Azulenium chemistry – towards new derivatives of photochromic dihydroazulenes

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ELECTRONIC SUPPLEMENTARY INFORMATION

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Synthesis – *Reactions of azulenium salts 4-7 with lithium triisopropylsilylacetylide*

*Reaction of **4** with lithium triisopropylsilylacetylide:* To a degassed solution of triisopropylsilylacetylene (1.60 mL, 7.13 mmol) in Et_2O (30 mL) at -40 °C was added a solution of LiHMDS (3.2 mL, 1.0 M in toluene, 3.2 mmol) and the contents of the vessel allowed to reach -20 °C. The solution was cooled to -78 °C and then added via cannula to a degassed suspension of **4** (1.01 g, 2.69 mmol) in THF (80 mL) at -78 °C. The reaction mixture was stirred for 2 h at -78 °C, quenched with saturated aqueous NH_4Cl (50 mL) and allowed to reach ambient temperature. The reaction mixture was diluted with Et_2O (100 mL) and water (50 mL) and the phases separated. The aqueous phase was extracted with Et_2O (50 mL) and dried over $MgSO_4$ and filtered. The solvent was removed under reduced pressure to give a crude residue, which was purified by flash chromatography (toluene/heptane 4:1) to give a regioisomeric mixture of **16** (715 mg, 57%). M.p. = 67-73 °C. R_f = 0.52 (toluene/heptane 4:1). Anal. calcd (%) for $C_{30}H_{34}N_2OSi$ (466.70): C 77.21, H 7.34, N 6.00; found C 77.04, H 7.12, N 6.09. HRMS (MALDI +ve) calcd for $C_{30}H_{33}N_2OSi$ [$(M-H)^+$]: *m/z* = 465.2357; found *m/z* = 465.2374. Mixture **16** was subject to repeated flash column chromatography (EtOAc/heptane) to isolate small portions of the following regioisomers.

*2-(4-Methoxyphenyl)-4-[(triisopropylsilyl)ethynyl]-1,4-dihydroazulene-1,1-dicarbonitrile (**16a**):* A pale yellow solid. M.p. = 65-68 °C. R_f = 0.39 (3:17 EtOAc/heptane). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.60 (d, *J* = 8.9 Hz, 2H), 7.12 (s, 1H), 6.99 (d, *J* = 8.9 Hz, 2H), 6.92 (d, *J* = 11.2 Hz, 1H), 6.79 (dd, *J* = 11.2, 6.1 Hz, 1H), 6.27 (ddd, *J* = 9.7, 6.1, 1.2 Hz, 1H), 5.43 (dd, *J* = 9.7, 4.9 Hz, 1H), 3.86 (s, 3H), 3.44 (dd, *J* = 4.9, 1.2 Hz, 1H), 1.14 (br s, 21H). ^{13}C NMR (125 MHz, $CDCl_3$) δ = 160.9, 142.2, 139.8, 132.9, 131.6, 130.4, 127.2, 127.1, 124.7, 123.1, 122.5, 115.1, 112.4, 112.2, 105.4, 85.0, 55.6, 43.4, 32.3, 18.8, 11.4 ppm. HRMS (MALDI +ve) calcd for $C_{30}H_{33}N_2OSi$ [$(M-H)^+$]: *m/z* = 465.2357; found *m/z* = 465.2355. Anal. calcd (%) for $C_{30}H_{34}N_2OSi$ (466.70): C 77.21, H 7.34, N 6.00; found C 77.16, H 7.50, N 5.96.

*2-(4-Methoxyphenyl)-5-[(triisopropylsilyl)ethynyl]-1,4-dihydroazulene-1,1-dicarbonitrile (**16b**):* A yellow oil. R_f = 0.36 (3:17 EtOAc/heptane). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.64 (d, *J* = 8.9 Hz, 2H), 7.15 (d, *J* = 6.5 Hz, 1H), 6.99 (d, *J* = 8.9 Hz, 2H), 6.86 (s, 1H), 6.33 (ddd, *J* = 9.5, 6.5, 1.3 Hz, 1H), 5.54 (dd, *J* = 9.5, 5.4 Hz, 1H), 5.47 (d, *J* = 5.4 Hz, 1H), 3.86 (s, 3H), 3.22 (ddd, *J* = 5.4, 5.4, 1.3 Hz, 1H), 1.10-1.09 (m, 21H). ^{13}C NMR (125 MHz, $CDCl_3$) δ = 161.0, 139.6, 138.5, 136.4, 129.7, 129.3, 127.6, 125.9, 123.5, 122.9, 117.0, 114.9, 114.3, 113.6, 107.9, 82.1, 55.6, 44.0, 32.4, 18.8, 11.3 ppm. HRMS (MALDI +ve) calcd for $C_{30}H_{33}N_2OSi$ [$(M-H)^+$]: *m/z* = 465.2357; found *m/z* = 465.2354.

*2-(4-Methoxyphenyl)-6-[(triisopropylsilyl)ethynyl]-1,4-dihydroazulene-1,1-dicarbonitrile (**16c**):* A yellow oil. R_f = 0.33 (3:17 EtOAc/heptane). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.67 (d, *J* = 8.9 Hz, 2H), 7.00 (d, *J* = 8.9 Hz, 2H), 6.97 (s, 1H), 6.72 (br d, *J* = 9.3 Hz, 1H), 6.48 (dd, *J* = 9.2, 1.2 Hz, 1H), 5.57 (dd, *J* = 9.2, 5.7 Hz, 1H), 5.52 (dd, *J* = 9.3, 5.7 Hz, 1H), 3.87 (s, 3H), 2.90 (dddd, *J* = 5.7, 5.7, 1.2, 1.2 Hz, 1H), 1.10 (m, 21H). ^{13}C NMR (125 MHz, $CDCl_3$) δ = 161.0, 146.5, 139.5, 136.3, 131.2, 127.5, 126.7, 124.4, 122.7, 121.6, 119.7, 115.0, 112.6, 112.6, 107.9, 82.1, 55.6, 44.3, 33.3, 18.8, 11.3 ppm. HRMS (MALDI +ve) calcd for $C_{30}H_{33}N_2OSi$ [$(M-H)^+$]: *m/z* = 465.2357; found *m/z* = 465.2354.

2-(4-Methoxyphenyl)-7-[(triisopropylsilyl)ethynyl]-1,4-dihydroazulene-1,1-dicarbonitrile ***(16d)****:* A yellow oil. R_f = 0.28 (3:17 EtOAc/heptane). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.64 (d, J = 9.0 Hz, 2H), 7.00 (d, J = 9.0 Hz, 2H), 6.99 (s, 1H), 6.64 (d, J = 6.5 Hz, 1H), 6.32 (ddd, J = 9.7, 6.5, 1.0 Hz, 1H), 6.18 (d, J = 5.4 Hz, 1H), 5.41 (dd, J = 9.7, 5.4 Hz, 1H), 3.87 (s, 3H), 3.39 (td, J = 5.4, 1.0 Hz, 1H), 1.10-1.09 (m, 21H). ^{13}C NMR (125 MHz, $CDCl_3$) δ = 161.0, 141.4, 137.0, 136.1, 132.8, 127.8, 126.5, 126.1, 125.8, 123.7, 122.9, 115.0, 114.1, 113.5, 107.1, 82.5, 55.6, 42.5, 32.2, 18.8, 11.3 ppm. HRMS (MALDI +ve) calcd for $C_{30}H_{33}N_2OSi$ [$(M-H)^+$]: m/z = 465.2357; found m/z = 465.2354.

2-(4-Methoxyphenyl)-8-[(triisopropylsilyl)ethynyl]-1,4-dihydroazulene-1,1-dicarbonitrile ***(16e)****:* A yellow solid. M.p. = 94-96 °C. R_f = 0.25 (3:17 EtOAc/heptane). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.63 (d, J = 8.9 Hz, 2H), 6.97 (d, J = 8.9 Hz, 2H), 6.87 (s, 1H), 6.75 (dd, J = 10.6, 6.3 Hz, 1H), 6.68 (d, J = 10.6 Hz, 1H), 6.20 (dddd, J = 9.1, 6.3, 0.9, 0.9 Hz, 1H), 5.34 (dd, J = 9.2, 6.3 Hz, 1H), 3.85 (s, 3H), 3.70 (dd, J = 6.3, 0.9 Hz, 1H), 1.12 (s, 21H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$) δ = 160.6, 141.3, 138.5, 133.3, 130.4, 127.4, 125.7, 124.0, 122.9, 114.8, 112.4, 112.2, 102.2, 86.9, 55.6, 43.8, 28.7, 18.8, 11.4 ppm, 2Cs masked. HRMS (MALDI +ve) calcd for $C_{30}H_{33}N_2OSi$ [$(M-H)^+$]: m/z = 465.2357; found m/z = 465.2362.

Reaction of ***5*** *with lithium triisopropylsilylacetylide:* To a degassed solution of triisopropylsilylacetylene (1.2 mL, 5.35 mmol) at -40 °C in Et_2O (25 mL) was added LiHMDS (2.4 mL, 1.0 M in toluene, 2.4 mmol) and the vessel allowed to warm to -20 °C. The reaction contents were cooled to -78 °C and added via cannula to a vessel containing a degassed suspension of **3** (620 mg, 1.69 mmol) in THF (50 mL) at -78 °C. The reaction mixture was stirred for 1 h at -78 °C, quenched with saturated aqueous NH_4Cl (50 mL) and allowed to warm to ambient temperature. The reaction mixture was diluted with Et_2O (100 mL) and water (50 mL) and the phases separated. The aqueous component was extracted with Et_2O (50 mL) and the combined organic extracts were dried over $MgSO_4$ and filtered. The solvent was removed under reduced pressure and the crude residue was purified by flash column chromatography (toluene) to give a regioisomeric mixture of **17** (315 mg, 40%) as a yellow oil. Anal. calcd (%) for $C_{30}H_{31}N_3Si$ (461.68): C 78.05, H 6.77, N 9.10; found C 77.93, H 6.63, N 9.04. Mixture **17** was subject to repeated flash column chromatography (EtOAc/heptane) to isolate small portions of the following regioisomers.

2-(4-Cyanophenyl)-4-[(triisopropylsilyl)ethynyl]-1,4-dihydroazulene-1,1-dicarbonitrile ***(17a)****:* A yellowish oil. R_f = 0.33 (1:9 EtOAc/heptane). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.77 (d, J = 8.5 Hz, 2H), 7.73 (d, J = 8.5 Hz, 2H), 7.46 (s, 1H), 6.96 (d, J = 11.2 Hz, 1H), 6.91 (dd, J = 11.2, 5.9 Hz, 1H), 6.33 (ddd, J = 9.7, 5.9, 1.3 Hz, 1H), 5.49 (dd, J = 9.7, 4.9 Hz, 1H), 3.47 (dd, J = 4.9, 1.3 Hz, 1H), 1.15 (s, 21H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$) δ = 139.8, 138.7, 136.4, 134.9, 134.2, 134.1, 133.3, 127.3, 125.7, 125.6, 122.2, 118.2, 112.9, 111.5, 111.3, 104.7, 85.7, 43.2, 32.1, 18.8, 11.3 ppm. HRMS (MALDI +ve) calcd for $C_{30}H_{30}N_3Si$ [$(M-H)^+$]: m/z = 460.2204; found m/z = 460.2209.

2-(4-Cyanophenyl)-5-[(triisopropylsilyl)ethynyl]-1,4-dihydroazulene-1,1-dicarbonitrile ***(17b)****:* A yellow solid. M.p. = 107.5-112 °C (decomposes). R_f = 0.21 (EtOAc/heptane 1:9). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.80 (d, J = 8.5 Hz, 2H), 7.77 (d, J = 8.5 Hz, 2H), 7.21 (d, J = 6.6 Hz, 1H), 7.17 (s, 1H), 6.39 (ddd, J = 9.6, 6.6, 1.2 Hz, 1H), 5.63 (d, J = 5.5 Hz, 1H), 5.54 (dd, J = 9.6, 5.5 Hz, 1H), 3.22 (ddd, J = 5.5, 5.5, 1.2 Hz, 1H), 1.09 (s, 21H) ppm. ^{13}C

NMR (125 MHz, $CDCl_3$) δ = 138.8, 137.5, 135.4, 134.7, 134.6, 133.2, 130.0, 126.5, 125.4, 123.9, 119.5, 118.2, 113.6, 113.3, 112.9, 107.1, 82.7, 43.7, 32.4, 18.8, 11.3 ppm. HRMS (MALDI +ve) calcd for $C_{30}H_{30}N_3Si$ [$(M-H)^+$]: *m/z* = 460.2204; found *m/z* = 460.2217.

2-(4-Cyanophenyl)-6-[(triisopropylsilyl)ethynyl]-1,4-dihydroazulene-1,1-dicarbonitrile ***(17c)****:* A yellowish solid. M.p. = 151-153 °C. R_f = 0.19 (EtOAc/heptane 1:9). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.83 (d, *J* = 8.6 Hz, 1H), 7.77 (d, *J* = 8.6 Hz, 1H), 7.31 (s, 1H), 6.77 (d, *J* = 9.2 Hz, 1H), 6.54 (d, *J* = 9.2 Hz, 1H), 5.63 (dd, *J* = 9.2, 5.8 Hz, 2H), 2.94 (dddd, *J* = 5.8, 5.8, 1.2, 1.2 Hz, 1H), 1.09 (s, 21H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$) δ = 145.6, 138.4, 137.3, 137.0, 133.9, 133.2, 127.3, 126.3, 126.2, 121.4, 119.6, 118.2, 113.1, 111.7, 111.7, 107.2, 82.5, 44.1, 33.3, 18.7, 11.3 ppm. HRMS (MALDI +ve) calcd for $C_{30}H_{30}N_3Si$ [$(M-H)^+$]: *m/z* = 460.2204; found *m/z* = 460.2214.

2-(4-Cyanophenyl)-7-[(triisopropylsilyl)ethynyl]-1,4-dihydroazulene-1,1-dicarbonitrile ***(17d)****:* A yellowish solid. M.p. = 126-135 °C (decomposes). R_f = 0.10 (EtOAc/heptane 1:9). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.79 (s, 4H), 7.28 (s, 1H), 6.81 (d, *J* = 6.5 Hz, 1H), 6.39 (dd, *J* = 9.8, 6.5 Hz, 1H), 6.22 (d, *J* = 5.5 Hz, 1H), 5.50 (dd, *J* = 9.8, 5.5 Hz, 1H), 3.42 (dd, *J* = 5.5, 5.5 Hz, 1H), 1.08 (s, 21H). ^{13}C NMR (125 MHz, $CDCl_3$) δ = 140.4, 138.2, 135.5, 135.2, 134.4, 133.2, 128.7, 126.6, 126.6, 126.4, 125.2, 118.2, 113.4, 113.3, 112.8, 106.3, 83.0, 42.2, 32.1, 18.8, 11.3 ppm. HRMS (MALDI +ve) calcd for $C_{30}H_{30}N_3Si$ [$(M-H)^+$]: *m/z* = 460.2204; found *m/z* = 460.2210.

2-(4-Cyanophenyl)-8-[(triisopropylsilyl)ethynyl]-1,4-dihydroazulene-1,1-dicarbonitrile ***(17e)****:* A yellow solid. M.p. = 152.5-154 °C. R_f = 0.05 (EtOAc/heptane 1:9). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.78 (d, *J* = 6.6 Hz, 2H), 7.75 (d, *J* = 6.6 Hz, 2H), 7.20 (s, 1H), 6.84 (dd, *J* = 10.7, 6.3 Hz, 1H), 6.75 (d, *J* = 10.7 Hz, 1H), 6.26 (ddd, *J* = 9.2, 6.3, 0.7 Hz, 1H), 5.42 (dd, *J* = 9.2, 6.0 Hz, 1H), 3.73 (dd, *J* = 6.0, 0.7 Hz, 1H), 1.13 (s, 21H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$) δ = 140.8, 136.8, 136.0, 134.3, 134.1, 133.2, 126.3, 124.0, 118.3, 112.8, 111.5, 111.4, 101.7, 87.8, 29.4, 18.8, 11.4 ppm, 4Cs masked. HRMS (MALDI +ve) calcd for $C_{30}H_{30}N_3Si$ [$(M-H)^+$]: *m/z* = 460.2204; found *m/z* = 460.2209.

Reaction of ***6*** *with lithium triisopropylsilylacetylide:* To a degassed solution of triisopropylsilylacetylene (1.6 mL, 7.13 mmol) at -40 °C in Et_2O (30 mL) was added LiHMDS (3.2 mL, 1.0 M in toluene, 3.2 mmol) and the vessel allowed to warm to -20 °C. The reaction contents were cooled to -78 °C and added via cannula to a vessel containing a degassed suspension of **6** (1.00 g, 2.39 mmol) in THF (80 mL) at -78 °C. The reaction mixture was stirred for 1 h at -78 °C, quenched with saturated aqueous NH_4Cl (50 mL) and allowed to warm to ambient temperature. The reaction mixture was diluted with Et_2O (100 mL) and water (50 mL) and the phases separated. The aqueous component was extracted with Et_2O (50 mL) and the combined organic extracts were dried over Na_2SO_4 and filtered. The solvent was removed under reduced pressure and the crude residue was purified by flash column chromatography (toluene/heptane 1:1) to give a regioisomeric mixture of **18** (544 mg, 44%) as a yellow oil. Anal. calcd (%) for $C_{29}H_{32}N_2Si$ (436.67): C 81.98, H 7.08, N 5.46; found C 81.84, H 6.99, N 5.45. This mixture was then subjected to further flash chromatography (EtOAc/heptane 1:19) to give a pure sample of **18c**. Compounds **18b** and **18d** were isolated as a mixture (R_f = 0.57 in EtOAc/heptane 1:9) and small amounts could be separated by flash column chromatography (chlorobenzene/heptane 2:1). Compounds **18a** and **18e** were isolated as a mixture (R_f = 0.50 in

EtOAc/heptane 1:9) and small amounts could be separated by flash column chromatography (chlorobenzene/CS_2 1:1).

2,3-Diphenyl-4-[(triisopropylsilyl)ethynyl]-1,4-dihydroazulene-1,1-dicarbonitrile ***(18a)****:* A yellowish oil. R_f = 0.52 (chlorobenzene/CS_2 1:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.45-7.43 (m, 3H), 7.37-7.35 (m, 2H), 7.29-7.26 (m, 5H), 6.98 (d, *J* = 11.3 Hz, 1H), 6.87 (dd, *J* = 11.3, 6.5 Hz, 1H), 6.38 (dd, *J* = 9.3, 6.5 Hz, 1H), 5.61 (dd, *J* = 9.3, 9.3 Hz, 1H), 4.18 (d, *J* = 9.3 Hz, 1H), 0.99-0.98 (m, 21H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$) δ = 147.8, 141.4, 136.5, 134.0, 133.4, 132.6, 131.1, 129.5, 129.3, 129.2, 129.0, 128.9, 128.8, 128.5, 123.3, 122.1, 112.6, 111.9, 102.7, 83.1, 45.4, 28.5, 18.7, 11.2 ppm. HRMS (MALDI +ve) calcd for $C_{35}H_{36}N_2Si$ [M^+]: *m/z* = 511.2564; found *m/z* = 511.2570.

2,3-Diphenyl-5-[(triisopropylsilyl)ethynyl]-1,4-dihydroazulene-1,1-dicarbonitrile ***(18b)****:* A yellowish oil. R_f = 0.36 (chlorobenzene/heptane 7:3). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.37-7.35 (m, 5H), 7.33-7.28 (m, 3H), 7.23-7.19 (m, 3H), 6.37 (ddd, *J* = 9.9, 6.5, 1.3 Hz, 1H), 5.52 (dd, *J* = 9.9, 5.5 Hz, 1H), 5.28 (d, *J* = 5.5 Hz, 1H), 3.18 (ddd, *J* = 5.5, 5.5, 1.3 Hz, 1H), 1.05 (m, 21H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$) δ = 145.7, 140.9, 138.0, 132.1, 131.7, 131.3, 129.3, 129.2, 129.0, 129.0, 128.9, 128.9, 125.0, 123.6, 117.7, 114.0, 113.9, 107.8, 82.3, 46.4, 32.0, 18.7, 11.3 ppm, 1C masked. HRMS (MALDI +ve) calcd for $C_{35}H_{36}N_2Si$ [M^+]: *m/z* = 511.2564; found *m/z* = 511.2562.

2,3-Diphenyl-6-[(triisopropylsilyl)ethynyl]-1,4-dihydroazulene-1,1-dicarbonitrile ***(18c)****:* A yellowish oil. R_f = 0.59 (EtOAc/heptane 1:9). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.44-7.42 (m, 2H), 7.39-7.37 (m, 3H), 7.33-7.27 (m, 5H), 6.79 (br d, *J* = 9.3 Hz, 1H), 6.23 (br d, *J* = 9.3 Hz, 1H), 5.64 (dd, *J* = 9.3, 5.8 Hz, 1H), 5.53 (dd, *J* = 9.3, 5.8 Hz, 1H), 2.98 (dddd, *J* = 5.8, 5.8, 1.3, 1.3 Hz, 1H), 1.11-1.10 (m, 21H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$) δ = 147.9, 136.6, 133.2, 132.4, 131.0, 129.4, 129.1, 129.1, 129.0, 125.6, 121.7, 119.9, 112.8, 112.3, 107.7, 82.1, 47.0, 33.3, 18.8, 11.3 ppm, 4Cs masked. HRMS (MALDI +ve) calcd for $C_{35}H_{36}N_2Si$ [M^+]: *m/z* = 511.2564; found *m/z* = 511.2569.

2,3-Diphenyl-7-[(triisopropylsilyl)ethynyl]-1,4-dihydroazulene-1,1-dicarbonitrile ***(18d)****:* A yellowish oil. R_f = 0.40 (chlorobenzene/heptane 7:3). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.42-7.37 (m, 5H), 7.35-7.31 (m, 3H), 7.26-7.24 (m, 2H), 6.52 (d, *J* = 6.6 Hz, 1H), 6.30 (ddd, *J* = 9.6, 6.6, 1.1 Hz, 1H), 6.21 (d, *J* = 5.4 Hz, 1H), 5.50 (dd, *J* = 9.6, 5.4 Hz, 1H), 3.35 (ddd, *J* = 5.4, 1.1 Hz, 1H), 1.11-1.10 (m, 21H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$) δ = 148.2, 143.0, 135.5, 132.3, 132.1, 131.4, 129.7, 129.4, 129.4, 129.1, 129.0, 128.9, 127.0, 126.3, 125.3, 124.8, 113.8, 113.8, 107.1, 82.5, 44.7, 32.4, 18.8, 11.4 ppm. HRMS (MALDI +ve) calcd for $C_{35}H_{36}N_2Si$ [M^+]: *m/z* = 511.2564; found *m/z* = 511.2576.

2,3-Diphenyl-8-[(triisopropylsilyl)ethynyl]-1,4-dihydroazulene-1,1-dicarbonitrile ***(18e)****:* A yellowish oil. R_f = 0.59 (chlorobenzene/CS_2 1:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.39-7.35 (m, 5H), 7.29-7.27 (m, 3H), 7.22-7.20 (m, 2H), 6.72 (dd, *J* = 10.5, 6.5 Hz, 1H), 6.46 (d, *J* = 10.5 Hz, 1H), 6.24 (br dd, *J* = 8.8, 6.5 Hz, 1H), 5.27 (dd, *J* = 8.8, 6.4 Hz, 1H), 3.67 (dd, *J* = 6.4, 0.7 Hz, 1H), 1.13 (br s, 21H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$) δ = 147.0, 142.0, 132.8, 132.7, 132.7, 131.1, 129.2, 129.1, 129.0, 129.0, 129.0, 128.9, 125.8, 123.8, 112.5, 112.1, 102.0, 87.0, 46.0, 28.0, 18.8, 11.4 ppm, 2Cs masked. HRMS (MALDI +ve) calcd for $C_{35}H_{36}N_2Si$ [M^+]: *m/z* = 511.2564; found *m/z* = 511.2569.

Reaction of 7 with lithium triisopropylsilylacetylide: To a degassed solution of triisopropylsilylacetylene (1.5 mL, 6.7 mmol) in Et_2O (25 mL) at -40 °C was added LiHMDS (3.5 mL, 1M in toluene, 3.5 mmol). The reaction contents were allowed to warm to -20 °C, then cooled to -78 °C and added via cannula to a vessel containing a degassed suspension of **7** (1.33 g, 2.69 mmol) in THF (50 mL) at -78 °C. The reaction mixture was stirred for 30 min at -78 °C, quenched with saturated aqueous NH_4Cl (20 mL) and water (80 mL) and allowed to warm to ambient temperature. The reaction mixture was diluted with Et_2O (100 mL) and the phases separated. The aqueous component was extracted with Et_2O (100 mL). The combined organic phases were dried over $MgSO_4$ and filtered. The solvent was removed under reduced pressure and the crude residue was purified by flash column chromatography (toluene/heptane 1:1) to give a regioisomeric mixture of **19** (391 mg, 25%) as a brilliant yellow oil. Anal. calcd (%) for $C_{40}H_{41}N_2Si$ (588.87): C 83.63, H 6.85, N 4.76; found C 83.44, H 6.74, N 4.47. Further purification by flash column chromatography (acetone/heptane 3:47) allowed for the isolation of **19a**, whereas **19c** and **20**, which were isolated as a mixture (R_f = 0.37), could each be obtained pure by flash column chromatography (chlorobenzene/cyclohexane 6:4).

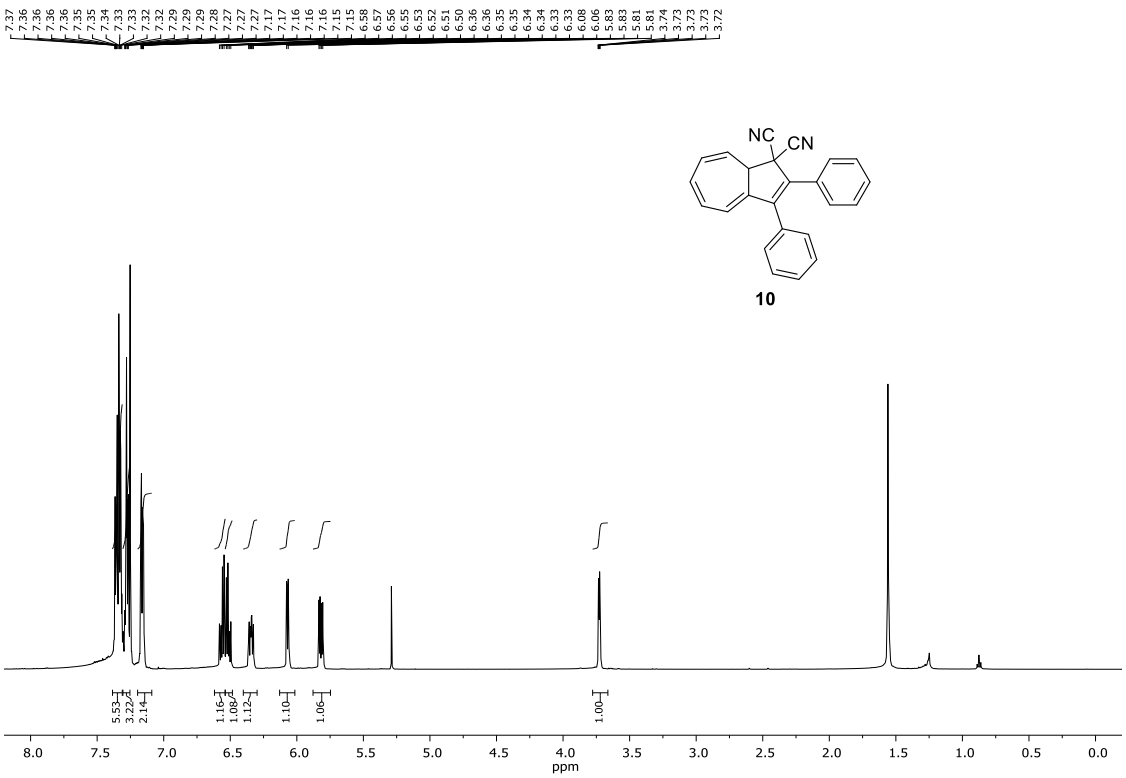
*2,3,7-Triphenyl-4-((triisopropylsilyl)ethynyl)azulene-1,1(4H)-dicarbonitrile (**19a**):* R_f = 0.34 (acetone/heptane 3:47). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.58-7.56 (m, 2H), 7.49-7.36 (m, 8H), 7.31-7.27 (m, 6H), 6.63 (d, *J* = 10.0 Hz, 1H), 5.79 (ddd, *J* = 10.0, 8.8, 0.8 Hz, 1H), 4.22 (d, *J* = 8.8 Hz, 1H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$) δ = 147.8, 146.1, 141.5, 140.8, 136.2, 134.2, 132.6, 131.1, 130.4, 129.6, 129.3, 129.2, 129.0, 128.8, 128.7, 128.6, 128.5, 127.1, 123.7, 119.0, 112.7, 112.1, 102.8, 82.8, 45.7, 28.3, 18.6 (2 signals, rotamers), 11.2 ppm. HRMS (ESP +ve) calcd for $C_{41}H_{40}N_2Si$ [$(M-H)^+$]: *m/z* = 587.2877; found *m/z* = 587.2866.

*2,3,7-triphenyl-6-((triisopropylsilyl)ethynyl)azulene-1,1(6H)-dicarbonitrile (**19c**):* R_f = 0.43 (chlorobenzene/cyclohexane 6:4). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.60-7.58 (m, 2H), 7.45–7.30 (m, 13H), 7.01 (s, 1H), 6.35 (d, *J* = 9.5 Hz, 1H), 5.79 (dd, *J* = 9.5, 7.7 Hz, 1H), 4.40 (br d, *J* = 7.7 Hz, 1H), 0.99-0.98 (m, 21H). ^{13}C NMR (125 MHz, $CDCl_3$) δ = 148.1, 146.4, 139.7, 136.9, 136.2, 132.8, 132.6, 131.3, 129.4, 129.3, 129.2, 129.1, 129.0, 129.0, 128.7, 128.6, 124.3, 123.1, 118.5, 113.3, 112.2, 104.8, 83.3, 47.4, 35.7, 18.8 (2 signals, rotamers), 11.2 ppm; 1C masked. HRMS (ESP +ve) calcd for $C_{41}H_{40}N_2Si$ [$(M-H)^+$]: *m/z* = 587.2877; found *m/z* = 587.2874.

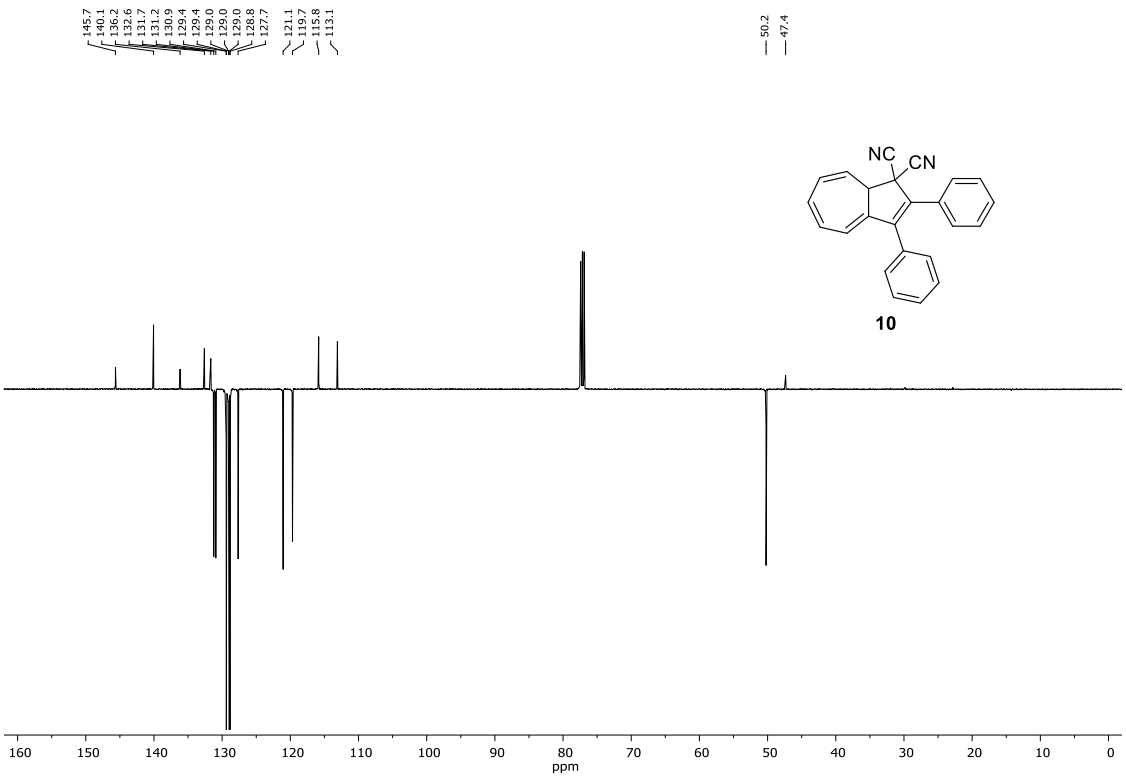
*2,5,6-Triphenyl-1-((triisopropylsilyl)ethynyl)-1a,6b-dihydrocyclopropa[e]indene-4,4(1H)-dicarbonitrile (**20**):* R_f = 0.41 (chlorobenzene/cyclohexane 6:4). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 7.57-7.55 (m, 2H), 7.45-7.30 (m, 13H), 7.24 (s, 1H), 4.47 (ddd, *J* = 5.8, 4.0, 1.1 Hz, 1H), 4.24 (dd, *J* = 5.8, 4.0 Hz, 1H), 2.59 (dd, *J* = 5.8, 5.8 Hz, 1H), 1.07 (br s, 21H) ppm. ^{13}C NMR (125 MHz, C_6D_6) δ = 146.3, 141.7, 139.2, 138.1, 135.7, 132.2, 132.1, 131.3, 129.3, 129.3, 129.1, 129.0, 128.9, 128.9, 128.6, 127.5, 122.8, 113.4, 113.1, 106.8, 83.5 (br), 83.1, 81.3 (br), 45.7, 22.3, 18.8, 18.8 (2 signals, rotamers), 11.2 ppm, 1C masked. HRMS (ESP +ve) calcd for $C_{41}H_{40}N_2Si$ [$(M-H)^+$]: *m/z* = 587.2877; found *m/z* = 587.2871.

