5.08753200 | -0.41024500 |

| | | | |
|---|---|---|---|
| H | -6.72485600 | -5.33144500 | -0.74224300 |
| S | -4.31085600 | 4.18311400 | 1.36183200 |
| C | -4.32771900 | 6.15726200 | -0.30204800 |
| H | -4.62076300 | 7.05684900 | -0.83201300 |

Cartesian Coordinates (Å) and Energies at 298.15 K/1 atm for the Optimized Structures of **5m**.

B3LYP/6-31G* SCF energy: -2974.057696 a.u.

**Table 35**. Cartesian coordinates (Å) of **5m**

| | x | y | z |
|---|---|---|---|
| O | 1.77289600 | -0.61143700 | -1.58170100 |
| O | -2.01788500 | -0.14726400 | 1.88079200 |
| C | -6.35781500 | -2.14793000 | 0.13833100 |
| C | -5.74963500 | -1.76175200 | 1.34490400 |
| H | -6.06605500 | -2.22554100 | 2.27400400 |
| C | -4.75251600 | -0.79540300 | 1.36020000 |
| H | -4.30135300 | -0.51848700 | 2.30438700 |
| C | -4.30965100 | -0.17183400 | 0.17481000 |
| C | -4.92730300 | -0.57689200 | -1.02688500 |
| H | -4.60543600 | -0.13292300 | -1.96417600 |
| C | -5.93087800 | -1.53672300 | -1.05191700 |
| H | -6.38826300 | -1.81987500 | -1.99471300 |
| C | -3.28090700 | 0.89028800 | 0.15680200 |
| C | -2.13949500 | 0.89808600 | 0.99919000 |
| C | -1.19396000 | 1.91729900 | 0.90806900 |
| H | -0.34010400 | 1.91770100 | 1.57099200 |
| C | -1.32036400 | 2.96981500 | -0.02158300 |
| C | -0.33851400 | 4.06327500 | -0.11785100 |
| C | 1.05873300 | 3.92453200 | 0.26844900 |
| C | 1.79196000 | 2.64235500 | 0.20227900 |

| | | | |
|---|---|---|---|
| C | 1.42443800 | 1.60844600 | -0.67803200 |
| H | 0.55668300 | 1.75140100 | -1.30531500 |
| C | 2.14705600 | 0.41941800 | -0.76232800 |
| C | 3.30772500 | 0.22010900 | 0.03090600 |
| C | 3.68407100 | 1.28558400 | 0.87678800 |
| H | 4.60121400 | 1.18987400 | 1.45272100 |
| C | 2.97453900 | 2.47203700 | 0.97063700 |
| C | 3.43074000 | 3.63231000 | 1.81787000 |
| H | 2.81979000 | 3.69543700 | 2.73206900 |
| C | 1.83305900 | 5.07045900 | 0.53771800 |
| C | -0.03315400 | 6.45167600 | -0.26414900 |
| C | -0.84645600 | 5.33574600 | -0.45890700 |
| C | -2.26831500 | 5.47069600 | -0.96213300 |
| H | -2.34997500 | 6.36700700 | -1.58095900 |
| H | -2.94829500 | 5.62458200 | -0.11009800 |
| C | -2.68565000 | 4.20479500 | -1.72046700 |
| H | -3.72844600 | 4.27017700 | -2.05181500 |
| H | -2.06503500 | 4.11449000 | -2.62599200 |
| C | -2.48716900 | 3.00609100 | -0.82629900 |
| C | -3.41431800 | 1.97765500 | -0.73011400 |
| H | -4.31094000 | 2.03292900 | -1.34284800 |
| C | -0.86499900 | -0.21139900 | 2.70423000 |
| H | -0.80663000 | 0.64445200 | 3.38934400 |
| H | 0.05559300 | -0.25557200 | 2.10820000 |
| H | -0.96701800 | -1.13067500 | 3.28521600 |
| C | 0.54987800 | -0.50373900 | -2.30214100 |
| H | -0.29803700 | -0.33910200 | -1.62728000 |
| H | 0.58729500 | 0.30611600 | -3.04118400 |
| C | 4.11627300 | -1.01066100 | 0.00088400 |
| H | 4.47106100 | 3.49467100 | 2.13505300 |
| C | 3.26086600 | 4.93197100 | 1.02347100 |
| C | 1.27574400 | 6.32722000 | 0.28722100 |

| | | | |
|---|---|---|---|
| C | -0.30665100 | 7.87492800 | -0.48406500 |
| H | 0.42846100 | -1.45810500 | -2.81847400 |
| C | 4.31456900 | -1.77283600 | -1.17483400 |
| C | 4.76866500 | -1.46386100 | 1.17202200 |
| H | 3.52735700 | 5.81049600 | 1.61535400 |
| H | 3.94680800 | 4.92740900 | 0.16213100 |
| C | 1.84347100 | 7.66398400 | 0.44298000 |
| O | -1.30356800 | 8.44941500 | -0.93872000 |
| N | 0.85174700 | 8.54216300 | -0.04802700 |
| H | 3.85065000 | -1.44894600 | -2.09663100 |
| C | 5.10864900 | -2.90727200 | -1.18097900 |
| C | 5.56584000 | -2.59642700 | 1.17851600 |
| H | 4.60922400 | -0.93371000 | 2.10496300 |
| O | 2.93367400 | 8.03710400 | 0.89429400 |
| C | 0.98633200 | 9.98766100 | -0.05305200 |
| H | 5.26654700 | -3.45146400 | -2.10645600 |
| C | 5.74798800 | -3.34116800 | -0.00286400 |
| H | 6.02449200 | -2.93335800 | 2.10238100 |
| H | 1.78201900 | 10.22516600 | 0.65985600 |
| H | 0.04370600 | 10.41143100 | 0.30994400 |
| C | 1.30900000 | 10.57293500 | -1.43707000 |
| H | 1.30995100 | 11.66818800 | -1.34184300 |
| H | 0.48907400 | 10.31709100 | -2.11851100 |
| C | 2.64677800 | 10.10152400 | -2.01371400 |
| H | 3.47867900 | 10.34836800 | -1.34396100 |
| H | 2.84093100 | 10.56786700 | -2.98713800 |
| H | 2.65483100 | 9.01558600 | -2.15493700 |
| N | -7.37982200 | -3.13472800 | 0.12259300 |
| N | 6.55382100 | -4.50199900 | -0.00567200 |
| C | 7.75016700 | -4.53837900 | 0.75608300 |
| C | 8.59394400 | -3.41393900 | 0.80009200 |
| C | 8.10018300 | -5.69766600 | 1.47137000 |

| | | | |
|---|---|---|---|
| C | 9.76503900 | -3.45435600 | 1.55050800 |
| H | 8.33231300 | -2.52595900 | 0.23471300 |
| C | 9.27668200 | -5.72638700 | 2.21371100 |
| H | 7.44067400 | -6.55883500 | 1.45181000 |
| C | 10.11350400 | -4.60766900 | 2.25901400 |
| H | 10.41456800 | -2.58426000 | 1.57164200 |
| H | 9.53422400 | -6.62279200 | 2.77026500 |
| H | 11.02931700 | -4.63438100 | 2.84165400 |
| C | 6.17012500 | -5.63232900 | -0.77112100 |
| C | 7.13518900 | -6.36931500 | -1.48132600 |
| C | 4.82000500 | -6.02404000 | -0.82525400 |
| C | 6.75048000 | -7.47813200 | -2.22847600 |
| H | 8.17395000 | -6.05775700 | -1.45474800 |
| C | 4.44844100 | -7.13198500 | -1.58031400 |
| H | 4.07797100 | -5.46547900 | -0.26497800 |
| C | 5.40834600 | -7.86488800 | -2.28393700 |
| H | 7.50154900 | -8.03504900 | -2.78105500 |
| H | 3.40481800 | -7.43121000 | -1.60902500 |
| H | 5.11326200 | -8.72962800 | -2.87052000 |
| C | -8.39055600 | -3.12146600 | 1.11978900 |
| C | -8.94875200 | -1.90532300 | 1.54935300 |
| C | -8.84282500 | -4.32184100 | 1.69428200 |
| C | -9.93265000 | -1.89546300 | 2.53498900 |
| H | -8.60933100 | -0.97609300 | 1.10375100 |
| C | -9.83730800 | -4.30105500 | 2.66915400 |
| H | -8.40716000 | -5.26344100 | 1.37620800 |
| C | -10.38632000 | -3.09044000 | 3.09862100 |
| H | -10.35594600 | -0.94683500 | 2.85391200 |
| H | -10.17398900 | -5.23765900 | 3.10561900 |
| H | -11.15752100 | -3.07833000 | 3.86332900 |
| C | -7.39040600 | -4.12804500 | -0.89002200 |
| C | -8.59964900 | -4.53490400 | -1.48054400 |

| | | | |
|---|---|---|---|
| C | -6.18895400 | -4.71804200 | -1.32003200 |
| C | -8.60212100 | -5.51447600 | -2.47042900 |
| H | -9.52973300 | -4.07494300 | -1.16315900 |
| C | -6.20226200 | -5.68683700 | -2.32035600 |
| H | -5.25334000 | -4.41454100 | -0.86197100 |
| C | -7.40611000 | -6.09479200 | -2.89986900 |
| H | -9.54542500 | -5.81441600 | -2.91901300 |
| H | -5.26474100 | -6.13496500 | -2.63887200 |
| H | -7.41229800 | -6.85407300 | -3.67652400 |

Cartesian Coordinates (Å) and Energies at 298.15 K/1 atm for the Optimized Structures of **5n**.

B3LYP/6-31G* SCF energy: -2207.094165 a.u.

**Table 36**. Cartesian coordinates (Å) of **5n**

| | x | y | z |
|---|---|---|---|
| O | -1.86659300 | 2.05326600 | 1.77019600 |
| O | -2.43289000 | -1.64081600 | -1.75260300 |
| C | -5.22860800 | -5.57232100 | -0.08057700 |
| C | -4.78706700 | -4.94664600 | -1.27418500 |
| H | -5.33908200 | -5.08065500 | -2.19690400 |
| C | -3.64318200 | -4.16774000 | -1.29594100 |
| H | -3.33893100 | -3.71477200 | -2.23040500 |
| C | -2.85299800 | -3.96257800 | -0.14207800 |
| C | -3.30025700 | -4.59190200 | 1.04156400 |
| H | -2.74506000 | -4.44223000 | 1.96246700 |
| C | -4.44620900 | -5.36719300 | 1.08395700 |
| H | -4.74292200 | -5.80705100 | 2.02863800 |
| C | -1.60528500 | -3.18110600 | -0.14410700 |
| C | -1.39432900 | -2.02807900 | -0.94907500 |
| C | -0.18964000 | -1.33040800 | -0.89277800 |

| | | | |
|---|---|---|---|
| H | -0.03895400 | -0.47014300 | -1.52916200 |
| C | 0.85381100 | -1.71681700 | -0.02945900 |
| C | 2.14374500 | -1.00321000 | 0.02379000 |
| C | 2.29329000 | 0.39840200 | -0.34072200 |
| C | 1.20878100 | 1.38796000 | -0.19820500 |
| C | 0.17505000 | 1.24535600 | 0.74726000 |
| H | 0.17533700 | 0.36917400 | 1.37979300 |
| C | -0.83161800 | 2.19864800 | 0.88627100 |
| C | -0.83513700 | 3.37386500 | 0.08551900 |
| C | 0.23842500 | 3.51926500 | -0.82066900 |
| H | 0.30061000 | 4.43660400 | -1.40039400 |
| C | 1.24792600 | 2.58142900 | -0.96799400 |
| C | 2.43209700 | 2.78887100 | -1.87811400 |
| H | 2.31459900 | 2.19116300 | -2.79572600 |
| C | 3.56325000 | 0.90534300 | -0.68291000 |
| C | 4.54298600 | -1.23733600 | 0.01885800 |
| C | 3.28639000 | -1.78990300 | 0.27473200 |
| C | 3.13485900 | -3.22108100 | 0.74528600 |
| H | 4.02017900 | -3.50965200 | 1.31625800 |
| H | 3.10137700 | -3.89529700 | -0.12446300 |
| C | 1.84687100 | -3.37968000 | 1.56185000 |
| H | 1.69874900 | -4.42169200 | 1.86784900 |
| H | 1.93632700 | -2.78298100 | 2.48333600 |
| C | 0.67720900 | -2.89656500 | 0.74195800 |
| C | -0.52794100 | -3.57800700 | 0.67791100 |
| H | -0.63297100 | -4.49190800 | 1.25685100 |
| C | -2.30798400 | -0.43894500 | -2.50046600 |
| H | -1.50747200 | -0.50851900 | -3.24792400 |
| H | -2.11790300 | 0.42168100 | -1.84739000 |
| H | -3.26545700 | -0.30758700 | -3.00862800 |
| C | -1.96080500 | 0.85075100 | 2.52167300 |
| H | -2.02124500 | -0.02736400 | 1.86704000 |

| | | | |
|---|---|---|---|
| H | -1.11060900 | 0.73363700 | 3.20546300 |
| C | -1.86771500 | 4.41984300 | 0.16729100 |
| H | 2.50305000 | 3.83853200 | -2.18546600 |
| C | 3.70716000 | 2.33637100 | -1.15637900 |
| C | 4.67619000 | 0.07855500 | -0.51437000 |
| C | 5.87876100 | -1.82153300 | 0.14627300 |
| H | -2.88137000 | 0.93791600 | 3.10231900 |
| C | -2.50590300 | 4.79048200 | 1.37299900 |
| C | -2.24199800 | 5.14559600 | -0.98636600 |
| H | 4.59017300 | 2.41836700 | -1.79390900 |
| H | 3.89213100 | 2.99543400 | -0.29404100 |
| C | 6.09622300 | 0.34176300 | -0.75088900 |
| O | 6.24578800 | -2.93059700 | 0.55711100 |
| N | 6.75831400 | -0.82824000 | -0.32469200 |
| H | -2.24894500 | 4.27083500 | 2.28666700 |
| C | -3.43819400 | 5.81194500 | 1.42689200 |
| C | -3.17807600 | 6.16453000 | -0.95271000 |
| H | -1.80379600 | 4.88020000 | -1.94350600 |
| O | 6.67008500 | 1.33462700 | -1.21675000 |
| C | 8.19617000 | -1.01550400 | -0.40401900 |
| H | -3.87854000 | 6.05985100 | 2.38535100 |
| C | -3.80653100 | 6.53445700 | 0.26340300 |
| H | -3.43142600 | 6.66990600 | -1.87698900 |
| H | 8.56345100 | -0.28504200 | -1.13149300 |
| H | 8.37838900 | -2.02513700 | -0.78734600 |
| C | 8.91629000 | -0.84472600 | 0.94307200 |
| H | 9.97690700 | -1.08636800 | 0.78385600 |
| H | 8.52438900 | -1.59477200 | 1.64021400 |
| C | 8.78926000 | 0.55808400 | 1.54350100 |
| H | 9.17471500 | 1.32162900 | 0.85807400 |
| H | 9.34452100 | 0.63239200 | 2.48624500 |
| H | 7.74298700 | 0.80624000 | 1.75066800 |

| | | | |
|---|---|---|---|
| N | -6.36956000 | -6.34458600 | -0.05287700 |
| N | -4.73550500 | 7.55076200 | 0.31201800 |
| C | -7.15868900 | -6.52858200 | -1.26070600 |
| H | -8.02749200 | -7.14663000 | -1.03130300 |
| H | -7.51756100 | -5.56950300 | -1.65698000 |
| H | -6.58170800 | -7.02945400 | -2.05001400 |
| C | -6.78582600 | -6.99236500 | 1.18094600 |
| H | -6.01344000 | -7.67558900 | 1.55841200 |
| H | -7.00707200 | -6.25917800 | 1.96857600 |
| H | -7.69025600 | -7.57269000 | 0.99471100 |
| C | -5.08291600 | 8.28470700 | -0.89480700 |
| H | -4.20668500 | 8.78232000 | -1.33143000 |
| H | -5.51712300 | 7.62546700 | -1.65863600 |
| H | -5.82038100 | 9.04983500 | -0.64985700 |
| C | -5.36691000 | 7.90654100 | 1.57327200 |
| H | -6.06813200 | 8.72467800 | 1.40536600 |
| H | -5.92427000 | 7.06108100 | 1.99823600 |
| H | -4.62851900 | 8.23664900 | 2.31629400 |

Cartesian Coordinates (Å) and Energies at 298.15 K/1 atm for the Optimized Structures of **5o**.

B3LYP/6-31G* SCF energy: -3615.567277 a.u.

**Table 37**. Cartesian coordinates (Å) of **5o**

| | x | y | z |
|---|---|---|---|
| O | -7.64157400 | -4.01008300 | -1.14864600 |
| C | -0.16610300 | -2.36295400 | 0.57350600 |
| C | 0.19622500 | -3.28839700 | -0.44037800 |
| C | -0.84306000 | -3.69691700 | -1.30902400 |
| H | -0.62808100 | -4.45705900 | -2.05401800 |
| C | -2.13413400 | -3.20105000 | -1.23902400 |

| | | | |
|---|---|---|---|
| C | -2.46074500 | -2.22103500 | -0.26378200 |
| C | -1.45748200 | -1.85390100 | 0.65857200 |
| H | -1.71304600 | -1.17499200 | 1.46038200 |
| C | -3.24016600 | -3.68858600 | -2.14225900 |
| H | -2.95738600 | -4.63285400 | -2.62126800 |
| H | -3.42310100 | -2.96178500 | -2.94933200 |
| C | -4.52647400 | -3.85356700 | -1.32404500 |
| H | -5.37093300 | -4.16138600 | -1.94436400 |
| H | -4.38411600 | -4.65384600 | -0.58168000 |
| C | -4.86743700 | -2.56118700 | -0.61348000 |
| C | -3.82790100 | -1.69248900 | -0.19815800 |
| C | -4.16546200 | -0.40796100 | 0.39044100 |
| C | -5.48999400 | -0.12185000 | 0.76740500 |
| C | -6.49046800 | -1.04252100 | 0.43513300 |
| C | -6.17846900 | -2.22041600 | -0.29846200 |
| C | -7.43539400 | -2.94788200 | -0.55469800 |
| C | -5.82233800 | 1.17634400 | 1.47244900 |
| H | -6.08571400 | 1.94810600 | 0.73274200 |
| C | -4.62158300 | 1.65011900 | 2.30075700 |
| H | -4.83025400 | 2.60820600 | 2.79032600 |
| H | -4.42855100 | 0.91388100 | 3.09595800 |
| C | -3.42086100 | 1.76556900 | 1.39635200 |
| C | -3.21394400 | 0.72981200 | 0.44369700 |
| C | -2.17769800 | 0.88668100 | -0.48941000 |
| H | -2.05041900 | 0.13533000 | -1.25530900 |
| O | 0.82818300 | -2.02323500 | 1.45037700 |
| C | -7.93026400 | -1.00828500 | 0.67304000 |
| N | -8.43617000 | -2.17106800 | 0.04249600 |
| H | -6.71232700 | 1.03370500 | 2.08936500 |
| C | -2.56584600 | 2.85222100 | 1.42268700 |
| C | -1.31903200 | 1.98378800 | -0.44742300 |
| C | 0.54014000 | -1.13178700 | 2.51485800 |

| | | | |
|---|---|---|---|
| O | -8.63402400 | -0.19148400 | 1.27713500 |
| C | -9.83930600 | -2.54900700 | 0.05448700 |
| C | -1.47792200 | 3.00148200 | 0.52852700 |
| H | -2.74773200 | 3.62233700 | 2.16560300 |
| O | -0.29219700 | 2.15529500 | -1.32502500 |
| H | 1.47484400 | -1.01834100 | 3.06710400 |
| H | -0.23039400 | -1.53853000 | 3.18198200 |
| H | 0.21332800 | -0.15306900 | 2.14031200 |
| H | -10.30321400 | -1.97858700 | 0.86488900 |
| H | -9.89568400 | -3.61658500 | 0.29294400 |
| C | -10.56149900 | -2.28304200 | -1.27534300 |
| C | -0.60498400 | 4.15932800 | 0.62907600 |
| C | -0.00587200 | 1.13748200 | -2.28255900 |
| H | -10.07569500 | -2.87764700 | -2.05791400 |
| H | -11.58601300 | -2.66894300 | -1.17681700 |
| C | -10.60052200 | -0.80562800 | -1.67608500 |
| C | -0.71935600 | 5.21956900 | 1.53333500 |
| H | 0.19247600 | 0.17836700 | -1.79185000 |
| H | 0.88701400 | 1.47581800 | -2.81013900 |
| H | -0.83137900 | 1.02434700 | -2.99451100 |
| H | -9.59073100 | -0.41088800 | -1.83141900 |
| H | -11.07317900 | -0.19437500 | -0.89860600 |
| H | -11.16068000 | -0.66704300 | -2.60842800 |
| H | -1.51563500 | 5.28278500 | 2.26378500 |
| C | 1.21708800 | 5.90186400 | 0.44282200 |
| C | 1.54288400 | -3.82109800 | -0.61137300 |
| C | 2.01632700 | -4.53640900 | -1.70211500 |
| C | 3.33874300 | -5.01679600 | -1.56782400 |
| H | 1.41669600 | -4.72329000 | -2.58516900 |
| H | 3.85577000 | -5.59258700 | -2.32742100 |
| S | 2.81671100 | -3.69837900 | 0.60594500 |
| C | 3.91806000 | -4.66865600 | -0.36828600 |

| | | | |
|---|---|---|---|
| S | 0.81380700 | 4.39922000 | -0.39113800 |
| C | 0.28822400 | 6.18844800 | 1.43728400 |
| H | 0.35091600 | 7.06437700 | 2.07130100 |
| N | 5.23339200 | -4.91195600 | 0.04756900 |
| C | 6.30688900 | -4.65920600 | -0.85139500 |
| C | 7.39819600 | -5.54043000 | -0.92528000 |
| C | 6.28293400 | -3.53079700 | -1.68723800 |
| C | 8.44474900 | -5.28739500 | -1.80982800 |
| H | 7.41888400 | -6.42145800 | -0.29215700 |
| C | 7.32852400 | -3.29511100 | -2.57664300 |
| H | 5.44167700 | -2.84744600 | -1.63453800 |
| C | 8.41772500 | -4.16732600 | -2.64325100 |
| H | 9.27980700 | -5.98159600 | -1.85628000 |
| H | 7.29457900 | -2.41618200 | -3.21538900 |
| H | 9.23246200 | -3.97809500 | -3.33630000 |
| C | 5.47932100 | -5.43189600 | 1.34967100 |
| C | 4.62061400 | -6.39733700 | 1.89787200 |
| C | 6.56968300 | -4.97469700 | 2.10761200 |
| C | 4.84793700 | -6.88850300 | 3.18169700 |
| H | 3.78126400 | -6.75698900 | 1.31150500 |
| C | 6.79674500 | -5.48461200 | 3.38388500 |
| H | 7.23064600 | -4.22039400 | 1.69309500 |
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| C | 3.45714100 | 6.09440000 | -0.51714800 |
| C | 4.03703100 | 6.65619300 | -1.66489700 |
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| | | | |
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S1. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, Revision A.1, Gaussian, Inc., Wallingford CT, 2009.

