ELECTRONIC SUPPORTING INFORMATION

Engineering the HOMO-LUMO gap of indeno[1,2-b]fluorene

Raquel Casares,[a] Álvaro Martínez-Pinel,[a] Sandra Rodríguez-González,[b] Irene R. Márquez,[c] Luis Lezama,[d] M. Teresa González,[e] Edmund Leary,[e] Víctor Blanco,[a] Joel G. Fallaque,[e,f] Cristina Díaz,[g] Fernando Martín,[e,f,h] Juan M. Cuerva,[*a] Alba Millán,[*a]

[a.] *Departamento de Química Orgánica, Facultad de Ciencias, Unidad de Excelencia de Química Aplicada a Biomedicina y Medioambiente (UEQ), Universidad de Granada, 18071 Granada, Spain.*
[b.] *Departamento de Química Física Aplicada, Universidad Autónoma de Madrid, 28049 Madrid, Spain*
[c.] *Centro de Instrumentación Científica, Universidad de Granada, 18071 Granada, Spain.*
[d.] *Departamento de Química Orgánica e Inorgánica, Facultad de Ciencia y Tecnología, Universidad del País Vasco, 48940, Leioa, Spain.*
[e.] *Fundación IMDEA Nanociencia, 28049, Madrid, Spain.*
[f.] *Departamento de Química, Módulo 13, Universidad Autónoma de Madrid, 28049, Madrid, Spain.*
[g.] *Departamento de Química Física, Facultad de Ciencias Químicas, Universidad Complutense de Madrid, 28040, Madrid, Spain*
[h.] *Condensed Matter Physics Center (IFIMAC), 28049, Madrid, Spain.*

TABLE OF CONTENTS

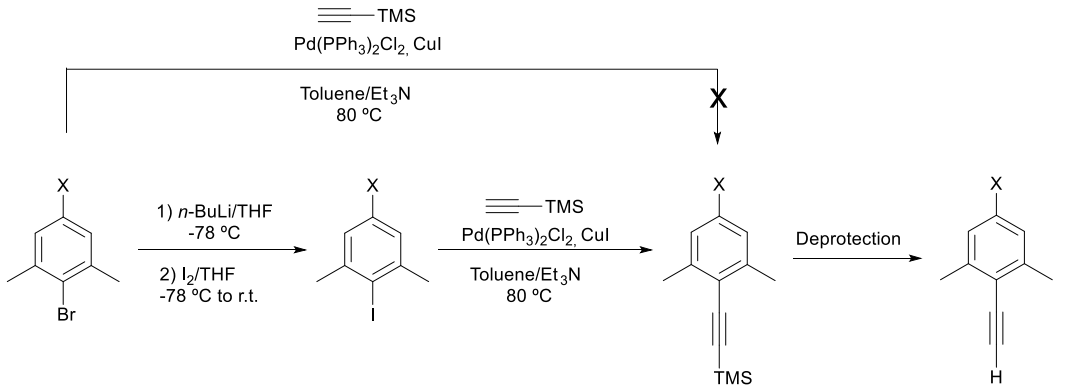
1. General Details

Unless otherwise stated, all reagents and solvents (DMF, DDQ, acetonitrile, CH2Cl2, EtOAc, Hexane, MeOH, toluene, Et_2O) were purchased from commercial sources and used without further purification. Anhydrous THF was freshly distilled over Na/benzophenone. Compound **5** was synthesized following the reported procedure.[S1] 2-bromo-5-fluoro-1,3-dimethylbenzene (**S1a**), 2-bromo-5-chloro-1,3-dimethylbenzene (**S2b**), 5-(tert-butyl)-2-iodo-1,3-dimethylbenzene (**S2e**), 2-bromo-5-methoxy-1,3-dimethylbenzene (**S1f**) and 2,4,6-trimethylphenyl acetylene (**6d**) are commercially available. Flash column chromatography was carried out using silica gel (40-63 µm) as the stationary phase. Analytical TLC was performed on aluminum sheets coated with silica gel with fluorescent indicator UV254 (Alugram SIL G/UV254, Mackerey-Nagel, Germany) and observed under UV light (254 nm) and/or stained with phosphomolybdic acid (5% methanol solution). All ^{1}H-, ^{13}C- and ^{19}F-NMR spectra were recorded on Bruker Avance Neo (400 MHz or 500 MHz) spectrometers at a constant temperature of 298 K or at 378 K. Chemical shifts are reported in ppm and referenced to residual solvent. Coupling constants (*J*) are reported in Hertz (Hz). Multiplicities are abbreviated as follow: s = singlet, br s = broad singlet, d = doublet, t =triplet m = multiplet, dd = doublet of doublets, td = triplet of doublets, ddd = doublet of doublet of doublets, dt = doublet of triplets. Assignment of the ^{13}C-NMR multiplicities was accomplished by DEPT techniques. HRMS spectra were obtained using ESI-TOF or GC-EI techniques. IR-ATR spectra were recorded on a Perkin Elmer Spectrum Two IR Spectrometer.

2. Synthetic procedures

2.1. General strategy and procedures for the synthesis of alkynes 6a-c, 6e, 6f and 6h

Alkynes **6a-c**, **6e**, **6f** and **6h** were prepared in three steps following a strategy based on lithiation-iodination of the corresponding Br-arenes **S1**, followed by Sonogashira cross-coupling reaction using TMS-acetylene and final deprotection. Sonogashira cross-coupling reactions on Br-arenes **S1** were unsuccessful, obtaining unaltered starting materials **S1**.



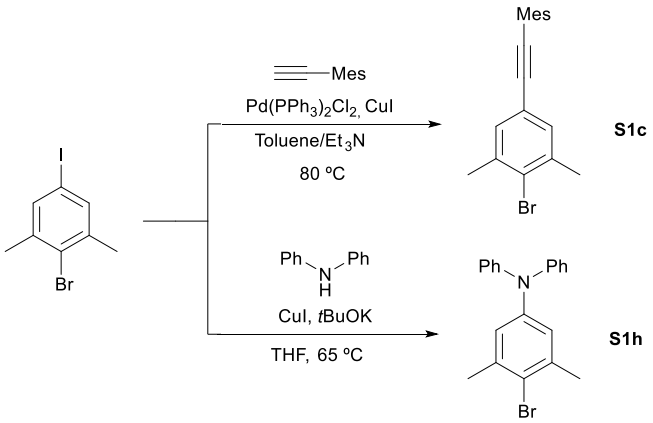
S1a, X = F
S1b, X = Cl
S1c, X = alk-Mes
S1f, X = OMe
S1h, X = $N(Ph)_2$

S2a, X = F
S2b, X = Cl
S2c, X = alk-Mes
S2e, X = *t*-Bu
S2f, X = OMe
S2h, X = $N(Ph)_2$

S2a, X = F
S3b, X = Cl
S3c, X = alk-Mes
S3e, X = *t*-Bu
S3f, X = OMe
S3h, X = $N(Ph)_2$

6a, X = F
6b, X = Cl
6c, X = alk-Mes
6e, X = *t*-Bu
6f, X = OMe
6h, X = $N(Ph)_2$

Procedures for the synthesis of bromoarenes S1c and S1h.



S1c. To a degassed mixture of 2-bromo-5-iodo-1,3-dimethylbenzene (2 g, 6.43 mmol, 1 equiv.), $Pd(PPh_3)_2Cl_2$ (0.21 g, 0.32 mmol, 5 mol%) and CuI (0.11 g, 0.6 mmol, 10 mol%) in toluene (35 mL) and triethylamine (Et_3N) (17.5 mL) was added a solution of 2,4,6-trimethylphenyl acetylene (1.43 mL, 9.16 mmol, 1.4 equiv.) in toluene (17.5 mL) and Et_3N (17.5 mL) at 80 °C.

The reaction mixture was heated to reflux for 18h, allowed to cool to room temperature and diluted with CH_2Cl_2 (150 mL). The mixture was washed with 10% aqueous NH_4OH, water and brine. The organic phase was dried over Na_2SO_4, filtered, and evaporated under reduced pressure. The residue was purified by column chromatography (SiO_2, Hexane/EtOAc, 9/1) to give **S1c** (1.4 g, 67%) as a white solid. **^{1}H NMR (500 MHz, $CDCl_3$)** δ(ppm): 7.24 (s, 2H), 6.90 (s, 2H), 2.48 (s, 6H), 2.43 (s, 6H), 2.30 (s, 3H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ: 140.1 (C), 138.4 (C), 137.8 (C), 130.7 (C), 127.6 (CH), 127.5 (CH), 122.4 (C), 119.8 (C), 96.3 (C), 87.6 (C), 23.7 (CH_3), 21.3 (CH_3), 21.0 (CH_3). **HRMS (ESI)** $C_{19}H_{19}Br$ $[M+H]^+$ calcd: 327.0748; found: 327.0746. **IR ν_{max} (neat)/cm^{-1}**: 2915, 2852, 1727, 1434, 1024, 863, 696, 569.

S1h. 2-Bromo-5-iodo-1,3-dimethyl benzene (2 g, 6.43 mmol, 1 equiv.), diphenylamine (1.63 g, 9.64 mmol, 1.5 equiv.), CuI (0.122 g, 0.643 mmol, 0.1 equiv.), and *t*-BuOK (1.76 g, 15.7 mmol, 2.5 equiv.) were dissolved in tetrahydrofuran (THF) (9 mL), and the mixture was degassed. Then, the resulting solution was stirred under argon and refluxed for 24 h. After cooling, the reaction mixture was filtered through a Celite® pad. The solvent was evaporated under reduced pressure, and the mixture was purified by column chromatography (SiO_2, Hexane/DCM, 9:1). Compound **S1h** was isolated as a white solid (1.04 g, 42% yield). **^{1}H NMR (500 MHz, $CDCl_3$)** δ(ppm): 7.19-7.15 (m, 4H), 7.00-6.96 (m, 4H), 6.94 (tt, *J* = 7.2, 1.2 Hz, 2H), 6.73 (s, 2H), 2.23 (s, 6H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ: 147.6 (C), 146.3 (C), 139.0 (C), 129.2 (CH), 124.1 (CH), 123.9 (CH), 122.7 (CH), 120.8 (C), 23.8 (CH_3). **HRMS (ESI)** $C_{20}H_{18}NBr$ $[M]^+$ calcd: 351.0623; found: 351.0619. **IR ν_{max} (neat)/cm^{-1}**: 3032, 2920, 2855, 1578, 1464, 1341, 1278, 1174, 1015, 858, 766, 693, 635.

General procedure for the synthesis of iodoarenes S2a-S2c, S2f and S2h (GP1)

***GP1*.** The corresponding bromoarene **S1** (1 equiv.) was dissolved in anhydrous THF (0.25 M) and deoxygenated. Then, *n*-BuLi (1.05 equiv.) was added dropwise under argon at –78°C over 10 min. The resulting white suspension was stirred for 30 min at –78°C, then a deoxygenated 1 M solution of iodine (1.1 equiv.) in anhydrous THF was added dropwise at –78°C over 15 min. The reaction mixture was allowed to warm up to room temperature and stirred overnight. The solvent was evaporated under reduced pressure and the residue was dissolved in CH_2Cl_2 (50 mL), washed with 10% $Na_2S_2O_3$ aqueous solution (50 mL), water and brine. The organic phase was dried over Na_2SO_4, filtered and solvent evaporated under reduced pressure. Compounds **S2** were obtained as colorless oils without further purification.

S2a. 2-bromo-5-fluoro-1,3-dimethylbenzene (1.00 g, 4 mmol), *n*-BuLi (2.50 M in hexane, 1.67 mL, 4.19 mmol) and iodine (1.11 g, 4.4 mmol) were reacted according to GP1 to afford **S2a** (1.19 g, 97% yield) as a brownish oil. **^{1}H NMR (500 MHz, $CDCl_3$)** δ(ppm): 6.85 (d, *J* = 9.5 Hz, 2H), 2.49 (s, 6H).**^{13}C NMR (126 MHz, $CDCl_3$)** δ: 162.3 (d, $J^1_{C\text{-}F}$ = 245.7 Hz, C), 143.8 (d, $J^3_{C\text{-}F}$ = 7.9 Hz, C), 113.9 (d, $J^2_{C\text{-}F}$ = 21.6 Hz, CH), 101.1 (d, $J^4_{C\text{-}F}$ = 2.7 Hz, C), 29.7 (d, $J^4_{C\text{-}F}$ = 1.7 Hz, CH_3). **^{19}F NMR (376 MHz, $CDCl_3$)** δ: –115.47. **HRMS (GC-EI)** C_8H_8FI $[M]^+$ calcd: 249.9655; found: 249.9648. **IR ν_{max} (neat)/cm^{-1}**: 2956, 2924, 1591, 1459, 1304, 1009, 854, 578.

S2b. 2-bromo-5-chloro-1,3-dimethylbenzene (1.00 g, 4.55 mmol), *n*-BuLi (2.50 M in hexane, 1.9 mL, 4.76 mmol) and iodine (1.25 g, 5 mmol) were reacted according to GP1 to afford **S2b** (1.18 g, 98% yield) as a brownish oil. **^{1}H NMR (500 MHz, $CDCl_3$)** δ(ppm): 6.94 (s, 2H), 2.34 (s, 6H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ: 143.6 (C), 133.5 (C), 126.7 (CH), 105.5 (C), 29.5 (CH_3). **HRMS (GC-EI)** C_8H_9ClI $[M+H]^+$ calcd: 266.5244; found: 266.5213. **IR ν_{max} (neat)/cm^{-1}**: 2975, 1702, 1430, 1260, 1121, 996, 849, 685, 545.

S2c. Compound **S1c** (1.4 g, 4.27 mmol), *n*-BuLi (2.50 M in hexane, 1.8 mL, 4.46 mmol) and iodine (1.17 g, 4.7 mmol) were reacted according to GP1 to afford **S2c** (1.24 g, 78% yield) as a brownish oil. **^{1}H NMR (500 MHz, $CDCl_3$)** δ(ppm): 7.21 (s, 2H), 6.90 (s, 2H), 2.40 (s, 6H), 2.47 (s, 6H), 2.30 (s, 3H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ: 142.2 (C), 140.1 (C), 137.9 (C), 129.3 (CH), 127.6 (CH), 123.3 (C), 119.8 (C), 108.0 (C), 96.3 (C), 87.9 (C), 29.5 (CH_3), 21.3 (CH_3), 21.0 (CH_3). **HRMS (ESI)** $C_{19}H_{20}I$ $[M+H]^+$ calcd: 375.0610; found: 375.0609. **IR ν_{max} (neat)/cm^{-1}**: 3745, 2915, 2852, 1727, 1434, 1024, 863, 696, 569.

S2f. 2-bromo-5-methoxy-1,3-dimethylbenzene (1.00 g, 4.64 mmol), a solution of *n*-BuLi (2.50 M in hexane, 1.95 mL, 4.87 mmol) and iodine (1.29 g, 5.10 mmol) were reacted according to GP1 to afford **S2f** (1.14 g, 94% yield) as a brownish solid. **^{1}H NMR (500 MHz, $CDCl_3$)** δ(ppm): 6.67 (s, 2H), 3.77 (s, 3H), 2.45 (s, 6H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ: 159.1 (C), 142.8 (C), 112.9 (CH), 97.0 (C), 55.2 (CH_3), 29.7 (CH_3). **HRMS (GC-EI)** $C_9H_{11}OI$ $[M]^+$ calcd: 261.9855; found: 261.9866. **IR ν_{max} (neat)/cm^{-1}**: 2952, 1583, 1462, 1313, 1159, 1003, 851, 689, 608.

S2h. Compound **S1h** (1.04 g, 2.95 mmol), a solution of *n*-BuLi (2.50 M in hexane, 1.4 mL, 3.5 mmol) and iodine (1.15 g, 3.68 mmol) were reacted according to GP1 to afford **S2h** (1.1 g, 95% yield) as a brownish solid. **^{1}H NMR (500 MHz, $CDCl_3$)** δ(ppm): 7.27-7.23 (m, 4H), 7.08-7.05 (m,

4H), 7.02 (tt, *J* = 7.1, 1.2 Hz, 2H), 6.80 (s, 2H), 2.36 (s, 6H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ: 147.5 (C), 147.4 (C), 142.7 (C), 129.2 (CH), 124.3 (CH), 122.9 (CH), 122.5 (CH), 99.8 (C), 29.5 (CH_3). **HRMS (ESI)** $C_{20}H_{18}NI$ $[M]^+$ calcd: 399.0484; found: 399.0479. **IR ν_{max} (neat)/cm^{-1}**: 3032, 2920, 2855, 1578, 1464, 1341, 1278, 1174, 1015, 858, 766, 693, 635.

General procedure for the synthesis of protected alkynes S3(a-c), S3(e-f) and S3h (GP2)

***GP2*.** To a degassed mixture of the corresponding iodoarenes **S2** (1 equiv.), $Pd(PPh_3)_2Cl_2$ (0.05 equiv.) and CuI (0.1 equiv.) in a 2:1 mixture of toluene and triethylamine (0.15 M) was added a solution of trimethylsilylacetylene (1.4 equiv.) in a 1:1 mixture of toluene and triethylamine (0.25 M).The reaction mixture was refluxed for 18h, allowed to cool to room temperatura and diluted with CH_2Cl_2. The mixture was washed with 10% aqueus NH_4OH, water and brine. The organic phase was dried over Na_2SO_4, filtered and evaporated under reduced pressure. The residue was purified by column chromatography (SiO_2, Hexane or Hexane/EtOAc, 95/5) to give corresponding **S3**.

