

Supplementary Information

Conjugated Figure-of-eight Macrocycles Derived from Anthracene Photodimer: Synthetic Execution through Intramolecular Cyclization and Topological Manipulation through Ring Expansion

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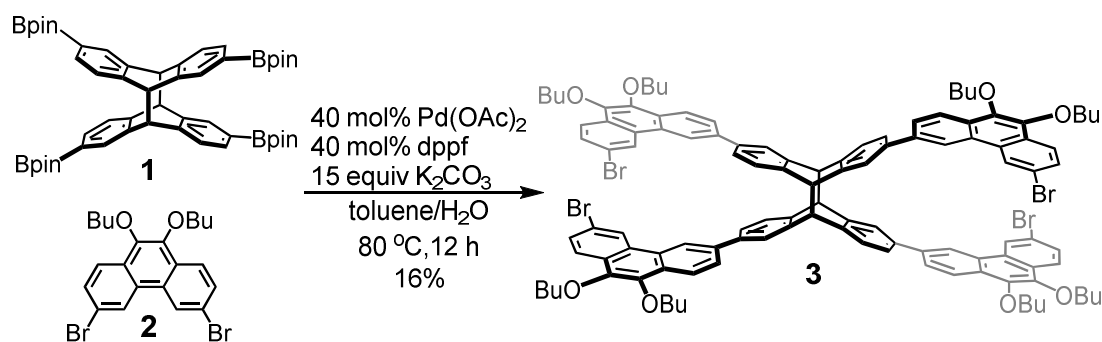
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I. General Information

^1H and ^{13}C NMR spectra were recorded with a Bruker Avance 400 or Ascend 600 spectrometer at 25 °C and were internally referenced to residual protio solvent signals (for example, CDCl_3 was referenced at 7.26 and 77.16 ppm, respectively)^[S1]. Data for ^1H NMR were reported as follows: chemical shift (δ ppm), integration, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), and coupling constant (Hz) when applicable. ^{13}C NMR spectra were recorded with complete proton decoupling. Infrared spectra were recorded on a Varian 3100 FT-IR. High-resolution mass spectra were obtained on a Bruker SolariX XR Fourier transform ion cyclotron mass spectrometer. UV-Vis spectra were recorded in 1 cm quartz cuvette using a Varian Cary 5000 UV-Vis spectrometer. The absolute singlet quantum yield, emission lifetime and fluorescence spectra were measured using an Edinburgh FLS1000 or FLSP920 spectrometer. The electronic circular dichroism spectra were measured using a Jasco J-815 spectrometer. The circularly polarized luminescence spectra were measured using a Jasco CPL-200 spectrometer. The specific rotations were measured using an SGW-2 Polarimeter.

All reactions were carried out using flame-dried glassware under a nitrogen atmosphere unless otherwise noted. The microwave reactions were conducted using a Biotage Initiator microwave reactor. Analytical thin layer chromatography (TLC) was performed using 0.25 mm silica gel 60-F plates. Flash chromatography was performed using 200-400 mesh silica gel. HPLC-grade tetrahydrofuran, dichloromethane, toluene, and hexanes were purified and dried by passing through a PURE SOLV® solvent purification system (Innovative Technology, Inc.). Deionized water was degassed by bubbling with nitrogen balloon for 20 min prior to use as reaction solvent. Chemical reagents were purchased from Strem, Adamas, Acros, Energy Chemicals, J&K, and Alfa Aesar, and were used as received.

II. Experimental Procedures and Compound Characterization



In a nitrogen-filled glove box, Pd(OAc)₂ (1.8 mg, 0.008 mmol, 40 mol%), dppf (4.4 mg, 0.008 mmol, 40 mol%), and anhydrous toluene (5 mL) were added to a 40 mL glass vial equipped with a stir bar. The mixture was stirred in the glove box at room temperature for 30 min. Then compound **1** (17.2 mg, 0.020 mmol, 1.0 equiv, prepared according to literature^[S2]), compound **2** (95 mg, 0.20 mmol, 10 equiv, prepared according to literature^[S3]), K₂CO₃ (41.4 mg, 0.30 mmol, 15 equiv) and anhydrous toluene (25 mL) were added to the 40 mL glass vial. The vial was sealed with a Teflon-lined septum cap then transferred out of glove box. Degassed water (3 mL) was subsequently added to the vial via a syringe, and the puncture in the septum cap was covered with vacuum grease. The reaction mixture was stirred at 80 °C for 12 h, and cooled to room temperature. Four reactions were carried out in parallel using identical procedures, and all the reaction mixtures were combined during work-up. The combined reaction mixture was extracted with ethyl acetate (30 mL × 3). The combined organic layers were washed with brine, and dried over sodium sulfate. The solvents were removed under reduced pressure. Purification using silica gel column chromatography (CH₂Cl₂: petroleum ether = 1:2) afforded compound **3** (25.1 mg, 16% yield) as a white solid.

Compound **3**

R_f = 0.30 (CH₂Cl₂: petroleum ether = 1:2);

¹H NMR (400 MHz, CDCl₃) δ 8.78 (s, 4H), 8.59 (s, 4H), 8.29 (d, *J* = 8.5 Hz, 4H), 8.12 (d, *J* = 8.7 Hz, 4H), 7.80 (d, *J* = 8.5 Hz, 4H), 7.70 (d, *J* = 8.7 Hz, 4H), 7.53 (s, 4H), 7.31 (d, *J* = 7.7 Hz, 4H), 7.25 (d, *J* = 7.7 Hz, 4H), 4.98 (s, 4H), 4.27–4.19 (m, 16H), 1.96–1.85 (m, 16H), 1.69–1.57 (m, 16H), 1.09–1.01 (m, 24H);

^{13}C NMR (151 MHz, CDCl_3) δ 144.3, 143.6, 143.0, 142.9, 139.0, 138.9, 130.2, 130.0, 129.1, 128.8, 128.1, 127.9, 126.8, 126.5, 125.5, 125.1, 124.3, 123.0, 120.8, 120.2, 73.6, 73.5, 53.9, 32.72, 32.68, 19.63, 19.61, 14.19, 14.16;

IR (film): 2957, 2931, 2871, 1591, 1480, 1434, 1318, 820 cm^{-1} ;

HRMS (MALDI): $[\text{M}]^+$ calcd. for $\text{C}_{116}\text{H}_{112}\text{Br}_4\text{O}_8$ 1948.5085, found 1948.4990.

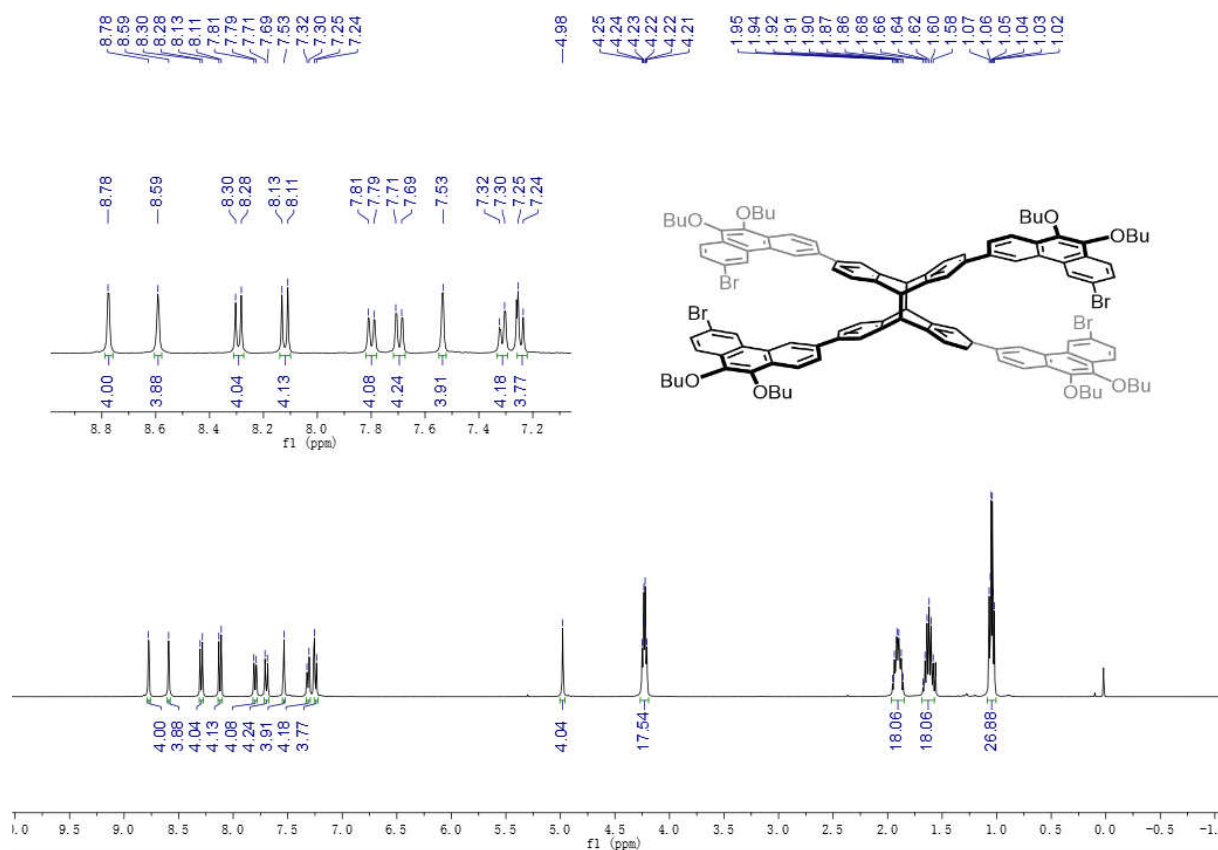


Figure S1. ^1H NMR spectrum (CDCl_3 , 400 MHz) of compound **3**.

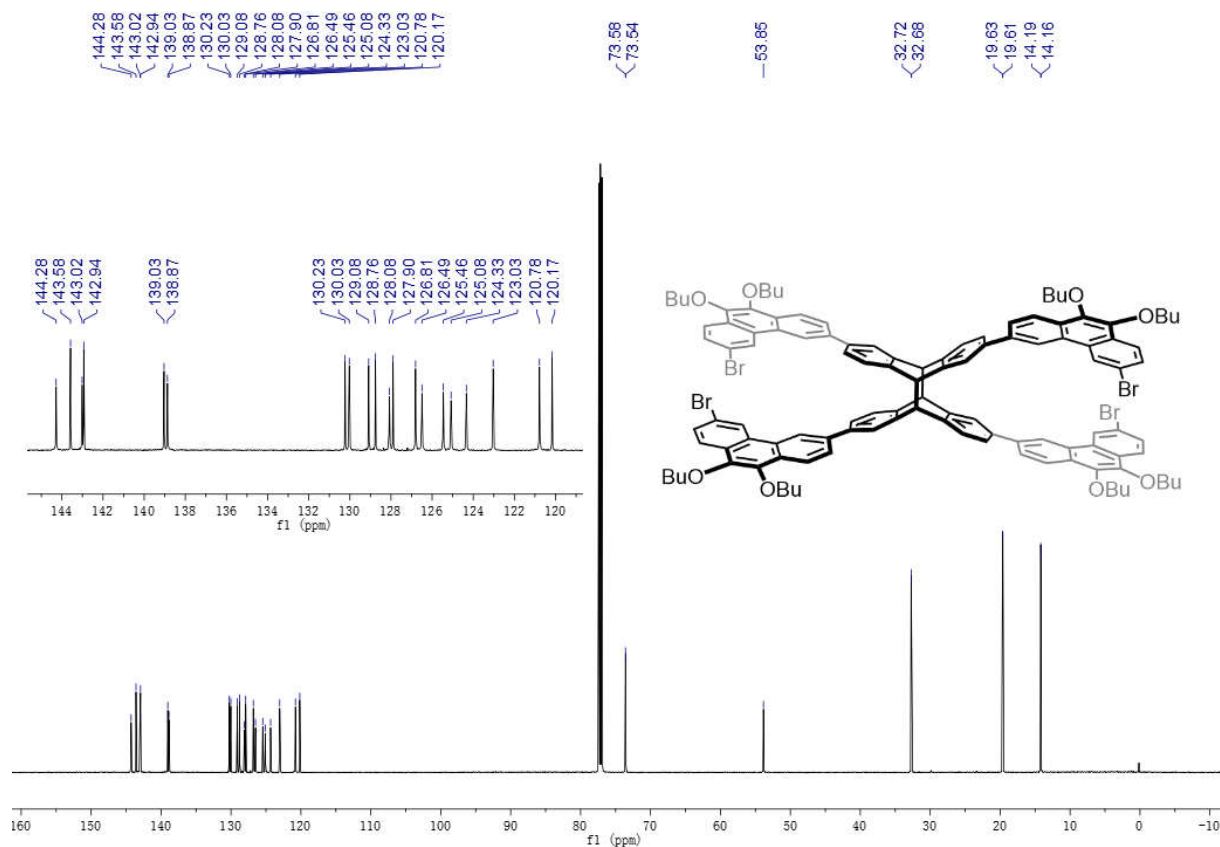
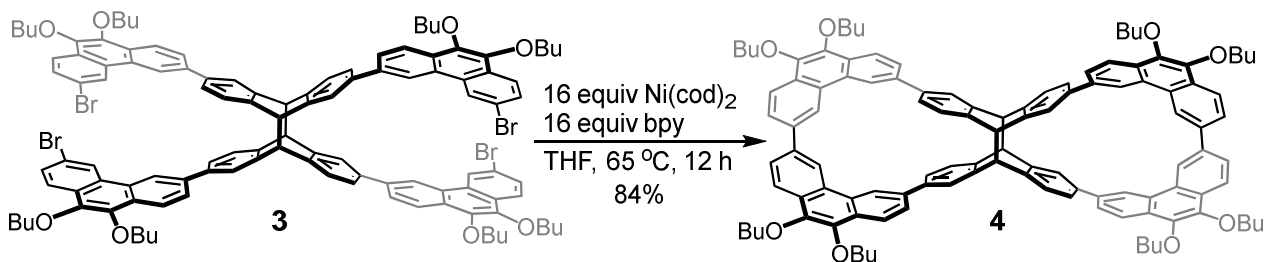


Figure S2. ¹³C NMR spectrum (CDCl₃, 151 MHz) of compound **3**.



In a nitrogen-filled glove box, Ni(cod)_2 (868 mg, 3.9 mmol, 16 equiv), 2,2'-bipyridyl (602 mg, 3.9 mmol, 16 equiv), and anhydrous THF (390 mL) were sequentially added to a 500 mL round-bottom flask equipped with a stir bar. The flask was capped with a rubber septum, transferred out of glove box, and stirred at 65 °C for 15 min. Meanwhile, compound **3** (471 mg, 0.24 mmol, 1.0 equiv) and anhydrous THF (10 mL) were mixed in a 40 mL glass vial in the glove box. The vial was capped, and transferred out of the glove box. The solution of compound **3** was added to the flask containing nickel complex. The mixture was stirred at 65 °C for 12 h, and cooled to room temperature, and filtered through a short pad of silica gel with the aid of mixed solvents (CH_2Cl_2 : ethyl acetate = 2:1). The solvents were removed under reduced pressure. Purification using silica gel column chromatography (CH_2Cl_2 : petroleum ether = 2:3) afforded compound **4** (331 mg, 84% yield) as a white solid.

Compound **4**

$R_f = 0.30$ (CH_2Cl_2 : petroleum ether = 2:3);

$^1\text{H NMR}$ (600 MHz, CDCl_3) δ 9.34 (s, 4H), 8.75 (s, 4H), 8.34 (d, $J = 8.6$ Hz, 4H), 8.27 (d, $J = 8.3$ Hz, 4H), 8.15 (d, $J = 8.7$ Hz, 4H), 7.68 (d, $J = 8.2$ Hz, 4H), 7.28 (s, 4H), 7.13 (d, $J = 8.6$ Hz, 4H), 7.06 (d, $J = 7.5$ Hz, 4H), 4.80 (s, 4H), 4.38–4.24 (m, 16H), 2.01–1.90 (m, 16H), 1.72–1.60 (m, 16H), 1.11–1.03 (m, 24H);

$^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 144.1, 144.0, 143.6, 142.8, 141.0, 140.5, 137.9, 129.2, 128.92, 128.89, 128.61, 128.56, 126.7, 126.1, 125.9, 124.4, 124.1, 123.6, 123.00, 122.95, 73.74, 73.69, 53.9, 32.8, 19.69, 19.67, 14.22, 14.21;

IR (film): 2958, 2931, 2871, 1596, 1440, 1323, 821 cm^{-1} ;

HRMS (MALDI): $[\text{M}]^+$ calcd. for $\text{C}_{116}\text{H}_{112}\text{O}_8$ 1632.8352, found 1632.8314.

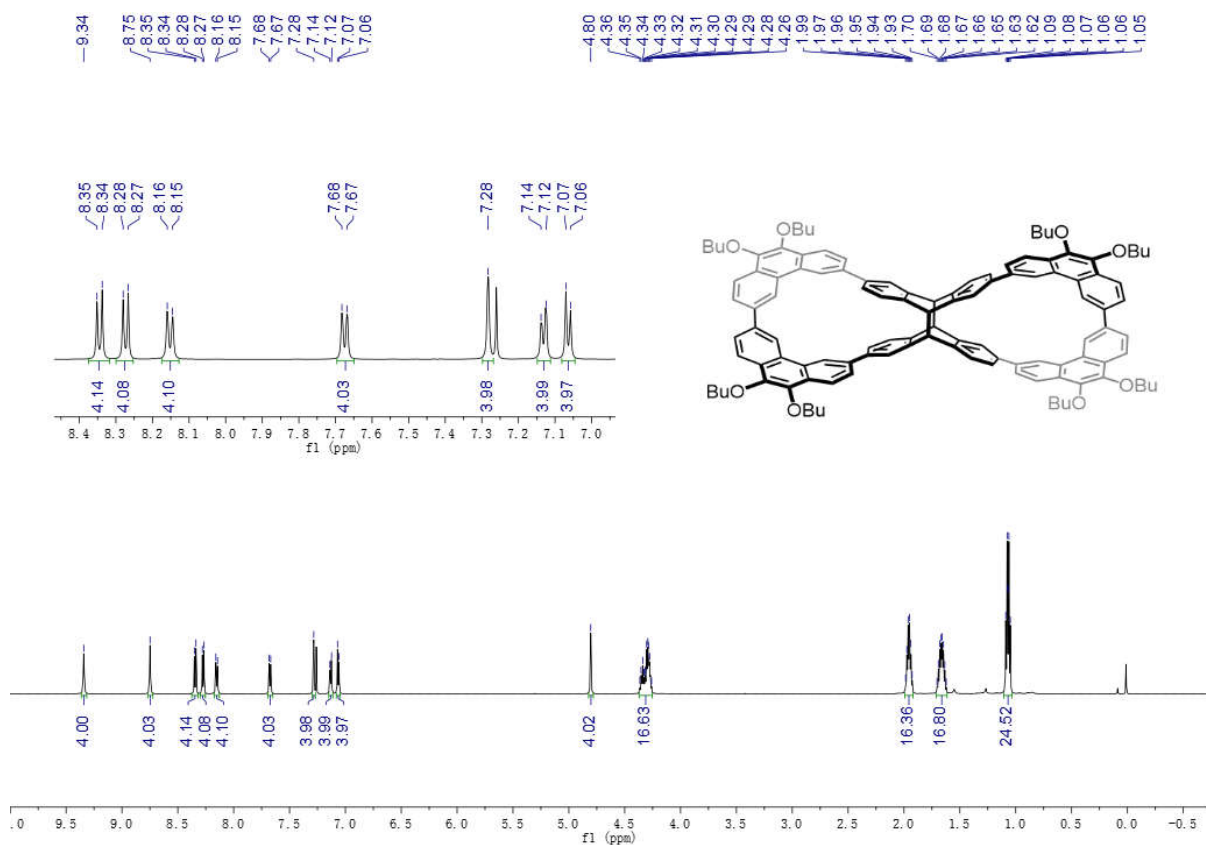


Figure S3. ¹H NMR spectrum (CDCl₃, 600 MHz) of compound 4.

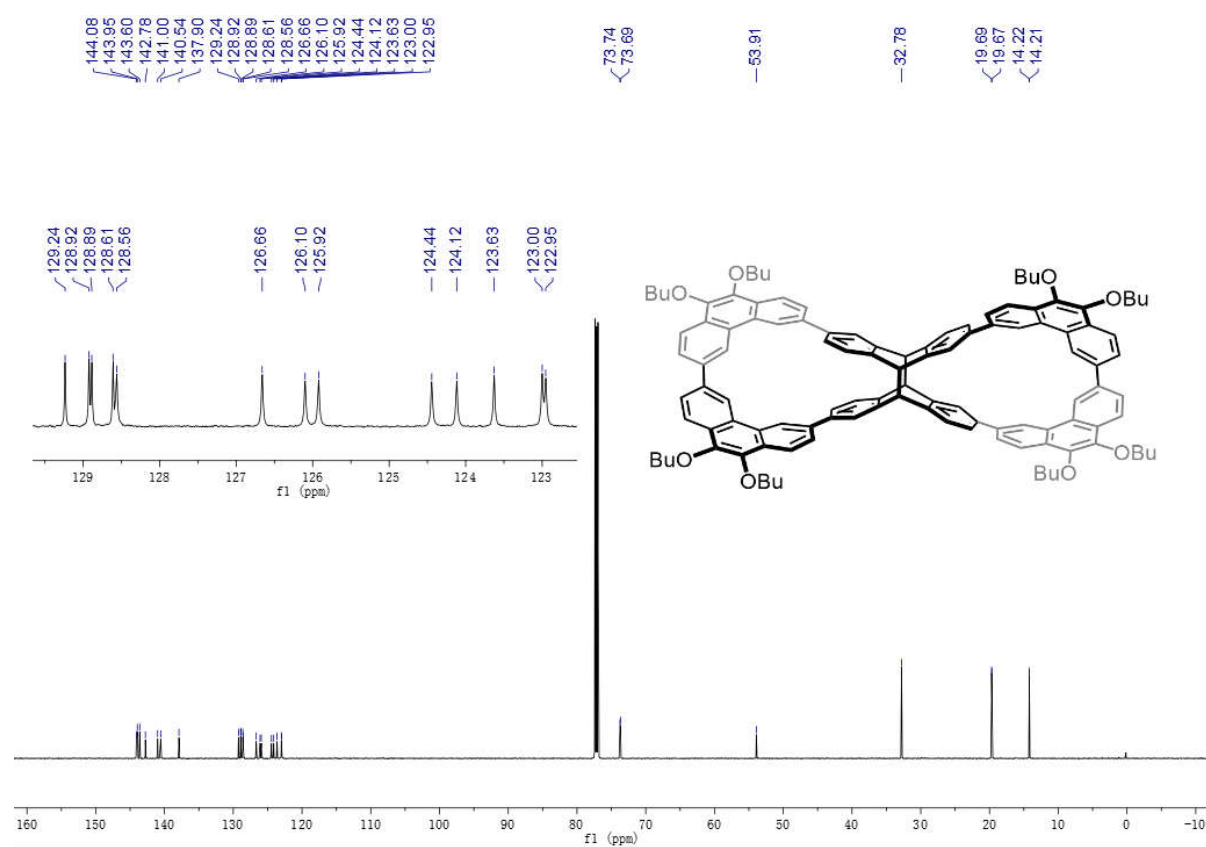


Figure S4. ¹³C NMR spectrum (CDCl₃, 151 MHz) of compound 4.

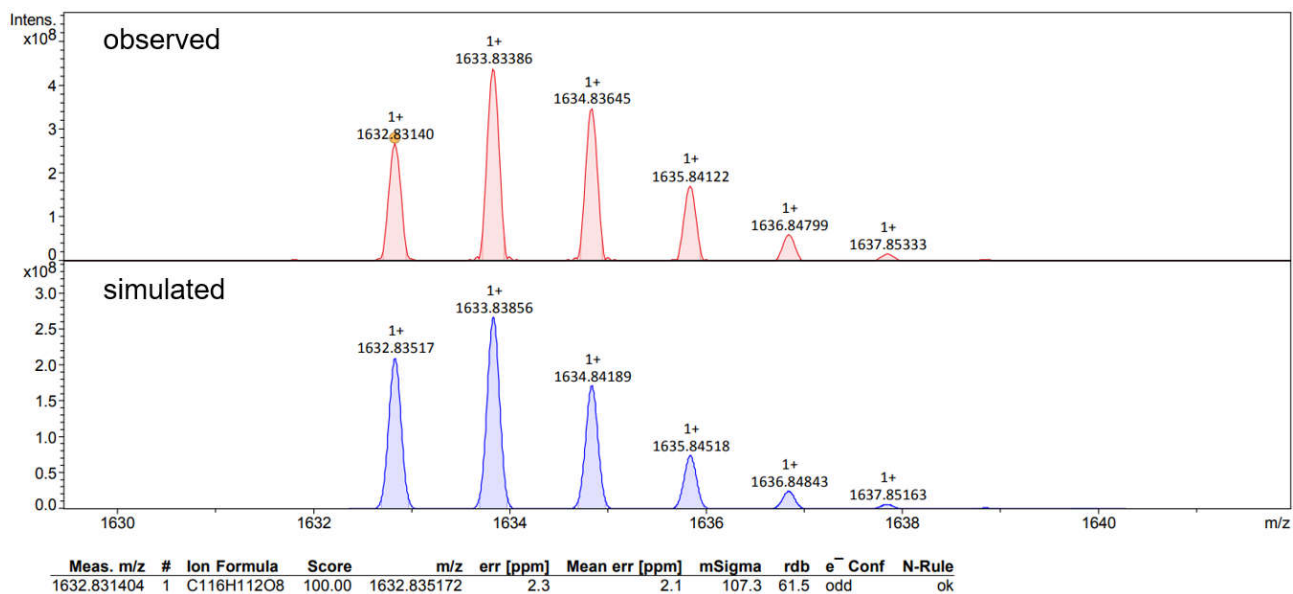
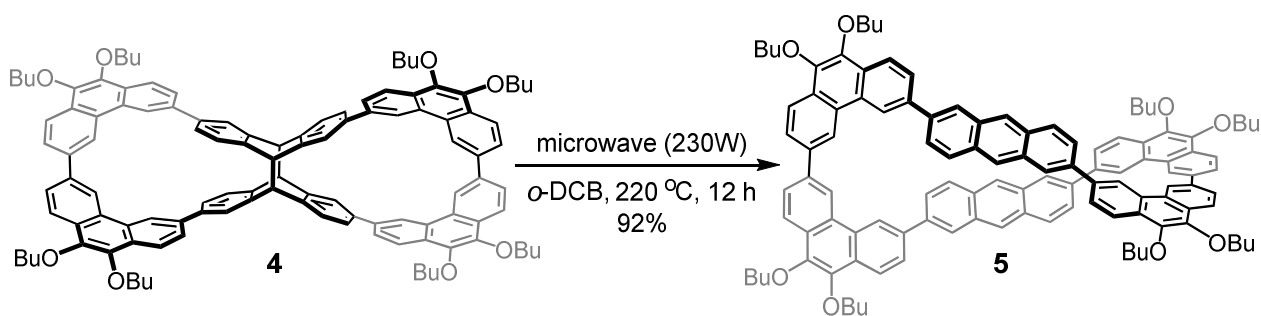


Figure S5. HRMS data for compound 4.



