Supporting Information

Synthesis of Cyclobutadienoid-Fused Phenazines with Strongly Modulated Degrees of Antiaromaticity

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1. General Information

Materials. All chemicals were obtained from commercial sources and used as received unless otherwise noted. Dry toluene and THF were obtained from solvent purification columns. Anhydrous 1,4-dioxane was purchased from Acros Organics and used as received. Compounds **2a**[1] and **2b**[2] were prepared according to literature procedures. All CANAL reactions were performed under nitrogen in flame-dried glassware. Flash chromatography (FC) was carried out with Silica 60 (230-400 mesh; Fisher). Analytical thin-layer chromatography (TLC) was carried out using 0.2 mm silica gel plate (silica gel 60, F254, EMD chemical).

Characterizations. ^{1}H and ^{13}C NMR spectra were recorded using 300 MHz, 400 MHz, or 500 MHz Varian NMR spectrometers. Chemical shifts are reported in ppm using the residual protiated solvent as an internal standard ($CDCl_3$ ^{1}H: 7.26 ppm and ^{13}C: 77.16 ppm; THF-d_8 ^{1}H: 3.58 ppm and ^{13}C: 67.57 ppm). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, dd = doublet of doublets, t = triplet, q = quartet, m = multiplet, br = broad signal, and associated combinations), coupling constant(s) (Hz), and integration. ESI MS was obtained using Waters Acquity QDa or SQ mass spectrometers. HRMS was obtained from Thermo Exactive Orbitrap mass spectrometer. UV–Vis spectra were recorded on a Thermo Scientific Genesys 10S spectrophotometer with background correction using pure solvent. Fluorescence spectra were recorded on a Fluorolog-3 fluorimeter (450W Xenon lamp) using right-angle detection. Quantum yields (QY) in Chloroform ($CHCl_3$) were determined relative to perylene in ethanol (EtOH) or fluorescein in 0.1 M NaOH as indicated, and are corrected for solvent refractive index and absorption differences at the excitation wavelength. Cyclic voltammetry (CV) was performed on a computer-controlled Nanowave in a three-electrode cell in a CH_2Cl_2 solution of $TBAPF_6$ (0.1 M) with a scan rate of 100 mV/s at room temperature. A Pt wire as counter electrode, $Ag/AgNO_3$(0.01 M), $TBAPF_6$(0.1 M)/MeCN as reference electrode, and a glassy carbon electrode as working electrode. The Ferrocene/Ferrocenium redox couple served as an external reference.

2. Synthetic Procedures

2.1. Syntheses of bromophenazines

Mono/dibromo-phenazines **1a**-**1e** were prepared following a reported procedure[3] with slight modifications.

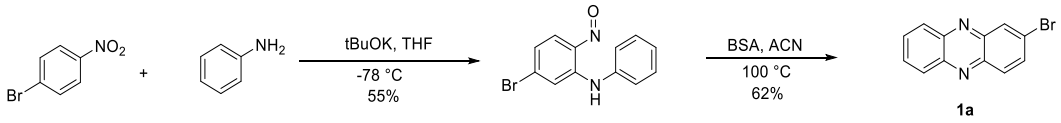
General procedure for bromophenazine synthesis

1. Synthesis of *N*-aryl-2-nitrosoanilines

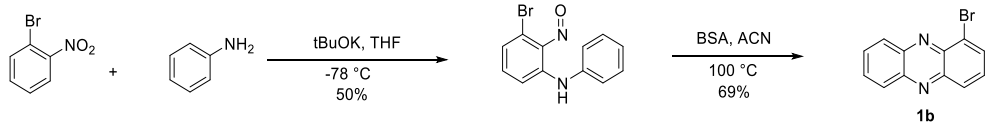
To a cooled solution of *t*-BuOK (18 mmol, 2.02 g) in THF (25 mL) was added dropwise at –78 °C a solution of aniline (6 mmol), followed by nitroarene (6 mmol) in THF (5 mL each). The mixture was stirred at this temperature for 1 hour. The reaction mixture was then poured into a concentrated NH_4Cl solution (ca. 70 mL) and extracted with EtOAc.
The combined organic layers were washed with water and brine, and dried over Na_2SO_4. The solvent was evaporated, and the remaining residual was purified by silica gel chromatography (1:9 EA/Hex) to obtain the product.

2. Cyclization of N-aryl-nitrosoanilines

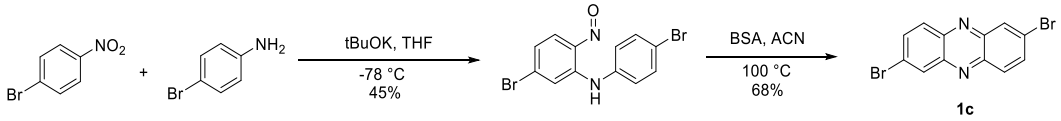
To a solution of nitrosoaniline (1 mmol) in MeCN (4 mL) was added N,O-bis(trimethylsilyl)acetamide (BSA) (1.2 mL, 5 mmol) and the reaction mixture was heated in a sealed tube at 100 °C for 12 h. The precipitated product was filtered off, washed with cold MeOH, and dried under vacuum.



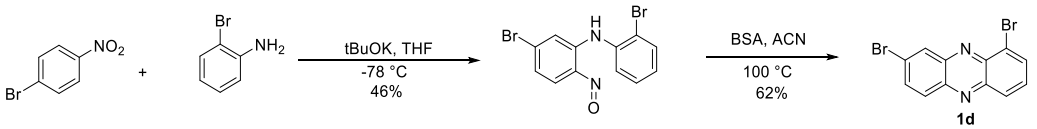
2-bromophenazine[3] **(1a).** Pale yellow solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.47 (d, *J* = 2.0 Hz, 1H), 8.24 (dd, *J* = 6.8, 3.3 Hz, 2H), 8.13 (d, *J* = 9.2 Hz, 1H), 7.92 – 7.84 (m, 3H).



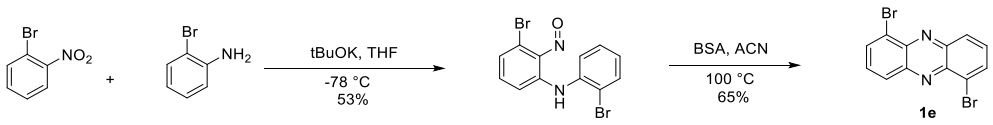
1-bromophenazine[4] **(1b).** Pale yellow solid. ^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.43 (dd, *J* = 7.1, 3.1 Hz, 1H), 8.34 – 8.20 (m, 3H), 7.97 – 7.89 (m, 2H), 7.77 – 7.68 (m, 1H).



2,7-dibromophenazine (1c). Bright yellow solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.43 (s, 2H), 8.09 (d, *J* = 9.2 Hz, 2H), 7.91 (d, *J* = 9.3 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 143.80, 142.49, 135.07, 131.87, 131.03, 125.51. HRMS (ESI): m/z calculated for $C_{12}H_7Br_2N_2$ [M+H$^+$]: 336.8971; found: 336.8979.

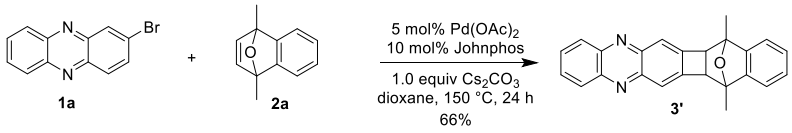


1,8-dibromophenazine (1d). Brown solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.62 (s, 1H), 8.21 (d, *J* = 8.0 Hz, 2H), 8.13 (d, *J* = 9.2 Hz, 1H), 7.93 (d, *J* = 9.1 Hz, 1H), 7.71 (t, *J* = 8.0 Hz, 1H).^{13}C NMR (101 MHz, Chloroform-*d*) δ 144.03, 143.85, 142.49, 141.23, 135.24, 134.42, 132.18, 130.86, 130.70, 129.87, 125.88, 124.49. HRMS (ESI): m/z calculated for $C_{12}H_7Br_2N_2$ [M+H$^+$]: 336.8971; found: 336.8980.

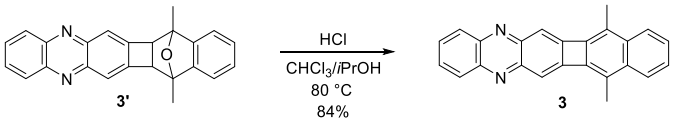


1,6-dibromophenazine (1e). Bright yellow solid. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.38 (d, *J* = 8.8 Hz, 2H), 8.24 (d, *J* = 7.3 Hz, 2H), 7.75 (t, *J* = 8.0 Hz, 2H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 144.05, 141.23, 134.48, 131.04, 130.14, 124.23. MS (ESI): m/z calculated for $C_{12}H_7Br_2N_2$ [M+H$^+$]: 336.8971; found: 336.8976.

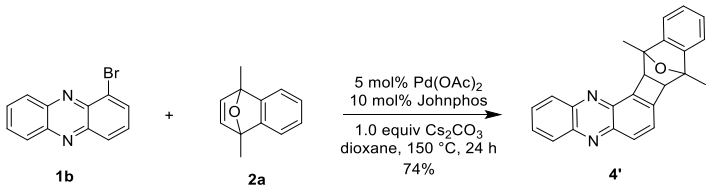
2.2. Syntheses of CBD-fused phenazines



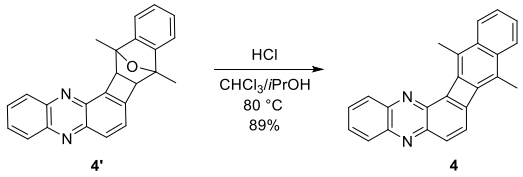
***exo*-7,12-dimethyl-6b,7,12,12a-tetrahydro-7,12-epoxynaphtho[2',3':3,4] cyclobuta[1,2-b]phenazine (3'):** To a flame-dried 15 mL pressure tube was added **1a** (65 mg, 0.25 mmol), **2a** (43 mg, 0.25 mmol), palladium acetate (2.8 mg, 0.0125 mmol) and Johnphos ligand (7.5 mg, 0.025 mmol). The tube was then transferred to a glovebox, and cesium carbonate (81.5 mg, 0.25 mmol) and 1 mL 1,4-dioxane were added. The tube was closed and taken outside glovebox. The mixture was stirred at room temperature for 5 min, and then heated to 150 °C. After 24 h, the reaction was cooled to room temperature, and was passed through a thin layer of Celite to remove the inorganic salt. The solution was concentrated *in vacuo* and the residue was purified by column chromatography (1:5 EA/Hex) to yield **3'** as a yellow solid (58 mg, 66%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.23 (dd, *J* = 6.7, 3.4 Hz, 2H), 7.96 (s, 2H), 7.82 (dd, *J* = 6.7, 3.4 Hz, 2H), 7.35 – 7.27 (m, 4H), 3.76 (s, 2H), 1.95 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 147.97, 147.30, 145.14, 142.36, 130.13, 129.50, 127.26, 122.44, 118.68, 85.24, 56.29, 14.21. HRMS (ESI): m/z calculated for $C_{24}H_{19}N_2O$ [M+H$^+$]: 351.1492; found: 351.1493.



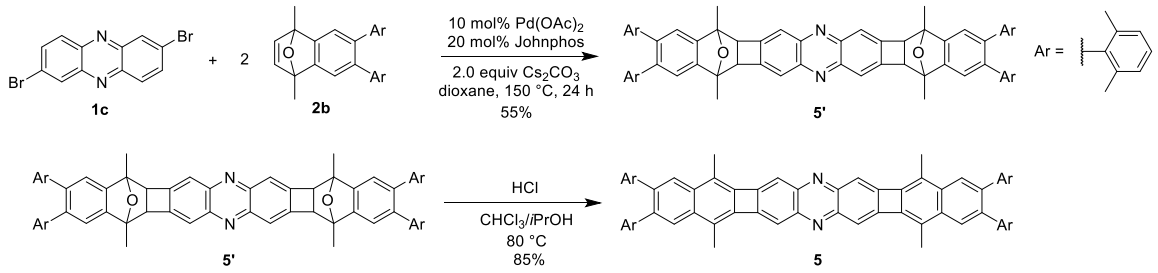
7,12-dimethylnaphtho[2',3':3,4]cyclobuta[1,2-b]phenazine (3): Compound **3'** (20.0 mg, 0.057 mmol) was dissolved in 0.6 mL isopropanol, 0.15 mL chloroform, and 0.1 ml HCl (37%). The solution was heated at 80°C for 24 h. The reaction mixture was cooled, washed with sat'd $NaHCO_3$ solution and extracted with chloroform. The combined organic layer was dried over Na_2SO_4 and concentrated. The solid was washed with MeOH, collected by filtration, and washed with cold MeOH to obtain **3** as a bright yellow solid (16 mg, 84%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.06 (dd, *J* = 6.5, 3.4 Hz, 2H), 7.85 (dd, *J* = 6.3, 3.4 Hz, 2H), 7.71 (dd, *J* = 6.6, 3.4 Hz, 2H), 7.51 (s, 2H), 7.45 (dd, *J* = 6.3, 3.3 Hz, 2H), 2.62 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.83, 147.54, 142.29, 142.13, 136.04, 129.72, 129.15, 126.77, 126.27, 125.40, 116.66, 15.02. MS (ESI): m/z calculated for $C_{24}H_{17}N_2$ [M+H$^+$]: 333.14; found: 333.06.



***exo*-8,13-dimethyl-7b,8,13,13a-tetrahydro-8,13-epoxynaphtho[2',3':3,4] cyclobuta[1,2-a]phenazine (4'):** To a flame-dried 15 mL pressure tube was added **1b** (65 mg, 0.25 mmol), **2a** (43 mg, 0.25 mmol), palladium acetate (2.8 mg, 0.0125 mmol) and Johnphos ligand (7.5 mg, 0.025 mmol). The tube was then transferred to a glovebox, and cesium carbonate (81.5 mg, 0.25 mmol) and 1 mL dioxane were added. The tube was closed and taken outside glovebox. The mixture was stirred at room temperature for 5 min, and then heated to 150 °C. After 24 h, the reaction was cooled to room temperature, and was passed through a thin layer of Celite to remove the inorganic salt. DCM (2×5 mL) was then used to wash the residue on Celite. The solution was concentrated *in vacuo* and the residue was purified by column chromatography (1:5 EA/Hex) to yield **4'** as a yellow solid (65 mg, 74%). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.32 – 8.23 (m, 3H), 7.89 – 7.79 (m, 2H), 7.75 (d, *J* = 8.5 Hz, 1H), 7.41 – 7.35 (m, 1H), 7.35 – 7.27 (m, 3H), 4.02 (d, *J* = 3.3 Hz, 1H), 3.63 (d, *J* = 3.3 Hz, 1H), 2.04 (s, 3H), 1.89 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.17, 147.89, 147.73, 144.30, 143.05, 140.96, 131.76, 130.78, 130.13, 130.10, 129.92, 127.12, 127.01, 126.29, 118.88, 118.56, 83.98, 83.03, 55.42, 54.94, 15.49, 14.64. HRMS (ESI): m/z calculated for $C_{24}H_{19}N_2O$ [M+H$^+$]: 351.1492; found: 351.1493.

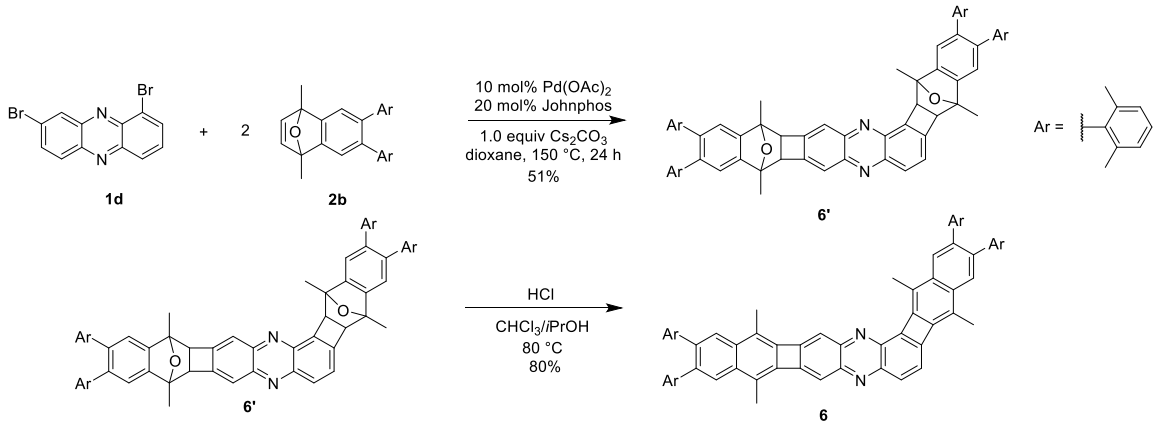


8,13-dimethylnaphtho[2',3':3,4]cyclobuta[1,2-a]phenazine (4): Compound **4'** (20.0 mg, 0.057 mmol) was dissolved in 0.6 mL isopropanol, 0.15 mL chloroform, and 0.1 ml HCl (37%). The solution was heated at 80°C for 24 h. The reaction mixture was cooled and washed with sat'd $NaHCO_3$ solution, and extracted with chloroform. The combined organic layer was dried over Na_2SO_4 and concentrated. The solid was washed with MeOH, collected by filtration, and washed with cold MeOH to obtain **4** as a red solid (17 mg, 89%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.04 – 7.96 (m, 2H), 7.89 (d, *J* = 8.3 Hz, 1H), 7.69 – 7.62 (m, 2H), 7.50 (dd, *J* = 8.8, 1.5 Hz, 2H), 7.45 – 7.39 (m, 1H), 7.24 – 7.18 (m, 2H), 2.67 (s, 3H), 2.26 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 152.88, 147.47, 144.64, 144.62, 143.46, 143.21, 142.90, 136.72, 136.69, 136.08, 131.87, 130.86, 130.33, 130.27, 130.04, 126.38, 126.13, 125.00, 124.70, 122.90, 121.36, 121.09, 15.37, 14.50. MS (ESI): m/z calculated for $C_{24}H_{17}N_2$ [M+H$^+$]: 333.14; found: 333.14.



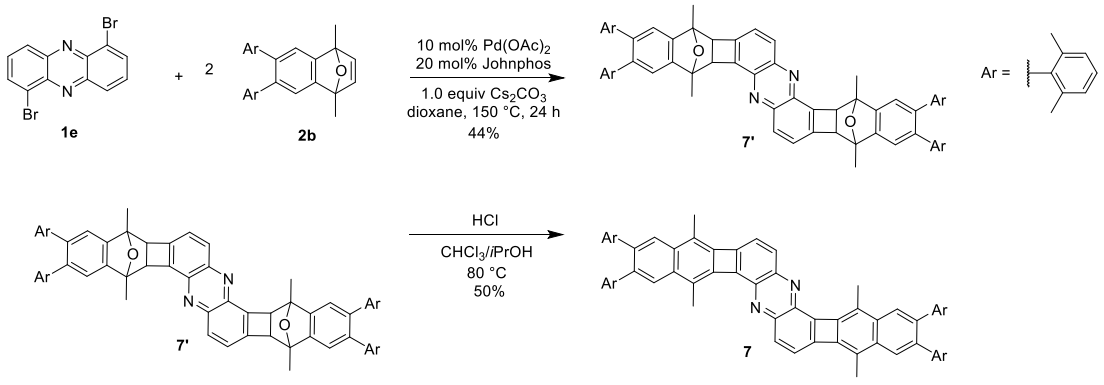
(5'): To a flame-dried 15 mL pressure tube was added **1c** (42 mg, 0.125 mmol), **2b** (95 mg, 0.25 mmol), palladium acetate (2.8 mg, 0.0125 mmol) and Johnphos ligand (7.5 mg, 0.025 mmol). The tube was then transferred to a glovebox, and cesium carbonate (81.3 mg, 0.25 mmol and 1.5 mL 1,4-dioxane were added. The tube was closed and taken outside glovebox. The mixture was stirred at room temperature for 5 min, and then heated to 150 °C. After 24 h, the reaction was cooled to room temperature, and was passed through a thin layer of Celite to remove the inorganic salt. The solution was concentrated *in vacuo* and the residue was purified by column chromatography (1:3 EA/Hex) to yield **5'** as a yellow solid (mixture of syn/anti isomers, 64 mg, 55%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (s, 4H), 7.22 (s, 4H), 7.05 (t, *J* = 7.5 Hz, 4H), 6.94 (d, *J* = 7.6 Hz, 8H), 3.89 (d, *J* = 5.6 Hz, 4H), 2.00 (m, 36H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.77, 146.41, 146.36, 143.98, 140.31, 138.79, 138.78, 136.93, 136.89, 136.71, 136.68, 127.66, 127.64, 127.59, 127.56, 127.08, 122.37, 122.33, 122.26, 85.38, 85.36, 56.62, 56.53, 21.52, 21.51, 21.43, 21.42, 14.30, 14.28. MS (ESI): m/z calculated for $C_{68}H_{61}N_2O_2$ [M+H$^+$]: 937.47; found: 937.94.

(5): Compound **5'** (20 mg, 0.021 mmol) was dissolved in 0.6 mL isopropanol, 0.15 mL chloroform, and 0.1 ml HCl (37%). The solution was heated at 80°C for 24 h. The reaction mixture was cooled, washed with sat'd $NaHCO_3$ solution and extracted with DCM. The combined organic layer was dried over Na_2SO_4 and concentrated. The solid was washed with MeOH, collected by filtration, and washed with cold MeOH to yield **5** as an orange solid (16 mg, 85%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (s, 4H), 7.48 (s, 4H), 7.09 (t, *J* =7.6 Hz, 4H), 6.98 (d, *J* = 7.6 Hz, 8H), 2.60 (s, 12H), 2.02 (s, 24H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.44, 146.15, 142.73, 140.19, 138.94, 136.96, 134.63, 128.78, 127.68, 127.27, 125.33, 117.06, 21.54, 15.05. HRMS (ESI): m/z calculated for $C_{68}H_{57}N_2$ [M+H$^+$]: 901.4516; found: 901.4538.