S3a. Trimethylsilylacetylene (0.9 mL, 6.3 mmol), compound **S2a** (1.19 g, 4.75 mmol), $Pd(PPh_3)_2Cl_2$ (0.158 g, 0.29 mmol), CuI (0.085 g, 0.44 mmol), were used following GP2 to afford **S3a** (0.93 g, 90% yield) as a brownish oil.**^{1}H NMR (500 MHz, $CDCl_3$)** δ(ppm): 6.53 (d, $J^3_{H\text{-}F}$ = 9.3 Hz, 2H), 2.22 (s, 6H), 0.07 (s, 9H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ: 161.7 (d, $J^1_{C\text{-}F}$ = 248.3 Hz, C), 143.0 (d, $J^3_{C\text{-}F}$ = 8.7 Hz, C), 118.9 (d, $J^4_{C\text{-}F}$ = 3 Hz, C), 113.5 (d, $J^2_{C\text{-}F}$ = 21.8 Hz, CH), 102.2 (d, $J^5_{C\text{-}F}$ = 1.7 Hz, C), 101.7 (C), 20.9 (d, $J^4_{C\text{-}F}$ = 1.8 Hz, CH_3), 0.0 (CH_3). **^{19}F NMR (376 MHz, $CDCl_3$)** δ: –112.43. **HRMS (GC-EI)** $C_{13}H_{17}FSi$ $[M]^+$ calcd: 220.1084; found: 220.1088. **IR ν_{max} (neat)/cm^{-1}:** 2963, 2150, 2066, 1606, 1473, 1249, 837, 758, 647, 541.

S3b. Trimethylsilylacetylene (0.9 mL, 6.3 mmol), compound **S2b** (1.18 g, 4.42 mmol), $Pd(PPh_3)_2Cl_2$ (0.147 g, 0.27 mmol), CuI (0.08 g, 0.44 mmol), were used following GP2 to afford **S3b** (0.68 g, 68% yield) as a brownish oil.**^{1}H NMR (500 MHz, $CDCl_3$)** δ(ppm): 7.02 (s, 2H), 2.40 (s, 6H), 0.27 (s, 9H).**^{13}C NMR (126 MHz, $CDCl_3$)** δ: 142.2 (C), 133.3 (C), 126.5 (CH), 121.4 (C), 103.6 (C), 101.6 (C), 20.7 (CH_3) 0.0 (CH_3). **HRMS (ESI)** $C_{13}H_{17}ClSi$ $[M]^+$ calcd: 236.0865; found: 236.0869. **IR ν_{max} (neat)/cm^{-1}**: 2959, 2150, 2067, 1586, 1249, 836, 759, 646, 556.

S3c. Trimethylsilylacetylene (0.67 mL, 4.71 mmol), compound **S2c** (1.24 g, 3.31 mmol), $Pd(PPh_3)_2Cl_2$ (0.11g, 0.2 mmol), CuI (0.088 g, 0.3 mmol), were used following GP2 to afford **S3 c**

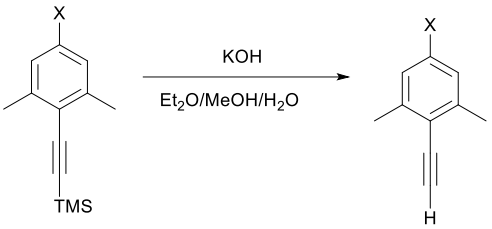
(0.65 g, 57% yield) as a brownish oil. **^{1}H NMR (500 MHz, $CDCl_3$)** δ(ppm): 7.20 (s, 2H), 6.89 (s, 2H), 2.47 (s, 6H), 2.43 (s, 6H), 2.29 (s, 3H), 0.29 (s, 9H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ: 140.5 (C), 140.0 (C), 137.7 (C), 129.2 (CH), 127.4 (CH), 123.0 (C), 122.6 (C), 119. 8 (C), 104.2 (C), 102.3 (C), 97.0 (C), 88.3 (C), 21.2 (CH_3), 20.8 (CH_3), 20.7 (CH_3), 0.0 (CH_3). **HRMS (ESI)** $C_{24}H_{29}Si$ $[M+H]^+$ calcd: 345.2039; found: 345.2031. **IR ν_{max} (neat)/cm^{-1}**: 2914, 2851, 2206, 1731, 1434, 1376, 999, 852, 727, 569.

S3e. Trimethylsilylacetylene (0.75 mL, 5.30 mmol), compound **S2e** (1 g, 3.80 mmol), $Pd(PPh_3)_2Cl_2$ (0.13 g, 0.19 mmol), CuI (0.072 g, 0.37 mmol), were used following GP2 to afford **S3e** (0.84 g, 93% yield) as a brownish oil. **^{1}H NMR (500 MHz, $CDCl_3$)** δ(ppm): 7.05 (s, 2H), 2.43 (s, 6H), 1.29 (s, 9H), 0.26 (s, 9H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ: 150.7 (C), 139.9 (C), 123.5 (CH), 119.9 (C), 102.8 (C), 101.5 (C), 34.4 (C), 30.9 (CH_3), 21.0 (CH_3), 0.0 (CH_3). **HRMS (GC-EI)** $C_{17}H_{26}Si$ $[M]^+$ calcd: 258.1804; found: 258.1805. **IR ν_{max} (neat)/cm^{-1}**: 2958, 2148, 1606, 1479, 1249, 837, 758, 630.

S3f. Trimethylsilylacetylene (0.86 mL, 6.05 mmol), compound **S2f** (1.14 g, 4.34 mmol), $Pd(PPh_3)_2Cl_2$ (0.15 g, 0.21 mmol), CuI (0.082 g, 0.43 mmol), were used following GP2 to afford **S3f** (0.9 g, 89% yield) as a brown oil. This compound was obtained pure after the work up and was not further purified by column chromatography **^{1}H NMR (500 MHz, $CDCl_3$)** δ(ppm): 6.61 (s, 2H), 3.80 (s, 3H), 2.44 (s, 6H), 0.29 (s, 9H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ: 158.7 (C), 142.1 (C), 115.2 (C), 112.7 (CH), 102.7 (C), 100.5 (C), 54.8 (CH_3), 21.0 (CH_3), 0.0 (CH_3). **HRMS (GC-EI)** $C_{14}H_{20}OSi$ $[M]^+$ calcd: 232.1283 found: 232.1272. **IR ν_{max} (neat)/cm^{-1}**: 2960, 2144, 1603, 1466, 1318, 1248, 1149, 836, 758, 624.

S3h. Trimethylsilylacetylene (0.52 mL, 3.60 mmol), compound **S2h** (1.10 g, 2.75 mmol), $Pd(PPh_3)_2Cl_2$ (0.092 g, 0.17 mmol), CuI (0.040 g, 0.25 mmol), were used following GP2 to afford **S3h** (0.84 g, 83% yield) as a dark yellow oil. **^{1}H NMR (500 MHz, $CDCl_3$)** δ(ppm): 7.26-7.23 (m, 4H), 7.07-7.05 (m, 4H), 7.02 (tt, *J* = 7.4, 1.1 Hz, 2H), 6.71 (s, 2H), 2.32 (s, 6H), 0.25 (s, 9H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ: 147.2 (C), 147.0 (C), 141.5 (C), 129.0 (CH), 124.4 (CH), 122.8 (CH), 121.1 (CH), 116.4 (C), 102.8 (C), 101.3 (C), 20.8 (CH_3), 0.0 (CH_3). **HRMS (ESI)** $C_{25}H_{27}NSi$ $[M]^+$ calcd: 369.1913; found: 369.1914. **IR ν_{max} (neat)/cm^{-1}**: 3064, 2960, 2855, 2145, 1588, 1491, 1340, 1231, 839, 752, 693, 650.

General procedure for the synthesis of alkynes 6a and 6b (GP3)



S3a, X = F
S3b, X = Cl

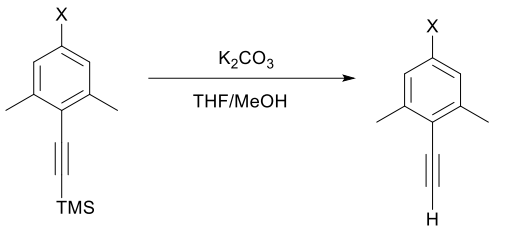
6a, X = F
6b, X = Cl

***GP3*.** To a solution of the corresponding **S3** (1 equiv.) in a 2:3 mixture of Et_2O and MeOH (0.3 M) was added a 3.5 M solution of KOH in H_2O. The resulting mixture was stirred at room temperature for 30 min. The reaction was diluted with water (50 mL) and extracted with pentane. The organic phase was dried over Na_2SO_4, filtered and evaporated under reduced pressure to give **6a** or **6b** without further purification.

6a. Compound **S3a** (0.9 g, 4.08 mmol), and 0.3 mL of KOH aqueous solution were reacted according to GP3 to afford **6a** (0.46 g, 74%) as a yellow oil . **^{1}H NMR (500 MHz, $CDCl_3$)** δ(ppm): 6.67 (d, $J^3_{H\text{-}F}$ = 9.4 Hz, 2H), 3.38 (s, 1H), 2.35 (s, 6H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ: 162.2 (d, $J^1_{C\text{-}F}$ = 248.4 Hz, C), 143.8 (d, $J^3_{C\text{-}F}$ = 8.7 Hz, C), 118.3 (d, $J^4_{C\text{-}F}$ = 2.8 Hz, C), 113.9 (d, $J^2_{C\text{-}F}$ = 21.8 Hz, CH), 85.2 (d, $J^5_{C\text{-}F}$ = 1.7 Hz, CH), 80.0 (C), 21.3 (d, $J^4_{C\text{-}F}$ = 1.8 Hz, CH_3). **^{19}F NMR** (376 MHz, $CDCl_3$) δ: –113.56. **HRMS (CG-EI)** $C_{10}H_9F$ $[M]^+$ calcd: 148.0688; found: 148.0692. **IR ν_{max} (neat)/cm^{-1}**: 3306, 2924, 2862, 2149, 1713, 1605, 1305, 1022, 856, 721, 540.

6b. Compound **S3b** (0.68 g, 2.9 mmol), and 0.2 mL of KOH aqueous solution were reacted according to GP3 to afford **6b** (0.35 g, 75%) as a yellow oil. **^{1}H NMR (500 MHz, $CDCl_3$)** δ(ppm): 7.04 (s, 2H), 3.53 (s, 1H), 2.42 (s, 6H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ: 142.6 (C), 133.7 (C), 126.7 (CH), 120.5 (C), 86.1 (CH), 80.2 (C), 20.8 (CH_3). **HRMS (ESI)** $C_{10}H_9Cl$ $[M]^+$ calcd: 164.0453; found: 164.0477. **IR ν_{max} (neat)/cm^{-1}**: 3296, 2923, 2102, 1586, 1464, 1263, 1103, 857, 725, 608, 575.

General procedure for the synthesis of alkynes 6c, 6e and 6h (GP4)



S3c, X = alk-Mes
S3e, X = *t*-Bu
S3h, X = $N(Ph)_2$

6c, X = alk-Mes
6e, X = *t*-Bu
6f, X = $N(Ph)_2$

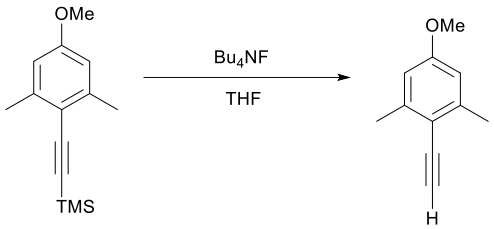
***GP4*.** To a degassed solution of the corresponding **S3** (1 equiv.) in a 1:1 mixture of THF and methanol (0.4 M) was added K_2CO_3 (0.4 equiv.). The resulting mixture was stirred at room temperature for 2 h. After addition of water, the mixture was extracted with DCM, washed with water and a 10% NH_4OH aqueous solution. The organic phase were dried over Na_2SO_4, filtered and evaporated under reduced pressure.The crude was purified by flash column chromatography (SiO_2, hexane/EtOAc, 9/1).

6c. Compound **S3c** (0.65 g, 3 mmol), K_2CO_3 (0.17 g, 1.2 mmol) were reacted according to the general procedure GP4 to afford **6c** (0.40 g, 91% yield) as a yellow oil. **^{1}H NMR (500 MHz, $CDCl_3$)** δ(ppm): 7.23 (s, 2H), 6.90 (s, 2H), 3.59 (s, 1H), 2.48 (s, 6H), 2.46 (s, 6H), 2.30 (s, 3H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ: 140.0 (C), 140.2 (C), 137.9 (C), 129.4 (CH), 127.6 (CH), 123.5 (C), 121.7 (C), 119.9 (C), 96.9 (C), 88.5 (C), 86.6 (CH), 81.0 (C), 21.3 (CH_3), 21.0 (CH_3), 20.8 (CH_3). **HRMS (ESI)** $C_{21}H_{21}$ $[M+H]^+$ calcd: 273.1643; found: 273.1656. **IR ν_{max} (neat)/cm-^{1}**: 3275, 2916, 2188, 1741, 1594, 1436, 1249, 1032, 868, 726, 630.

6e. Compound **S3e** (0.84 g, 3 mmol), K_2CO_3 (0.17 g, 1.2 mmol) were reacted according to the general procedure GP4 to afford **6e** (0.48 g, 79%) as a yellow oil. **^{1}H NMR (500 MHz, $CDCl_3$)** δ(ppm): 7.12 (s, 2H), 3.49 (s, 1H), 2.50 (s, 6H), 1.35 (s, 9H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ: 151.3 (C), 140.5 (C), 123.8 (CH), 119.1 (C), 84.5 (CH), 81.4 (C), 34.5 (C), 31.2 (CH_3), 21. 3 (CH_3). **HRMS (GC-EI)** $C_{14}H_{18}$ $[M]^+$ calcd: 186.1409; found: 186.1402. **IR ν_{max} (neat)/cm-^{1}**: 3311, 2962, 2098, 1480, 1362, 1232, 1004, 868, 732, 595.

6h. Compound **S3h** (0.84 g, 2.27 mmol, 1eq), K_2CO_3 (0.13 g, 0.91 mmol) were reacted according to the general procedure GP4 to afford **6h** (0.30 g, 44%) as a brown solid. **^{1}H NMR (500 MHz, $CDCl_3$)** δ(ppm): 7.28-7.24 (m, 4H), 7.09-7.02 (m, 6H), 6.72 (s, 2H), 3.44 (s, 1H), 2.33 (s, 6H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ: 147.5 (C), 147.4 (C), 142.0 (C), 129.2 (CH), 124.8 (CH), 124.0 (C), 123.1 (CH), 121.2 (CH), 84.1 (CH), 81.5 (C), 21.1 (CH_3). **HRMS (ESI)** $C_{22}H_{19}N$ $[M]^+$ calcd: 297.1517; found: 297.1515. **IR ν_{max} (neat)/cm^{-1}**: 3313, 2924, 2859, 2098, 1731, 1587, 1484, 1338, 1229, 1135, 860, 758, 695.

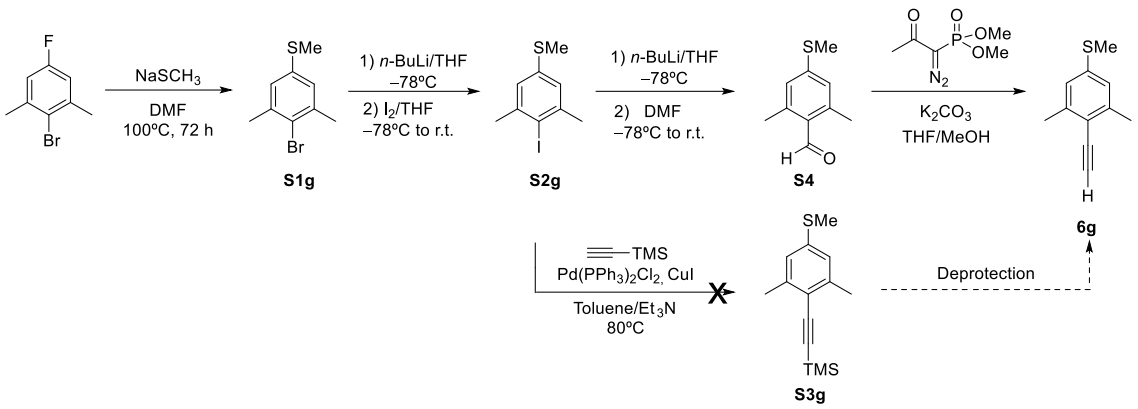
Procedure for the synthesis of alkyne 6f.