In a nitrogen-filled glove box, compound **4** (99.5 mg, 0.061 mmol, 1.0 equiv) and 1,2-dichlorobenzene (15 mL) were added to a 20 mL microwave tube equipped with a stir bar. The tube was sealed with a Teflon-lined septum cap and transferred to the microwave reactor (conditions: 230 W, 220 °C, 12 h). After the reaction, the solvent was removed under reduced pressure. Purification using silica gel column chromatography (CH₂Cl₂: petroleum ether = 2:3) afforded compound **5** (92.1 mg, 92% yield) as a yellow solid.

Compound **5**

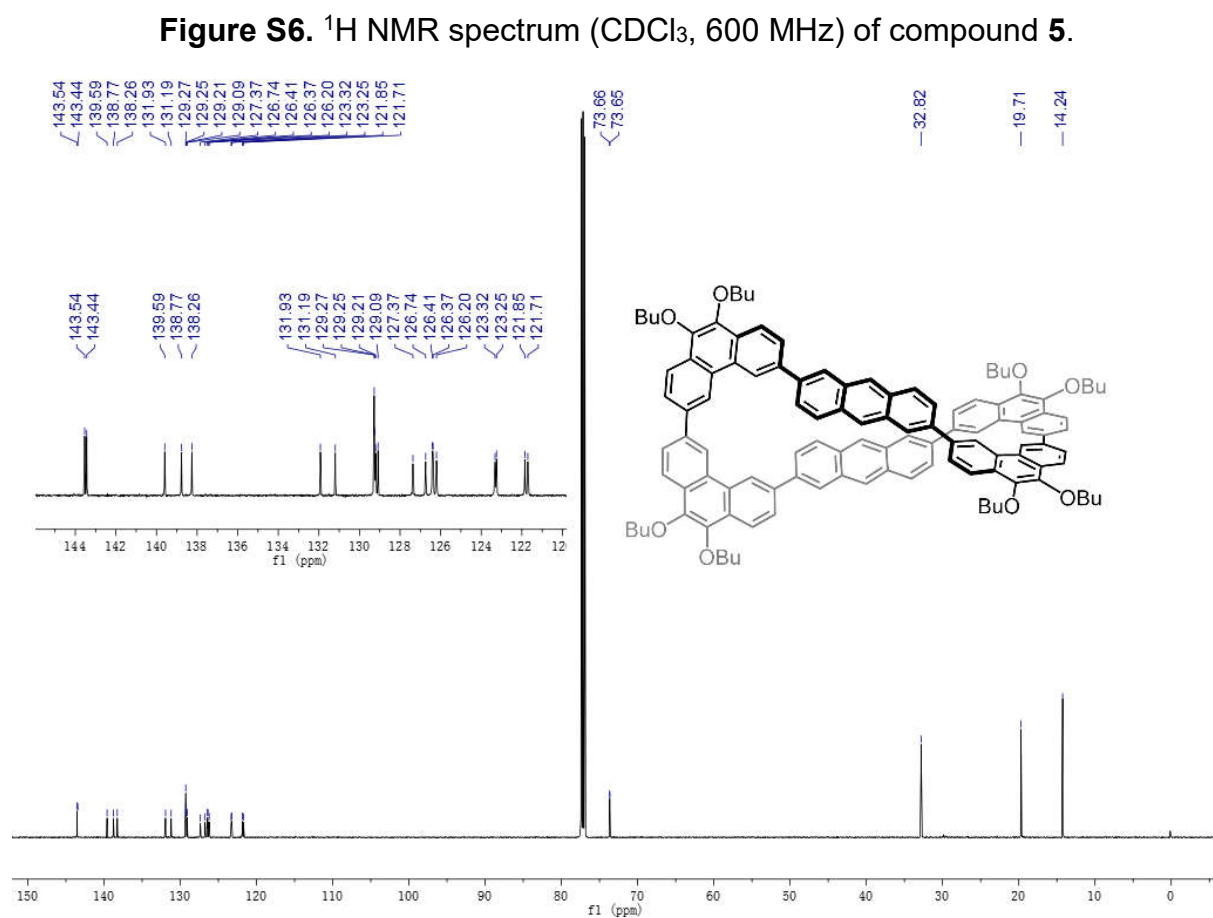
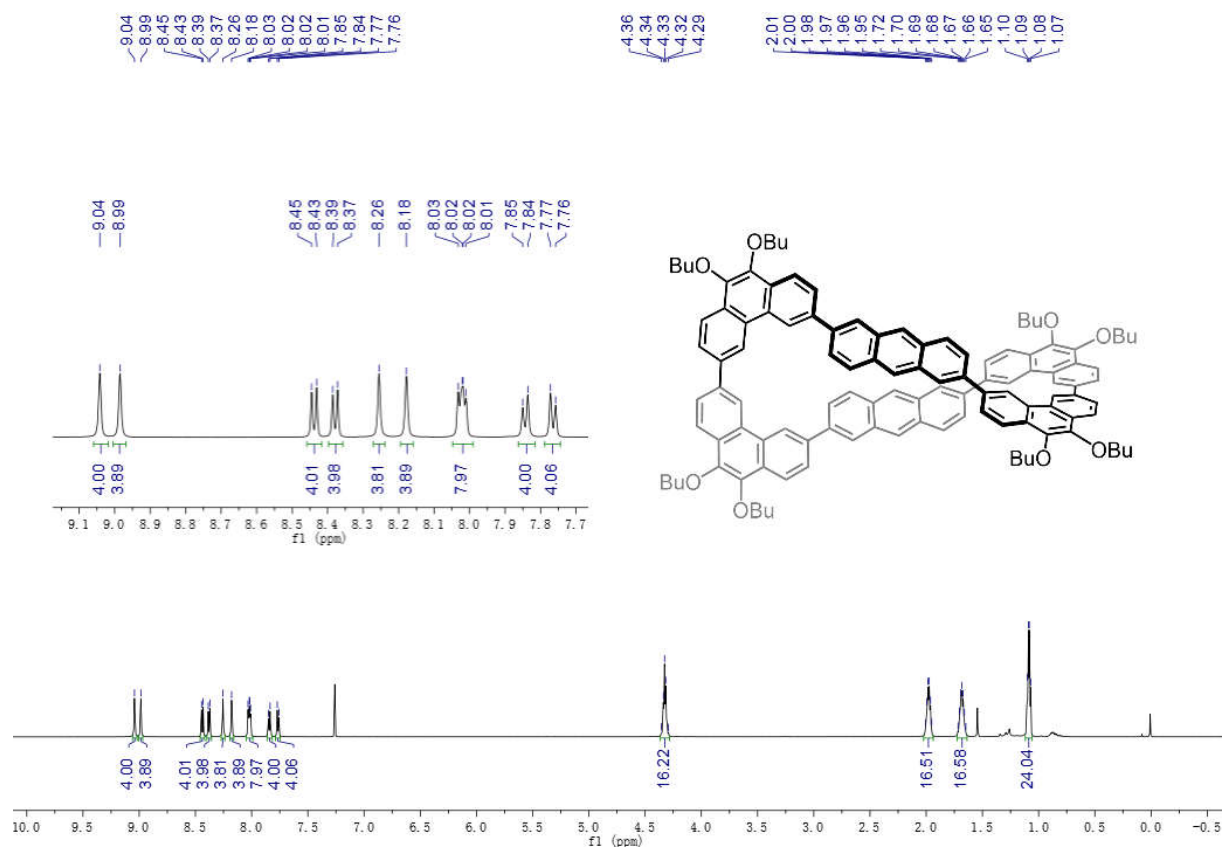
R_f = 0.25 (CH₂Cl₂: petroleum ether = 2:3);

¹H NMR (600 MHz, CDCl₃) δ 9.04 (s, 4H), 8.99 (s, 4H), 8.44 (d, *J* = 8.5 Hz, 4H), 8.38 (d, *J* = 8.2 Hz, 4H), 8.26 (s, 4H), 8.18 (s, 4H), 8.05–7.99 (m, 8H), 7.84 (d, *J* = 8.6 Hz, 4H), 7.76 (d, *J* = 8.6 Hz, 4H), 4.38–4.27 (m, 16H), 2.03–1.92 (m, 16H), 1.75–1.63 (m, 16H), 1.12–1.04 (m, 24H);

¹³C NMR (151 MHz, CDCl₃) δ 143.5, 143.4, 139.6, 138.8, 138.3, 131.9, 131.2, 129.27, 129.25, 129.21, 129.1, 127.4, 126.7, 126.41, 126.37, 126.2, 123.32, 123.25, 121.8, 121.7, 73.7, 73.6, 32.8, 19.7, 14.2;

IR (film): 2957, 2931, 2871, 1604, 1438, 1314, 823 cm⁻¹;

HRMS (MALDI): [M]⁺ calcd. for C₁₁₆H₁₁₂O₈ 1632.8352, found 1632.8369.



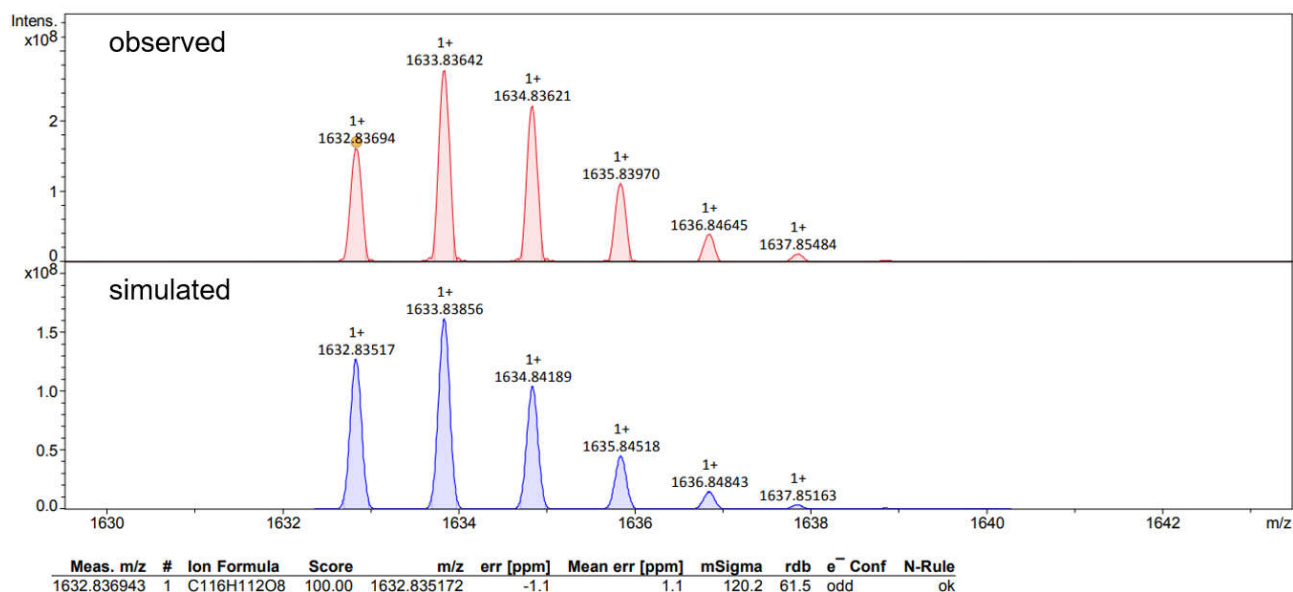
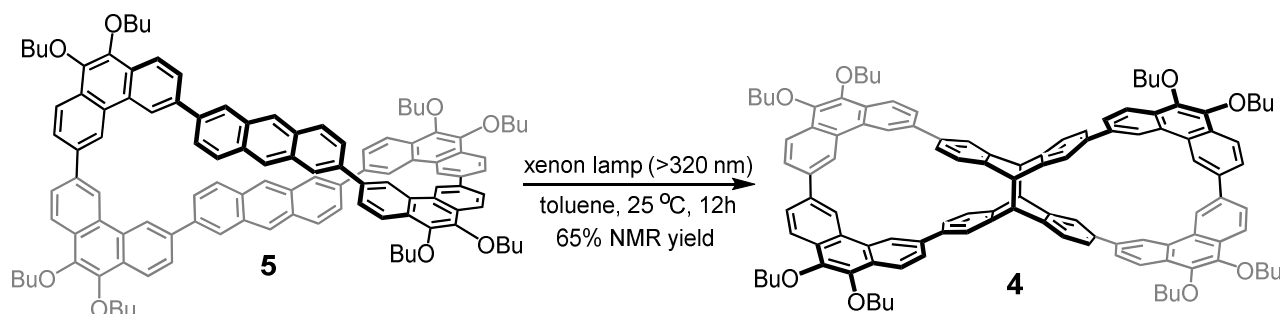


Figure S8. HRMS data for compound **5**.

Note: Compound **4** can be re-formed via photo-induced [4+4]-cycloaddition from **5**. However, the reaction also afforded by-products (probably intermolecular [4+4] cycloadducts) that complicated the purification of **4**.



In a nitrogen-filled glove box, compound **5** (5.0 mg, 0.0031 mmol, 1.0 equiv) and toluene (40 mL) were added to a 75 mL glass heavy-wall pressure vessel equipped with a stir bar. The vessel was capped, transferred out of the glove box, and stirred under the irradiation of a xenon lamp (Beijing PerfectLight Technology PLS-SXE300, equipped with a Vis-Ref filter) at 25 °C for 12 h. After the reaction, the solvent was removed under reduced pressure. The crude reaction mixture showed complete conversion of **5**, with 65% NMR yield of **4** as a single diastereomer, employing DMF (0.25 M in CDCl₃, 20 μL, 0.0050 mmol) as internal standard.

The NMR yield of **4** was calculated according to Figure S9: $1.60 \div 4 \times 0.0050 \div 0.0031 = 65\%$.

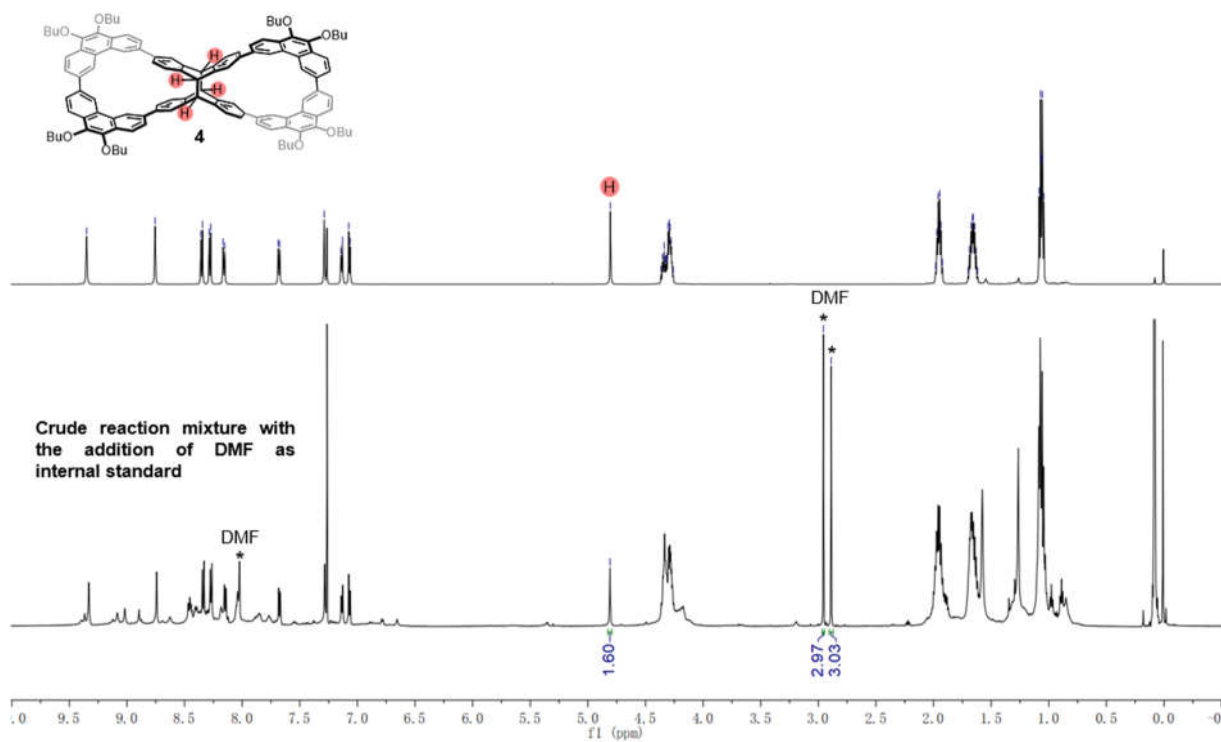
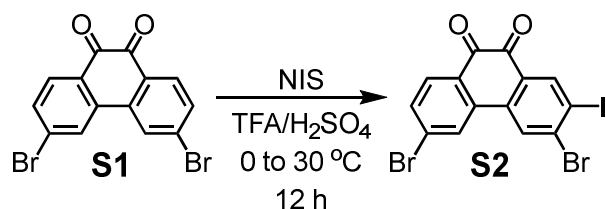
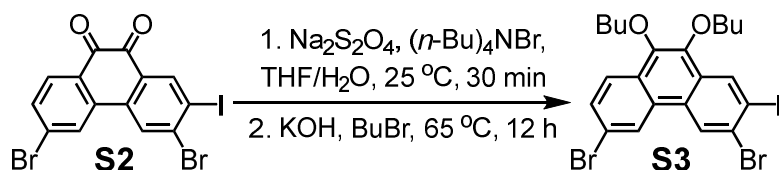


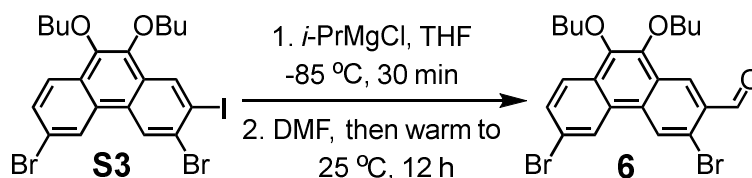
Figure S9. ¹H NMR spectra (CDCl₃, 600 MHz) of compound **4** and the crude reaction mixture after irradiation of **5**.



In air, a 100 mL round-bottom flask was charged with compound **S1** (732 mg, 2.0 mmol, 1.0 equiv) and TFA (45 mL), and cooled in an ice bath. Concentrated H₂SO₄ (20 mL) was added slowly to the mixture at 0 °C. NIS (360 mg, 1.6 mmol, 0.8 equiv) was added portionwise to the vigorously stirring solution at 0 °C. After stirring for 30 min at 0 °C, the reaction mixture was warmed to 25 °C and stirred for 12 h. The combined mixtures were poured into ice water (1 L) and the resulting orange precipitate was collected by filtration. The precipitate was added to a mixture of aq. Na₂S₂O₃ (0.2 M, 100 mL) and MeOH (100 mL), and stirred for 20 min. After filtration, the precipitate was washed with H₂O and MeOH, then dried to afford crude compound **S2** as orange powder, which was used in the next step without further purification.



To a nitrogen-purged flask containing tetrahydrofuran (20 mL) and water (10 mL) was added crude **S2** (prepared from 732 mg of **S1**), tetra-*n*-butylammonium bromide (179 mg, 0.56 mmol, 0.28 equiv), and sodium dithionite (2.58 g, 15 mmol, 7.5 equiv), and stirred at 25 °C for 30 minutes. Then a solution of potassium hydroxide (1.04 g, 19 mmol, 9.5 equiv, in 5 mL of water) was added to the reaction mixture, followed by the addition of 1-bromobutane (1.1 mL, 9.3 mmol, 4.6 equiv). The reaction mixture was stirred at 65 °C for 12 h. After cooled to room temperature, the volume of the reaction mixture was reduced to about 15 mL. At the same time, the crude product **S3** precipitated as a white solid which was collected by filtration, washed with water, and dried in air. The crude **S3** was used in the next step without further purification.



The crude **S3** from the previous step was dissolved in THF (120 mL) under nitrogen. To the solution was added dropwise isopropylmagnesium chloride (1.2 mL, 2.4 mmol, 1.2 equiv, 2.0 M solution in THF) at $-85\text{ }^\circ\text{C}$, and the reaction mixture was kept at the same temperature for 30 minutes. Then, anhydrous *N,N*-dimethylformamide (1.8 mL) was added to the reaction mixture, which was subsequently warmed to room temperature and stirred for 12 h. The reaction mixture was quenched with ammonium chloride solution (10 mL), and the aqueous layer was extracted with ethyl acetate (30 mL \times 3). The combined organic layer was washed with brine, dried over anhydrous sodium sulfate, and the solvents were removed under reduced pressure. Purification using silica gel column chromatography (CH_2Cl_2 : petroleum ether = 1:3) afforded compound **6** (257 mg, 25% yield, based on **S1** over three steps) as a yellow solid.

Compound **6**

$R_f = 0.30$ (CH_2Cl_2 : petroleum ether = 1:3);

$^1\text{H NMR}$ (600 MHz, CDCl_3) δ 10.52 (s, 1H), 8.77 (s, 1H), 8.73 (s, 1H), 8.65 (s, 1H), 8.11 (d, $J = 8.7$ Hz, 1H), 7.77 (d, $J = 8.7$ Hz, 1H), 4.25–4.17 (m, 4H), 1.93–1.81 (m, 4H), 1.65–1.53 (m, 4H), 1.07–1.00 (m, 6H);

$^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 191.8, 144.0, 143.4, 132.1, 131.9, 131.6, 130.3, 129.34, 128.3, 128.1, 126.3, 125.8, 124.6, 122.1, 120.9, 73.9, 73.6, 32.6, 32.5, 19.6, 19.5, 14.11, 14.09;

IR (film): 2956, 2932, 2871, 1689, 1545, 1348, 818 cm^{-1} ;

HRMS (MALDI): $[M]^+$ calcd. for $\text{C}_{23}\text{H}_{24}\text{Br}_2\text{O}_3$ 506.0087, found 506.0104.