(6'): To a flame-dried 15 mL pressure tube was added **1d** (42 mg, 0.125 mmol), **2b** (95 mg, 0.25 mmol), palladium acetate (2.8 mg, 0.0125 mmol) and Johnphos ligand (7.5 mg, 0.025 mmol). The tube was then transferred to a glovebox, and cesium carbonate (81.3 mg, 0.25 mmol and 1.5 mL 1,4-dioxane were added. The tube was closed and taken outside glovebox. The mixture was stirred at room temperature for 5 min, and then heated to 150 °C. After 24 h, the reaction was cooled to room temperature, and was passed through a thin layer of Celite to remove the inorganic salt. The solution was concentrated *in vacuo* and the residue was purified by column chromatography (1:3 EA/Hex) to yield **6'** as a yellow solid (mixture of syn/anti isomers, 60 mg, 51%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (dd, *J* = 8.5, 2.9 Hz, 1H), 8.08 (d, *J* = 16.6 Hz, 1H), 8.04 (s, 1H), 7.80 (d, *J* = 8.4 Hz, 1H), 7.34 – 7.24 (m, 4H), 7.09 (dd, *J* = 9.3, 5.7 Hz, 4H), 7.05 – 6.93 (m, 8H), 4.20 (dd, *J* = 8.6, 3.3 Hz, 1H), 3.95-3.91 (m, 2H), 3.79 (dd, *J* = 6.1, 3.4 Hz, 1H), 2.12 – 1.95 (m, 36H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.73, 147.40, 146.95, 146.92, 146.71, 146.57, 146.49, 146.43, 146.41, 146.36, 145.36, 145.28, 144.77, 143.22, 143.17, 140.76, 140.72, 140.58, 140.37, 138.92, 138.69, 138.65, 138.58, 138.51, 137.13, 137.08, 137.04, 137.02, 137.00, 136.98, 136.95, 136.91, 136.86, 136.79, 136.77, 131.67, 131.56, 127.76, 127.68, 127.19, 127.12, 125.97, 122.99, 122.94, 122.82, 122.56, 122.38, 122.27, 85.58, 85.56, 85.54, 84.30, 83.39, 83.29, 56.82, 56.71, 55.79, 55.23, 21.79, 21.66, 21.63, 21.60, 21.57, 21.54, 21.49, 21.47, 21.43, 15.64, 15.61, 14.85, 14.83, 14.54, 14.41, 14.39, 14.33. MS (ESI): m/z calculated for $C_{68}H_{61}N_2O_2$ [M+H$^+$]: 937.47; found: 937.23.

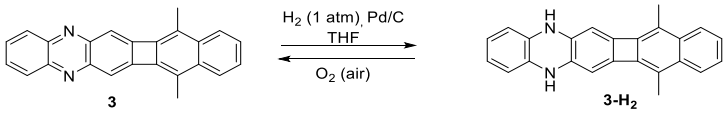
(6): Compound **6'** (18 mg, 0.019 mmol) was dissolved in 0.5 mL isopropanol, 1.5 mL chloroform, and 0.1 ml HCl (37%). The solution was heated at 80°C for 24 h. The reaction mixture was cooled, washed with sat'd $NaHCO_3$ solution, and extracted with chloroform. The combined organic layer was dried over Na_2SO_4 and concentrated. The solid was washed with MeOH, collected by filtration, and washed with cold MeOH to yield **6** as a bright red solid (14 mg, 80%). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.83 (d, *J* = 8.0 Hz, 1H), 7.78 (d, *J* = 10.7 Hz, 2H), 7.53 (s, 1H), 7.47 (d, *J* = 8.1 Hz, 1H), 7.44 – 7.36 (m, 3H), 7.07 (dt, *J* = 12.1, 6.5 Hz, 4H), 7.01 – 6.92 (m, 8H), 2.74 (s, 3H), 2.62 (s, 3H), 2.56 (s, 3H), 2.24 (s, 3H), 2.06 (s, 6H), 2.01 (s, 12H), 2.00 (s, 6H). ^{13}C NMR (126 MHz, CDCl3) δ 151.78, 150.84, 150.36, 148.50, 147.38, 147.07, 143.53, 143.43, 143.15, 142.50, 140.29, 139.85, 139.06, 137.95, 137.77, 136.67, 136.63, 135.21, 134.98, 134.53, 134.48, 131.35, 128.69, 128.50, 128.19, 127.64, 127.56, 127.25, 126.94, 126.09, 126.03, 121.75, 121.14, 120.53, 117.29, 117.14, 21.48, 15.48, 15.44, 14.99, 14.54. HRMS (ESI): m/z calculated for $C_{68}H_{57}N_2$ [M+H$^+$]: 901.4516; found: 901.4541.



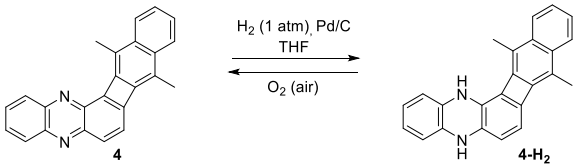
(7'): To a flame-dried 15 mL pressure tube was added **2e** (42 mg, 0.125 mmol), **1b** (95 mg, 0.25 mmol), palladium acetate (2.8 mg, 0.0125 mmol) and Johnphos ligand (7.5 mg, 0.025 mmol). The tube was then transferred to a glovebox, and cesium carbonate (81.3 mg, 0.25 mmol and 1.5 mL 1,4-dioxane were added. The tube was closed and taken outside glovebox. The mixture was stirred at room temperature for 5 min, and then heated to 150 °C. After 24 h, the reaction was cooled to room temperature, and was passed through a thin layer of Celite to remove the inorganic salt. The solution was concentrated *in vacuo* and the residue was purified by column chromatography (1:3 EA/Hex) to yield **7'** as a yellow solid (mixture of syn/anti isomers, 52 mg, 44%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (dd, *J* = 8.5, 2.6 Hz, 2H), 7.80 (dd, *J* = 8.5, 1.9 Hz, 2H), 7.27 (s, 2H), 7.21 (s, 2H), 7.06 (td, *J* = 7.5, 4.9 Hz, 4H), 7.01 – 6.90 (m, 8H), 4.17 (dd, *J* = 5.3, 3.4 Hz, 2H), 3.76 (dd, *J* = 3.5, 1.3 Hz, 2H), 2.08 – 2.02 (m, 18H), 1.99 – 1.92 (m, 18H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.48, 147.35, 146.54, 146.45, 146.23, 144.29, 141.25, 141.22, 140.46, 139.26, 138.62, 138.58, 138.49, 138.44, 137.00, 136.96, 136.92, 136.88, 136.83, 136.78, 136.75, 131.99, 131.91, 127.67, 127.48, 127.01, 126.59, 126.52, 122.47, 122.15, 84.20, 84.17, 83.25, 83.17, 55.24, 55.17, 21.68, 21.65, 21.54, 21.53, 21.37, 21.34, 21.32, 15.54, 15.45, 14.75, 14.72. MS (ESI): m/z calculated for $C_{68}H_{61}N_2O_2$ [M+H$^+$]: 937.47; found: 937.85.

(7): Compound **7'** (10 mg, 0.010 mmol) was dissolved in 0.5 mL isopropanol, 0.5 mL chloroform, and 0.1 ml HCl (37%). The solution was heated at 80°C for 24 h. The reaction mixture was cooled and the solid collected by filtration. The solid was re-dissolved in chloroform, washed with sat'd $NaHCO_3$ solution, dried over Na_2SO_4 and concentrated to obtain **7** as a dark purple solid (5 mg, 50%). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.96 (d, *J* = 8.4 Hz, 2H), 7.62 (d, *J* = 8.4 Hz, 2H), 7.51 (s, 2H), 7.43 (s, 2H), 7.07 (t, *J* = 7.5 Hz, 4H), 7.00 – 6.94 (m, 8H), 2.73 (s, 6H), 2.36 (s, 6H), 2.05 (d, *J* = 4.1 Hz, 24H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 152.75, 147.72, 145.64, 143.25, 142.88, 140.19, 138.17, 137.91, 136.62, 135.01, 134.45, 132.72, 128.59, 128.27, 127.57, 127.47, 126.97, 123.45, 121.22, 120.96, 21.47, 15.47, 14.57. HRMS (ESI): m/z calculated for $C_{68}H_{57}N_2$ [M+H$^+$]: 901.4516; found: 901.4541.

2.3. Reduction of linear and bent CBD-fused phenazines



7,12-dimethyl-5,14-dihydronaphtho[2',3':3,4]cyclobuta[1,2-b]phenazine (3-H2). A vial containing **3** (10 mg), 10 wt% Pd/C catalyst (2 mg) and 1.5 mL of THF was bubbled with nitrogen followed by hydrogen gas for 3 min each. The reaction mixture was stirred under H_2 (1 atm) at room temperature for 15 min, during which the fluorescence of the solution was gradually turned off by monitoring using 365 nm light irradiation. The reaction vial was then transferred to a glovebox and the mixture passed through a thin layer of Celite to remove the Pd/C catalyst. The solution was concentrated *in vacuo* to yield **3-H2** as an orange solid. ^{1}H NMR (400 MHz, THF-d_8, under N_2) δ 7.31 (dd, J = 6.0, 3.4 Hz, 2H), 7.02 (dd, J = 6.1, 3.3 Hz, 2H), 6.49 (s, 2H), 6.15 (dd, J = 5.6, 3.4 Hz, 2H), 5.84 (dd, J = 5.5, 3.4 Hz, 2H), 5.70 (s, 2H), 2.04 (s, 6H). ^{13}C NMR (101 MHz, THF-d_8) δ 145.83, 144.19, 137.95, 136.30, 135.58, 126.56, 125.30, 122.61, 117.51, 113.17, 106.48, 15.37. **3-H2** is spontaneously oxidized back to **3** upon exposure to air.



8,13-dimethyl-5,14-dihydronaphtho[2',3':3,4]cyclobuta[1,2-a]phenazine (4-H2). A vial containing **4** (10 mg), 10 wt% Pd/C catalyst (2 mg) and 1.5 mL of THF was bubbled with nitrogen followed by hydrogen gas for 3 min each. The reaction mixture was stirred under H_2 (1 atm) at room temperature for 15 min, during which the fluorescence of the solution was gradually turned on by monitoring using 365 nm light irradiation. The reaction vial was then transferred to a glovebox and the mixture passed through a thin layer of Celite to remove the Pd/C catalyst. The solution was concentrated in vacuo to yield **4-H2** as a yellow solid. ^{1}H NMR (400 MHz, THF-d_8, under N_2) δ 7.48 (ddt, J = 21.2, 5.0, 2.4 Hz, 2H), 7.11 (dt, J = 7.1, 2.1 Hz, 2H), 6.81 (s, 1H), 6.30 – 6.19 (m, 2H), 6.18 – 6.11 (m, 1H), 5.96 (td, J = 6.4, 2.0 Hz, 2H), 5.79 (s, 1H), 5.48 (dd, J = 7.1, 2.0 Hz, 1H), 2.29 (s, 3H), 2.14 (s, 3H). ^{13}C NMR (101 MHz, THF-d_8) δ 144.60, 144.06, 141.49, 137.75, 137.05, 136.81, 134.50, 133.37, 130.40, 127.84, 126.55, 126.26, 125.70, 125.38, 122.87, 121.68, 119.79, 119.14, 114.72, 114.24, 113.39, 111.14, 16.87, 15.12. A minute amount of byproduct was noticeable in crude NMR spectrum, which may correspond to reduction of fused benzenoid in phenazine. **4-H2** is spontaneously oxidized back to **4** upon exposure to air.

3. Supporting Figures

3.1. UV–vis and Fluorescence Spectra of CBD-fused phenazines

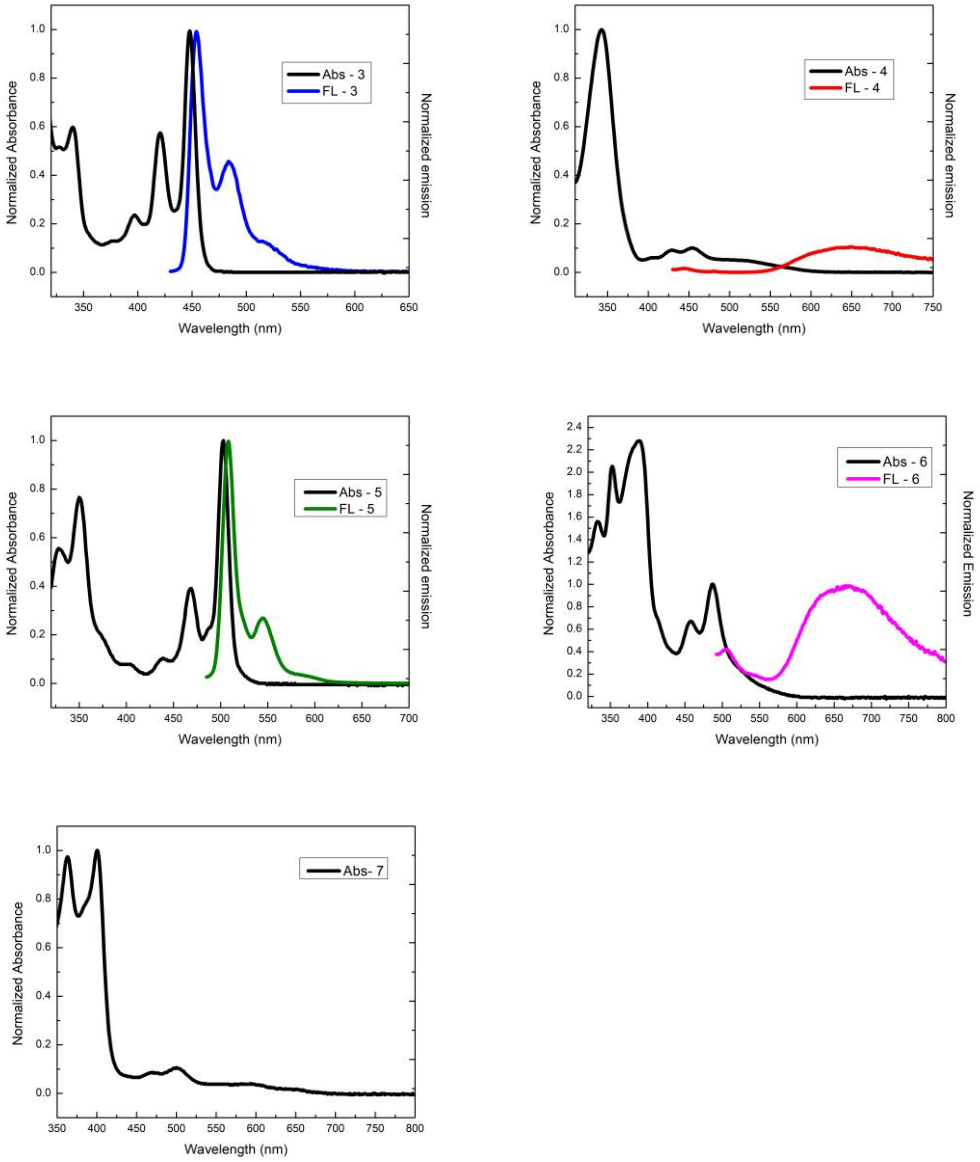


Figure S1. Normalized UV–vis and fluorescence spectra of **3-7** in chloroform. Perylene/EtOH was used as standard for QY calculation of **3**. Fluorescein/0.1 M NaOH was used as standard for QY calculations of **4-6**.

Table S1. Optical, Electrochemical and Calculation Data for 3-4

Comp.	optical					electrochemical[c]		calculation[d]	
	λ_{max} [nm]	λ_{onset} [nm]	$\lambda_{em,max}$ [nm]	QY	E_{gap} [eV]	E_{red} [V]	LUMO [eV]	HOMO [eV]	LUMO [eV]
3	448[a]	461	454	0.72	2.67	-1.72	-3.38	-6.04	-2.72
4	455[a]	590	648	0.02	2.10	-1.50	-3.60	-5.57	-2.98
3-H_2	470[b]	535	502	0.02	2.32	n.d	-	-4.40	-1.35
4-H_2	437[b]	496	544	0.74	2.50	n.d	-	-4.82	-1.42

[a]Optical spectra were obtained in $CHCl_3$ solution at 298K; the optical gap was estimated from the absorption edge (λ_{onset}). [b]Optical spectra were obtained in THF solution at 298K. [c]Electrochemical data were obtained at a scan rate of 100 mV s^{-1} in DCM containing 0.1 M $n$$Bu_4NPF_6$ using a glassy carbon working electrode and Fc^+/Fc as an external standard. LUMO energy levels in eV were calculated from the reversible half-potential waves using the equation, LUMO = -(5.10 + E_{red}). [d]DFT calculations were performed at the B3LYP/6-311+G* level of theory.

Table S2. Transition energies (ΔE), oscillator strengths (*f*), and orbital assignments for 3-7[a]

Comp.	Excited state	ΔE [eV]	*f*	Assignments
3	1	2.93	0.000	H → L
	2	3.03	0.479	H-1 → L; H → L+1
4	1	2.09	0.019	H → L
	2	2.68	0.095	H-1 → L; H → L+1
3-H_2	1	2.39	0.002	H → L
	2	2.73	0.511	H-1 → L; H → L+1
4-H_2	1	2.85	0.005	H → L
	2	2.93	0.098	H-1 → L; H → L+1
5	1	2.57	1.83	H → L
	2	2.77	0.0004	H-1 → L; H → L+1
6	1	2.05	0.025	H → L
	2	2.54	0.547	H-1 → L; H → L+1
7	1	1.67	0.016	H → L
	2	2.08	0.000	H-1 → L

[a] TD-DFT calculations were performed at the B3LYP/6-311+G* level of theory and xylyl groups were replaced by phenyl groups.

3.2. UV–vis and Fluorescence Spectra of N,N-dihydro derivatives

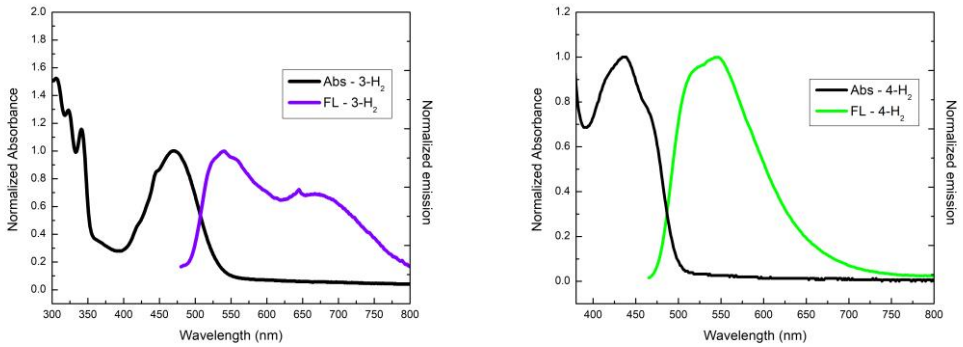


Figure S2a. Normalized UV–vis and fluorescence spectra of **3**-H_2 and **4**-H_2 in THF. Fluorescein/0.1 M NaOH was used as standard for QY calculations.

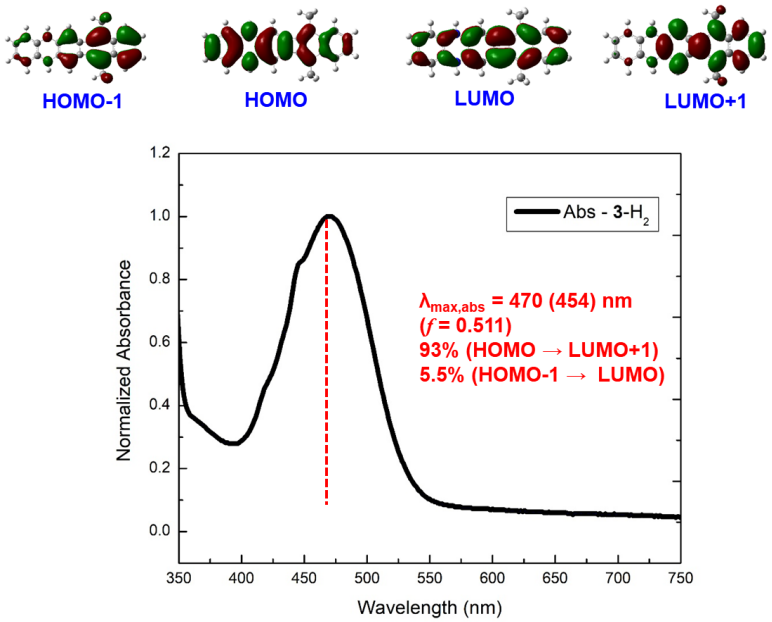


Figure S2b. Frontier MOs and normalized UV-vis spectrum of **3**-H_2 with theoretically assigned percentage contributions of various transitions to the observed absorption peak. $\lambda_{max,abs}$ and oscillator strength (*f*) values predicted at the TDDFT B3LYP/6-311+G* level of theory are shown in parentheses.

TDDFT calculations of **3**-H_2 predict that the lower energy excitation possesses HOMO-LUMO character with low oscillator strength (0.002) (Table S2). The second excitation is predicted to have a maximum wavelength of 454 nm, f = 0.511, and contributions of 93% from the HOMO−LUMO+1 and 5.5% from the HOMO-1−LUMO transitions. The HOMO−LUMO+1 transition is of charge transfer (CT) character, where the electron occupying a π orbital localized on the dihydrophenazine core is promoted into the π^* LUMO+1 orbital.