NMR Spectra

Compound 10

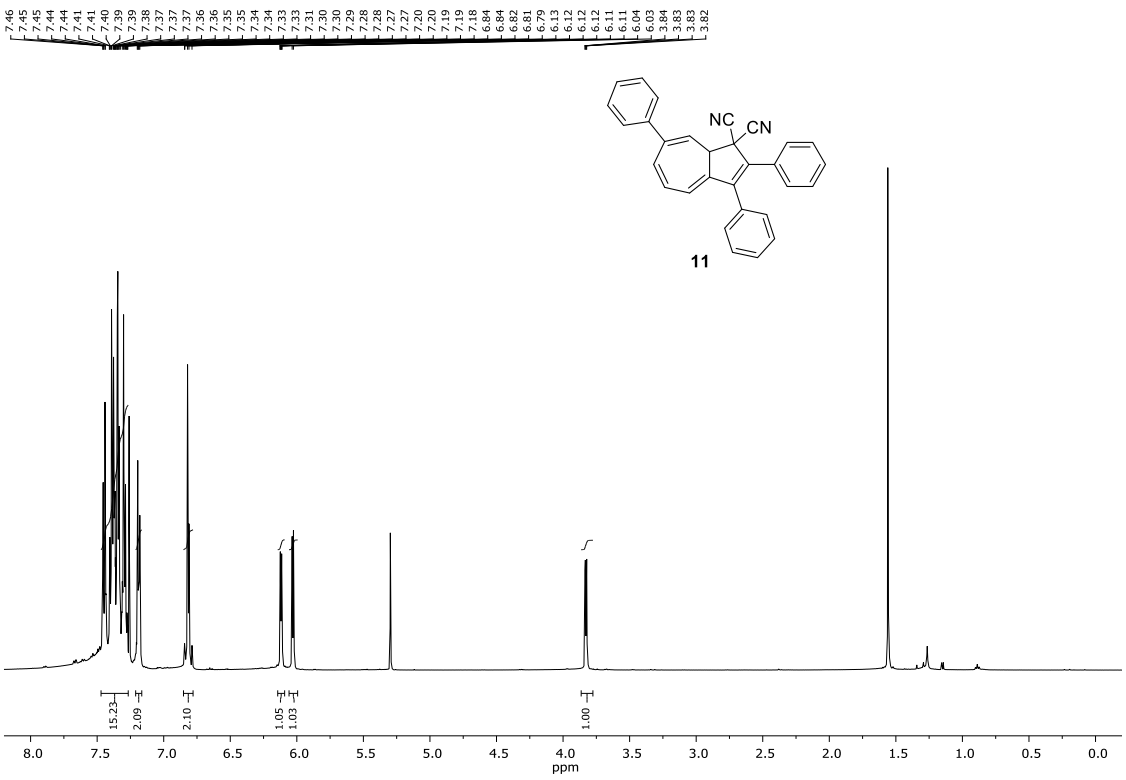


^{1}H NMR (500 MHz) spectrum of **10** in $CDCl_3$

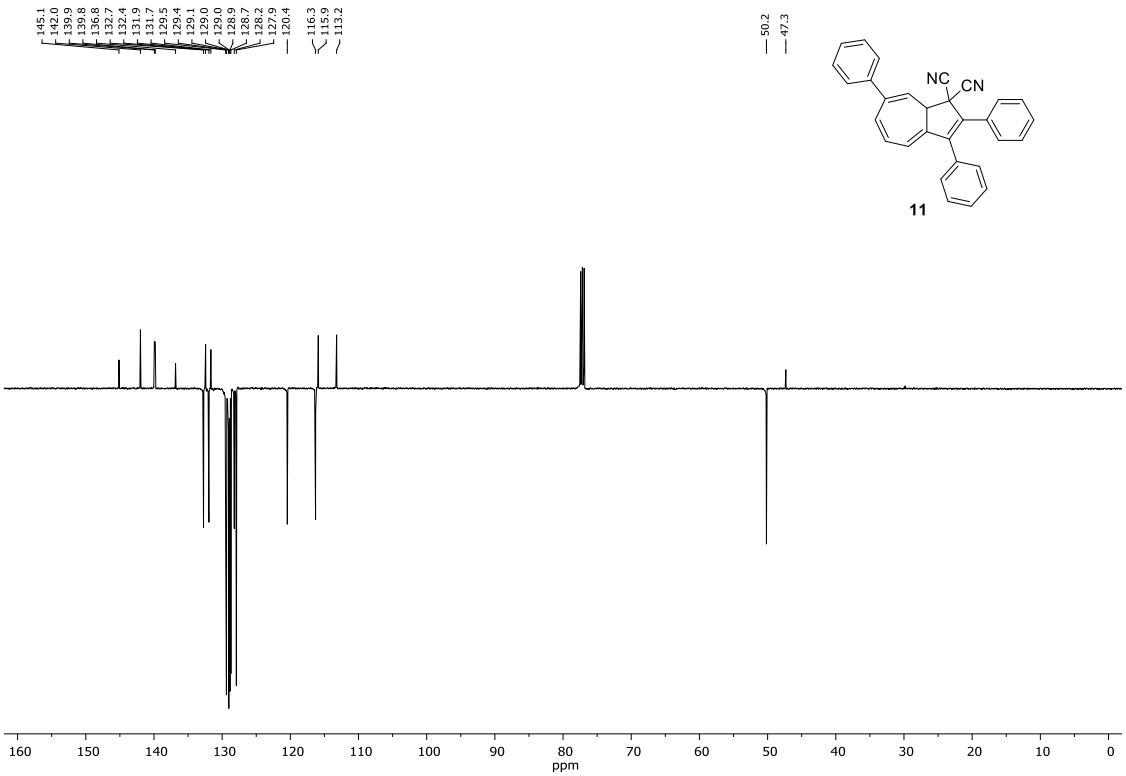


^{13}C NMR APT (125 MHz) spectrum of **10** in $CDCl_3$

Compound 11

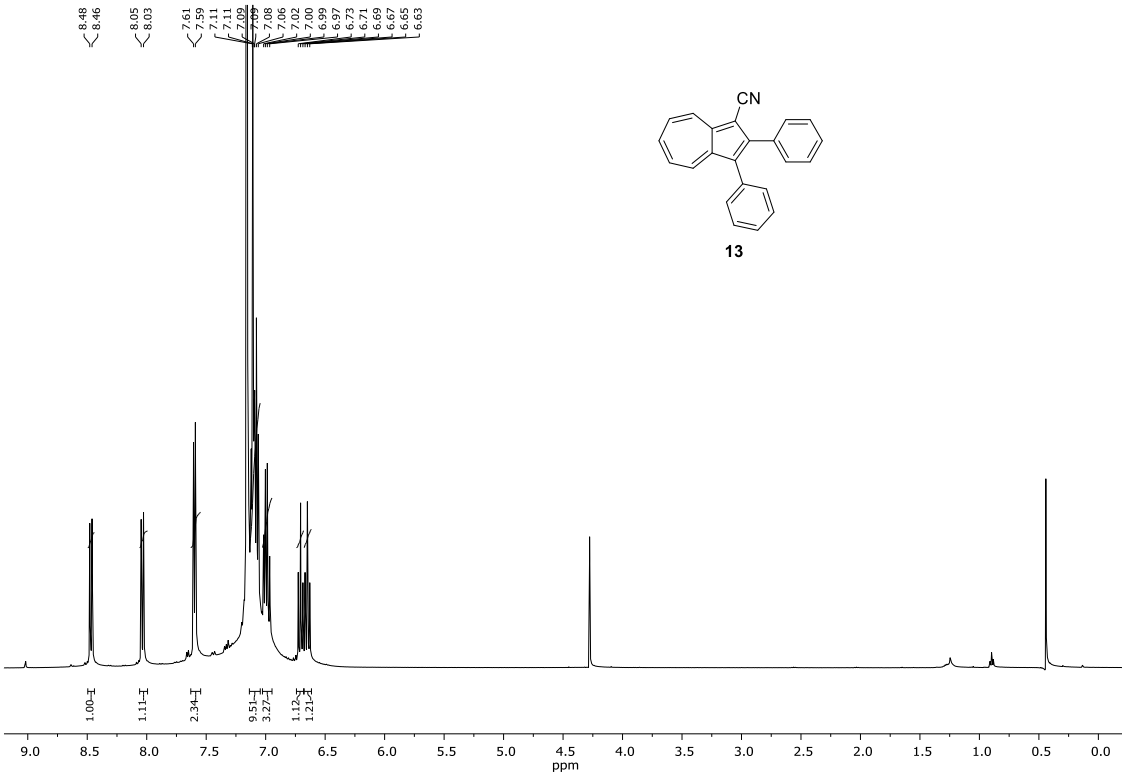


^{1}H NMR (500 MHz) spectrum of **11** in $CDCl_3$

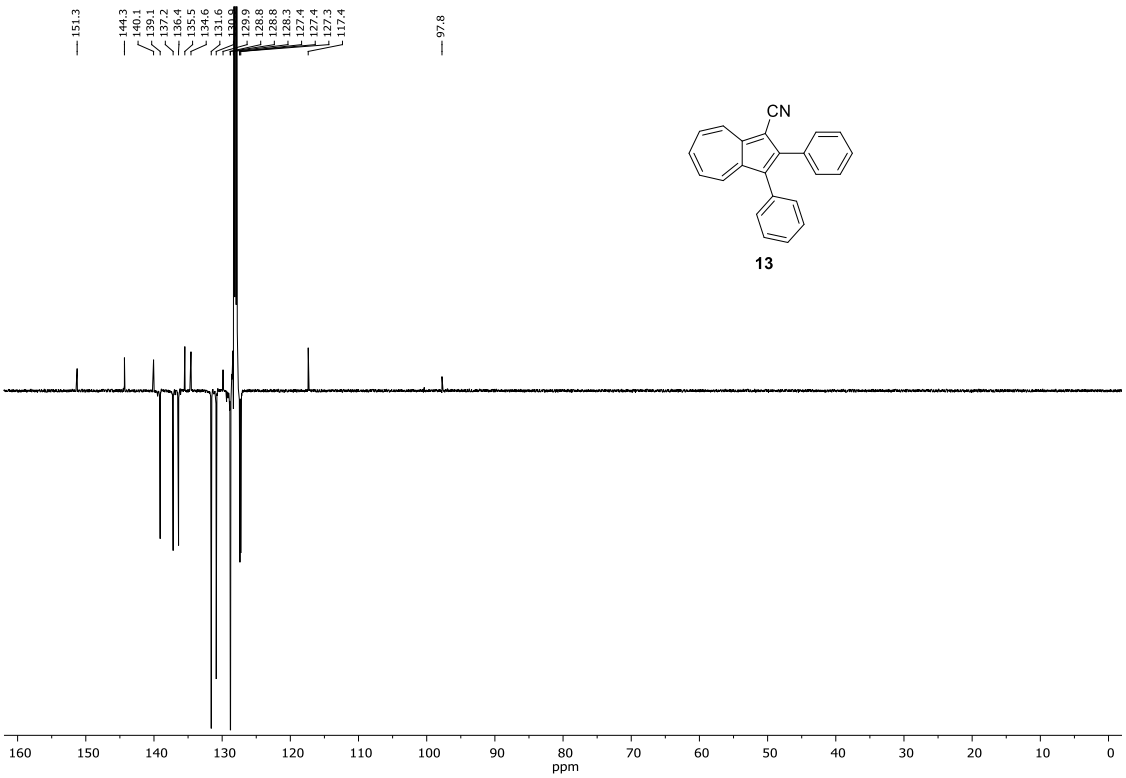


^{13}C NMR APT (125 MHz) spectrum of **11** in $CDCl_3$

Compound 13

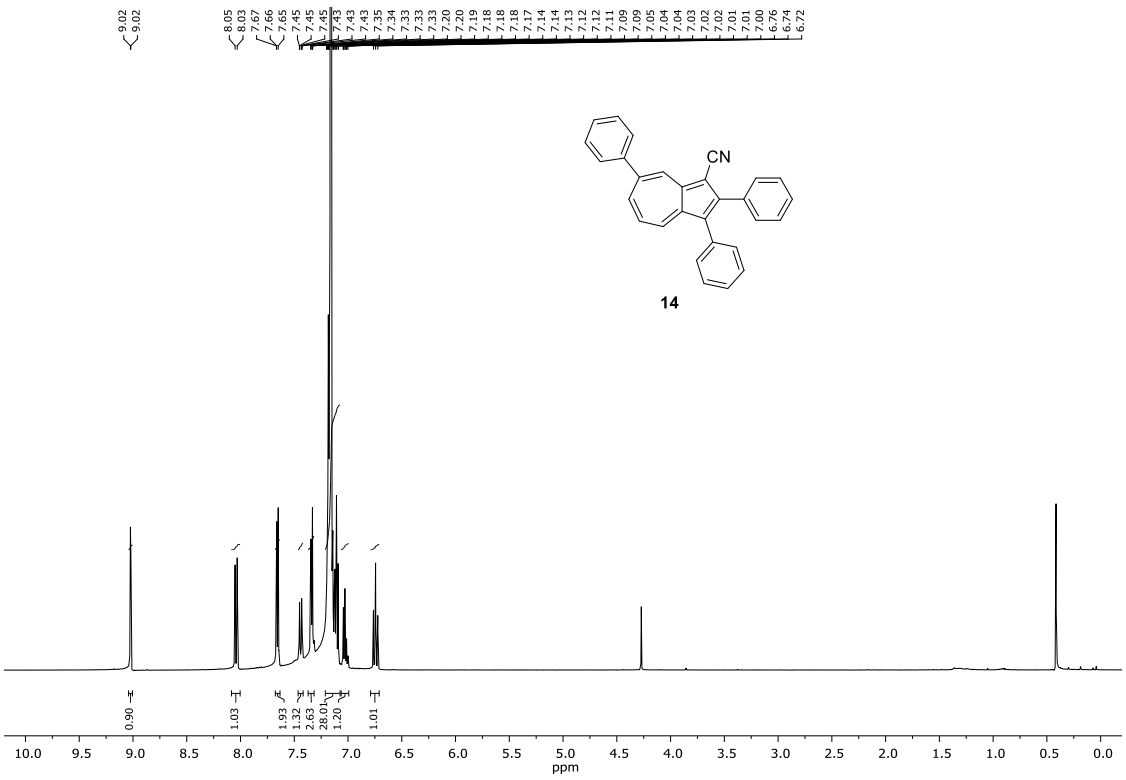


^{1}H NMR (500 MHz) spectrum of **13** in C_6D_6

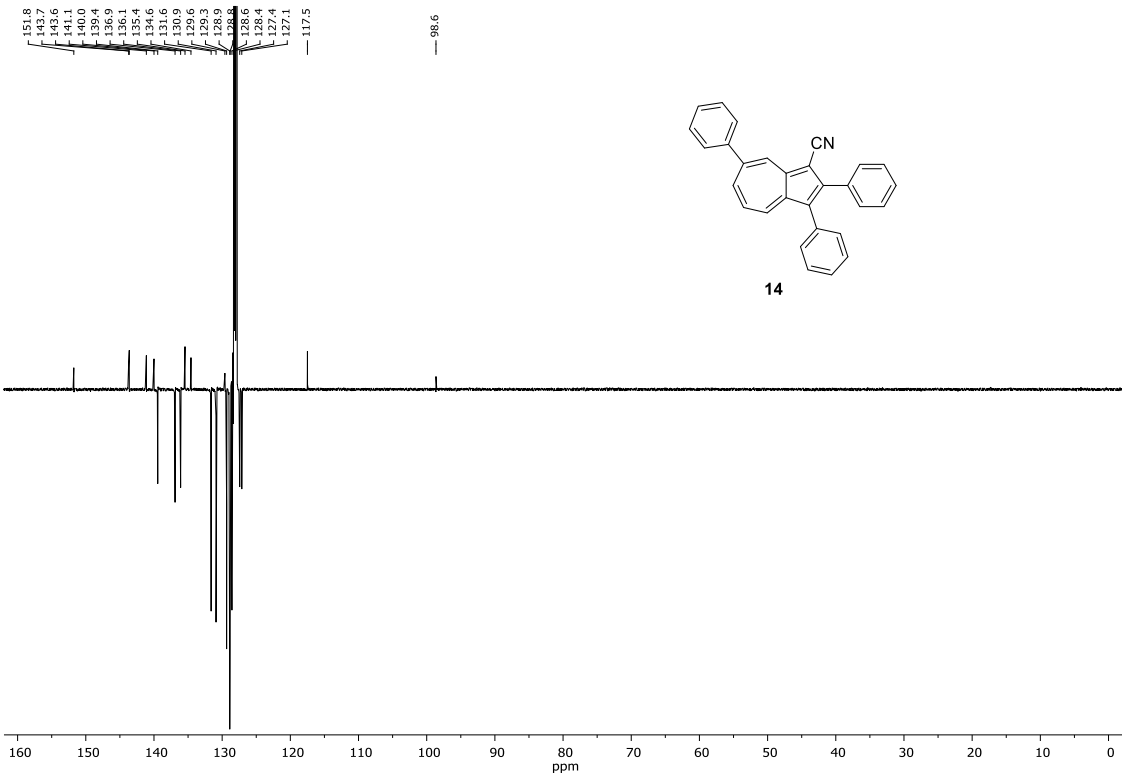


^{13}C NMR APT (125 MHz) spectrum of **13** in C_6D_6

Compound 14

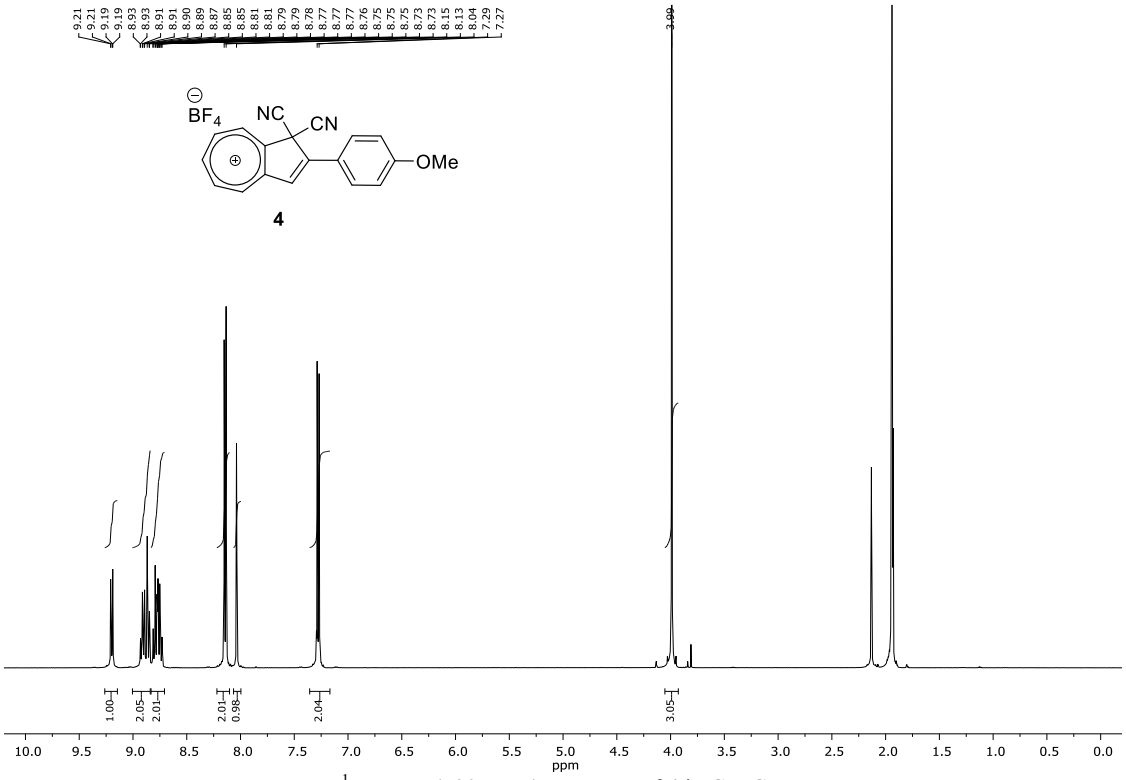


^{1}H NMR (500 MHz) spectrum of **14** in C_6D_6

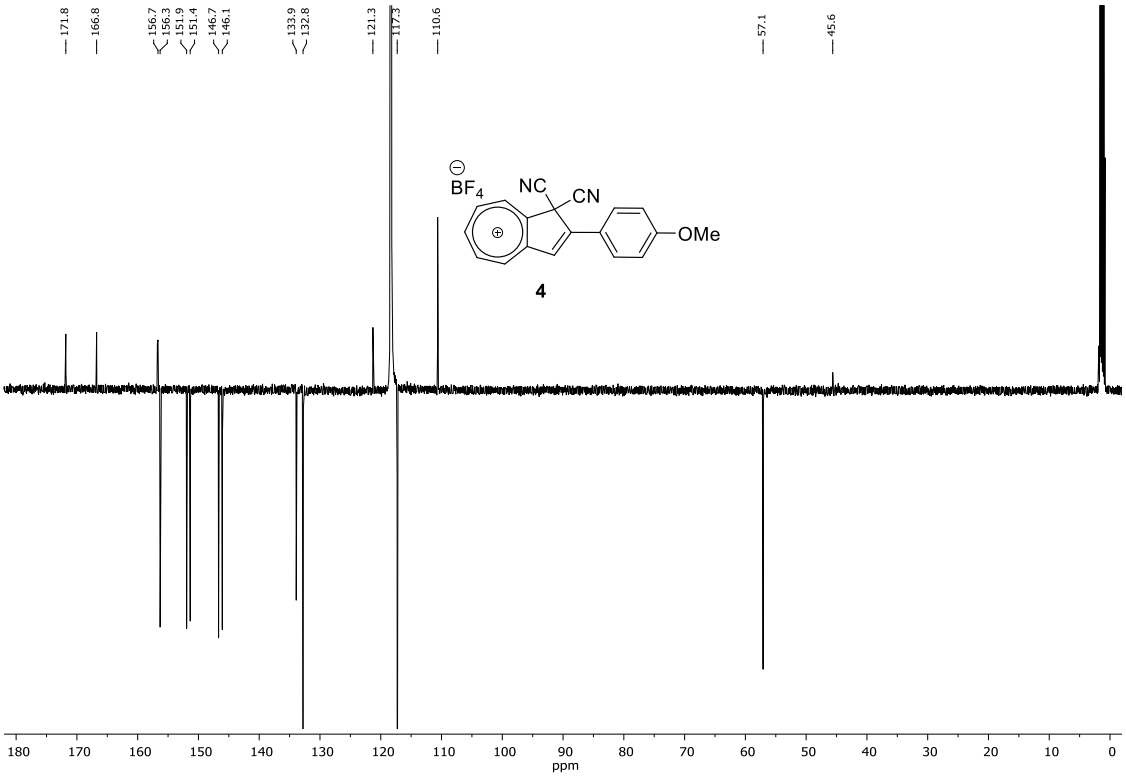


^{13}C NMR APT (125 MHz) spectrum of **14** in C_6D_6

Compound 4

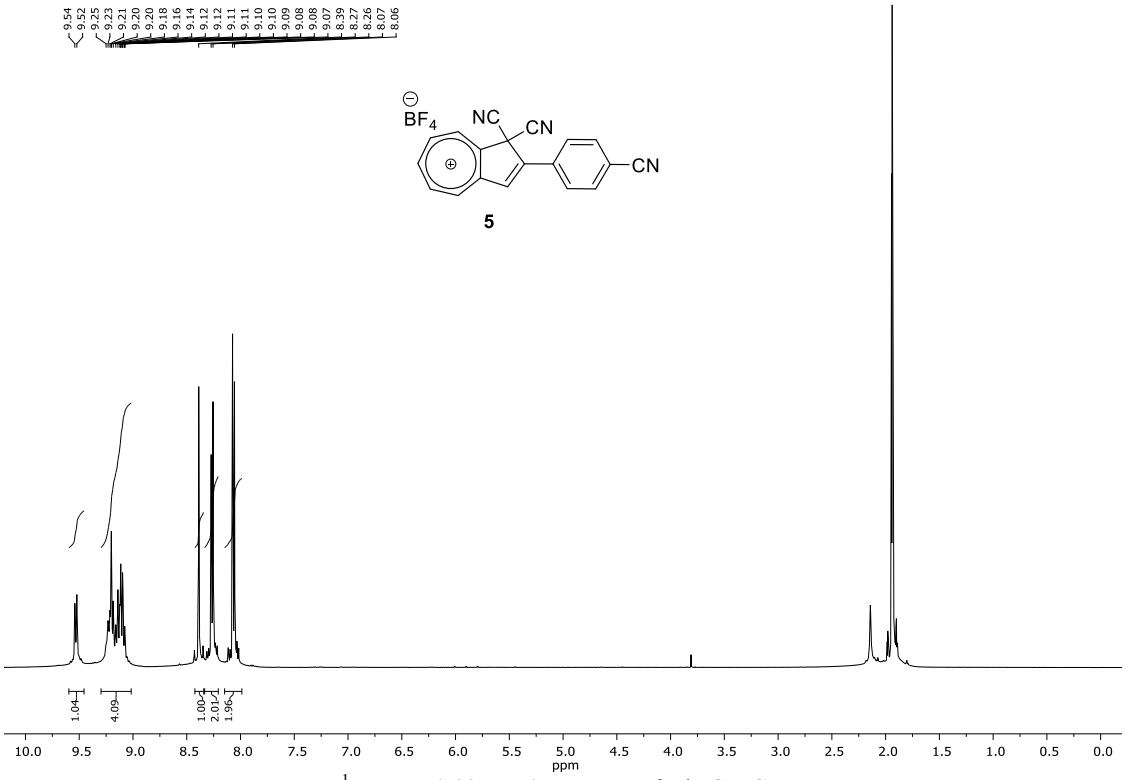


^{1}H NMR (500 MHz) spectrum of **4** in CD_3CN

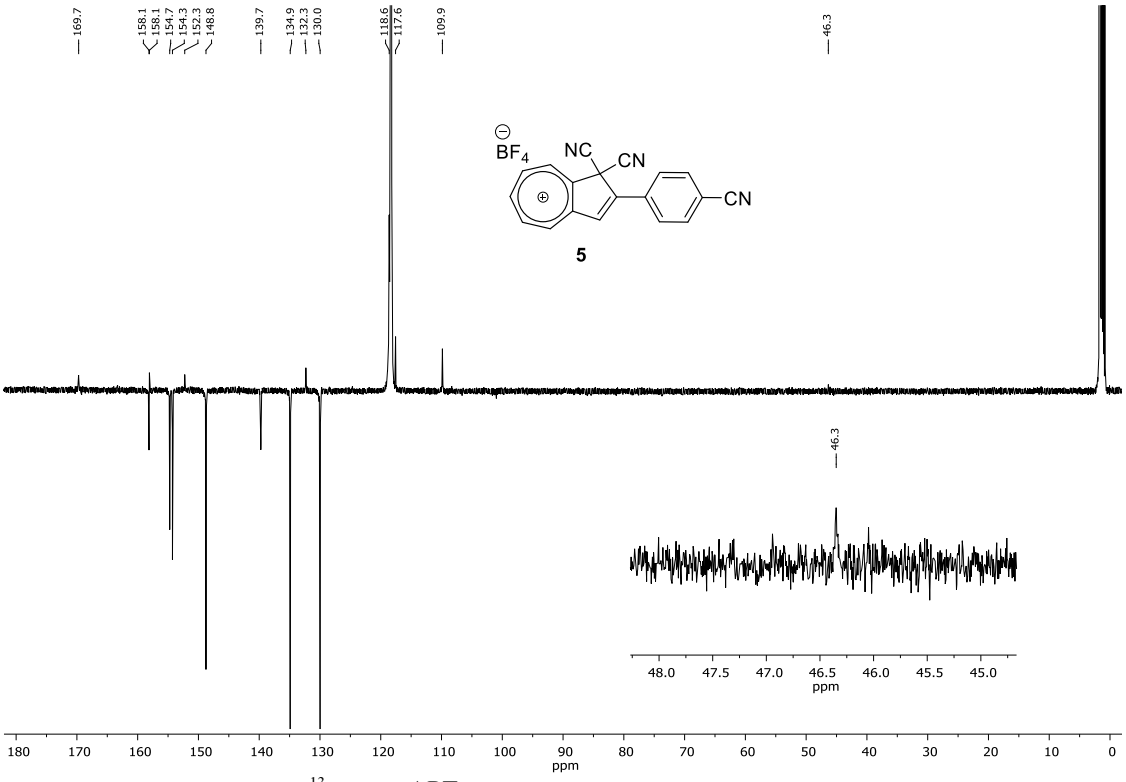


^{13}C NMR APT (125 MHz) spectrum of **4** in CD_3CN

Compound 5

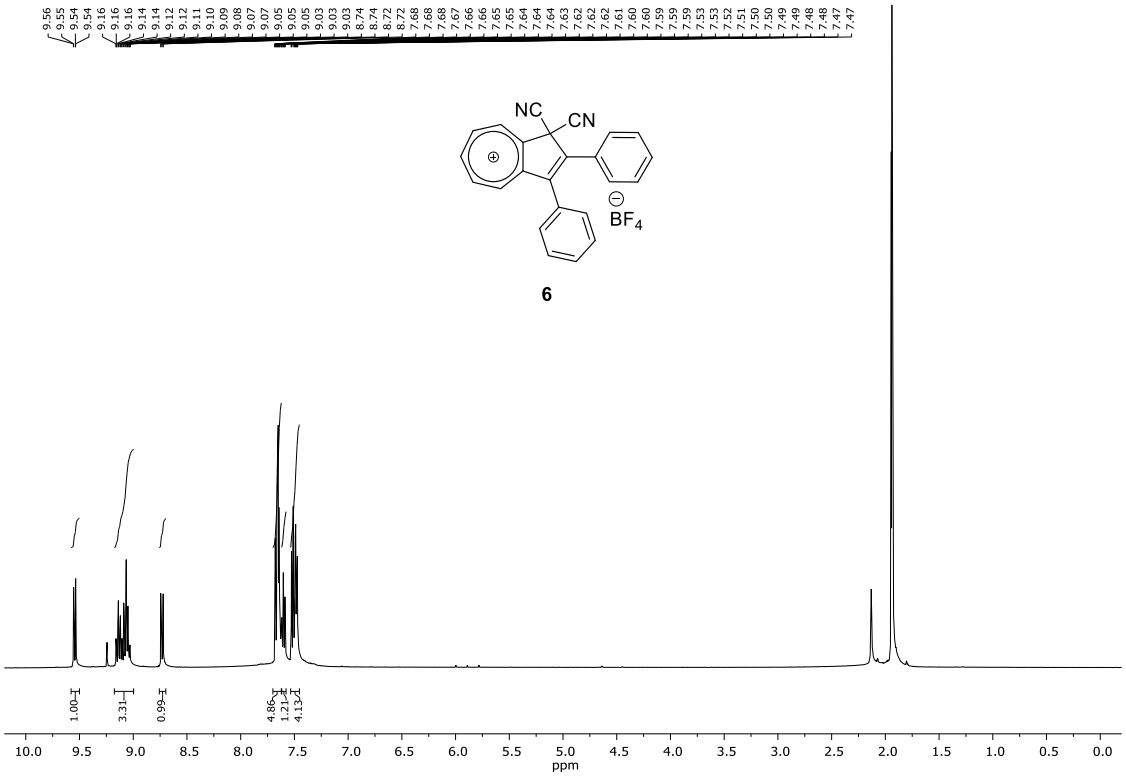


^{1}H NMR (500 MHz) spectrum of **5** in CD_3CN

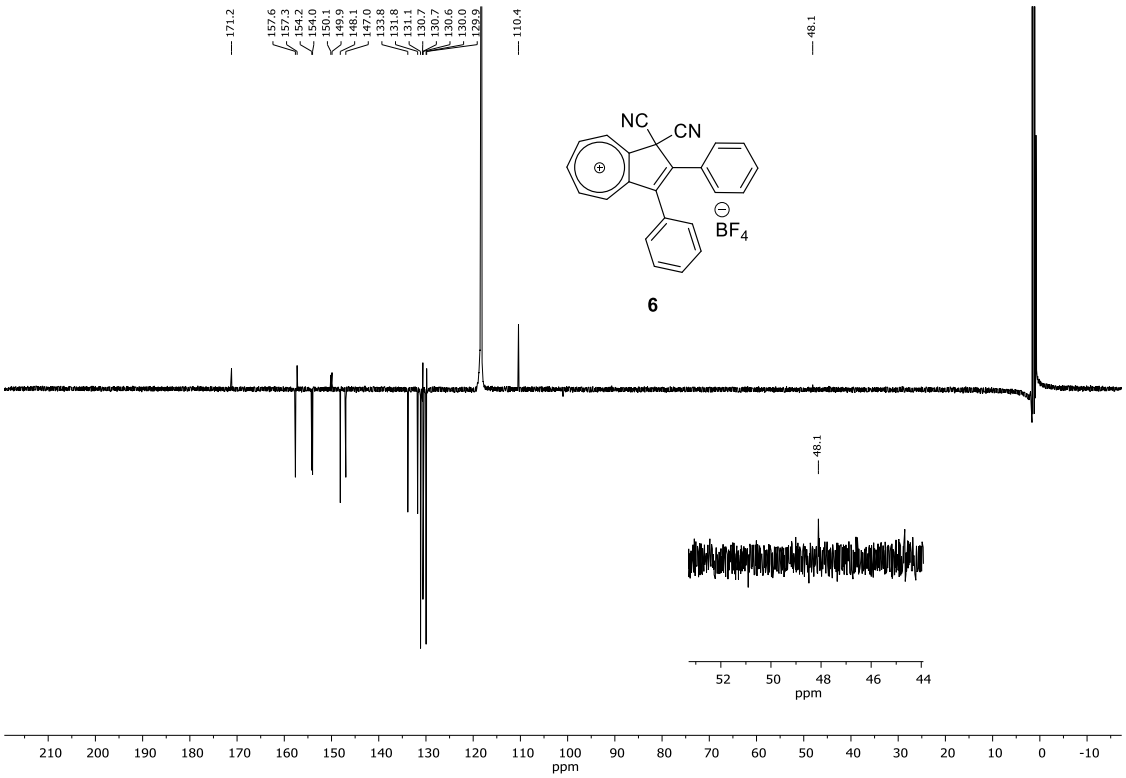


^{13}C NMR APT (125 MHz) spectrum of **5** in CD_3CN

Compound 6

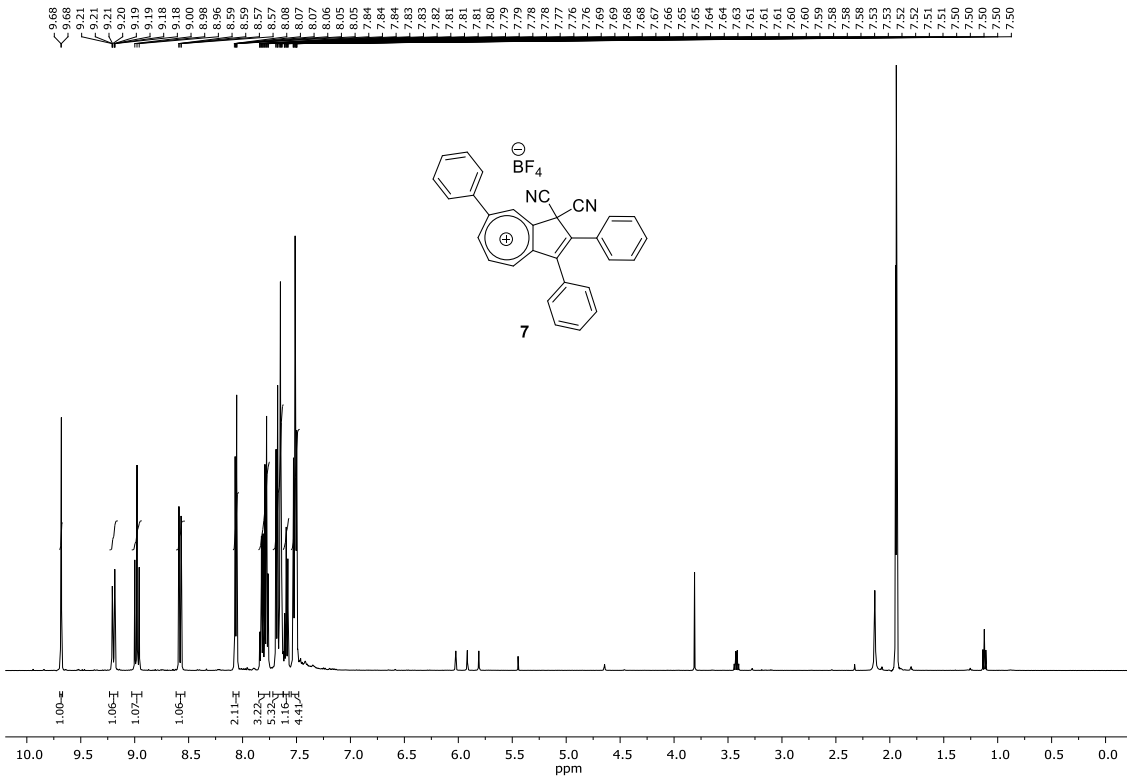


^{1}H NMR (500 MHz) spectrum of **6** in CD_3CN

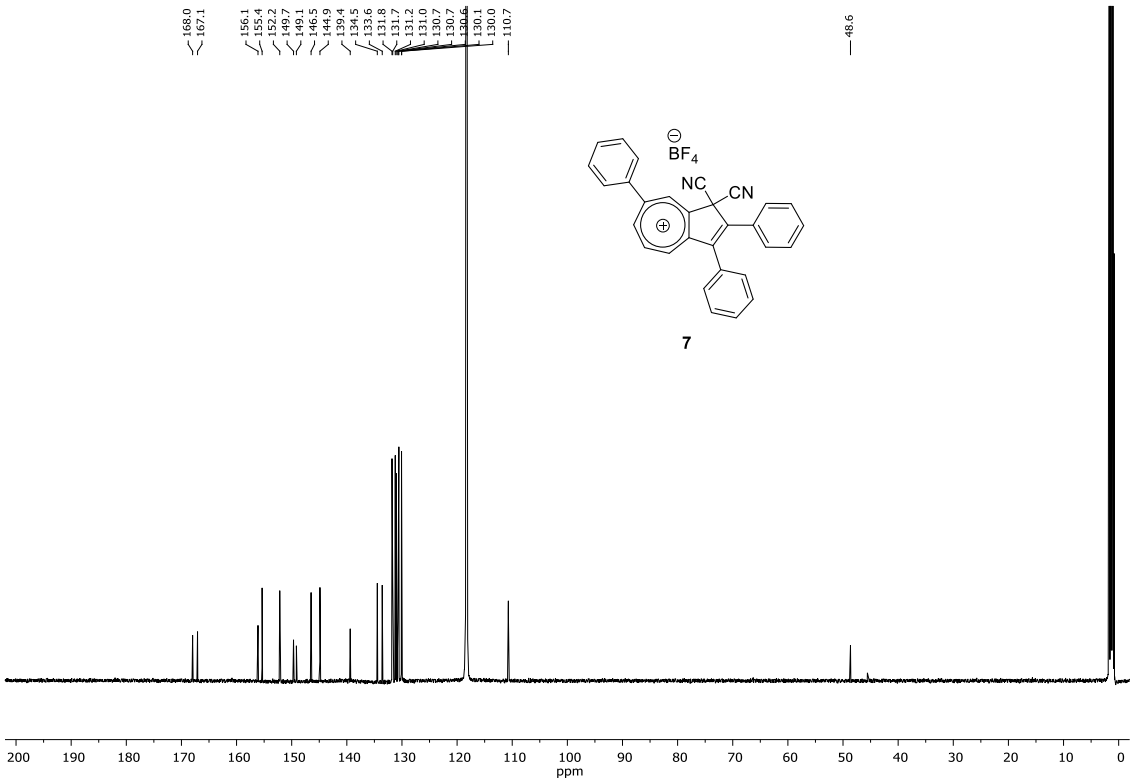


^{13}C NMR APT (125 MHz) spectrum of **6** in CD_3CN

Compound 7

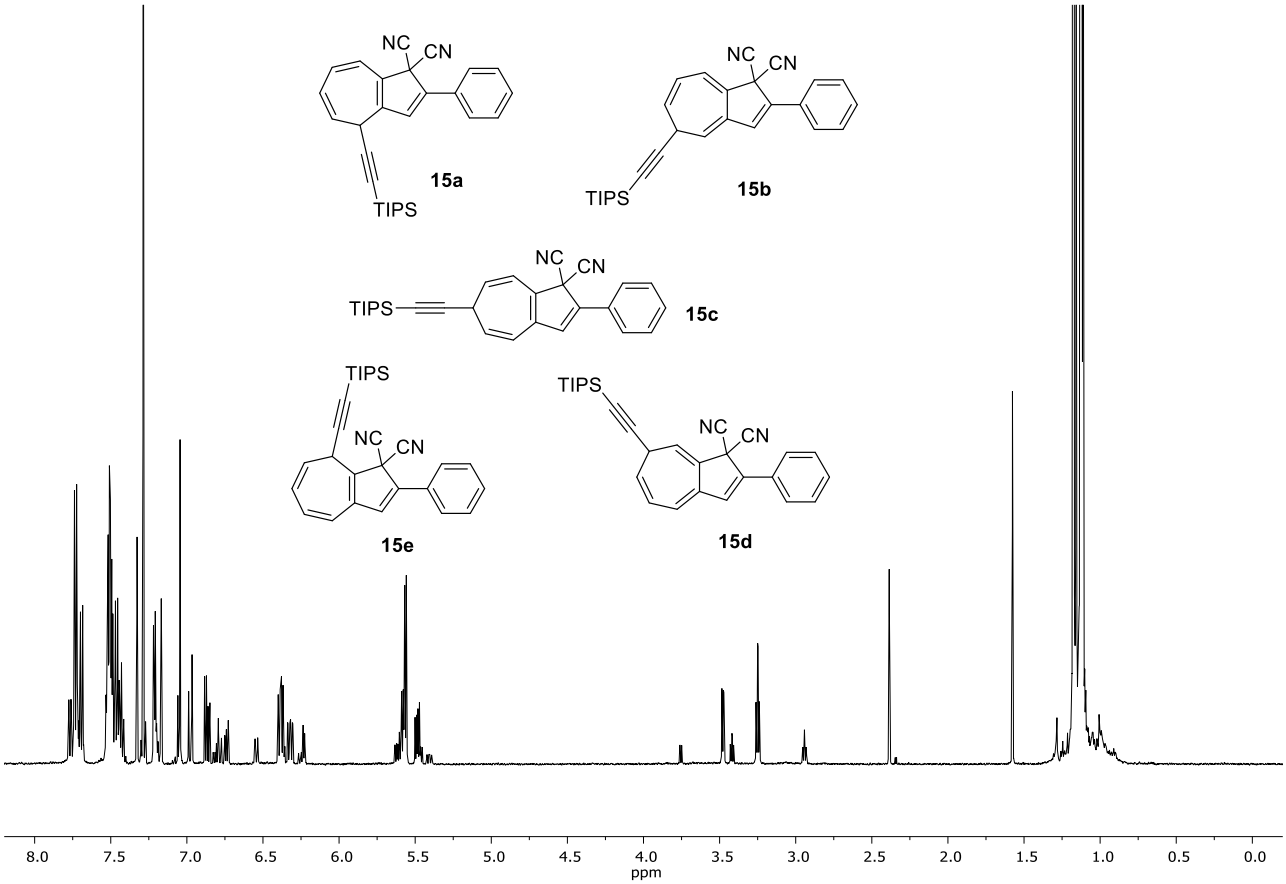


^{1}H NMR (500 MHz) spectrum of **7** in CD_3CN

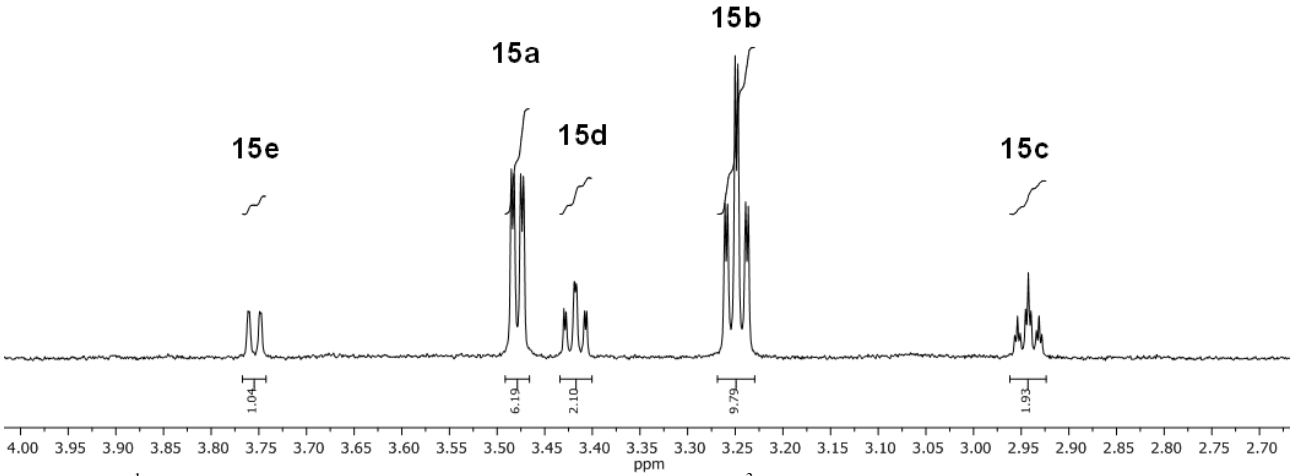


^{13}C NMR (125 MHz) spectrum of **7** in CD_3CN

Regioisomeric mixture 15 (Table 3 Entry 1)

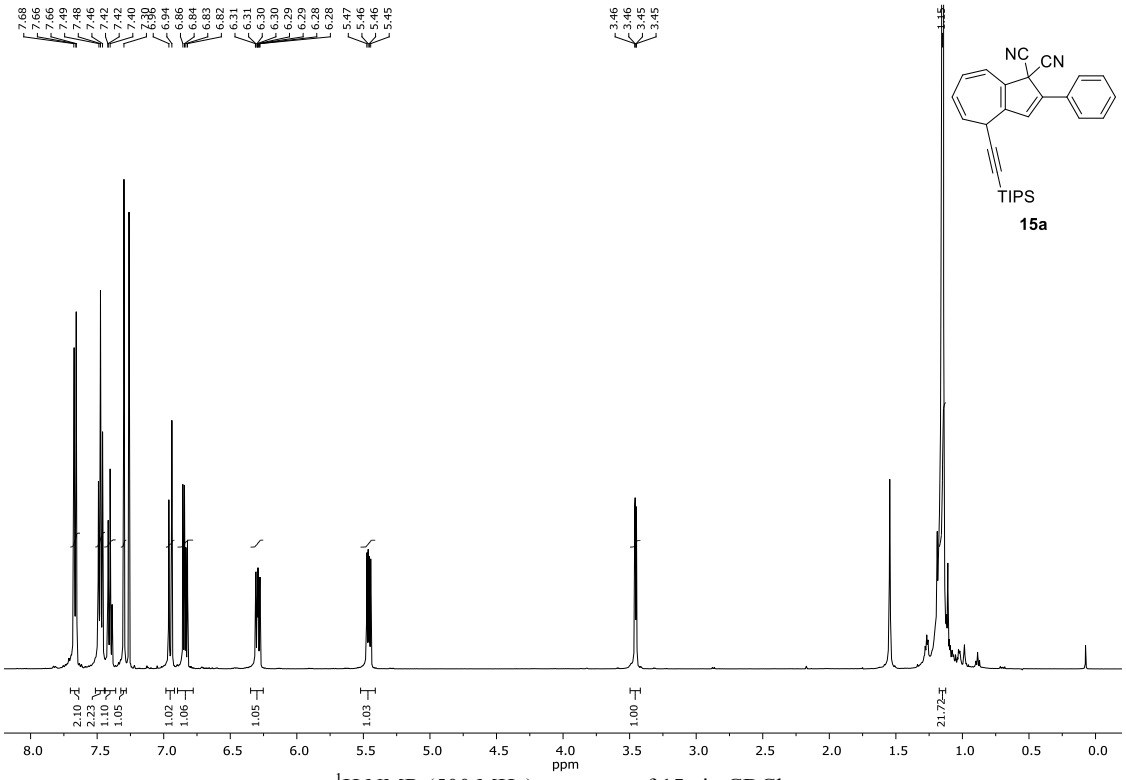


^{1}H NMR (500 MHz) spectra of **15** in $CDCl_3$

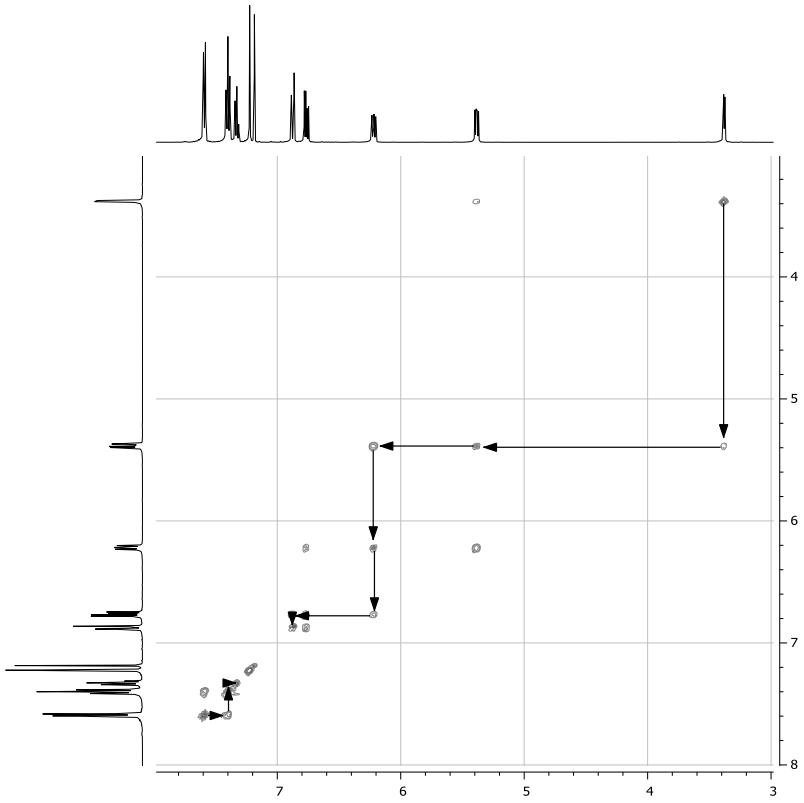


^{1}H NMR (500 MHz) spectra of **15** in $CDCl_3$ zoomed into the sp^3 region for the point of nucleophilic attack

Compound 15a

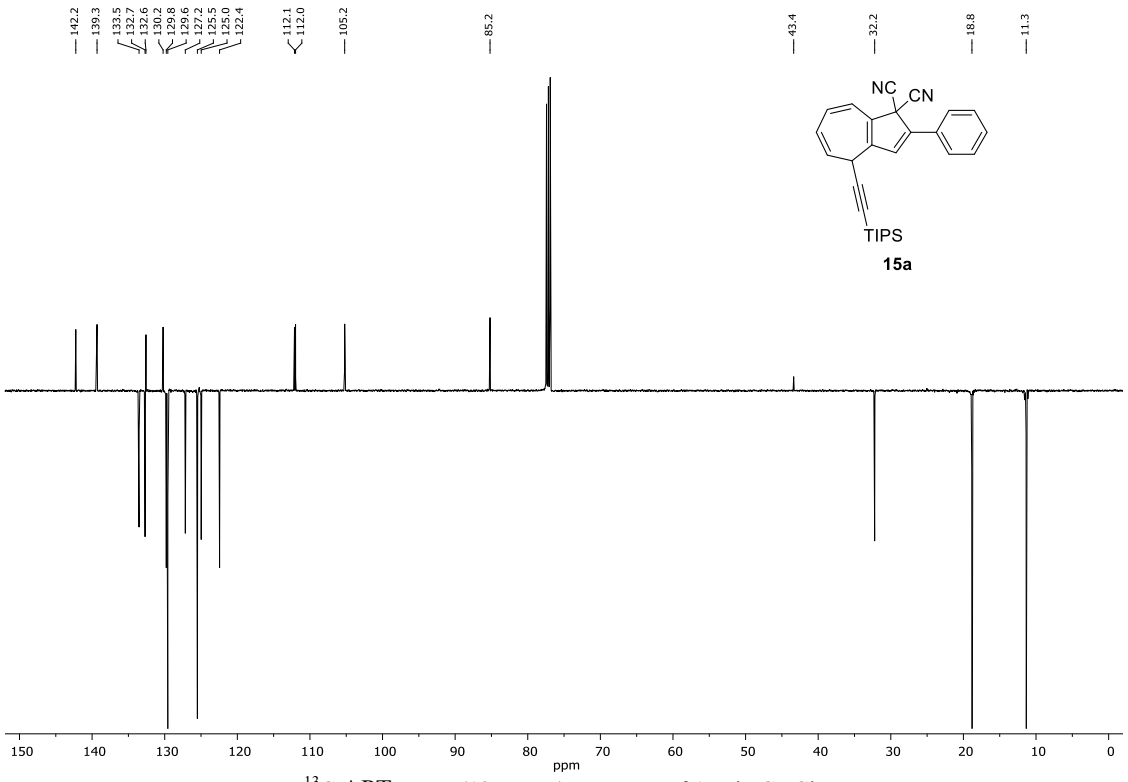


^{1}H NMR (500 MHz) spectrum of **15a** in $CDCl_3$

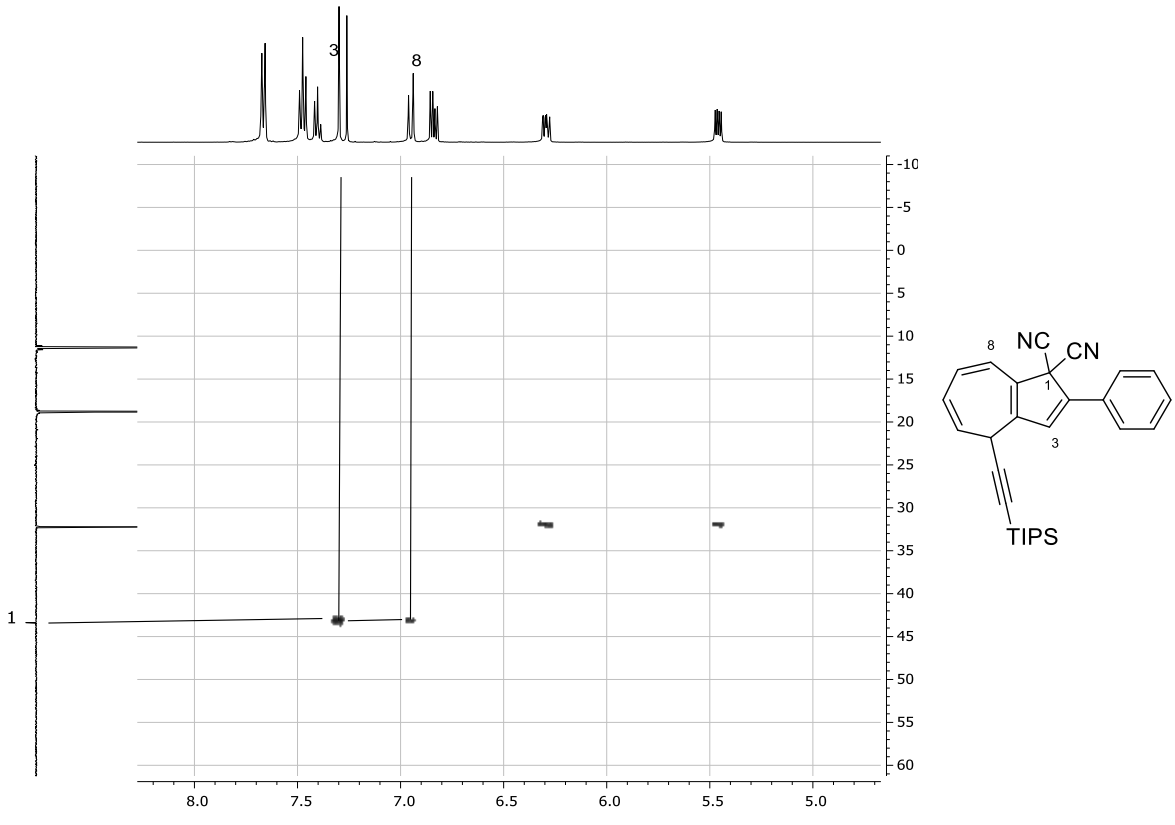


COSY spectrum (500 MHz) of **15a** in $CDCl_3$.

