

Supporting Information

Synthesis of Fused *N*-Bridged [3.3.1]nonadiquinoline Multicyclic Skeleton *via* Metal-Free Formal [4+2] Cycloaddition/ Mannich/ Dearomatization Domino Reaction

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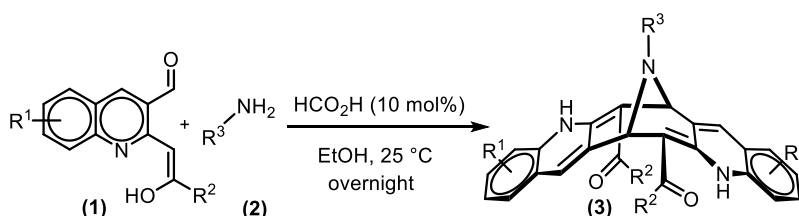
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General Information

All reagents were purchased from commercials including TCI, Alfa Aesar, and Sigma-Aldrich (Merck), and were used without further purification. Melting points (m.p.) were determined in capillary tubes with an Electrothermal 9100 digital melting point apparatus and are uncorrected. All experiments were monitored by thin layer chromatography (TLC Silica Gel 60 F₂₅₄) plate was visualized under UV light at 254 nm for UV active materials. All ¹H NMR and ¹³C NMR spectra were recorded using 400, 300, and 250 MHz Bruker spectrometers. The chemical shifts (δ) were reported in parts per million (ppm) and also coupling constants (J) are reported in Hertz (Hz). Multiplicities are indicated as s = singlet, br s = broad singlet, d = doublet, t = triplet, q = quartet, m = multiplet. High-resolution ESI-MS (HRMS-ESI) data were obtained using a Waters LCT Premier XE™ TOF (Time of Flight) mass spectrometer in positive ionization mode. Merck silica gel 60® (230-400 mesh) was used for column chromatography. Single-crystal X-ray diffraction data were collected on a Bruker APEX-II Quazar area detector at room temperature. The ratio of the products was determined by the analytical HPLC (Rigol L3400 Column Aven).

General procedure for the synthesis of fused azabicyclo[3.3.1]nonadiquinoline skeletons (3a-ag)



To a round bottom flask, a solution of enolized-*o*-alkenylquinoline carbaldehyde¹ **1** (0.2 mmol) and amine **2** (0.1 mmol) in EtOH (2.0 mL) was added formic acid (10 mol%) at 25 °C overnight. After the completion of the reactions (monitored by TLC), the solution was then concentrated under reduced pressure and the resulting residue was purified by column chromatography on silica gel (*n*-hexane/ethyl acetate) to obtain the desired product **3a-ag**.

Procedure for the scale-up reaction for the synthesis of compound 3a:

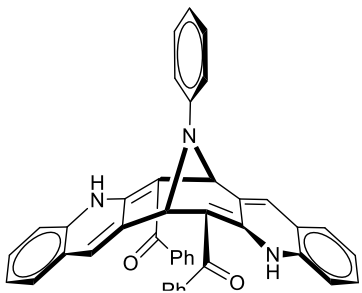
Supporting Information

To a round bottom flask, a solution of (Z)-2-(2-hydroxy-2-phenylvinyl)quinoline-3-carbaldehyde **1a** (4 mmol, 2 equiv.) and aniline **2a** (2 mmol, 1 equiv.) in EtOH (20.0 mL) was added formic acid (10 mol%) at 25 °C overnight. After the completion of the reactions (monitored by TLC), the solution was then concentrated under reduced pressure, and the resulting residue was purified by column chromatography on silica gel (*n*-hexane/ethyl acetate= 3/1) to obtain the desired product **3a** (80%).

Procedure for the synthesis of the asymmetric structural product compound

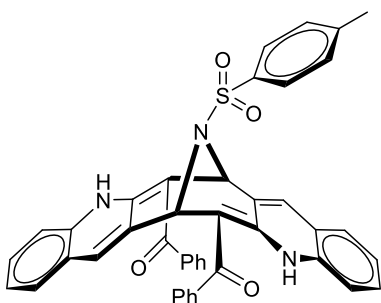
To a round bottom flask, a solution of (Z)-2-(2-hydroxy-2-phenylvinyl)-6-isopropylquinoline-3-carbaldehyde (0.1 mmol), (Z)-2-(2-hydroxy-2-phenylvinyl)quinoline-3-carbaldehyde (0.1 mmol) and 4-fluoroaniline (0.1 mmol) in EtOH (2.0 mL) was added formic acid (10 mol%) at 25 °C overnight. After the completion of the reactions (monitored by TLC), the solution was then concentrated under reduced pressure, but the products were not separated by column chromatography, because of their similar polarity. Therefore, the type, and ratio of the products were determined by the analytical HPLC chromatogram and Mass spectrometry. At first, the crud of the reaction was characterized by Mass and analytical HPLC techniques. Subsequently, analytical HPLC yielded three fractions, and the chemical structure of the purified compounds was determined by mass spectrometry. Based on the obtained results, the yield of the desired product **3ah** was 37%.

((7R,15S)-17-Phenyl-5,7,13,15-tetrahydro-7,15-epiminocycloocta[1,2-b:5,6-b']diquinoline-6,14-diyl)bis(phenylmethanone) (3a)



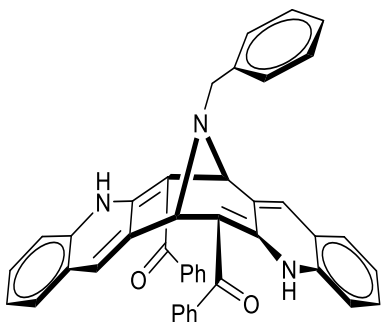
Yellow solid (56 mg, Yield 92%, m.p. 195-198 °C), (*n*-hexane/EtOAc = 3:1, R_f = 0.3); ¹H NMR (400 MHz, CDCl₃) δ 7.71 – 7.61 (m, 7H), 7.56 – 7.45 (m, 7H), 7.40 (d, *J* = 8.2 Hz, 2H), 7.31 (t, *J* = 8.2 Hz, 2H), 7.23 (t, *J* = 7.5 Hz, 2H), 7.19 – 7.13 (m, 4H), 6.92 (t, *J* = 7.8 Hz, 1H), 6.15 (s, 2H), 6.01 (s, 2H); ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 187.6, 150.1, 148.5, 141.8, 136.1, 130.6, 130.5, 130.4, 129.4, 129.1, 129.0, 127.3, 127.2, 124.0, 122.9, 120.9, 118.1, 117.9, 99.3, 56.1; HRMS-ESI (*m/z*): [M + H]⁺ calcd for C₄₂H₂₉N₃O₂ 608.2330; found: 608.2334.

((7S)-17-Tosyl-5,7,13,15-tetrahydro-7,15-epiminocycloocta[1,2-b:5,6-b']diquinoline-6,14-diyl)bis(phenylmethanone) (3b)



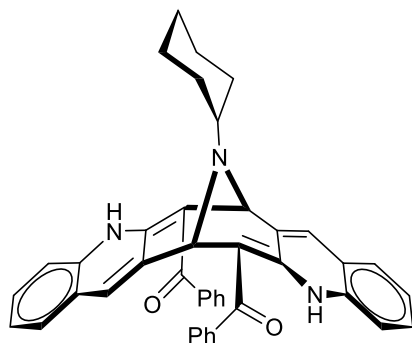
Yellow solid (50 mg, Yield 73%, m.p. 227-231 °C), (*n*-hexane/EtOAc = 3:1, R_f = 0.3); ¹H NMR (250 MHz, CDCl₃) δ 7.68 – 7.51 (m, 9H), 7.51 – 7.43 (m, 5H), 7.42 (s, 1H), 7.38 (s, 1H), 7.15 (d, *J* = 2.8 Hz, 1H), 7.12 (d, *J* = 2.7 Hz, 1H), 7.09 – 6.97 (m, 3H), 6.96 (s, 1H), 6.55 (d, *J* = 2.7 Hz, 2H), 6.09 (s, 2H), 6.00 (s, 2H), 1.25 (s, 3H). ¹³C{¹H} NMR (63 MHz, CDCl₃) δ 182.0, 156.4, 149.5, 145.2, 141.0, 132.4, 131.0, 130.4, 129.0, 127.5, 124.4, 122.3, 120.8, 120.1, 120.0, 116.1, 115.7, 107.5, 99.6, 56.9, 29.7.; HRMS-ESI (*m/z*): [M + H]⁺ calcd for C₄₃H₃₁N₃O₄S 686.2114; found: 686.2122.

((7R,15S)-17B-5,7,13,15-Tetrahydro-7,15-epiminocycloocta[1,2-b:5,6-b']diquinoline-6,14-diyl)bis(phenylmethanone) (3c)



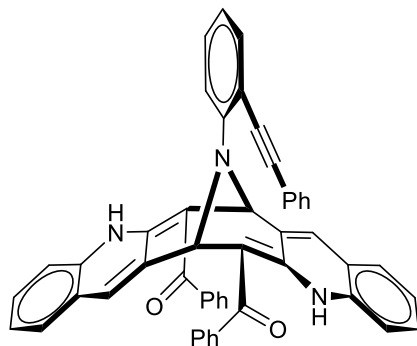
Yellow solid (49 mg, Yield 79%, m.p. 314-317 °C), (*n*-hexane/EtOAc = 3:1, R_f = 0.3); ¹H NMR (250 MHz, CDCl₃) δ 7.49 – 7.36 (m, 18H), 7.24 – 7.10 (m, 7H), 5.94 (s, 2H), 5.26 (s, 2H), 3.92 – 3.70 (m, 2H). ¹³C{¹H} NMR (63 MHz, CDCl₃) δ 187.7, 150.0, 141.5, 138.0, 137.6, 136.3, 130.8, 130.4, 130.0, 129.3, 128.9, 128.6, 127.7, 127.4, 127.2, 123.9, 123.1, 118.0, 98.8, 56.4, 29.7.; HRMS-ESI (*m/z*): [M + H]⁺ calcd for C₄₃H₃₁N₃O₂ 622.2495; found: 622.2507.

((7R,15S)-17-Cyclohexyl-5,7,13,15-tetrahydro-7,15-epiminocycloocta[1,2-b:5,6-b']diquinoline-6,14-diyl)bis(phenylmethanone) (3d)



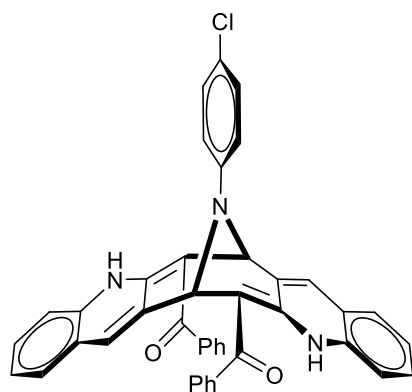
Yellow solid (49 mg, Yield 81%, m.p. 212-215 °C), (*n*-hexane/EtOAc = 4:1, R_f = 0.3); ¹H NMR (300 MHz, CDCl₃) δ 7.75-7.55 (m, 7H), 7.54-7.35 (m, 9H), 7.23 (t, *J* = 7.4 Hz, 2H), 7.16 (d, *J* = 7.5 Hz, 2H), 5.93 (br s, 2H), 5.58 (br s, 2H), 2.48-2.37 (m, 1H), 2.34-2.24 (m, 1H), 2.03 – 1.90 (m, 2H), 1.87 – 1.78 (m, 1H), 1.72-1.61 (m, 1H), 1.48 – 1.34 (m, 2H), 1.28-1.16 (m, 1H), 0.96 – 0.86 (m, 2H).; ¹³C{¹H} NMR (76 MHz, CDCl₃) δ 188.3, 150.3, 142.1, 136.1, 130.8, 130.3, 130.2, 129.0, 128.9, 127.3, 127.2, 123.8, 123.0, 117.8, 99.0, 56.4, 53.5, 31.5, 30.6, 25.9, 25.2, 25.1; HRMS-ESI (*m/z*): [M + H]⁺ calcd for C₄₂H₃₆N₃O₂ 614.2805; found: 614.2808.

((7R,15S)-17-(2-(phenylethynyl)phenyl)-5,7,13,15-tetrahydro-7,15-epiminocycloocta[1,2-b:5,6-b']diquinoline-6,14-diyl)bis(phenylmethanone) (3e)



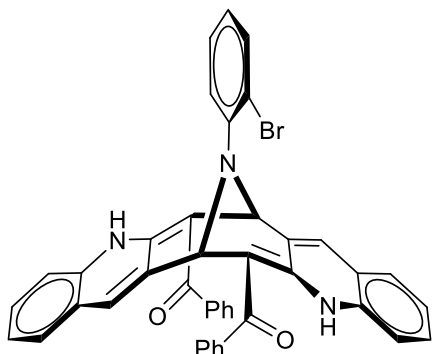
Yellow solid (53 mg, Yield 75%, m.p. 269-271 °C), (*n*-hexane/EtOAc = 3:1, R_f = 0.3); ¹H NMR (300 MHz, CDCl₃) δ 7.56 (d, *J* = 7.6 Hz, 1H), 7.49 – 7.41 (m, 7H), 7.40 – 7.31 (m, 8H), 7.23 – 7.02 (m, 9H), 6.99 – 6.94 (m, 3H), 6.89 (d, *J* = 8.2 Hz, 1H), 6.28 (s, 2H), 5.77 (s, 2H); ¹³C NMR (75 MHz, CDCl₃) δ 187.4, 151.1, 150.2, 141.7, 136.2, 134.5, 131.6, 131.4, 131.0, 130.4, 130.1, 129.6, 128.9, 128.8, 128.2, 128.1, 127.4, 127.3, 123.9, 123.2, 122.9, 122.2, 119.1, 118.0, 116.8, 99.8, 95.9, 88.1, 56.7; HRMS-ESI (*m/z*): [M + H]⁺ calcd for C₅₀H₃₃N₃O₂ 708.2645; found: 708.2646.

((7R,15S)-17-(4-Chlorophenyl)-5,7,13,15-tetrahydro-7,15-epiminocycloocta[1,2-b:5,6-b']diquinoline-6,14-diyl)bis(phenylmethanone) (3f)



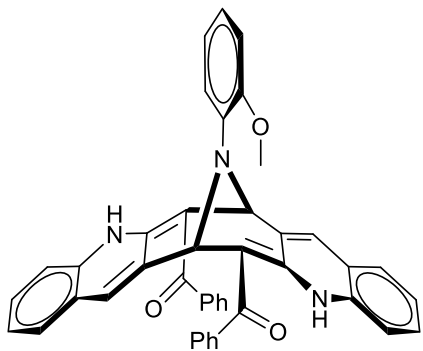
Yellow solid (58 mg, Yield 91%, m.p. 216-219 °C), (*n*-hexane/EtOAc = 3:1, R_f = 0.3); ¹H NMR (300 MHz, CDCl₃) δ 7.77 – 7.60 (m, 7H), 7.57 – 7.45 (m, 7H), 7.41 (d, *J* = 8.2 Hz, 2H), 7.31 – 7.22 (m, 4H), 7.18 (d, *J* = 7.8 Hz, 2H), 7.08 (d, *J* = 8.2 Hz, 2H), 6.08 (s, 2H), 6.01 (s, 2H); ¹³C{¹H} NMR (75 MHz, CDCl₃) δ 187.7, 149.9, 147.3, 141.8, 136.1, 130.7, 130.5, 130.1, 129.4, 129.2, 129.1, 127.4, 127.2, 125.8, 124.1, 122.8, 119.4, 118.0, 99.1, 56.3; HRMS-ESI (*m/z*): [M + H]⁺ calcd for C₄₂H₂₈³⁵ClN₃O₂ 642.1947; found: 642.1947.

((7R,15S)-17-(2-Bromophenyl)-5,7,13,15-tetrahydro-7,15-epiminocycloocta[1,2-b:5,6-b']diquinoline-6,14-diyl)bis(phenylmethanone) (3g)



Yellow solid (52 mg, Yield 77%, m.p. 318-320 °C), (*n*-hexane/EtOAc = 3:1, R_f = 0.3); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.67 (d, J = 8.0 Hz, 1H), 7.64-7.54 (m, 7H), 7.53 – 7.40 (m, 9H), 7.37 (d, J = 8.0 Hz, 1H), 7.23 (t, J = 8.1 Hz, 2H), 7.18 (t, J = 8.1 Hz, 1H), 7.12 (d, J = 8.4 Hz, 2H), 6.95 (t, J = 7.6 Hz, 1H), 5.92 (s, 2H), 5.84 (s, 2H); $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 187.3, 162.7, 150.3, 147.9, 141.6, 136.1, 134.1, 130.5, 130.0, 129.0, 128.9, 128.5, 127.4, 127.3, 124.9, 124.0, 122.9, 122.5, 120.1, 118.0, 99.6, 57.2; HRMS-ESI (m/z): $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{42}\text{H}_{29}^{79}\text{BrN}_3\text{O}_2$ 686.1563; found: 686.1563.

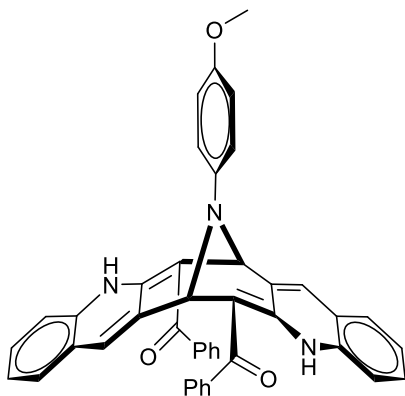
((7R,15S)-17-(2-Methoxyphenyl)-5,7,13,15-tetrahydro-7,15-epiminocycloocta[1,2-b:5,6-b']diquinoline-6,14-diyl)bis(phenylmethanone) (3h)



found: 638.2441.

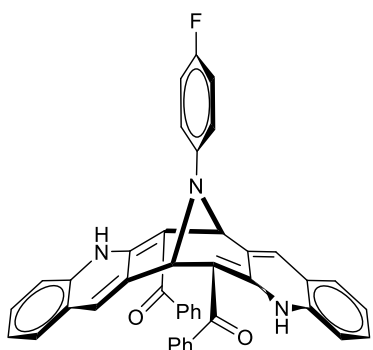
Yellow solid (53 mg, Yield 84%, m.p. 307-309 °C), (*n*-hexane/EtOAc = 3:1, R_f = 0.3); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.67 – 7.56 (m, 7H), 7.55 – 7.43 (m, 7H), 7.40 (d, J = 8.2 Hz, 2H), 7.32 (d, J = 7.9 Hz, 1H), 7.20 (t, J = 7.5 Hz, 2H), 7.11 (d, J = 8.0 Hz, 2H), 7.04 (t, J = 7.8 Hz, 1H), 6.97 (d, J = 8.1 Hz, 1H), 6.87 (t, J = 7.6 Hz, 1H), 6.13 (s, 2H), 5.88 (s, 2H), 4.06 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 187.5, 152.0, 150.0, 141.9, 138.0, 136.1, 131.0, 130.3, 130.1, 129.0, 128.7, 127.4, 127.3, 123.8, 123.4, 123.0, 121.1, 119.8, 117.8, 111.1, 99.8, 55.9, 55.5; HRMS-ESI (m/z): $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{43}\text{H}_{32}\text{N}_3\text{O}_3$ 638.2440;

((7R,15S)-17-(4-Methoxyphenyl)-5,7,13,15-tetrahydro-7,15-epiminocycloocta[1,2-b:5,6-b']diquinoline-6,14-diyl)bis(phenylmethanone) (3i)



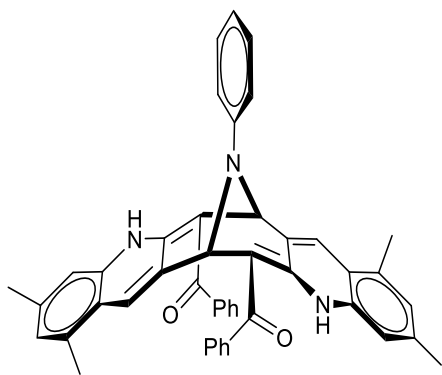
Yellow solid (55 mg, Yield 87%, m.p. 302-306 °C), (*n*-hexane/EtOAc = 3:1, R_f = 0.3); $^1\text{H NMR}$ (250 MHz, CDCl_3) δ 7.66 – 7.55 (m, 7H), 7.54 – 7.37 (m, 8H), 7.22 – 7.05 (m, 7H), 6.84 (s, 1H), 6.81 (s, 1H), 5.96 (s, 4H), 3.73 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (63 MHz, CDCl_3) δ 187.5, 150.1, 148.5, 142.5, 141.8, 136.2, 130.7, 130.4, 130.2, 129.0, 127.8, 127.2, 123.9, 122.9, 120.0, 118.0, 115.9, 114.6, 99.4, 56.9, 55.5; HRMS-ESI (m/z): $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{43}\text{H}_{31}\text{N}_3\text{O}_3$ 638.2444; found: 638.2435.

((7R,15S)-17-(4-Fluorophenyl)-5,7,13,15-tetrahydro-7,15-epiminocycloocta[1,2-b:5,6-b']diquinoline-6,14-diyl)bis(phenylmethanone) (3j)



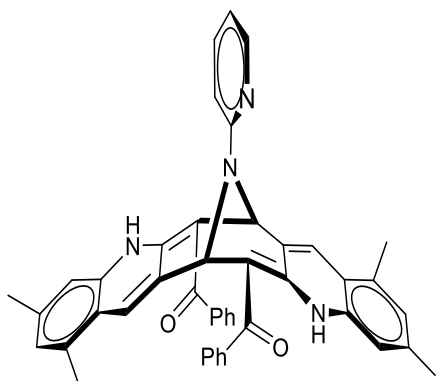
Yellow solid (50 mg, Yield 81%, m.p. 219-221 °C), (*n*-hexane/EtOAc = 3:1, $R_f = 0.3$); $^1\text{H NMR}$ (300 MHz, DMSO- d_6) δ 7.83-7.61 (m, 9H), 7.59-7.51 (m, 4H), 7.50-7.37 (m, 5H), 7.33-7.25 (m, 2H), 7.24-7.08 (m, 4H), 5.96 (s, 2H), 5.76 (s, 2H); $^{13}\text{C}\{^1\text{H}\}$ NMR (76 MHz, DMSO- d_6) δ 186.9, 158.6, 155.5 ($^1J_{\text{C-F}} = 240.0$ Hz), 149.6, 145.2, 141.4, 136.3, 131.3, 130.2, 129.8, 129.7, 127.6, 127.4, 124.8, 122.4, 120.0, 119.9, 118.7, 116.6, 116.3 ($^2J_{\text{C-F}} = 21.8$ Hz), 99.0, 56.2; **HRMS-ESI** (m/z): $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{42}\text{H}_{29}\text{FN}_3\text{O}_2$ 626.5152; found: 626.5156.

((7R,15S)-1,3,9,11-Tetramethyl-17-phenyl-5,7,13,15-tetrahydro-7,15-epiminocycloocta[1,2-b:5,6-b']diquinoline-6,14-diyl)bis(phenylmethanone) (3k)



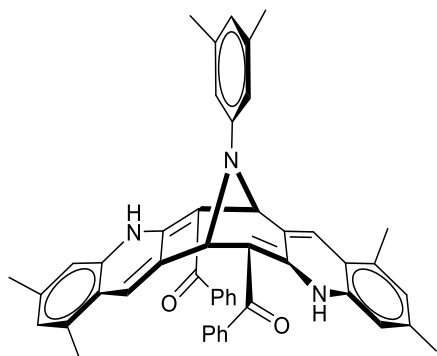
Yellow solid (61 mg, Yield 93%, m.p. 286-288 °C), (*n*-hexane/EtOAc = 3:1, $R_f = 0.3$); $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.70 – 7.52 (m, 11H), 7.33 (t, $J = 8.7$ Hz, 2H), 7.14 (d, $J = 8.2$ Hz, 2H), 7.07 (br s, 2H), 6.94 (d, $J = 7.4$ Hz, 1H), 6.91 (br s, 2H), 6.69 (s, 2H), 6.24 (s, 2H), 2.39 (s, 6H), 2.24 (s, 6H); $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 185.8, 149.9, 148.9, 142.0, 141.0, 136.6, 134.5, 130.1, 129.3, 129.1, 129.0, 127.4, 127.2, 127.1, 120.8, 120.3, 118.4, 116.0, 99.8, 56.3, 21.7, 18.3; **HRMS-ESI** (m/z): $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{46}\text{H}_{38}\text{N}_3\text{O}_2$ 664.3248; found: 664.3248.

((7R,15S)-1,3,9,11-Tetramethyl-17-(pyridin-2-yl)-5,7,13,15-tetrahydro-7,15-epiminocycloocta[1,2-b:5,6-b']diquinoline-6,14-diyl)bis(phenylmethanone) (3l)



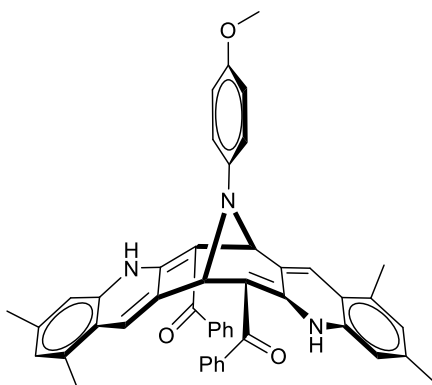
Yellow solid (45 mg, Yield 68%, m.p. 229-231 °C), (*n*-hexane/EtOAc = 3:1, $R_f = 0.3$); $^1\text{H NMR}$ (300 MHz, CDCl_3) δ 8.43 (d, $J = 6.0$ Hz, 1H), 7.96-7.77 (m, 5H), 7.74-7.65 (m, 5H), 7.63-7.54 (m, 3H), 7.07 (br s, 2H), 7.01 (s, 2H), 6.90 (br s, 2H), 6.81 (d, $J = 8.5$ Hz, 1H), 6.74 (d, $J = 8.4$ Hz, 1H), 6.72 (s, 2H), 2.39 (s, 6H), 2.23 (s, 6H); $^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, CDCl_3) δ 186.1, 162.9, 157.4, 150.1, 148.5, 142.0, 141.0, 137.9, 136.6, 134.6, 129.9, 129.1, 127.7, 127.5, 127.1, 120.2, 116.0, 114.4, 108.3, 100.1, 52.3, 21.7, 18.3; **HRMS-ESI** (m/z): $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{45}\text{H}_{37}\text{N}_4\text{O}_2$ 665.2905; found: 665.2906.

((7R,15S)-17-(3,5-Dimethylphenyl)-1,3,9,11-tetramethyl-5,7,13,15-tetrahydro-7,15-epiminocycloocta[1,2-b:5,6-b']diquinoline-6,14-diyl)bis(phenylmethanone) (3m)



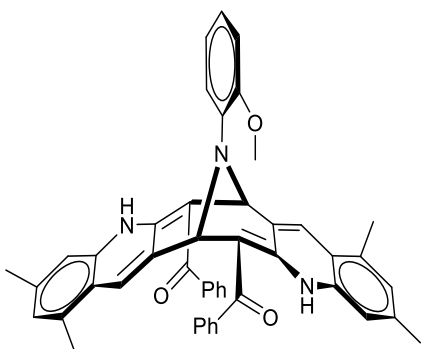
Yellow solid (65 mg, Yield 95%, m.p. 273-275 °C), (*n*-hexane/EtOAc = 4:1, R_f = 0.3); ¹H NMR (300 MHz, CDCl₃) δ 7.92-7.39 (m 12H), 7.08 (s, 2H), 6.92 (s, 2H), 6.79 (s, 2H), 6.73 (s, 2H), 6.61 (s, 1H), 6.24 (s, 2H), 2.41 (s, 6H), 2.34 (s, 6H), 2.27 (s, 6H); ¹³C{¹H} NMR (75 MHz, CDCl₃) δ 185.66, 150.05, 148.9, 142.1, 140.8, 138.8, 136.7, 134.5, 130.4, 129.0 (2C), 127.3 (2C), 127.0, 122.6, 120.3, 116.2, 116.0, 100.1, 56.2, 21.8, 21.7, 18.3; HRMS-ESI (*m/z*): [M + H]⁺ calcd for C₄₈H₄₂N₃O₂ 692.2114; found: 692.2117.

((7R,15S)-17-(4-Methoxyphenyl)-1,3,9,11-tetramethyl-5,7,13,15-tetrahydro-7,15-epiminocycloocta[1,2-b:5,6-b']diquinoline-6,14-diyl)bis(phenylmethanone) (3n)



Yellow solid (62 mg, Yield 90%, m.p. 199-201 °C), (*n*-hexane/EtOAc = 3:1, R_f = 0.3); ¹H NMR (300 MHz, CDCl₃) δ 7.99 – 7.33 (m, 12H), 7.13 (d, *J* = 8.6 Hz, 2H), 7.08 (br s, 2H), 6.91 (br s, 2H), 6.89 (d, *J* = 8.4 Hz, 2H), 6.67 (s, 2H), 6.10 (s, 2H), 3.79 (s, 3H), 2.40 (s, 6H), 2.24 (s, 6H); ¹³C{¹H} NMR (75 MHz, CDCl₃) δ 185.7, 154.3, 149.9, 142.9, 142.0, 140.8, 136.7, 134.5, 130.3, 129.0, 128.9, 127.3, 127.2, 127.0, 120.4, 120.3, 116.0, 114.5, 99.8, 57.1, 55.5, 21.7, 18.3; HRMS-ESI (*m/z*): [M + H]⁺ calcd for C₄₇H₄₀N₃O₃ 694.3060; found: 694.3062.

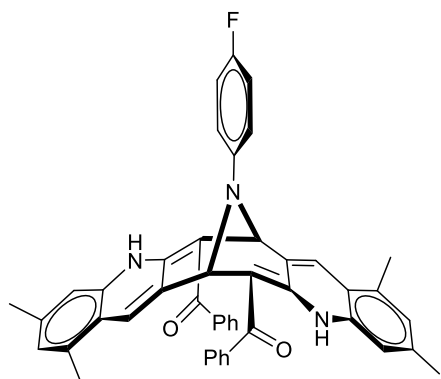
((7R,15S)-17-(2-Methoxyphenyl)-1,3,9,11-tetramethyl-5,7,13,15-tetrahydro-7,15-epiminocycloocta[1,2-b:5,6-b']diquinoline-6,14-diyl)bis(phenylmethanone) (3o)



found: 694.3058.

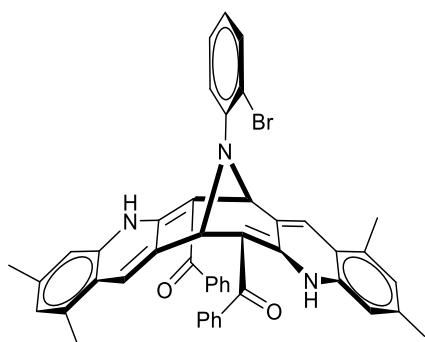
Yellow solid (57 mg, Yield 83%, m.p. 308-310 °C), (*n*-hexane/EtOAc = 3:1, R_f = 0.3); ¹H NMR (400 MHz, CDCl₃) δ 7.65 – 7.47 (m, 12H), 7.31 (d, *J* = 7.9 Hz, 1H), 7.07 (br s, 2H), 7.03 (d, *J* = 7.9 Hz, 1H), 6.99 (d, *J* = 8.0 Hz, 1H), 6.87 (br s, 2H), 6.84 (d, *J* = 8.0 Hz, 1H), 6.51 (s, 2H), 6.19 (s, 2H), 4.05 (s, 3H), 2.38 (s, 6H), 2.16 (s, 6H); ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 185.7, 152.2, 149.8, 142.2, 140.6, 138.5, 136.6, 134.5, 130.5, 128.9, 128.8, 127.3, 127.0, 126.9, 123.3, 121.0, 120.3, 120.1, 115.9, 110.9, 100.2, 56.1, 55.5, 21.7, 18.2; HRMS-ESI (*m/z*): [M + H]⁺ calcd for C₄₇H₄₀N₃O₃ 694.3063;

((7R,15S)-17-(4-Fluorophenyl)-1,3,9,11-tetramethyl-5,7,13,15-tetrahydro-7,15-epimino cycloocta[1,2-b:5,6-b']diquinoline-6,14-diyl)bis(phenylmethanone) (3p)



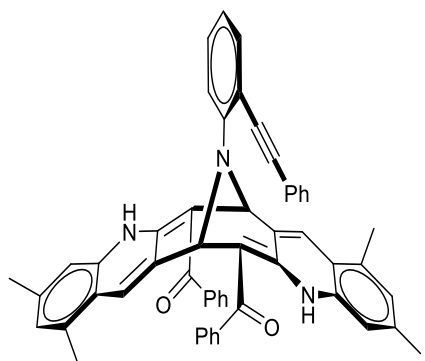
Yellow solid (53 mg, Yield 79%, m.p. 220-223 °C), (*n*-hexane/EtOAc = 3:1, $R_f = 0.3$); $^1\text{H NMR}$ (300 MHz, CDCl_3) δ 7.72-7.51 (m, 10H), 7.19-6.97 (m, 6H), 6.92 (br s, 2H), 6.69 (br s, 2H), 6.12 (br s, 2H), 2.41 (br s, 6H), 2.25 (br s, 6H); $^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, CDCl_3) δ 185.7, 158.6, 155.9 ($^1J_{\text{C-F}} = 244.0$ Hz), 149.8, 145.5, 141.9, 141.0, 136.7, 134.6, 130.0, 129.1, 129.0, 127.4, 127.2, 127.1, 120.3, 120.2, 120.1, 116.1, 116.0, 115.7 ($^2J_{\text{C-F}} = 22.0$ Hz), 99.6, 57.0, 21.7, 18.3; **HRMS-ESI** (m/z): $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{46}\text{H}_{37}\text{FN}_3\text{O}_2$ 682.2701; found: 682.2704.

((7R,15S)-17-(2-Bromophenyl)-1,3,9,11-tetramethyl-5,7,13,15-tetrahydro-7,15-epiminocycloocta[1,2-b:5,6-b']diquinoline-6,14-diyl)bis(phenylmethanone) (3q)



Yellow solid (62 mg, Yield 84%, m.p. 313-316 °C), (*n*-hexane/EtOAc = 3:1, $R_f = 0.3$); $^1\text{H NMR}$ (300 MHz, CDCl_3) δ 7.71 (d, $J = 7.9$ Hz, 1H), 7.65 – 7.48 (m, 12H), 7.35 (d, $J = 7.9$ Hz, 1H), 7.19 (t, $J = 7.6$ Hz, 1H), 7.11 (br s, 2H), 6.98 (t, $J = 7.6$ Hz, 1H), 6.91 (br s, 2H), 6.52 (s, 2H), 6.04 (s, 2H), 2.41 (s, 6H), 2.19 (s, 6H); $^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, CDCl_3) δ 185.7, 150.1, 148.3, 141.9, 140.8, 136.7, 134.7, 134.1, 130.1, 128.9, 128.8, 128.5, 127.3, 127.0, 126.8, 124.8, 122.8, 120.4, 120.3, 116.0, 100.0, 57.4, 21.7, 18.3; **HRMS-ESI** (m/z): $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{46}\text{H}_{37}^{79}\text{BrN}_3\text{O}_2$ 742.2055; found: 742.2054.

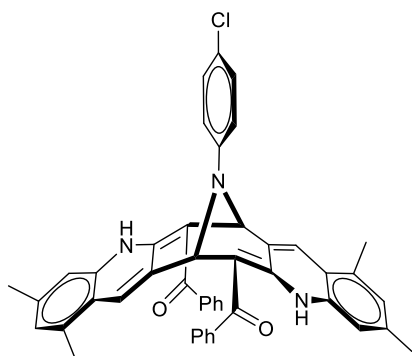
((7R,15S)-1,3,9,11-Tetramethyl-17-(2-(phenylethynyl)phenyl)-5,7,13,15-tetrahydro-7,15-epiminocycloocta[1,2-b:5,6-b']diquinoline-6,14-diyl)bis(phenylmethanone) (3r)



$\text{C}_{54}\text{H}_{41}\text{N}_3\text{O}_2$ 764.3271; found: 764.3273.

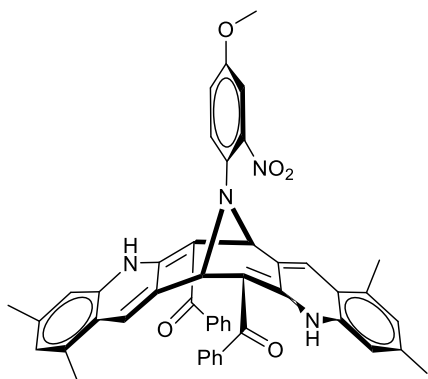
Yellow solid (53 mg, Yield 70%, m.p. 314-318 °C), (*n*-hexane/EtOAc = 3:1, $R_f = 0.3$); $^1\text{H NMR}$ (300 MHz, CDCl_3) δ 7.70 (d, $J = 7.6$ Hz, 1H), 7.65 – 7.52 (m, 9H), 7.52 – 7.43 (m, 3H), 7.23 – 7.14 (m, 5H), 7.12-7.09 (m, 3H), 7.03 (t, $J = 7.4$ Hz, 1H), 6.95 (d, $J = 8.1$ Hz, 1H), 6.90 (s, 2H), 6.63 (s, 2H), 6.55 (s, 2H), 2.41 (s, 6H), 2.10 (s, 6H); $^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, CDCl_3) δ 185.6, 151.4, 150.0, 141.8, 140.8, 136.8, 134.6, 134.4, 131.4, 130.9, 129.6, 128.9, 128.8, 128.1, 128.0, 127.5, 127.1, 127.0, 123.2, 121.9, 120.3, 119.1, 116.7, 116.1, 100.3, 95.9, 88.1, 56.7, 21.8, 18.2; **HRMS-ESI** (m/z): $[\text{M} + \text{H}]^+$ calcd for

((7R,15S)-17-(4-Chlorophenyl)-1,3,9,11-tetramethyl-5,7,13,15-tetrahydro-7,15-epiminocycloocta[1,2-b:5,6-b']diquinoline-6,14-diyl)bis(phenylmethanone) (3s)



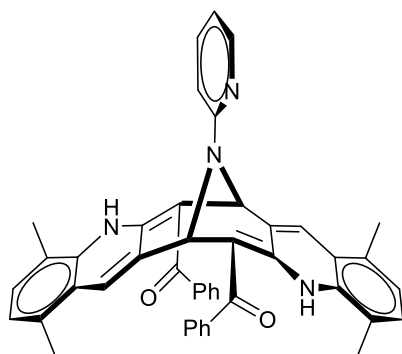
Yellow solid (62 mg, Yield 89%, m.p. 221-224 °C), (*n*-hexane/EtOAc = 4:1, R_f = 0.3); $^1\text{H NMR}$ (300 MHz, CDCl_3) 7.79 – 7.50 (m, 12H), 7.30 (s, 1H), 7.08 (br s, 4H), 6.92 (s, 2H), 6.69 (s, 2H), 6.18 (s, 2H), 2.41 (s, 6H), 2.26 (s, 6H); $^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, CDCl_3) δ 185.9, 149.7, 147.6, 141.9, 141.1, 136.7, 134.6, 129.8, 129.3, 129.2, 129.1, 127.5, 127.2, 127.1, 125.7, 120.2, 119.7, 116.0, 99.5, 56.5, 21.7, 18.3; HRMS-ESI (m/z): $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{46}\text{H}_{37}^{35}\text{ClN}_3\text{O}_2$ 698.2566; found: 698.2568.

((7R,15S)-17-(4-methoxy-2-nitrophenyl)-1,3,9,11-tetramethyl-5,7,13,15-tetrahydro-7,15-epiminocycloocta[1,2-b:5,6-b']diquinoline-6,14-diyl)bis(phenylmethanone) (3t)



Yellow solid (46 mg, Yield 63%, m.p. 282-285 °C), (*n*-hexane/EtOAc = 3:1, R_f = 0.3); $^1\text{H NMR}$ (300 MHz, CDCl_3) δ 7.72 – 7.41 (m, 13H), 7.40 (d, J = 3.1 Hz, 1H), 7.10 (s, 2H), 6.98 (dd, J = 8.9, 3.1 Hz, 1H), 6.90 (s, 2H), 6.43 (s, 2H), 5.78 (s, 2H), 3.84 (s, 3H), 2.41 (s, 6H), 2.17 (s, 6H); $^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, CDCl_3) δ 186.0, 155.7, 149.8, 146.4, 141.9, 140.9, 137.3, 136.6, 134.7, 129.7, 129.0, 128.9, 127.1, 127.0, 126.7, 125.2, 120.2, 119.5, 116.0, 110.1, 99.9, 58.9, 55.9, 21.7, 18.2; HRMS-ESI (m/z): $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{47}\text{H}_{39}\text{N}_4\text{O}_5$ 739.1302; found: 739.1304.

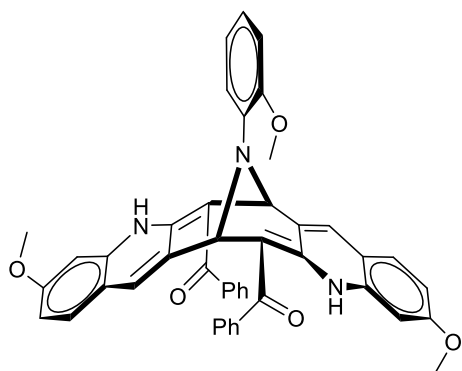
((7R,15S)-1,4,9,12-Tetramethyl-17-(pyridin-2-yl)-5,7,13,15-tetrahydro-7,15-epiminocycloocta[1,2-b:5,6-b']diquinoline-6,14-diyl)bis(phenylmethanone) (3u)



Yellow solid (46 mg, Yield 70%, m.p. 194-197 °C), (*n*-hexane/EtOAc = 3:1, R_f = 0.3); $^1\text{H NMR}$ (300 MHz, CDCl_3) δ 8.32 (d, J = 6.9 Hz, 1H), 7.81-7.66 (m, 5H), 7.65 – 7.55 (m, 5H), 7.52 (d, J = 7.0 Hz, 2H), 7.45 (t, J = 6.9 Hz, 1H), 7.11 (d, J = 7.3 Hz, 2H), 6.98 (br s, 2H), 6.86 (d, J = 7.3 Hz, 2H), 6.73 (d, J = 8.6 Hz, 1H), 6.70 (br s, 2H), 6.62 (dd, J = 7.2, 4.9 Hz, 1H), 2.42 (s, 6H), 2.13 (s, 6H); $^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, CDCl_3) 186.1, 157.4, 149.7, 148.4, 141.9, 138.0, 135.6, 132.4, 130.7, 130.5, 129.2, 129.1, 127.8, 127.5, 124.7, 123.9, 122.1, 114.4, 108.3, 100.3, 52.3, 18.2, 17.0; HRMS-ESI (m/z): $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{45}\text{H}_{37}\text{N}_4\text{O}_2$ 665.2906; found: 665.2908.

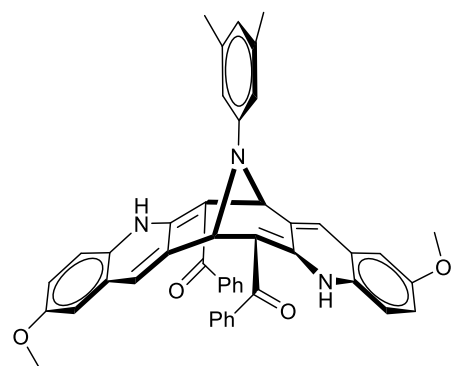
665.2906; found: 665.2908.

((7R,15S)-3,11-Dimethoxy-17-(2-methoxyphenyl)-5,7,13,15-tetrahydro-7,15-epiminocycloocta[1,2-b:5,6-b']diquinoline-6,14-diyl)bis(phenylmethanone) (3v)



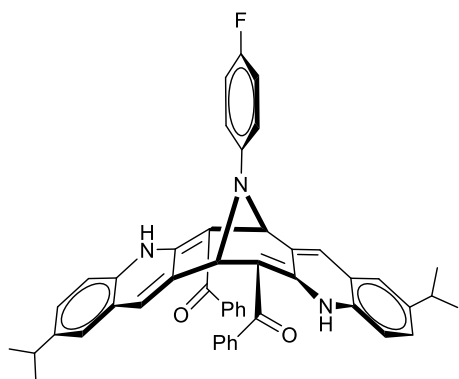
Yellow solid (59 mg, Yield 86%, m.p. 310-311 °C), (*n*-hexane/EtOAc = 3:1, R_f = 0.3); ¹H NMR (300 MHz, CDCl₃) δ 7.51 – 7.41 (m, 7H), 7.40 – 7.35 (m, 4H), 7.14 (d, *J* = 8.4 Hz, 1H), 6.97 – 6.75 (m, 5H), 6.73 – 6.66 (m, 5H), 5.96 (s, 2H), 5.76 (s, 2H), 3.91 (s, 3H), 3.71 (s, 6H); ¹³C{¹H} NMR (75 MHz, CDCl₃) δ 185.8, 161.5, 152.0, 150.4, 141.9, 138.3, 137.9, 130.4, 128.9, 128.8, 128.7, 128.5, 127.5, 123.3, 121.1, 119.8, 117.7, 114.8, 111.0, 100.3, 99.3, 55.8, 55.6, 55.5; HRMS-ESI (*m/z*): [M + H]⁺ calcd for C₄₅H₃₆N₃O₅ 698.2650; found: 698.2651.

((7R,15S)-17-(3,5-Dimethylphenyl)-2,10-dimethoxy-5,7,13,15-tetrahydro-7,15-epiminocycloocta[1,2-b:5,6-b']diquinoline-6,14-diyl)bis(phenylmethanone) (3w)



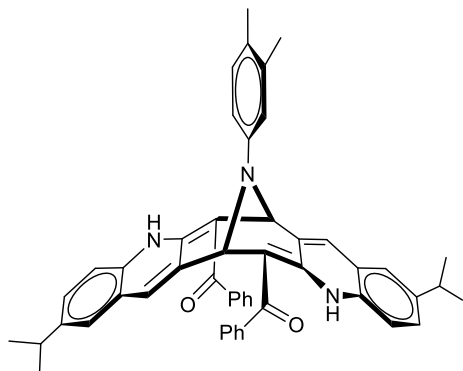
Yellow solid (62 mg, Yield 90%, m.p. 206-207 °C), (*n*-hexane/EtOAc = 3:1, R_f = 0.3); ¹H NMR (250 MHz, CDCl₃) δ 7.68 – 7.48 (m, 12H), 7.39 (d, *J* = 9.2 Hz, 2H), 7.12 (d, *J* = 9.4 Hz, 2H), 6.71 (s, 2H), 6.61 – 6.50 (m, 3H), 6.19 (s, 2H), 6.12 (s, 2H), 3.84 (s, 6H), 2.28 (s, 6H). ¹³C{¹H} NMR (63 MHz, CDCl₃) δ 181.5, 156.4, 149.8, 148.7, 141.1, 138.8, 132.5, 131.5, 130.3, 129.0, 128.9, 127.7, 124.5, 122.7, 120.9, 120.7, 116.1, 107.4, 100.2, 56.1, 55.6, 21.8.; HRMS-ESI (*m/z*): [M + H]⁺ calcd for C₄₆H₃₈N₃O₄ 696.2863; found: 696.2867.

((7R,15S)-17-(4-Fluorophenyl)-2,10-diisopropyl-5,7,13,15-tetrahydro-7,15-epiminocycloocta[1,2-b:5,6-b']diquinoline-6,14-diyl)bis(phenylmethanone) (3x)



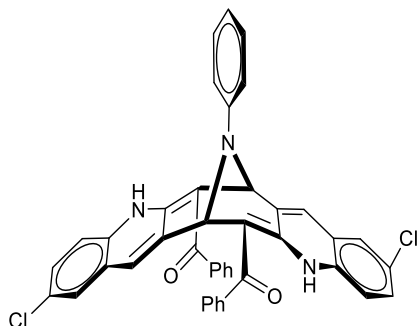
Yellow solid (51 mg, Yield 73%, m.p. 212-215 °C), (*n*-hexane/EtOAc = 3:1, R_f = 0.3); ¹H NMR (300 MHz, CDCl₃) δ 7.83 – 7.62 (m, 7H), 7.55 – 7.47 (m, 4H), 7.44 – 7.34 (m, 4H), 7.20 – 6.85 (m, 7H), 6.06 (br s, 2H), 6.03 (br s, 2H), 3.16-2.83 (m, 2H), 1.33 (s, 6H), 1.31 (s, 6H); ¹³C{¹H} NMR (75 MHz, CDCl₃) δ 186.3, 159.5, 156.3 (¹J_{C-F} = 242.2 Hz), 149.8, 145.0, 141.8, 139.2, 134.7, 130.6, 130.4, 129.8, 129.1, 129.0, 127.3, 124.2, 123.0, 120.0, 119.9, 118.2, 116.0, 115.7 (²J_{C-F} = 22.5 Hz), 99.1, 56.9, 33.7, 23.9; HRMS-ESI (*m/z*): [M + H]⁺ calcd for C₄₈H₄₁FN₃O₂ 710.3178; found: 710.3179.

((7R,15S)-17-(3,4-Dimethylphenyl)-2,10-diisopropyl-5,7,13,15-tetrahydro-7,15-epiminocycloocta[1,2-b:5,6-b']diquinoline-6,14-diyl)bis(phenylmethanone) (3y)



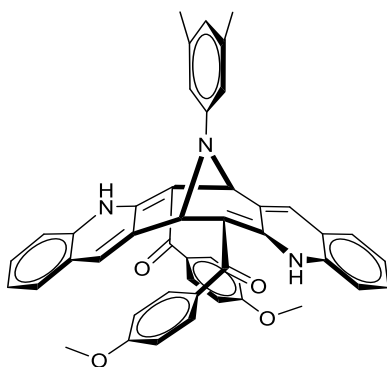
Yellow solid (63 mg, Yield 89%, m.p. 277-280 °C), (*n*-hexane/EtOAc = 3:1, R_f = 0.3); ¹H NMR (300 MHz, CDCl₃) δ 7.70 – 7.47 (m, 8H), 7.46 – 7.36 (m, 4H), 7.32 – 7.20 (m, 4H), 6.91 (d, *J* = 8.4 Hz, 1H), 6.90 – 6.83 (br s, 3H), 6.73 (d, *J* = 8.2 Hz, 1H), 5.98 (br s, 2H), 5.97 (br s, 2H), 2.98-2.80 (m, 2H), 2.17 (s, 3H), 2.07 (s, 3H), 1.20 (s, 6H), 1.18 (s, 6H); ¹³C{¹H} NMR (75 MHz, CDCl₃) δ 186.1, 150.0, 146.7, 144.8, 141.9, 137.3, 134.7, 130.8, 130.5, 130.3, 129.6, 129.1, 129.0, 128.9, 127.4, 124.1, 123.1, 120.1, 118.1, 115.5, 99.5, 56.3, 33.7, 23.9, 20.4, 18.8; HRMS-ESI (*m/z*): [M + H]⁺ calcd for C₅₀H₄₆N₃O₂ 720.3580; found: 720.3582.

((7R,15S)-2,10-Dichloro-17-phenyl-5,7,13,15-tetrahydro-7,15-epiminocycloocta[1,2-b:5,6-b']diquinoline-6,14-diyl)bis(phenylmethanone) (3z)



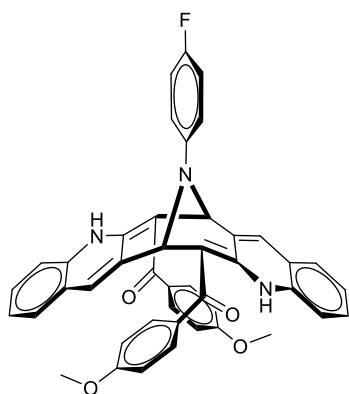
Yellow solid (62 mg, Yield 92%, m.p. 206-209 °C), (*n*-hexane/EtOAc = 3:1, R_f = 0.3); ¹H NMR (300 MHz, CDCl₃) δ 7.99 – 7.92 (m, 3H), 7.89 – 7.78 (m, 8H), 7.74 – 7.74 (m, 2H), 7.45 (s, 5H), 7.32 (s, 2H), 7.08 (s, 3H), 6.09 (s, 2H), 5.87 (s, 2H). ¹³C{¹H} NMR (75 MHz, CDCl₃) δ 186.7, 150.1, 148.4, 141.2, 135.1, 131.5, 130.9, 129.6, 129.5, 129.4, 129.2, 129.1, 127.3, 126.2, 125.8, 123.8, 119.8, 118.2, 99.8, 77.5, 77.1, 76.7, 56.0; HRMS-ESI (*m/z*): [M + H]⁺ calcd for C₄₂H₂₇³⁷Cl₂N₃O₂ 676.1559; found: 676.1558.

((7R,15S)-17-(3,5-Dimethylphenyl)-5,7,13,15-tetrahydro-7,15-epiminocycloocta[1,2-b:5,6-b']diquinoline-6,14-diyl)bis((4-methoxyphenyl)methanone) (3aa)



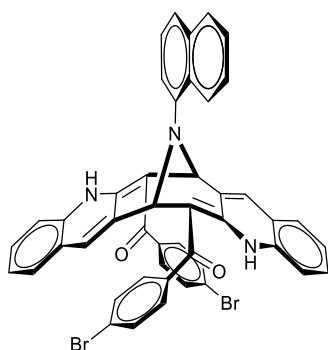
Yellow solid (56 mg, Yield 82%, m.p. 291-293 °C), (*n*-hexane/EtOAc = 3:1, R_f = 0.4); ¹H NMR (300 MHz, CDCl₃) δ 7.80 – 7.46 (m, 7H), 7.44 – 7.32 (m, 3H), 7.31 – 7.05 (m, 8H), 6.77 (br s, 2H), 6.60 (br s, 1H), 6.28 (br s, 2H), 6.19 (br s, 2H), 4.03 (br s, 6H), 2.34 (br s, 6H); ¹³C{¹H} NMR (75 MHz, CDCl₃) δ 186.8, 160.3, 150.1, 148.7, 138.9, 136.4, 134.4, 131.2, 130.4, 130.0, 128.9, 127.2, 123.8, 123.0, 122.8, 118.0, 116.1, 114.1, 100.2, 56.2, 55.5, 21.8; HRMS-ESI (*m/z*): [M + H]⁺ calcd for C₄₆H₃₈N₃O₄ 696.2808; found: 696.2809.

((7R,15S)-17-(4-Fluorophenyl)-5,7,13,15-tetrahydro-7,15-epiminocycloocta[1,2-b:5,6-b']diquinoline-6,14-diyl)bis((4-methoxyphenyl)methanone) (3ab)



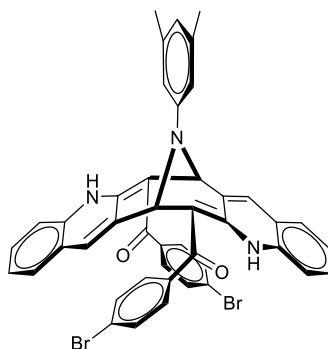
Yellow solid (51 mg, Yield 75%, m.p. 269-271 °C), (*n*-hexane/EtOAc = 3:1, R_f = 0.3); ¹H NMR (300 MHz, DMSO-*d*₆) (mixture of two rotamers (66:34)) δ 8.72 (s, 1H, minor rotamer), 8.72 (s, 1H, major rotamer), 8.41-8.22 (m, 1H, mixture of two rotamers), 8.21 – 8.04 (m, 2H, major rotamer), 8.02 – 7.92 (m, 2H, minor rotamer), 7.86 – 7.60 (m, 4H, mixture of two rotamers), 7.58 – 7.38 (m, 4H, mixture of two rotamers), 7.34 – 6.96 (m, 9H, mixture of two rotamers), 6.84 – 6.57 (m, 1H, mixture of two rotamers), 6.32-6.18 (m, 2H, minor rotamer), 6.05 (d, *J* = 11.0 Hz, 2H, major rotamer), 5.59 (s, 1H, major rotamer), 5.47 (s, 1H, minor rotamer), 3.97 (s, 4H, major rotamer), 3.92 (s, 2H, minor rotamer); ¹³C{¹H} NMR (75 MHz, DMSO-*d*₆) (mixture of two rotamers (66:34)) δ 185.9, 185.8, 163.9, 163.8, 160.6, 160.5 (¹*J*_{C-F} = 247.2 Hz), 149.7, 147.2, 146.8, 136.7, 133.7, 131.9, 131.7, 131.5, 131.3, 131.2, 130.3, 130.2, 129.7, 129.1, 128.7, 128.5, 128.3, 127.6, 127.0, 124.8, 122.6, 121.4, 120.2, 120.1, 119.0, 117.2, 116.6, 116.4, 116.1, 114.8 (²*J*_{C-F} = 23.2 Hz), 101.6, 99.7, 99.2, 56.4, 56.1, 55.9, 55.8; HRMS-ESI (*m/z*): [M + H]⁺ calcd for C₄₄H₃₃FN₃O₄ 686.2446; found: 686.2449.

((7R,15S)-17-(Naphthalen-1-yl)-5,7,13,15-tetrahydro-7,15-epiminocycloocta[1,2-b:5,6-b']diquinoline-6,14-diyl)bis((4-bromophenyl)methanone) (3ac)



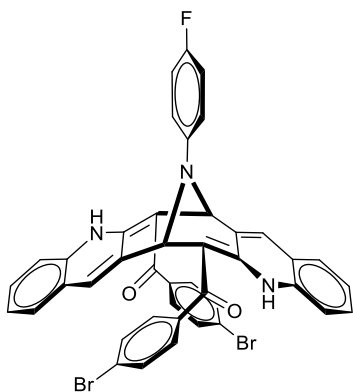
Yellow solid (71 mg, Yield 88%, m.p. 229-231 °C), (*n*-hexane/EtOAc = 3:1, R_f = 0.3); ¹H NMR (300 MHz, CDCl₃) δ 8.26 (d, *J* = 8.4, 2.8 Hz, 1H), 8.04 – 7.82 (m, 2H), 7.79 – 7.36 (m, 14H), 7.36 -7.22 (M, 5H), 7.22 – 6.92 (m, 3H), 6.17 (s, 1H), 6.09 (s, 1H), 6.01 (s, 1H), 5.89 (s, 1H); ¹³C{¹H} NMR (75 MHz, CDCl₃) δ 187.8, 185.8, 146.2, 140.3, 136.3, 134.8, 133.1, 132.0, 130.7, 129.0, 128.9, 128.8, 127.4, 126.3, 126.0, 125.9, 124.4, 124.2, 123.5, 123.2, 123.1, 118.2, 116.5, 102.1, 98.1, 58.7, 58.0; HRMS-ESI (*m/z*): [M + H]⁺ calcd for C₄₆H₃₀⁷⁹Br₂N₃O₂ 814.0692; found: 814.0693.

((7R,15S)-17-(3,5-Dimethylphenyl)-5,7,13,15-tetrahydro-7,15-epiminocycloocta[1,2-b:5,6-b']diquinoline-6,14-diyl)bis((4-bromophenyl)methanone) (3ad)



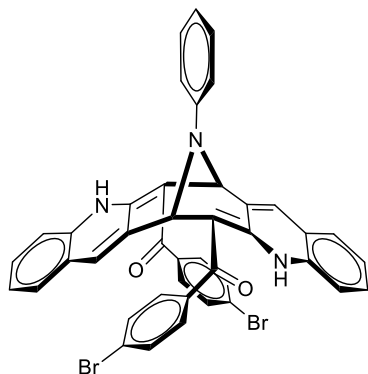
Yellow solid (71 mg, Yield 90%, m.p. 203-206 °C), (*n*-hexane/EtOAc = 3:1, R_f = 0.3); ¹H NMR (300 MHz, CDCl₃) δ 7.90 – 7.70 (m, 5H), 7.58 – 7.47 (m, 3H), 7.46-7.37 (m, 6H), 7.36 – 7.23 (m, 4H), 6.71 (s, 2H), 6.62 (s, 1H), 6.29 (s, 2H), 6.07 (s, 2H), 2.33 (s, 6H); ¹³C{¹H} NMR (75 MHz, CDCl₃) δ 185.6, 150.2, 148.5, 140.6, 139.0, 136.1, 132.1, 130.9, 130.7, 130.4, 129.1, 127.4, 124.4, 123.3, 123.1, 123.0, 118.1, 116.1, 99.8, 56.2, 21.8; HRMS-ESI (*m/z*): [M + H]⁺ calcd for C₄₄H₃₂⁷⁹Br₂N₃O₂ 792.0587; found: 792.0586.

((7R,15S)-17-(4-Fluorophenyl)-5,7,13,15-tetrahydro-7,15-epiminocycloocta[1,2-b:5,6-b']diquinoline-6,14-diyl)bis((4-bromophenyl)methanone) (3ae)



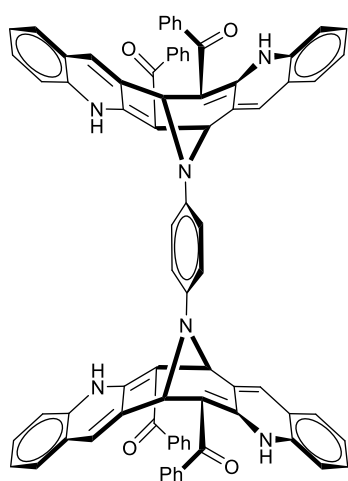
Yellow solid (57 mg, Yield 74%, m.p. 238-240 °C), (*n*-hexane/EtOAc = 3:1, R_f = 0.3); ¹H NMR (300 MHz, CDCl₃) δ 7.82 – 7.69 (m, 5H), 7.50 – 7.29 (m, 10H), 7.25 – 7.20 (m, 3H), 7.02 (s, 4H), 6.16 (s, 2H), 5.90 (s, 2H); ¹³C{¹H} NMR (75 MHz, CDCl₃) δ 185.8, 159.5, 156.3 (¹J_{C-F} = 241.8 Hz), 149.9, 145.0, 140.5, 136.1, 132.2, 130.8, 130.4, 129.0, 127.4, 124.4, 123.3, 122.9, 120.6, 112.0, 118.1, 116.2, 115.9 (²J_{C-F} = 21.3 Hz), 99.3, 57.0.; HRMS-ESI (*m/z*): [M + H]⁺ calcd for C₄₂H₂₆⁷⁹Br₂FN₃O₂ 782.0455; found: 782.0442.

((7R,15S)-17-Phenyl-5,7,13,15-tetrahydro-7,15-epiminocycloocta[1,2-b:5,6-b']diquinoline-6,14-diyl)bis((4-bromophenyl)methanone) (3af)



Yellow solid (70 mg, Yield 93%, m.p. 278-281 °C), (*n*-hexane/EtOAc = 3:1, R_f = 0.3); ¹H NMR (300 MHz, CDCl₃) δ 7.75 (s, 5H), 7.58 – 7.34 (m, 10H), 7.26 – 6.89 (m, 8H), 6.17 (s, 2H), 6.02 (s, 2H); ¹³C{¹H} NMR (75 MHz, CDCl₃) δ 186.0, 150.1, 148.5, 140.6, 136.1, 132.2, 130.9, 130.6, 130.5, 129.6, 129.1, 127.4, 124.5, 123.3, 122.9, 121.3, 118.2, 118.1, 99.5, 77.5, 77.1, 76.7, 56.3.; HRMS-ESI (*m/z*): [M + H]⁺ calcd for C₄₂H₂₇⁷⁹Br₂N₃O₂ 764.0549; found: 764.0540.

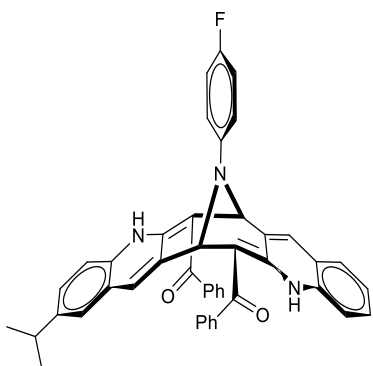
((7R,7'R,15S,15'S)-1,4-Phenylenebis(5,7,13,15-tetrahydro-7,15-epiminocycloocta[1,2-b:5,6-b']diquinoline-17,6,14-triyl))tetrakis(phenylmethanone) (3ag)



Yellow solid (60 mg, Yield 53%, m.p. 235-237 °C), (*n*-hexane/EtOAc = 3:1, R_f = 0.3); ¹H NMR (300 MHz, CDCl₃) δ 7.85-7.58 (m, 15H), 7.56 – 7.34 (m, 11H), 7.21-6.93 (m, 18H), 6.18-5.88 (m, 8H); ¹³C{¹H} NMR (75 MHz, CDCl₃) δ 187.1, 149.8, 142.8, 141.8, 141.7, 135.8, 130.6, 130.4, 130.3, 129.2, 129.0, 127.2, 127.1, 124.0, 123.9, 122.6, 119.5, 117.6, 99.4, 56.3; HRMS-ESI (*m/z*): [M + H]⁺ calcd for C₇₈H₅₃N₆O₄ 1137.4115; found: 1137.4119.

Supporting Information

((7S,15R)-17-(4-fluorophenyl)-2-isopropyl-5,7,13,15-tetrahydro-7,15-epiminocycloocta[1,2-b:5,6-b']diquinoline-6,14-diyl)bis(phenylmethanone) (3ah)



Yellow solid (Yield 37%, m.p. 229-231 °C), (*n*-hexane/EtOAc = 3:1, R_f = 0.3); ¹H NMR (300 MHz, CDCl₃) δ 8.20-7.99 (m, 1H), 7.82-7.70 (m, 1H), 7.69-7.56 (m, 6H), 7.51 – 7.41 (m, 5H), 7.39 – 7.32 (m, 2H), 7.24-7.12 (m, 4H), 7.11-7.03 (m, 1H), 7.02 – 6.94 (m, 3H), 6.92 – 6.73 (m, 2H), 5.99 (br s, 2H), 3.10-2.95 (m, 1H), 1.22 (d, *J* = 6.7 Hz, 6H); ¹³C{¹H} NMR (75 MHz, CDCl₃) δ 196.8, 159.0, 155.8 (¹J_{C-F} = 241.0 Hz), 149.5, 145.0, 141.2, 135.6, 134.1, 132.1, 131.3, 130.3, 129.6, 129.3, 128.5, 128.3, 127.7, 127.3, 127.1, 126.7, 123.6, 122.9, 120.5, 119.4, 119.3, 118.1, 117.6, 115.6, 115.5, 115.3 (²J_{C-F} = 21.1 Hz), 115.2, 56.4, 33.2,

23.4.; HRMS-ESI (*m/z*): [M + H]⁺ calcd for C₄₅H₃₅FN₃O₂ 668.7071; found: 668.7078.