3.3. Electrochemistry of CBD-fused phenazines

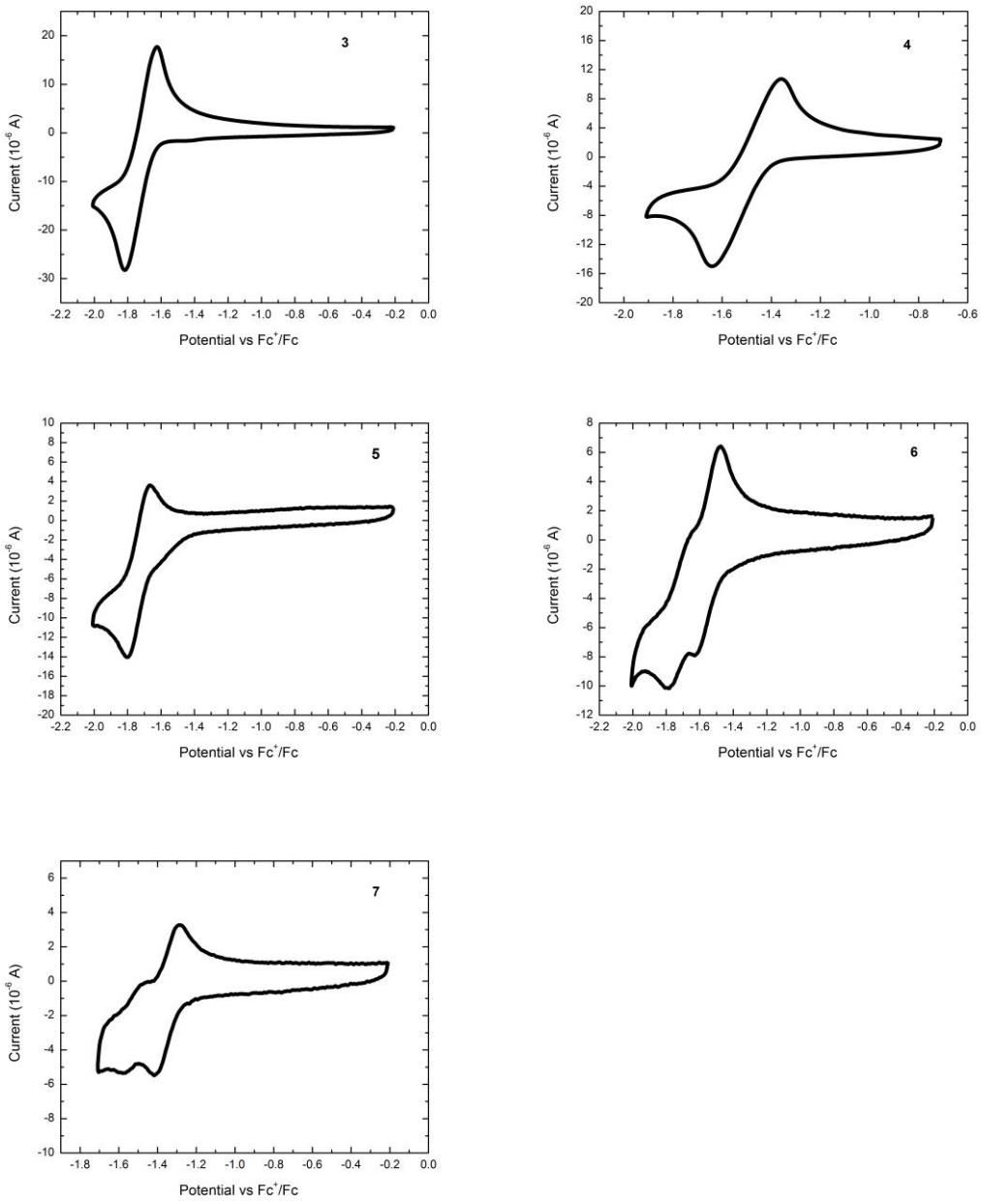


Figure S3. Cyclic voltammograms of compounds **3-7** recorded in DCM with ferrocene as an external standard. Experimental Parameters: Glassy carbon (3 mm dia) working electrode, $Ag/AgNO_3$(0.01 M), $TBAPF_6$(0.1 M)/MeCN reference electrode, Pt wire counter electrode, scan rate 100 mVs^{-1}.

3.4. Stability of 5-7 in solution

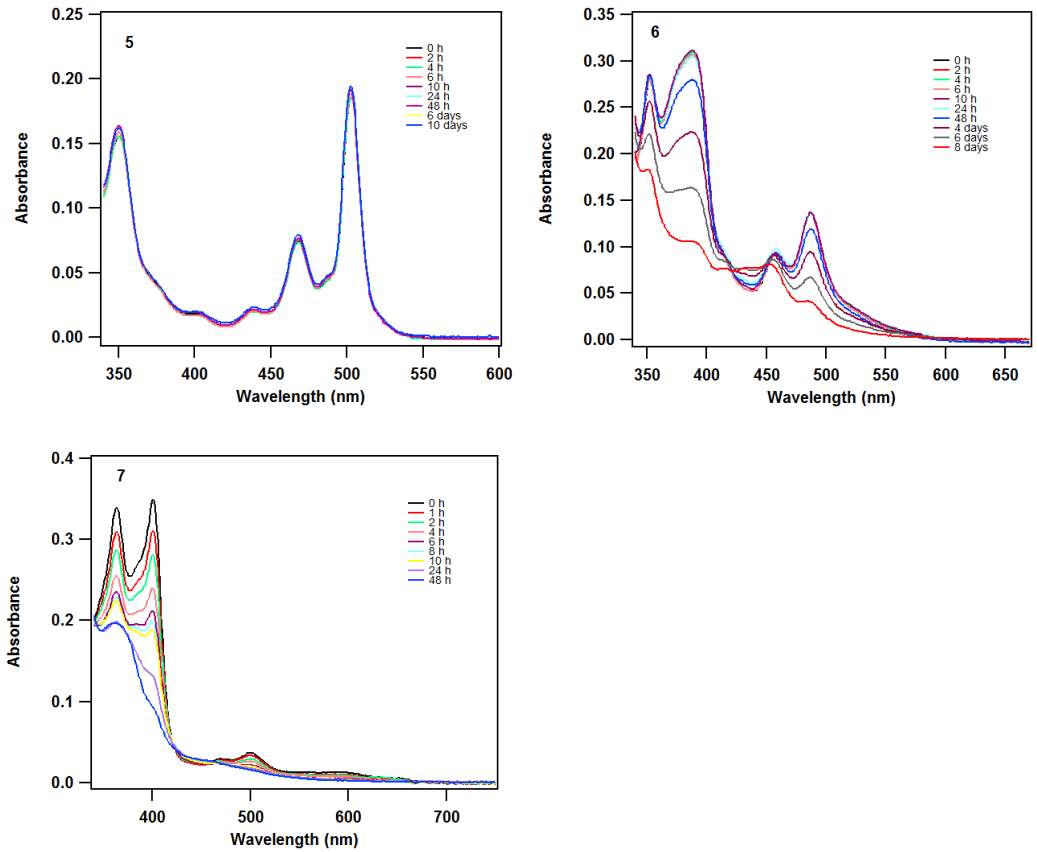


Figure S4. UV–vis spectra of compounds **5-7** recorded after different time periods at 298 K in $CHCl_3$ solution under ambient conditions and light. The half-life was estimated by monitoring the intensity of the maximum absorption peak in the 450-550 nm region**.**

3.5. ^{1}H NMR of 5 and 7

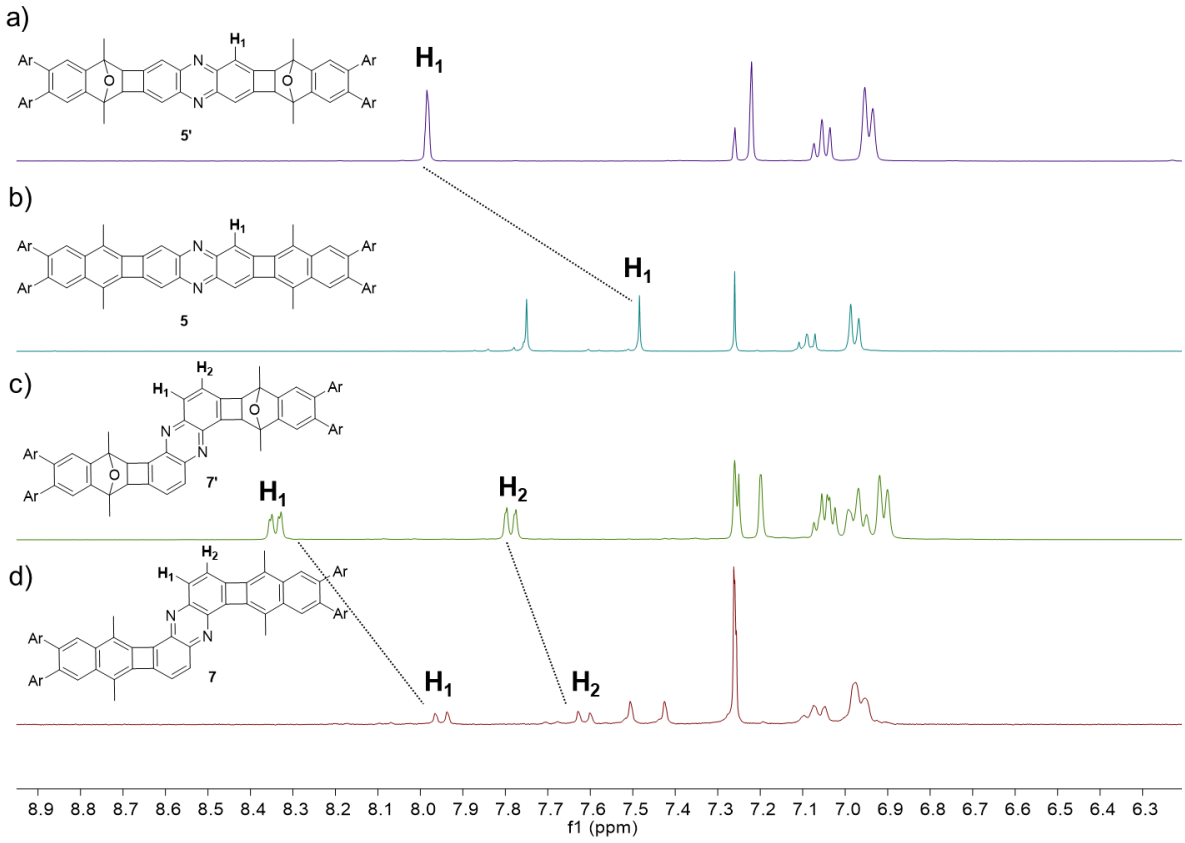
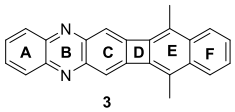
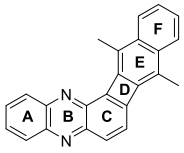


Figure S5. Partial ^{1}H NMR spectra (400MHz, $CDCl_3$, 298K) of compound (a) **5'**, (b) **5**, (c) **7'**, (d) **7**.

3.6. HOMA of 3 and 4



3



4

Table S3. HOMA values of **3** and **4**.

	HOMA					
Comp.	A	B	C	D	E	F
3	0.782	0.724	0.242	-0.780	0.416	0.785
4	0.619	0.713	0.657	-0.829	0.150	0.869

3.7. Resonance structures of 3 and 4

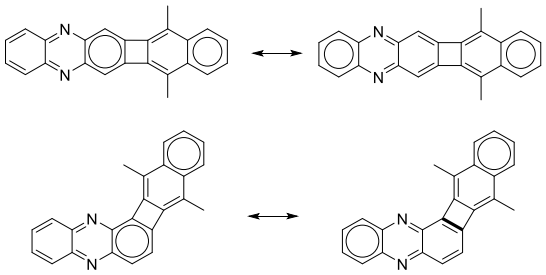


Figure S6. Resonance structures of **3** and **4** using Clar's sextet rule, showing more double bond character in the CBD of **4** as compared to **3**.

4. X-ray crystallographic analysis

4.1. General X-Ray data collection

A crystal was coated with Paratone-N oil, attached to a Mitegen® loop or micromesh mount, and transferred to a Bruker D85 diffractometer equipped with a Photon 100 CMOS detector at Beamline 11.3.1 at the Advanced Light Source at the Lawrence Berkeley National Lab. Synchrotron X-rays of wavelength λ = 0.7749 Å were monochormated using silicon (111). Frames were collected using ω and ϕ and scans and the unit-cell parameters were refined against all data. Data were integrated and corrected for Lorentz and polarization effects using SAINT v8.34A and were corrected for absorption effects using SADABS V2014/2.[5] The structure was solved using the intrinsic phasing method implemented in APEX2. It was refined against all data using SHELXTL[6,7] and OLEX2[8] software.[9] Hydrogen atoms were inserted at idealized positions and refined using a riding model with an isotropic thermal parameter 1.2 or 1.5 times that of the attached non-methyl carbon or methyl carbon, respectively. Thermal parameters for all non-hydrogen atoms were refined anisotropically.

The X-ray crystallographic coordinates for structures reported in this article have been deposited at the Cambridge Crystallographic Data Centre (CCDC), under deposition number CCDC 1586460 (**3**), 1586464 (**4**). These data can be obtained free of charge from CCDC via http://www.ccdc.cam.ac.uk/data_request/cif.

4.2. Crystallographic Data

Table S4. Crystal data and structure refinement for **3**.

	3
Empirical formula	$C_{24}H_{16}N_2$
Formula weight	332.39
Temperature/K	100.0
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	6.8981(4)
b/Å	13.8999(9)
c/Å	17.4205(11)
α/°	90
β/°	99.144(2)
γ/°	90
Volume/Å^3	1649.10(18)
Z	4
ρ_{calc}g/cm^3	1.339
μ/mm^{-1}	0.095
F(000)	696.0
Crystal size/mm^3	0.25 × 0.1 × 0.02
Radiation	Synchotron (λ = 0.7749)
2Θ range for data collection/°	4.108 to 67.168
Index ranges	$-9 \le h \le 9$, $-19 \le k \le 19$, $-24 \le l \le 24$
Reflections collected	25535
Independent reflections	5022 [R_{int} = 0.0900, R_{sigma} = 0.0691]
Data/restraints/parameters	5022/0/237
Goodness-of-fit on F^2	1.050
Final R indexes [I>=2σ (I)]	R_1 = 0.0658, wR_2 = 0.1748
Final R indexes [all data]	R_1 = 0.0806, wR_2 = 0.1925
Largest diff. peak/hole / e Å^{-3}	0.52/-0.43

Table S5. Crystal data and structure refinement for **4**.

	4
Empirical formula	$C_{24}H_{16}N_2$
Formula weight	332.39
Temperature/K	100.0
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	14.8902(7)
b/Å	6.8039(3)
c/Å	17.2784(8)
α/°	90
β/°	113.073(2)
γ/°	90
Volume/Å^3	1610.47(13)
Z	4
ρ_{calc}g/cm^3	1.371
μ/mm^{-1}	0.097
F(000)	696.0
Crystal size/mm^3	0.6 × 0.1 × 0.005
Radiation	Synchrotron (λ = 0.7749)
2Θ range for data collection/°	5.248 to 69.498
Index ranges	$-21 \leq h \leq 21$, $-10 \leq k \leq 9$, $-25 \leq l \leq 25$
Reflections collected	27064
Independent reflections	5343 [R_{int} = 0.0504, R_{sigma} = 0.0404]
Data/restraints/parameters	5343/0/237
Goodness-of-fit on F^2	1.062
Final R indexes [I>=2σ (I)]	R_1 = 0.0536, wR_2 = 0.1490
Final R indexes [all data]	R_1 = 0.0774, wR_2 = 0.1653
Largest diff. peak/hole / e Å^{-3}	0.38/-0.30

5. Computational Details

5.1. Computational Methods

All calculations were performed using the Gaussian 09[10] program package. In model compounds, dixylyl groups are replaced with phenyl groups. The geometries of these molecules were first optimized at the B3LYP level of density functional theory (DFT) with the 6-31+G(d) basis set, and the energy were then calculated with the 6-311+G(d) basis set. All structures are ground-state minima according to the analysis of their harmonic vibrational analytical frequencies computed at the same level, which show no imaginary frequencies. The first six vertical transition energies were calculated by time-dependent density functional theory (TD-DFT) at the B3LYP/6-311+G(d) level of theory. NICS calculations of the compounds are at the GIAO-B3LYP/6-311+G(d) computational level and were all carried out using the Aroma package[11] according to published procedures.[12] The NICS(1)$_{\pi,ZZ}$ values are derived from the sigma only model.

5.2. Quantum Chemical Calculations of the FMOs of 3-7

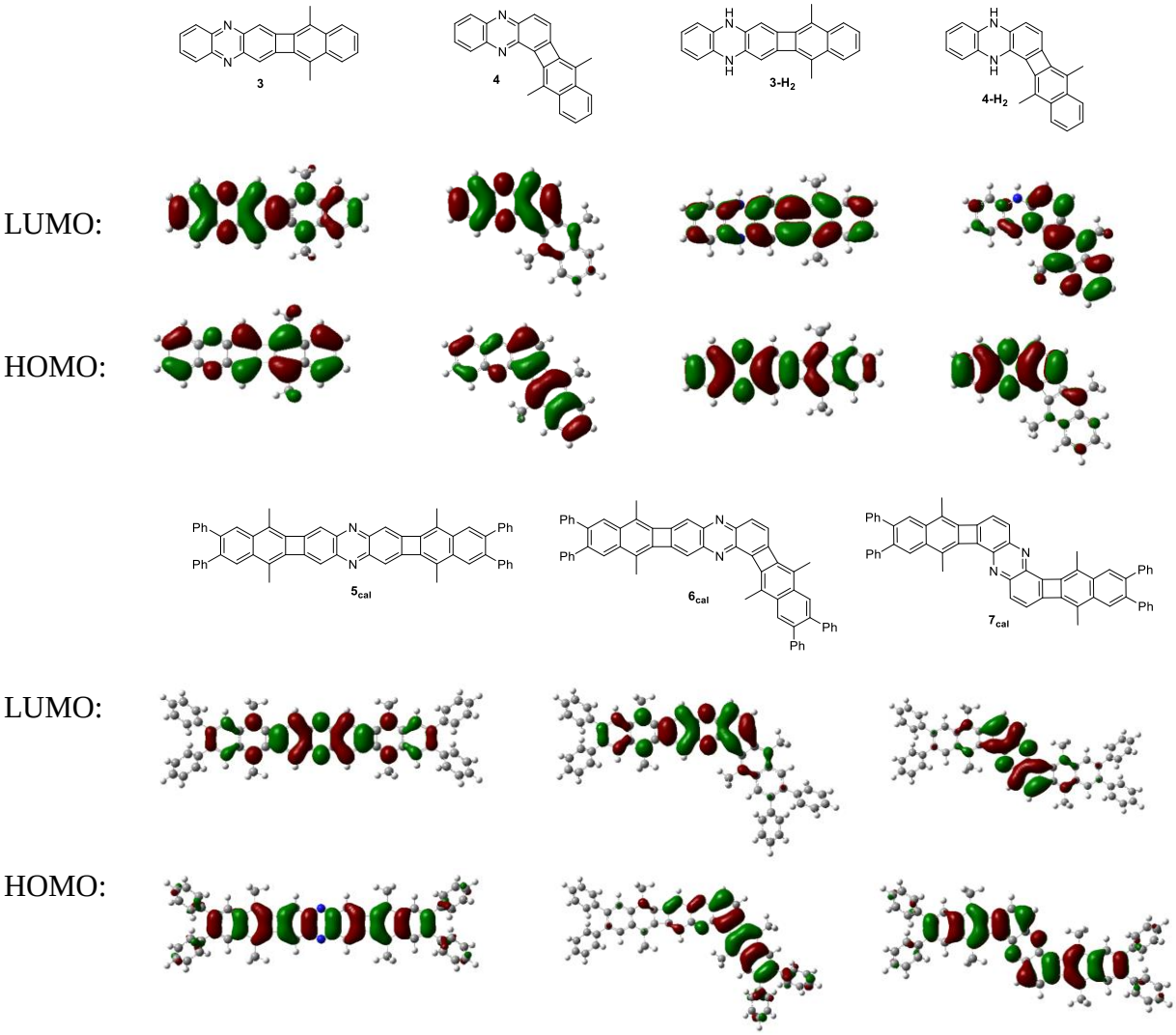


Figure S7. Quantum-chemical calculations (B3LYP 6-311+G(d)) of the FMOs for compounds **3-7**.

5.3 Calculated Cartesian Coordinates of 3-7

3

C	-6.9206600000	-0.7108830000	-0.0002230000
C	-5.7413750000	-1.4106580000	-0.0001450000
C	-4.4993220000	-0.7178440000	-0.0000570000
C	-4.4993220000	0.7178440000	-0.0000570000
C	-5.7413750000	1.4106580000	-0.0001450000
C	-6.9206600000	0.7108830000	-0.0002230000
C	-2.2059710000	0.7308630000	0.0000820000
C	-2.2059710000	-0.7308630000	0.0000820000
C	-0.9609760000	-1.4656880000	0.0001940000
H	-1.0073950000	-2.5486790000	0.0001120000
C	0.1740190000	-0.7298910000	0.0004000000
C	0.1740190000	0.7298910000	0.0004000000
C	-0.9609760000	1.4656880000	0.0001940000
H	-5.7176600000	-2.4949040000	-0.0001470000
H	-5.7176600000	2.4949040000	-0.0001470000
H	-1.0073950000	2.5486790000	0.0001120000
N	-3.3451750000	1.4150950000	0.0000160000
N	-3.3451750000	-1.4150950000	0.0000160000
C	1.6623330000	-0.7202680000	0.0002190000
C	2.7920310000	-1.4796260000	0.0000420000
C	4.0275800000	-0.7227670000	-0.0000440000
C	4.0275800000	0.7227670000	-0.0000440000
C	2.7920310000	1.4796260000	0.0000420000
C	1.6623330000	0.7202680000	0.0002190000
H	5.2928230000	-2.4740000000	-0.0002270000
C	5.2755310000	-1.3903030000	-0.0001920000
C	5.2755310000	1.3903030000	-0.0001910000
C	6.4715090000	0.7021960000	-0.0002770000
C	6.4715090000	-0.7021960000	-0.0002770000
H	5.2928230000	2.4740000000	-0.0002260000
H	7.4102660000	1.2466530000	-0.0003600000
H	7.4102660000	-1.2466530000	-0.0003610000
C	2.7650350000	-2.9837060000	0.0000890000
H	3.2645800000	-3.3998750000	-0.8806960000
H	3.2645760000	-3.3998340000	0.8808910000
H	1.7374070000	-3.3496270000	0.0000810000
C	2.7650350000	2.9837060000	0.0000890000
H	3.2645760000	3.3998340000	0.8808910000
H	3.2645800000	3.3998750000	-0.8806960000

H	1.7374070000	3.3496270000	0.0000810000
H	-7.8667720000	-1.2424260000	-0.0002890000
H	-7.8667720000	1.2424260000	-0.0002890000

4

C	6.3506660000	-0.9912020000	-0.0000110000
C	5.7413110000	0.2320340000	-0.0000340000
C	4.3163990000	0.3268300000	-0.0000100000
C	3.5320700000	-0.8901820000	0.0000390000
C	4.2116960000	-2.1470940000	0.0000620000
C	5.5774670000	-2.1918010000	0.0000370000
C	1.6140980000	0.3487330000	0.0000410000
C	2.3990860000	1.5789170000	-0.0000140000
C	1.7587700000	2.8593190000	-0.0000480000
H	2.4079550000	3.7278380000	-0.0000890000
C	-0.3652690000	1.7986600000	0.0000240000
C	0.2181430000	0.5315050000	0.0000620000
H	3.6082070000	-3.0480250000	0.0000990000
H	6.0882210000	-3.1492850000	0.0000550000
N	2.1955860000	-0.8598360000	0.0000650000
N	3.7372710000	1.5330300000	-0.0000360000
C	-1.7369400000	1.1880410000	0.0000250000
C	-3.0713420000	1.4022850000	-0.0000330000
C	-3.8825880000	0.1844840000	-0.0000320000
C	-3.2728300000	-1.1208090000	0.0000100000
C	-1.8187160000	-1.2842850000	0.0000530000
C	-1.1260100000	-0.1237390000	0.0000650000
H	-5.7630290000	1.2398000000	-0.0001020000
C	-5.2886580000	0.2649570000	-0.0000720000
C	-4.1153690000	-2.2494110000	0.0000080000
C	-5.4967080000	-2.1339750000	-0.0000330000
C	-6.0880190000	-0.8676160000	-0.0000730000
H	-3.6720830000	-3.2385040000	0.0000400000
H	-6.1146090000	-3.0262620000	-0.0000340000
H	-7.1687420000	-0.7678820000	-0.0001040000
C	0.3855570000	2.9887340000	-0.0000320000
H	-0.0783660000	3.9690030000	-0.0000610000
C	-3.6912120000	2.7727940000	-0.0000910000
H	-4.3216550000	2.9339700000	-0.8806370000
H	-4.3216650000	2.9340370000	0.8804370000
H	-2.9207020000	3.5456080000	-0.0001150000
C	-1.1605110000	-2.6363140000	0.0000790000
H	-0.0751570000	-2.5289390000	0.0000950000
H	-1.4430910000	-3.2233220000	0.8805970000
H	-1.4430640000	-3.2233440000	-0.8804320000