S3f **6f**

6f. To a solution of compound **S3f** (0.9 g, 3.87 mmol, 1 equiv.) in THF (0.27 M) was added Bu_4NF (4 g, 5.80 mmol, 1.5 equiv.). The resulting mixture was stirred at room temperature for 1 h. Solvent was evaporated and the crude redissolved in EtOAc and washed with water and brine. The organic phase was dried over Na_2SO_4, filtered and evaporated under reduced pressure. The residue was purified by column chromatography (SiO_2, Hexane/EtOAc, 95/5) to give **S3f** (0.35 g, 56%) as a brownish oil. **^{1}H NMR (500 MHz, $CDCl_3$)** δ(ppm): 6.44 (s, 2H), 3.63 (s, 3H), 3.27 (s, 1H), 2.28 (s, 6H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ: 159.2 (C), 142.7 (C), 114.3 (C), 112.4 (CH), 83.7 (CH), 81.3 (C), 55.1 (CH_3), 21.2 (CH_3). **HRMS (GC-EI)** $C_{11}H_{12}O$ $[M]^+$ calcd: 160.0888; found: 160.0890. **IR ν_{max} (neat)/cm^{-1}**: 3280, 2913, 2841, 2095, 1603, 1317, 1142, 1059, 855, 580.

2.2. Synthetic route and procedures for the preparation of 6g



S1g. In a Schlenk tube, a mixture of 2-bromo-5-fluoro-1,3-dimethylbenzene **S1a** (0.1 g, 0.49 mmol, 1equiv.) and $NaSCH_3$ (0.069 g, 0.98 mmol, 2 equiv.) was degassed. Then, the mixture was dissolved in DMF (0.9 mL) and heated to 100 ºC for 72 h. The reaction was cooled to room temperature and diluted with EtOAc (150 mL). The mixture was washed with water and brine several times. The organic phase was dried over Na_2SO_4, filtered and evaporated under reduced pressure. The residue was purified by column chromatography (SiO_2, hexane) to give **S1g** (0.075 g, 62**%** yield) as a colorless oil. This reaction is only scalable up to 0.1 g. **^{1}H NMR (500 MHz, $CDCl_3$)** δ(ppm): 6.97(s, 2H), 2.46 (s, 3H), 2.39 (s, 6H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ: 138.6 (C), 136.7 (C), 126.3 (CH), 124.1 (C), 23.8 (CH_3), 16.0 (CH_3). **HRMS (GC-EI)** $C_9H_{11}BrS$ $[M]^+$ calcd: 229.9765; found: 229.9759. **IR ν_{max} (neat)/cm^{-1}**: 2978, 2919, 2848, 1567, 1458, 1265, 1131, 1009, 842, 693, 568.

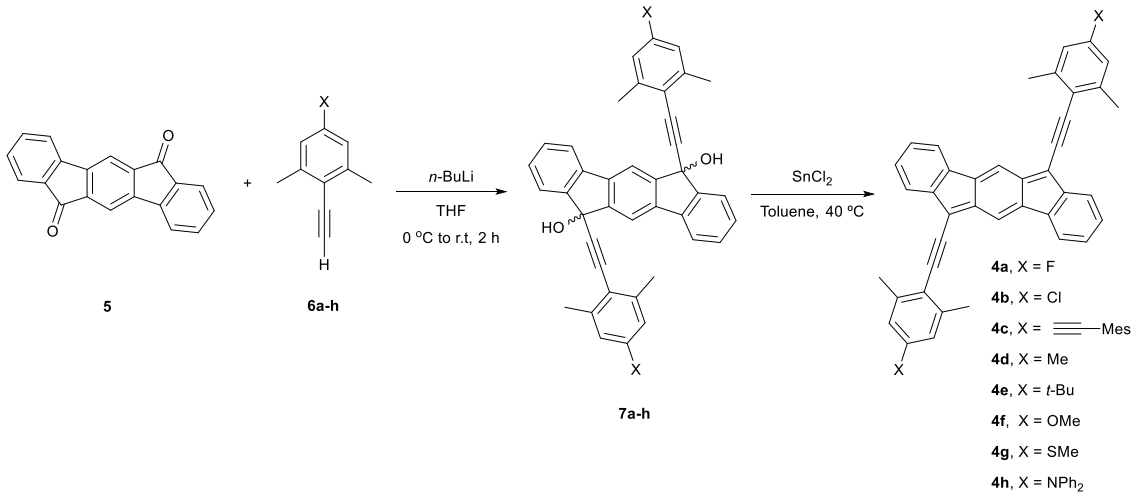
S2g. Bromoarene **S1g** (3 g, 13 mmol.), *n*-BuLi (5.5 mL, 13.6 mmol) and iodine (3.63 g, 14.3 mmol) were reacted according to GP1 to afford **S2g** (1.27 g, 94% yield) as a yellow oil without further purification. **^{1}H NMR (500 MHz, $CDCl_3$)** δ(ppm): 6.98 (s, 2H), 2.50 (s, 3H), 2.48 (s, 6H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ:142.3 (C), 138.1 (C),124.9 (CH), 103,9 (C), 29.7 (CH_3), 15.8 (CH_3). **HRMS (GC-EI)** $C_9H_{11}IS$ $[M]^+$ calcd: 277.9626; found: 277.9621. **IR ν_{max} (neat)/cm^{-1}**: 2978, 2917, 2859, 1774, 1566, 1432, 1131, 998, 841, 731, 555.

S4. Compound **S2g** (1.27 g, 4.56 mmol, 1 equiv.) was dissolved in anhydrous THF (47 mL). Then, a solution of *n*-BuLi (5.5 mL, 5.28 mmol, 1.05 eq) was added at –78ºC. After 30 min, DMF (1.4 mL, 18.24 mmol, 4 equiv.) was added dropwise under argon at –78ºC over 10 min. The mixture was stirred for 3h at –78ºC. The reaction was quenched with NH_4Cl and extracted with EtOAc (100 mL), The organic layer was dried over Na_2SO_4, filtered and evaporated under reduced pressure. The crude was purified by flash column chromatography (SiO_2, Hexane/AcOEt 8:2) to

give **S4** (0.50 g, 62% yield) as a colorless oil. **^{1}H NMR (500 MHz, $CDCl_3$)** δ(ppm): 10.52 (s, 1H), 6.89 (s, 2H), 2.59 (s, 6H), 2.50 (s, 3H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ: 192.2 (C=O), 145.6 (C), 141.9 (C),128.9 (C), 125.8 (CH), 20.7 (CH_3), 14.4 (CH_3). **HRMS (GC-EI)** $C_{10}H_{12}OS$ $[M]^+$ calcd: 180.0609; found: 180.0605. **IR ν_{max} (neat)/cm^{-1}**: 2967, 2924, 2772, 1679, 1581, 1433, 1097, 894, 730, 684.

6g. To a solution of compound **S3g** (0.5 g, 3.27 mmol, 1 equiv.) in MeOH (5.8 mL) and THF (41 mL) was added K_2CO_3 (2.72 g, 19.6 mmol, 6 equiv.) and Bestmann-Ohira reagent (1.48 mL, 9,86 mmol, 3 equiv.). The resulting mixture was stirred at room temperature for 18h. Water was added and the mixture was extracted with DCM. The organic layer was dried over Na_2SO_4, filtered and evaporated under reduced pressure. The crude was purified by column chromatography (SiO_2, Hexane/EtOAC, 95/5) to give **6g** (0.23 g, 40%) as a colorless oil. **^{1}H NMR (500 MHz, $CDCl_3$)** δ(ppm): 6.92 (s, 2H), 3.49 (s, 1H), 2.47 (s, 3H), 2.42 (s, 6H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ: 141.3 (C), 138.8 (C), 124.1 (CH), 118.6 (CH), 85.1 (CH), 81.0 (C), 21.0 (CH_3), 15.3 (CH_3). **HRMS (ESI)** $C_{11}H_{12}S$ $[M]^+$ calcd: 176.0660; found: 176.0654. **IR ν_{max} (neat)/cm^{-1}**: 3285, 2919, 2098, 1588, 1435, 1204, 1098, 846, 725, 646, 579.

2.3. Synthetic route and procedures for the preparation of compounds 4a-4h



General procedure for the synthesis of compounds 7a-h (GP5)

GP5. The corresponding compound **6** (6.5 equiv.) was dissolved in THF (0.25 M), degassed with Ar for 10 min, and cooled to 0 °C. *n*-BuLi (3.3 equiv.) was added and the mixture stirred at 0 °C for 20 min. In a separate flask, compound **5** (1 equiv.) was dissolved in THF (0.01 M), and also

degassed with Ar for 10 min, and cooled to 0 °C. The lithiated alkyne was transferred to the cold solution containing compound **5** and then stirred at room temperature for 1 h. Then the reaction was quenched with 10% aq. HCl and extracted with EtOAc. The organic layer was dried with Na_2SO_4, filtered, and evaporated to dryness. The crude was purified by flash column chromatography (SiO_2, Hexane/AcOEt 1:1) (**7b**, **7d**, **7e**) or directly submitted to the next reaction.

7b. Compound **6b** (0.4 g, 2.43 mmol), *n*-BuLi (2.5 M in hexane, 0.1 mL, 1.15 mmol) and compound **5** (0.1 g, 0.35 mmol) were reacted according to GP5 to afford **7b** (0.08 g, 37% yield) as a brown solid. **^{1}H NMR (500 MHz, $CDCl_3$)** δ(ppm): 7.95 (s, 2H), 7.71 (dd, *J* = 7.5, 1.1 Hz, 2H), 7.61 (dd, *J* = 7.1, 0.8 Hz, 2H), 7.38 (td, *J* = 7.5, 1.3 Hz, 2H), 7.33 (td, *J* = 7.4, 1.2 Hz, 2H), 7.19 (s, 2H), 6.92 (m, 4H), 2.29 (s, 12H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ: 149.3 (C), 147.5 (C), 142.6 (CH), 139.9 (C), 138.6 (C), 133.8 (C), 130.0 (C), 128.8 (C), 126.8 (CH), 124.2 (CH), 120.5 (CH), 120.3 (CH), 116.3 (C), 97.6 (C), 80.4 (C), 75.1 (C), 20.9 (CH_3). **HRMS (ESI)** $C_{40}H_{28}O_2NaCl$ $[M + Na]^+$ calcd: 633.1364; found: 633.1422. **IR ν_{max} (neat)/cm^{-1}**: 2922, 2851, 1717, 1584, 1444, 1244, 1007, 875, 761.

7d. 2,4,6-trimethylphenyl acetylene (0.35 mL, 2.43 mmol), *n*-BuLi (2.5 M in hexane, 0.1 mL, 1.15 mmol) and compound **5** (0.1 g, 0.35 mmol) were reacted according to GP5 to afford **7d** (0.095 g, 48% yield) as a brownish solid. **^{1}H NMR (500 MHz, $CDCl_3$)** δ(ppm): 7.96 (s, 2H), 7.71 (dd, *J* = 7.4, 1.0, 2H), 7.61 (dd, *J* = 7.4, 0.9, 2H), 7.37 (td, *J* = 7.2, 1.0 Hz, 2H), 7.30 (td, *J* = 7.2, 1.1 Hz, 2H), 7.18 (s, 2H), 6.73 (s, 4H), 2.28 (s, 12H), 2.16 (s, 6H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ: 149.4 (C), 147.7 (C), 140.7 (CH), 139.8 (C), 138.7 (C), 138.2 (C), 129.8 (C), 128.6 (C), 127.5 (CH), 124.2 (CH), 120.2 (CH), 118.8 (CH), 116.3 (C), 96.0 (C), 81.6 (C), 75.2 (C), 31.6 (CH_3), 22.6 (CH_3), 14.1 (CH_3). **HRMS (ESI)** $C_{42}H_{24}O_2Na$ $[M + Na]^+$ calcd: 593.2509; found: 570.2656. **IR ν_{max} (neat)/cm^{-1}**: 3412, 2918, 2852, 2218, 1736, 1609, 1444, 1376, 1257, 1036, 852, 747.

7e. Compound **6e** (0.45 g, 2.43 mmol), *n*-BuLi, (2.5M in hexane, 0.1 mL, 1.15 mmol) and compound **5** (0.1 g, 0.35 mmol) were reacted according to GP5 to afford **7e** (0.11 g, 48% yield) as a brownish solid. **^{1}H NMR (500 MHz, $CDCl_3$)** δ(ppm): 8.03 (s, 2H), 7.78 (dd, *J* = 6.9, 1.2 Hz, 2H), 7.68 (dd, *J* = 7.8, 1.1 Hz, 2H), 7.43 (td, *J* = 7.4, 0.8 Hz, 2H), 7.40 (td, *J* = 7.4, 0.8 Hz, 2H), 7.01 (s, 4H), 2.39 (s, 12H), 1.26 (s, 18H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ: 151.4 (C), 149.4 (C), 147.8 (C), 140.4 (CH), 139.7 (C), 138.7 (C), 129.7 (CH), 128.6 (CH), 124.2 (C), 123.8 (CH), 120.2 (CH), 118.9 (C), 116.2 (CH), 96.1 (C), 81.7 (C), 75.1 (C), 34.5 (C), 31.1 (CH_3), 21.3 (CH_3). **HRMS (ESI)**

$C_{48}H_{46}O_2Na$ $[M + Na]^+$ calcd: 677.3396; found: 677.3411. **IR ν_{max} (neat)/cm^{-1}**: 2961, 2853, 2214, 1716, 1605, 1444, 1365, 1223, 1032, 869, 759, 734.

General procedure for the synthesis of compounds 4a-h (GP6)

GP6. The corresponding either crude or purified diol **7** (1 equiv.) was dissolved in dry toluene (0.07 M) and degassed with Ar for 10 min. $SnCl_2$ (4 equiv.) was added and mixture stirred at 40 °C for 15 min. The solvent was evaporated under reduced pressure. The residue was purified by column chromatography (SiO_2, DCM)to give compound **4**.

4a. Compound **6a** (0.15 g, 1.10 mmol), *n*-BuLi (2.5 M in hexane, 0.22 mL, 0.56 mmol), compound **5** (0.05 g, 0.17 mmol) were used according to GP5 and then crude diol **7a** and $SnCl_2$ (0.15 g, 0.68 mmol) were reacted according to GP6 to afford **4a** (0.010 g, 21% yield) as a dark blue solid. **^{1}H NMR (500 MHz, $CDCl_3$)** δ(ppm): 7.50-7.48 (m, 2H), 7.48 (s, 2H), 7.42-7.40 (m, 2H), 7.20-7.18 (m, 4H), 6.94 (d, *J* = 10.4 Hz, 4H). A good-quality ^{13}C-NMR could not be obtained due to poor solubility. **^{19}F NMR** (376 MHz, $CDCl_3$) δ: –110.60. **HRMS (ESI)** $C_{40}H_{26}F_2$ $[M]^+$ calcd: 544.2003; found: 544.1995. **IR ν_{max} (neat)/cm^{-1}**: 2922, 2877, 1739, 1473, 1378, 1215, 1028, 840, 557.

4b. Compound **7b** (0.05 g, 0.082 mmol) and $SnCl_2$ (0.074 g, 0.32 mmol) were reacted according to the general procedure GP6 to afford **4b** (0.030 g, 64% yield) as a dark blue solid **^{1}H NMR (500 MHz, $C_2D_2Cl_4$)** δ(ppm): 7.54-7.52 (m, 2H),7.52 (s, 2H), 7.48-7.46 (m, 2H), 7.30 (s, 4H), 7.30-7.26 (m, 4H), 2.75 (s, 12H). A good-quality ^{13}C-NMR could not be obtained due to poor solubility. **HRMS (ESI)** $C_{40}H_{26}Cl_2$ $[M]^+$ calcd: 576.1412; found: 576.1390. **IR ν_{max} (neat)/cm^{-1}**: 2963, 2877, 1738, 1473, 1365, 1216, 1066, 840, 557.

4c. Compound **6c** (0.3 g, 1.10 mmol), *n*-BuLi (2.5 M in hexane, 0.22 mL, 0.56 mmol), compound **5** (0.05 g, 0.17 mmol) were used according to GP5 and then crude diol **7c** and $SnCl_2$ (0.15 g, 0.68 mmol,) were reacted according to GP6 (reaction time is 2 h in this case) to afford **4c** (0.035 g, 74% yield) as a blue solid. **^{1}H NMR (500 MHz, $C_2D_2Cl_4$, 375 K)** δ(ppm): 7.54 (s, 2H), 7.52-7.51 (m, 2H), 7.48-7.47 (m, 2H), 7.41 (s, 4H), 7.25-7.24 (m, 4H), 7.00 (s, 4H), 2.75 (s, 12H), 2.60 (s, 12H), 2.40 (s, 6H). A good-quality ^{13}C-NMR could not be obtained due to poor solubility. **HRMS (ESI)** $C_{62}H_{48}$ $[M]^+$ calcd: 792.3856; found: 792.3748. **IR ν_{max} (neat)/cm^{-1}**: 3015, 2969, 1738, 1365, 1216, 1091, 515.

4d. Compound **7d** (0.05 g, 0.087 mmol) and $SnCl_2$ (0.079 g, 0.35 mmol) were reacted according to the general procedure GP6 to afford **4d** (0.018 g, 38% yield) as a dark blue solid. **^{1}H NMR (500 MHz, $C_2D_2Cl_4$, 375 K)** δ(ppm): 7.47 (s, 2H), 7.40-7.45 (m, 4H), 7.18-7.15 (m, 4H), 7.01 (s, 4H), 2.65 (s, 12H), 2.38 (s, 6H). A good-quality ^{13}C-NMR could not be obtained due to poor solubility. **HRMS (ESI)** $C_{42}H_{32}$ $[M]^+$ calcd: 536.2504; found: 536.2495. **IR ν_{max} (neat)/cm^{-1}**: 3005, 2970, 1738, 1365, 1216, 1091, 515.