Supporting Information

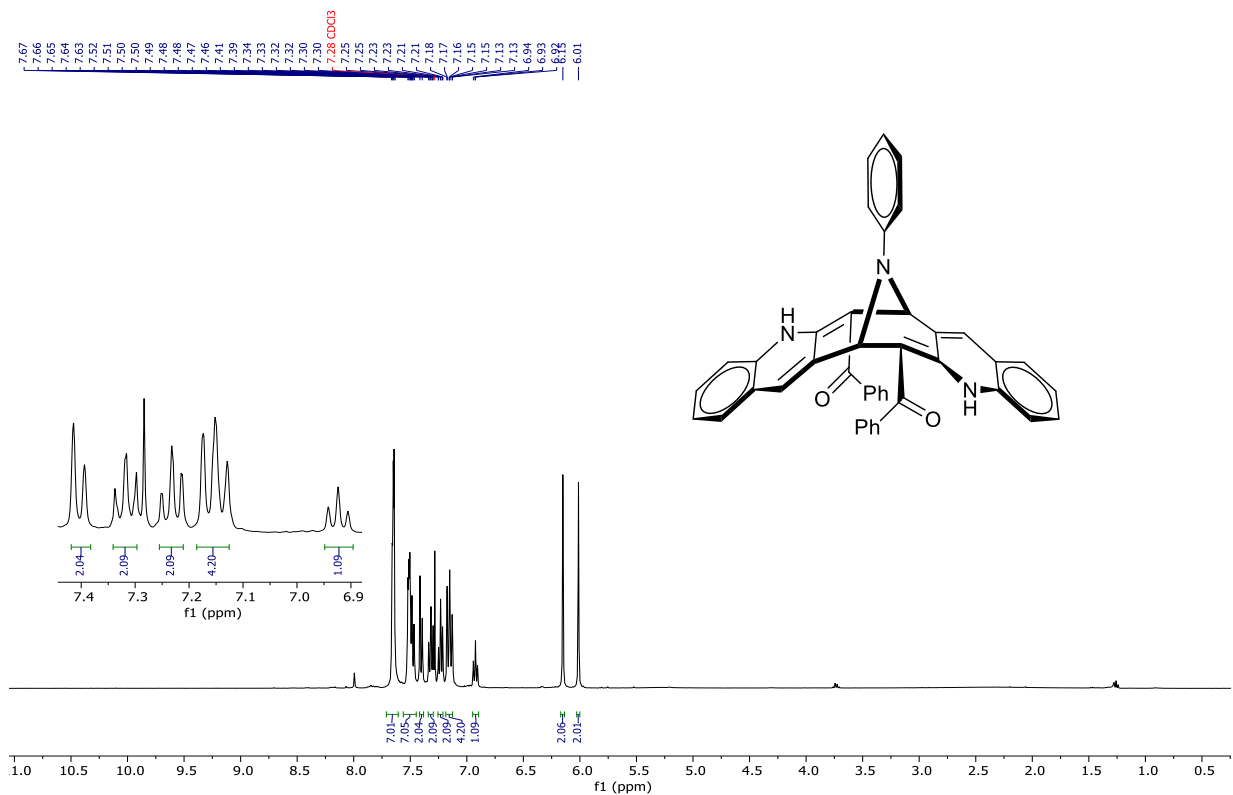


Figure S1: $^1\text{H NMR}$ Compound 3a (400 MHz, CDCl_3)

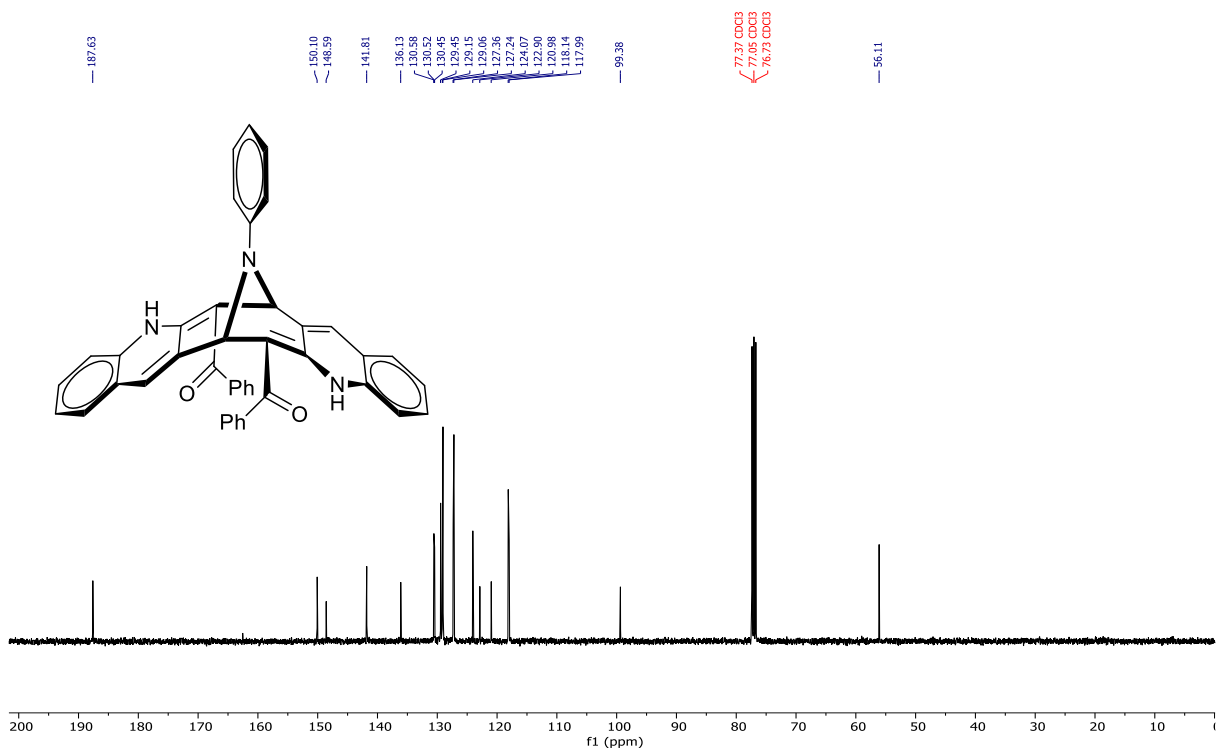
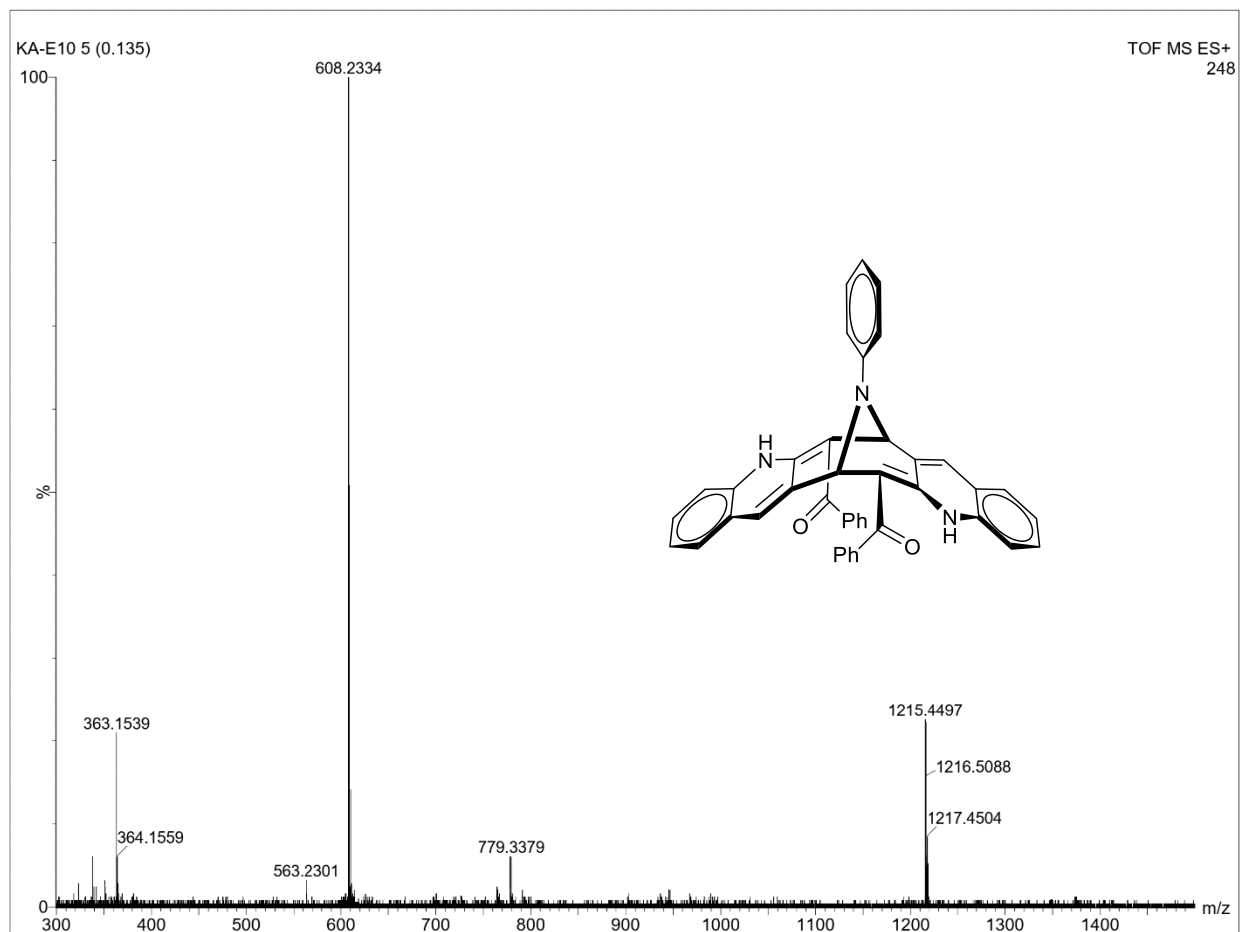


Figure S2: $^{13}\text{C}\{^1\text{H}\}$ NMR Compound 3a (101 MHz, CDCl_3)

Figure S3: HRMS (ESI) of **3a**

Supporting Information

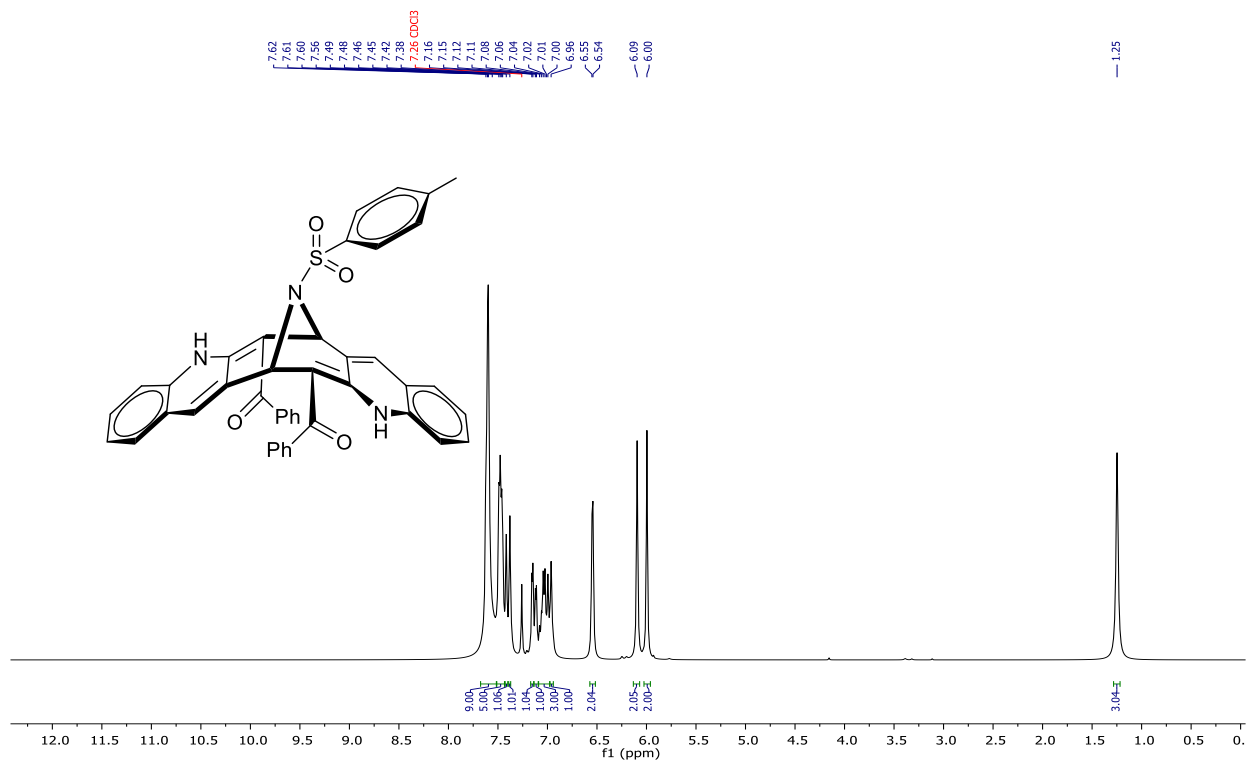


Figure S4: ¹H NMR Compound **3b** (250 MHz, CDCl₃)

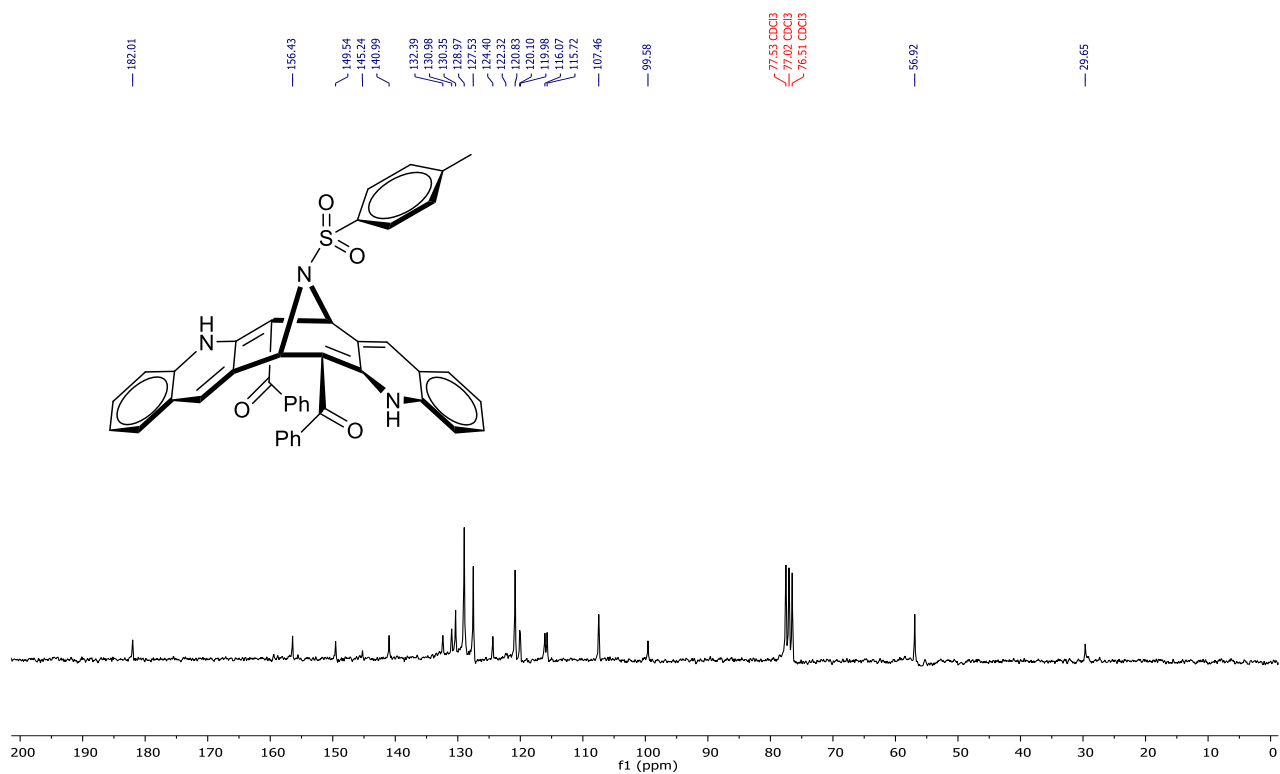


Figure S5: ¹³C{¹H}NMR Compound **3b** (63 MHz, CDCl₃)

Supporting Information

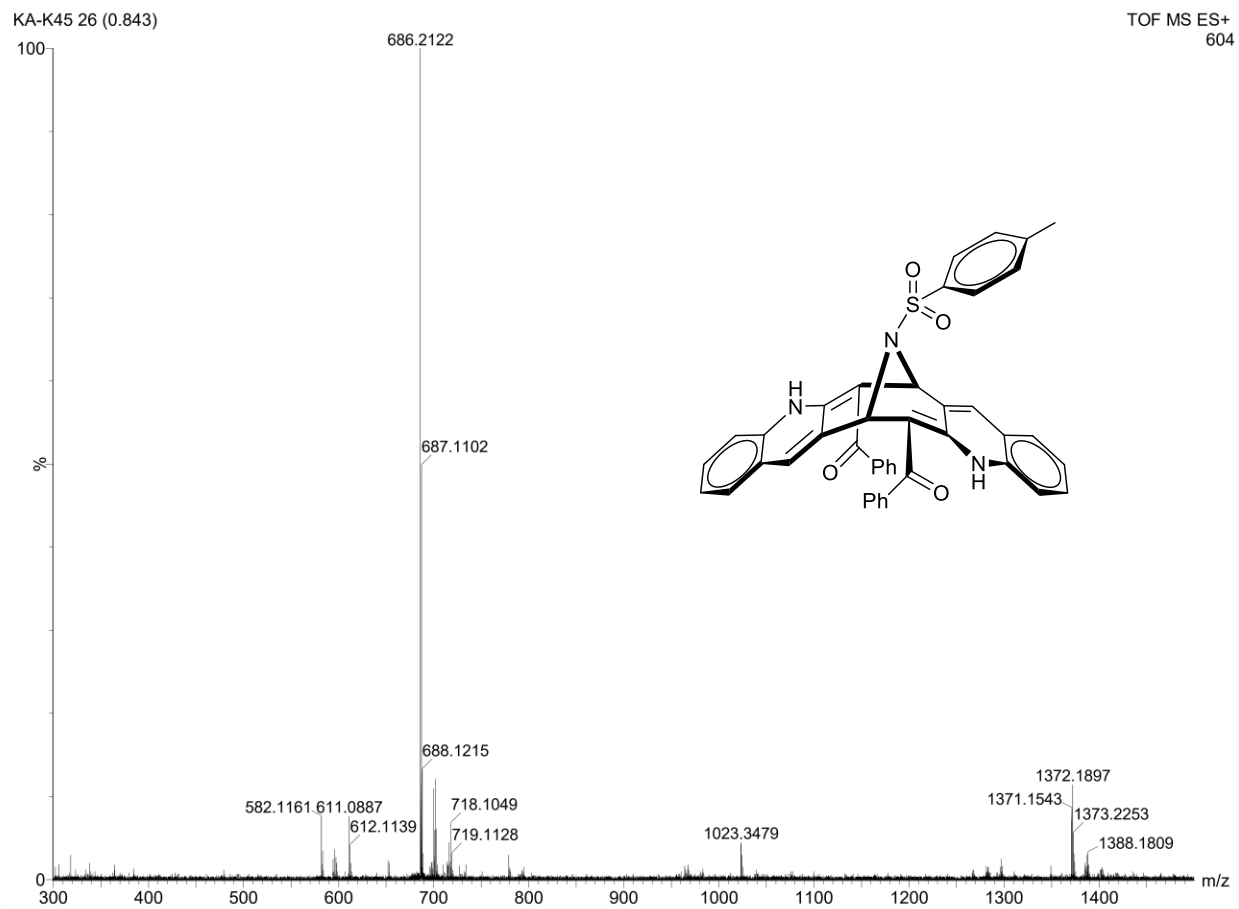


Figure S6: HRMS (ESI) of **3b**

Supporting Information

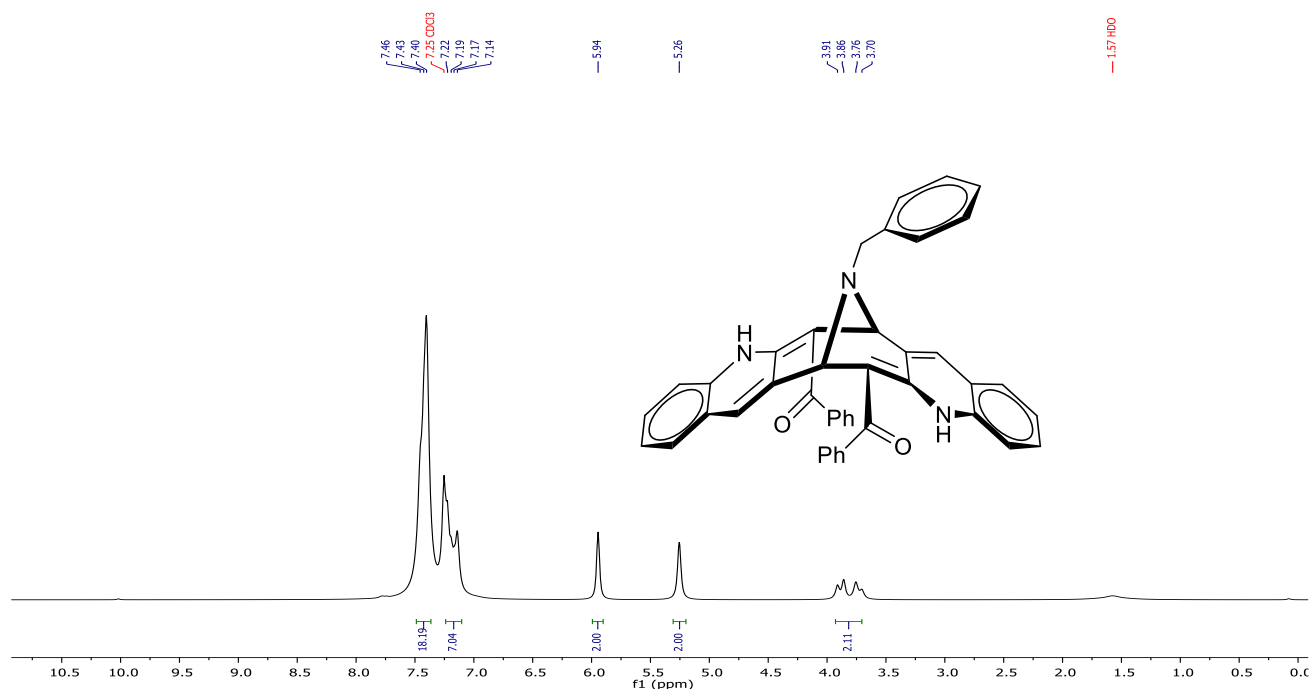


Figure S7: ^1H NMR Compound 3c (250 MHz, CDCl₃)

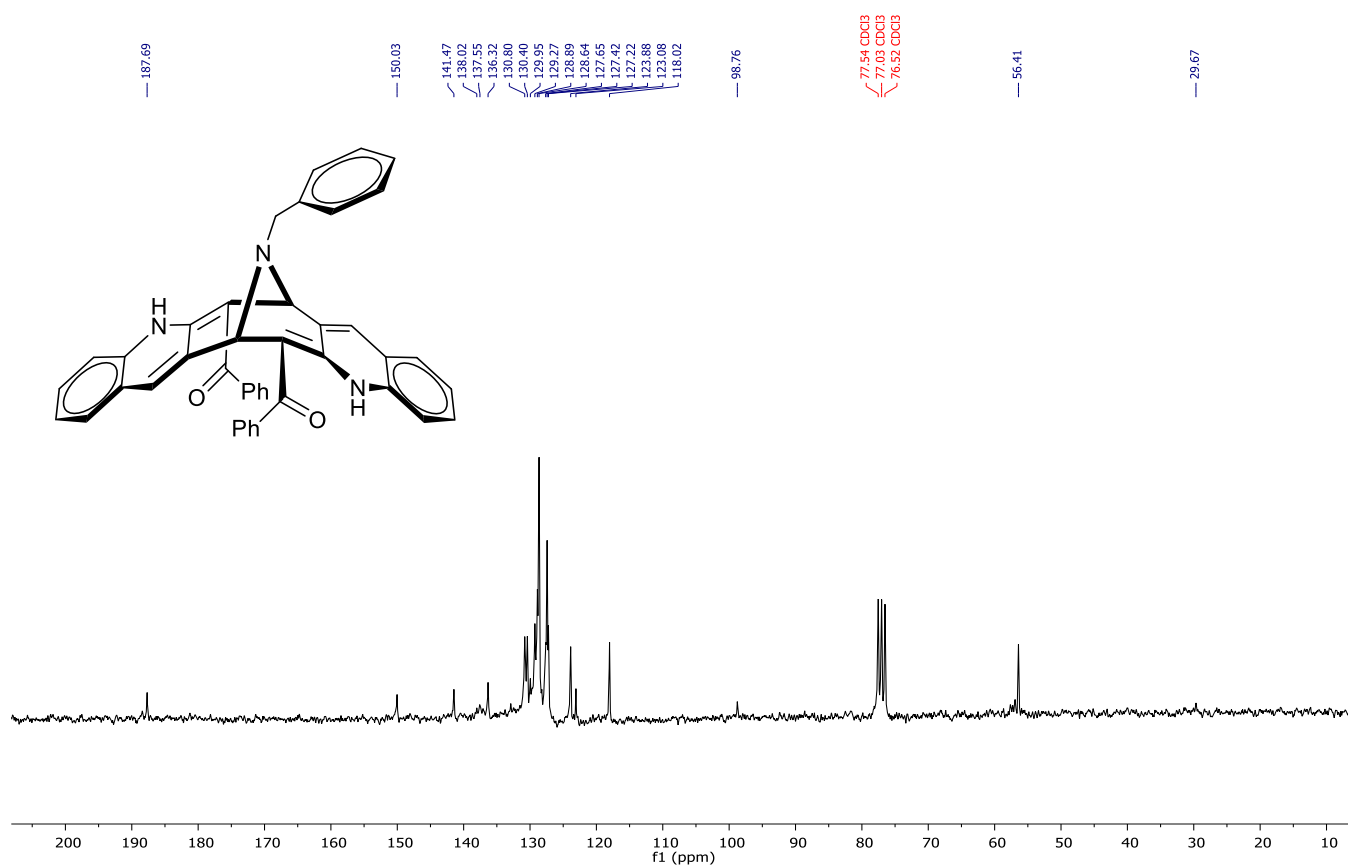


Figure S8: $^{13}\text{C}\{^1\text{H}\}$ NMR Compound 3c (63 MHz, CDCl₃)

Supporting Information

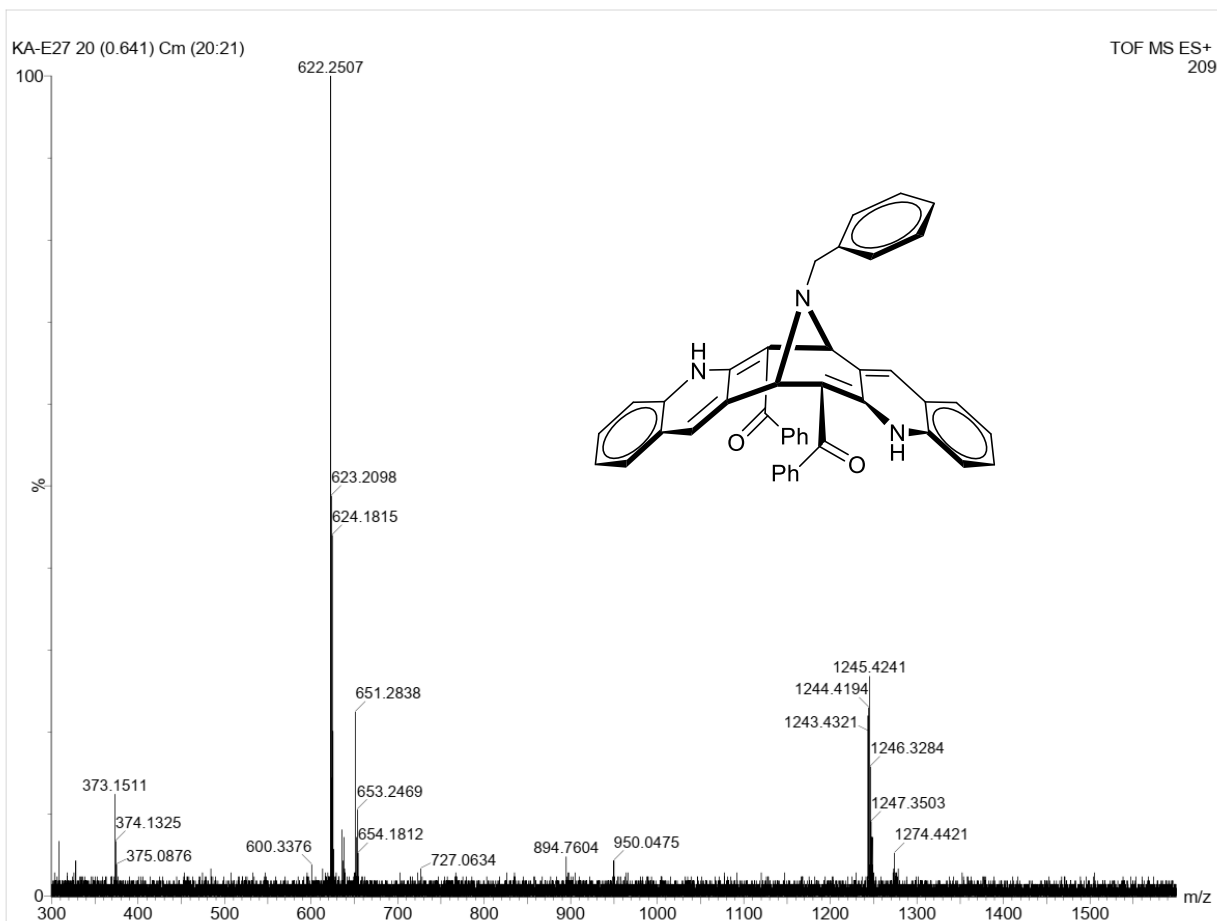


Figure S9: HRMS (ESI) of 3c

Supporting Information

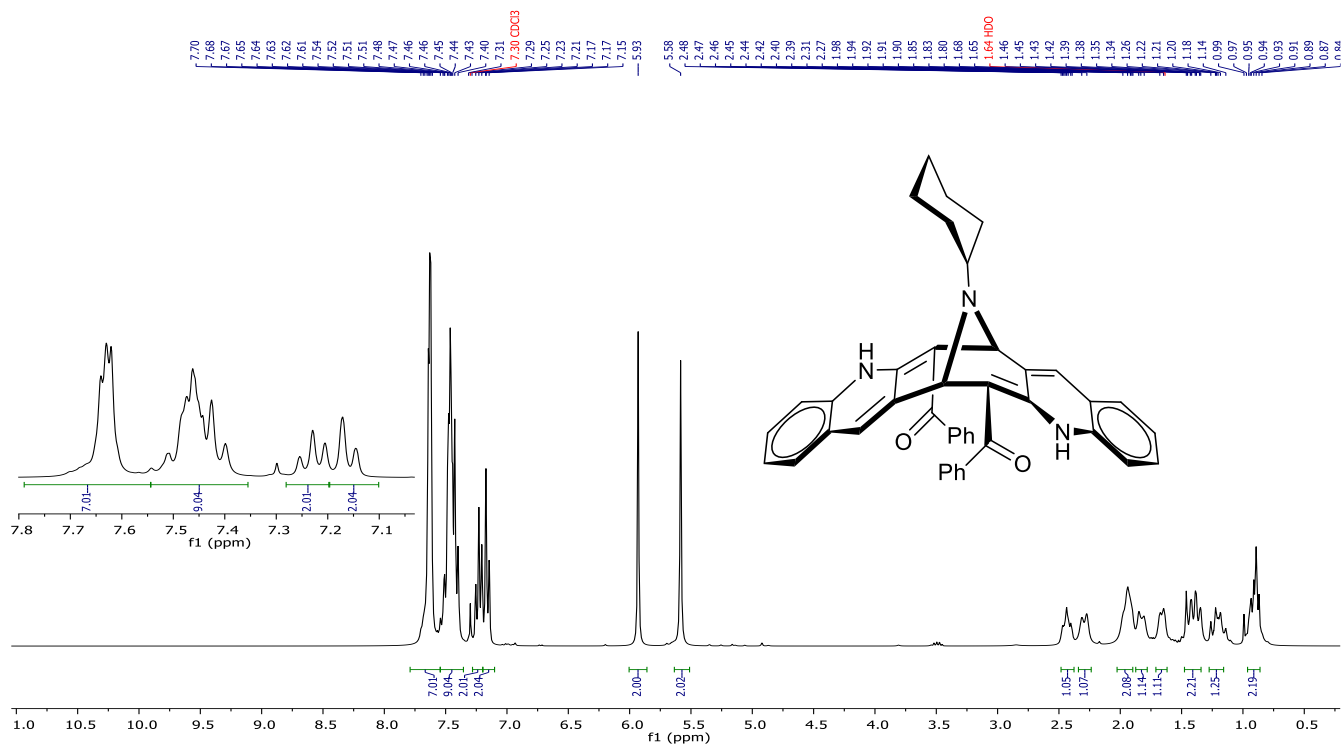


Figure S10: ^1H NMR Compound 3d (300 MHz, CDCl_3)

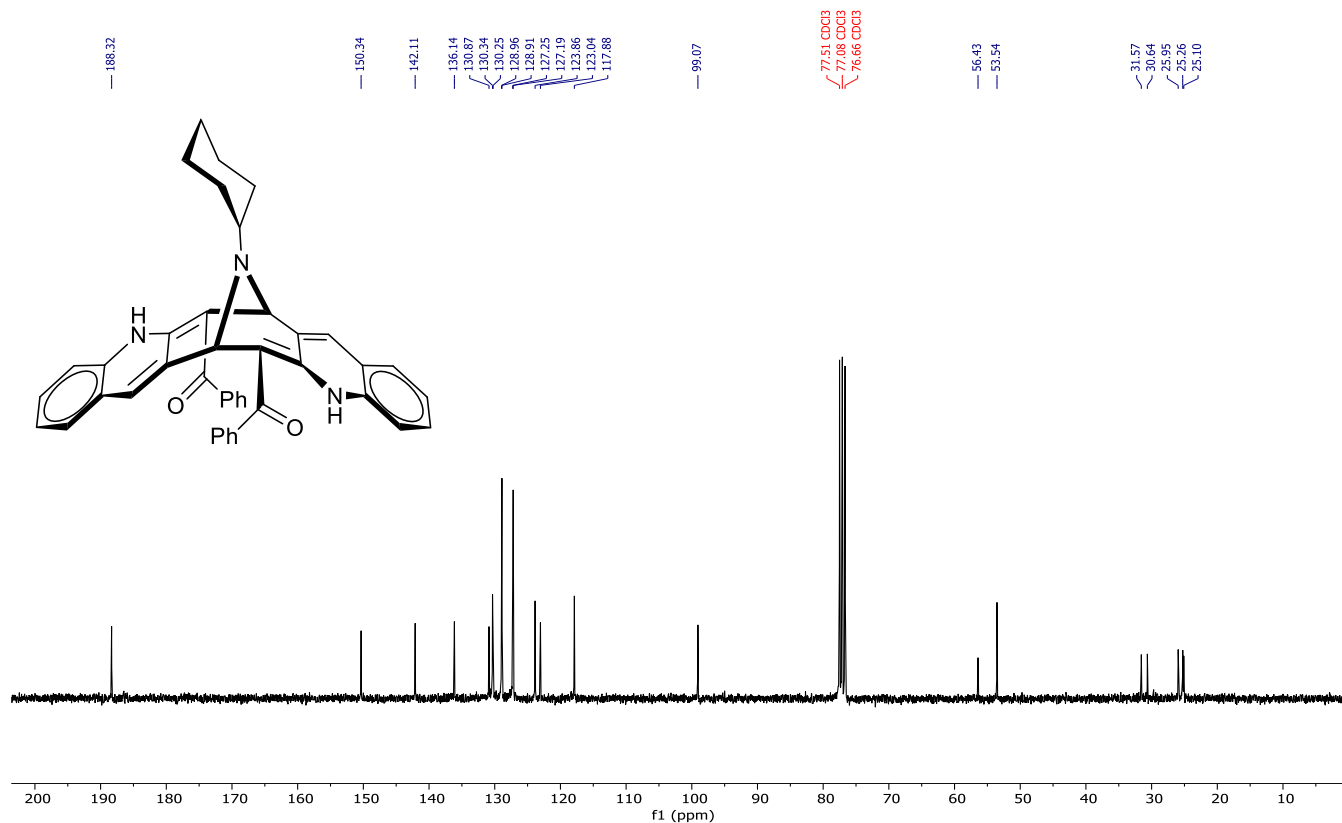
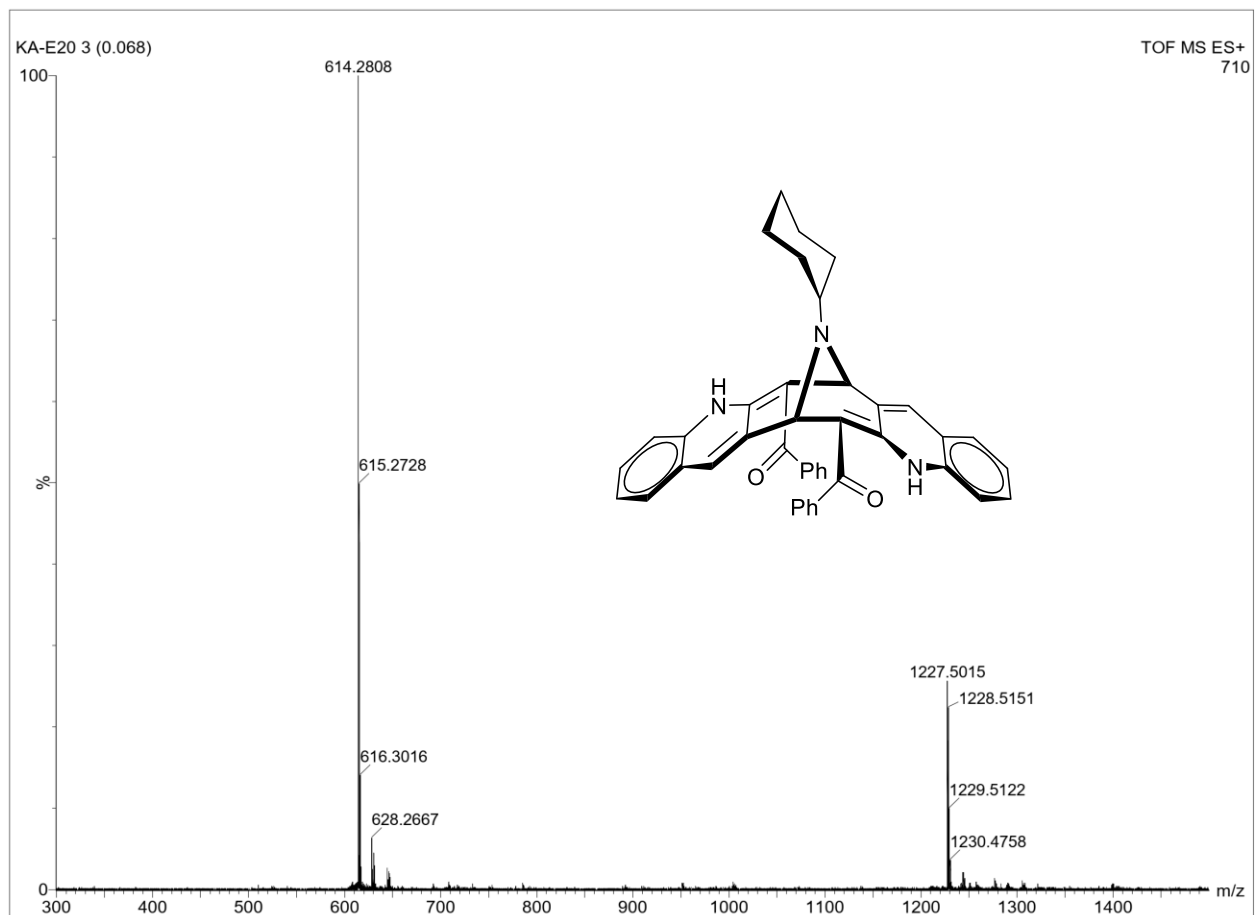


Figure S11: $^{13}\text{C}\{^1\text{H}\}$ NMR Compound 3d (75 MHz, CDCl_3)

Figure S12: HRMS (ESI) of **3d**

Supporting Information

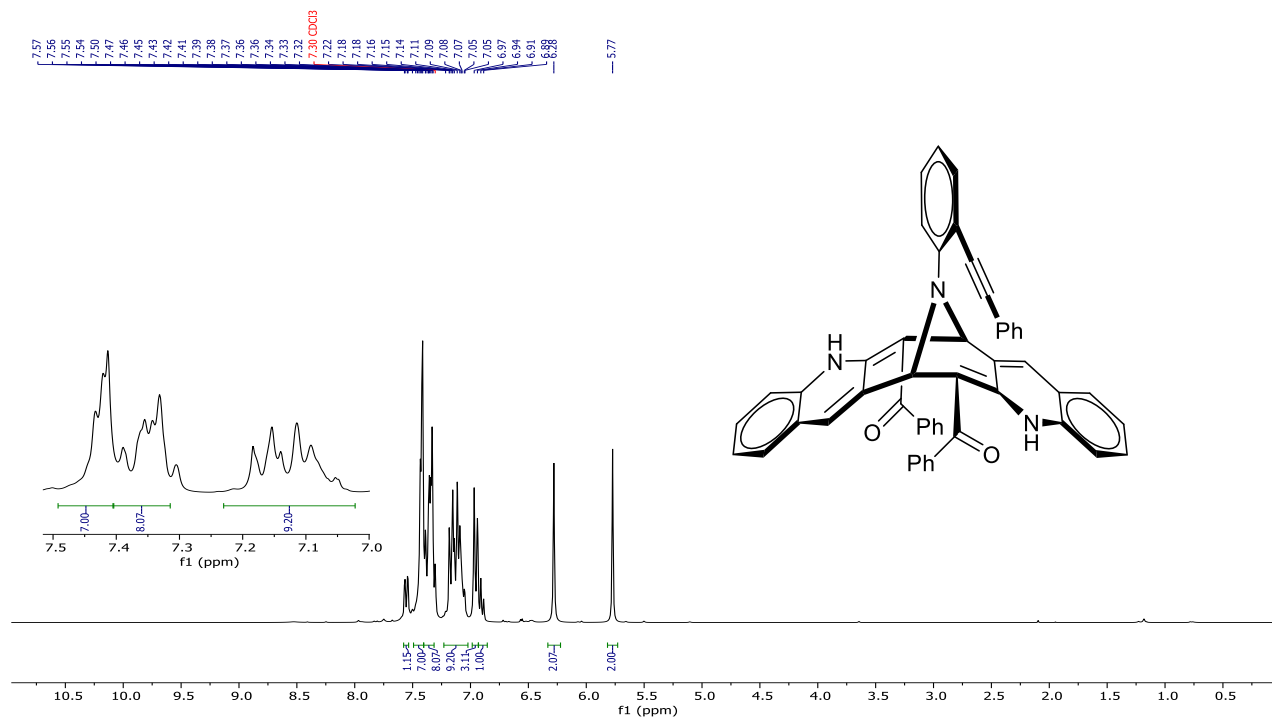


Figure S13: ^1H NMR Compound **3e** (300 MHz, CDCl_3)

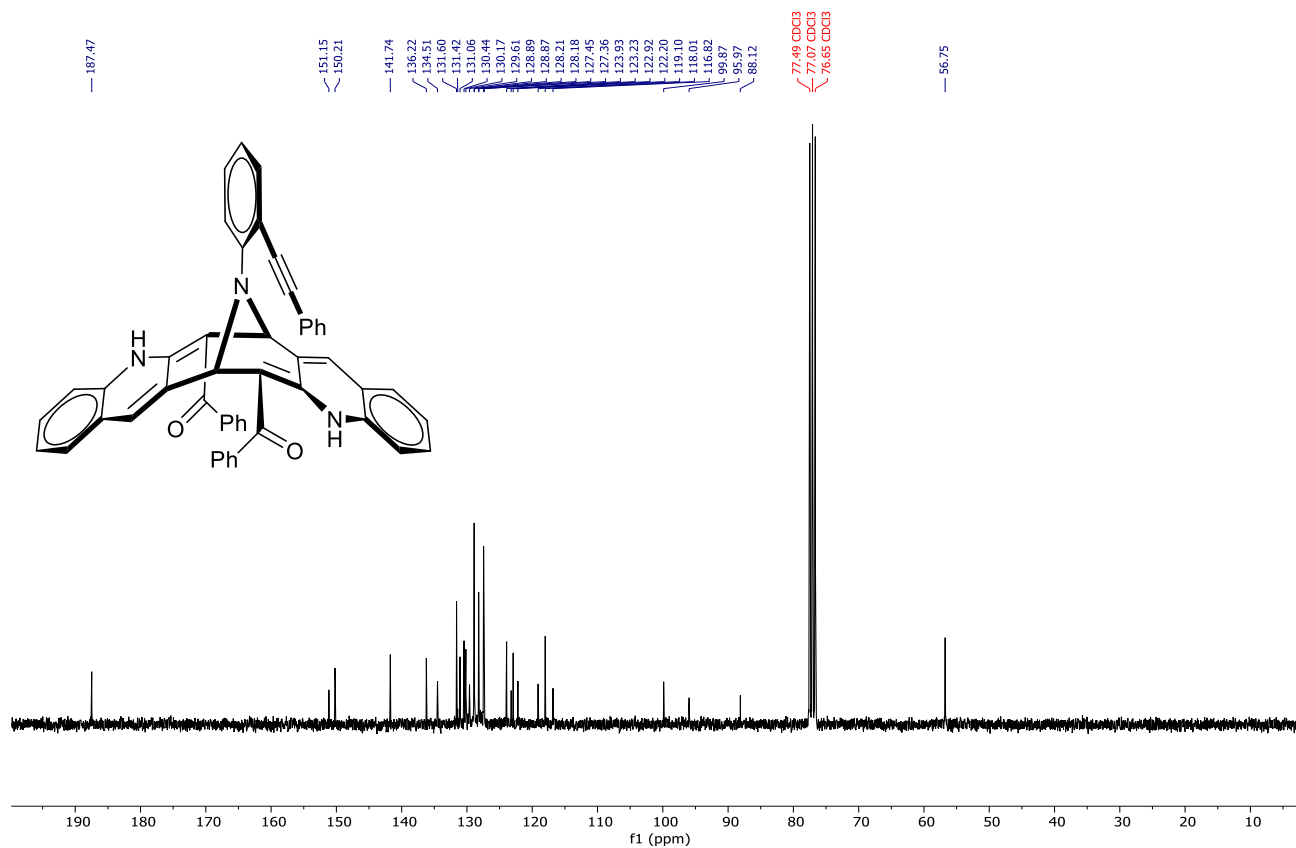
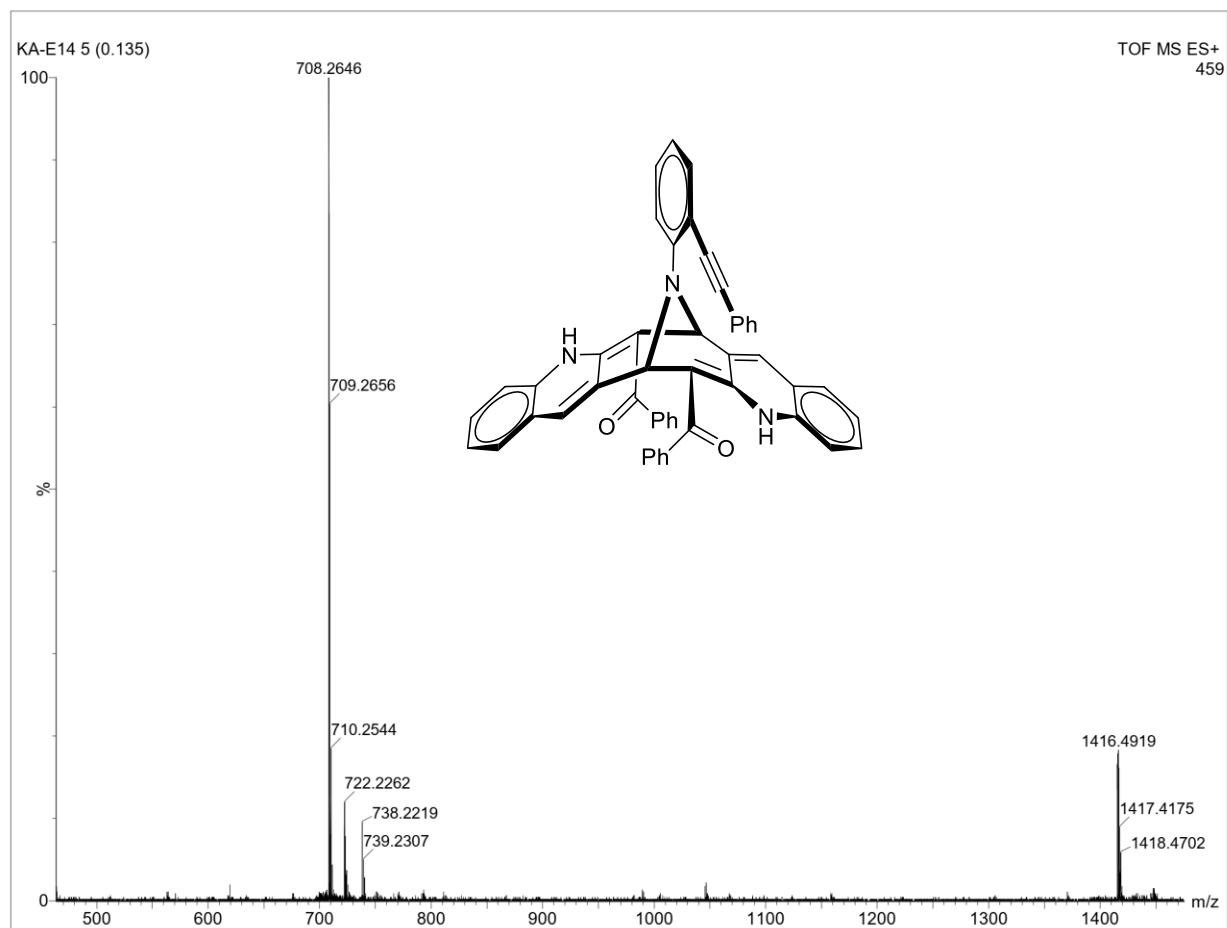
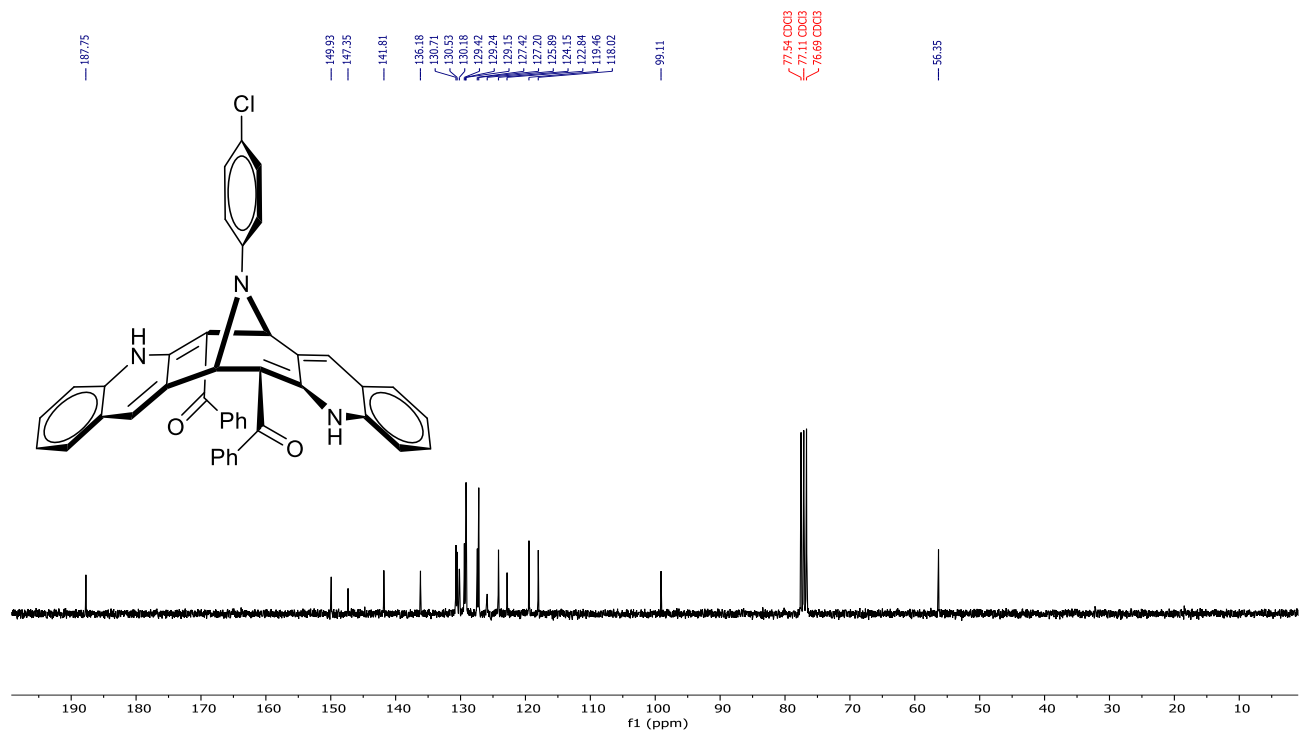
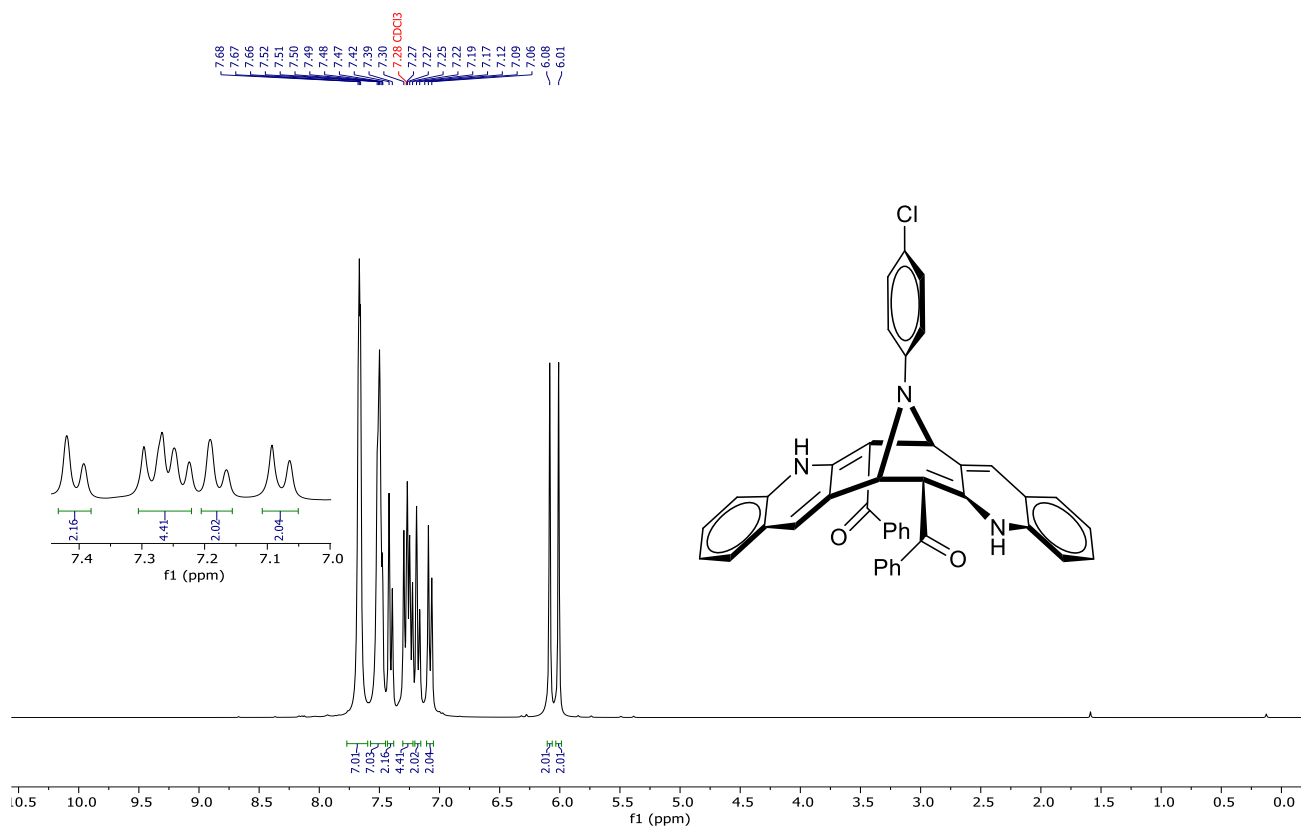


Figure S14: $^{13}\text{C}\{^1\text{H}\}$ NMR Compound **3e** (75 MHz, CDCl_3)

Figure S15: HRMS (ESI) of **3e**

Supporting Information



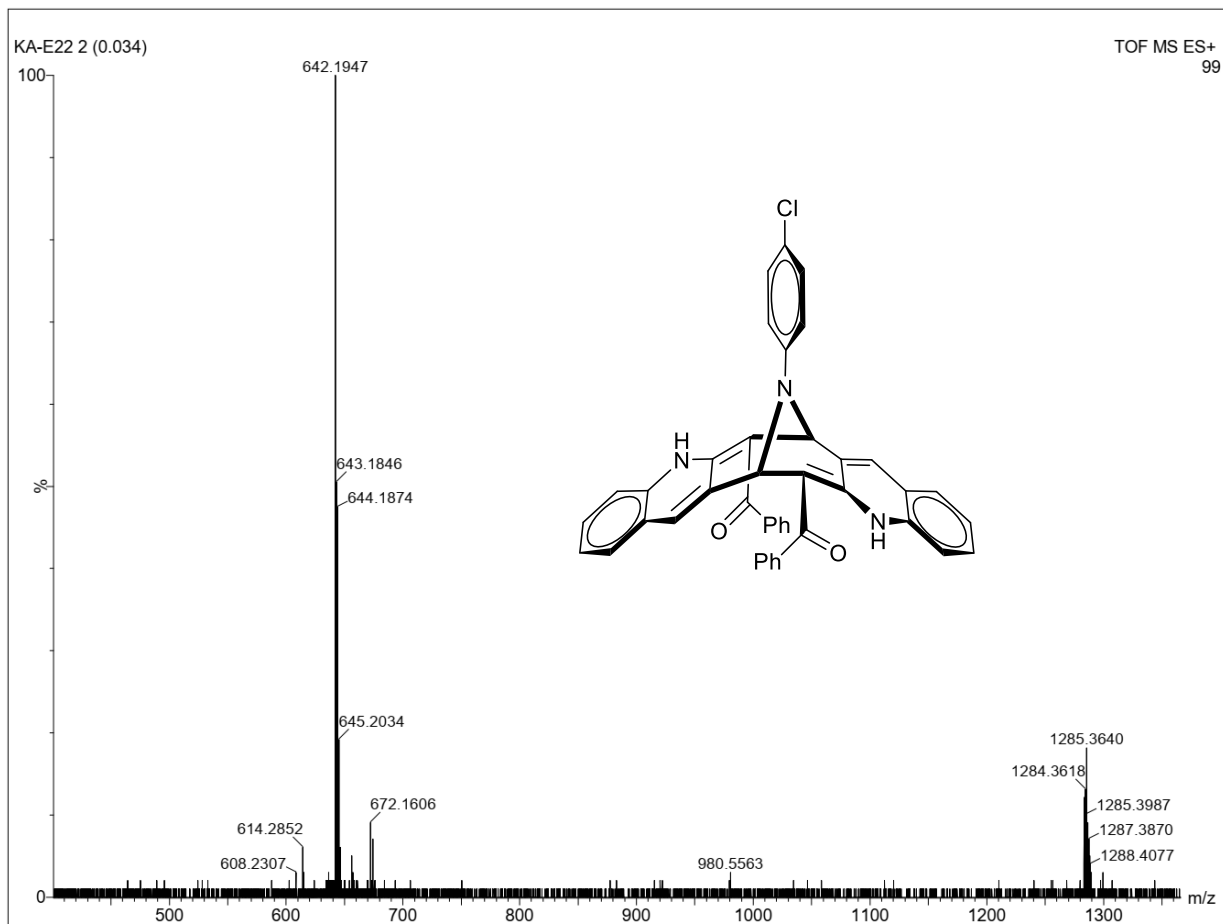


Figure S18: HRMS (ESI) of 3f

Supporting Information

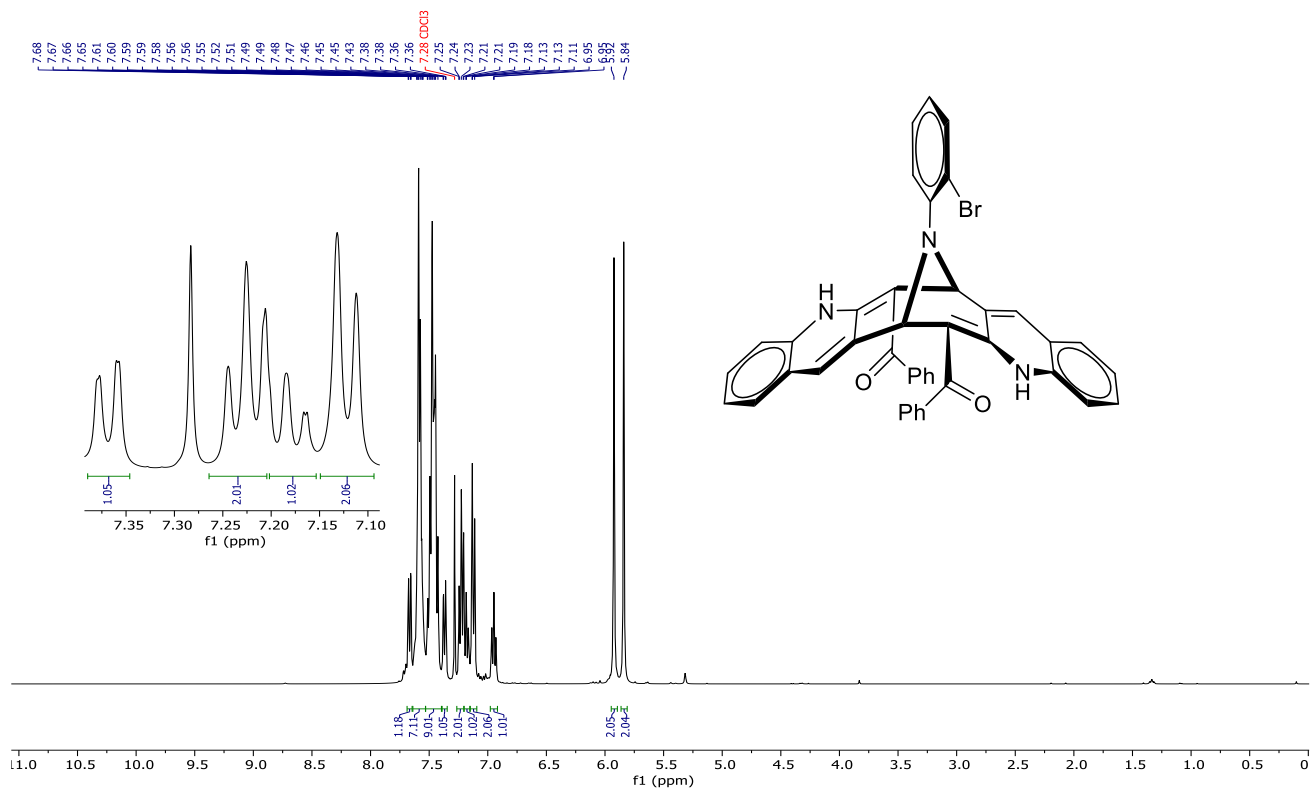


Figure S19: $^1\text{H NMR}$ Compound **3g** (400 MHz, CDCl_3)

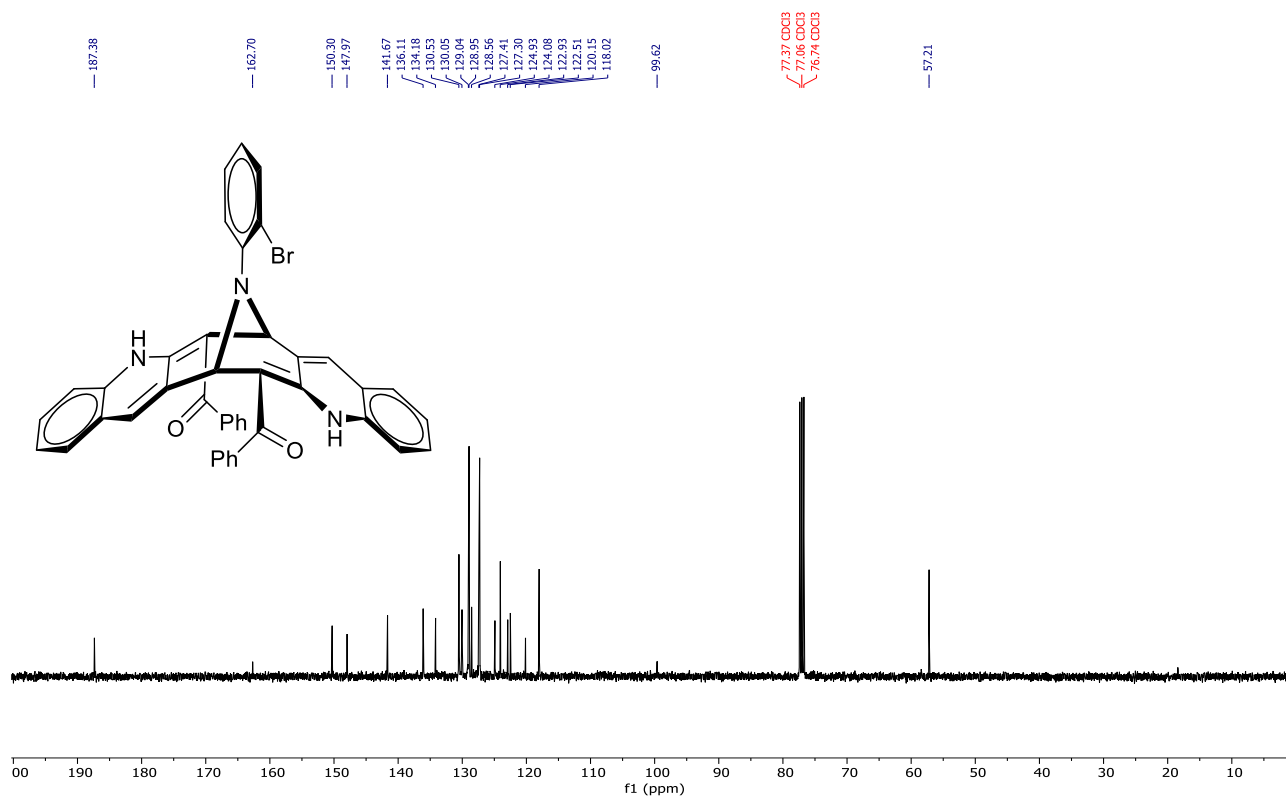
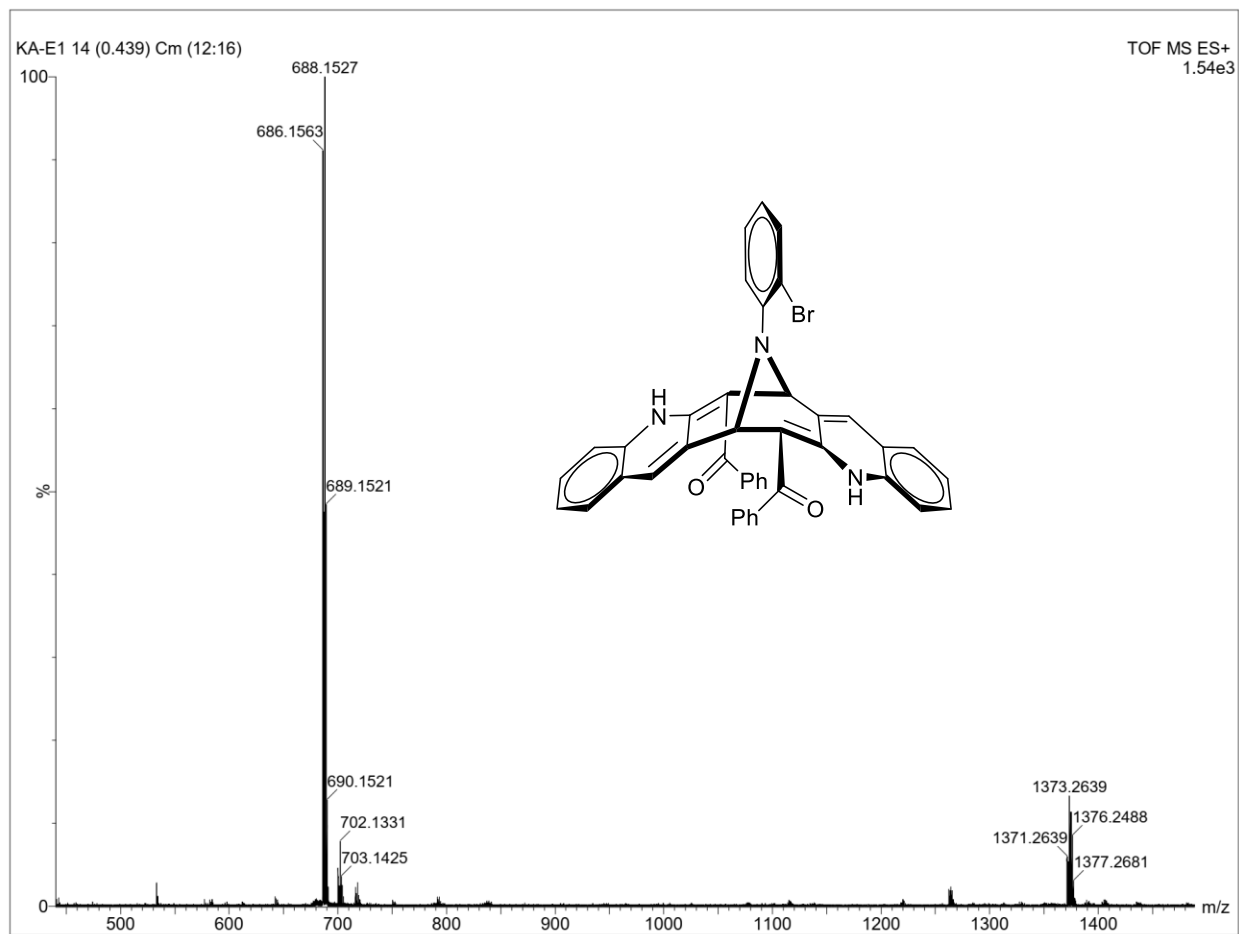