H	6.3076240000	1.1568060000	-0.0000720000
H	7.4336100000	-1.0590420000	-0.0000300000

3-H_2

C	7.0127270000	-0.6934920000	-0.0018810000
C	5.7973480000	-1.3892540000	-0.0007400000
C	4.5871930000	-0.7051410000	0.0004600000
C	4.5871930000	0.7051410000	0.0004600000
C	5.7973480000	1.3892540000	-0.0007410000
C	7.0127270000	0.6934920000	-0.0018810000
C	2.1225650000	0.7064920000	0.0011850000
C	2.1225650000	-0.7064920000	0.0011850000
C	0.9179460000	-1.4348790000	0.0007320000
H	0.9467650000	-2.5207100000	0.0007550000
C	-0.2555700000	-0.7070680000	0.0003440000
C	-0.2555700000	0.7070680000	0.0003440000
C	0.9179460000	1.4348790000	0.0007320000
H	5.7929160000	-2.4759810000	-0.0007310000
H	5.7929160000	2.4759810000	-0.0007320000
H	0.9467650000	2.5207100000	0.0007540000
C	-1.7508370000	-0.7231390000	-0.0000990000
C	-2.8740470000	-1.4791320000	-0.0001660000
C	-4.1219030000	-0.7206880000	-0.0003540000
C	-4.1219030000	0.7206880000	-0.0003540000
C	-2.8740470000	1.4791320000	-0.0001660000
C	-1.7508370000	0.7231390000	-0.0000990000
H	-5.3812500000	-2.4711810000	-0.0004920000
C	-5.3640680000	-1.3871690000	-0.0004960000
C	-5.3640680000	1.3871690000	-0.0004960000
C	-6.5669250000	0.6991790000	-0.0006310000
C	-6.5669250000	-0.6991790000	-0.0006310000
H	-5.3812500000	2.4711810000	-0.0004920000
H	-7.5043030000	1.2464380000	-0.0007350000
H	-7.5043030000	-1.2464380000	-0.0007350000
C	-2.8545360000	-2.9838690000	-0.0000420000
H	-3.3557560000	-3.3998240000	0.8804830000
H	-3.3557590000	-3.3999790000	-0.8804900000
H	-1.8278100000	-3.3542920000	-0.0000170000
C	-2.8545360000	2.9838690000	-0.0000420000
H	-3.3557580000	3.3999790000	-0.8804900000
H	-3.3557560000	3.3998240000	0.8804830000
H	-1.8278100000	3.3542920000	-0.0000170000
H	7.9456910000	-1.2461680000	-0.0027640000
H	7.9456910000	1.2461680000	-0.0027640000
N	3.3550180000	1.3649380000	0.0018950000

H	3.3550150000	2.3718990000	0.0008620000
N	3.3550180000	-1.3649380000	0.0018960000
H	3.3550150000	-2.3718990000	0.0008560000

4-H_2

C	6.3510640000	-1.0271840000	0.3966460000
C	5.7246840000	0.2043970000	0.1851540000
C	4.3568350000	0.2701200000	-0.0630480000
C	3.5984820000	-0.9156580000	-0.0854050000
C	4.2246860000	-2.1366400000	0.1420300000
C	5.6017500000	-2.1971300000	0.3757800000
C	1.5450080000	0.3936960000	-0.2217890000
C	2.3093070000	1.6022990000	-0.1923820000
C	1.6981010000	2.8445680000	-0.0697980000
H	2.3268670000	3.7305470000	-0.0478340000
C	-0.4360830000	1.8293800000	-0.0180220000
C	0.1803480000	0.5448380000	-0.1316390000
H	3.6342260000	-3.0487680000	0.1272450000
H	6.0758110000	-3.1581470000	0.5422720000
C	-1.7826220000	1.1895720000	0.0237770000
C	-3.1191780000	1.3918160000	0.1166800000
C	-3.9259820000	0.1805800000	0.0902760000
C	-3.3169880000	-1.1196880000	-0.0338280000
C	-1.8705180000	-1.2737200000	-0.1368120000
C	-1.1666330000	-0.1141440000	-0.0960870000
H	-5.8046160000	1.2245250000	0.2805030000
C	-5.3320970000	0.2533490000	0.1863770000
C	-4.1609540000	-2.2509850000	-0.0516440000
C	-5.5372540000	-2.1418110000	0.0455820000
C	-6.1281710000	-0.8783170000	0.1651950000
H	-3.7223430000	-3.2381610000	-0.1424750000
H	-6.1539470000	-3.0348190000	0.0287970000
H	-7.2067770000	-0.7839860000	0.2413210000
C	0.2927260000	2.9898650000	0.0151340000
H	-0.1489820000	3.9759040000	0.1037430000
C	-3.7337200000	2.7600080000	0.2383530000
H	-4.4186700000	2.9752150000	-0.5886210000
H	-4.3054100000	2.8701860000	1.1659730000
H	-2.9608920000	3.5303650000	0.2345390000
C	-1.2439810000	-2.6349190000	-0.2787880000
H	-0.1611550000	-2.5585570000	-0.3902660000
H	-1.4401440000	-3.2707270000	0.5909140000
H	-1.6187390000	-3.1670690000	-1.1587530000
H	6.3065870000	1.1219910000	0.2041990000
H	7.4194730000	-1.0607200000	0.5796390000

N	3.6988080000	1.4793410000	-0.3307130000
H	4.2380280000	2.3214750000	-0.1968940000
N	2.2275330000	-0.8162800000	-0.3735260000
H	1.6834320000	-1.6564260000	-0.2550870000

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C	-3.5339080000	0.7279240000	0.0072880000
C	-2.3919710000	1.4655340000	0.0103110000
C	-1.1524540000	0.7266860000	0.0025700000
C	-1.1524540000	-0.7266860000	-0.0025700000
C	-2.3919710000	-1.4655340000	-0.0103120000
C	-3.5339080000	-0.7279240000	-0.0072890000
C	1.1524540000	-0.7266860000	0.0025700000
C	1.1524540000	0.7266860000	-0.0025700000
C	2.3919710000	1.4655340000	-0.0103120000
H	2.3452080000	2.5503140000	-0.0175470000
C	3.5339080000	0.7279240000	-0.0072890000
C	3.5339080000	-0.7279240000	0.0072880000
C	2.3919710000	-1.4655340000	0.0103110000
H	-2.3452080000	2.5503140000	0.0175470000
H	-2.3452080000	-2.5503140000	-0.0175470000
H	2.3452080000	-2.5503140000	0.0175470000
N	0.0000000000	-1.4127640000	0.0000000000
N	0.0000000000	1.4127640000	0.0000000000
C	-9.8657930000	0.7139090000	0.0092570000
C	-8.6426850000	1.3783210000	0.0270760000
C	-7.3917020000	0.7214780000	0.0165140000
C	-7.3917020000	-0.7214780000	-0.0165140000
C	-8.6426850000	-1.3783210000	-0.0270760000
C	-9.8657930000	-0.7139090000	-0.0092570000
H	-8.6584710000	2.4635080000	0.0146590000
C	-6.1555120000	1.4836880000	0.0241820000
C	-6.1555120000	-1.4836880000	-0.0241820000
H	-8.6584710000	-2.4635080000	-0.0146590000
C	-5.0243140000	-0.7217960000	-0.0095830000
C	-5.0243140000	0.7217960000	0.0095830000
C	5.0243140000	0.7217960000	-0.0095830000
C	6.1555120000	1.4836880000	-0.0241820000
C	7.3917020000	0.7214780000	-0.0165140000
C	7.3917020000	-0.7214780000	0.0165140000
C	6.1555120000	-1.4836880000	0.0241820000
C	5.0243140000	-0.7217960000	0.0095830000
H	8.6584710000	2.4635080000	-0.0146590000
C	8.6426850000	1.3783210000	-0.0270760000
C	8.6426850000	-1.3783210000	0.0270760000

C	9.8657930000	-0.7139090000	0.0092570000
C	9.8657930000	0.7139090000	-0.0092570000
H	8.6584710000	-2.4635080000	0.0146590000
C	6.1313460000	2.9899220000	-0.0484520000
H	6.6369070000	3.4195890000	0.8260600000
H	6.6301330000	3.3906970000	-0.9404930000
H	5.1004670000	3.3558270000	-0.0506170000
C	6.1313460000	-2.9899220000	0.0484520000
H	6.6369070000	-3.4195890000	-0.8260600000
H	6.6301340000	-3.3906970000	0.9404930000
H	5.1004670000	-3.3558270000	0.0506170000
C	-6.1313460000	2.9899220000	0.0484520000
H	-6.6369070000	3.4195890000	-0.8260600000
H	-6.6301340000	3.3906970000	0.9404930000
H	-5.1004670000	3.3558270000	0.0506170000
C	-6.1313460000	-2.9899220000	-0.0484520000
H	-6.6369070000	-3.4195890000	0.8260600000
H	-6.6301330000	-3.3906970000	-0.9404930000
H	-5.1004670000	-3.3558270000	-0.0506170000
C	-11.1117390000	-1.5344630000	0.0301390000
C	-13.4073090000	-3.1716860000	0.1425880000
C	-12.0788160000	-1.3506130000	1.0333920000
C	-11.3175110000	-2.5550680000	-0.9140380000
C	-12.4549490000	-3.3647710000	-0.8612540000
C	-13.2127090000	-2.1622340000	1.0906430000
H	-12.5972380000	-4.1429770000	-1.6071970000
H	-13.9450130000	-2.0065990000	1.8790510000
H	-14.2928900000	-3.8005740000	0.1863110000
C	-11.1117390000	1.5344630000	-0.0301380000
C	-13.4073090000	3.1716860000	-0.1425880000
C	-11.3175110000	2.5550680000	0.9140380000
C	-12.4549490000	3.3647710000	0.8612540000
C	-13.2127090000	2.1622340000	-1.0906430000
H	-12.5972380000	4.1429770000	1.6071970000
H	-13.9450130000	2.0065990000	-1.8790510000
H	-14.2928900000	3.8005740000	-0.1863110000
C	11.1117390000	-1.5344630000	-0.0301380000
C	13.4073090000	-3.1716860000	-0.1425880000
C	11.3175110000	-2.5550680000	0.9140380000
C	13.2127090000	-2.1622340000	-1.0906430000
C	12.4549490000	-3.3647710000	0.8612540000
H	13.9450130000	-2.0065990000	-1.8790510000
H	12.5972380000	-4.1429770000	1.6071970000
H	14.2928900000	-3.8005740000	-0.1863110000
C	11.1117390000	1.5344630000	0.0301390000
C	13.4073090000	3.1716860000	0.1425880000

C	11.3175110000	2.5550680000	-0.9140380000
C	12.0788160000	1.3506130000	1.0333920000
C	13.2127090000	2.1622340000	1.0906430000
C	12.4549490000	3.3647710000	-0.8612540000
H	13.9450130000	2.0065990000	1.8790510000
H	12.5972380000	4.1429770000	-1.6071970000
H	14.2928900000	3.8005740000	0.1863110000
H	10.5864720000	2.7035100000	-1.7053330000
H	11.9359460000	0.5724360000	1.7777090000
H	-10.5864720000	2.7035100000	1.7053330000
H	-11.9359460000	-0.5724360000	1.7777090000
H	-10.5864720000	-2.7035100000	-1.7053330000
H	10.5864720000	-2.7035100000	1.7053330000
C	12.0788160000	-1.3506130000	-1.0333920000
H	11.9359460000	-0.5724360000	-1.7777090000
C	-12.0788160000	1.3506130000	-1.0333920000
H	-11.9359460000	0.5724360000	-1.7777090000

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C	-3.9669450000	-3.4929790000	-0.0149730000
C	-3.1239840000	-2.3724890000	-0.0201300000
C	-1.7253650000	-2.4877330000	-0.0206340000
C	-1.2166780000	-3.8467050000	-0.0148170000
C	-2.1030250000	-4.9641340000	-0.0108880000
C	-3.4818530000	-4.8091520000	-0.0107230000
C	0.9322910000	-3.0277280000	-0.0143290000
C	0.4109310000	-1.6559320000	-0.0224900000
C	1.3148770000	-0.5262920000	-0.0272400000
H	0.8863810000	0.4707670000	-0.0340030000
C	2.6389800000	-0.8128270000	-0.0218540000
C	3.1589630000	-2.1793330000	-0.0110160000
C	2.3579590000	-3.2720930000	-0.0080800000
H	-1.6457450000	-5.9487210000	-0.0069790000
H	-4.1382620000	-5.6742460000	-0.0066980000
H	2.6980880000	-4.3026510000	-0.0010420000
N	0.1153320000	-4.0791800000	-0.0115710000
N	-0.8978220000	-1.4169330000	-0.0250920000
C	4.0327410000	-0.2930250000	-0.0196560000
C	4.8199960000	0.8212100000	-0.0248110000
C	6.2434060000	0.5482540000	-0.0165170000
C	6.7562350000	-0.8004440000	0.0020930000
C	5.8742950000	-1.9504970000	0.0032250000
C	4.5455100000	-1.6414580000	-0.0077230000
H	6.8081700000	2.6252240000	0.0159120000
C	7.1793220000	1.6062220000	-0.0127550000

C	8.1586440000	-0.9693890000	0.0067960000
C	9.0647390000	0.0845710000	-0.0004590000
C	8.5567690000	1.4204960000	0.0024240000
H	8.5579070000	-1.9777640000	-0.0203380000
C	-8.1431020000	1.4838850000	-0.0064500000
C	-6.7645610000	1.2631280000	-0.0123860000
C	-6.1762180000	-0.0138530000	-0.0096010000
C	-7.0519000000	-1.1555530000	-0.0074380000
C	-8.4378400000	-0.9187430000	0.0073460000
C	-9.0081840000	0.3556750000	0.0168380000
H	-6.1153470000	2.1314320000	-0.0552770000
C	-4.7217360000	-0.1637150000	-0.0188550000
C	-6.5276830000	-2.5215040000	-0.0071510000
H	-9.1101380000	-1.7695790000	0.0493080000
C	-5.1751830000	-2.6015580000	-0.0133650000
C	-4.2966230000	-1.4497650000	-0.0192000000
C	6.3894290000	-3.3654150000	0.0169340000
H	7.0087250000	-3.5799940000	-0.8630250000
H	7.0069810000	-3.5637120000	0.9018820000
H	5.5592790000	-4.0769840000	0.0225790000
C	4.2642680000	2.2207300000	-0.0389520000
H	4.5791450000	2.7911680000	0.8438430000
H	4.5987020000	2.7811070000	-0.9209420000
H	3.1711180000	2.2003330000	-0.0508940000
C	-7.4339130000	-3.7241670000	-0.0006930000
H	-8.0771440000	-3.7432090000	0.8882890000
H	-8.0955310000	-3.7386590000	-0.8761290000
H	-6.8484940000	-4.6481150000	-0.0091260000
C	-3.7845420000	1.0146130000	-0.0242210000
H	-3.9354260000	1.6534740000	0.8556680000
H	-2.7466080000	0.6699690000	-0.0240850000
H	-3.9370100000	1.6466330000	-0.9087640000
C	-8.6249130000	2.8936040000	-0.0707710000
C	-9.4300380000	5.5904620000	-0.2400310000
C	-8.0960610000	3.8615570000	0.7993610000
C	-9.5655990000	3.3058200000	-1.0294570000
C	-9.9617400000	4.6393660000	-1.1138950000
C	-8.4954800000	5.1959090000	0.7180350000
H	-10.6856180000	4.9371800000	-1.8680660000
H	-8.0780350000	5.9257130000	1.4070910000
H	-9.7421590000	6.6293870000	-0.3057600000
C	-10.4940220000	0.4550590000	0.0983030000
C	-13.3051490000	0.5324710000	0.2992530000
C	-11.3017710000	-0.2822700000	-0.7832840000
C	-11.1245750000	1.2311170000	1.0852080000
C	-12.5141740000	1.2676020000	1.1852130000

C	-12.6932000000	-0.2425520000	-0.6865330000
H	-12.9806390000	1.8696150000	1.9607420000
H	-13.2981100000	-0.8153280000	-1.3848860000
H	-14.3886730000	0.5642700000	0.3770990000
C	9.4266660000	2.6299040000	0.0667820000
C	10.9756280000	4.9778300000	0.2365450000
C	10.4200820000	2.7667560000	1.0506950000
C	9.2254430000	3.6932430000	-0.8286680000
C	9.9937660000	4.8550600000	-0.7471690000
C	11.1837910000	3.9293830000	1.1356620000
H	9.8261630000	5.6621660000	-1.4556160000
H	11.9418880000	4.0178500000	1.9094170000
H	11.5746050000	5.8821440000	0.3025140000
C	10.5189660000	-0.2409480000	-0.0548070000
C	13.2384780000	-0.9627860000	-0.2038400000
C	11.0692950000	-1.1683150000	0.8451320000
C	11.3586710000	0.3174120000	-1.0329060000
C	12.7029320000	-0.0424430000	-1.1078640000
C	12.4166240000	-1.5239320000	0.7741480000
H	13.3334930000	0.3955790000	-1.8771060000
H	12.8234300000	-2.2374350000	1.4860800000
H	14.2878580000	-1.2391400000	-0.2616270000
H	-10.5187810000	1.8011410000	1.7827810000
H	-10.8307210000	-0.8788450000	-1.5602010000
H	-9.9804400000	2.5758970000	-1.7176170000
H	-7.3764630000	3.5581130000	1.5553130000
H	10.9508060000	1.0301810000	-1.7429450000
H	10.4358930000	-1.6000010000	1.6157160000
H	10.5861970000	1.9600030000	1.7578010000
H	8.4700960000	3.5981700000	-1.6044500000

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C	-2.4770060000	2.6919440000	0.0063480000
C	-1.0793480000	2.5440570000	0.0052540000
C	-0.4604020000	1.2829180000	0.0055280000
C	-1.3728280000	0.1377140000	0.0060170000
C	-2.7928160000	0.3294730000	0.0069090000
C	-3.3611650000	1.5948420000	0.0073410000
C	0.4604020000	-1.2829180000	0.0055280000
C	1.3728280000	-0.1377140000	0.0060170000
C	2.7928160000	-0.3294730000	0.0069090000
H	3.4023480000	0.5669430000	0.0073020000
C	3.3611650000	-1.5948420000	0.0073410000
C	2.4770060000	-2.6919440000	0.0063480000
C	1.0793480000	-2.5440570000	0.0052540000

H	-3.4023480000	-0.5669430000	0.0073020000
H	-4.4383090000	1.7183860000	0.0082570000
N	-0.8864970000	-1.1248520000	0.0057660000
N	0.8864970000	1.1248520000	0.0057660000
C	0.8864970000	-4.0299690000	0.0036090000
C	-0.0011050000	-5.0550560000	0.0010510000
C	0.6139320000	-6.3872580000	0.0023260000
C	2.0468070000	-6.5555640000	0.0014060000
C	2.9542650000	-5.4011480000	0.0054690000
C	2.3327030000	-4.1951750000	0.0056120000
H	-1.2626360000	-7.4326090000	-0.0493150000
C	-0.1855030000	-7.5464740000	-0.0085030000
C	2.5552980000	-7.8688140000	0.0089730000
C	1.7486750000	-9.0132100000	0.0105530000
C	0.3333500000	-8.8467090000	-0.0136380000
H	3.6290510000	-8.0116160000	0.0499110000
C	-0.3333500000	8.8467090000	-0.0136380000
C	0.1855030000	7.5464740000	-0.0085030000
C	-0.6139320000	6.3872580000	0.0023260000
C	-2.0468070000	6.5555640000	0.0014060000
C	-2.5552980000	7.8688140000	0.0089730000
C	-1.7486750000	9.0132100000	0.0105530000
H	1.2626360000	7.4326090000	-0.0493150000
C	0.0011050000	5.0550560000	0.0010510000
C	-2.9542650000	5.4011480000	0.0054690000
H	-3.6290510000	8.0116160000	0.0499110000
C	-2.3327030000	4.1951750000	0.0056120000
C	-0.8864970000	4.0299690000	0.0036090000
C	4.4520510000	-5.5692830000	0.0077810000
H	4.7979490000	-6.1166410000	0.8940540000
H	4.7995750000	-6.1269030000	-0.8713880000
H	4.9500940000	-4.5955530000	0.0027400000
C	-1.4942560000	-4.8526670000	-0.0017390000
H	-1.7284360000	-3.7843380000	0.0036790000
H	-1.9610330000	-5.3013460000	-0.8884620000
H	-1.9659680000	-5.3119670000	0.8768800000
C	-4.4520510000	5.5692830000	0.0077810000
H	-4.7979490000	6.1166410000	0.8940540000
H	-4.7995750000	6.1269030000	-0.8713880000
H	-4.9500940000	4.5955530000	0.0027400000
C	1.4942560000	4.8526670000	-0.0017390000
H	1.9659680000	5.3119670000	0.8768800000
H	1.7284360000	3.7843380000	0.0036790000
H	1.9610330000	5.3013460000	-0.8884620000
C	0.6302250000	9.9843720000	-0.0902400000
C	2.5349380000	12.0620900000	-0.2835520000