4e. Compound **7e** (0.05 g, 0.076 mmol) and $SnCl_2$ (0.068 g, 0.30 mmol) were reacted according to the general procedure GP6 to afford **4e** (0.030 g, 66% yield) as a dark blue solid. **^{1}H NMR (500 MHz, $CDCl_3$)** δ(ppm): 7.42 (s, 2H), 7.42-7.41 (m, 2H), 7.38-7.36 (m, 2H), 7.17 (s, 4H), 7.14-7.12 (m, 4H), 2.64 (s, 12H), 1.34 (s, 18H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ: 152.3 (C), 143.3 (C), 140.1 (C), 139.5 (CH), 138.8 (C), 137.7 (C), 128.1 (CH), 127.9 (CH), 126.4 (CH), 124.3 (CH), 122.3 (C), 120.3 (C), 120.2 (CH), 118.6 (C), 104.9 (C), 93.9 (C), 34.8 (C), 31.2 (CH_3), 21.8 (CH_3). **HRMS (ESI)** $C_{48}H_{44}$ $[M]^+$ calcd: 620.3443; found: 620.3442. **IR ν_{max} (neat)/cm^{-1}**: 3452, 3015, 2970, 1738, 1434, 1365, 1216, 1091, 514.

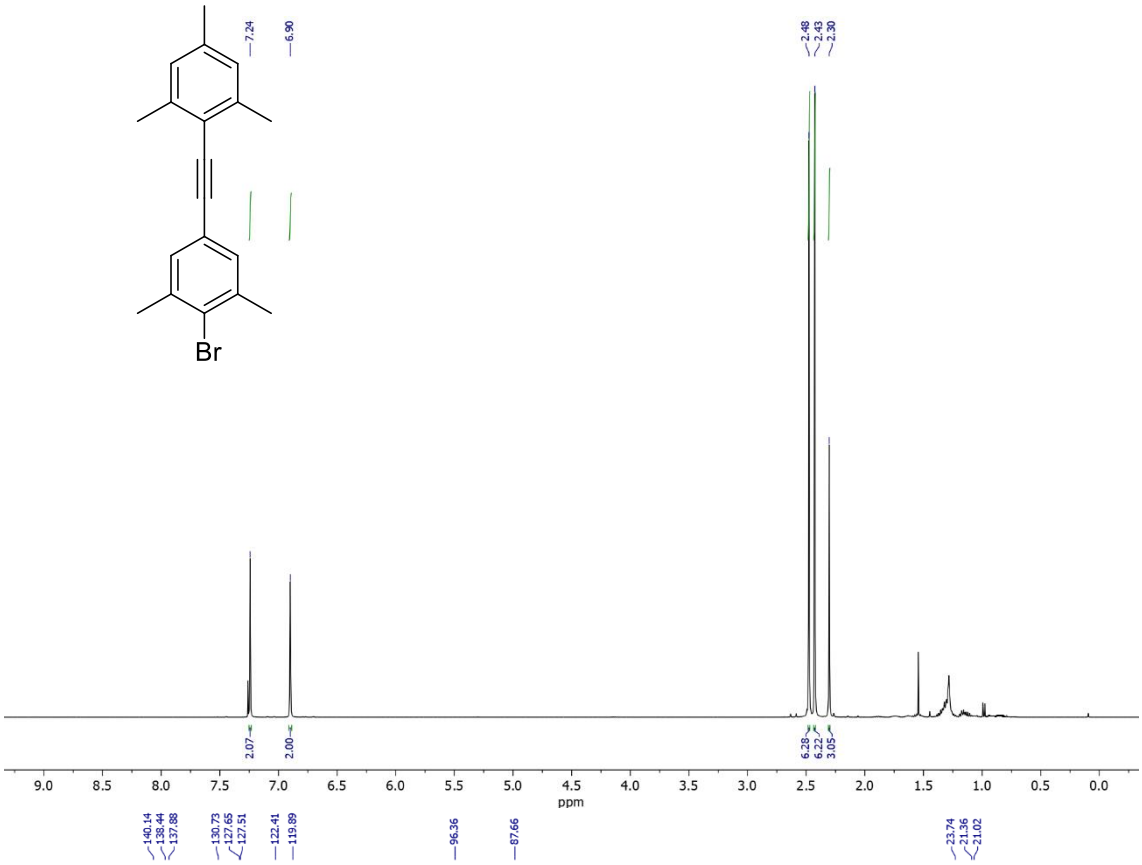
4f. Compound **6f** (0.17 g, 1.10 mmol), *n*-BuLi (2.5 M in hexane, 0.22 mL, 0.56 mmol), compound **5** (0.05 g, 0.17 mmol) were used according to GP5 and then crude diol **7f** and $SnCl_2$ (0.15 g, 0.68 mmol) were reacted according to GP6 to afford **4f** (0.015 g, 32% yield) as a dark blue solid. **^{1}H NMR (500 MHz, $C_2D_2Cl_4$, 375 K)** δ(ppm): 7.54 (s, 2H), 7.52-7.50 (m, 2H), 7.48-7.46 (m, 2H), 7.23-7.22 (m, 4H), 6.81 (s, 4H), 3.94 (s, 6H), 2.73 (s, 12H). A good-quality ^{13}C-NMR could not be obtained due to poor solubility. **HRMS (ESI)** $C_{42}H_{32}O_2$ $[M]^+$ calcd: 568.2402; found: 568.2414. **IR ν_{max} (neat)/cm^{-1}**: 3010, 2974, 1738, 1442, 1365, 1216, 1065, 748, 515.

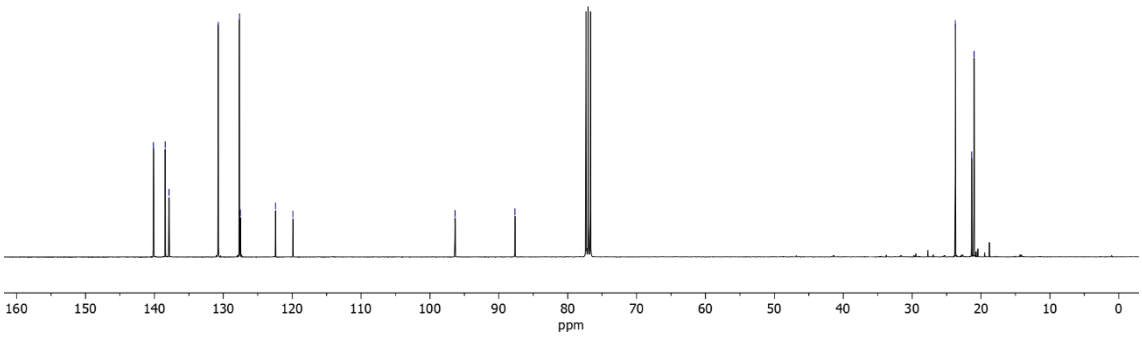
4g. Compound **6g** (0.19 g, 1.10 mmol), *n*-BuLi (2.5 M in hexane, 0.22 mL, 0.56 mmol), compound **5** (0,05 g, 0.17 mmol)) were used according to GP5 and then crude diol **7g** and $SnCl_2$ (0.15 g, 0.68 mmol) were reacted following procedure GP6 to afford **4g** (0.030 g, 69%) as blue solid.**^{1}H NMR (500 MHz, $C_2D_2Cl_4$, 375 K)** δ(ppm): 7.53 (s, 2H), 7.52-7.50 (m, 2H), 7.48-7.46 (m, 2H), 7.25-7.23 (m, 4H), 7.15 (s, 4H), 2.73 (s, 12H), 2.62 (s, 6H). A good-quality ^{13}C-NMR could not be obtained due to poor solubility. **HRMS (ESI)** $C_{42}H_{32}S_2$ $[M]^+$ calcd: 600.1945; found: 600.1938. **IR ν_{max} (neat)/cm^{-1}**: 3453, 3015, 2970, 2150, 1738, 1435, 1365, 1216, 1091, 748, 516.

4h. Compound **6h** (0.0.32 g, 1.10 mmol), *n*-BuLi (0.22 mL, 0.56 mmol), compound **5** (0.05 g, 0.17 mmol) and $SnCl_2$ (0.15 g, 0.68 mmol) were reacted according to GP6 to afford **4h** (0.025 g, 52**%** yield) as a blue solid. **^{1}H NMR (500 MHz, $C_2D_2Cl_4$, 375 K)** δ(ppm):7.54 (s, 2H), 7.51-7.49 (m, 2H), 7.47-7.46 (m, 2H), 7.41-7.37 (m, 8H), 7.25-7.17 (m, 16H), 6.89 (s, 4H), 2.64 (s, 12 H). A good-quality ^{13}C-NMR could not be obtained due to poor solubility. **HRMS (ESI)** $C_{64}H_{46}N_2$ $[M]^+$ calcd: 842.3661; found: 842.3663. **IR ν_{max} (neat)/cm^{-1}**: 2923, 2852, 2182, 1738, 1587, 1738, 1365, 1216, 1021, 795.

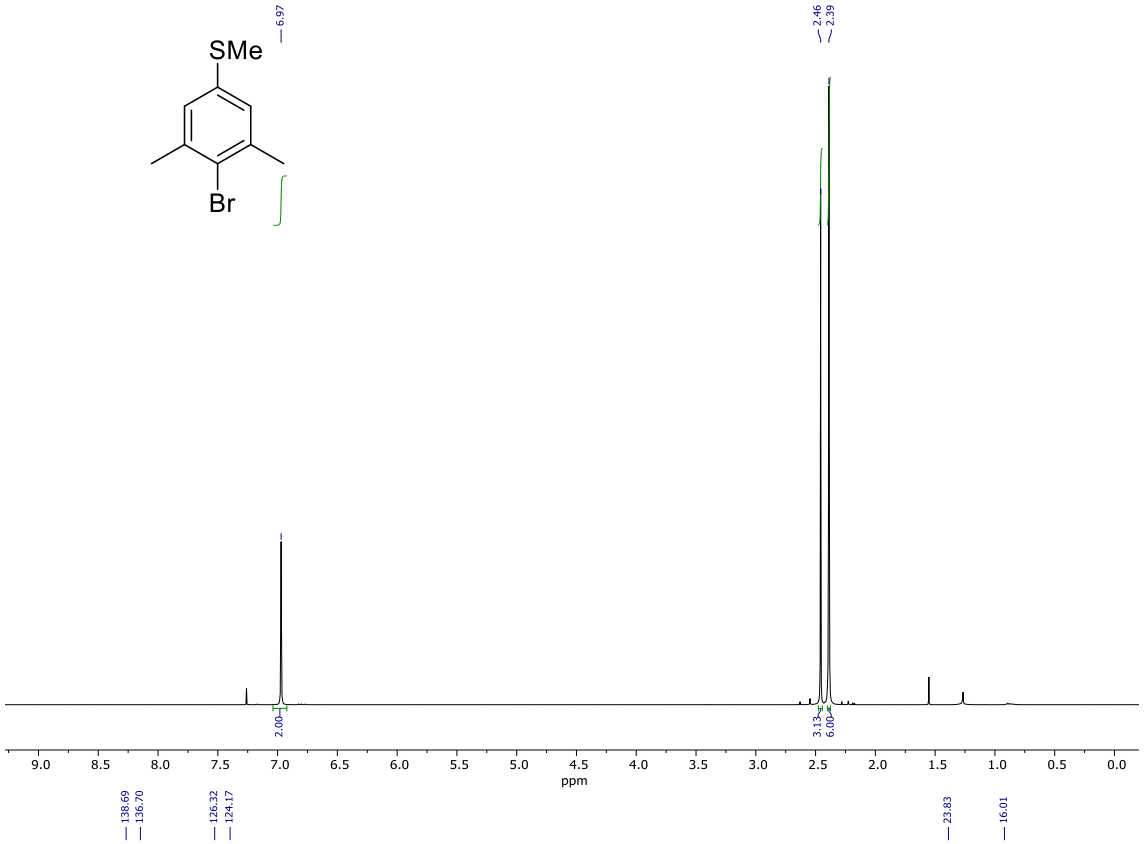
3. NMR spectra of new compounds

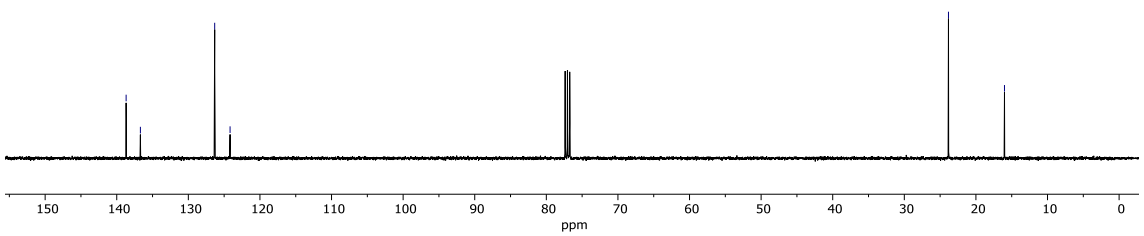
^{1}H-NMR (500 MHz, $CDCl_3$) and ^{13}C-NMR (126 MHz, $CDCl_3$) of compound S1c



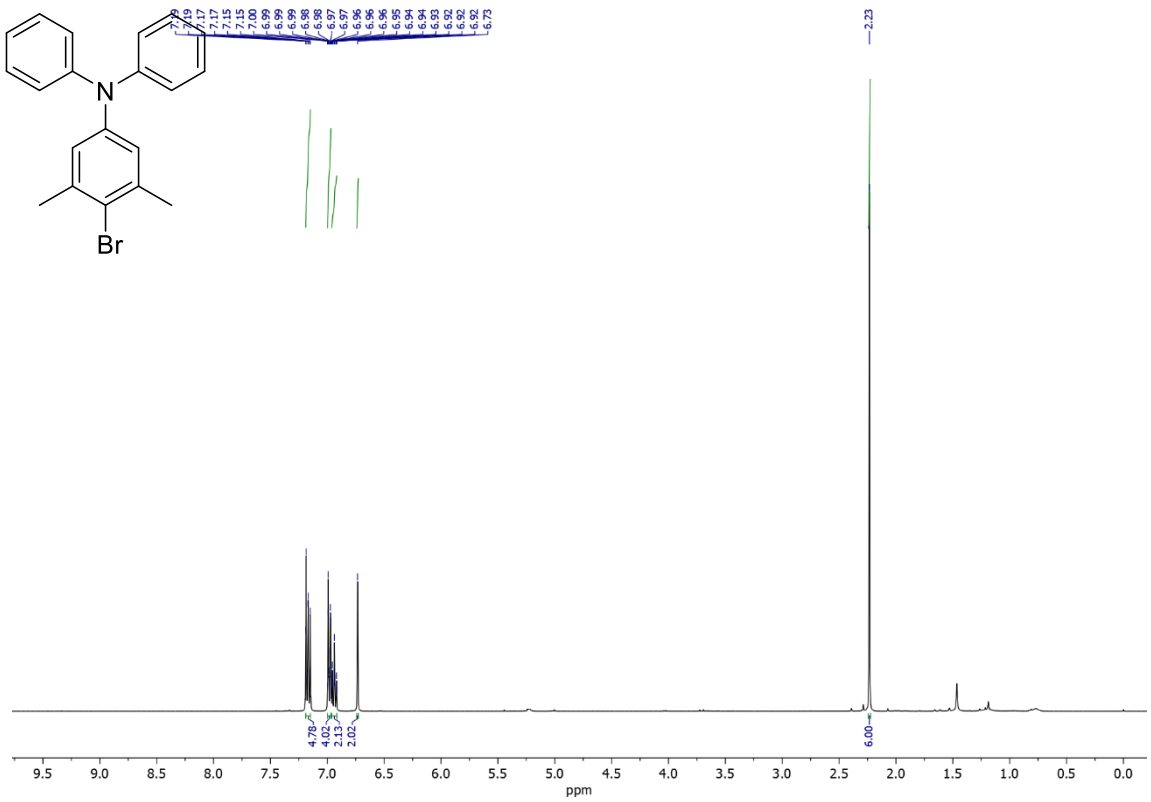


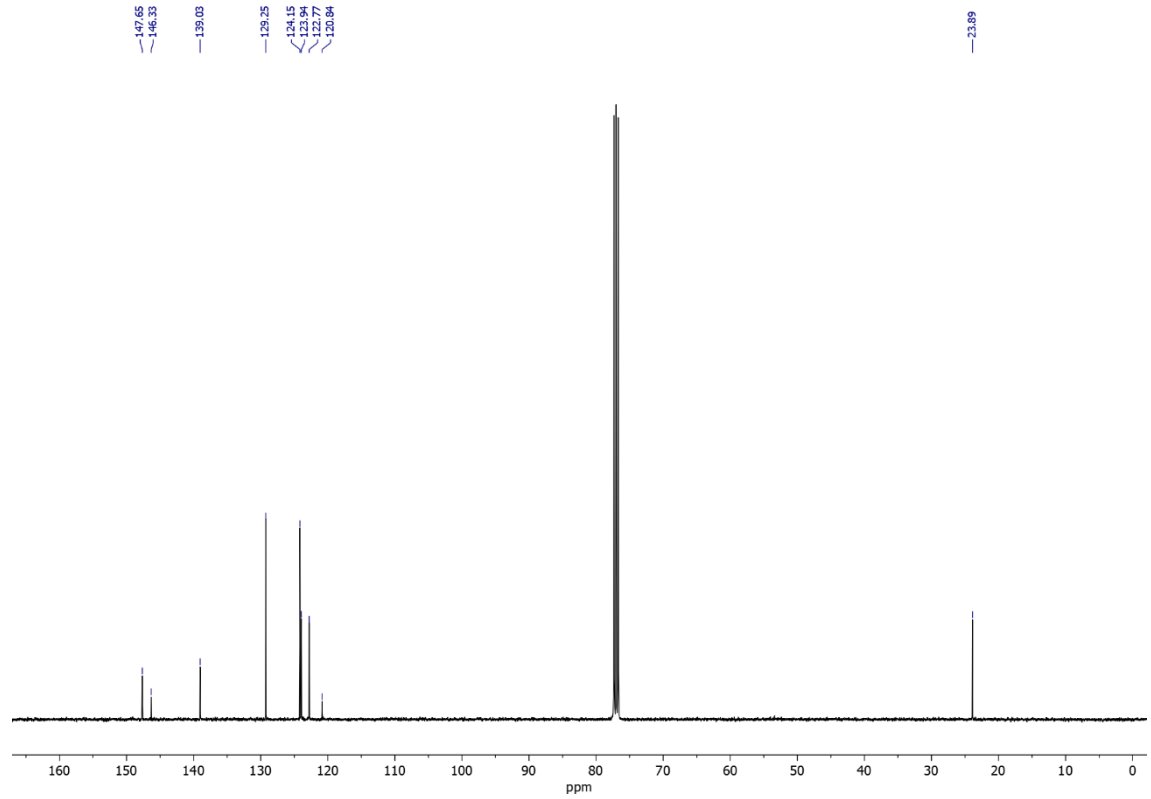
^{1}H-NMR (500 MHz, $CDCl_3$) and ^{13}C-NMR (126 MHz, $CDCl_3$) of compound S1g