Figure S20: $^{13}\text{C}\{^1\text{H}\}$ NMR Compound **3g** (101 MHz, CDCl_3)

Figure S21: HRMS (ESI) of **3g**

Supporting Information

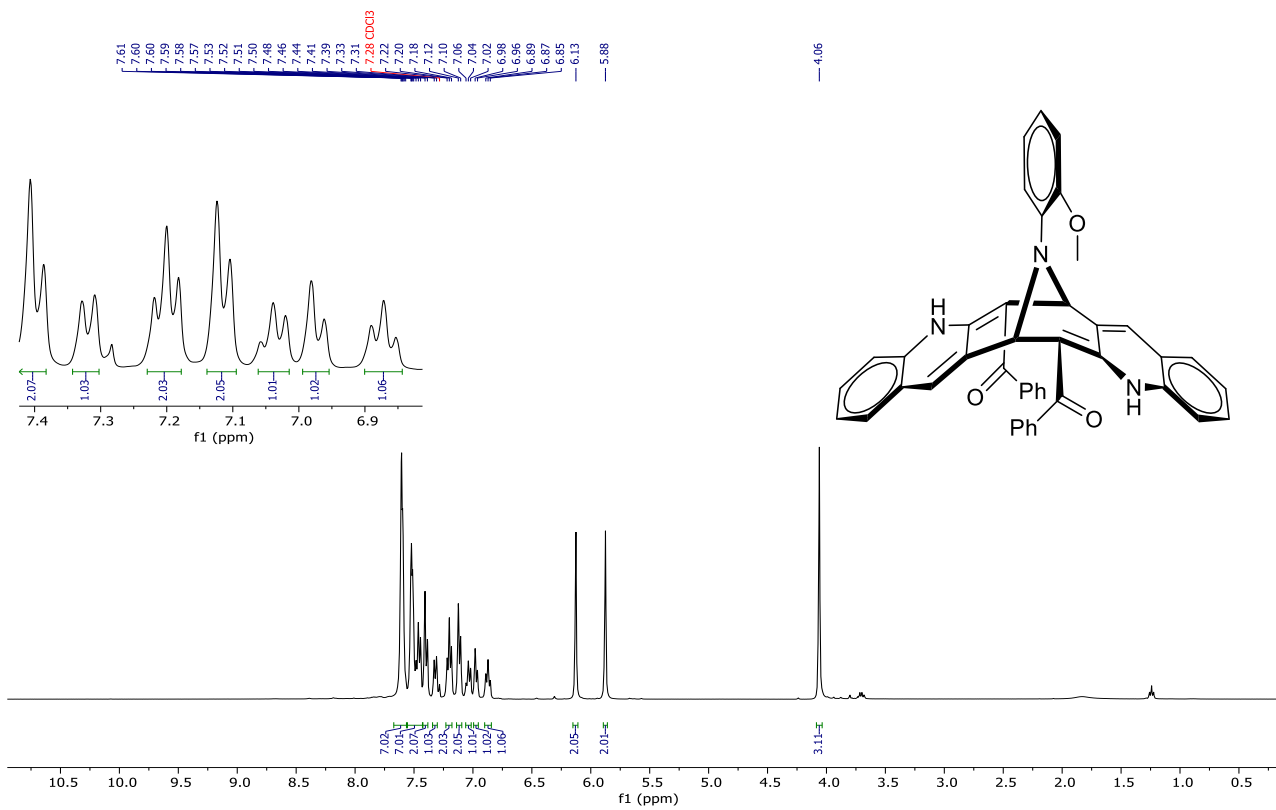


Figure S22: $^1\text{H NMR}$ Compound 3h (400 MHz, CDCl_3)

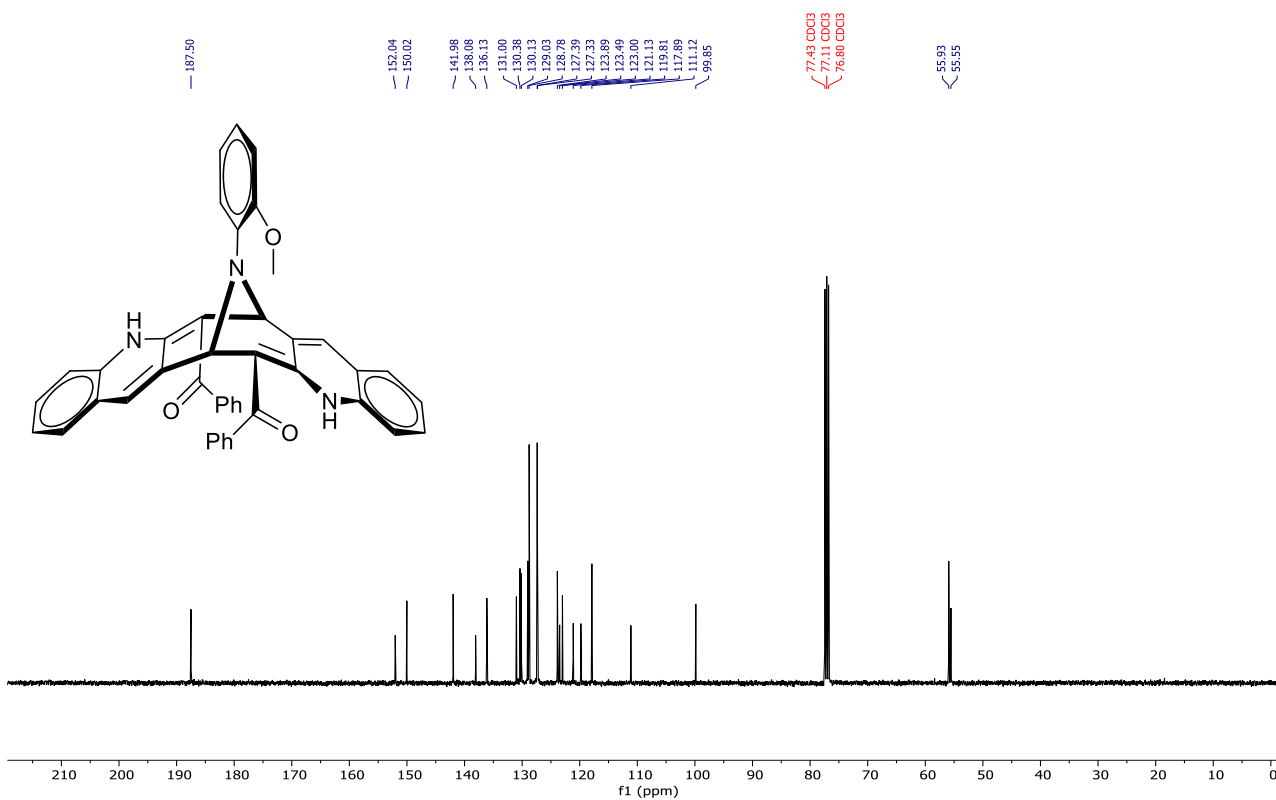
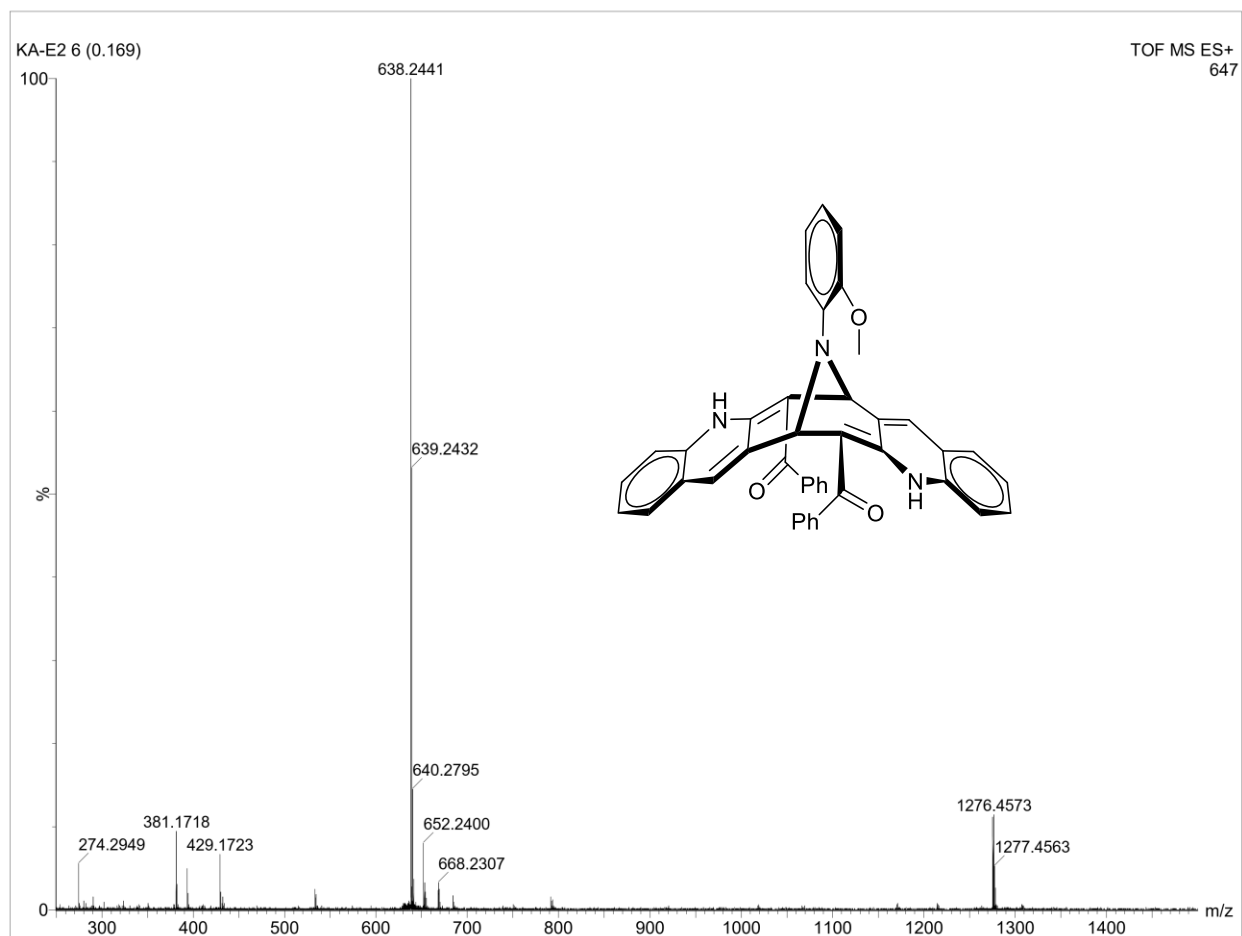


Figure S23: $^{13}\text{C}\{^1\text{H}\}$ NMR Compound 3h (101 MHz, CDCl_3)

Figure S24: HRMS (ESI) of **3h**

Supporting Information

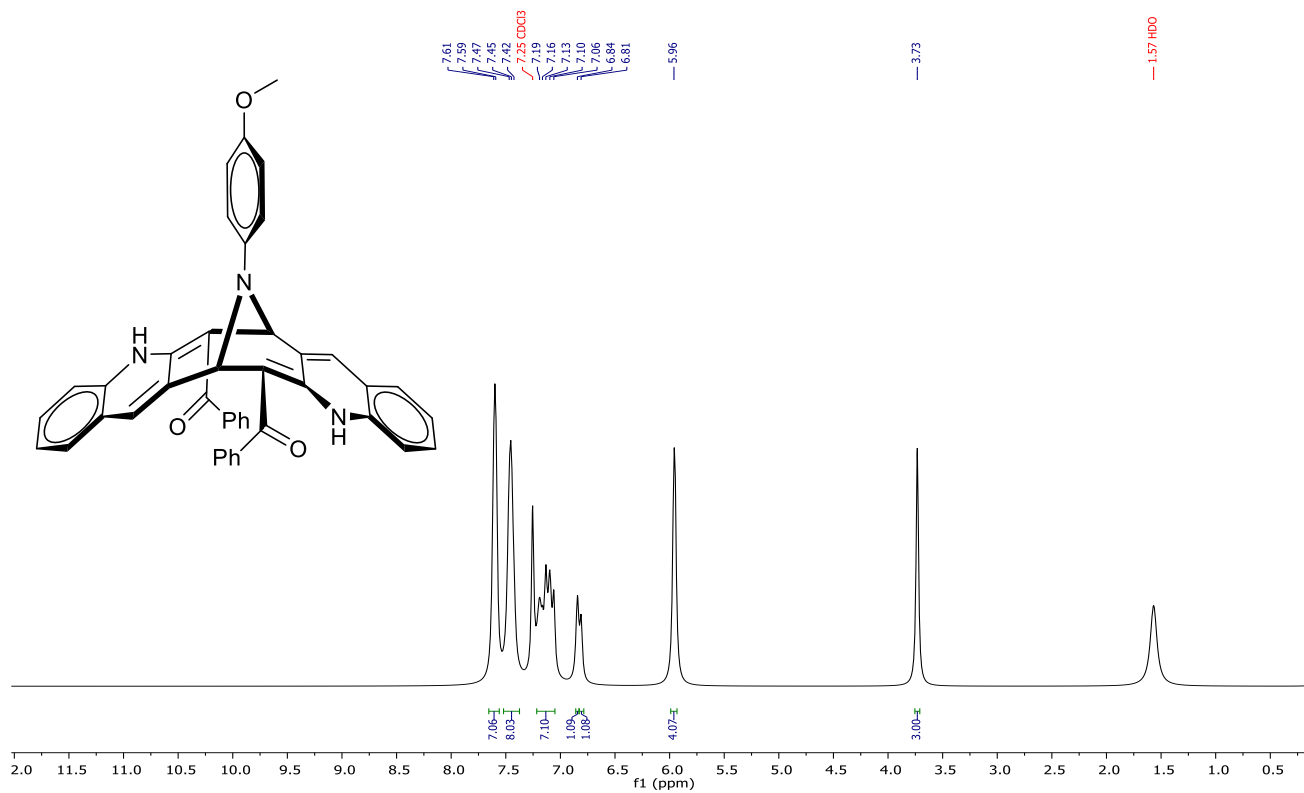


Figure S25: ¹H NMR Compound **3i** (250 MHz, CDCl₃)

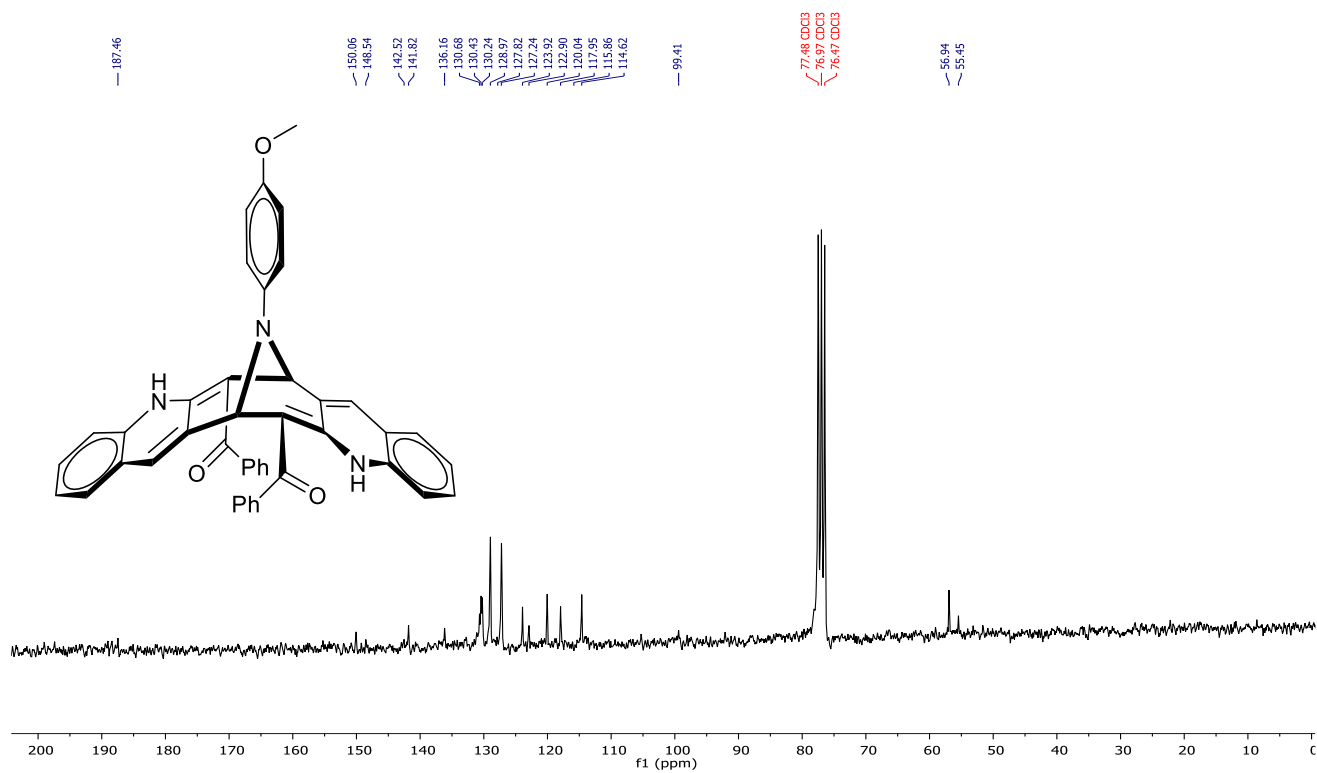


Figure S26: ¹³C{¹H}NMR Compound **3i** (63 MHz, CDCl₃)

Supporting Information

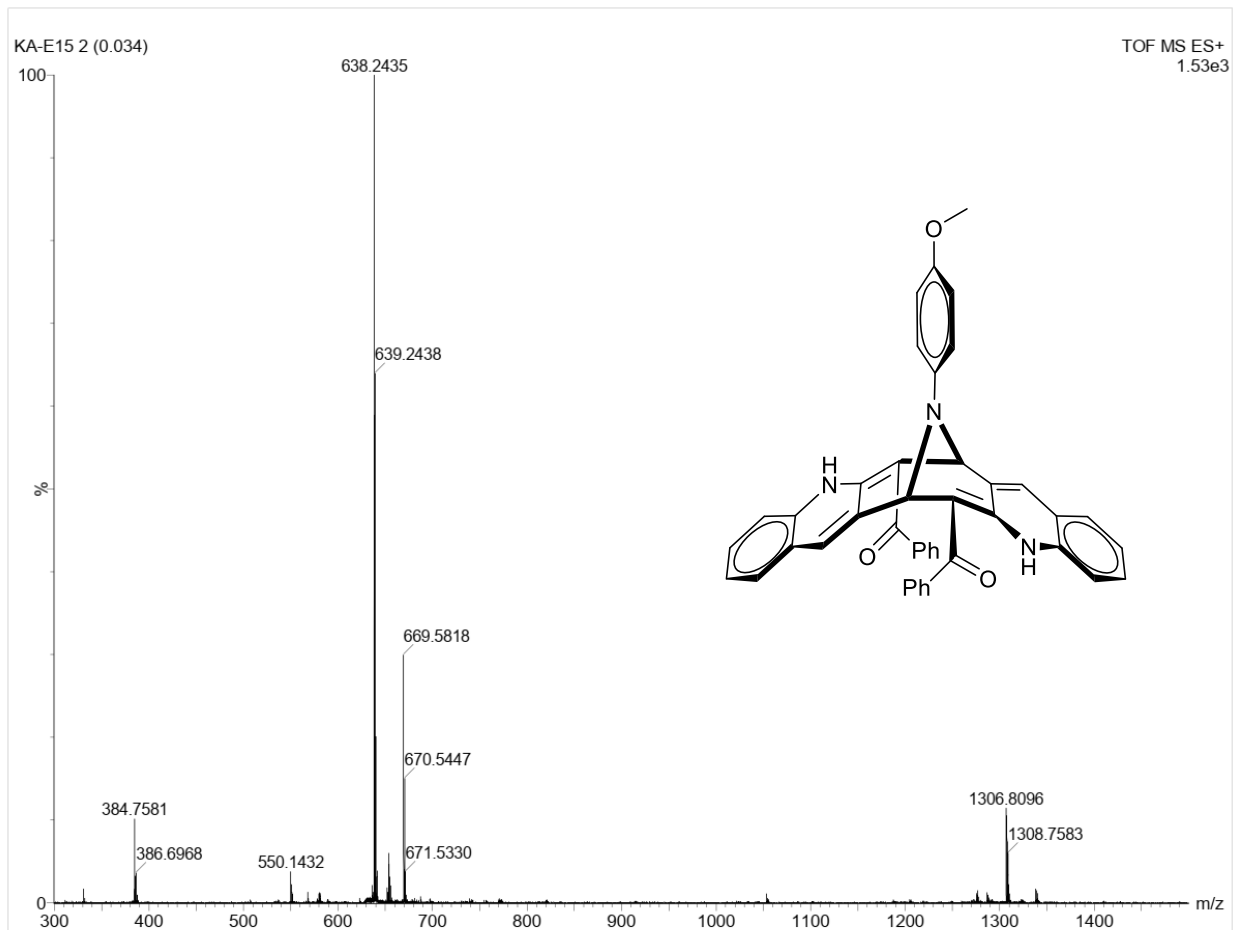


Figure S27: HRMS (ESI) of **3i**

Supporting Information

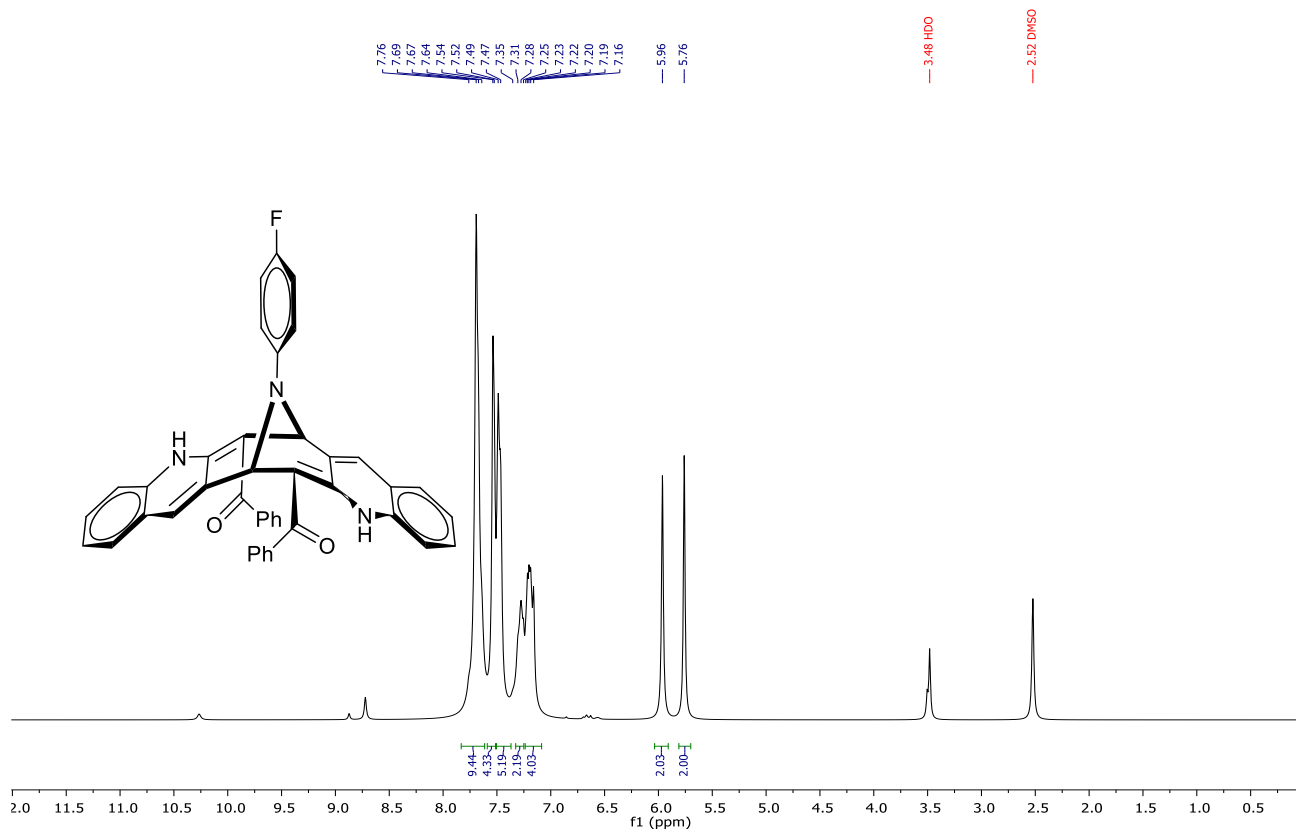


Figure S28: ¹H NMR Compound 3j (300 MHz, DMSO-*d*₆)

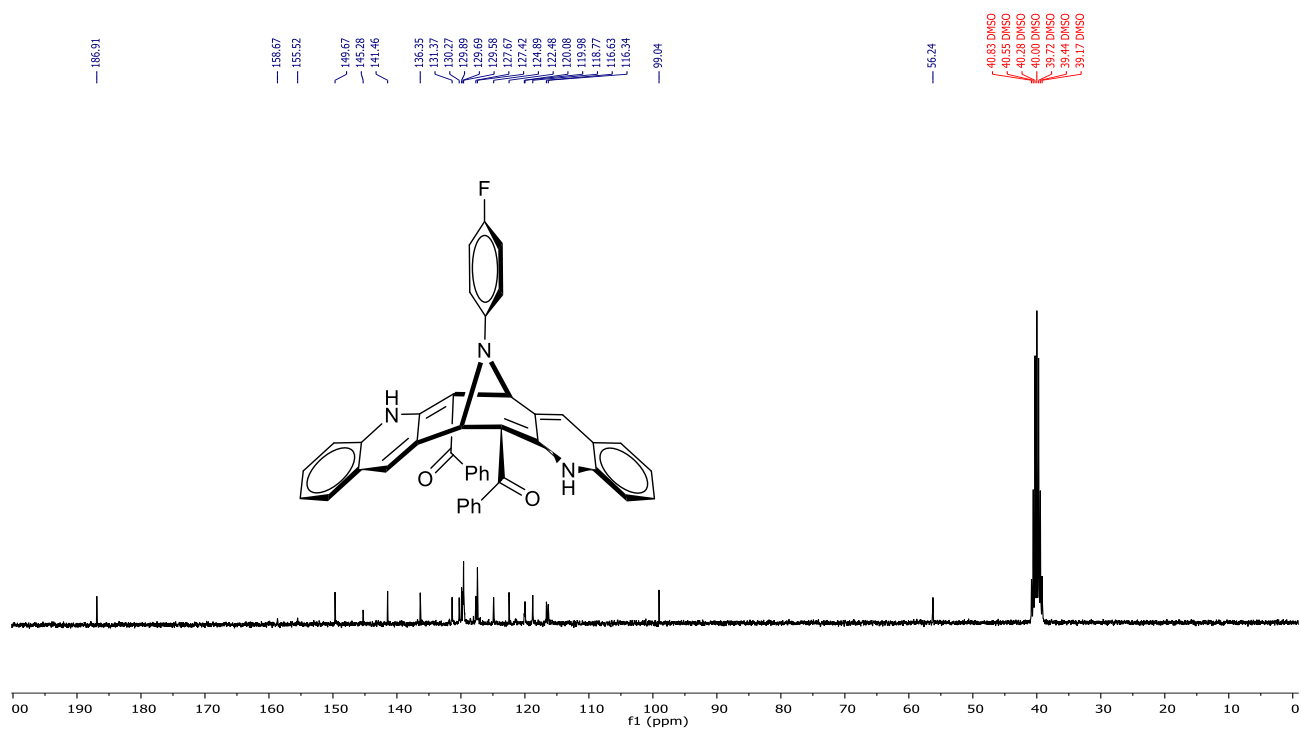
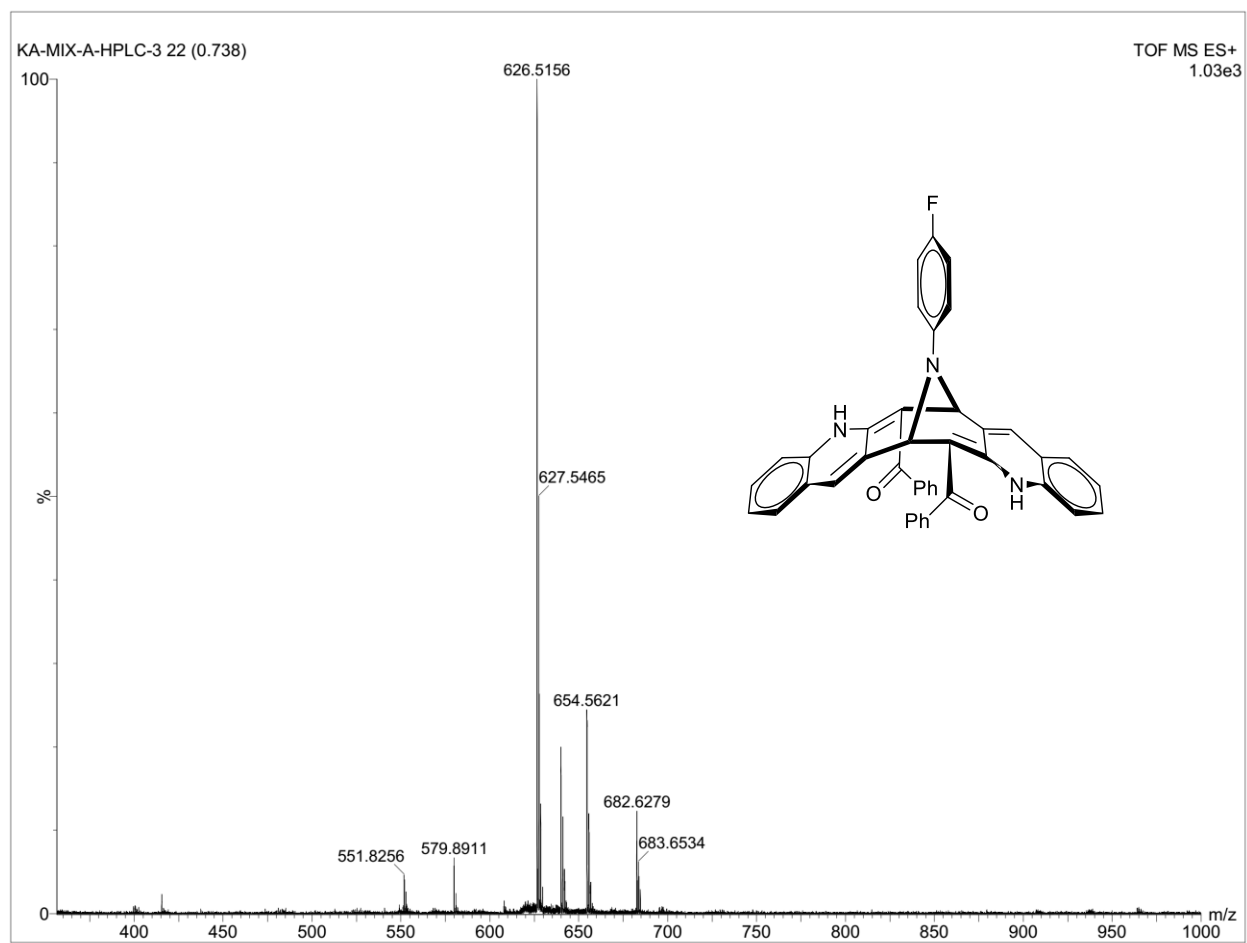


Figure S29: ¹³C{¹H} NMR Compound 3j (76 MHz, DMSO-*d*₆)

Figure S30: HRMS (ESI) of **3j**

Supporting Information

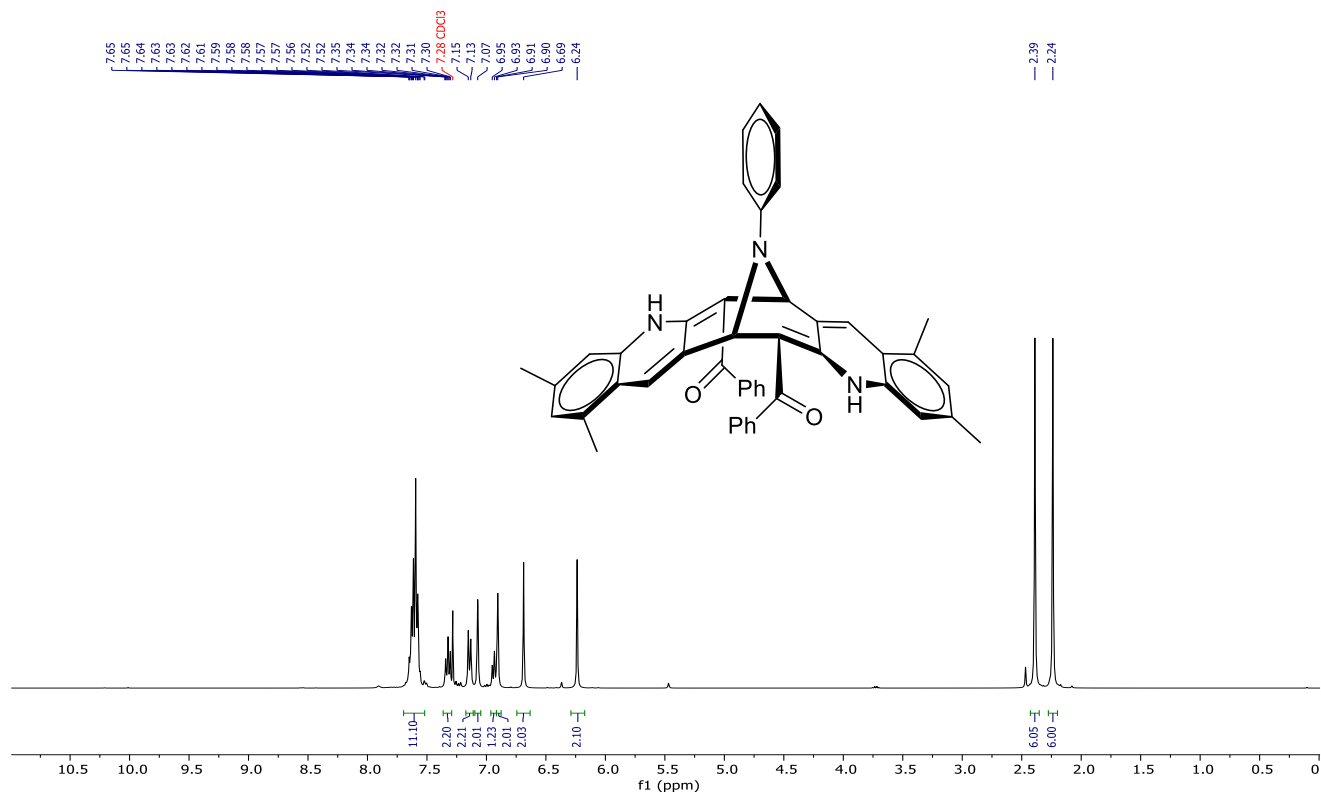


Figure S31: ^1H NMR Compound 3k (400 MHz, CDCl_3)

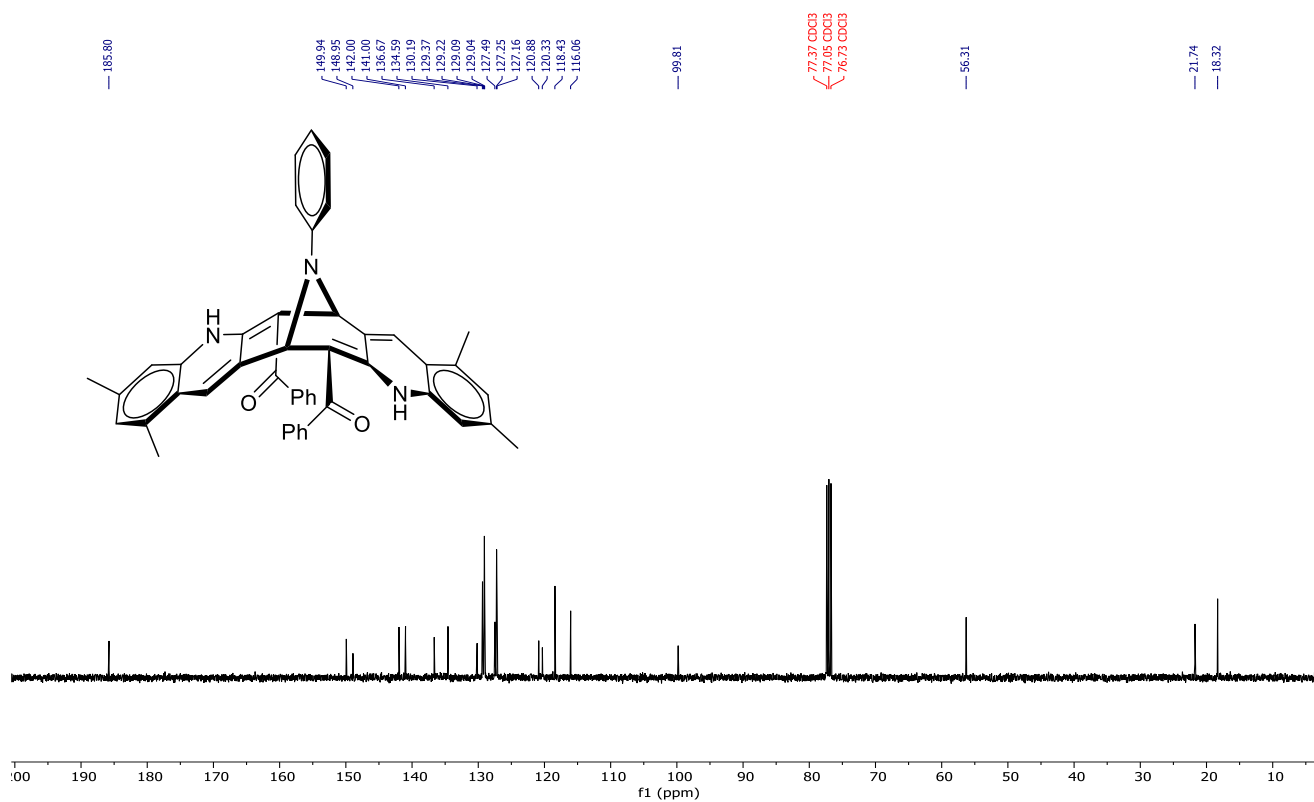
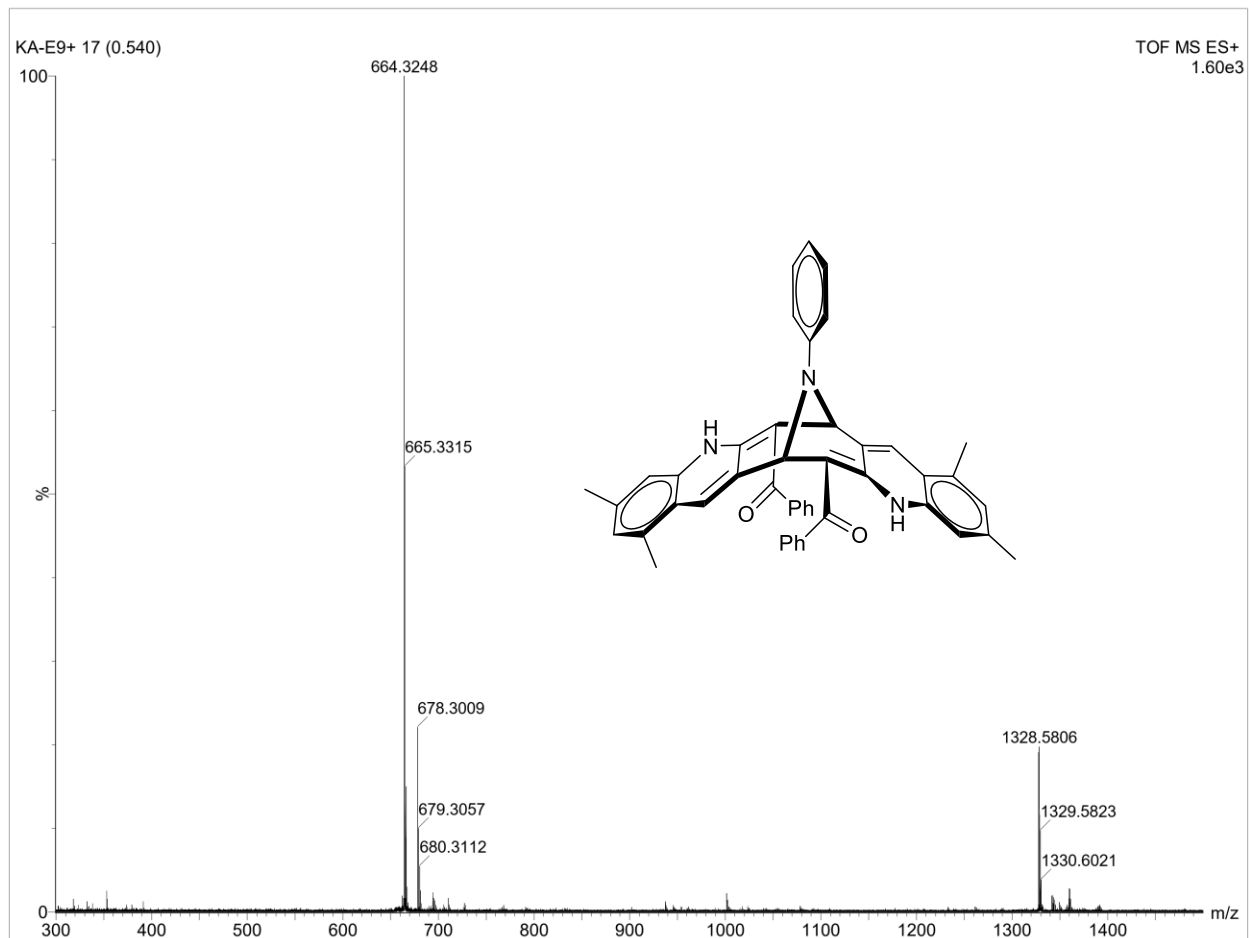


Figure S32: $^{13}\text{C}\{^1\text{H}\}$ NMR Compound 3k (101 MHz, CDCl_3)

Figure S33: HRMS (ESI) of **3k**

Supporting Information

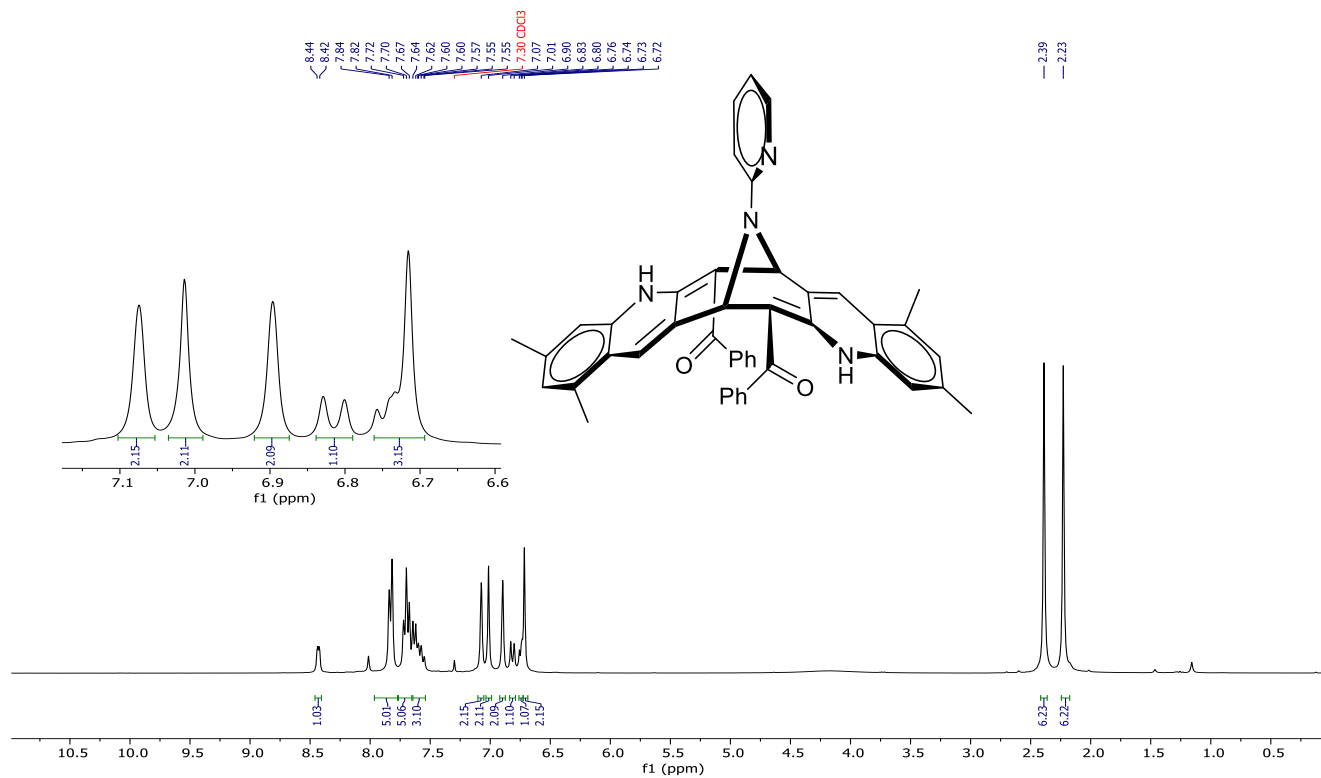


Figure S34: ^1H NMR Compound 31 (300 MHz, CDCl_3)

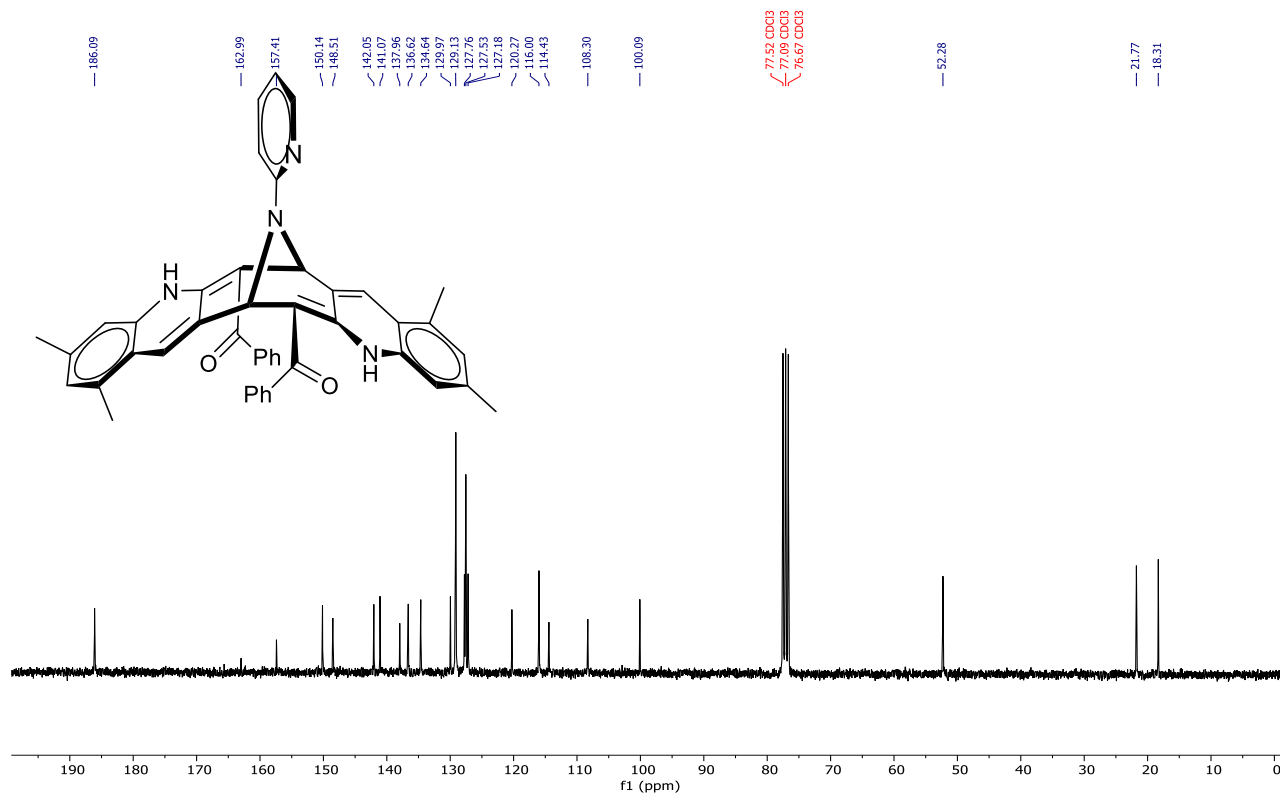
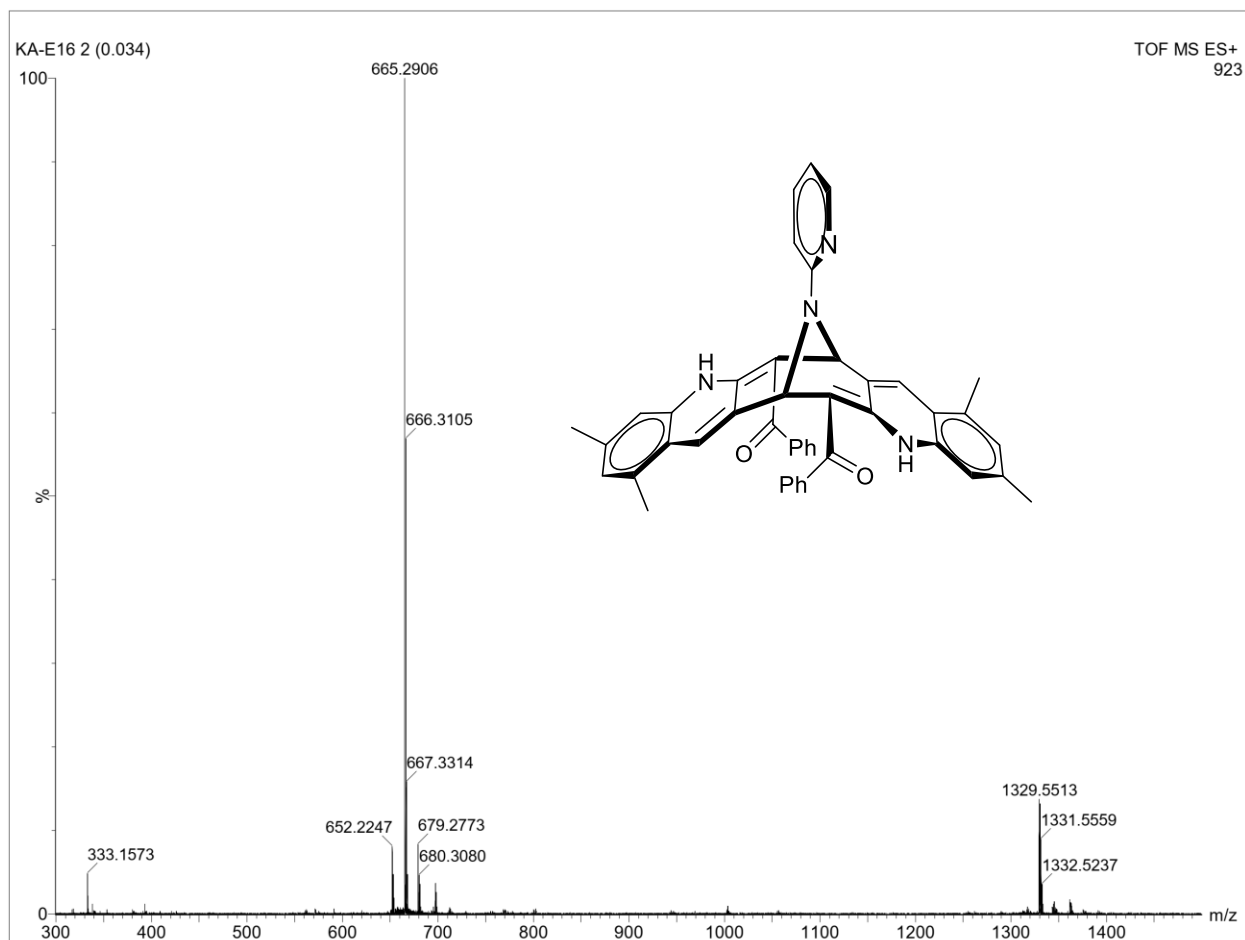


Figure S35: $^{13}\text{C}\{^1\text{H}\}$ NMR Compound 31 (75 MHz, CDCl_3)

Figure S36: HRMS (ESI) of **31**

Supporting Information

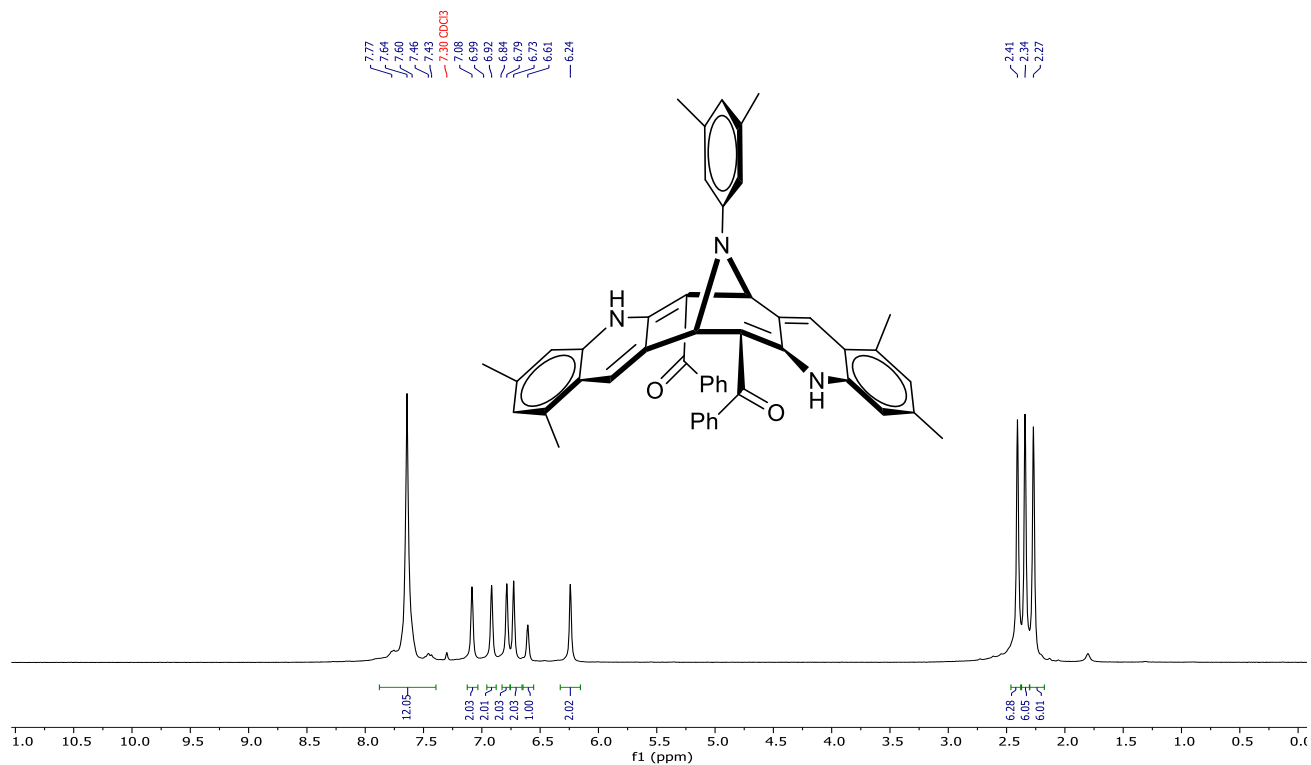


Figure S37: ^1H NMR Compound **3m** (300 MHz, CDCl_3)

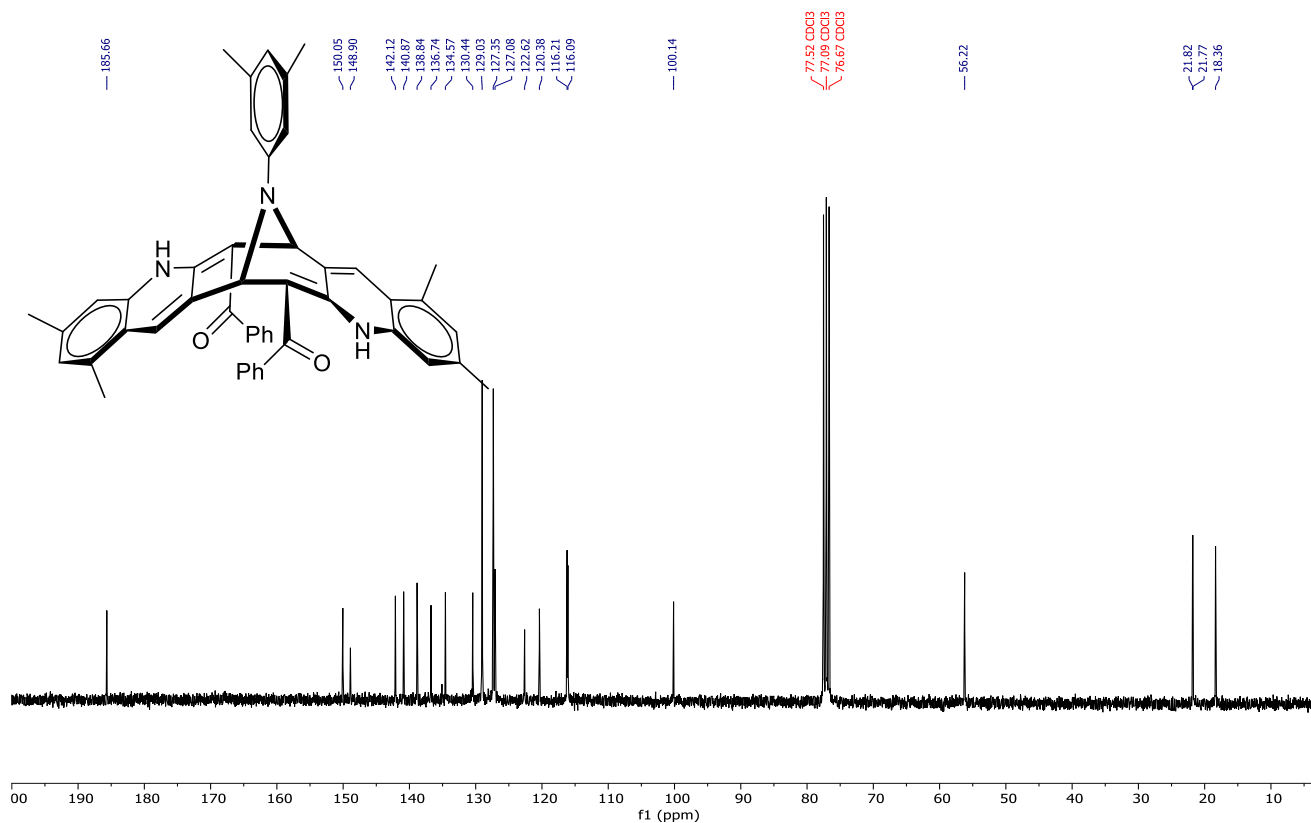


Figure S38: $^{13}\text{C}\{^1\text{H}\}$ NMR Compound **3m** (75 MHz, CDCl_3)