C	1.7342400000	10.0370430000	0.7831730000
C	0.5013400000	10.9927180000	-1.0655190000
C	1.4443040000	12.0193220000	-1.1610390000
C	2.6763050000	11.0667690000	0.6895470000
H	1.3299840000	12.7837420000	-1.9233820000
H	3.5158830000	11.0925930000	1.3774890000
H	3.2652660000	12.8616520000	-0.3581000000
C	-2.4225260000	10.3433960000	0.0835020000
C	-3.7939340000	12.8068240000	0.2694960000
C	-3.4830440000	10.6489870000	-0.7920080000
C	-2.0647220000	11.2966720000	1.0571120000
C	-2.7440280000	12.5141960000	1.1489290000
C	-4.1609060000	11.8692570000	-0.7019870000
H	-2.4563510000	13.2330660000	1.9098780000
H	-4.9703940000	12.0877200000	-1.3918190000
H	-4.3188850000	13.7541960000	0.3411580000
C	-0.6302250000	-9.9843720000	-0.0902400000
C	-2.5349380000	-12.0620900000	-0.2835520000
C	-0.5013400000	-10.9927180000	-1.0655190000
C	-2.6763050000	-11.0667690000	0.6895470000
C	-1.4443040000	-12.0193220000	-1.1610390000
H	-3.5158830000	-11.0925930000	1.3774890000
H	-1.3299840000	-12.7837420000	-1.9233820000
H	-3.2652660000	-12.8616520000	-0.3581000000
C	2.4225260000	-10.3433960000	0.0835020000
C	3.7939340000	-12.8068240000	0.2694960000
C	3.4830440000	-10.6489870000	-0.7920080000
C	2.0647220000	-11.2966720000	1.0571120000
C	2.7440280000	-12.5141960000	1.1489290000
C	4.1609060000	-11.8692570000	-0.7019870000
H	2.4563510000	-13.2330660000	1.9098780000
H	4.9703940000	-12.0877200000	-1.3918190000
H	4.3188850000	-13.7541960000	0.3411580000
H	4.4383090000	-1.7183860000	0.0082570000
C	-1.7342400000	-10.0370430000	0.7831730000
H	-3.7634800000	9.9298980000	-1.5557760000
H	-1.2567680000	11.0769580000	1.7462200000
H	1.8420720000	9.2732210000	1.5473220000
H	-0.3365660000	10.9647320000	-1.7532890000
H	1.2567680000	-11.0769580000	1.7462200000
H	3.7634800000	-9.9298980000	-1.5557760000
H	-1.8420720000	-9.2732210000	1.5473220000
H	0.3365660000	-10.9647320000	-1.7532890000

5.4. NICS calculations

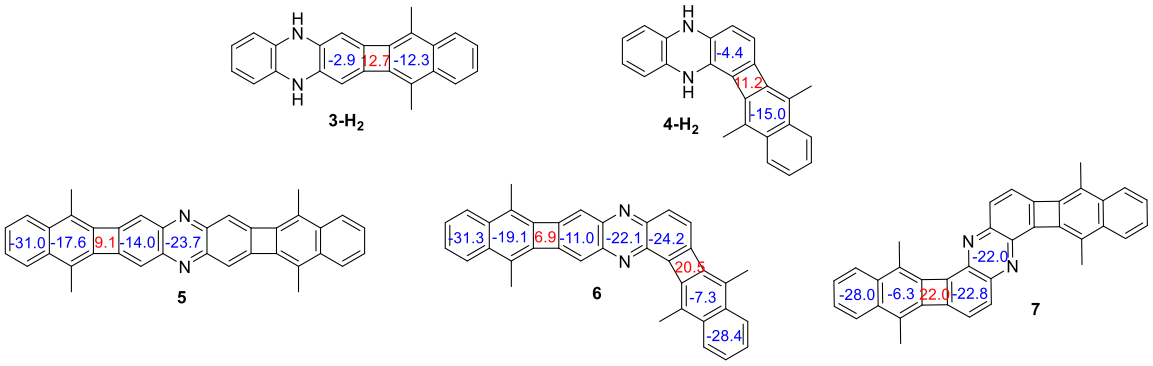

Figure S8. NICS(1)$_{\pi,ZZ}$ calculations on **3-H$_2$**, **4-H$_2$**, and **5-7** (GIAO-B3LYP/6-311+G(d)).

6. References

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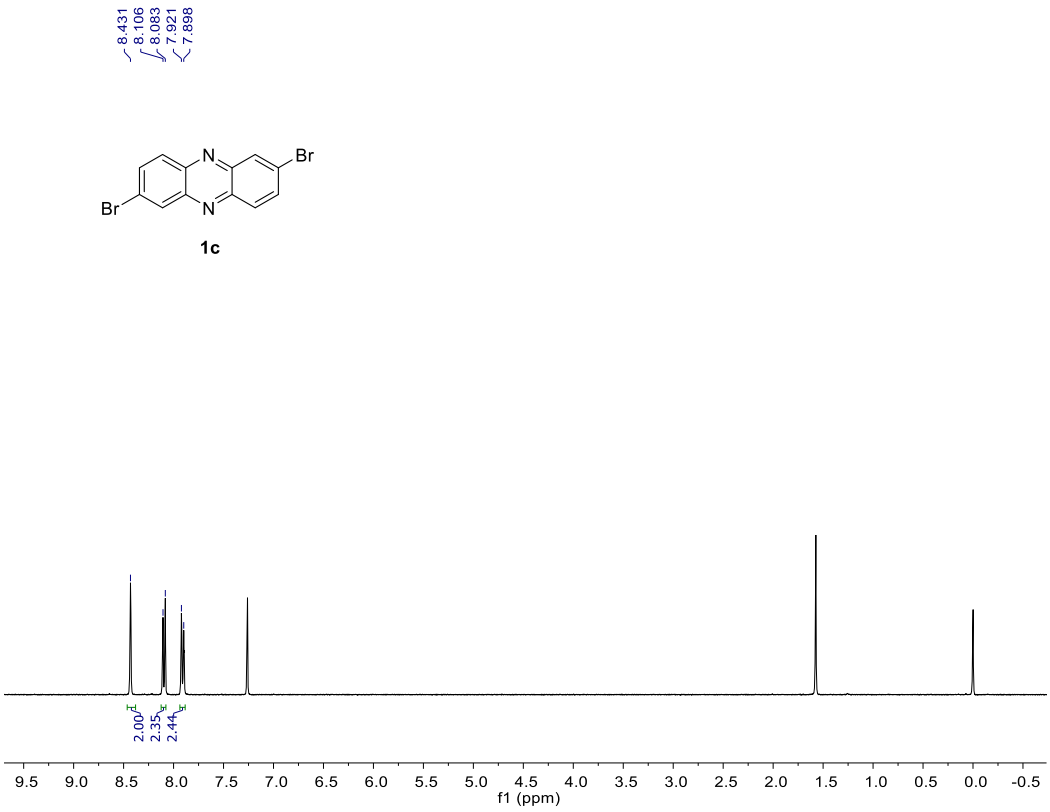
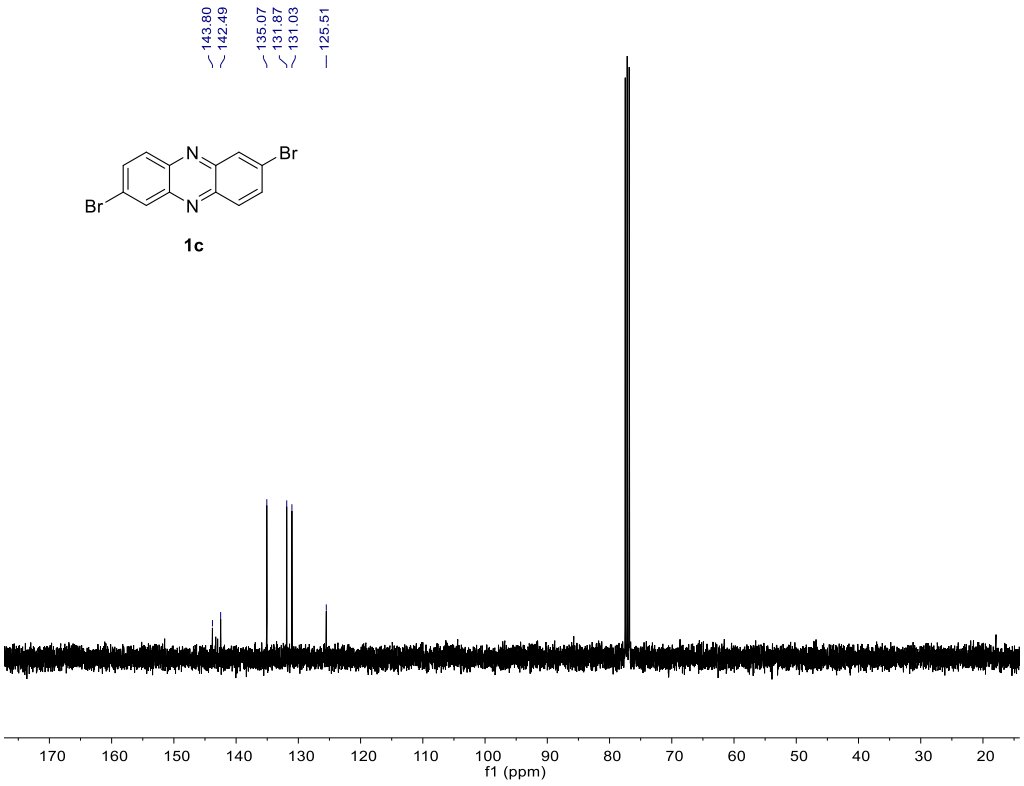
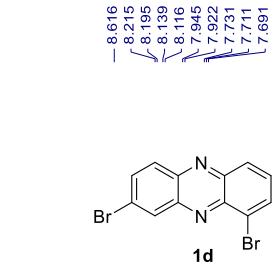
7. NMR Spectra of New Compounds



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7.922
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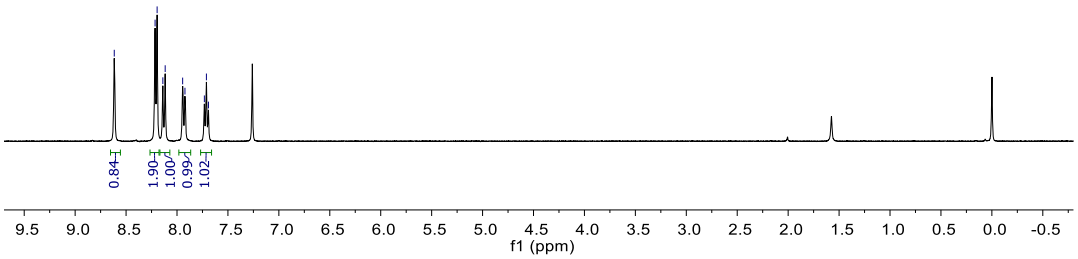
7.711
7.691
N
N
Br
Br
1d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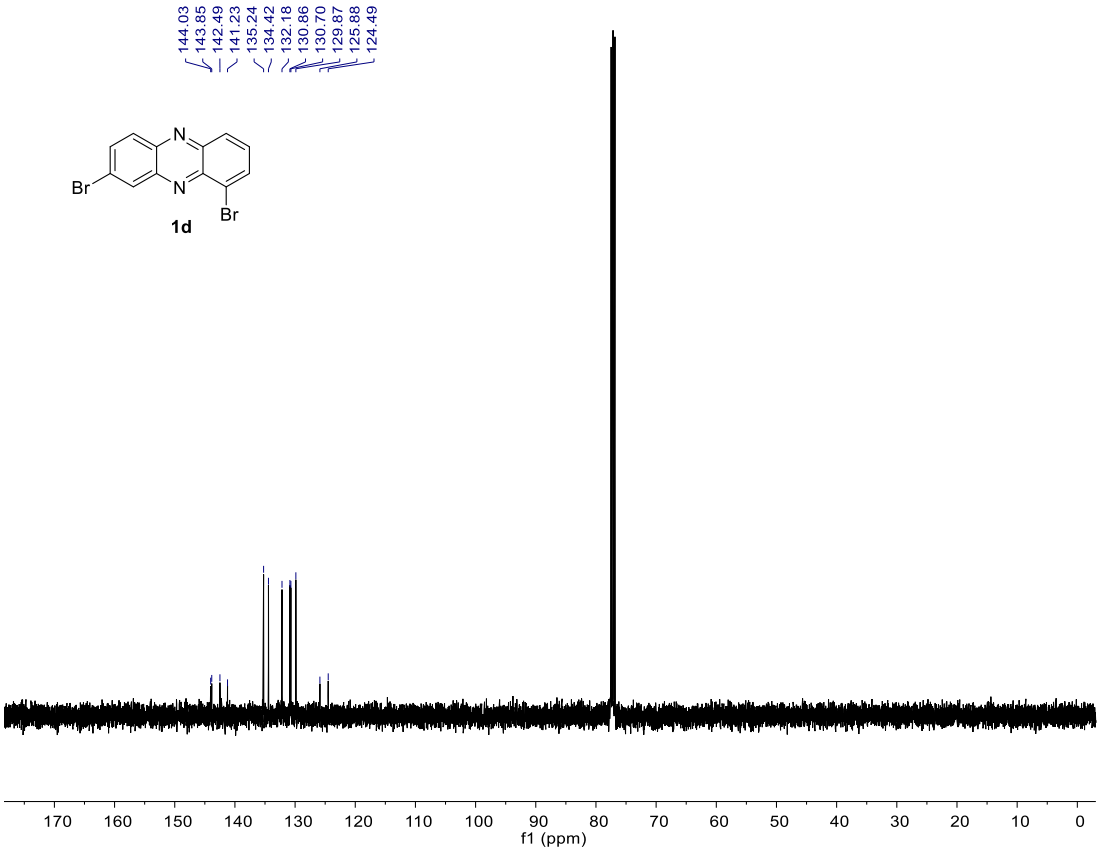
1.90
1.00
0.99
1.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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143.85
142.49
141.23
135.24
134.42
132.18
130.86
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129.87
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124.49
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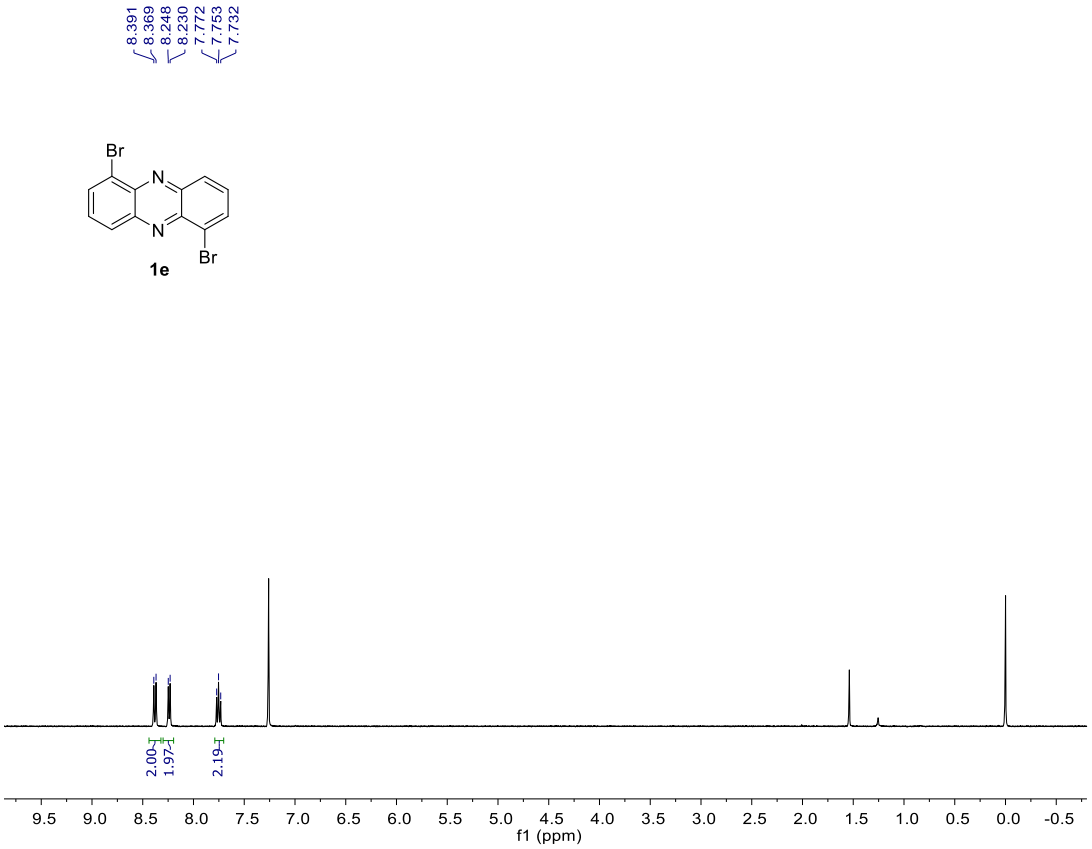
N
Br
Br
1d
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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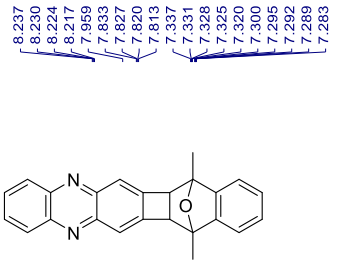
8.369
8.248
8.230
7.772
7.753
7.732
Br
N
N
Br
1e
2.00
1.97
2.19
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)
144.052
141.227
134.479
131.035
130.145
124.231
Br
N
N
Br
1e
160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25
f1 (ppm)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8.217
7.959
7.833
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7.820
7.813
7.337
7.331
7.328
7.325
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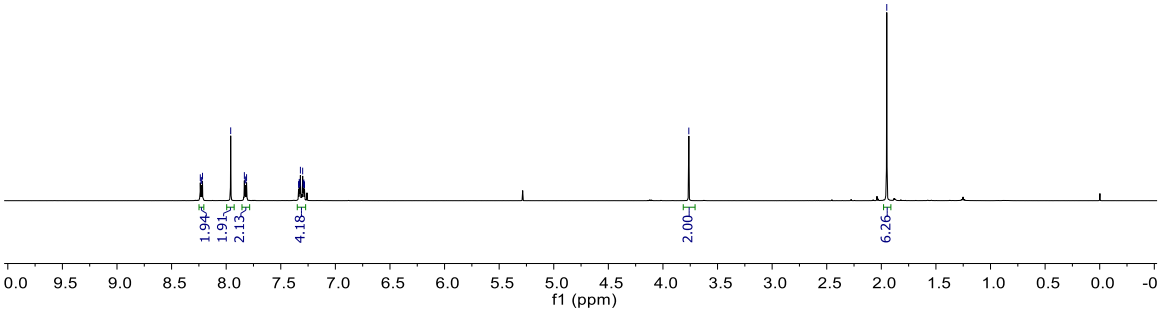
7.300
7.295
7.292
7.289
7.283
3.763
1.950
N
N
O

3'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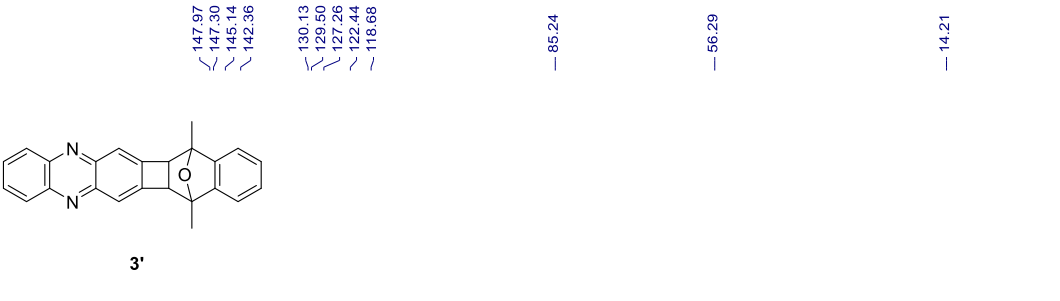
1.91
2.13
4.18
2.00
6.26
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)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56.29
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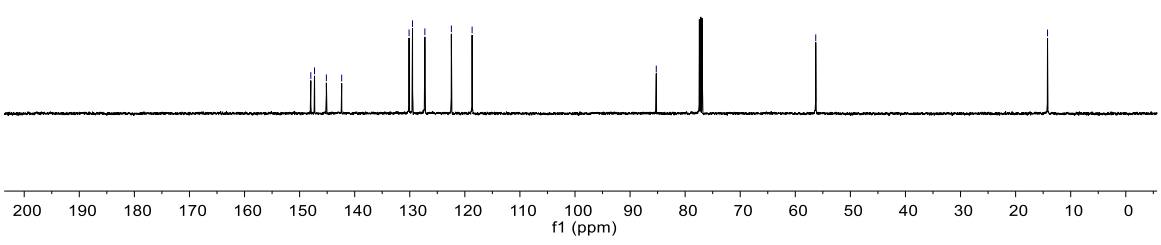
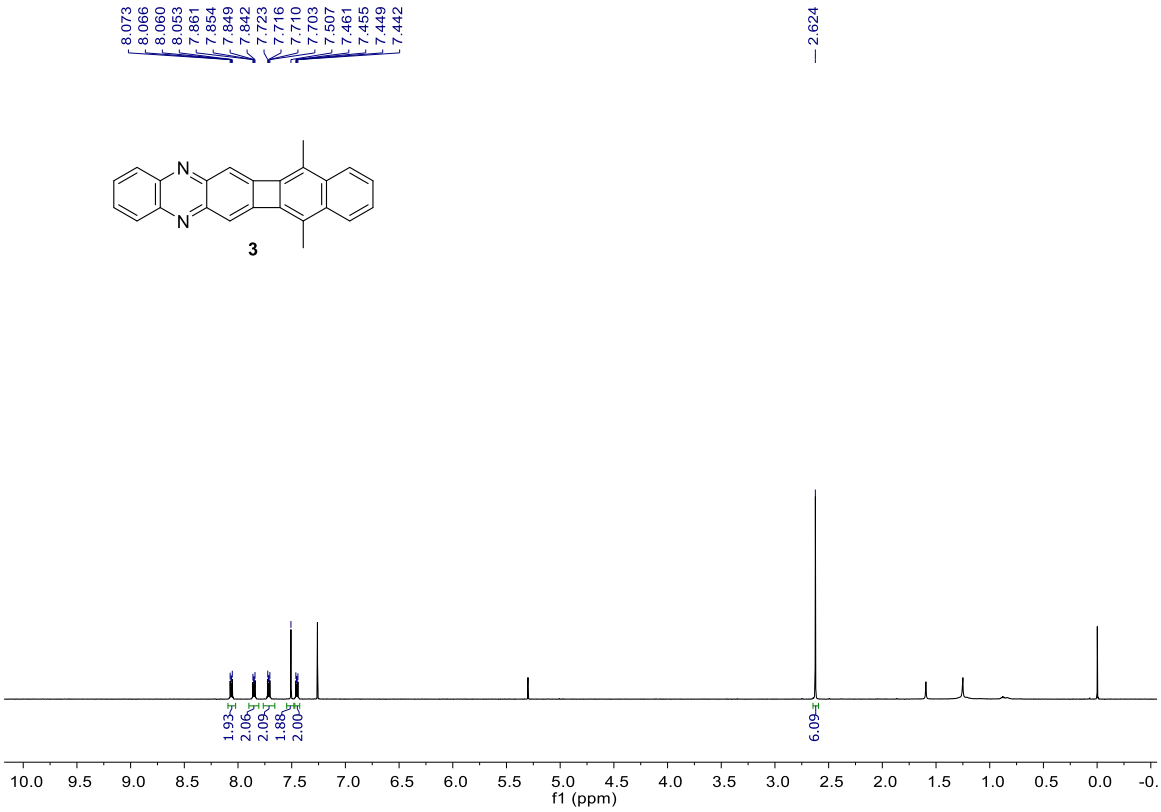
N
N
O