## 6. $^{1}$H NMR and $^{13}$C NMR spectra of new compounds

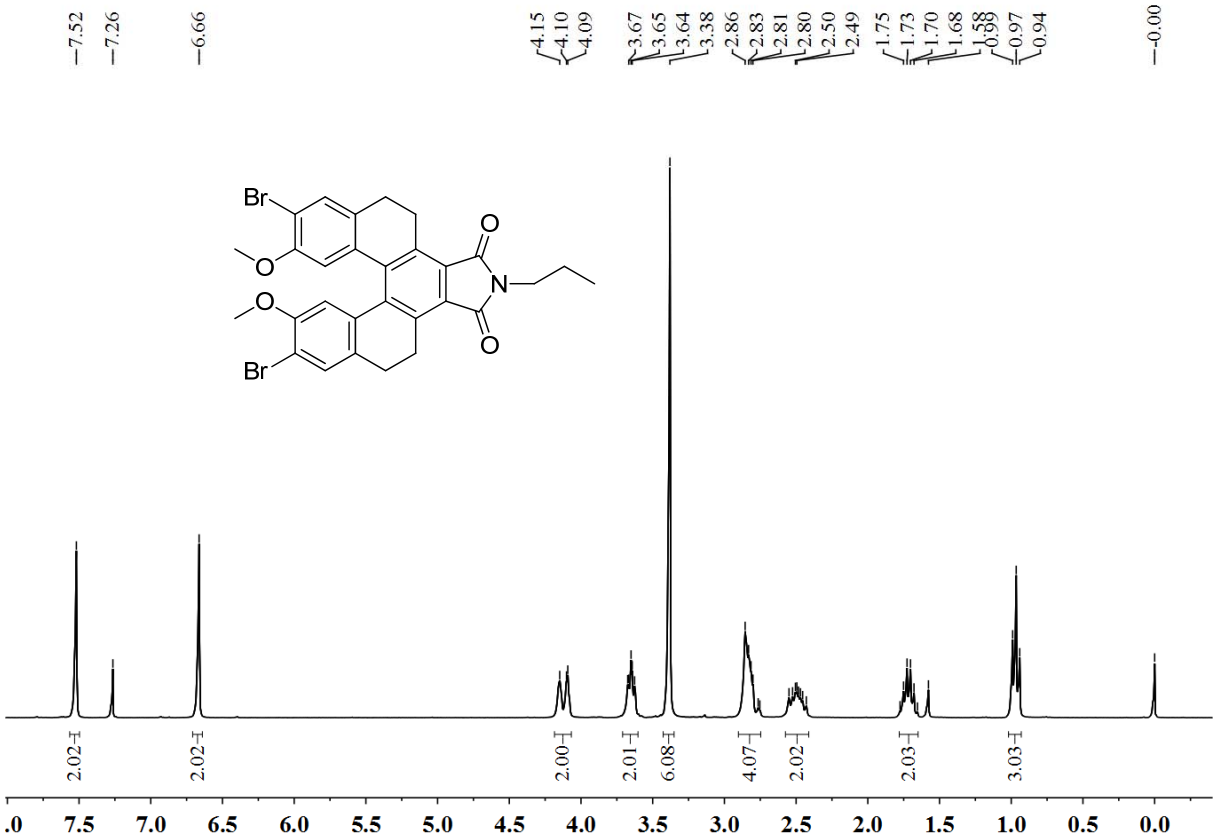


**Fig. S36** $^{1}$H NMR spectrum (300 MHz, $CDCl_3$) of **2**.

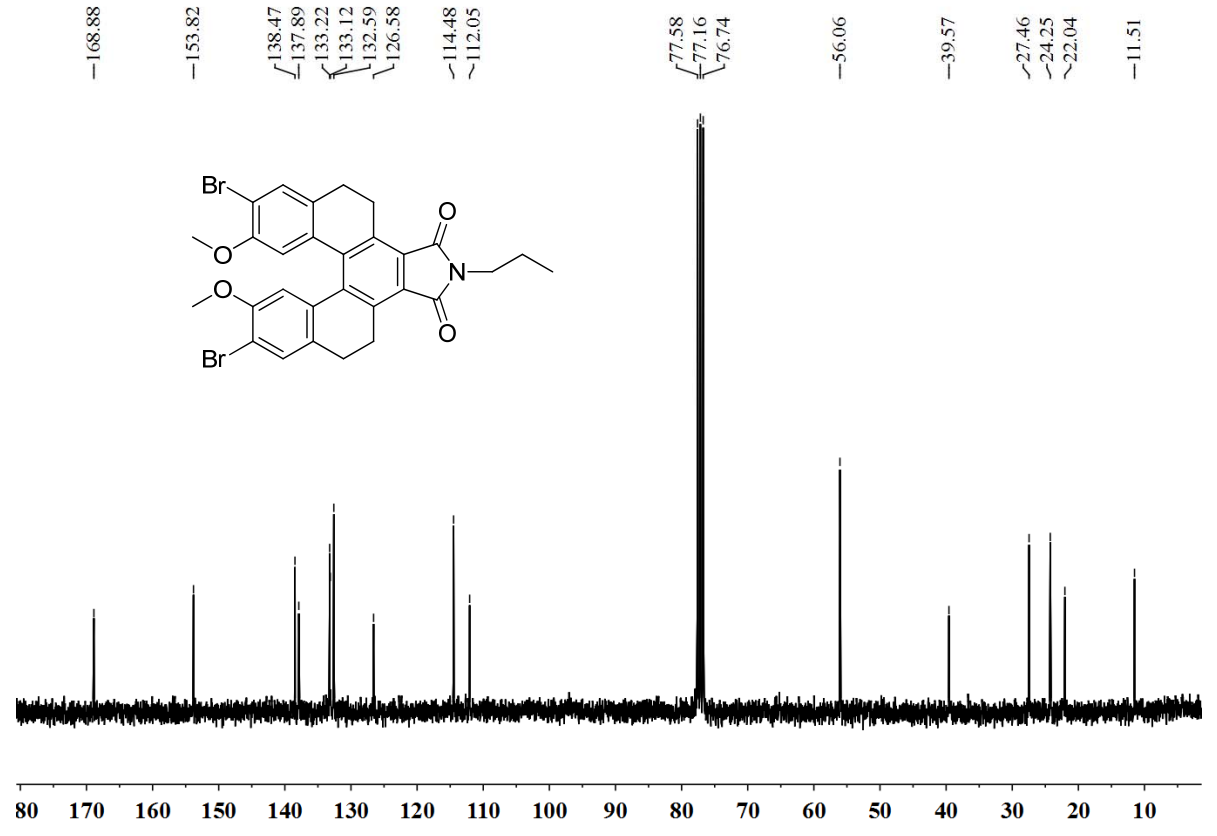


**Fig. S37** $^{13}$C NMR spectrum (75 MHz, $CDCl_3$) of **2**.

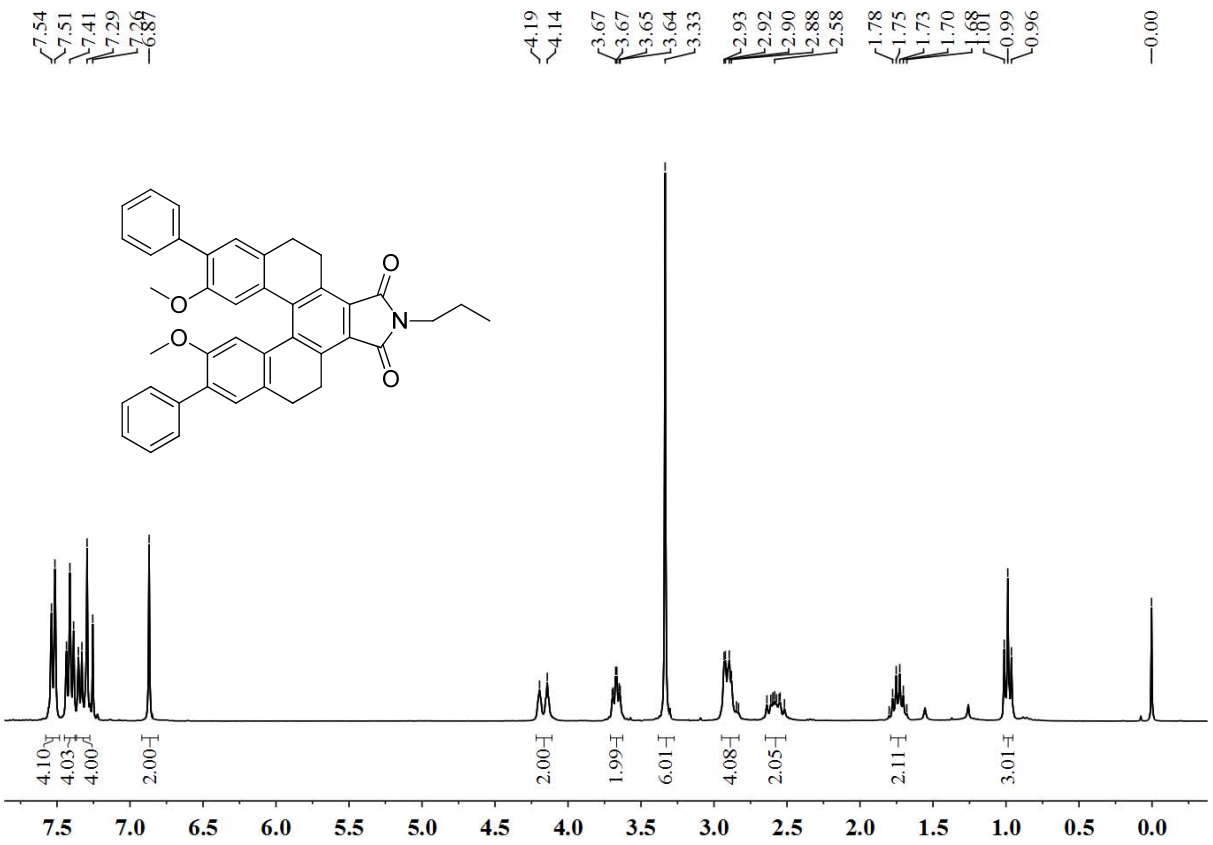


**Fig. S38** $^{1}$H NMR spectrum (300 MHz, $CDCl_3$) of **4a**.

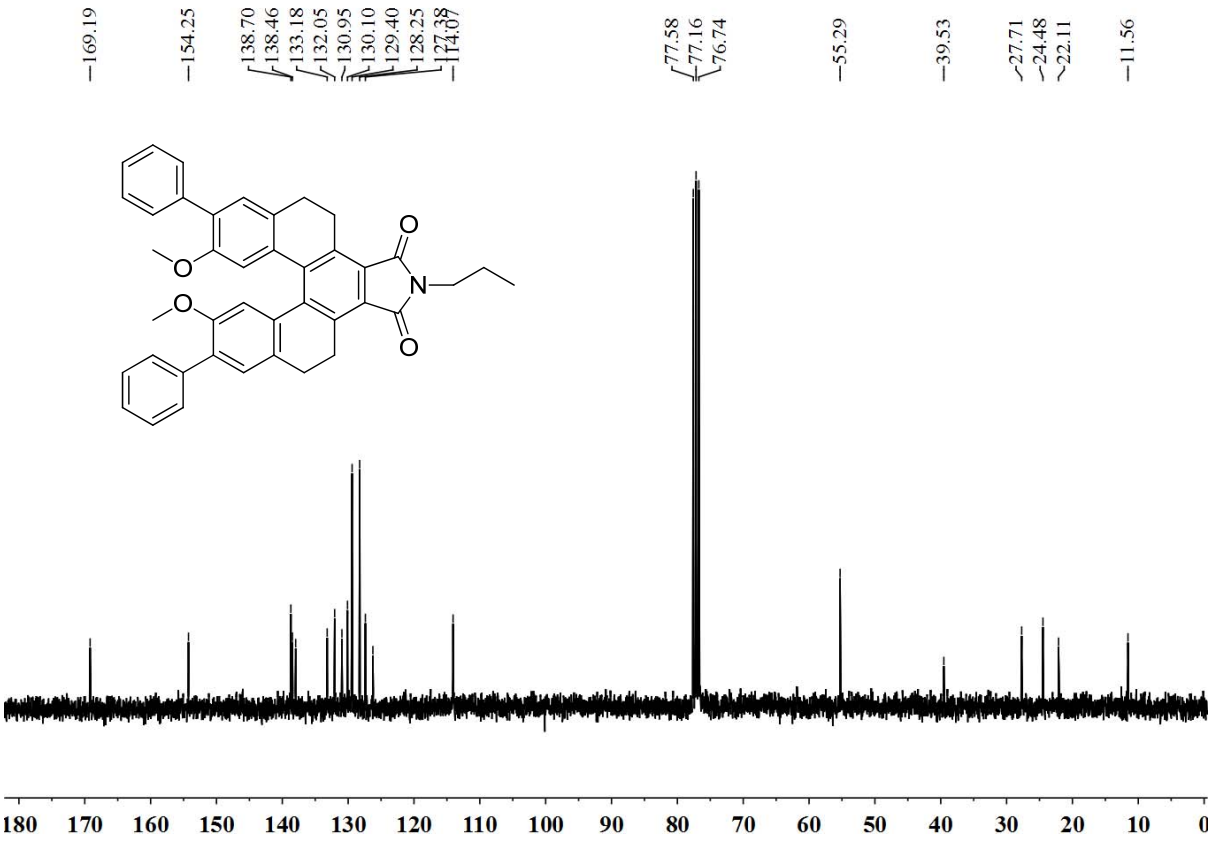


**Fig. S39** $^{13}$C NMR spectrum (75 MHz, $CDCl_3$) of **4a**.

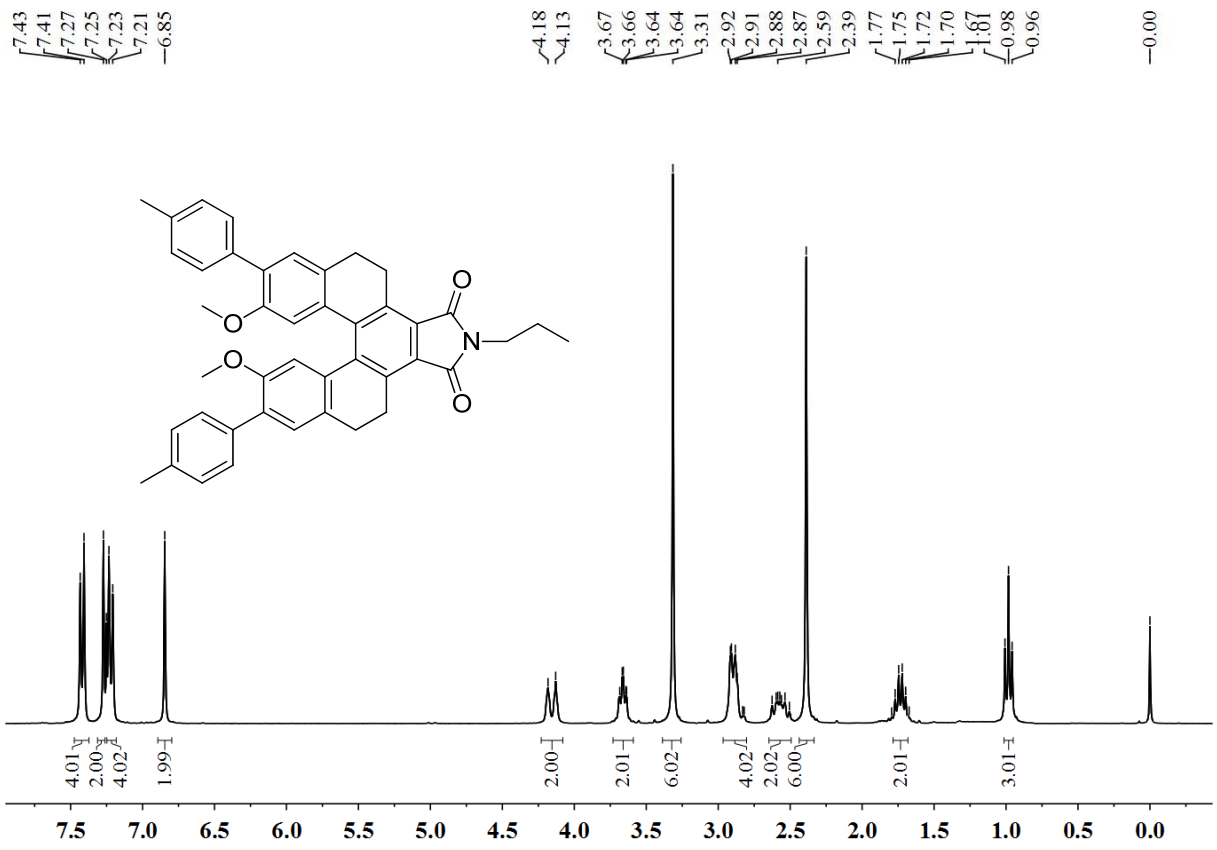


**Fig. S40** $^{1}$H NMRspectrum (300 MHz, $CDCl_3$) of **4b**.

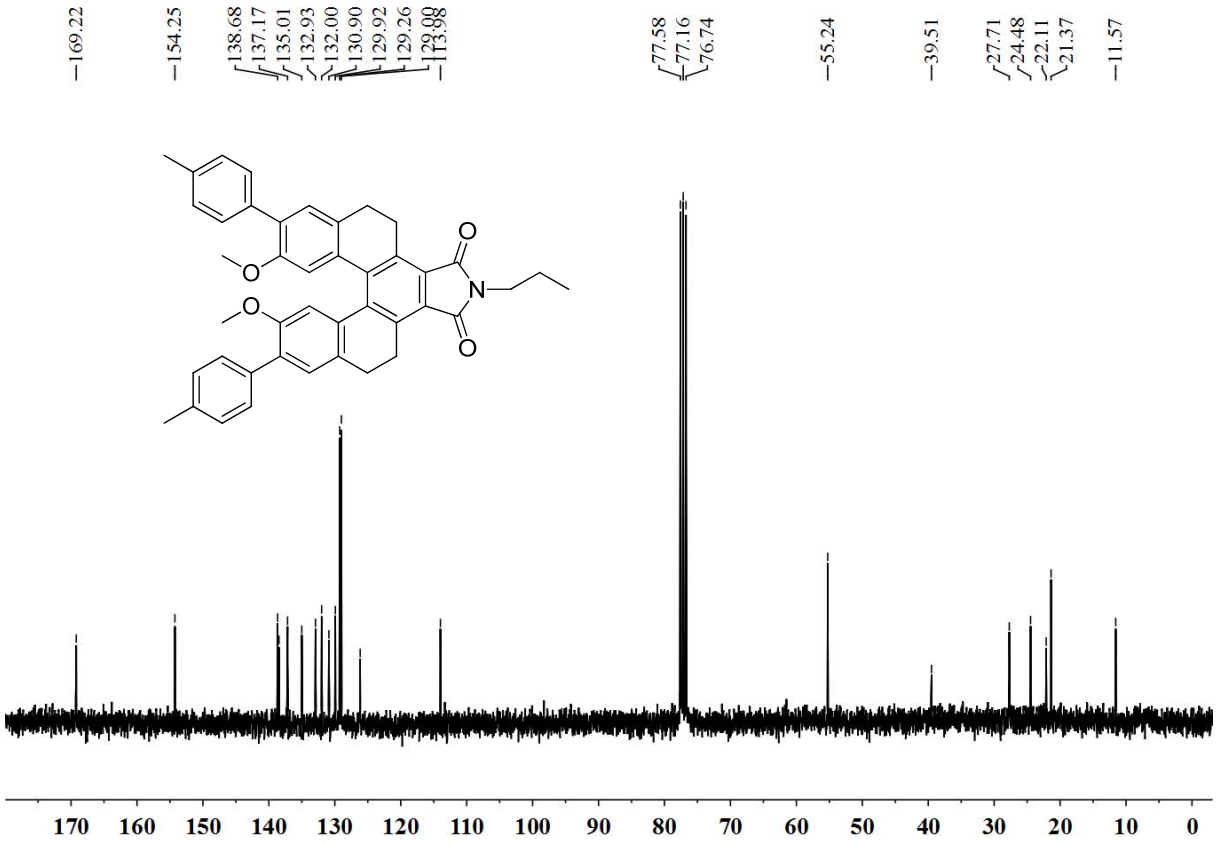


**Fig. S41** $^{13}$C NMR spectrum (75 MHz, $CDCl_3$) of **4b**.

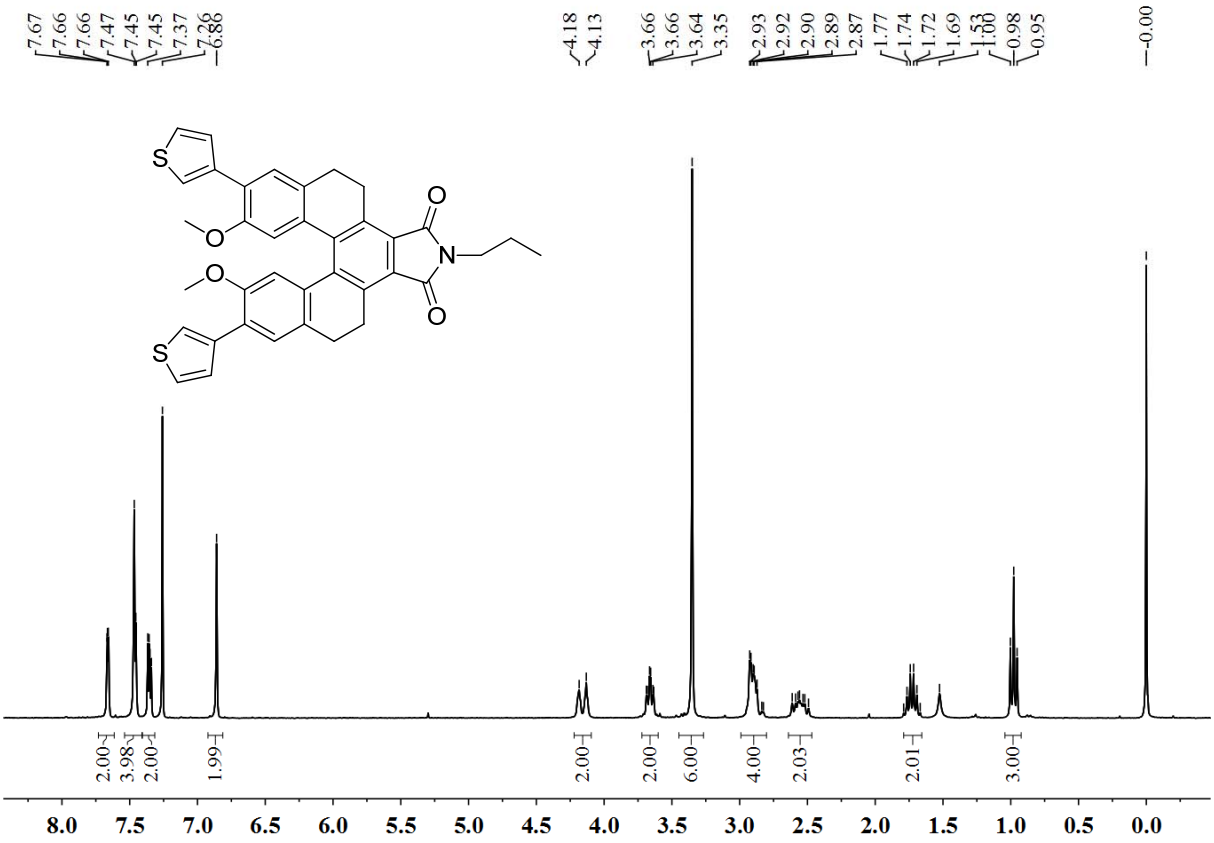