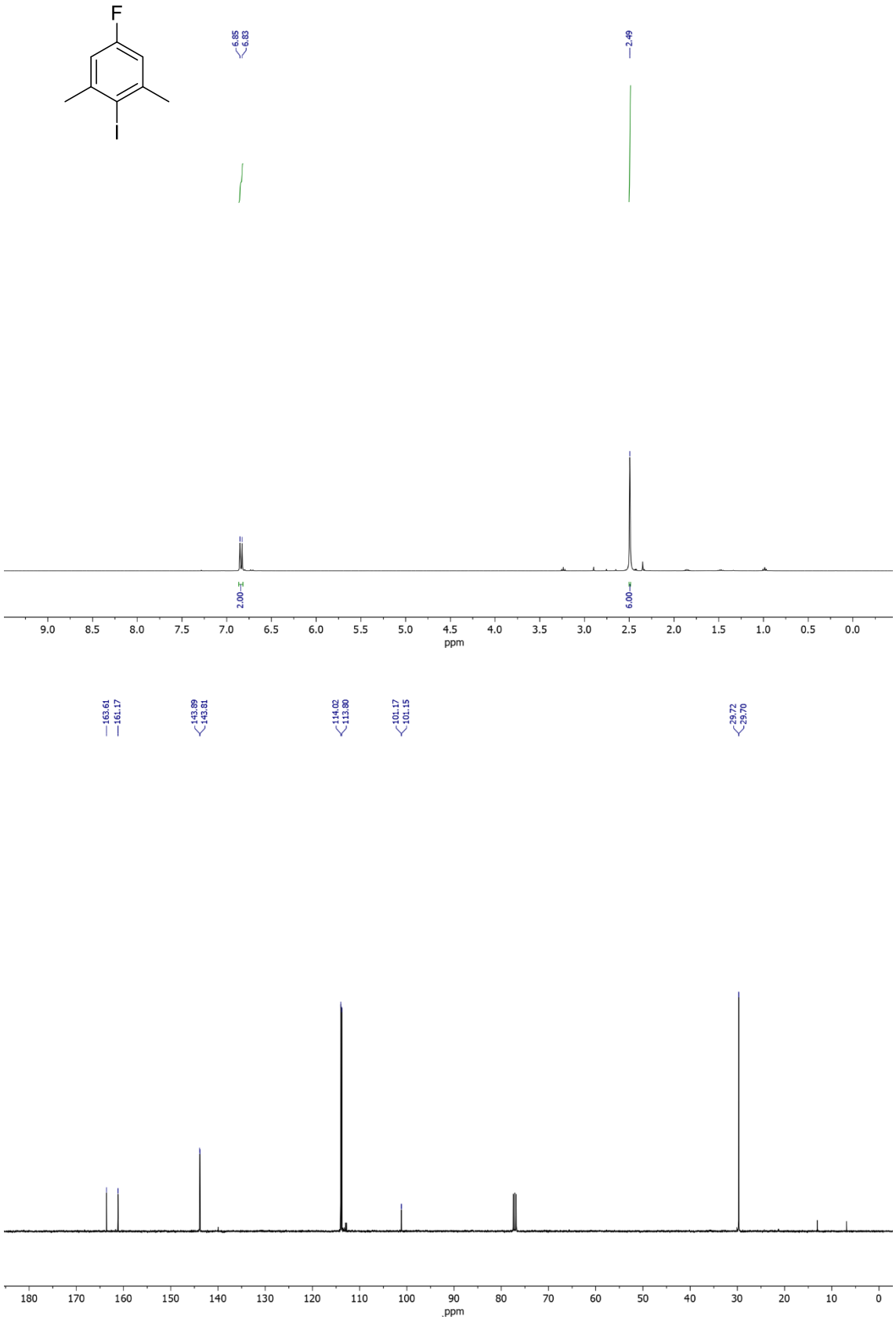


^{1}H-NMR (500 MHz, $CDCl_3$) and ^{13}C-NMR (126 MHz, $CDCl_3$) of compound S1h

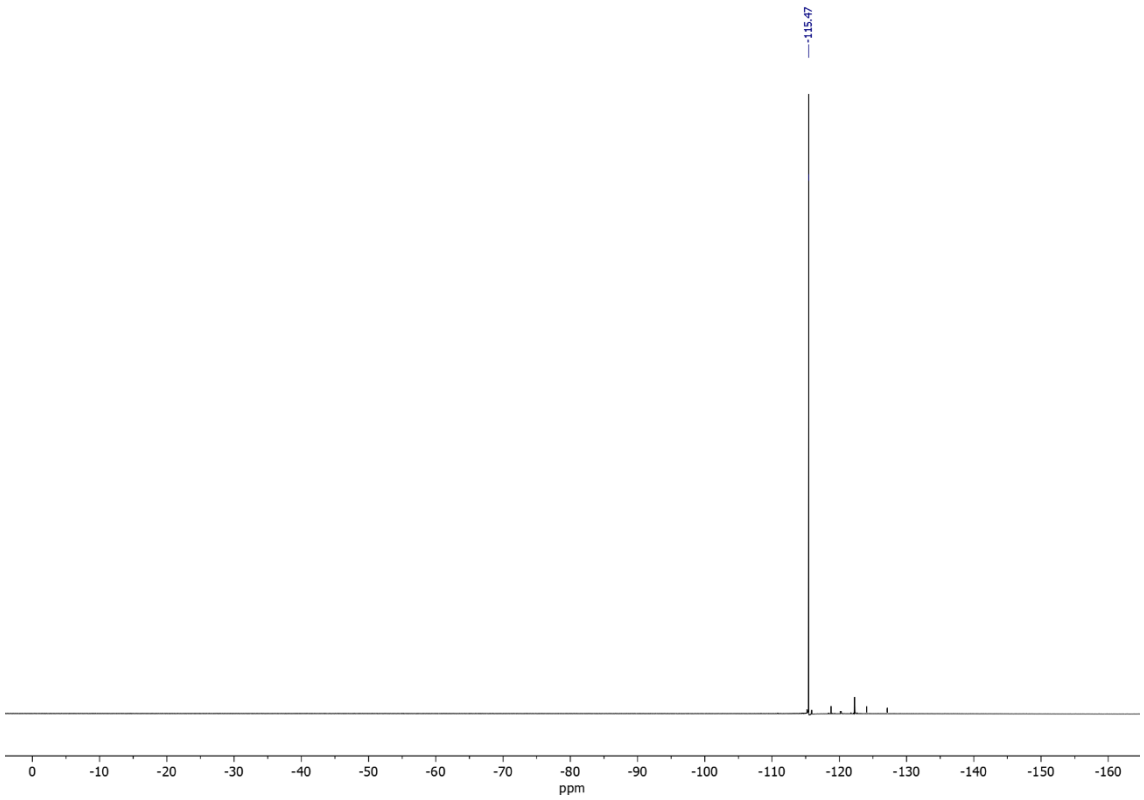




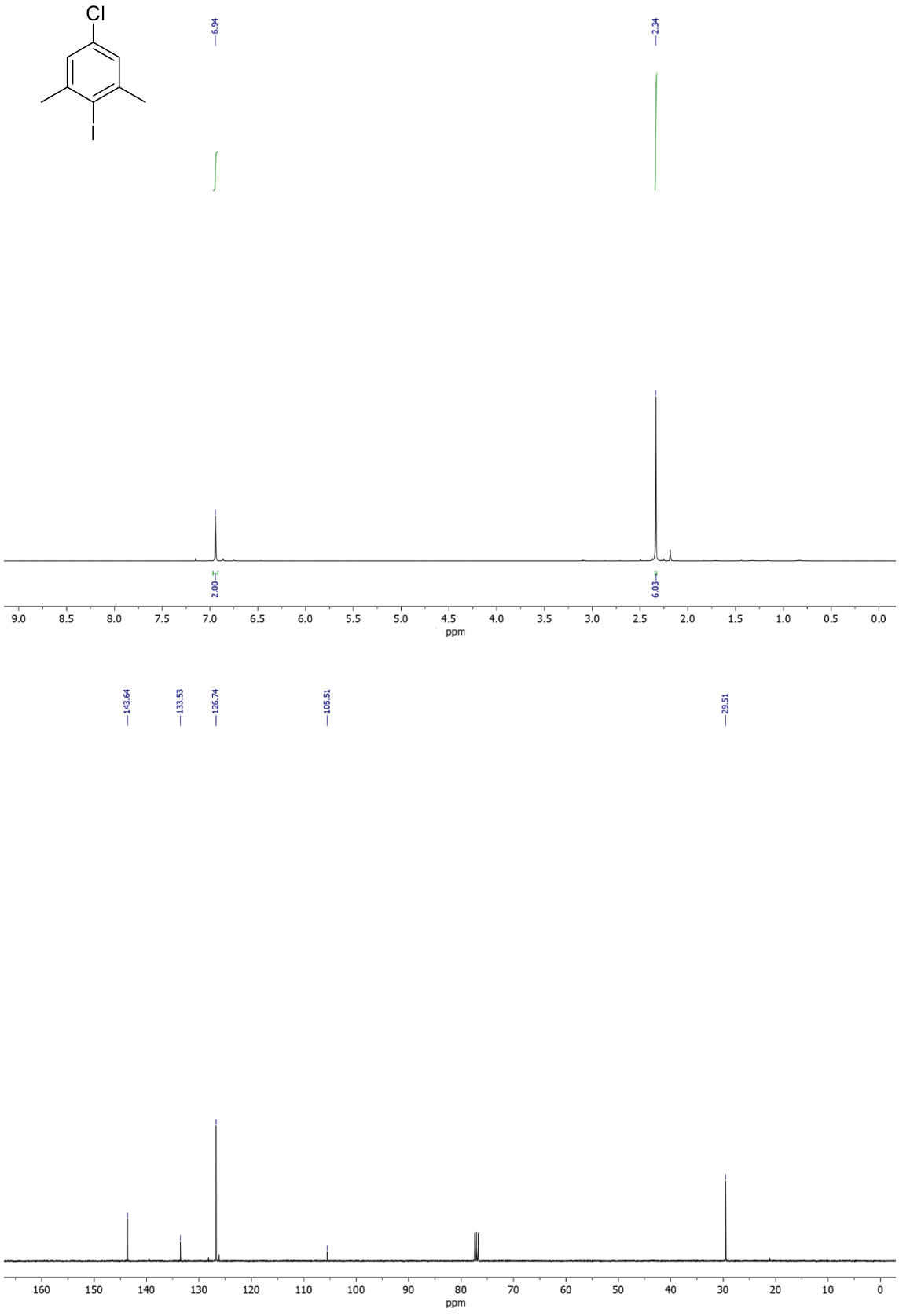
^{1}H-NMR (500 MHz, $CDCl_3$) and ^{13}C-NMR (126 MHz, $CDCl_3$) of compound S2a



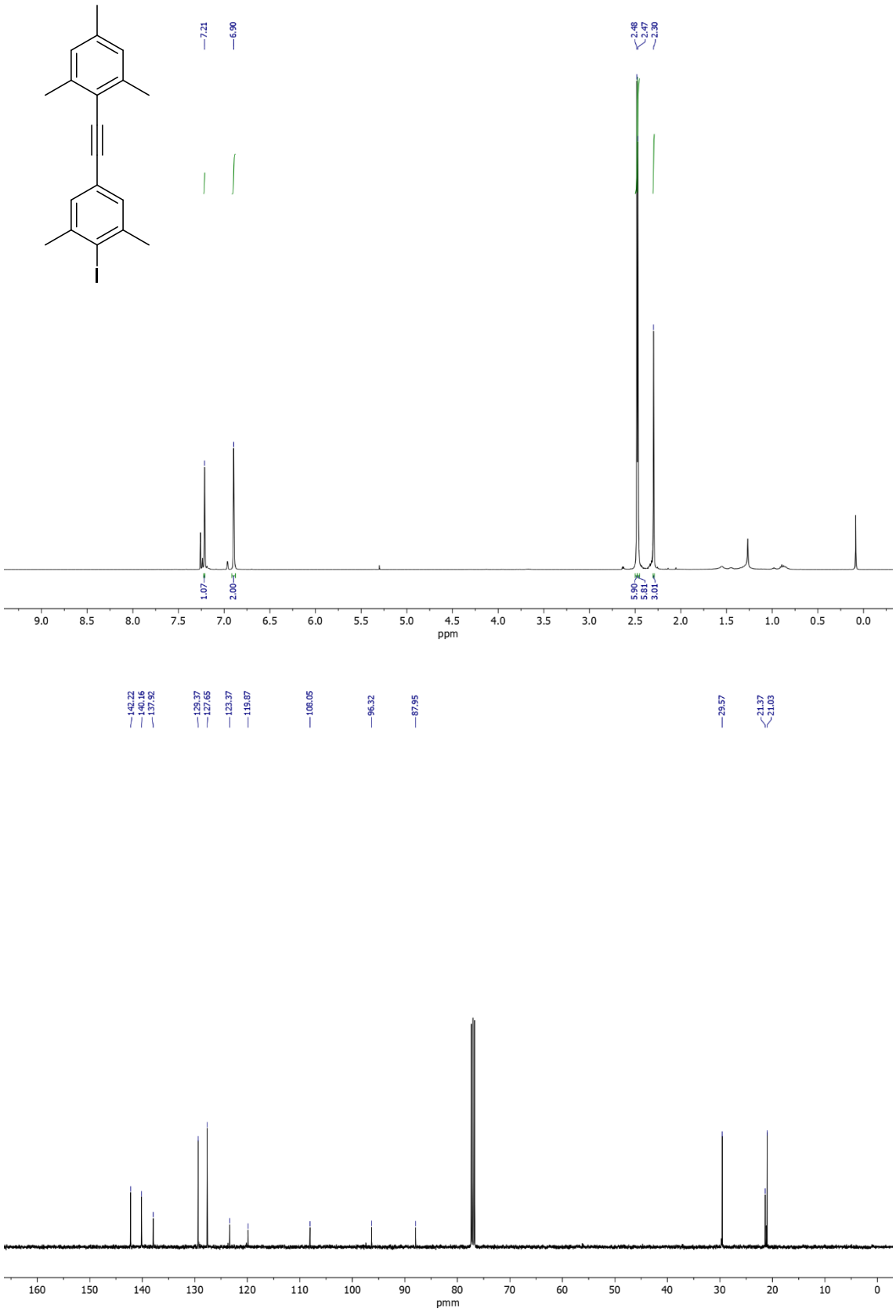
^{19}F-NMR (376 MHz, $CDCl_3$) of compound S2a