Supporting Information

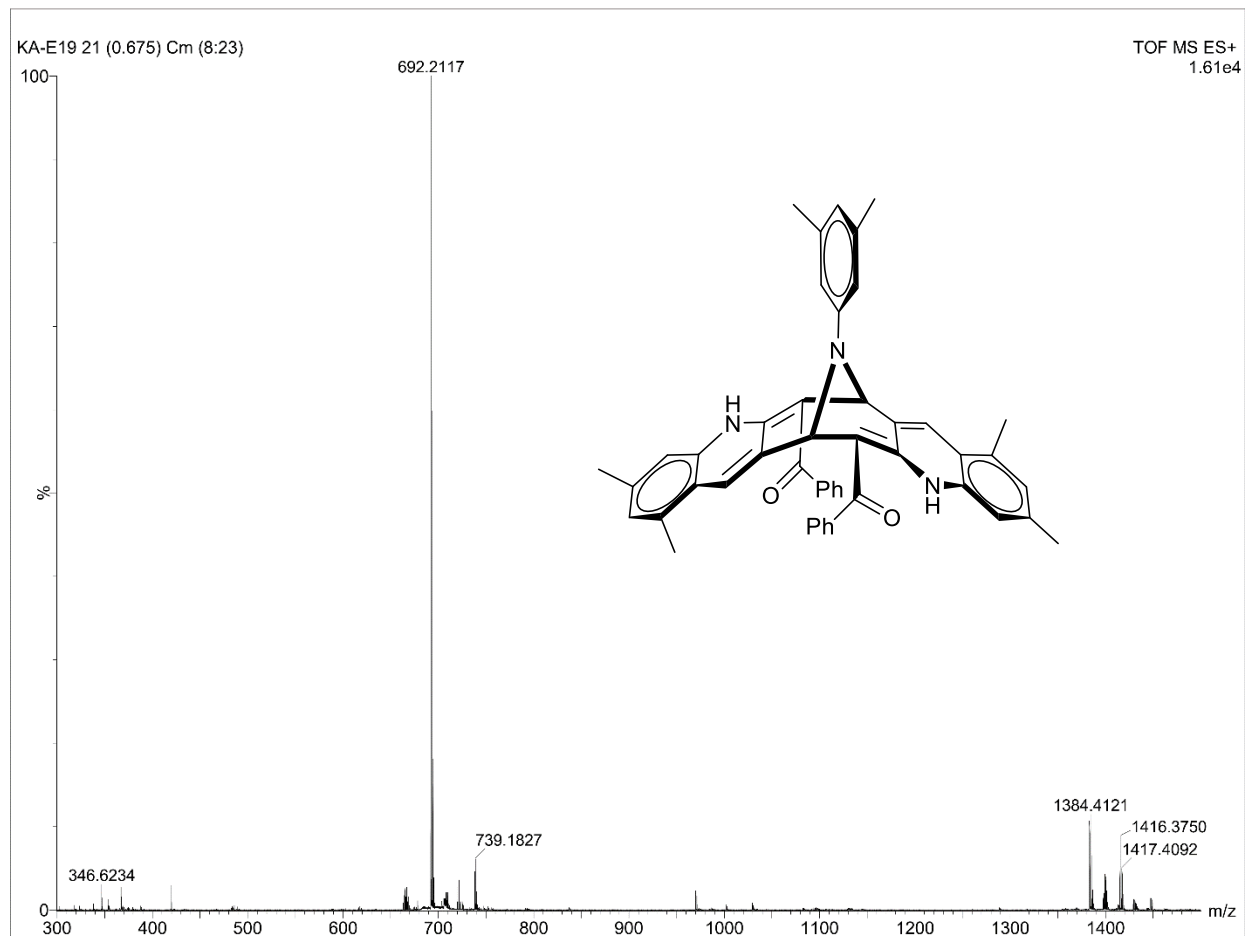
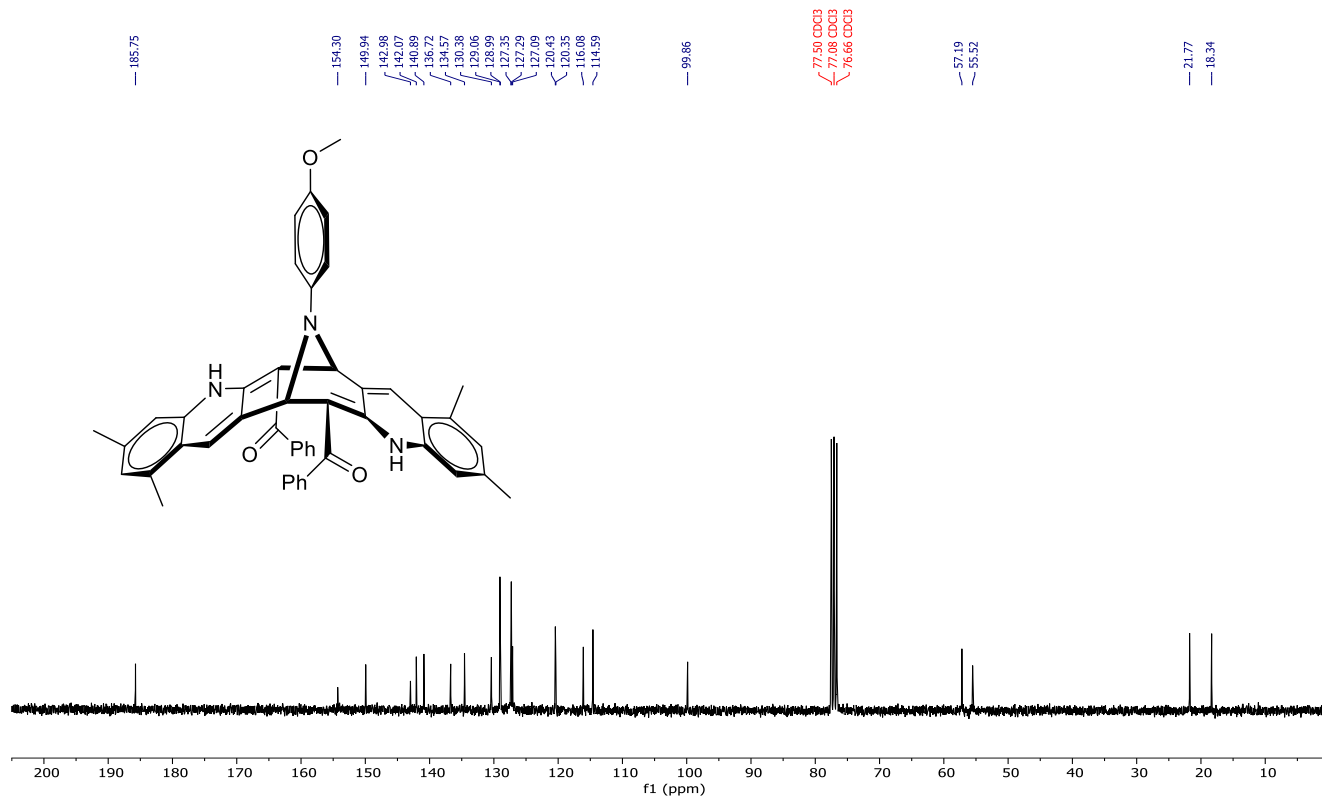
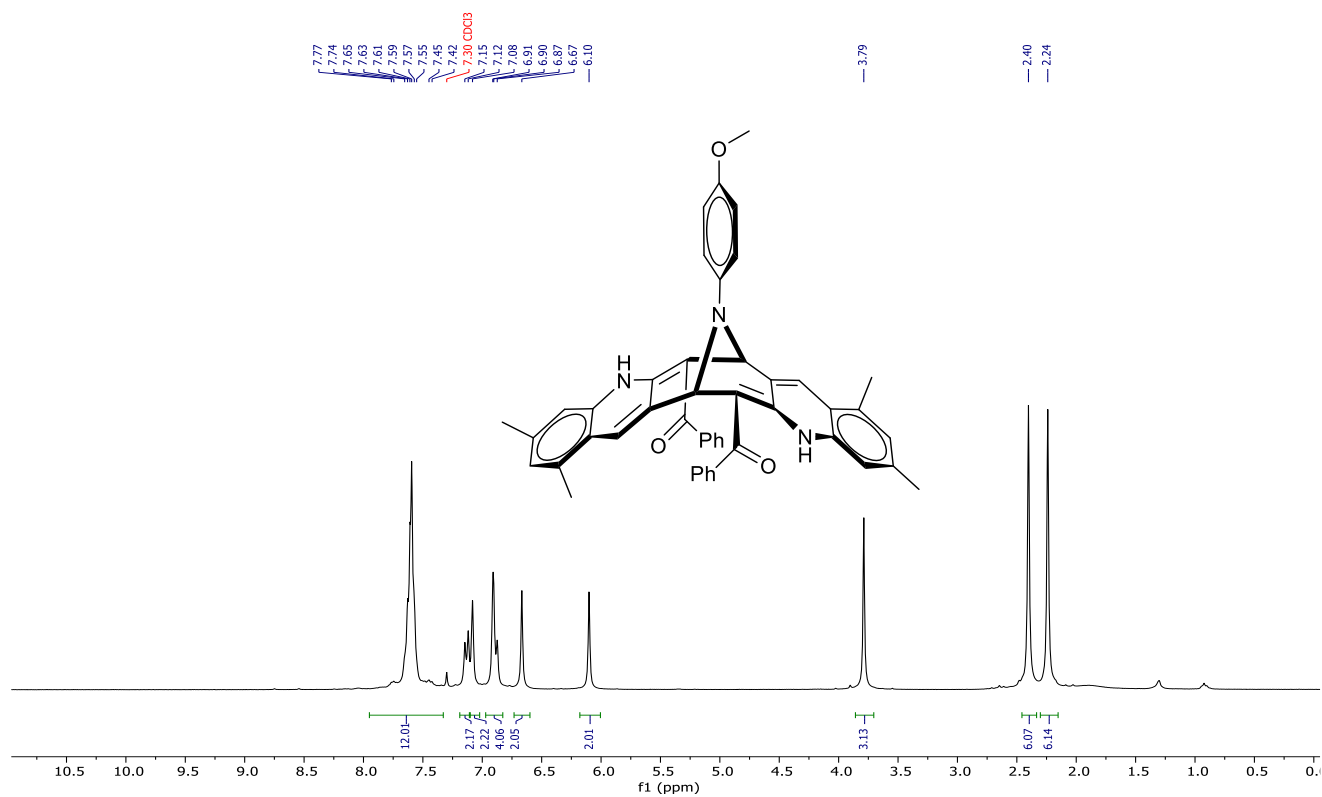
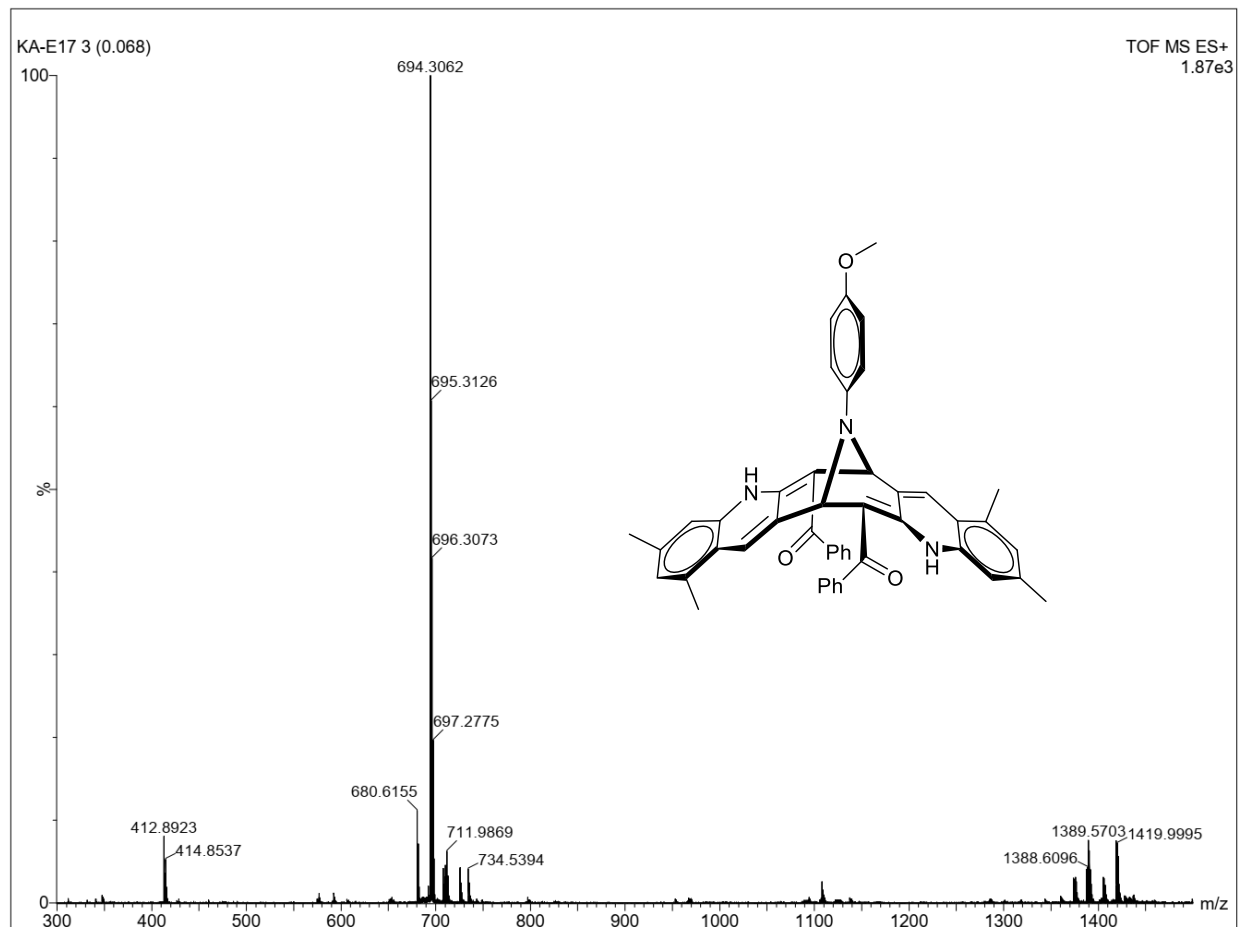


Figure S39 : HRMS (ESI) of **3m**

Supporting Information



Figure S42: HRMS (ESI) of **3n**

Supporting Information

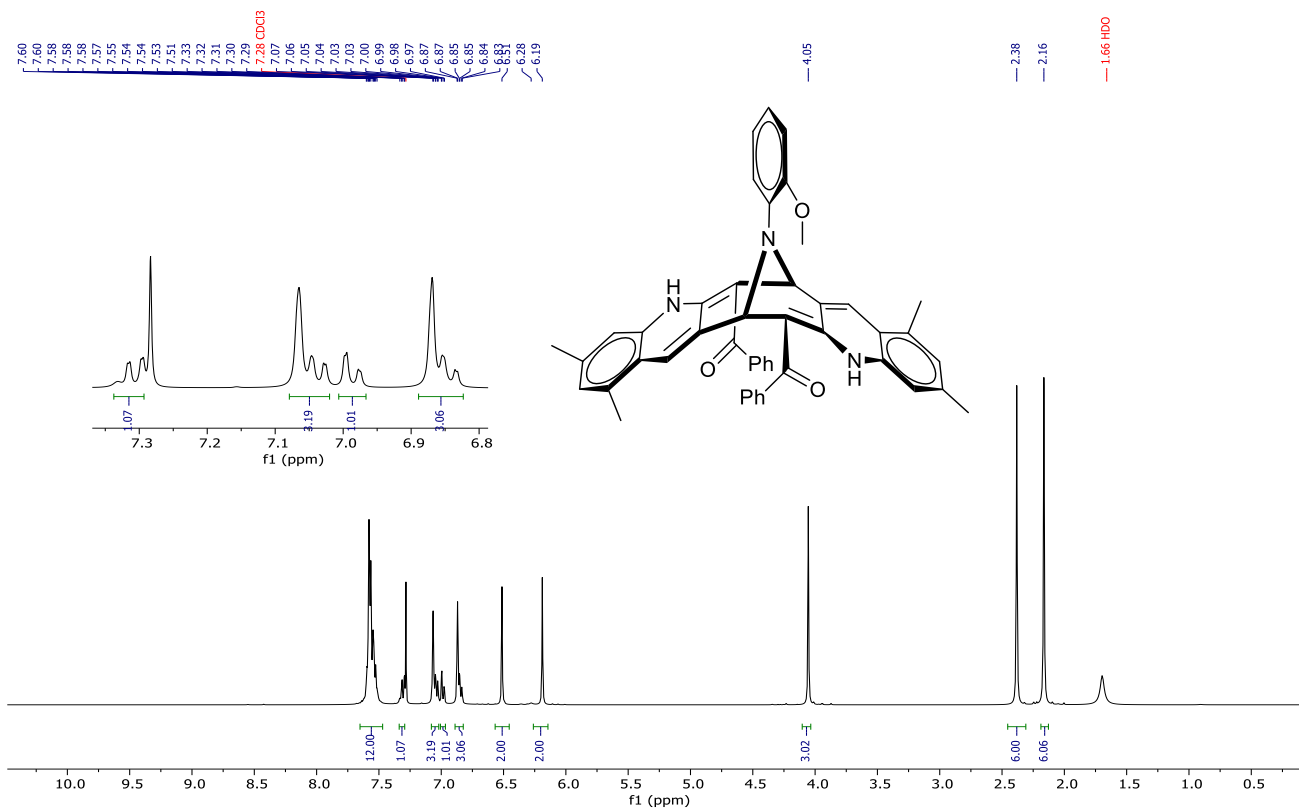


Figure S43: ^1H NMR Compound **3o** (400 MHz, CDCl_3)

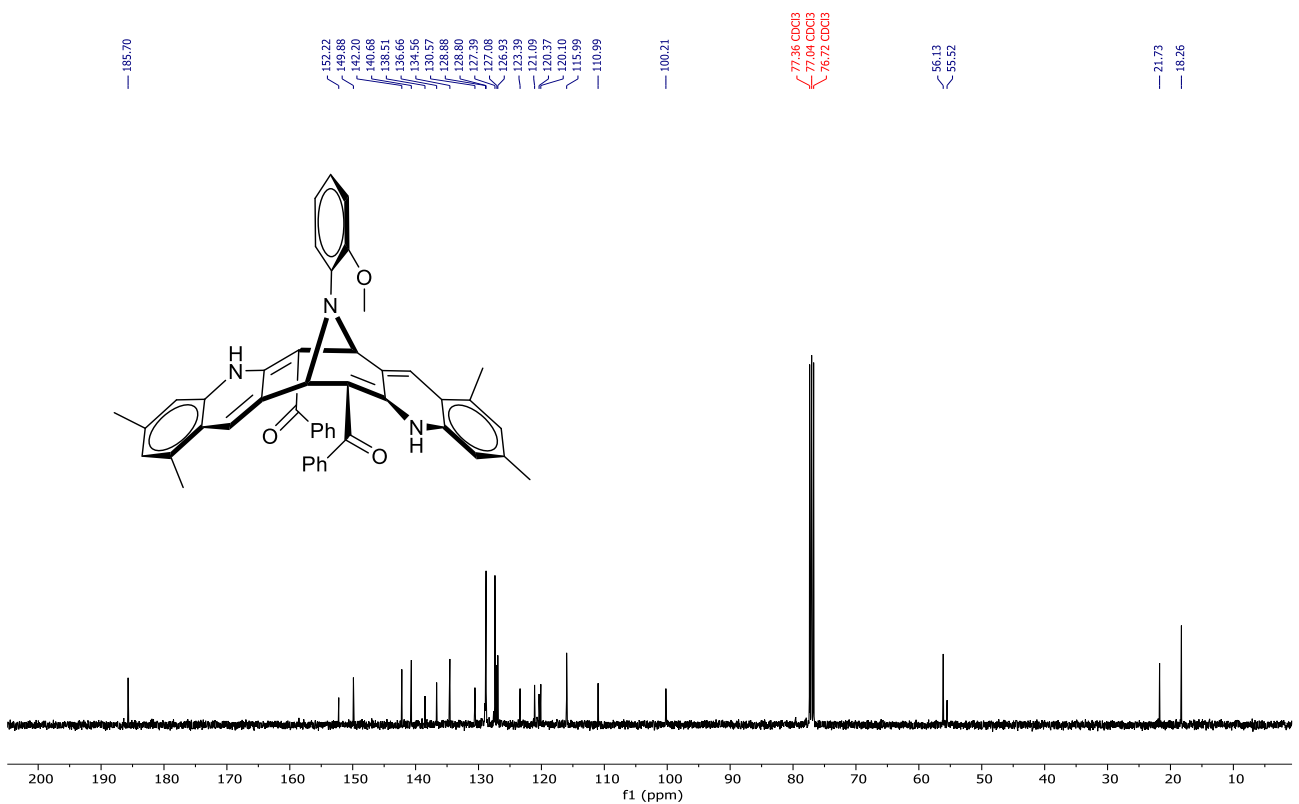
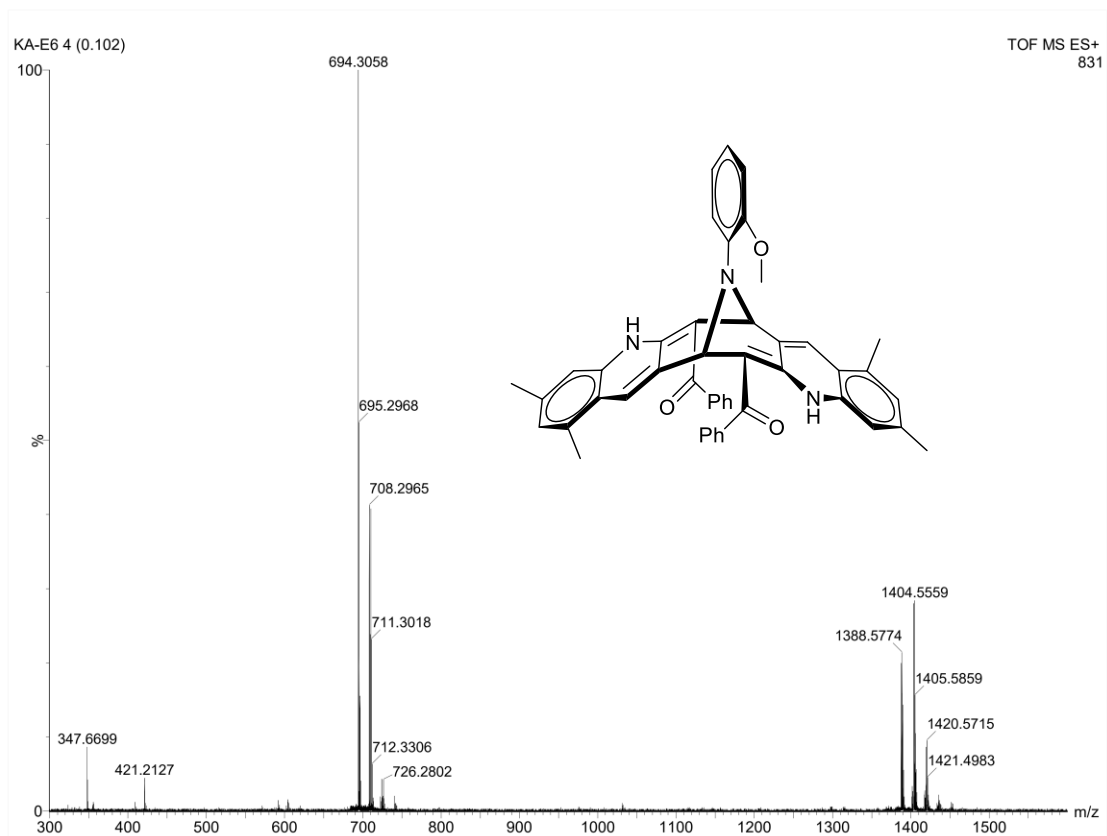


Figure S44: $^{13}\text{C}\{^1\text{H}\}$ NMR Compound **3o** (101 MHz, CDCl_3)

Figure S45: HRMS (ESI) of **3o**

Supporting Information

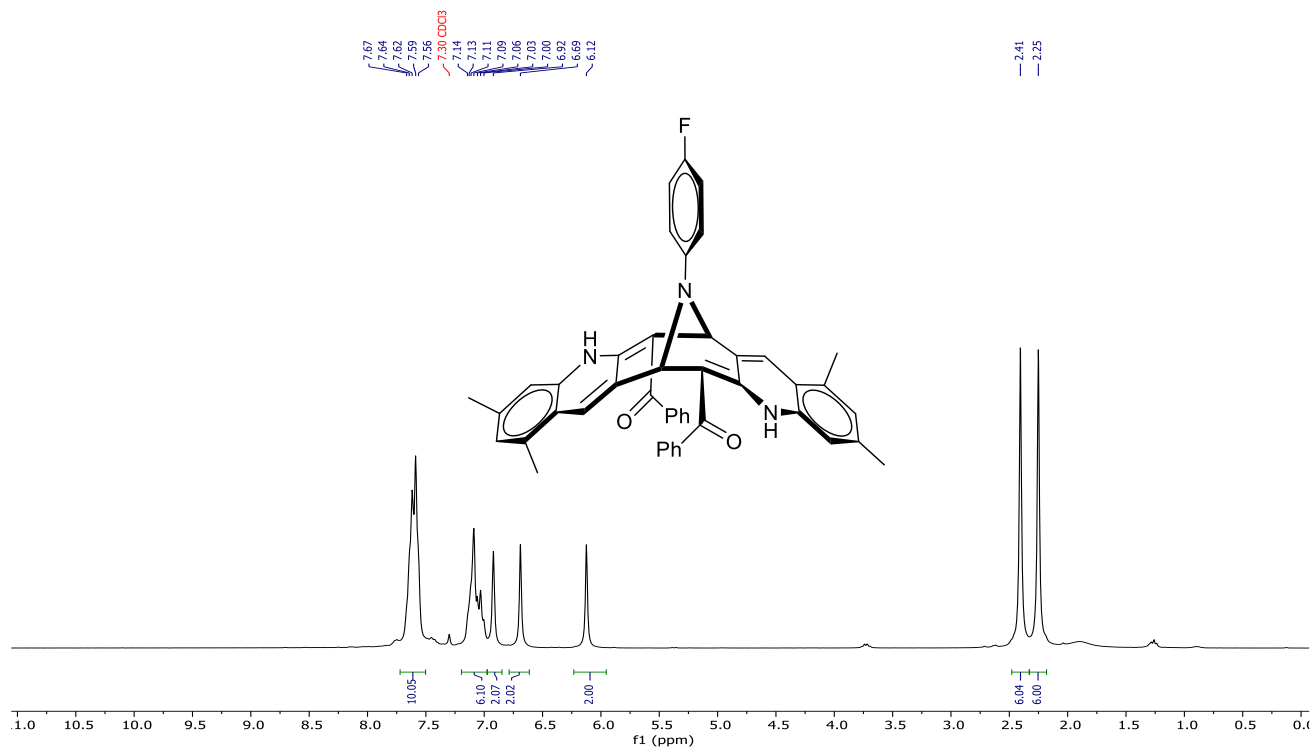


Figure S46: ¹H NMR Compound 3p (300 MHz, CDCl₃)

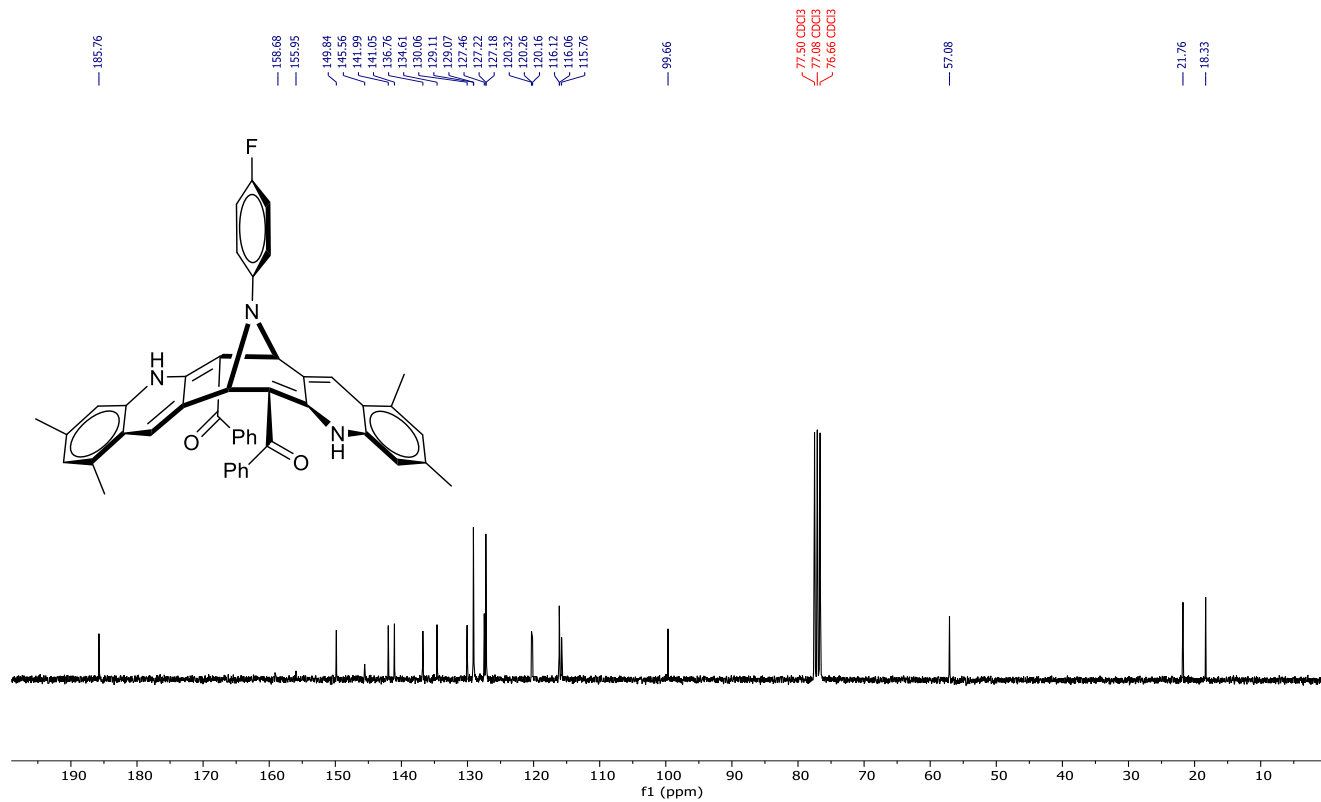


Figure S47: ¹³C {¹H} NMR Compound 3p (75 MHz, CDCl₃)

Supporting Information

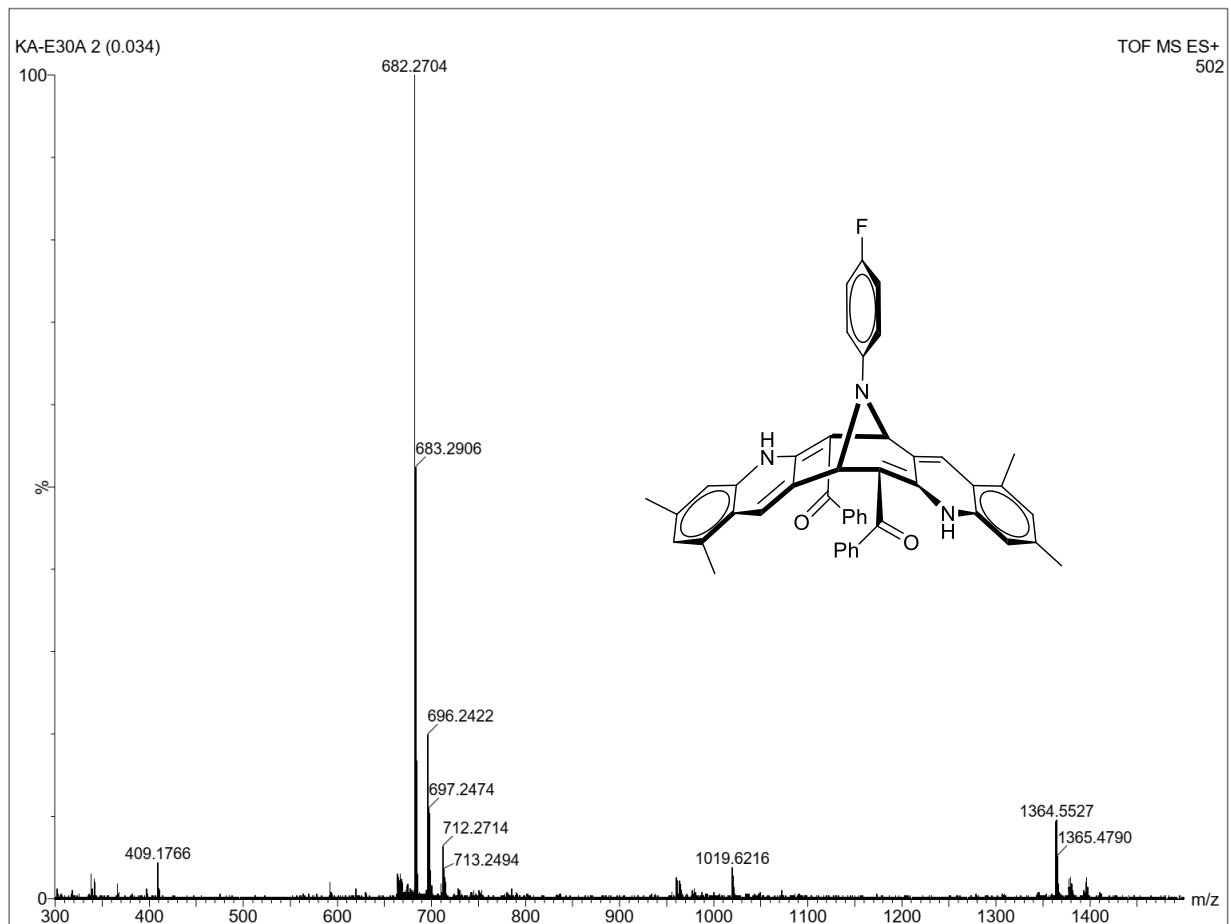


Figure S48: HRMS (ESI) of **3p**

Supporting Information

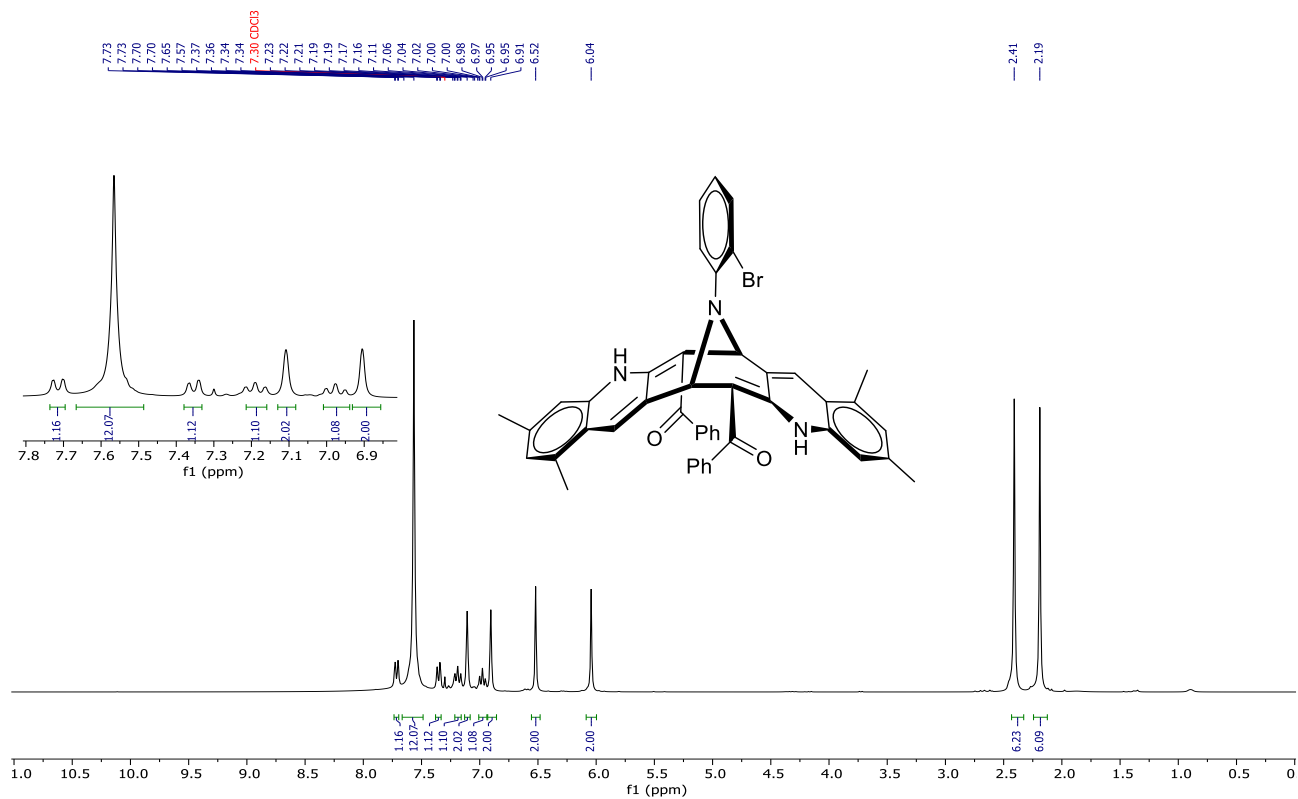


Figure S49: ^1H NMR Compound **3q** (300 MHz, CDCl_3)

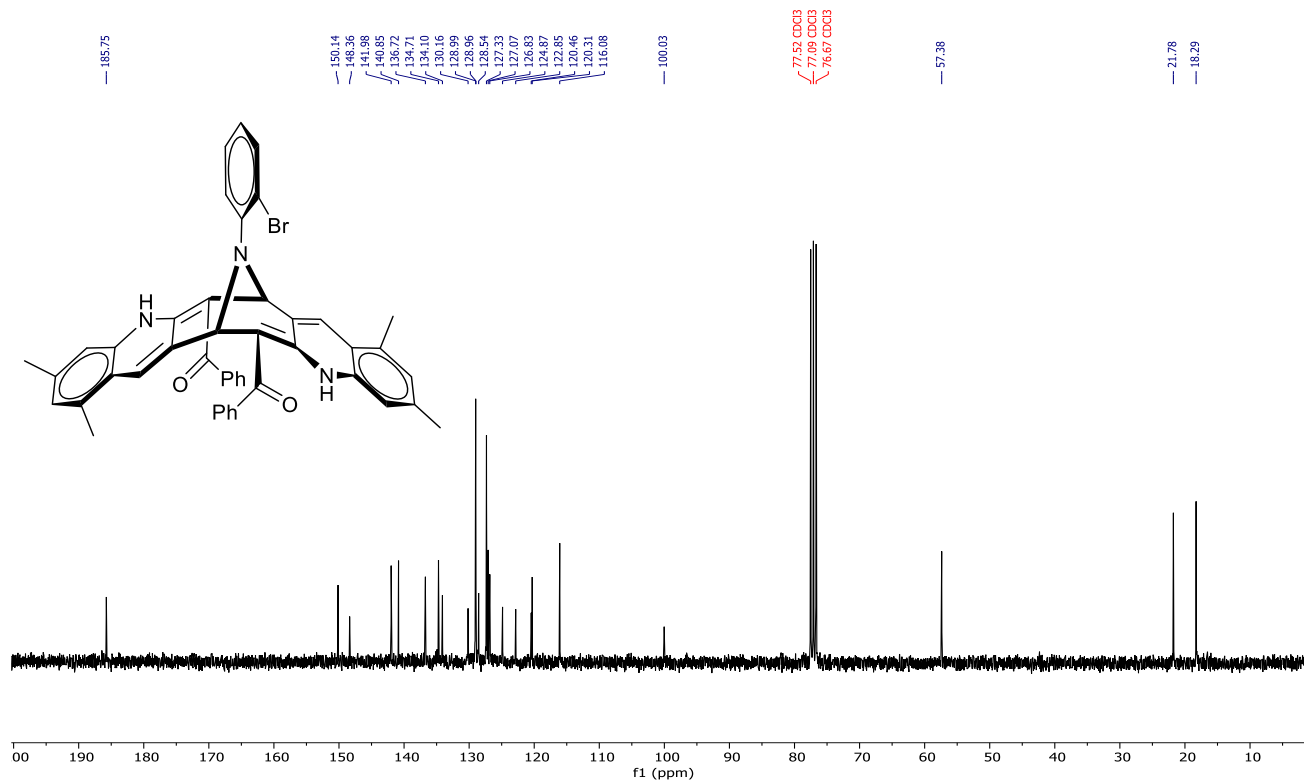
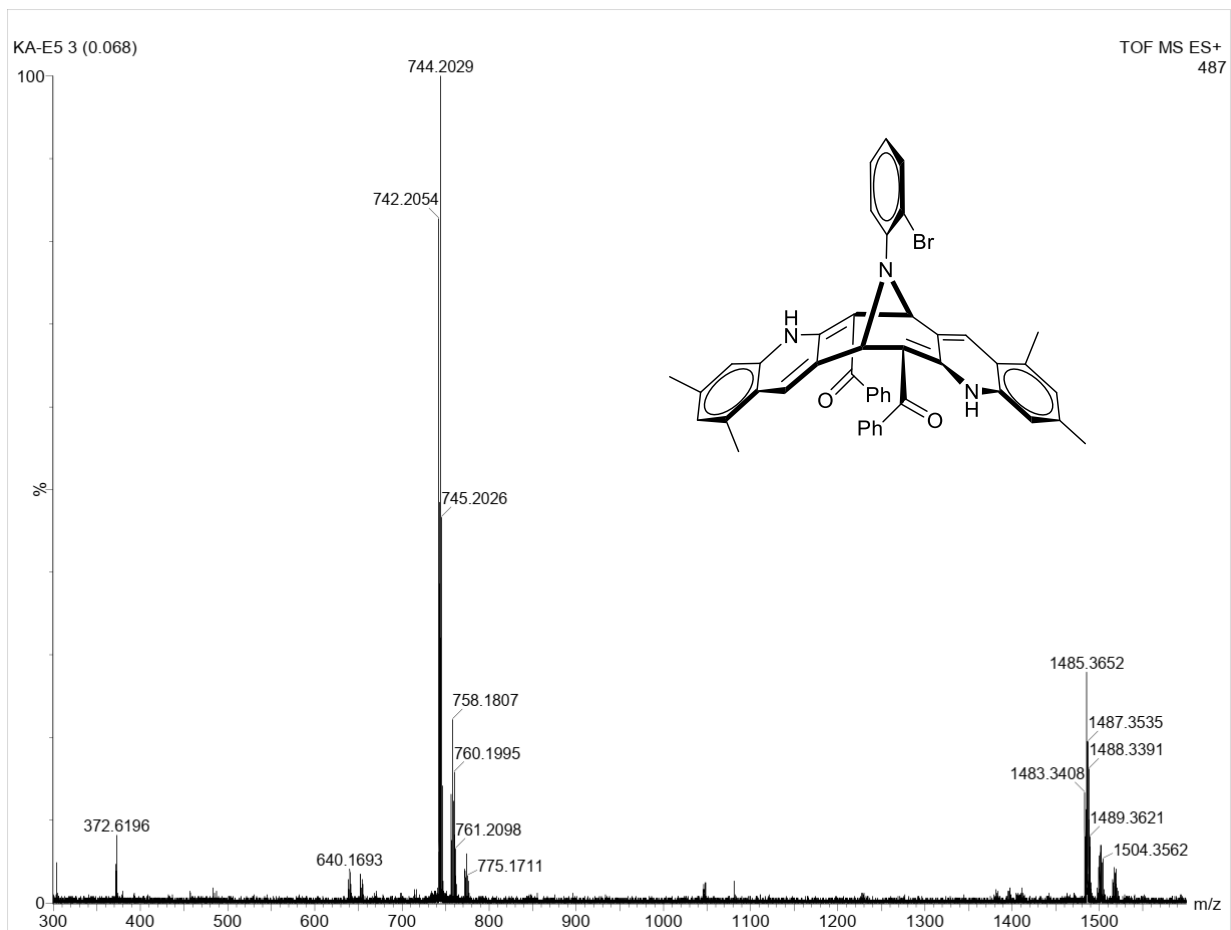


Figure S50: $^{13}\text{C}\{^1\text{H}\}$ NMR Compound **3q** (75 MHz, CDCl_3)

Figure S51: HRMS (ESI) of **3q**

Supporting Information

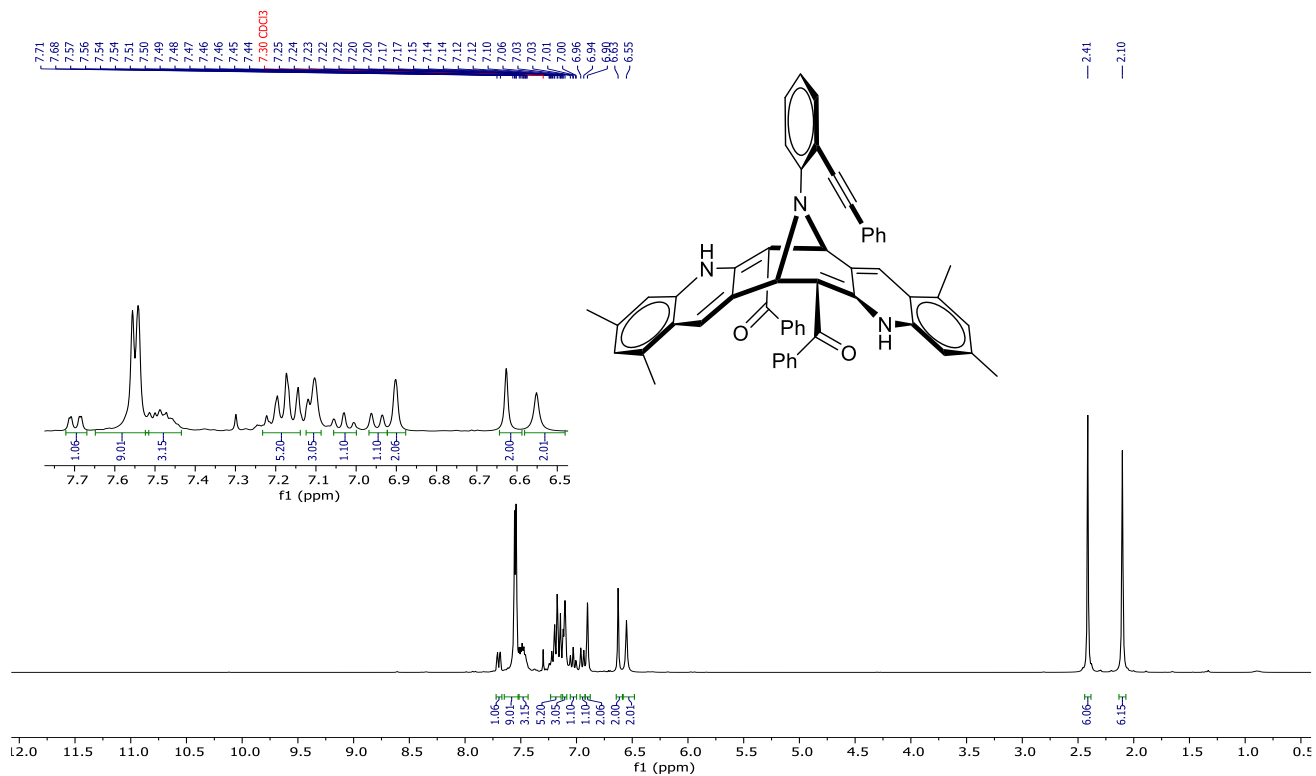


Figure S52: ¹H NMR Compound 3r (300 MHz, CDCl₃)

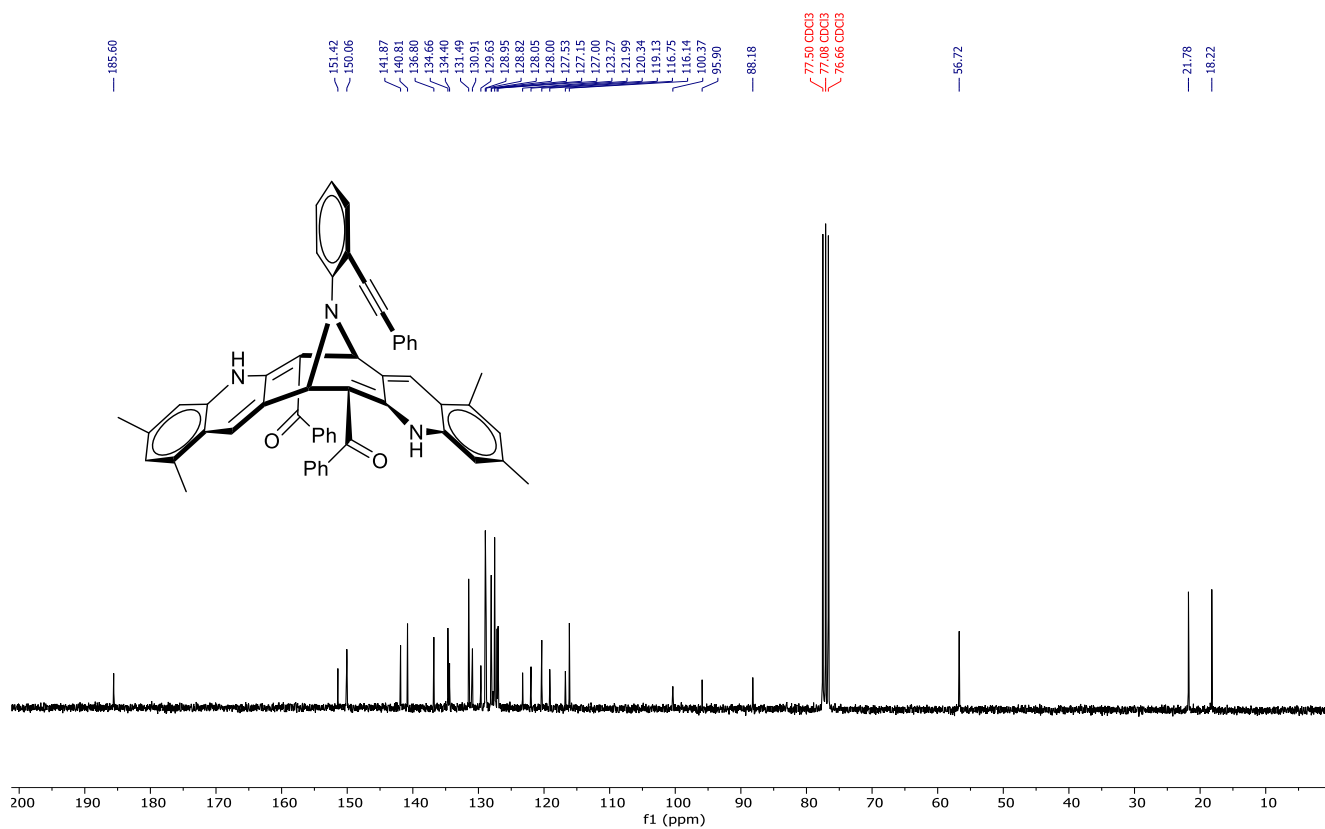


Figure S53: ¹³C{¹H}NMR Compound 3r (75 MHz, CDCl₃)

Supporting Information

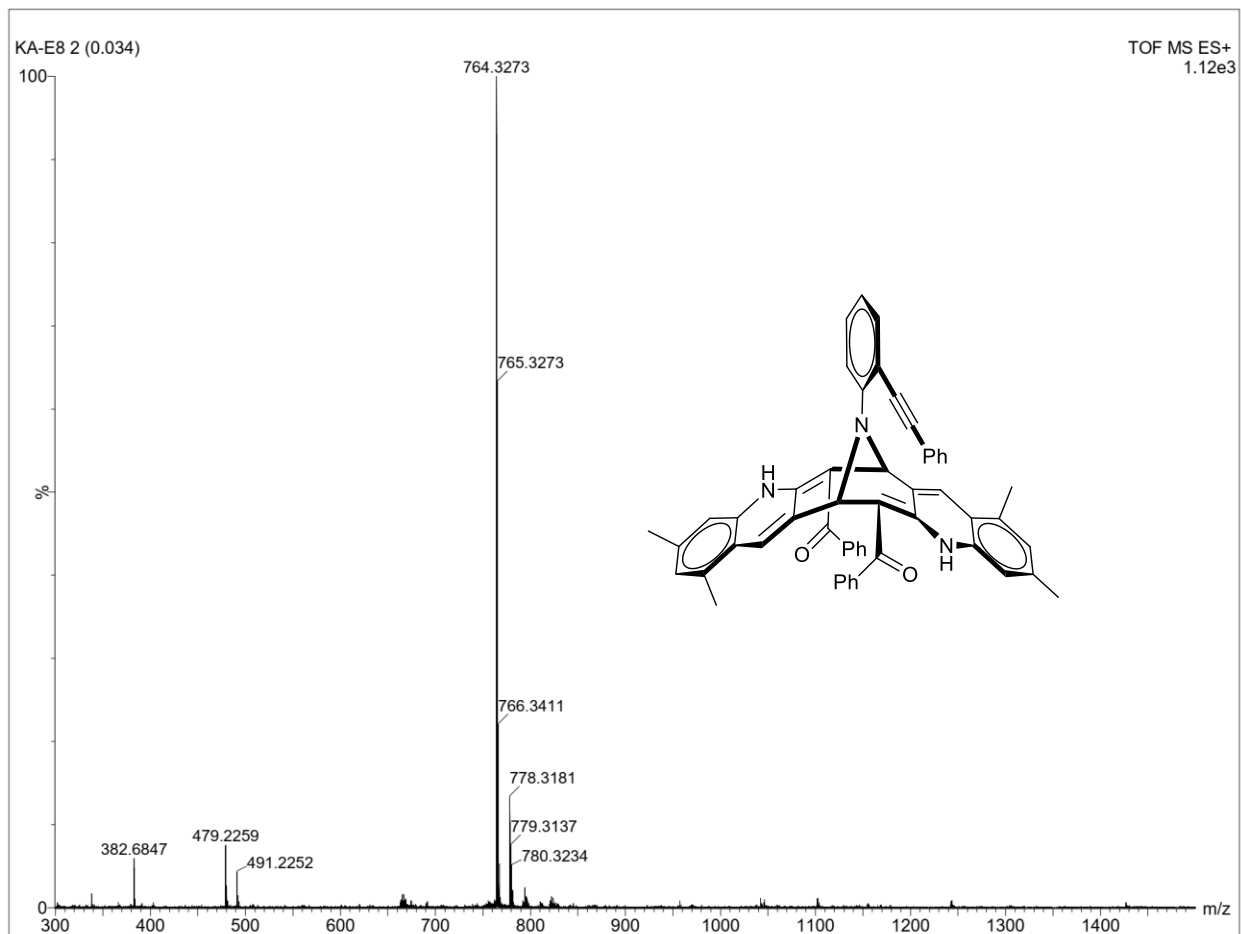
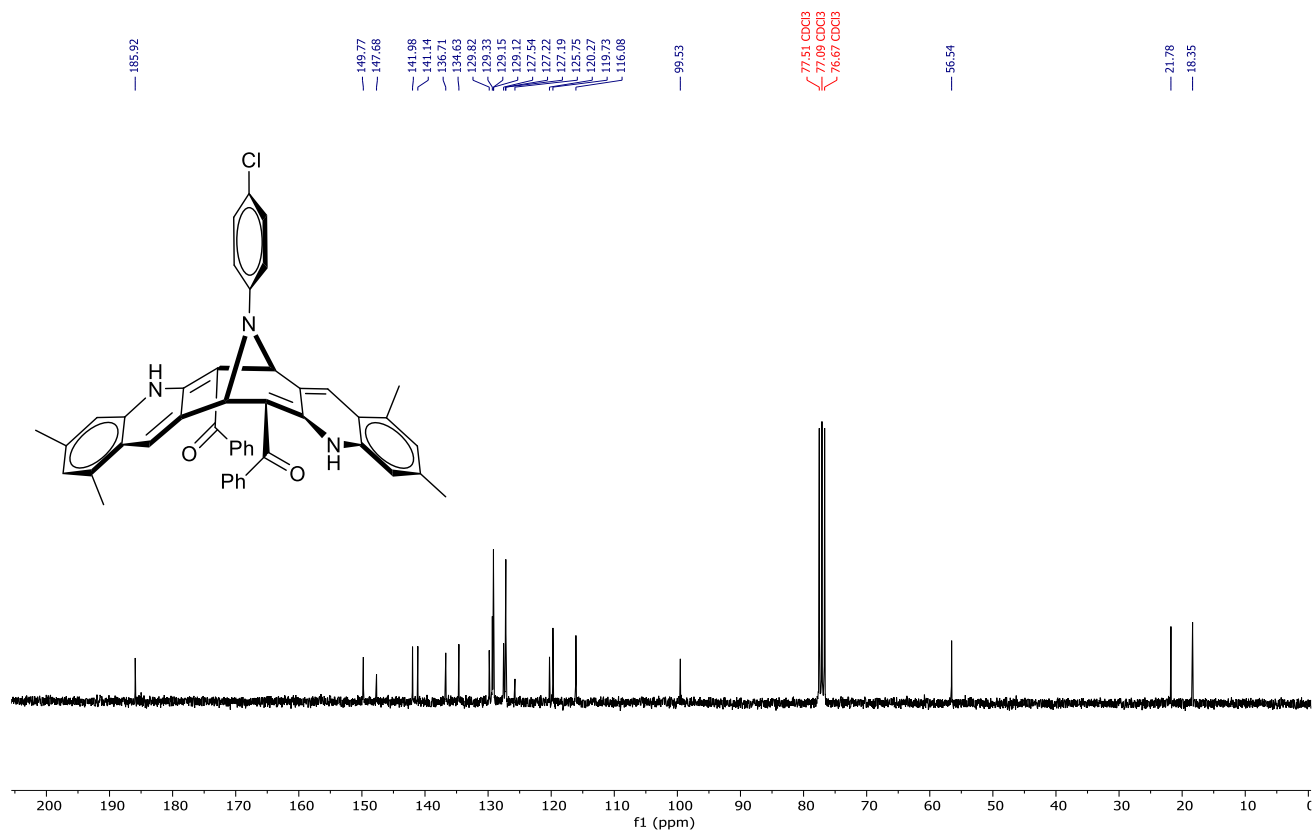
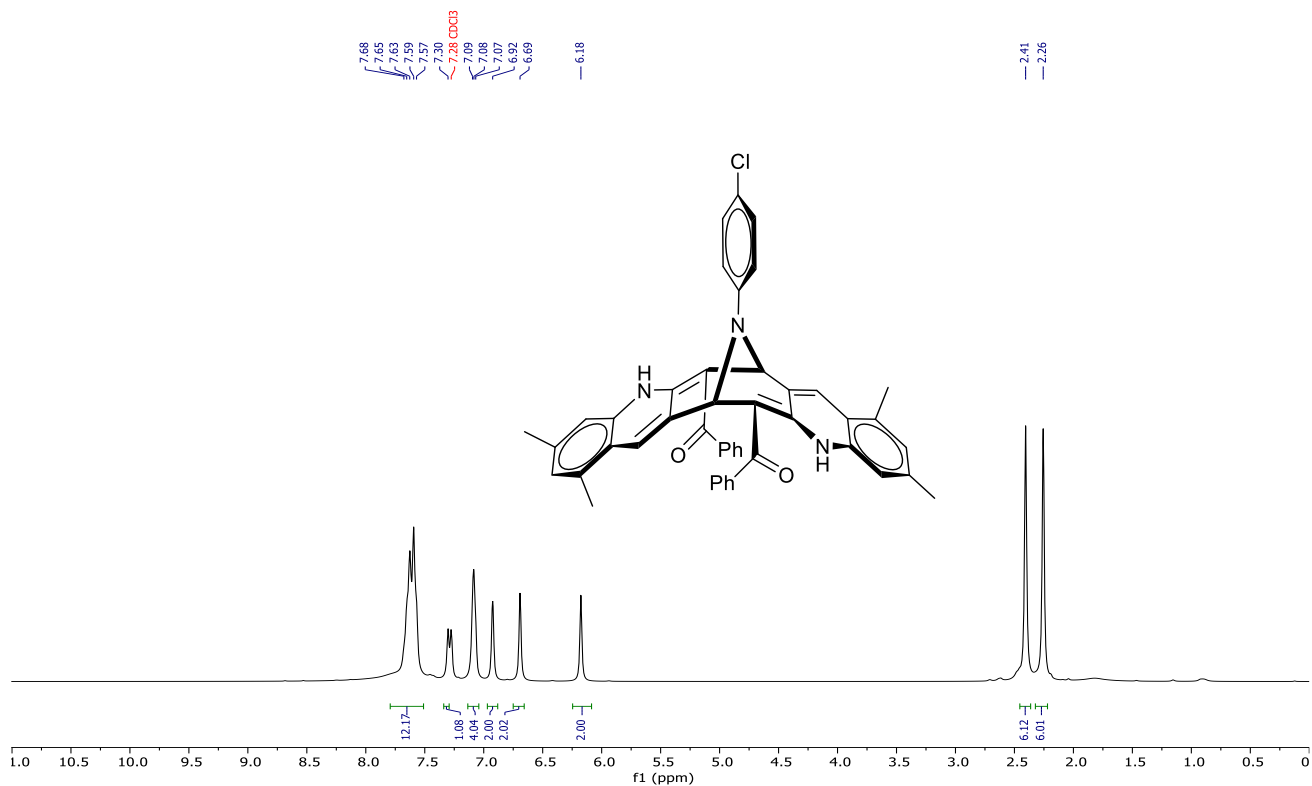
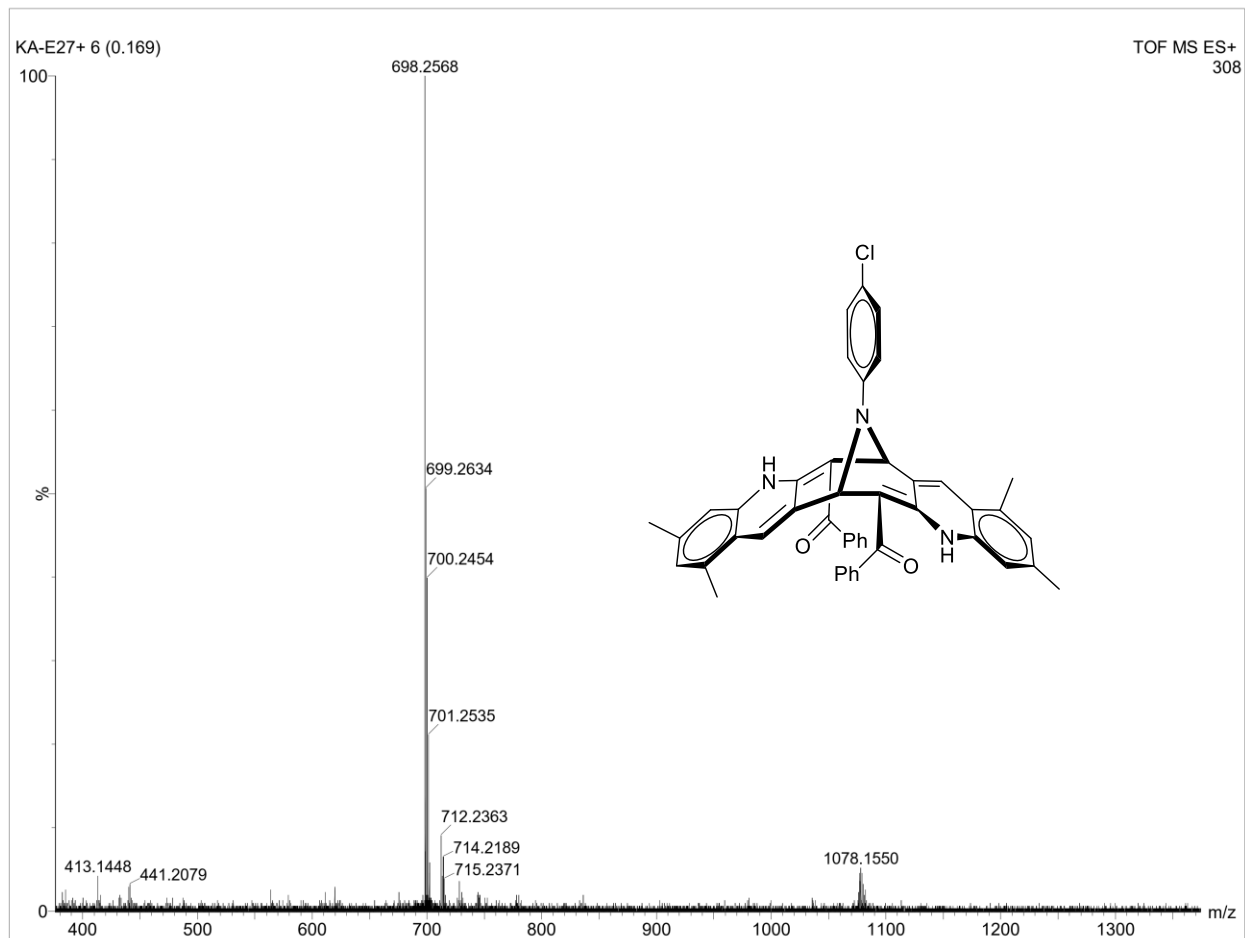


Figure S54: HRMS (ESI) of **3r**

Supporting Information



Figure S57: HRMS (ESI) of **3s**

Supporting Information

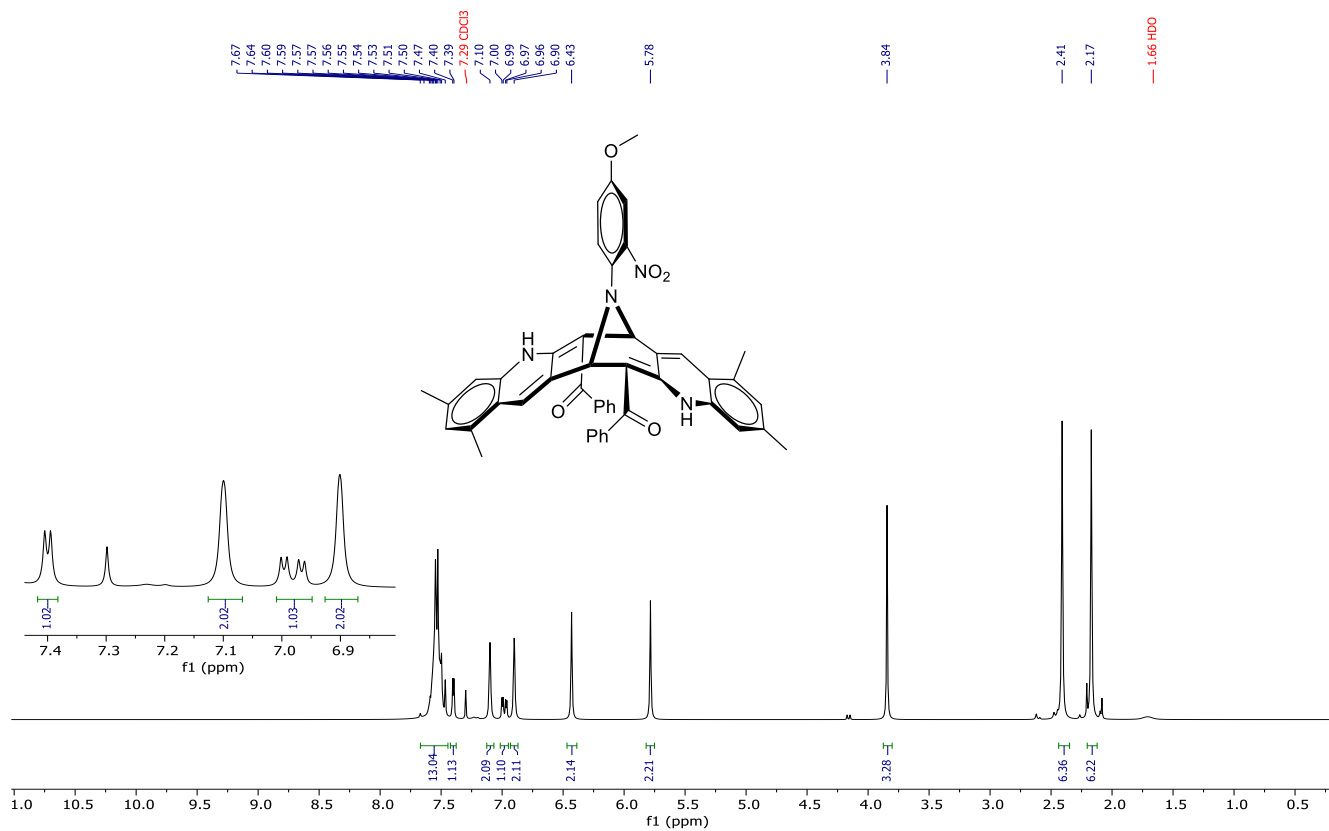


Figure S58: ¹H NMR Compound 3t (300 MHz, CDCl₃)

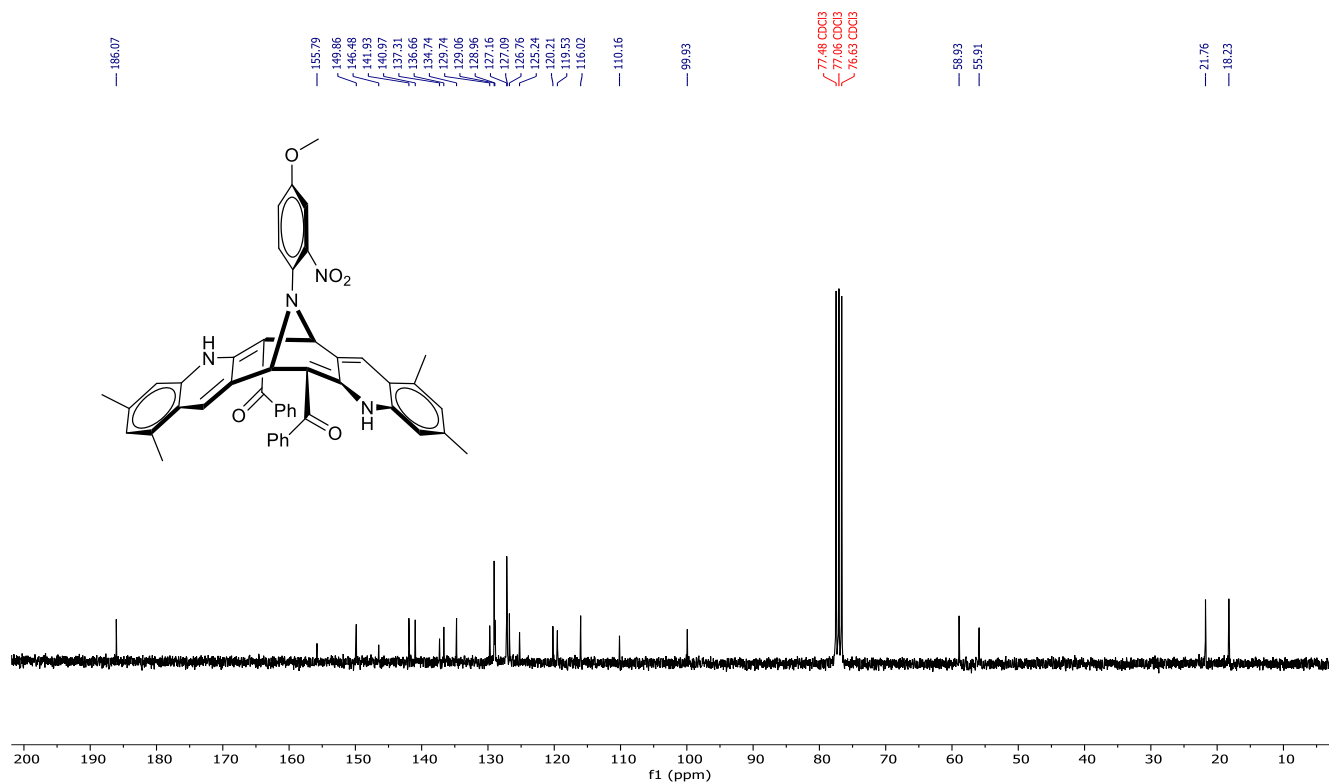


Figure S59: ¹³C{¹H}NMR Compound 3t (75 MHz, CDCl₃)