Compound 15a

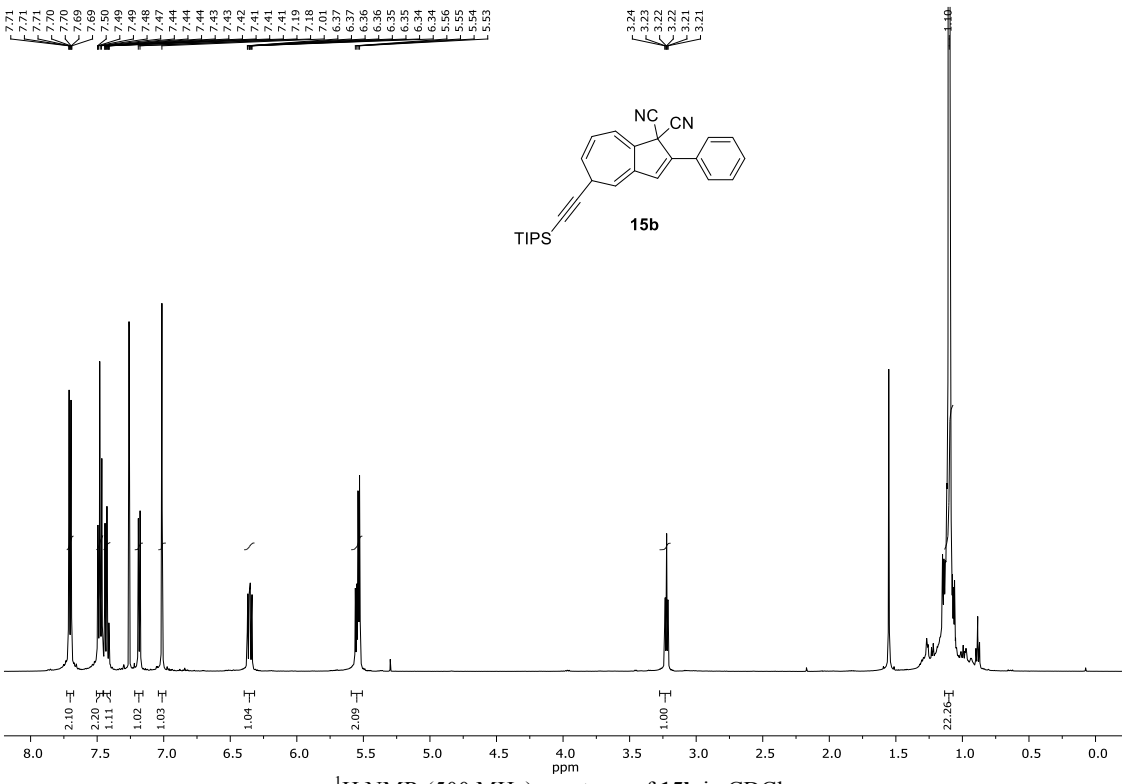


^{13}C APT NMR (125 MHz) spectrum of **15a** in $CDCl_3$

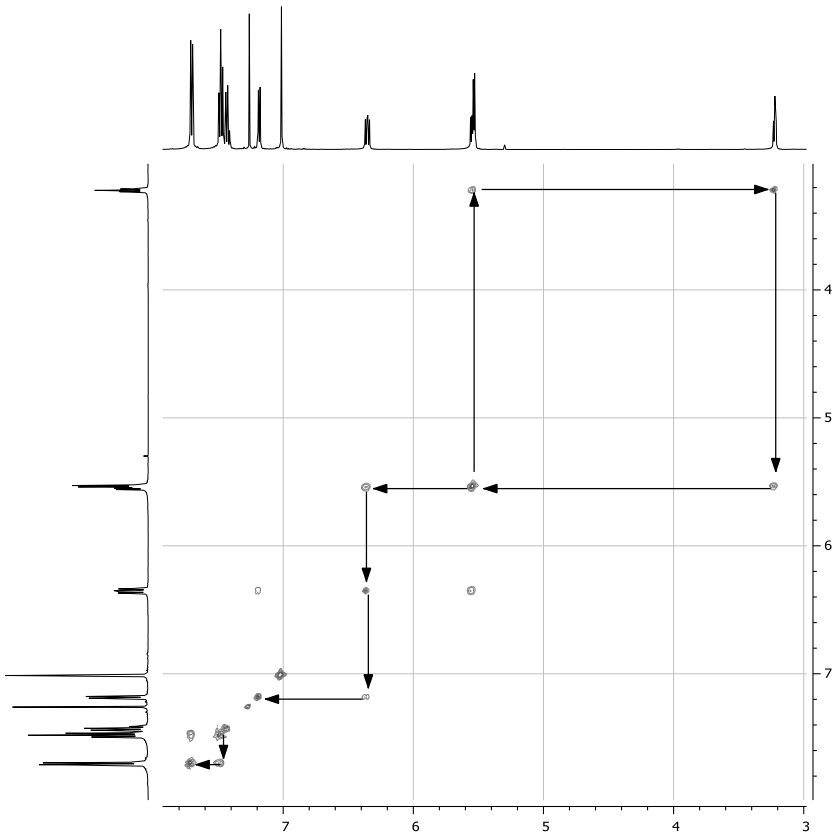


HMBC spectrum (500 MHz / 125 MHz) of 15a in $CDCl_3$

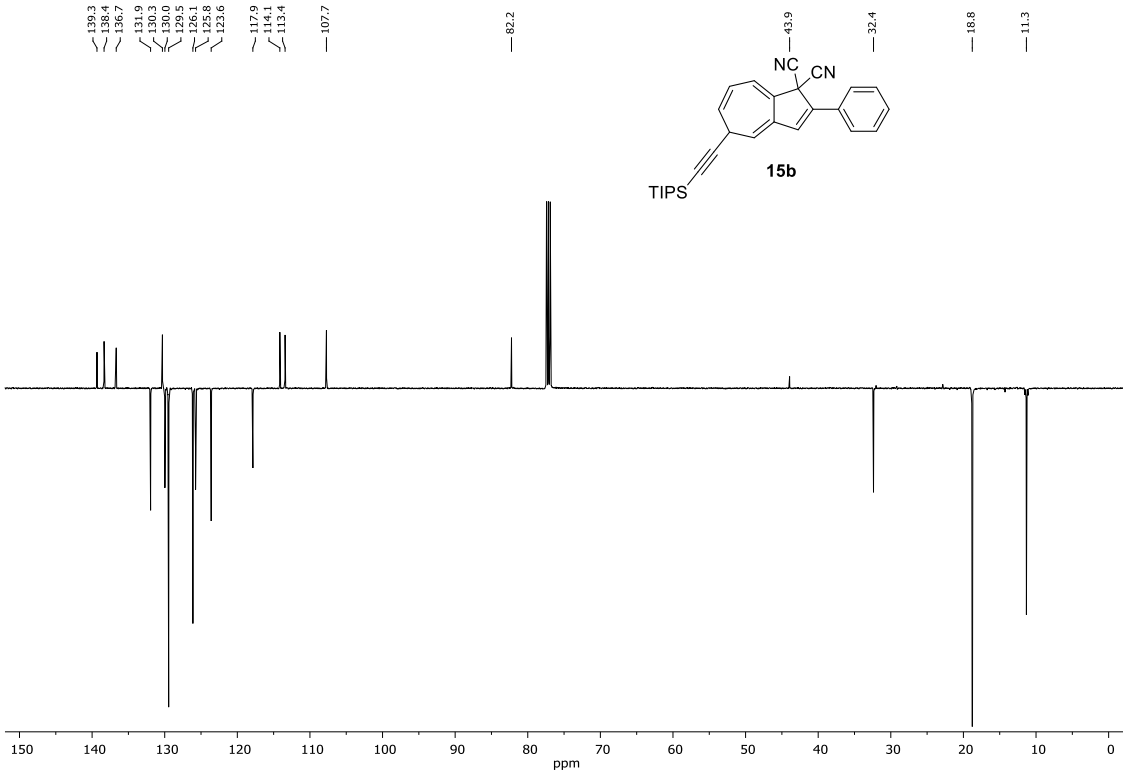
Compound 15b



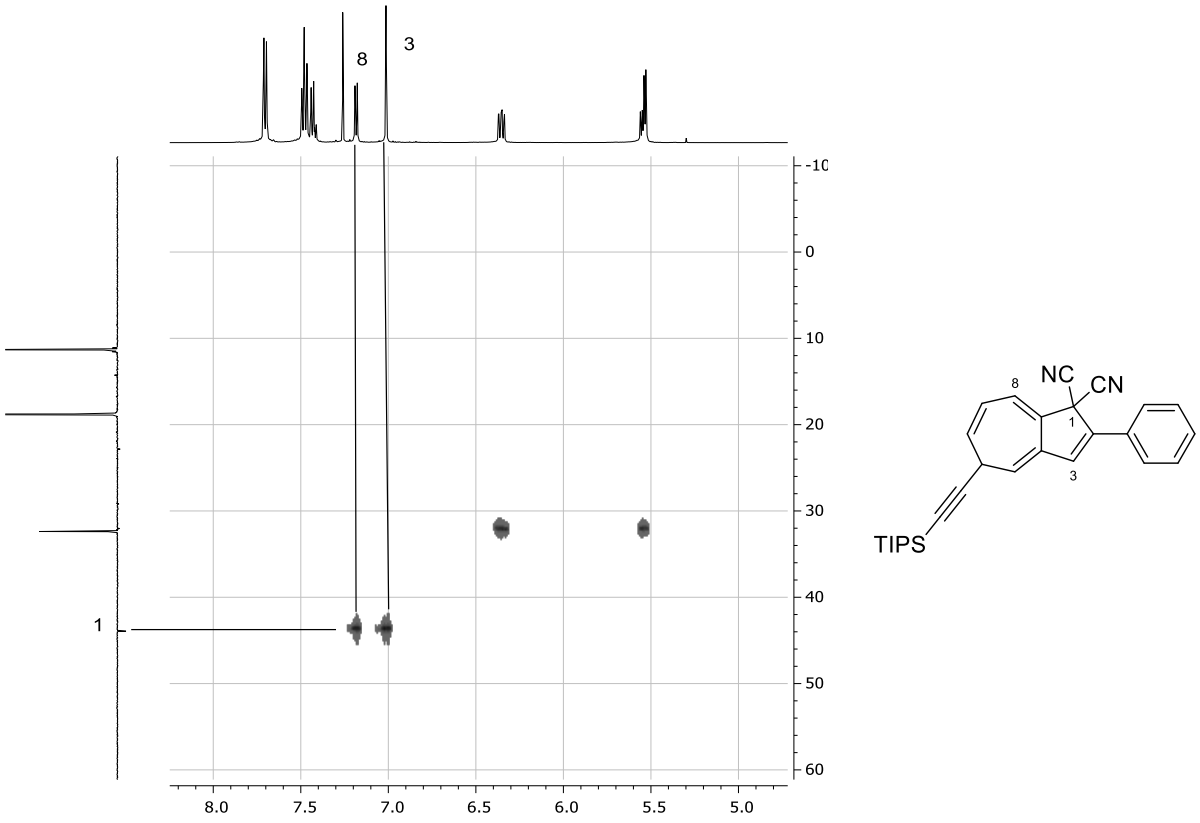
^{1}H NMR (500 MHz) spectrum of **15b** in $CDCl_3$



COSY spectrum (500 MHz) of **15b** in $CDCl_3$

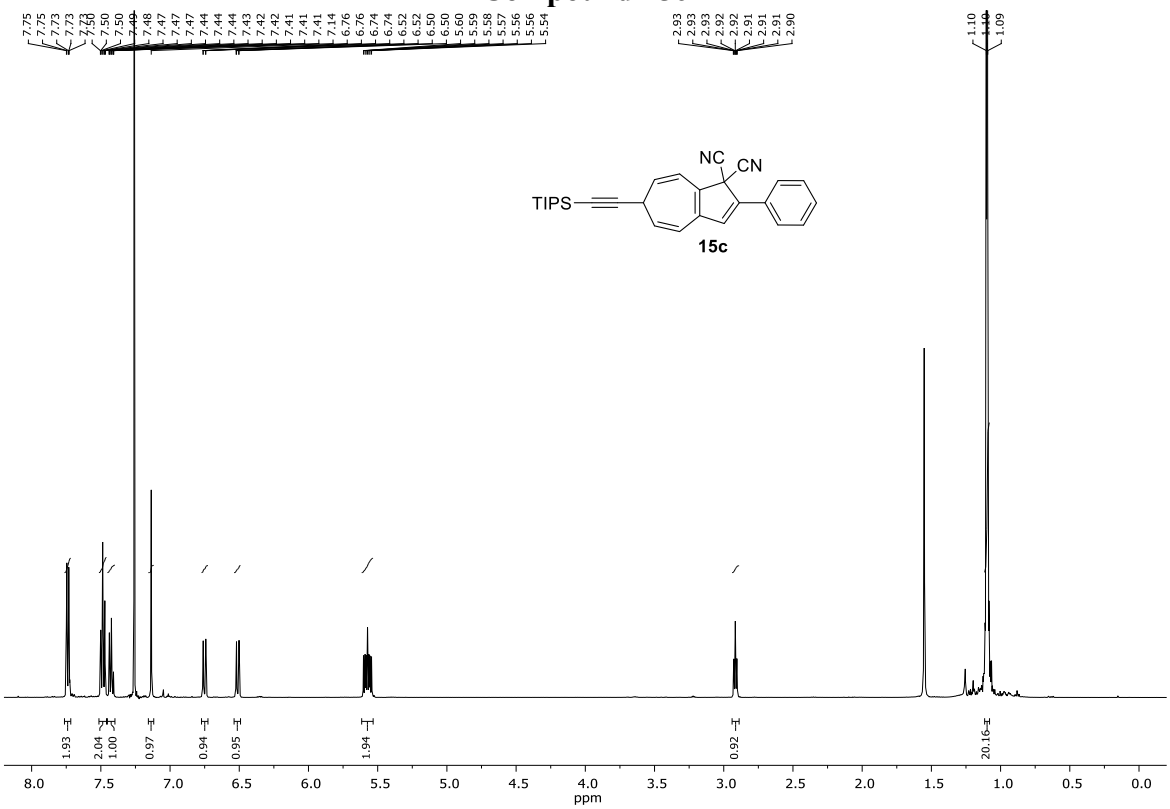


^{13}C NMR APT (125 MHz) spectrum of **15b** in $CDCl_3$

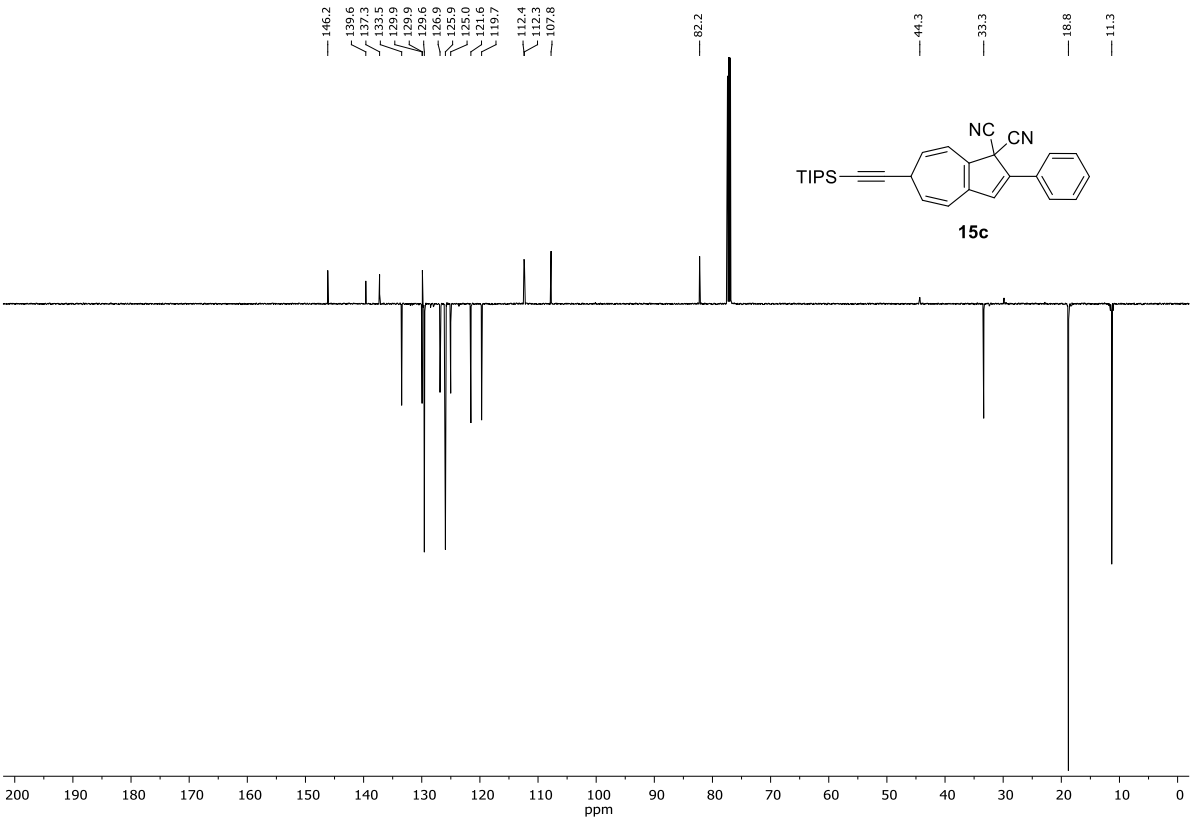


HMBC spectrum (500 MHz / 125 MHz) of **15b** in $CDCl_3$

Compound 15c

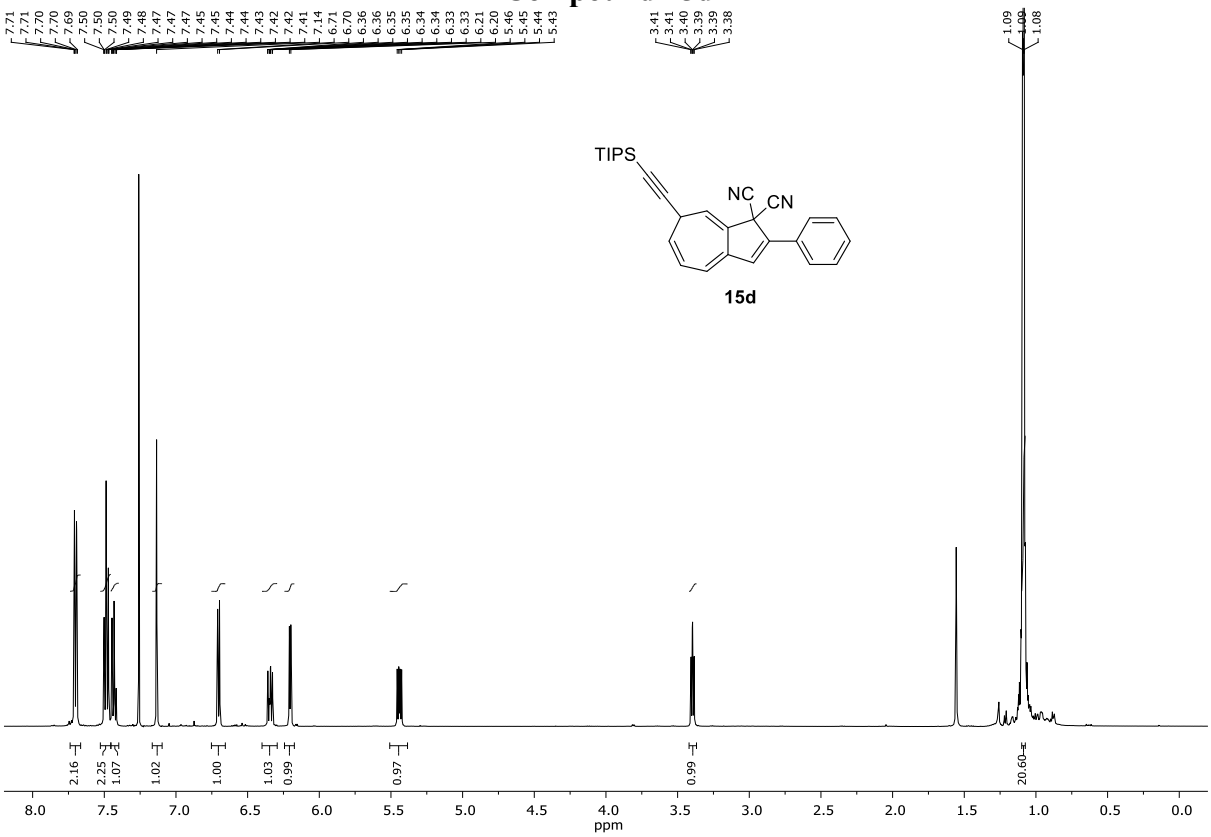


^{1}H NMR (500 MHz) spectrum of **15c** in $CDCl_3$

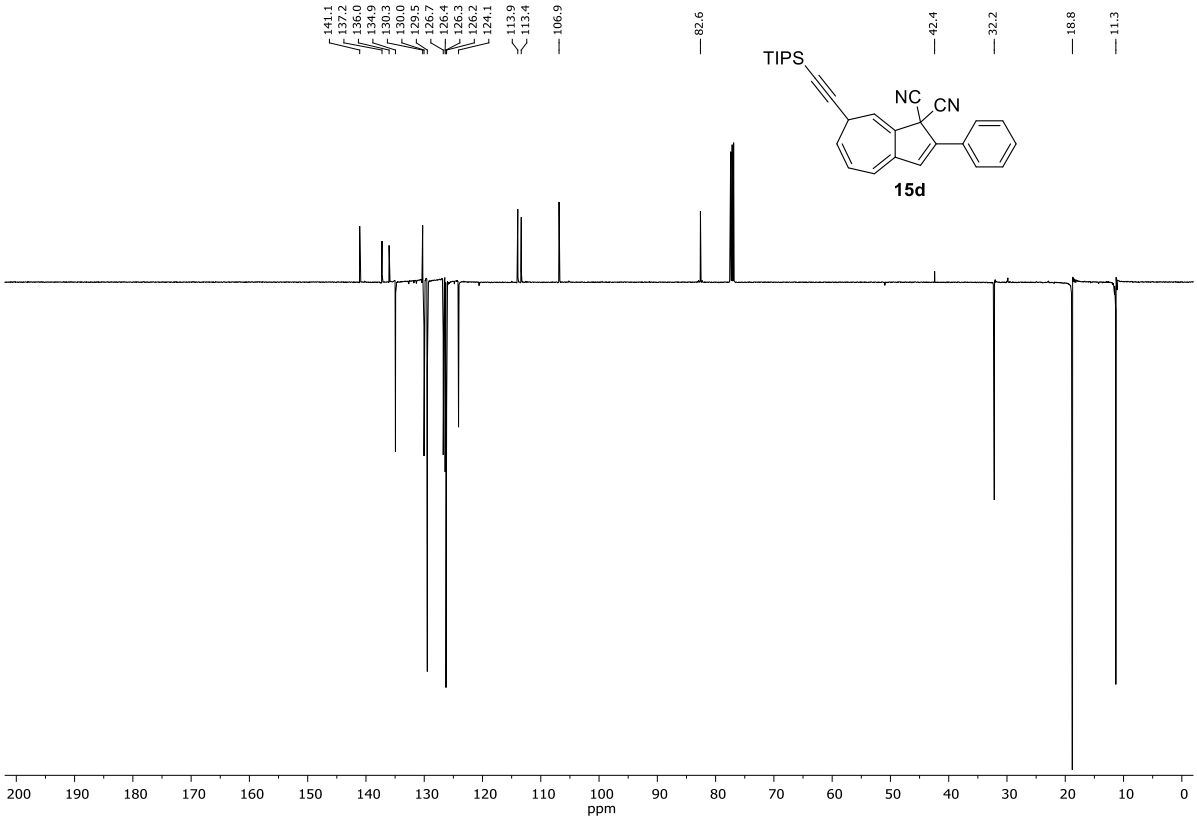


^{13}C NMR APT (125 MHz) spectrum of **15c** in $CDCl_3$

Compound 15d

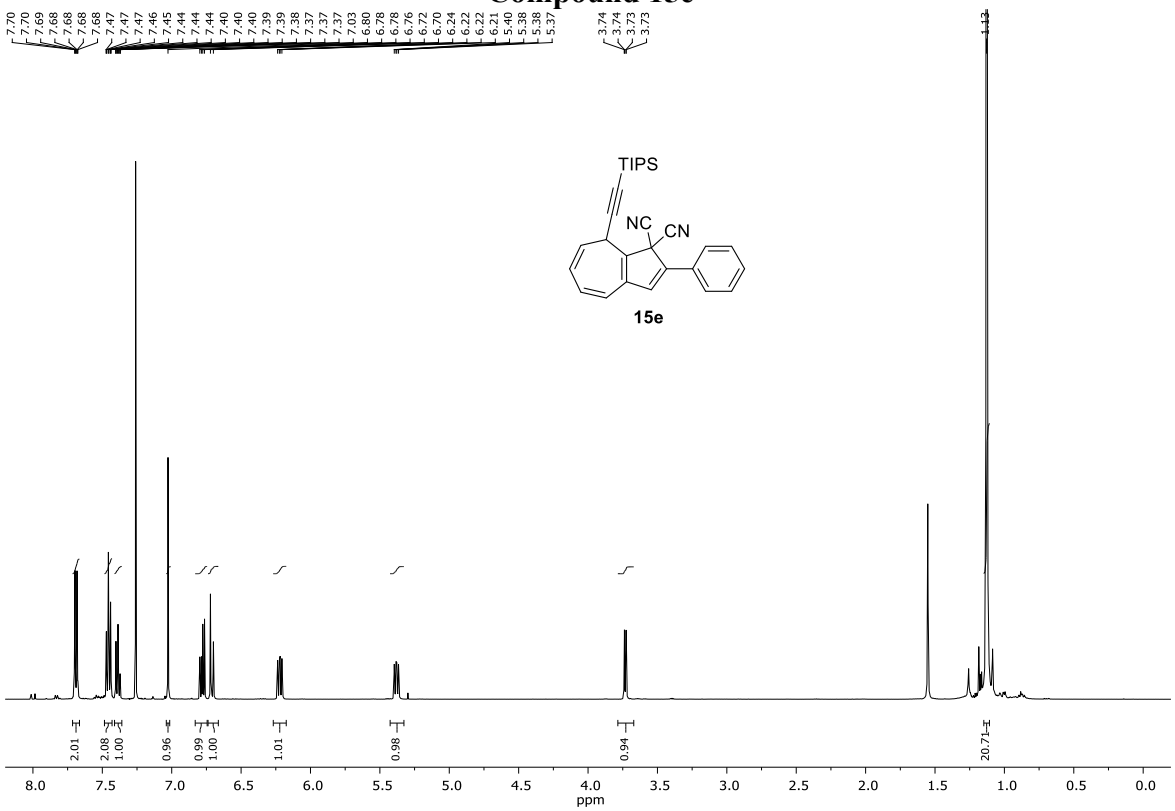


^{1}H NMR (500 MHz) spectrum of **15d** in $CDCl_3$

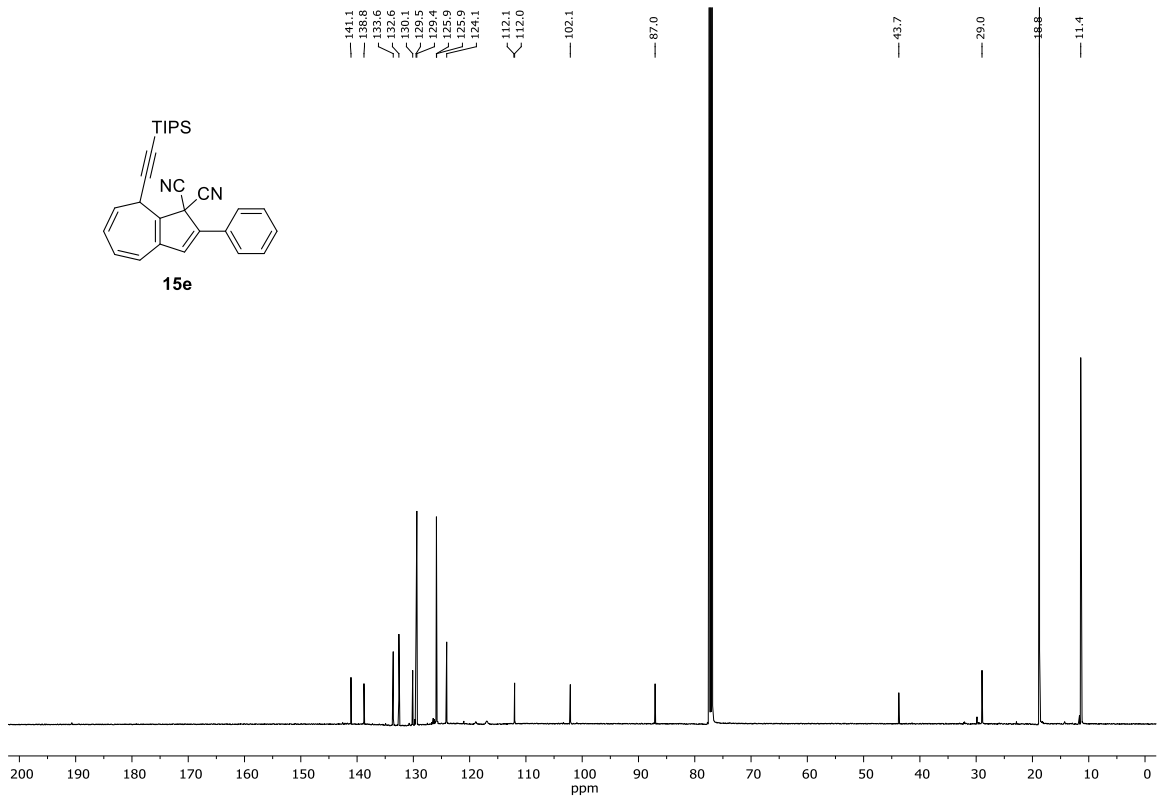


^{13}C NMR APT (125 MHz) spectrum of **15d** in $CDCl_3$

Compound 15e

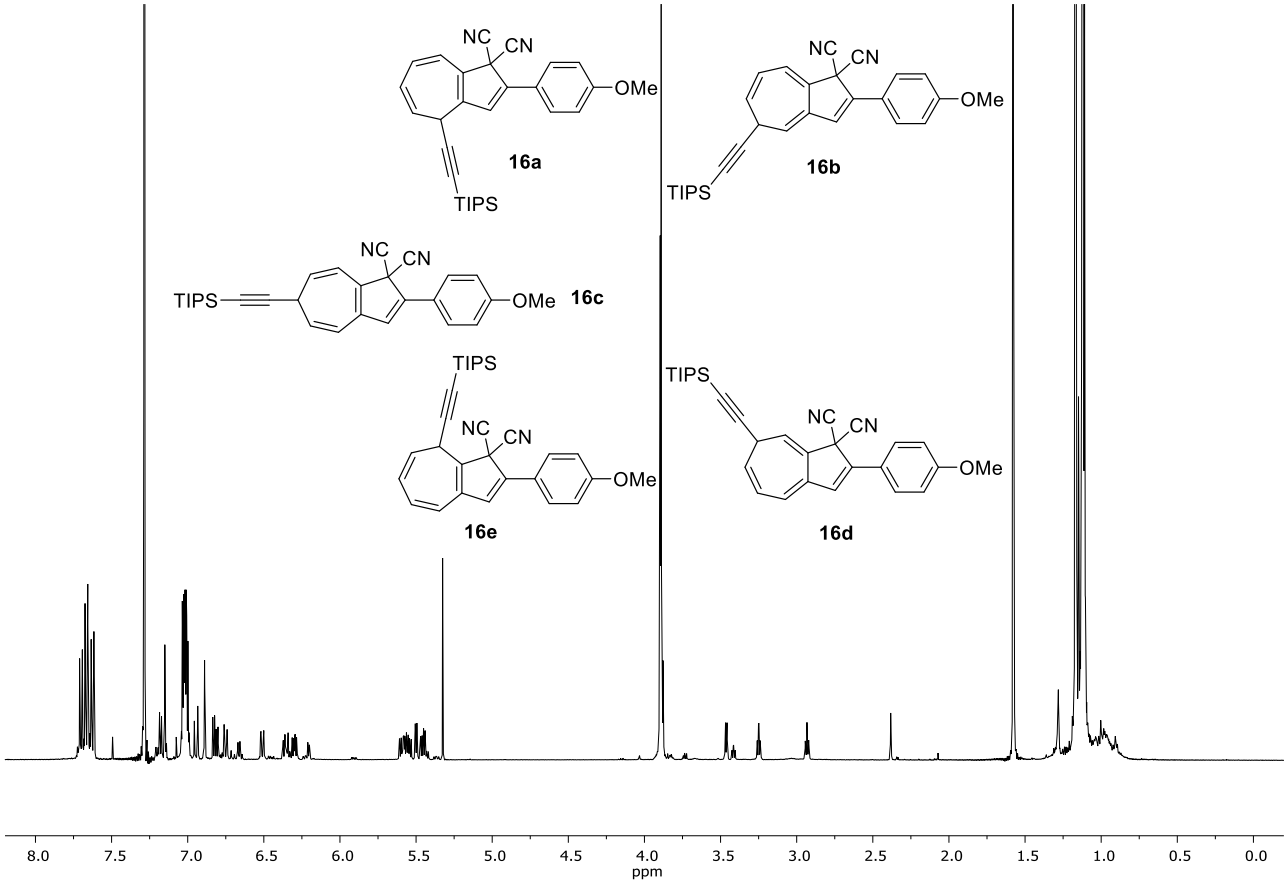


^{1}H NMR (500 MHz) spectrum of **15e** in $CDCl_3$

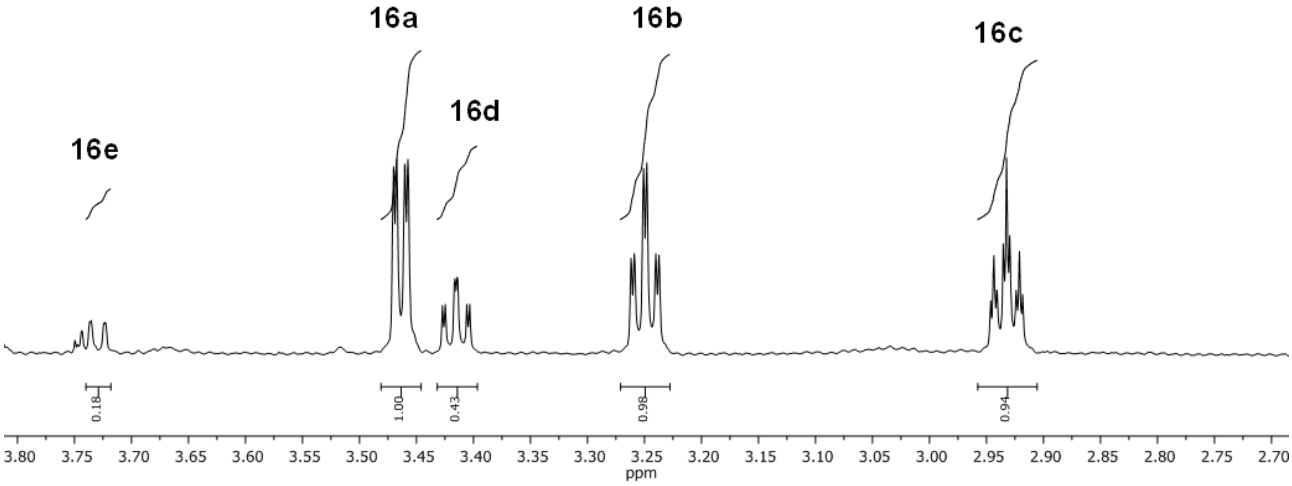


^{13}C NMR (125 MHz) spectrum of **15e** in $CDCl_3$

Regioisomeric mixture 16 (Table 3 Entry 2)

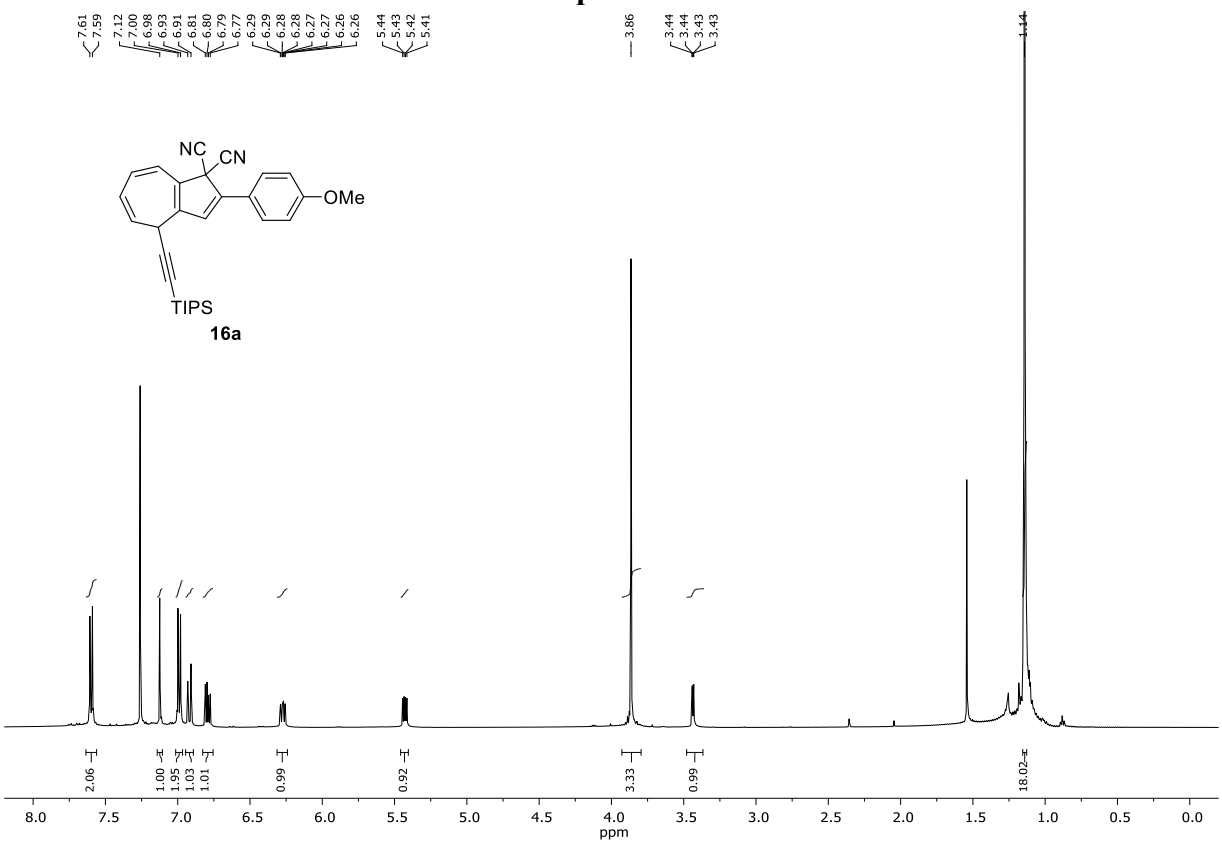


^{1}H NMR (500 MHz) spectrum of **16** in $CDCl_3$

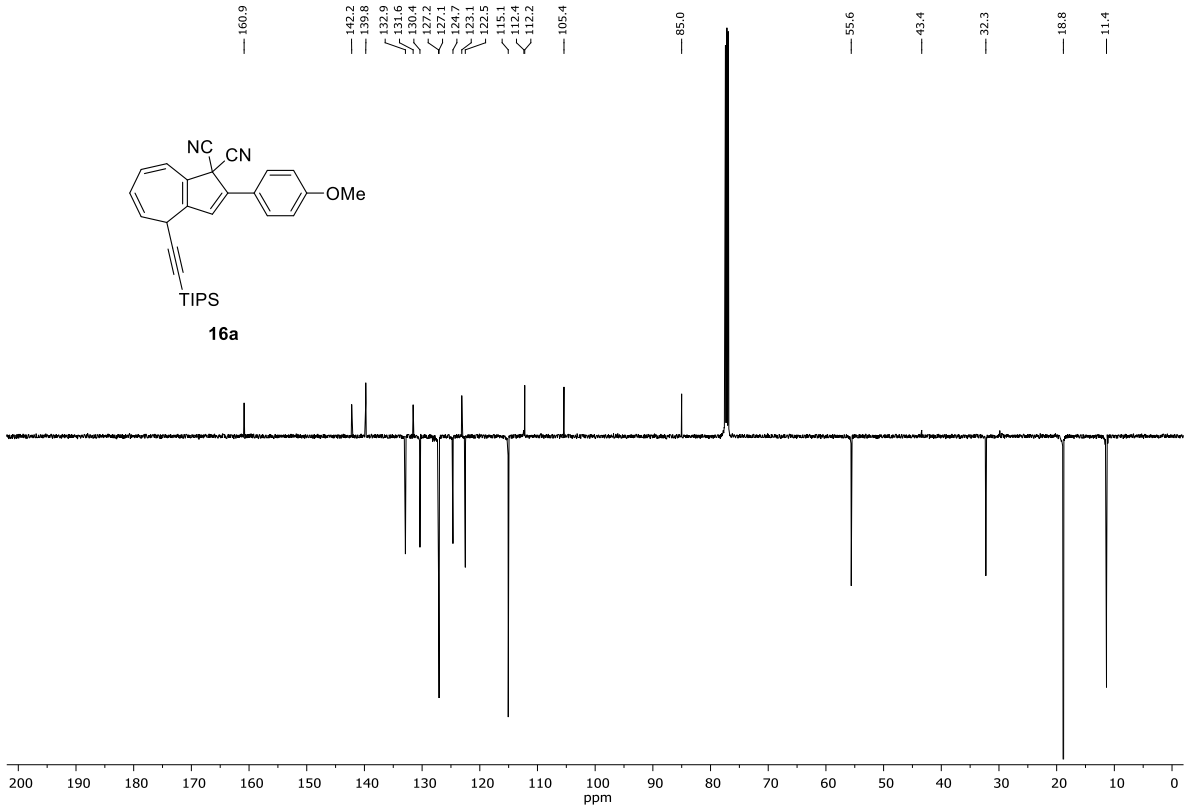


^{1}H NMR (500 MHz) spectrum of **16** in $CDCl_3$ zoomed into the sp^3 region for the point of nucleophilic attack