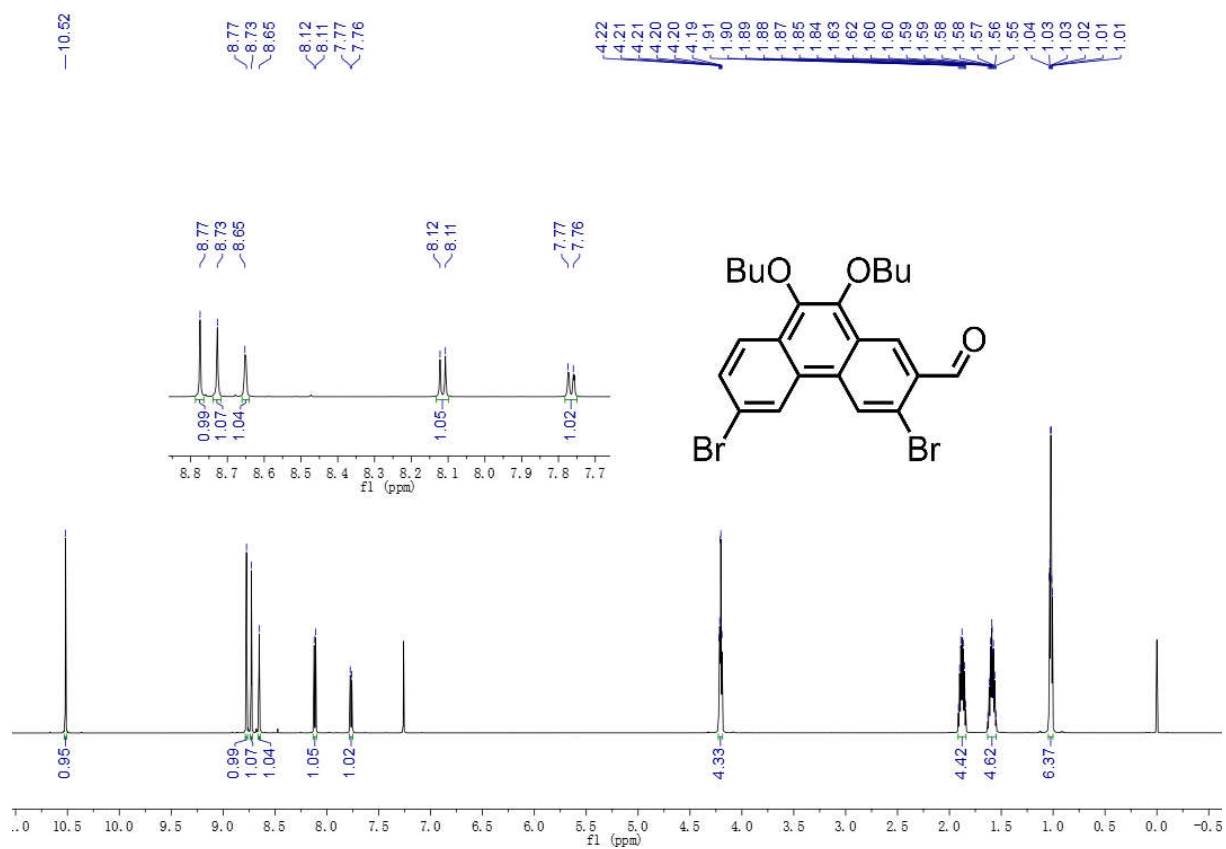


Figure S10. ¹H NMR spectrum (CDCl₃, 600 MHz) of compound 6.

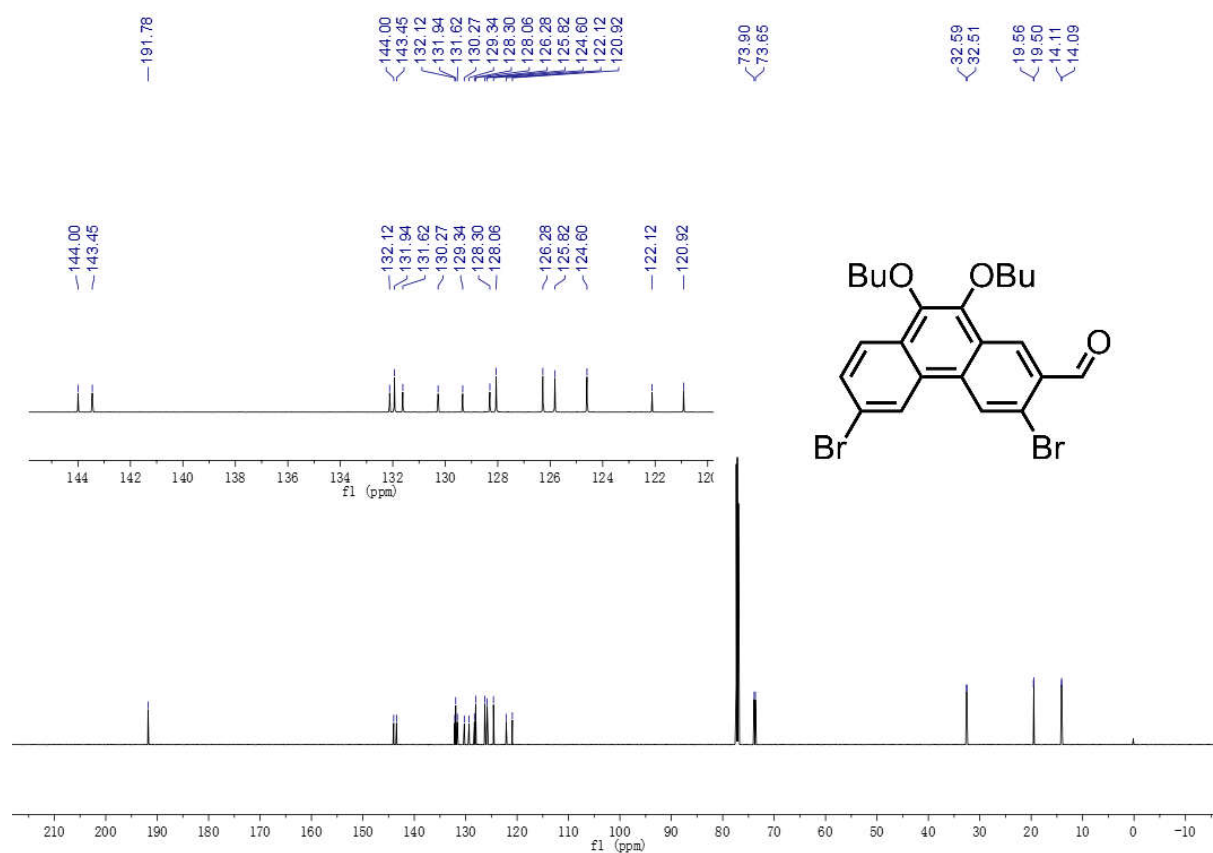
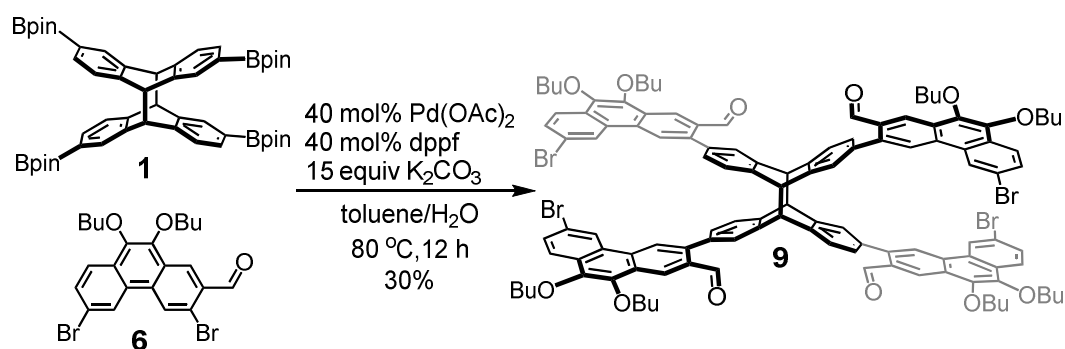


Figure S11. ¹³C NMR spectrum (CDCl₃, 151 MHz) of compound 6.



In a nitrogen-filled glove box, Pd(OAc)₂ (1.8 mg, 0.008 mmol, 40 mol%), dppf (4.4 mg, 0.008 mmol, 40 mol%), and anhydrous toluene (5 mL) were added to a 40 mL glass vial equipped with a stir bar. The mixture was stirred in the glove box at room temperature for 30 min. Then **1** (17.2 mg, 0.020 mmol, 1.0 equiv), **6** (122 mg, 0.24 mmol, 12 equiv), K₂CO₃ (41.4 mg, 0.30 mmol, 15 equiv) and anhydrous toluene (25 mL) were added to the 40 mL glass vial. The vial was sealed with a Teflon-lined septum cap then transferred out of glove box. Degassed water (3 mL) was subsequently added to the vial via a syringe, and the puncture in the septum cap was covered with vacuum grease. The reaction mixture was stirred at 80 °C for 12 h, and cooled to room temperature. Four reactions were carried out in parallel using identical procedures, and all the reaction mixtures were combined during work-up. The combined reaction mixture was extracted with ethyl acetate (30 mL × 3). The combined organic layers were washed with brine, and dried over sodium sulfate. The solvents were removed under reduced pressure. Purification using silica gel column chromatography with CH₂Cl₂ afforded compound **9** (49.4 mg, 30% yield) as a yellow solid.

Note: Based on our experience, regioisomers, if any, of analogous cross-coupling reactions with **1** have almost identical polarities on silica. During the above reaction, the NMR spectra of the isolated fraction from silica gel column chromatography showed a single regioisomer which was characterized as **9**. Other possible regioisomers were not observed. In addition, the reaction generated significant amount of insoluble polymeric by-products, which should account for the observed loss of mass balance.

Compound **9**

R_f = 0.35 (CH₂Cl₂);

¹H NMR (600 MHz, CDCl₃) δ 9.92 (s, 4H), 8.92 (s, 4H), 8.77 (s, 4H), 8.47 (s, 4H), 8.12 (d, *J* = 8.7 Hz, 4H), 7.73 (d, *J* = 8.6 Hz, 4H), 7.31–7.27 (m, 8H), 7.19 (s, 4H), 4.87 (s, 4H), 4.28–4.20 (m, 16H), 1.97–1.91 (m, 8H), 1.91–1.85 (m, 8H), 1.67–1.56 (m, 16H), 1.08–1.00 (m, 24H);

¹³C NMR (151 MHz, CDCl₃) δ 192.4, 143.8, 143.7, 143.4, 143.2, 141.4, 136.5, 132.9, 131.4, 130.7, 130.00, 129.95, 129.5, 129.3, 127.7, 127.6, 126.5, 124.9, 124.4, 123.5, 120.7, 73.8, 73.6, 53.4, 32.6, 19.58, 19.56, 14.2, 14.1;

IR (film): 2957, 2932, 2871, 1693, 1589, 1347, 822 cm⁻¹;

HRMS (MALDI): [M+Na]⁺ calcd. for C₁₂₀H₁₁₂Br₄NaO₁₂ 2083.4780, found 2083.4786.

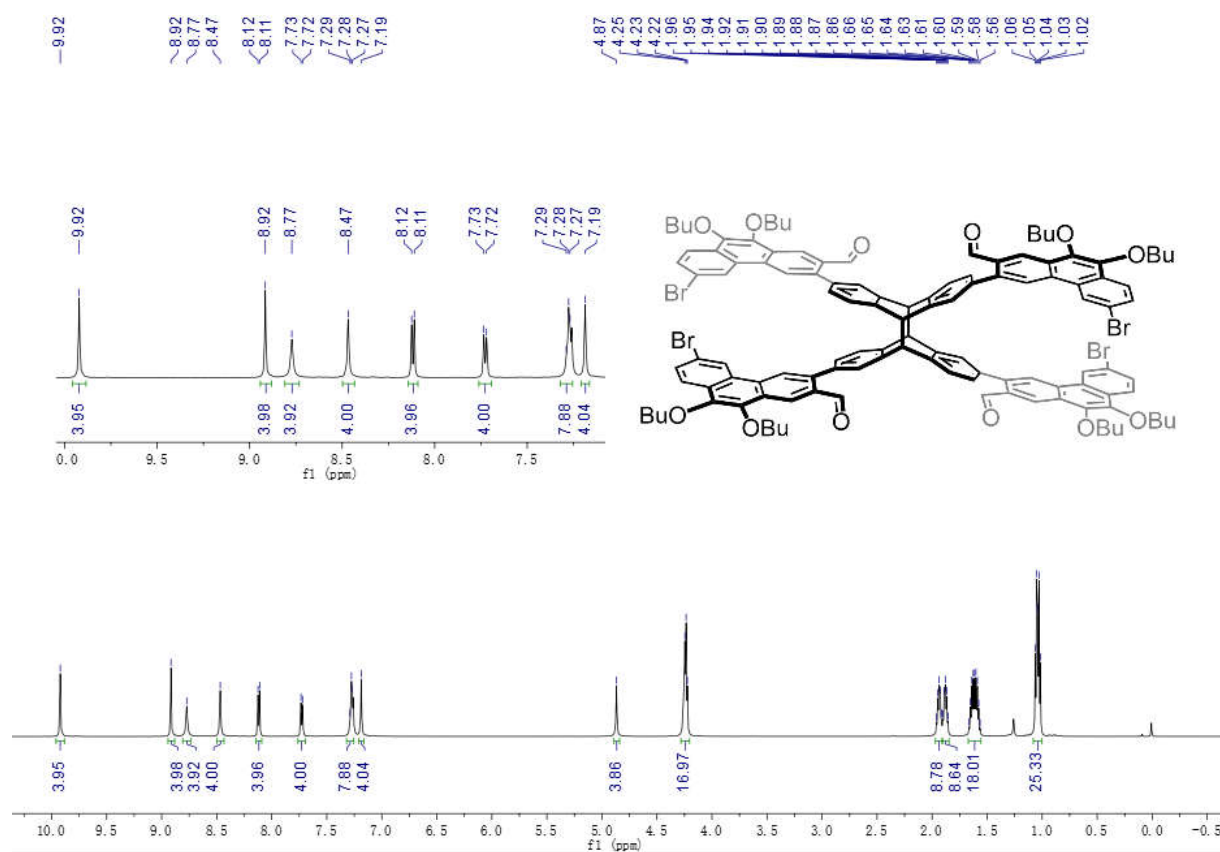


Figure S12. ¹H NMR spectrum (CDCl₃, 600 MHz) of compound **9**.

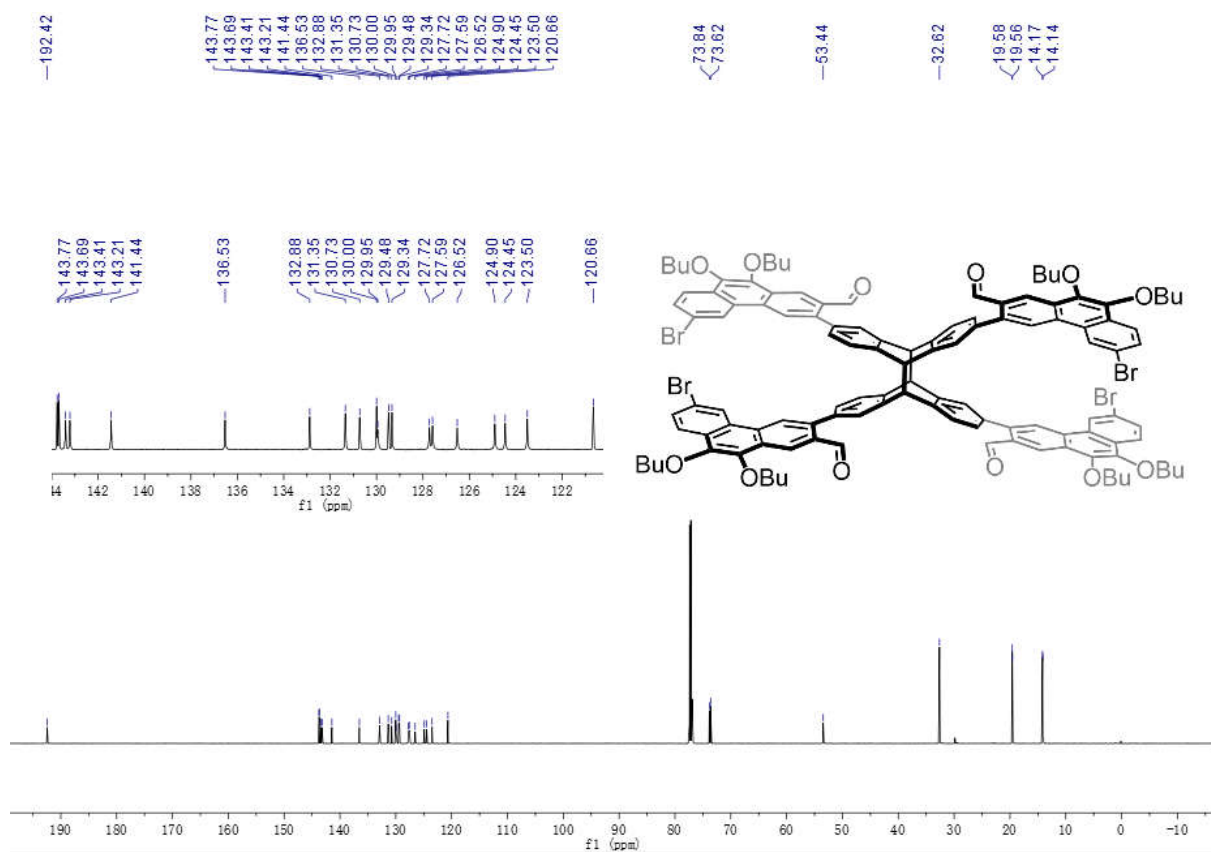
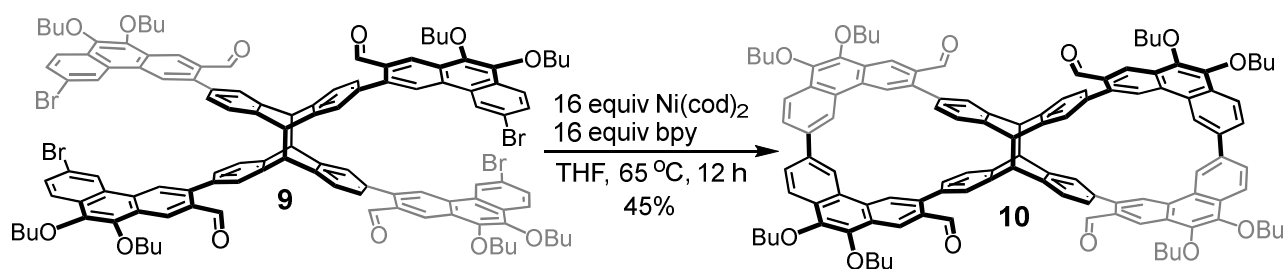


Figure S13. ^{13}C NMR spectrum (CDCl₃, 151 MHz) of compound **9**.



In a nitrogen-filled glove box, Ni(cod)_2 (306 mg, 1.4 mmol, 16 equiv), 2,2'-bipyridyl (212 mg, 1.4 mmol, 16 equiv), and anhydrous THF (150 mL) were sequentially added to a 250 mL round-bottom flask equipped with a stir bar. The flask was capped with a rubber septum, transferred out of glove box, and stirred at 65 °C for 15 min. Meanwhile, compound **9** (176 mg, 0.088 mmol, 1.0 equiv) and anhydrous THF (10 mL) were mixed in a 40 mL glass vial. The vial was capped, and transferred out of the glove box. The solution of compound **9** was added to the flask containing nickel complex. The mixture was stirred at 65 °C for 12 h, and cooled to room temperature, and filtered through a short pad of silica gel with the aid of mixed solvents (CH_2Cl_2 : ethyl acetate = 2:1). The solvents were removed under reduced pressure. Purification using silica gel column chromatography with CH_2Cl_2 afforded compound **10** (69.0 mg, 45% yield) as a yellow solid.

Compound **10**

$R_f = 0.40$ (CH_2Cl_2 : ethyl acetate = 100:1);

$^1\text{H NMR}$ (400 MHz, $\text{CHloroform-}d$) δ 10.22 (s, 4H), 9.33 (s, 4H), 8.91 (s, 4H), 8.71 (s, 4H), 8.38 (d, $J = 8.5$ Hz, 4H), 8.21 (d, $J = 8.5$ Hz, 4H), 7.25–7.17 (m, 12H), 4.85 (s, 4H), 4.39–4.27 (m, 16H), 2.00–1.91 (m, 16H), 1.72–1.60 (m, 16H), 1.10–1.03 (m, 24H);

$^{13}\text{C NMR}$ (151 MHz, CDCl_3) δ 192.5, 144.3, 144.1, 143.6, 141.8, 137.7, 137.0, 132.0, 131.7, 130.6, 129.6, 129.2, 128.9, 128.2, 127.4, 126.5, 125.7, 124.1, 123.5, 123.4, 74.0, 73.7, 53.6, 32.7, 32.6, 19.7, 19.6, 14.20, 14.16;

IR (film): 2957, 2930, 2870, 1692, 1591, 1346, 823 cm^{-1} ;

HRMS (MALDI): $[\text{M}+\text{Na}]^+$ calcd. for $\text{C}_{120}\text{H}_{112}\text{NaO}_{12}$ 1767.8046, found 1767.8047.

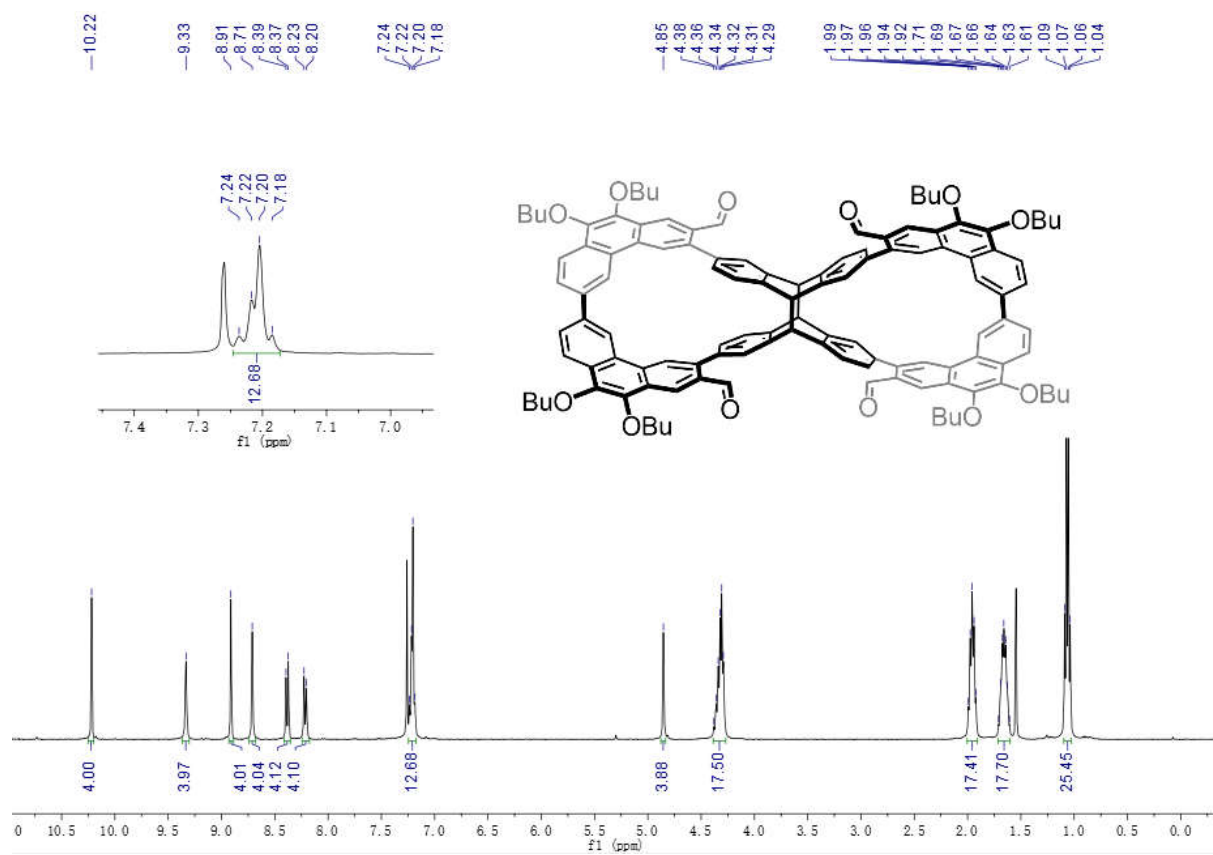


Figure S14. ^1H NMR spectrum (CDCl_3 , 400 MHz) of compound **10**.

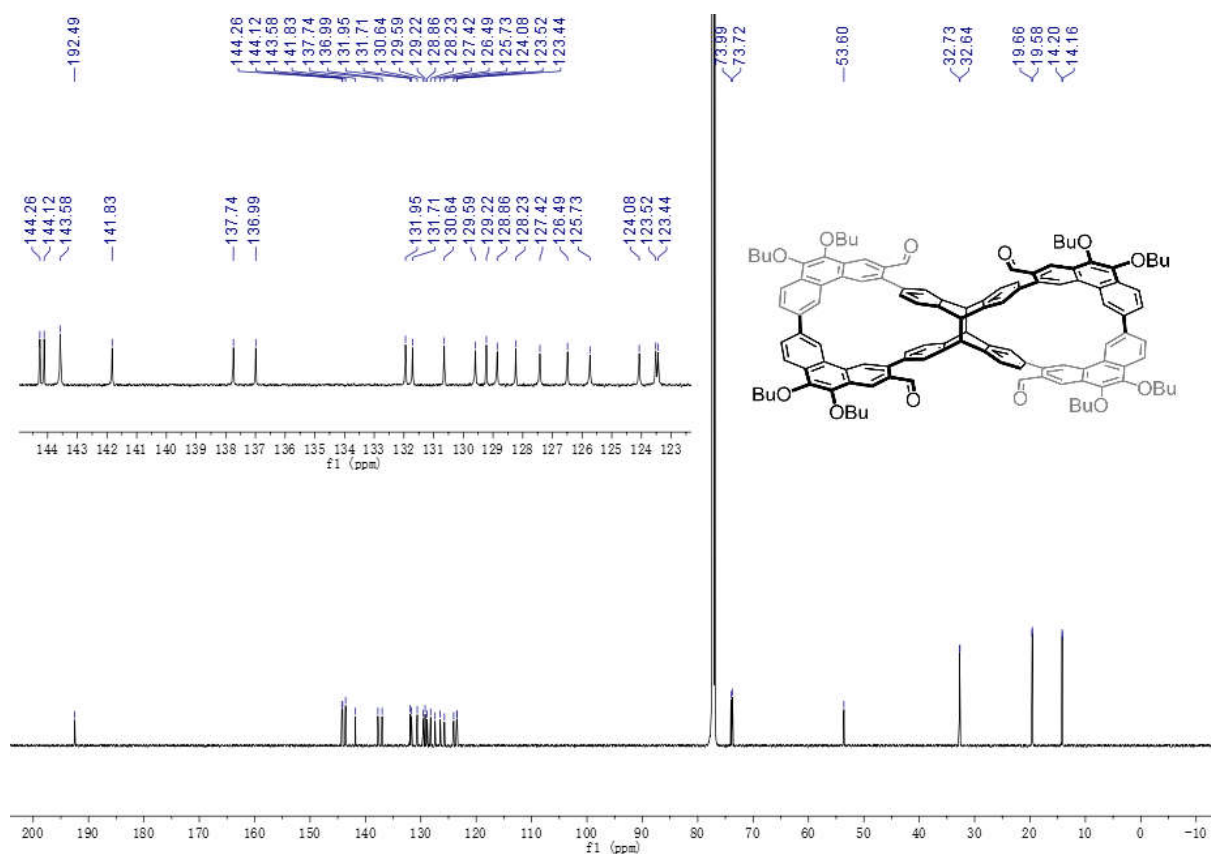


Figure S15. ^{13}C NMR spectrum (CDCl_3 , 151 MHz) of compound 10.