3'


200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.716
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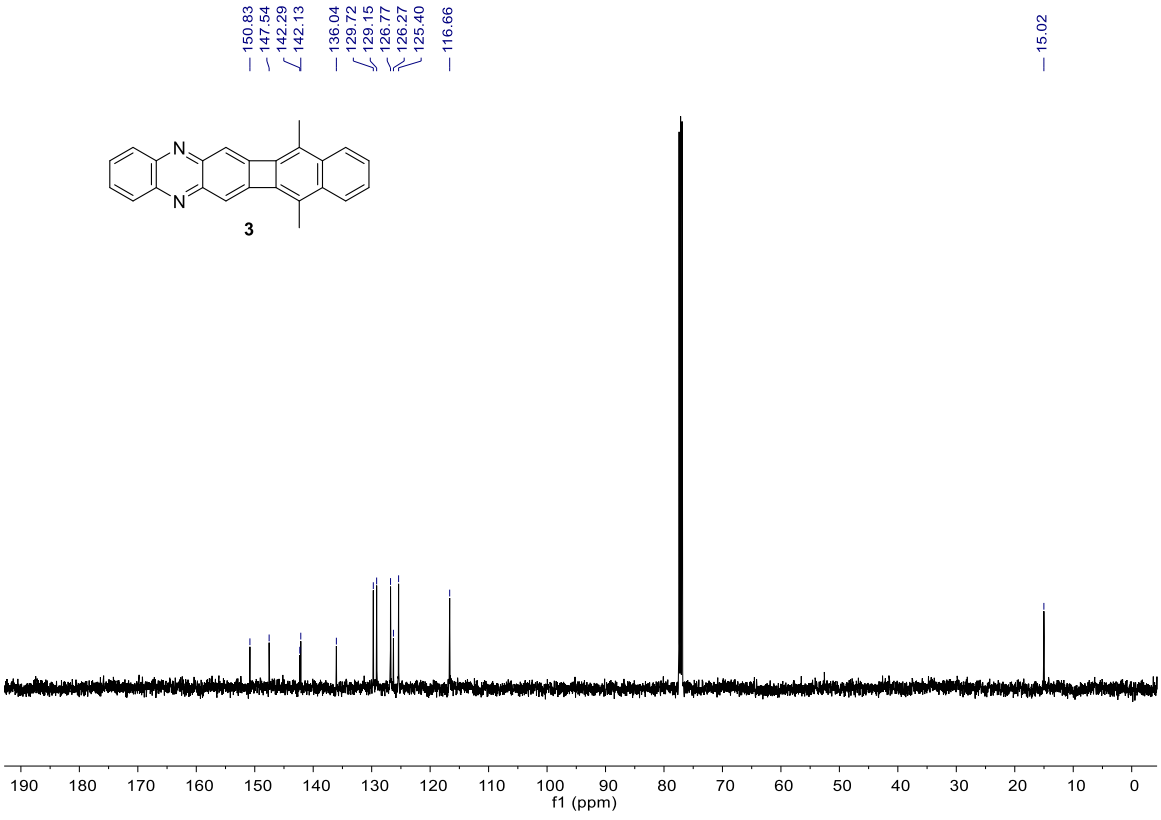
7.703
7.507
7.461
7.455
7.449
7.442
2.624
N
N
3
1.93
2.06
2.09
1.88
2.00
6.09
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)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N
N
3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.298
8.290
8.278
8.268
8.248
7.868
7.856
7.851
7.845
7.838
7.830
7.824
7.819
7.760
7.739
7.395
7.389
7.379
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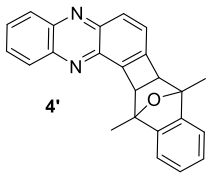
1.891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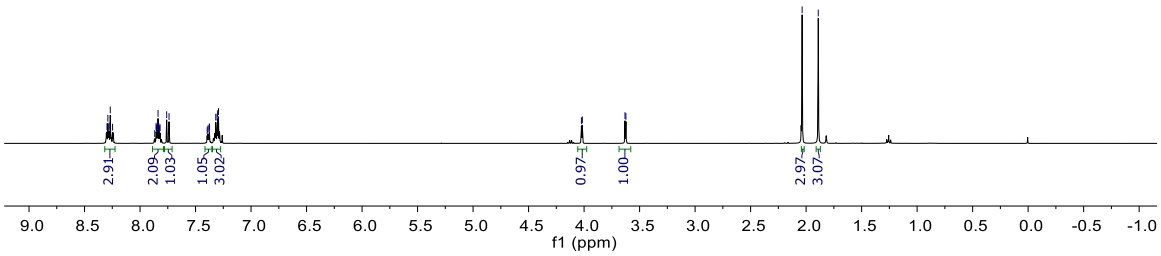
N
O

4'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0.97
1.00
2.97
3.07
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)


148.17
147.89
147.73
144.30
143.05
140.96
131.76
130.78
130.13
130.10
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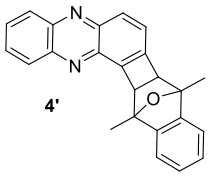
54.94
15.49
14.64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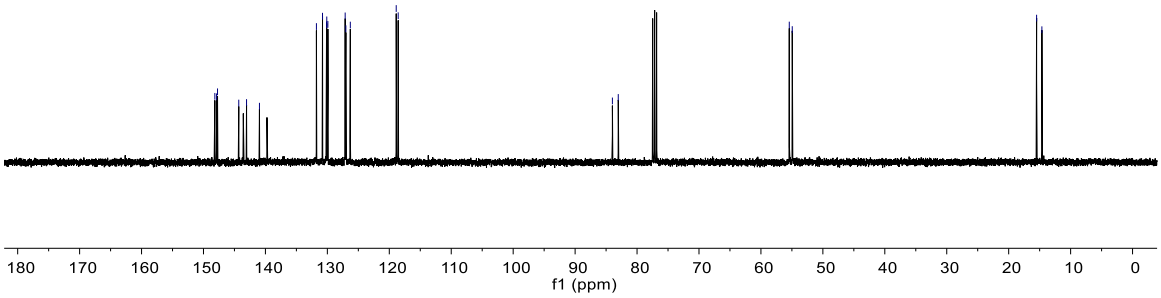
N
O

4'


180
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150
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110
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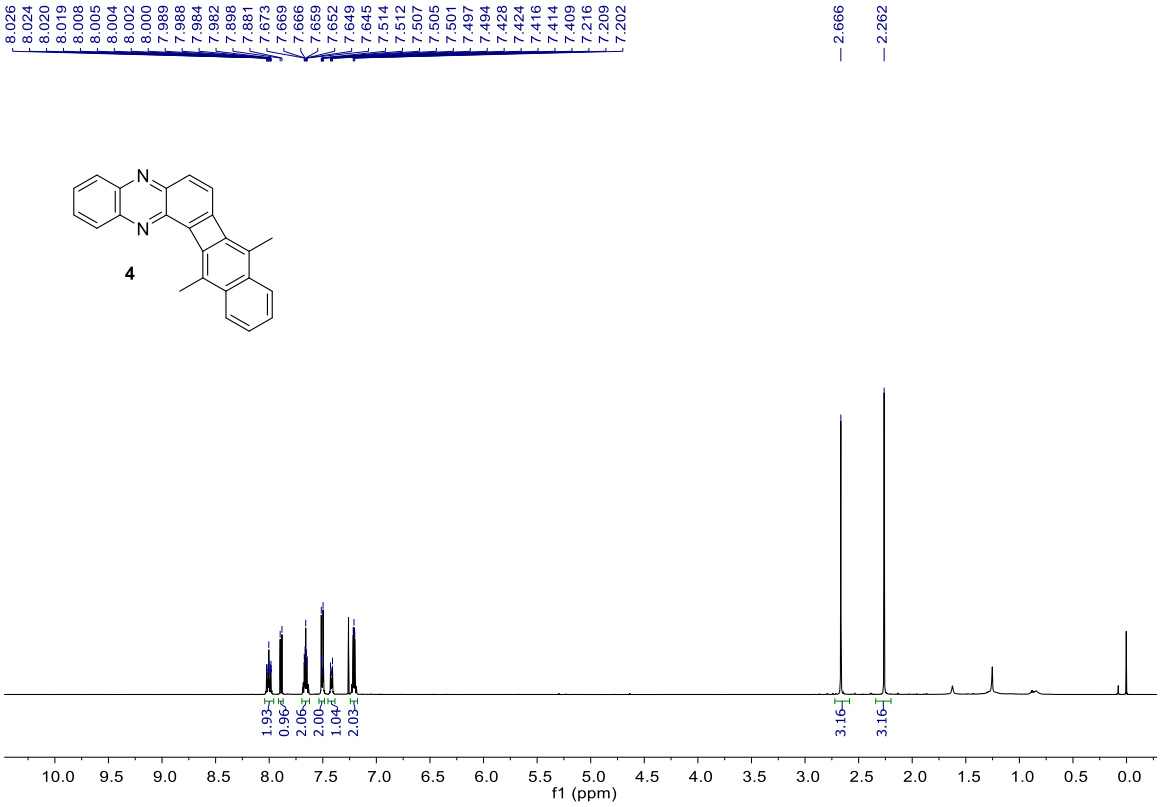
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.416
7.414
7.409
7.216
7.209
7.202
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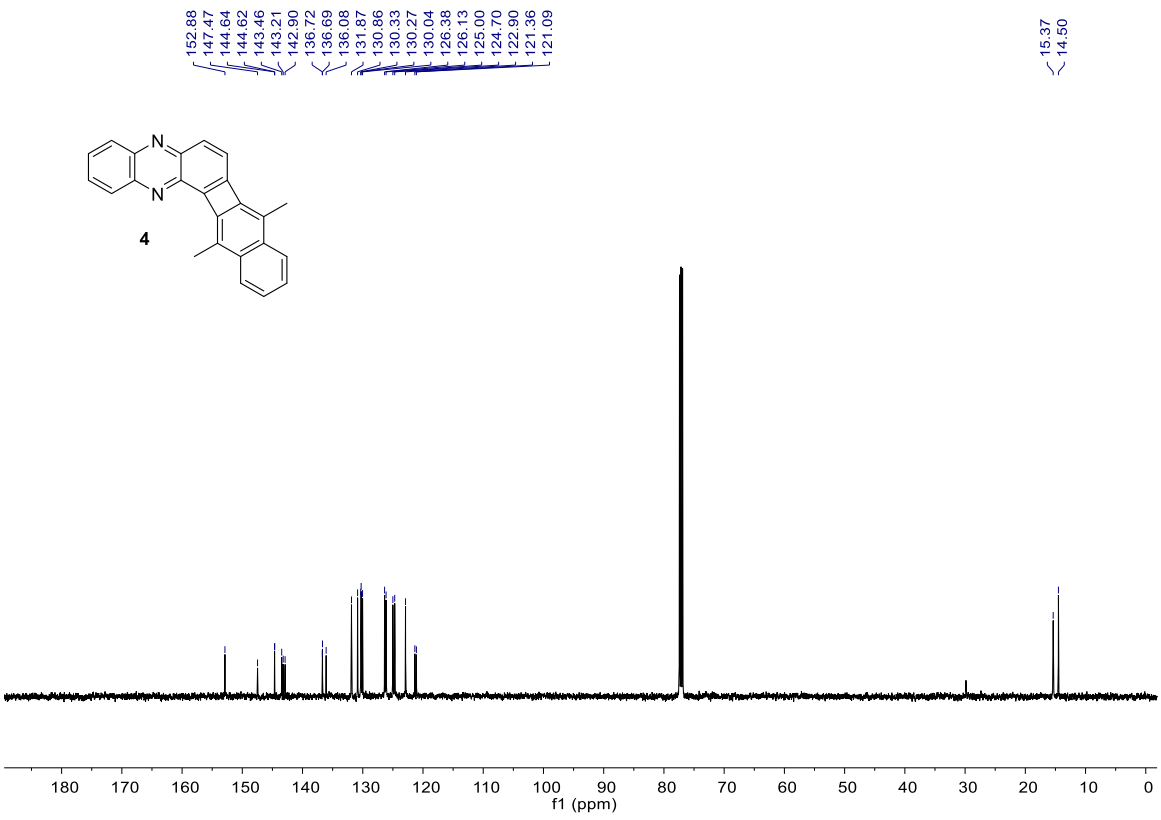
2.262
4
1.93
0.96
2.06
2.00
1.04
2.03
3.16
3.16
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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130.33
130.27
130.04
126.38
126.13
125.00
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121.36
121.09
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14.50
4
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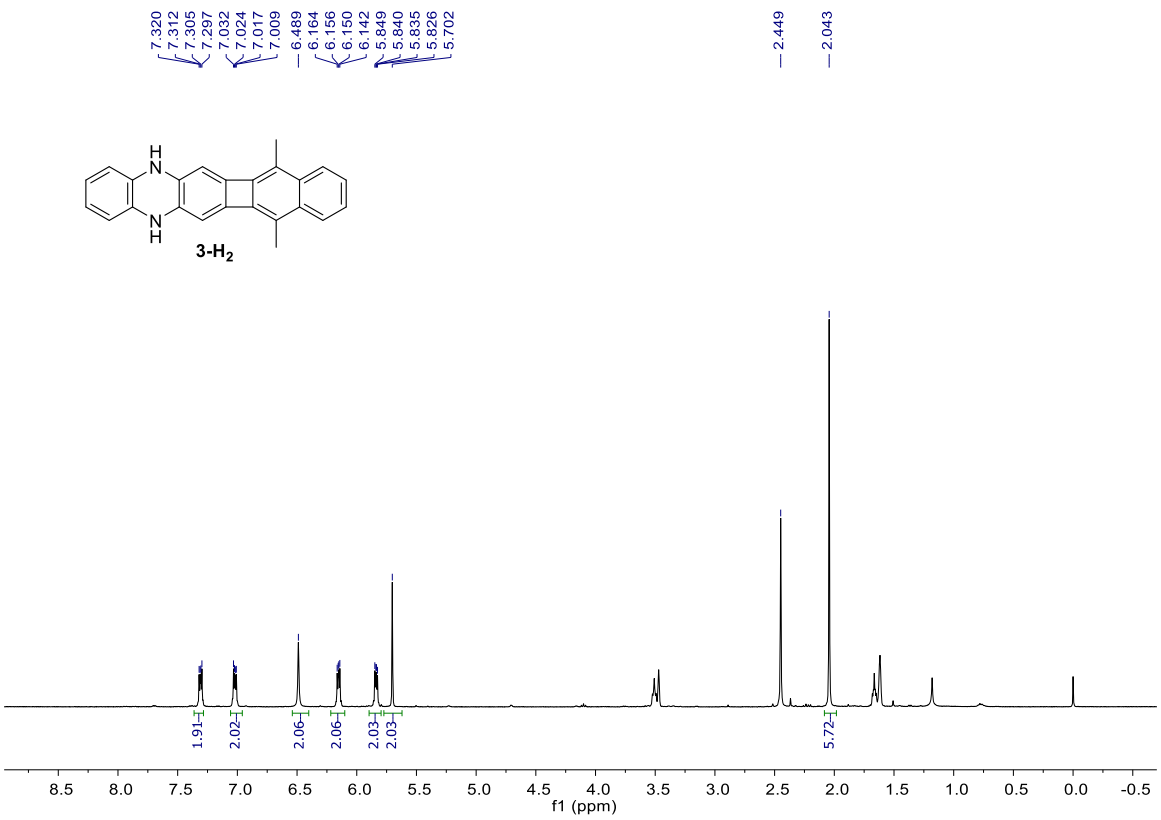
f1 (ppm)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7.032
7.024
7.017
7.009
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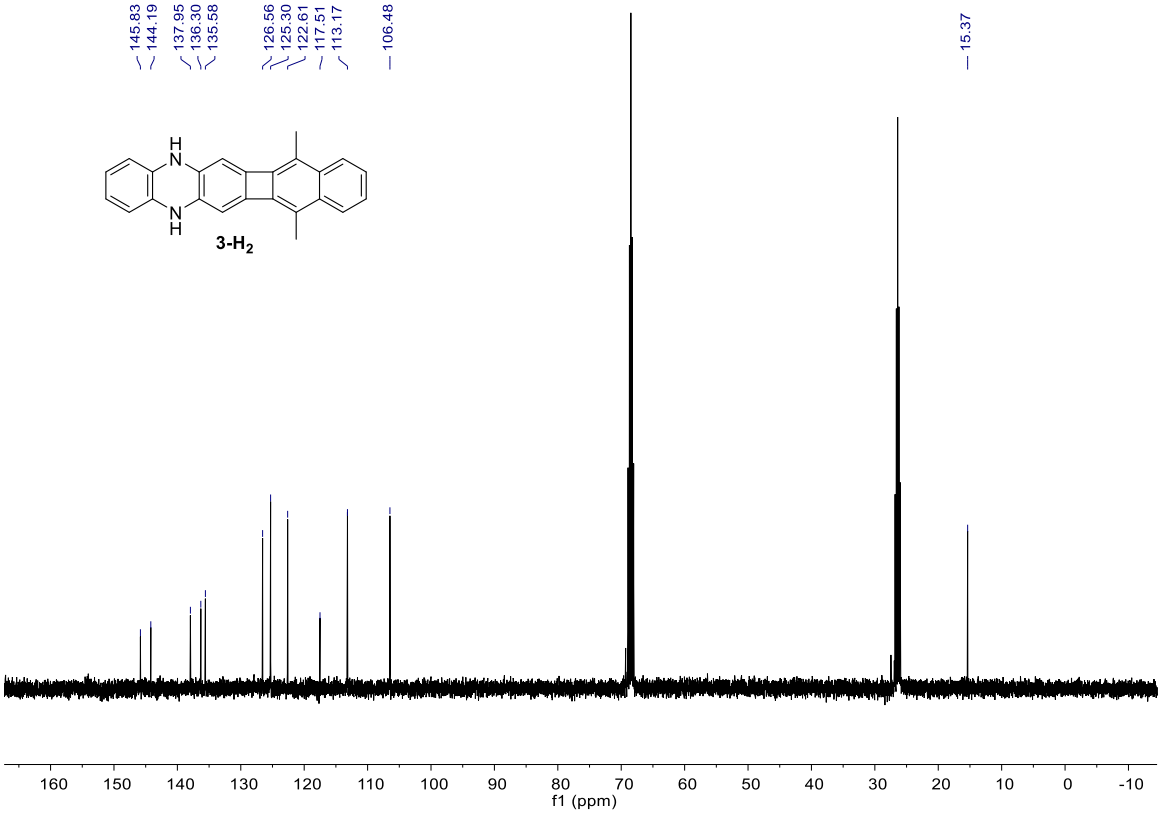
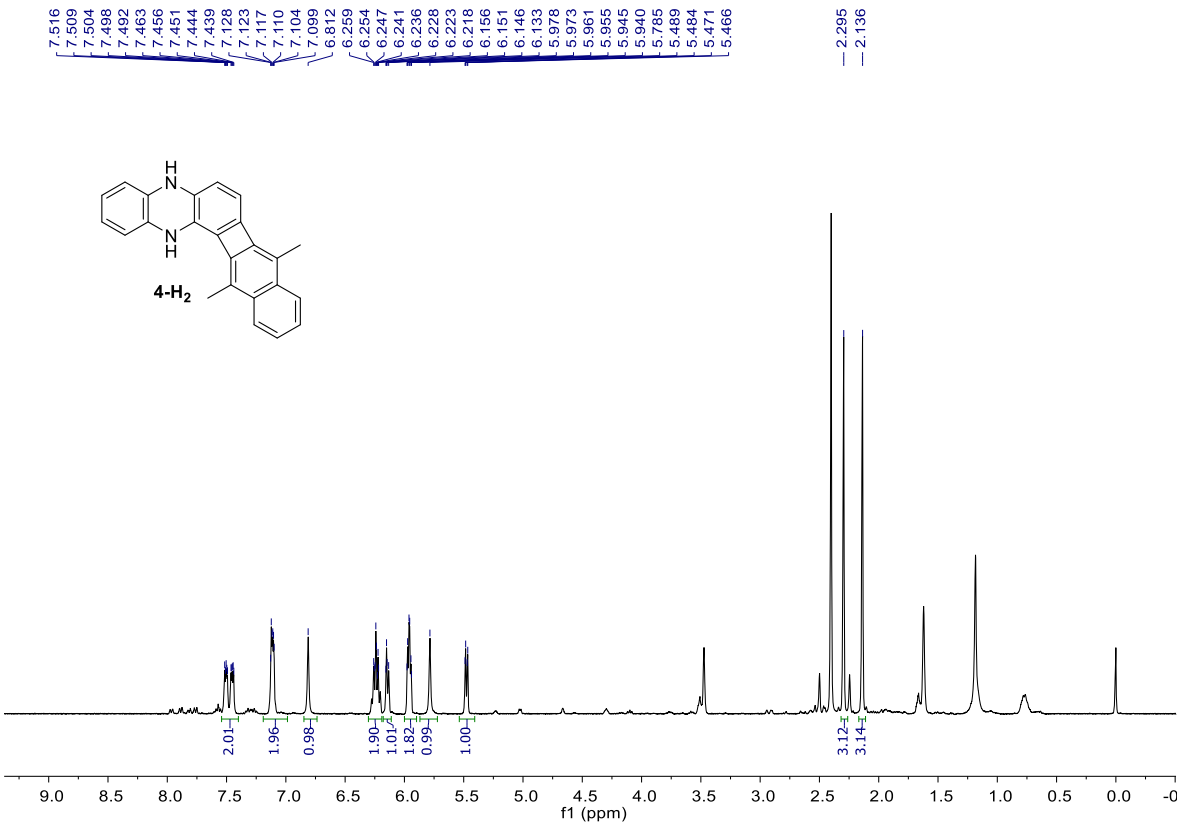
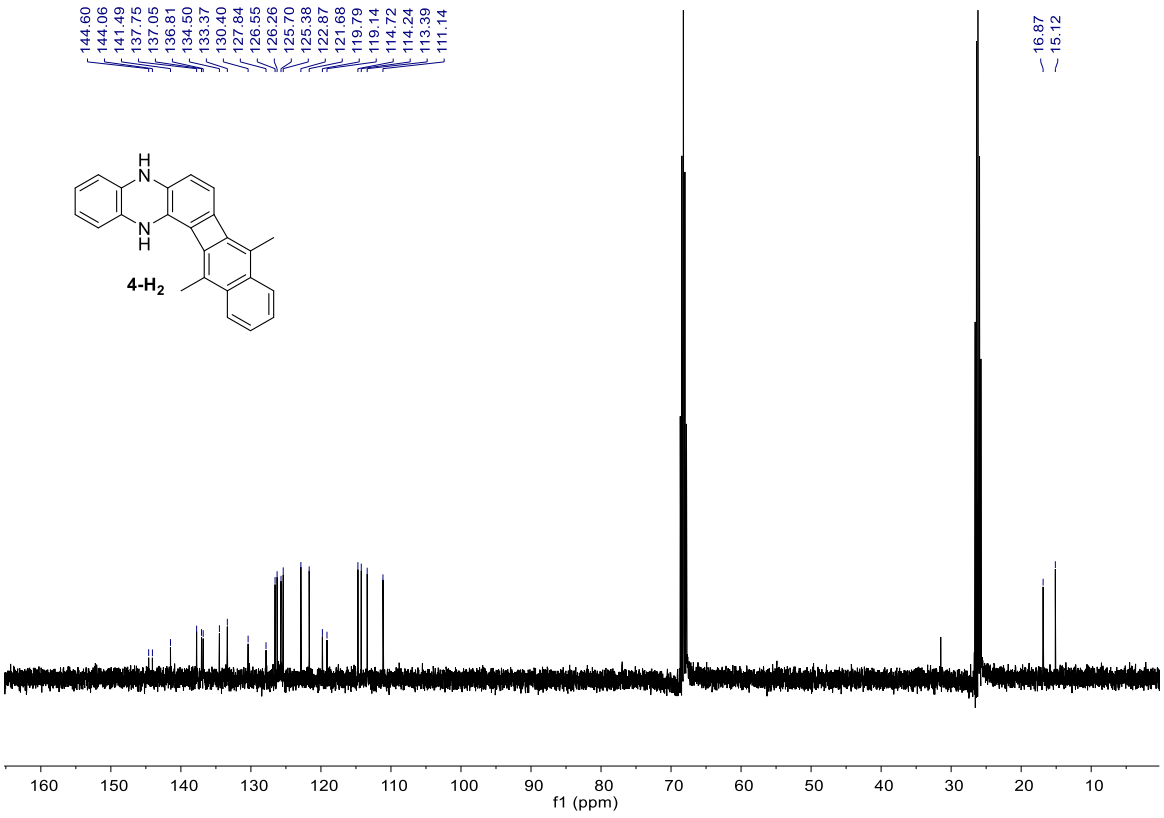
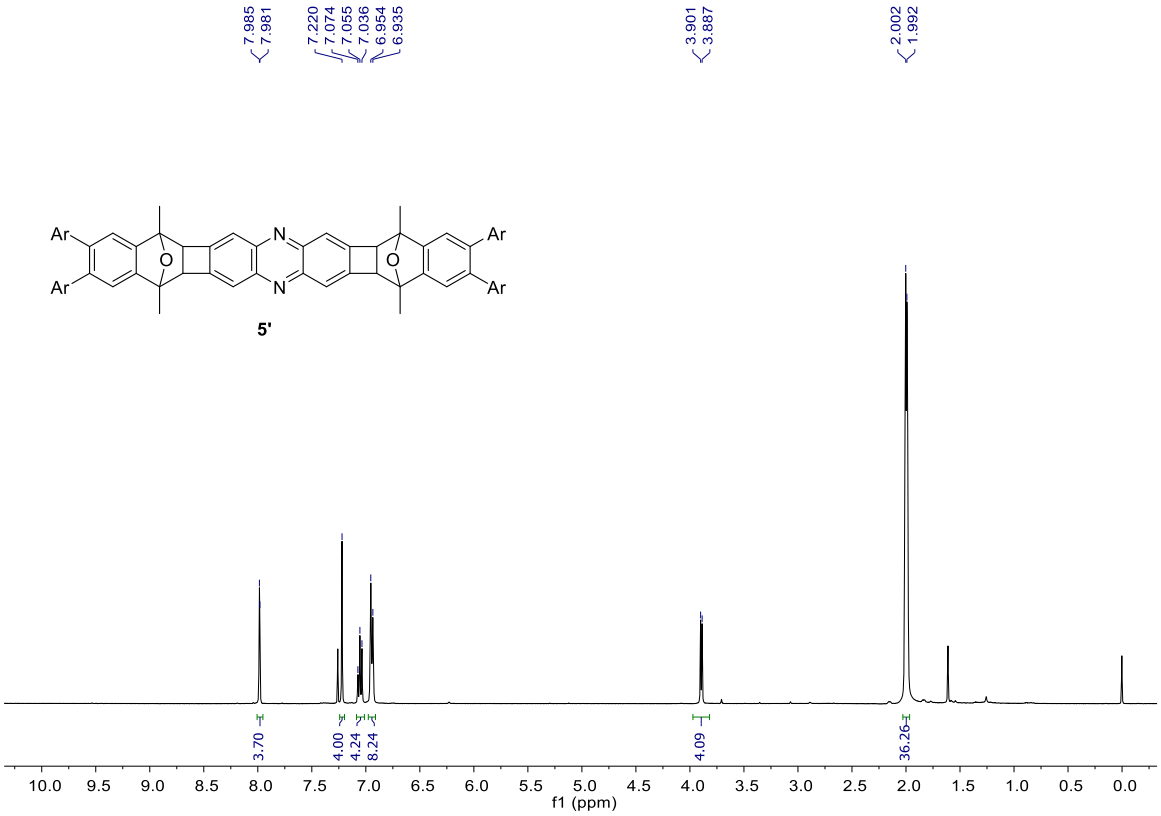
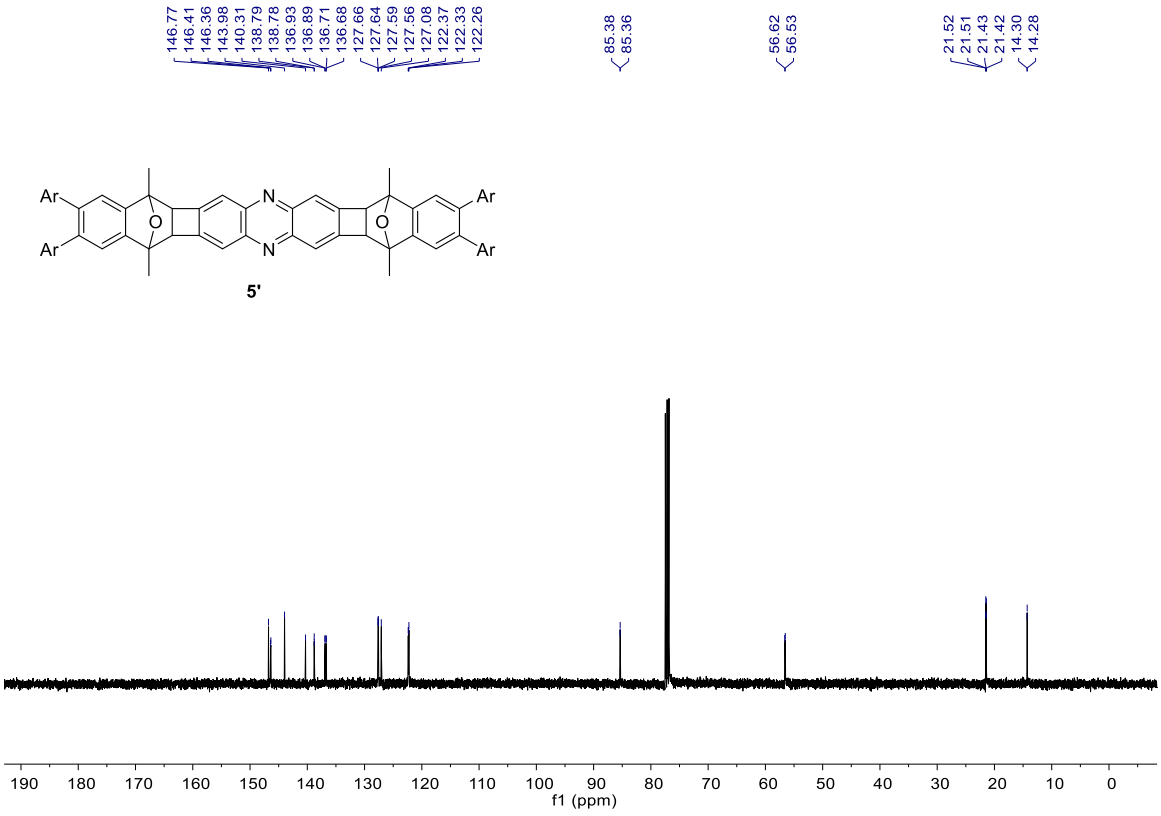
6.164
6.156
6.150
6.142
5.849
5.840
5.835
5.826
5.702
2.449
2.043
3-H2
1.91
2.02
2.06
2.06
2.03
2.03
5.72
f1 (ppm)