Compound 16a

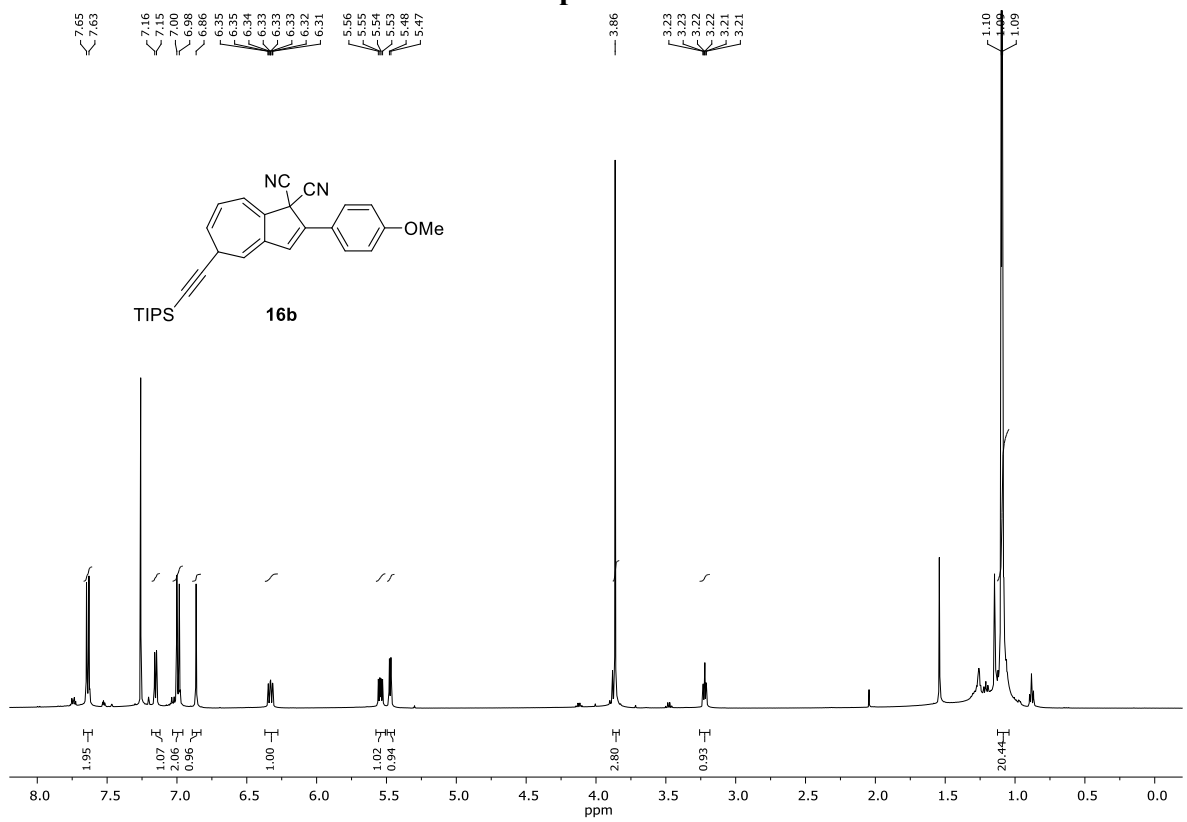


^{1}H NMR (500 MHz) spectrum of **16a** in $CDCl_3$

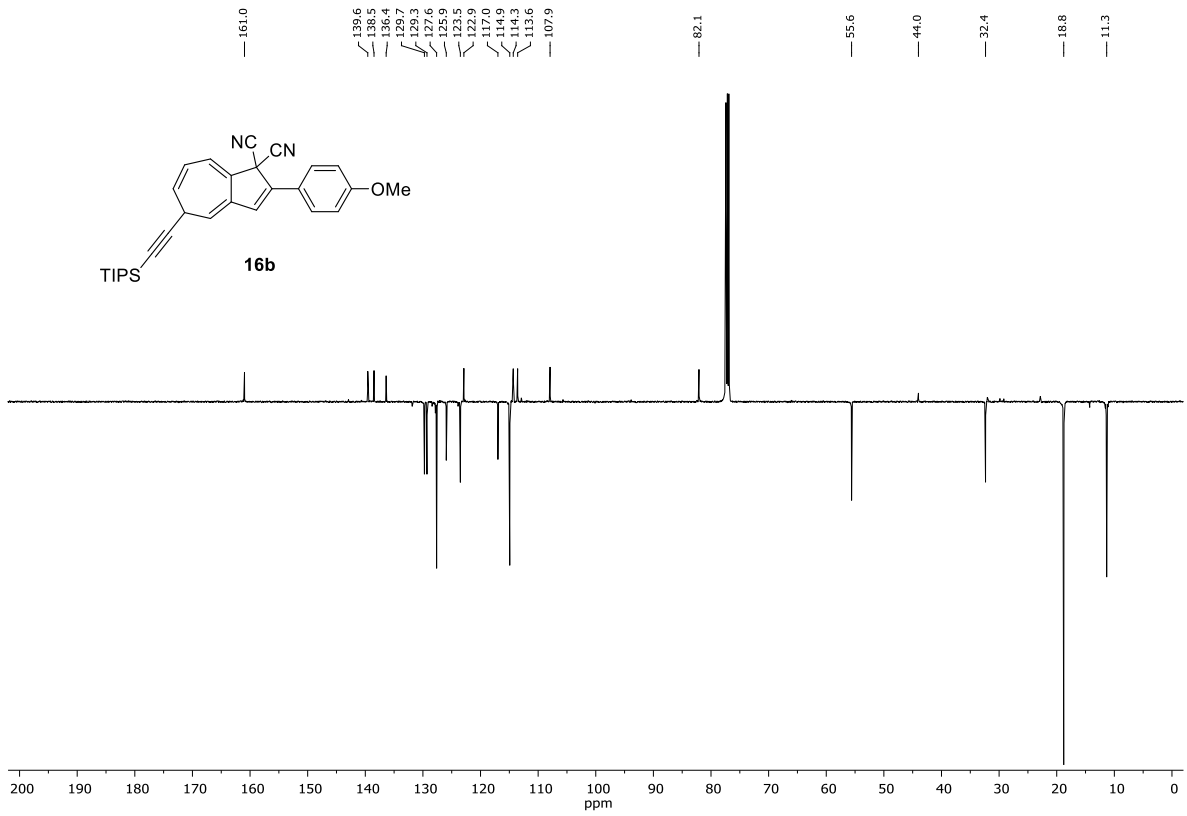


^{13}C NMR APT (125 MHz) spectrum of **16a** in $CDCl_3$

Compound 16b

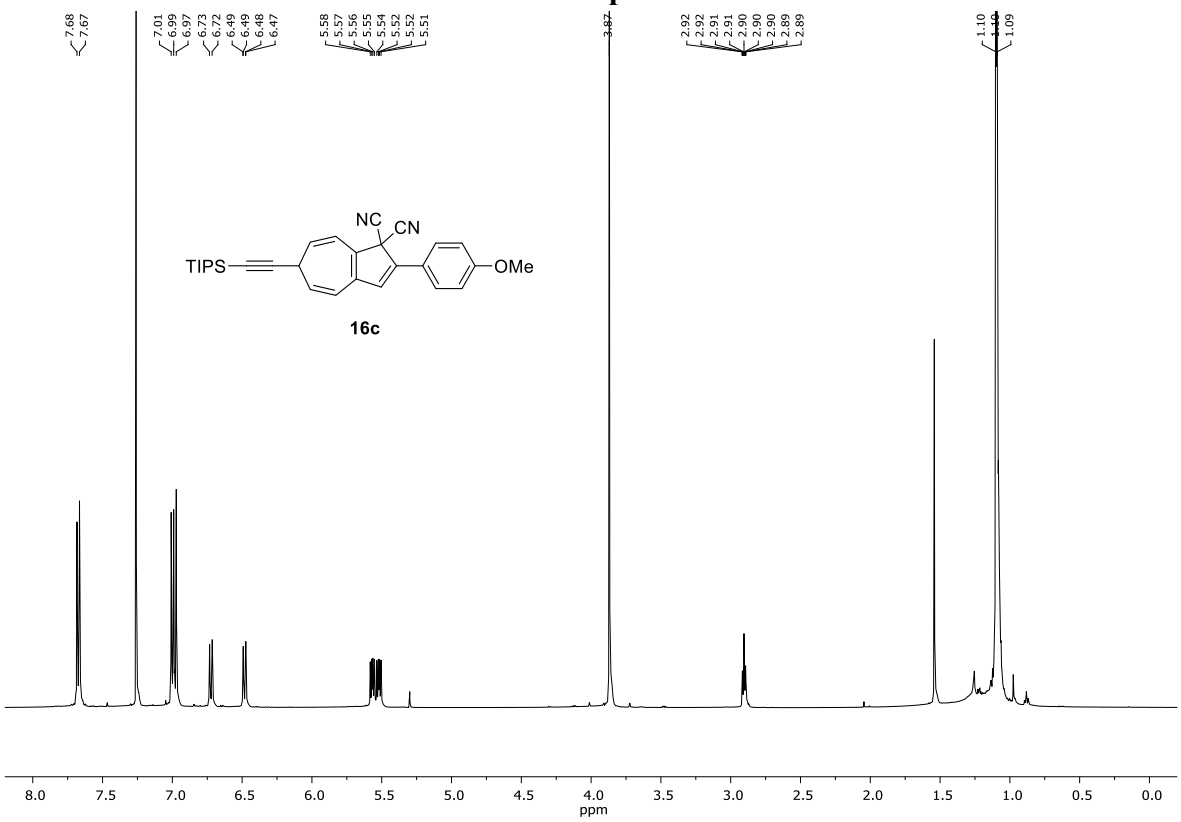


^{1}H NMR (500 MHz) spectrum of **16b** in $CDCl_3$

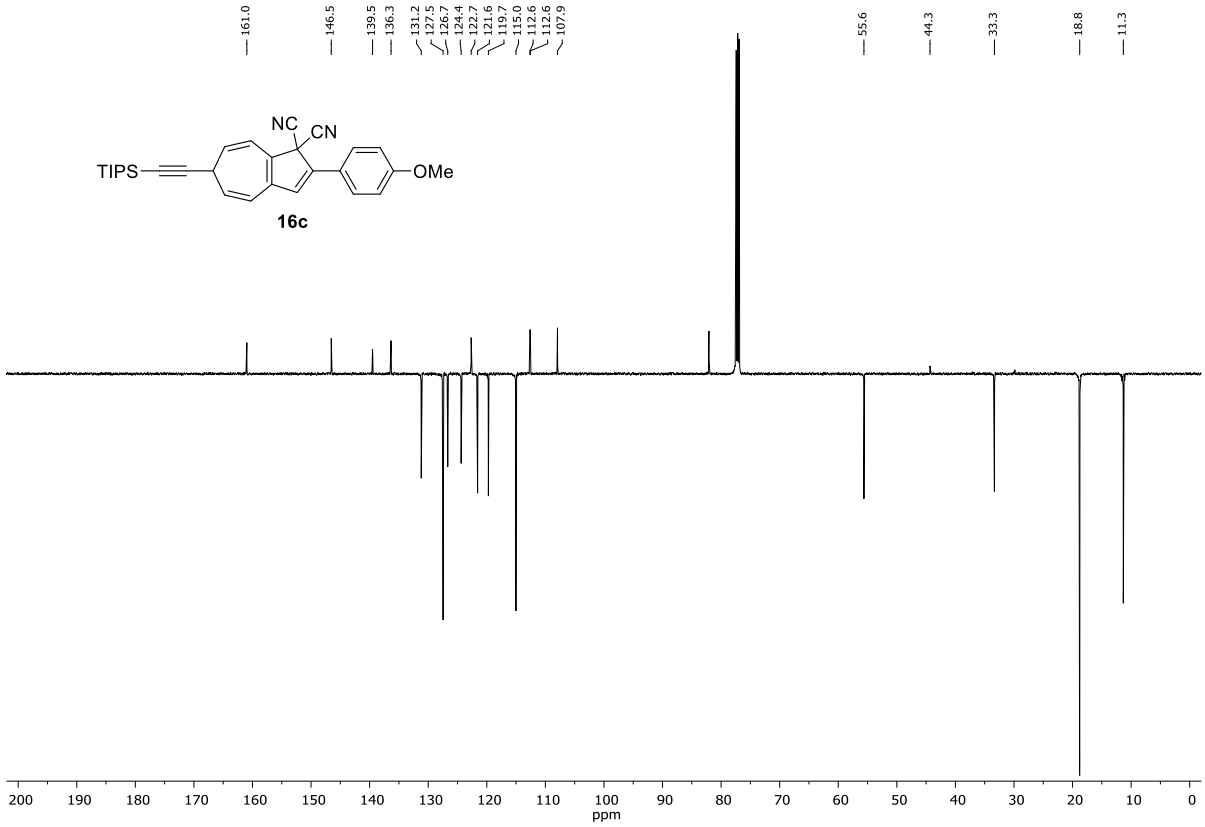


^{13}C NMR APT (125 MHz) spectrum of **16b** in $CDCl_3$

Compound 16c

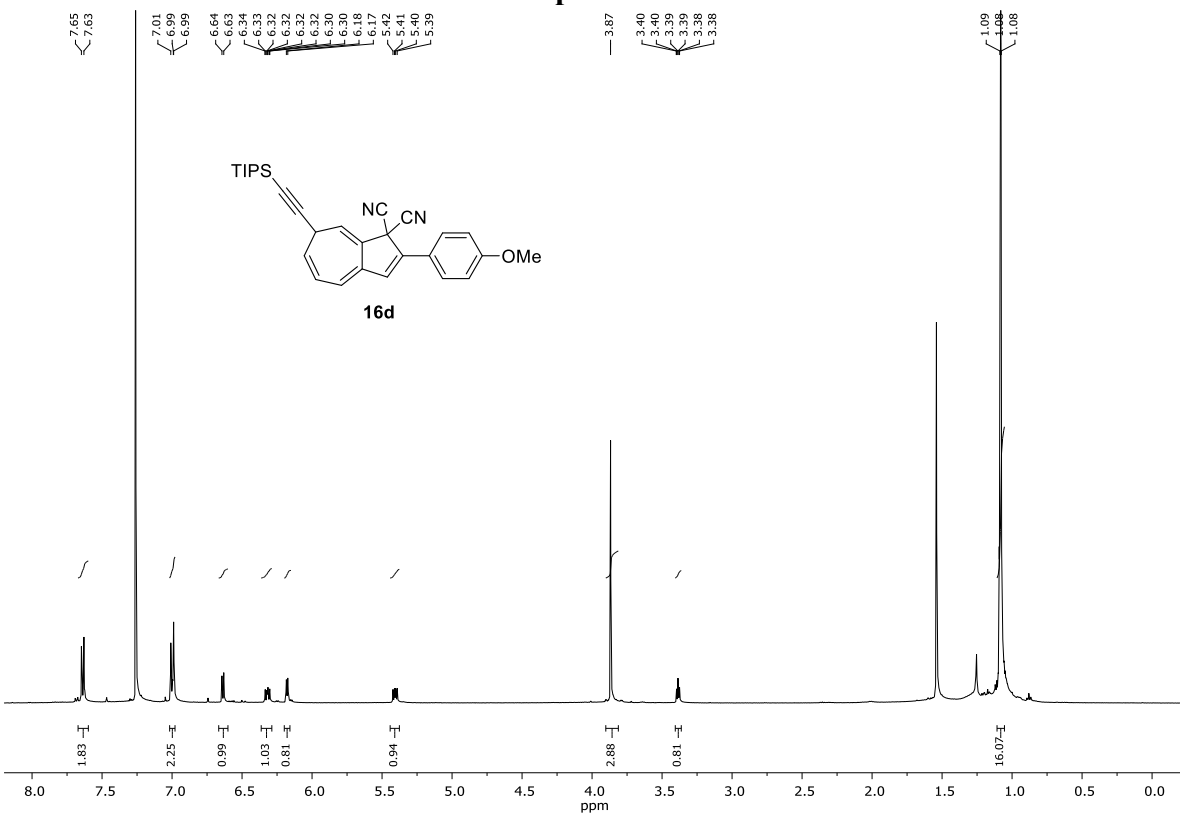


^{1}H NMR (500 MHz) spectrum of **16c** in $CDCl_3$

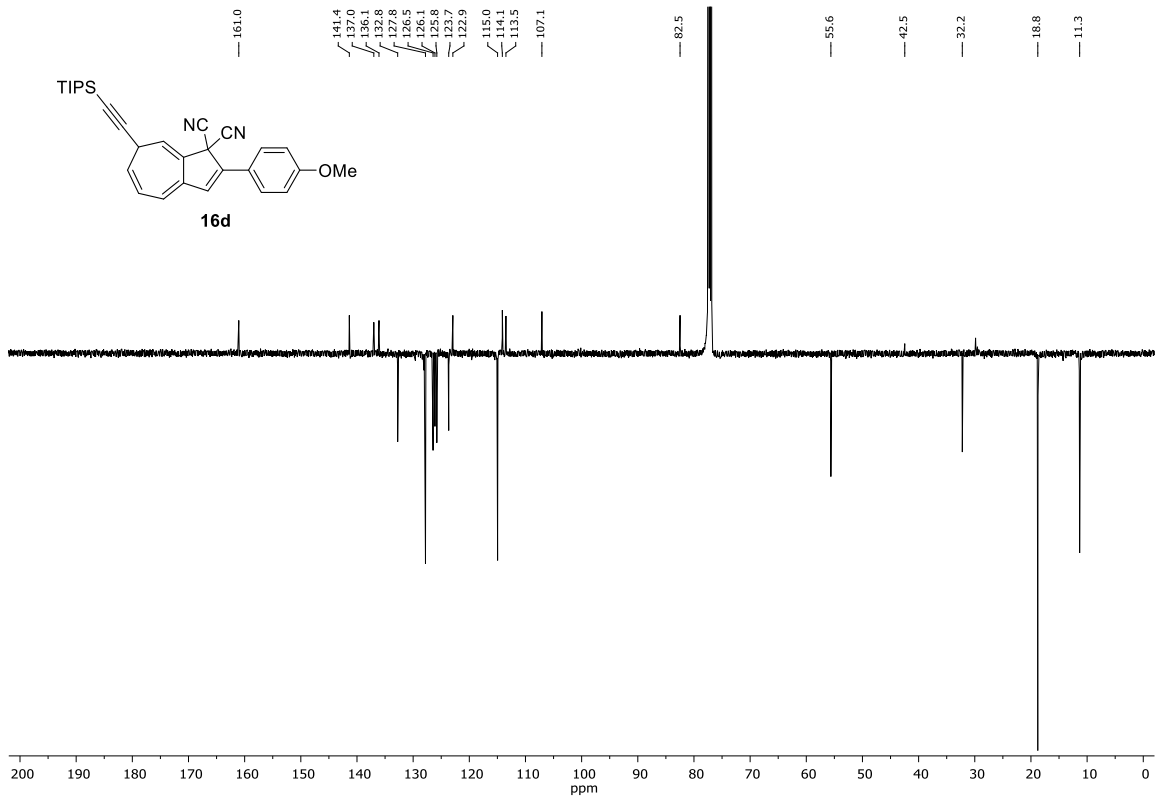


^{13}C NMR APT (125 MHz) spectrum of **16c** in $CDCl_3$

Compound 16d

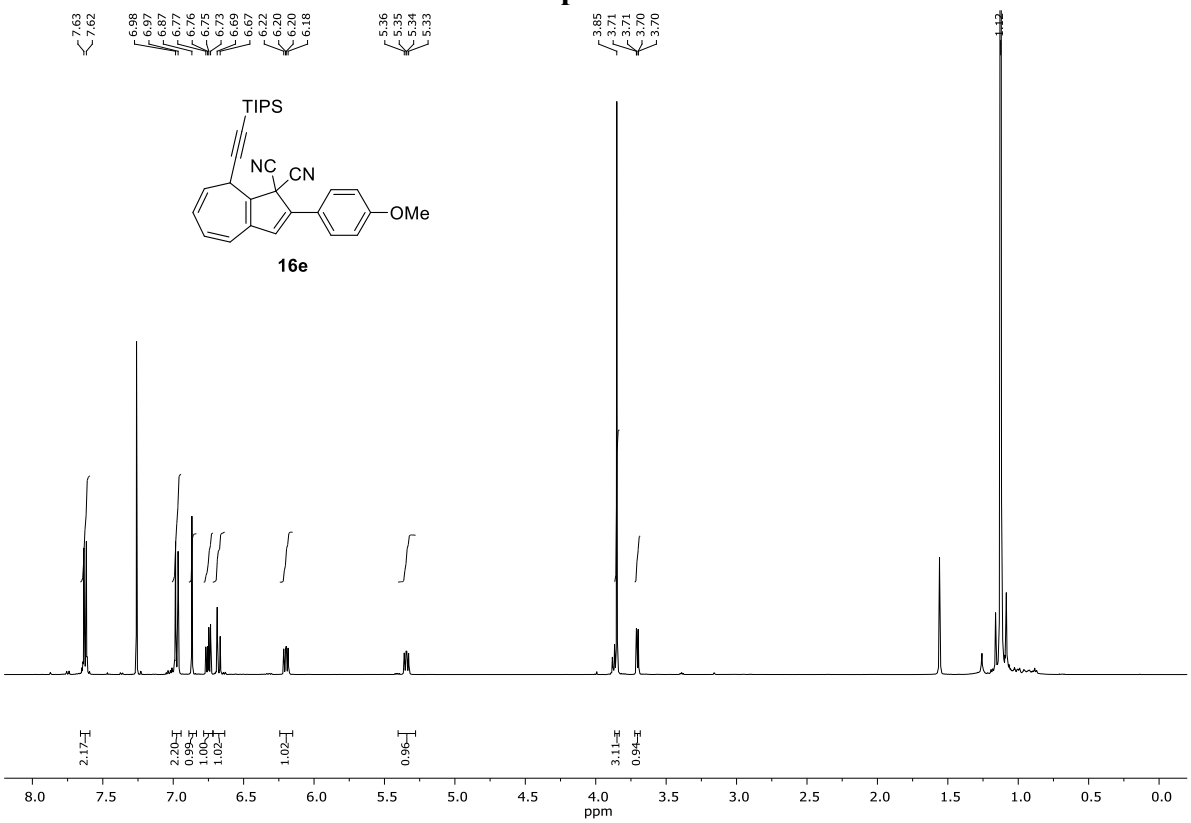


^{1}H NMR (500 MHz) spectrum of **16d** in $CDCl_3$

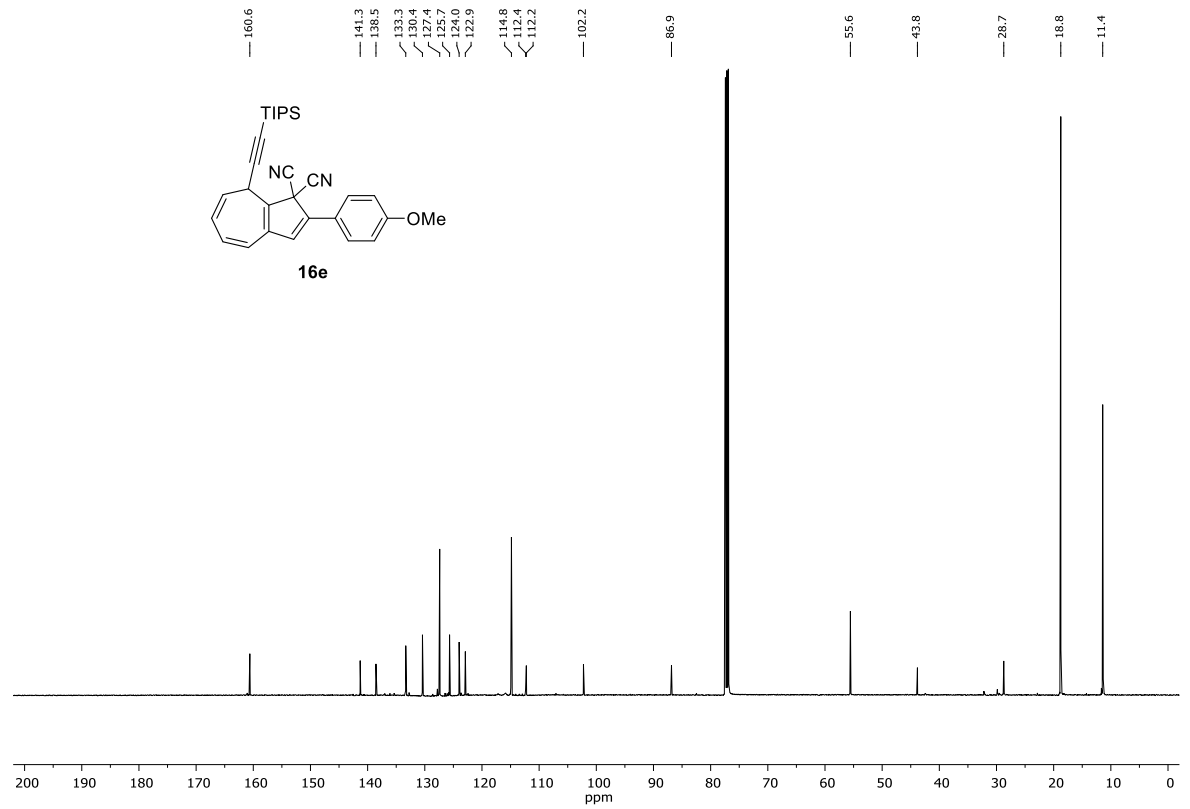


^{13}C NMR APT (125 MHz) spectrum of **16d** in $CDCl_3$

Compound 16e

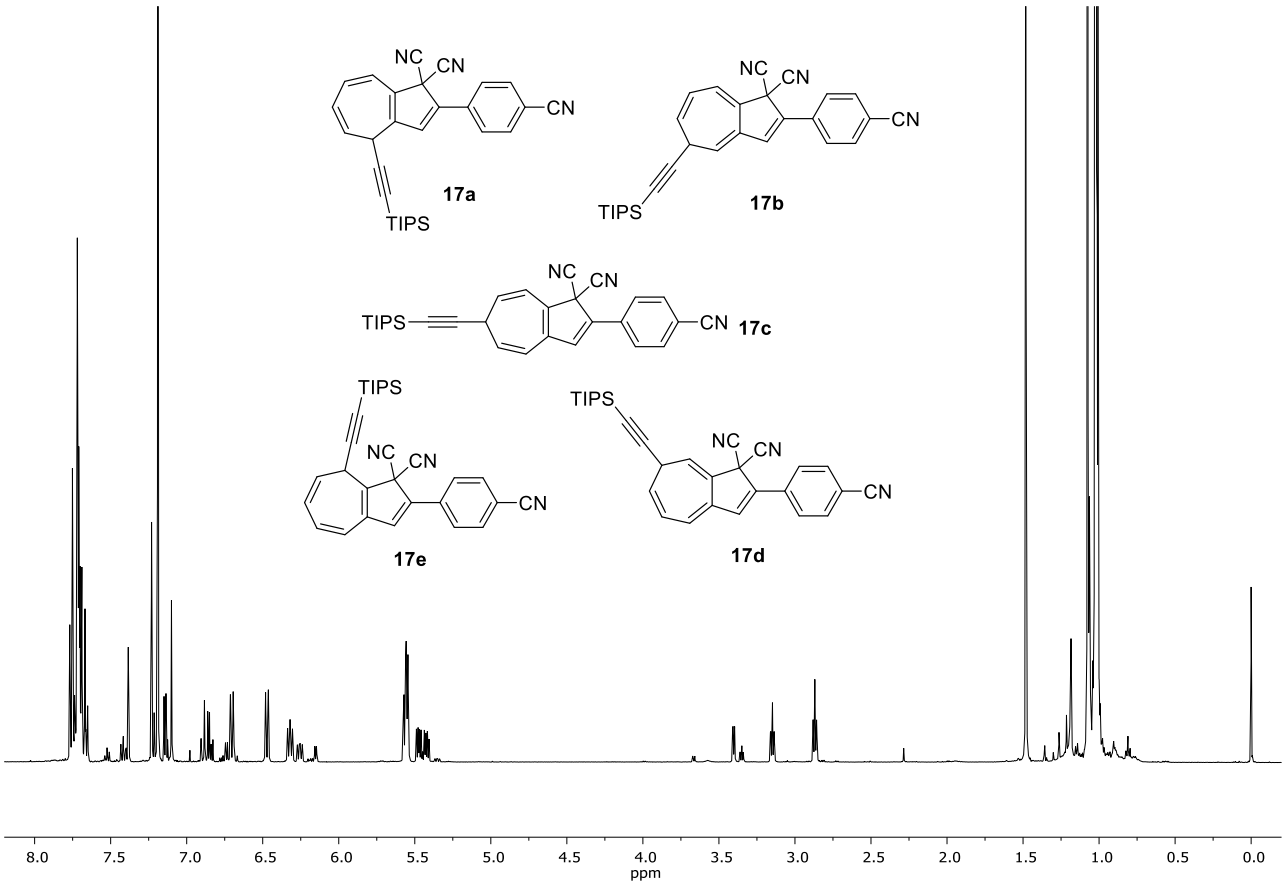


^{1}H NMR (500 MHz) spectrum of **16e** in $CDCl_3$

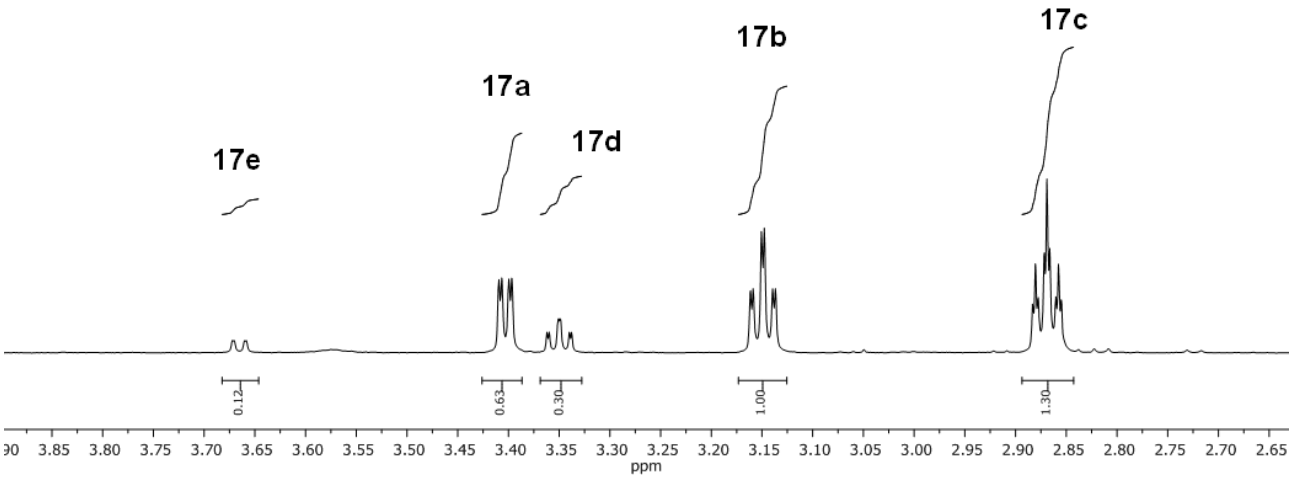


^{13}C NMR (125 MHz) spectrum of **16e** in $CDCl_3$

Regioisomeric mixture 17 (Table 3 Entry 3)

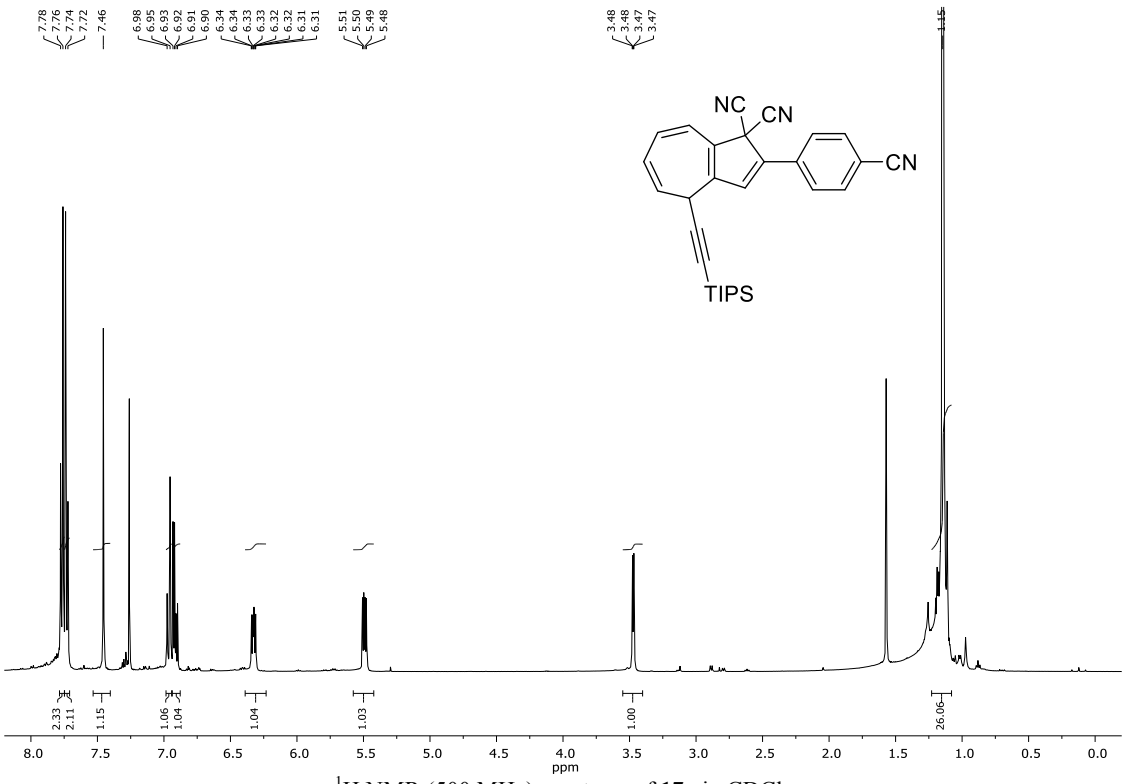


^{1}H NMR (500 MHz) spectrum of **17** in $CDCl_3$

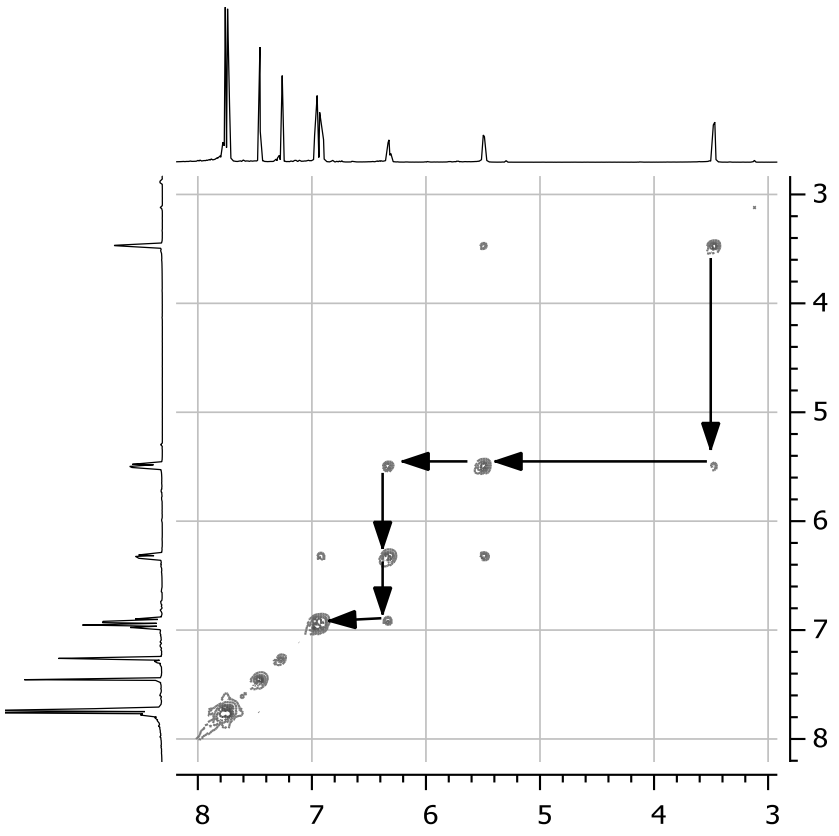


^{1}H NMR (500 MHz) spectrum of **17** in $CDCl_3$ zoomed into the sp^3 region for the point of nucleophilic attack

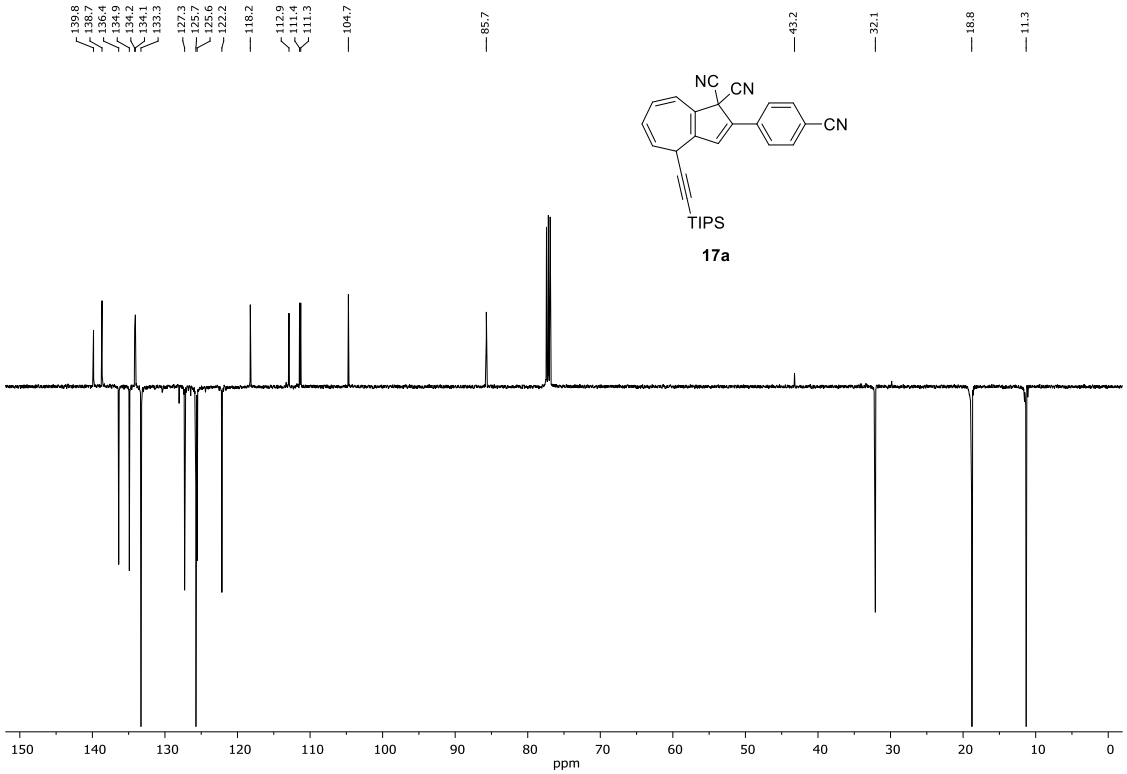
Compound 17a



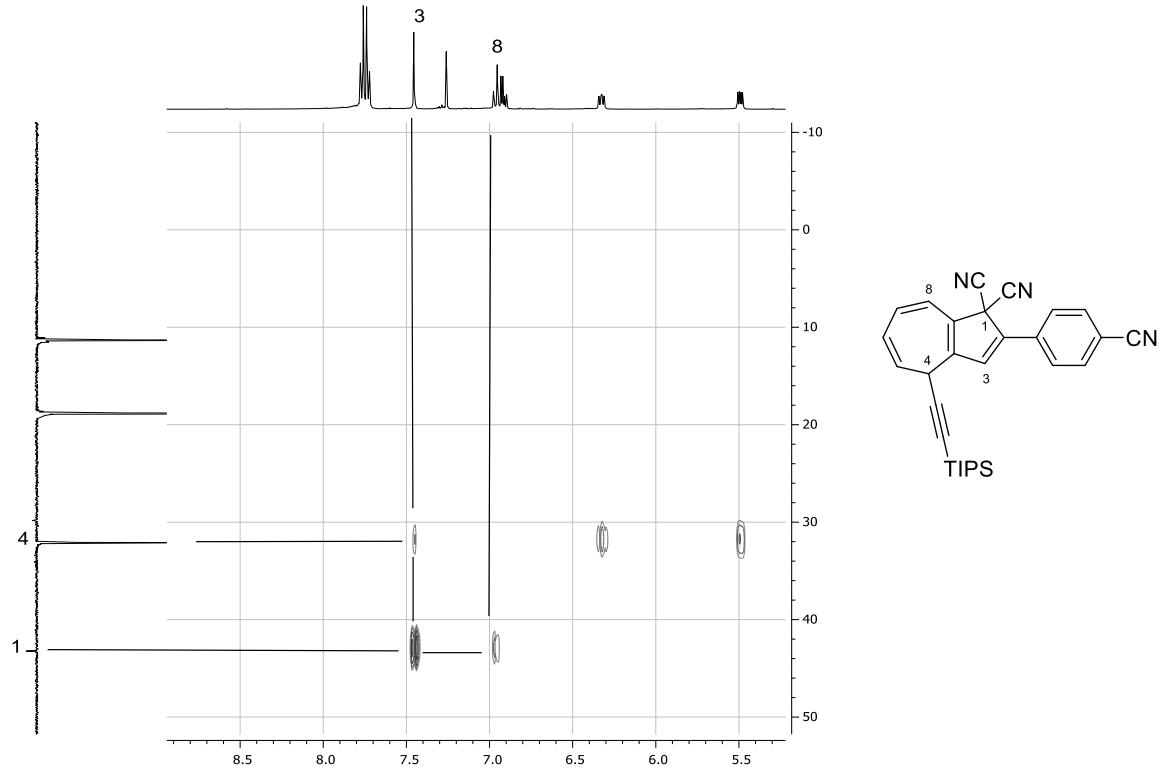
^{1}H NMR (500 MHz) spectrum of **17a** in $CDCl_3$



COSY spectrum (500 MHz) of **17a** in $CDCl_3$.

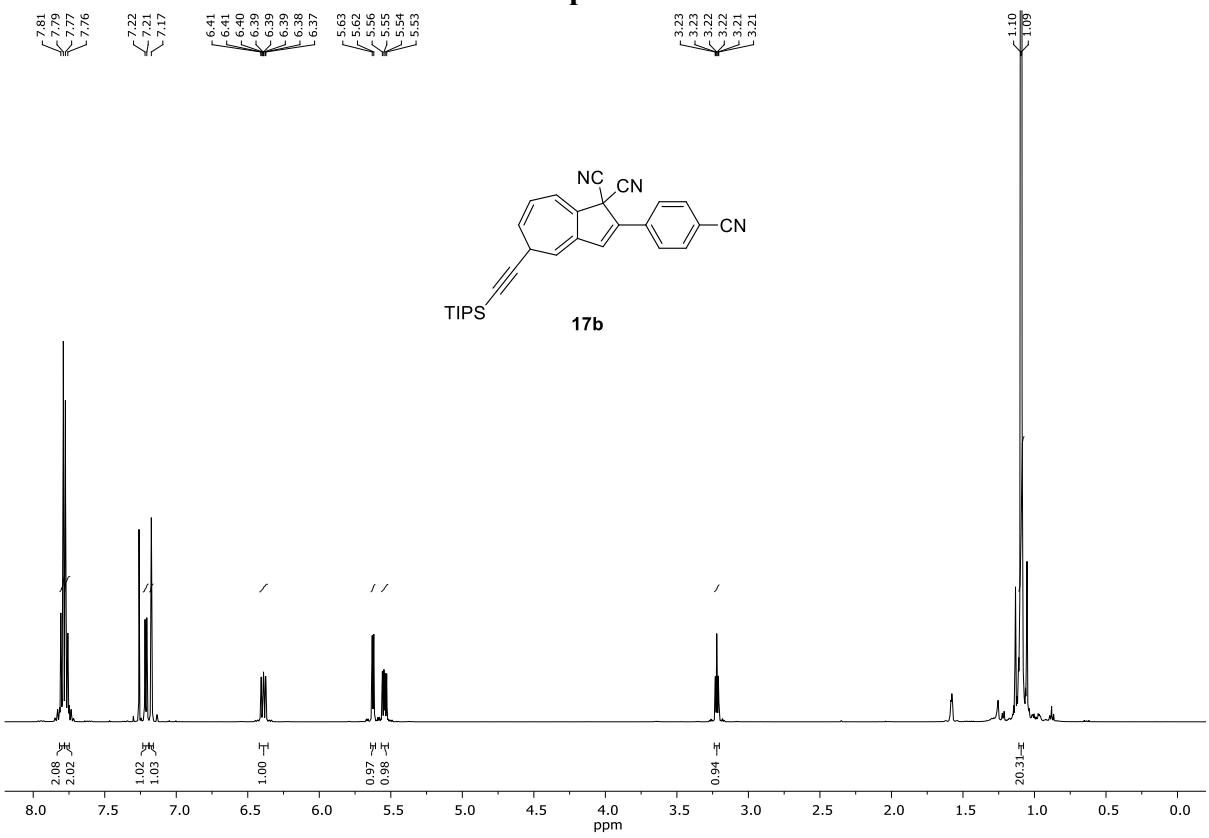


^{13}C APT NMR (125 MHz) spectrum of **17a** in $CDCl_3$

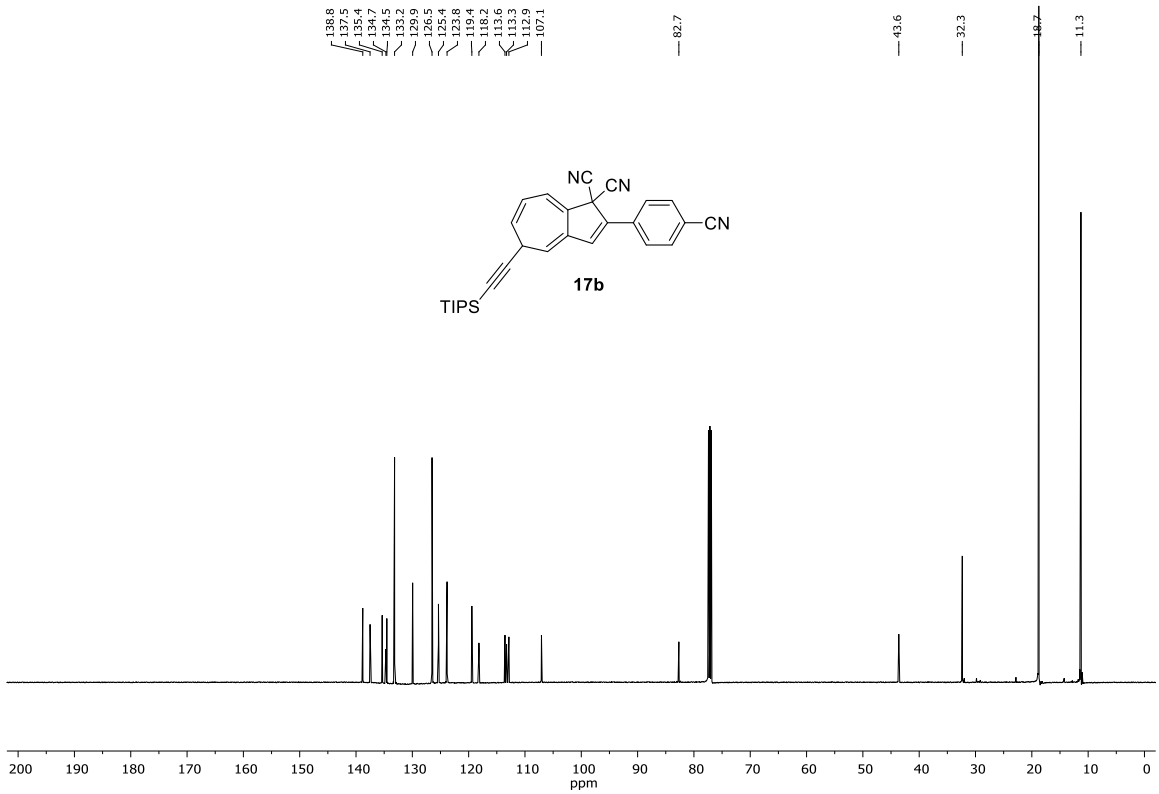


HMBC spectrum (500 MHz / 125 MHz) of **17a** in $CDCl_3$

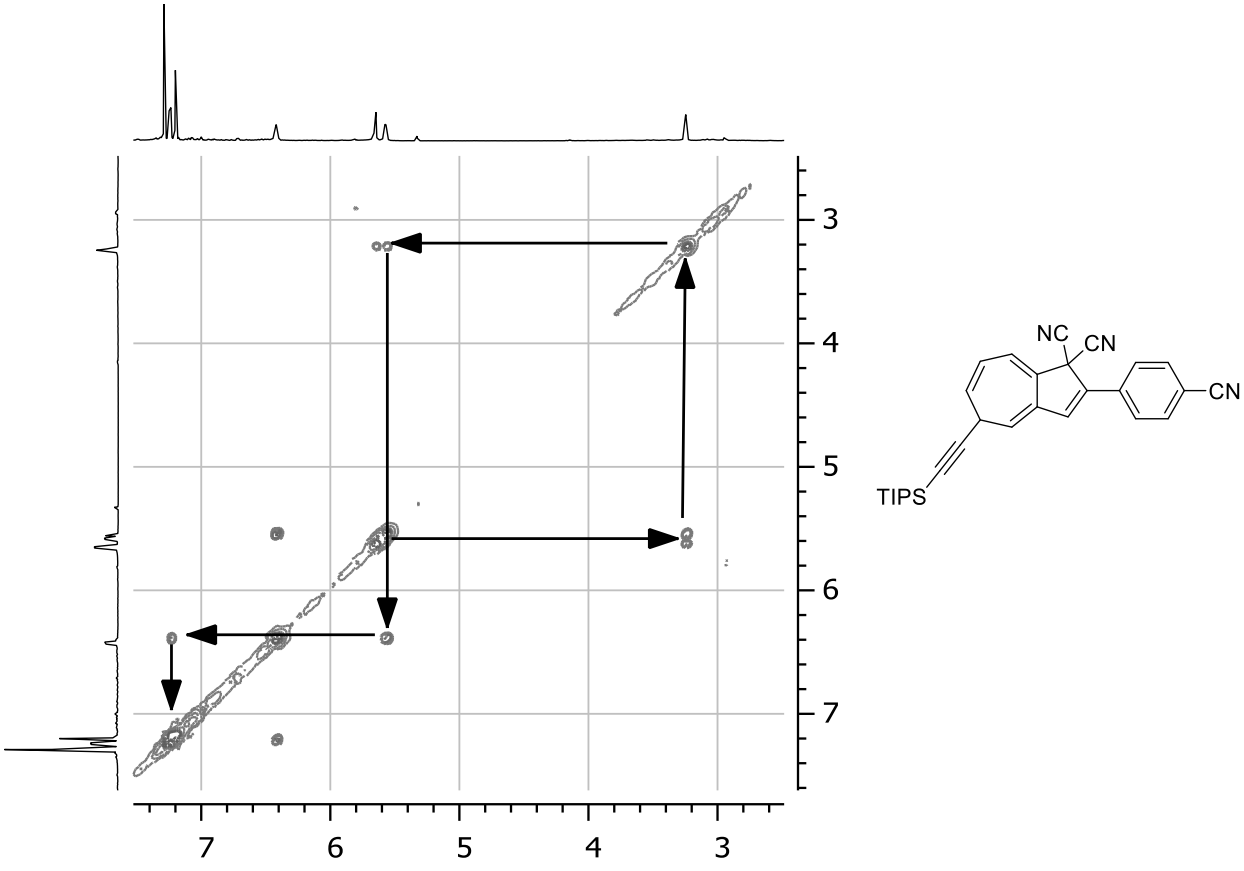
Compound 17b



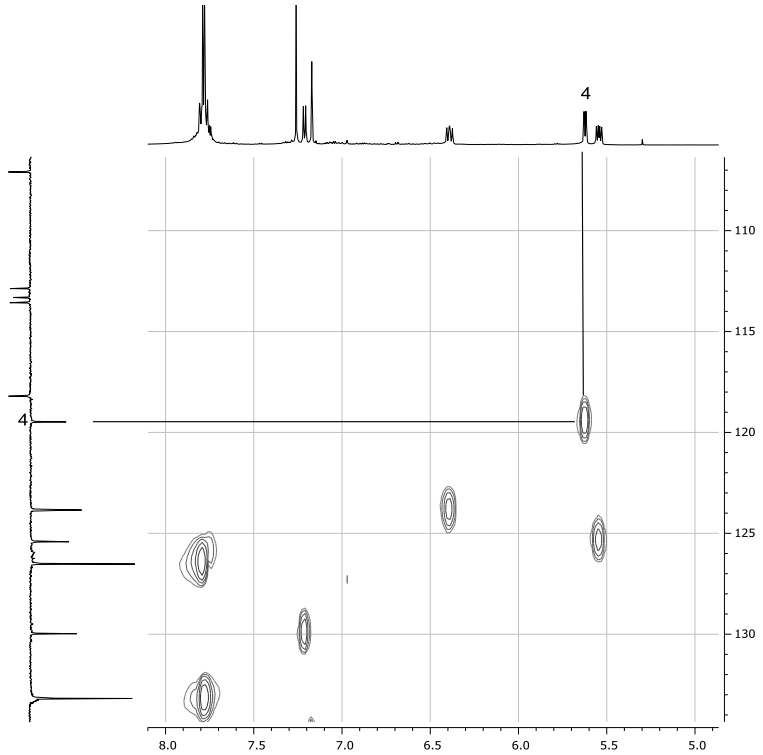
^{1}H NMR (500 MHz) spectrum of **17b** in $CDCl_3$



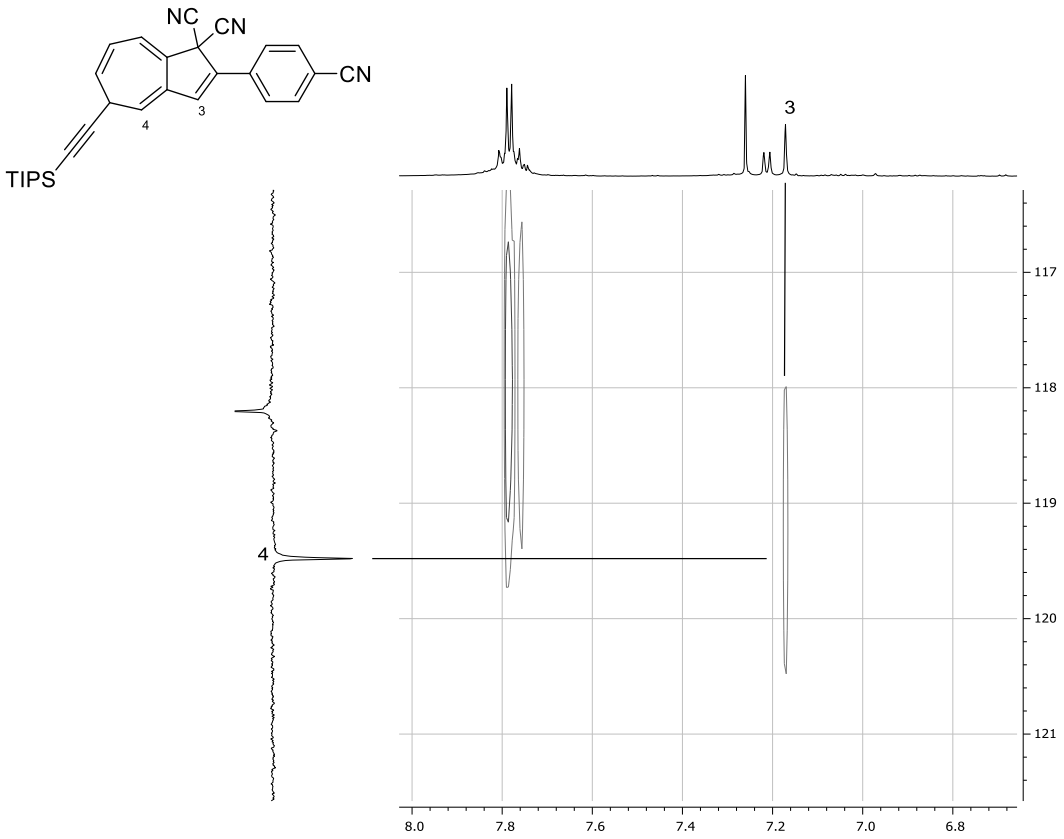
^{13}C NMR (125 MHz) spectrum of **17b** in $CDCl_3$