Supporting Information

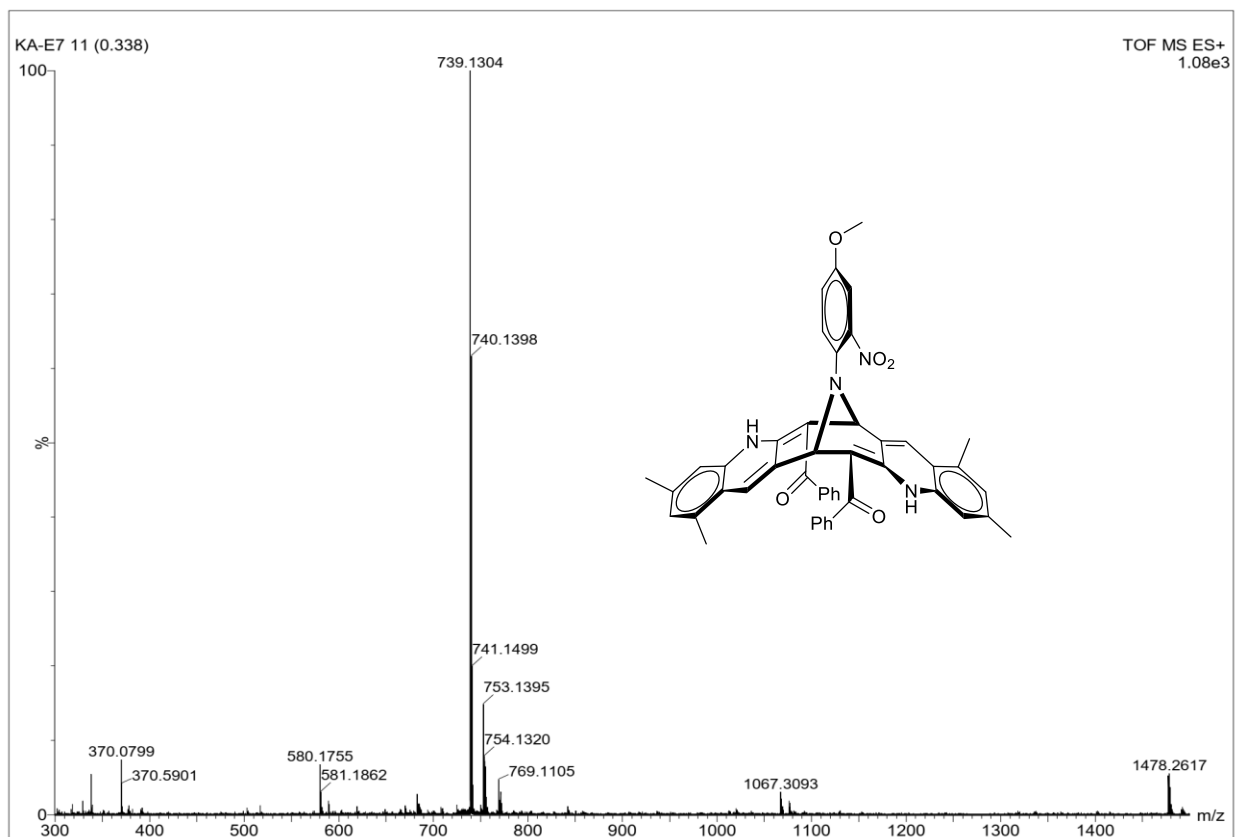
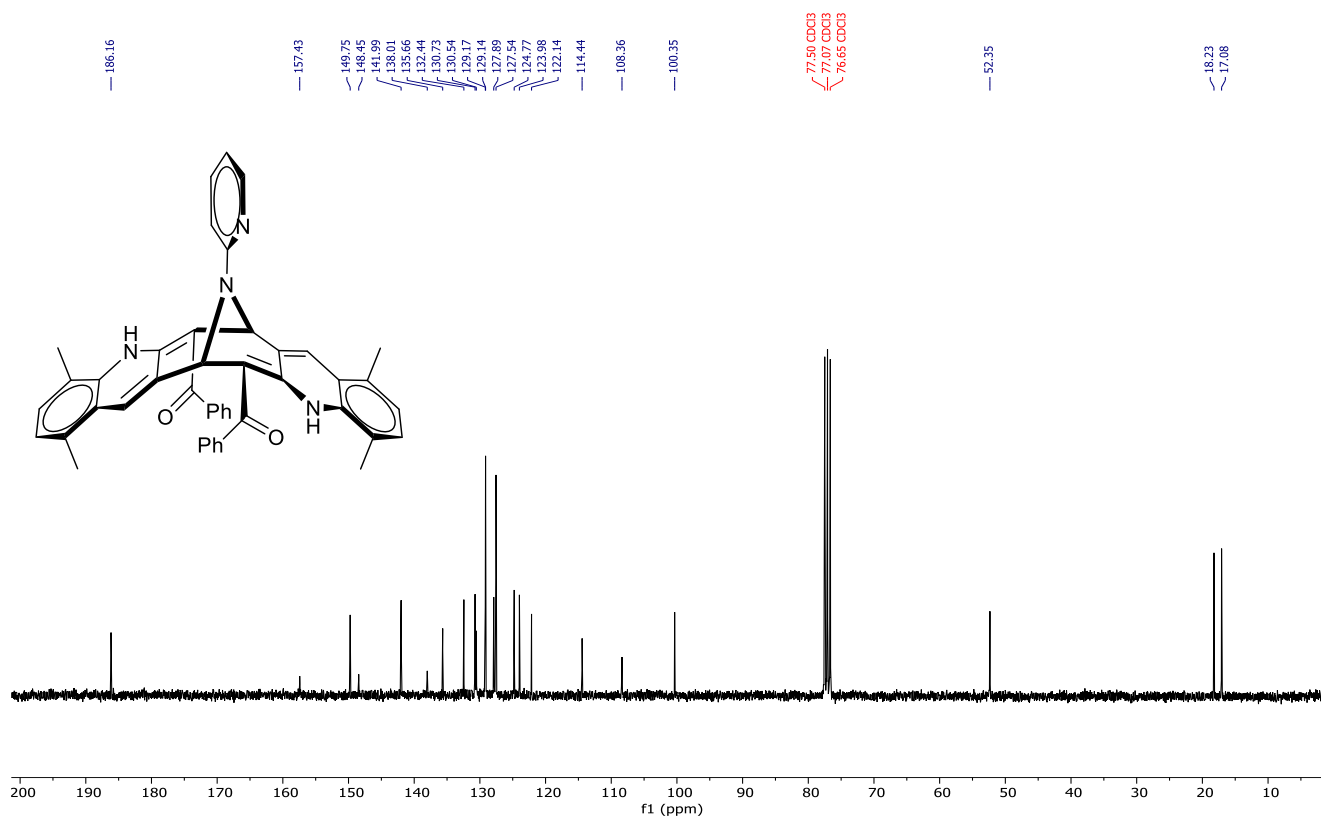
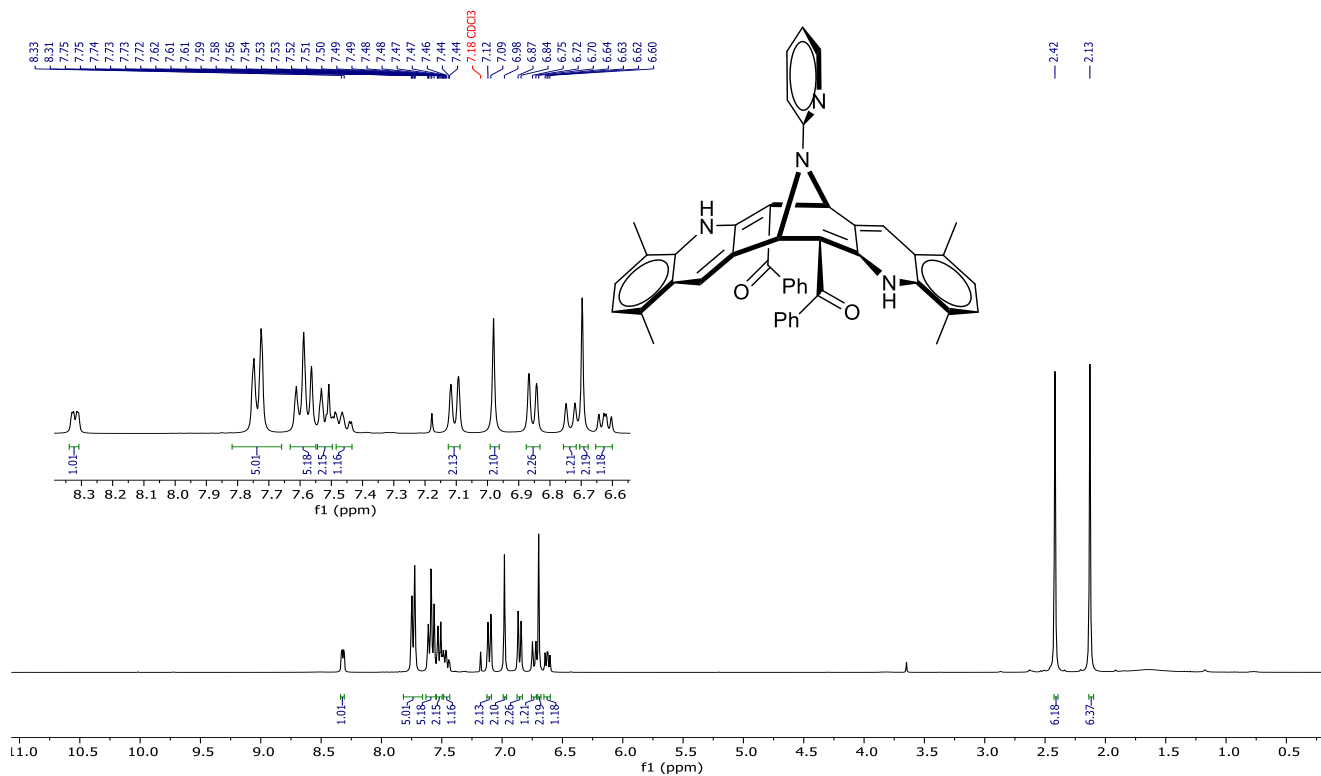
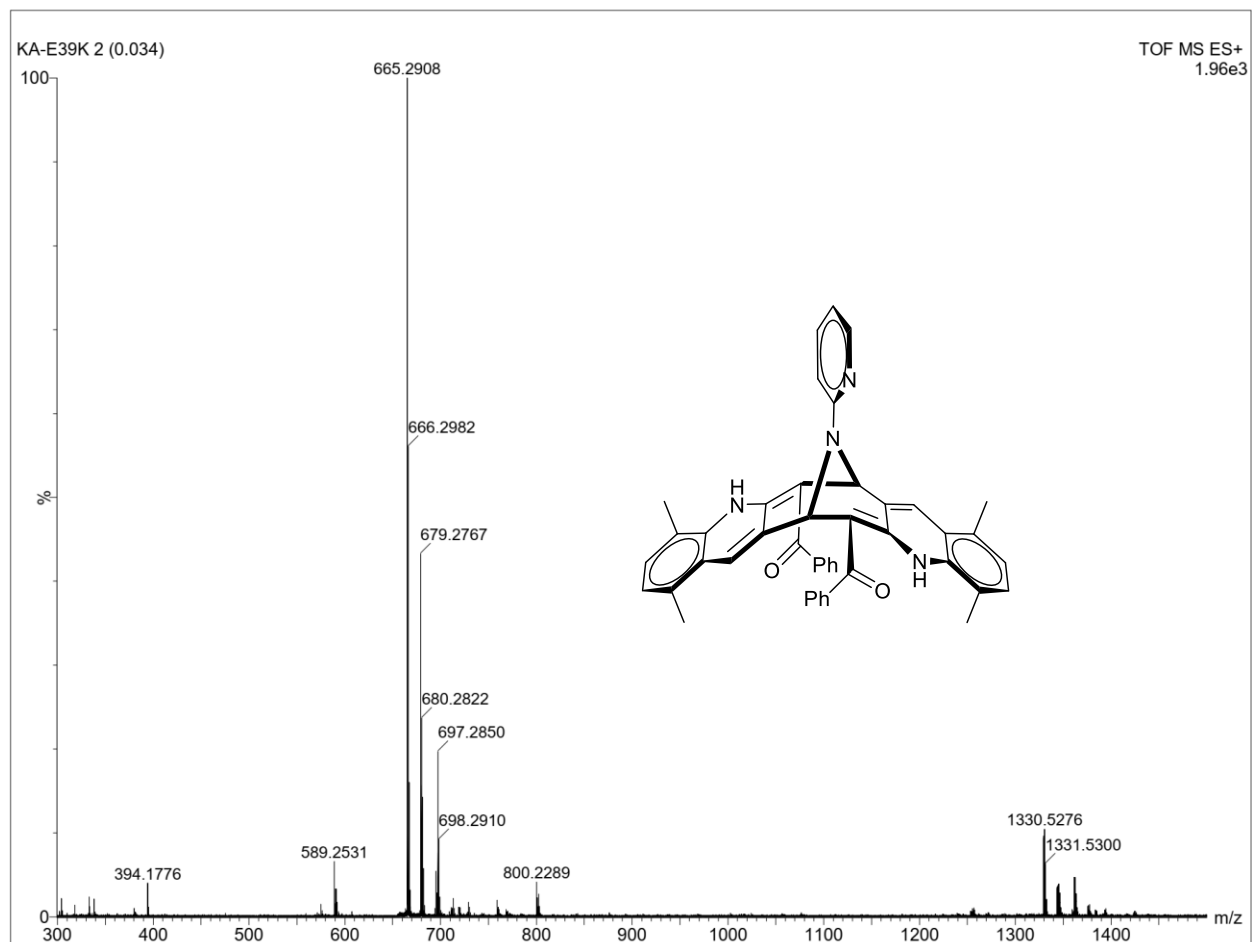


Figure S60: HRMS (ESI) of **3t**

Supporting Information



Figure S63: HRMS (ESI) of **3u**

Supporting Information

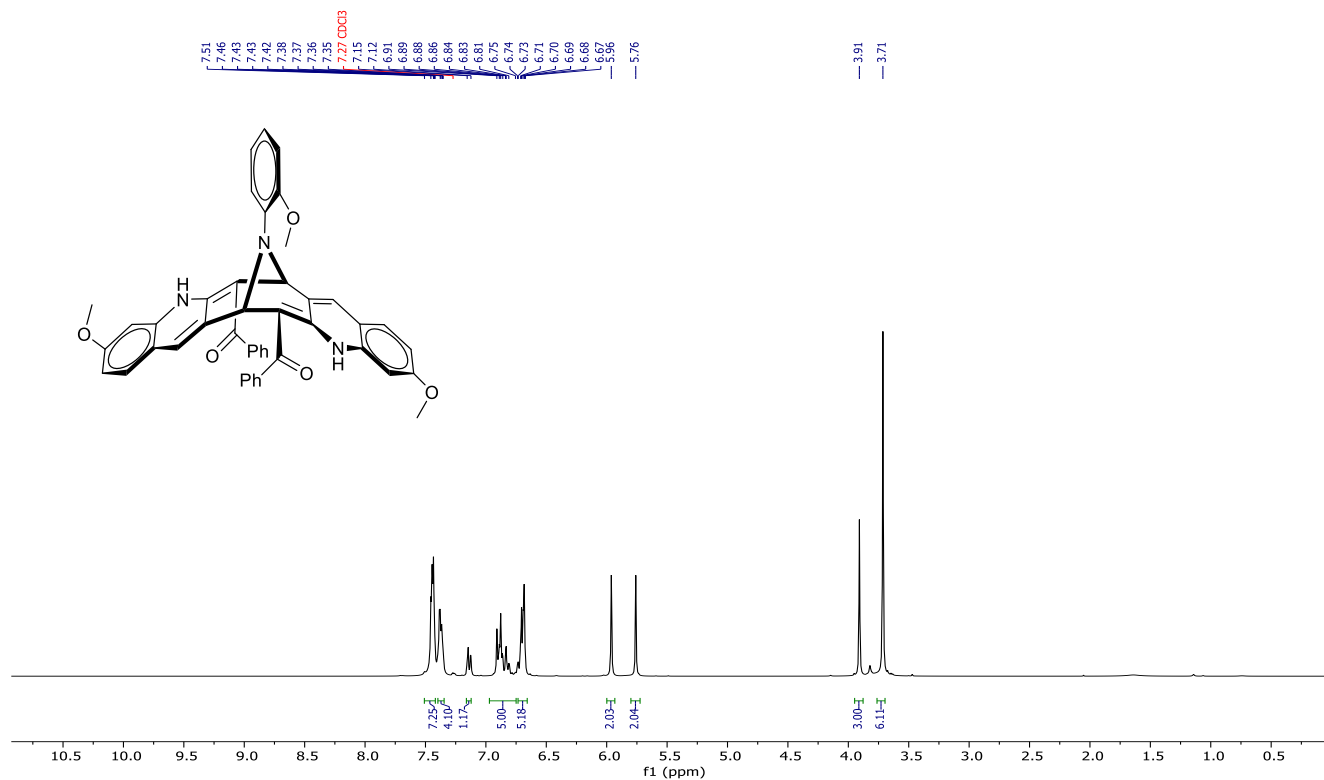


Figure S64: ^1H NMR Compound 3v (300 MHz, CDCl_3)

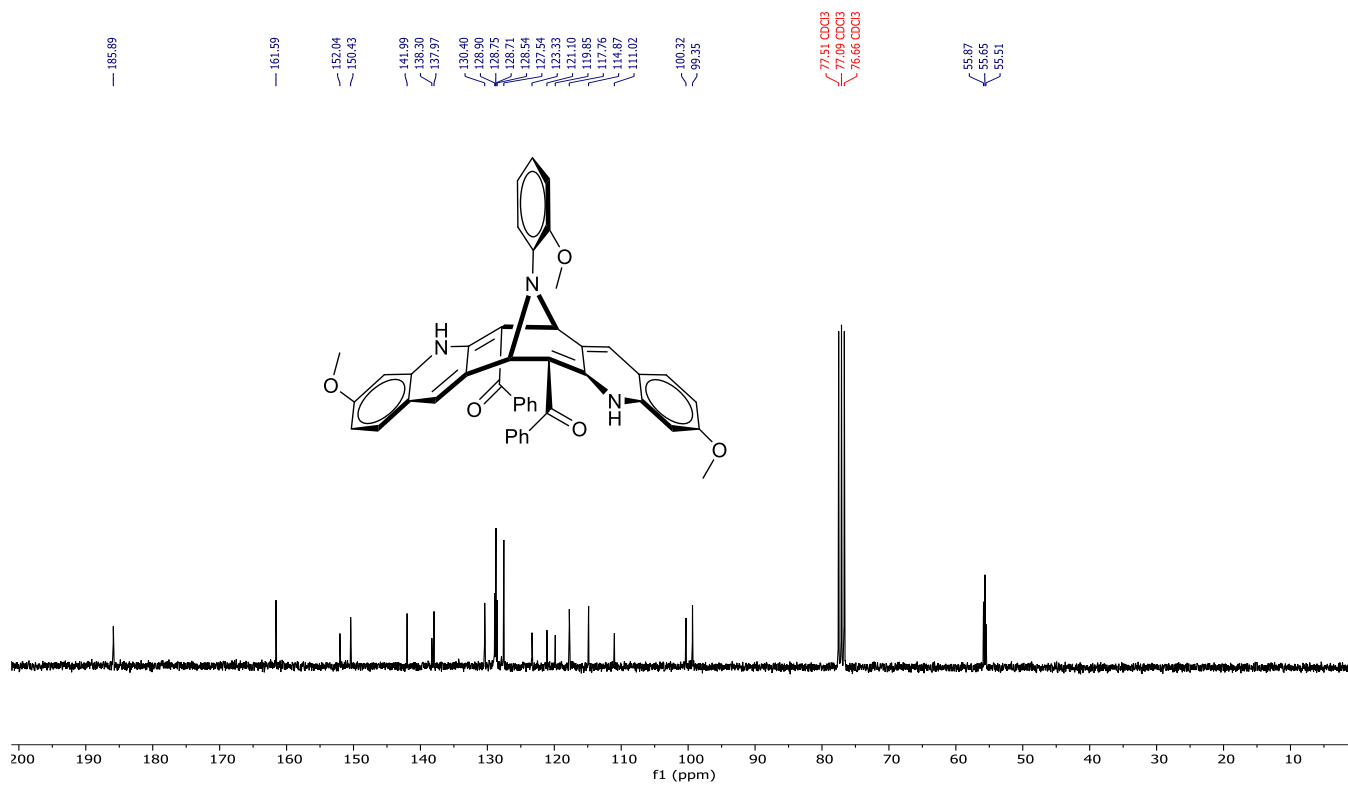
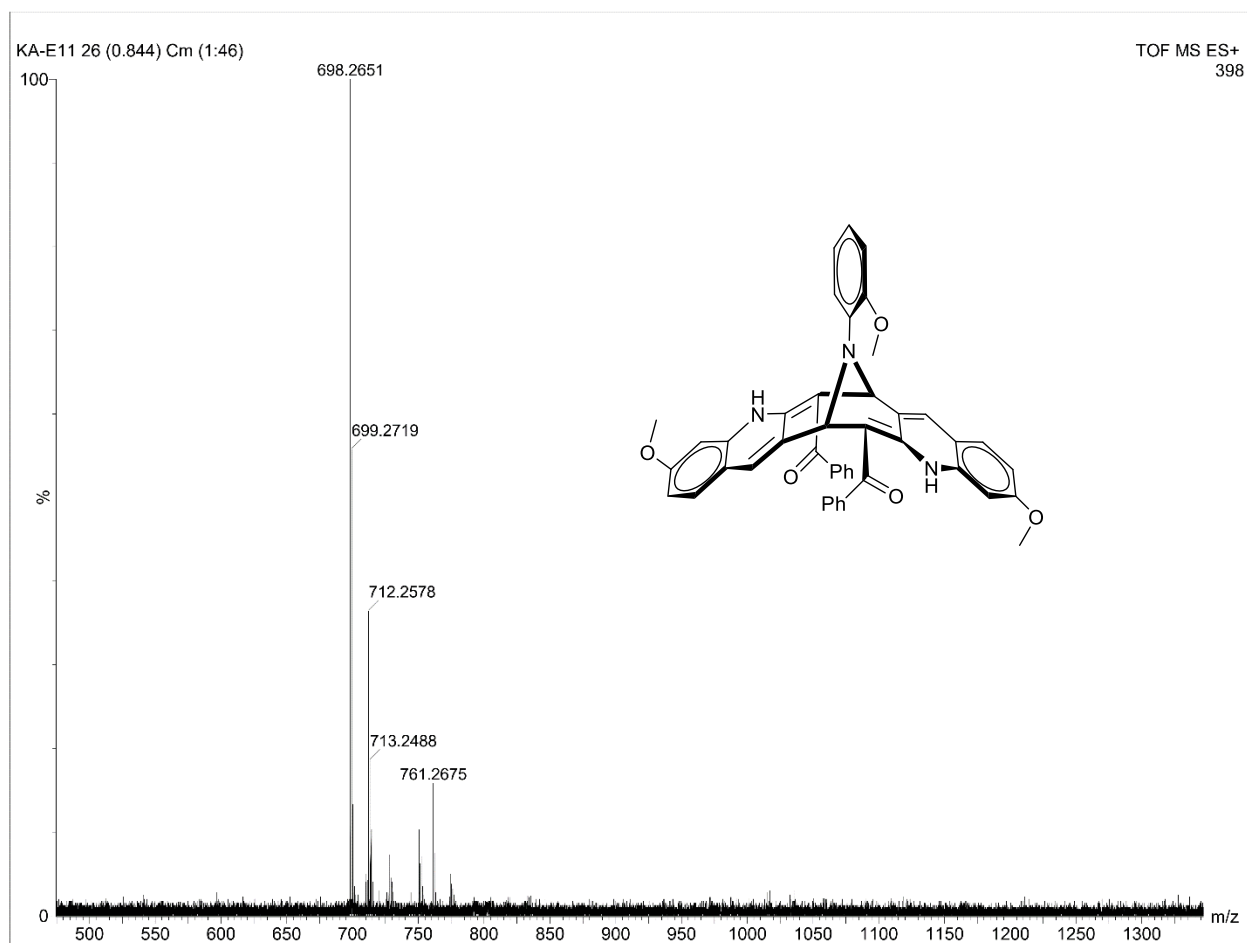


Figure S65: $^{13}\text{C}\{^1\text{H}\}$ NMR Compound 3v (75 MHz, CDCl_3)

Figure S66: HRMS (ESI) of **3v**

Supporting Information

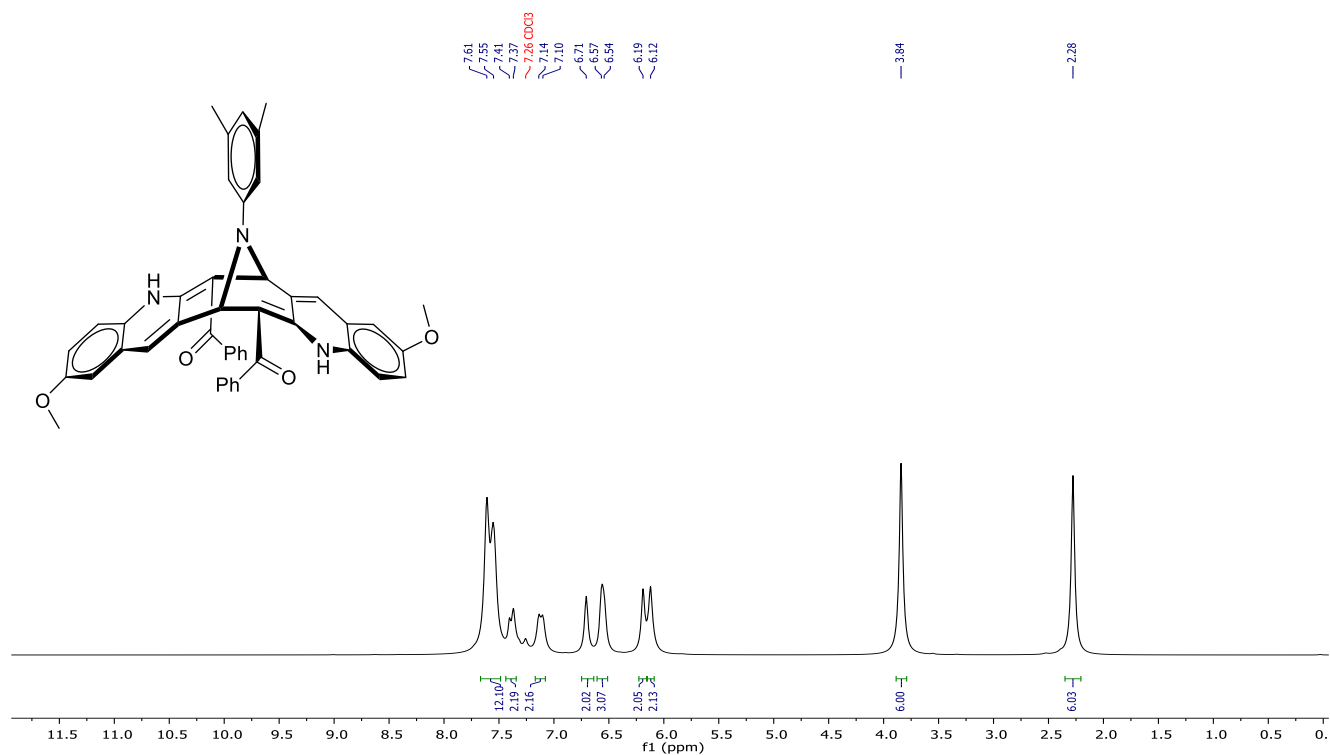


Figure S67: ¹H NMR Compound 3w (250 MHz, CDCl₃)

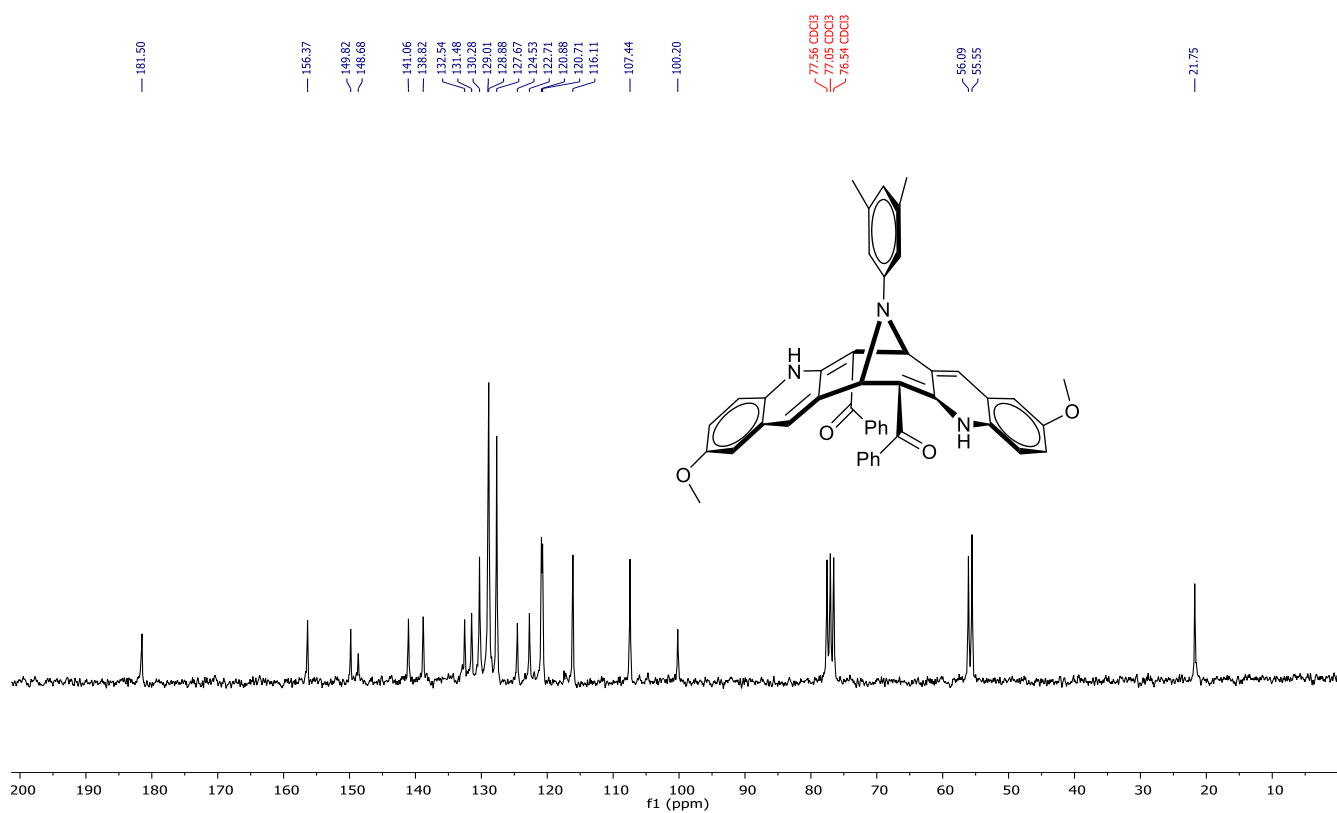


Figure S68: ¹³C{¹H}NMR Compound 3w (63 MHz, CDCl₃)

Supporting Information

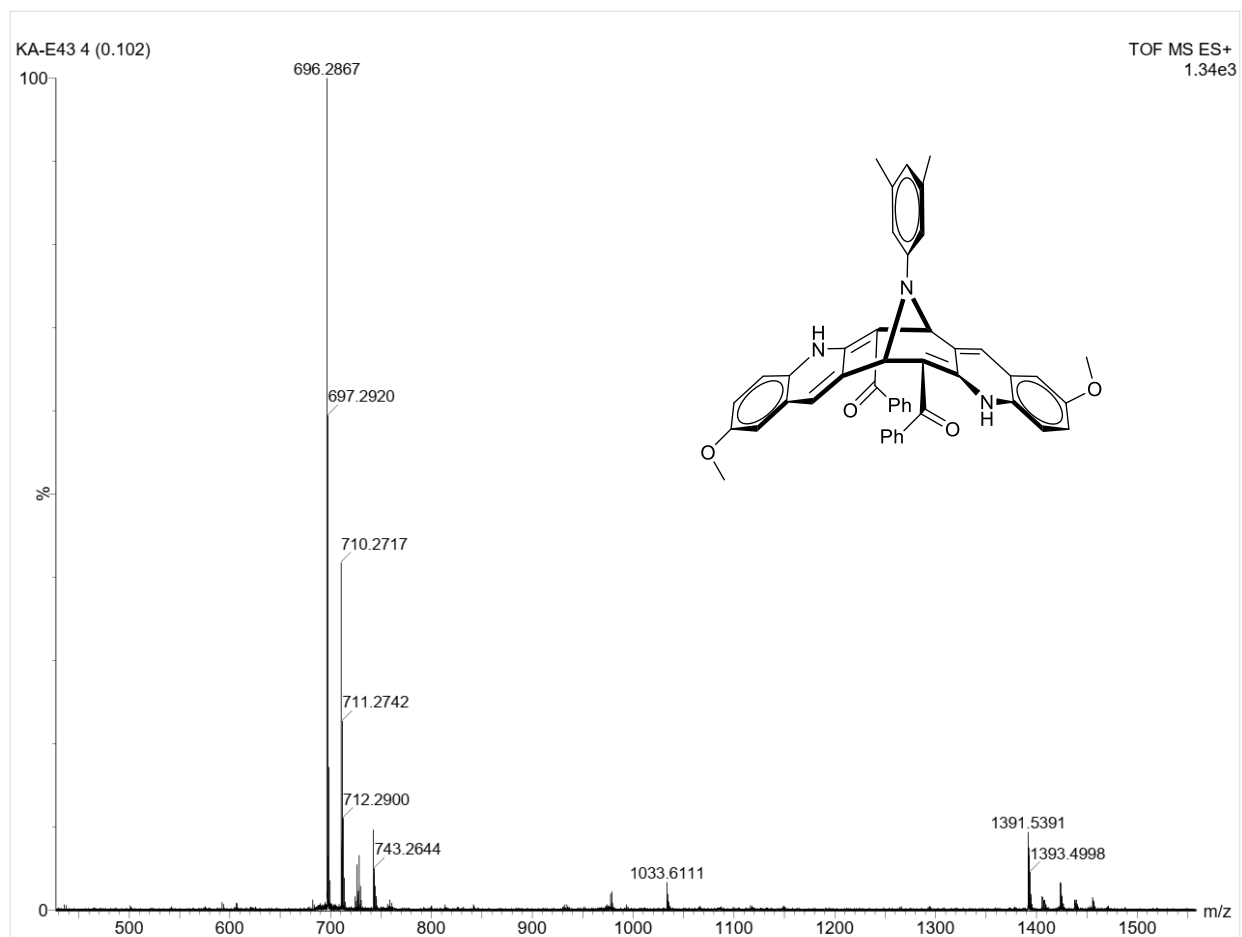
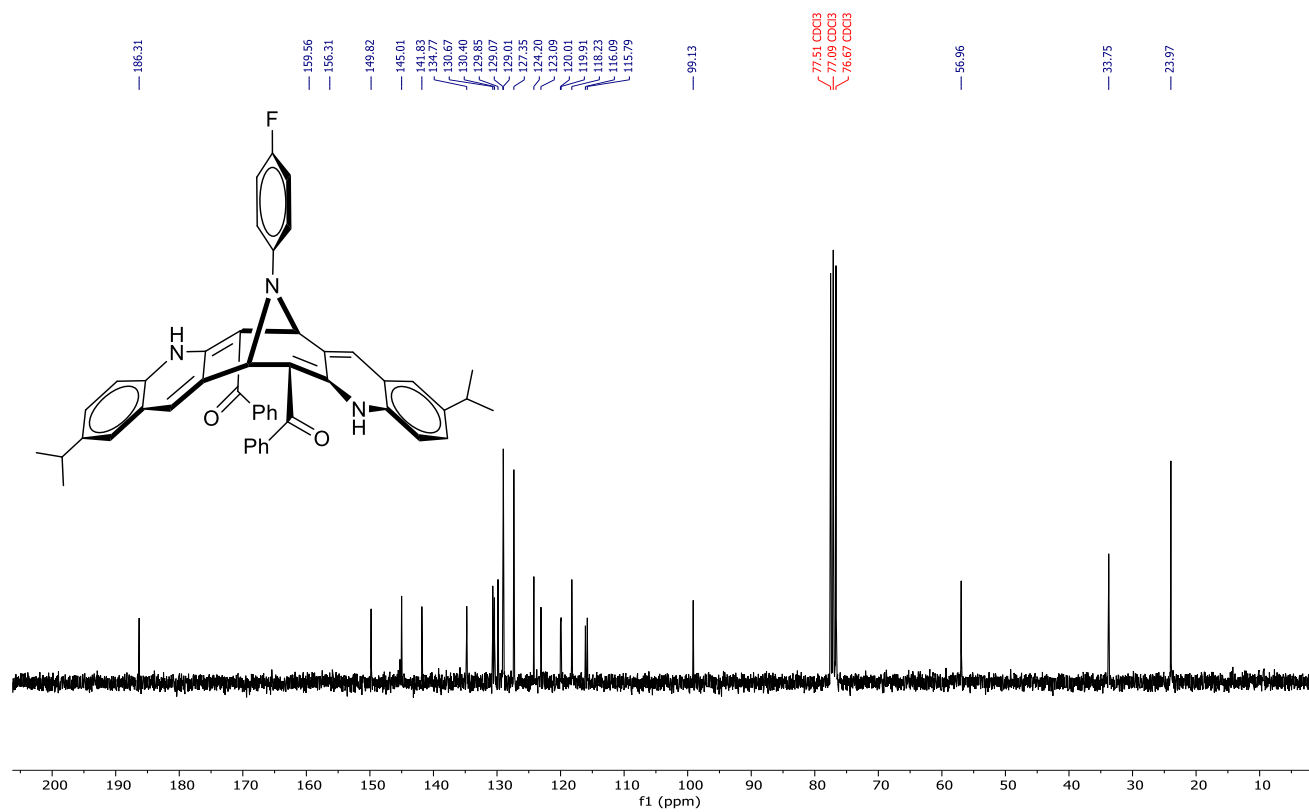
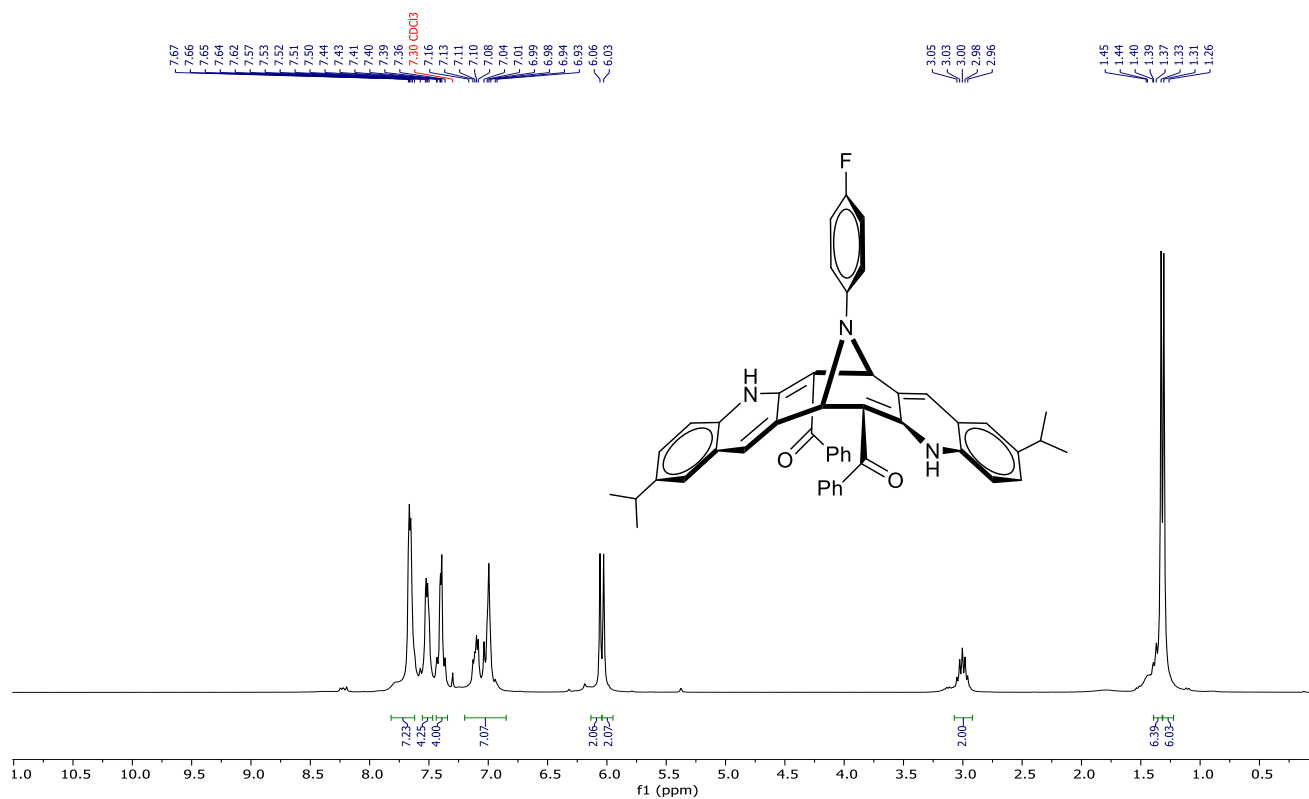
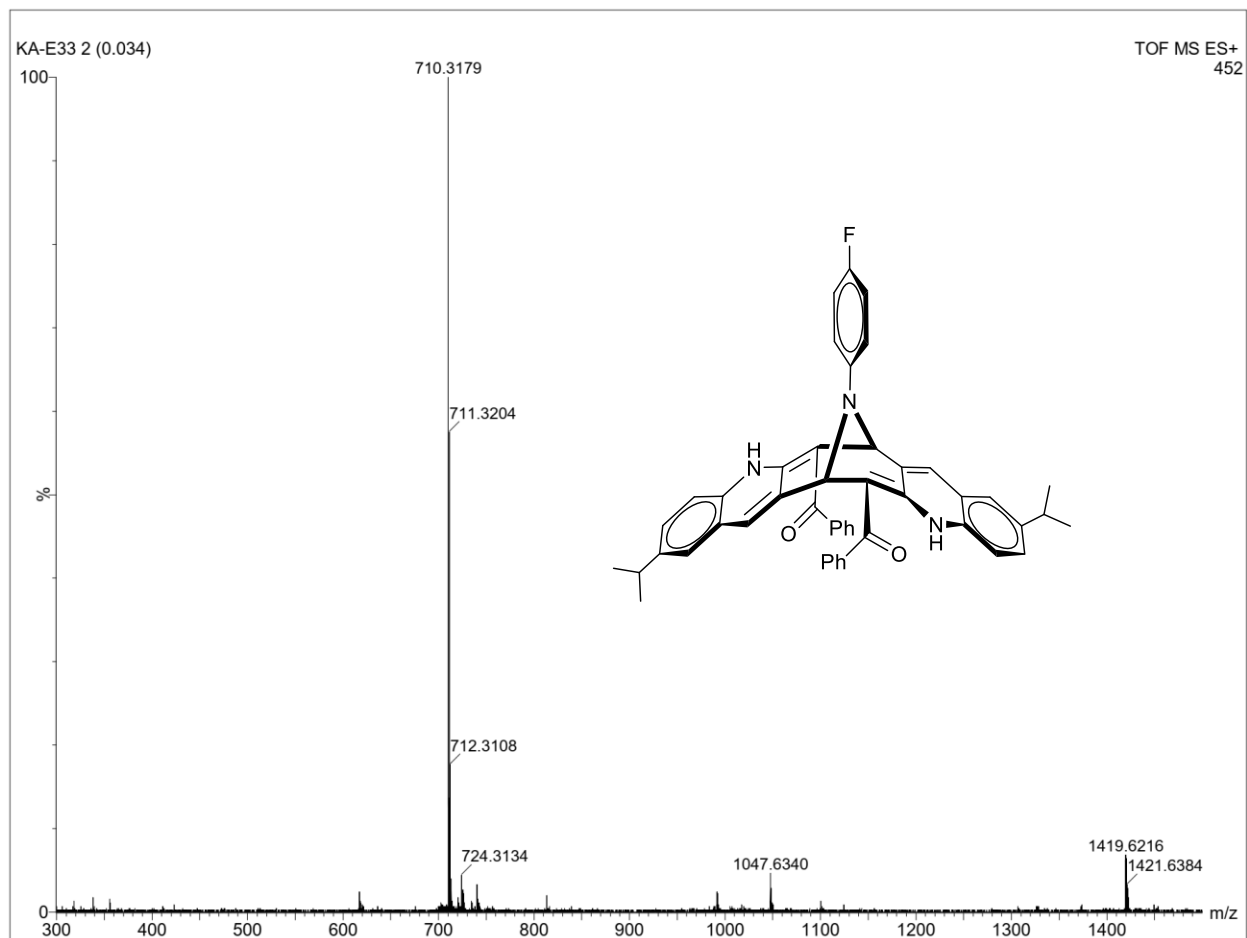


Figure S69: HRMS (ESI) of **3w**

Supporting Information



Figure S72: HRMS (ESI) of **3x**

Supporting Information

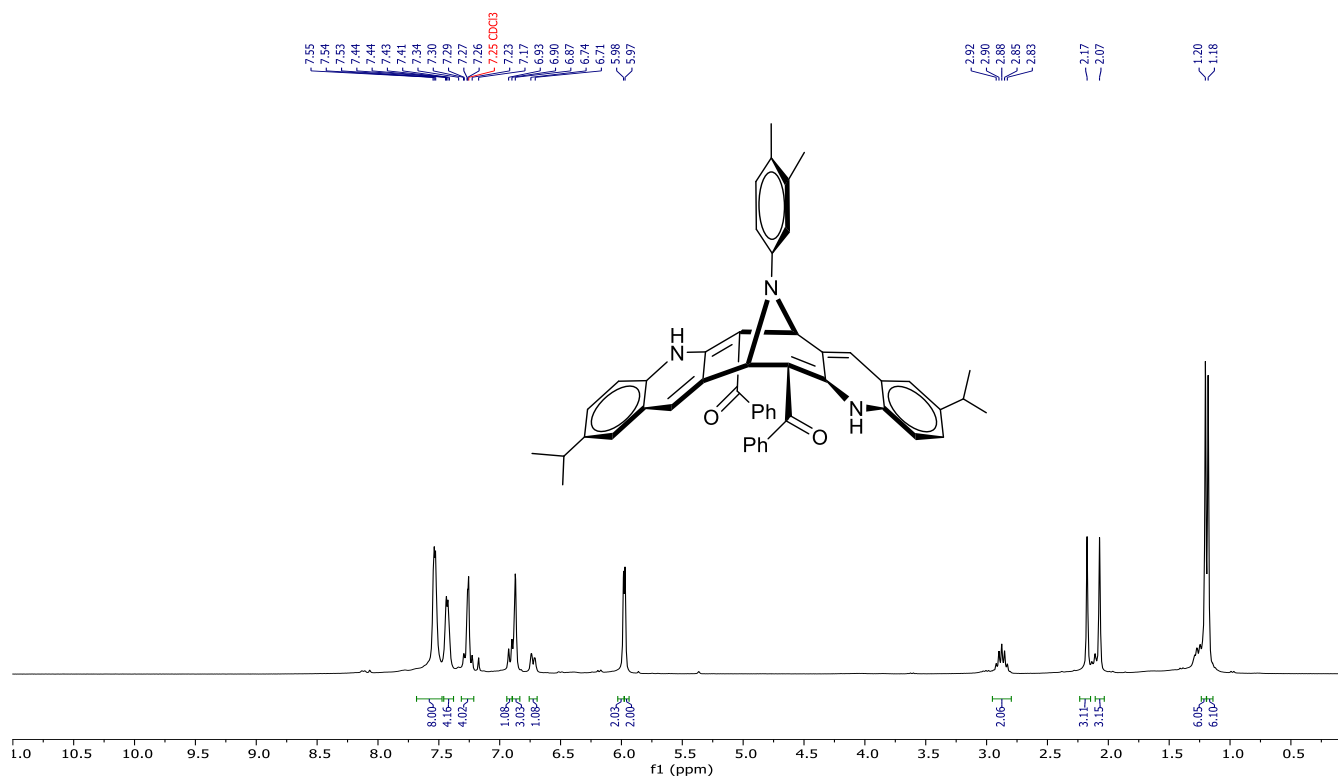


Figure S73: ^1H NMR Compound **3y** (300 MHz, CDCl_3)

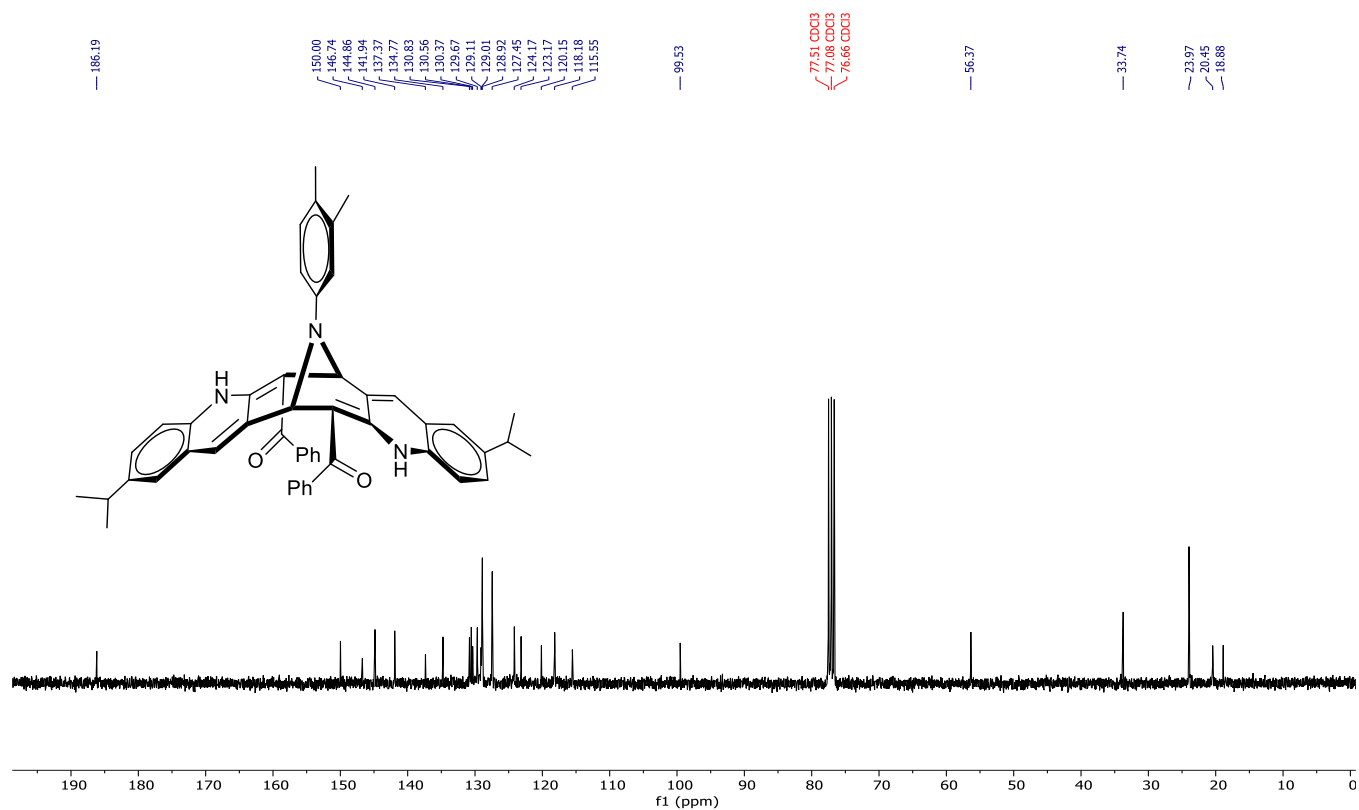


Figure S74: $^{13}\text{C}\{^1\text{H}\}$ NMR Compound **3y** (75 MHz, CDCl_3)

Supporting Information

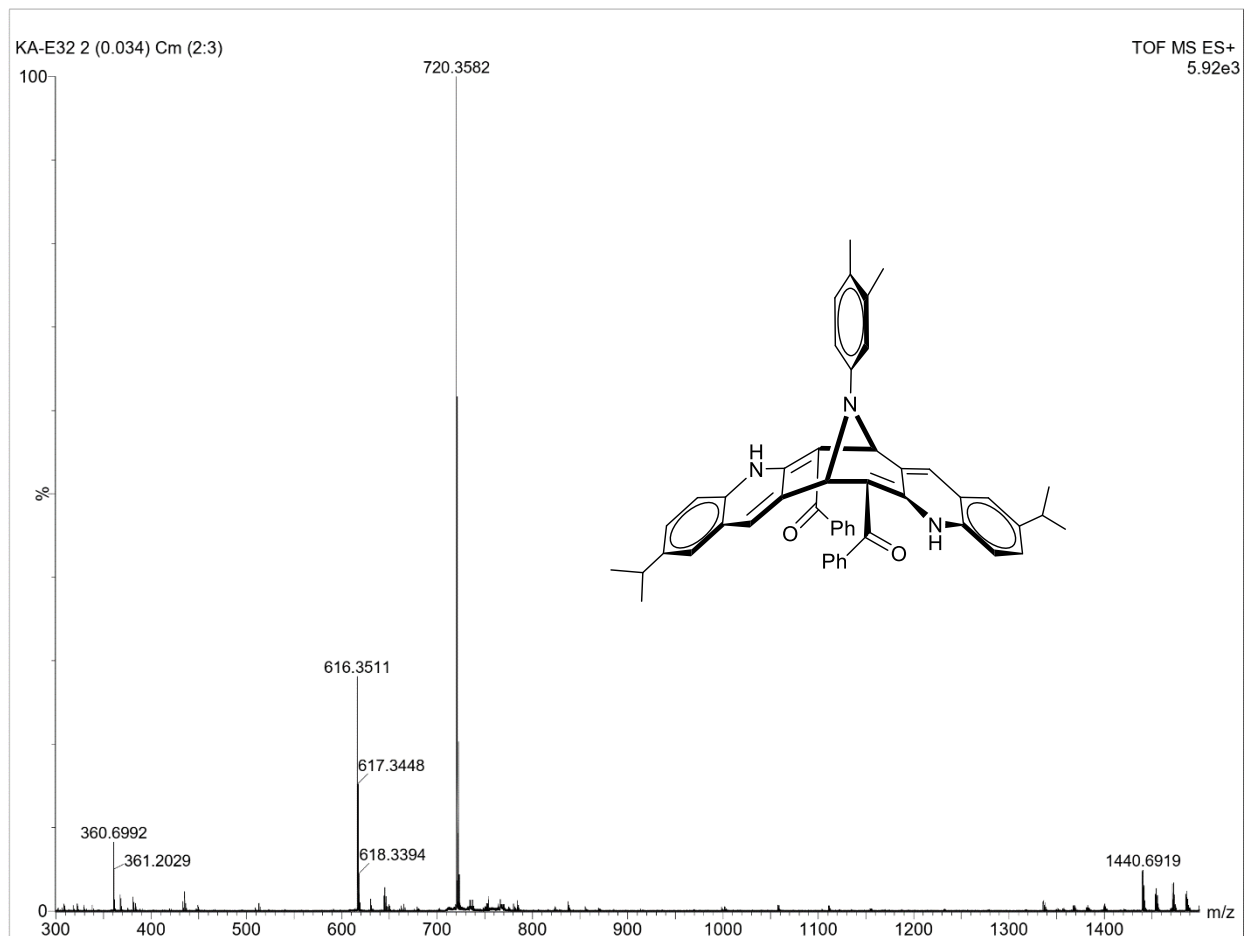


Figure S75: HRMS (ESI) of **3y**

Supporting Information

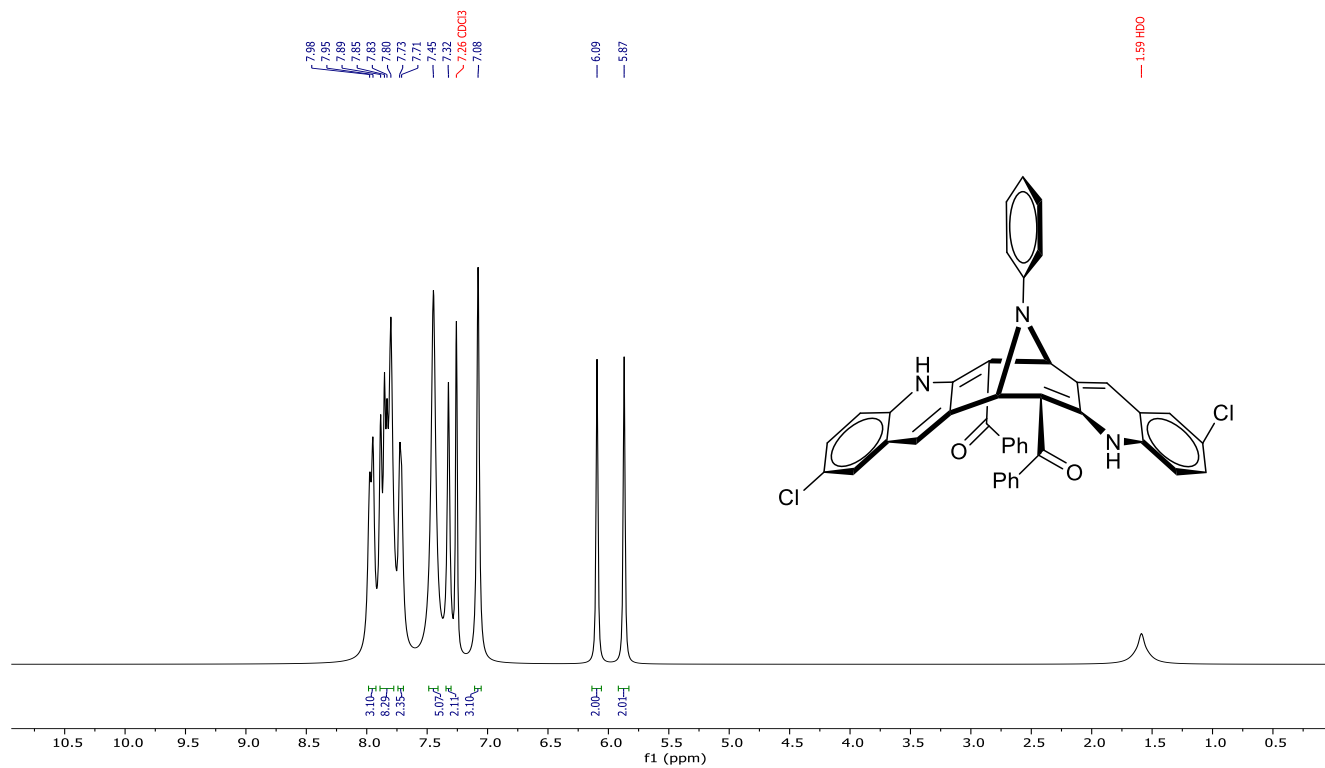


Figure S76: ^1H NMR Compound **3z** (300 MHz, CDCl_3)

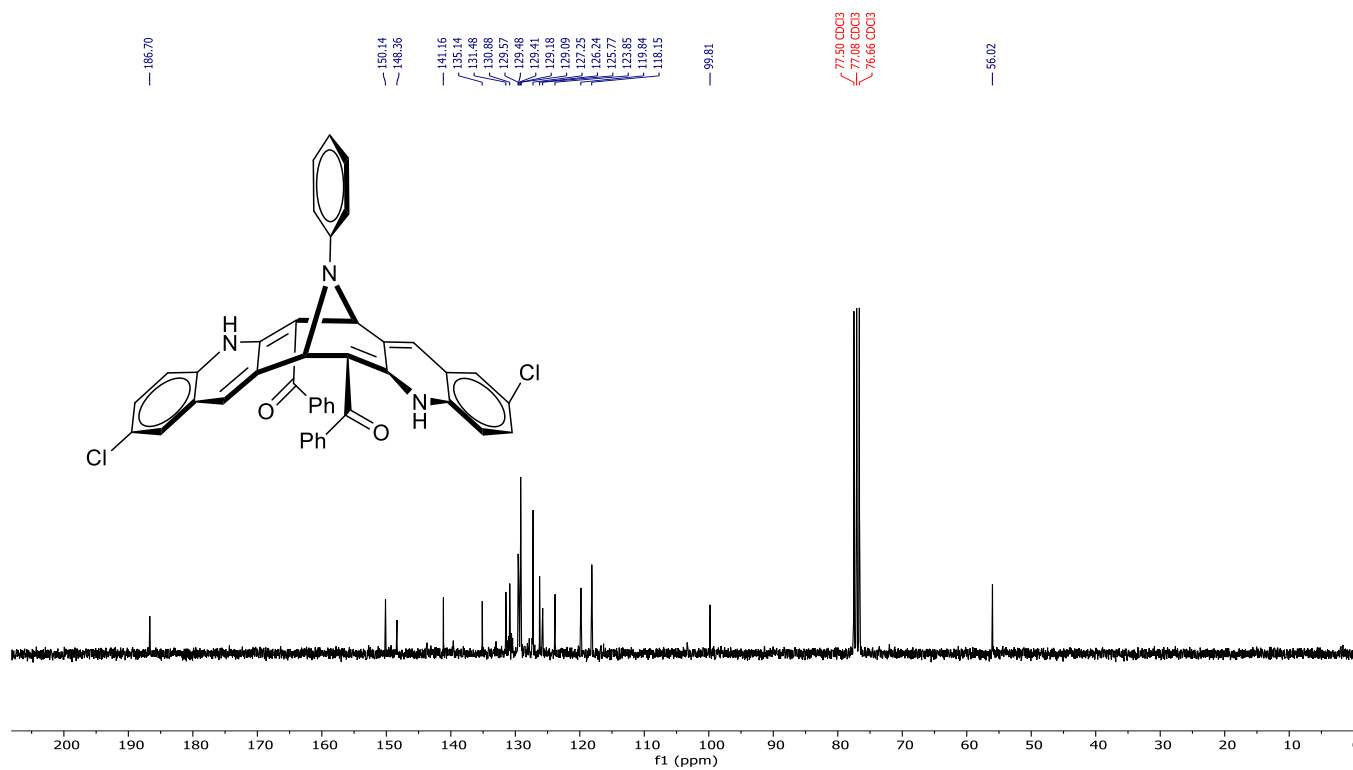
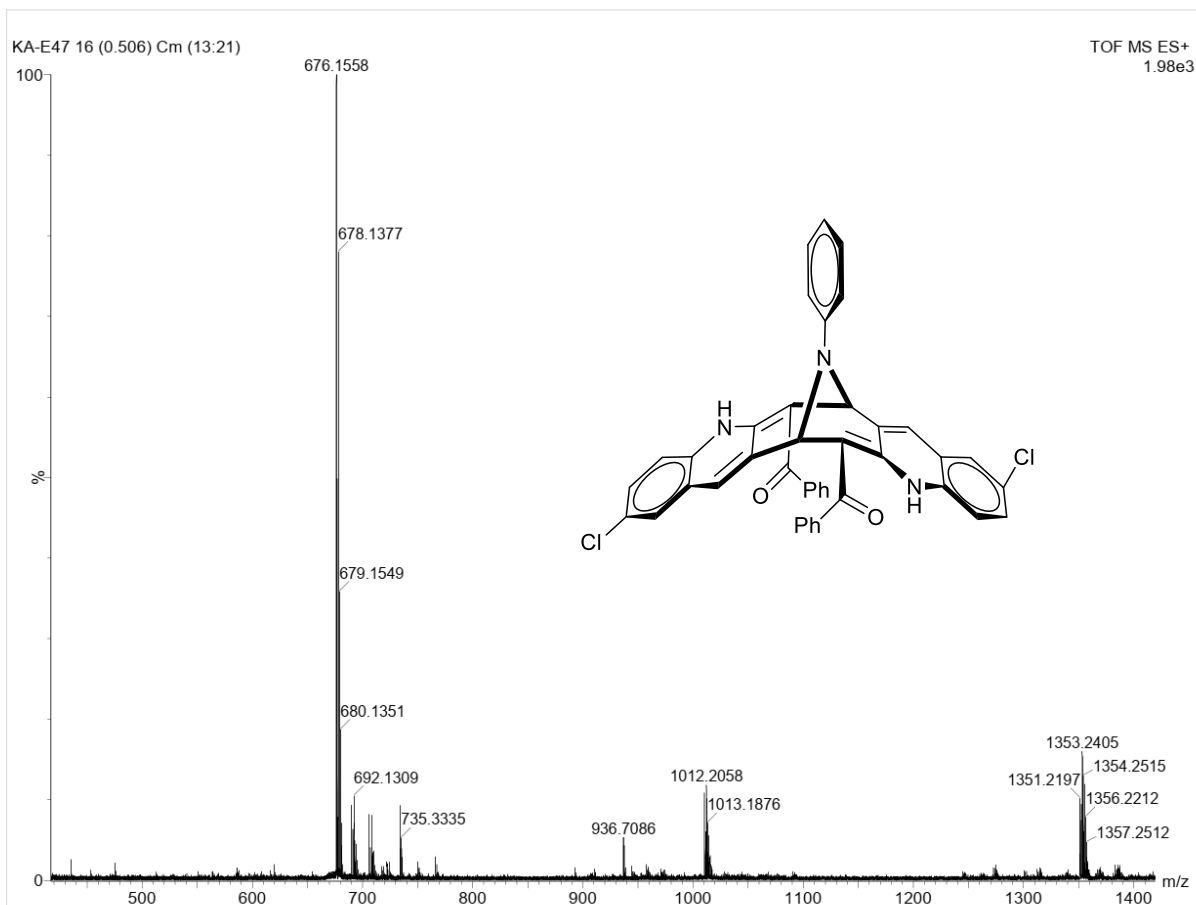


Figure S77: $^{13}\text{C}\{^1\text{H}\}$ NMR Compound **3z** (75 MHz, CDCl_3)

Figure S78: HRMS (ESI) of **3z**

Supporting Information

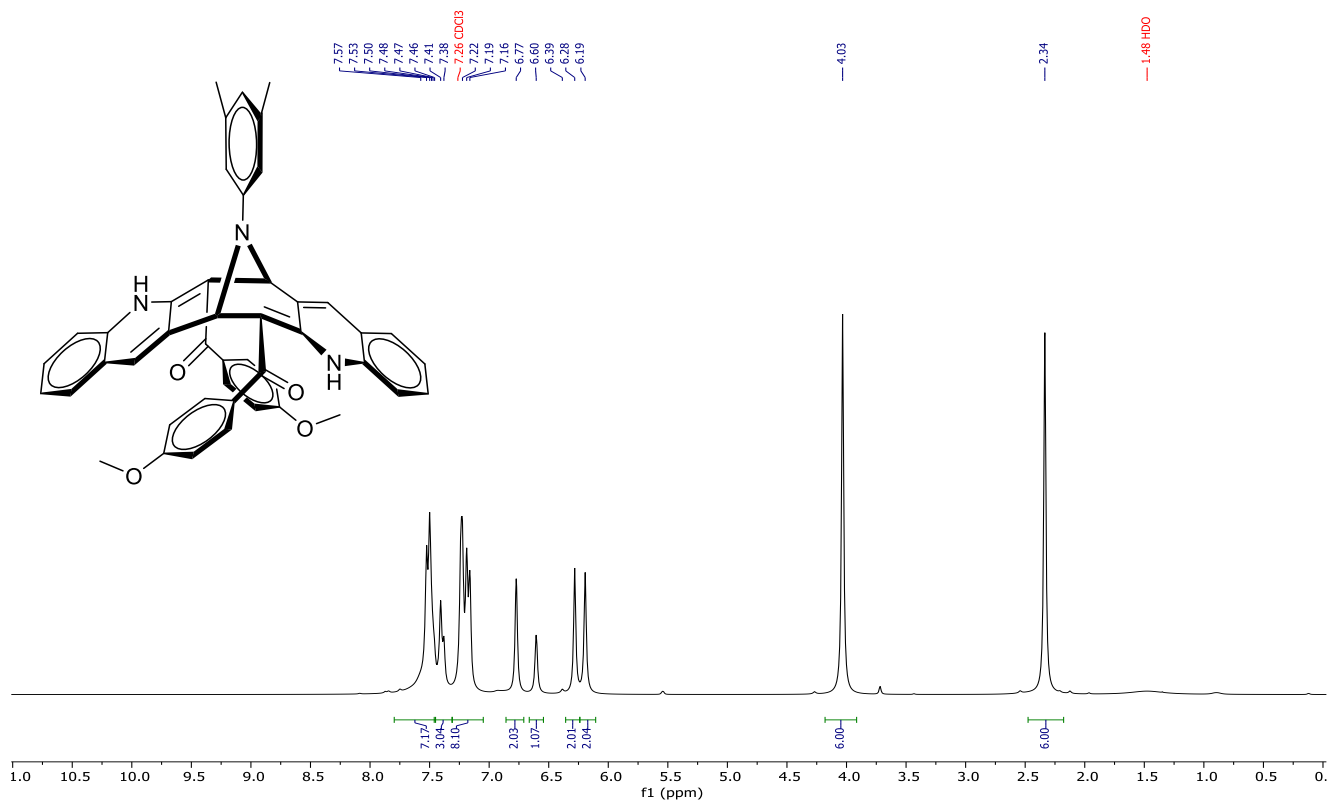


Figure S79: ^1H NMR Compound 3aa (300 MHz, CDCl_3)