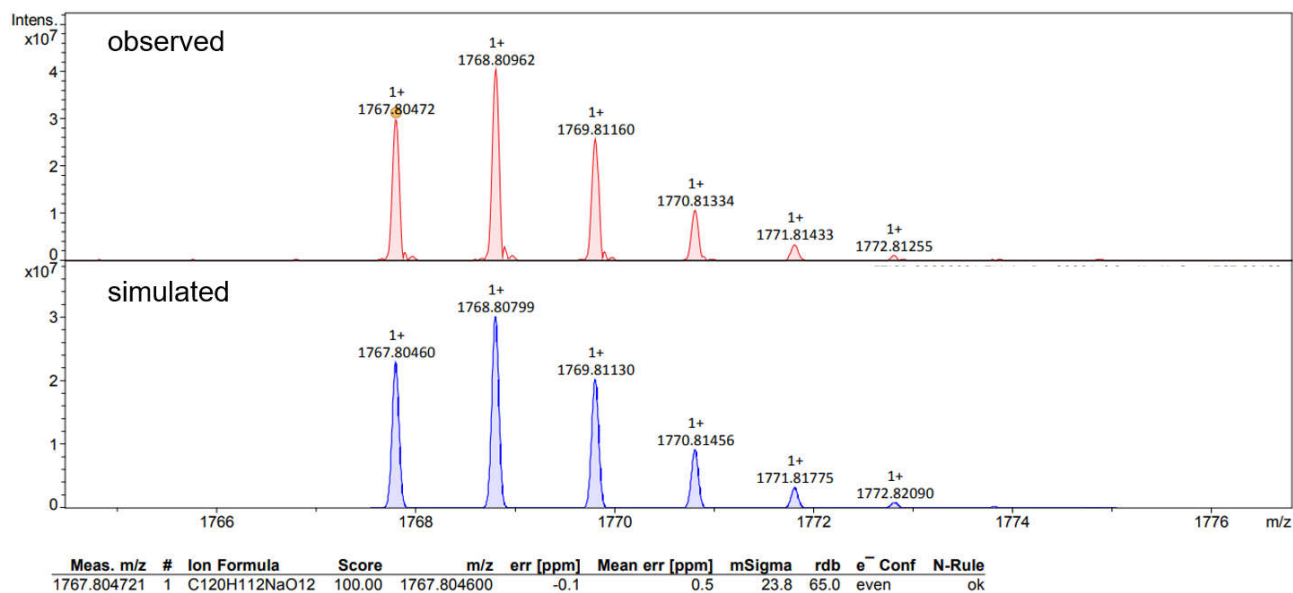
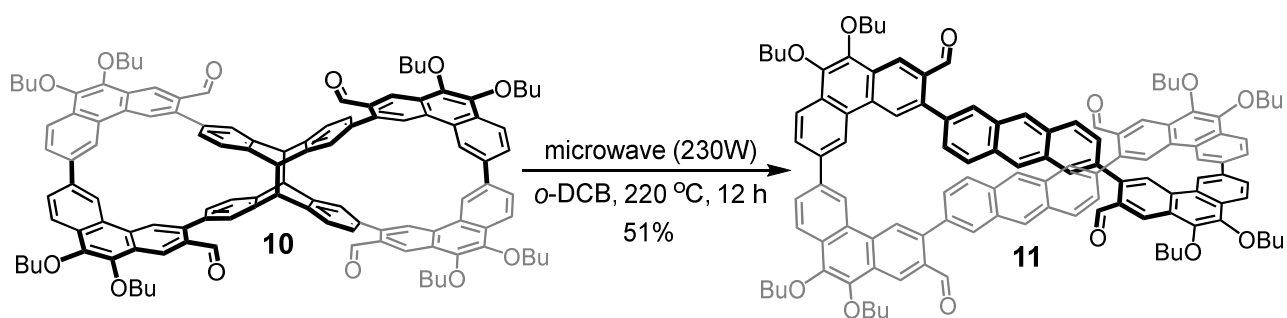


Figure S16. HRMS data for compound 10.



In a nitrogen-filled glove box, compound **10** (78.5 mg, 0.045 mmol, 1.0 equiv) and 1,2-dichlorobenzene (15 mL) were added to a 20 mL microwave tube equipped with a stir bar. The tube was sealed with a Teflon-lined septum cap and transferred to the microwave reactor (conditions: 230 W, 220 °C, 12 h). After the reaction, the solvent was removed under reduced pressure. Purification using silica gel column chromatography with CH₂Cl₂ afforded compound **11** (40.0 mg, 51% yield) as a yellow solid.

Compound **11**

R_f = 0.30 (CH₂Cl₂: ethyl acetate = 100:1);

¹H NMR (600 MHz, CDCl₃) δ 10.24 (s, 4H), 9.06 (s, 4H), 9.02–8.93 (m, 8H), 8.44 (d, *J* = 8.5 Hz, 4H), 8.28 (s, 4H), 8.05 (d, *J* = 8.6 Hz, 4H), 7.94–7.83 (m, 8H), 7.75 (d, *J* = 8.1 Hz, 4H), 4.38–4.27 (m, 16H), 2.02–1.92 (m, 16H), 1.71–1.62 (m, 16H), 1.13–1.01 (m, 24H);

¹³C NMR (151 MHz, CDCl₃) δ 192.6, 144.1, 143.7, 140.6, 139.6, 134.8, 132.8, 131.8, 131.3, 131.2, 130.7, 129.4, 129.3, 128.5, 127.5, 126.8, 125.2, 124.3, 123.7, 122.5, 73.9, 73.7, 32.8, 32.7, 19.7, 19.6, 14.21, 14.19;

IR (film): 2957, 2931, 2871, 1691, 1607, 1440, 1346, 1074 cm⁻¹;

HRMS (MALDI): [M+Na]⁺ calcd. for C₁₂₀H₁₁₂NaO₁₂ 1767.8046, found 1767.8053.

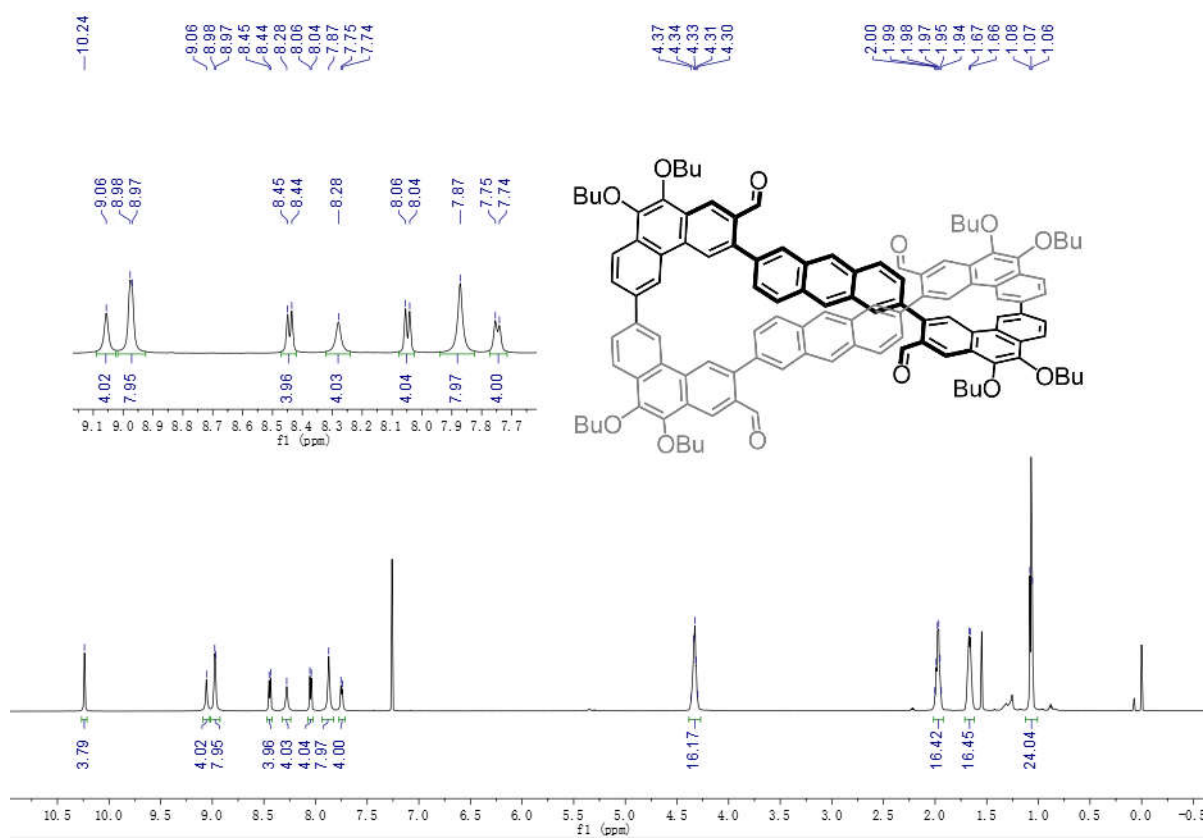


Figure S17. ^1H NMR spectrum (CDCl_3 , 600 MHz) of compound **11**.

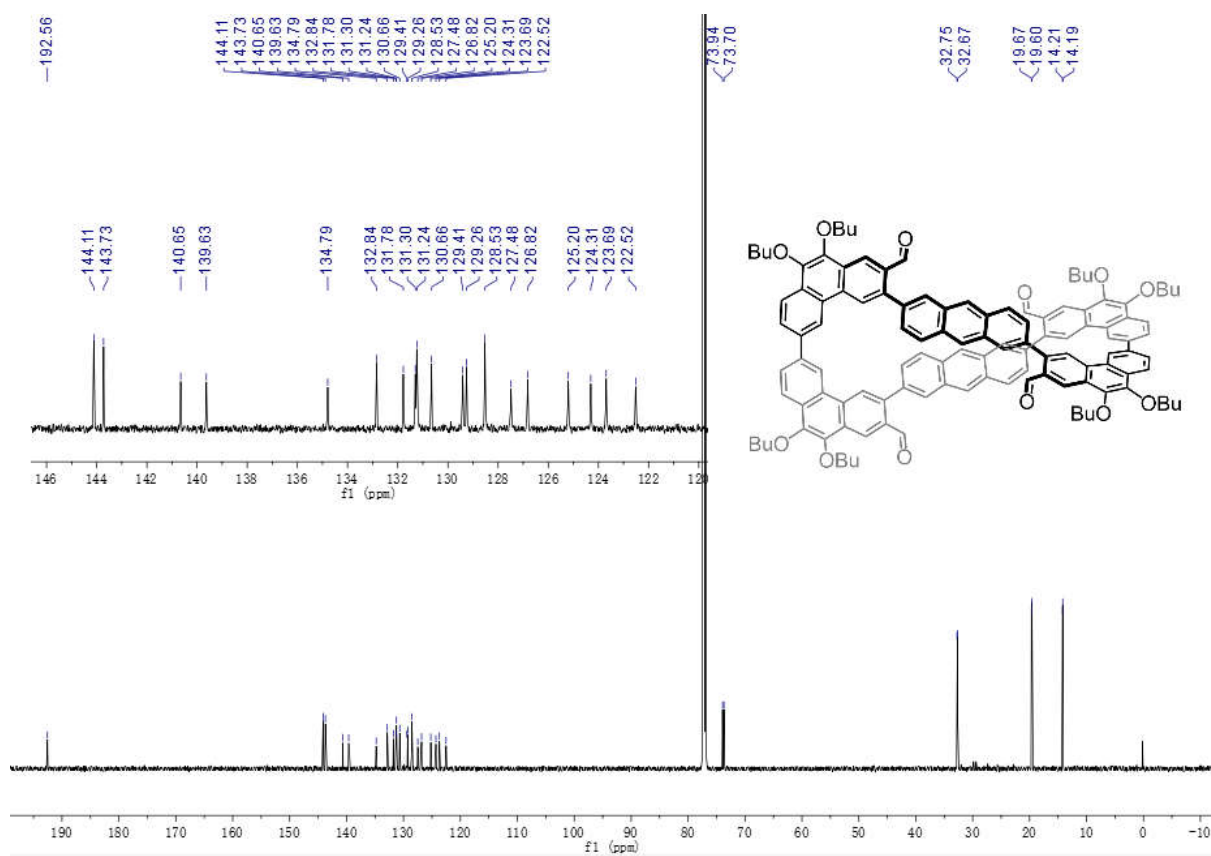


Figure S18. ^{13}C NMR spectrum (CDCl_3 , 151 MHz) of compound **11**.

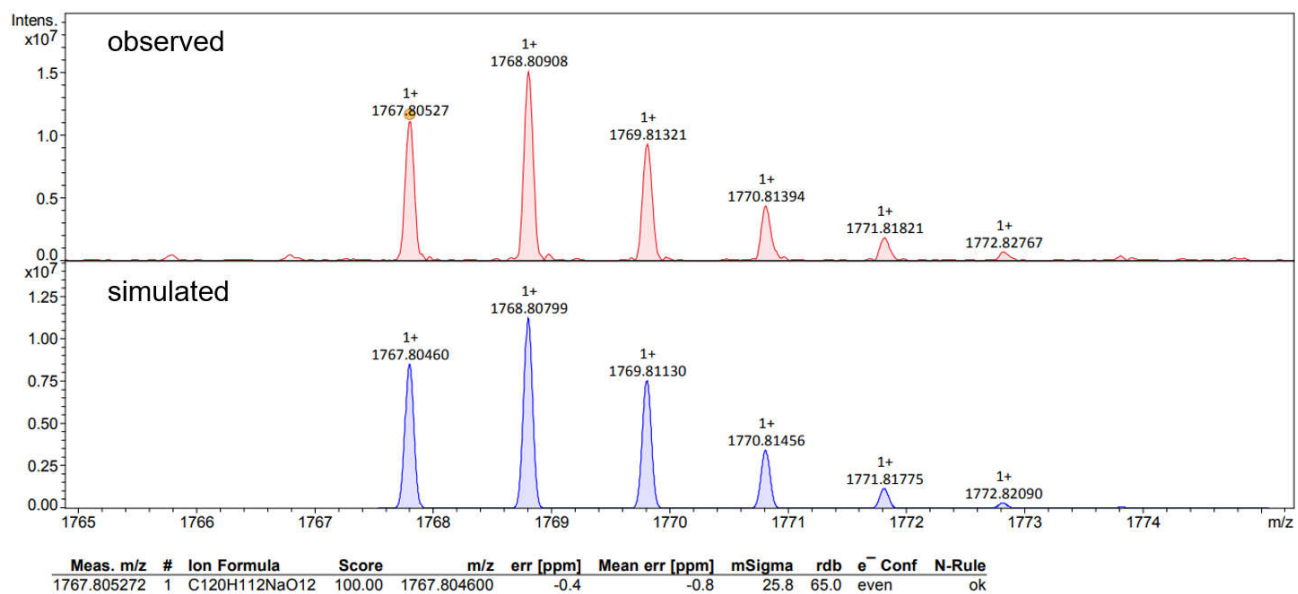
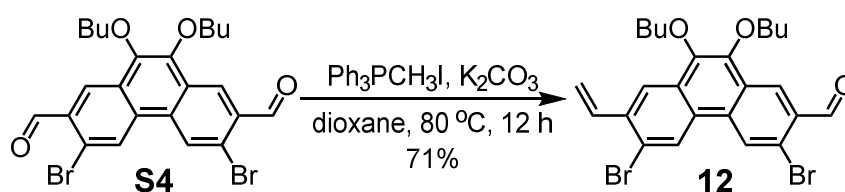


Figure S19. HRMS data for compound 11.



In a nitrogen-filled glove box, compound **S4** (804 mg, 1.5 mmol, 1.0 equiv, prepared according to literature^[S4]), $\text{Ph}_3\text{PCH}_3\text{I}$ (546 mg, 1.4 mmol, 0.90 equiv), K_2CO_3 (310 mg, 2.2 mmol, 1.5 equiv) and anhydrous dioxane (25 mL) were sequentially added to a 40 mL glass vial equipped with a stir bar. The vial was sealed with a Teflon-lined septum cap then transferred out of glove box. The reaction mixture was stirred at 80 °C for 12 h, and cooled to room temperature before quenched with saturated aq. NH_4Cl (5 mL) and diluted with ethyl acetate (20 mL). The aqueous layer was extracted with ethyl acetate (30 mL \times 3). The combined organic layers were washed with brine, and dried over sodium sulfate. The solvents were removed under reduced pressure. Purification using silica gel column chromatography (CH_2Cl_2 : petroleum ether = 2:3) afforded compound **12** (568 mg, 71% yield) as a yellow solid.

Compound **12**

R_f = 0.30 (CH_2Cl_2 : petroleum ether = 2:3);

^1H NMR (600 MHz, CDCl_3) δ 10.51 (s, 1H), 8.76 (s, 1H), 8.69–8.68 (m, 2H), 8.40 (s, 1H), 7.22 (dd, J = 17.3, 10.9 Hz, 1H), 5.92 (d, J = 17.3 Hz, 1H), 5.52 (d, J = 11.0 Hz, 1H), 4.25–4.19 (m, 4H), 1.91–1.86 (m, 4H), 1.65–1.57 (m, 4H), 1.06–1.00 (m, 6H);

^{13}C NMR (151 MHz, CDCl_3) δ 191.6, 143.7, 143.4, 131.9, 131.4, 130.6, 129.2, 127.8, 127.6, 127.3, 125.7, 122.17, 122.16, 120.4, 118.2, 73.7, 73.5, 32.45, 32.38, 19.5, 19.4, 13.96, 13.95;

IR (film): 2957, 2931, 2871, 1686, 1579, 1461 1351, 895 cm^{-1} ;

HRMS (MALDI): $[\text{M}]^+$ calcd. for $\text{C}_{25}\text{H}_{26}\text{Br}_2\text{O}_3$ 532.0243, found 532.0268.

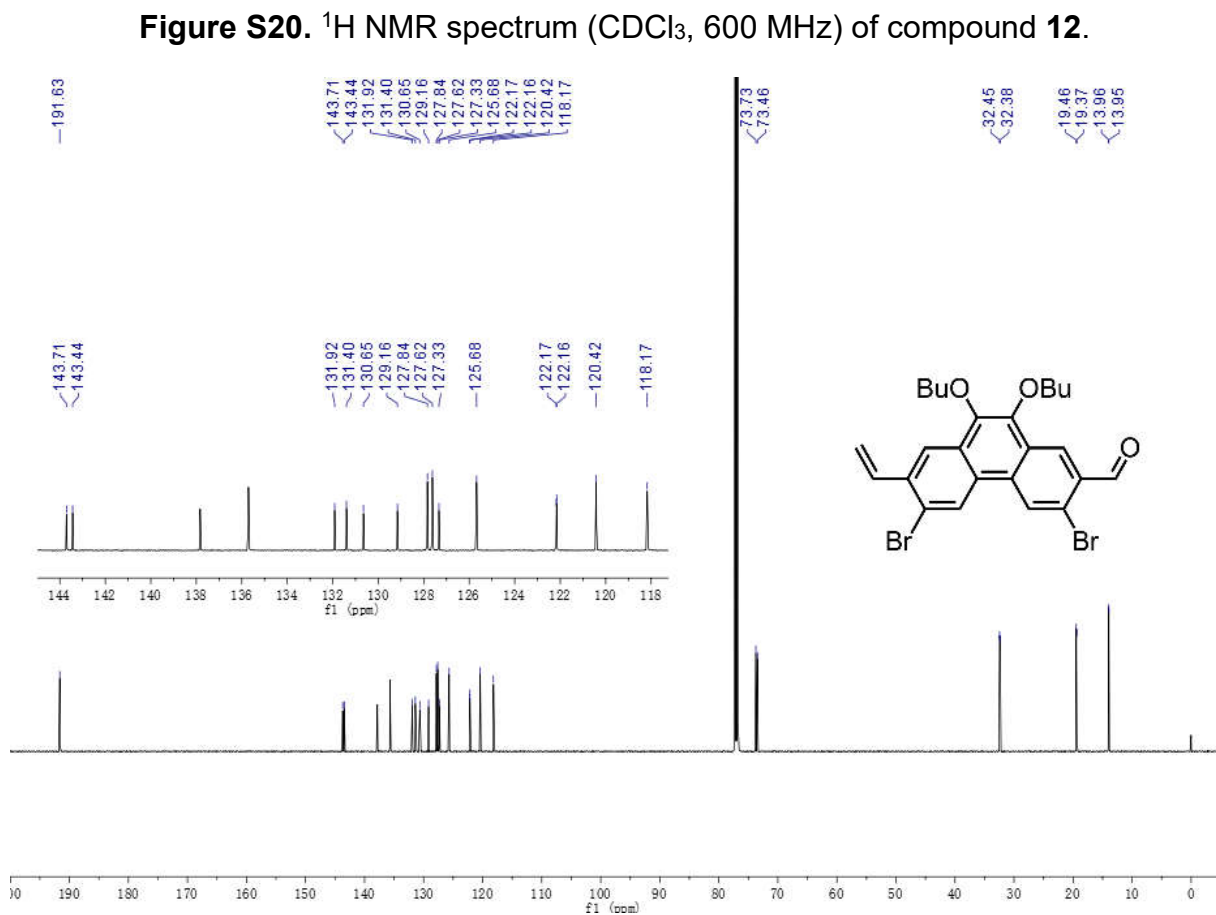
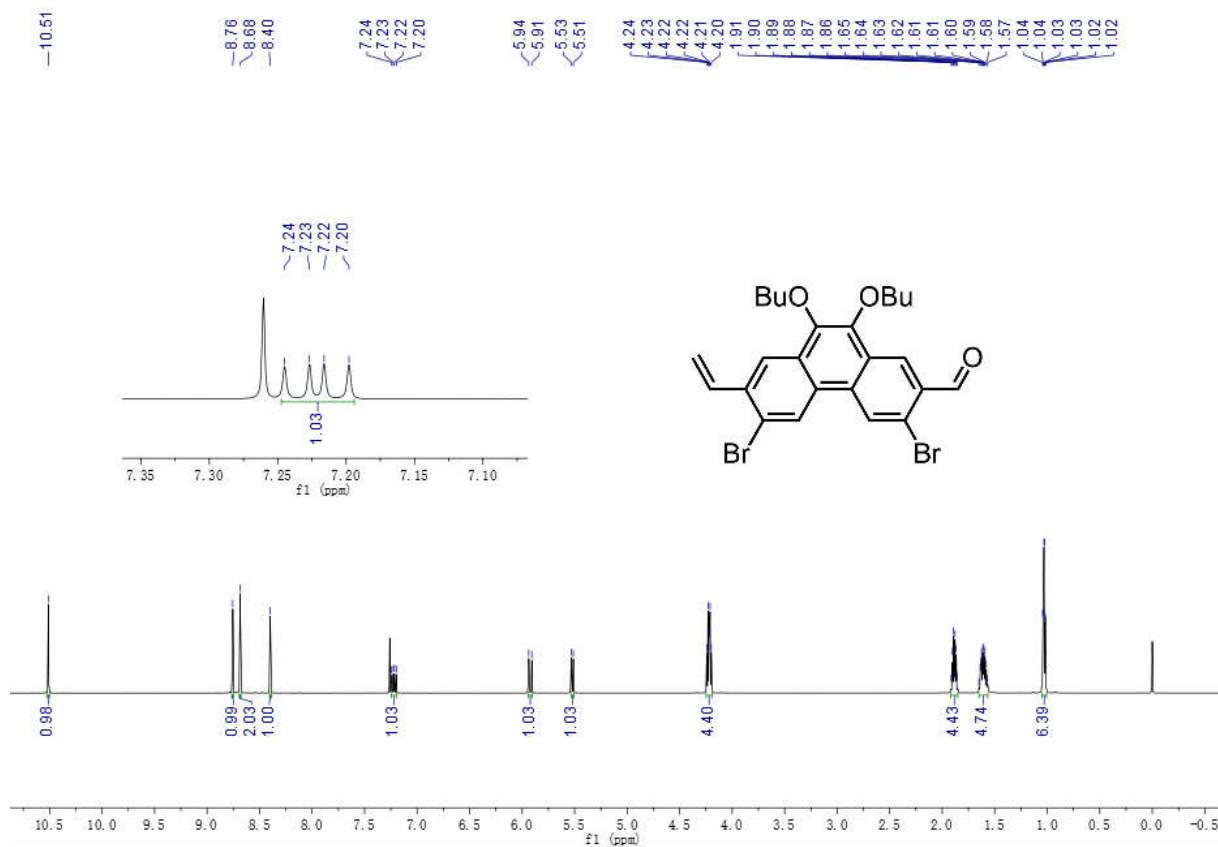
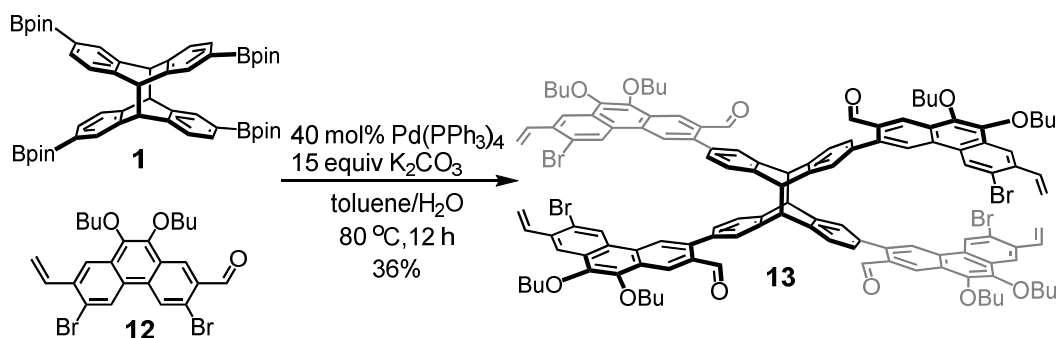


Figure S21. ¹³C NMR spectrum (CDCl₃, 151 MHz) of compound 12.