COSY spectrum (500 MHz) of **17b** in $CDCl_3$

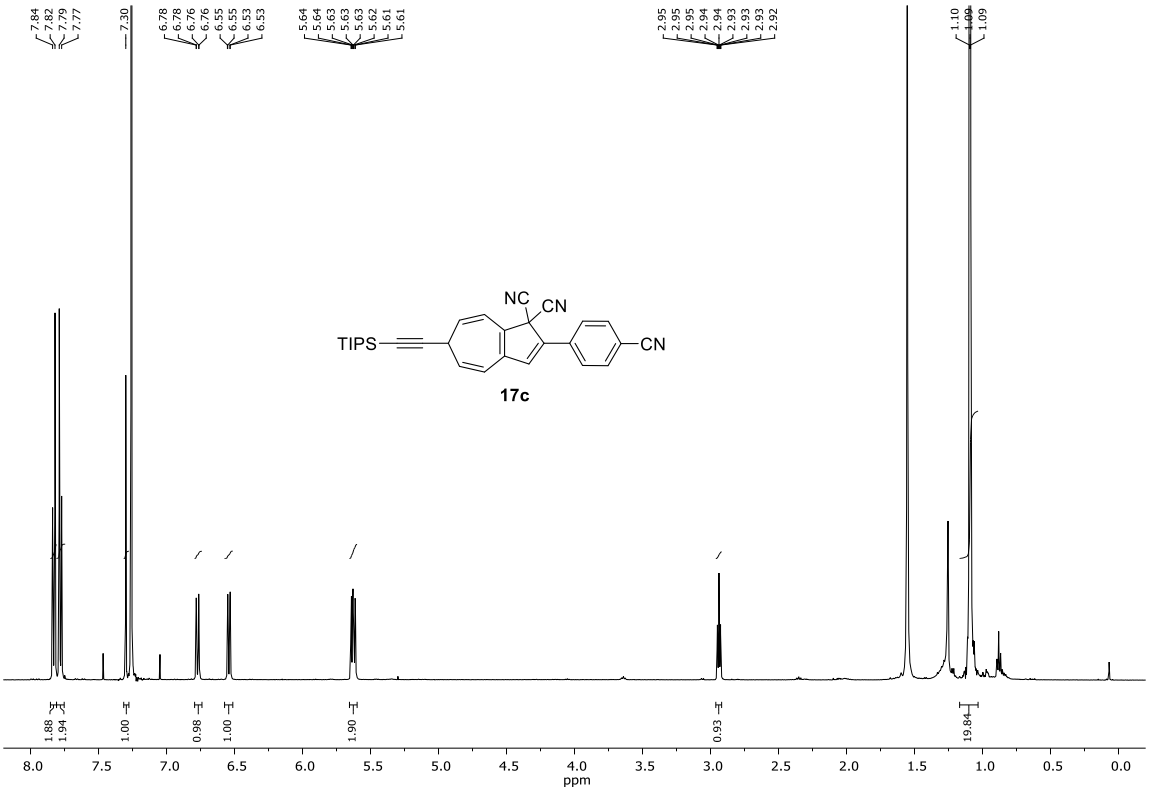


HSQC spectrum (500 MHz / 125 MHz) of **17b** in $CDCl_3$

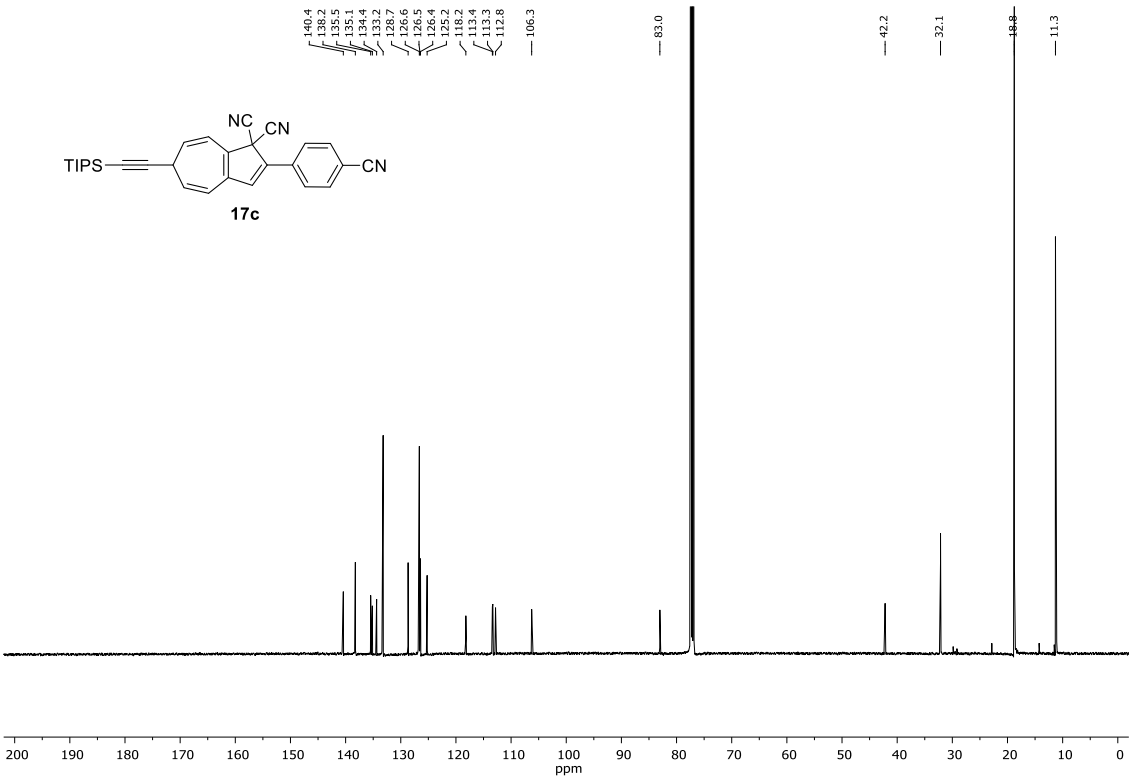


HMBC spectrum (500 MHz / 125 MHz) of **17b** in $CDCl_3$

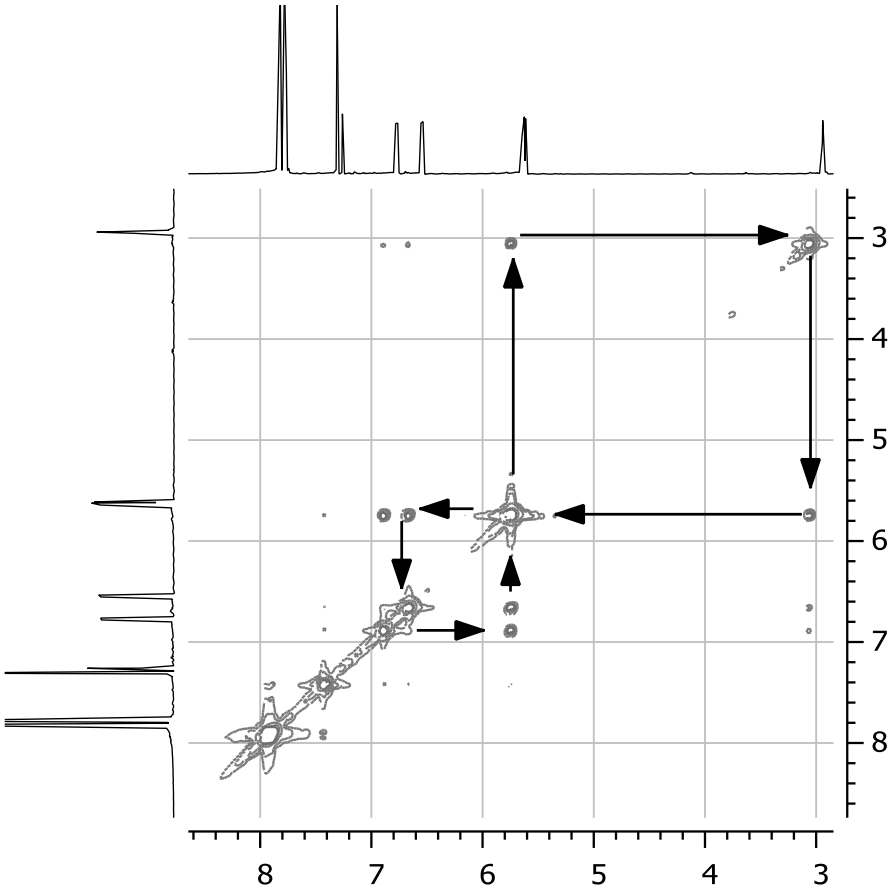
Compound 17c



^{1}H NMR (500 MHz) spectrum of **17c** in $CDCl_3$

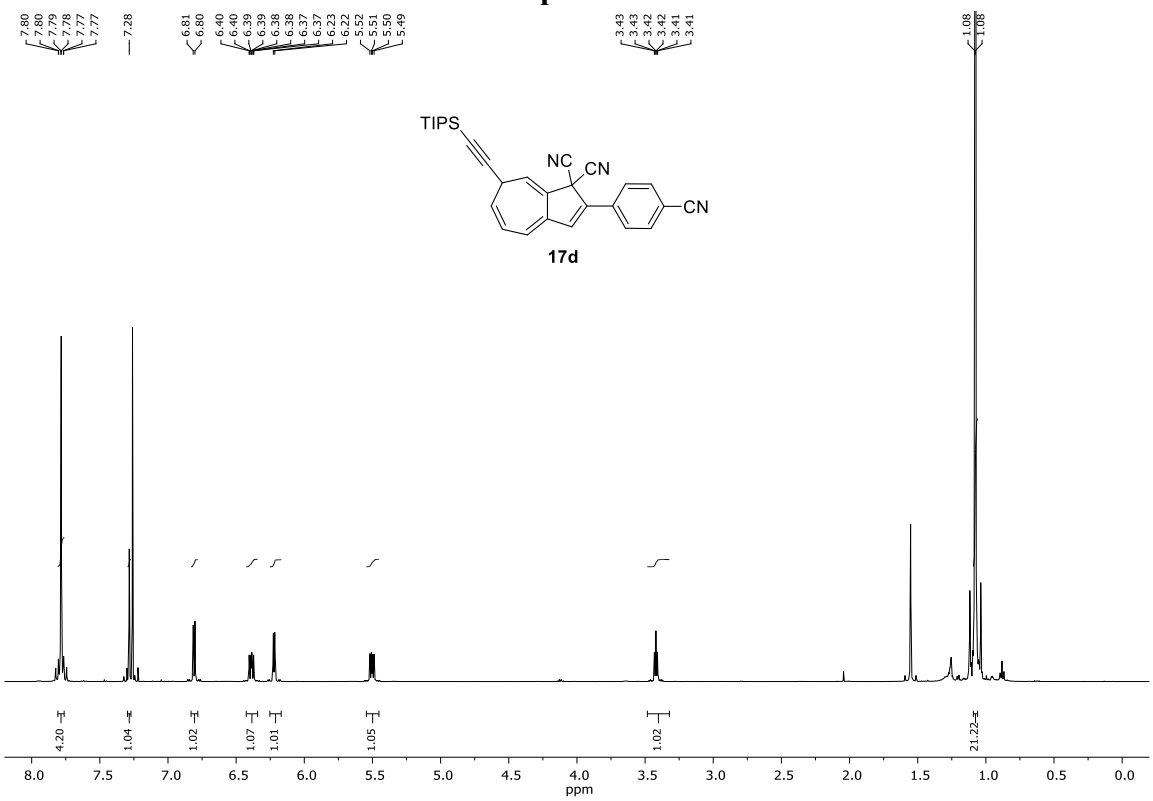


^{13}C NMR (125 MHz) spectrum of **17c** in $CDCl_3$

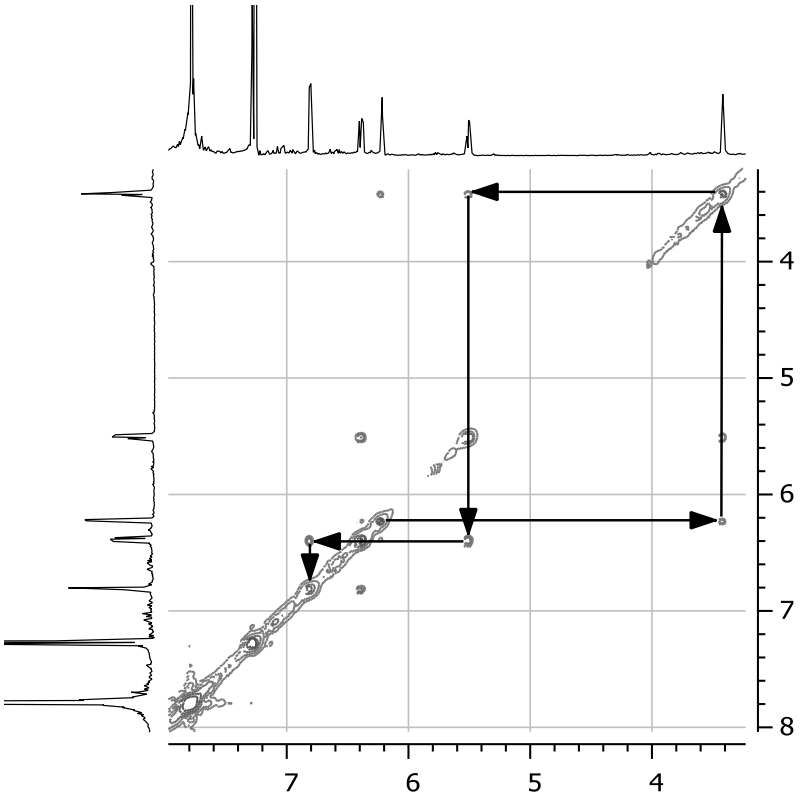


COSY spectrum (500 MHz) of **17c** in $CDCl_3$

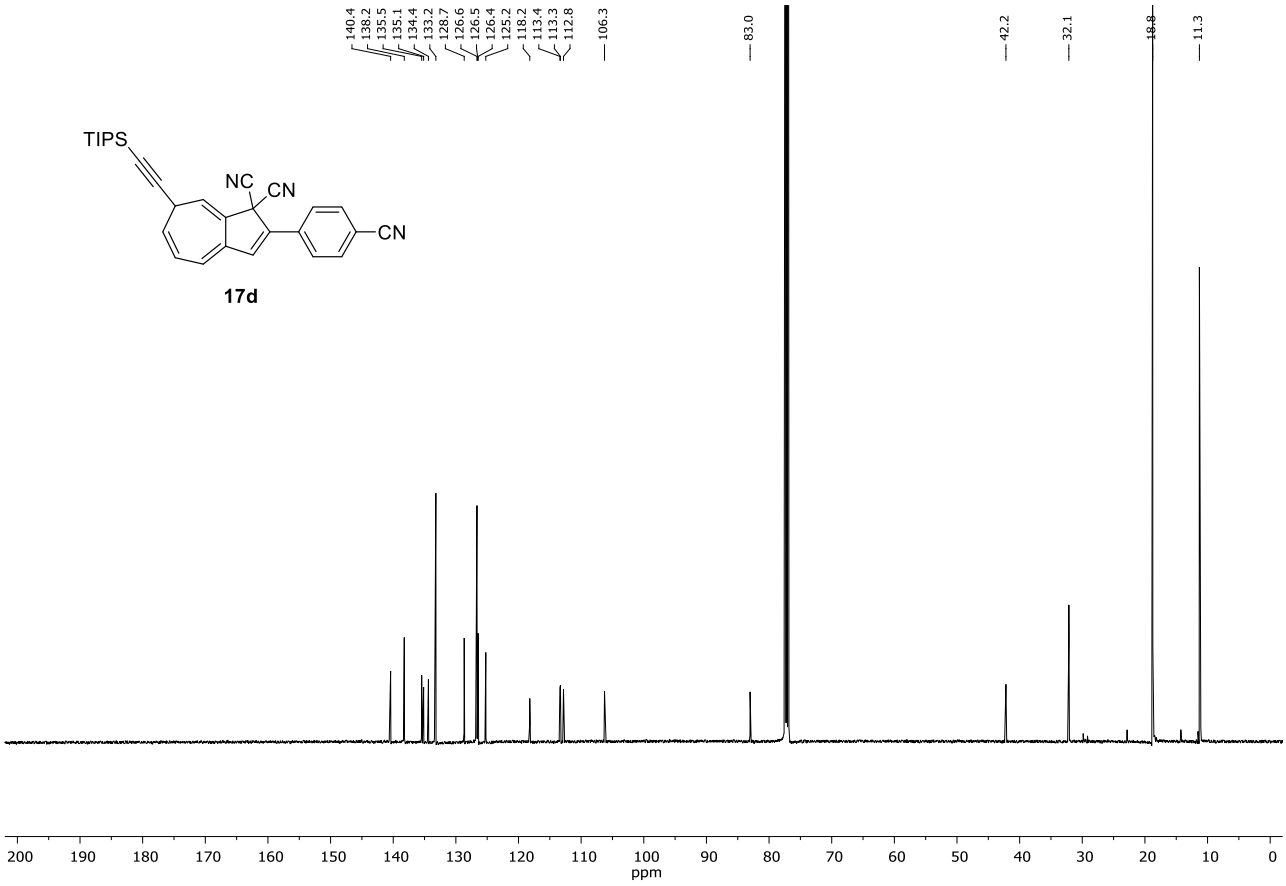
Compound 17d



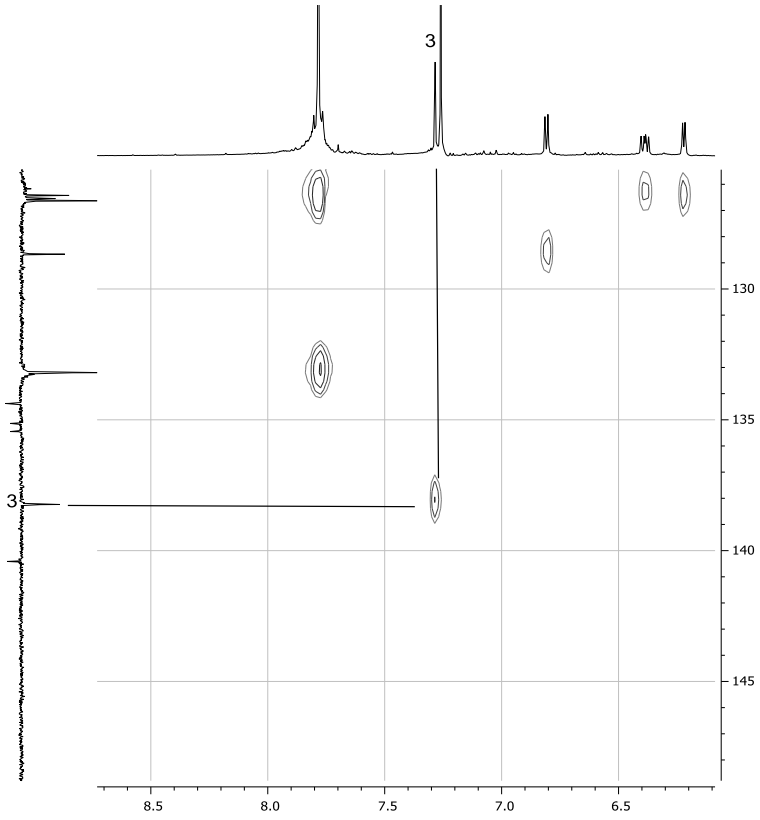
^{1}H NMR (500 MHz) spectrum of **17d** in $CDCl_3$



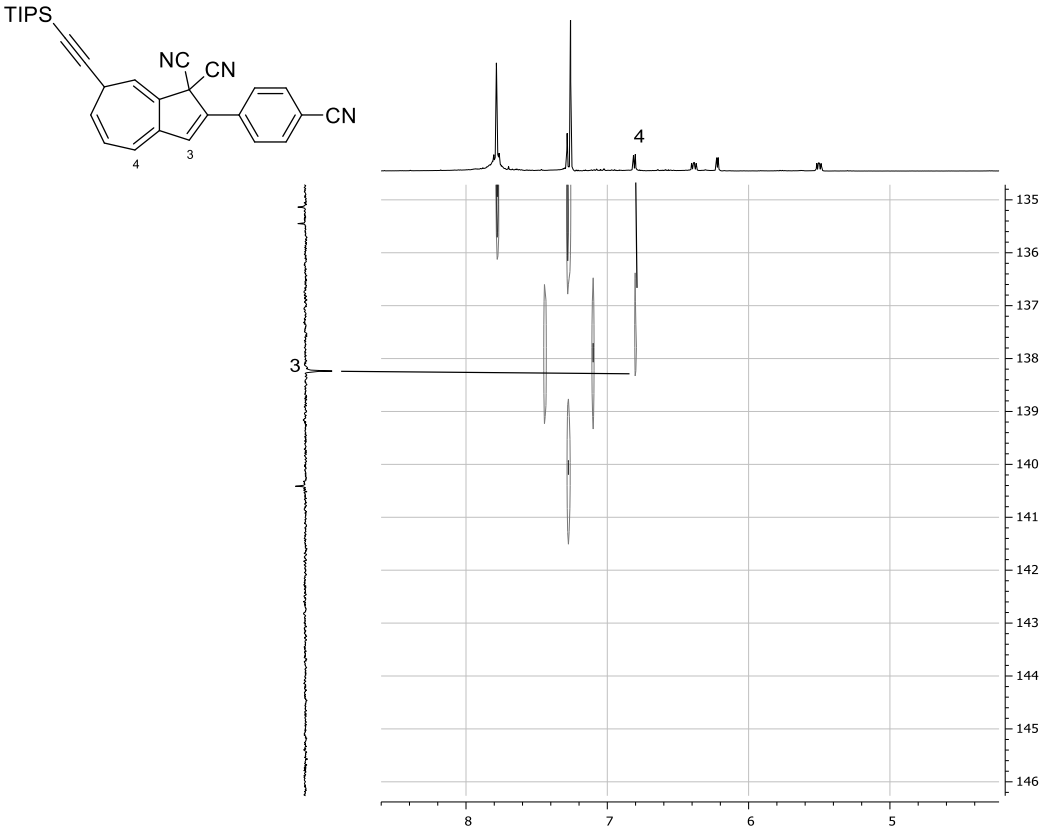
COSY spectrum (500 MHz) of **17d** in $CDCl_3$



^{13}C NMR (125 MHz) spectrum of **17d** in $CDCl_3$

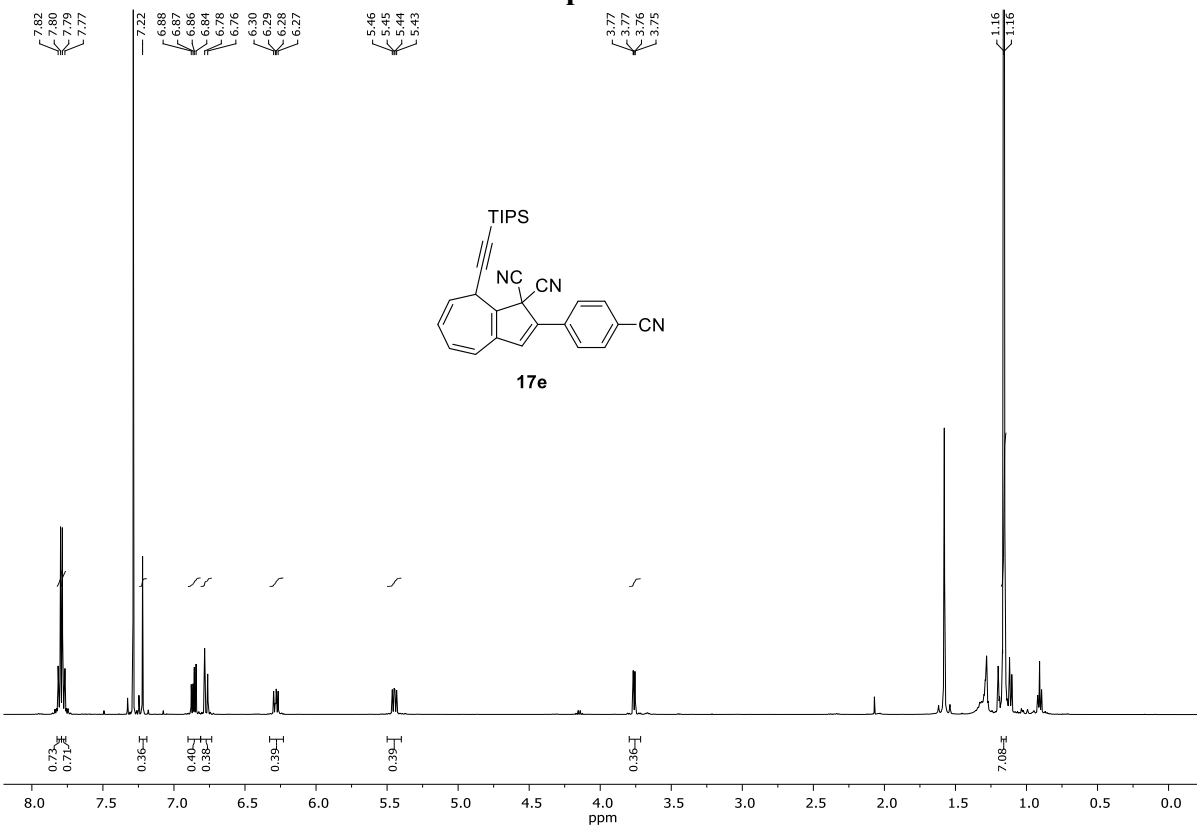


HSQC spectrum (500 MHz / 125 MHz) of **17d** in $CDCl_3$

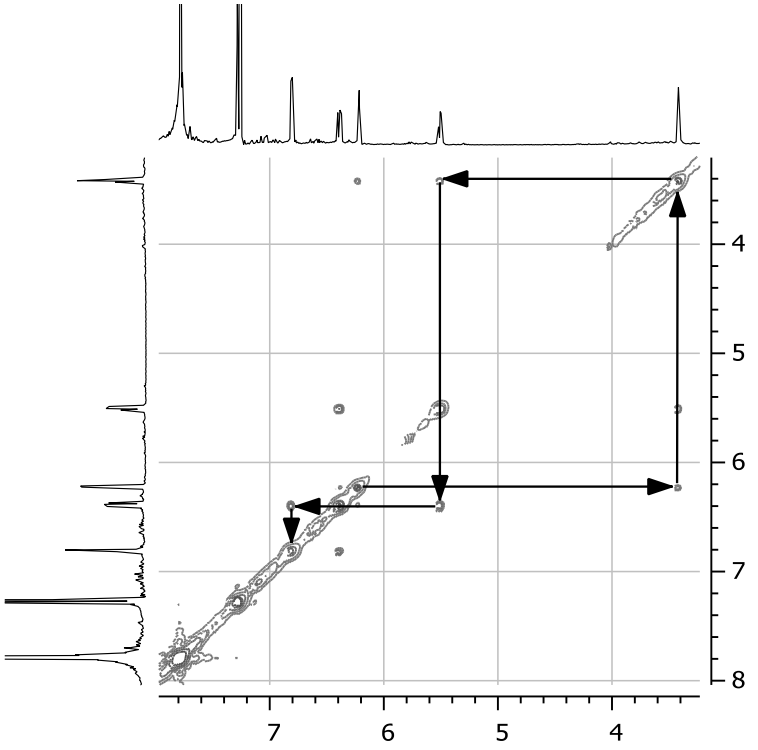


HMBC spectrum (500 MHz / 125 MHz) of **17d** in $CDCl_3$

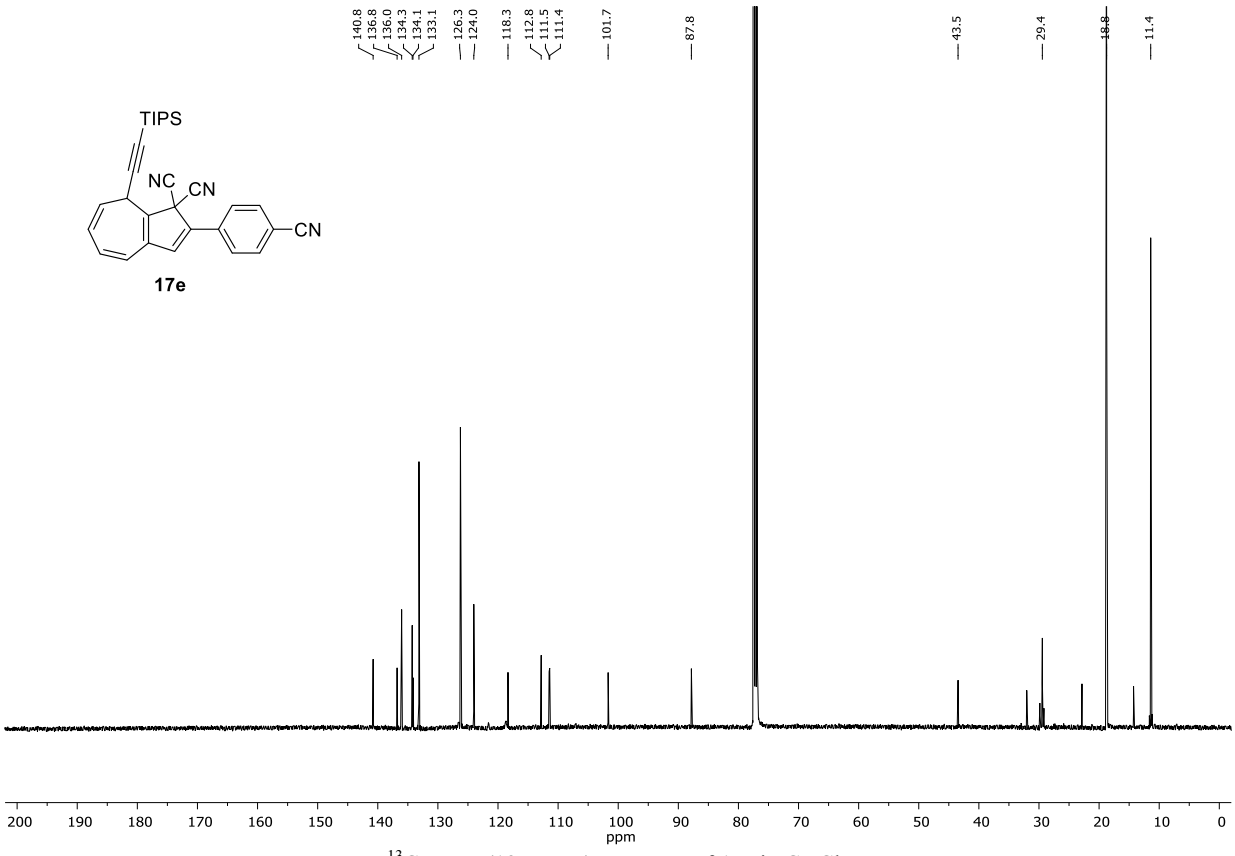
Compound 17e



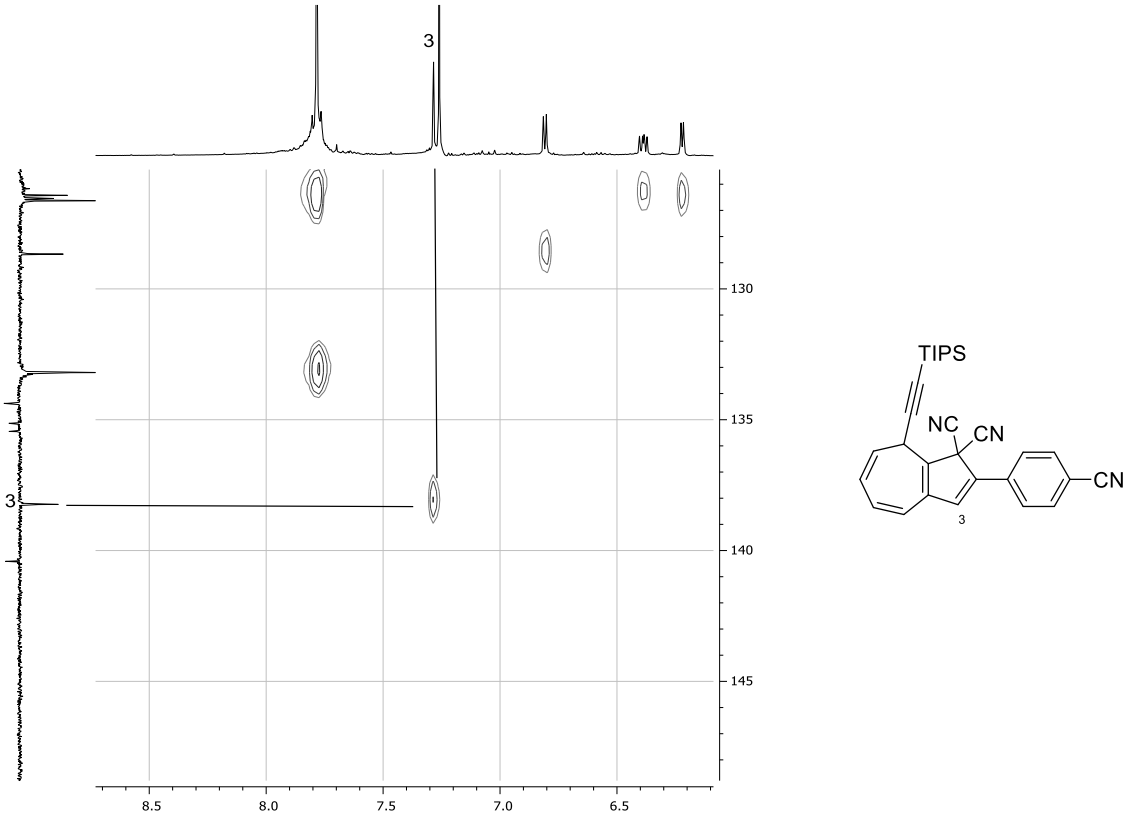
^{1}H NMR (500 MHz) spectrum of **17e** in $CDCl_3$



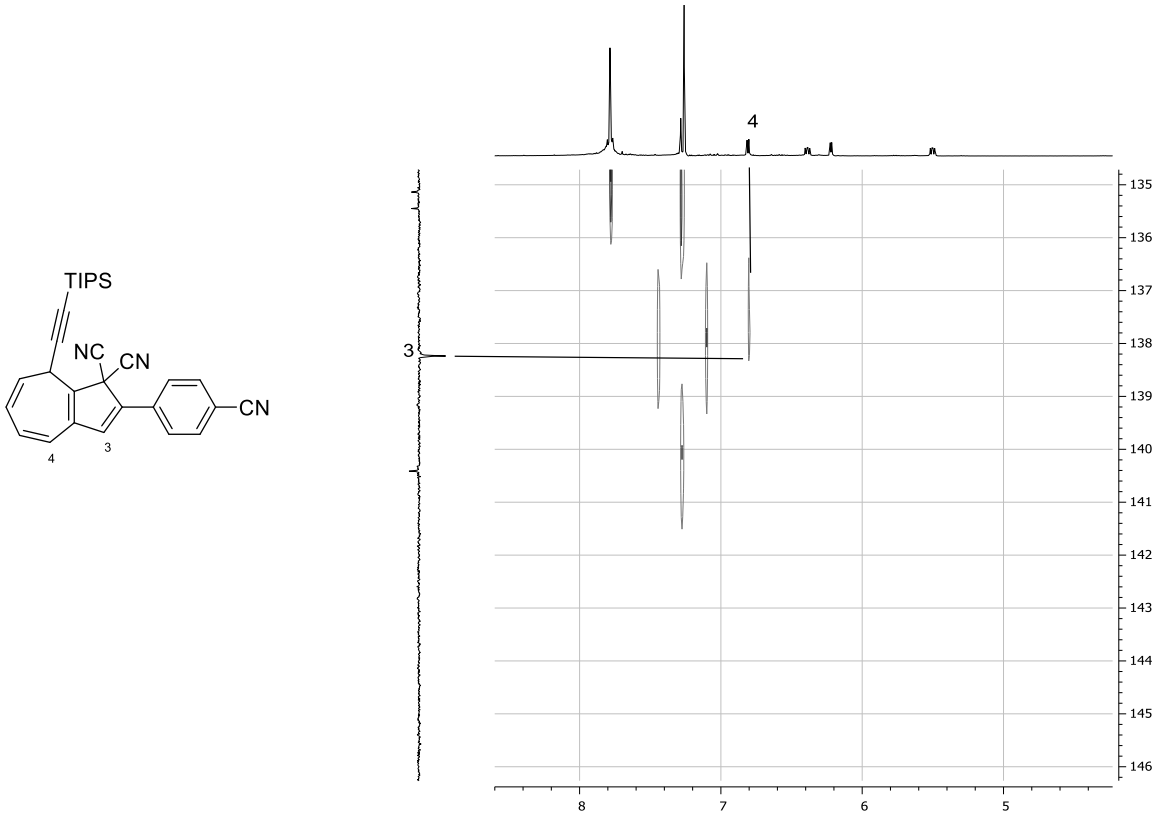
COSY spectrum (500 MHz) of **17e** in $CDCl_3$



^{13}C NMR (125 MHz) spectrum of **17e** in $CDCl_3$

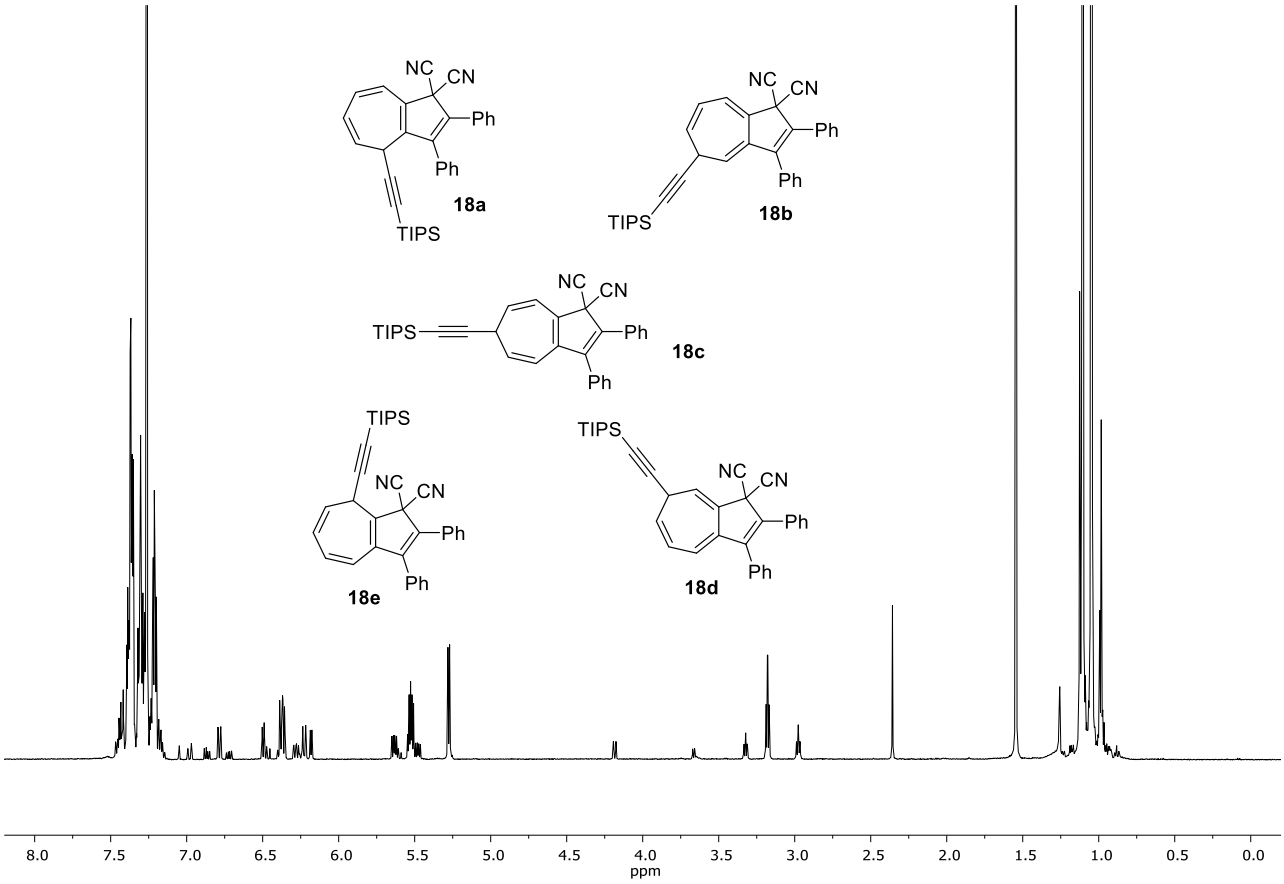


HSQC spectrum (500 MHz / 125 MHz) of **17e** in $CDCl_3$

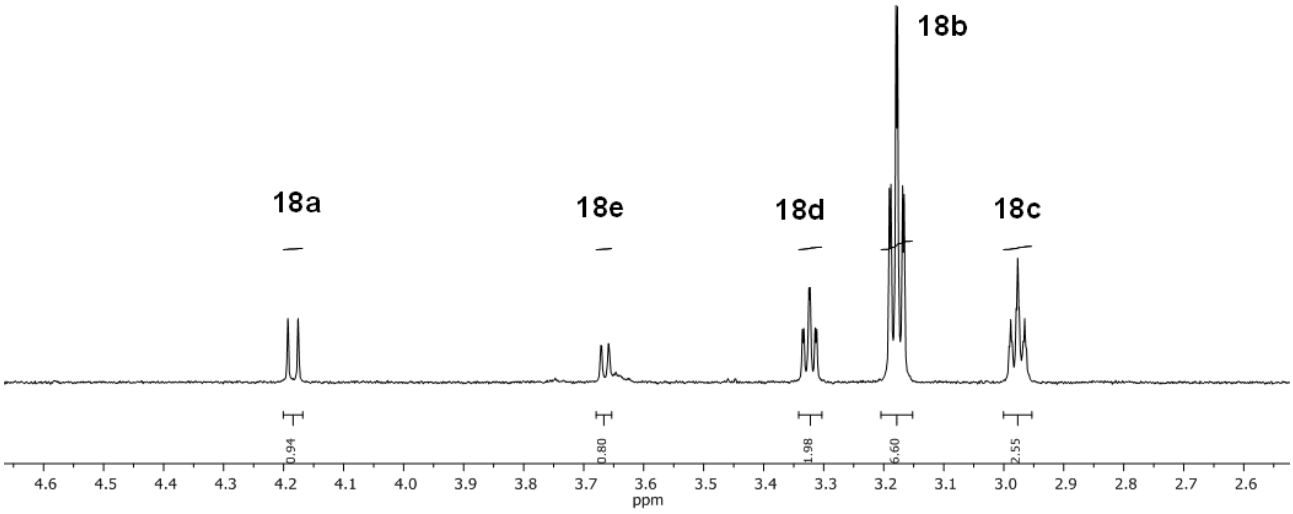


HMBC spectrum (500 MHz / 125 MHz) of **17e** in $CDCl_3$

Regioisomeric mixture 18 (Table 3 Entry 4)

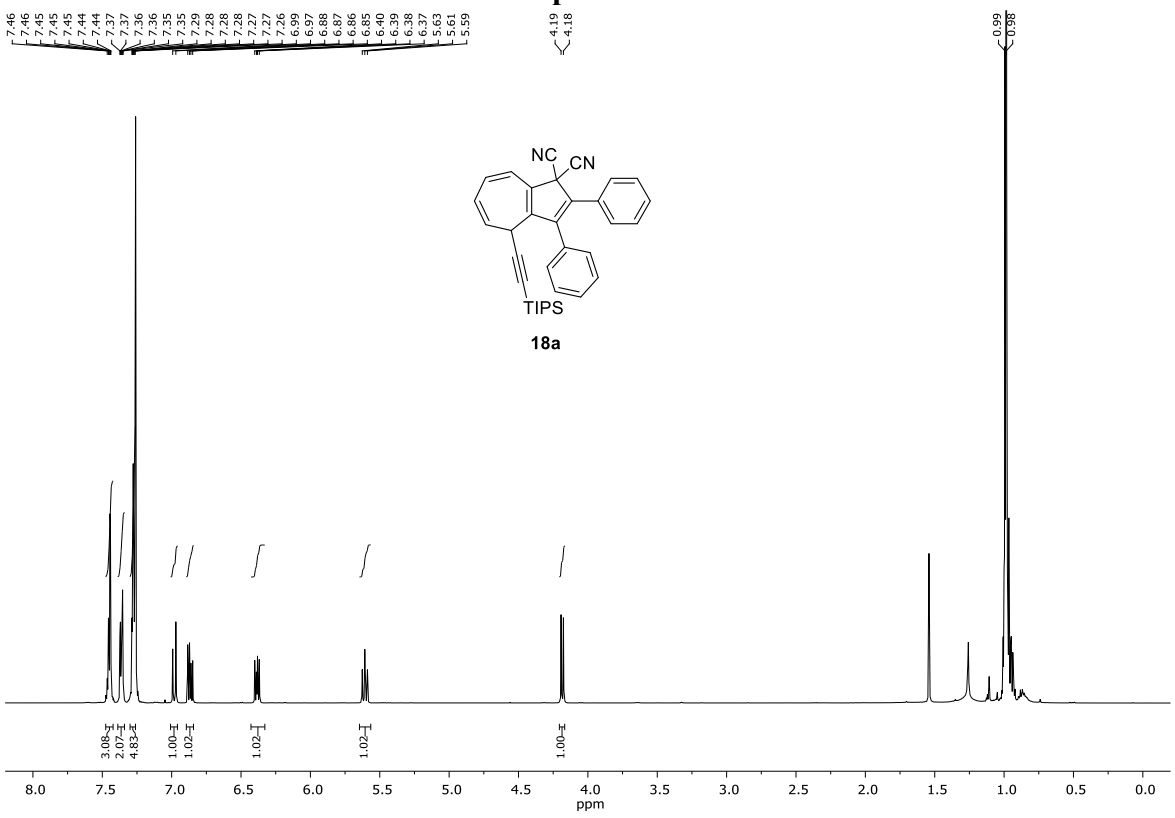


^{1}H NMR (500 MHz) spectrum of **18** in $CDCl_3$

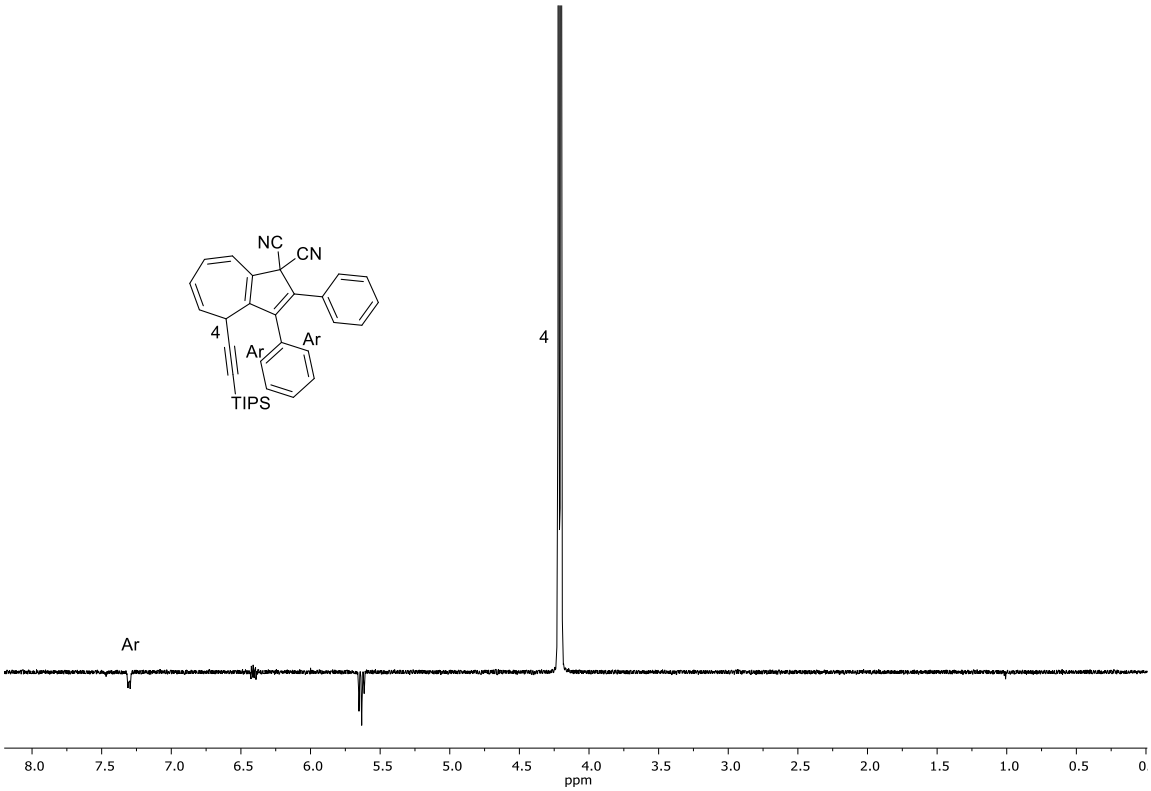


^{1}H NMR (500 MHz) spectrum of **18** in $CDCl_3$ zoomed into the sp^3 region for the point of nucleophilic attack