**Fig. S42** $^{1}$H NMR spectrum (300 MHz, $CDCl_3$) of **4c**.

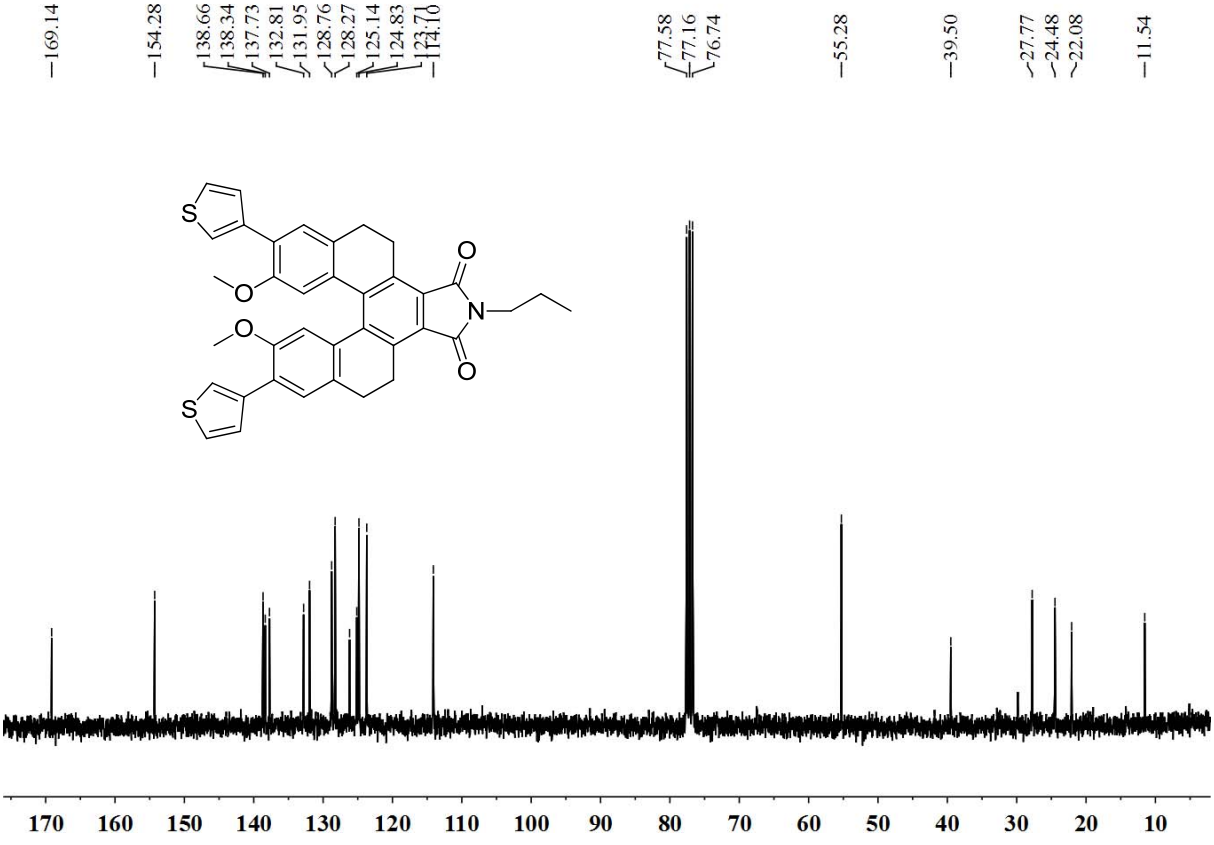


**Fig. S43** $^{13}$C NMR spectrum (75 MHz, $CDCl_3$) of **4c**.

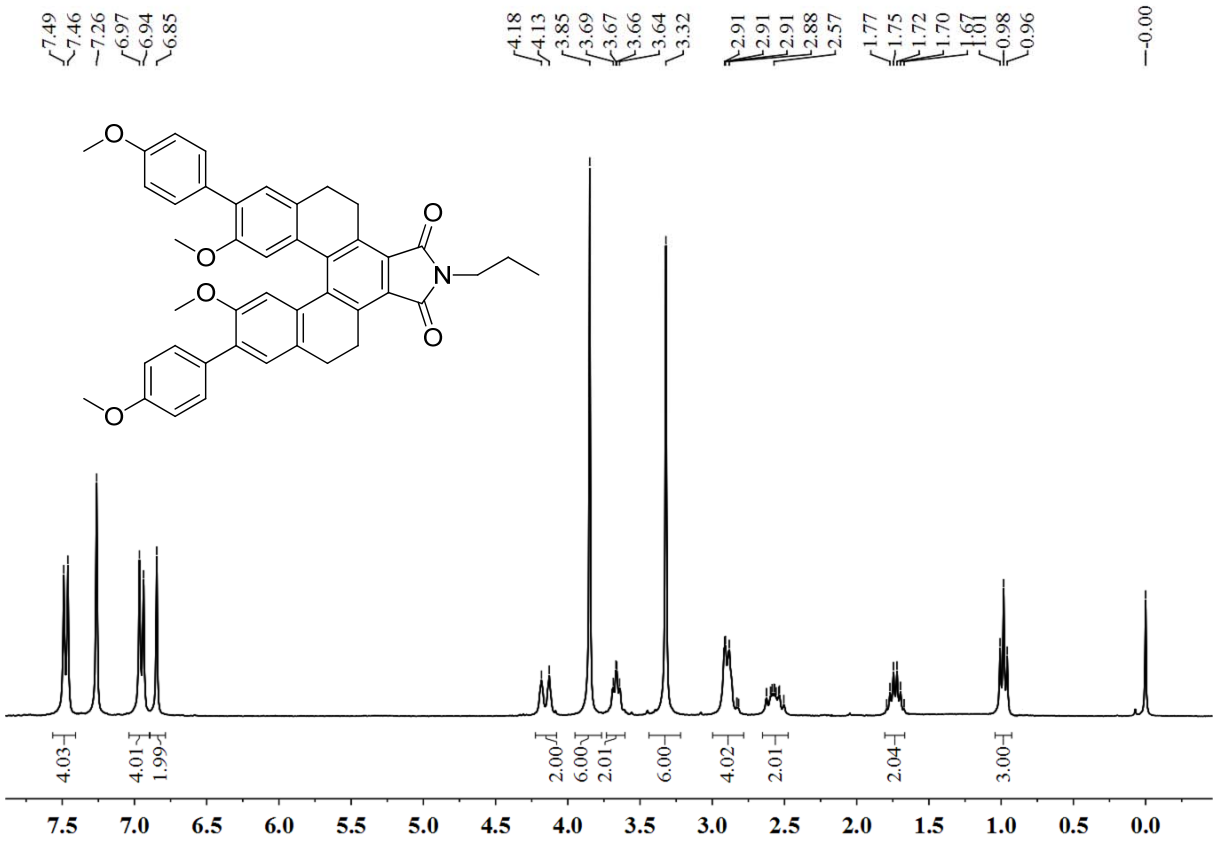


**Fig. S44** $^{1}$H NMR spectrum (300 MHz, $CDCl_3$) of **4d**.

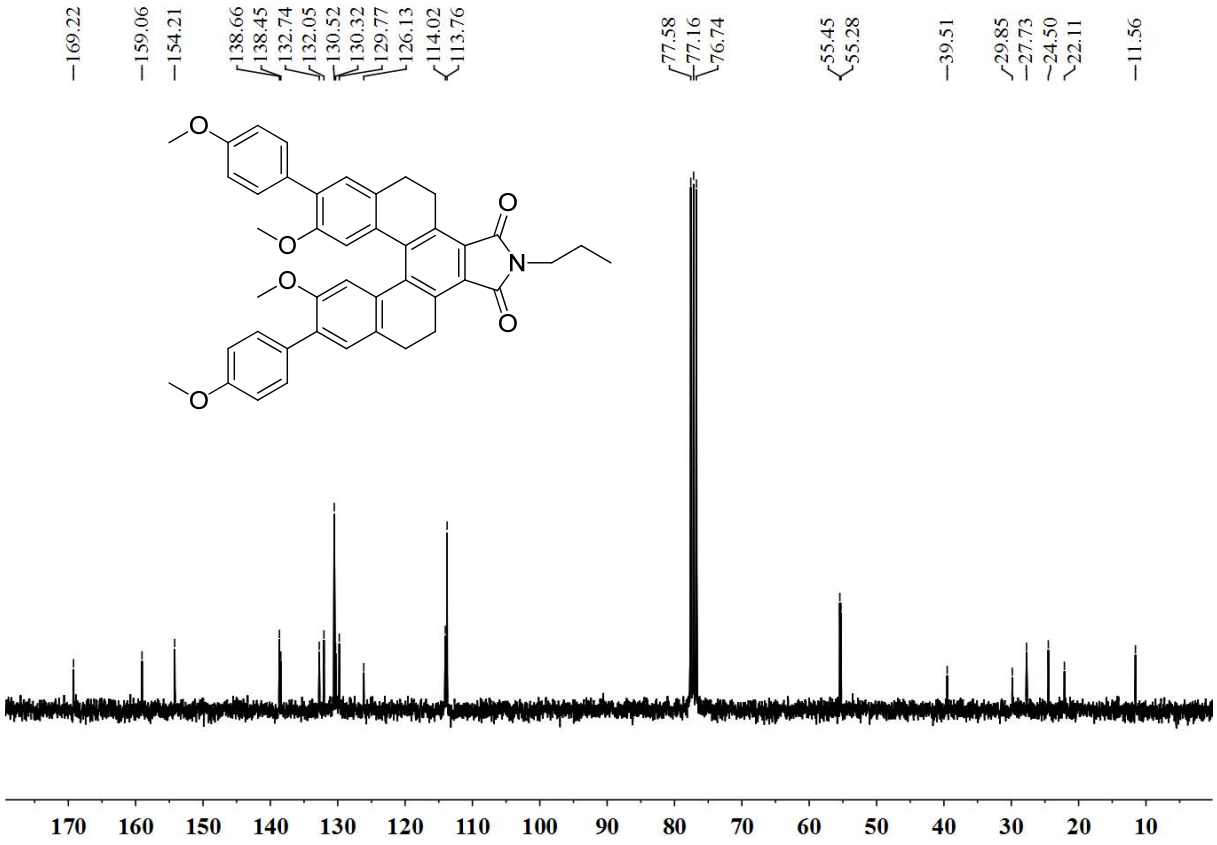


**Fig. S45** $^{13}$C NMR spectrum (75 MHz, $CDCl_3$) of **4d**.

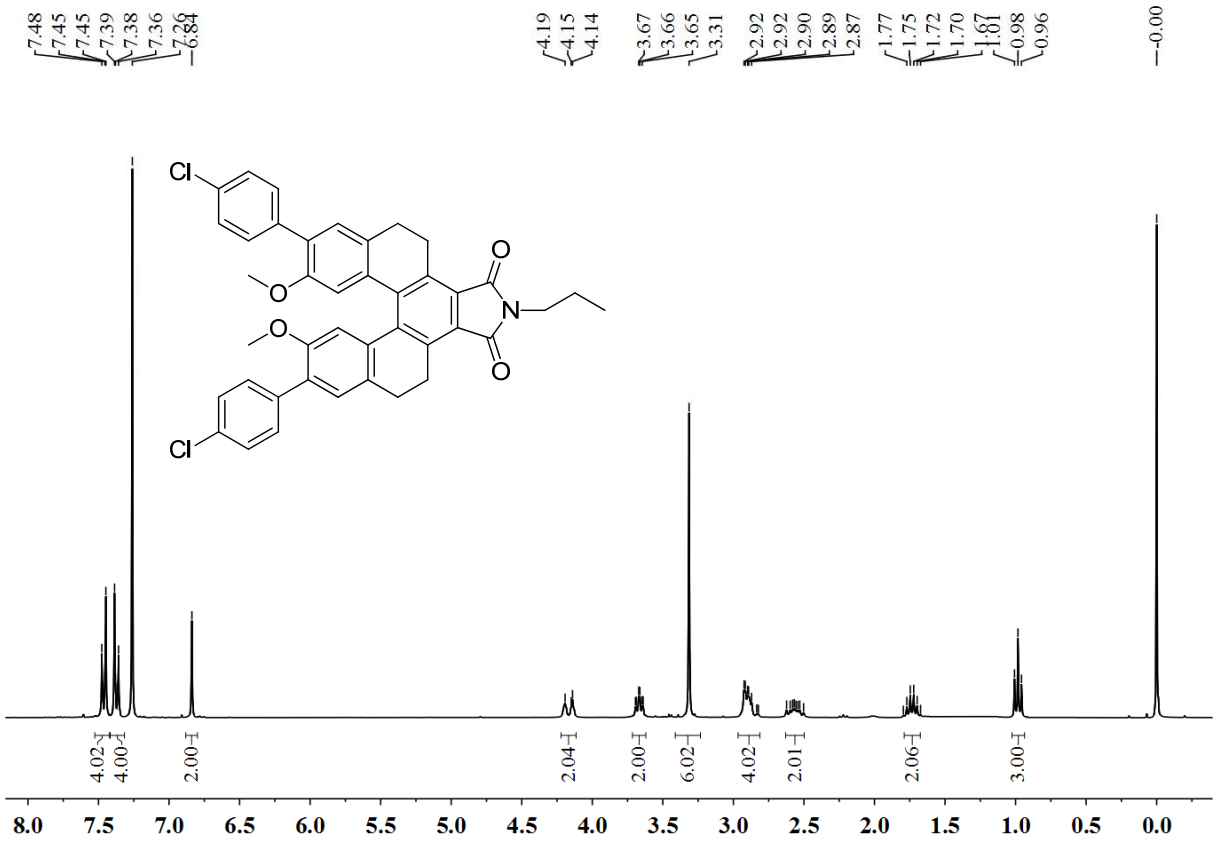


**Fig. S46** $^{1}$H NMR spectrum (300 MHz, $CDCl_3$) of **4e**.

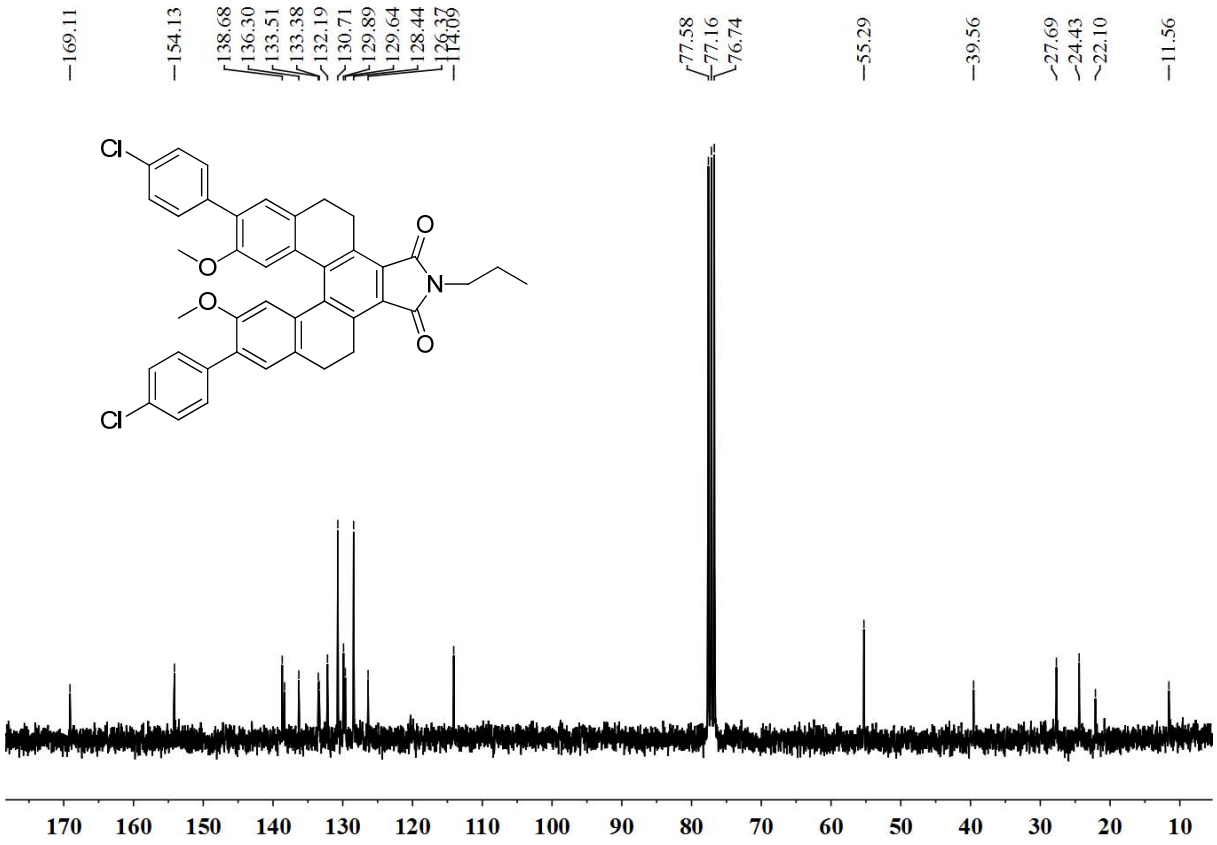


**Fig. S47** $^{13}$C NMR spectrum (75 MHz, $CDCl_3$) of **4e**.

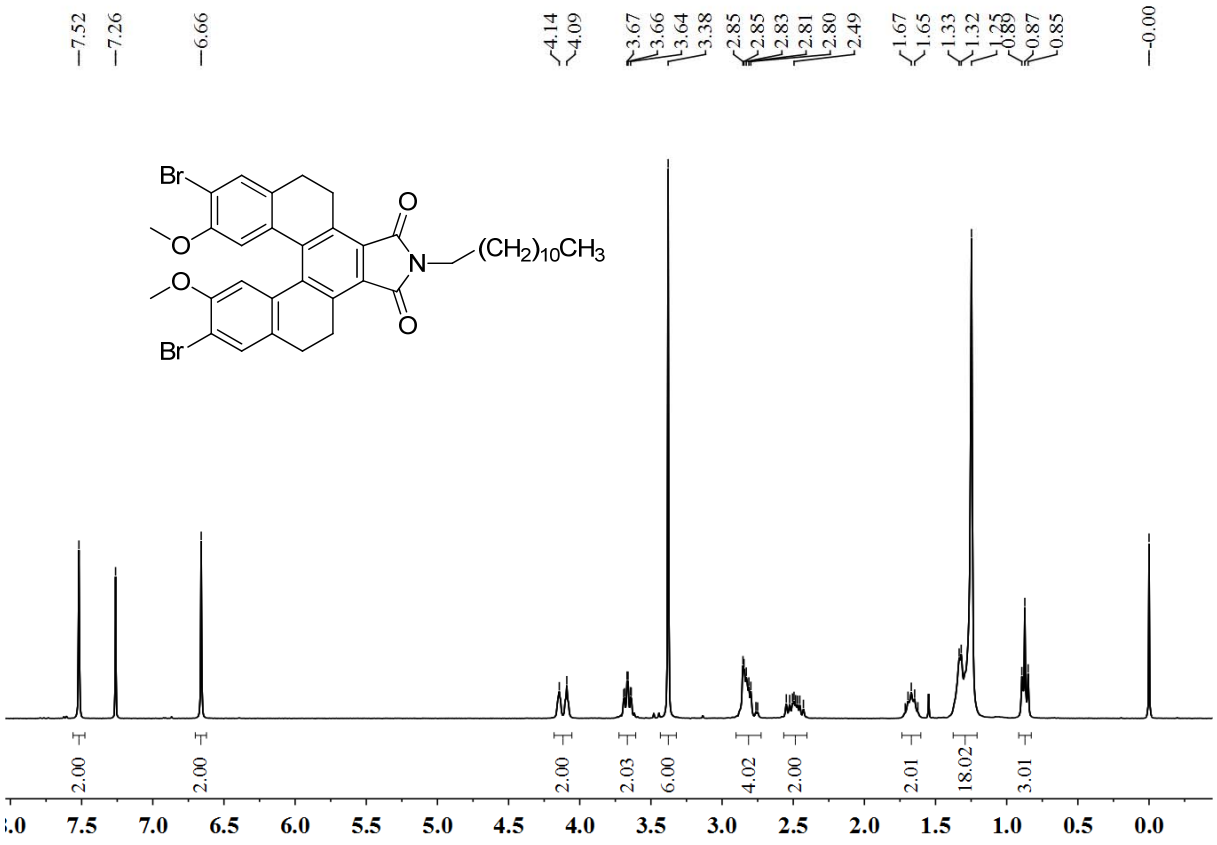


**Fig. S48** $^{1}$H NMR spectrum (300 MHz, $CDCl_3$) of **3**.

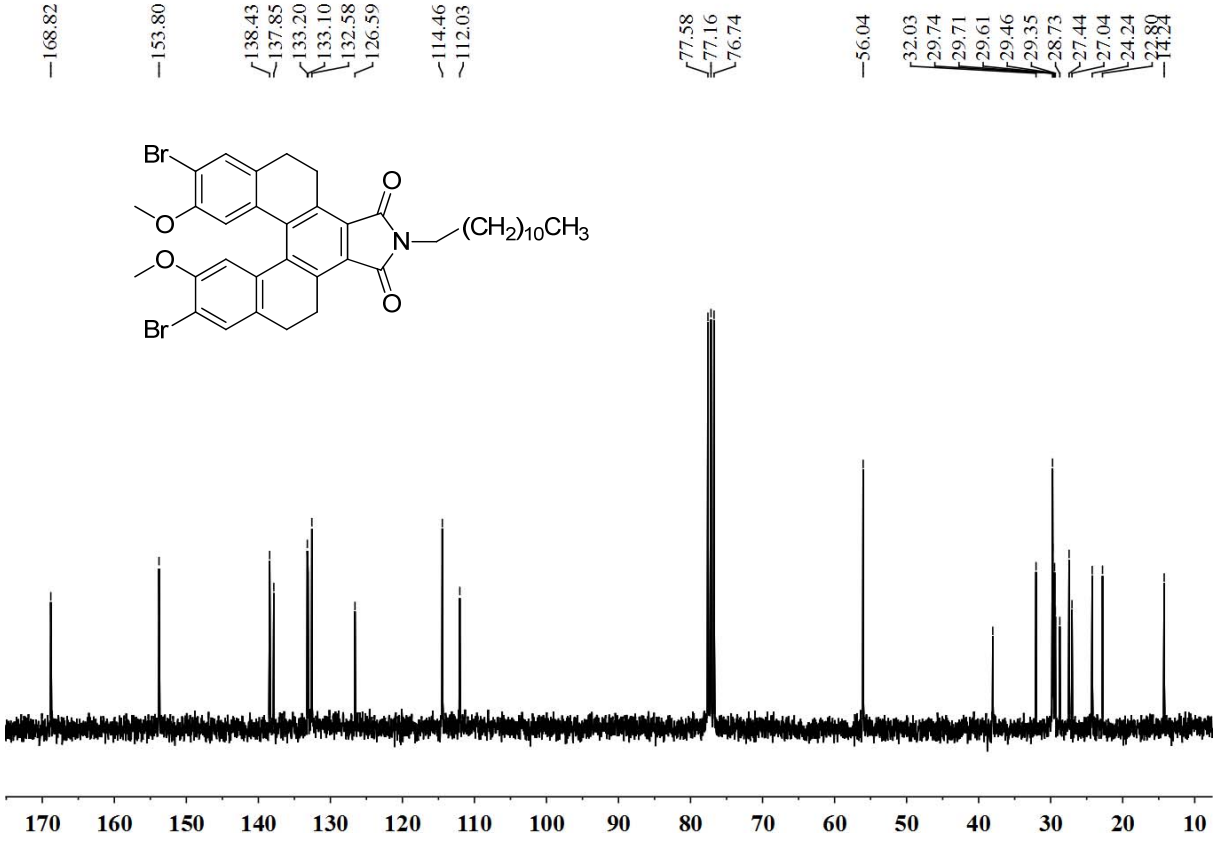