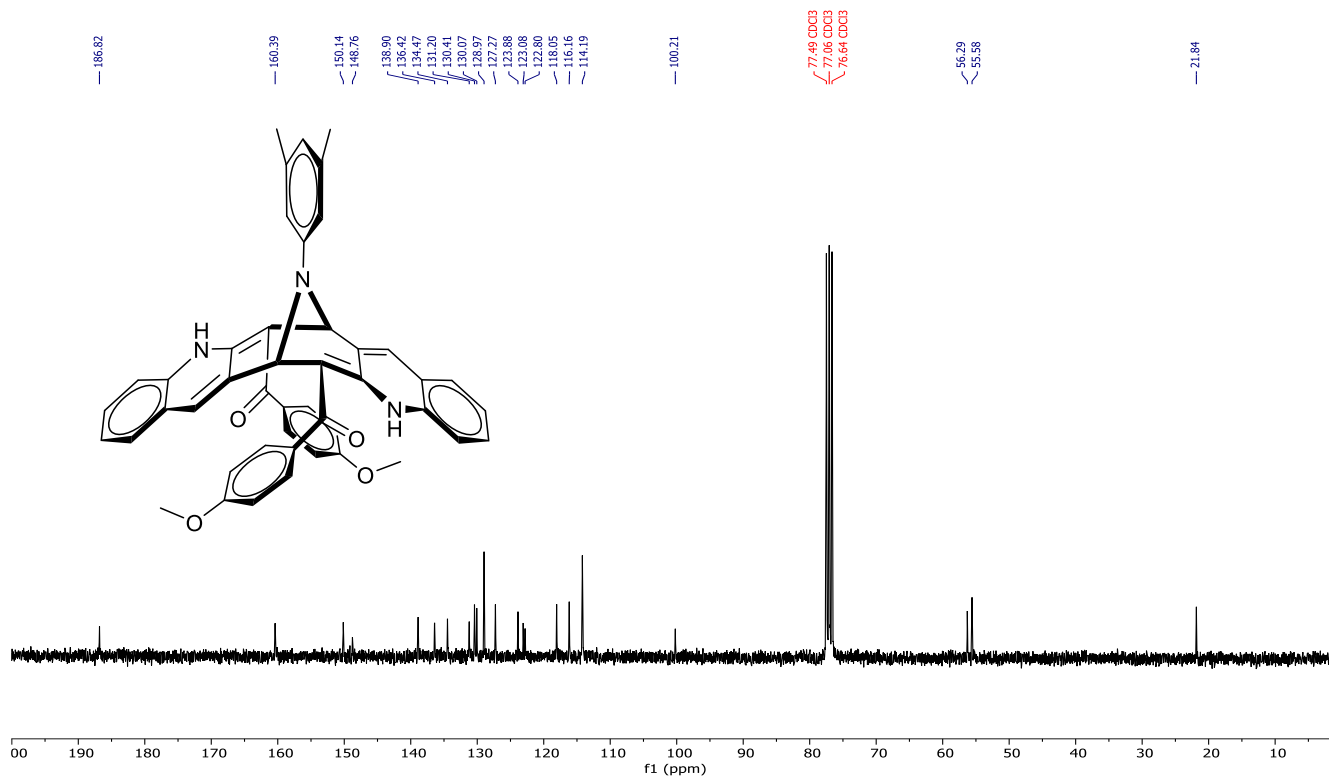
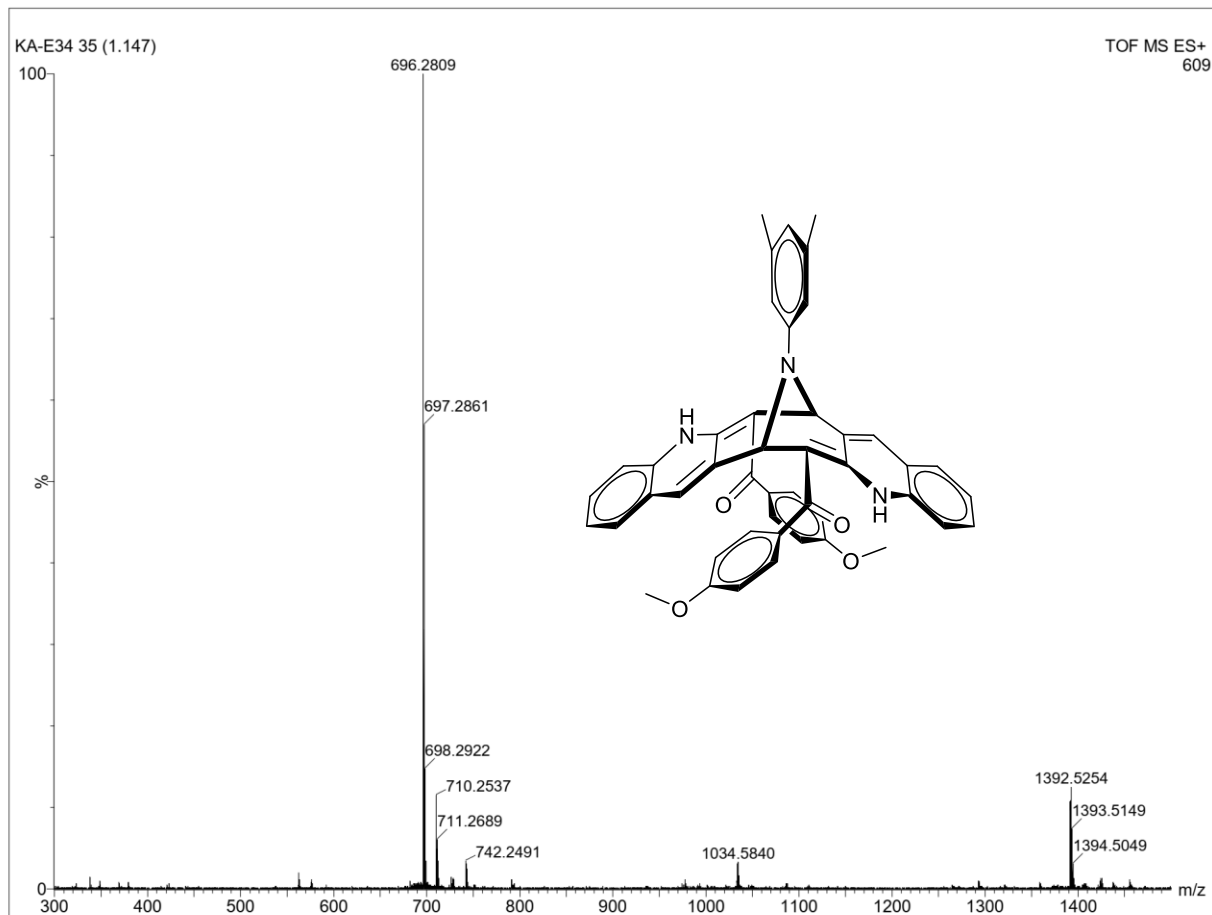


Figure S80: $^{13}\text{C}\{^1\text{H}\}$ NMR Compound 3aa (75 MHz, CDCl_3)

Figure S81: HRMS (ESI) of **3aa**

Supporting Information

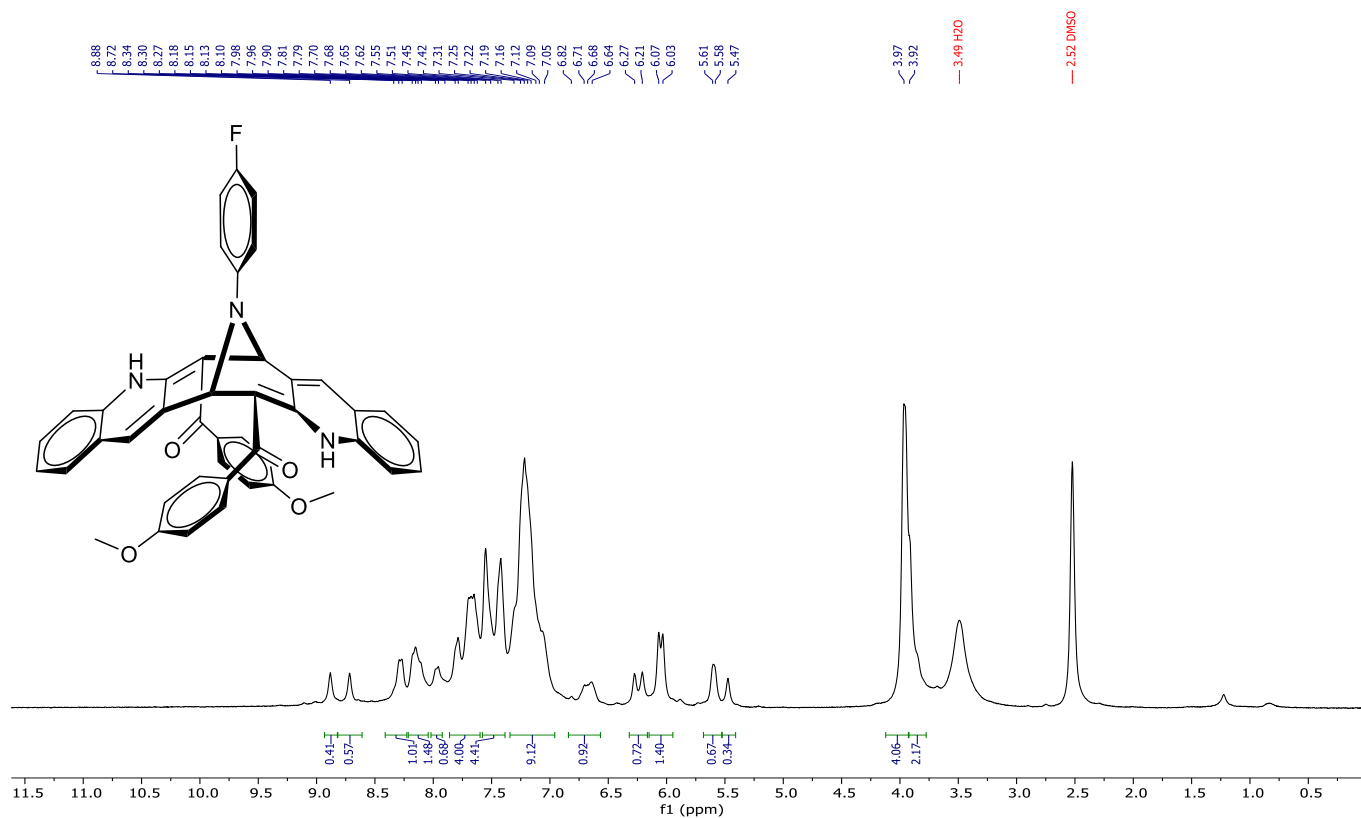


Figure S82: ^1H NMR Compound **3ab** (300 MHz, CDCl_3)

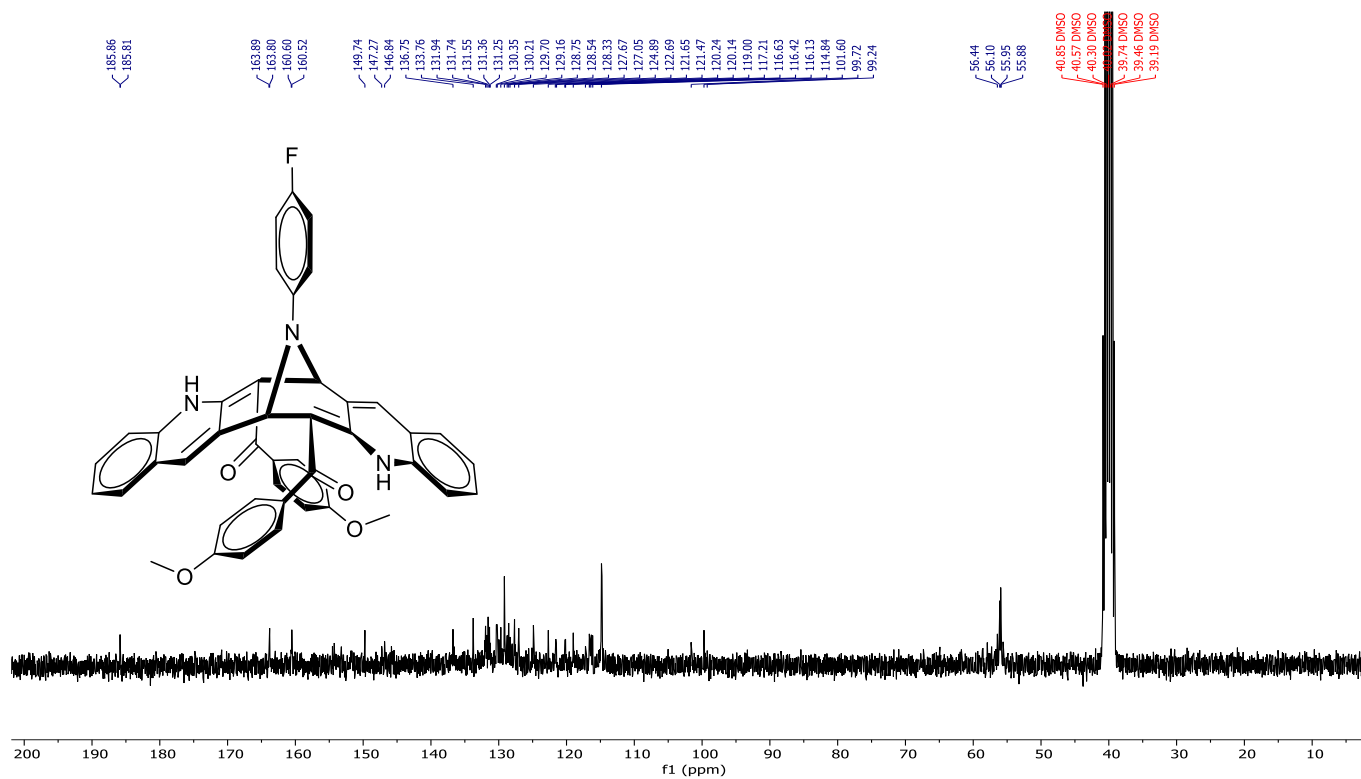
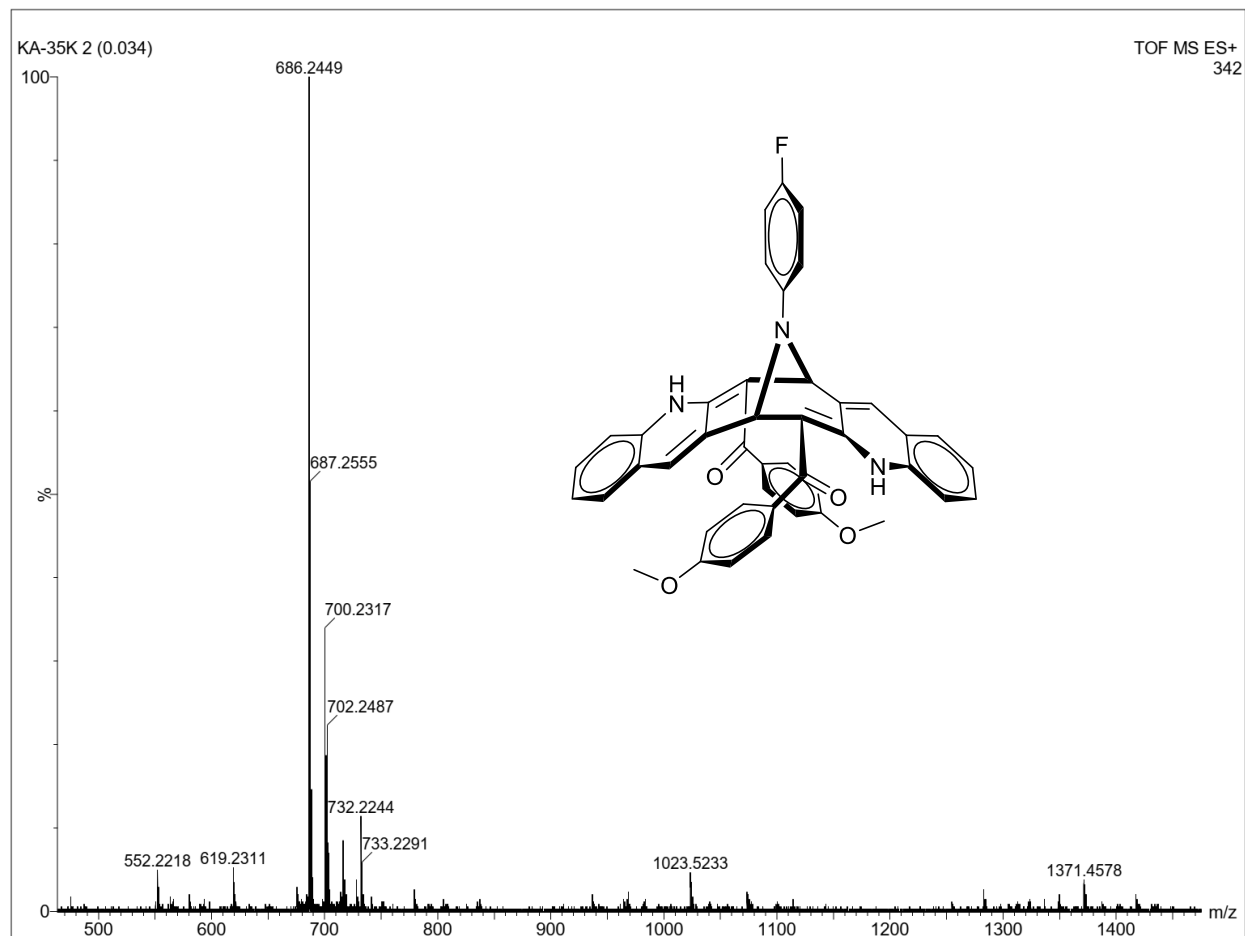


Figure S83: $^{13}\text{C}\{^1\text{H}\}$ NMR Compound **3ab** (75 MHz, CDCl_3)

Figure S84: HRMS (ESI) of **3ab**

Supporting Information

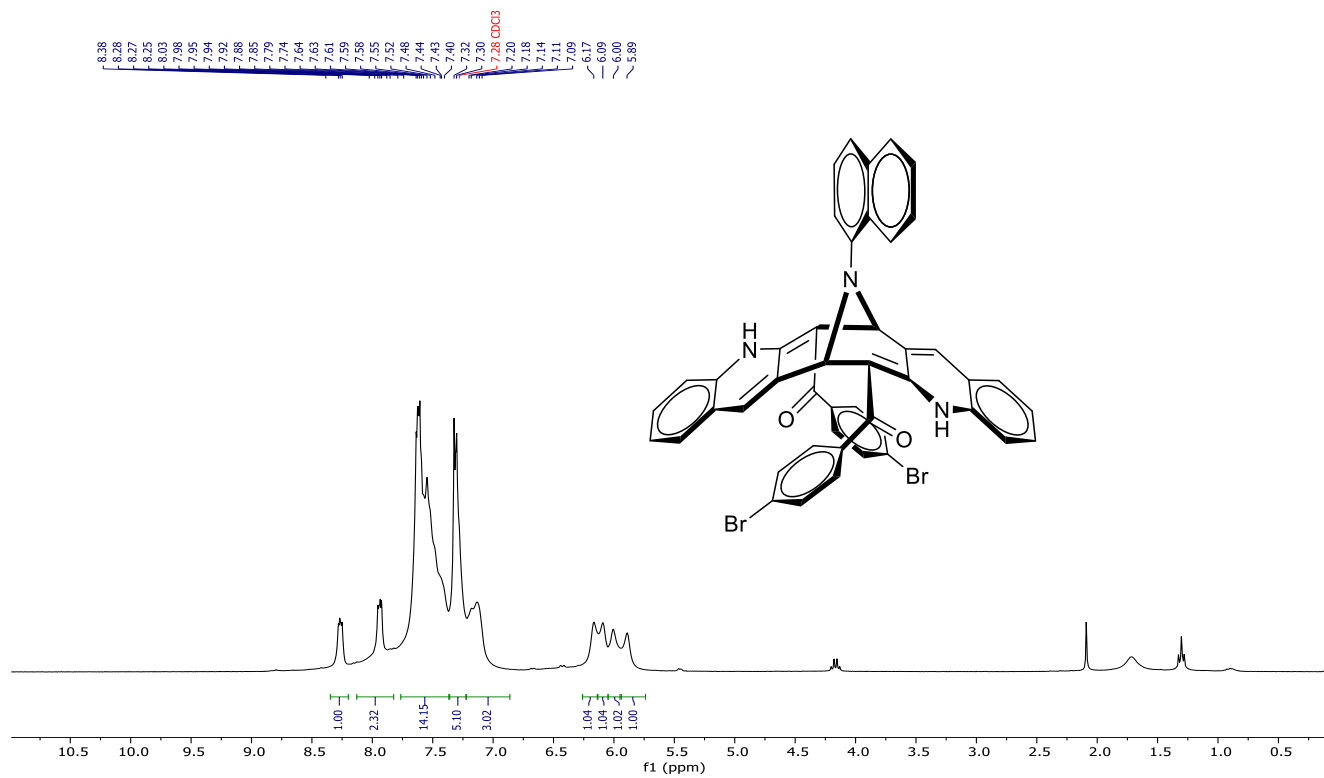


Figure S85: ¹H NMR Compound 3ac (300 MHz, CDCl₃)

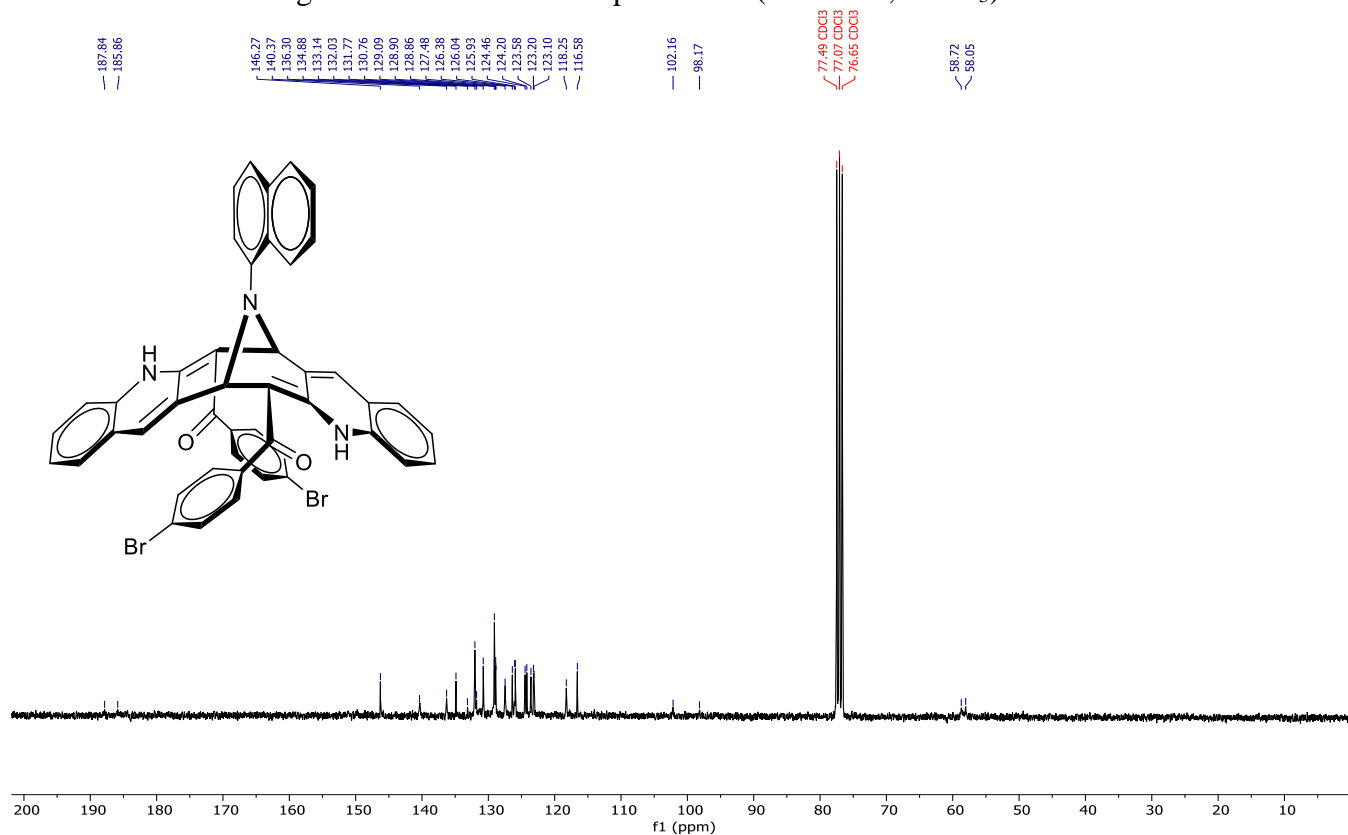


Figure S86: ¹³C{¹H}NMR Compound 3ac (75 MHz, CDCl₃)

Supporting Information

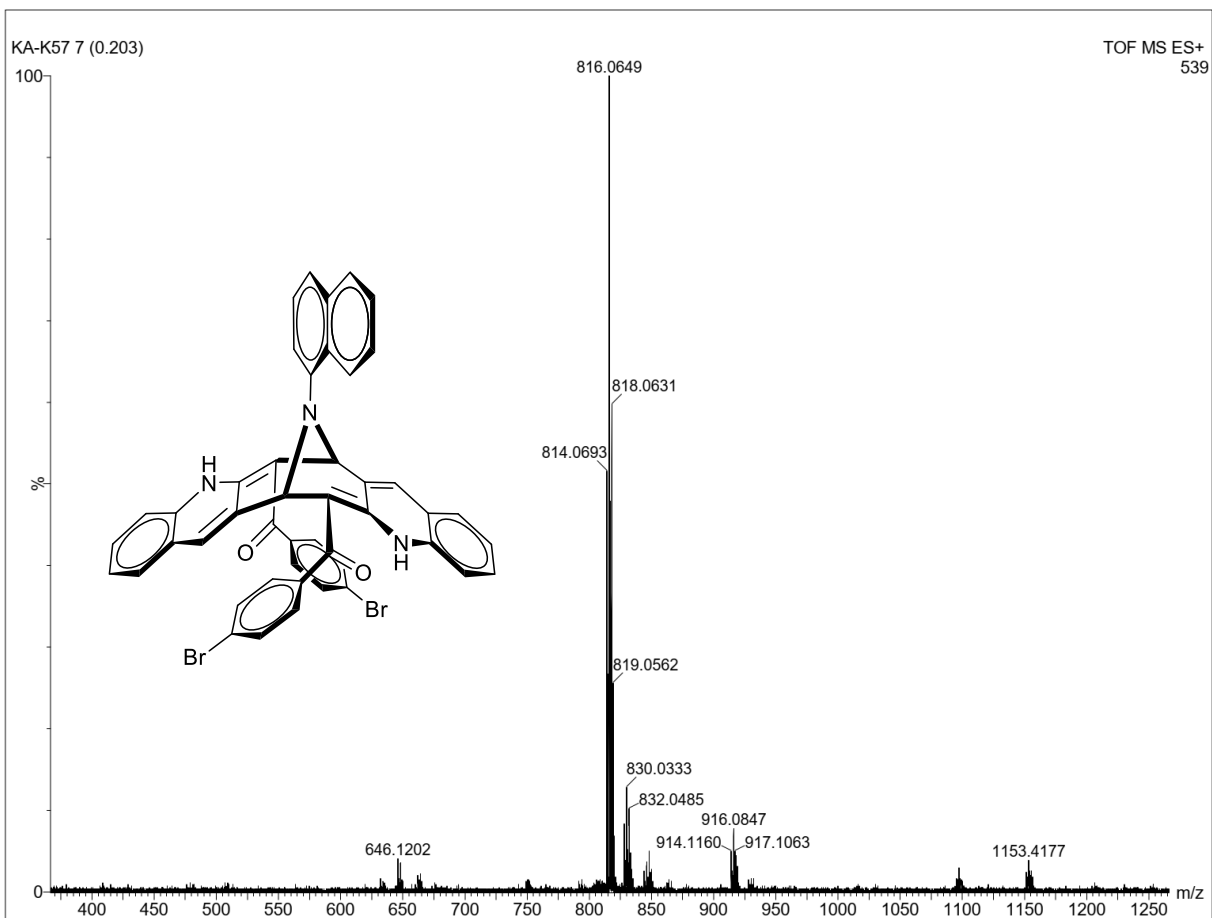


Figure S87: HRMS (ESI) of **3ac**

Supporting Information

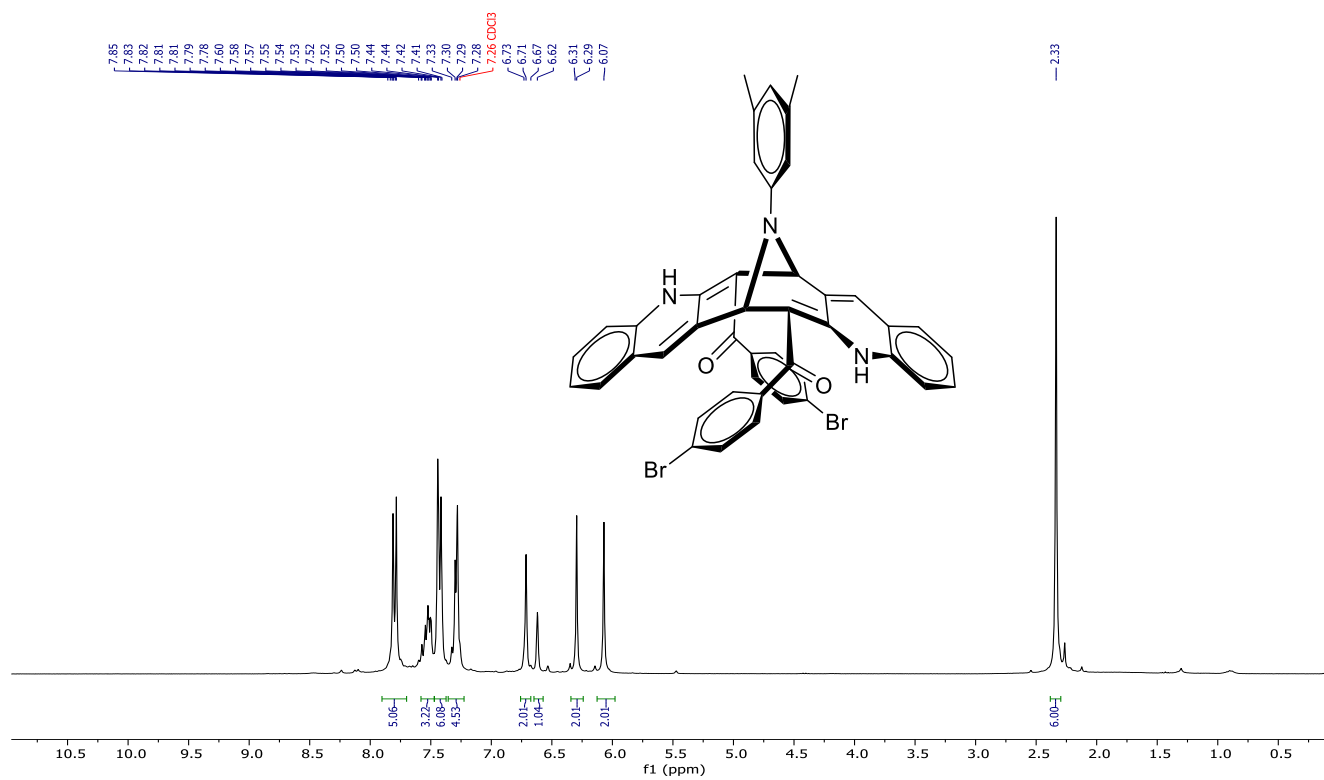


Figure S88: ^1H NMR Compound **3ad** (300 MHz, CDCl_3)

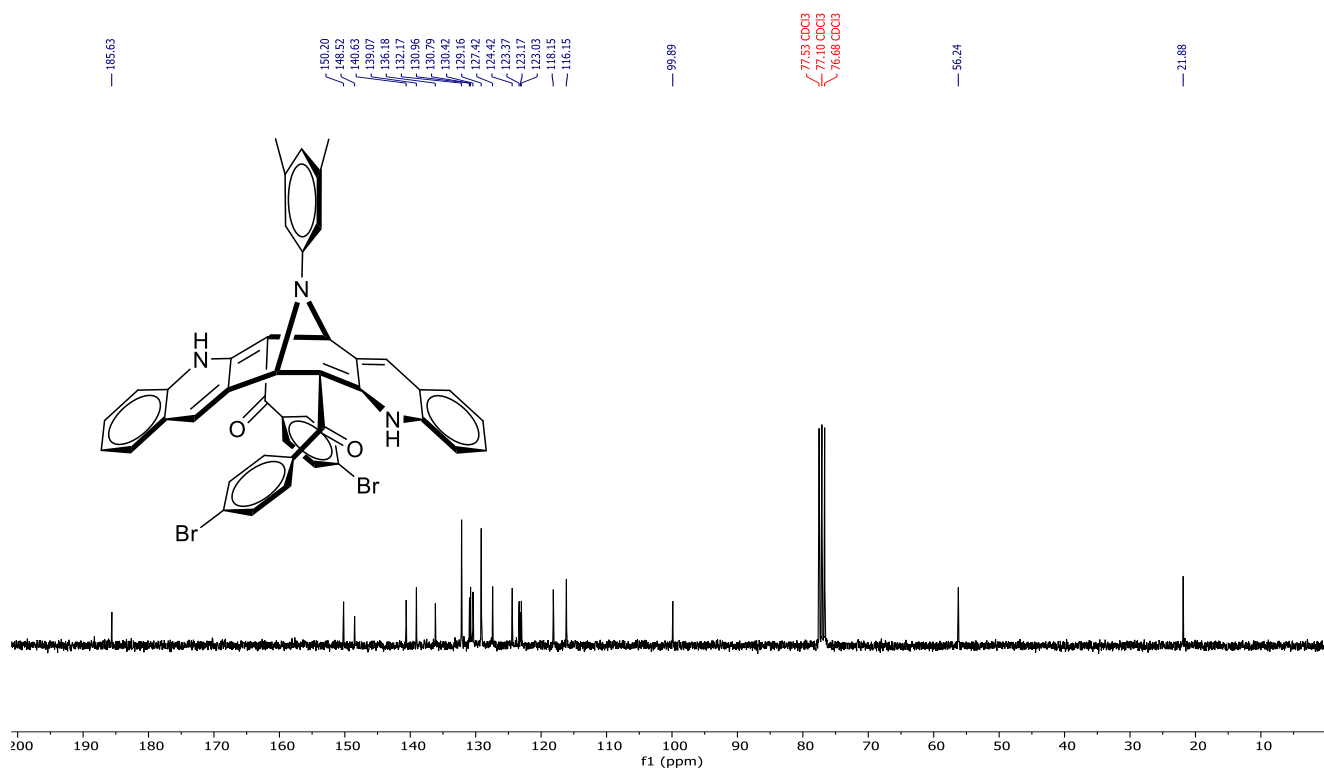
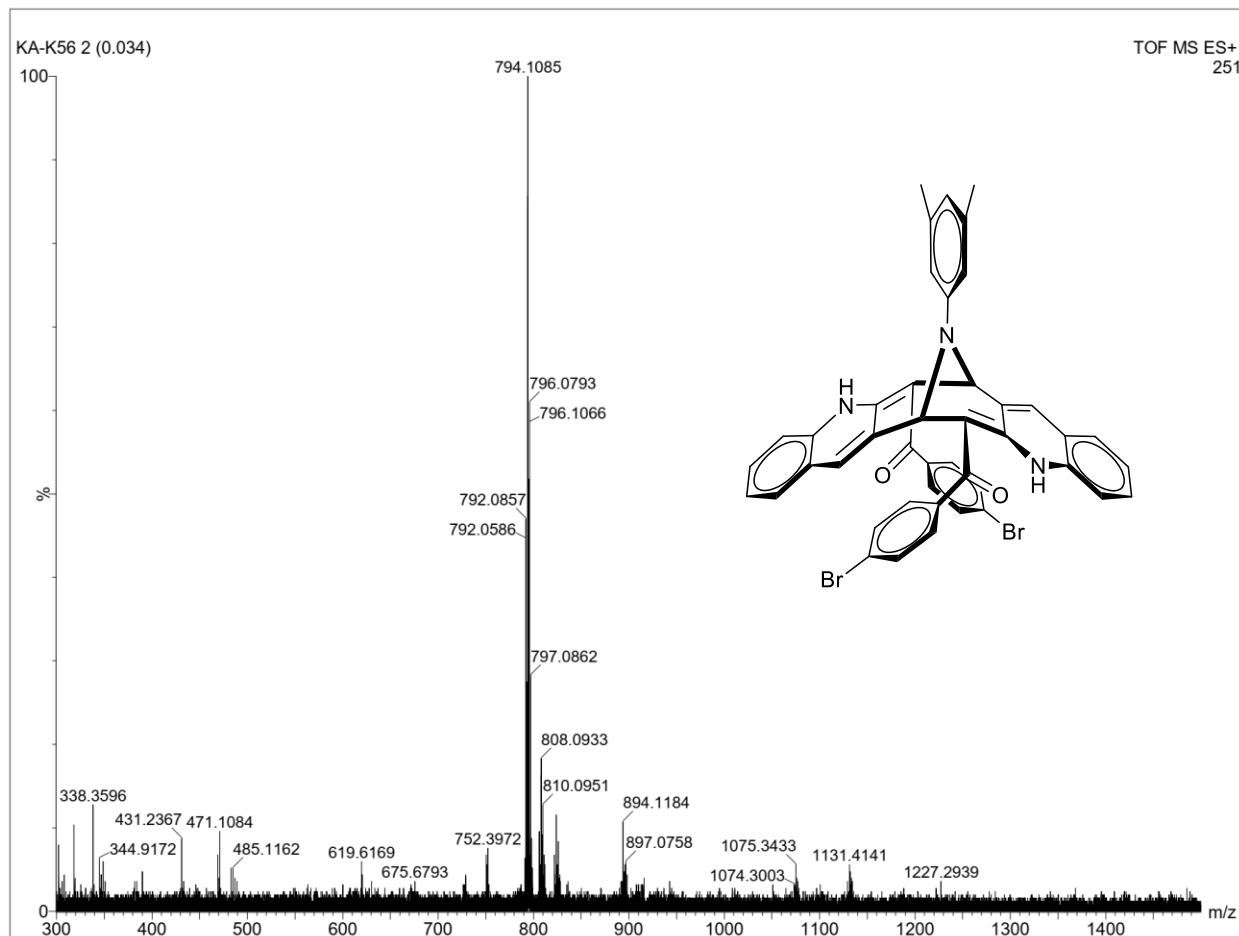


Figure S89: $^{13}\text{C}\{^1\text{H}\}$ NMR Compound **3ad** (75 MHz, CDCl_3)

Figure S90: HRMS (ESI) of **3ad**

Supporting Information

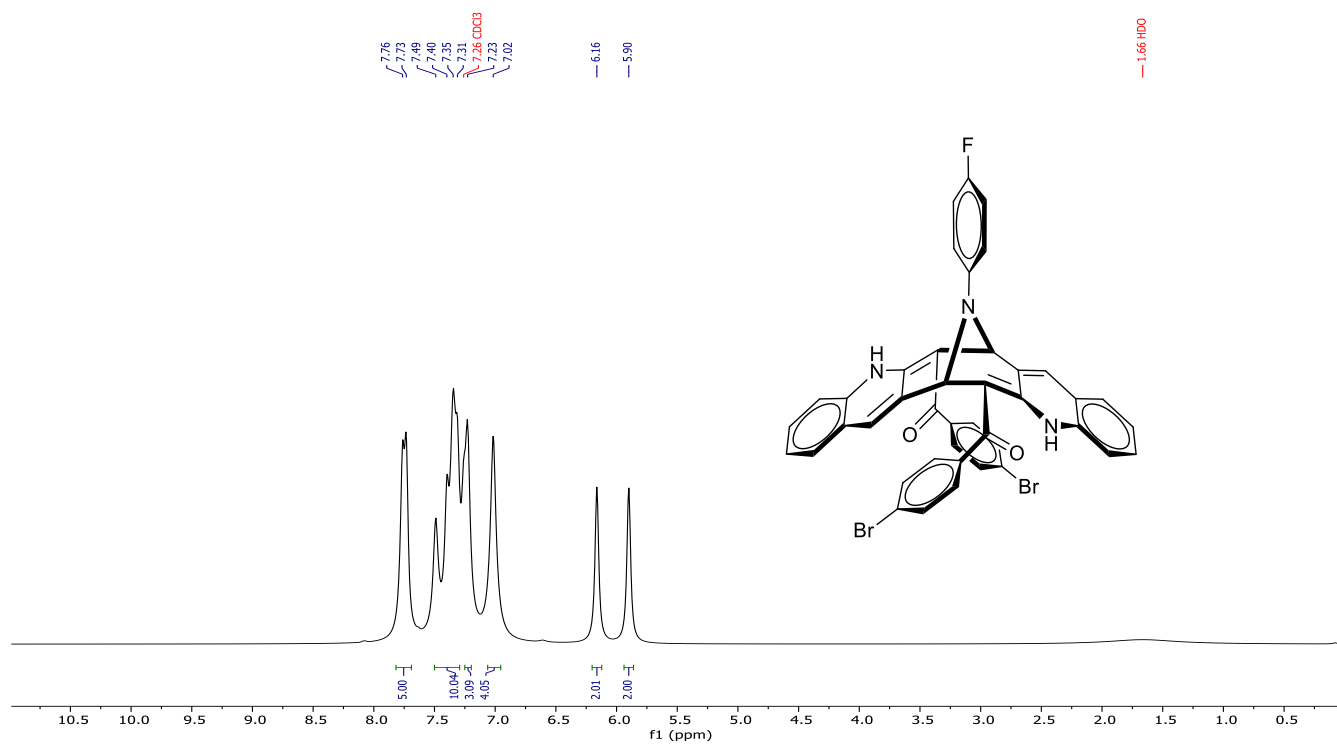


Figure S91: ^1H NMR Compound 3ae (300 MHz, CDCl₃)

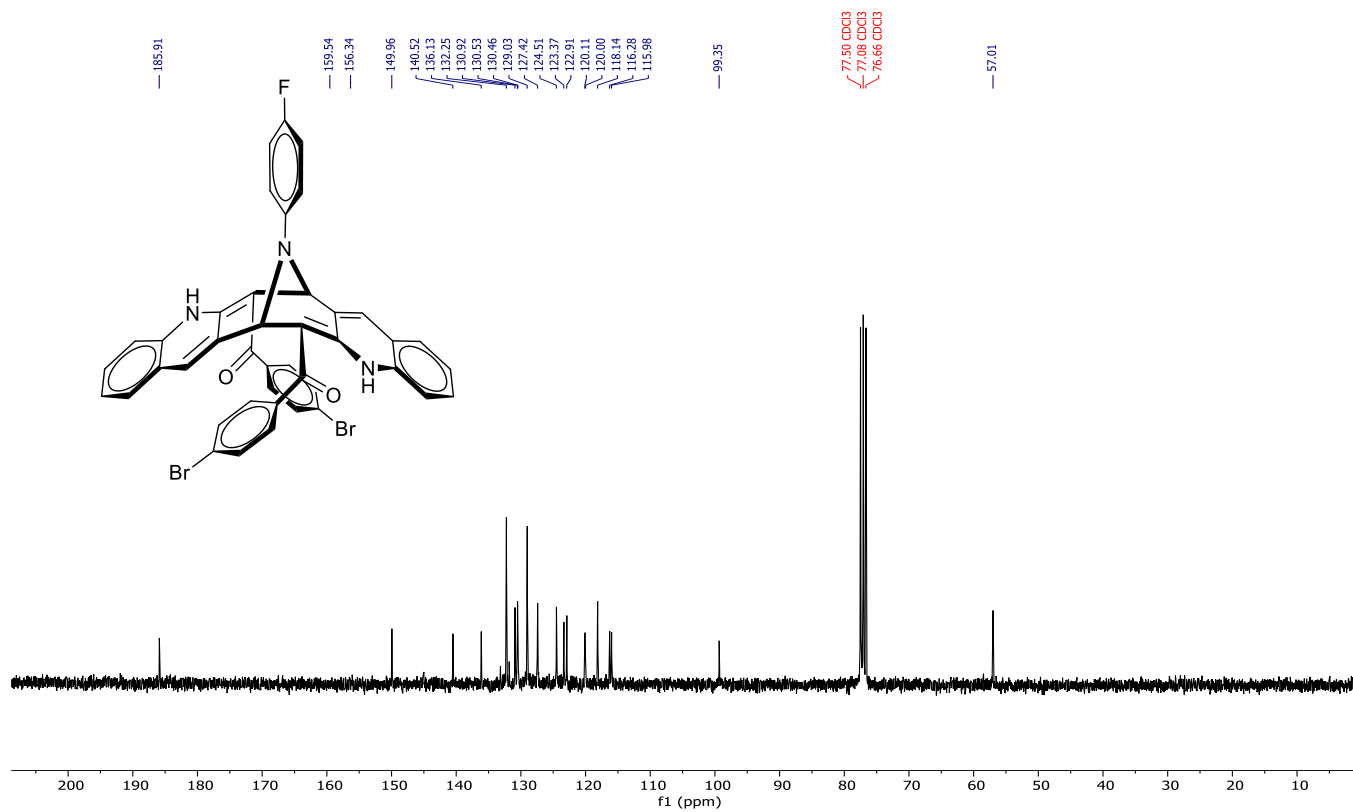


Figure S92: $^{13}\text{C}\{^1\text{H}\}$ NMR Compound 3ae (75 MHz, CDCl₃)

Supporting Information

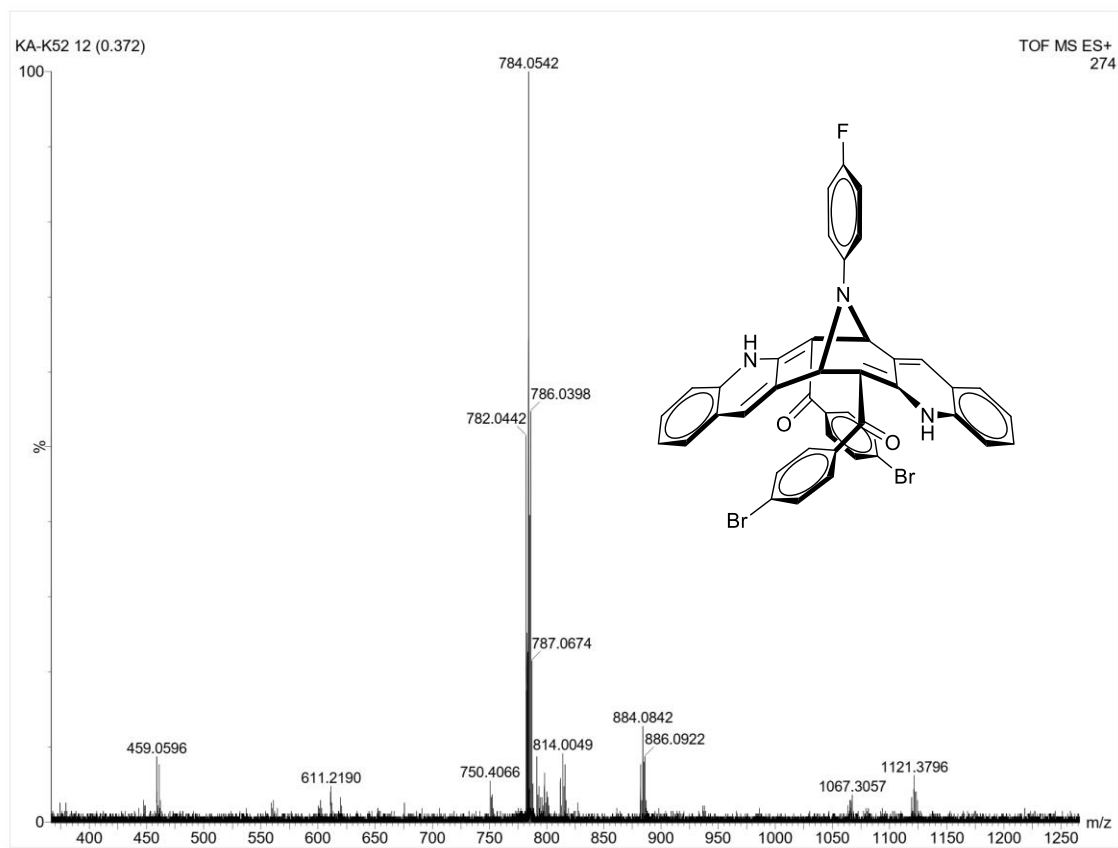


Figure S93: HRMS (ESI) of **3ae**

Supporting Information

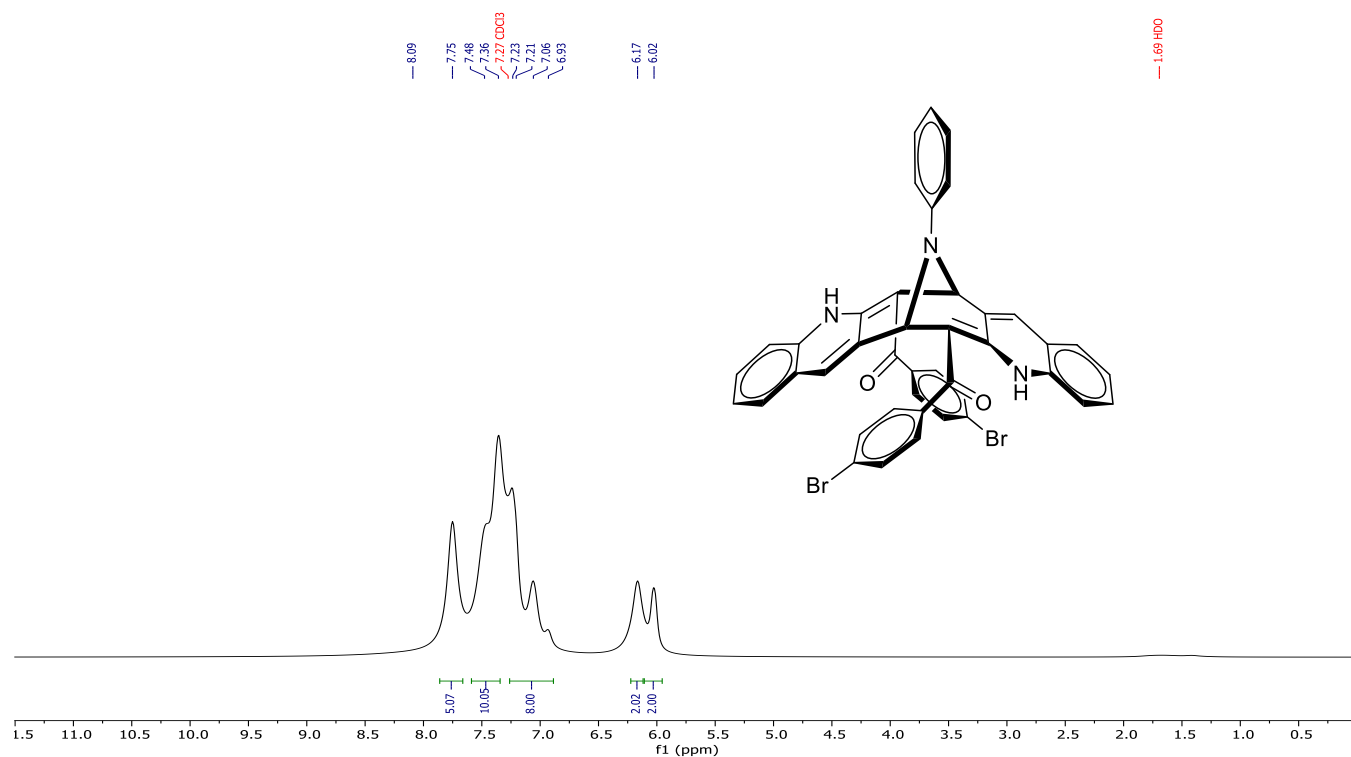


Figure S94: ^1H NMR Compound **3af** (300 MHz, CDCl_3)

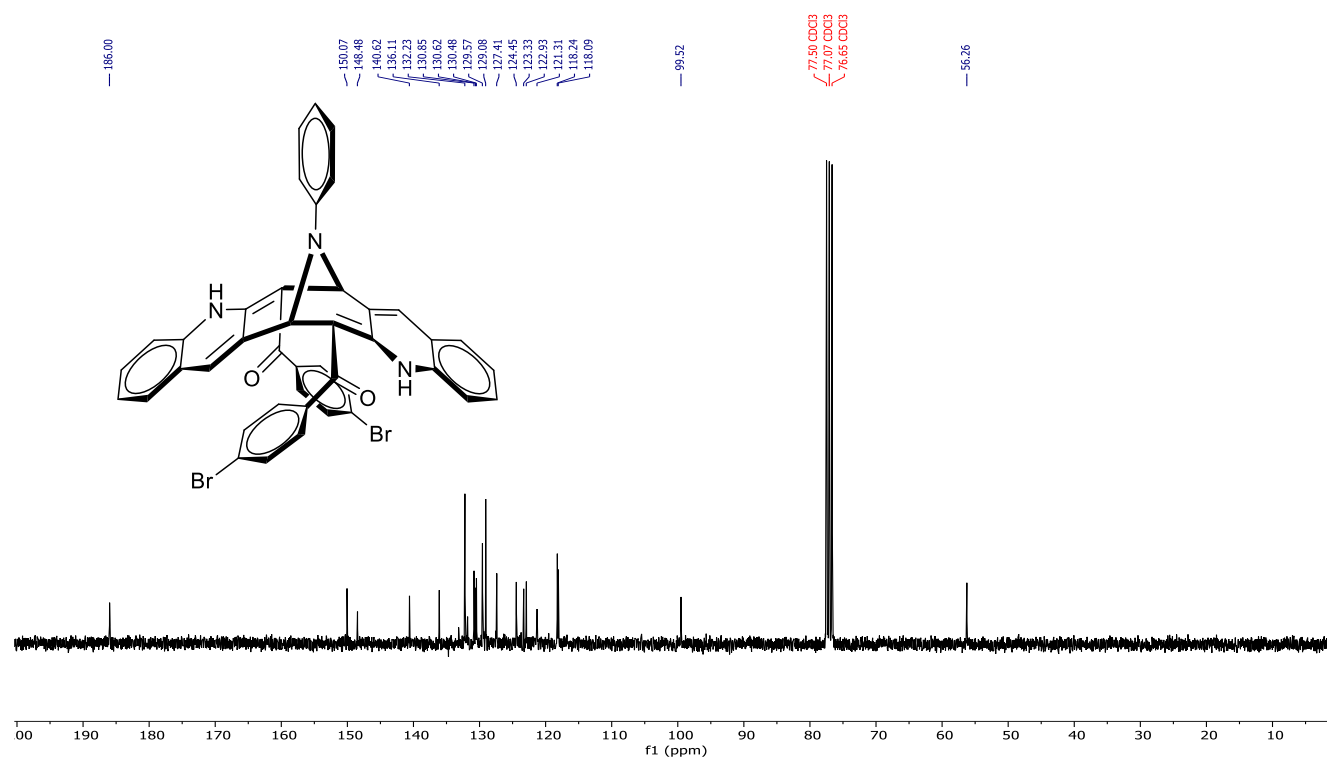


Figure S95: $^{13}\text{C}\{^1\text{H}\}$ NMR Compound **3af** (75 MHz, CDCl_3)

Supporting Information

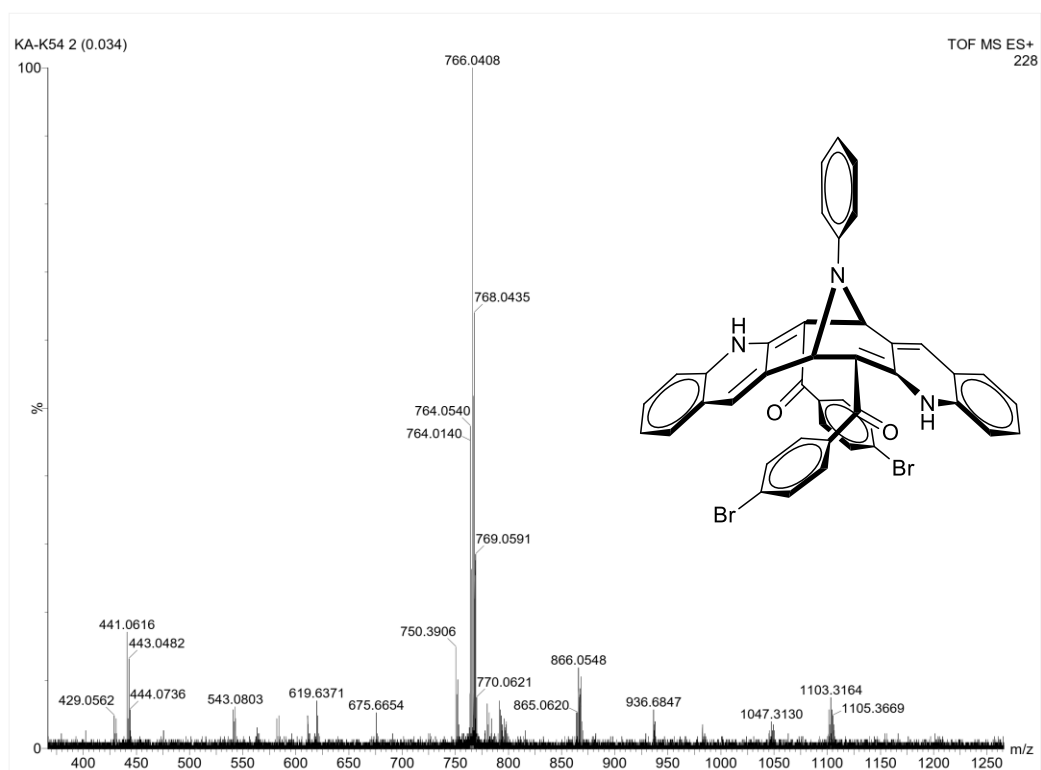


Figure S96: HRMS (ESI) of 3af

Supporting Information

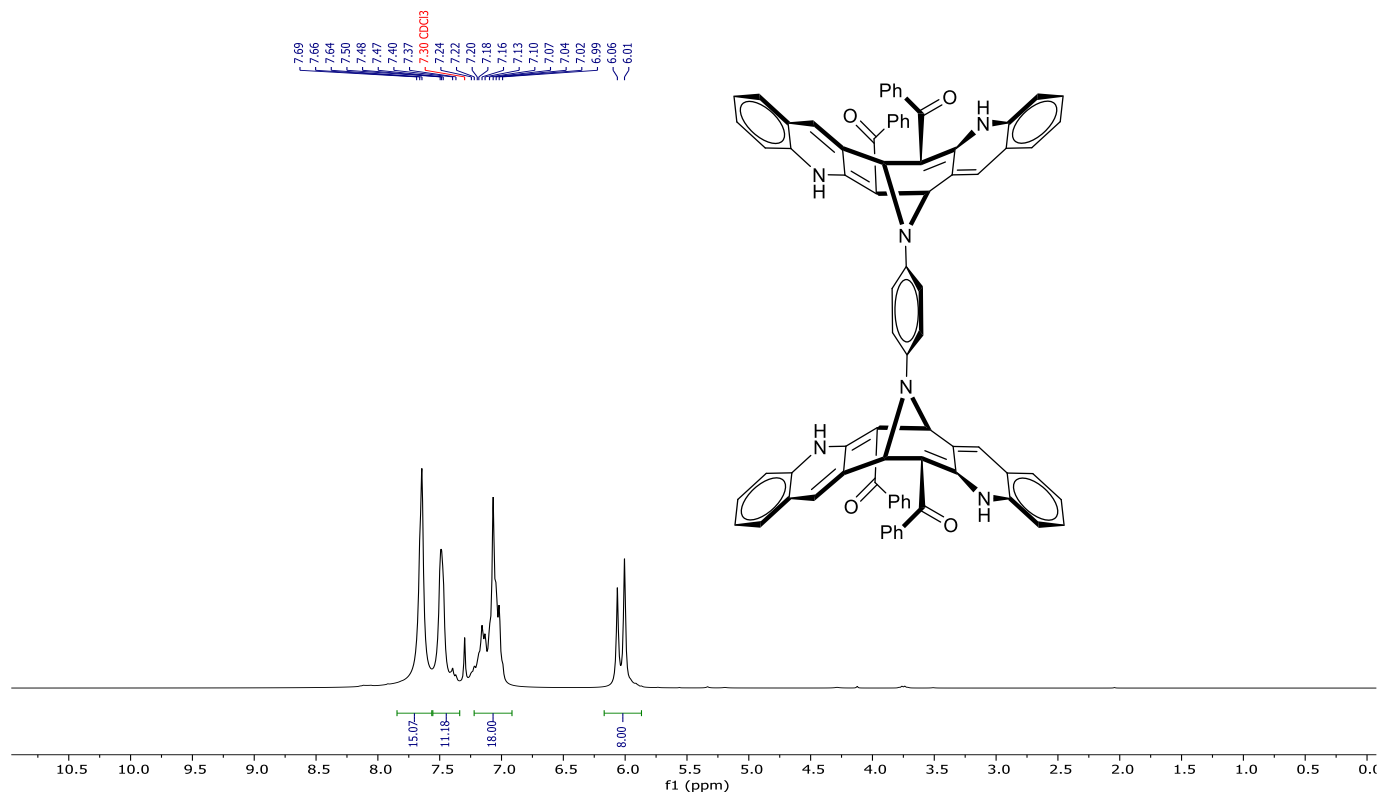


Figure S97: $^1\text{H NMR}$ Compound **3ag** (300 MHz, CDCl_3)

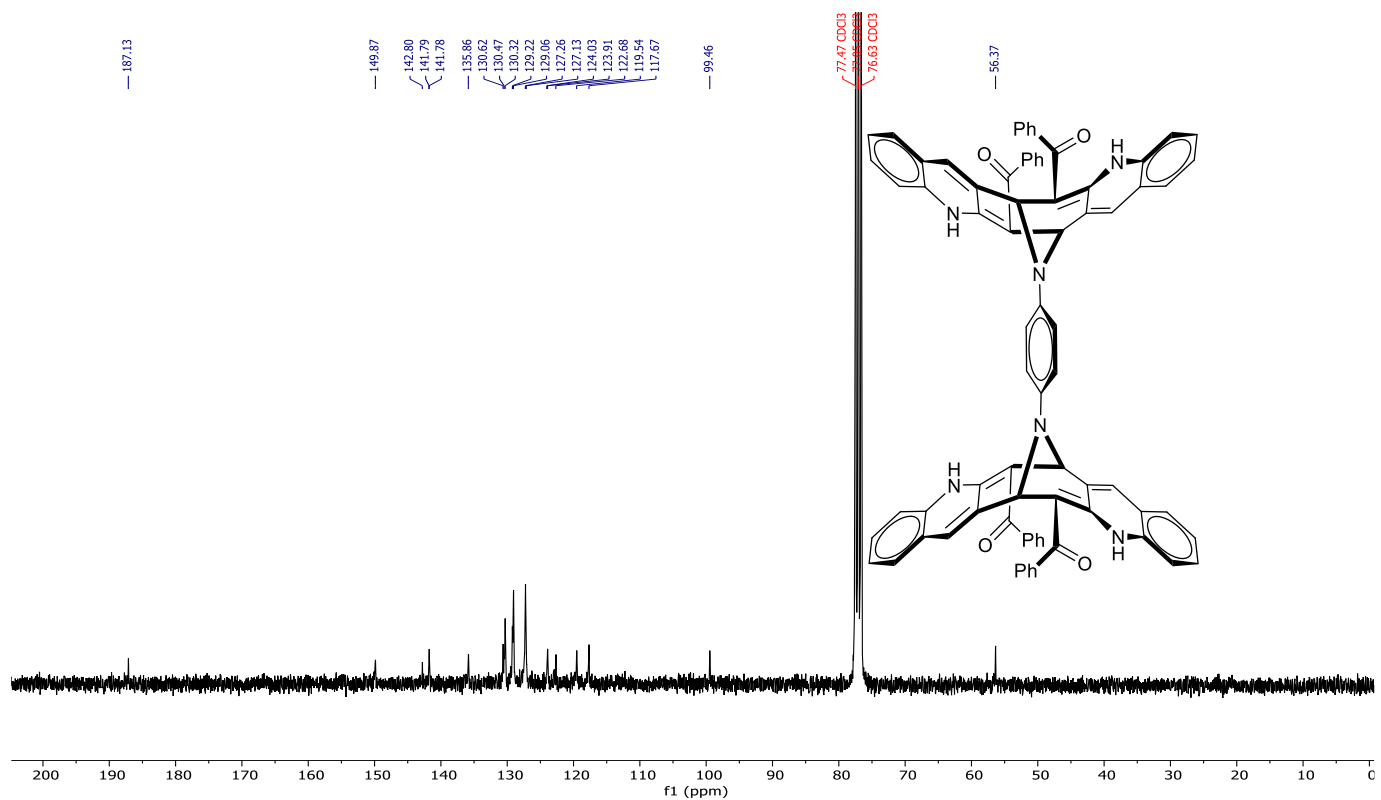
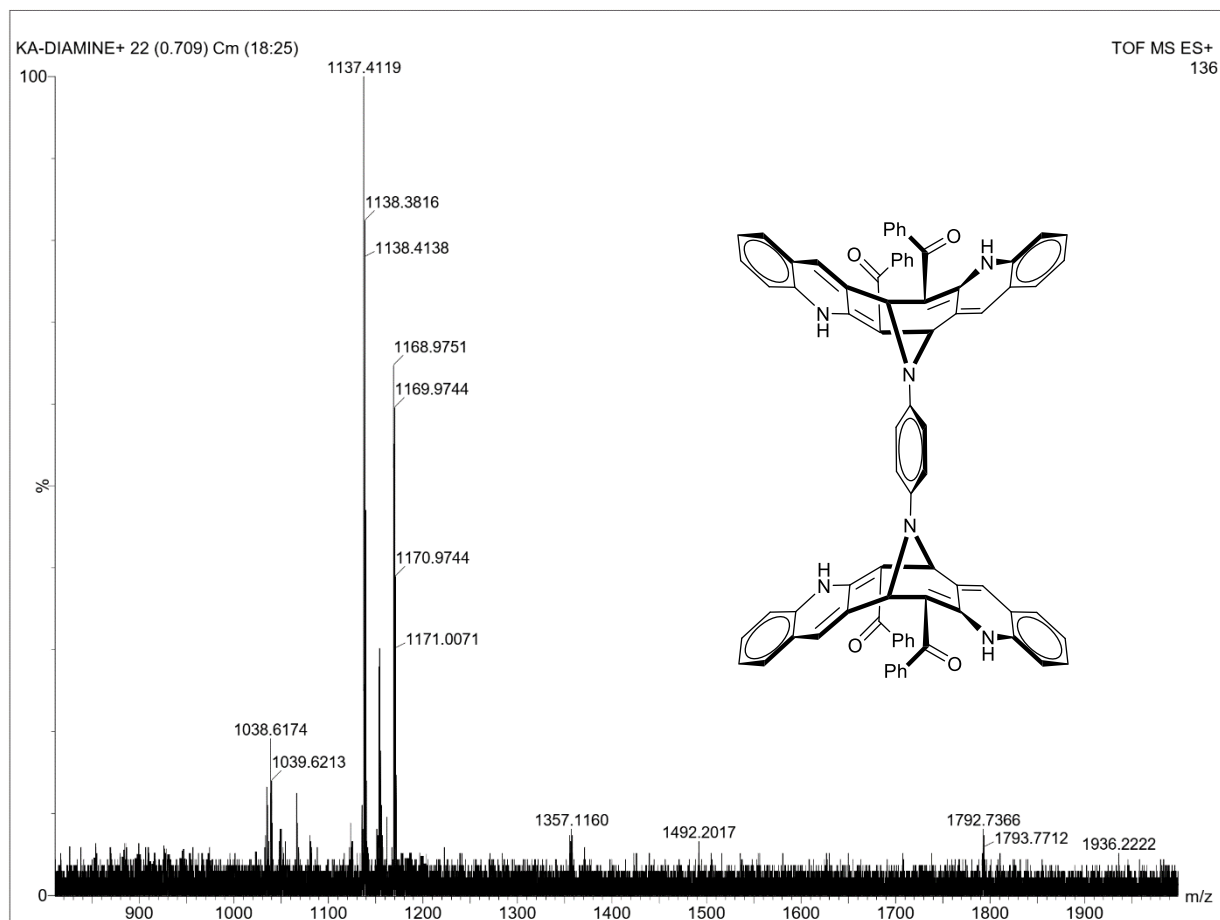