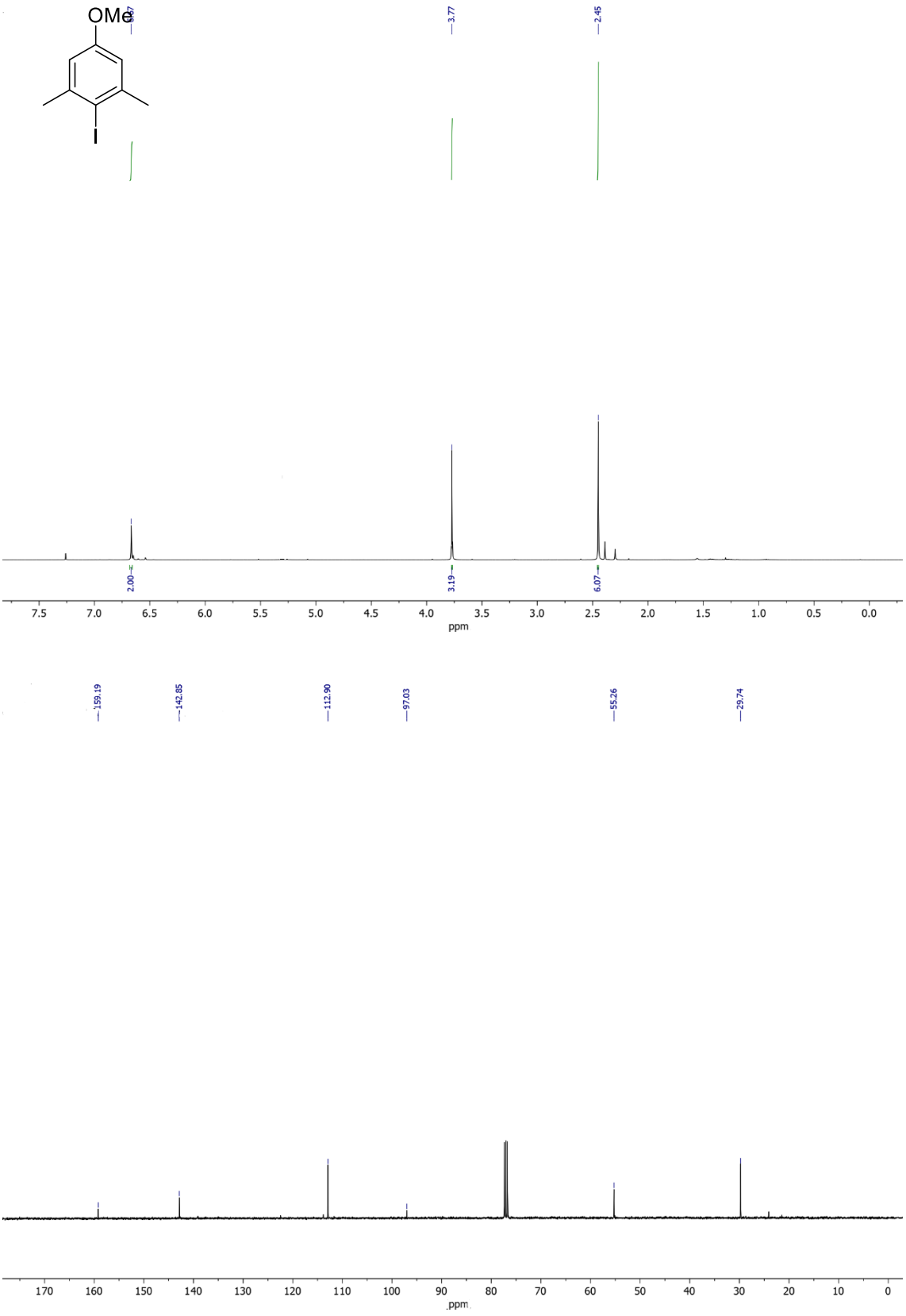
^{1}H-NMR (500 MHz, $CDCl_3$) and ^{13}C-NMR (126 MHz, $CDCl_3$) of compound S2b



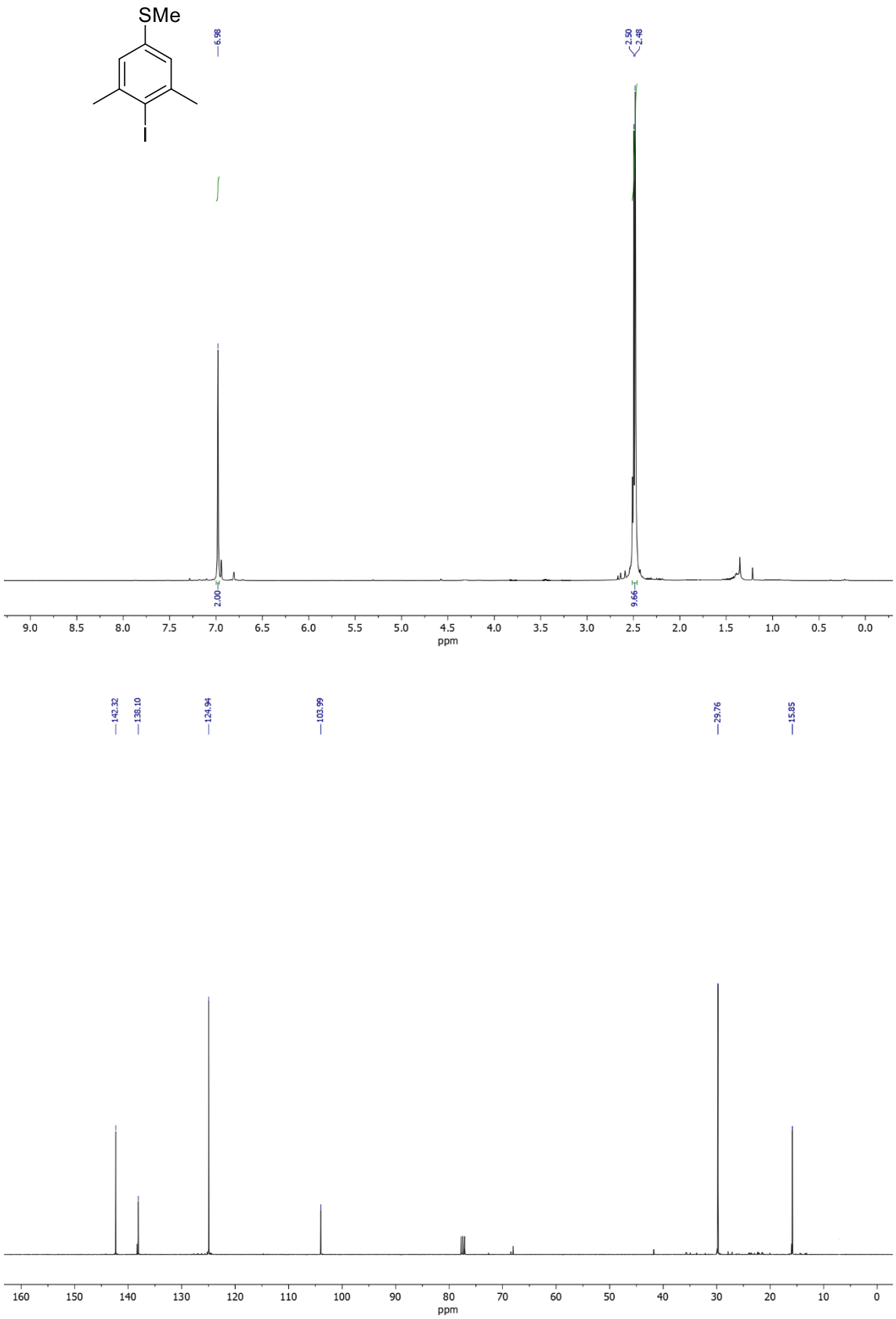
^{1}H-NMR (500 MHz, $CDCl_3$) and ^{13}C-NMR (126 MHz, $CDCl_3$) of compound S2c



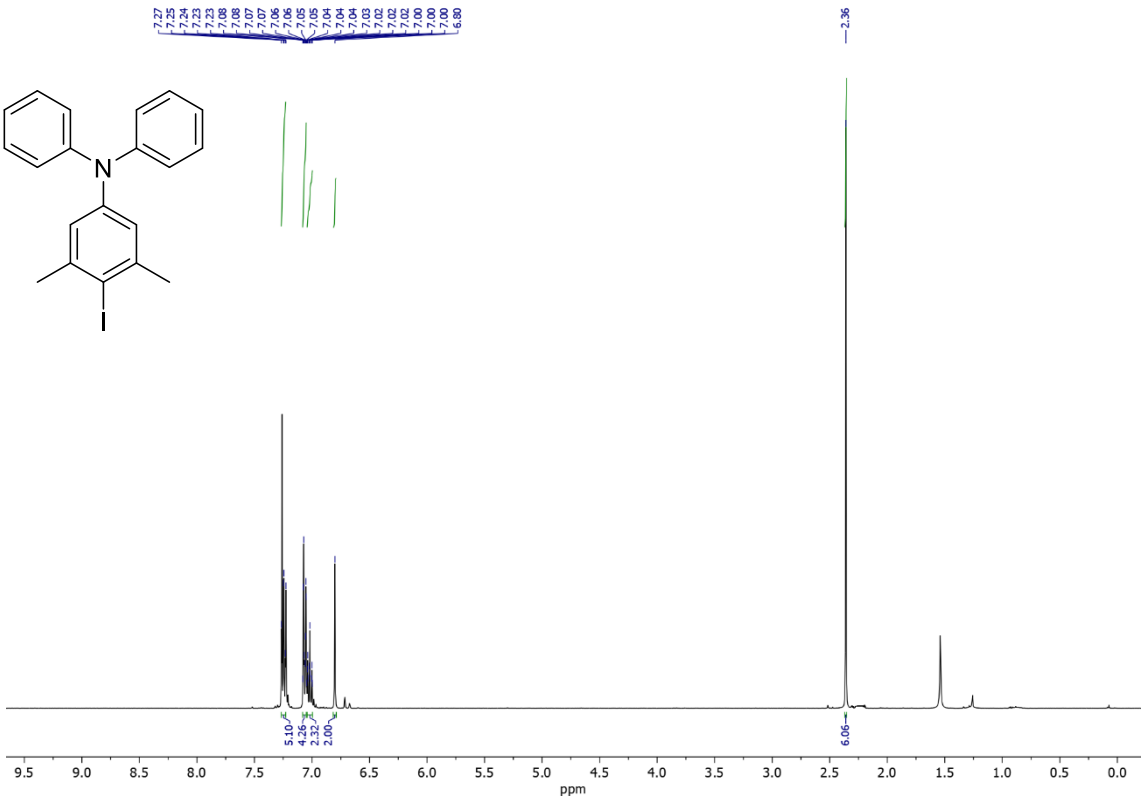
^{1}H-NMR (500 MHz, $CDCl_3$) and ^{13}C-NMR (126 MHz, $CDCl_3$) of compound S2f