**Fig. S49** $^{13}$C NMR spectrum (75 MHz, $CDCl_3$) of **3**.

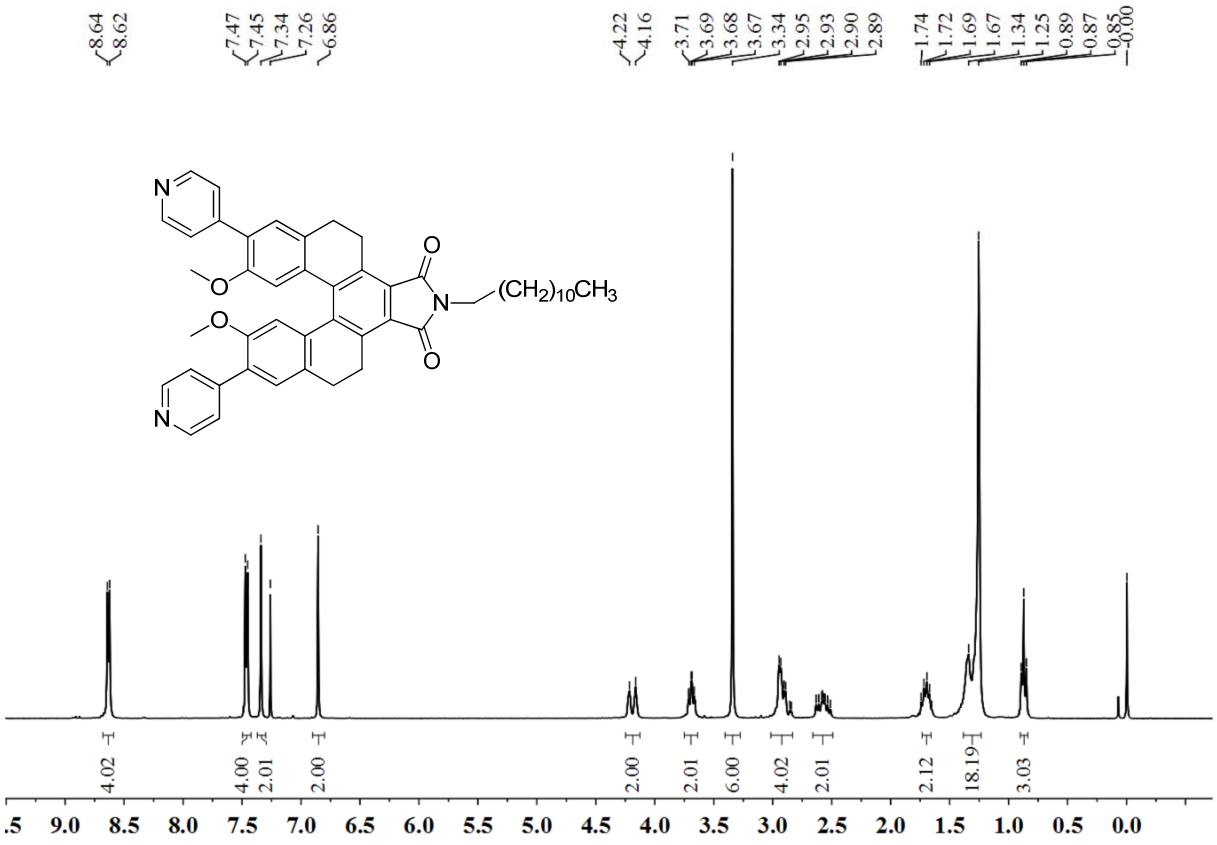


**Fig. S50** $^{1}$H NMR spectrum (300 MHz, $CDCl_3$) of **5a**.

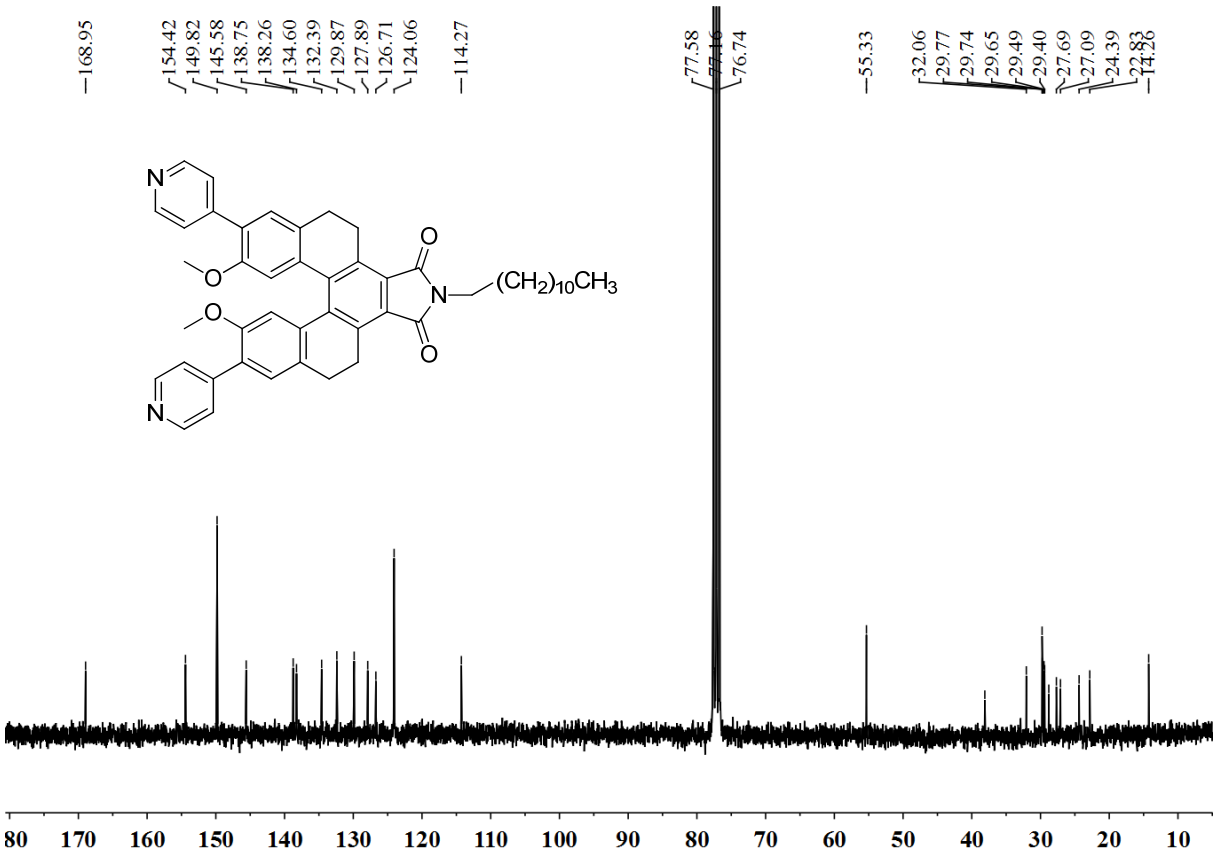


**Fig. S51** $^{13}$C NMR spectrum (75 MHz, $CDCl_3$) of **5a**.

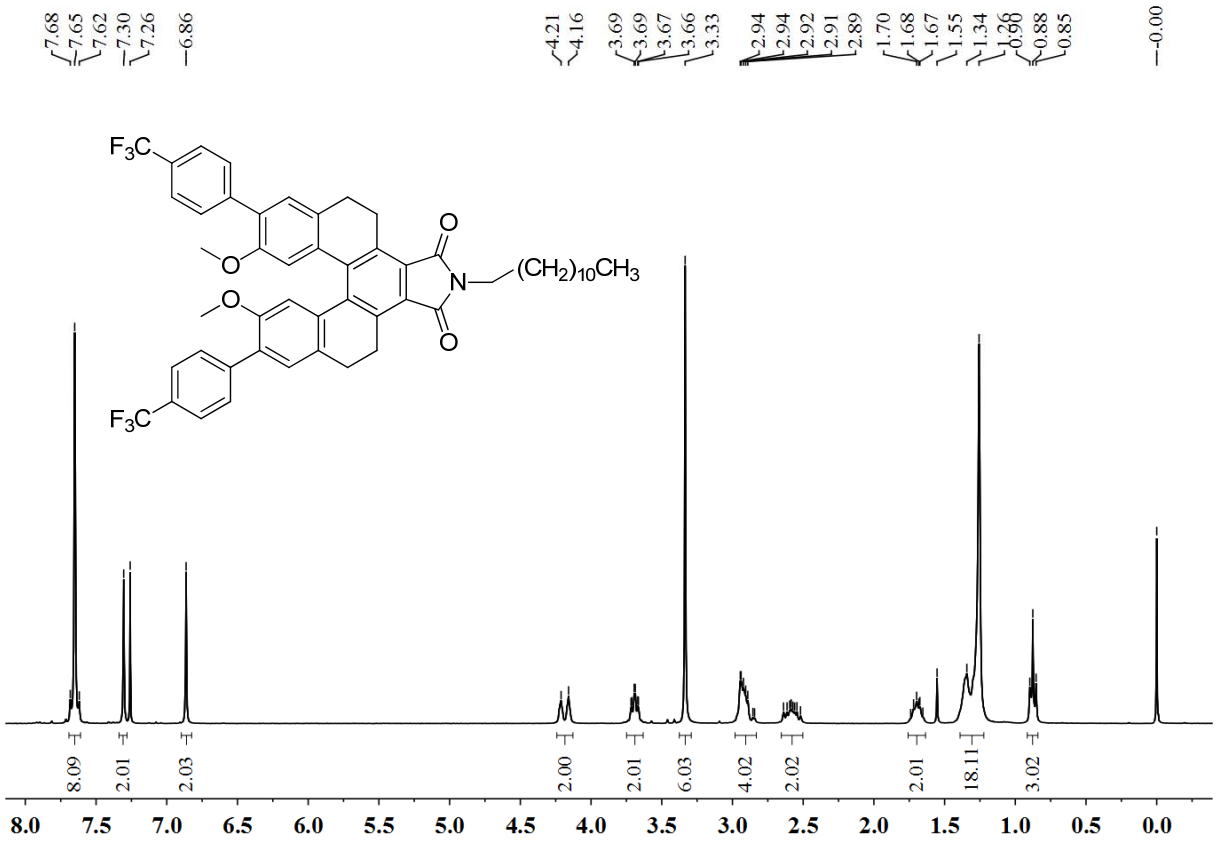


**Fig. S52** $^{1}$H NMR spectrum (300 MHz, $CDCl_3$) of **5b**.

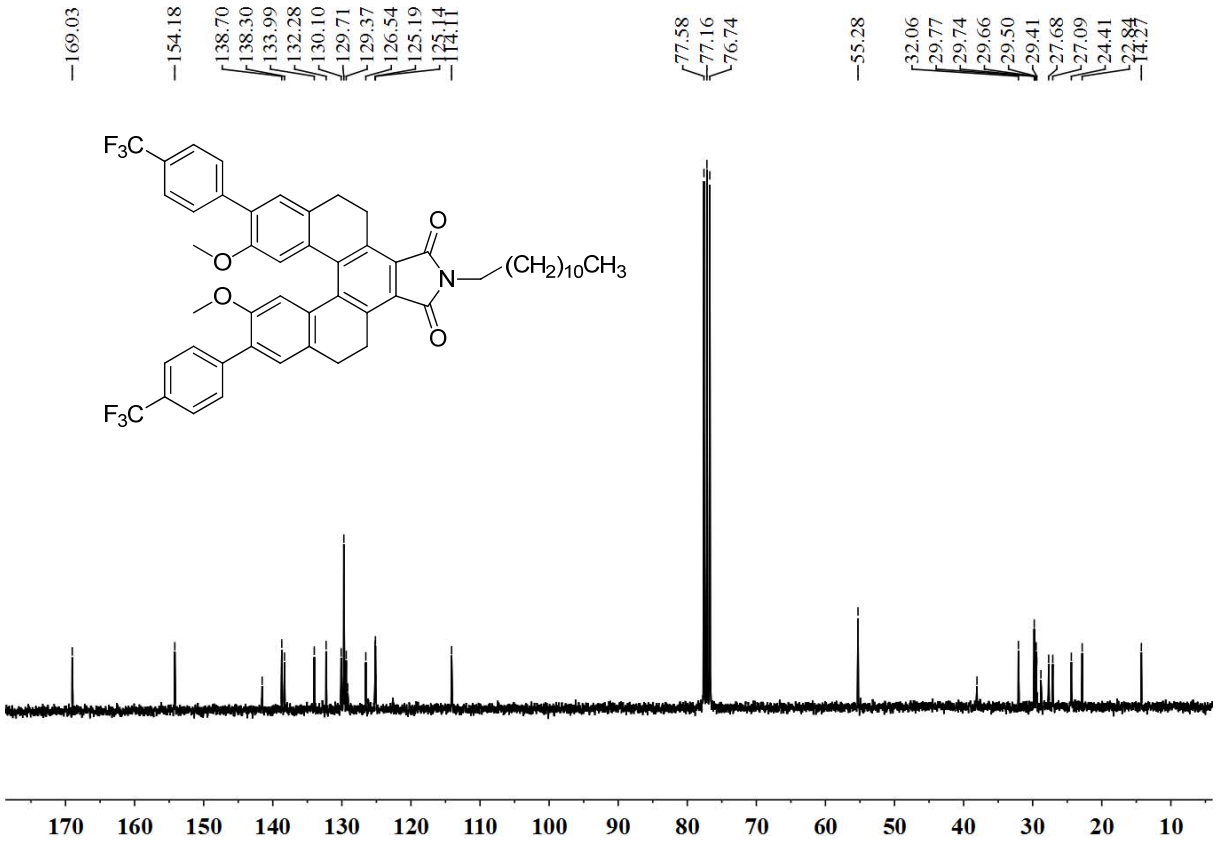


**Fig. S53** $^{13}$C NMR spectrum (75 MHz, $CDCl_3$) of **5b**.

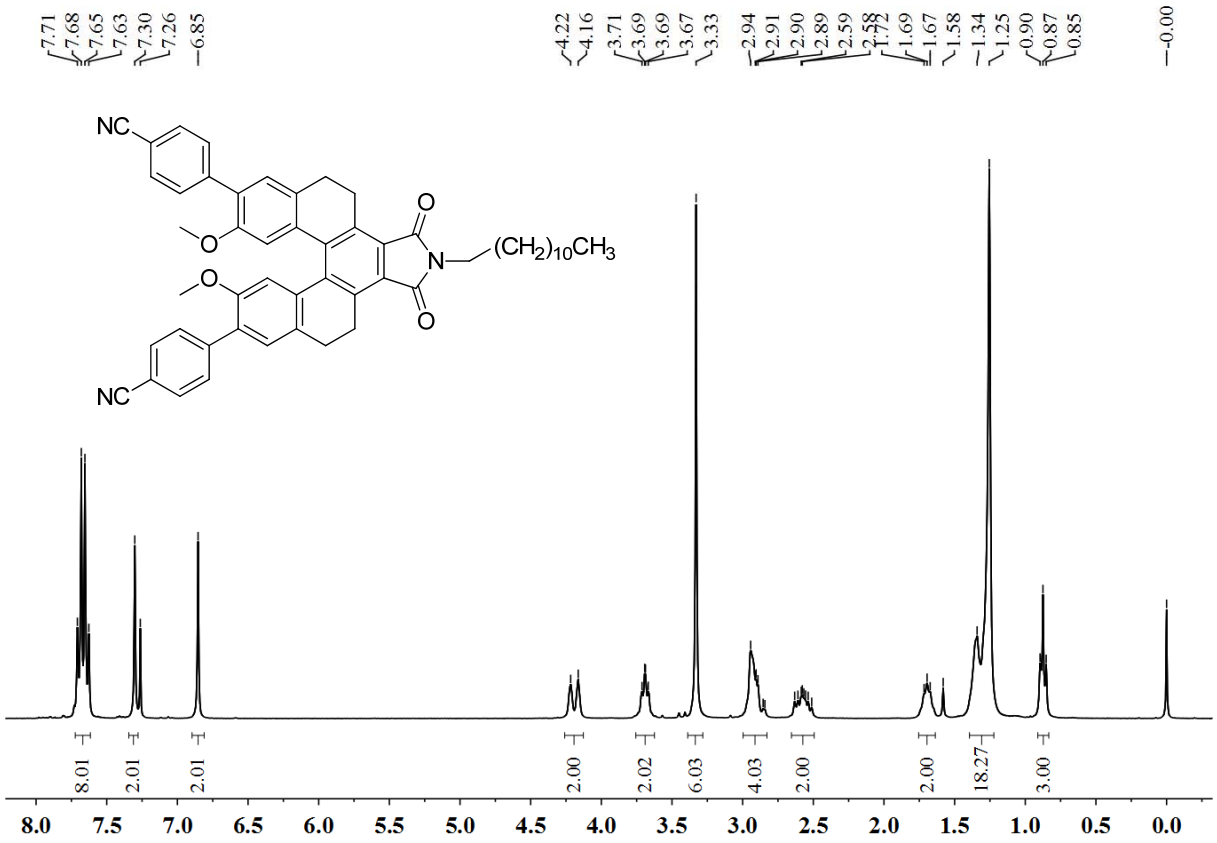


**Figure S54**. $^{1}$H NMR spectrum (300 MHz, $CDCl_3$) of **5c**.

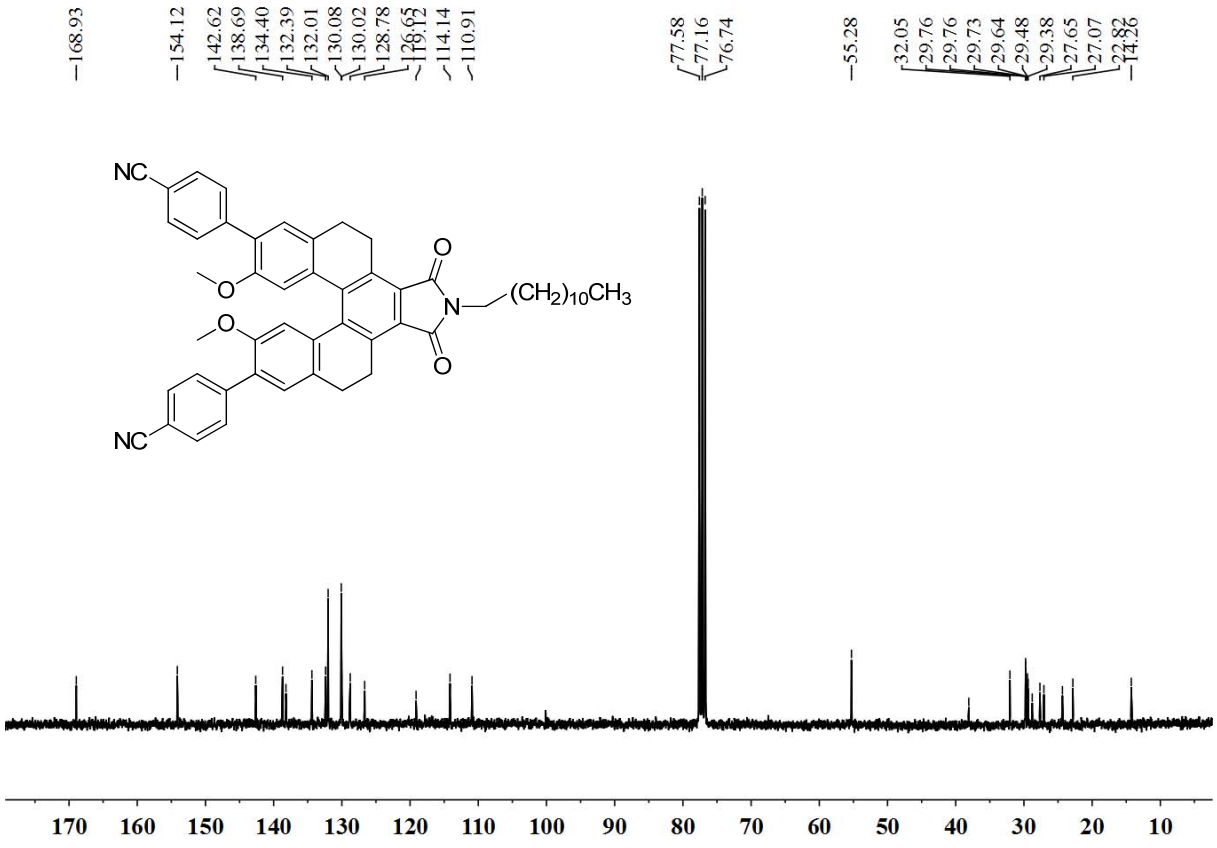


**Fig. S55** $^{13}$C NMR spectrum (75 MHz, $CDCl_3$) of **5c**.

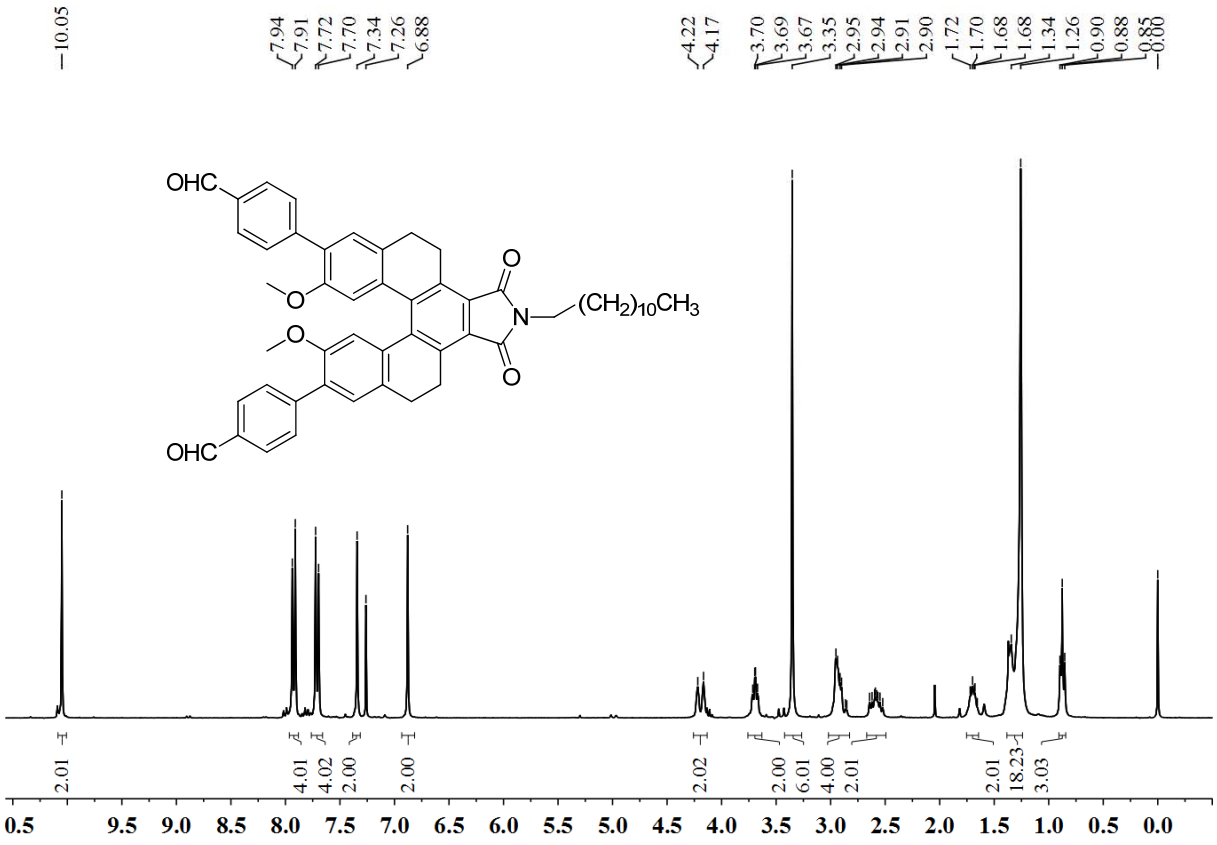


**Fig. S56** $^{1}$H NMR spectrum (300 MHz, $CDCl_3$) of **5d**.

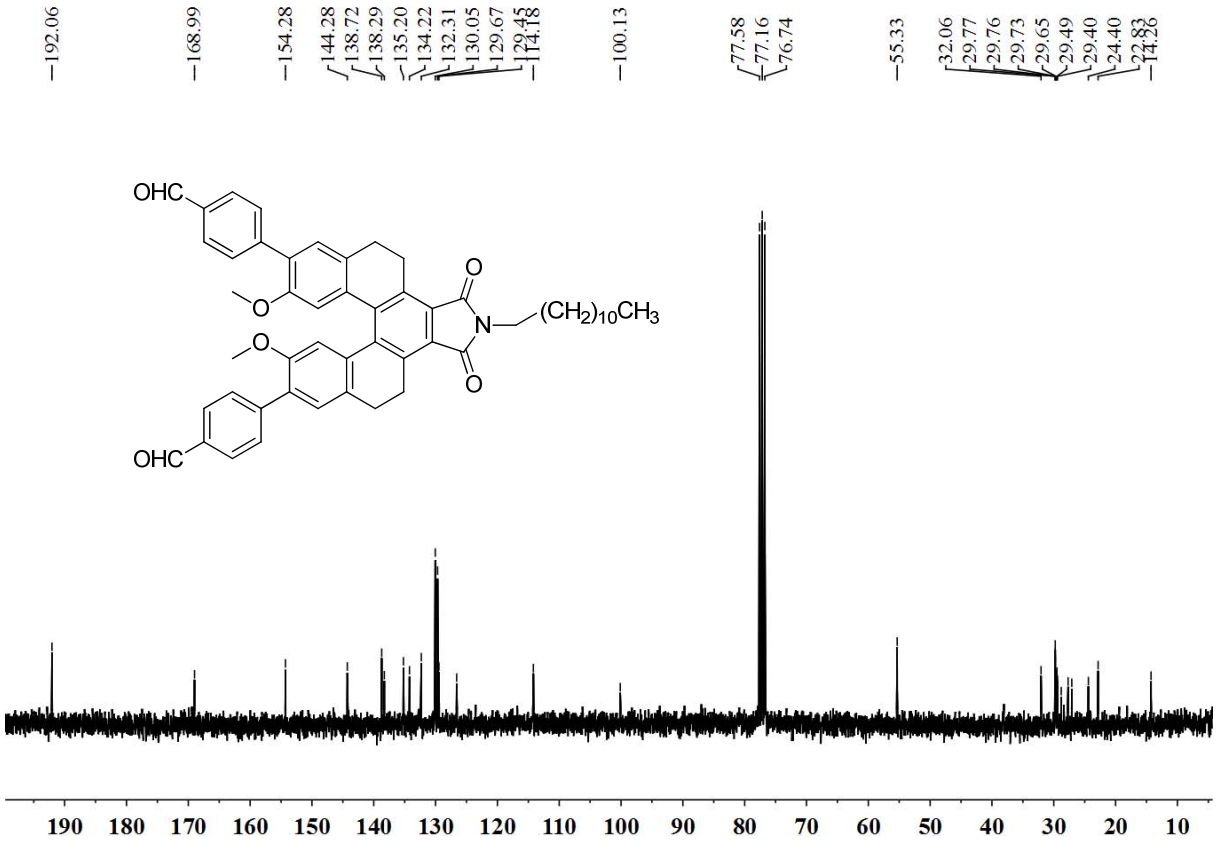