In a nitrogen-filled glove box, compound **1** (11.2 mg, 0.013 mmol, 1.0 equiv), compound **12** (114 mg, 0.21 mmol, 16 equiv), Pd(PPh₃)₄ (6.2 mg, 0.0052 mmol, 40 mol%), anhydrous K₂CO₃ (27.0 mg, 0.20 mmol, 15 equiv), and anhydrous toluene (20 mL) were added to a 40 mL glass vial equipped with a stir bar. The vial was sealed with a Teflon-lined septum cap then transferred out of glove box. Degassed water (2 mL) was subsequently added to the vial via a syringe, and the puncture in the septum cap was covered with vacuum grease. The reaction mixture was stirred at 80 °C for 12 h, and cooled to room temperature. Eight reactions were carried out in parallel using identical procedures, and all the reaction mixtures were combined during work-up. The combined reaction mixture was extracted with ethyl acetate (30 mL × 3). The combined organic layers were washed with brine, and dried over sodium sulfate. The solvents were removed under reduced pressure. Purification using silica gel column chromatography with CH₂Cl₂ afforded **13** (81.0 mg, 36% yield) as a yellow solid.

Compound **13**

R_f = 0.35 (CH₂Cl₂);

¹H NMR (400 MHz, CDCl₃) δ 9.92 (s, 4H), 8.89 (s, 4H), 8.80 (s, 4H), 8.43 (s, 4H), 8.41 (s, 4H), 7.33–7.27 (m, 8H), 7.25–7.17 (m, 8H), 5.92 (d, J = 17.3 Hz, 4H), 5.49 (d, J = 11.6 Hz, 4H), 4.91 (s, 4H), 4.28–4.23 (m, 16H), 1.98–1.84 (m, 16H), 1.69–1.58 (m, 16H), 1.09–1.01 (m, 24H);

¹³C NMR (151 MHz, CDCl₃) δ 192.4, 143.9, 143.5, 143.4, 143.2, 141.6, 137.3, 136.5, 136.0, 132.8, 130.7, 130.5, 130.0, 129.3, 128.7, 128.0, 127.7, 127.6, 124.9, 123.5, 122.1, 120.4, 117.8, 73.8, 73.6, 53.5, 32.6, 19.63, 19.56, 14.2, 14.1;

IR (film): 2957, 2931, 2870, 1691, 1610, 1584, 1440, 1074 cm⁻¹;

HRMS (MALDI): [M+Na]⁺ calcd. For C₁₂₈H₁₂₀Br₄NaO₁₂ 2187.5406, found 2187.5307.

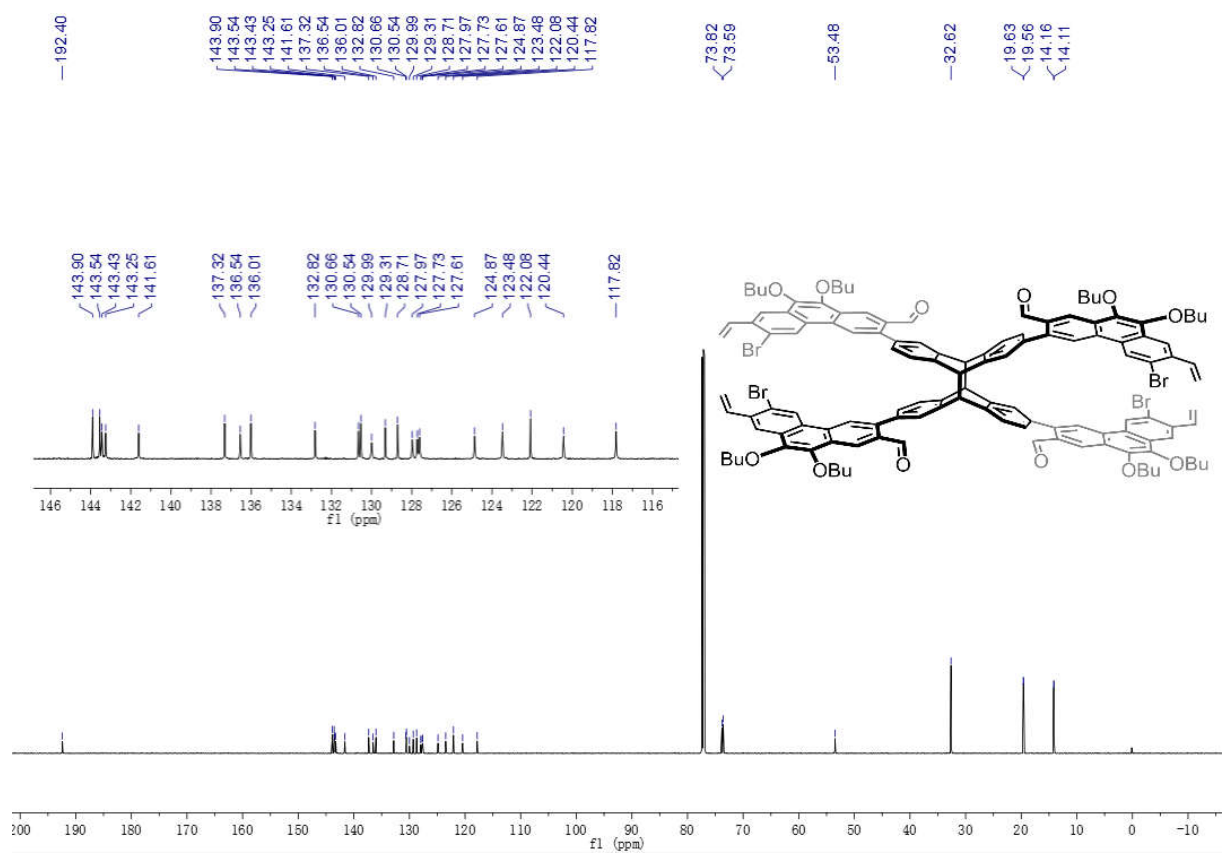
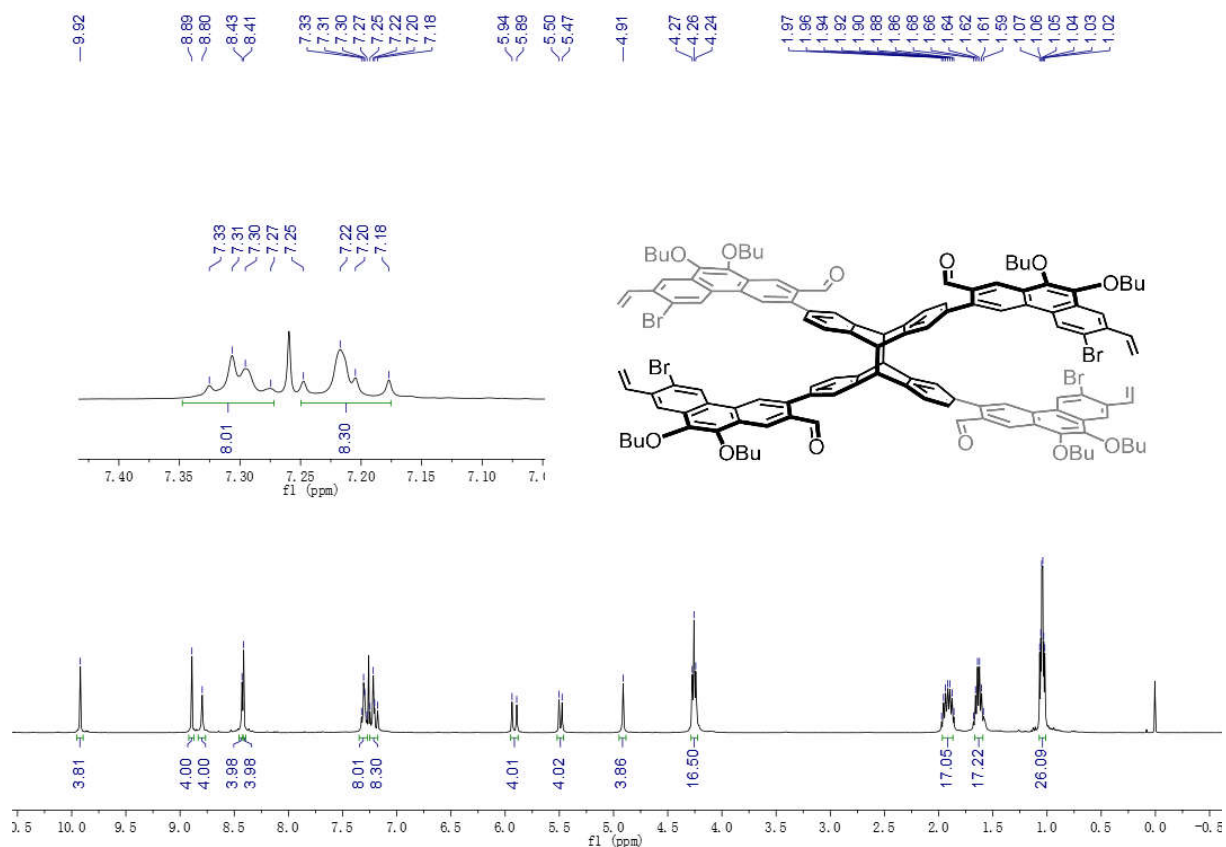
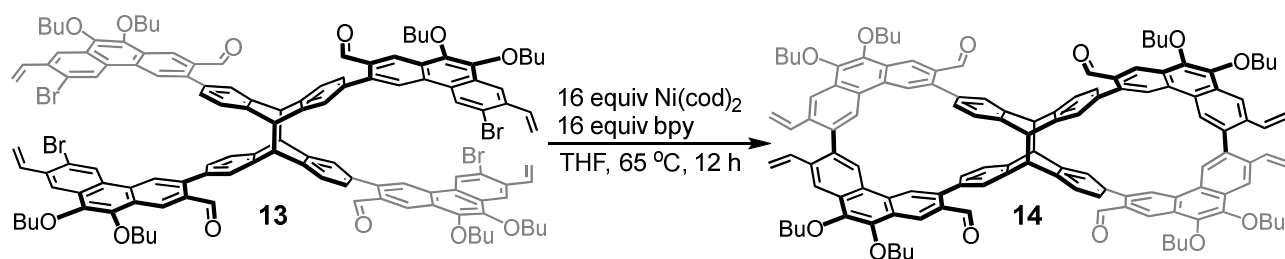
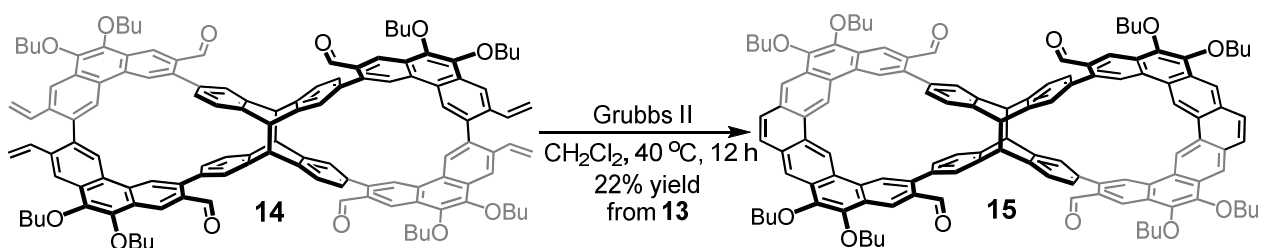


Figure S23. ^{13}C NMR spectrum (CDCl_3 , 151 MHz) of compound **13**.



In a nitrogen-filled glove box, Ni(cod)₂ (33.0 mg, 0.15 mmol, 16 equiv), 2,2'-bipyridyl (23.0 mg, 0.15 mmol, 16 equiv), and anhydrous THF (15 mL) were sequentially added to a 40 mL glass vial equipped with a stir bar. The vial was sealed with a Teflon-lined septum cap, transferred out of glove box, and stirred at 65 °C for 15 min. Meanwhile, compound **13** (20.0 mg, 0.0092 mmol, 1.0 equiv) and anhydrous THF (5 mL) were mixed in another 40 mL glass vial in the glove box. The vial was capped, and transferred out of the glove box. The solution of compound **13** was added to the first vial containing nickel complex. The mixture was stirred at 65 °C for 12 h, and cooled to room temperature. Eight reactions were carried out in parallel using identical procedures, and all the reaction mixtures were combined during work-up. The mixtures were filtered through a short pad of silica gel with the aid of mixed solvents (CH₂Cl₂: ethyl acetate = 2:1). The solvents were removed under reduced pressure. Crude **14** was found unstable on silica gel, and was used in the next step without further purification.



In a nitrogen-filled glove box, crude compound **14** (prepared from 8 × 20.0 mg of **13**), Grubbs II catalyst (16.0 mg, 0.019 mmol, 26 mol%), and anhydrous CH₂Cl₂ (120 mL) were sequentially added to a 250 mL round-bottom flask equipped with a stir bar. The flask was capped with a rubber septum and transferred out of glove box. The reaction mixture was stirred at 40 °C for 12 h, and cooled to room temperature. The solvents were removed under reduced pressure. Purification using silica gel column chromatography with CH₂Cl₂ afforded compound **15** (29.7 mg, 22% yield, based on **13** over two steps) as a yellow solid.

Compound 15

R_f = 0.30 (CH₂Cl₂: ethyl acetate = 100:1);

¹H NMR (600 MHz, Chloroform-*d*) δ 10.43 (s, 4H), 10.32 (s, 4H), 8.88 (s, 4H), 8.86 (s, 4H), 8.64 (s, 4H), 8.01 (s, 4H), 7.45 (s, 4H), 7.33 (d, *J* = 7.5 Hz, 4H), 7.18 (d, *J* = 7.5 Hz, 4H), 4.99 (s, 4H), 4.44–4.37 (m, 8H), 4.36–4.32 (m, 8H), 2.04–1.95 (m, 16H), 1.74–1.63 (m, 16H), 1.12–1.05 (m, 24H);

¹³C NMR (151 MHz, CDCl₃) δ 192.3, 144.5, 144.2, 144.0, 143.9, 142.7, 137.6, 132.13, 132.06, 131.6, 130.2, 129.4, 128.9, 128.8, 128.4, 128.2, 128.0, 127.8, 126.2, 123.0, 120.7, 118.7, 73.9, 73.7, 54.0, 32.8, 32.7, 19.7, 19.6, 14.23, 14.18;

IR (film): 2957, 2931, 2870, 1694, 1599, 1548, 1440, 1074 cm⁻¹;

HRMS (MALDI): [M]⁺ calcd. For C₁₂₄H₁₁₂O₁₂ 1792.8148, found 1792.8159.

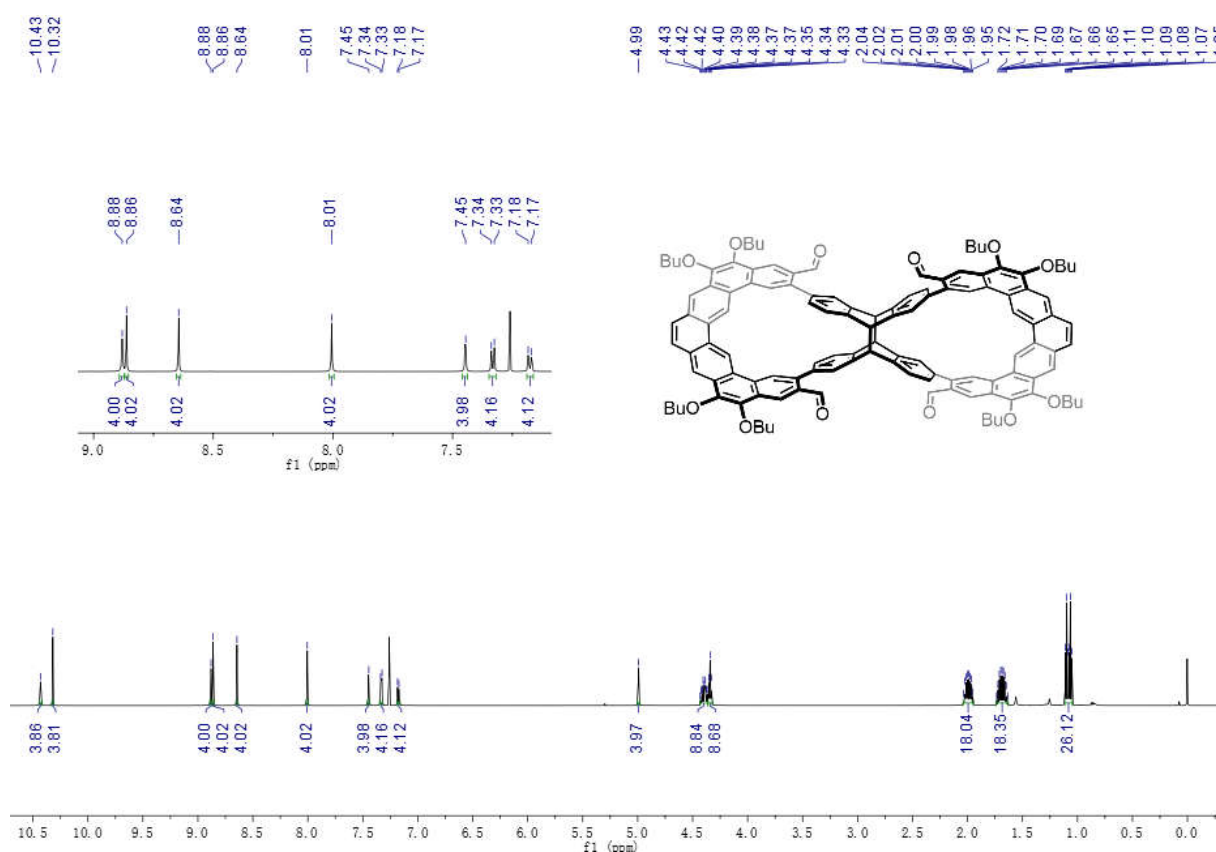


Figure S24. ¹H NMR spectrum (CDCl₃, 400 MHz) of compound 15.

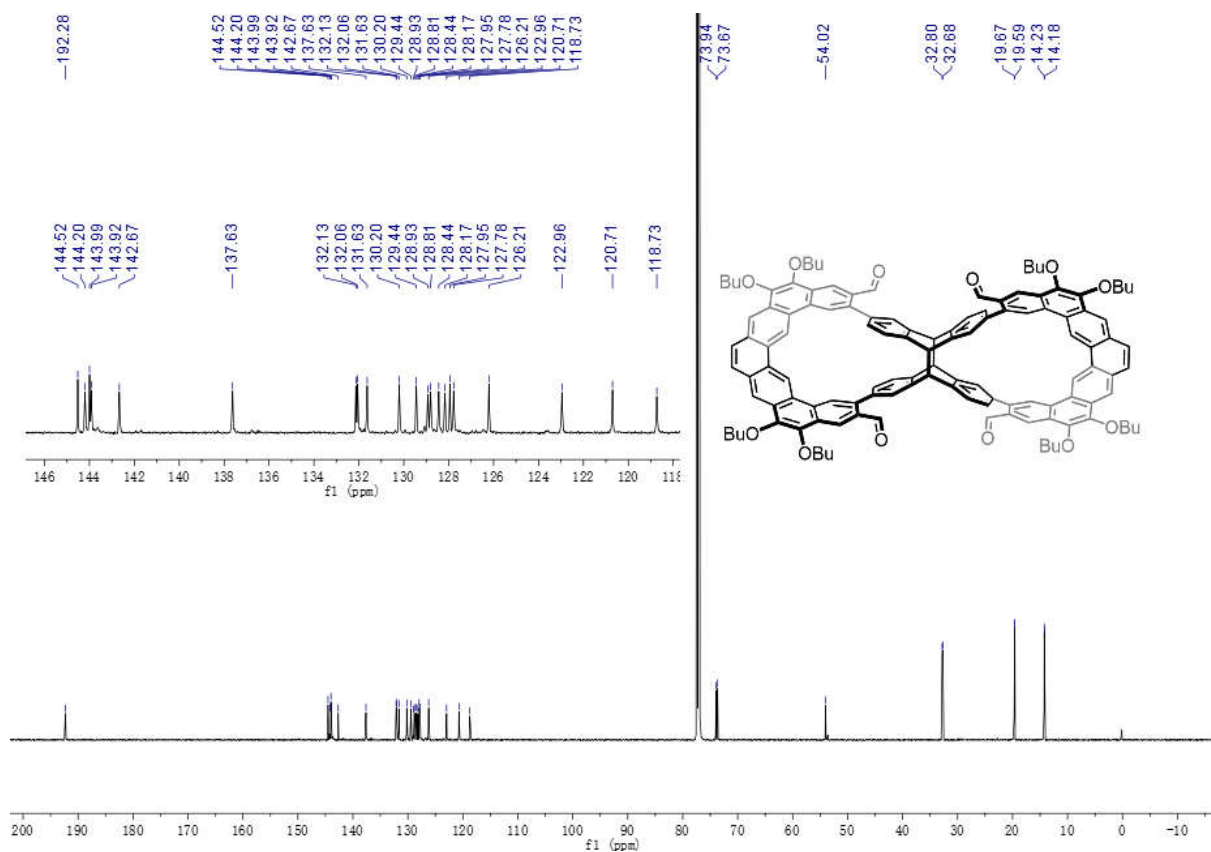


Figure S25. ^{13}C NMR spectrum (CDCl_3 , 151 MHz) of compound **15**.

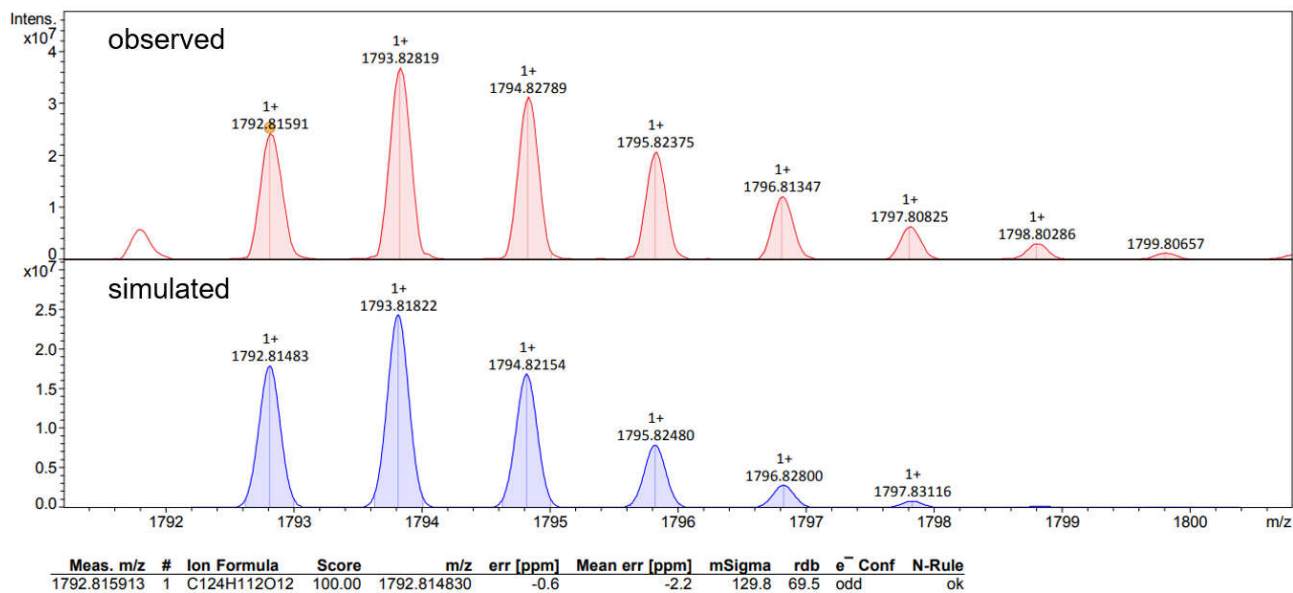
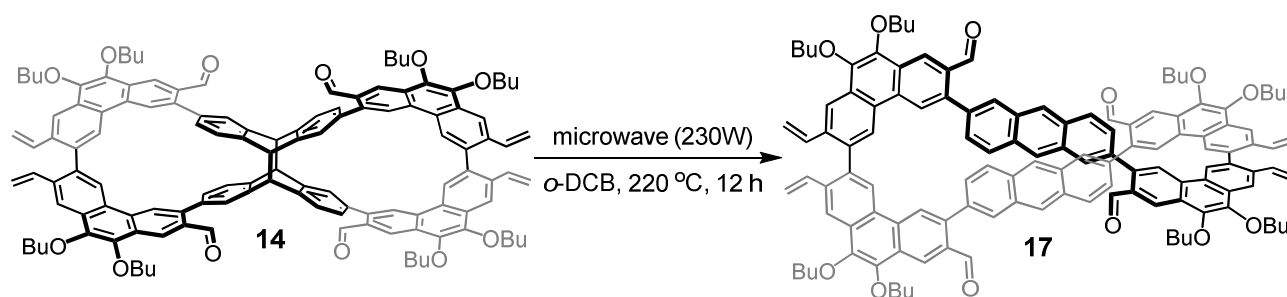
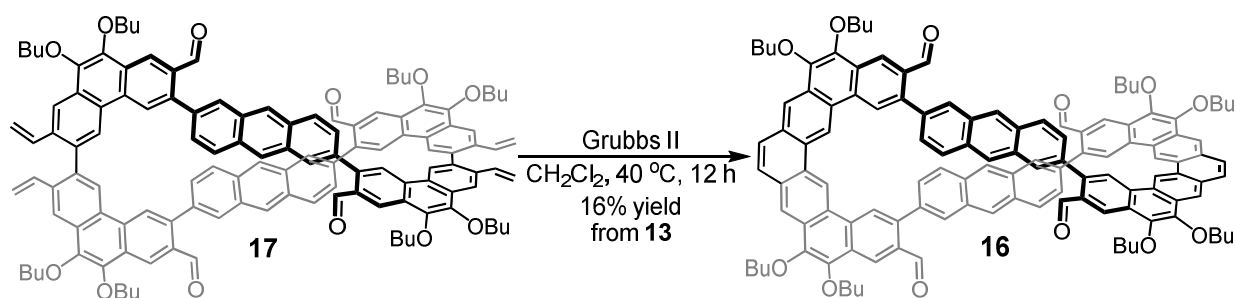


Figure S26. HRMS data for compound **15**.