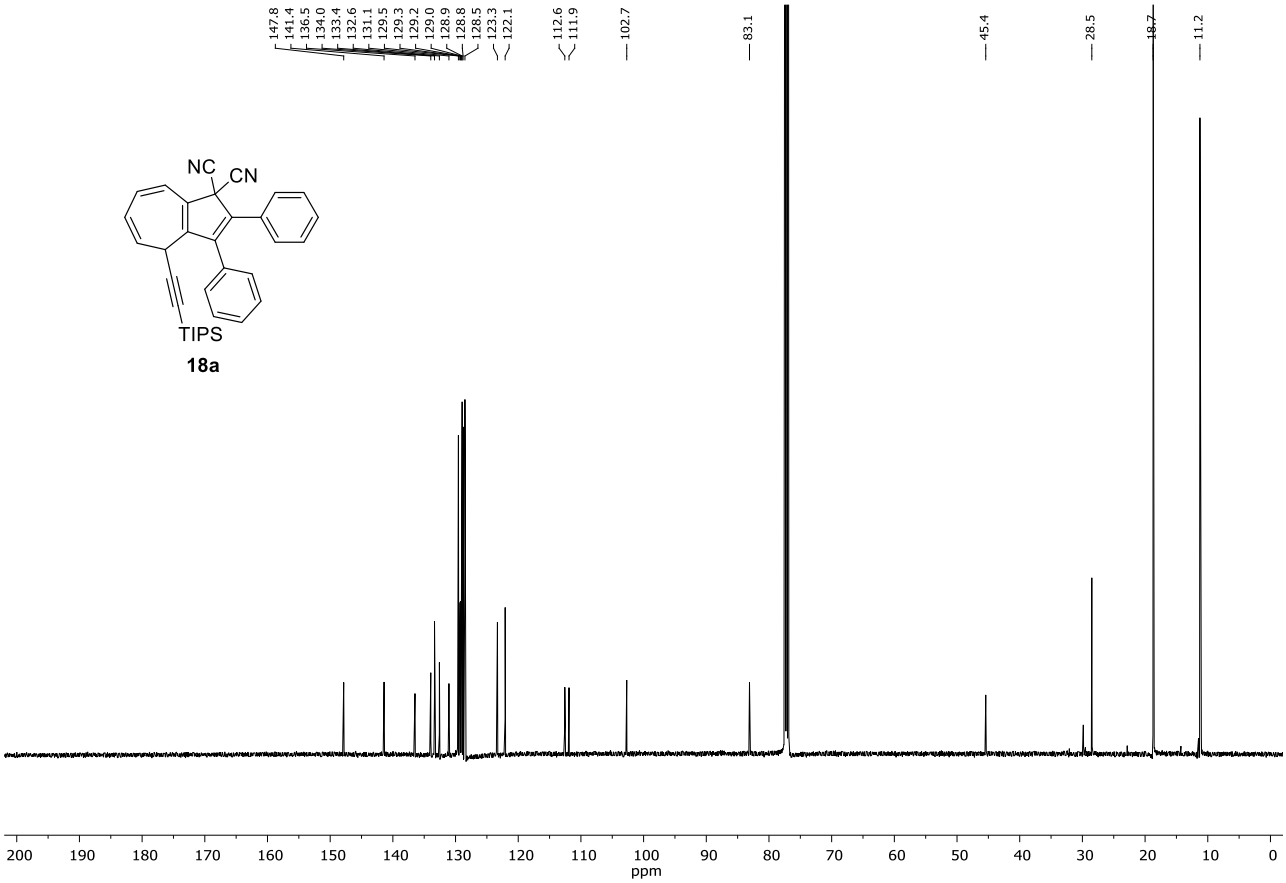
Compound 18a



^{1}H NMR (500 MHz) spectrum of **18a** in $CDCl_3$

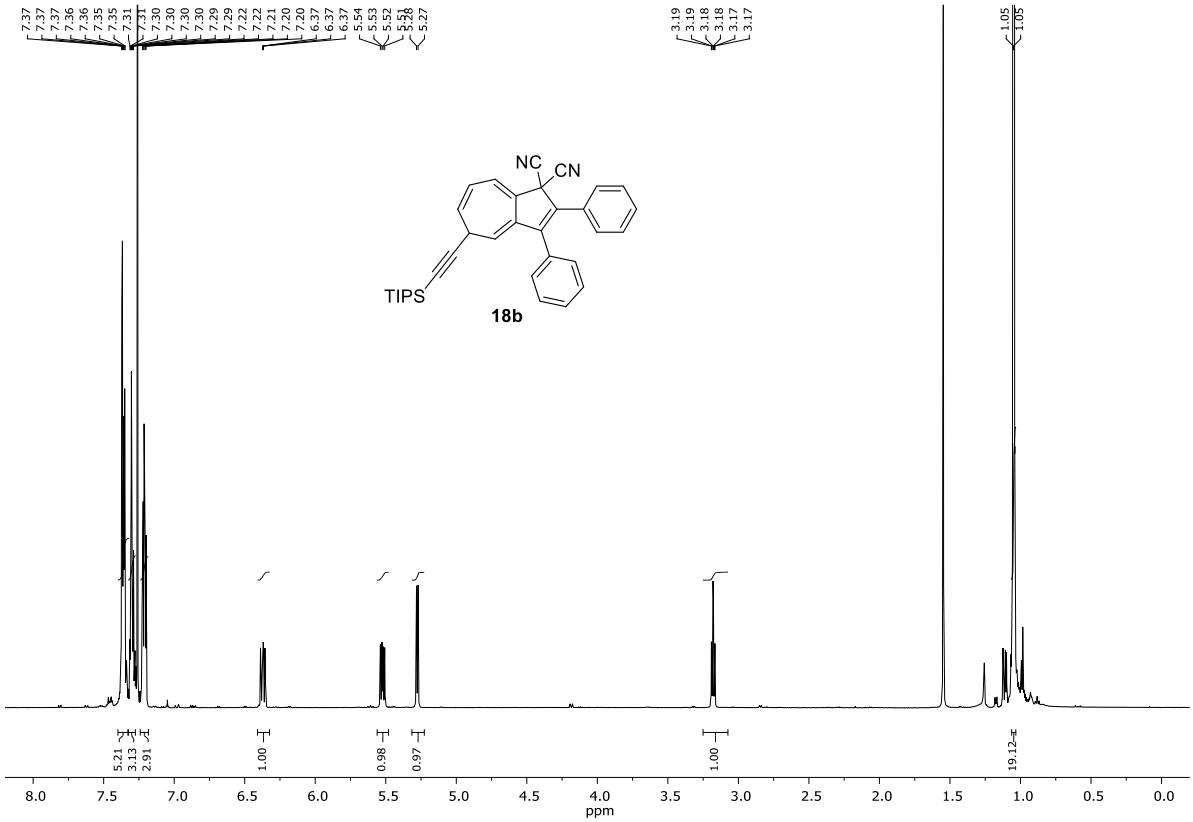


^{1}H NMR (500 MHz) NOE spectrum of **18a** in $CDCl_3$ irradiating at δ 4.18 ppm

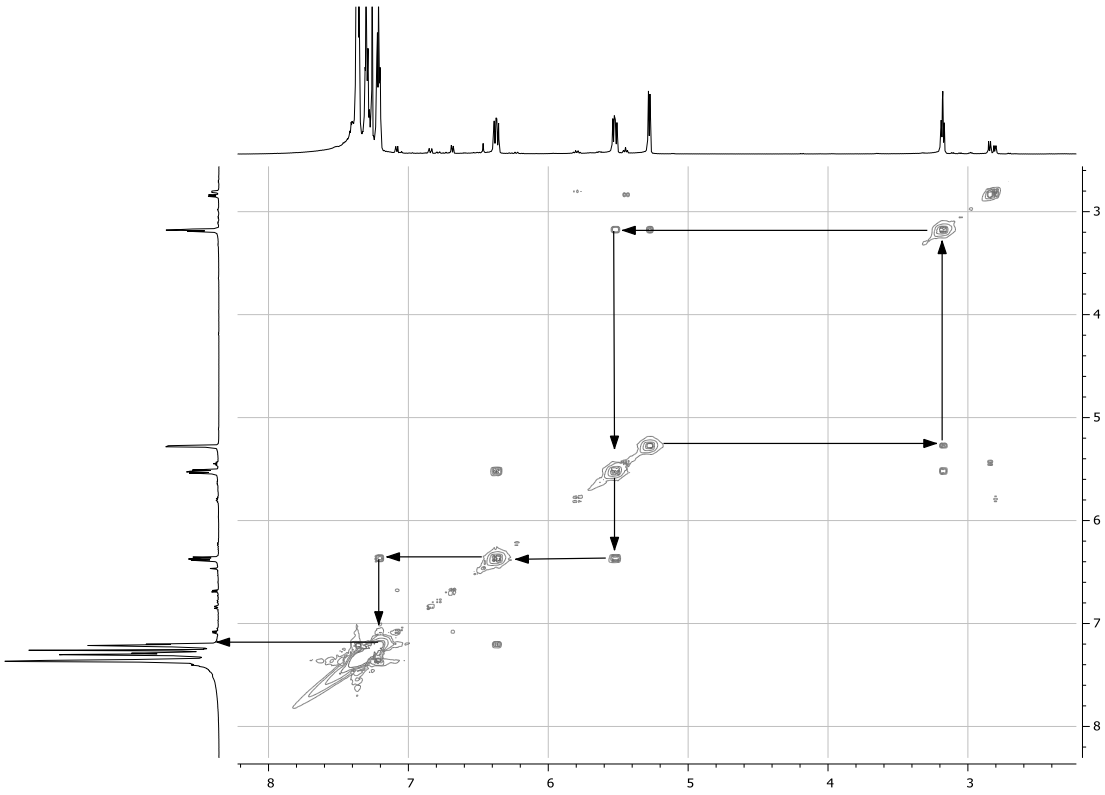


^{13}C NMR (125 MHz) spectrum of **18a** in $CDCl_3$

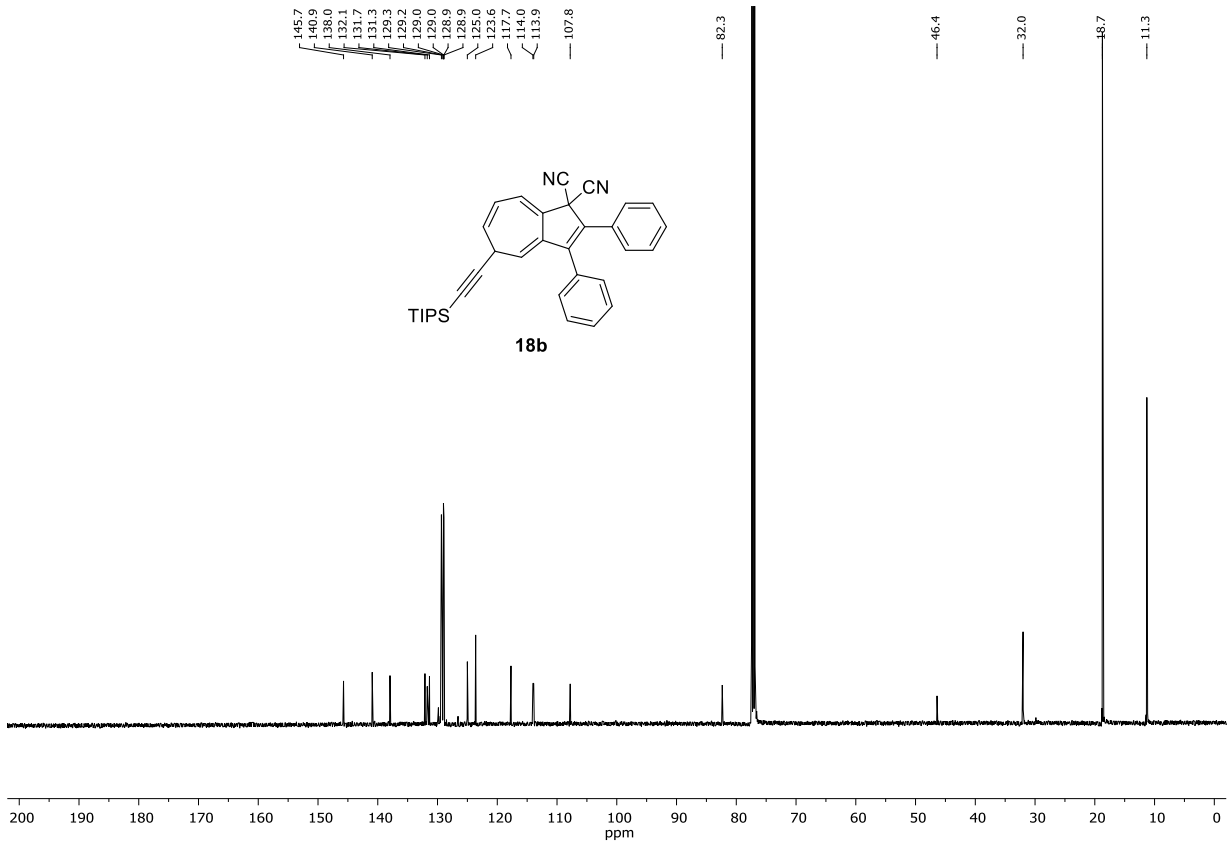
Compound 18b



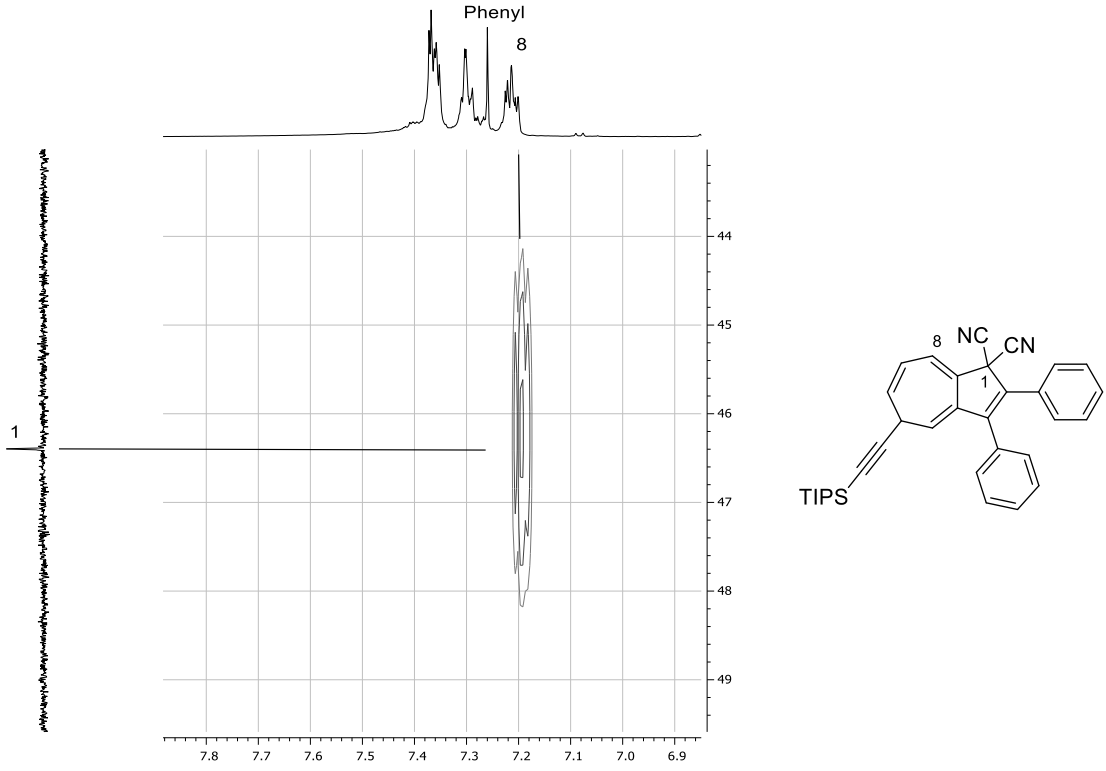
^{1}H NMR (500 MHz) spectrum of **18b** in $CDCl_3$



COSY spectrum (500 MHz) of **18b** in $CDCl_3$

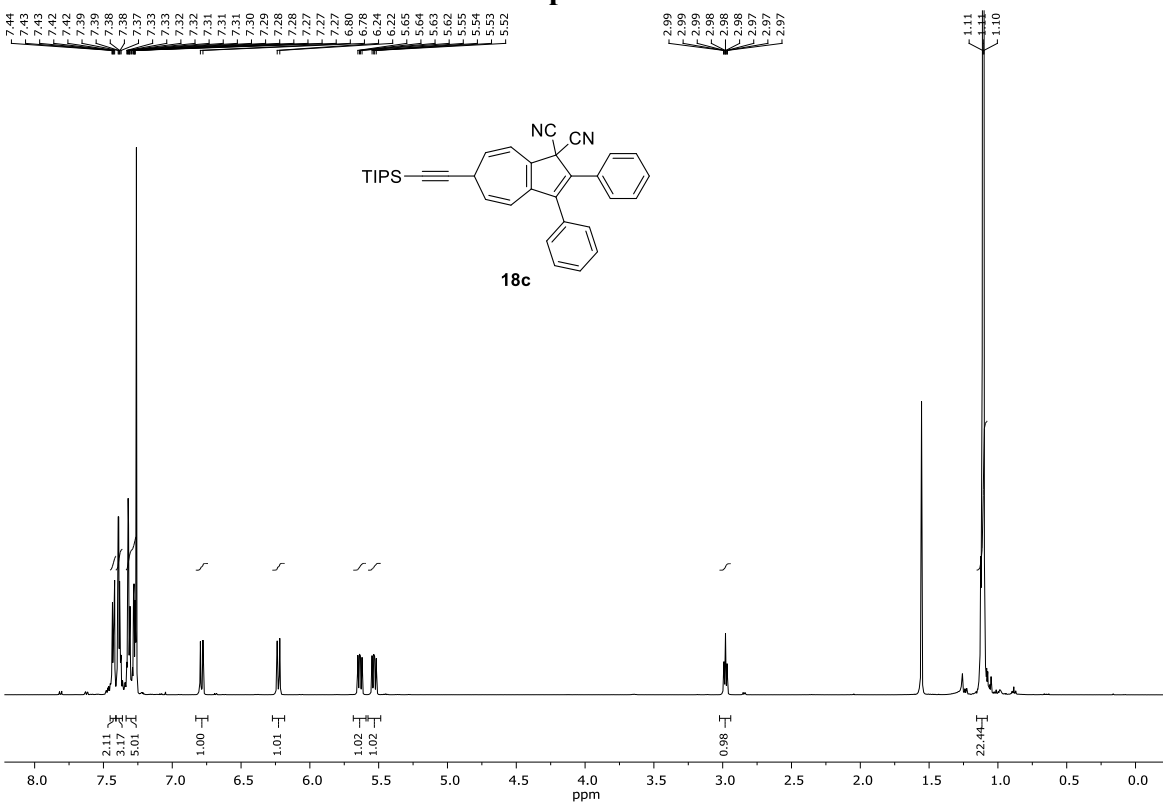


^{13}C NMR (125 MHz) spectrum of **18b** in $CDCl_3$.

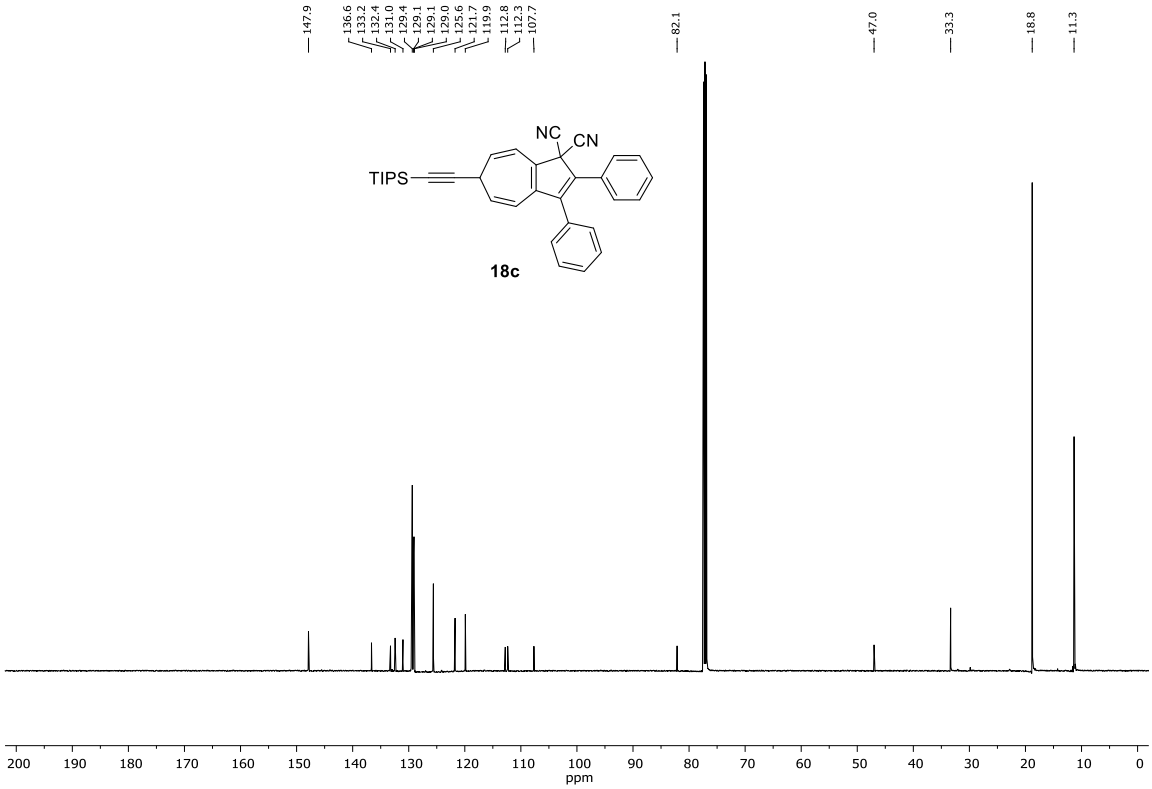


HMBC spectrum (500 MHz / 125 MHz) of **18b** in $CDCl_3$.

Compound 18c

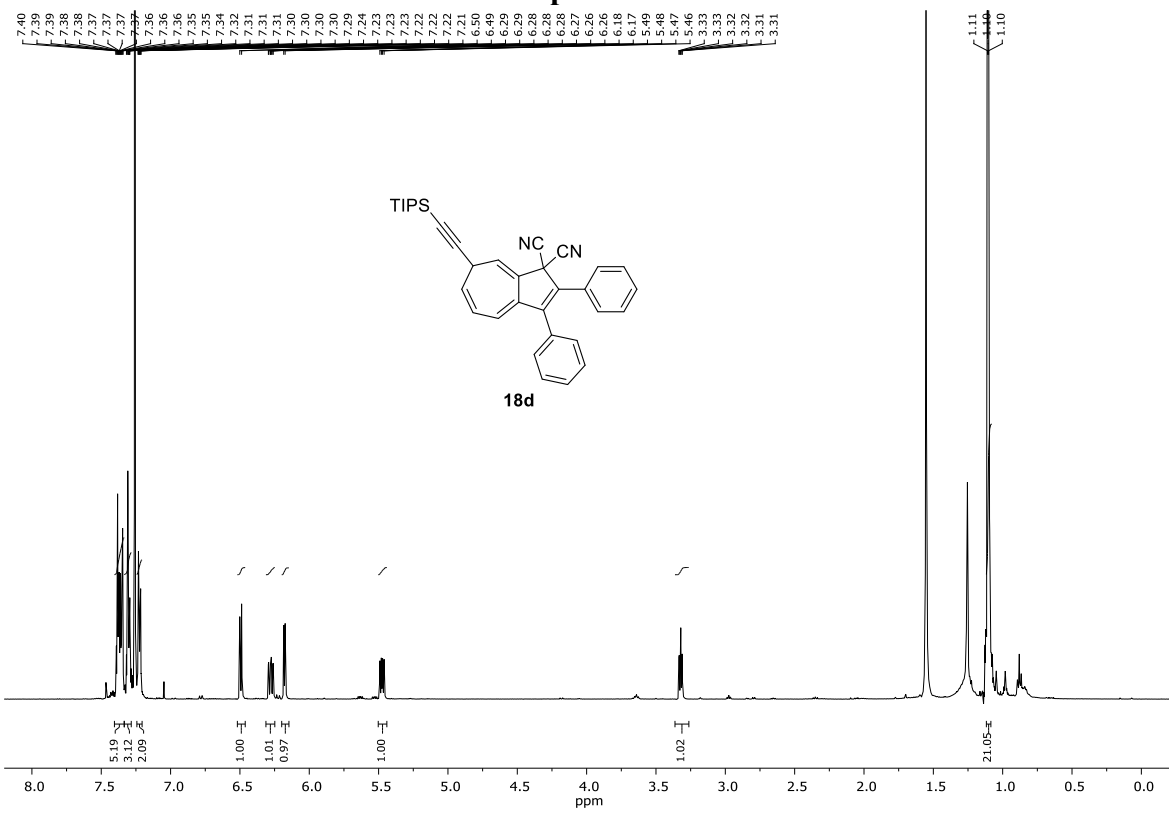


^{1}H NMR (500 MHz) spectrum of **18c** in $CDCl_3$

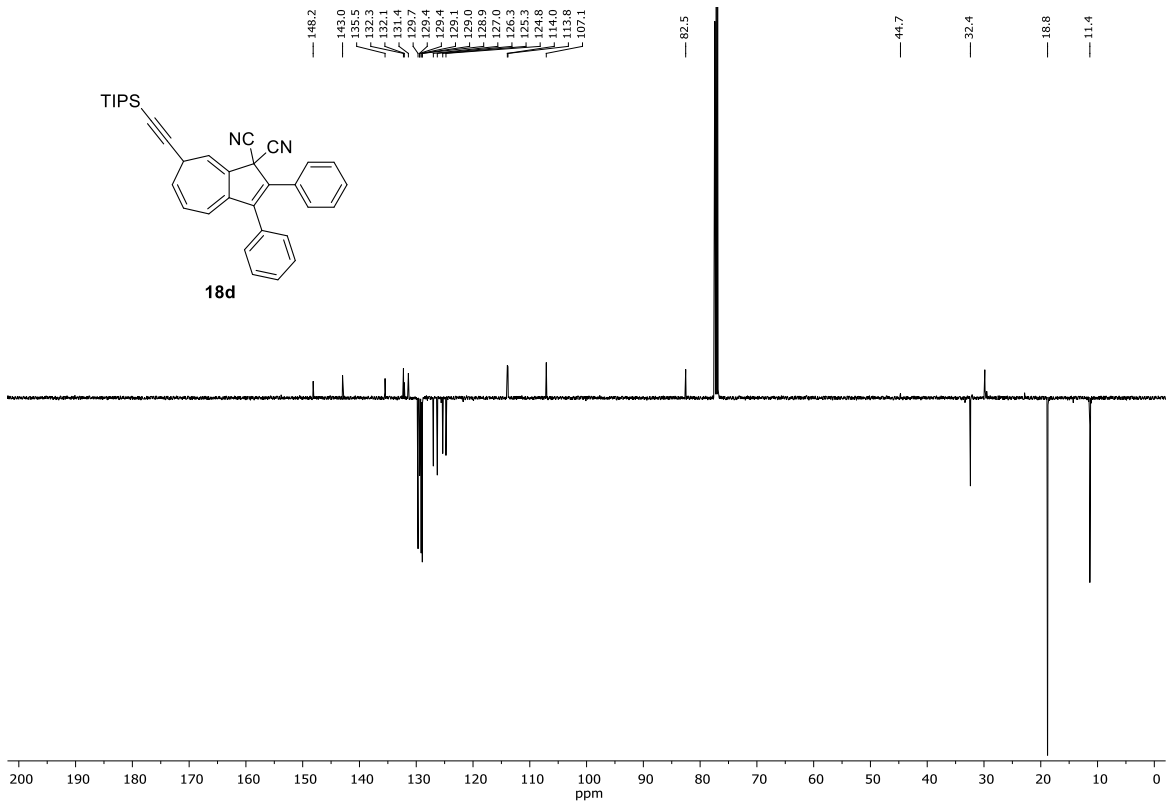


^{13}C NMR (125 MHz) spectrum of **18c** in $CDCl_3$

Compound 18d

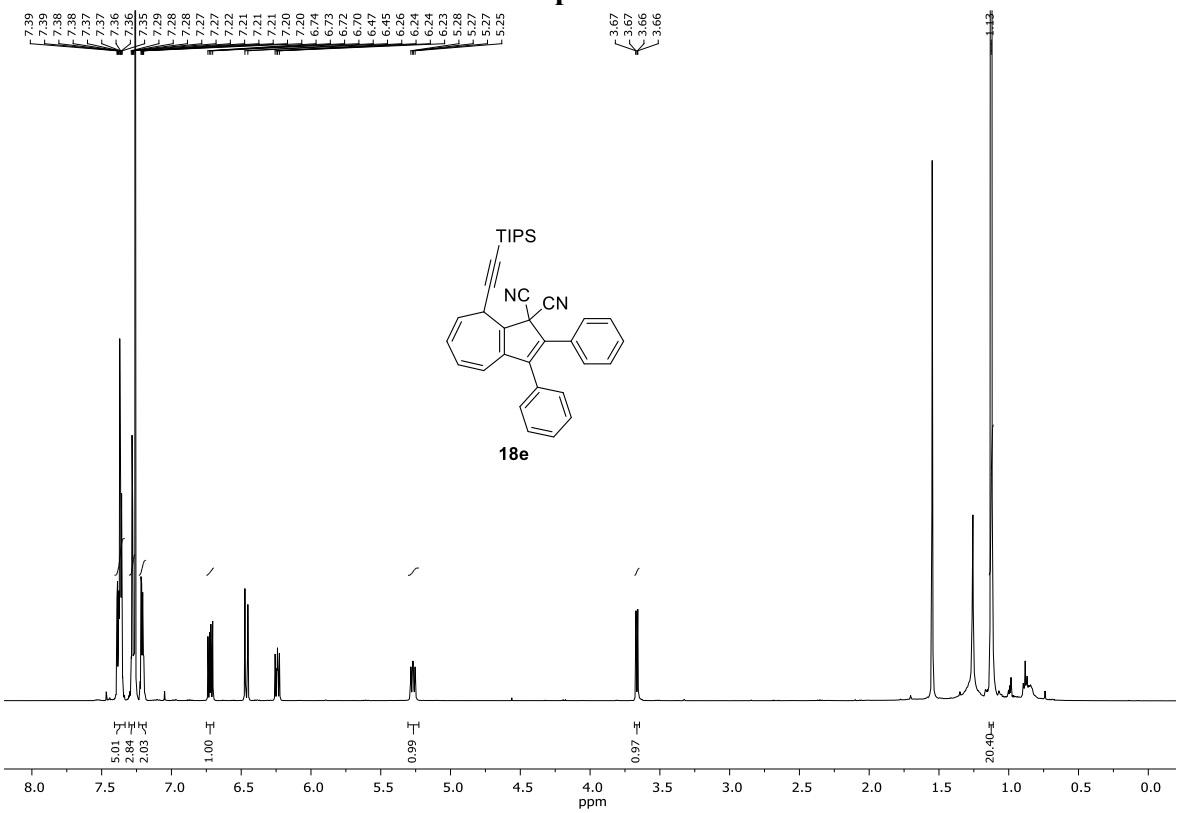


^{1}H NMR (500 MHz) spectrum of **18d** in $CDCl_3$

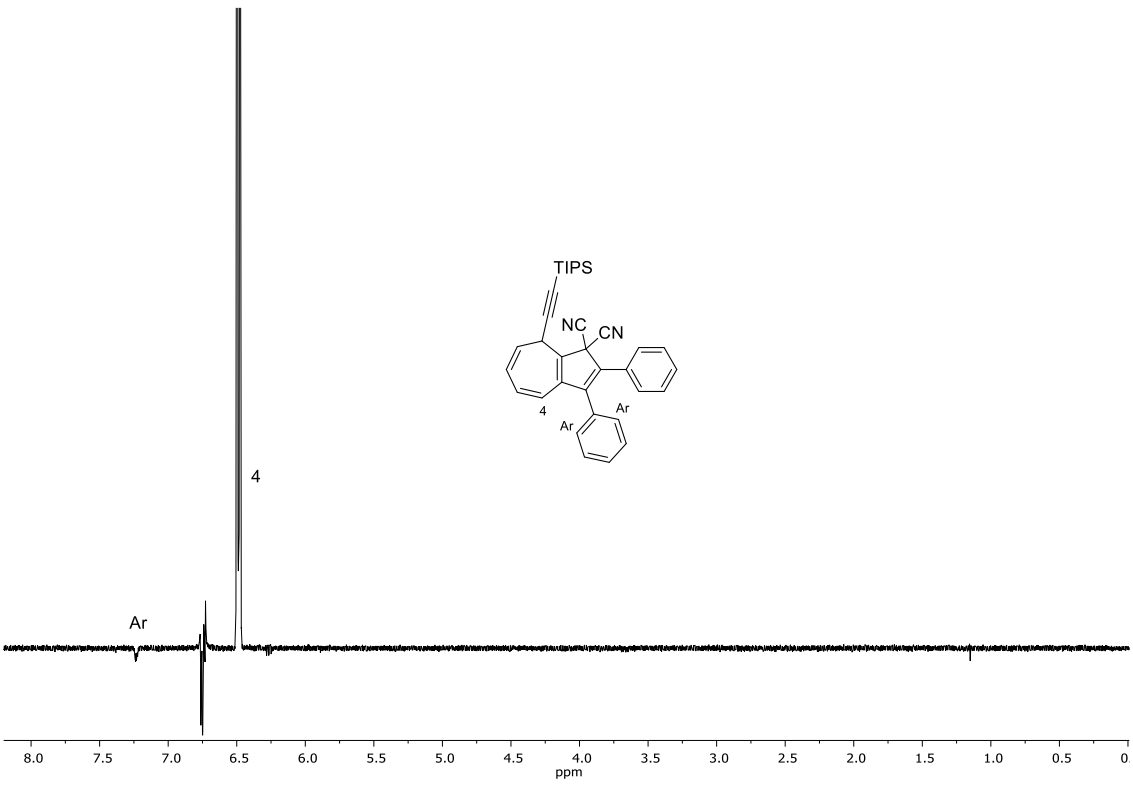


^{13}C NMR APT (125 MHz) spectrum of **18d** in $CDCl_3$

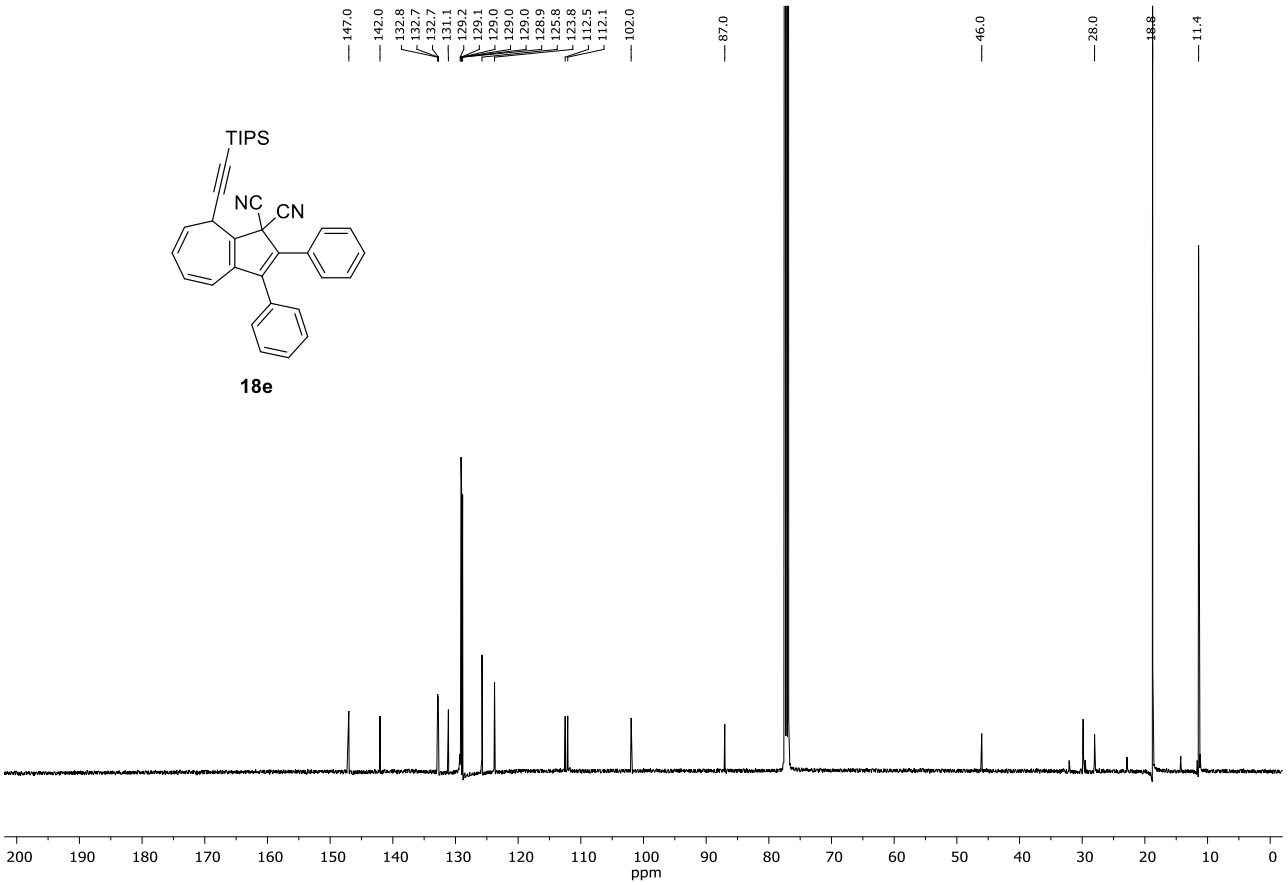
Compound 18e



^{1}H NMR (500 MHz) spectrum of **18e** in $CDCl_3$

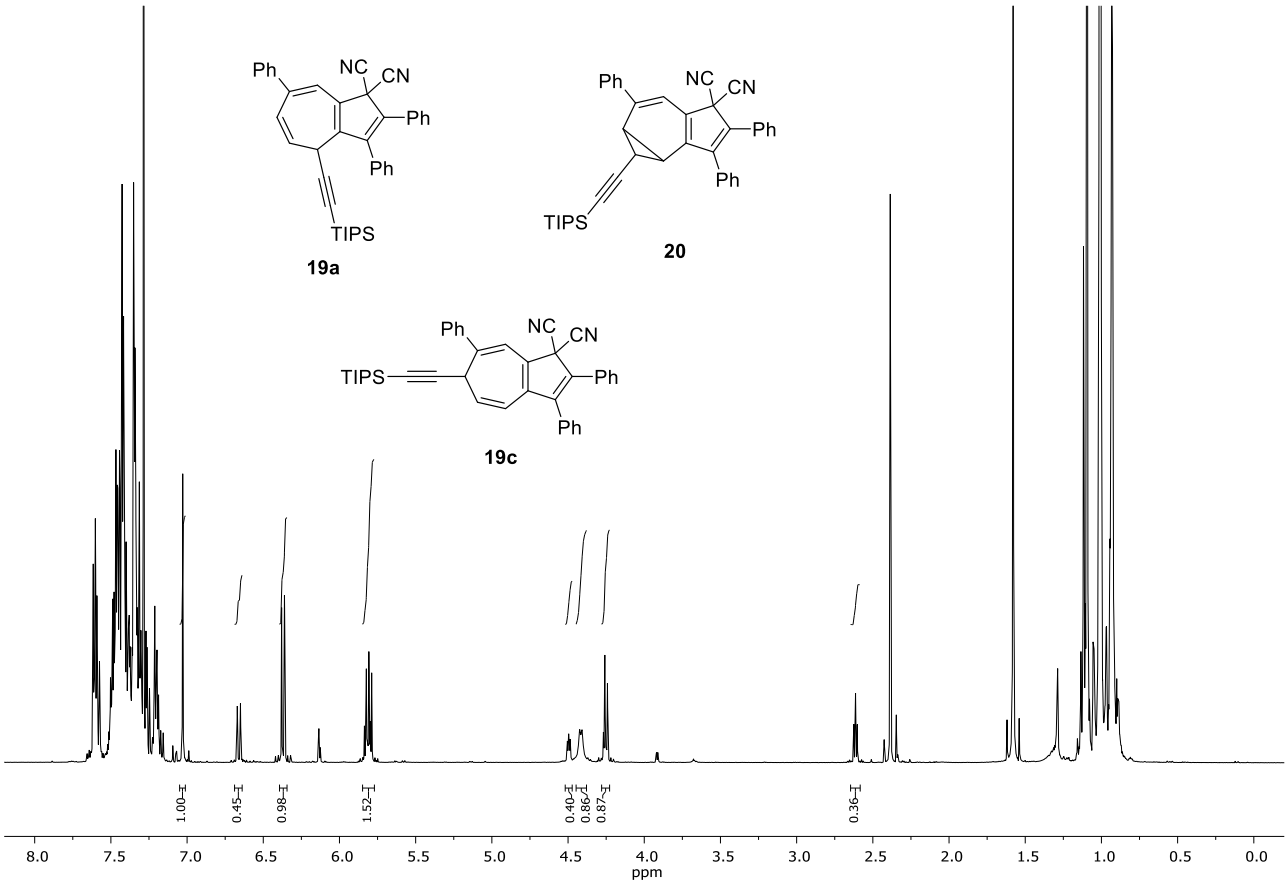


^{1}H NMR (500 MHz) NOE spectrum of **18e** in $CDCl_3$ irradiating at δ 6.46 ppm



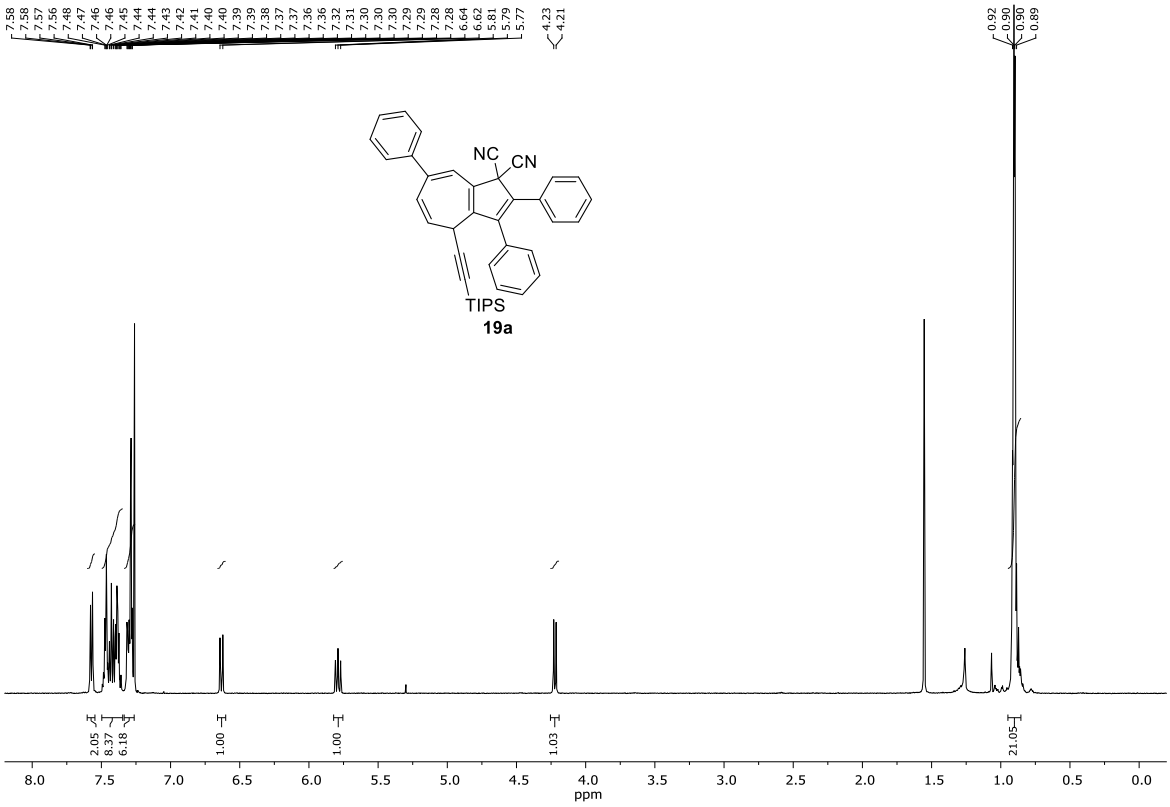
^{13}C NMR (125 MHz) spectrum of **18e** in $CDCl_3$

Regioisomeric mixture 19 and 20 (Table 3 Entry 5)