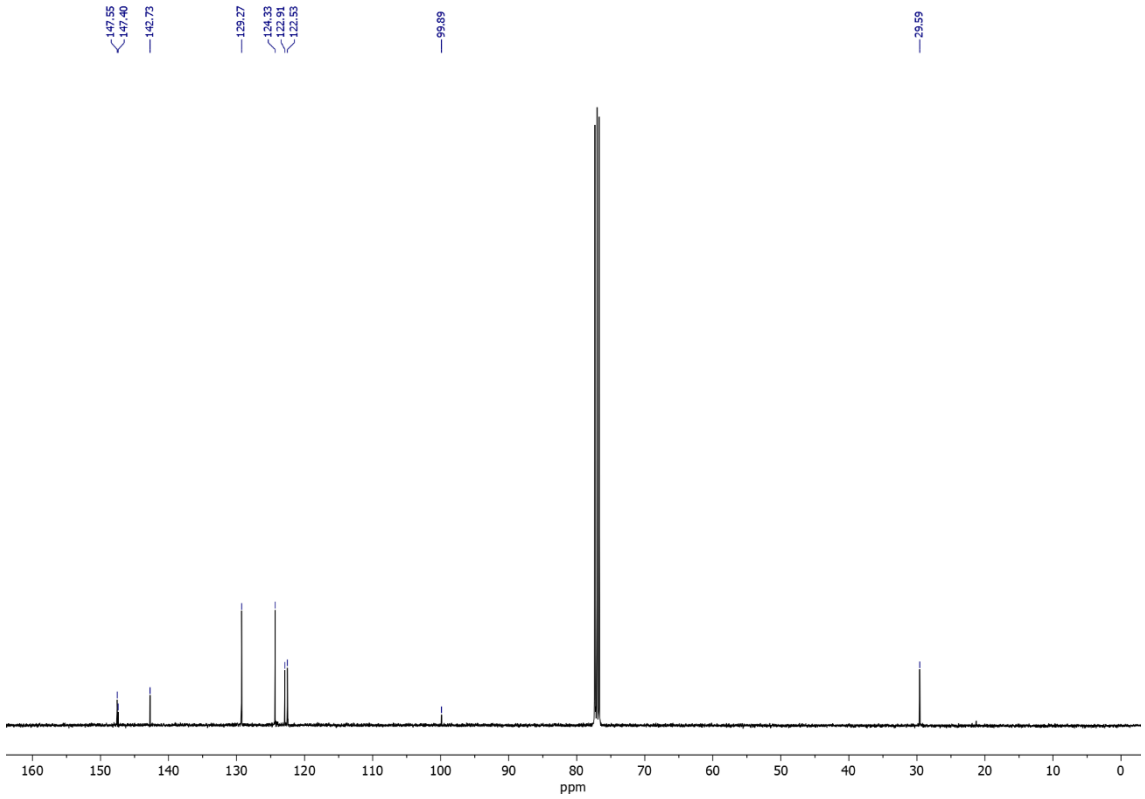


^{1}H-NMR (500 MHz, $CDCl_3$) and ^{13}C-NMR (126 MHz, $CDCl_3$) of compound S2g

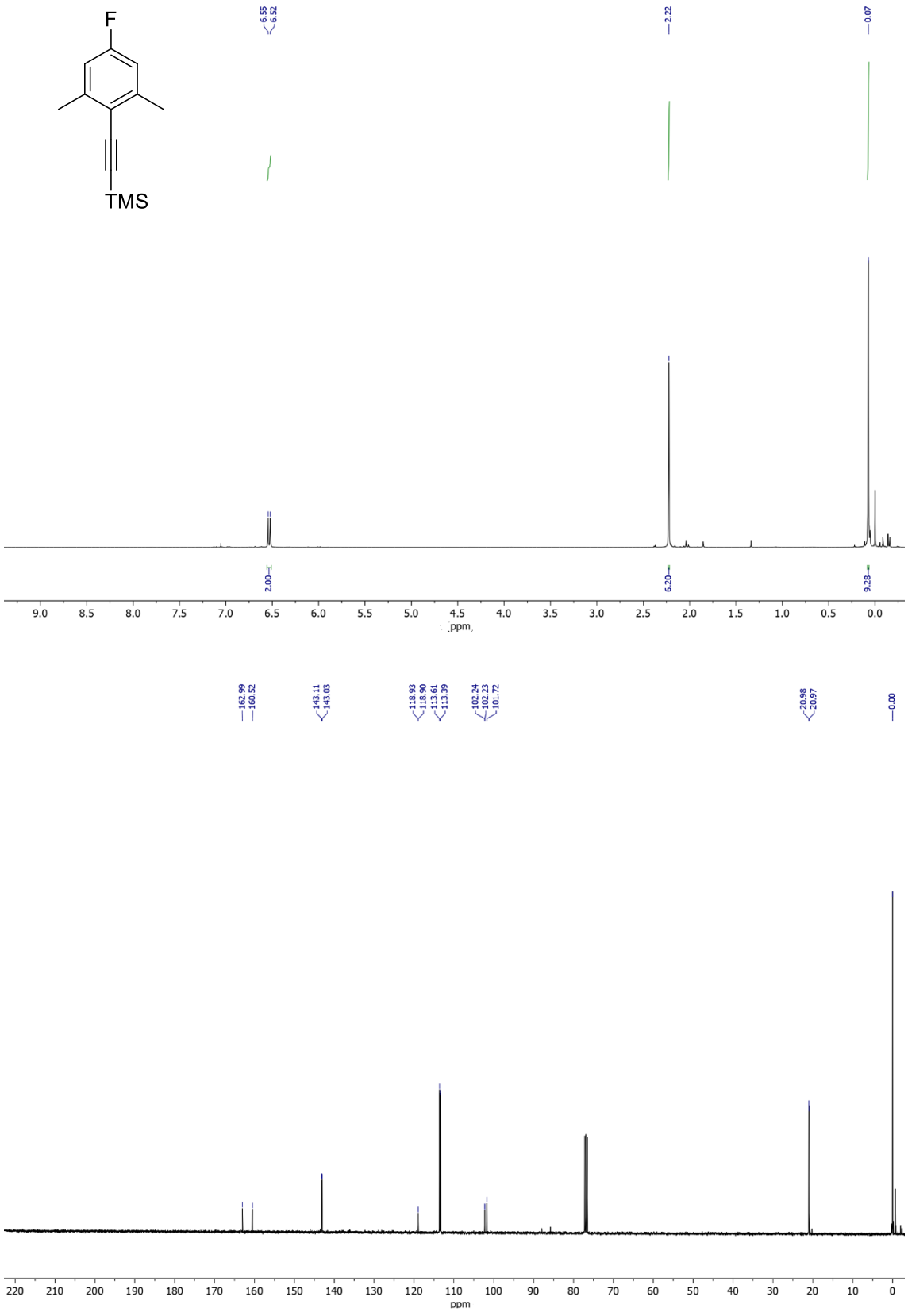


^{1}H-NMR (500 MHz, $CDCl_3$) and ^{13}C-NMR (126 MHz, $CDCl_3$) of compound S2h

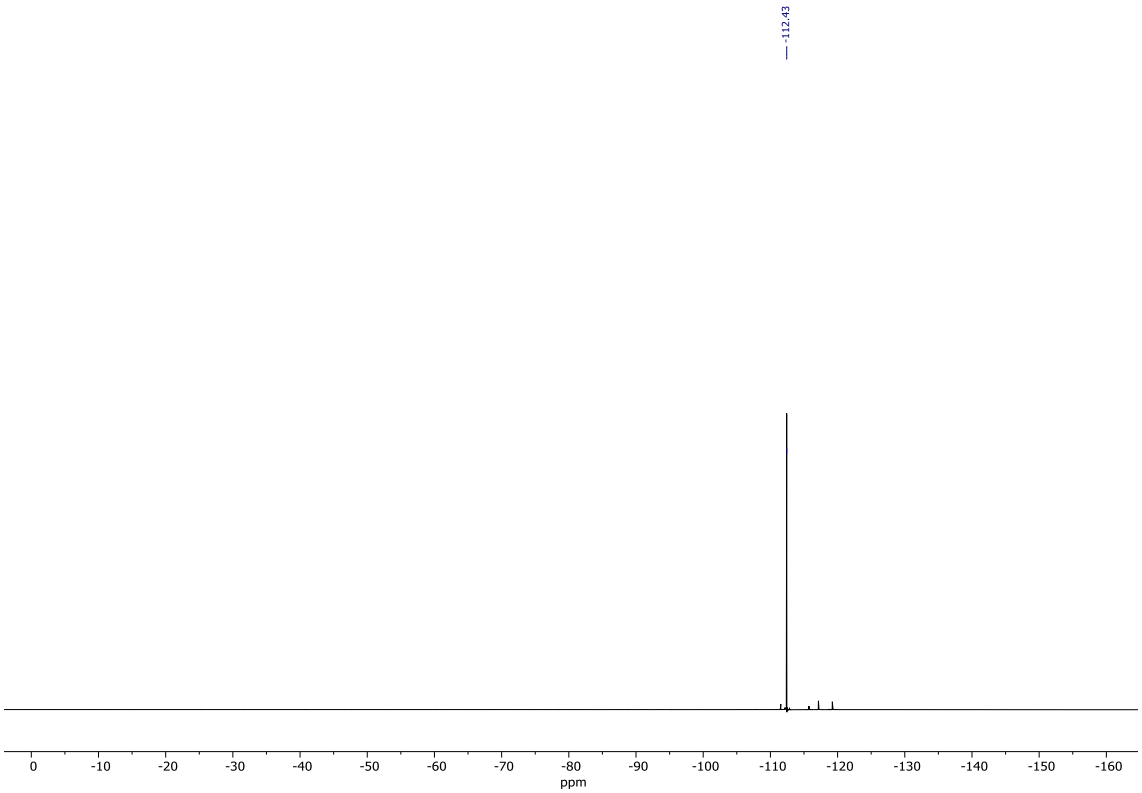




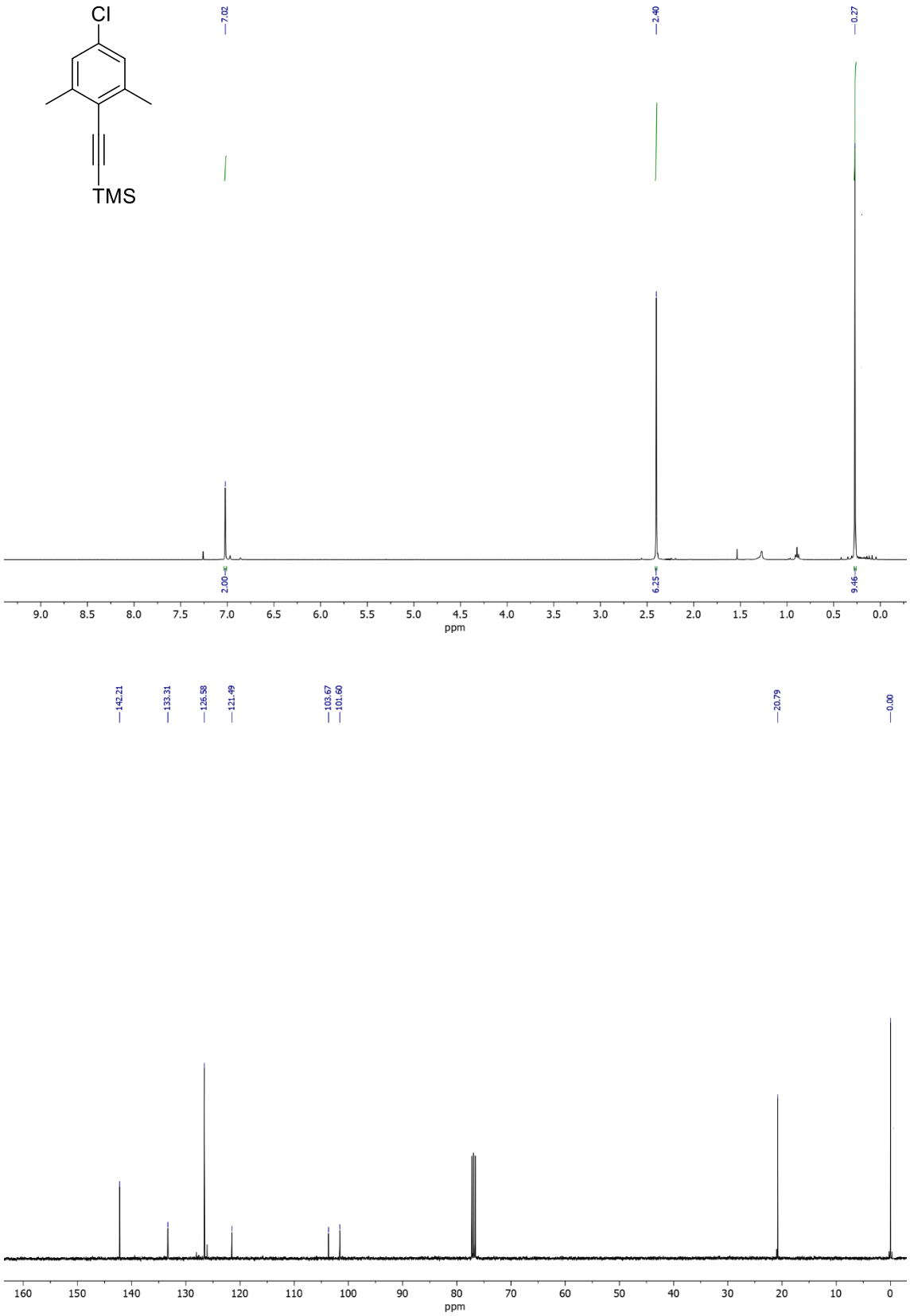
^{1}H-NMR (500 MHz, $CDCl_3$) and ^{13}C-NMR (126 MHz, $CDCl_3$) of compound S3a



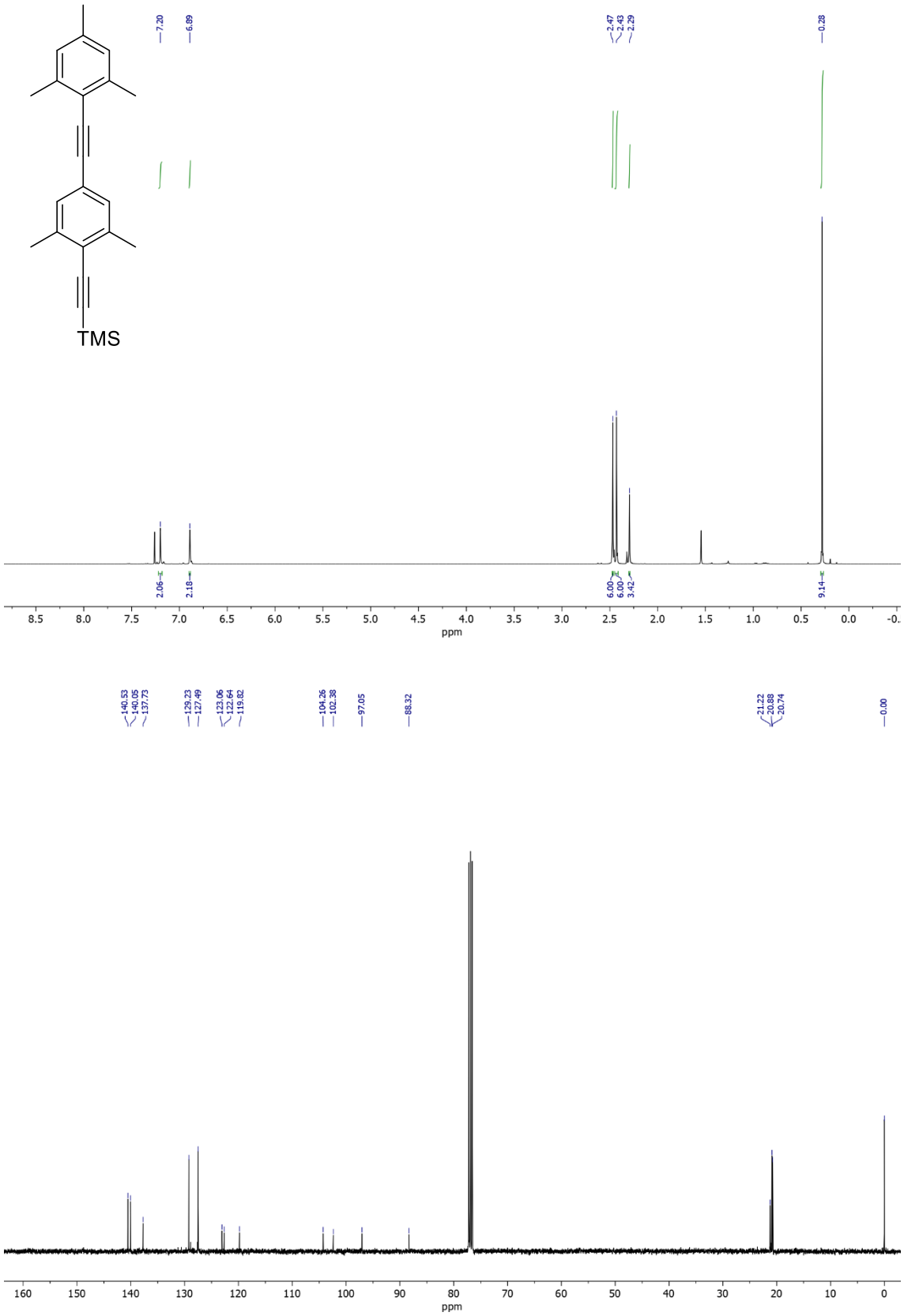
^{19}F-NMR (376 MHz, $CDCl_3$) of compound S3a



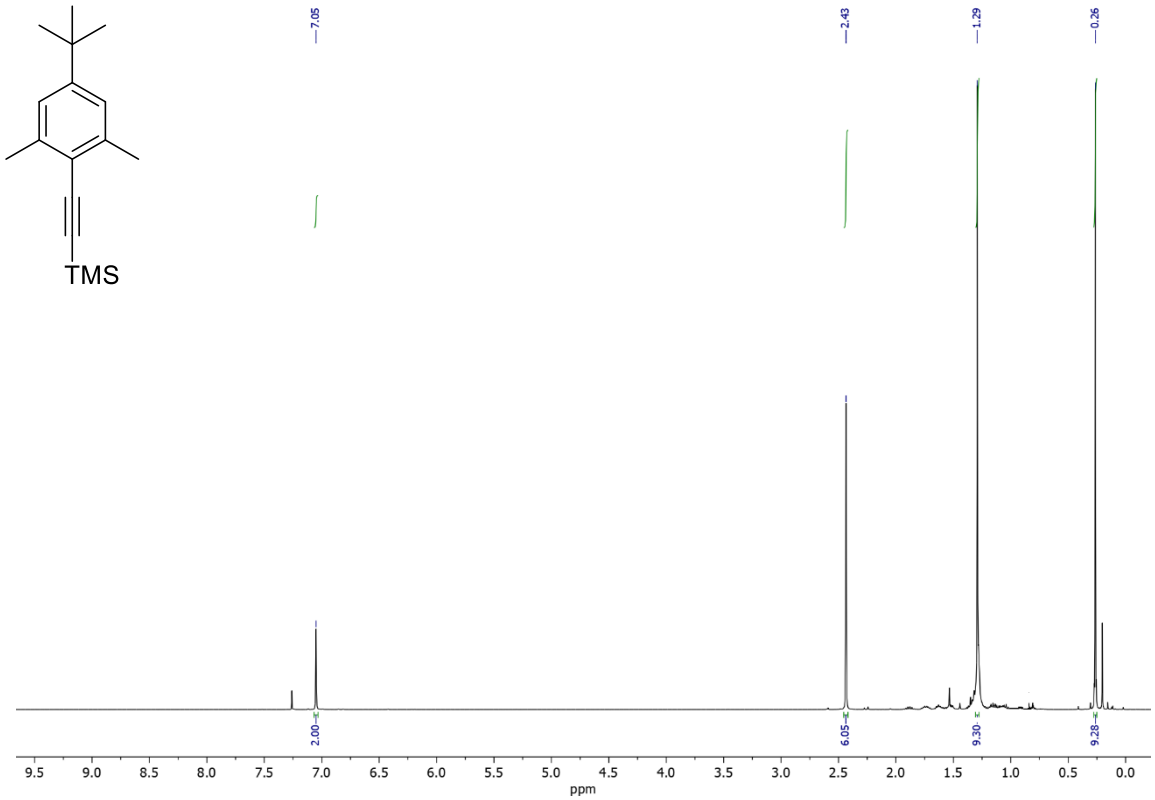
^{1}H-NMR (500 MHz, $CDCl_3$) and ^{13}C-NMR (126 MHz, $CDCl_3$) of compound S3b