In a nitrogen-filled glove box, the crude compound **14** (prepared from 12×20.0 mg of **13**) and 1,2-dichlorobenzene (15 mL) were added to a 20 mL microwave tube equipped with a stir bar. The tube was sealed with a Teflon-lined septum cap and transferred to the microwave reactor (conditions: 230 W, 220 °C, 12 h). Then, the reaction mixture was diluted with 20 mL of petroleum ether and filtered through a short pad of silica gel with the aid of CH_2Cl_2 . The solvents were removed under reduced pressure, affording crude **17** which was unstable on silica gel and was used in the next step without further purification.



In a nitrogen-filled glove box, the crude compound **17** (prepared from the previous step), Grubbs II catalyst (18.7 mg, 0.022 mmol, 0.20 equiv), and anhydrous CH_2Cl_2 (150 mL) were sequentially added to a 250 mL round-bottom flask equipped with a stir bar. The flask was capped with a rubber septum and transferred out of glove box. The reaction mixture was stirred at 40 °C for 12 h, and cooled to room temperature. The solvents were removed under reduced pressure. Purification using silica gel column chromatography with CH_2Cl_2 afforded compound **16** (32.0 mg, 16% yield, based on **13** over three steps) as a yellow solid.

Compound **16**

$R_f = 0.30$ (CH_2Cl_2 : ethyl acetate = 50:1);

$^1\text{H NMR}$ (400 MHz, Chloroform- d) δ 10.27 (s, 4H), 10.23 (s, 4H), 9.20 (s, 4H), 9.00 (s, 4H), 8.75 (s, 4H), 8.36 (s, 4H), 8.16 (s, 4H), 7.98 (s, 4H), 7.85–7.68 (m, 8H), 4.50–4.31 (m, 16H), 2.07–1.97 (m, 16H), 1.78–1.62 (m, 16H), 1.17–1.01 (m, 24H);

^{13}C NMR (151 MHz, CDCl_3) δ 192.2, 143.7, 143.2, 141.1, 135.4, 132.7, 132.3, 132.0, 131.5, 131.4, 130.2, 129.8, 129.5, 129.0, 128.6, 128.4, 128.2, 127.0, 126.8, 125.4, 124.2, 122.0, 118.2, 73.7, 73.5, 32.7, 32.5, 19.6, 19.5, 14.1, 14.0;

IR (film): 2956, 2930, 2870, 1690, 1605, 1440, 1344, 1074 cm^{-1} ;

HRMS (MALDI): $[\text{M}]^+$ calcd. for $\text{C}_{124}\text{H}_{112}\text{O}_{12}$ 1792.8148, found 1792.8147.

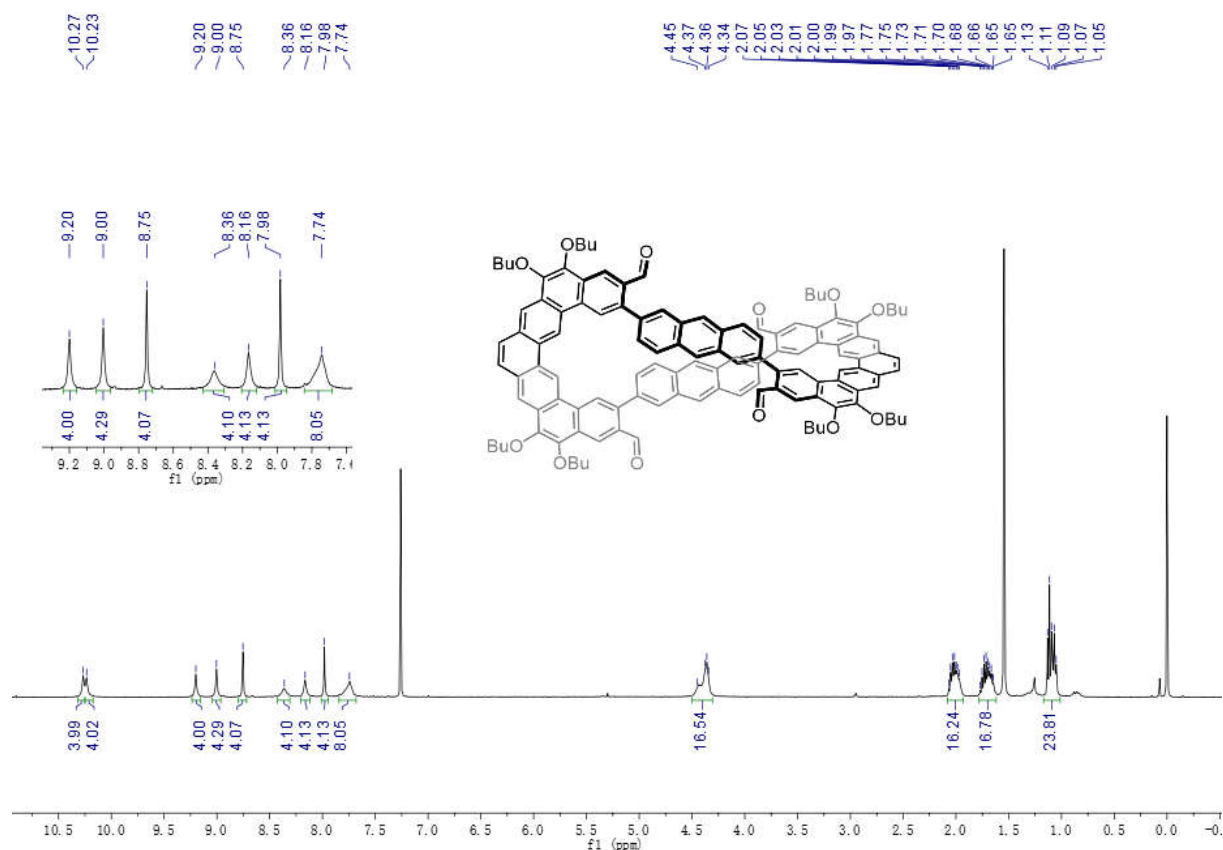


Figure S27. ^1H NMR spectrum (CDCl_3 , 400 MHz) of compound 16.

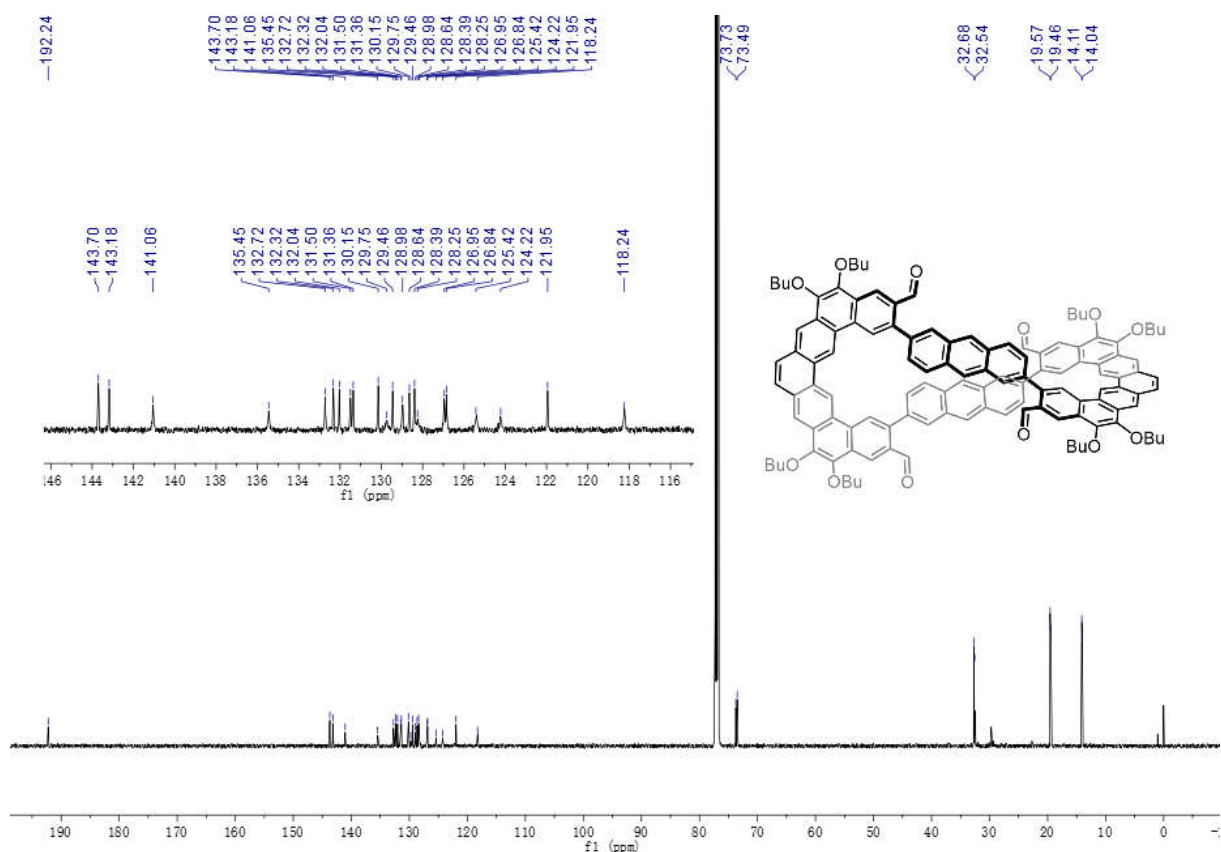


Figure S28. ^{13}C NMR spectrum (CDCl_3 , 151 MHz) of compound **16**.

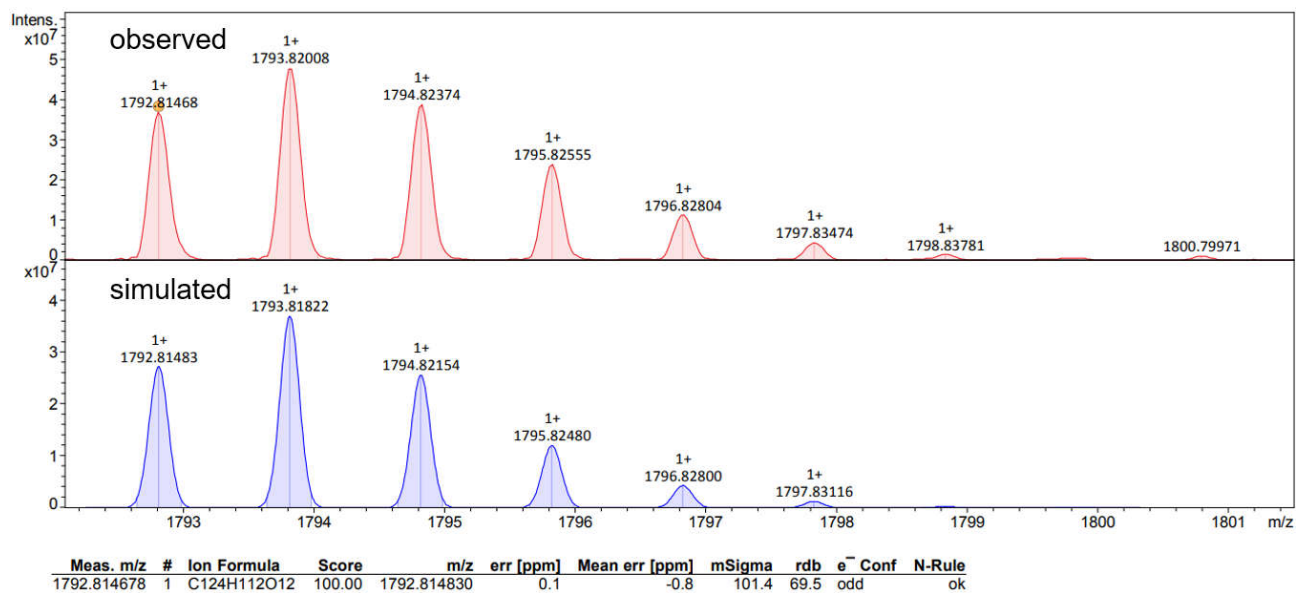


Figure S29. HRMS data for compound **16**.

III. X-ray Crystallography

X-ray diffraction data collection of the compounds were recorded by Bruker D8 VENTURE system with PHOTON II CPAD detector and a Ga-target Liquid METALJET D2 PLUS X-ray Source ($\lambda = 1.34139 \text{ \AA}$). The structure was solved by SHELXT (version 2018/2)^[S5] and refined by full-matrix least-squares procedures using the SHELXL program (version 2018/3)^[S6] through the Olex2 graphical interface.^[S7] Crystallographic data were deposited at the Cambridge Crystallographic Data Center. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures.

Compound **5** (CCDC #2288403)

Single crystals suitable for X-ray crystallography were obtained by slowly evaporation of CH₂Cl₂/ethyl acetate solution of **5** at 25 °C.

Table S1. Crystal data and structure refinement for **5**.

Identification code	5
Empirical formula	C ₁₂₀ H ₁₂₀ O ₁₀
Formula weight	1722.15
Temperature/K	200.00
Crystal system	monoclinic
Space group	P2 ₁ /n
a/Å	16.664(3)
b/Å	21.413(3)
c/Å	29.794(5)
α /°	90
β /°	100.271(7)
γ /°	90
Volume/Å ³	10461(3)
Z	4
$\rho_{\text{calc}}/\text{cm}^3$	1.093
μ/mm^{-1}	0.339
F(000)	3680.0
Crystal size/mm ³	0.2 × 0.12 × 0.1
Radiation	GaK α ($\lambda = 1.34139$)
2 θ range for data collection/°	4.446 to 116.03
Index ranges	-20 ≤ h ≤ 20, -26 ≤ k ≤ 26, -37 ≤ l ≤ 37
Reflections collected	146326
Independent reflections	21580 [R _{int} = 0.0853, R _{sigma} = 0.0543]
Data/restraints/parameters	21580/3275/1230
Goodness-of-fit on F ₂	1.141
Final R indexes [I >= 2 σ (I)]	R ₁ = 0.1001, wR ₂ = 0.2640
Final R indexes [all data]	R ₁ = 0.1236, wR ₂ = 0.2775
Largest diff. peak/hole / e Å ⁻³	0.66/-0.73

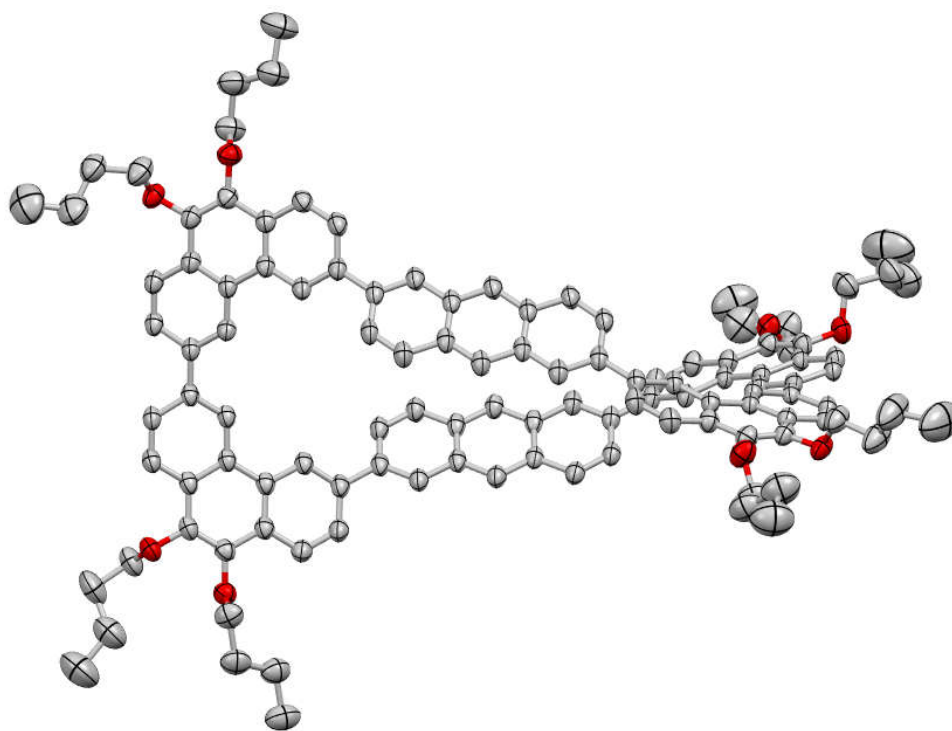


Figure S30. ORTEP drawing of **5** with the thermal ellipsoids shown at a 50% probability. (Color codes: red, O; black, C. Hydrogen atoms and solvent molecules are omitted for clarity.)

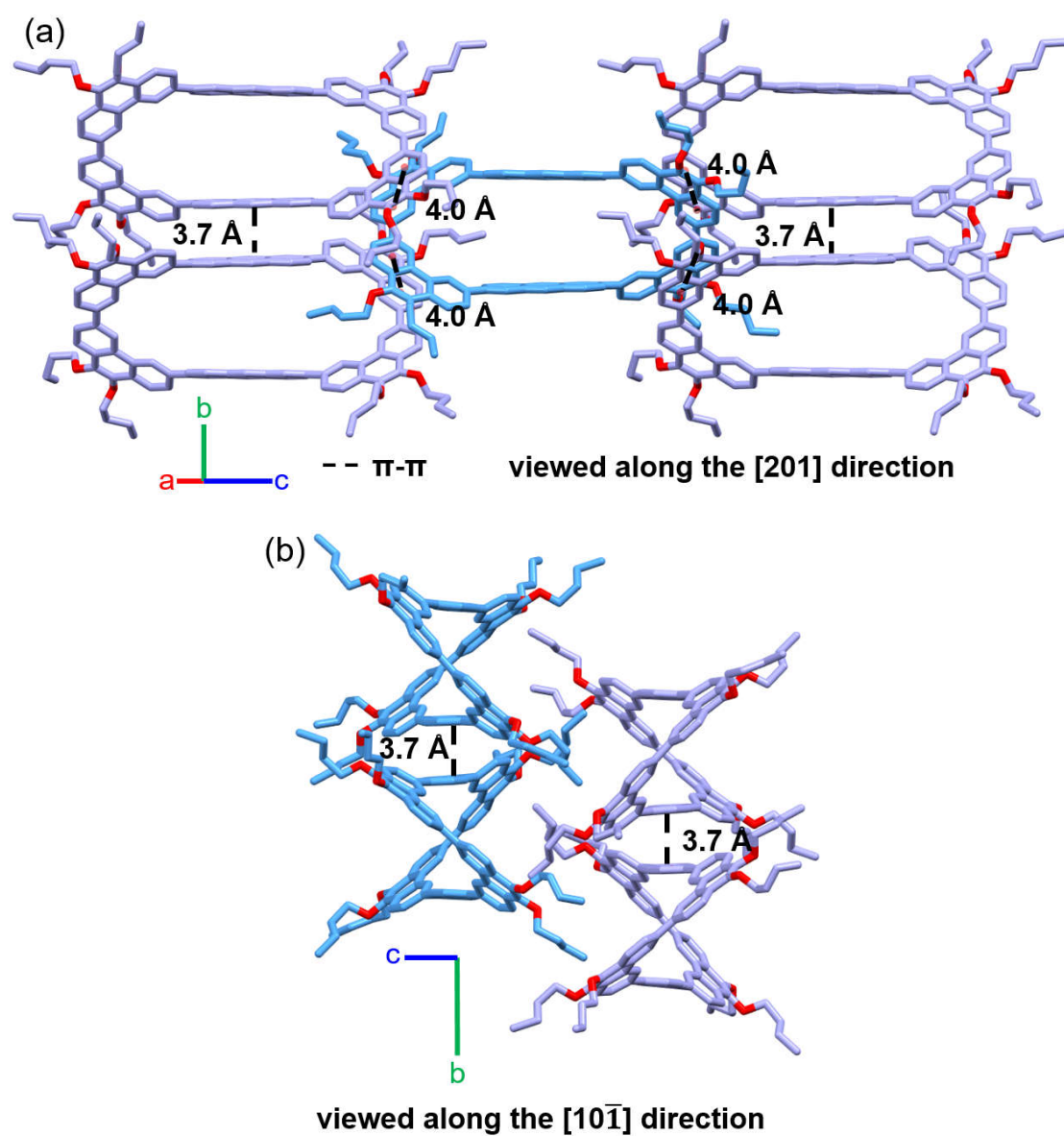


Figure S31. Molecular packing and intermolecular π - π interactions in the crystal structure of **5**. Hydrogen atoms and solvent molecules are omitted for clarity.

Compound **11** (CCDC #2288404)

Single crystals suitable for X-ray crystallography were obtained by slowly evaporation of CH₂Cl₂/ethyl acetate solution of **11** at 25 °C.

Table S2. Crystal data and structure refinement for **11**.

Identification code	11
Empirical formula	C ₁₂₀ H ₁₁₂ O ₁₂
Formula weight	1746.09
Temperature/K	200.00
Crystal system	triclinic
Space group	P-1
a/Å	11.8063(18)
b/Å	17.510(3)
c/Å	33.608(5)
α/°	88.500(4)
β/°	82.347(5)
γ/°	73.448(6)
Volume/Å ³	6599.9(17)
Z	2
ρ _{calc} /cm ³	0.879
μ/mm ⁻¹	0.280
F(000)	1856.0
Crystal size/mm ³	0.2 × 0.15 × 0.1
Radiation	GaKα (λ = 1.34139)
2θ range for data collection/°	4.58 to 112.042
Index ranges	-14 ≤ h ≤ 14, -21 ≤ k ≤ 21, 0 ≤ l ≤ 41
Reflections collected	29188
Independent reflections	29188 [R _{int} = 0.1586, R _{sigma} = 0.2496]
Data/restraints/parameters	29188/180/1218
Goodness-of-fit on F ²	0.993
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.1691, wR ₂ = 0.4003
Final R indexes [all data]	R ₁ = 0.2036, wR ₂ = 0.4448
Largest diff. peak/hole / e Å ⁻³	0.64/-0.60

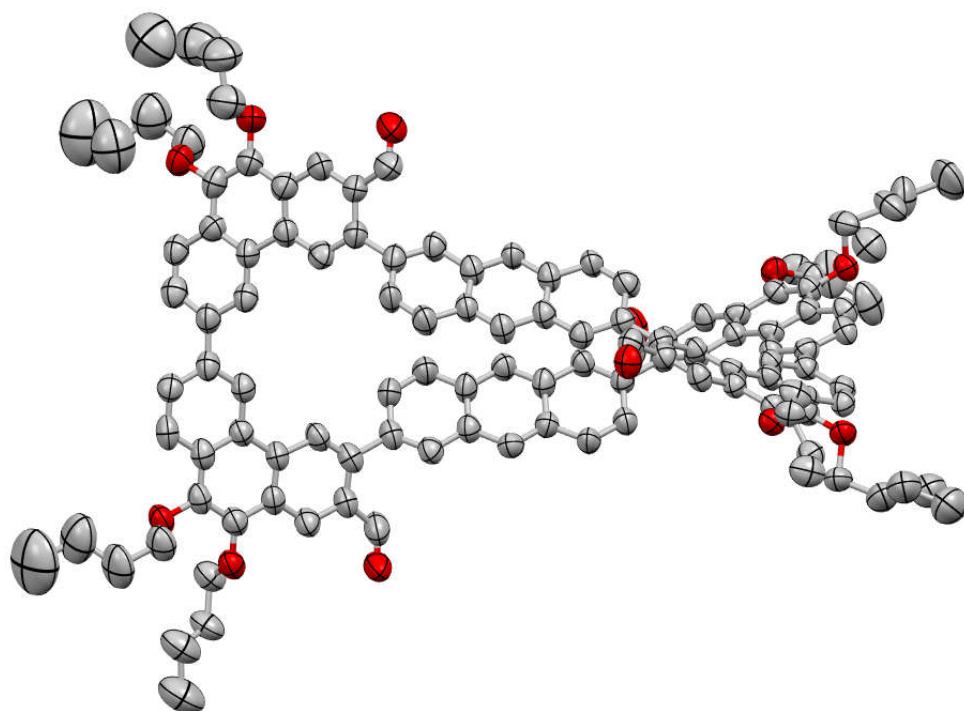


Figure S32. ORTEP drawing of **11** with the thermal ellipsoids shown at a 50% probability. (Color codes: red, O; black, C. Hydrogen atoms and solvent molecules are omitted for clarity.)