**Fig. S57** $^{13}$C NMR spectrum (75 MHz, $CDCl_3$) of **5d**.

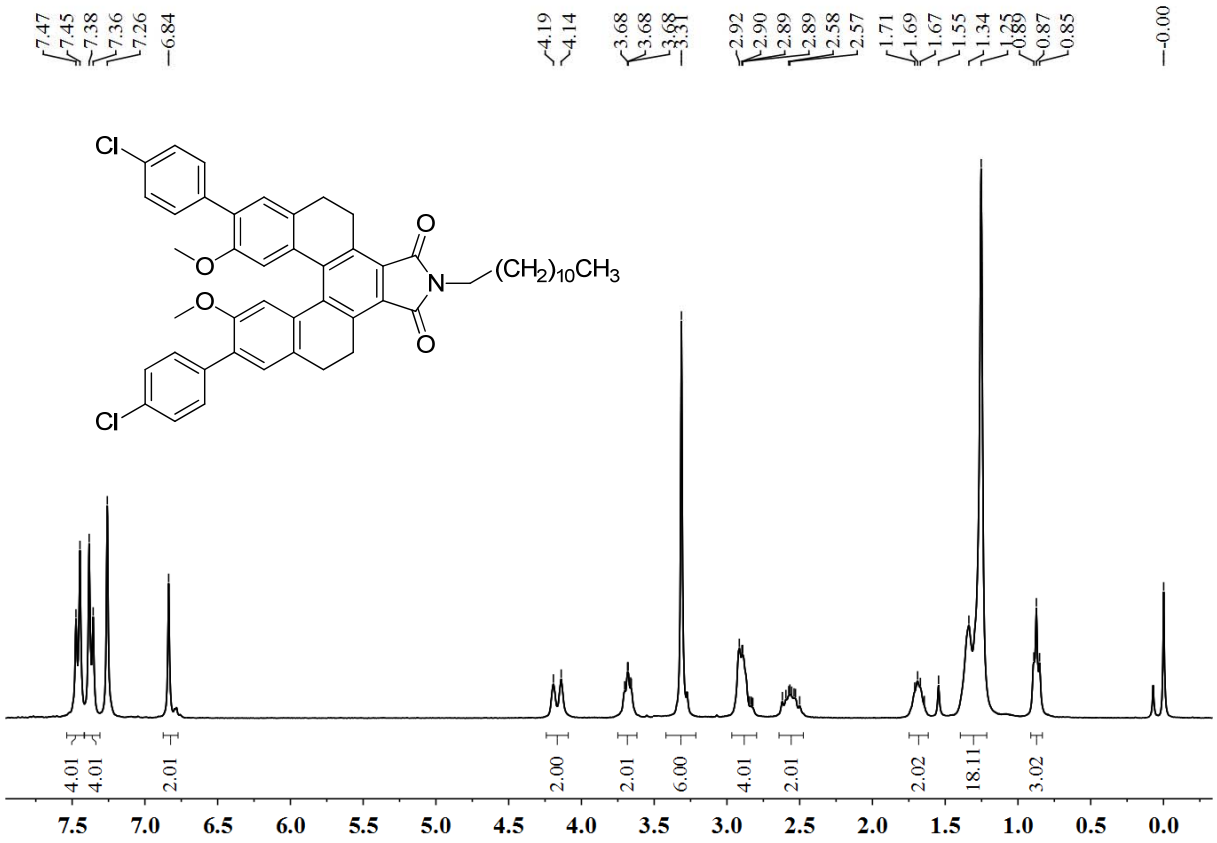


**Fig. S58** $^{1}$H NMR spectrum (300 MHz, $CDCl_3$) of **5e**.

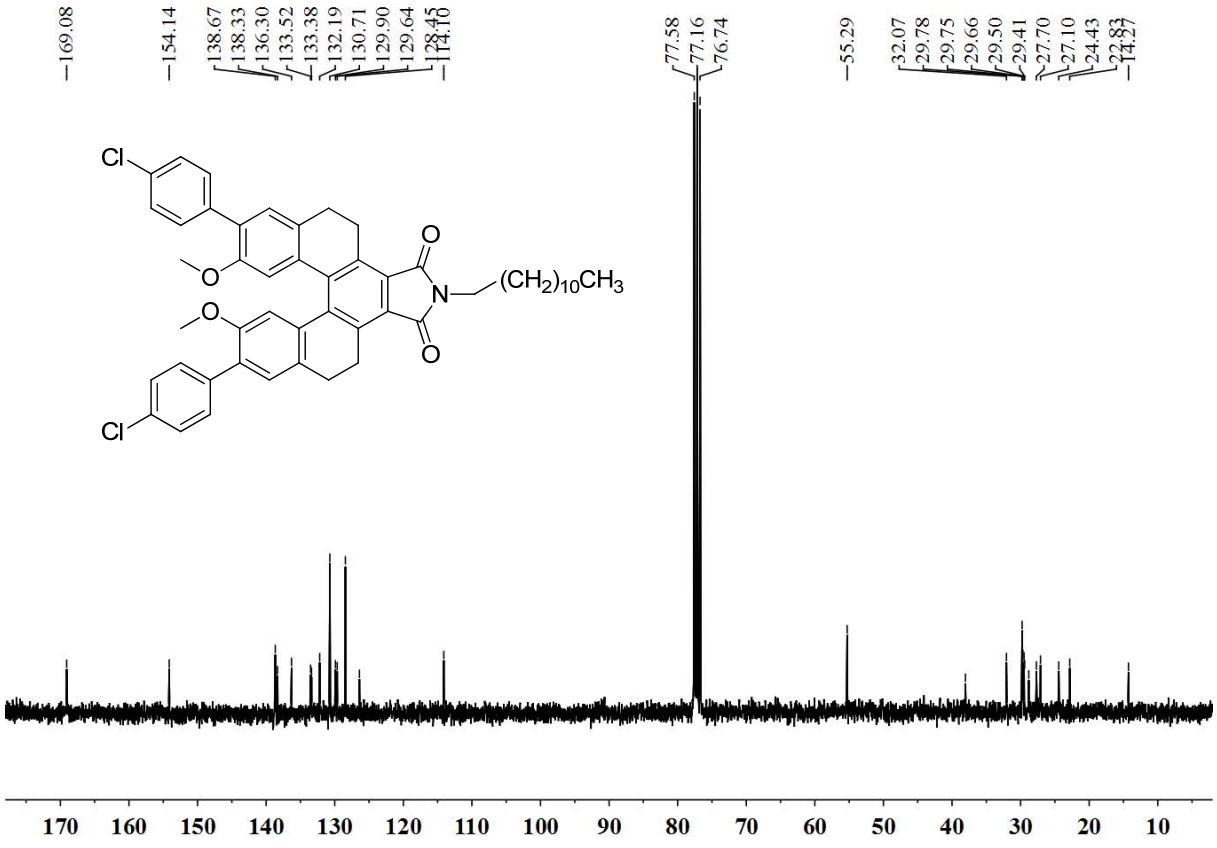


**Fig. S59** $^{13}$C NMR spectrum (75 MHz, $CDCl_3$) of **5e**.

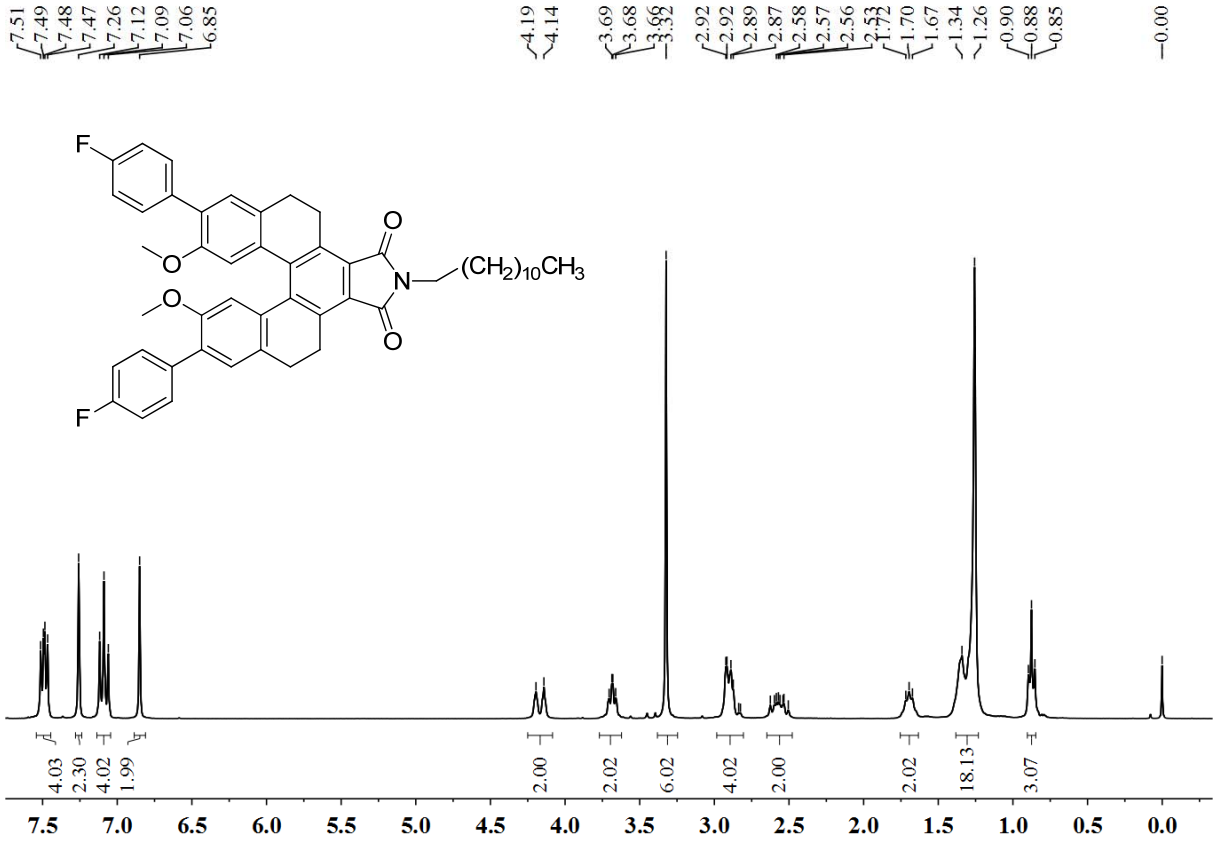


**Fig. S60** $^{1}$H NMR spectrum (300 MHz, $CDCl_3$) of **5f**.

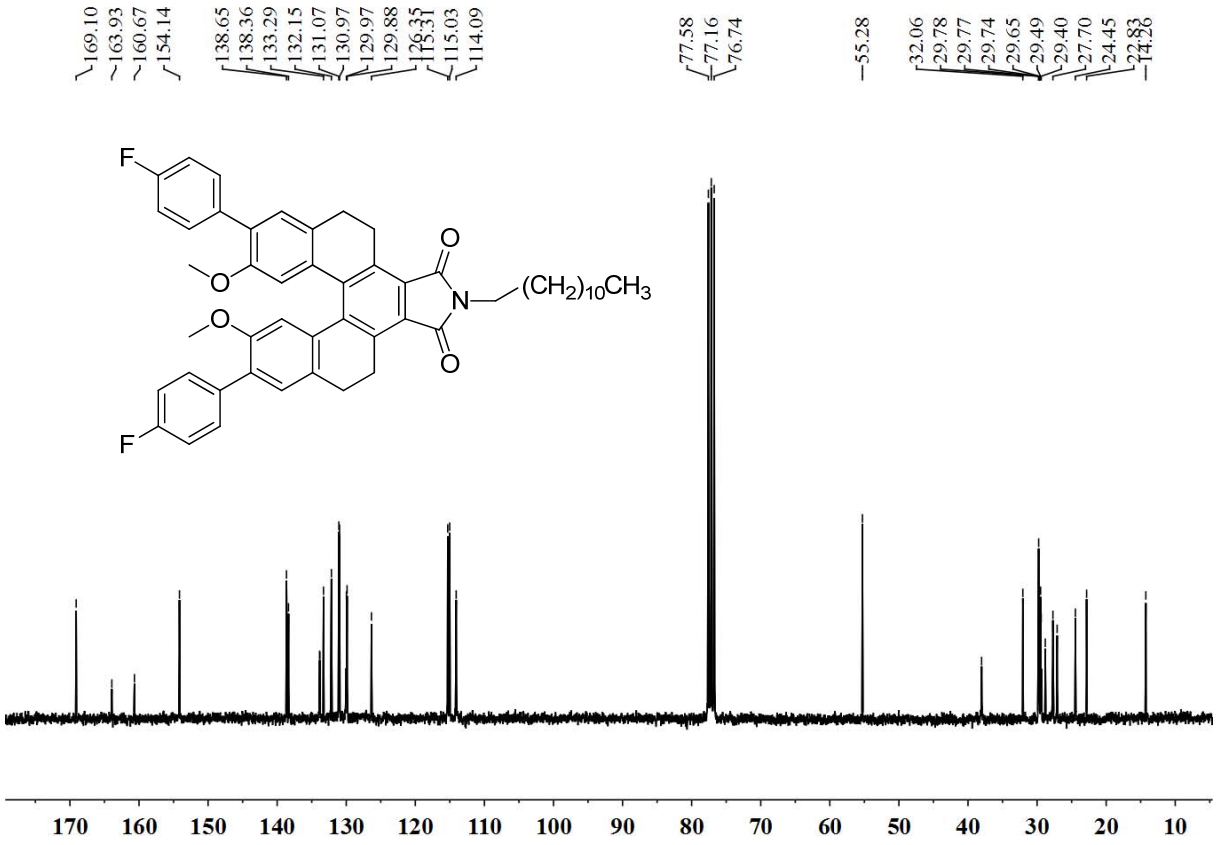


**Fig. S61** $^{13}$C NMR spectrum (75 MHz, $CDCl_3$) of **5f**.

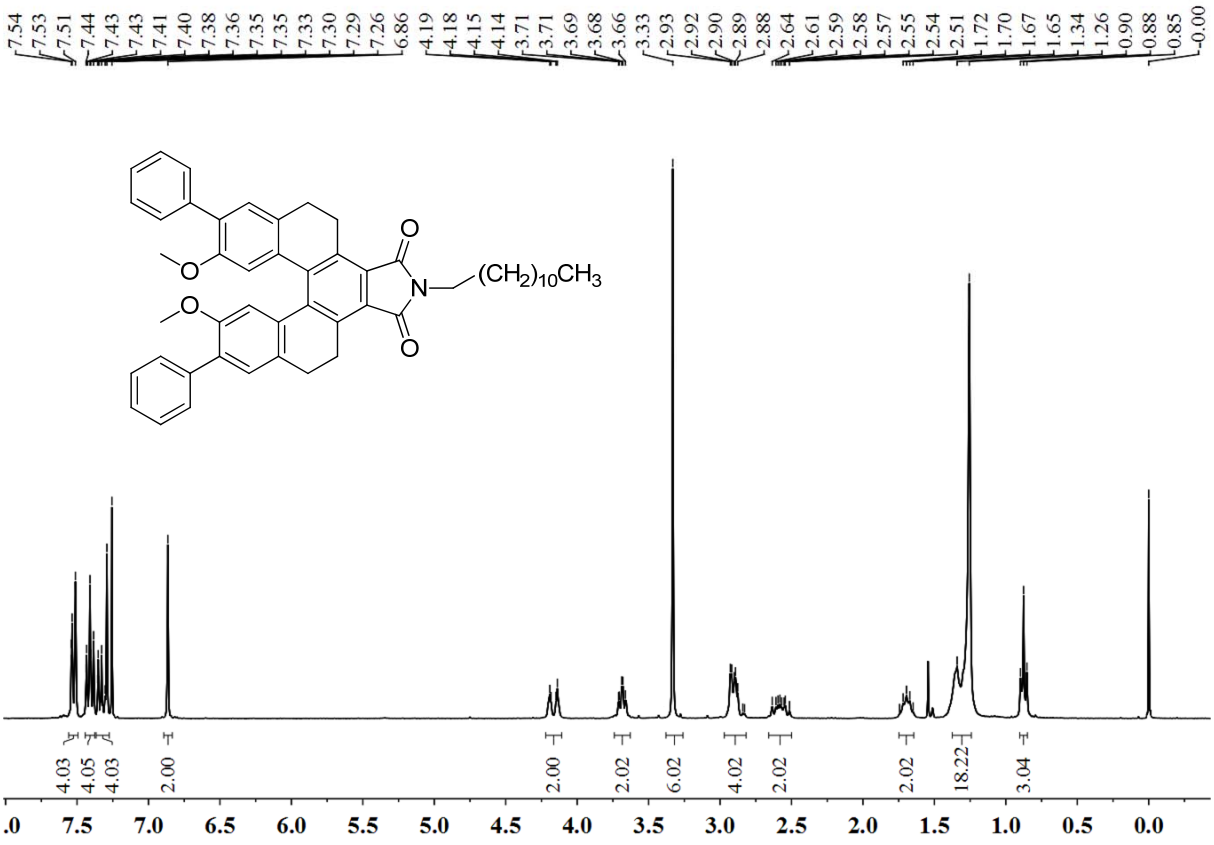


**Fig. S62** $^{1}$H NMR spectrum (300 MHz, $CDCl_3$) of **5g**.

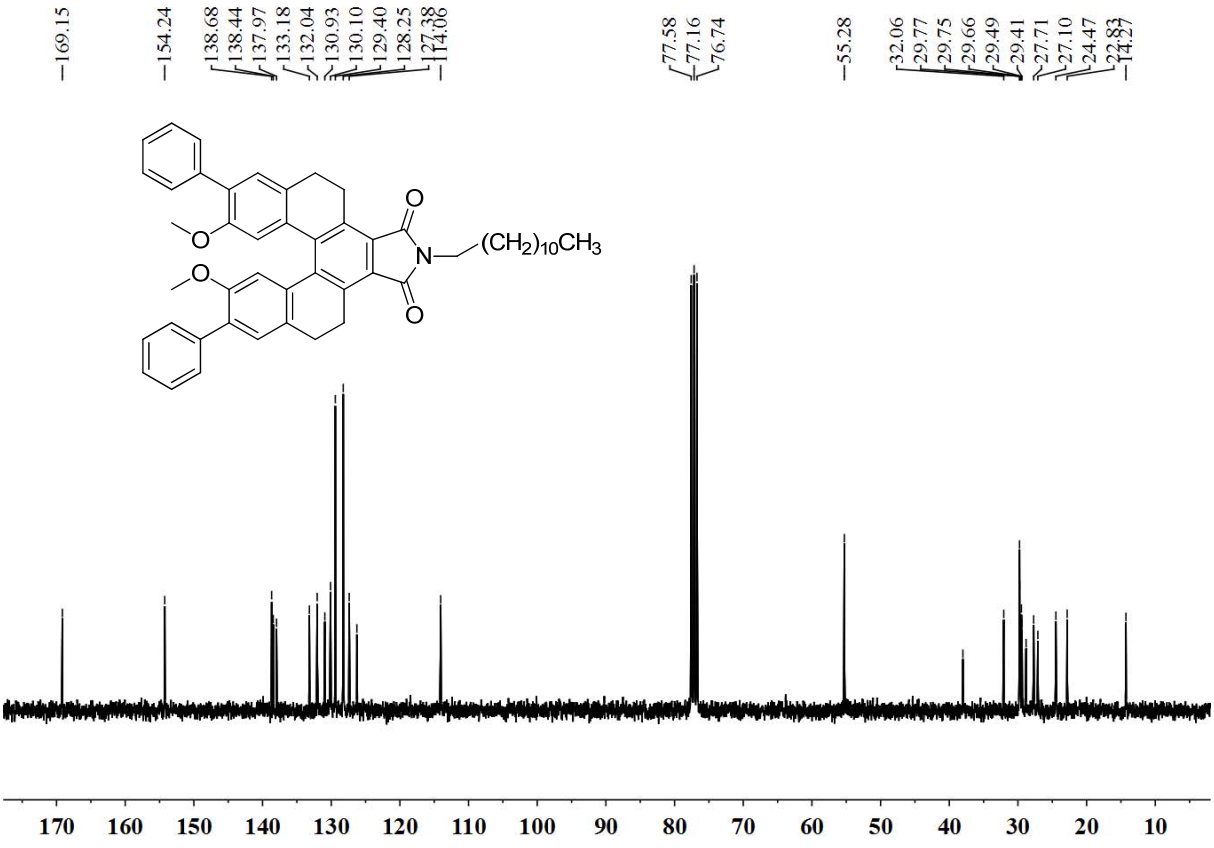


**Fig. S63** $^{13}$C NMR spectrum (75 MHz, $CDCl_3$) of **5g**.

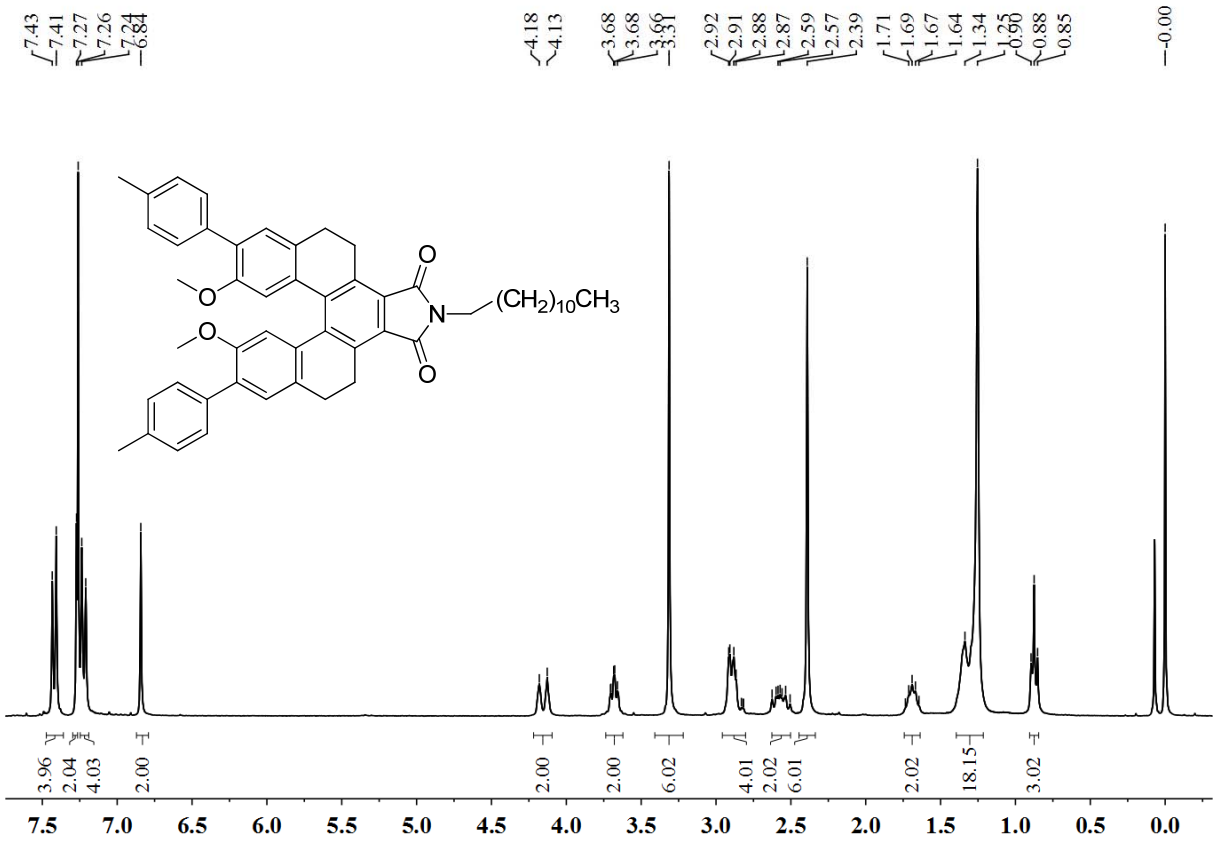