Figure S98: $^{13}\text{C}\{^1\text{H}\}$ NMR Compound **3ag** (75 MHz, CDCl_3)

Figure S99: HRMS (ESI) of **3ag**

Supporting Information

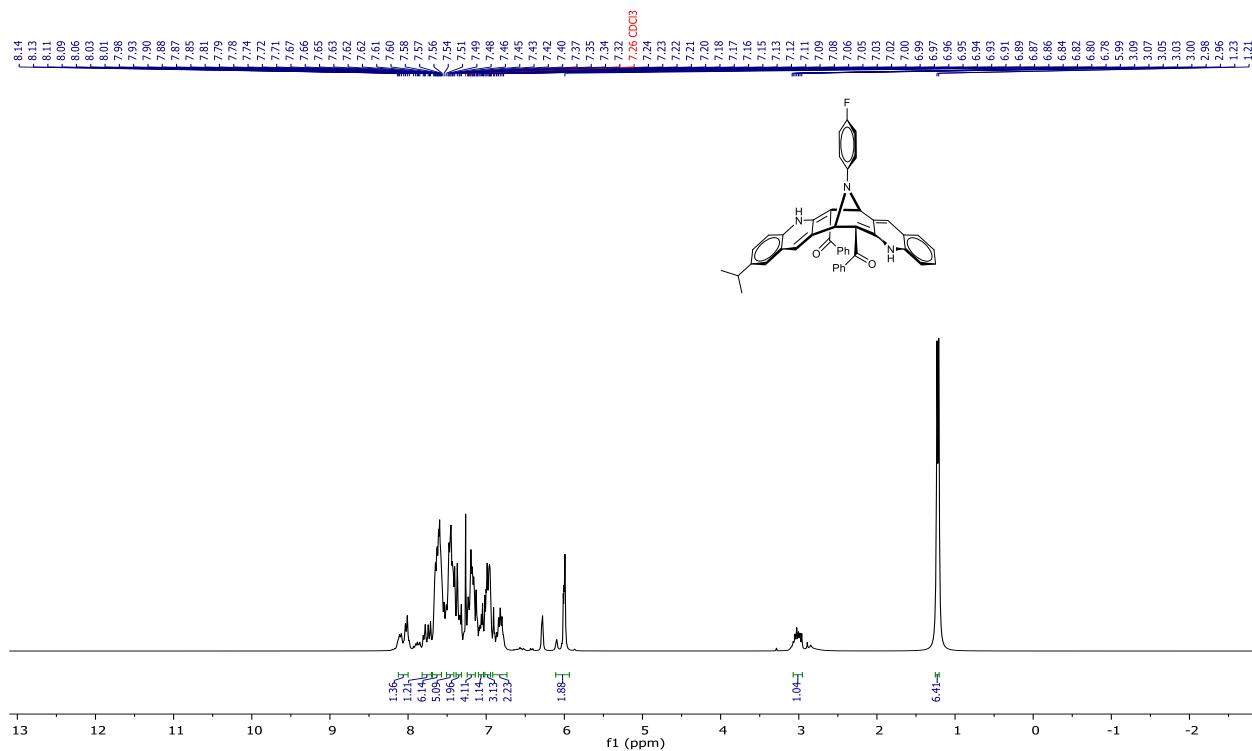


Figure S100: $^1\text{H NMR}$ Compound 3ah (300 MHz, CDCl_3)

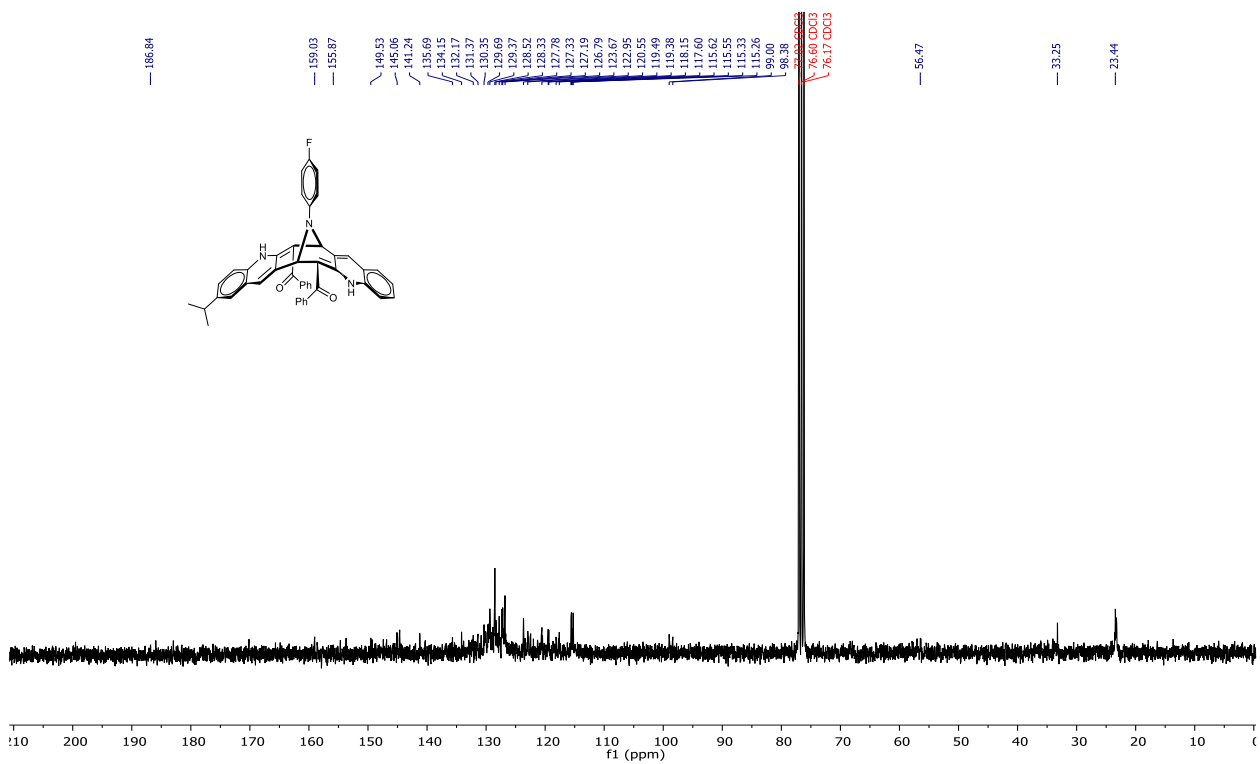


Figure S101: $^{13}\text{C}\{^1\text{H}\}$ NMR Compound 3ah (75 MHz, CDCl_3)

Supporting Information

07/22/2023 02:05 طاب

Chromatogram D:\RIGOL HPLC Data\1402\Nayebzadeh\QC-02123.0000.PRM

Page 1 of 1



Clarity - Chromatography SW

DataApex

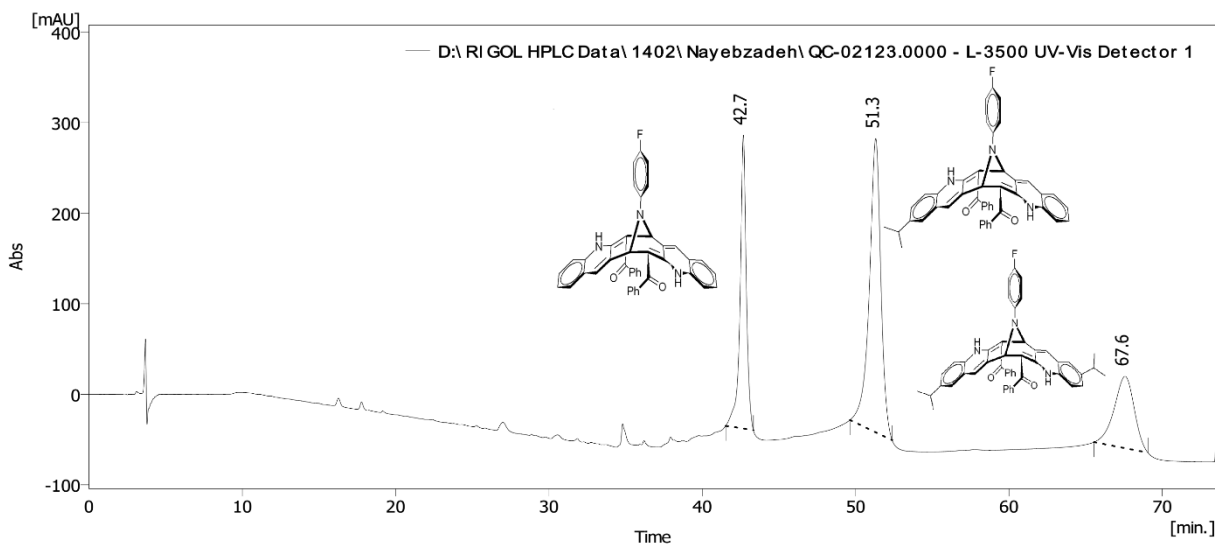
www.dataapex.com

Chromatogram Info:

File Name	: D:\RIGOL HPLC Data\1402\Nayebzadeh\QC-02123.0000.PRM	File Created	: 07/15/2023 04:44:55 طاب
Origin	: Acquired, Acquisition started 07/15/2023 03:26:33 طاب	Acquired Date	: 07/15/2023 04:44:55 طاب
Project	: D:\RIGOL HPLC Data\Projects\sohbatl.PRJ	By	: GLA

Sample Info:

Sample ID	: QC-02123-2	Amount	: 0
Sample	: enol-min-04-24	ISTD Amount	: 0
Inj. Volume [mL]	: 0	Dilution	: 1



Result Table (Uncal - D:\RIGOL HPLC Data\1402\Nayebzadeh\QC-02123.0000 - L-3500 UV-Vis Detector 1)

	Reten. Time [min]	Area [mAU.s]	Height [mAU]	Area [%]	Height [%]	W05 [min]	Compound Name
1	42.677	9191.350	323.847	27.5	44.5	0.39	
2	51.307	17010.090	324.535	50.9	44.6	0.76	
3	67.563	7217.435	79.399	21.6	10.9	1.43	
	Total	33418.876	727.781	100.0	100.0		

Figure S102: Analytical HPLC of crude compound (3ah)

Supporting Information

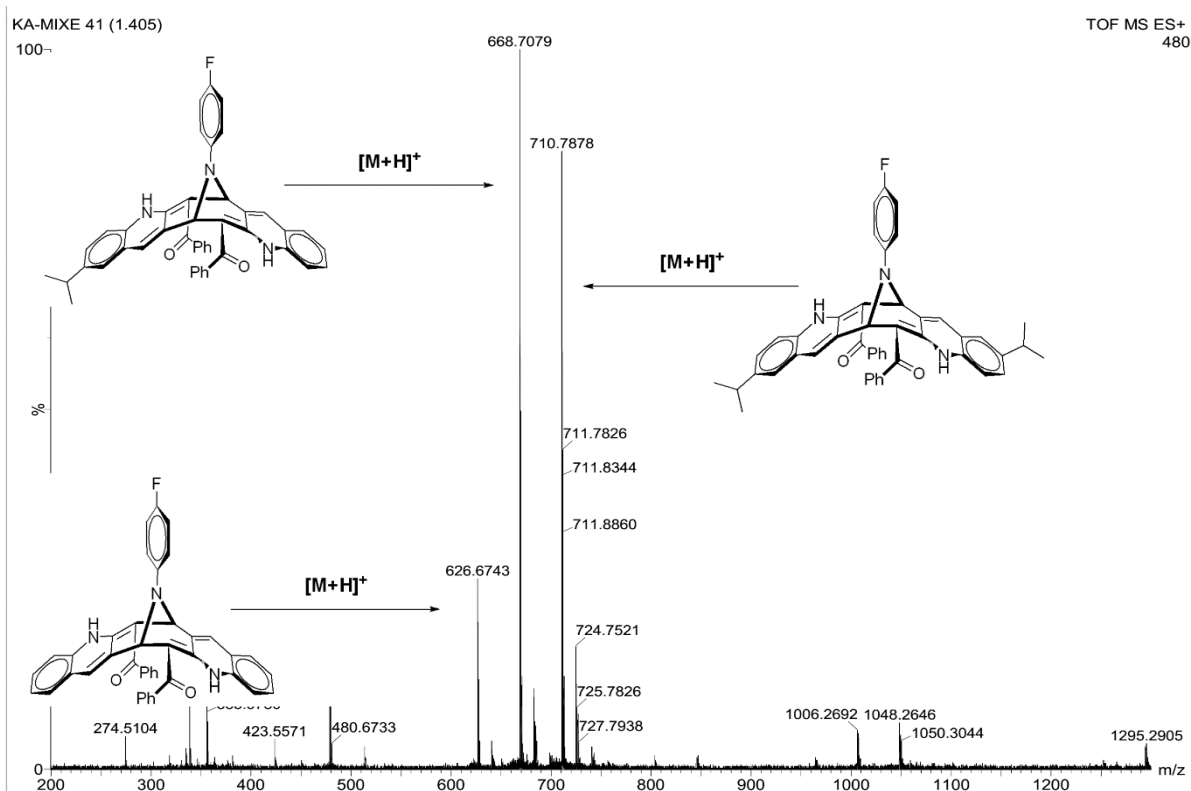
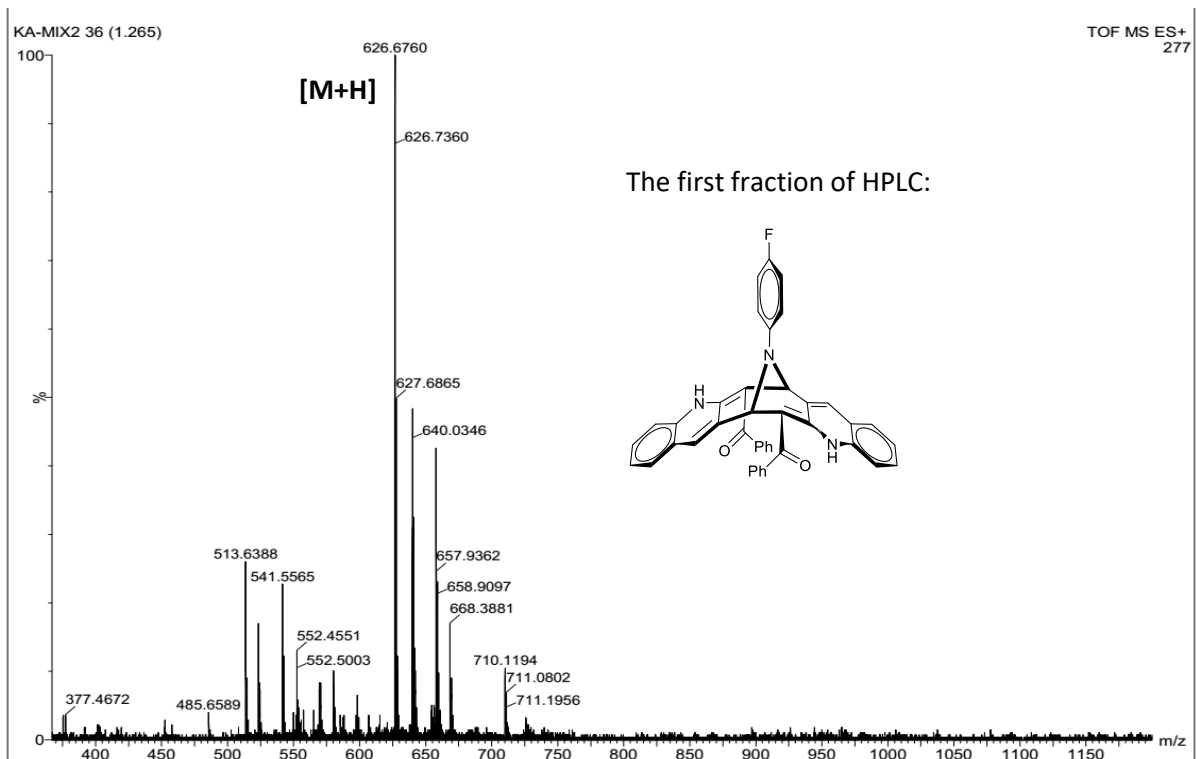
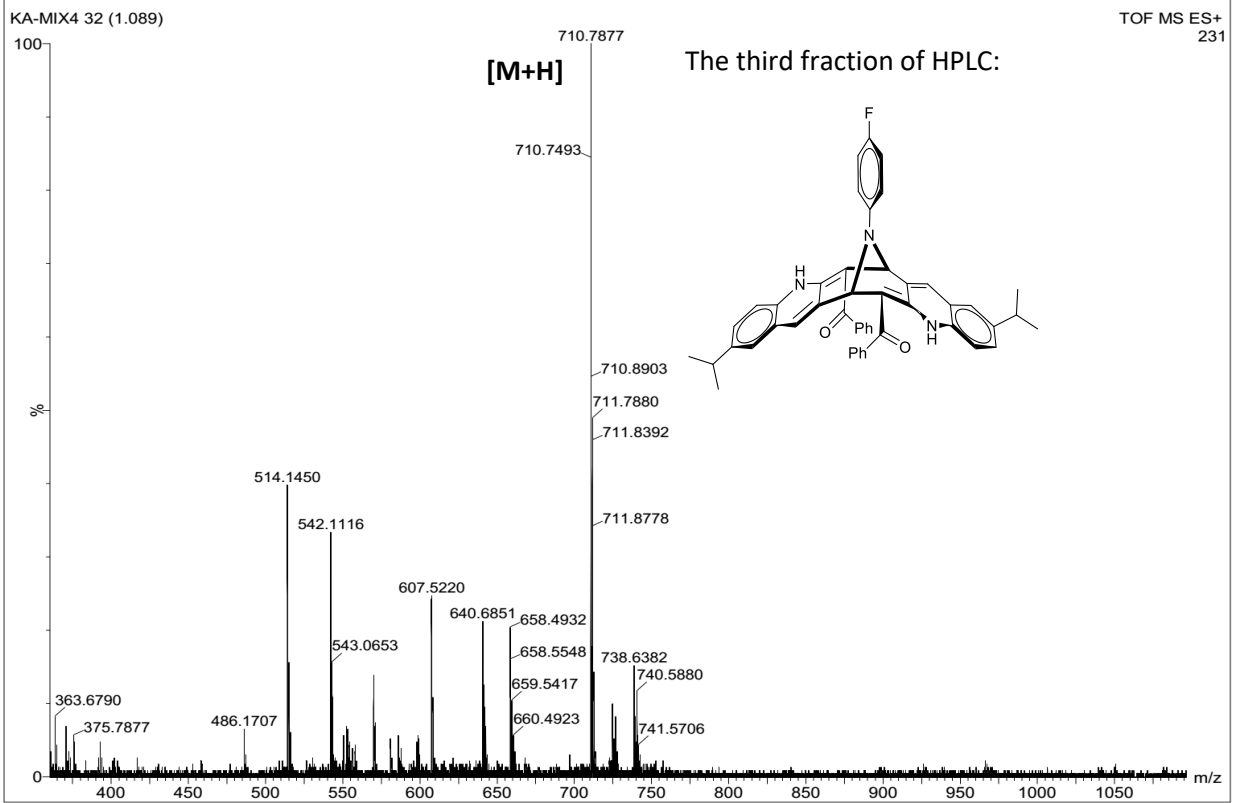
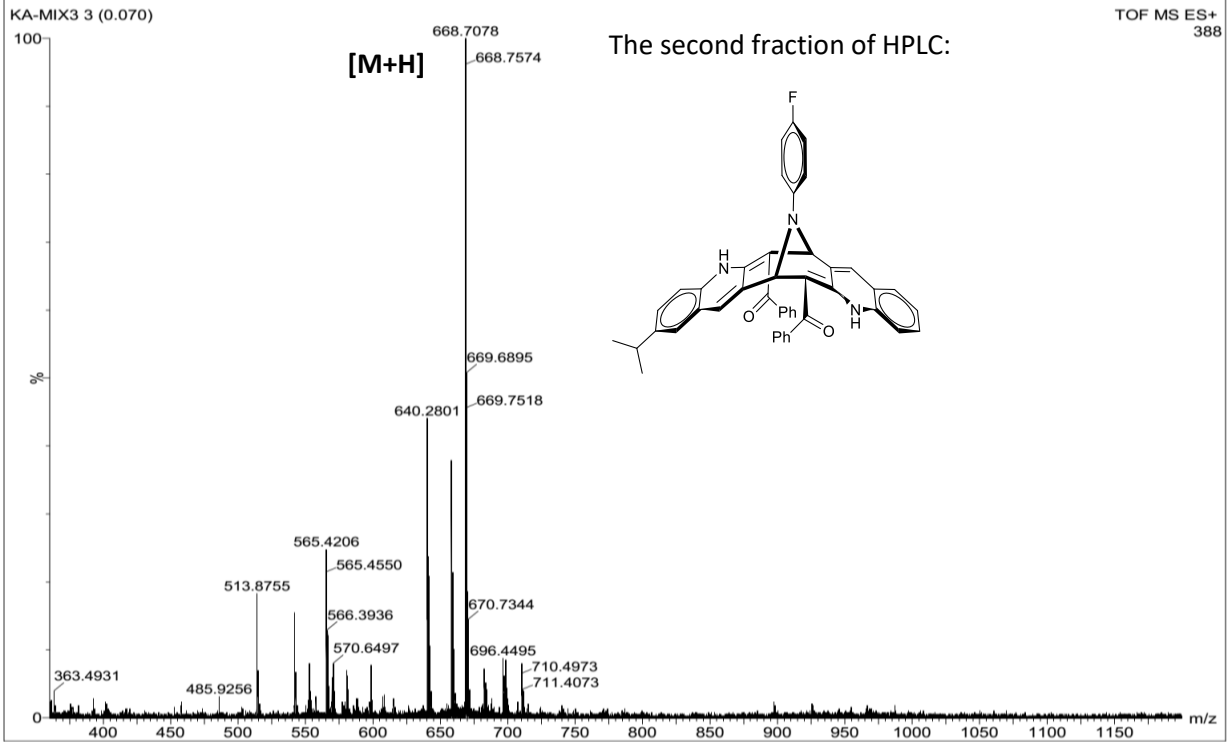


Figure S103: Mass of crude compound (3ah)



Supporting Information



Supporting Information

Chemie : Saeed Balalaie
 Probe : KA4000
 Dateinamen : **3e**
 Operateur : F. Rominger
 Gerät : Bruker APEX-II Quazar area detector

Table S1: Crystal data and structure refinement for **3e**.

Identification code	3e	
Empirical formula	C ₅₀ H ₃₃ N ₃ O ₂	
Formula weight	707.79	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	trigonal	
Space group	R $\bar{3}$	
Z	18	
Unit cell dimensions	a = 39.4459(15) Å	$\alpha = 90$ deg.
	b = 39.4459(15) Å	$\beta = 90$ deg.
	c = 12.5093(8) Å	$\gamma = 120$ deg.
Volume	16856.5(17) Å ³	
Density (calculated)	1.25 g/cm ³	
Absorption coefficient	0.08 mm ⁻¹	
Crystal shape	hexagonal	
Crystal size	0.157 x 0.082 x 0.066 mm ³	
Crystal colour	yellow	
Theta range for data collection	2.0 to 24.1 deg.	
Index ranges	-45 ≤ h ≤ 39, -38 ≤ k ≤ 45, -14 ≤ l ≤ 14	
Reflections collected	34031	
Independent reflections	5968 (R(int) = 0.0717)	
Observed reflections	3507 (I > 2σ(I))	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.96 and 0.93	
Refinement method	Full-matrix least-squares on F ²	
Data/restraints/parameters	5968 / 0 / 502	
Goodness-of-fit on F ²	1.04	
Final R indices (I > 2σ(I))	R1 = 0.053, wR2 = 0.113	
Largest diff. peak and hole	0.22 and -0.20 eÅ ⁻³	

Table S2: Atomic coordinates and equivalent isotropic displacement parameters (Å²) for 3e. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U _{eq}
N1	0.5637(1)	0.7394(1)	0.6842(2)	0.0323(6)
C11	0.5707(1)	0.7745(1)	0.7427(2)	0.0332(7)
H11	0.5766	0.7717	0.8189	0.040
C12	0.5360(1)	0.7817(1)	0.7404(2)	0.0331(7)
C13	0.5096(1)	0.7654(1)	0.6554(2)	0.0333(7)
N14	0.4776(1)	0.7699(1)	0.6496(2)	0.0365(6)
H14	0.4780(8)	0.7868(8)	0.706(2)	0.044
C15	0.4493(1)	0.7534(1)	0.5720(2)	0.0384(7)
C16	0.4178(1)	0.7603(1)	0.5719(3)	0.0520(9)
H16	0.4157	0.7761	0.6260	0.062
C17	0.3901(1)	0.7442(1)	0.4935(3)	0.0668(11)
H17	0.3688	0.7491	0.4930	0.080

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C18	0.3928(1)	0.7209(1)	0.4144(3)	0.0676(11)
H18	0.3734	0.7100	0.3602	0.081
C19	0.4234(1)	0.7136(1)	0.4142(3)	0.0523(9)
H19	0.4250	0.6976	0.3600	0.063
C20	0.4523(1)	0.7297(1)	0.4941(2)	0.0390(8)
C21	0.4854(1)	0.7240(1)	0.4986(2)	0.0347(7)
H21	0.4876	0.7073	0.4480	0.042
C22	0.5137(1)	0.7420(1)	0.5731(2)	0.0315(7)
C23	0.5513(1)	0.7403(1)	0.5733(2)	0.0331(7)
H23	0.5465	0.7158	0.5360	0.040
C24	0.5843(1)	0.7755(1)	0.5154(2)	0.0324(7)
C25	0.6110(1)	0.8073(1)	0.5797(2)	0.0325(7)
N26	0.6420(1)	0.8390(1)	0.5341(2)	0.0382(6)
H26	0.6425(8)	0.8369(8)	0.464(2)	0.046
C27	0.6688(1)	0.8716(1)	0.5902(2)	0.0370(7)
C28	0.6991(1)	0.9035(1)	0.5366(3)	0.0465(8)
H28	0.7014	0.9031	0.4611	0.056
C29	0.7253(1)	0.9354(1)	0.5945(3)	0.0539(9)
H29	0.7458	0.9573	0.5586	0.065
C30	0.7224(1)	0.9363(1)	0.7048(3)	0.0497(9)
H30	0.7408	0.9587	0.7437	0.060
C31	0.6932(1)	0.9052(1)	0.7578(3)	0.0426(8)
H31	0.6916	0.9059	0.8335	0.051
C32	0.6655(1)	0.8720(1)	0.7011(2)	0.0367(7)
C33	0.6338(1)	0.8388(1)	0.7512(2)	0.0364(7)
H33	0.6316	0.8381	0.8269	0.044
C34	0.6067(1)	0.8080(1)	0.6932(2)	0.0321(7)
C40	0.5315(1)	0.8050(1)	0.8172(2)	0.0389(7)
O40	0.5044(1)	0.8137(1)	0.8140(2)	0.0533(6)
C41	0.5595(1)	0.8224(1)	0.9087(2)	0.0393(8)
C42	0.5629(1)	0.7993(1)	0.9862(2)	0.0482(8)
H42	0.5474	0.7716	0.9815	0.058
C43	0.5887(1)	0.8162(1)	1.0706(3)	0.0665(11)
H43	0.5906	0.8001	1.1238	0.080
C44	0.6113(1)	0.8559(2)	1.0777(3)	0.0839(13)
H44	0.6293	0.8674	1.1351	0.101
C45	0.6082(1)	0.8795(1)	1.0018(4)	0.0805(12)
H45	0.6238	0.9071	1.0072	0.097
C46	0.5822(1)	0.8628(1)	0.9174(3)	0.0583(10)
H46	0.5800	0.8791	0.8653	0.070
C50	0.5866(1)	0.7780(1)	0.4035(2)	0.0398(8)
O50	0.6139(1)	0.8072(1)	0.3529(2)	0.0547(6)
C51	0.5554(1)	0.7475(1)	0.3329(2)	0.0441(8)
C52	0.5484(1)	0.7097(1)	0.3253(2)	0.0501(9)
H52	0.5634	0.7017	0.3664	0.060
C53	0.5191(1)	0.6830(1)	0.2570(3)	0.0653(11)
H53	0.5145	0.6570	0.2517	0.078
C54	0.4969(1)	0.6940(1)	0.1976(3)	0.0726(12)
H54	0.4768	0.6756	0.1521	0.087
C55	0.5039(1)	0.7318(1)	0.2045(3)	0.0740(11)
H55	0.4887	0.7397	0.1634	0.089
C56	0.5331(1)	0.7584(1)	0.2716(3)	0.0568(9)
H56	0.5380	0.7845	0.2756	0.068
C61	0.5453(1)	0.7029(1)	0.7384(2)	0.0333(7)
C62	0.5557(1)	0.6750(1)	0.7078(2)	0.0365(7)
C63	0.5396(1)	0.6396(1)	0.7634(3)	0.0476(8)
H63	0.5458	0.6203	0.7417	0.057
C64	0.5148(1)	0.6320(1)	0.8489(3)	0.0518(9)
H64	0.5042	0.6078	0.8861	0.062
C65	0.5056(1)	0.6600(1)	0.8798(2)	0.0484(8)
H65	0.4891	0.6552	0.9397	0.058
C66	0.5203(1)	0.6949(1)	0.8245(2)	0.0392(7)
H66	0.5132	0.7136	0.8459	0.047

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C67	0.5842(1)	0.6839(1)	0.6259(3)	0.0431(8)
C68	0.6083(1)	0.6914(1)	0.5583(3)	0.0479(8)
C71	0.6374(1)	0.7009(1)	0.4769(3)	0.0513(9)
C72	0.6496(1)	0.6747(1)	0.4503(3)	0.0841(13)
H72	0.6383	0.6498	0.4843	0.101
C73	0.6787(2)	0.6847(2)	0.3736(4)	0.1064(17)
H73	0.6876	0.6670	0.3572	0.128
C74	0.6943(1)	0.7196(2)	0.3219(4)	0.0918(14)
H74	0.7139	0.7261	0.2691	0.110
C75	0.6820(1)	0.7454(1)	0.3459(3)	0.0697(11)
H75	0.6932	0.7699	0.3103	0.084
C76	0.6532(1)	0.7359(1)	0.4223(3)	0.0583(10)
H76	0.6441	0.7537	0.4372	0.070

Table S3: Hydrogen coordinates and isotropic displacement parameters (\AA^2) for 3e.

Atom	x	y	z	U_{eq}
H11	0.5766	0.7717	0.8189	0.040
H14	0.4780(8)	0.7868(8)	0.706(2)	0.044
H16	0.4157	0.7761	0.6260	0.062
H17	0.3688	0.7491	0.4930	0.080
H18	0.3734	0.7100	0.3602	0.081
H19	0.4250	0.6976	0.3600	0.063
H21	0.4876	0.7073	0.4480	0.042
H23	0.5465	0.7158	0.5360	0.040
H26	0.6425(8)	0.8369(8)	0.464(2)	0.046
H28	0.7014	0.9031	0.4611	0.056
H29	0.7458	0.9573	0.5586	0.065
H30	0.7408	0.9587	0.7437	0.060
H31	0.6916	0.9059	0.8335	0.051
H33	0.6316	0.8381	0.8269	0.044
H42	0.5474	0.7716	0.9815	0.058
H43	0.5906	0.8001	1.1238	0.080
H44	0.6293	0.8674	1.1351	0.101
H45	0.6238	0.9071	1.0072	0.097
H46	0.5800	0.8791	0.8653	0.070
H52	0.5634	0.7017	0.3664	0.060
H53	0.5145	0.6570	0.2517	0.078
H54	0.4768	0.6756	0.1521	0.087
H55	0.4887	0.7397	0.1634	0.089
H56	0.5380	0.7845	0.2756	0.068
H63	0.5458	0.6203	0.7417	0.057
H64	0.5042	0.6078	0.8861	0.062
H65	0.4891	0.6552	0.9397	0.058
H66	0.5132	0.7136	0.8459	0.047
H72	0.6383	0.6498	0.4843	0.101
H73	0.6876	0.6670	0.3572	0.128
H74	0.7139	0.7261	0.2691	0.110
H75	0.6932	0.7699	0.3103	0.084
H76	0.6441	0.7537	0.4372	0.070

Table S4: Anisotropic displacement parameters (\AA^2) for 3e. The anisotropic displacement factor exponent takes the form: $-2 \pi^2 (h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12})$

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Atom	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
N1	0.0347(14)	0.0294(14)	0.0350(14)	-0.0001(11)	0.0003(11)	0.0176(12)
C11	0.0374(18)	0.0325(18)	0.0328(16)	-0.0021(13)	-0.0025(13)	0.0198(15)
C12	0.0335(18)	0.0318(17)	0.0375(17)	0.0009(13)	0.0030(14)	0.0190(15)
C13	0.0297(17)	0.0286(17)	0.0420(18)	0.0056(13)	0.0031(14)	0.0149(15)
N14	0.0332(15)	0.0341(15)	0.0448(16)	-0.0044(12)	-0.0034(12)	0.0188(13)
C15	0.0295(18)	0.0299(18)	0.052(2)	0.0021(15)	0.0011(15)	0.0123(15)
C16	0.036(2)	0.050(2)	0.073(2)	-0.0114(18)	-0.0094(17)	0.0240(18)
C17	0.046(2)	0.066(3)	0.097(3)	-0.022(2)	-0.020(2)	0.035(2)
C18	0.046(2)	0.074(3)	0.084(3)	-0.021(2)	-0.026(2)	0.032(2)
C19	0.039(2)	0.050(2)	0.063(2)	-0.0113(17)	-0.0113(17)	0.0183(18)
C20	0.0334(19)	0.0333(18)	0.0473(19)	0.0019(14)	-0.0004(14)	0.0144(15)
C21	0.0346(18)	0.0299(17)	0.0370(17)	0.0012(13)	0.0038(14)	0.0144(15)
C22	0.0302(17)	0.0267(16)	0.0372(17)	0.0025(13)	0.0018(13)	0.0140(14)
C23	0.0323(17)	0.0310(17)	0.0356(16)	-0.0012(13)	-0.0024(13)	0.0155(14)
C24	0.0320(17)	0.0345(18)	0.0327(17)	0.0019(13)	0.0014(13)	0.0182(15)
C25	0.0292(17)	0.0337(18)	0.0392(17)	0.0047(14)	0.0033(14)	0.0191(15)
N26	0.0354(15)	0.0395(16)	0.0358(14)	0.0003(13)	0.0010(13)	0.0158(14)
C27	0.0322(18)	0.0338(19)	0.0463(19)	-0.0018(15)	-0.0064(15)	0.0174(16)
C28	0.039(2)	0.042(2)	0.049(2)	0.0048(16)	0.0020(16)	0.0132(17)
C29	0.038(2)	0.041(2)	0.069(3)	0.0047(18)	-0.0036(18)	0.0092(17)
C30	0.041(2)	0.039(2)	0.062(2)	-0.0010(17)	-0.0123(17)	0.0145(18)
C31	0.0374(19)	0.041(2)	0.0486(19)	0.0000(16)	-0.0085(15)	0.0193(17)
C32	0.0299(18)	0.0338(18)	0.0471(19)	0.0016(15)	-0.0054(14)	0.0164(16)
C33	0.0384(19)	0.0410(19)	0.0369(17)	-0.0004(15)	-0.0035(14)	0.0251(17)
C34	0.0306(17)	0.0313(17)	0.0410(17)	-0.0003(14)	-0.0020(14)	0.0204(15)
C40	0.0368(19)	0.0399(19)	0.0429(18)	0.0000(15)	-0.0007(14)	0.0214(16)
O40	0.0540(15)	0.0640(16)	0.0605(15)	-0.0172(12)	-0.0116(11)	0.0435(13)
C41	0.0406(19)	0.043(2)	0.0405(18)	-0.0053(15)	-0.0001(14)	0.0260(17)
C42	0.056(2)	0.054(2)	0.045(2)	0.0002(17)	0.0029(17)	0.0347(19)
C43	0.080(3)	0.093(3)	0.048(2)	-0.004(2)	-0.008(2)	0.060(3)
C44	0.086(3)	0.099(4)	0.078(3)	-0.038(3)	-0.038(2)	0.055(3)
C45	0.079(3)	0.060(3)	0.095(3)	-0.031(2)	-0.030(3)	0.029(2)
C46	0.071(3)	0.048(2)	0.060(2)	-0.0068(18)	-0.0111(19)	0.033(2)
C50	0.0378(19)	0.0348(19)	0.046(2)	0.0027(15)	0.0014(15)	0.0177(16)
O50	0.0544(15)	0.0499(14)	0.0429(13)	0.0035(11)	0.0042(11)	0.0133(12)
C51	0.042(2)	0.048(2)	0.0354(18)	0.0015(15)	0.0045(15)	0.0168(17)
C52	0.053(2)	0.044(2)	0.046(2)	-0.0044(16)	0.0029(16)	0.0182(18)
C53	0.068(3)	0.054(2)	0.052(2)	-0.0066(19)	0.009(2)	0.015(2)
C54	0.063(3)	0.074(3)	0.053(2)	-0.005(2)	-0.009(2)	0.014(2)
C55	0.068(3)	0.083(3)	0.055(2)	0.005(2)	-0.009(2)	0.026(2)
C56	0.056(2)	0.059(2)	0.045(2)	0.0047(17)	-0.0030(18)	0.021(2)
C61	0.0279(17)	0.0281(17)	0.0405(17)	-0.0006(14)	-0.0057(13)	0.0113(14)
C62	0.0403(19)	0.0334(18)	0.0373(17)	-0.0049(14)	-0.0077(14)	0.0196(16)
C63	0.058(2)	0.0307(19)	0.052(2)	-0.0021(16)	-0.0086(17)	0.0202(17)
C64	0.052(2)	0.036(2)	0.053(2)	0.0073(16)	-0.0092(18)	0.0118(18)
C65	0.043(2)	0.042(2)	0.048(2)	0.0074(16)	0.0026(15)	0.0122(18)
C66	0.0347(18)	0.0346(19)	0.0451(19)	0.0011(15)	0.0009(15)	0.0151(15)
C67	0.051(2)	0.039(2)	0.048(2)	-0.0057(15)	-0.0045(17)	0.0292(18)
C68	0.048(2)	0.047(2)	0.053(2)	-0.0089(17)	-0.0051(18)	0.0271(18)
C71	0.055(2)	0.063(2)	0.048(2)	-0.0062(18)	-0.0044(17)	0.038(2)
C72	0.114(4)	0.096(3)	0.078(3)	0.013(2)	0.027(3)	0.080(3)
C73	0.144(5)	0.153(5)	0.087(3)	0.019(3)	0.040(3)	0.124(4)
C74	0.092(3)	0.138(4)	0.076(3)	0.018(3)	0.026(3)	0.081(4)
C75	0.053(2)	0.090(3)	0.072(3)	0.007(2)	0.003(2)	0.040(2)
C76	0.042(2)	0.069(3)	0.070(2)	-0.004(2)	-0.0010(18)	0.033(2)

Table S5: Bond lengths (Å) and angles (deg) for 3e.

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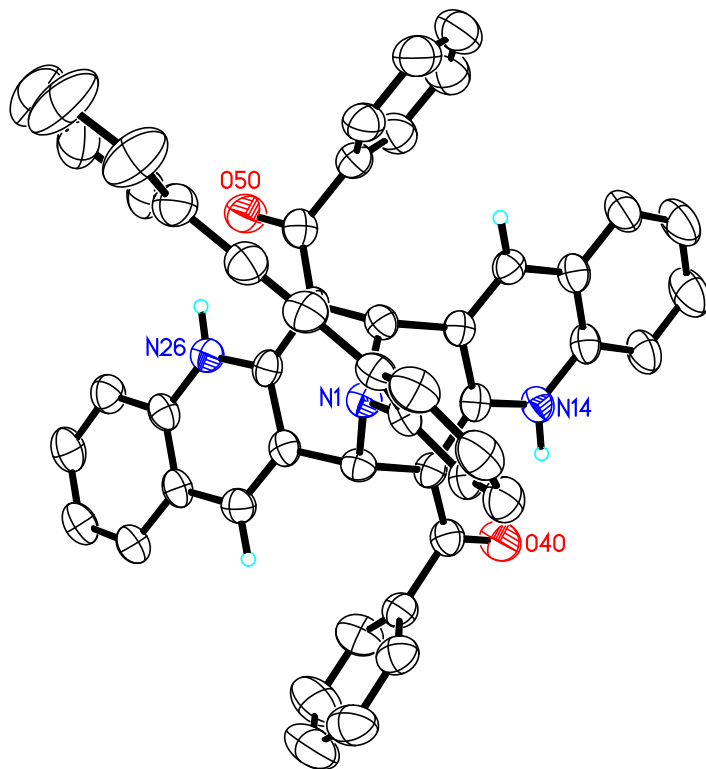
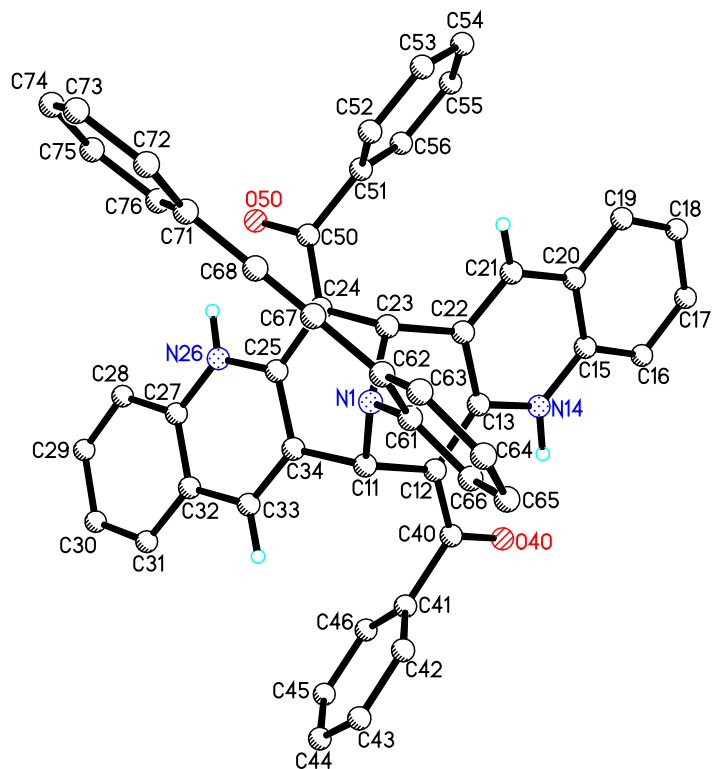
N1-C61	1.419(3)	C51-C56	1.387(4)
N1-C11	1.465(3)	C52-C53	1.398(4)
N1-C23	1.478(3)	C52-H52	0.9500
C11-C34	1.508(4)	C53-C54	1.372(5)
C11-C12	1.531(4)	C53-H53	0.9500
C11-H11	1.0000	C54-C55	1.378(5)
C12-C13	1.400(4)	C54-H54	0.9500
C12-C40	1.402(4)	C55-C56	1.388(5)
C13-N14	1.362(3)	C55-H55	0.9500
C13-C22	1.444(4)	C56-H56	0.9500
N14-C15	1.373(4)	C61-C66	1.386(4)
N14-H14	0.97(3)	C61-C62	1.406(4)
C15-C20	1.396(4)	C62-C63	1.397(4)
C15-C16	1.398(4)	C62-C67	1.430(4)
C16-C17	1.367(4)	C63-C64	1.377(4)
C16-H16	0.9500	C63-H63	0.9500
C17-C18	1.390(5)	C64-C65	1.377(4)
C17-H17	0.9500	C64-H64	0.9500
C18-C19	1.373(4)	C65-C66	1.383(4)
C18-H18	0.9500	C65-H65	0.9500
C19-C20	1.408(4)	C66-H66	0.9500
C19-H19	0.9500	C67-C68	1.192(4)
C20-C21	1.432(4)	C68-C71	1.439(5)
C21-C22	1.350(4)	C71-C76	1.377(4)
C21-H21	0.9500	C71-C72	1.384(5)
C22-C23	1.520(4)	C72-C73	1.390(5)
C23-C24	1.530(4)	C72-H72	0.9500
C23-H23	1.0000	C73-C74	1.358(6)
C24-C50	1.403(4)	C73-H73	0.9500
C24-C25	1.418(4)	C74-C75	1.361(5)
C25-N26	1.360(3)	C74-H74	0.9500
C25-C34	1.432(4)	C75-C76	1.386(5)
N26-C27	1.380(4)	C75-H75	0.9500
N26-H26	0.88(3)	C76-H76	0.9500
C27-C32	1.395(4)	C61-N1-C11	118.6(2)
C27-C28	1.400(4)	C61-N1-C23	117.7(2)
C28-C29	1.370(4)	C11-N1-C23	110.8(2)
C28-H28	0.9500	N1-C11-C34	105.9(2)
C29-C30	1.386(4)	N1-C11-C12	113.8(2)
C29-H29	0.9500	C34-C11-C12	111.4(2)
C30-C31	1.362(4)	N1-C11-H11	108.5
C30-H30	0.9500	C34-C11-H11	108.5
C31-C32	1.407(4)	C12-C11-H11	108.5
C31-H31	0.9500	C13-C12-C40	120.9(3)
C32-C33	1.427(4)	C13-C12-C11	117.2(2)
C33-C34	1.357(4)	C40-C12-C11	121.9(3)
C33-H33	0.9500	N14-C13-C12	120.3(3)
C40-O40	1.274(3)	N14-C13-C22	116.9(3)
C40-C41	1.499(4)	C12-C13-C22	122.8(3)
C41-C42	1.383(4)	C13-N14-C15	124.3(3)
C41-C46	1.386(4)	C13-N14-H14	111.0(16)
C42-C43	1.384(4)	C15-N14-H14	124.8(16)
C42-H42	0.9500	N14-C15-C20	119.3(3)
C43-C44	1.365(5)	N14-C15-C16	120.0(3)
C43-H43	0.9500	C20-C15-C16	120.7(3)
C44-C45	1.375(5)	C17-C16-C15	119.5(3)
C44-H44	0.9500	C17-C16-H16	120.2
C45-C46	1.387(5)	C15-C16-H16	120.2
C45-H45	0.9500	C16-C17-C18	120.7(3)
C46-H46	0.9500	C16-C17-H17	119.7
C50-O50	1.283(3)	C18-C17-H17	119.7
C50-C51	1.504(4)	C19-C18-C17	120.3(3)
C51-C52	1.377(4)	C19-C18-H18	119.8

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C17-C18-H18	119.8	C42-C43-H43	119.9
C18-C19-C20	120.3(3)	C43-C44-C45	120.2(4)
C18-C19-H19	119.9	C43-C44-H44	119.9
C20-C19-H19	119.9	C45-C44-H44	119.9
C15-C20-C19	118.5(3)	C44-C45-C46	119.9(4)
C15-C20-C21	117.8(3)	C44-C45-H45	120.1
C19-C20-C21	123.7(3)	C46-C45-H45	120.1
C22-C21-C20	121.6(3)	C41-C46-C45	120.4(3)
C22-C21-H21	119.2	C41-C46-H46	119.8
C20-C21-H21	119.2	C45-C46-H46	119.8
C21-C22-C13	120.1(3)	O50-C50-C24	123.4(3)
C21-C22-C23	123.1(3)	O50-C50-C51	114.4(3)
C13-C22-C23	116.8(2)	C24-C50-C51	122.1(3)
N1-C23-C22	110.2(2)	C52-C51-C56	118.9(3)
N1-C23-C24	108.9(2)	C52-C51-C50	123.3(3)
C22-C23-C24	111.4(2)	C56-C51-C50	117.8(3)
N1-C23-H23	108.8	C51-C52-C53	120.0(3)
C22-C23-H23	108.8	C51-C52-H52	120.0
C24-C23-H23	108.8	C53-C52-H52	120.0
C50-C24-C25	120.7(3)	C54-C53-C52	120.8(4)
C50-C24-C23	122.1(3)	C54-C53-H53	119.6
C25-C24-C23	117.0(2)	C52-C53-H53	119.6
N26-C25-C24	120.2(2)	C53-C54-C55	119.5(4)
N26-C25-C34	117.3(3)	C53-C54-H54	120.2
C24-C25-C34	122.5(3)	C55-C54-H54	120.2
C25-N26-C27	124.0(3)	C54-C55-C56	119.8(4)
C25-N26-H26	112.6(19)	C54-C55-H55	120.1
C27-N26-H26	123.4(19)	C56-C55-H55	120.1
N26-C27-C32	119.0(3)	C51-C56-C55	121.0(4)
N26-C27-C28	120.4(3)	C51-C56-H56	119.5
C32-C27-C28	120.5(3)	C55-C56-H56	119.5
C29-C28-C27	119.1(3)	C66-C61-C62	119.0(3)
C29-C28-H28	120.5	C66-C61-N1	123.2(3)
C27-C28-H28	120.5	C62-C61-N1	117.6(2)
C28-C29-C30	121.0(3)	C63-C62-C61	118.9(3)
C28-C29-H29	119.5	C63-C62-C67	120.7(3)
C30-C29-H29	119.5	C61-C62-C67	120.3(3)
C31-C30-C29	120.3(3)	C64-C63-C62	121.5(3)
C31-C30-H30	119.8	C64-C63-H63	119.3
C29-C30-H30	119.8	C62-C63-H63	119.3
C30-C31-C32	120.4(3)	C63-C64-C65	119.1(3)
C30-C31-H31	119.8	C63-C64-H64	120.5
C32-C31-H31	119.8	C65-C64-H64	120.5
C27-C32-C31	118.6(3)	C64-C65-C66	120.8(3)
C27-C32-C33	118.0(3)	C64-C65-H65	119.6
C31-C32-C33	123.3(3)	C66-C65-H65	119.6
C34-C33-C32	121.5(3)	C65-C66-C61	120.7(3)
C34-C33-H33	119.2	C65-C66-H66	119.6
C32-C33-H33	119.2	C61-C66-H66	119.6
C33-C34-C25	120.0(3)	C68-C67-C62	179.3(3)
C33-C34-C11	122.7(3)	C67-C68-C71	179.4(3)
C25-C34-C11	117.3(2)	C76-C71-C72	118.6(3)
O40-C40-C12	123.6(3)	C76-C71-C68	120.9(3)
O40-C40-C41	115.3(3)	C72-C71-C68	120.5(3)
C12-C40-C41	121.1(3)	C71-C72-C73	119.9(4)
C42-C41-C46	118.9(3)	C71-C72-H72	120.1
C42-C41-C40	121.7(3)	C73-C72-H72	120.1
C46-C41-C40	119.4(3)	C74-C73-C72	120.7(4)
C41-C42-C43	120.4(3)	C74-C73-H73	119.7
C41-C42-H42	119.8	C72-C73-H73	119.7
C43-C42-H42	119.8	C73-C74-C75	120.0(4)
C44-C43-C42	120.3(4)	C73-C74-H74	120.0
C44-C43-H43	119.9	C75-C74-H74	120.0

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C74-C75-C76	120.1(4)
C74-C75-H75	119.9
C76-C75-H75	119.9
C71-C76-C75	120.7(3)
C71-C76-H76	119.7
C75-C76-H76	119.7



Supporting Information

Suggestion for a short experimental part:

3e: yellow crystal (hexagonal), dimensions 0.157 x 0.082 x 0.066 mm³, crystal system trigonal, space group $R\bar{3}$, Z=18, a=39.4459(15) Å, b=39.4459(15) Å, c=12.5093(8) Å, alpha=90 deg, beta=90 deg, gamma=120 deg, V=16856.5(17) Å³, rho=1.255 g/cm³, T=200(2) K, Theta_{max}= 24.108 deg, radiation MoK α , lambda=0.71073 Å, 0.5 deg omega-scans with CCD area detector, covering the asymmetric unit in reciprocal space with a mean redundancy of 5.7 and a completeness of 99.9% to a resolution of 0.89 Å, 34031 reflections measured, 5968 unique (R(int)=0.0717), 3507 observed (I > 2 σ (I)), intensities were corrected for Lorentz and polarization effects, an empirical scaling and absorption correction was applied using SADABS^[1] based on the Laue symmetry of the reciprocal space, mu=0.08mm⁻¹, T_{min}=0.93, T_{max}=0.96, structure solved with SHELXT-2018/2 (Sheldrick 2015)^[2] and refined against F² with a Full-matrix least-squares algorithm using the SHELXL-2018/3 (Sheldrick, 2018) software^[3], 502 parameters refined, hydrogen atoms were treated using appropriate riding models, goodness of fit 1.04 for observed reflections, final residual values R1(F)=0.053, wR(F²)=0.113 for observed reflections, residual electron density -0.20 to 0.22 eÅ⁻³. CCDC 2249320 contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures.

Lit. 1: (SADABS-2016/2 - Bruker AXS area detector scaling and absorption correction)
Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10.

Lit. 2: (SHELXT - Integrated space-group and crystal structure determination)
Sheldrick G. M., Acta Cryst. A71 (2015) 3-8.

Lit. 3: (program SHELXL-2018/3 (Sheldrick, 2018) for structure refinement)
Sheldrick G. M., Acta Cryst. (2015). C71, 3-8

Lit. APEX, APEX2, SMART, SAINT, SAINT-Plus:
Bruker (2007). "Program name(s)". Bruker AXS Inc., Madison, Wisconsin, USA.

Computational details

Gaussian 16¹ was used to fully optimize all the structures reported in this paper at the M06-2X hybrid functional of Truhlar and Zhao² level of theory. For all of the calculations, solvent effects were considered using the SMD solvation model of Truhlar and workers³ with ethanol as the solvent. For geometry optimizations, the 6-31G(d) basis set was employed for all atoms. This basis set combination will be referred to as BS1. Frequency calculations were carried out at the same level of theory as those for structural optimization. Transition structures were located using the Berny algorithm. Intrinsic reaction coordinate (IRC) calculations were used to confirm the connectivity between transition structures and minima.⁴ To further refine the energies obtained from the SMD/M06-2X/6-31G(d) calculations, we carried out single-point energy calculations using the M06-2X functional method for all of the structures with a larger basis set def2-TZVP (BS2).⁵ Grimme empirical dispersion was added with the GD3 term on all the single-point energy calculations.⁶ A tight convergence criterion and ultrafine integral grid were also employed to increase the accuracy of the calculations. The free energy for each species in the solution was calculated using the equation,

$$G = E(\text{BS2}) + G(\text{BS1}) - E(\text{BS1}) + \Delta G^{1\text{atm} \rightarrow 1\text{M}} \quad (1)$$

where $\Delta G^{1\text{atm} \rightarrow 1\text{M}} = 1.89$ kcal/mol is the free-energy change for compression of 1 mol of an ideal gas from 1 atm to the 1 M solution phase standard state.⁷

(1) Gaussian 16, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

(2) Zhao, Y.; Truhlar, D. G. The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two

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new functionals and systematic testing of four M06-class functionals and 12 other functionals. *Theor. Chem. Acc.* **2008**, 120 (1), 215-241.

(3) Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. Universal solvation model based on solute electron density and on a continuum model of the solvent defined by the bulk dielectric constant and atomic surface tensions. *The Journal of Physical Chemistry B* **2009**, 113 (18), 6378-6396.

(4) Fukui, K. The path of chemical reactions-the IRC approach. *Acc. Chem. Res.* **1981**, 14 (12), 363-368.

(5) Weigend, F.; Furche, F.; Ahlrichs, R. Gaussian basis sets of quadruple zeta valence quality for atoms H–Kr. *The Journal of chemical physics* **2003**, 119 (24), 12753-12762.

(6) Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. *The Journal of chemical physics* **2010**, 132 (15), 154104.

(7) Cramer, C. J. *Essentials of computational chemistry: theories and models*; John Wiley & Sons, 2013.

Total potential (E), enthalpy (H) and Gibbs free energies (G) of all structures optimized at the SMD/M06/BS1 level of theory along with the total potential energies calculated by SMD/M06-2X/BS2//SMD/M06-2X/BS1 in dichloromethane.

BS1 = 6-31G(d)