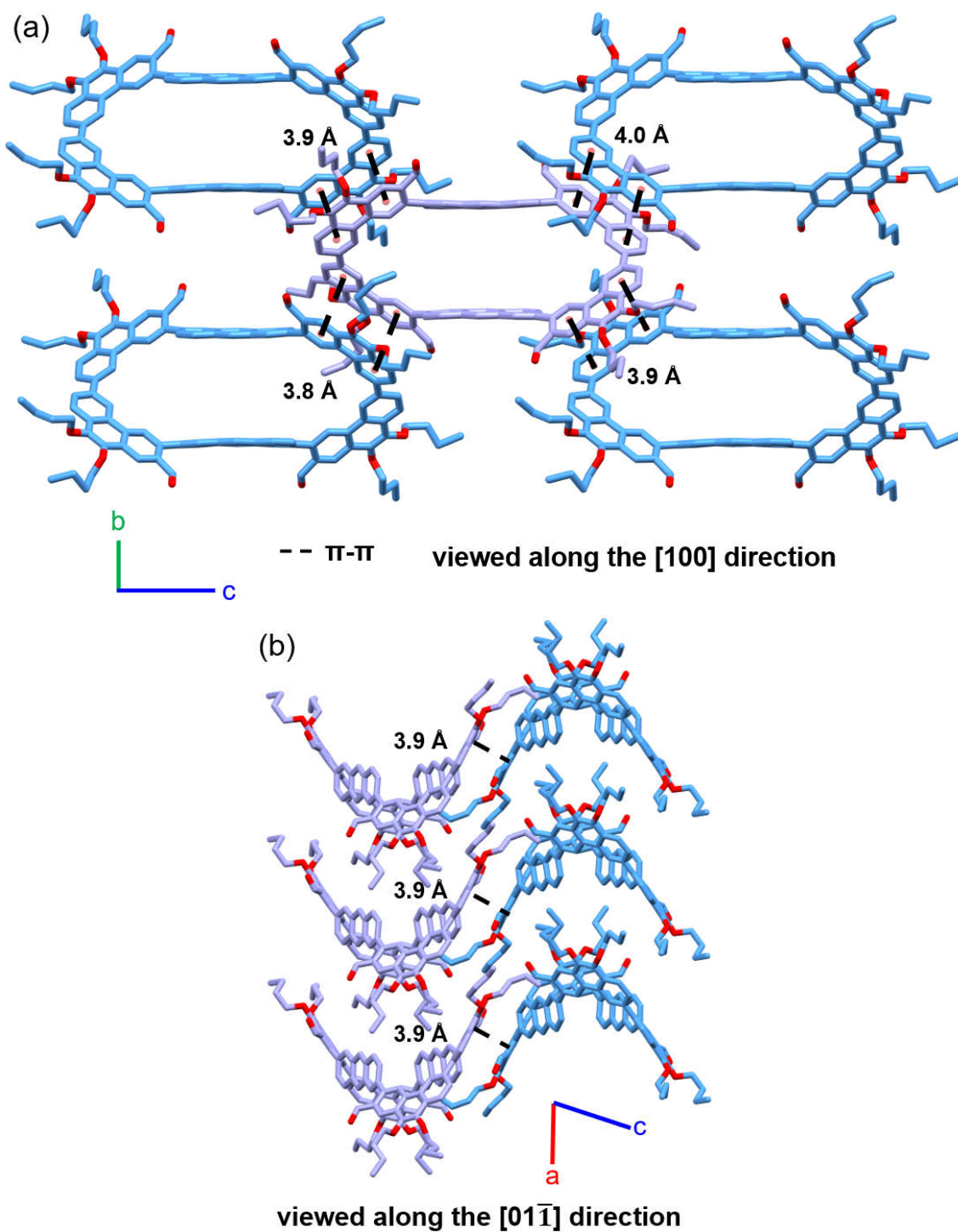


Figure S33. Molecular packing and intermolecular π - π interactions in the crystal structure of **11**. Hydrogen atoms and solvent molecules are omitted for clarity.

IV. Photophysical Properties

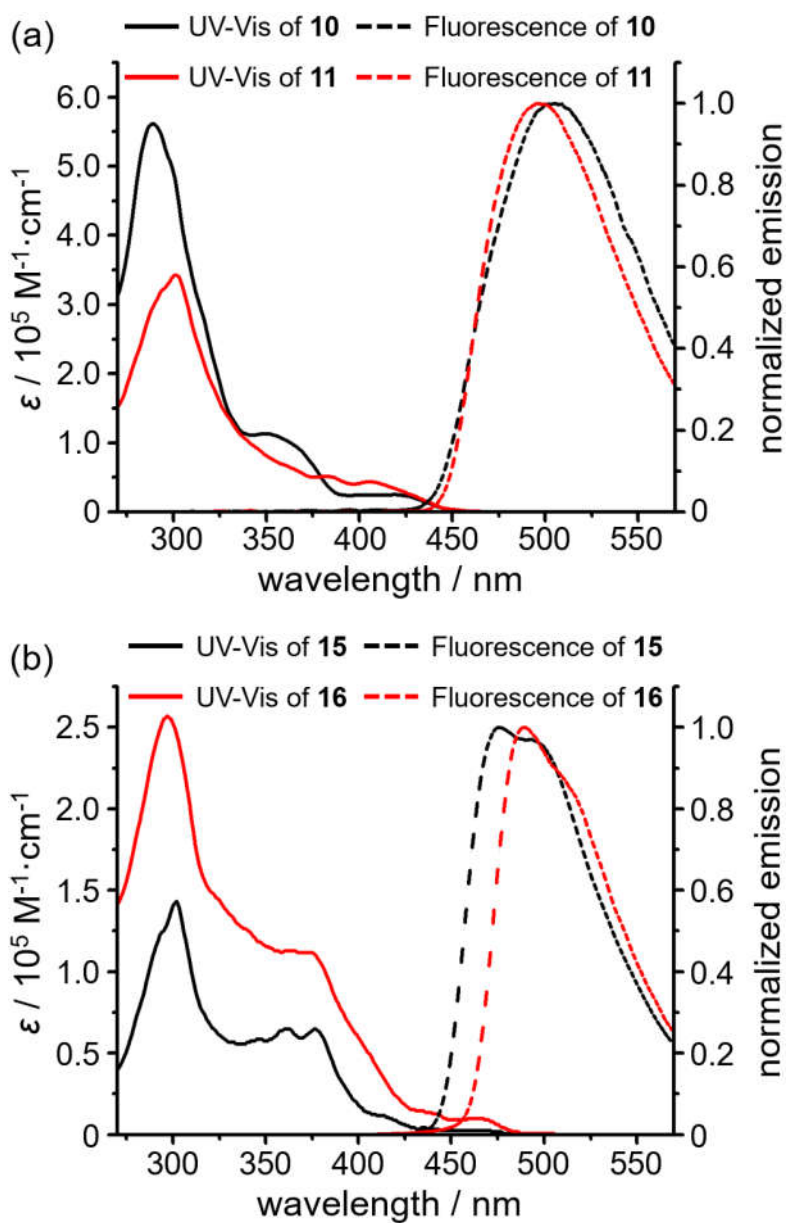


Figure S34. UV-Vis and fluorescence spectra of (a) **10** ($\lambda_{\text{ex}} = 289 \text{ nm}$) and **11** ($\lambda_{\text{ex}} = 301 \text{ nm}$), (b) **15** ($\lambda_{\text{ex}} = 302 \text{ nm}$) and **16** ($\lambda_{\text{ex}} = 297 \text{ nm}$) in CH_2Cl_2 ($1.1 \times 10^{-6} \text{ mol/L}^{-1}$) at $25 \text{ }^\circ\text{C}$.

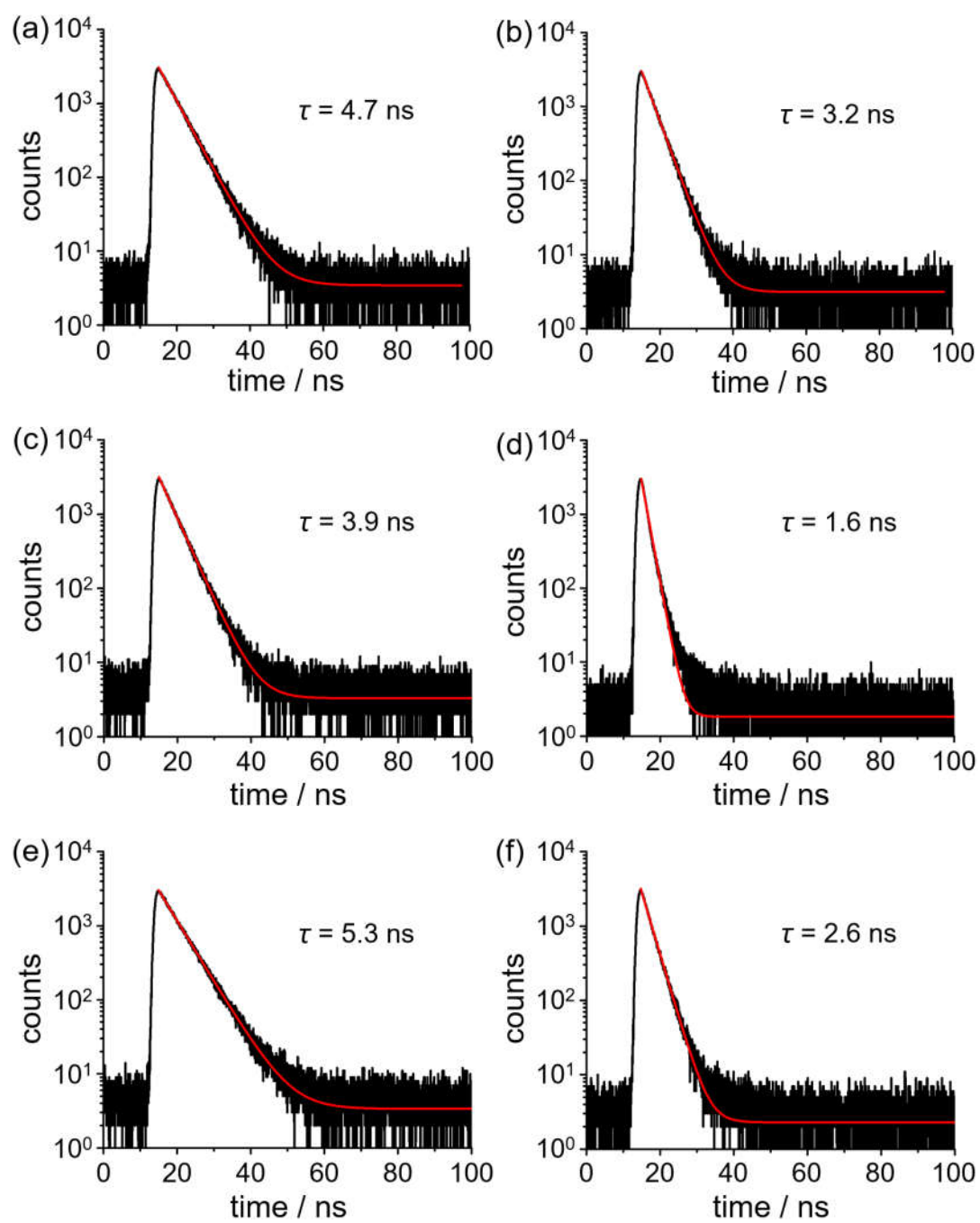


Figure S35. Emission lifetimes of (a) **4**, (b) **5**, (c) **10**, (d) **11**, (e) **15** and (f) **16** in CH_2Cl_2 at 25°C

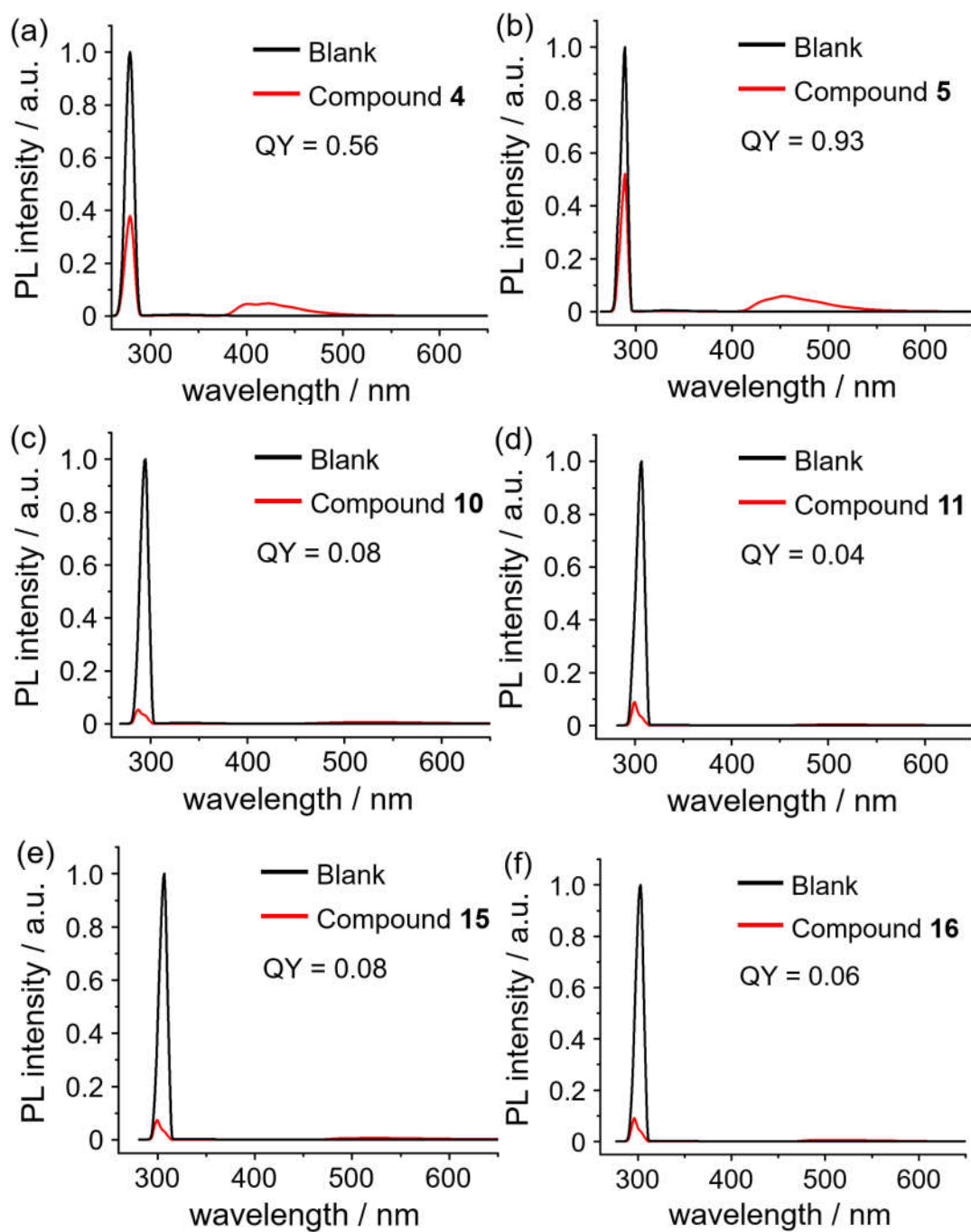


Figure S36. Quantum yields of (a) **4**, (b) **5**, (c) **10**, (d) **11**, (e) **15** and (f) **16** in CH_2Cl_2 at 25 °C.

V. Enantiomer Resolution and Chiroptic Properties

Preparative chromatographic resolution was outsourced under a contract with Daicel Chiral Technologies (China) Co. Ltd.

Conditions for preparative HPLC resolution were optimized as follows:

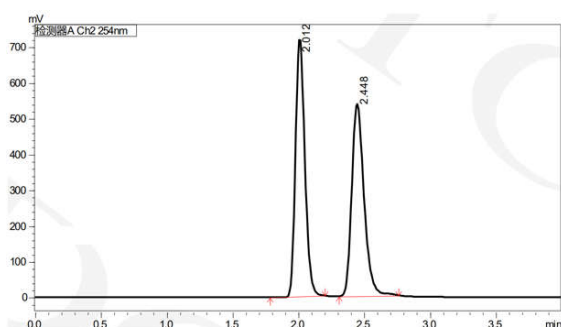
HPLC column: CHIRALPAK ID (2 cm I.D. × 25 cm L, 10 μm);

eluent: heptane/CH₂Cl₂ = 80/20 (V/V);

flow rate: 60.0 mL/min;

detection wavelength: 254 nm;

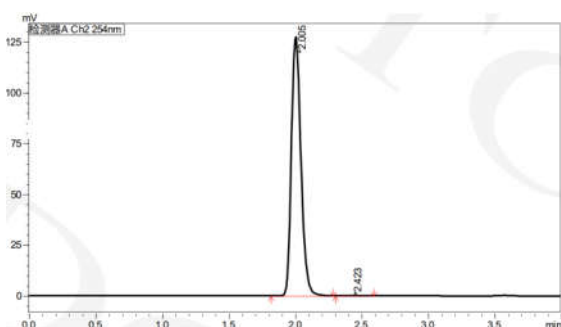
column temperature: 38 °C.



Racemic of **4**

<Peak Table>

Peak#	Ret. Time	Area	Area%
1	2.012	3565657	50.596
2	2.448	3481617	49.404



Peak 1

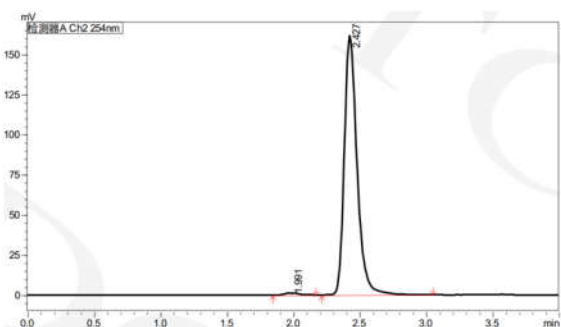
Assigned as (*P*)-**6** (99.7% ee);

retention time: 2.0 min;

[α]³⁰_D = -4471 (c = 0.31, in CH₂Cl₂).

<Peak Table>

Peak#	Ret. Time	Area	Area%
1	2.005	638037	99.845
2	2.423	990	0.155



Peak 2

Assigned as (*M*)-**6** (98.4% ee);

retention time: 2.4 min;

[α]³⁰_D = +4114 (c = 0.28, in CH₂Cl₂).

<Peak Table>

Peak#	Ret. Time	Area	Area%
1	1.991	8903	0.819
2	2.427	1078445	99.181

Figure S37. HPLC separation of enantiomers of **4**.

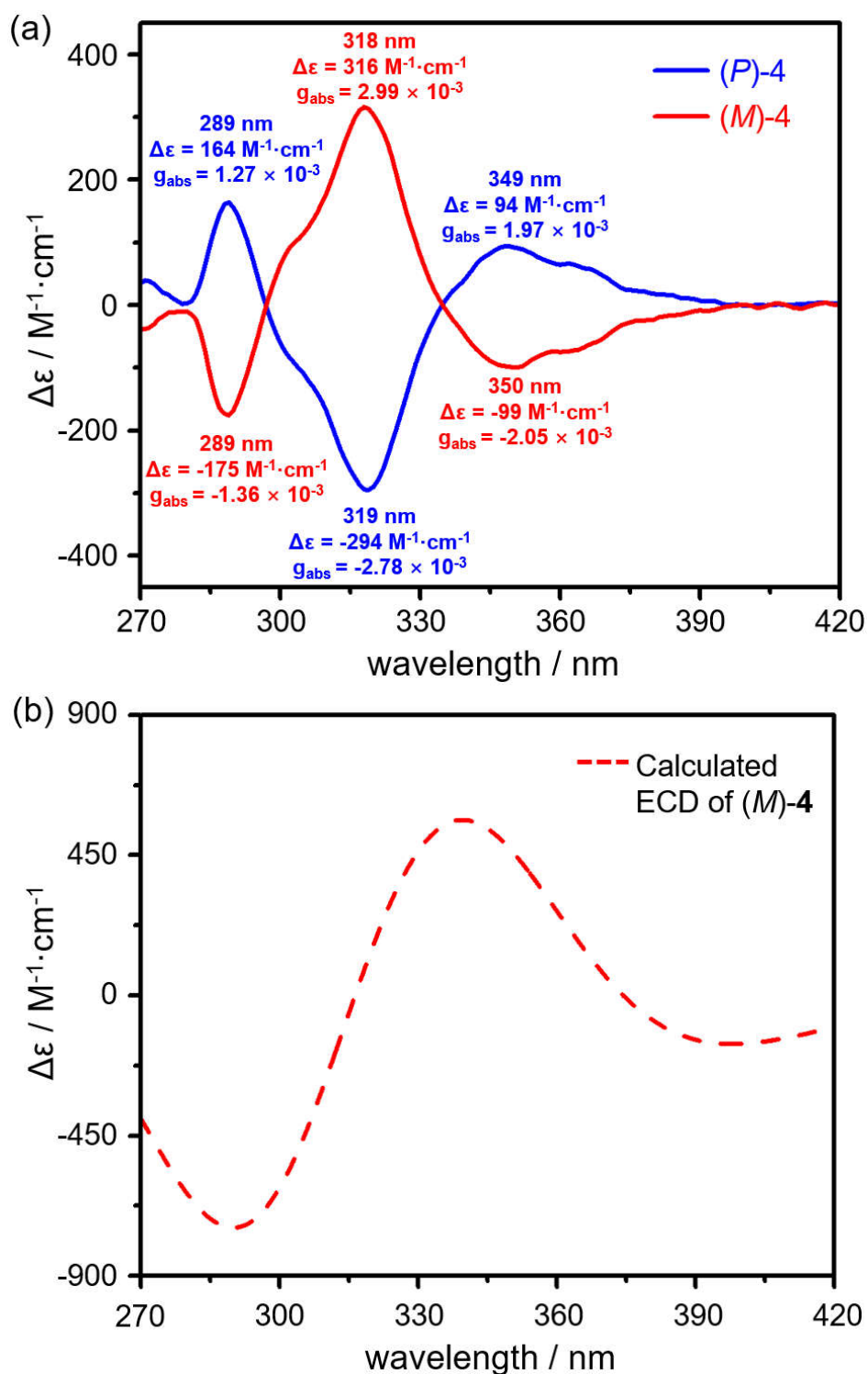


Figure S38. The electronic circular dichroism (ECD) spectra of **4** in CH_2Cl_2 . (a) Experimental ECD spectra of enantiomers of **4**. (b) Calculated ECD spectrum of (*M*)-**4**.

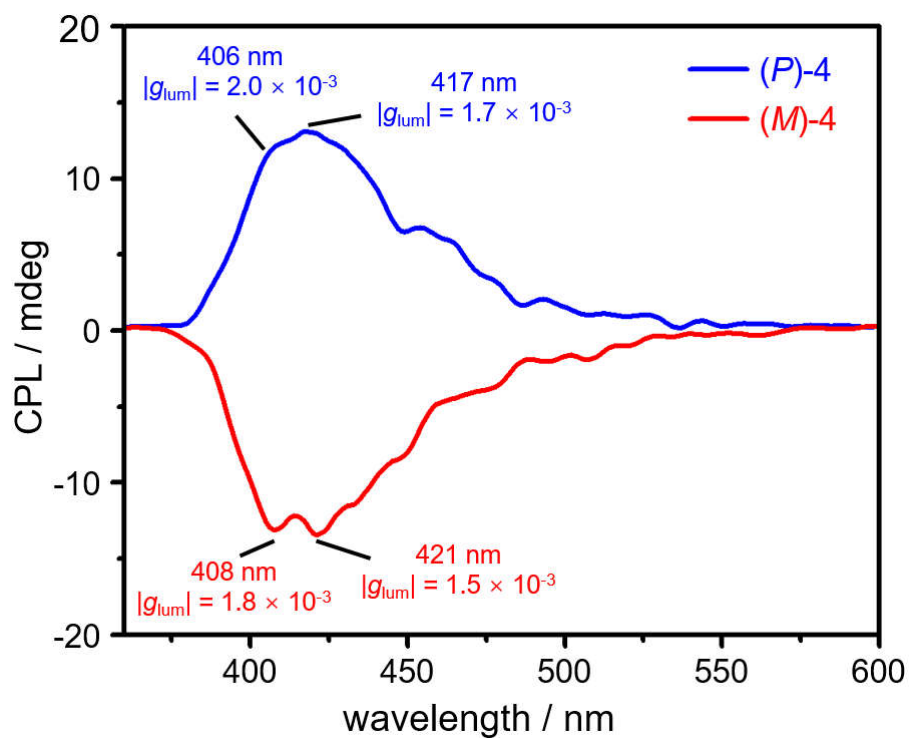


Figure S39. The circularly polarized luminescence (CPL) spectra of **4** in CH₂Cl₂.