145.83
144.19
137.95
136.30
135.58
126.56
125.30
122.61
117.51
113.17
106.48
15.37
3-H2
f1 (ppm)


7.516
7.509
7.504
7.498
7.492
7.463
7.456
7.451
7.444
7.439
7.128
7.123
7.117
7.110
7.104
7.099
6.812
6.259
6.254
6.247
6.241
6.236
6.228
6.223
6.218
6.156
6.151
6.146
6.133
5.978
5.973
5.961
5.955
5.945
5.940
5.785
5.489
5.484
5.471
5.466
2.295
2.136
4-H2
2.01
1.96
0.98
1.90
1.01
1.82
0.99
1.00
3.12
3.14
f1 (ppm)


144.60
144.06
141.49
137.75
137.05
136.81
134.50
133.37
130.40
127.84
126.55
126.26
125.70
125.38
122.87
121.68
119.79
119.14
114.72
114.24
113.39
111.14
16.87
15.12
4-H2
f1 (ppm)


7.985
7.981
7.220
7.074
7.055
7.036
6.954
6.935
3.901
3.887
2.002
1.992
Ar
Ar
O
N
N
O
Ar
Ar
5'
3.70
4.00
4.24
8.24
4.09
36.26
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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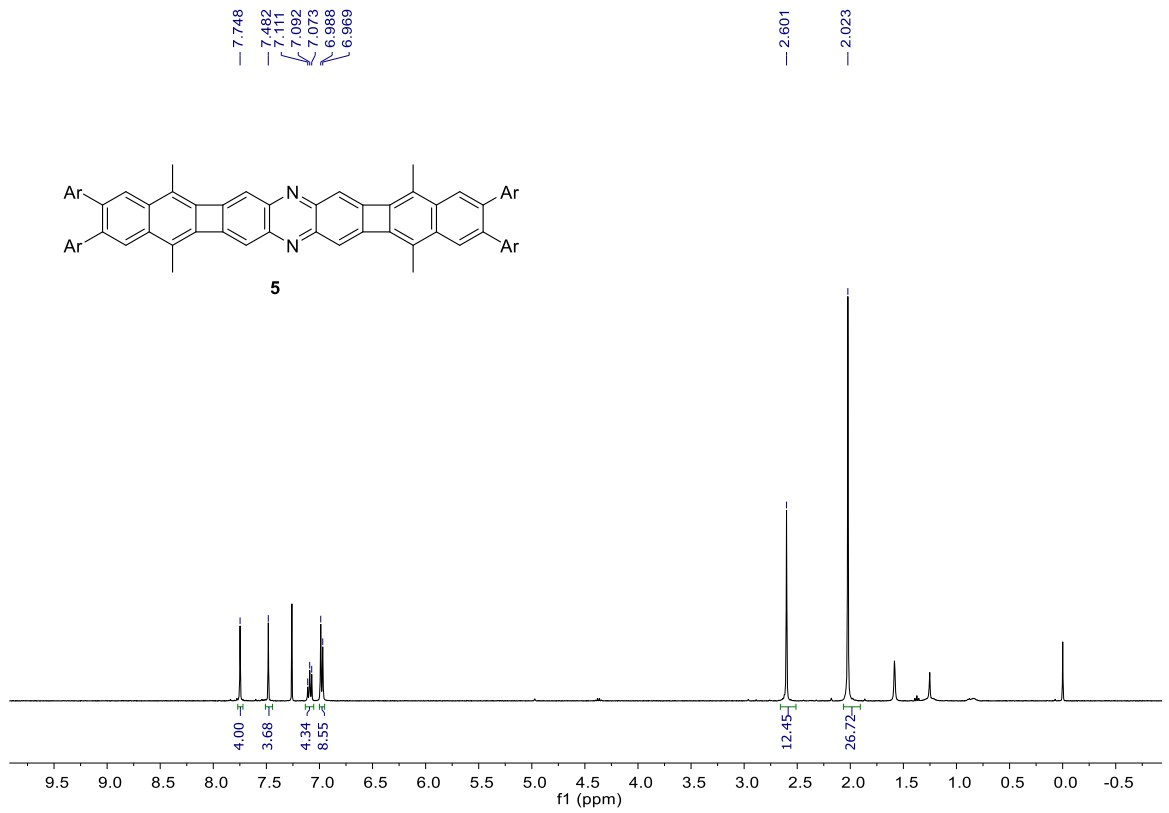
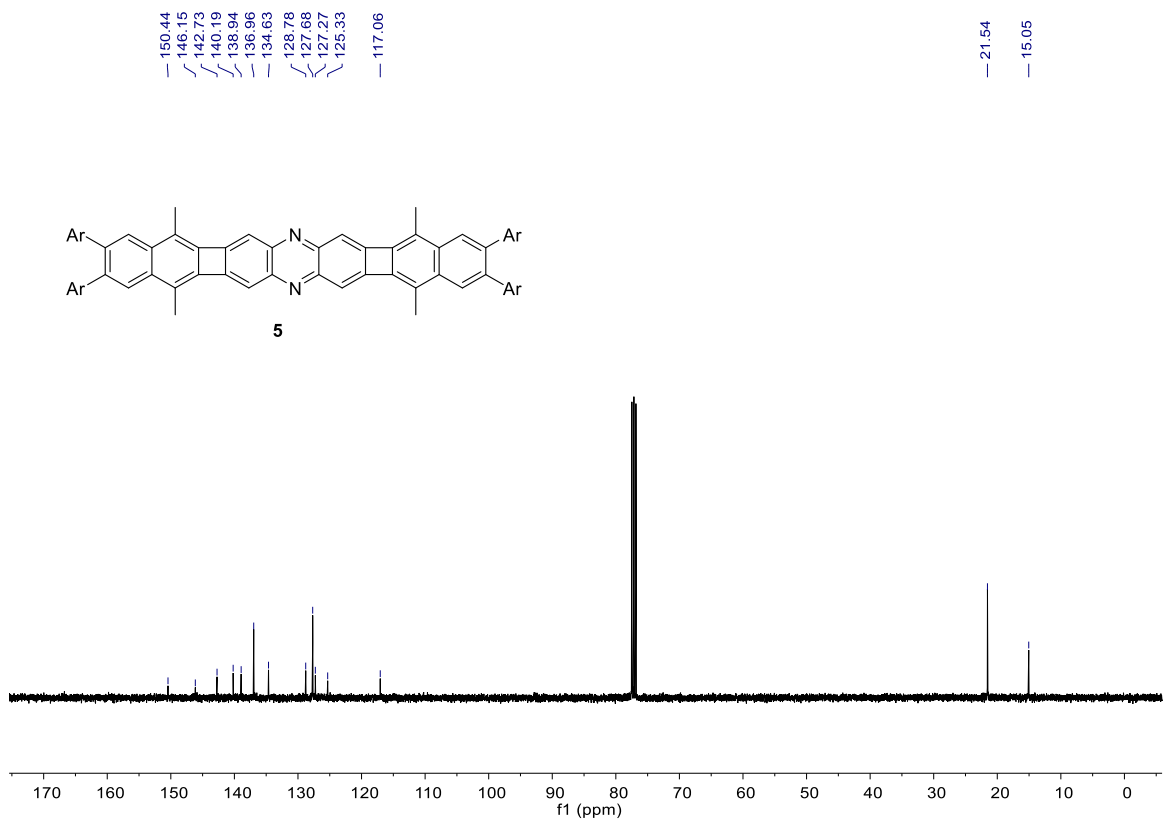
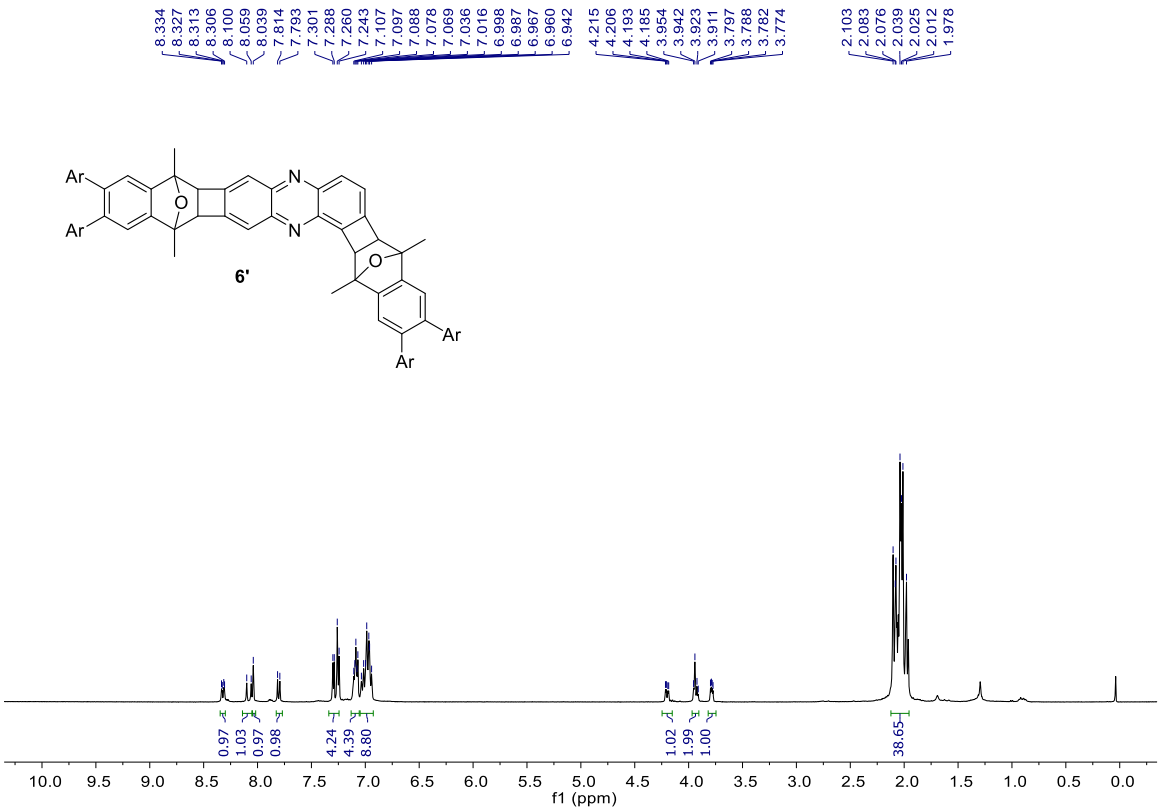
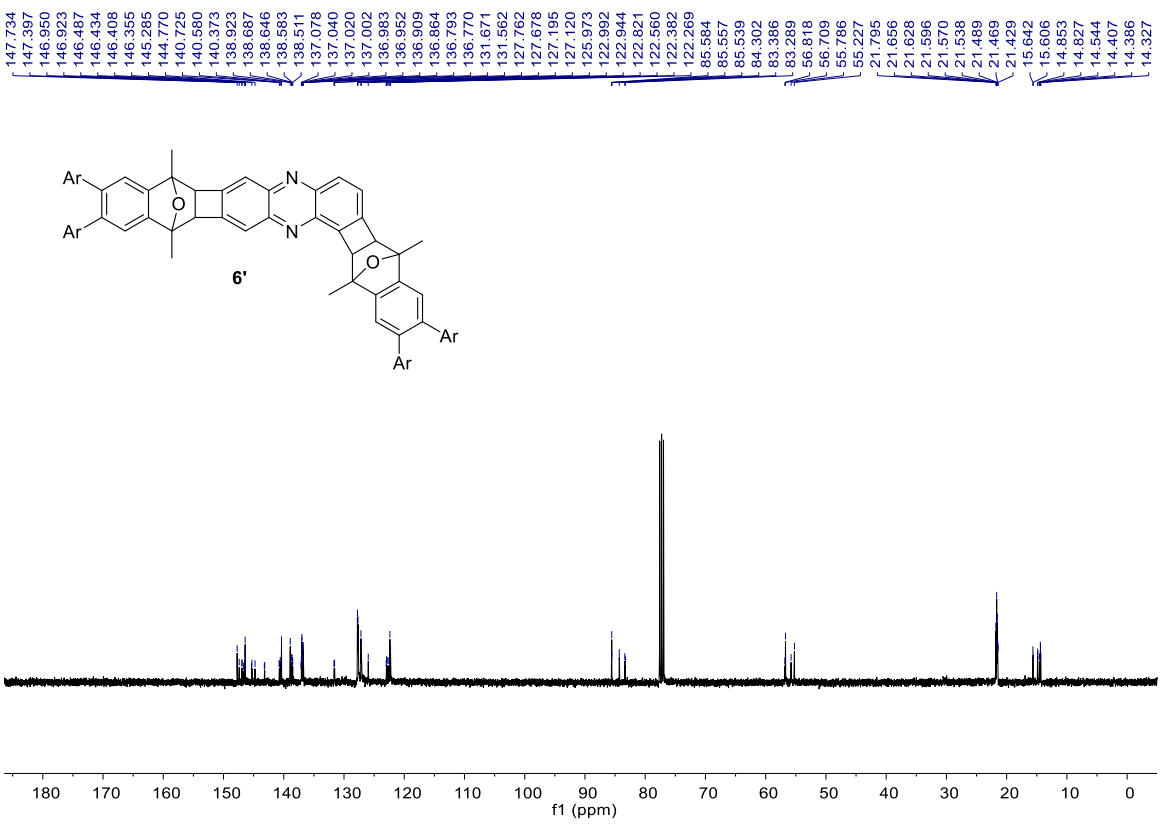
146.41
146.36
143.98
140.31
138.79
138.78
136.93
136.89
136.71
136.68
127.66
127.64
127.59
127.56
127.08
122.37
122.33
122.26
85.38
85.36
56.62
56.53
21.52
21.51
21.43
21.42
14.30
14.28
Ar
Ar
O
N
N
O
Ar
Ar
5'
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.748
7.482
7.111
7.092
7.073
6.988
6.969
2.601
2.023
Ar
Ar
N
N
Ar
Ar
5
4.00
3.68
4.34
8.55
12.45
26.72
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