BS2 = def2-TZVP

```
1
E (M062x-SMD/BS1) = -898.588794 au
H (M062x-SMD/BS1) = -898.304186 au
G (M06-SMD/6-31G(d)) = -898.366816 au
E (M062x-SMD/BS2//M062x-SMD/BS1) = -
898.941994 au
C -4.33386200 -2.42999400 -0.09703000
C -2.97526300 -2.22523100 -0.09340600
C -2.45978300 -0.90644300 -0.03611300
C -3.36499800 0.18677300 0.01671300
C -4.76212000 -0.05396000 0.01129700
C -5.23828200 -1.34004700 -0.04439800
H -4.72428600 -3.44224300 -0.14077500
H -2.27611800 -3.05499900 -0.13329500
C -2.80537500 1.48168600 0.07010200
H -5.43861900 0.79537600 0.05155600
H -6.30669500 -1.52968700 -0.04860100
C -1.44302500 1.66019200 0.07077800
C -0.58642200 0.50176800 0.02140300
H -3.45621600 2.35201300 0.10627600
N -1.11274000 -0.72049700 -0.03087100
C 0.85990900 0.60559300 0.03145300
H 1.31732400 1.57849500 0.12945700
C 1.68806700 -0.47616300 -0.04371500
O 1.24415000 -1.73422600 -0.10967700
H 0.23618800 -1.68095200 -0.08083400
C 3.16466600 -0.36667600 -0.03438100
C 3.81724900 0.81166600 -0.41988800
C 3.92931000 -1.47050700 0.36349000
C 5.20539100 0.88759100 -0.38901100
H 3.24419300 1.66505500 -0.76883100
C 5.31816000 -1.39010200 0.39491200
H 3.43019200 -2.38784000 0.65704700
C 5.96019700 -0.21109200 0.02116400
H 5.69965200 1.80426100 -0.69588300
H 5.89938000 -2.25048900 0.71236900
H 7.04404400 -0.14962400 0.04262600
C -0.92785300 3.04779700 0.11118100
H 0.16183400 3.19220200 0.06781400
O -1.65883700 4.01857500 0.18341100
HCOOH
E (M062x-SMD/BS1) = -189.68377 au
H (M062x-SMD/BS1) = -189.64528 au
G (M06-SMD/6-31G(d)) = -189.67344 au
E (M062x-SMD/BS2//M062x-SMD/BS1) = -
189.77829 au
C 0.00000000 0.42083400 0.00000000
H -0.35251200 1.45925400 0.00000000
O 1.16106400 0.09001500 0.00000000
O -1.03089900 -0.42081700 0.00000000
H -0.68881400 -1.33783600 0.00000000
1-O
E (M062x-SMD/BS1) = -1088.28556 au
H (M062x-SMD/BS1) = -1087.96044 au
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G (M06-SMD/6-31G(d)) = -1088.03632 au
E (M062x-SMD/BS2//M062x-SMD/BS1) = -1088.72950 au
C -4.82808600 -2.66442500 -0.09534300
C -3.45430600 -2.63868600 -0.09644000
C -2.77083000 -1.39911000 -0.03521800
C -3.52681200 -0.19700300 0.02491200
C -4.94369900 -0.25381300 0.02412000
C -5.58324400 -1.46650100 -0.03432300
H -5.34716000 -3.61697100 -0.14184200
H -2.86937900 -3.55217800 -0.14205000
C -2.80532300 1.01431600 0.07541500
H -5.50343100 0.67627900 0.07019000
H -6.66719300 -1.51567100 -0.03480400
C -1.42994800 1.01054600 0.06984900
C -0.73002900 -0.24997900 0.02311200
H -3.33799600 1.96163500 0.11024900
N -1.41081200 -1.39262000 -0.03178900
C 0.71648500 -0.32904700 0.04115100
H 1.29083800 0.57751500 0.15673600
C 1.40348200 -1.50489600 -0.04327800
O 0.80436200 -2.69519000 -0.12942400
H -0.18801700 -2.51720500 -0.09926900
C 2.88194100 -1.58086400 -0.02562500
C 3.67978200 -0.47285900 -0.34152900
C 3.49987700 -2.79182200 0.31091200
C 5.06599800 -0.57309700 -0.30440500
H 3.22270600 0.46607000 -0.63809200
C 4.88765300 -2.88763700 0.34805200
H 2.88817000 -3.65461900 0.55182600
C 5.67469000 -1.77910200 0.04263900
H 5.67273700 0.29122900 -0.55633500
H 5.35458300 -3.83028000 0.61693400
H 6.75752400 -1.85483300 0.06890900
C -0.72328700 2.29911800 0.08594100
H 0.37058100 2.30256800 0.01569400
O -1.31228300 3.37180200 0.16178500
C 1.60377800 5.12296200 -0.04237500
H 2.29521400 5.97457800 -0.07112700
O 1.96244200 3.96813700 -0.13915200
O 0.35583100 5.52475600 0.10920900
H -0.25503000 4.73557600 0.13075600

1-N

E (M062x-SMD/BS1) = -1088.28296 au
H (M062x-SMD/BS1) = -1087.95713 au
G (M06-SMD/6-31G(d)) = -1088.03177 au
E (M062x-SMD/BS2//M062x-SMD/BS1) = -1088.72673 au
C -4.42404700 -1.78765700 -0.54675200
C -3.05874900 -1.65091300 -0.46352200
C -2.49422500 -0.37112000 -0.24523000
C -3.35036900 0.75311500 -0.11155600
C -4.75445300 0.58203300 -0.20266200
C -5.28154100 -0.66736200 -0.41657800

H -4.85579400 -2.76964200 -0.71509100
H -2.39096300 -2.50172800 -0.56280700
C -2.73707700 2.00623500 0.10560900
H -5.39486600 1.45364300 -0.10022400
H -6.35569200 -0.80418100 -0.48680200
C -1.36909000 2.11546400 0.17620600
C -0.56471100 0.92912800 0.04935800
H -3.34869000 2.90042600 0.19985200
N -1.13664700 -0.25682300 -0.15044100
C 0.88442000 0.97676900 0.13897300
H 1.34462500 1.84144800 0.59532500
C 1.71562700 0.00363300 -0.32311100
O 1.30385600 -1.14135500 -0.88731500
H 0.31797400 -1.17380600 -0.85438200
C 3.19019200 0.10747400 -0.25352700
C 3.83520000 1.34966400 -0.19596500
C 3.95921800 -1.06313500 -0.25025600
C 5.22185700 1.41641600 -0.11636000
H 3.25652300 2.26727600 -0.23926300
C 5.34646600 -0.99177100 -0.16896000
H 3.46547000 -2.02793300 -0.29985600
C 5.98132600 0.24685400 -0.09981700
H 5.71123800 2.38472600 -0.07864200
H 5.93217300 -1.90585300 -0.15896900
H 7.06405600 0.30189000 -0.03997200
C -0.78506000 3.46818100 0.32992500
H 0.30492200 3.56795300 0.21254100
O -1.46283600 4.45394600 0.55123600
C -0.01229300 -3.39606600 1.06162500
H 0.36649300 -4.17069100 1.74034000
O -0.21015700 -3.57390500 -0.12070000
O -0.22171600 -2.25741800 1.70394000
H -0.55024800 -1.57755900 1.05935900

H₂O

E (M062x-SMD/BS1) = -76.38523 au
H (M062x-SMD/BS1) = -76.36021 au
G (M06-SMD/6-31G(d)) = -76.38166 au
E (M062x-SMD/BS2//M062x-SMD/BS1) = -76.43881 au
O 0.00000000 0.00000000 0.12019800
H 0.00000000 0.75987200 -0.48079100
H 0.00000000 -0.75987200 -0.48079100

A

E (M062x-SMD/BS1) = -1109.67773 au
H (M062x-SMD/BS1) = -1109.29416 au
G (M06-SMD/6-31G(d)) = -1109.36816 au
E (M062x-SMD/BS2//M062x-SMD/BS1) = -1110.10443 au
C 5.93613900 -0.24485700 -0.07955000
C 4.78916900 0.51209200 -0.05909000
C 3.52334400 -0.12427400 -0.04420300
C 3.46081700 -1.54035500 -0.05143000
C 4.65818300 -2.29714400 -0.07282300

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C 5.87505600 -1.66012400 -0.08645300
H 6.90469300 0.24576800 -0.09044600
H 4.82506700 1.59739200 -0.05320500
C 2.17311400 -2.12469200 -0.03768300
H 4.59208200 -3.38177900 -0.07814800
H 6.79441300 -2.23646700 -0.10252300
C 1.03181300 -1.35653400 -0.01764500
C 1.18269600 0.08499700 -0.00573700
H 2.08988300 -3.20979600 -0.04685400
N 2.39571600 0.63499200 -0.02047300
C 0.04883900 0.98421800 0.02570300
H -0.93476200 0.54812700 0.08350100
C 0.17078700 2.34325300 -0.00015400
O 1.34818600 2.97505900 -0.02907300
H 2.05163400 2.24893100 -0.01687600
C -0.99647500 3.25357300 0.02110000
C -2.27280400 2.81649300 -0.35844900
C -0.82378600 4.58362100 0.42406800
C -3.35423400 3.68940200 -0.31874300
H -2.42000700 1.79861000 -0.70694900
C -1.90914800 5.45395900 0.46431100
H 0.16256100 4.92937600 0.71466000
C -3.17714400 5.00980500 0.09494200
H -4.33690800 3.34039300 -0.62092000
H -1.76335600 6.48085600 0.78555600
H -4.02328100 5.68975900 0.12298700
C -0.23601300 -2.10164700 -0.01317000
H -0.09686400 -3.19058800 0.00761100
N -1.40657100 -1.59336500 -0.05199800
C -2.51701900 -2.46330500 0.00091200
C -3.63096300 -2.14619100 -0.78545100
C -2.56170600 -3.58603600 0.83737800
C -4.75465400 -2.96518600 -0.77000300
H -3.59345800 -1.26046200 -1.41320300
C -3.69619100 -4.39332400 0.85884600
H -1.72096000 -3.80595500 1.48923100
C -4.79186800 -4.09228200 0.05181200
H -5.60796400 -2.71810700 -1.39456500
H -3.72532300 -5.25690100 1.51678600
H -5.67466600 -4.72379400 0.07230300

AB

E (M062x-SMD/BS1) = -2197.99629 au
H (M062x-SMD/BS1) = -2197.28652 au
G (M06-SMD/6-31G(d)) = -2197.40917 au
E (M062x-SMD/BS2//M062x-SMD/BS1) = -
2198.86332 au
C 3.32043000 4.14727600 1.47808600
C 2.00716500 3.77287600 1.63073200
C 1.65838800 2.39966200 1.61990300
C 2.68787300 1.42754600 1.48776600
C 4.03442700 1.84289800 1.32719700
C 4.34442400 3.17988000 1.31645500
H 3.58055000 5.20177300 1.47438200
H 1.21631300 4.50819000 1.74396900
C 2.30281700 0.07108600 1.55049600

H 4.80441800 1.08393700 1.21564800
H 5.37253300 3.50364000 1.19133800
C 0.97711800 -0.27367300 1.68634200
C -0.01895100 0.76978100 1.70116000
H 3.05788800 -0.71135000 1.49852500
N 0.34842000 2.04912100 1.71191000
C -1.43354500 0.47679700 1.61939400
H -1.75804300 -0.55223400 1.55372000
C -2.38126500 1.44037900 1.43316000
O -2.11177000 2.74738100 1.41858700
H -1.11272500 2.83196400 1.53355200
C -3.79859700 1.11207800 1.16539500
C -4.38812200 -0.04887400 1.68051600
C -4.55920900 1.96978300 0.36017100
C -5.71356400 -0.35156400 1.38577300
H -3.81630200 -0.70580200 2.32934200
C -5.88255000 1.65808500 0.06031000
H -4.10529300 2.87161200 -0.03818500
C -6.46261200 0.49716400 0.57109500
H -6.16295200 -1.25113500 1.79545300
H -6.46203600 2.32386400 -0.57213300
H -7.49665700 0.25834300 0.34097600
C 0.63548900 -1.70088100 1.78108000
H -0.42045100 -1.99676200 1.81574800
O 1.50000200 -2.56874000 1.82895300
C -0.58894100 -5.12792100 1.24382900
H -0.96064500 -6.11316600 0.93441400
O -1.30689300 -4.23394500 1.64001800
O 0.72494300 -5.05117700 1.13088000
H 1.02281400 -4.14564500 1.43122800
C -4.77988600 -2.46697200 -1.46551600
C -4.01324200 -1.32991900 -1.54235900
C -2.60007200 -1.42544400 -1.48200400
C -1.99505600 -2.70172100 -1.33630500
C -2.81209800 -3.85900700 -1.26419200
C -4.17840100 -3.74373900 -1.33002000
H -5.86254700 -2.38917300 -1.50500500
H -4.46298600 -0.34487600 -1.63817700
C -0.58430600 -2.74444200 -1.26615200
H -2.33451500 -4.82964800 -1.15934700
H -4.80531000 -4.62793800 -1.27535200
C 0.16447900 -1.59216600 -1.34633100
C -0.52747100 -0.33240400 -1.48260100
H -0.07753500 -3.70000200 -1.15086000
N -1.85651800 -0.29156300 -1.55361500
C 0.17482800 0.93648300 -1.50208000
H 1.25044800 0.95130100 -1.40239700
C -0.46341000 2.14151400 -1.53177000
O -1.79214900 2.26800600 -1.57677100
H -2.16332200 1.32598200 -1.56690200
C 0.26279300 3.43004700 -1.48033000
C 1.57819800 3.54646100 -1.94873500
C -0.37696600 4.55762200 -0.95014900
C 2.24314600 4.76607400 -1.87753200
H 2.07474500 2.69035300 -2.39566000
C 0.29376100 5.77576700 -0.87722800

Supporting Information

H -1.39643700 4.47177100 -0.58774000
C 1.60476300 5.88343600 -1.33869500
H 3.26020700 4.84585900 -2.24945300
H -0.20907900 6.64207500 -0.45785400
H 2.12546900 6.83481200 -1.28455600
C 1.63253500 -1.66106000 -1.24555800
H 2.19419500 -0.72803800 -1.33741000
N 2.22742100 -2.76656000 -1.01366700
C 3.63258400 -2.75961700 -0.88832200
C 4.47264600 -1.96272300 -1.67773100
C 4.19396500 -3.61840200 0.06473000
C 5.85142300 -2.00628600 -1.48857500
H 4.04741200 -1.33437700 -2.45518400
C 5.57106400 -3.64546600 0.25783500
H 3.53308000 -4.24970800 0.65185200
C 6.40502100 -2.83853500 -0.51669700
H 6.49597100 -1.39228300 -2.11071400
H 5.99533700 -4.30489900 1.00905000
H 7.48068200 -2.86889300 -0.37326000

TS_{AB-B}

E (M062x-SMD/BS1) = -2197.97512 au
H (M062x-SMD/BS1) = -2197.26723 au
G (M06-SMD/6-31G(d)) = -2197.38766 au
E (M062x-SMD/BS2//M062x-SMD/BS1) = -2198.84863 au
C -5.78990200 2.77840400 -2.13934000
C -4.41752800 2.72137500 -2.10020700
C -3.76906700 1.52812500 -1.69402600
C -4.55456200 0.40281400 -1.33226500
C -5.96750300 0.48955300 -1.38178800
C -6.57498500 1.65624000 -1.77795900
H -6.28248200 3.69458700 -2.45091800
H -3.80619500 3.57555700 -2.37586400
C -3.86559600 -0.75839000 -0.90204300
H -6.55390900 -0.38012300 -1.09735700
H -7.65748400 1.72468400 -1.81520900
C -2.49942900 -0.77547900 -0.84217200
C -1.76971200 0.38828300 -1.27171300
H -4.42596900 -1.63794800 -0.59429300
N -2.40875000 1.48745700 -1.66742900
C -0.31869400 0.39939300 -1.32442200
H 0.22732400 -0.48133400 -1.02099400
C 0.41187300 1.44197500 -1.81302300
O -0.13750600 2.59749700 -2.20033700
H -1.13278500 2.49239700 -2.07614900
C 1.88281300 1.39107600 -1.97442100
C 2.56957900 0.17069500 -2.04860300
C 2.60477000 2.58664400 -2.08257600
C 3.94883500 0.15124900 -2.22864800
H 2.02757800 -0.77018300 -1.99700200
C 3.98484400 2.56210900 -2.26371900
H 2.08067100 3.53497400 -2.02074100
C 4.66070900 1.34547600 -2.34079300
H 4.46580600 -0.80187700 -2.29333000
H 4.53204300 3.49671900 -2.34530400

H 5.73636200 1.32723400 -2.48836300
C -1.80984600 -1.97589200 -0.25029500
H -0.75814000 -2.06773200 -0.52832900
O -2.48118600 -3.06850600 -0.16279700
C -0.09543100 -4.71827200 -1.52635000
H 0.46286600 -5.61054800 -1.84786100
O 0.13869000 -3.61289900 -1.98738400
O -0.99835100 -5.00137700 -0.62393000
H -1.62019600 -4.15440700 -0.39475400
C 4.84416500 -4.20871600 -0.08433000
C 4.65110900 -2.88041100 0.21205800
C 3.37132200 -2.42410800 0.61429500
C 2.30295800 -3.35525300 0.70214000
C 2.53304000 -4.72073000 0.40490700
C 3.78155600 -5.13988700 0.01449400
H 5.82589700 -4.55324000 -0.39471100
H 5.46096900 -2.15987200 0.14701300
C 1.03675100 -2.86155400 1.10087100
H 1.70756600 -5.42207000 0.49819800
H 3.96060700 -6.18492500 -0.21648700
C 0.88306600 -1.53078100 1.39515600
C 2.01188500 -0.64182000 1.27615400
H 0.19792900 -3.54935800 1.19592200
N 3.19874800 -1.10459000 0.90094600
C 1.85302200 0.77809600 1.49950500
H 0.86493800 1.15235700 1.72954400
C 2.86235300 1.67978500 1.32068300
O 4.09240200 1.31871000 0.95178600
H 4.07962000 0.31993500 0.82464800
C 2.69119800 3.14091000 1.48381800
C 1.57177200 3.68713000 2.12608000
C 3.67118500 4.00363600 0.97505300
C 1.42971500 5.06538200 2.23998000
H 0.81464400 3.04018700 2.55751400
C 3.52470100 5.38273100 1.08971100
H 4.54372800 3.58861100 0.48259200
C 2.40285800 5.91809700 1.71920900
H 0.55914600 5.47486200 2.74297500
H 4.28899400 6.03961600 0.68570200
H 2.28872700 6.99408000 1.80963200
C -0.39391800 -1.02836700 1.91628400
H -0.36931200 -0.42851700 2.83032300
N -1.53449700 -1.29784300 1.40234700
C -2.72895400 -0.83720600 2.03466400
C -2.95151900 0.53122700 2.18641700
C -3.69485800 -1.77394800 2.39762900
C -4.15971900 0.96610200 2.72253300
H -2.19304500 1.23914900 1.86112800
C -4.89922700 -1.32444800 2.93460600
H -3.49894100 -2.83133400 2.25903800
C -5.13420100 0.04020900 3.09415400
H -4.34283500 2.02960500 2.83934400
H -5.65572900 -2.04561300 3.22757700
H -6.07788900 0.38321800 3.50650700

Supporting Information

B

E (M062x-SMD/BS1) = -2197.98310 au
H (M062x-SMD/BS1) = -2197.27133 au
G (M06-SMD/6-31G(d)) = -2197.39155 au
E (M062x-SMD/BS2//M062x-SMD/BS1) = -2198.85735 au
C 6.28302600 -2.50970500 -2.21830500
C 4.90999500 -2.49885000 -2.26592300
C 4.18801400 -1.43560800 -1.66774800
C 4.90090500 -0.39155600 -1.02270300
C 6.31639400 -0.42758900 -0.98998200
C 6.99574200 -1.46756600 -1.57656600
H 6.83176800 -3.32543400 -2.67918000
H 4.35294900 -3.29061300 -2.75787900
C 4.14095400 0.64017600 -0.41391300
H 6.84746200 0.37911500 -0.49195200
H 8.08041500 -1.49579900 -1.55156500
C 2.77661000 0.61395800 -0.46959200
C 2.12612800 -0.45473300 -1.17797700
H 4.64746100 1.44821300 0.10755800
N 2.82834800 -1.43740400 -1.73473700
C 0.68216100 -0.48910900 -1.32106200
H 0.08563700 0.31157700 -0.90876700
C 0.01267200 -1.45930700 -2.00453800
O 0.61243500 -2.52323900 -2.54663100
H 1.59744100 -2.41386900 -2.37114100
C -1.45404500 -1.42630500 -2.18446600
C -2.15076000 -0.20993300 -2.21315100
C -2.16009500 -2.62731200 -2.31366600
C -3.53451600 -0.20135000 -2.35039500
H -1.60988700 0.73116200 -2.14584700
C -3.54567000 -2.61357700 -2.44858000
H -1.62158100 -3.56953200 -2.29261500
C -4.23556000 -1.40258000 -2.46570100
H -4.06609100 0.74561800 -2.37299500
H -4.08745700 -3.55089200 -2.53412300
H -5.31669400 -1.39341600 -2.56932600
C 1.95447100 1.65384900 0.25800900
H 1.08494800 1.93877300 -0.33715600
O 2.67303500 2.75677400 0.63574900
C 0.75289900 4.42259000 -1.45713200
H 0.36394500 5.28494900 -2.04023900
O 0.46051300 3.28061100 -1.85136000
O 1.45414600 4.73760000 -0.44517800
H 2.20219600 3.57224300 0.22607900
C -4.36703200 4.85706100 -0.36726200
C -4.40440000 3.51108700 -0.09089600
C -3.22921900 2.84563300 0.33509600
C -2.02690200 3.58937000 0.47062600
C -2.01784600 4.97801500 0.18723600
C -3.16890300 5.60026600 -0.22823700
H -5.26991700 5.36265700 -0.69601300
H -5.31907000 2.93495300 -0.19254500
C -0.87583900 2.89801500 0.91012400
H -1.08781900 5.52781000 0.30403600
H -3.16786000 6.66235300 -0.45000800

C -0.94934900 1.55203300 1.18746100
C -2.20199300 0.85435400 1.00280200
H 0.04615700 3.45362500 1.06637800
N -3.28197800 1.51099600 0.59838700
C -2.28923400 -0.57528500 1.19806000
H -1.37629500 -1.12901800 1.37505300
C -3.45587200 -1.27600400 1.07094600
O -4.61634700 -0.69531400 0.76470600
H -4.42054600 0.27772100 0.59745600
C -3.54549500 -2.74317900 1.23888700
C -2.54376600 -3.47206900 1.89309500
C -4.65582700 -3.42284600 0.72122500
C -2.64286800 -4.85427900 2.00787600
H -1.69375000 -2.96151300 2.33476800
C -4.75101500 -4.80600500 0.83739600
H -5.43671500 -2.86399800 0.21645500
C -3.74392300 -5.52605500 1.47751200
H -1.86187100 -5.40727800 2.52048800
H -5.61289800 -5.32191500 0.42532600
H -3.81893900 -6.60537300 1.56896200
C 0.16219300 0.85411700 1.81631400
H -0.06377500 0.20458500 2.66246300
N 1.41336300 0.95160500 1.50900100
C 2.39033600 0.24848300 2.31386500
C 2.38790200 -1.14338700 2.30306100
C 3.33077100 0.98138500 3.02986200
C 3.35441000 -1.81999200 3.04119700
H 1.64843700 -1.67857100 1.71236700
C 4.29282300 0.28849200 3.76160300
H 3.30550200 2.06482900 3.01107000
C 4.30653500 -1.10519100 3.76669000
H 3.36621900 -2.90508700 3.04122800
H 5.03145400 0.84355600 4.33082500
H 5.06192600 -1.63633000 4.33711600

TS_{B-C}

E (M062x-SMD/BS1) = -2197.96183 au
H (M062x-SMD/BS1) = -2197.25220 au
G (M06-SMD/6-31G(d)) = -2197.36610 au
E (M062x-SMD/BS2//M062x-SMD/BS1) = -2198.83439 au
C -5.54193700 -2.45583500 1.92506900
C -4.17155900 -2.51915200 2.01880600
C -3.37732400 -1.47907100 1.47661200
C -4.01458600 -0.38380600 0.83999600
C -5.42754700 -0.34031500 0.76051600
C -6.17887100 -1.35964700 1.29436800
H -6.14707800 -3.25658000 2.33932000
H -3.67368300 -3.35557500 2.50009600
C -3.17996200 0.58300000 0.22981000
H -5.89811700 0.50291400 0.26170500
H -7.26198000 -1.33210100 1.23187400
C -1.81419900 0.47808800 0.30226600
C -1.24090200 -0.63982800 1.01260900
H -3.63259600 1.40216200 -0.32565000

Supporting Information

N -2.02096800 -1.56927800 1.55470100
C 0.19409700 -0.83457300 1.08524800
H 0.84706200 -0.07266300 0.68719800
C 0.77575400 -1.97179300 1.56197000
O 0.08029600 -3.01321700 2.02743800
C 2.24180500 -2.17169400 1.57986000
C 3.11773800 -1.08538500 1.70563800
C 2.76565400 -3.46696500 1.49160600
C 4.49273600 -1.29152600 1.73990200
H 2.72003600 -0.08097900 1.81774900
C 4.14304100 -3.66873600 1.51427300
H 2.09086800 -4.31210900 1.40034300
C 5.00899600 -2.58376000 1.64150100
H 5.16157500 -0.44292100 1.84941600
H 4.53991200 -4.67638900 1.43638700
H 6.08302400 -2.74374900 1.66419400
C -1.02406900 1.38933500 -0.55488200
H -1.61729600 1.87288700 -1.32602500
C 5.51699000 -1.81765400 -1.68108000
C 4.15186900 -1.88022400 -1.81174800
C 3.38435500 -0.69262000 -1.72644300
C 4.03006800 0.55141900 -1.49404700
C 5.44098300 0.58094400 -1.35440600
C 6.16823800 -0.57975900 -1.44972000
H 6.10793300 -2.72614400 -1.74737400
H 3.63679200 -2.82043200 -1.98517000
C 3.21403000 1.70238800 -1.34925000
H 5.92834600 1.53465000 -1.17158600
H 7.24826800 -0.55607200 -1.34485100
C 1.85592600 1.61208700 -1.51096400
C 1.30216900 0.33834300 -1.84388600
H 3.67382400 2.65065200 -1.07627600
N 2.03389200 -0.76267100 -1.88255900
C -0.14918400 0.22874500 -2.05815500
H -0.54864400 0.95432500 -2.75535400
C -0.76239900 -1.05227700 -2.07646900
O -0.09123400 -2.12733300 -1.79419200
C -2.19996900 -1.23547700 -2.28547100
C -2.99008500 -0.24002400 -2.88034100
C -2.80435700 -2.40051500 -1.78621700
C -4.36596300 -0.41430900 -2.97459500
H -2.53722500 0.66124800 -3.28284000
C -4.18141200 -2.55959400 -1.87016900
H -2.19286200 -3.15925900 -1.30867800
C -4.96272100 -1.56761900 -2.46427100
H -4.97370800 0.35298800 -3.44311500
H -4.64775500 -3.45134300 -1.46309700
H -6.03964500 -1.69225400 -2.52684600
C 0.90919500 2.73068100 -1.12668300
H 1.45047600 3.54234000 -0.63026000
N 0.00721400 2.14187900 -0.08682900
H -1.78651300 2.70328400 1.77314200
C 0.28377200 2.35112100 1.29231700
C 1.59503600 2.35269000 1.77424200
C 1.83889500 2.61158500 3.12145700
C 0.78421000 2.86085800 3.99533000

C -0.52239300 2.87660600 3.50785100
C -0.77507200 2.63989300 2.16157100
H 2.42434300 2.13836400 1.10855700
H 2.86181600 2.60615800 3.48533600
H 0.97819300 3.05389500 5.04560800
H -1.35120500 3.09739700 4.17337100
C -1.33020000 5.09847800 -0.13739300
O -1.79836500 4.43767700 -1.11453200
O -0.13647600 5.34964900 0.09746000
H -2.09367100 5.49290100 0.57107000
H -0.89018200 -2.75318100 1.97593800
O 0.17515800 3.16809700 -2.21381800
H -0.55430200 3.78093600 -1.85236200
H 0.91292400 -1.86844700 -1.77761400

TS_{B-c}

E (M062x-SMD/BS1) = -2197.94919 au
H (M062x-SMD/BS1) = -2197.23796 au
G (M06-SMD/6-31G(d)) = -2197.34945 au
E (M062x-SMD/BS2//M062x-SMD/BS1) = -
2198.82009 au
C -2.52316800 -4.21680600 3.50575200
C -1.25968900 -3.68063700 3.43487700
C -1.07187400 -2.39174000 2.88344800
C -2.19935200 -1.66432800 2.41808700
C -3.49431100 -2.23561400 2.51447700
C -3.65033900 -3.49088100 3.04552900
H -2.66482200 -5.21016000 3.92041500
H -0.38852400 -4.22422200 3.78663200
C -1.96759200 -0.40638400 1.82492400
H -4.34518000 -1.67061500 2.14351200
H -4.63692100 -3.93814900 3.11028100
C -0.67311000 0.02606600 1.62526300
C 0.37963800 -0.72643900 2.23136500
H -2.81148900 0.20099500 1.51542600
N 0.18590600 -1.86536500 2.83772100
C 1.79720500 -0.19812100 2.24568300
C 2.38533900 -0.31477400 0.81538300
O 2.30990200 -1.65851500 0.42990600
C 3.87068600 0.05029700 0.83742800
C 4.33689900 1.14264400 1.57755000
C 4.78919700 -0.69641900 0.09567200
C 5.68543000 1.49136900 1.55930300
H 3.65262800 1.73320700 2.18049700
C 6.13915300 -0.34768600 0.07781300
H 4.44901200 -1.56271000 -0.46047200
C 6.59268700 0.74854900 0.80617900
H 6.02621700 2.34173900 2.14241000
H 6.83707800 -0.94136500 -0.50528100
H 7.64426800 1.01855200 0.79369700
C -0.42873800 1.30294800 0.96776600
H -1.12318900 2.09851900 1.21469600
C 0.02916900 -3.53882800 -4.85315300
C -0.75994900 -2.66080900 -4.15274200
C -0.16657900 -1.72970600 -3.26015500

Supporting Information

C 1.23925400 -1.73525000 -3.08787300
C 2.03529400 -2.63842900 -3.83846000
C 1.43987800 -3.52323700 -4.70252600
H -0.42532100 -4.25309900 -5.53314000
H -1.84076300 -2.65300700 -4.25758900
C 1.76915800 -0.85484100 -2.11789400
H 3.11348900 -2.62754200 -3.70164500
H 2.04546300 -4.22247800 -5.27066300
C 0.94604400 -0.05457600 -1.36232000
C -0.44566300 -0.02481400 -1.71664500
H 2.84224600 -0.85392500 -1.94592400
N -0.96109200 -0.83382000 -2.62082300
C -1.38900500 0.98548400 -1.18635800
H -1.11006000 2.02169100 -1.33623200
C -2.71670100 0.72745200 -0.94371200
O -3.24256600 -0.46548500 -0.77512700
C -3.68607100 1.83227000 -0.72129400
C -3.49390100 3.10425700 -1.27907400
C -4.82825700 1.59749700 0.05599700
C -4.40993000 4.12350300 -1.03973600
H -2.64225400 3.29622700 -1.92511400
C -5.74104500 2.62007400 0.29598900
H -4.99531900 0.60990400 0.47389300
C -5.53288100 3.88634800 -0.24747600
H -4.25199200 5.10170500 -1.48348300
H -6.61721000 2.42606900 0.90704800
H -6.24689500 4.68317100 -0.06291800
C 1.62799200 0.67775600 -0.20883100
H 2.41390900 1.27275800 -0.66568600
N 0.73611600 1.67504100 0.45203300
H -1.13564100 3.64580600 0.04043200
C 0.96312600 3.07459800 0.15833100
C 2.27503900 3.55044600 0.08020300
C 2.51467800 4.89531300 -0.18164600
C 1.45726900 5.78116400 -0.36932800
C 0.15208800 5.30756000 -0.28210800
C -0.10172900 3.96476600 -0.01690900
H 3.11949900 2.89087800 0.24318500
H 3.54042600 5.24598600 -0.23201200
H 1.64847100 6.82869600 -0.57799900
H -0.68801500 5.97984800 -0.42510700
C -1.16742100 -3.19757600 -0.55289700
O -2.32304300 -2.77092800 -0.84036600
O -0.22611000 -2.54860600 -0.06535400
H -1.00104600 -4.27590300 -0.76062100
H -2.63536800 -1.32022000 -0.83264200
H 1.78760500 0.84755700 2.56996300
O 2.58872200 -0.92557000 3.14466000
H 2.17101800 -1.80550200 3.22005100
H 1.37945000 -1.93736700 0.26682400

C
E (M062x-SMD/BS1) = -2198.00270 au
H (M062x-SMD/BS1) = -2197.28878 au

G (M06-SMD/6-31G(d)) = -2197.40442 au
E (M062x-SMD/BS2//M062x-SMD/BS1) = -2198.87452 au
C 4.99109900 -3.44490900 -2.10945100
C 3.62967600 -3.29769700 -2.22161600
C 2.98484000 -2.19169800 -1.61243000
C 3.76098400 -1.24757100 -0.89495700
C 5.16241900 -1.42460800 -0.79140300
C 5.76720700 -2.50375500 -1.38900200
H 5.48177000 -4.29360000 -2.57630600
H 3.02435000 -4.01332700 -2.77004000
C 3.06490100 -0.19939100 -0.24253500
H 5.74076800 -0.69840400 -0.22603200
H 6.84064600 -2.64295300 -1.30959800
C 1.70245300 -0.09064100 -0.32602800
C 0.99949500 -1.05007000 -1.13891200
H 3.62970000 0.49158800 0.38171600
N 1.63521500 -2.06142500 -1.72464500
C -0.44212200 -0.98578600 -1.28825600
H -0.94341700 -0.08573000 -0.96743000
C -1.19498500 -2.01304000 -1.76781600
O -0.67351200 -3.16738800 -2.19962800
C -2.67291300 -1.96842000 -1.80220700
C -3.36359000 -0.75107000 -1.86679000
C -3.39811100 -3.16550800 -1.75688600
C -4.75437900 -0.73422400 -1.87658100
H -2.81521000 0.18465300 -1.93635000
C -4.78968600 -3.14379400 -1.75637000
H -2.86663500 -4.11050400 -1.71229400
C -5.47135200 -1.92934000 -1.81586500
H -5.27963500 0.21424100 -1.93773900
H -5.34243200 -4.07724800 -1.71002500
H -6.55740200 -1.91276200 -1.81740200
C 0.98961000 0.89577500 0.58920500
H 1.76947300 1.40865200 1.16754900
C -5.78012700 -1.55101200 1.63414700
C -4.41839300 -1.72488200 1.71912000
C -3.58590700 -0.60657000 1.52352600
C -4.11939800 0.66643200 1.22192200
C -5.52638600 0.80722800 1.14554500
C -6.33829000 -0.28073400 1.35460000
H -6.43745600 -2.40176600 1.78214700
H -3.97579900 -2.69281000 1.93449200
C -3.21414800 1.72801500 0.96572500
H -5.94035600 1.78429300 0.91538300
H -7.41639900 -0.17388400 1.29672000
C -1.86157100 1.53169400 1.06247600
C -1.36838100 0.26319400 1.43768500
H -3.60550400 2.70251200 0.68282300
N -2.22107700 -0.73369900 1.62500200
C 0.11134400 0.14586600 1.68857800
H 0.25032500 0.73405300 2.60495700
C 0.64786000 -1.25618700 1.96358800
O -0.01981000 -2.25316100 1.73152400
C 2.03961900 -1.38144400 2.47370200
C 2.69663700 -0.34451400 3.14486700

Supporting Information

C 2.71724500 -2.57552500 2.19651100
C 4.02507700 -0.50352000 3.52986700
H 2.18347800 0.58361100 3.37937000
C 4.04829300 -2.72185000 2.56545500
H 2.19899200 -3.36651800 1.66273900
C 4.70327300 -1.68423100 3.23109800
H 4.53164700 0.29797000 4.05783700
H 4.57885400 -3.63861300 2.32779900
H 5.74451900 -1.79678400 3.51779300
C -0.80962400 2.55700400 0.72061800
H -1.24752800 3.35940900 0.11983100
N 0.16075900 1.85474300 -0.13510900
H 2.79040300 2.60736800 -0.32461900
C 0.78991700 2.64338400 -1.14020400
C -0.01268400 3.13607500 -2.17725600
C 0.52809900 3.95405800 -3.16254600
C 1.88706700 4.26787300 -3.14686700
C 2.69403200 3.75773800 -2.13287400
C 2.15271100 2.95487400 -1.13019700
H -1.06754200 2.87352700 -2.19697700
H -0.11178700 4.33546000 -3.95281600
H 2.31298300 4.89859100 -3.92105400
H 3.75340600 3.99608500 -2.10783300
C 0.92753200 5.64090800 0.39222000
O 1.44367300 4.91612300 1.29423500
O -0.25587900 5.64472100 0.01027600
H 1.62924800 6.35652800 -0.09492400
H 0.32410300 -3.05826700 -2.15933800
O -0.26255900 3.04744600 1.90786700
H 0.37175400 3.80578900 1.67804700
H -1.82496500 -1.65918600 1.82019100

D

E (M062x-SMD/BS1) = -2198.00587 au
H (M062x-SMD/BS1) = -2197.29209 au
G (M06-SMD/6-31G(d)) = -2197.41147 au
E (M062x-SMD/BS2//M062x-SMD/BS1) = -2198.87310 au
C 4.82914600 -3.56526700 -2.37543100
C 3.48037600 -3.33380600 -2.50281100
C 2.87089300 -2.28081300 -1.77582100
C 3.66794700 -1.47520000 -0.92595200
C 5.05393600 -1.73780900 -0.80791600
C 5.62535200 -2.76433300 -1.52128300
H 5.29279900 -4.37309800 -2.93350400
H 2.85861400 -3.94270300 -3.15251200
C 3.00719600 -0.45345400 -0.19550700
H 5.64972700 -1.11717500 -0.14355200
H 6.68779500 -2.96753500 -1.43214500
C 1.66004800 -0.24685200 -0.31821500
C 0.92844500 -1.09641700 -1.22634800
H 3.58975200 0.15065800 0.49900000
N 1.53283400 -2.06787100 -1.90510200
C -0.50874600 -0.97571400 -1.37273000
H -0.99895000 -0.12937100 -0.92014600
C -1.28692600 -1.92863300 -1.95397000

O -0.79745900 -3.03467900 -2.52796700
C -2.76367400 -1.85761300 -1.93364100
C -3.43072000 -0.62743500 -1.88329800
C -3.50973800 -3.04251100 -1.93152500
C -4.81942900 -0.58585500 -1.81490100
H -2.86383800 0.29914000 -1.91837800
C -4.89793400 -2.99690900 -1.84777700
H -2.99568900 -3.99714700 -1.97661600
C -5.55641000 -1.76948700 -1.78545600
H -5.32727800 0.37336200 -1.78573000
H -5.46675900 -3.92162900 -1.82984900
H -6.64007700 -1.73409300 -1.72095400
C 0.99133600 0.76427600 0.60509900
H 1.80324800 1.23285600 1.17754500
C -5.85760300 -1.33648300 1.82997500
C -4.50226900 -1.54334300 1.92610500
C -3.59625300 -0.49030100 1.64380200
C -4.11108500 0.77020400 1.24005900
C -5.51281800 0.96257500 1.16240900
C -6.36978800 -0.07071200 1.45442600
H -6.54578300 -2.14849100 2.04478400
H -4.09269400 -2.50588100 2.21719700
C -3.17236200 1.77607200 0.89141800
H -5.89160500 1.93479600 0.85756000
H -7.44360100 0.07603700 1.39092100
C -1.83823600 1.50345000 0.99140600
C -1.41874500 0.22115400 1.46368600
H -3.52082100 2.74521300 0.53909000
N -2.25498600 -0.73510400 1.77422700
C 0.07203200 0.08927700 1.70843600
H 0.23814700 0.68777400 2.61050700
C 0.61150300 -1.31264500 1.97267000
O 0.06887000 -2.31127300 1.54208200
C 1.92823400 -1.41965500 2.68345800
C 2.49276600 -0.37555900 3.42425600
C 2.64469600 -2.61273500 2.52051100
C 3.75351000 -0.52844900 3.99762100
H 1.96238300 0.56055700 3.56872500
C 3.90623200 -2.75869400 3.08239800
H 2.20651000 -3.41021700 1.92839200
C 4.46258000 -1.71481400 3.82373100
H 4.18223500 0.28300900 4.57721700
H 4.45978300 -3.68151600 2.93895300
H 5.44940900 -1.82645100 4.26286100
C -0.76811000 2.47606600 0.57842000
H -1.18769800 3.25474000 -0.06313600
N 0.24707600 1.77129200 -0.15358600
H 2.89416400 2.47142400 -0.14635500
C 0.96657300 2.53479500 -1.12026000
C 0.26013800 3.01184100 -2.23107700
C 0.89102800 3.80753100 -3.18000400
C 2.24529600 4.11531200 -3.04884300
C 2.95899300 3.61333200 -1.96340200
C 2.32748600 2.82589800 -1.00097100
H -0.79118800 2.75531000 -2.33570300
H 0.32607500 4.17828500 -4.03006600

Supporting Information

H 2.74164100 4.73154700 -3.79210600
H 4.01527400 3.84106000 -1.85345700
C 1.20285800 5.68911900 0.10922300
O 1.67528300 4.98205400 1.12099900
O 0.08416500 5.58857700 -0.34790300
H 1.94900400 6.40275800 -0.26439000
H 0.20322400 -2.96013100 -2.46764400
O -0.16275200 3.09554000 1.73356500
H -0.86154300 3.54074700 2.24634700
H 0.99189000 4.29978900 1.38033500

TS_{D-E}

E (M062x-SMD/BS1) = -2197.94951 au
H (M062x-SMD/BS1) = -2197.23804 au
G (M06-SMD/6-31G(d)) = -2197.36051 au
E (M062x-SMD/BS2//M062x-SMD/BS1) = -
2198.82983 au
C 0.94372800 5.23126200 -3.31566700
C 1.33551500 3.91001800 -3.33610800
C 0.55576800 2.96879200 -2.64283000
C -0.59880300 3.35544100 -1.93752500
C -0.97269600 4.71725200 -1.93273900
C -0.21139500 5.63987000 -2.61366000
H 1.53392500 5.97010700 -3.84818600
H 2.22045100 3.58482500 -3.87458700
C -1.29371700 2.34828400 -1.21426800
H -1.85763300 5.01488700 -1.37797400
H -0.49285300 6.68744200 -2.61093400
C -0.88660700 1.03956000 -1.18918800
C 0.22164200 0.64281400 -2.01845900
H -2.14706900 2.66005200 -0.61340300
N 0.86681000 1.63130700 -2.67188700
C 0.68093100 -0.70162800 -2.22357900
H -0.04267500 -1.39269200 -2.63780600
C 2.03046100 -1.15834200 -2.25365600
O 2.30915400 -2.27623800 -2.73401600
C 3.13286200 -0.42284000 -1.51918400
C 2.92015300 0.60373600 -0.58847300
C 4.43533500 -0.91178700 -1.68399200
C 3.97781400 1.11592700 0.15871800
H 1.92808500 0.99393800 -0.38640000
C 5.49390100 -0.39833800 -0.94245700
H 4.60111100 -1.71807200 -2.39039200
C 5.26655300 0.61391200 -0.01020400
H 3.78425600 1.89495300 0.89059400
H 6.49459700 -0.79659100 -1.08162600
H 6.08685000 1.00440300 0.58507600
C -1.54327300 0.14980800 -0.12878100
H -2.59180200 0.44394000 -0.06946200
C 4.54878500 -0.78497600 3.64542500
C 3.32891100 -0.16812800 3.49986300
C 2.40695600 -0.63621500 2.53338600
C 2.75383400 -1.76340100 1.73637800
C 4.01912100 -2.38121600 1.90638100
C 4.90046700 -1.89667000 2.84109400
H 5.25618800 -0.41589400 4.38172700

H 3.04916000 0.69051200 4.10231500
C 1.81746900 -2.19731300 0.77298900
H 4.27431900 -3.23083900 1.27892300
H 5.87224100 -2.36309000 2.96806800
C 0.65251400 -1.48123400 0.61288900
C 0.40047800 -0.35588800 1.45015000
H 2.02973900 -3.06245400 0.14765500
N 1.22262200 0.03423000 2.38680300
C -0.94781300 0.31652000 1.30601100
H -1.62742300 -0.23626200 1.96423800
C -0.91625900 1.79383800 1.69206700
O 0.05997600 2.46779200 1.41552100
C -2.11854600 2.41272400 2.32288000
C -3.28343500 1.69385200 2.61826900
C -2.07076700 3.78841200 2.59125100
C -4.37975100 2.34321000 3.18007300
H -3.35318700 0.62948500 2.41806100
C -3.16363400 4.43161800 3.15555900
H -1.16723200 4.33960600 2.35130200
C -4.32054800 3.70809400 3.45131900
H -5.27912200 1.78003300 3.40755500
H -3.11783100 5.49570200 3.36488000
H -5.17630500 4.21016700 3.89251200
C -0.35086600 -1.90684800 -0.33874800
H -0.28845800 -2.92392700 -0.72099800
N -1.49333900 -1.27352700 -0.48796100
H -4.02808200 -1.03366000 0.23431400
C -2.60738300 -1.88671000 -1.15101300
C -2.41283000 -2.74690300 -2.23107900
C -3.51328200 -3.38669900 -2.79664000
C -4.79358500 -3.17006800 -2.29433200
C -4.97544300 -2.30931500 -1.21329800
C -3.88594600 -1.66675200 -0.63603100
H -1.42127400 -2.94309700 -2.62559300
H -3.36081500 -4.05804000 -3.63566800
H -5.64567400 -3.67396400 -2.73905300
H -5.96700000 -2.14710000 -0.80311500
C -2.08925000 -5.16402800 -0.19481300
O -3.06406500 -4.74090900 0.47849400
O -0.88422100 -4.84076700 -0.08412900
H -2.33512200 -5.92393100 -0.97391700
H 1.63915100 1.34896000 -3.27526500
O -1.76386500 -2.94314900 2.07517900
H -0.89419900 -3.35727200 1.96218900
H -2.32900000 -3.52790400 1.51002600

E

E (M062x-SMD/BS1) = -2121.62575 au
H (M062x-SMD/BS1) = -2120.93890 au
G (M06-SMD/6-31G(d)) = -2121.05284 au
E (M062x-SMD/BS2//M062x-SMD/BS1) = -
2122.44481 au
C -1.64176200 0.98547400 5.67517400
C -0.56506700 1.06451900 4.82858300
C -0.75998500 1.02932700 3.42264000

Supporting Information

C -2.07847600 0.91297500 2.90983200
C -3.17546500 0.83720200 3.80772900
C -2.95970900 0.87107000 5.16183100
H -1.48949300 1.01050000 6.74991800
H 0.45026700 1.15334500 5.20288100
C -2.22954600 0.88408500 1.50447700
H -4.17943600 0.74737700 3.40131600
H -3.79728900 0.80955600 5.84965000
C -1.12800200 0.94081300 0.68672400
C 0.14894600 1.06536000 1.30617000
H -3.23285800 0.82368200 1.08519000
N 0.32610400 1.12082100 2.60711400
C 1.38460000 1.23224700 0.44951800
H 1.59089400 2.30616100 0.40216000
C 2.60411500 0.52153100 1.00254700
O 2.50173700 -0.53034400 1.62222200
C 3.95794100 1.05169300 0.67571800
C 4.18506300 2.38460500 0.31133800
C 5.03714600 0.15826100 0.73908300
C 5.47625900 2.81465900 0.01649300
H 3.37228900 3.10295000 0.28125100
C 6.32124400 0.58851700 0.43245300
H 4.85049600 -0.87398700 1.01908900
C 6.54176800 1.91881300 0.07154100
H 5.64862900 3.85151500 -0.25381800
H 7.15101200 -0.11004300 0.47327100
H 7.54610800 2.25647100 -0.16573300
C -1.27647200 0.89340200 -0.82729600
H -2.14617600 1.49541100 -1.08689300
C 1.68022000 -5.65693100 -1.75074300
C 0.57461600 -4.84527600 -1.71733400
C 0.72596200 -3.44180300 -1.56801100
C 2.03029800 -2.89425500 -1.45954700
C 3.15774900 -3.75446400 -1.50633000
C 2.98445100 -5.10813600 -1.64488800
H 1.56188200 -6.73094800 -1.85784800
H -0.43134100 -5.24664200 -1.79483800
C 2.13356700 -1.49665900 -1.28036200
H 4.15093200 -3.32199900 -1.41695400
H 3.84556700 -5.76863300 -1.67129200
C 1.00264300 -0.72234800 -1.19241400
C -0.26016900 -1.37195400 -1.32572300
H 3.12310600 -1.04526200 -1.22585100
N -0.39078800 -2.66538600 -1.51839900
C -1.52364300 -0.54104800 -1.37385500
H -1.77003200 -0.41546700 -2.43409700
C -2.70999400 -1.19183100 -0.66939300
O -2.54789300 -1.97252900 0.25033200
C -4.09384700 -0.78413800 -1.07527500
C -4.36021200 0.05284000 -2.16596200
C -5.15935600 -1.25365300 -0.29478200
C -5.67238800 0.40486000 -2.47299900
H -3.55788300 0.43540600 -2.78907600
C -6.46674000 -0.90070400 -0.60224800
H -4.94396800 -1.89441900 0.55425200
C -6.72498600 -0.07061900 -1.69432200

H -5.87074900 1.05113000 -3.32214100
H -7.28545800 -1.26955600 0.00774200
H -7.74671900 0.20624000 -1.93624000
C 1.11541400 0.78312400 -1.02812800
H 1.95812800 1.10786100 -1.64265100
N -0.09827500 1.42064800 -1.51187900
H -2.16495700 2.82061900 -2.49072100
C -0.06732000 2.76257900 -1.93588000
C 1.12215000 3.51111200 -1.95608000
C 1.13195800 4.82088100 -2.43259000
C -0.03063700 5.42549000 -2.89683000
C -1.21143600 4.68405500 -2.89520600
C -1.23404200 3.37451900 -2.43240400
H 2.05750700 3.09007500 -1.60616700
H 2.06949700 5.36944300 -2.42937500
H -0.01813000 6.44771100 -3.26045800
H -2.13120100 5.12209700 -3.27196100
C 0.34993200 -3.11515100 1.63656600
O 0.10842400 -1.84601400 1.92673700
O 1.45345500 -3.59906800 1.51102000
H -0.58356700 -3.68403500 1.53507500
H 0.96714700 -1.34575100 1.93506200

F

E (M062x-SMD/BS1) = -1931.92353 au
H (M062x-SMD/BS1) = -1931.27753 au
G (M06-SMD/6-31G(d)) = -1931.38084 au
E (M062x-SMD/BS2//M062x-SMD/BS1) = -
1932.65169 au
C -2.33075200 1.07268000 5.37693300
C -1.45045200 1.64802700 4.49583400
C -1.46098500 1.26950800 3.12746500
C -2.39214400 0.29048300 2.68759300
C -3.29378300 -0.28622800 3.62023200
C -3.26171600 0.09655000 4.93700600
H -2.31925300 1.36395400 6.42280300
H -0.73203900 2.39719700 4.81437500
C -2.37132500 -0.06154200 1.31754700
H -4.00059000 -1.03391600 3.27033200
H -3.94923100 -0.34616600 5.65094000
C -1.46414900 0.52273900 0.46923900
C -0.58353700 1.49878900 1.01154400
H -3.08116600 -0.80106200 0.94877800
N -0.58146700 1.86430100 2.27484700
C 0.38601100 2.23566700 0.11831600
H -0.00222600 3.25650900 0.03453700
C 1.77431100 2.43164200 0.73546500
O 2.28590000 3.53466600 0.62674500
C 2.55538400 1.30596300 1.35147500
C 2.04598600 0.01803600 1.56078100
C 3.91450900 1.54502100 1.59232200
C 2.88679500 -1.01233900 1.96887300
H 1.00374800 -0.21497100 1.37774800
C 4.75273000 0.51660200 2.00885500
H 4.31093200 2.54010200 1.41869900

Supporting Information

C 4.24245700 -0.76904700 2.18657100
H 2.47917800 -2.01051300 2.10012300
H 5.80717500 0.71344400 2.17699100
H 4.89895700 -1.57924800 2.48996300
C -1.40226900 0.15956300 -1.00559200
H -2.42006400 -0.06187900 -1.32590900
C 5.30066300 -2.63148000 -1.30069100
C 3.93974000 -2.80437000 -1.26217600
C 3.07396900 -1.68523800 -1.38315300
C 3.63732100 -0.39265800 -1.55499900
C 5.04791000 -0.24315200 -1.60283100
C 5.86183400 -1.33989700 -1.47262700
H 5.95929300 -3.48864200 -1.19844800
H 3.49304900 -3.78512000 -1.12925900
C 2.74474100 0.70159800 -1.61871500
H 5.46417400 0.75333800 -1.72661300
H 6.94099500 -1.22480600 -1.49780100
C 1.39798200 0.49466500 -1.46586700
C 0.93260900 -0.84295700 -1.33707100
H 3.14055700 1.71047700 -1.73069000
N 1.72885600 -1.88791900 -1.31698500
C -0.55732400 -1.11359900 -1.31458300
H -0.82672400 -1.40818200 -2.33420900
C -0.92675100 -2.23247300 -0.34572000
O -0.31057900 -2.37296800 0.69668600
C -2.10629000 -3.09935200 -0.64894400
C -2.88743900 -2.94888800 -1.80135800
C -2.44785000 -4.08358300 0.28921100
C -3.98882700 -3.77496300 -2.01152400
H -2.65317600 -2.19189200 -2.54314000
C -3.54284000 -4.90973700 0.07447100
H -1.84194400 -4.18830500 1.18338600
C -4.31532400 -4.75598600 -1.07816800
H -4.59002200 -3.65189200 -2.90671100
H -3.79760000 -5.67268800 0.80336400
H -5.17265200 -5.40068500 -1.24690300
C 0.44774200 1.66349400 -1.34118700
H 0.82644200 2.45791900 -1.98787200
N -0.87546400 1.26612000 -1.80585400
H -3.28546800 0.80484000 -2.85047700
C -1.77642100 2.24894500 -2.27216400
C -1.45445200 3.61505700 -2.30185300
C -2.35115100 4.54583700 -2.82502000
C -3.58740300 4.15082900 -3.32308400
C -3.90935600 2.79400300 -3.30824000
C -3.01962400 1.85567200 -2.80158200
H -0.50763200 3.97787000 -1.91971300
H -2.07050200 5.59510000 -2.82945700
H -4.28383200 4.88106400 -3.72217700
H -4.85957700 2.45377300 -3.70966200

3

E (M062x-SMD/BS1) = -1931.91997 au
H (M062x-SMD/BS1) = -1931.27371 au
G (M06-SMD/6-31G(d)) = -1931.37783 au

E (M062x-SMD/BS2//M062x-SMD/BS1) = -
1932.65806 au
C -4.49712900 3.00273500 2.04645200
C -3.24940900 3.13576500 1.46390000
C -2.63994300 2.01076000 0.88779600
C -3.28608800 0.76145300 0.90044900
C -4.55207700 0.65358400 1.50164700
C -5.15506900 1.76110600 2.06900600
H -4.97041500 3.87151700 2.49344000
H -2.73297000 4.09159700 1.44816900
C -2.59584600 -0.34781400 0.30214300
H -5.04157200 -0.31698600 1.51208300
H -6.13217600 1.67442900 2.53253800
C -1.34420700 -0.22053200 -0.20149000
C -0.68493500 1.07678100 -0.23773500
H -3.09502600 -1.31482500 0.28283300
N -1.40420800 2.11532900 0.28482600
C 0.55617300 1.21603500 -0.85219100
C 1.38028000 2.40360700 -0.87847100
O 2.25805100 2.55795900 -1.74237500
C 1.26402600 3.46048200 0.18449000
C 1.16082000 3.11873700 1.53783900
C 1.33244600 4.80645900 -0.18640200
C 1.11317300 4.11628000 2.50728600
H 1.12368300 2.07063400 1.82491600
C 1.26478400 5.80325100 0.78323100
H 1.43079300 5.06289700 -1.23742400
C 1.15628700 5.45870400 2.13018900
H 1.04388700 3.84693600 3.55675900
H 1.30193100 6.84781600 0.48945400
H 1.10957600 6.23614200 2.88692200
C -0.56628200 -1.39373000 -0.76706700
H -1.28382700 -2.16834300 -1.02861300
C 6.36768300 -2.11398600 1.53960300
C 5.02578500 -2.41652700 1.67152100
C 4.09969800 -1.82091800 0.79952200
C 4.52677200 -0.92109800 -0.19603300
C 5.89967800 -0.63131300 -0.30643900
C 6.81127300 -1.21998600 0.54828800
H 7.08635900 -2.57416000 2.21061400
H 4.67432400 -3.10666400 2.43302000
C 3.52343000 -0.32934200 -1.03618700
H 6.22491000 0.06457800 -1.07487300
H 7.86866800 -0.99366200 0.45860400
C 2.21094200 -0.63705700 -0.88955800
C 1.78900900 -1.59846400 0.10485000
H 3.82997900 0.39453900 -1.78695600
N 2.75801700 -2.11381700 0.90213700
C 0.44138700 -1.96951900 0.22517400
C 0.01905700 -2.81765900 1.29662200
O 0.78969200 -3.27232500 2.17533600
C -1.44027500 -3.15155500 1.45056600
C -2.13787200 -3.90771200 0.50545900
C -2.09847400 -2.70204700 2.59855600
C -3.49149200 -4.18271200 0.69191000
H -1.62169400 -4.28426800 -0.37442500

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C -3.45518500 -2.96107700 2.77501400
H -1.54783200 -2.12857500 3.33945400
C -4.15511400 -3.69690600 1.81825700
H -4.02801600 -4.77438600 -0.04373800
54546700 0.43246800 -2.58830600
N 0.11032600 -0.96159400 -2.00171700
H -1.68636600 -2.61006900 -3.01845800
C -0.76030300 -0.65989000 -3.08067900
C -0.72985200 0.56352800 -3.76459900
C -1.57372700 0.78442900 -4.85338900
C -2.47216200 -0.19108200 -5.27158900
C -2.51142600 -1.40809500 -4.58978200
C -1.66537200 -1.64371900 -3.51384300
H -0.06044300 1.35786400 -3.45208500
H -1.52822000 1.73999900 -5.36791400
H -3.13018700 -0.01034400 -6.11562600
H -3.19733000 -2.18879700 -4.90575700
H 2.42493100 -2.75589700 1.62870100
H -1.01200200 3.04959000 0.22676700

D*

E (M062x-SMD/BS1) = -2121.57554 au
H (M062x-SMD/BS1) = -2120.89192 au
G (M06-SMD/6-31G(d)) = -2121.00506 au
E (M062x-SMD/BS2//M062x-SMD/BS1) = -
2122.40466 au
C 5.25994800 1.77787500 2.51091300
C 3.90758000 1.63155000 2.69720700
C 3.15620100 0.78708900 1.83846200
C 3.82573400 0.10489100 0.78927200
C 5.22318300 0.27182000 0.61771800
C 5.92715500 1.09175200 1.46453300
H 5.82936400 2.42896200 3.16745200
H 3.37909300 2.15648600 3.48710100
C 3.02791800 -0.66378000 -0.09175300
H 5.71732600 -0.24985800 -0.19795900
H 6.99646200 1.22487200 1.33346100
C 1.66989100 -0.72580600 0.08230100
C 1.09169500 -0.05661700 1.21960800
H 3.49890700 -1.14664800 -0.94713200
N 1.81875100 0.66042000 2.05491200
C -0.34601500 -0.15049700 1.45603000
H -0.82586500 -1.10050000 1.27037900
C -1.15882200 0.86895000 1.83112200
O -0.82727500 2.13821100 2.03788000
C -2.62144900 0.63878200 1.97044100
C -3.13751800 -0.56859500 2.45635800
C -3.50414900 1.65636200 1.58882100
C -4.51351700 -0.75509200 2.55781300
H -2.45889400 -1.35269600 2.78169400
C -4.87988300 1.46370200 1.68075500
H -3.09958200 2.58999200 1.20915800
C -5.38758800 0.25984700 2.16932900
H -4.90344600 -1.69067500 2.94804900
H -5.55680700 2.25404900 1.36953900
H -6.46108300 0.11276100 2.24579400

H -3.96631600 -2.59039900 3.65864100
H -5.21290000 -3.90062700 1.95562700
C 1.11151900 0.04446100 -1.66511000
H 1.
C 0.83944900 -1.34397400 -1.03274400
H 1.55632700 -1.69131200 -1.78023200
C -5.98681700 1.19606500 -1.82191500
C -4.62678700 1.34631800 -1.96556200
C -3.75543400 0.29577100 -1.59622500
C -4.31026700 -0.90369700 -1.06519000
C -5.71651400 -1.03136000 -0.92506400
C -6.53950000 -0.00025400 -1.30297900
H -6.65001400 2.00626600 -2.10928700
H -4.19256400 2.25859300 -2.36165400
C -3.41347400 -1.92919500 -0.70586900
H -6.11932500 -1.95339300 -0.51475000
H -7.61575200 -0.09298000 -1.19991600
C -2.06116500 -1.72513900 -0.89291600
C -1.59828100 -0.48613600 -1.43506500
H -3.78308800 -2.86539500 -0.29322000
N -2.40947200 0.47234000 -1.78449200
C -0.13203200 -0.36827400 -1.78110100
H -0.07849900 -0.64887200 -2.84041700
C 0.43494800 1.05807900 -1.65533800
O -0.12595700 1.91456000 -1.00641400
C 1.77022800 1.31145800 -2.27953400
C 2.25294900 0.58024900 -3.36971300
C 2.58563700 2.27352900 -1.67023200
C 3.53846700 0.81825500 -3.85107700
H 1.63532300 -0.16759700 -3.85877700
C 3.87442000 2.49297600 -2.14117800
H 2.21714600 2.79986500 -0.79367200
C 4.35129500 1.76733500 -3.23406800
H 3.90597000 0.25785300 -4.70497300
H 4.51244900 3.22095700 -1.64928200
H 5.35869600 1.93862900 -3.60154700
C -1.12571300 -2.74665200 -0.52966700
H -1.49218900 -3.70662100 -0.17222500
N 0.16048400 -2.59112800 -0.57438100
H 2.05338800 -3.88040000 -1.96004800
C 1.03127300 -3.63186200 -0.07554800
C 0.90384000 -4.02346800 1.25351600
C 1.74591700 -5.01911500 1.74175300
C 2.70025000 -5.59816200 0.90828600
C 2.81659900 -5.18680400 -0.41933700
C 1.98176300 -4.19412300 -0.92293500
H 0.16836500 -3.54362200 1.89327900
H 1.65932400 -5.33244900 2.77690900
H 3.35753100 -6.37100000 1.29375000
H 3.55550200 -5.64304900 -1.06983300
C 0.82054500 4.49373700 0.77350900
O 1.26363800 3.45303000 1.35263100
O -0.35862800 4.77405800 0.50885900
H 1.60753000 5.22746800 0.47989700
H 0.09407200 2.46327400 1.72611600

Supporting Information

TS_{D⁺-E}

E (M062x-SMD/BS1) = -2121.56701 au
H (M062x-SMD/BS1) = -2120.88509 au
G (M06-SMD/6-31G(d)) = -2120.99554 au
E (M062x-SMD/BS2//M062x-SMD/BS1) = -
2122.39572 au
C -2.15243300 -0.68541800 5.51575600
C -0.98370000 -0.41259300 4.85017700
C -1.02113200 0.04675400 3.50722900
C -2.27569900 0.21475200 2.87197000
C -3.47132800 -0.06464300 3.58263000
C -3.40829500 -0.50860900 4.87936300
H -2.12180300 -1.03899700 6.54189400
H -0.01455200 -0.53706400 5.32344900
C -2.25671500 0.63632800 1.52450700
H -4.42537000 0.06680300 3.07859400
H -4.31976700 -0.73087800 5.42544400
C -1.07246800 0.84514300 0.85872700
C 0.14378300 0.74218300 1.62269800
H -3.20885500 0.76585500 1.01214500
N 0.14644600 0.35383000 2.88339900
C 1.47732800 1.16305000 1.11785900
H 1.60142100 2.22577900 0.94483000
C 2.58985200 0.37529300 1.14589800
O 2.58084200 -0.93413300 1.32136800
C 3.94056400 0.93274100 0.85931500
C 4.22674700 2.29836400 0.99764500
C 4.95949800 0.06822800 0.43859300
C 5.49324400 2.78786300 0.69449300
H 3.46974600 2.98274200 1.36891600
C 6.22639300 0.56068000 0.13655300
H 4.74905700 -0.99258500 0.34914700
C 6.49622600 1.92205200 0.25867500
H 5.70088000 3.84719000 0.81146200
H 7.00399100 -0.12175700 -0.19307600
H 7.48465200 2.30638600 0.02567800
C -1.20702600 1.10188500 -0.64480200
H -2.06007500 1.76383500 -0.78371200
C 1.75825300 -5.24881000 -2.24959100
C 0.64061800 -4.45137900 -2.19659900
C 0.77237700 -3.05992200 -1.97466200
C 2.07528200 -2.50431900 -1.83446600
C 3.21337500 -3.34849100 -1.90372200
C 3.05503100 -4.69691500 -2.09912000
H 1.65131600 -6.31796500 -2.40533800
H -0.35873500 -4.86176700 -2.30180200
C 2.17152600 -1.11686000 -1.61490200
H 4.19976900 -2.90778600 -1.78783600
H 3.92161300 -5.34887900 -2.13971500
C 1.01194100 -0.38102100 -1.48465200
C -0.24891800 -1.04149400 -1.59399300
H 3.14609800 -0.63724500 -1.55443000
N -0.36594400 -2.30894900 -1.87609500
C -1.48098000 -0.17545700 -1.49457300
H -1.70400700 0.17657700 -2.50929400
C -2.69402400 -0.92796600 -0.94282400

O -2.53955300 -1.83321300 -0.14718100
C -4.06313200 -0.47669400 -1.33796000
C -4.29418600 0.57111300 -2.23736300
C -5.15346100 -1.12348300 -0.73950900
C -5.59768500 0.95764400 -2.53893100
H -3.47048300 1.09614000 -2.71138100
C -6.45189300 -0.73801900 -1.04427100
H -4.96547000 -1.92737400 -0.03517300
C -6.67537900 0.30369000 -1.94633300
H -5.76948800 1.76969400 -3.23815300
H -7.29106600 -1.24564600 -0.57922200
H -7.69058300 0.60615700 -2.18486300
C 1.06201600 1.05479200 -1.36702200
H 1.97955500 1.56503200 -1.64542700
N -0.02103800 1.78184000 -1.20921800
H -2.04915300 3.35609600 -1.95144700
C 0.00743400 3.21722200 -1.28698400
C 1.18015200 3.92407900 -1.00925700
C 1.18414600 5.31185900 -1.11521400
C 0.03343100 5.99676500 -1.49553600
C -1.12699200 5.28291500 -1.78571100
C -1.14594900 3.89589300 -1.68696000
H 2.09153400 3.41675400 -0.71073600
H 2.09649300 5.85469000 -0.89029900
H 0.04212600 7.07920400 -1.57117300
H -2.02574900 5.80293700 -2.10087600
C 0.62403800 -3.37175600 1.06166800
O 0.40362400 -2.12542500 1.22541800
O 1.72127100 -3.94354700 1.07687300
H -0.29500300 -3.97564400 0.89858700
H 1.61504100 -1.39942400 1.32257900

Supporting Information

TS_{D-D}*

E (M062x-SMD/BS1) = -2197.97614 au
H (M062x-SMD/BS1) = -2197.26606 au
G (M06-SMD/6-31G(d)) = -2197.38843 au
E (M062x-SMD/BS2//M062x-SMD/BS1) = -2198.85014 au
C 5.24279700 -2.44295500 -2.96002800
C 3.87335400 -2.36357600 -3.04462800
C 3.15245100 -1.57547200 -2.11338900
C 3.85945600 -0.87541700 -1.10540900
C 5.26982700 -0.97506600 -1.03874400
C 5.95014600 -1.74602200 -1.95057300
H 5.79250800 -3.04820000 -3.67450000
H 3.32019200 -2.89479900 -3.81344800
C 3.09211000 -0.10868900 -0.19079600
H 5.79645900 -0.43572800 -0.25580100
H 7.03139800 -1.82544800 -1.90117300
C 1.72685300 -0.05664000 -0.27574900
C 1.08510900 -0.79166300 -1.33831100
H 3.61097000 0.43069500 0.60040800
N 1.79650900 -1.50823900 -2.20402200
C -0.35487500 -0.80210100 -1.49727800
H -0.96135200 -0.23351700 -0.81270900
C -1.00795400 -1.53975900 -2.43957100
O -0.38412200 -2.32817500 -3.31877600
C -2.48322000 -1.56443400 -2.54002800
C -3.25603400 -0.47375100 -2.12214800
C -3.12199900 -2.70136000 -3.04898200
C -4.64429200 -0.53199600 -2.18410600
H -2.77003400 0.43205400 -1.77036600
C -4.51133800 -2.75676700 -3.10834000
H -2.52589200 -3.54480400 -3.38211600
C -5.27595900 -1.67601800 -2.67148300
H -5.23324200 0.32257800 -1.86375400
H -4.99796900 -3.64731500 -3.49429300
H -6.35979400 -1.72075400 -2.71918800
C 0.98384300 0.71883600 0.80393800
H 1.76184500 1.22802800 1.38082200
C -5.38154900 -2.46220700 2.38393500
C -4.01149000 -2.41959100 2.47252500
C -3.30356600 -1.28042800 2.01555500
C -4.03390900 -0.18645800 1.47564700
C -5.44828400 -0.25502600 1.39653000
C -6.10807400 -1.37323700 1.84142700
H -5.91853300 -3.33955200 2.73123000
H -3.44093300 -3.24668400 2.88315900
C -3.29454600 0.93209500 1.02477800
H -5.99093900 0.58949200 0.98037700
H -7.19024600 -1.42912100 1.78058000
C -1.92710700 0.90362200 1.11821700
C -1.28388900 -0.24193000 1.66792800
H -3.80741000 1.79401700 0.60211700
N -1.93923000 -1.28098500 2.11423100
C 0.21328800 -0.15426400 1.85795600
H 0.33698900 0.36494700 2.81435900
C 0.92500500 -1.50830500 1.91537000
O 0.50493700 -2.45553000 1.28010900

Supporting Information

C 2.21896400 -1.59502600 2.65722400
C 2.68574600 -0.58161900 3.50230400
C 3.01421700 -2.72717400 2.43324800
C 3.92833300 -0.70561700 4.11947500
H 2.09292600 0.30705700 3.69451100
C 4.25418800 -2.84611900 3.04621400
H 2.64996100 -3.50024100 1.76422100
C 4.71267300 -1.83398900 3.89159000
H 4.28274200 0.08152400 4.77732500
H 4.86713500 -3.72314800 2.86349300
H 5.68292900 -1.92521800 4.37047700
C -1.11276000 2.01381900 0.60785100
H -1.61748300 2.81465100 0.07182200
N 0.13796000 1.77710300 0.22145400
H 2.21168400 3.35859800 0.86713100
C 0.79500400 2.73164200 -0.63223500
C 0.32558100 2.89384700 -1.93349200
C 0.92237500 3.84076300 -2.76151400
C 1.99179000 4.60213900 -2.29325200
C 2.46631900 4.41703000 -0.99518600
C 1.86848400 3.48050300 -0.15606000
H -0.50260200 2.28338900 -2.28410800
H 0.55499600 3.97715300 -3.77366300
H 2.45839600 5.33795000 -2.94084800
H 3.29602200 5.01250900 -0.62747700
C -0.74126400 5.57424100 0.28923600
O -0.19521600 5.28932400 1.40236600
O -1.66303900 4.96204000 -0.27280400
H -0.33486600 6.48122000 -0.20676700
H 0.60168100 -2.23596800 -3.12581600
O -0.96956500 3.04648000 2.20980100
H -1.88001200 3.16490200 2.53793200
H -0.66297400 4.00630800 1.88097400

NH₂-Ph

E (M062x-SMD/BS1) = -287.478497 au
H (M062x-SMD/BS1) = -287.353394 au
G (M06-SMD/6-31G(d)) = -287.389075 au
E (M062x-SMD/BS2//M062x-SMD/BS1) = -287.597891 au
C 0.93797100 -0.00007000 -0.01016200
C 0.22189500 -1.20669600 -0.00498500
C -1.16913100 -1.20091100 0.00349300
C -1.87823200 0.00008000 0.00738600
C -1.16899500 1.20099900 0.00354400
C 0.22202200 1.20661800 -0.00503200
H 0.76809100 -2.14676700 -0.00792800
H -1.70295000 -2.14729200 0.00976600
H -2.96351900 0.00005400 0.01528800
H -1.70261800 2.14748300 0.00987200
H 0.76834300 2.14662000 -0.00812600
N 2.33053600 -0.00001100 -0.08291400
H 2.76288600 0.83515600 0.29814200
H 2.76283300 -0.83529800 0.29792000

TS'_{AB-B}

Supporting Information

E (M062x-SMD/BS1) = -2197.94849 au
H (M062x-SMD/BS1) = -2197.24188 au
G (M06-SMD/6-31G(d)) = -2197.35816 au
E (M062x-SMD/BS2//M062x-SMD/BS1) = -2198.82121au
C 6.31949000 1.42498400 1.23672900
C 5.03616800 1.91496000 1.18865800
C 3.94195900 1.01896300 1.09460700
C 4.18901700 -0.37520500 1.05963900
C 5.51978600 -0.85471700 1.11730700
C 6.56742800 0.03087500 1.20159500
H 7.15698000 2.11304500 1.30119100
H 4.83360200 2.98165500 1.21182300
C 3.07000200 -1.22607900 0.87907700
H 5.69260500 -1.92712200 1.07987300
H 7.58926200 -0.33283200 1.23970100
C 1.80259800 -0.72041500 0.74737900
C 1.63375400 0.71113100 0.83713400
H 3.24079100 -2.29720700 0.79404100
N 2.67960500 1.51546700 1.00644900
C 0.33622900 1.34158700 0.69476100
H -0.53789600 0.71863200 0.56764800
C 0.15010900 2.68889900 0.64982700
O 1.14452100 3.58210700 0.71530200
C -1.19408800 3.28544900 0.50466500
C -2.30523500 2.66823700 1.09092100
C -1.36237100 4.48028000 -0.20486700
C -3.56934200 3.23391300 0.96353700
H -2.16956300 1.76017200 1.67124300
C -2.63203400 5.03498400 -0.34348800
H -0.49983600 4.96482000 -0.65219000
C -3.73679700 4.41579500 0.24220800
H -4.42344500 2.75115700 1.42998700
H -2.75855600 5.95640000 -0.90387000
H -4.72394700 4.85720100 0.14137900
C 0.74185200 -1.69776200 0.32166400
H 1.20650600 -2.64971100 0.07676900
C -4.85193700 1.70969600 -2.01586600
C -3.49394500 1.51201100 -1.93220400
C -2.99295000 0.19703000 -1.80959800
C -3.88858900 -0.90319000 -1.78087500
C -5.28350800 -0.66635900 -1.86315800
C -5.75390400 0.61826800 -1.97936200
H -5.24115200 2.71943700 -2.10512700
H -2.79479200 2.34415000 -1.94653000
C -3.32868900 -2.19847700 -1.69628500
H -5.96086900 -1.51499800 -1.83750300
H -6.82073600 0.80521300 -2.04481300
C -1.96671600 -2.37775400 -1.62525500
C -1.12768200 -1.21987900 -1.63094500
H -3.98780600 -3.06499400 -1.69228800
N -1.64596700 -0.00660700 -1.72307400
C 0.34420300 -1.30933400 -1.49925600
H 0.72349400 -2.24594900 -1.88869200
C 1.10490500 -0.17938500 -2.00734400
O 0.54900400 0.95281600 -2.21543100
C 2.55406500 -0.25380500 -2.22367400

Supporting Information

C 3.22594100 -1.48064000 -2.34452800
C 3.28539800 0.94415600 -2.22269800
C 4.60958000 -1.50146800 -2.46411200
H 2.67897400 -2.41802200 -2.35731100
C 4.67079400 0.91427700 -2.32807700
H 2.76379700 1.88856700 -2.10209200
C 5.33295200 -0.30754400 -2.44870800
H 5.12616800 -2.45040100 -2.56489900
H 5.23421000 1.84158100 -2.30744300
H 6.41576000 -0.33076600 -2.52707000
C -1.46163700 -3.77093100 -1.58098800
H -2.24831200 -4.53278600 -1.70359200
N -0.39333500 -1.92469300 1.06652100
H 0.73355500 -0.66537700 3.18414700
C -1.03665200 -1.13507700 2.04518400
C -2.43251200 -1.02923900 1.99141500
C -3.12253400 -0.33974500 2.98511800
C -2.42797600 0.27556900 4.02557100
C -1.03784000 0.17175200 4.07720400
C -0.34254900 -0.54627400 3.10817100
H -2.96535100 -1.50576000 1.17351000
H -4.20555200 -0.27213300 2.93530000
H -2.96401000 0.82424200 4.79377400
H -0.48830700 0.63183200 4.89308700
C -2.31252200 -4.53798100 2.04209500
O -2.28659300 -4.03985200 0.88054700
O -1.49836900 -4.35944200 2.96565700
H -3.17568300 -5.21746400 2.24592200
H 1.98900700 3.04774900 0.83131300
O -0.29626800 -4.09496700 -1.45499400
H -0.92738800 -2.78634400 0.85976300
H -0.51732900 0.82220800 -1.99402500

References

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