**Fig. S64** $^{1}$H NMR spectrum (300 MHz, $CDCl_3$) of **5h**.

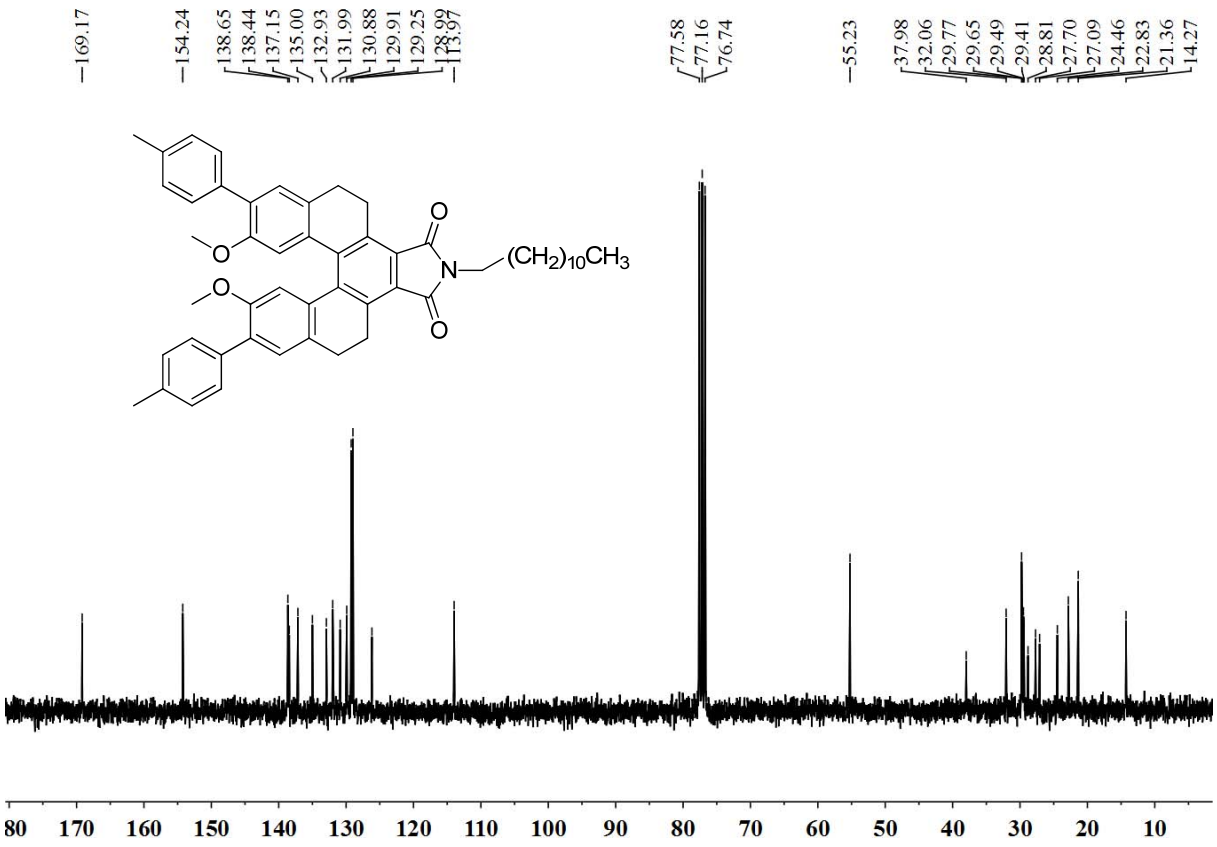


**Fig. S65** $^{13}$C NMR spectrum (75 MHz, $CDCl_3$) of **5h**.

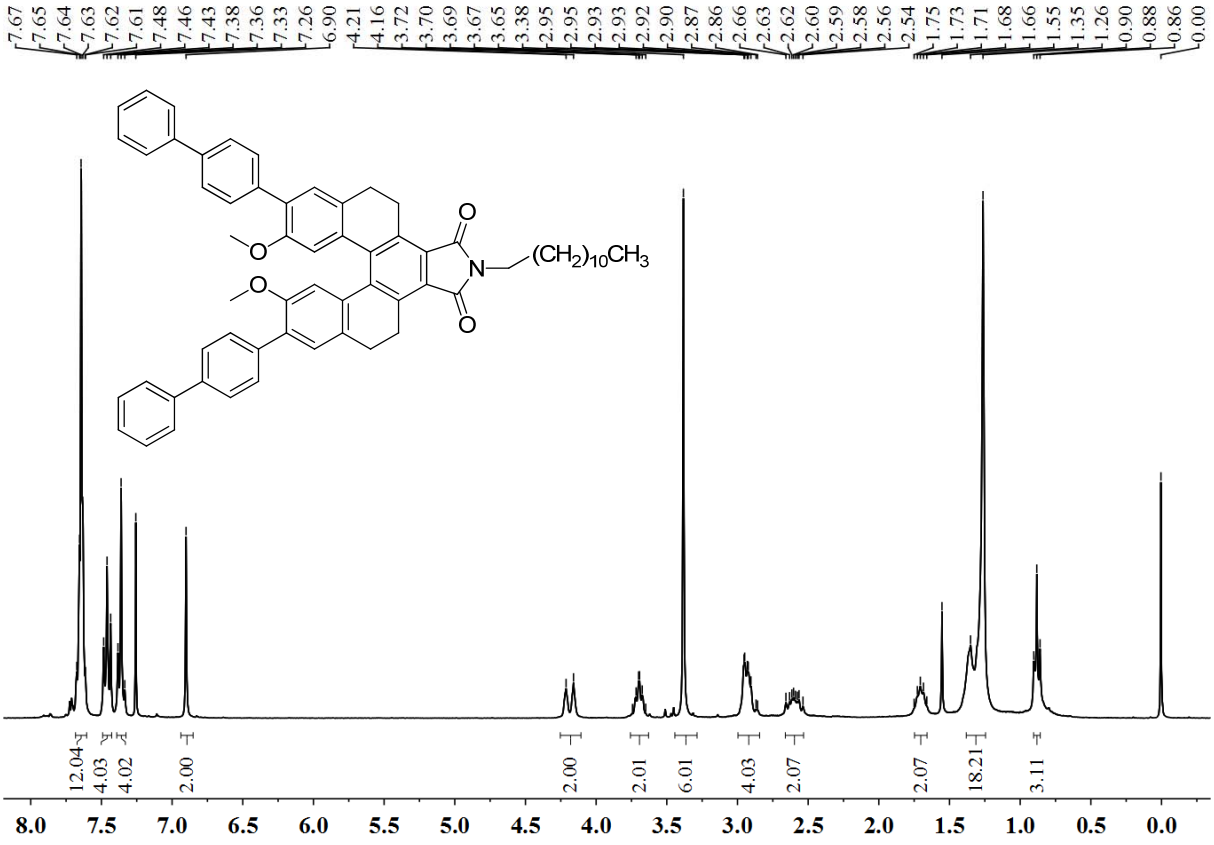


**Fig. S66** $^{1}$H NMR spectrum (300 MHz, $CDCl_3$) of **5i**.

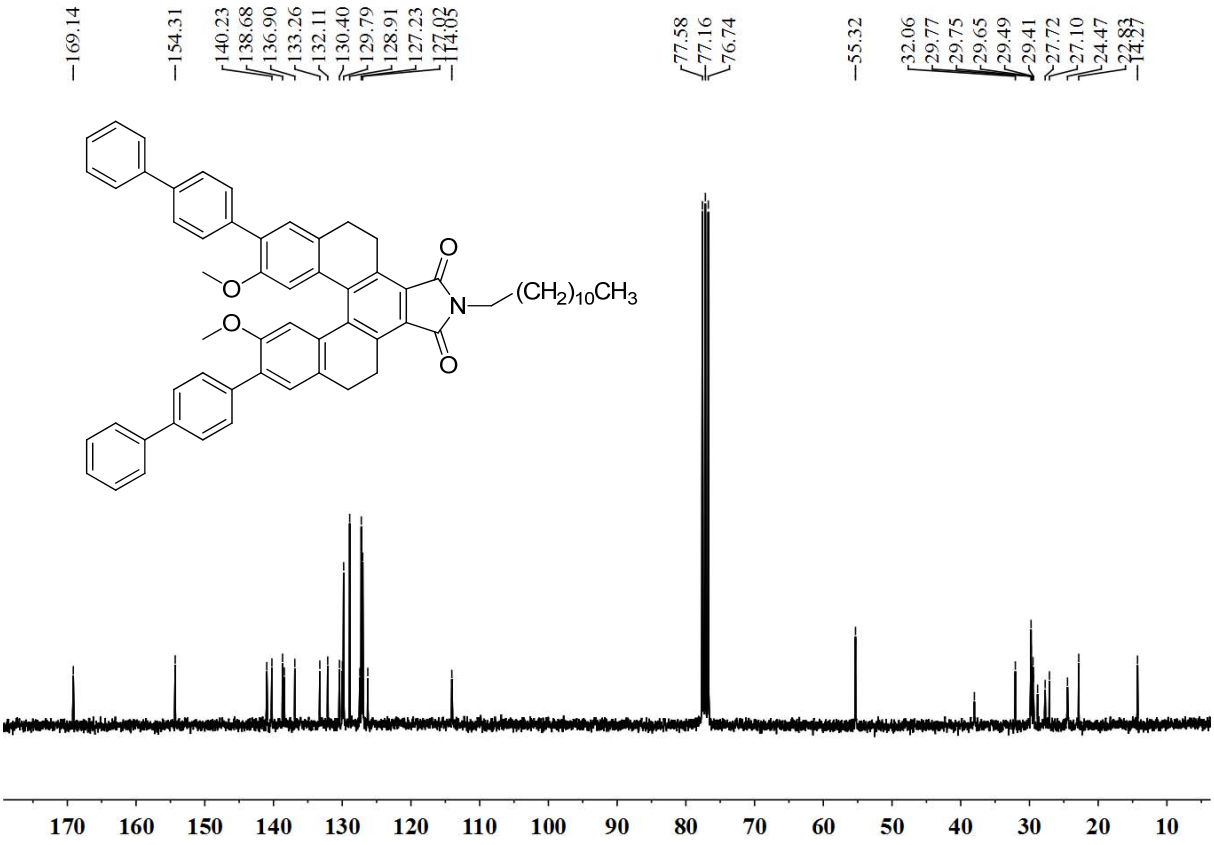


**Fig. S67** $^{13}$C NMR spectrum (75 MHz, $CDCl_3$) of **5i**.

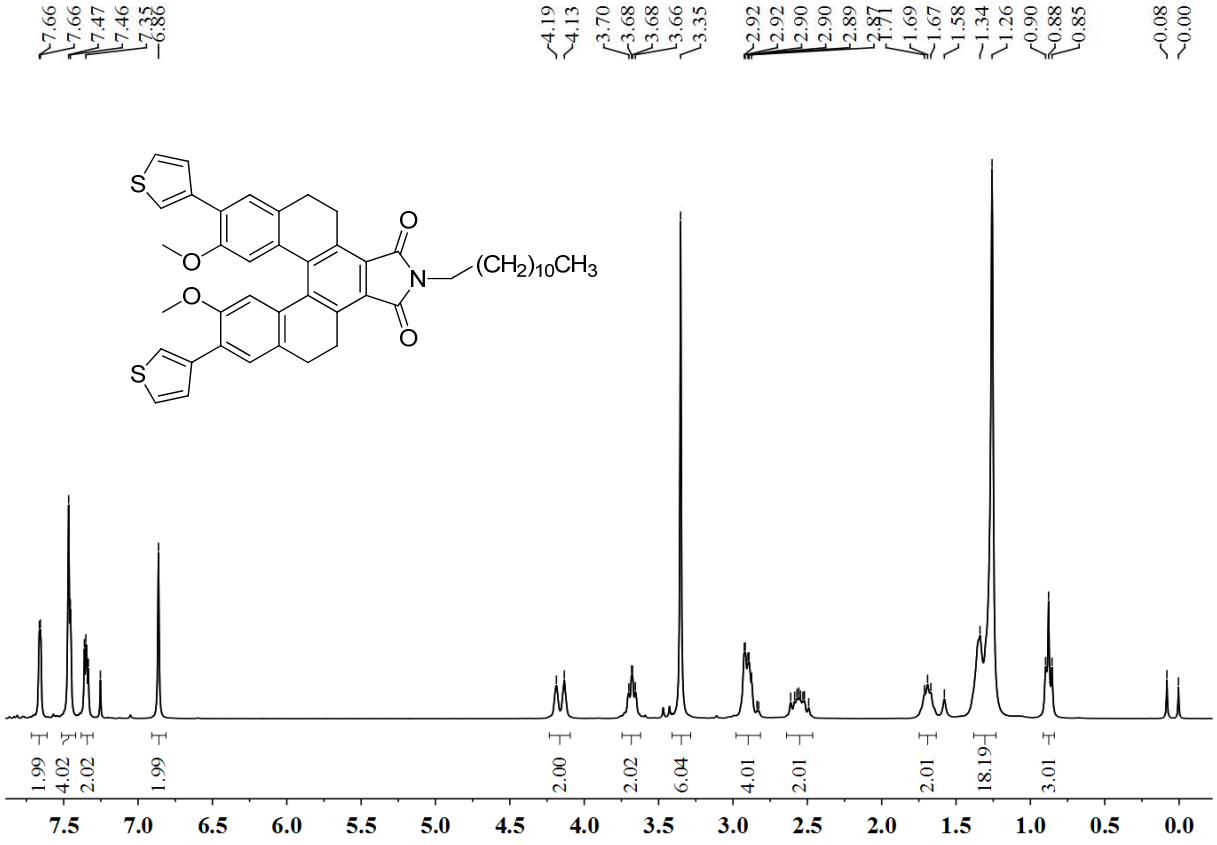


**Fig. S68** $^{1}$H NMR spectrum (300 MHz, $CDCl_3$) of **5j**.

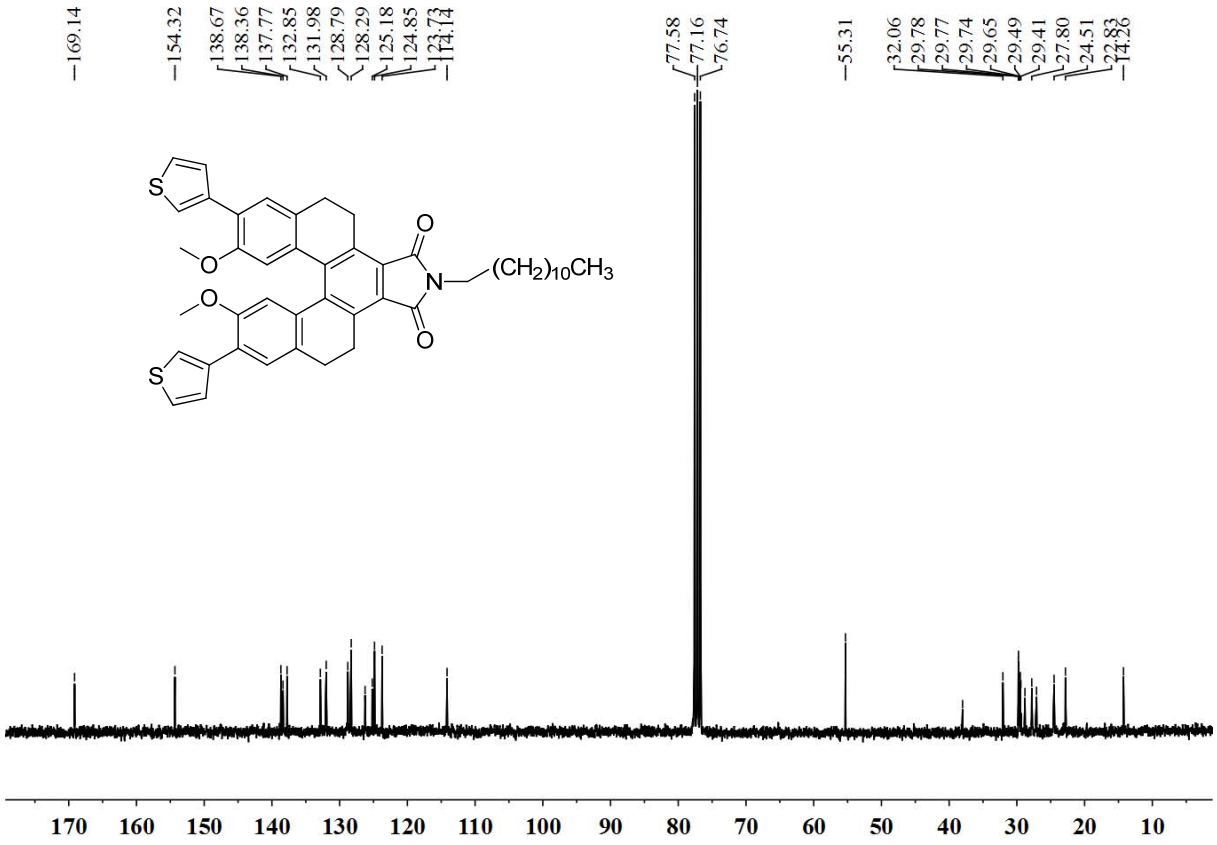


**Fig. S69** $^{13}$C NMR spectrum (75 MHz, $CDCl_3$) of **5j**.

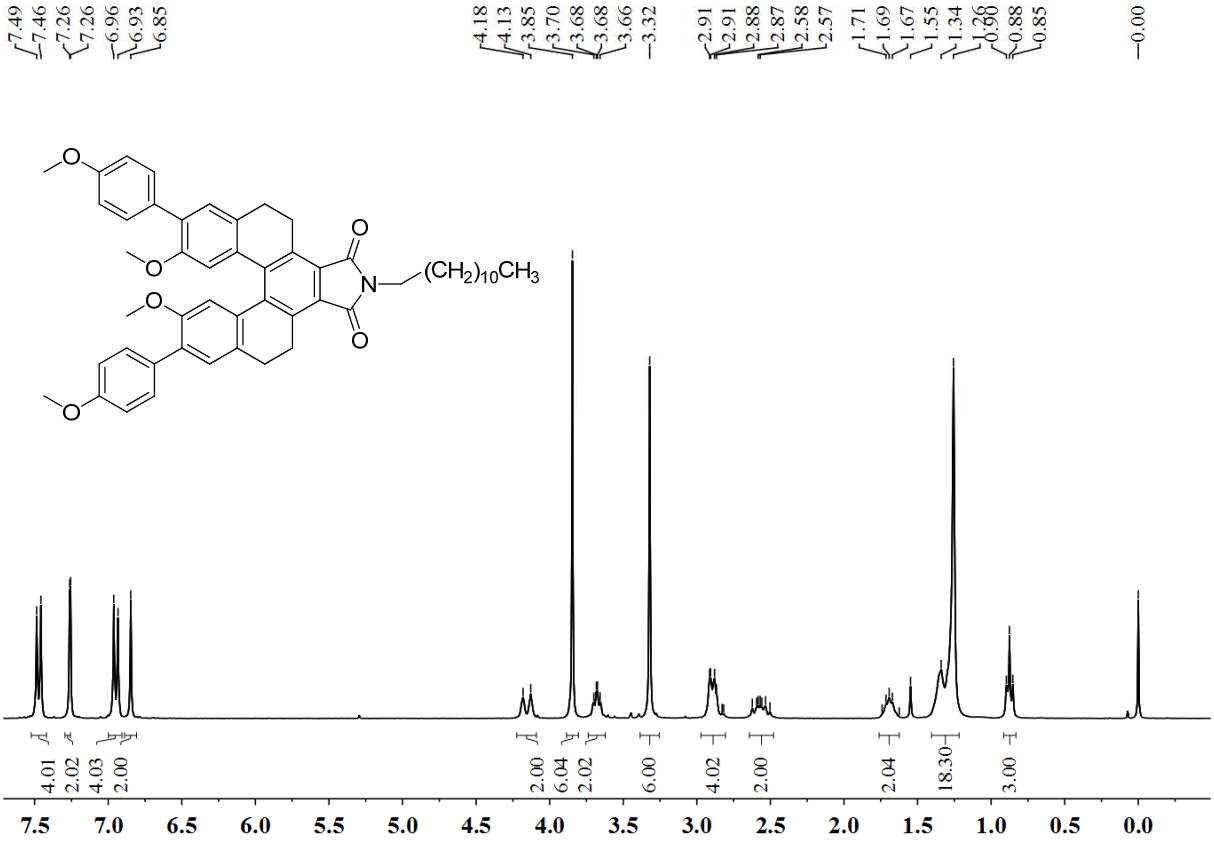


**Fig. S70** $^{1}$H NMR spectrum (300 MHz, $CDCl_3$) of **5k**.

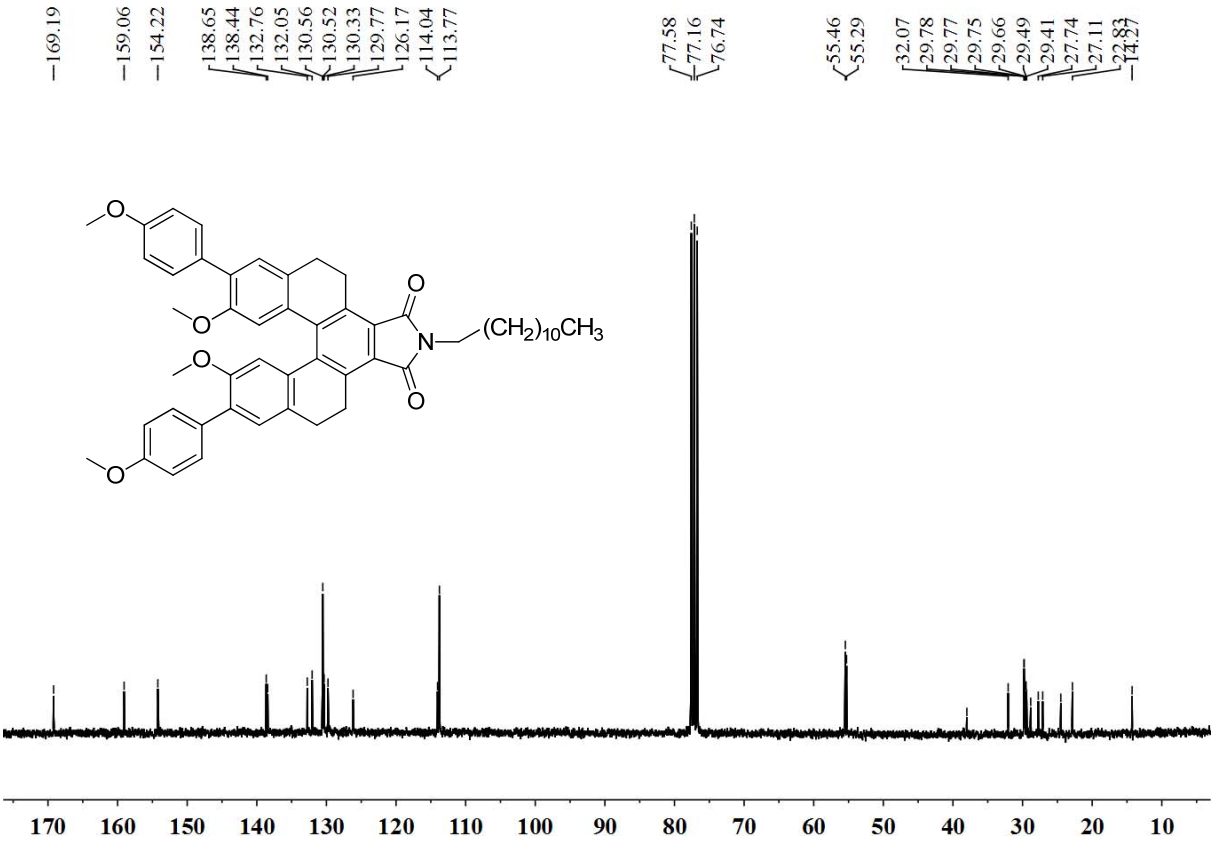