VI. Density Functional Theory Calculations

The structures were optimized at the B3LYP/6-31G* level. The dispersion correction with the Grimme's D3 version was considered. Considering the calculation cost and the reliability of the results, all butoxy groups were replaced by methyl groups. Based on the optimized structures, the time-dependent (TD) B3LYP/6-31G* method was used to calculate fifty singlet excited states in order to fit the electronic circular dichroism (ECD) spectrum. All the calculations were performed with Gaussian 16 software package.^[S8] Cartesian coordinates of the optimized structures were listed at the end. Simulated ECD spectrum was performed with the help of programs multiwfn^[S9] and VMD^[S10].

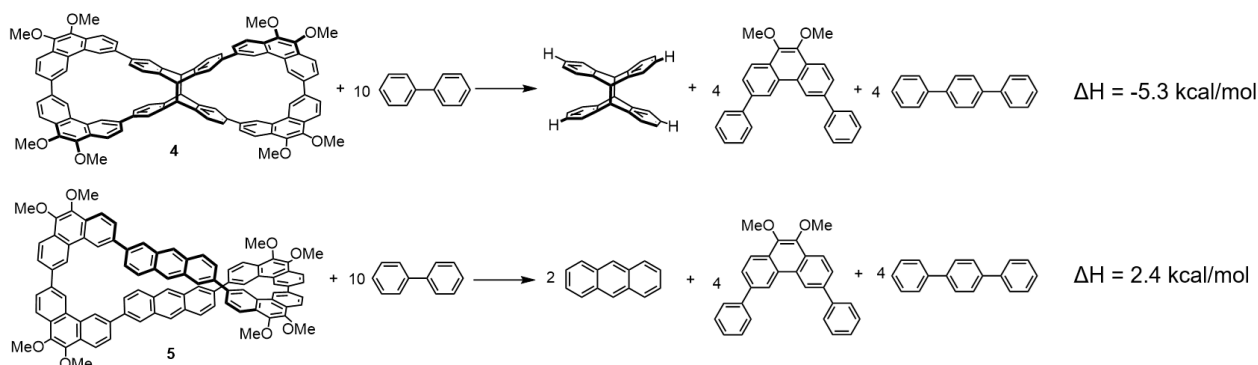


Figure S40. Internal strain enthalpy of compounds **4** and **5**.

Note: The results indicated that 7.7 kcal/mol of strain is released during the conversion of **4** into **5**.

Table S3. Cartesian coordinates (Å) of the optimized structures

Compound **4**

C	-5.598883	4.190103	-3.362446	C	-8.497483	1.223411	-0.68268
C	-4.480723	3.790713	-2.655019	C	-9.688515	0.528311	-0.494406
C	-4.596971	2.888856	-1.570172	C	-10.80009	0.897864	-1.288619
C	-5.859512	2.410746	-1.243812	C	-10.679483	1.887573	-2.248121
C	-7.017073	2.773317	-1.960522	C	0.030839	-0.812746	1.391724
C	-6.882546	3.687886	-3.041296	C	1.24885	-1.365616	0.668549
C	-8.317299	2.182084	-1.689509	C	1.205785	-1.40354	-0.736853
C	-9.440538	2.530511	-2.488736	C	-0.03084	0.812745	1.391725
C	-9.27901	3.508304	-3.531817	C	-1.24316	-1.37061	-0.667924
C	-8.047778	4.05281	-3.805572	C	-1.199818	-1.408811	0.737481
				C	-2.263294	-1.943557	1.456643

C	-3.411125	-2.422419	0.801514	C	9.686622	0.580872	0.48906
C	-3.448543	-2.366469	-0.599646	C	8.496569	1.279611	0.669742
C	-2.371576	-1.853836	-1.324753	C	8.309754	2.230618	1.682744
C	2.271811	-1.932897	-1.45614	C	9.427225	2.571929	2.493181
C	3.42166	-2.407394	-0.801313	C	7.004215	2.80552	1.961984
C	3.458147	-2.352944	0.599958	C	6.866134	3.726914	3.036527
C	2.379049	-1.844993	1.325196	C	8.031399	4.104339	3.794959
C	0.027411	0.812785	-1.391044	C	9.258096	3.538312	3.545404
C	-1.205785	1.403542	-0.736852	C	5.847913	2.433165	1.248108
C	-1.24885	1.365616	0.668551	C	4.584143	2.911152	1.569418
C	-0.02741	-0.812783	-1.391045	C	4.464535	3.82073	2.647381
C	1.199818	1.408811	0.737482	C	5.580806	4.227363	3.353727
C	1.24316	1.370611	-0.667922	O	-7.855148	-5.011532	4.818458
C	2.371576	1.853837	-1.324751	C	-8.489653	-6.279915	4.605623
C	3.448542	2.366471	-0.599644	O	-10.37311	-3.881301	4.280343
C	3.411124	2.42242	0.801517	C	-10.345728	-3.443911	5.646138
C	2.263294	1.943557	1.456645	O	-10.392018	3.83227	-4.278406
C	-2.379049	1.844993	1.325197	C	-10.853512	5.179234	-4.10721
C	-3.458147	2.352943	0.599959	O	-7.879923	4.977132	-4.815089
C	-3.421661	2.407394	-0.801312	C	-8.04461	4.450761	-6.139168
C	-2.271811	1.932899	-1.456139	O	7.87992	-4.977138	-4.815085
C	-10.66683	-1.928363	2.257892	C	8.044596	-4.450773	-6.139168
C	-10.792419	-0.942781	1.294818	O	10.392021	-3.832275	-4.278402
C	-9.686622	-0.580869	0.489065	C	10.853527	-5.179231	-4.107183
C	-8.49657	-1.279608	0.669746	O	7.855152	5.011531	4.818459
C	-8.309753	-2.230616	1.682746	C	8.48965	6.279917	4.605617
C	-9.427224	-2.571928	2.493183	O	10.373112	3.881303	4.280338
C	-7.004215	-2.805519	1.961984	C	10.345732	3.443918	5.646135
C	-6.866134	-3.726915	3.036526	H	-5.511567	4.896569	-4.180644
C	-8.031398	-4.104339	3.794959	H	-3.502093	4.18416	-2.91675
C	-9.258095	-3.538312	3.545406	H	-5.926941	1.691113	-0.436735
C	-5.847914	-2.433164	1.248107	H	-7.671237	1.000208	-0.022304
C	-4.584144	-2.911152	1.569416	H	-11.746256	0.377247	-1.166961
C	-4.464535	-3.820732	2.647377	H	-11.527532	2.160215	-2.866744
C	-5.580805	-4.227364	3.353724	H	0.073375	-1.115931	2.442082
C	5.598883	-4.190109	-3.362443	H	-0.073375	1.115929	2.442083
C	4.480723	-3.790718	-2.655017	H	-2.226867	-1.954315	2.543714
C	4.596971	-2.888857	-1.570174	H	-4.320235	-2.748091	-1.123946
C	5.859511	-2.410744	-1.243816	H	-2.41436	-1.831459	-2.41129
C	7.017072	-2.773316	-1.960525	H	2.235604	-1.942571	-2.54324
C	6.882546	-3.68789	-3.041295	H	4.330873	-2.731972	1.124398
C	8.317298	-2.182082	-1.689513	H	2.421562	-1.82329	2.411742
C	9.440537	-2.530509	-2.488739	H	0.068697	1.116254	-2.441396
C	9.279009	-3.508306	-3.531817	H	-0.068697	-1.116251	-2.441397
C	8.047778	-4.052813	-3.805571	H	2.41436	1.831461	-2.411288
C	8.497482	-1.223407	-0.682685	H	4.320234	2.748094	-1.123944
C	9.688514	-0.528308	-0.494411	H	2.226867	1.954313	2.543716
C	10.800089	-0.897862	-1.288624	H	-2.421562	1.823291	2.411744
C	10.679482	-1.887572	-2.248124	H	-4.330873	2.731971	1.1244
C	10.666831	1.928365	2.257888	H	-2.235603	1.942573	-2.543238
C	10.792419	0.942783	1.294813	H	-11.514629	-2.206062	2.87469

H	-11.738652	-0.421406	1.176898	H	-10.246807	-2.352098	5.699007
H	-7.675877	-1.064234	-0.0002	H	-11.302944	-3.744171	6.078879
H	-5.917576	-1.706035	0.447941	H	-11.755118	5.269669	-4.71763
H	-3.484233	-4.211458	2.90694	H	-11.102908	5.370903	-3.055707
H	-5.488999	-4.927273	4.176989	H	-10.101149	5.900298	-4.442355
H	5.511568	-4.896579	-4.180637	H	-7.837612	5.278593	-6.821476
H	3.502094	-4.184167	-2.916747	H	-7.329802	3.638238	-6.322326
H	5.92694	-1.691107	-0.436741	H	-9.063987	4.083567	-6.294751
H	7.671235	-1.000204	-0.02231	H	7.837597	-5.27861	-6.821471
H	11.746255	-0.377246	-1.166965	H	7.329784	-3.638253	-6.322326
H	11.527531	-2.160215	-2.866748	H	9.063971	-4.083576	-6.294761
H	11.51463	2.206062	2.874686	H	11.755132	-5.26967	-4.717604
H	11.738652	0.421409	1.176892	H	11.102931	-5.370878	-3.055677
H	7.675877	1.064238	-0.000203	H	10.10117	-5.900309	-4.44231
H	5.917575	1.706036	0.447941	H	8.227788	6.897517	5.467993
H	3.484233	4.211455	2.906946	H	9.576964	6.171268	4.539904
H	5.489	4.92727	4.176993	H	8.11143	6.75152	3.689593
H	-8.227777	-6.897519	5.467991	H	11.302958	3.744156	6.078866
H	-9.576969	-6.171264	4.53993	H	9.523253	3.913173	6.195188
H	-8.111452	-6.751516	3.68959	H	10.246786	2.352107	5.699008
H	-9.523234	-3.913146	6.195185				

Compound 5

O	8.255708	5.596493	-4.321826	C	8.276474	2.080089	-1.971792
O	10.550355	4.878443	-2.866352	C	-3.572953	-1.089495	-3.494075
O	-10.543022	4.842497	2.961914	C	-7.085809	-2.391524	-2.798285
O	-8.244836	-5.511688	-4.449517	C	7.082782	-2.455115	2.758652
O	10.530152	-4.905188	2.888956	C	-5.910959	-1.61151	-2.786245
O	8.232462	-5.611576	4.345192	H	-5.865435	-0.727757	-2.160417
O	-10.542887	-4.824037	-2.987828	C	-9.427978	2.890663	2.094788
O	-8.246043	5.529922	4.428521	C	10.602881	-1.451891	0.537824
C	-8.333367	0.928471	1.172562	H	11.492155	-1.215098	-0.039501
H	-7.47823	0.265793	1.107956	C	5.911869	-1.669184	2.767065
C	9.468095	0.588259	-0.425122	H	5.873045	-0.766113	2.169001
C	-8.336288	-0.909211	-1.194771	C	-4.78176	-1.946113	-3.527735
H	-7.486295	-0.239118	-1.139467	C	7.091201	-3.651523	3.532738
C	7.095081	2.439125	-2.745104	C	-10.602517	-1.426419	-0.555207
C	-8.272465	-2.044211	-2.027787	H	-11.48999	-1.200413	0.029192
C	1.295674	-0.553818	-3.471349	C	9.432911	2.910456	-2.039706
C	-3.578096	1.101358	3.490054	C	-4.784727	1.96128	3.516615
C	-9.466913	-0.588022	-0.449745	C	-10.608156	1.430342	0.551184
C	9.465221	-0.615381	0.439397	H	-11.497408	1.200531	-0.028995
C	-8.271815	2.06166	2.008129	C	8.330923	-0.953145	1.171529
C	-7.089185	2.404482	2.78688	H	7.478219	-0.286167	1.12083
C	1.144935	0.882534	-3.457234	C	3.582257	1.155701	-3.474804
C	-1.13551	-0.817025	-3.479755	C	-9.423954	-2.880505	-2.105777
C	-9.467566	0.600014	0.4361	C	1.289414	0.554519	3.465704
C	8.336034	0.930684	-1.158536	C	-3.714403	-0.32809	3.459915
H	7.480785	0.266855	-1.109372	H	-4.711066	-0.758874	3.4842
C	-1.141173	0.823253	3.474704	C	3.572244	-1.160233	3.479749

C	2.314766	1.698024	-3.461653	C	-10.578931	-2.544168	-1.362677
H	2.187295	2.777277	-3.428262	H	-11.446276	-3.190318	-1.438885
C	7.107655	3.63786	-3.515574	C	8.268607	-4.476388	3.563677
C	10.588761	2.553548	-1.30763	C	-8.284727	-4.38021	-3.662648
H	11.454405	3.204065	-1.363068	C	4.810265	-3.218853	4.249055
C	5.922223	1.656164	-2.757652	H	3.945739	-3.495093	4.845698
H	5.880501	0.750706	-2.16338	C	-4.81904	3.145876	4.292112
C	8.266301	-2.101321	1.986133	H	-3.95553	3.413052	4.894326
C	-1.286129	0.618985	-3.444501	C	3.708813	0.269482	3.475071
C	9.413188	4.099189	-2.848383	H	4.705495	0.69957	3.509353
C	-2.305487	-1.631985	-3.505635	C	5.955829	4.003785	-4.24944
H	-2.177988	-2.711736	-3.509317	H	5.989589	4.910582	-4.842857
C	9.419936	-2.935329	2.056952	C	-8.279725	4.408361	3.627453
C	1.135451	-0.881543	3.46283	C	-0.156476	-1.425109	3.448193
C	-3.706113	0.339896	-3.450497	H	-0.27679	-2.506623	3.437397
H	-4.701949	0.772926	-3.468687	C	-2.610147	1.15679	-3.427974
C	4.790389	2.013837	-3.484222	H	-2.732399	2.237208	-3.410219
C	-7.101611	-3.564903	-3.606726	C	4.825916	3.214305	-4.234775
C	8.28773	4.459006	-3.543432	H	3.962389	3.495062	-4.830772
C	4.778365	-2.021144	3.493882	C	-5.951641	-3.908866	-4.353985
C	10.608903	1.420741	-0.521342	H	-5.982247	-4.80504	-4.963524
H	11.496593	1.180152	0.056847	C	-2.62029	-1.147572	3.442512
C	-5.91697	1.620504	2.782517	H	-2.744972	-2.227825	3.434585
H	-5.876397	0.727822	2.169181	C	2.614784	1.089307	3.469336
C	5.937836	-4.011566	4.267098	H	2.73963	2.169514	3.480828
H	5.968528	-4.916465	4.863567	C	-5.947904	3.936389	4.322926
C	2.303424	-1.699633	3.471731	H	-5.980545	4.830714	4.935039
H	2.173271	-2.778763	3.446064	C	8.297526	6.82524	-3.583211
C	-7.100317	3.587041	3.581918	H	9.23524	6.919661	-3.026422
C	-0.145734	1.428844	-3.436247	H	7.450006	6.886547	-2.888546
H	-0.263591	2.510507	-3.416538	C	11.232835	4.90739	-4.127605
C	-10.585663	2.548109	1.358704	H	10.604102	5.34978	-4.906821
H	-11.451035	3.197579	1.428708	H	11.531687	3.894815	-4.427502
C	3.715696	-0.274278	-3.480415	C	-9.08629	-5.45889	-5.610001
H	4.711463	-0.7062	-3.518335	H	-8.80659	-4.612903	-6.250822
C	0.150809	1.366956	3.473258	H	-10.140829	-5.373359	-5.329079
H	0.271129	2.448495	3.481946	C	-11.223628	4.847065	4.224486
C	2.619798	-1.091634	-3.480034	H	-10.593507	5.27368	5.011336
H	2.742118	-2.17201	-3.49958	H	-11.522671	3.828965	4.504874
C	-1.295034	-0.612647	3.451822	C	-10.42135	-6.118189	-2.381341
C	-9.398917	-4.056467	-2.93282	H	-10.149874	-6.023641	-1.322096
C	0.155238	-1.36362	-3.484265	H	-9.673584	-6.727713	-2.898576
H	0.273081	-2.445318	-3.50175	C	8.270018	-6.842501	3.609977
C	-9.406321	4.063171	2.926814	H	9.207022	-6.9413	3.052751
C	10.577806	-2.583593	1.325559	H	7.421763	-6.903198	2.916151
H	11.441142	-3.236993	1.383001	C	11.212087	-4.932657	4.150512
C	-4.821099	-3.121004	-4.317568	H	10.581314	-5.369889	4.930993
H	-3.958656	-3.384555	-4.922917	H	11.514983	-3.920302	4.447098
C	-2.309326	1.640963	3.494836	C	-8.287844	6.773317	3.714845
H	-2.179261	2.720396	3.488576	H	-8.918106	-6.394666	-6.14821
C	9.395626	-4.122164	2.868302	H	-11.405753	-6.584713	-2.464698

H	-12.115041	5.463126	4.08494	H	8.220531	7.625367	-4.323141
H	-7.440372	6.848561	3.021489	H	12.124398	5.52006	-3.974702
H	-9.225612	6.879016	3.160177	H	12.101185	-5.54949	3.999997
H	-8.21073	7.558356	4.47075	H	8.19121	-7.640324	4.352197

Compound 16

O	-8.511194	-5.14011	4.908172	C	-10.818234	-1.975657	2.019401
O	-8.511125	5.140035	-4.908277	H	-11.757878	-2.296625	2.456636
O	-10.875693	-3.859949	4.080301	C	-4.913621	4.523578	-2.866217
O	-10.8756	3.860156	-4.0803	C	-5.95834	2.79626	-1.533482
O	10.875669	3.859859	4.08044	H	-5.875828	2.056107	-0.745451
O	8.511134	-5.139943	-4.908388	C	-2.582537	3.160375	1.193716
O	10.875614	-3.860185	-4.080307	H	-2.677168	3.141032	2.276669
O	3.817384	-6.208425	-4.158997	C	9.56682	-0.547003	-0.484835
O	-3.817408	6.208592	-4.158779	C	3.592891	-3.342025	-1.02478
O	-3.817603	-6.208753	4.158702	C	3.694065	-3.282061	0.406885
C	-7.257536	-3.943948	3.233436	H	4.674937	-3.376089	0.863678
O	8.511123	5.139861	4.90838	C	-7.187998	2.965108	-2.198921
C	-9.635484	-2.582959	2.45682	C	-4.825555	3.551358	-1.82672
C	-8.39342	-2.229524	1.837507	C	6.109453	4.681199	3.55998
C	-9.657769	-3.570986	3.507856	H	6.159985	5.431681	4.340444
C	-9.56682	0.547039	-0.484778	C	5.958342	-2.796232	-1.53354
C	-8.398994	-1.197063	0.891054	H	5.875843	-2.056123	-0.745466
H	-7.460717	-0.90582	0.436579	C	4.825607	3.551355	1.826777
C	-8.513369	4.21409	-3.891845	C	9.566828	0.547048	0.484673
C	-3.592914	-3.342011	1.02477	C	-3.827667	5.493739	-3.171431
C	8.39343	2.229547	1.83747	H	-3.020422	5.567889	-2.418596
C	8.399	1.197102	0.890996	C	-5.95836	-2.796221	1.533532
H	7.460721	0.905872	0.436515	H	-5.87582	-2.056043	0.745529
C	-8.513462	-4.21408	3.891819	C	7.257534	3.943907	3.233482
C	-10.816071	0.997596	-1.021866	C	-6.109462	-4.681284	3.559876
C	4.913609	-4.523494	-2.866339	H	-6.160004	-5.431824	4.340285
C	-7.188039	-2.965071	2.198932	C	-2.347698	3.222232	-1.604205
O	3.817512	6.208515	4.158948	H	-2.251385	3.223261	-2.687249
C	2.3477	-3.222089	-1.604246	C	-1.160398	-3.11918	0.819596
H	2.251383	-3.223008	-2.687289	C	9.657769	3.570932	3.507877
C	-6.109368	4.681259	-3.559913	C	-8.398974	1.197082	-0.891083
H	-6.15988	5.431757	-4.340365	H	-7.460699	0.905804	-0.436626
C	-3.694085	-3.281916	-0.406893	C	8.513362	-4.214014	-3.891938
H	-4.674963	-3.375868	-0.863689	C	8.398974	-1.197027	-0.891158
C	4.913689	4.523534	2.866309	H	7.460693	-0.905747	-0.436714
C	-4.825584	-3.551337	1.826765	C	7.187995	-2.965054	-2.198997
C	-9.566827	-0.547007	0.484739	C	3.827651	-5.493641	-3.171598
C	3.592938	3.34209	1.024768	H	3.020381	-5.567805	-2.418797
C	4.825551	-3.551312	-1.826802	C	7.257445	-3.943877	-3.233555
C	-3.592888	3.342055	-1.024716	C	5.958389	2.796277	1.533486
C	-7.257458	3.943962	-3.233451	H	5.875866	2.056163	0.745421
C	-4.913694	-4.523597	2.866222	C	-3.69405	3.281964	0.406943

H	-4.674926	3.375899	0.863749	H	4.674974	3.376089	-0.863694
C	6.109352	-4.681152	-3.560045	C	-3.827759	-5.493778	3.17144
H	6.159861	-5.431621	-4.340527	H	-3.020407	-5.567801	2.418711
C	2.347751	3.222205	1.60425	C	-9.177442	-6.37396	4.597769
H	2.251445	3.223165	2.687294	H	-8.70778	-6.856113	3.731329
C	-8.393384	2.229552	-1.837527	H	-10.240271	-6.207021	4.39619
C	-10.816085	-0.997544	1.021831	C	2.58259	3.160527	-1.193675
C	10.816078	-0.997576	-1.021907	H	2.677218	3.141251	-2.276629
C	8.513462	4.214004	3.891893	C	1.274931	3.105193	-0.619947
C	8.393382	-2.229509	-1.837591	C	10.818244	1.975662	2.019363
C	-9.635438	2.582995	-2.456851	H	11.757888	2.29662	2.456608
C	-2.347721	-3.222164	1.604247	C	-0.114273	3.0879	1.400927
H	-2.251401	-3.223188	2.68729	H	-0.203816	3.094966	2.485213
C	9.635442	-2.582972	-2.456895	C	1.160424	3.119253	0.819605
C	7.188059	2.965094	2.198916	C	2.582563	-3.160478	1.193677
C	-9.176939	6.374084	-4.597748	H	2.677203	-3.141226	2.27663
H	-8.706989	6.856111	-3.731391	C	11.009387	-3.441332	-5.447089
H	-10.239778	6.207434	-4.395975	H	10.86963	-2.356273	-5.53217
C	9.635491	2.582951	2.456799	H	10.288256	-3.956738	-6.08893
C	-2.582581	-3.160294	-1.193673	C	3.827717	5.49365	3.171608
H	-2.677217	-3.140946	-2.276625	H	3.02038	5.567726	2.418867
C	-1.160368	3.119264	-0.819565	C	9.176718	-6.374092	-4.597746
C	9.657706	-3.571028	-3.507902	H	8.70651	-6.856082	-3.731509
C	-1.274876	3.105114	0.619988	H	10.239534	-6.207578	-4.395735
C	-10.818201	1.975705	-2.019443	C	9.177544	6.373725	4.598395
H	-11.757838	2.296686	-2.456688	H	8.708087	6.856133	3.731986
C	1.274901	-3.105111	0.619962	H	10.240388	6.206737	4.396968
C	-1.274917	-3.105013	-0.619951	C	11.009196	3.440785	5.447171
C	-9.657701	3.571051	-3.507859	H	10.869085	2.355761	5.532106
C	0.114329	3.087981	-1.400889	H	10.28816	3.956318	6.089027
H	0.203874	3.09511	-2.485174	H	-9.056897	7.009837	-5.477426
C	-0.11432	-3.087772	-1.400902	H	-12.027565	3.702413	-5.743726
H	-0.203874	-3.094817	-2.485186	H	-12.027627	-3.702321	5.743752
C	0.114304	-3.087907	1.400913	H	-9.057418	-7.009741	5.477431
H	0.203856	-3.09506	2.485197	H	9.057404	7.009292	5.478193
C	-11.009252	3.441478	-5.447143	H	12.027494	3.701588	5.743919
H	-10.869207	2.356469	-5.532391	H	9.056793	-7.009802	-5.477471
H	-10.288249	3.957167	-6.088901	H	12.027634	-3.702492	-5.743702
C	10.816094	0.997575	1.02176	C	-12.04695	-0.458067	0.500705
C	1.160382	-3.119137	-0.819589	C	-12.046945	0.458162	-0.500716
C	10.818206	-1.975702	-2.019466	C	12.046952	-0.458134	-0.500772
H	11.757847	-2.296721	-2.456679	C	12.046957	0.458146	0.500586
C	-11.009236	-3.441596	5.447253	H	-12.982778	0.830095	-0.910172
H	-10.868896	-2.356651	5.532774	H	-12.982788	-0.829995	0.910155
H	-10.288381	-3.957614	6.08891	H	12.982784	-0.830151	-0.910153
C	3.6941	3.282097	-0.406896	H	12.982793	0.830116	0.910003

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