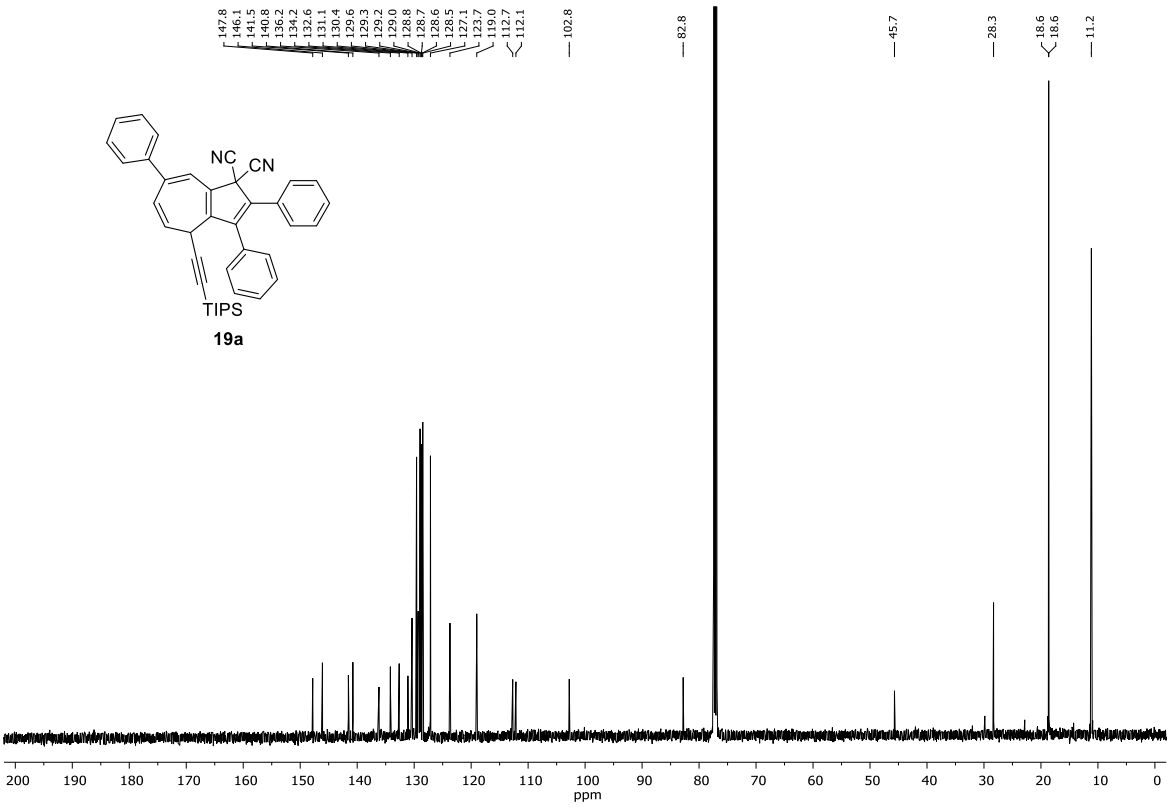


^{1}H NMR (500 MHz) spectrum of mixture of **19** and **20** in $CDCl_3$

Compound 19a

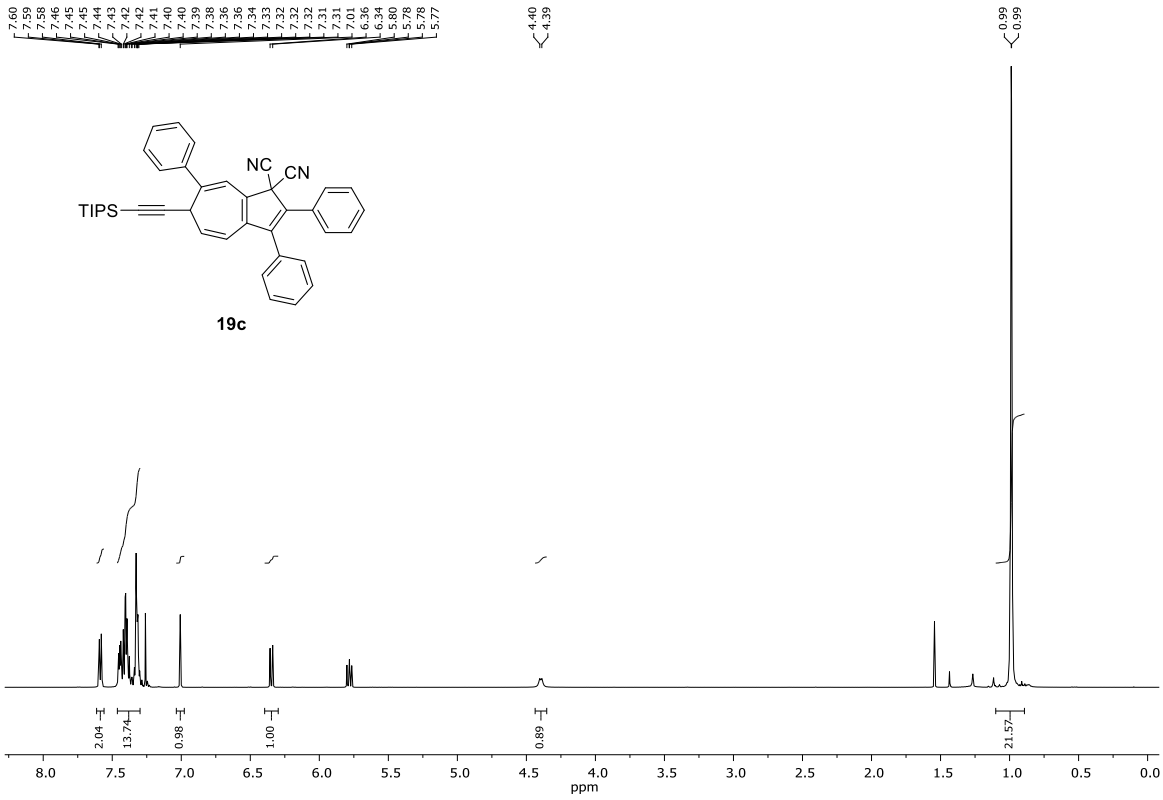


^{1}H NMR (500 MHz) spectrum of **19a** in $CDCl_3$

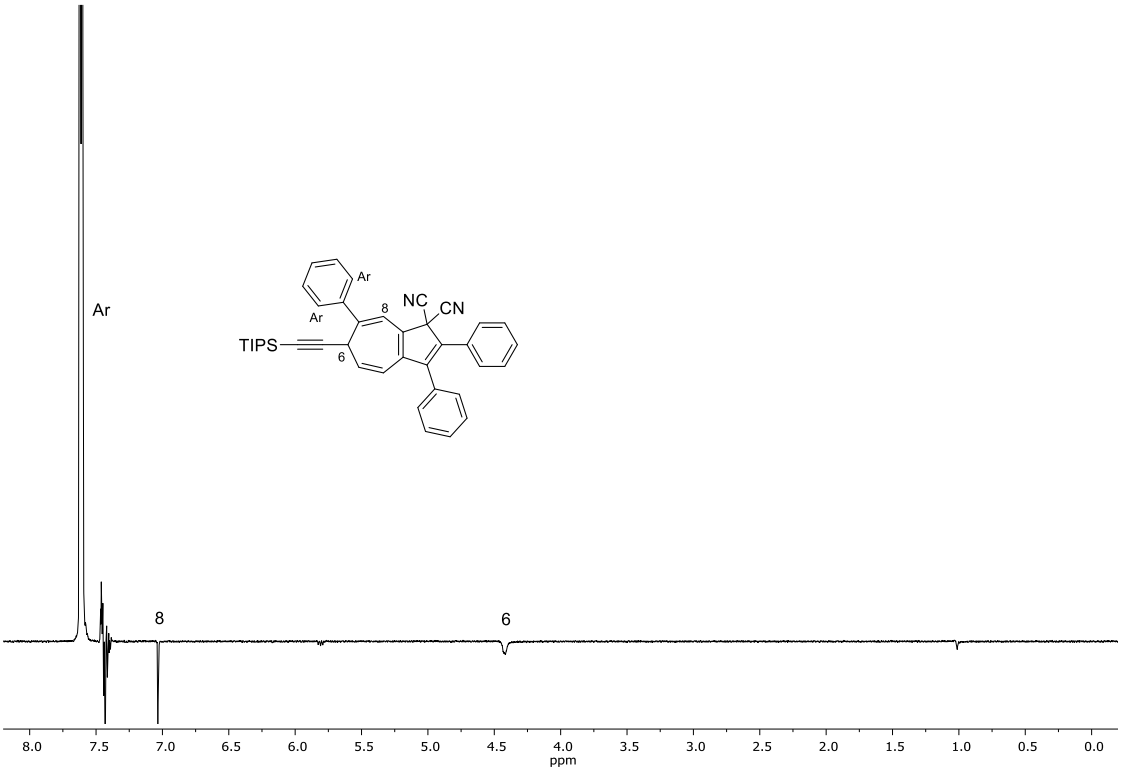


^{13}C NMR (125 MHz) spectrum of **19a** in $CDCl_3$

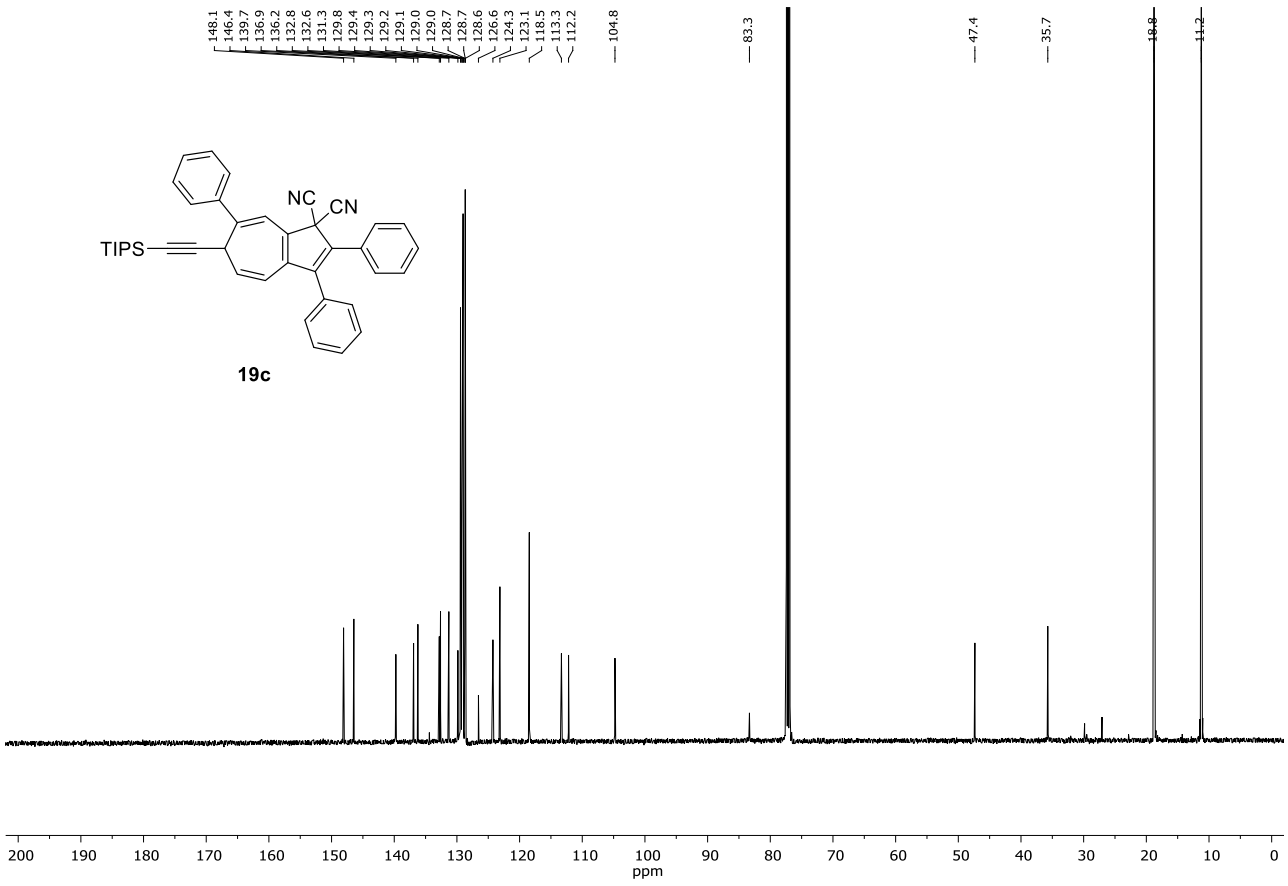
Compound 19c



^{1}H NMR (500 MHz) spectrum of **19c** in $CDCl_3$. (Contains some residual chlorobenzene from chromatography)

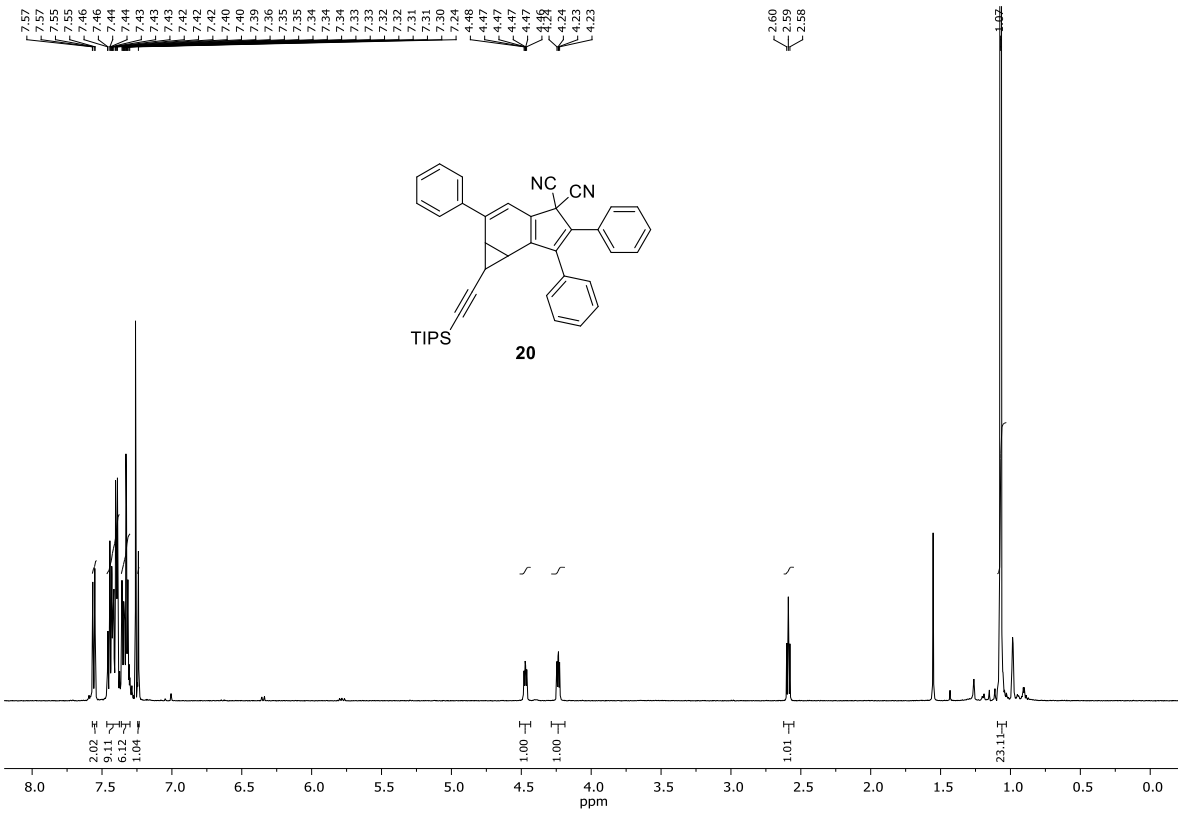


^{1}H NMR (500 MHz) NOE spectrum of **19c** in $CDCl_3$ irradiating at δ 7.59 ppm

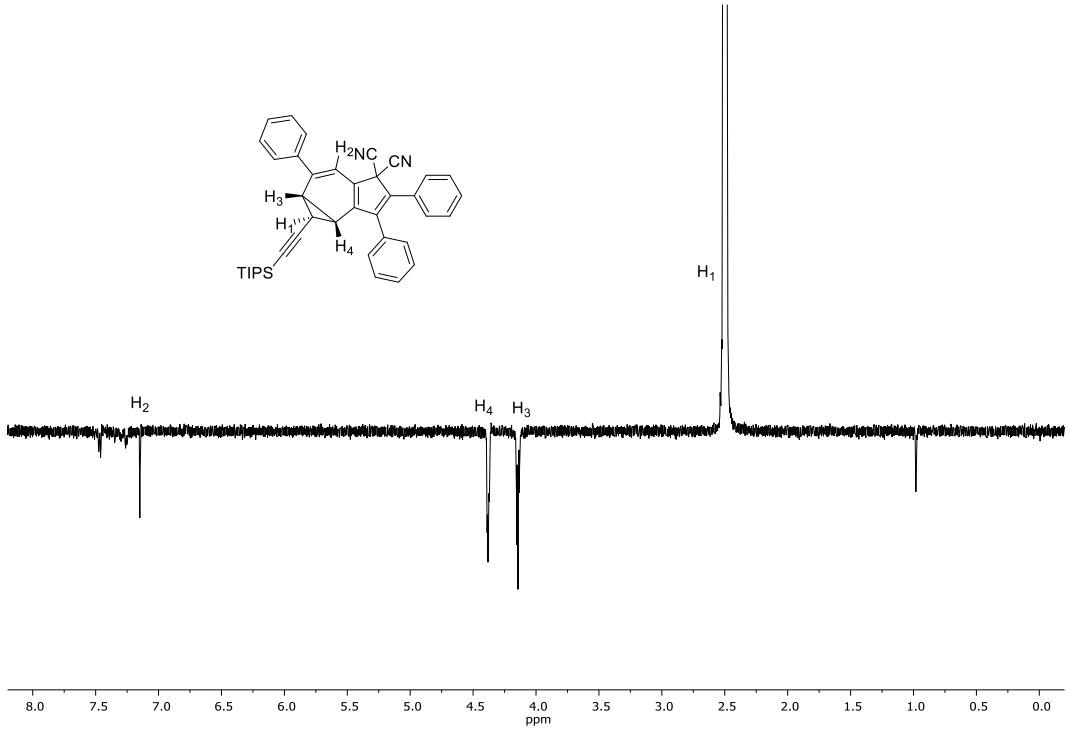


^{13}C NMR (125 MHz) spectrum of **19c** in $CDCl_3$. (Contains some residual chlorobenzene from chromatography)

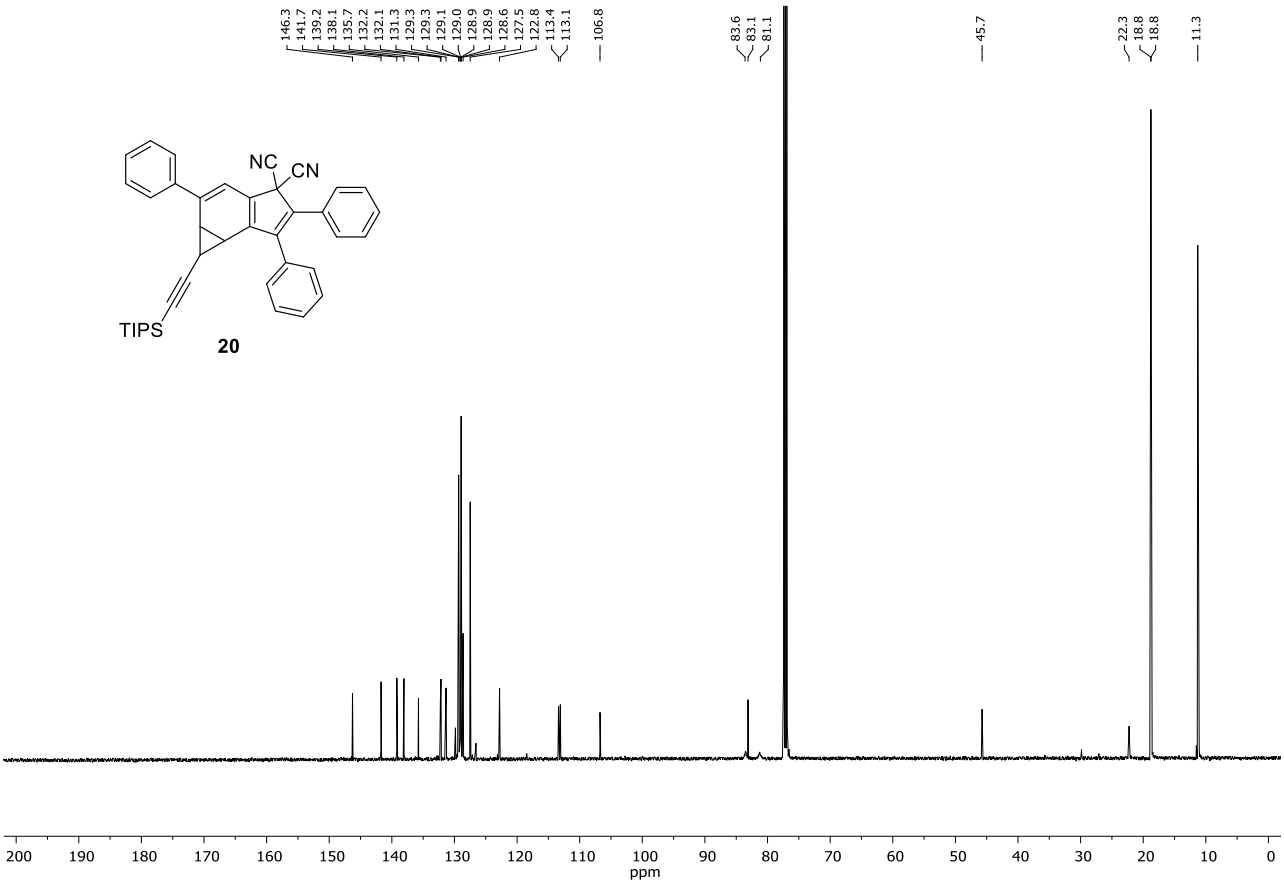
Compound 20



^{1}H NMR (500 MHz) spectrum of **20** in $CDCl_3$

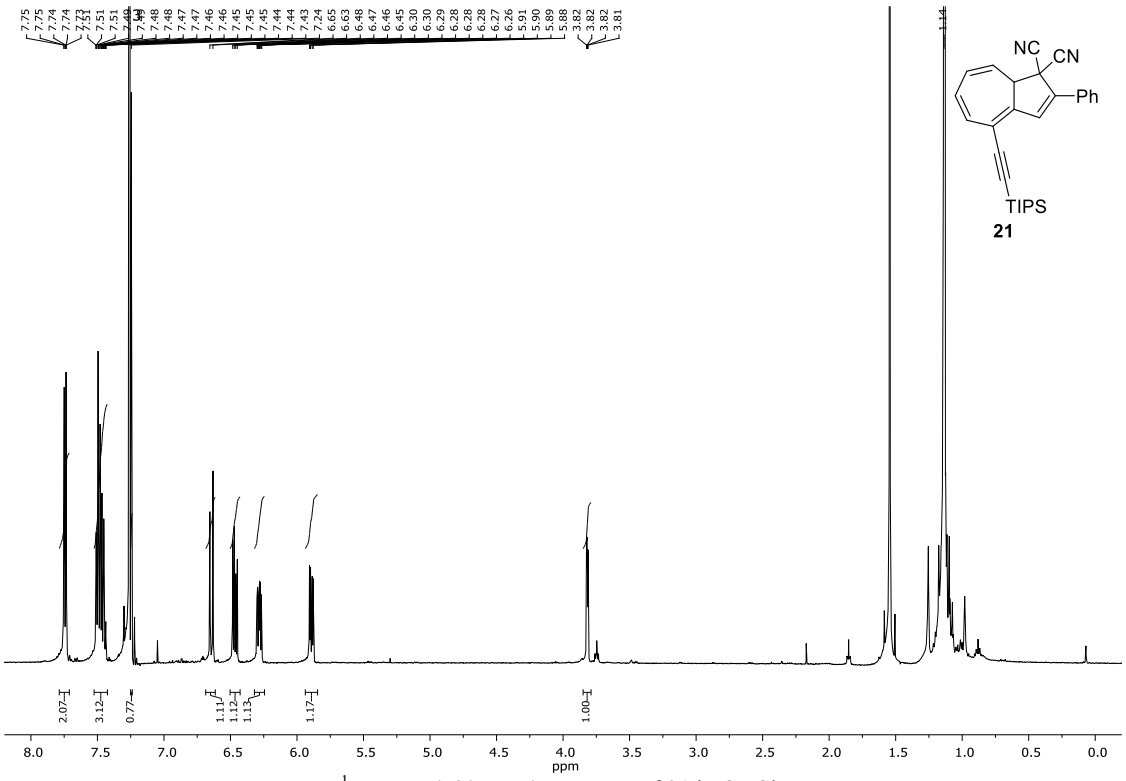


^{1}H NMR (500 MHz) NOE spectrum of **20** in $CDCl_3$ irradiating at δ 2.59 ppm

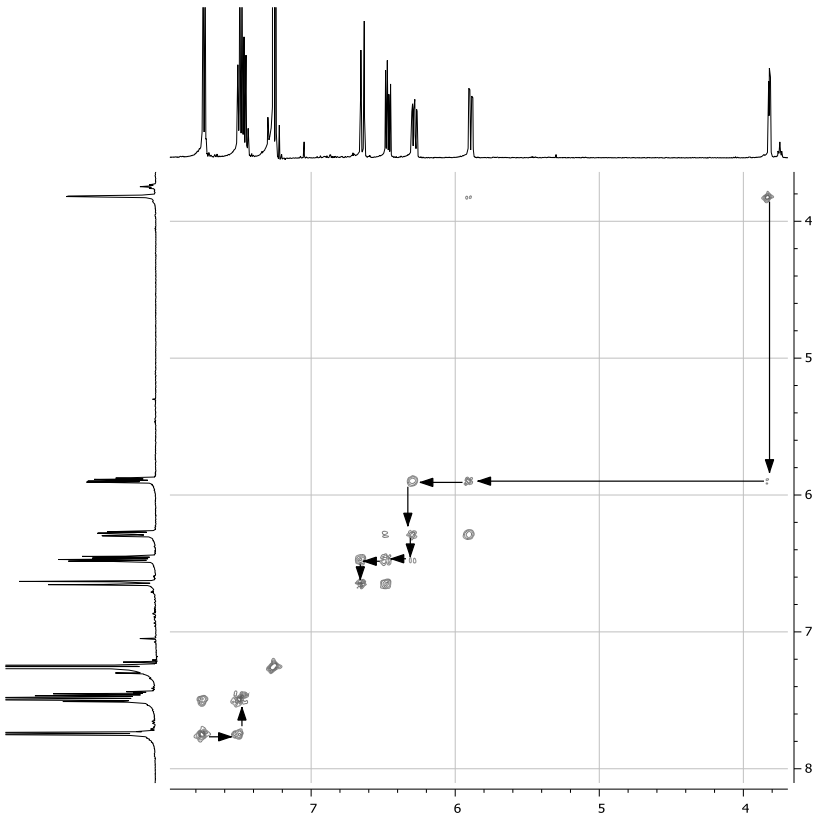


^{13}C NMR (125 MHz) spectrum of **20** in $CDCl_3$

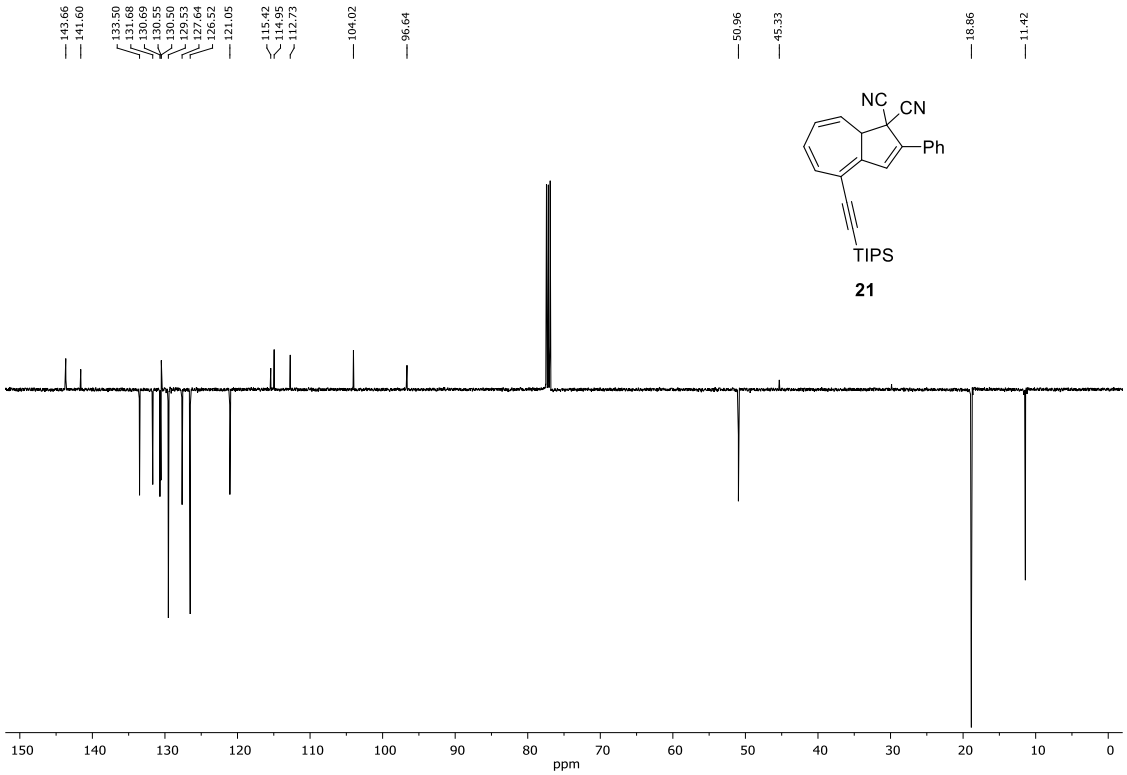
Compound 21



^{1}H NMR (500 MHz) spectrum of **21** in $CDCl_3$

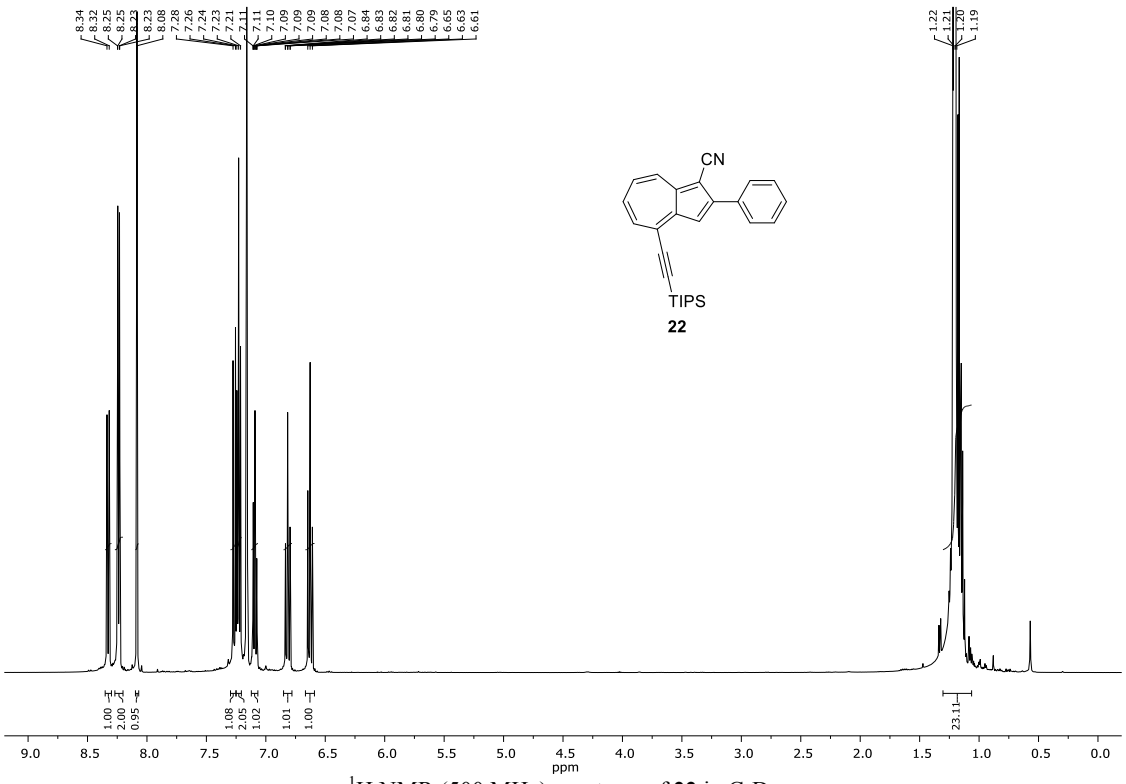


COSY spectrum (500 MHz) of **21** in $CDCl_3$

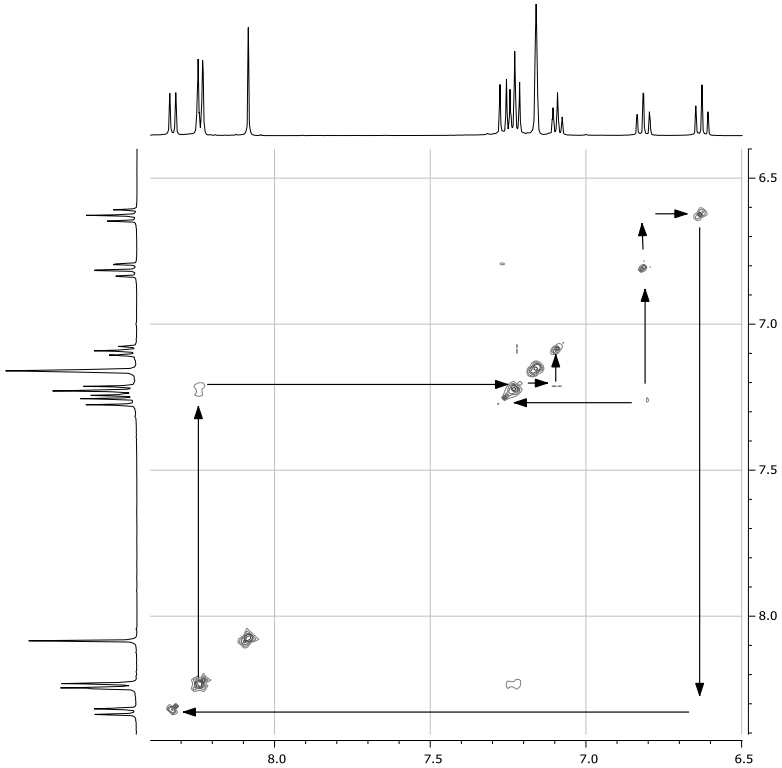


^{13}C NMR APT (125 MHz) spectrum of **21** in $CDCl_3$

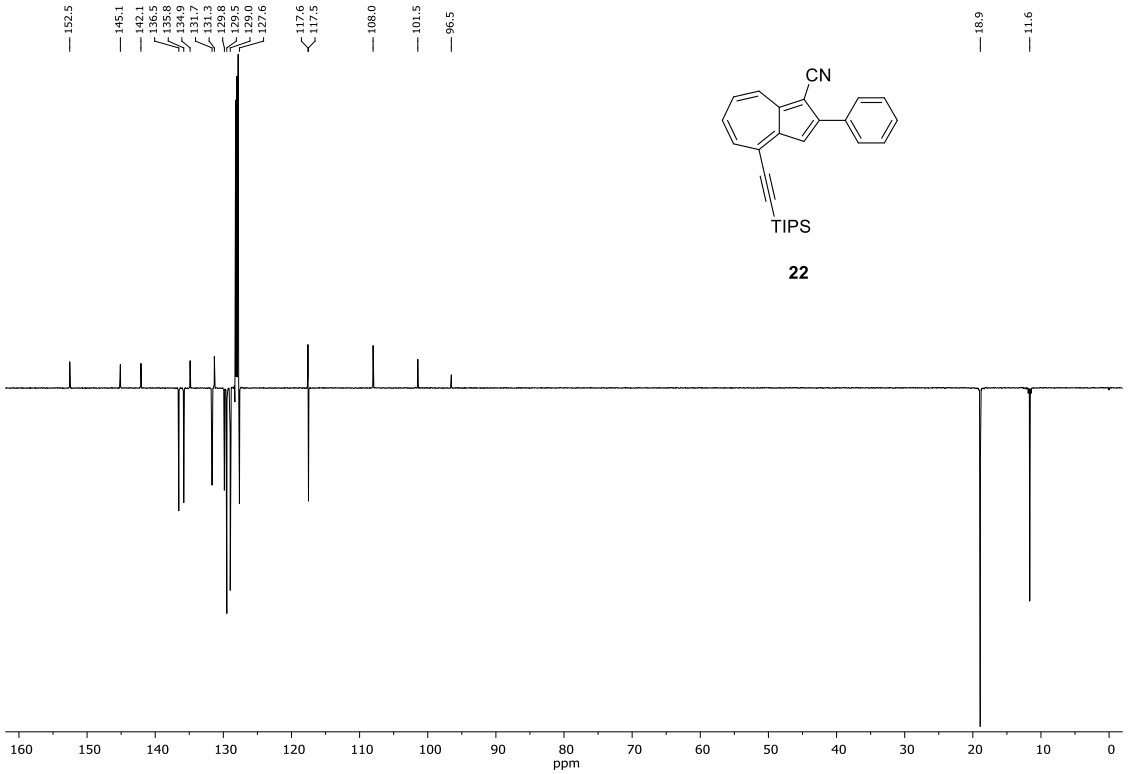
Compound 22



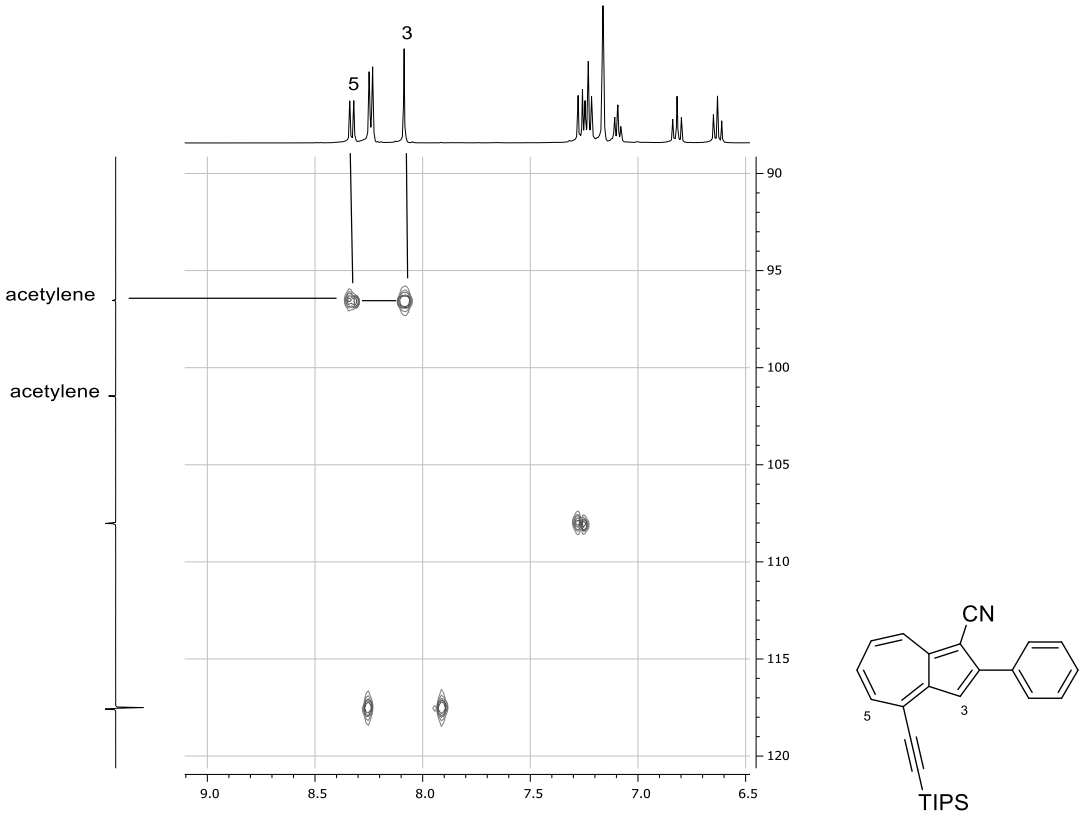
^{1}H NMR (500 MHz) spectrum of **22** in C_6D_6