**Fig. S71** $^{13}$C NMR spectrum (75 MHz, $CDCl_3$) of **5k**.

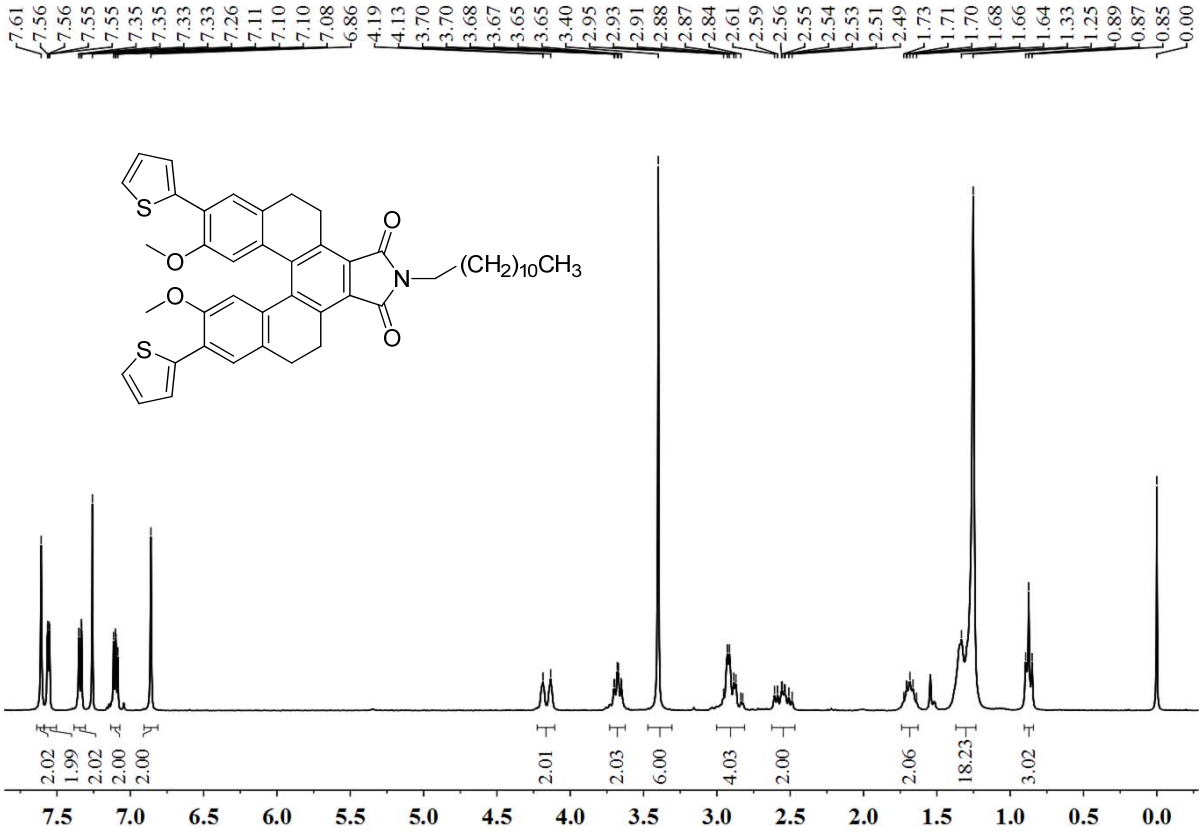


**Fig. S72** $^{1}$H NMR spectrum (300 MHz, $CDCl_3$) of **5l**.

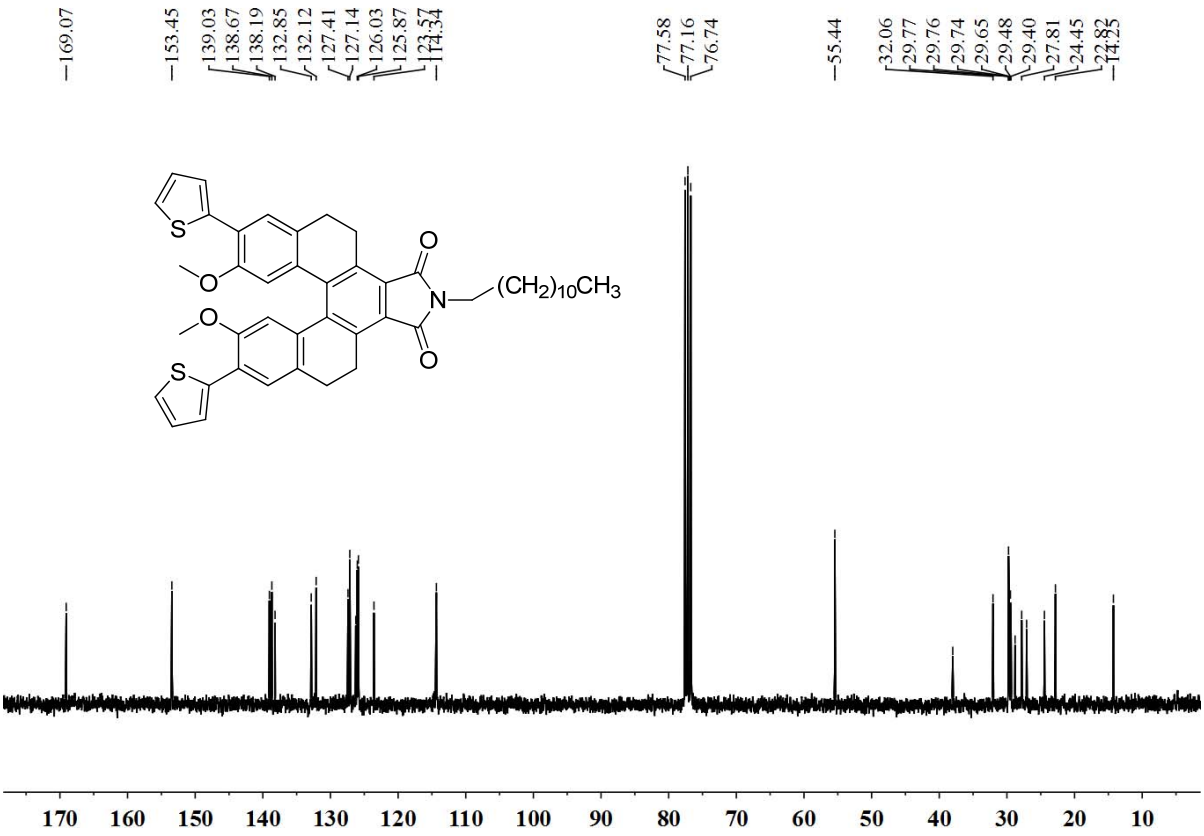


**Fig. S73** $^{13}$C NMR spectrum (75 MHz, $CDCl_3$) of **5l**.

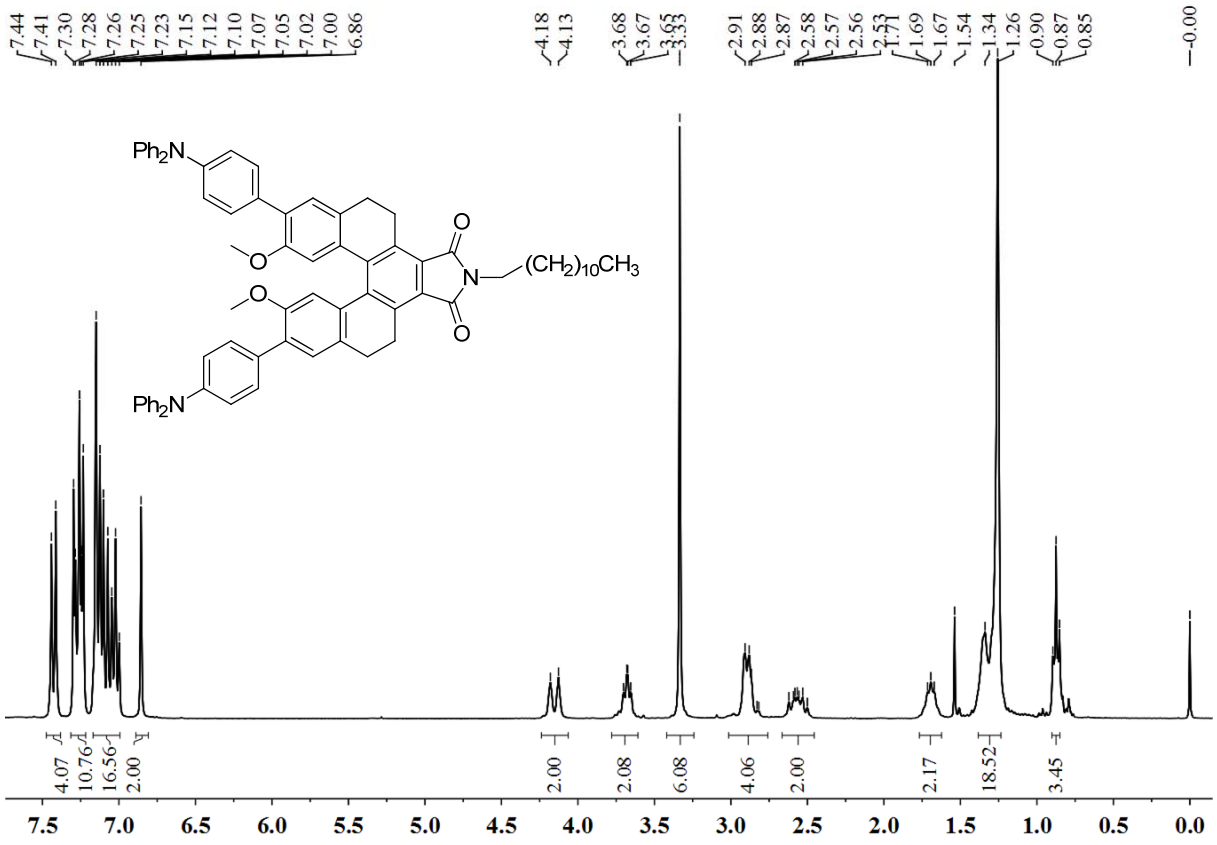


**Fig. S74** $^{1}$H NMR spectrum (300MHz, $CDCl_3$) of **5m**.

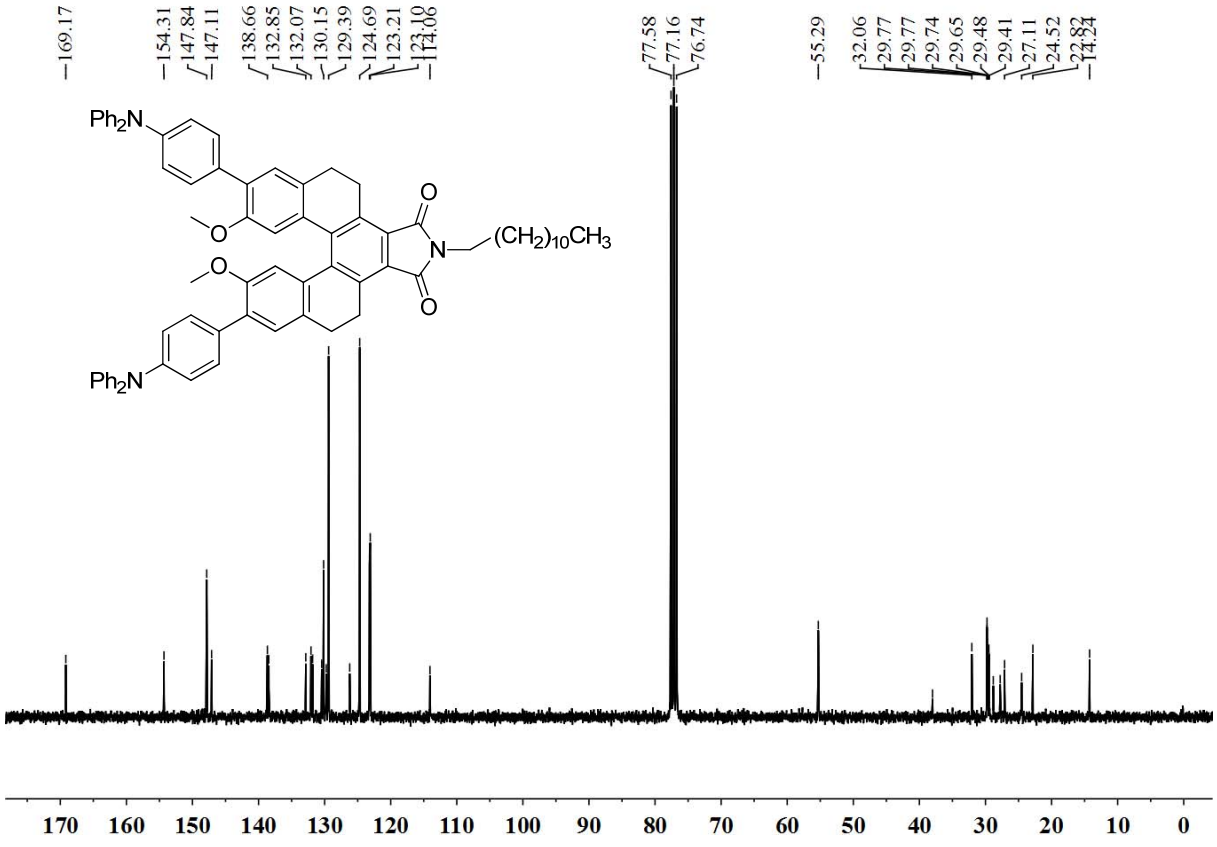


**Fig. S75** $^{13}$C NMR spectrum (75 MHz, $CDCl_3$) of **5m**.

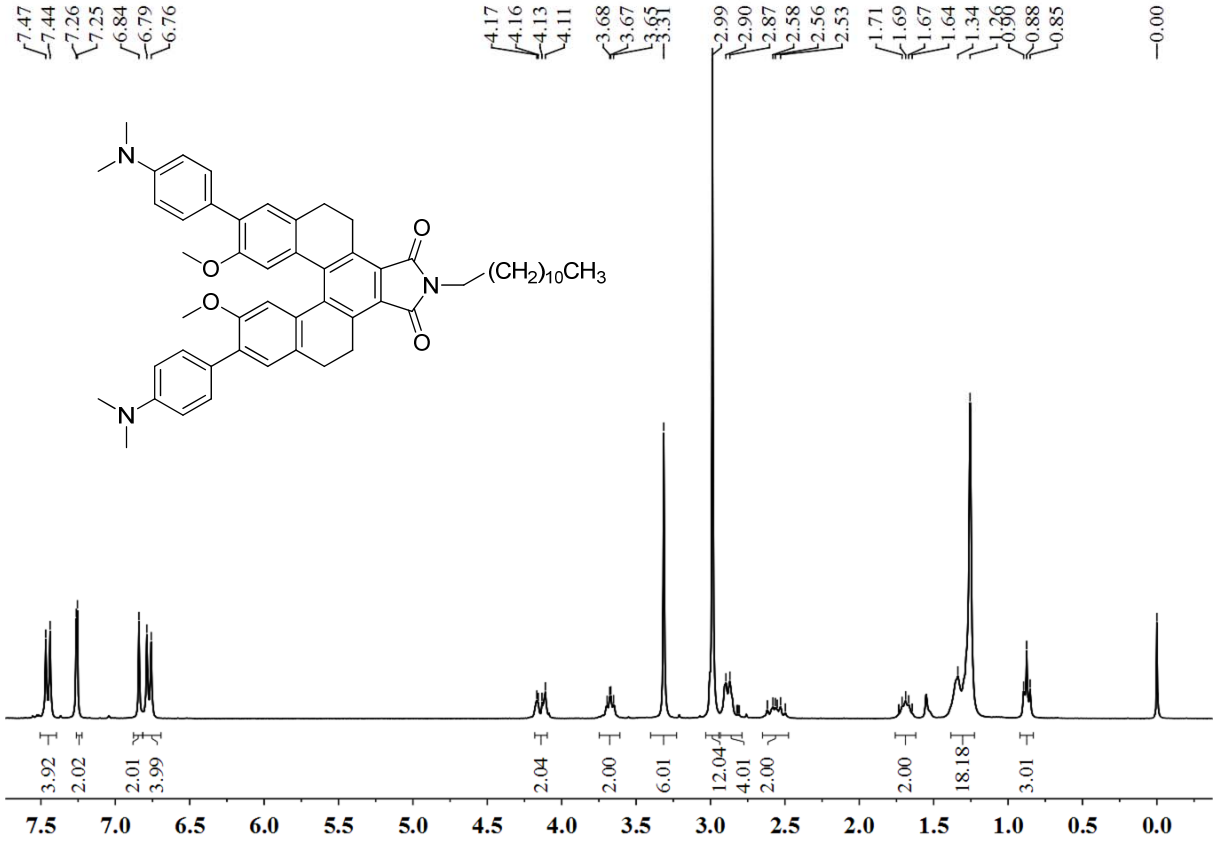


**Fig. S76** $^{1}$H NMR spectrum (300 MHz, $CDCl_3$) of **5n**.

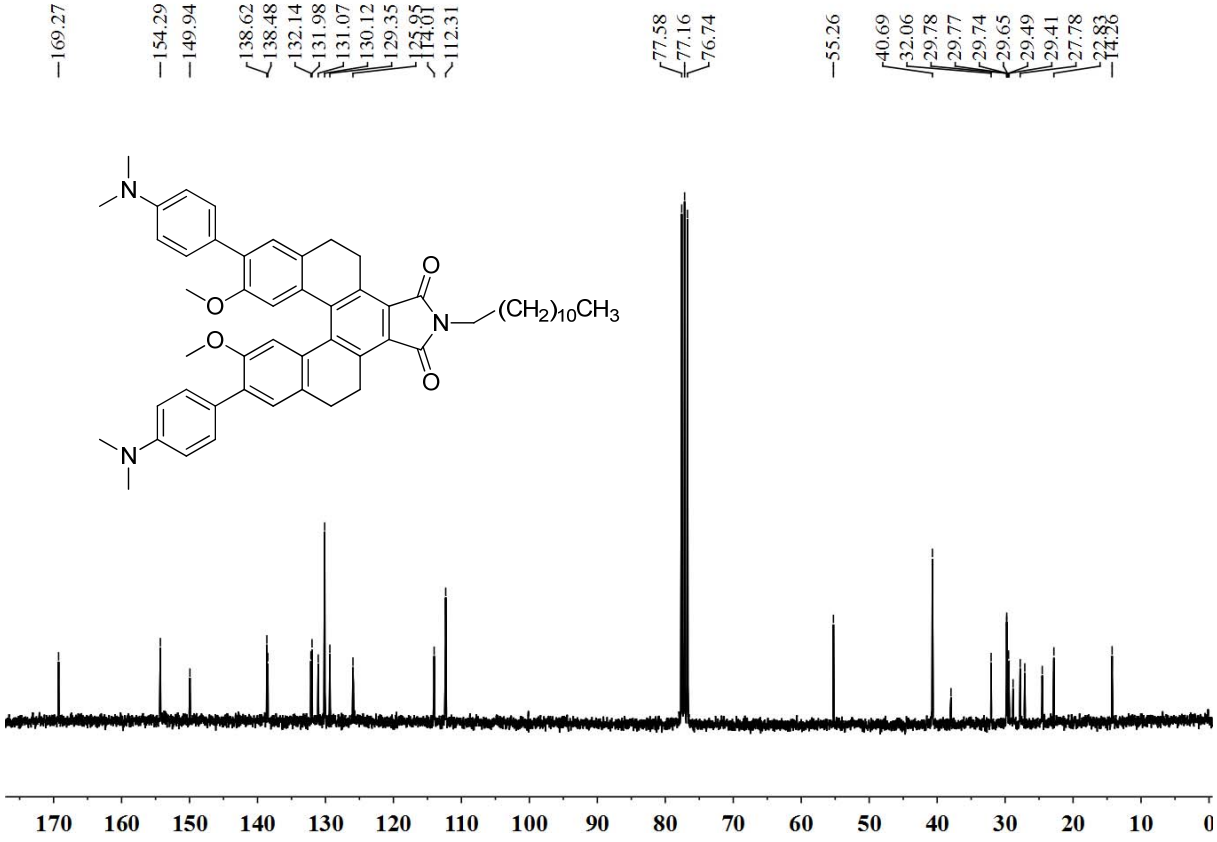


**Fig. S77** $^{13}$C NMR spectrum (75 MHz, $CDCl_3$) of **5n**.

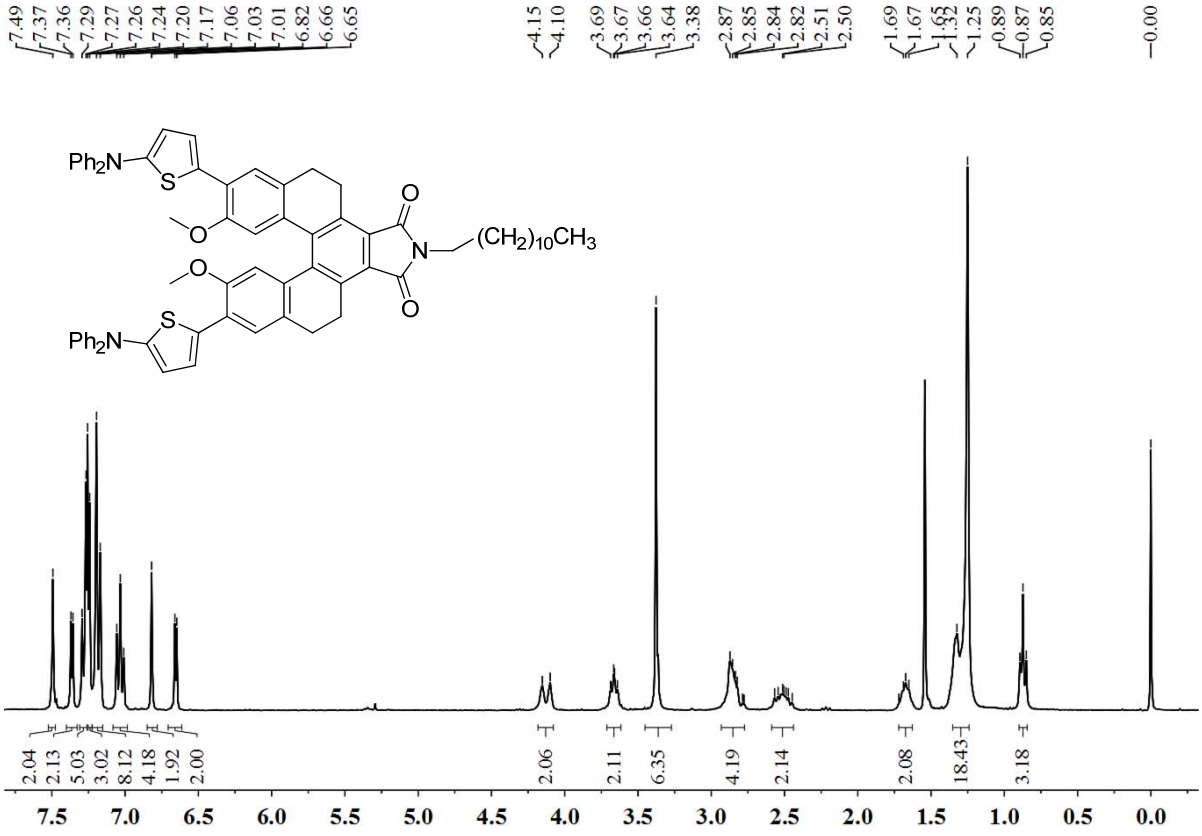