150.44
146.15
142.73
140.19
138.94
136.96
134.63
128.78
127.68
127.27
125.33
117.06
21.54
15.05
Ar
Ar
N
N
Ar
Ar
5
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.334
8.327
8.313
8.306
8.100
8.059
8.039
7.814
7.793
7.301
7.288
7.260
7.243
7.107
7.097
7.088
7.078
7.069
7.036
7.016
6.998
6.987
6.967
6.960
6.942
4.215
4.206
4.193
4.185
3.954
3.942
3.923
3.911
3.797
3.788
3.782
3.774
2.103
2.083
2.076
2.039
2.025
2.012
1.978
Ar
Ar
O
N
N
O
Ar
Ar
6'
0.97
1.03
0.97
0.98
4.24
4.39
8.80
1.02
1.99
1.00
38.65
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


147.734
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146.950
146.923
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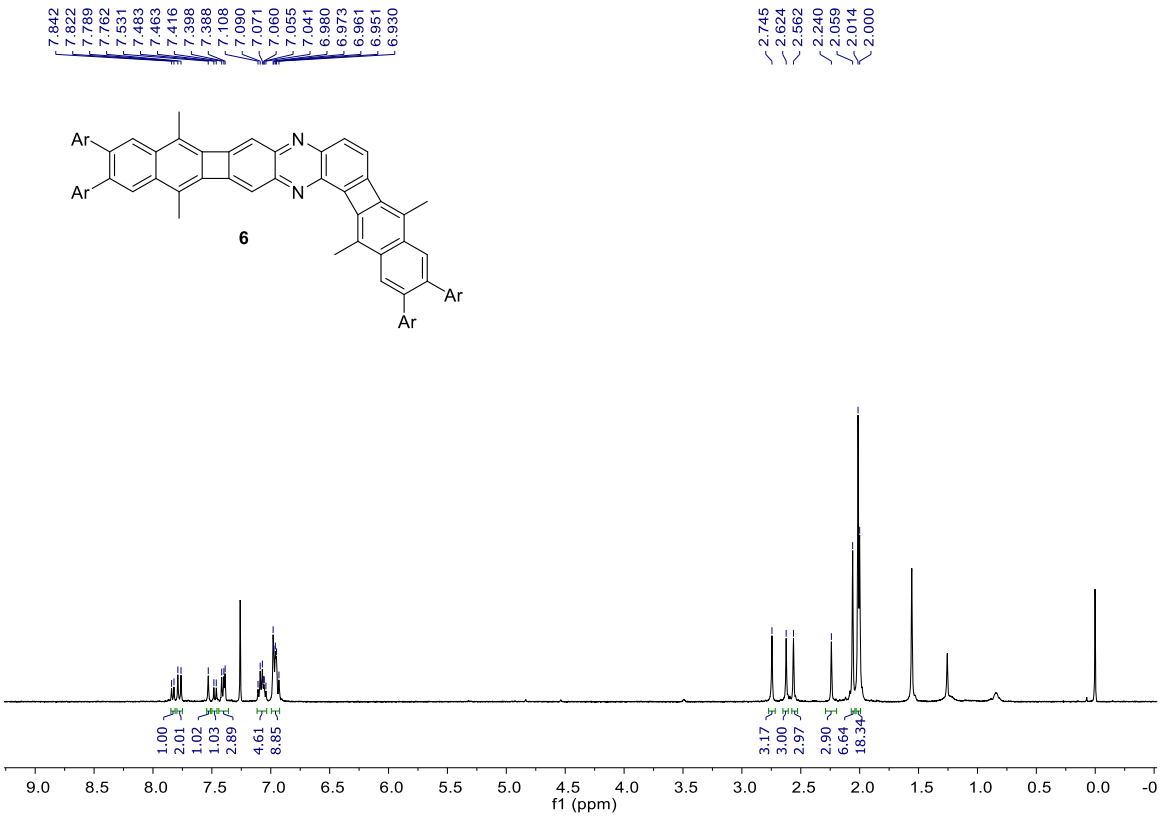
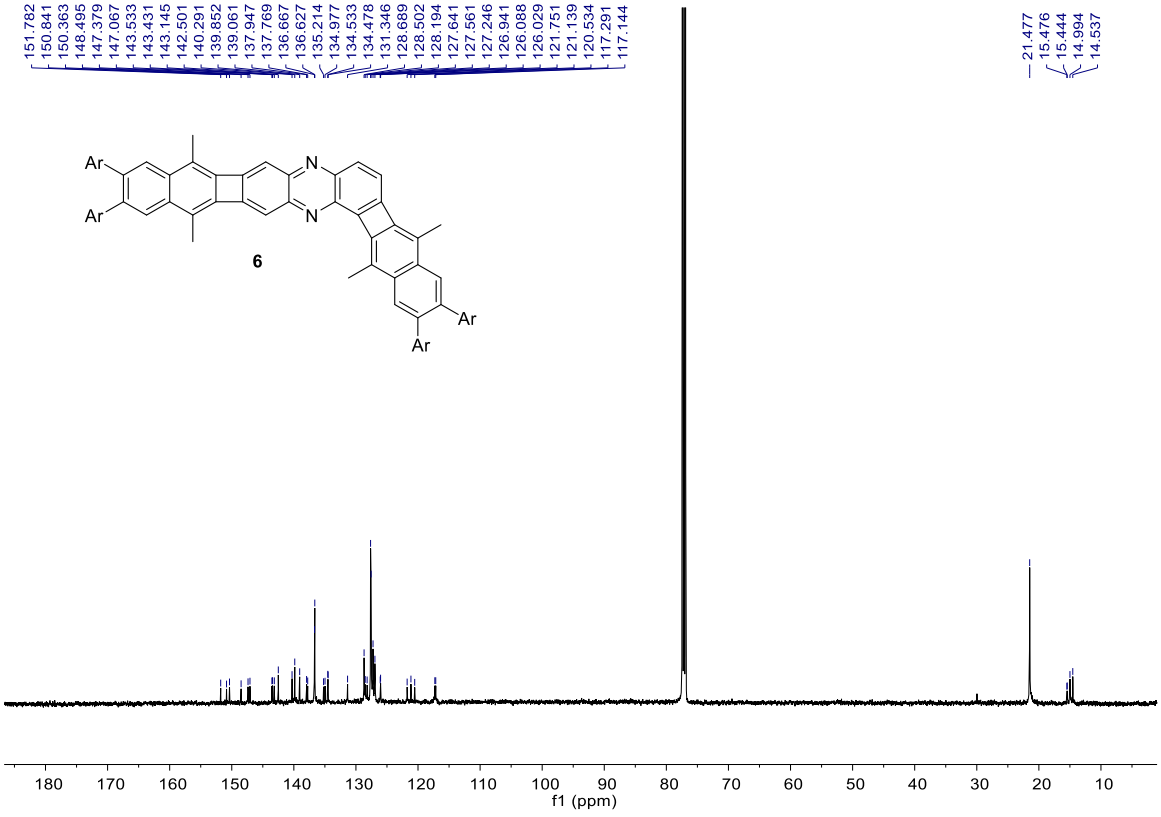
146.434
146.408
146.355
145.285
144.770
140.725
140.580
140.373
138.923
138.687
138.646
138.583
138.511
137.078
137.040
137.020
137.002
136.983
136.952
136.909
136.864
136.793
136.770
131.671
131.562
127.762
127.678
127.195
127.120
125.973
122.992
122.944
122.821
122.560
122.382
122.269
85.584
85.557
85.539
84.302
83.386
83.289
56.818
56.709
55.786
55.227
21.795
21.656
21.628
21.596
21.570
21.538
21.489
21.469
21.429
15.642
15.606
14.853
14.827
14.544
14.407
14.386
14.327
Ar
Ar
O
N
N
O
Ar
Ar
6'
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.842
7.822
7.789
7.762
7.531
7.483
7.463
7.416
7.398
7.388
7.108
7.090
7.071
7.060
7.055
7.041
6.980
6.973
6.961
6.951
6.930
2.745
2.624
2.562
2.240
2.059
2.014
2.000
Ar
Ar
N
N
6
Ar
Ar
1.00
2.01
1.02
1.03
2.89
4.61
8.85
3.17
3.00
2.97
2.90
6.64
18.34
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0
f1 (ppm)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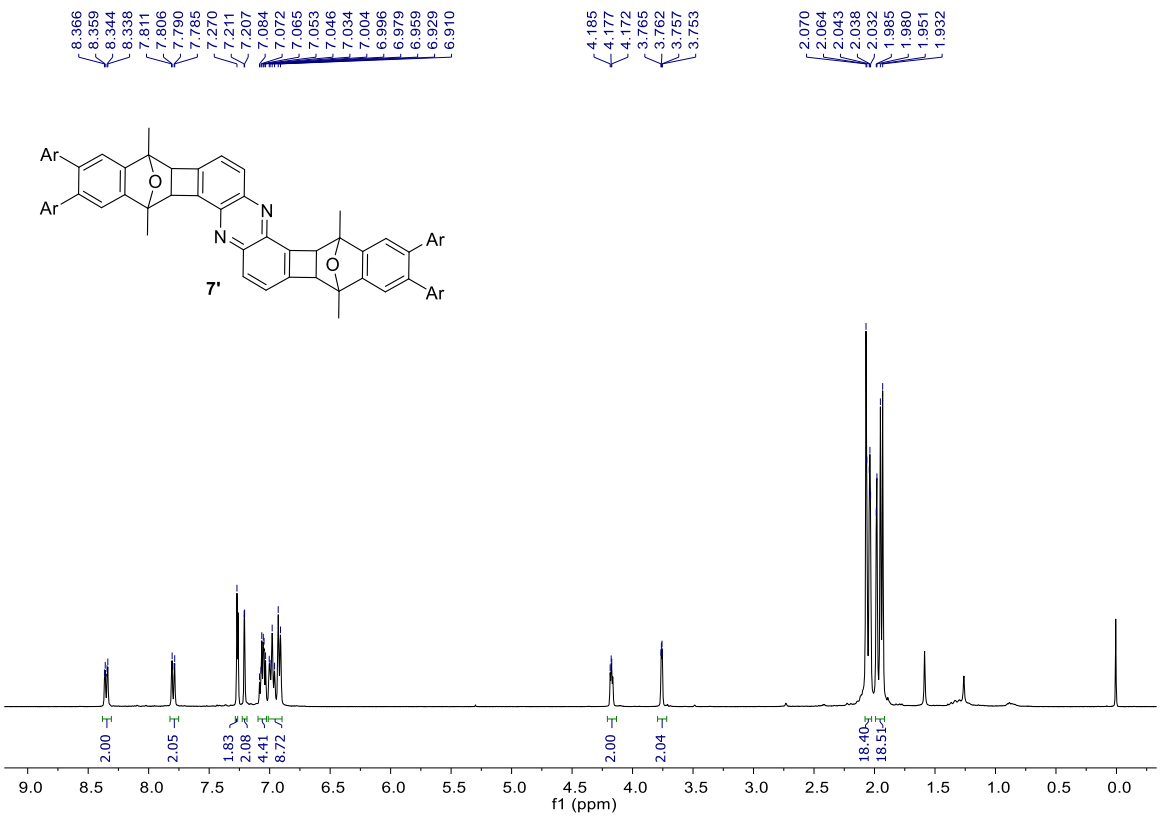
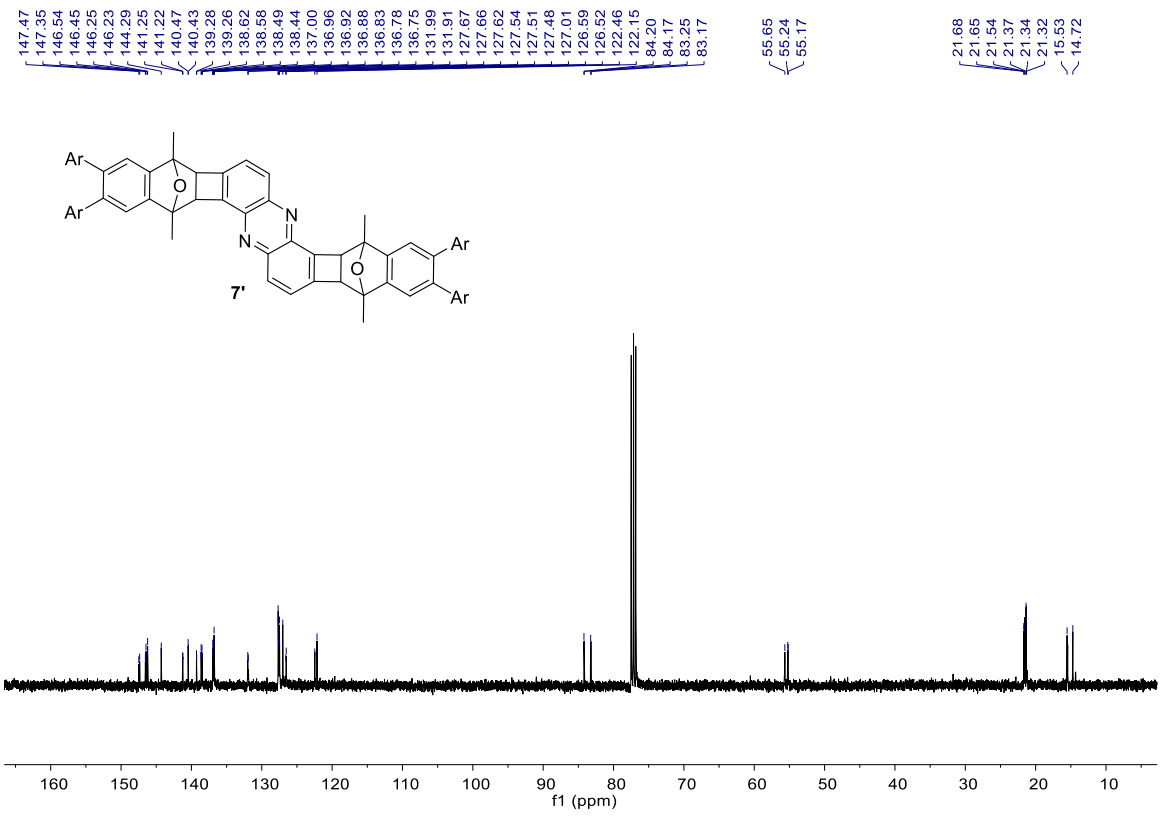
143.533
143.431
143.145
142.501
140.291
139.852
139.061
137.947
137.769
136.667
136.627
135.214
134.977
134.533
134.478
131.346
128.689
128.502
128.194
127.641
127.561
127.246
126.941
126.088
126.029
121.751
121.139
120.534
117.291
117.144
21.477
15.476
15.444
14.994
14.537
Ar
Ar
N
N
6
Ar
Ar
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


8.366
8.359
8.344
8.338
7.811
7.806
7.790
7.785
7.270
7.211
7.207
7.084
7.072
7.065
7.053
7.046
7.034
7.004
6.996
6.979
6.959
6.929
6.910
4.185
4.177
4.172
3.765
3.762
3.757
3.753
2.070
2.064
2.043
2.038
2.032
1.985
1.980
1.951
1.932
Ar
Ar
O
N
N
O
Ar
Ar
7'
2.00
2.05
1.83
2.08
4.41
8.72
2.00
2.04
18.40
18.51
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


147.47
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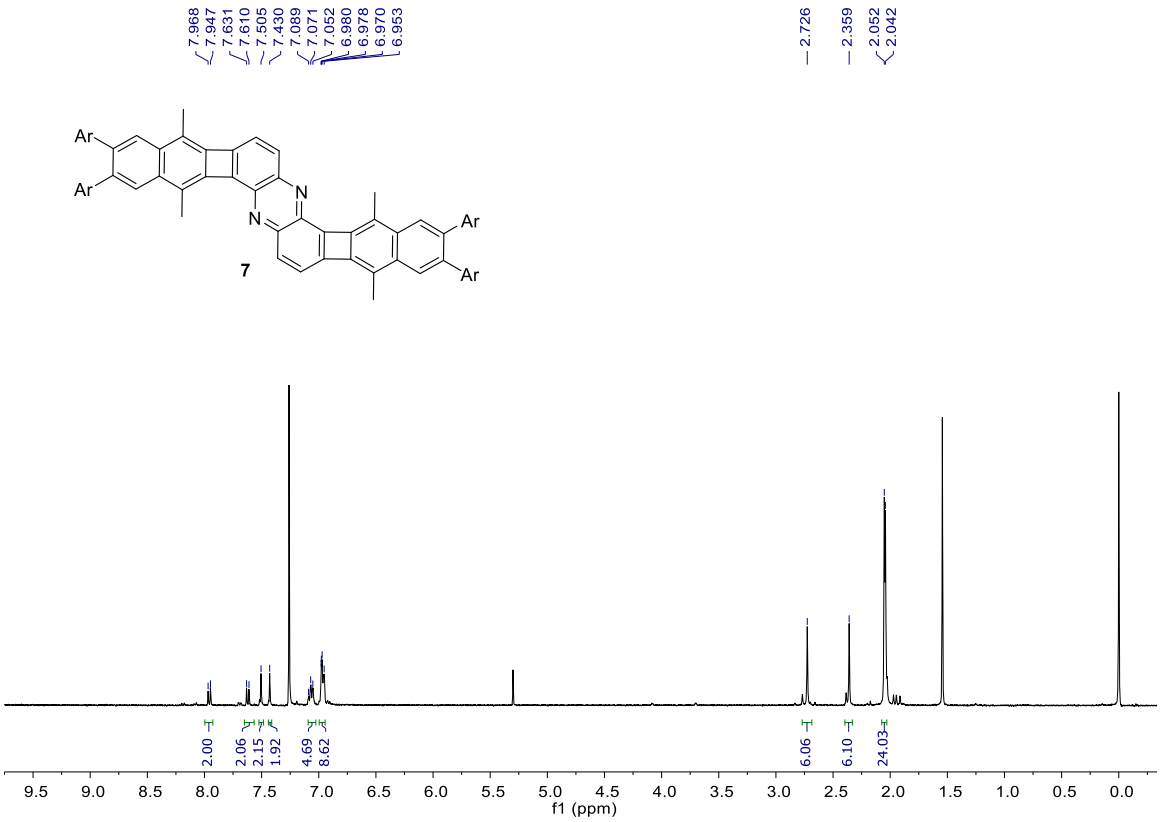
146.45
146.25
146.23
144.29
141.25
141.22
140.47
140.43
139.28
139.26
138.62
138.58
138.49
138.44
137.00
136.96
136.92
136.88
136.83
136.78
136.75
131.99
131.91
127.67
127.66
127.62
127.54
127.51
127.48
127.01
126.59
126.52
122.46
122.15
84.20
84.17
83.25
83.17
55.65
55.24
55.17
21.68
21.65
21.54
21.37
21.34
21.32
15.53
14.72
Ar
Ar
O
N
N
O
Ar
Ar
7'
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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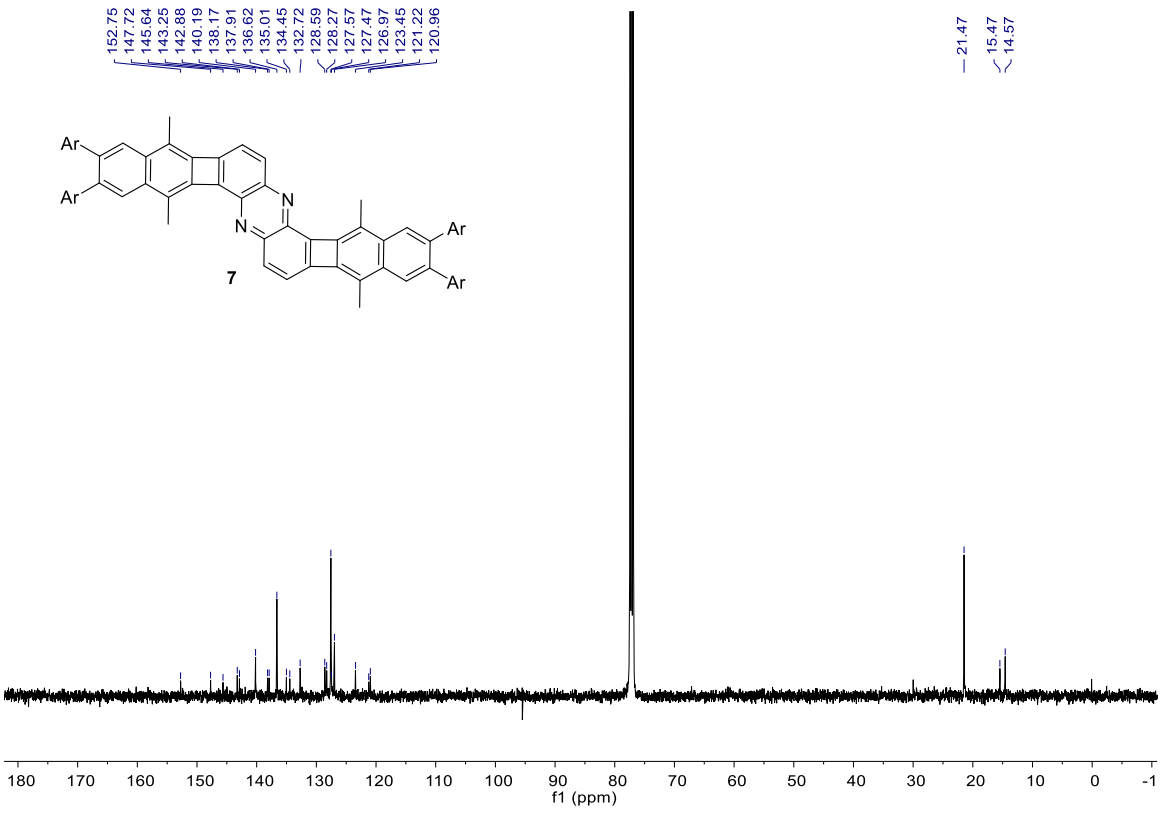
7.610
7.505
7.430
7.089
7.071
7.052
6.980
6.978
6.970
6.953
2.726
2.359
2.052
2.042
Ar
Ar
N
N
Ar
Ar
7
2.00
2.06
2.15
1.92
4.69
8.62
6.06
6.10
24.03
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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147.72
145.64
143.25
142.88
140.19
138.17
137.91
136.62
135.01
134.45
132.72
128.59
128.27
127.57
127.47
126.97
123.45
121.22
120.96
21.47
15.47
14.57
Ar
Ar
N
N
Ar
Ar
7
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)