COSY spectrum (500 MHz) of **22** in C_6D_6

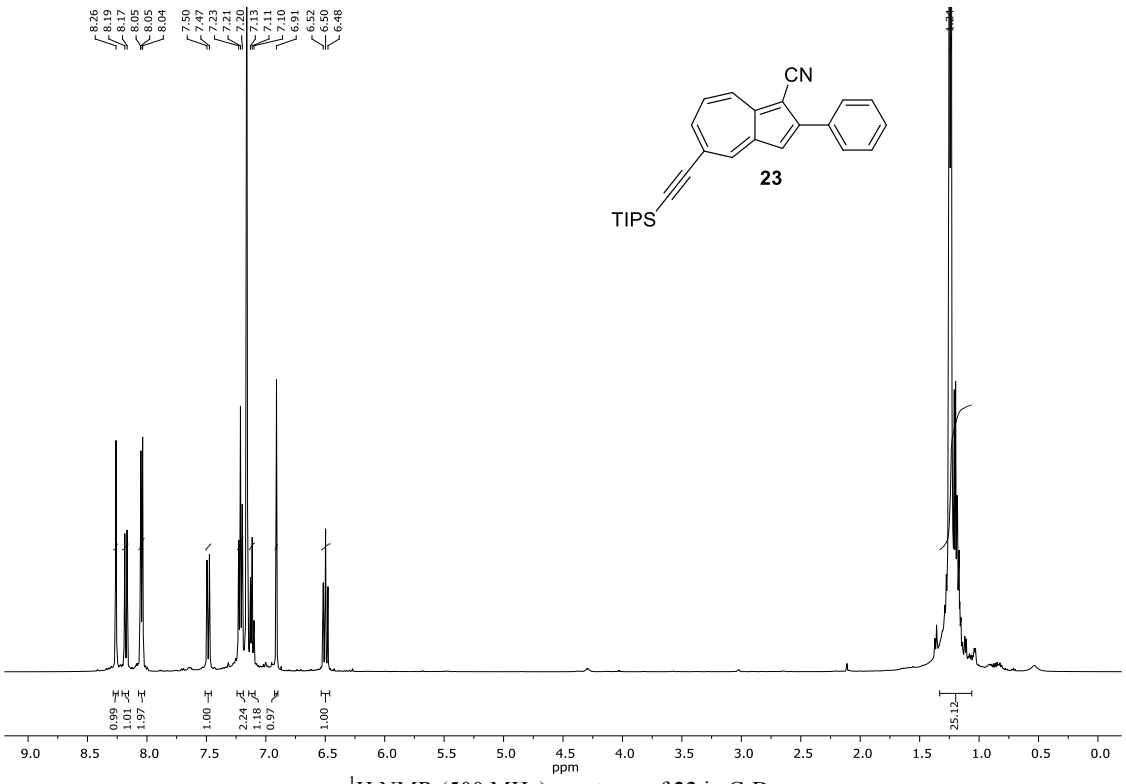


^{13}C NMR APT (125 MHz) spectrum of **22** in C_6D_6

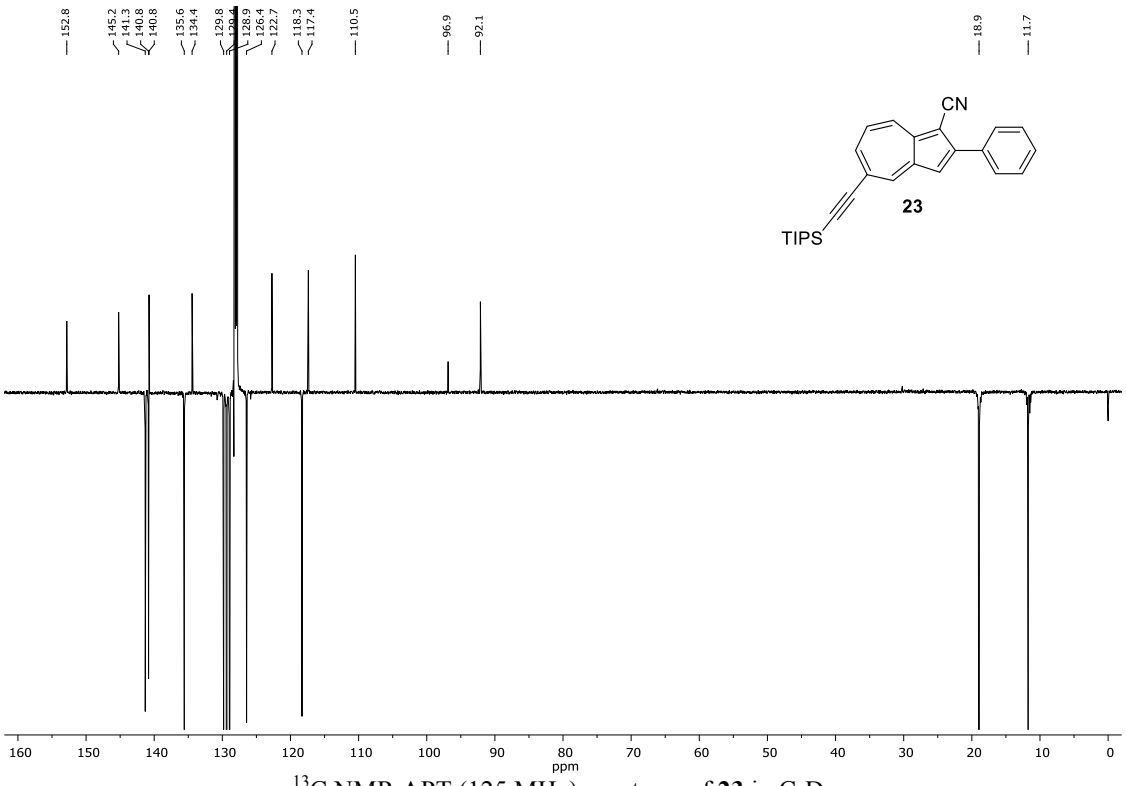


HMBC spectrum (500 /125 MHz) of **22** in C_6D_6

Compound 23

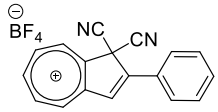


^{1}H NMR (500 MHz) spectrum of **23** in C_6D_6

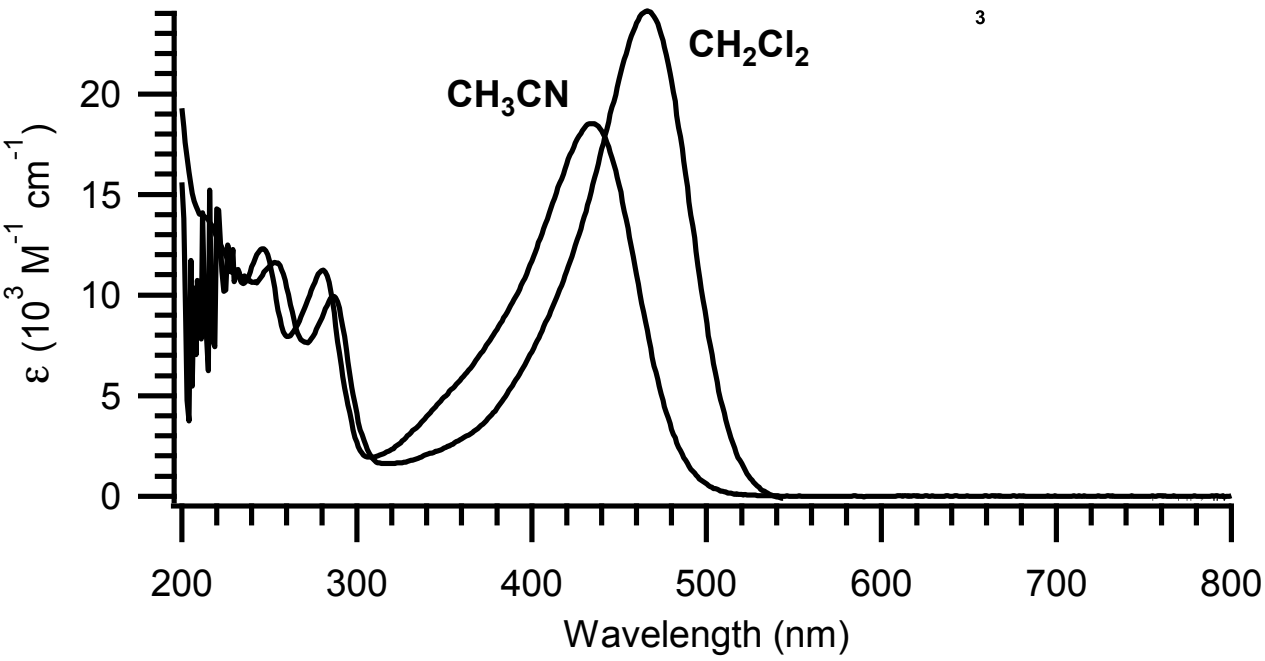


^{13}C NMR APT (125 MHz) spectrum of **23** in C_6D_6

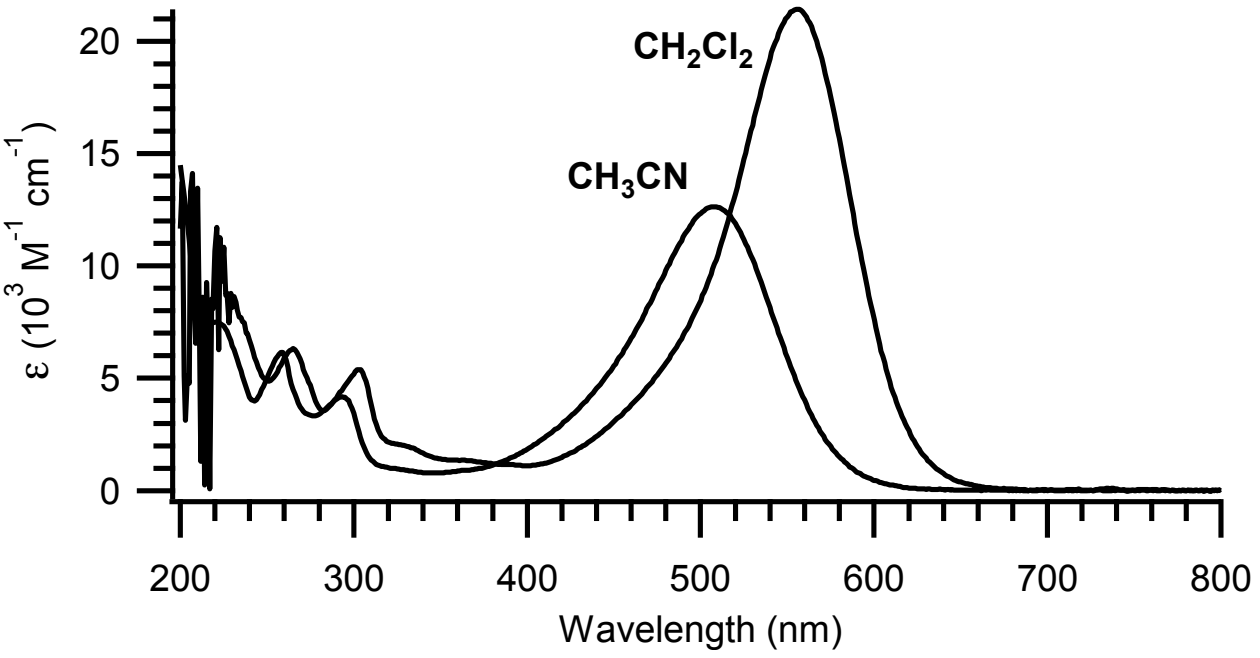
UV-Vis Absorption Spectra



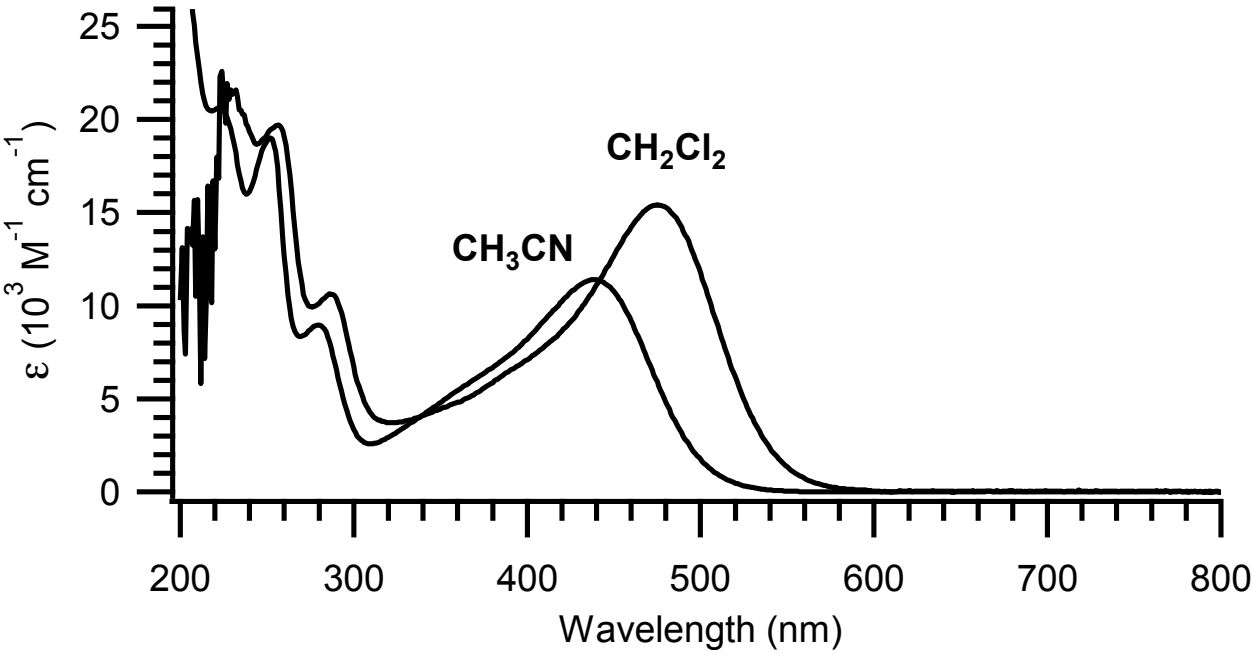
3



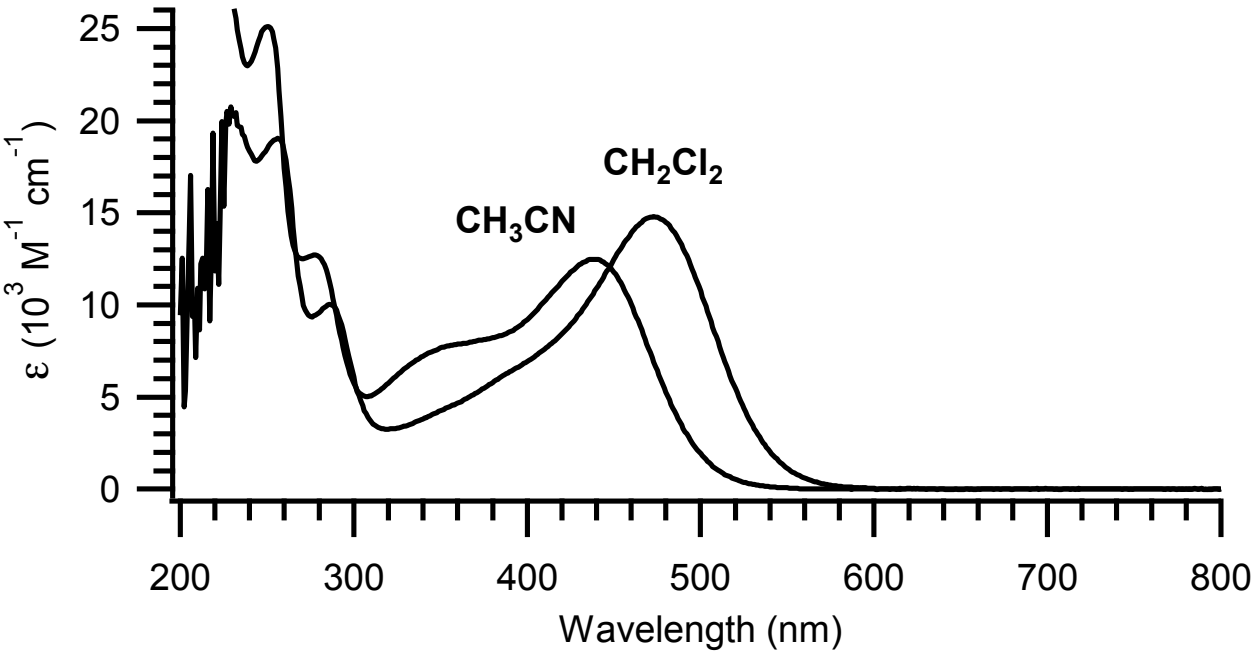
UV-Vis absorption spectra of compound **3**.



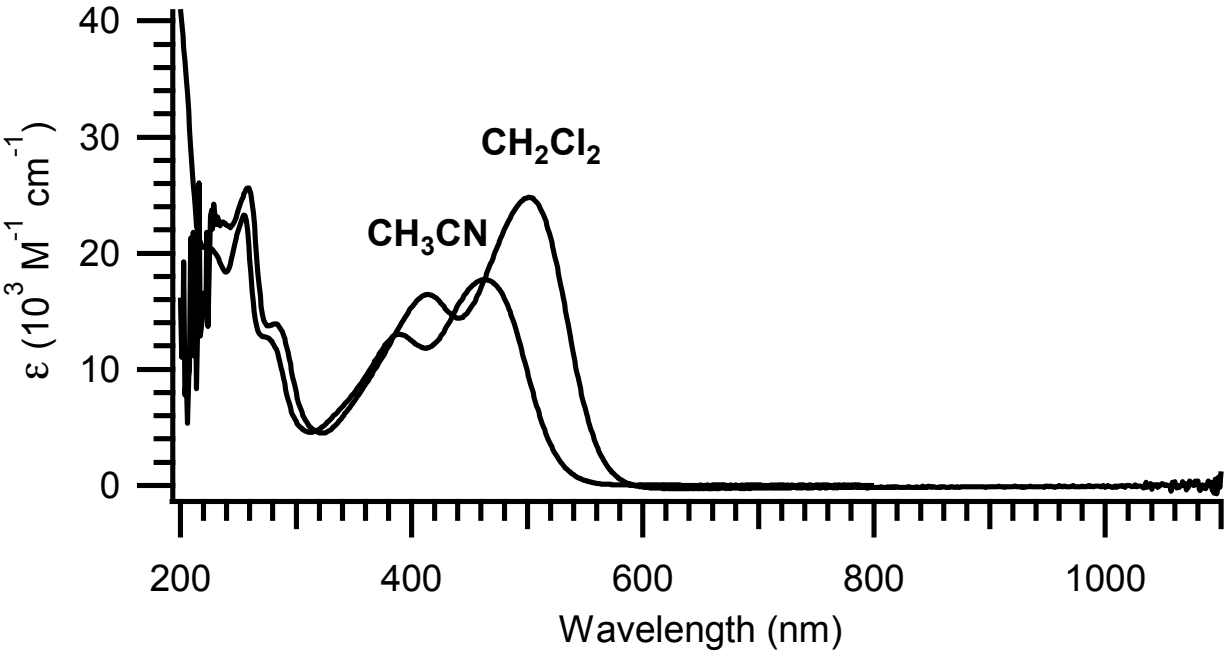
UV-Vis absorption spectra of compound **4**.



UV-Vis absorption spectra of compound **5**.



UV-Vis absorption spectra of compound **6**.



UV-Vis absorption spectra of compound **7**.

Calculational Data

Free energy differences (kJ/mol) between DHA **21** and **25** in MeCN:

CAM	38.8
M06-2X	30.6
PBE0	35.7

Free energy differences (kJ/mol) of s-*cis* and s-*tran*s conformers of *E*/*Z*-VHFs **24** and **26** in MeCN:

E-**24** (s-*cis vs* s-*trans*)

CAM	-2.9
M06-2X	-3.7
PBE0	-4.1

Z-**24** (s-*cis vs* s-*trans*)

CAM	-2.9
M06-2X	-5.0
PBE0	-5.8

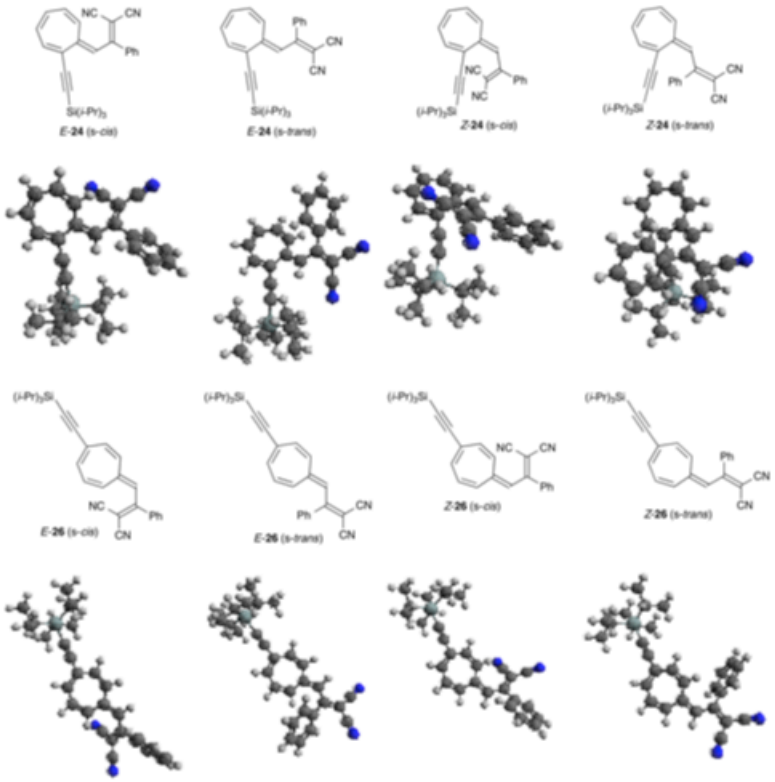
E-**26** (s-*cis vs* s-*trans*)

CAM	-11.5
M06-2X	-14.8
PBE0	-13.0

Z-**26** (s-*cis vs* s-*trans*)

CAM	-9.5
M06-2X	-10.8
PBE0	-10.5

Geometries of *E*/*Z*-VHFs 24 and 26 (s-*cis*/s-*trans*):



Coordinates at the CAM-B3LYP/6-311+G(d) level of theory

Compound 21

C	-0.77843	-4.37996	-0.28981
C	0.06920	-3.46646	0.22930
C	-0.05403	-2.01852	0.11965
C	-1.97160	-4.09760	-1.06359
C	-1.25141	-1.38358	0.06312
C	-2.77565	-3.04275	-0.89371
C	-2.56244	-2.09919	0.25911
H	-0.48415	-5.42278	-0.22129
H	0.99132	-3.82739	0.67301
H	-3.59967	-2.87779	-1.57800
C	-1.50389	0.02232	-0.12372
H	-0.71526	0.72975	-0.34070
C	-2.79790	0.34730	0.02056
C	-3.60072	-0.91688	0.40635
H	-2.54320	-2.67881	1.18578
C	-4.03388	-0.84142	1.81304
C	-4.79362	-1.08109	-0.43662
N	-4.33343	-0.79473	2.91835
N	-5.71229	-1.20744	-1.10957
H	-2.21433	-4.80644	-1.84972
C	-3.41014	1.67083	-0.13720
C	-2.73402	2.66744	-0.85396
C	-4.65863	1.98243	0.40957
C	-3.27886	3.93145	-0.99954
H	-1.78036	2.44723	-1.31807
C	-5.20389	3.25020	0.26148
H	-5.21980	1.24709	0.97232
C	-4.51687	4.23005	-0.44024
H	-2.73915	4.68534	-1.56099
H	-6.17083	3.46920	0.69926
H	-4.94470	5.21894	-0.55776
C	1.16066	-1.26762	0.06260
C	2.19619	-0.64297	0.02069
Si	3.76648	0.33992	-0.05212
C	3.33194	2.07152	0.59900
C	4.43416	3.11275	0.36829
H	5.32310	2.90087	0.96758
H	4.74838	3.16780	-0.67644
H	4.08545	4.10993	0.65512
C	2.86398	2.09933	2.05814
H	3.69002	1.91145	2.74788
H	2.45369	3.08211	2.31121
H	2.08797	1.35756	2.26144
C	4.28210	0.45893	-1.87655
H	5.19378	1.07002	-1.89222
H	2.47289	2.36448	-0.01911
C	3.23018	1.17439	-2.73201
H	3.01744	2.18495	-2.37603
H	3.56791	1.25965	-3.76966
H	2.28518	0.62362	-2.74351
C	4.62763	-0.90490	-2.48436
H	4.92649	-0.79666	-3.53180
H	5.45003	-1.39886	-1.96235
H	3.76860	-1.58199	-2.46178
C	5.06304	-0.64996	0.92048
H	5.13014	-1.59385	0.36369
C	4.65525	-1.00851	2.35361
H	5.37276	-1.70989	2.79143
H	4.63185	-0.12910	3.00066

H	3.66951	-1.47693	2.39749
C	6.45552	-0.00759	0.89877
H	6.47779	0.92220	1.47283
H	7.19601	-0.67781	1.34653
H	6.79722	0.22285	-0.11334

Compound 25

C	-0.66568	4.27925	-0.46659
C	-0.28741	3.80262	-1.67009
C	0.75555	2.84756	-1.94171
C	-0.09164	3.95546	0.82117
C	1.28910	1.94574	-1.09895
C	0.59679	2.86659	1.17921
C	0.82014	1.63769	0.32284
H	-1.42405	5.05559	-0.45639
H	-0.76549	4.23005	-2.54575
H	0.96381	2.81290	2.19813
C	2.31442	0.98972	-1.44384
H	2.71442	0.91362	-2.44686
C	2.71080	0.22903	-0.41392
C	2.03634	0.74674	0.86966
C	1.58925	-0.31591	1.77858
C	3.01387	1.58547	1.59338
N	1.25893	-1.14776	2.49364
N	3.79997	2.22440	2.12977
H	-0.24871	4.69964	1.59670
C	3.69171	-0.86182	-0.43212
C	3.90503	-1.57341	-1.61949
C	4.43067	-1.22108	0.69864
C	4.83821	-2.59474	-1.67690
H	3.32047	-1.33763	-2.50082
C	5.36484	-2.24601	0.63908
H	4.30096	-0.69673	1.63734
C	5.57413	-2.93516	-0.54707
H	4.98449	-3.13507	-2.60513
H	5.93105	-2.50391	1.52658
H	6.30117	-3.73786	-0.59083
H	1.13950	2.84383	-2.95792
C	-0.39742	0.82152	0.25582
C	-1.41118	0.17168	0.18320
Si	-2.97434	-0.82356	0.06042
C	-3.87331	-0.59546	1.71691
C	-3.04616	-1.07782	2.91341
C	-5.27106	-1.22538	1.73937
H	-3.99626	0.48994	1.82082
H	-2.05358	-0.62246	2.94049
H	-3.54756	-0.83131	3.85465
H	-2.91050	-2.16287	2.89866
H	-5.90074	-0.88384	0.91409
H	-5.22045	-2.31613	1.68559
H	-5.79129	-0.97692	2.66976
C	-3.98895	-0.08097	-1.36021
C	-3.24551	-0.10842	-2.70076
C	-4.46556	1.34207	-1.04549
H	-4.87817	-0.71677	-1.45905
H	-2.96984	-1.11967	-3.00615
H	-3.86891	0.31214	-3.49616
H	-2.32758	0.48480	-2.66003
H	-5.08553	1.38677	-0.14753
H	-3.62171	2.02254	-0.89807
H	-5.06153	1.74068	-1.87256
C	-2.50061	-2.64201	-0.24113

C	-1.20563	-2.83963	-1.03795
C	-3.64679	-3.44106	-0.87789
H	-2.32841	-3.05812	0.75942
H	-0.35455	-2.34461	-0.56728
H	-0.96687	-3.90489	-1.11948
H	-1.28838	-2.45007	-2.05595
H	-4.57796	-3.37217	-0.31151
H	-3.85821	-3.10004	-1.89478
H	-3.38468	-4.50162	-0.94272

Compound *E*-24 (s-*trans*)

C	1.53813	1.29550	-0.37410
C	2.50922	-1.03817	-0.18600
C	3.16169	-3.41896	-0.14892
N	3.88411	-4.29502	0.04463
C	3.90013	-0.67229	0.18569
C	4.13801	0.01312	1.37780
C	4.97599	-1.01561	-0.63235
C	5.43272	0.34467	1.74602
H	3.30554	0.27912	2.01875
C	6.26903	-0.66456	-0.27090
H	4.79991	-1.53689	-1.56622
C	6.50016	0.01256	0.91956
H	5.60897	0.86680	2.67935
H	7.09696	-0.92238	-0.92107
H	7.51113	0.28090	1.20420
C	2.46860	4.38888	-0.34498
H	3.04790	5.30537	-0.31777
C	3.15368	3.22939	-0.80698
H	4.15120	3.41026	-1.19459
C	2.75676	1.93376	-0.82081
H	3.48128	1.25100	-1.24205
C	2.22422	-2.37826	-0.39058
C	1.45815	-0.07680	-0.23347
H	0.46137	-0.48655	-0.13195
C	0.30659	2.07398	-0.19748
C	0.19123	3.42737	-0.02179
H	-0.82210	3.76857	0.15993
C	0.94103	-2.81139	-0.82310
N	-0.09368	-3.17009	-1.17976
C	1.16152	4.46664	0.00149
H	0.78069	5.44074	0.28817
C	-0.92894	1.35327	-0.13433
C	-1.98851	0.77354	-0.07022
Si	-3.62947	-0.09241	0.04362
C	-4.68655	0.95813	1.22094
H	-4.75577	1.92471	0.70506
C	-4.04901	1.22942	2.58797
H	-3.03450	1.62461	2.49967
H	-4.63990	1.96260	3.14627
H	-3.99936	0.32611	3.19969
C	-6.11523	0.42526	1.38594
H	-6.61531	0.25771	0.42883
H	-6.13076	-0.51968	1.93490
H	-6.72734	1.13418	1.95221
C	-4.39130	-0.08205	-1.69531
H	-5.34621	-0.61595	-1.60559
C	-4.69689	1.33161	-2.20267
H	-5.14427	1.29485	-3.20094
H	-5.39447	1.86678	-1.55481

H	-3.78755	1.93522	-2.27854
C	-3.52822	-0.84042	-2.71049
H	-2.55097	-0.36514	-2.83518
H	-3.35288	-1.87826	-2.41910
H	-4.00973	-0.85435	-3.69329
C	-3.24990	-1.87567	0.56950
H	-2.50679	-2.20589	-0.16706
C	-4.45382	-2.81955	0.45653
H	-4.15005	-3.85169	0.65795
H	-5.23585	-2.57012	1.17811
H	-4.90718	-2.80409	-0.53721
C	-2.59482	-2.00202	1.94919
H	-3.30098	-1.78012	2.75273
H	-2.23686	-3.02379	2.11079
H	-1.73869	-1.33334	2.06707

Compound *E*-24 (s-*cis*)

C	-1.69171	1.69740	-0.27947
C	-2.74870	-0.58210	0.13578
C	-5.09016	-1.17970	0.63071
N	-6.02405	-1.85133	0.57806
C	-2.45804	-1.97164	-0.29727
C	-2.75021	-3.06325	0.52251
C	-1.84055	-2.19384	-1.53028
C	-2.43929	-4.35119	0.11245
H	-3.19641	-2.90428	1.49696
C	-1.54683	-3.48364	-1.94641
H	-1.60513	-1.35113	-2.17000
C	-1.84421	-4.56443	-1.12483
H	-2.65773	-5.18967	0.76353
H	-1.08212	-3.64513	-2.91216
H	-1.60679	-5.57214	-1.44634
C	-2.45741	4.80957	-0.67961
H	-2.98530	5.75266	-0.77060
C	-3.22974	3.63611	-0.91923
H	-4.23761	3.81487	-1.27955
C	-2.90257	2.33418	-0.74054
H	-3.68969	1.63478	-0.99734
C	-3.97924	-0.29145	0.70019
C	-1.67069	0.34455	-0.00280
H	-0.69423	-0.11680	0.06289
C	-0.41315	2.42176	-0.26144
C	-0.21932	3.77547	-0.29617
H	0.81728	4.08121	-0.20406
C	-4.22157	0.89376	1.44321
N	-4.43097	1.83851	2.06759
C	-1.13370	4.86156	-0.40115
H	-0.68984	5.84421	-0.28524
C	0.77896	1.63871	-0.13968
C	1.78863	0.98030	-0.03995
Si	3.31921	-0.06334	0.10439
C	4.27397	0.11252	-1.52703
H	5.15693	-0.53181	-1.42811
C	4.76872	1.54242	-1.77174
H	5.43024	1.89716	-0.97854
H	5.32696	1.60222	-2.71129
H	3.93510	2.24694	-1.84613
C	3.46655	-0.38743	-2.73078
H	3.16723	-1.43298	-2.62975
H	2.55688	0.20317	-2.87263
H	4.05338	-0.30445	-3.65089
C	4.33043	0.67438	1.53134
H	4.53749	1.69778	1.19217
C	3.57585	0.79071	2.86044
H	4.15919	1.37258	3.58106
H	2.60863	1.28530	2.74587
H	3.39541	-0.18774	3.31071
C	5.68233	-0.02080	1.73669
H	5.55751	-1.03788	2.11683
H	6.26865	-0.08345	0.81664
H	6.28636	0.52274	2.46985
C	2.70559	-1.84980	0.30029
H	2.02894	-1.97890	-0.55478
C	1.88007	-2.10130	1.56701
H	1.40436	-3.08616	1.52542
H	2.50559	-2.08600	2.46232
H	1.08849	-1.36094	1.70521
C	3.81537	-2.89968	0.16504
H	4.52370	-2.84953	0.99581

H	3.39044	-3.90833	0.16740
H	4.38597	-2.79065	-0.75996

Compound *Z*-24 (s-*trans*)

C	2.48573	1.12007	-1.05558
C	2.13772	-1.30221	-0.42582
C	1.72718	-3.73218	-0.24270
N	1.56049	-4.72325	0.31779
C	1.99576	-1.13527	1.03844
C	0.88437	-1.62952	1.72208
C	3.01332	-0.50648	1.75993
C	0.78886	-1.49271	3.09781
H	0.07601	-2.09490	1.17237
C	2.92443	-0.38691	3.13812
H	3.88435	-0.12657	1.24001
C	1.81054	-0.87591	3.80961
H	-0.08780	-1.86537	3.61465
H	3.72679	0.09047	3.68854
H	1.73780	-0.77515	4.88654
C	2.84192	3.72636	0.62849
H	2.89092	4.39887	1.47829
C	1.70625	2.85962	0.59323
H	0.89612	3.13873	1.25926
C	1.48963	1.74840	-0.16219
C	1.94956	-2.54189	-0.99277
C	2.61679	-0.22018	-1.24916
H	3.20538	-0.52026	-2.11084
C	3.82254	3.18567	-1.59704
H	4.45394	3.63464	-2.35713
C	2.02663	-2.72728	-2.40346
N	2.08526	-2.88222	-3.54222
C	3.76310	3.88912	-0.34987
H	4.49692	4.67706	-0.21666
C	3.25678	2.00264	-1.91786
H	3.47679	1.60278	-2.90335
C	0.17366	1.18909	-0.15107
C	-0.97141	0.79877	-0.17932
Si	-2.75709	0.29731	-0.24227
C	-3.73177	1.90302	-0.53622
H	-3.31629	2.27606	-1.48163
C	-3.11491	-0.64596	1.36735
H	-2.37688	-1.45842	1.35720
C	-2.98321	-0.86103	-1.72915
H	-4.05000	-1.11889	-1.74645
C	-5.23253	1.67722	-0.75770
H	-5.73088	1.35253	0.15913
H	-5.71806	2.60613	-1.07307
H	-5.43703	0.92787	-1.52613
C	-3.50081	2.99718	0.51161
H	-3.95583	2.74107	1.47088
H	-2.43924	3.18471	0.68786
H	-3.95126	3.94019	0.18560
C	-2.87043	0.16321	2.64548
H	-1.88820	0.64111	2.65310
H	-3.62126	0.94563	2.77583
H	-2.92695	-0.48477	3.52599
C	-4.50307	-1.29776	1.39798
H	-4.61186	-1.92640	2.28738
H	-5.29957	-0.55067	1.43540
H	-4.68861	-1.93229	0.52812
C	-2.19450	-2.16712	-1.58399
H	-1.11806	-1.97880	-1.53952
H	-2.46910	-2.72517	-0.68605
H	-2.37220	-2.82370	-2.44142
C	-2.65000	-0.18186	-3.06232
H	-1.60300	0.13269	-3.09965

H	-2.81070	-0.87065	-3.89764
H	-3.26591	0.70084	-3.24736

Compound *Z*-24 (s-*cis*)

C	2.49712	1.60440	-0.56263
C	2.24436	-0.76080	0.39966
C	0.94493	-1.58694	2.32348
N	0.34116	-2.36917	2.91385
C	2.39572	-2.13378	-0.14083
C	2.85306	-3.18529	0.65568
C	2.11908	-2.37478	-1.48876
C	3.01638	-4.45327	0.11769
H	3.11162	-3.00761	1.69247
C	2.26774	-3.64617	-2.02100
H	1.76922	-1.56304	-2.11606
C	2.71726	-4.68808	-1.21854
H	3.38475	-5.25822	0.74299
H	2.03515	-3.82347	-3.06461
H	2.84187	-5.68056	-1.63640
C	1.88041	4.64213	0.10520
H	1.50528	5.53440	0.59445
C	0.99830	3.52325	0.12366
H	-0.01124	3.75528	0.44614
C	1.20944	2.21089	-0.19373
C	1.65938	-0.56628	1.63177
C	2.82403	0.28228	-0.39667
H	3.68397	-0.05321	-0.96760
C	3.69312	3.71811	-1.32168
H	4.52253	4.04744	-1.93919
C	1.74667	0.66268	2.33891
N	1.83095	1.63841	2.94389
C	3.06207	4.73950	-0.54809
H	3.56138	5.70250	-0.53526
C	3.44101	2.39015	-1.33896
H	4.09452	1.79493	-1.96930
C	0.04190	1.38509	-0.18592
C	-0.99998	0.76970	-0.20029
Si	-2.68918	-0.00088	-0.26063
C	-3.81381	1.25119	-1.13976
H	-4.80876	0.78845	-1.16687
C	-3.22948	-0.36909	1.52576
H	-2.73649	-1.31622	1.77707
C	-2.54191	-1.58078	-1.30469
H	-2.00998	-1.26158	-2.21013
C	-3.94252	2.58534	-0.39655
H	-2.97197	3.07692	-0.28474
H	-4.59198	3.27213	-0.94873
H	-4.36958	2.46879	0.60104
C	-3.37198	1.49364	-2.58823
H	-2.37503	1.94183	-2.62909
H	-3.34392	0.57564	-3.17927
H	-4.05772	2.18345	-3.09022
C	-2.76408	0.66414	2.55874
H	-1.68224	0.80700	2.53896
H	-3.22578	1.64128	2.39760
H	-3.03737	0.34219	3.56868
C	-4.74367	-0.59462	1.63868
H	-5.01293	-0.88949	2.65767
H	-5.30495	0.31506	1.40873
H	-5.10488	-1.37823	0.96955
C	-3.89154	-2.16065	-1.74682
H	-4.46300	-2.54824	-0.89930
H	-4.51929	-1.42758	-2.25812
H	-3.74085	-2.99736	-2.43617
C	-1.69229	-2.66383	-0.63214
H	-2.18377	-3.06315	0.25905

H	-1.52873	-3.50531	-1.31272
H	-0.71019	-2.29512	-0.32971

Compound *E*-26 (s-*trans*)

C	2.45018	0.66582	-0.34130
C	-0.71328	-0.08324	-0.47463
C	-0.05029	1.16731	-0.20462
H	-0.72386	1.98812	0.01670
C	1.26517	1.47514	-0.15626
H	1.47540	2.50938	0.09714
C	1.28428	-1.44388	-1.13236
H	1.50807	-2.41201	-1.56891
C	-0.10126	-1.23074	-0.88601
H	-0.74360	-2.08096	-1.08461
C	2.36700	-0.65678	-0.90847
H	3.30861	-1.08844	-1.21618
C	-2.13502	-0.08270	-0.32121
C	-3.33619	-0.05440	-0.18377
Si	-5.18092	-0.02552	0.02823
C	-5.76003	1.78440	-0.06788
H	-5.87650	1.98607	-1.14017
C	-4.75141	2.80454	0.47323
H	-5.12375	3.82356	0.32724
H	-4.57600	2.67705	1.54448
H	-3.78426	2.73043	-0.02693
C	-7.13264	1.99090	0.58886
H	-7.48645	3.01315	0.42322
H	-7.89690	1.31647	0.19674
H	-7.08758	1.83834	1.67043
C	-5.88246	-1.06847	-1.39454
H	-5.40590	-2.05049	-1.28249
C	-5.49466	-0.52811	-2.77521
H	-5.83456	-1.20582	-3.56464
H	-5.95261	0.44553	-2.97111
H	-4.41388	-0.41246	-2.88519
C	-7.39924	-1.27598	-1.30480
H	-7.73937	-1.96923	-2.08039
H	-7.71241	-1.68708	-0.34193
H	-7.94254	-0.33937	-1.45542
C	-5.56264	-0.83342	1.70193
H	-6.65015	-0.75543	1.82903
C	-4.90297	-0.10868	2.88085
H	-5.21486	0.93453	2.95946
H	-5.16130	-0.59642	3.82605
H	-3.81259	-0.12080	2.79727
C	-5.19651	-2.32223	1.72106
H	-5.44870	-2.76853	2.68812
H	-5.72279	-2.89288	0.95296
H	-4.12391	-2.47184	1.56631
C	3.65115	1.29183	-0.04186
H	3.57217	2.34971	0.18351
C	4.96910	0.76906	0.01879
C	6.05587	1.63171	0.04585
C	5.90192	3.03306	-0.13184
C	7.38424	1.19357	0.29268
N	5.77870	4.16897	-0.27882
N	8.47433	0.88225	0.49812
C	5.24198	-0.68591	0.15009
C	6.03295	-1.35276	-0.78400
C	4.71273	-1.39223	1.23053
C	6.27652	-2.71265	-0.64865
H	6.44107	-0.81192	-1.63015
C	4.97401	-2.74641	1.37349
H	4.10074	-0.87618	1.96135
C	5.75070	-3.41056	0.43085
H	6.88055	-3.22607	-1.38771

H	4.56780	-3.28553	2.22147
H	5.94659	-4.47119	0.53908

Compound *E*-26 (s-*cis*)

C	-2.37563	-0.15520	0.06638
C	0.83261	0.16749	0.42982
C	0.05998	-0.82759	-0.27327
H	0.65819	-1.57036	-0.78970
C	-1.27632	-0.96514	-0.41420
H	-1.58446	-1.80799	-1.02489
C	-1.03642	1.36006	1.59719
H	-1.17553	2.09721	2.38138
C	0.32694	1.12684	1.25609
H	1.04427	1.77652	1.74427
C	-2.18069	0.83465	1.09498
H	-3.09068	1.20051	1.55507
C	2.25057	0.09526	0.25645
C	3.44719	0.01773	0.09857
Si	5.28627	-0.09571	-0.13906
C	5.60613	-1.79081	-0.93363
H	4.94211	-1.78777	-1.80813
C	5.19862	-2.98587	-0.06495
H	5.23562	-3.91259	-0.64623
H	5.87493	-3.11386	0.78322
H	4.18519	-2.88769	0.33139
C	7.03909	-1.96657	-1.45160
H	7.13432	-2.90777	-2.00213
H	7.34309	-1.16413	-2.12753
H	7.76400	-1.99990	-0.63458
C	5.78202	1.28227	-1.34700
H	6.86608	1.18199	-1.48717
C	5.51499	2.68388	-0.78679
H	5.82536	3.45127	-1.50287
H	4.45045	2.83920	-0.58826
H	6.05466	2.87234	0.14378
C	5.11879	1.11977	-2.71966
H	5.44859	1.90753	-3.40412
H	5.35554	0.16218	-3.18860
H	4.02970	1.18994	-2.64612
C	6.05433	0.22944	1.56622
H	5.70202	1.23963	1.81239
C	7.58729	0.27433	1.54224
H	7.97658	0.96159	0.78703
H	7.97732	0.60210	2.51092
H	8.01592	-0.71113	1.34275
C	5.55759	-0.69853	2.68028
H	5.91522	-0.35139	3.65486
H	4.46706	-0.74147	2.72741
H	5.92305	-1.71928	2.54989
C	-3.63292	-0.49365	-0.40356
H	-3.69423	-1.42027	-0.96373
C	-4.89170	0.14447	-0.20463
C	-5.07682	1.51462	-0.09911
C	-4.07542	2.45310	-0.46023
C	-6.30614	2.09565	0.32251
N	-3.28162	3.22824	-0.76994
N	-7.27136	2.60979	0.68362
C	-6.07589	-0.74997	-0.18777
C	-6.05320	-1.91039	0.58900
C	-7.20163	-0.47541	-0.96642
C	-7.14519	-2.76500	0.60659
H	-5.18094	-2.13258	1.19289
C	-8.28537	-1.34087	-0.96188
H	-7.21984	0.40335	-1.60007
C	-8.26237	-2.48259	-0.17036
H	-7.12283	-3.65457	1.22538

H	-9.14784	-1.12510	-1.58175
H	-9.11242	-3.15531	-0.16349

Compound *Z*-26 (s-*trans*)

C	-2.74234	-1.63003	0.10006
C	-4.92438	-0.32109	-0.00301
C	-7.18306	0.65736	-0.16873
N	-7.93827	1.52739	-0.15607
C	-4.37005	1.05442	0.09369
C	-4.50186	1.95469	-0.96232
C	-3.72035	1.45602	1.26104
C	-3.97428	3.23441	-0.85852
H	-4.99854	1.64711	-1.87542
C	-3.21151	2.74132	1.36890
H	-3.61986	0.76037	2.08623
C	-3.33147	3.63071	0.30717
H	-4.06843	3.92302	-1.69016
H	-2.71718	3.04863	2.28321
H	-2.92522	4.63231	0.38948
C	0.49915	-1.42168	0.08888
C	-0.50817	-0.52934	-0.42767
H	-0.10640	0.36442	-0.89298
C	-1.85804	-0.61300	-0.42375
H	-2.35287	0.21714	-0.90742
C	-6.29474	-0.45086	-0.18048
C	-4.11923	-1.47716	0.16618
H	-4.66944	-2.38553	0.38625
C	-0.97032	-3.36016	0.68139
H	-0.88303	-4.39084	1.00921
C	-6.91009	-1.72097	-0.34489
N	-7.40975	-2.74995	-0.48133
C	0.27285	-2.67774	0.57070
H	1.14273	-3.24290	0.88512
C	-2.24020	-2.92808	0.47928
H	-3.01264	-3.66706	0.66705
C	1.84632	-0.94453	0.03743
C	2.98027	-0.52678	-0.01216
Si	4.73215	0.08662	-0.09505
C	4.74121	1.47569	-1.38817
H	4.39746	0.97014	-2.30010
C	6.14249	2.02934	-1.67651
H	6.11453	2.72070	-2.52453
H	6.53908	2.58654	-0.82401
H	6.86325	1.24533	-1.92135
C	3.75541	2.61734	-1.11615
H	3.69687	3.28470	-1.98181
H	2.74530	2.25380	-0.91382
H	4.06483	3.22612	-0.26379
C	5.21308	0.54191	1.68442
H	4.99207	-0.37434	2.24749
C	4.36990	1.66239	2.30282
H	4.57396	1.74839	3.37476
H	4.59999	2.63184	1.85513
H	3.29734	1.48973	2.18612
C	6.70865	0.83408	1.85863
H	6.95120	0.96996	2.91725
H	7.34130	0.02689	1.48245
H	7.00439	1.75113	1.34315
C	5.80096	-1.36178	-0.69869
H	6.82934	-0.98002	-0.73491
C	5.42697	-1.82176	-2.11231
H	5.53082	-1.02580	-2.85285
H	6.06956	-2.64814	-2.43197
H	4.39418	-2.17984	-2.15557
C	5.78027	-2.54847	0.27193
H	6.42832	-3.35338	-0.08864

H	6.12497	-2.27838	1.27254
H	4.77344	-2.96435	0.37145

Compound *Z*-26 (s-*cis*)

C	2.49438	-1.26189	-0.54966
C	4.61988	0.12531	-0.32476
C	4.88050	2.56188	-0.04002
N	5.38549	3.50997	0.37523
C	5.98817	-0.10785	0.20051
C	6.18122	-1.02230	1.23833
C	7.09562	0.54227	-0.34708
C	7.45329	-1.26136	1.73612
H	5.32666	-1.53392	1.66595
C	8.36923	0.28800	0.13963
H	6.96520	1.22901	-1.17501
C	8.54965	-0.60790	1.18626
H	7.58930	-1.96103	2.55263
H	9.22313	0.78790	-0.30269
H	9.54511	-0.80115	1.56954
C	-0.74254	-1.18567	-0.35919
C	0.25693	-0.31173	0.20580
H	-0.15048	0.50831	0.78720
C	1.60450	-0.33718	0.11427
H	2.10366	0.45895	0.65381
C	4.19457	1.42484	-0.55321
C	3.85895	-1.04272	-0.62237
H	4.46168	-1.90433	-0.88818
C	0.76320	-2.99860	-1.21192
H	0.69259	-3.99533	-1.63508
C	3.07311	1.73168	-1.36708
N	2.17920	1.99904	-2.04252
C	-0.49624	-2.37460	-0.97922
H	-1.36031	-2.93565	-1.31639
C	2.02528	-2.54173	-1.02480
H	2.81542	-3.22775	-1.31366
C	-2.10033	-0.76392	-0.20522
C	-3.24266	-0.39233	-0.06477
Si	-4.99002	0.19934	0.14402
C	-4.93305	1.70784	1.29341
H	-5.97683	2.01889	1.42901
C	-4.17521	2.88171	0.66207
H	-4.18039	3.74835	1.33054
H	-3.12855	2.62584	0.47302
H	-4.61232	3.20012	-0.28667
C	-4.35948	1.38682	2.67820
H	-4.35587	2.28026	3.31062
H	-4.93484	0.62154	3.20260
H	-3.32646	1.03393	2.61093
C	-5.57577	0.70463	-1.59069
H	-4.83399	1.43767	-1.93152
C	-6.94489	1.39519	-1.59568
H	-7.18380	1.76827	-2.59647
H	-7.74461	0.70480	-1.31484
H	-6.99005	2.24673	-0.91232
C	-5.55665	-0.46014	-2.58631
H	-5.79814	-0.11074	-3.59506
H	-4.57993	-0.94746	-2.63339
H	-6.29515	-1.22403	-2.32741
C	-6.02030	-1.23709	0.84823
H	-6.29804	-1.83849	-0.02660
C	-7.32131	-0.75199	1.50312
H	-7.92654	-0.13399	0.83657
H	-7.93902	-1.60323	1.80574
H	-7.12358	-0.16342	2.40300
C	-5.25471	-2.16184	1.80211
H	-5.88553	-3.00341	2.10597

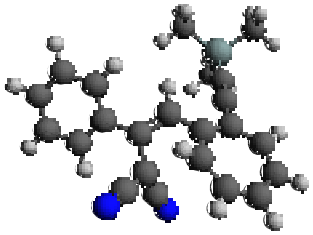
H	-4.35430	-2.57202	1.34148
H	-4.94848	-1.64464	2.71493

Transition State Calculations

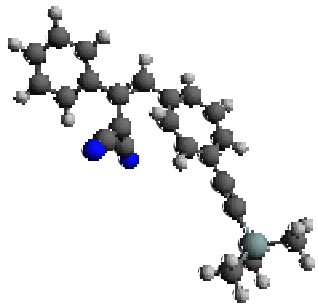
s-*cis*-VHF to TS activation energies (kJ/mol):

	"**24**-$SiMe_3$"	"**26**-$SiMe_3$"
CAM-B3LYP	91.5	94.9
M06-2X	92.4	93.4
PBE0	82.1	84.8

Geometries:



"**24**-$SiMe_3$"-TS



"**26**-$SiMe_3$"-TS

Coordinates:

"**24**-$SiMe_3$"-TS:

C	0.73132900	4.37204000	-0.07668200
C	1.48506800	3.24780600	-0.16984200
C	1.08025400	1.88735000	-0.38660600
C	-0.17712400	1.42808200	-0.72107000
C	-1.36517900	2.20483600	-0.95060900
C	-1.57767900	3.57822800	-0.65916600
C	-0.67380100	4.50822900	-0.24889300
C	-0.47957600	-0.00282800	-0.75730400
C	-1.67108600	-0.36611500	-0.25040500
C	-2.50773900	0.74318400	0.32421800
C	-2.19680500	1.21544600	1.61876000
N	-1.94252100	1.60166600	2.67744800
C	-3.86281600	0.85748100	-0.06342800
N	-4.95113500	0.97802500	-0.43021200
H	1.26494200	5.28847600	0.14849700
H	2.54965300	3.37265900	-0.00706000
H	-2.02961200	1.79175100	-1.69688300
H	-2.58876700	3.92939200	-0.83810900
H	0.26859400	-0.72203700	-1.06210400

C	-2.13816800	-1.76428500	-0.19430200
C	-2.99917100	-2.19209200	0.81941500
C	-1.72178400	-2.68969100	-1.15630000
C	-3.41016500	-3.51543600	0.88578700
H	-3.34106600	-1.48962300	1.57087300
C	-2.13763400	-4.01052600	-1.09230400
H	-1.08601200	-2.36674400	-1.97266100
C	-2.98020800	-4.42883300	-0.06864300
H	-4.07054100	-3.83314300	1.68454800
H	-1.81170900	-4.71385400	-1.85012100
H	-3.30785500	-5.46109800	-0.02087000
H	-1.05966500	5.51300800	-0.11146000
C	2.12352400	0.92267200	-0.22673400
C	3.02135000	0.12648900	-0.07675500
Si	4.39127800	-1.10170600	0.17068300
C	3.62902900	-2.67857600	0.83017200
H	2.96853900	-3.14337500	0.09434200
H	4.40781500	-3.40404900	1.08083000
H	3.04498100	-2.49371200	1.73456200
C	5.60248800	-0.36725100	1.39371100
H	5.93501800	0.62518500	1.08087800
H	5.16052200	-0.27395000	2.38850500
H	6.48931400	-1.00058800	1.48339900
C	5.20170200	-1.39024600	-1.49130600
H	4.46811900	-1.66336900	-2.25331500
H	5.73154900	-0.50058800	-1.83996600
H	5.92900400	-2.20408400	-1.42438000

"**26**-$SiMe_3$"-TS:

C	-1.74203000	2.48650000	0.19671300
C	-0.62282300	3.26366500	0.17596600
C	0.70359000	2.91449200	-0.17265000
C	1.17912600	1.73889700	-0.68221700
C	0.40042700	0.62407500	-1.14694900
C	-0.95818000	0.35994600	-0.88591200
C	-1.89764000	1.13632000	-0.23977100
C	2.60718300	1.46668700	-0.65914700
C	3.00164200	0.22100500	-0.32920500
C	1.92006900	-0.81933900	-0.17619100
C	1.53227200	-1.12629200	1.14759100
N	1.21669700	-1.29375800	2.24689300
C	1.77839900	-1.85092900	-1.12771000
N	1.63093100	-2.65320400	-1.94683600
H	-2.64353500	2.95113700	0.57844200
H	-0.74760900	4.27676100	0.54231000
H	1.44965400	3.67424400	0.03933800
H	0.79809900	0.12520300	-2.01930300

H	-1.31914700	-0.58457100	-1.27945000
H	3.30675000	2.29039300	-0.73297200
C	4.40415100	-0.11176200	0.01029800
C	4.86070400	-1.43225900	-0.03117500
C	5.31069600	0.88690300	0.38954300
C	6.18026000	-1.74162800	0.26983900
H	4.18906200	-2.23277400	-0.31231800
C	6.62698700	0.57813000	0.69032000
H	4.98215700	1.91532700	0.47556400
C	7.06953600	-0.73874800	0.62848500
H	6.51148100	-2.77278600	0.22320000
H	7.30795800	1.36764300	0.98727400
H	8.09887100	-0.98039900	0.86772700
C	-3.20755600	0.58009800	-0.09082900
C	-4.31237900	0.10628700	0.03674800
Si	-6.00167700	-0.65696900	0.21718300
C	-5.97392300	-1.73210500	1.74561300
H	-5.27446400	-2.56429500	1.63800100
H	-5.68432200	-1.16377500	2.63238500
H	-6.96546400	-2.15395200	1.93160700
C	-6.31667800	-1.66752300	-1.31586800
H	-7.29279400	-2.15743100	-1.26172400
H	-6.30954100	-1.04577300	-2.21417600
H	-5.56293600	-2.44786700	-1.44415900
C	-7.24629900	0.73433500	0.38859500
H	-7.03561100	1.35678600	1.26126000
H	-7.24787300	1.38098800	-0.49185600
H	-8.25588200	0.33091400	0.50537700