**Fig. S78** $^{1}$H NMR spectrum (300 MHz, $CDCl_3$) of **5o**.

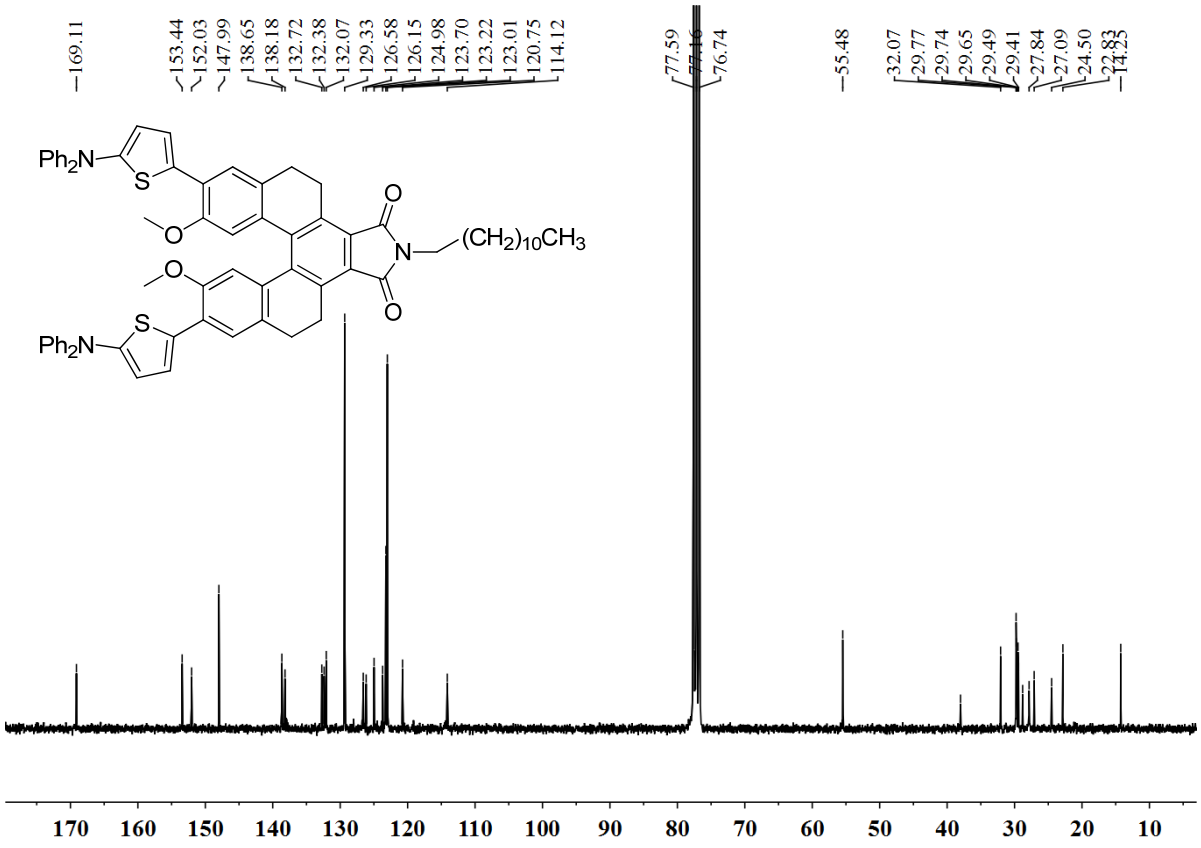


**Fig. S79** $^{13}$C NMR spectrum (75 MHz, $CDCl_3$) of **5o**.

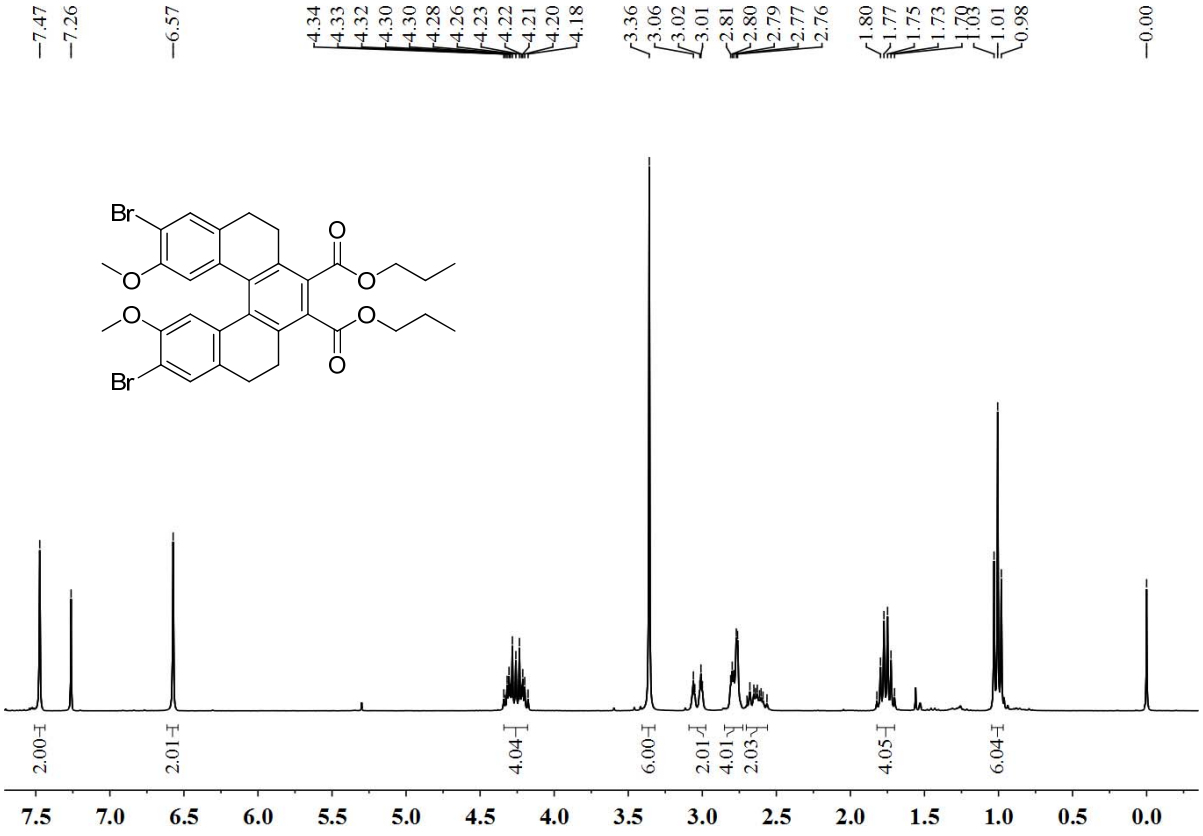


**Fig. S80** $^{1}$H NMR spectrum (300 MHz, $CDCl_3$) of **6**.

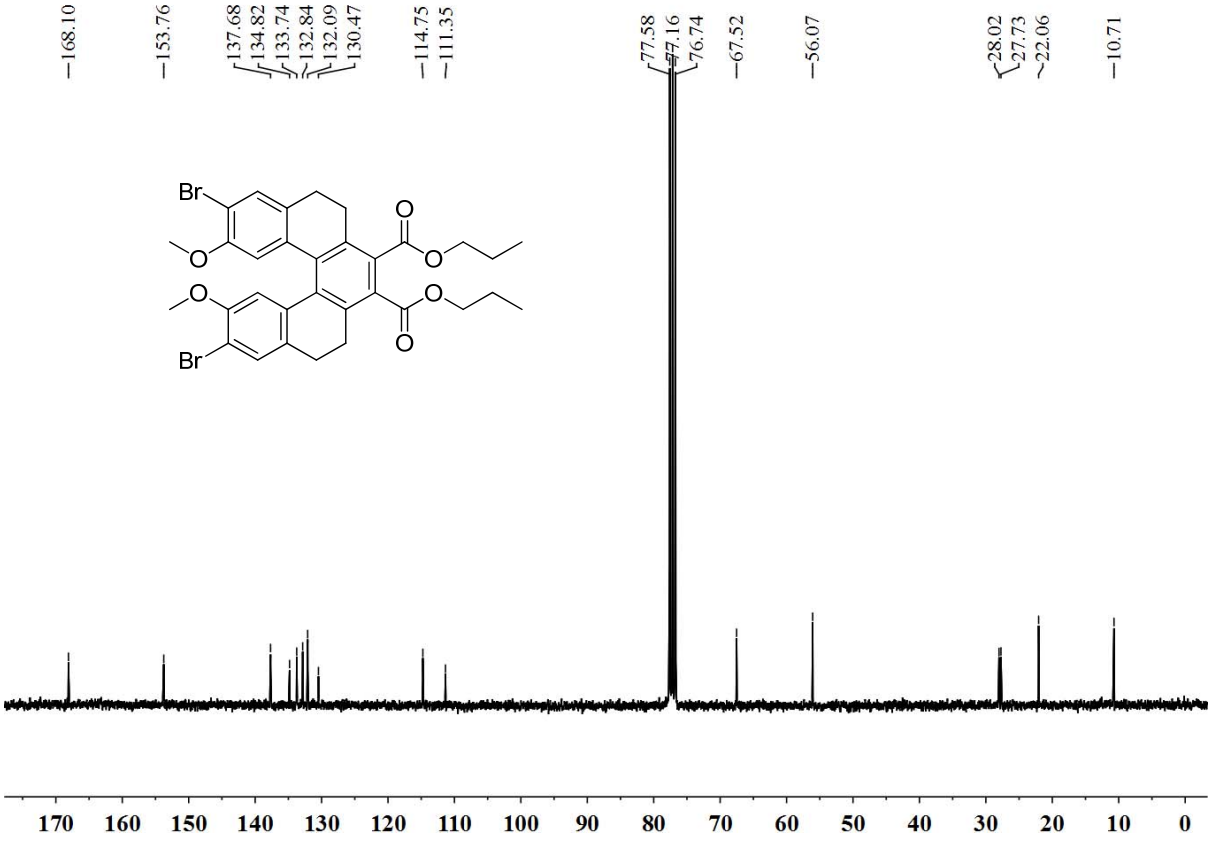


**Fig. S81** $^{13}$C NMR spectrum (75 MHz, $CDCl_3$) of **6**.

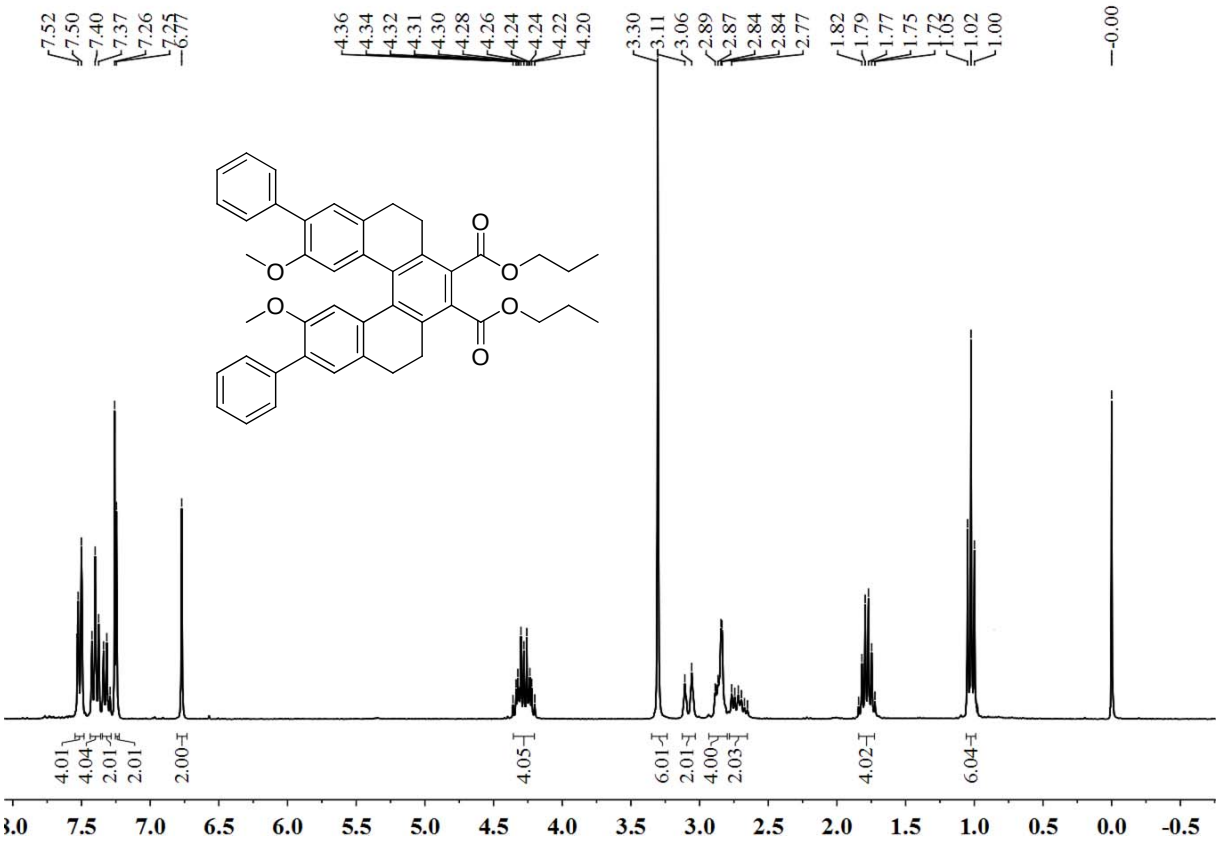

**Fig. S82** $^{1}$H NMR spectrum (300 MHz, $CDCl_3$) of **7**.

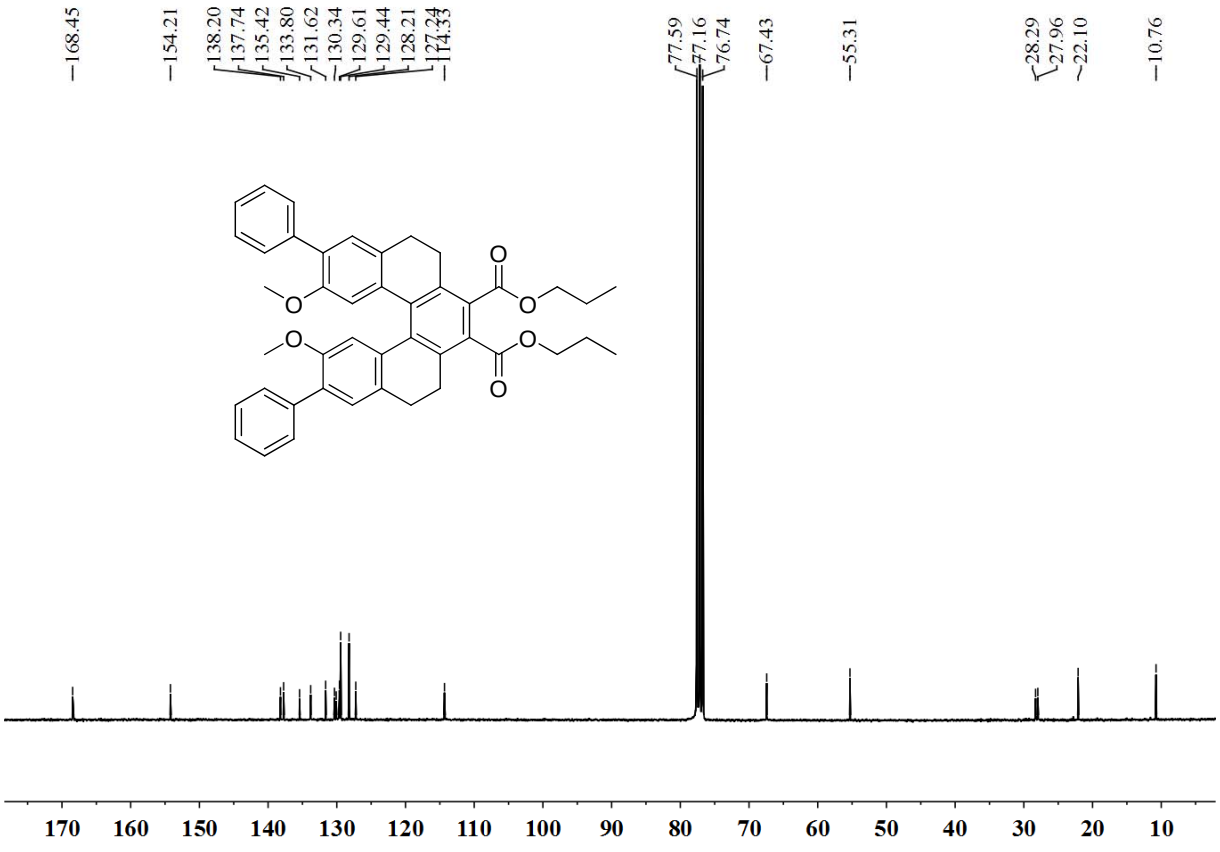

**Fig. S83** $^{13}$C NMR spectrum (75 MHz, $CDCl_3$) of **7**.

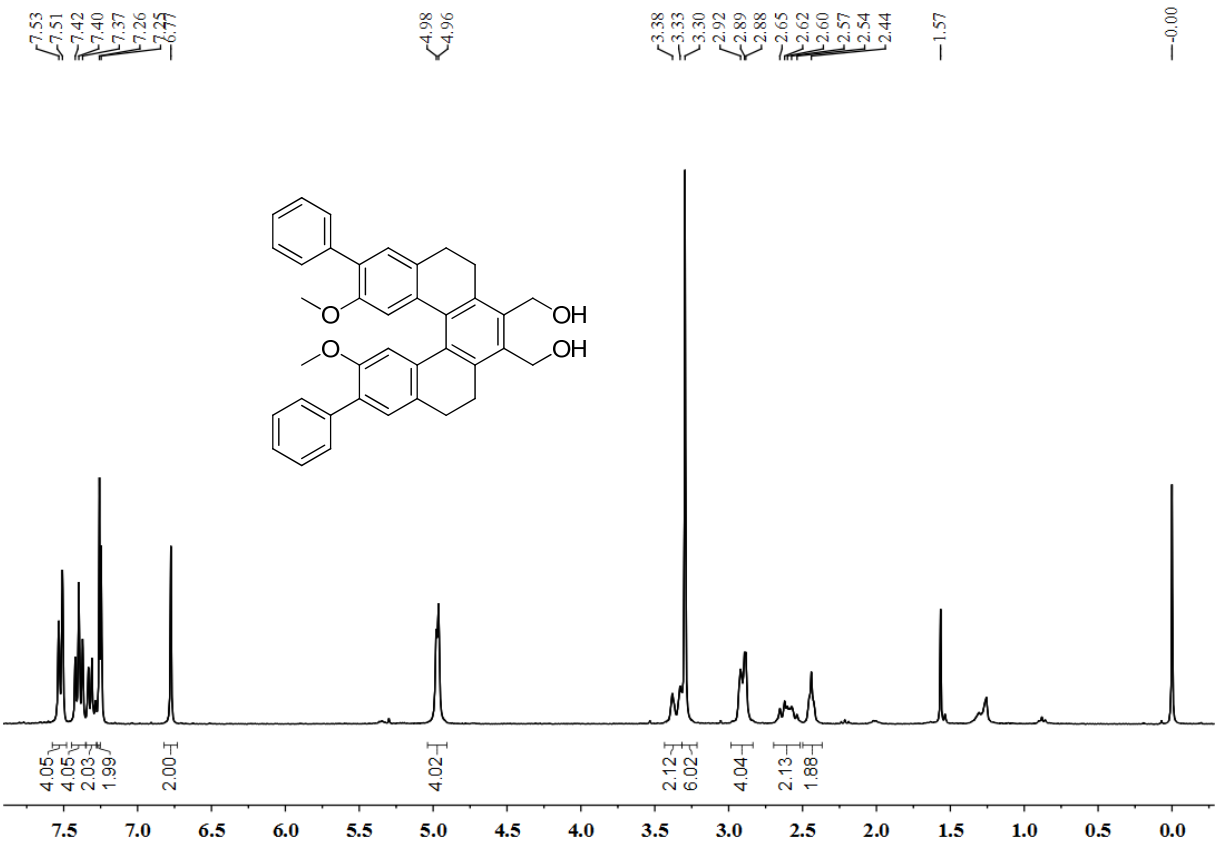


**Fig. S84** $^{1}$H NMR spectrum (300 MHz, $CDCl_3$) of **8**.

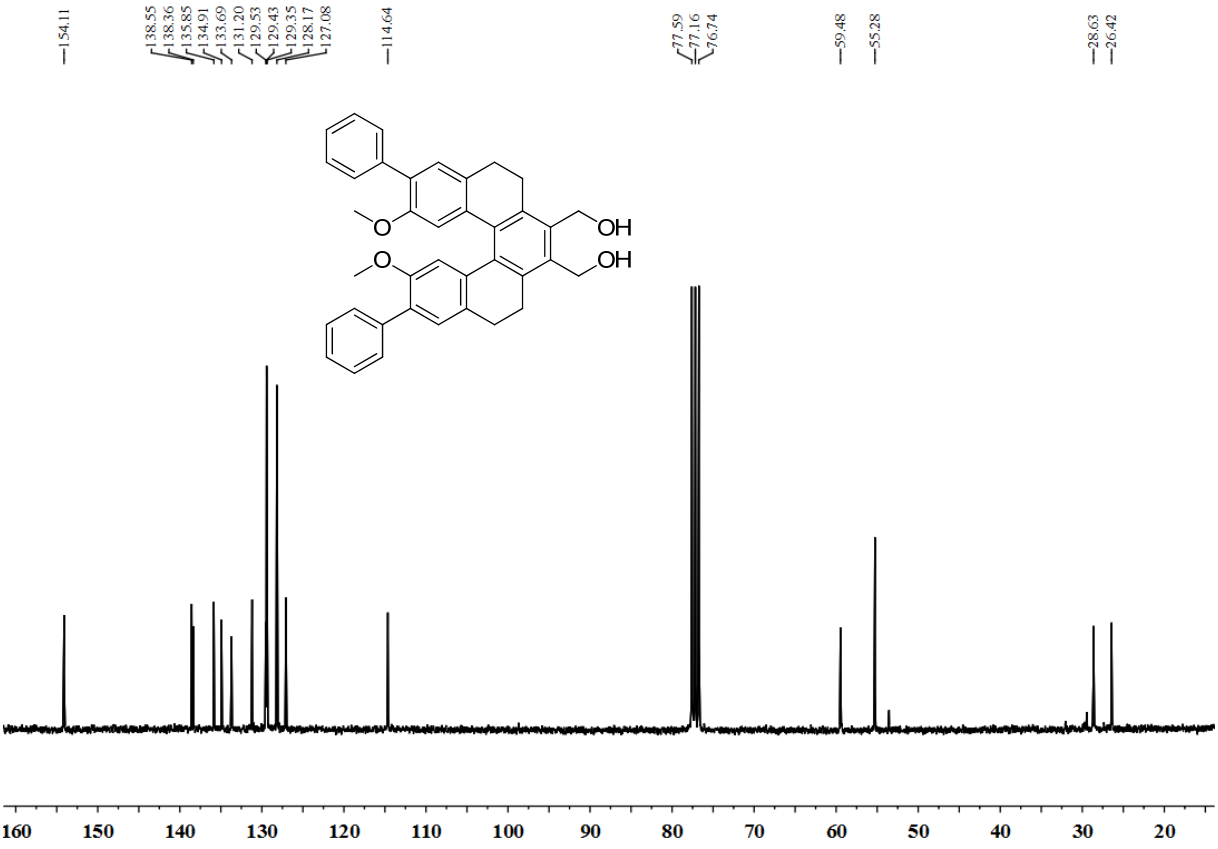


**Fig. S85** $^{13}$C NMR spectrum (75 MHz, $CDCl_3$) of **8**.