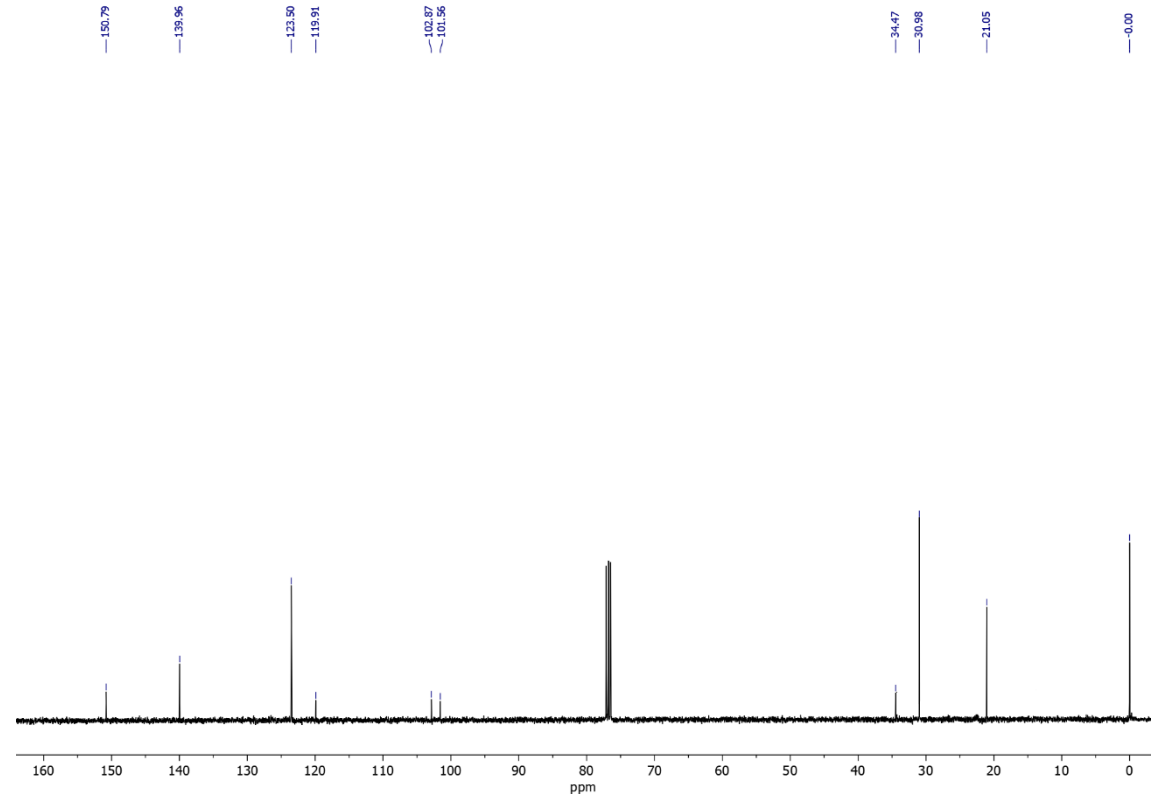


^{1}H-NMR (500 MHz, $CDCl_3$) and ^{13}C-NMR (126 MHz, $CDCl_3$) of compound S3c

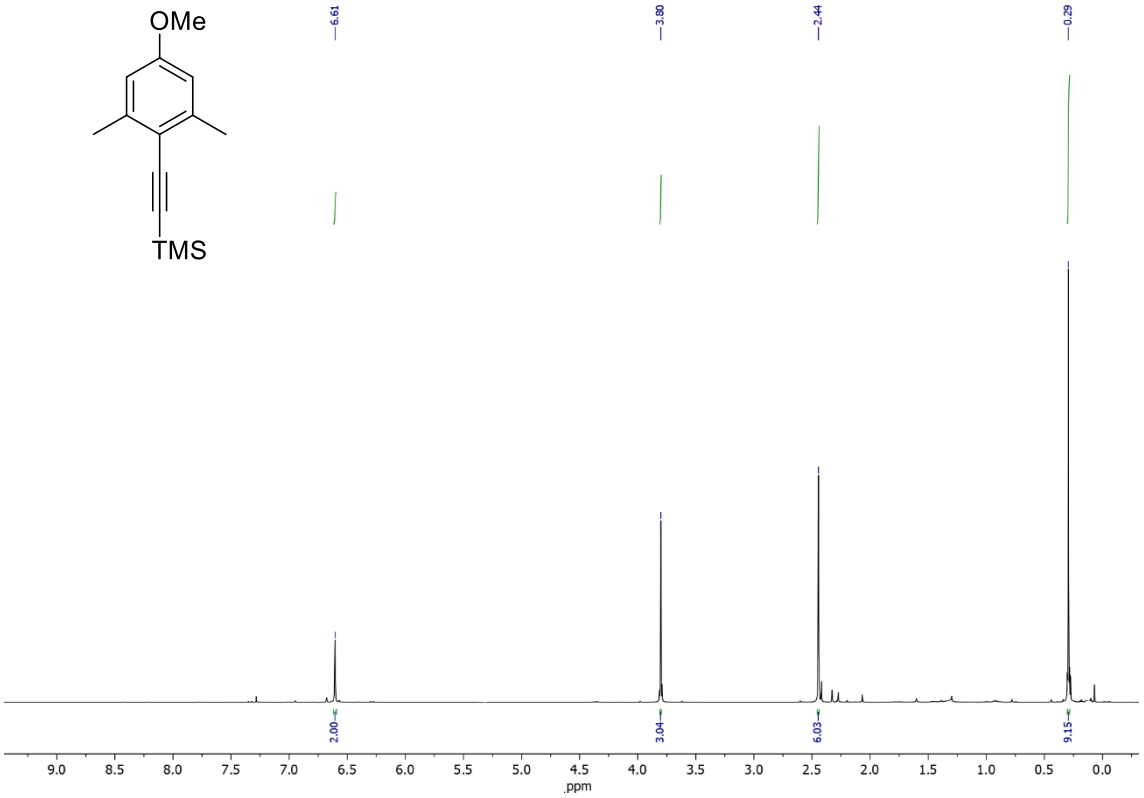


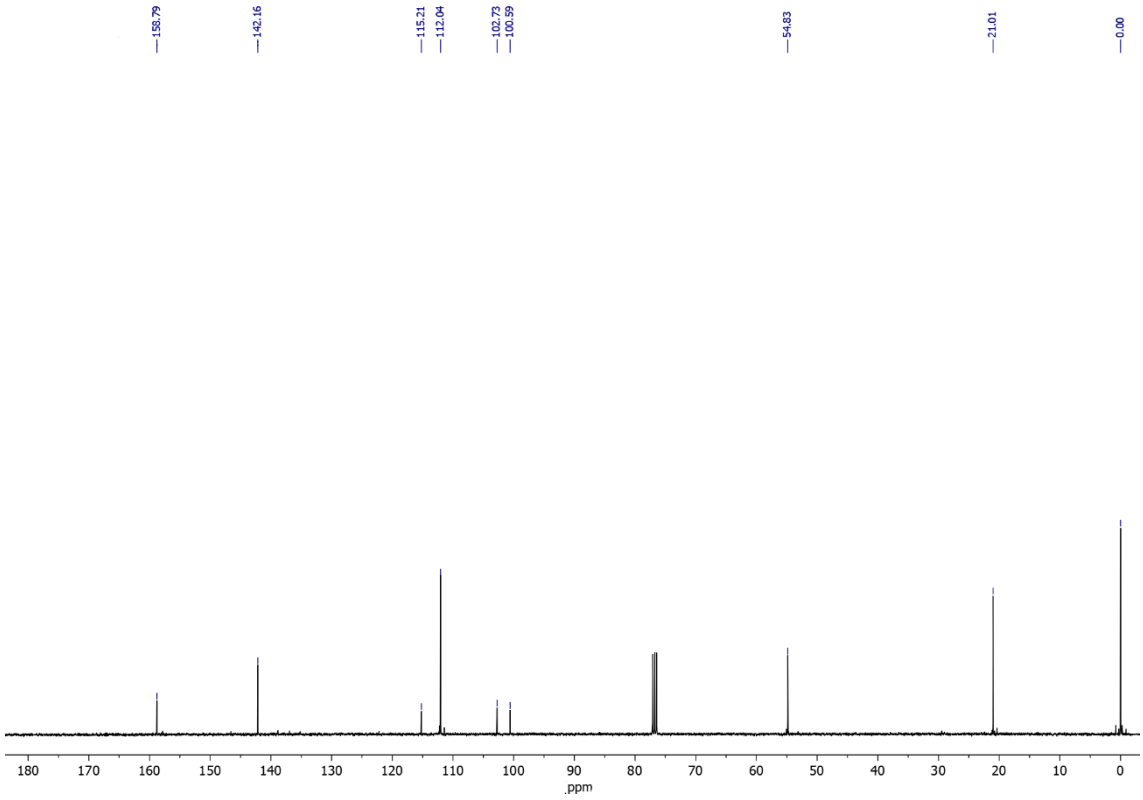
^{1}H-NMR (500 MHz, $CDCl_3$) and ^{13}C-NMR (126 MHz, $CDCl_3$) of compound S3e



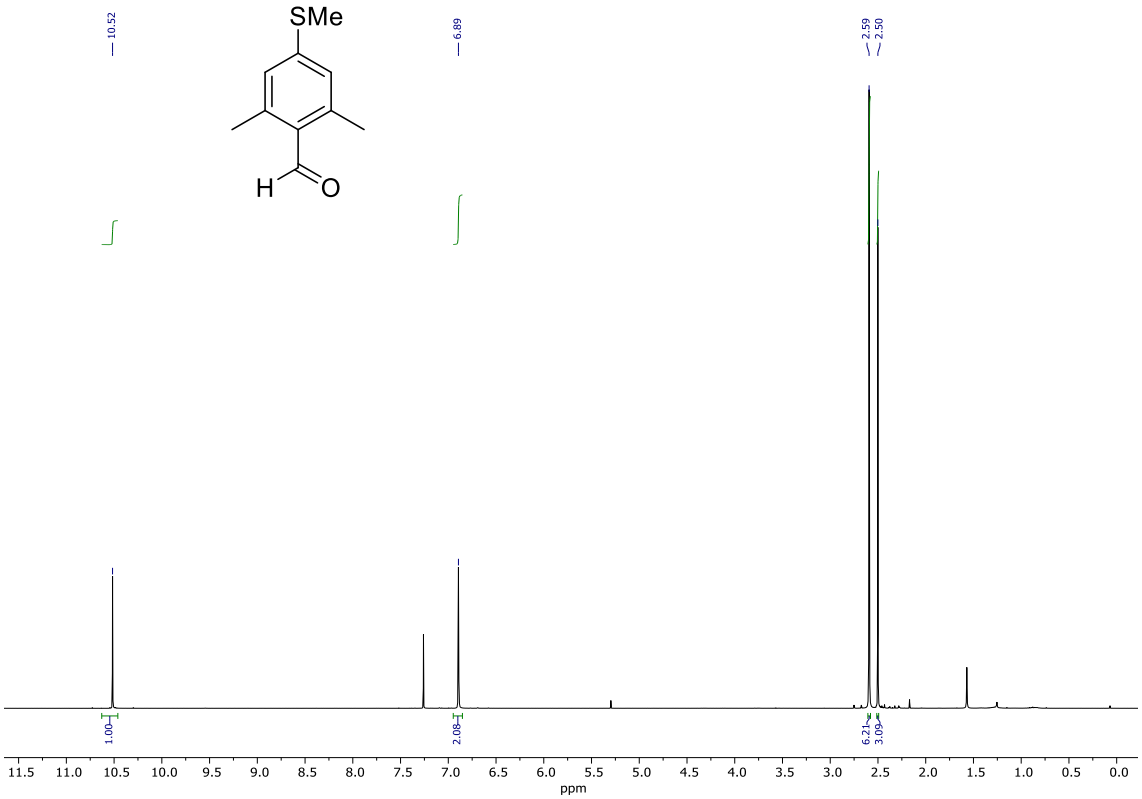


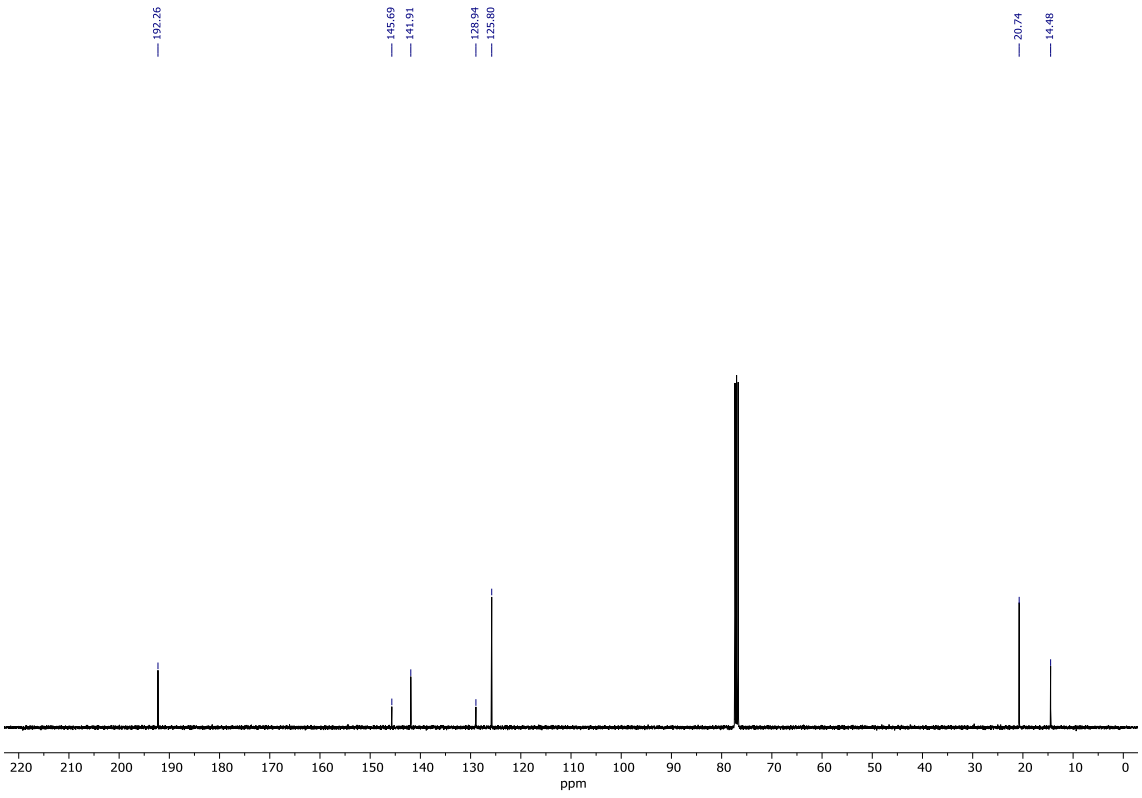
^{1}H-NMR (500 MHz, $CDCl_3$) and ^{13}C-NMR (126 MHz, $CDCl_3$) of compound S3f



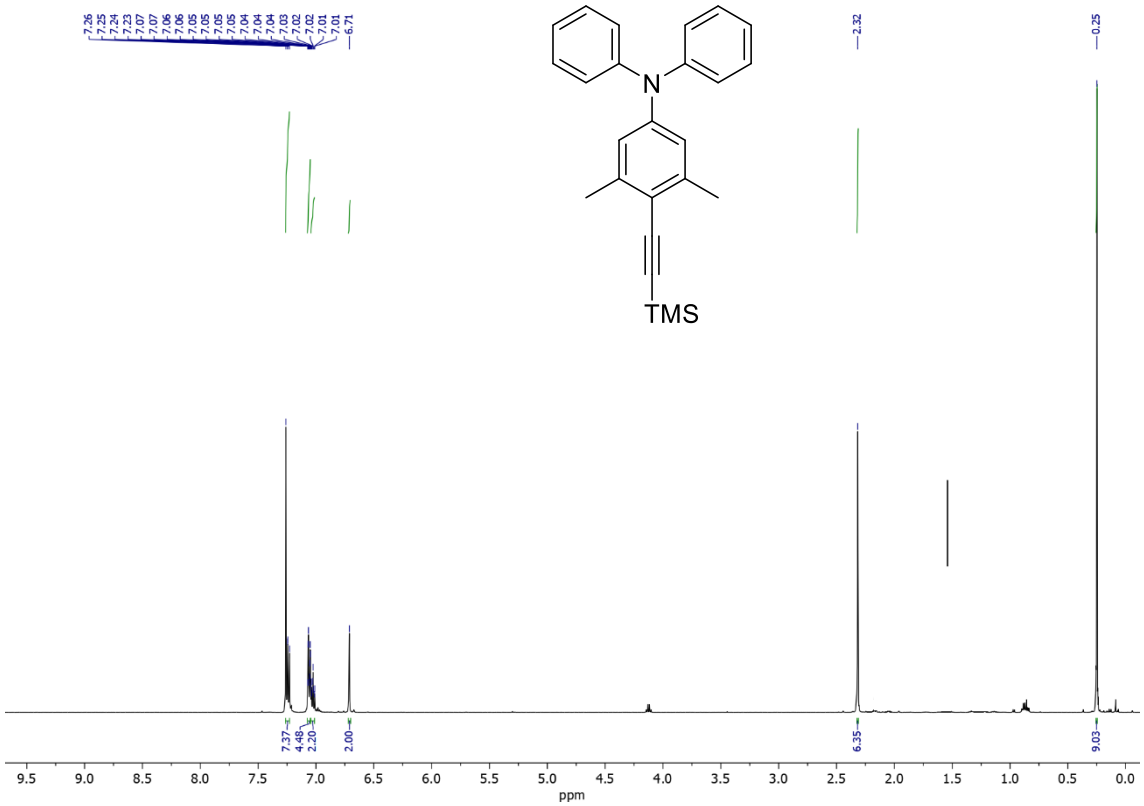


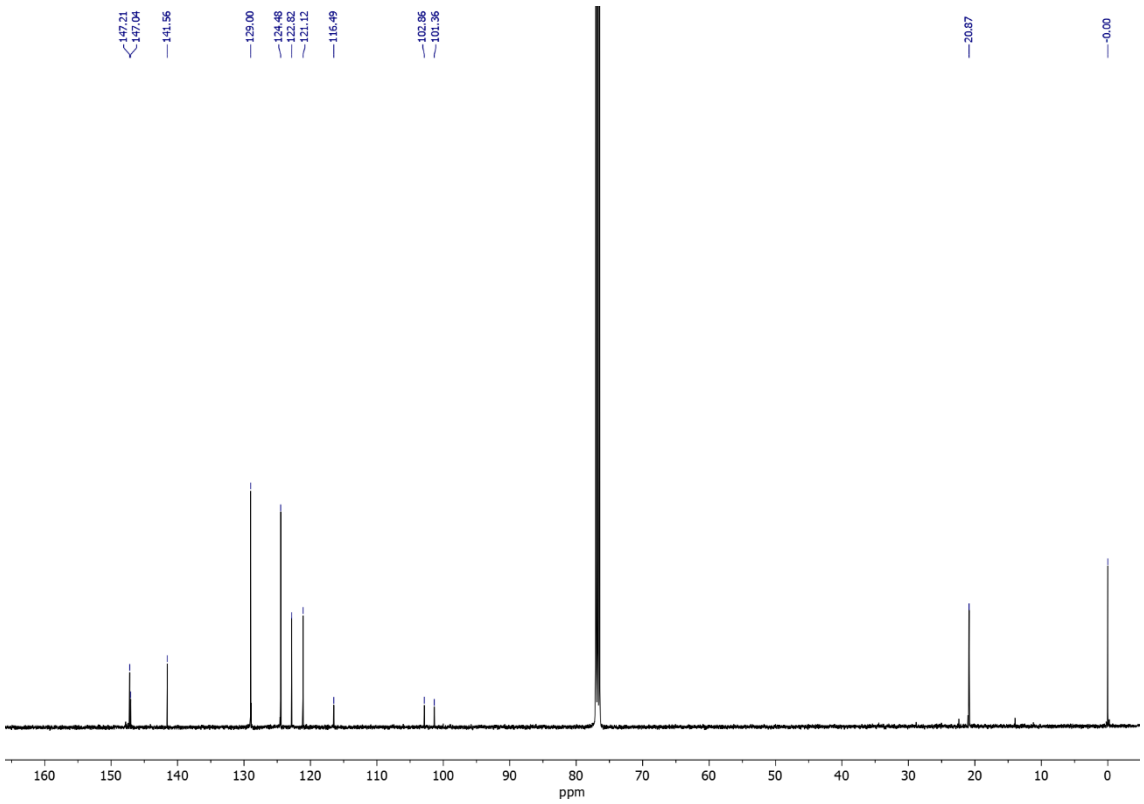
^{1}H-NMR (500 MHz, $CDCl_3$) and ^{13}C-NMR (126 MHz, $CDCl_3$) of compound S4



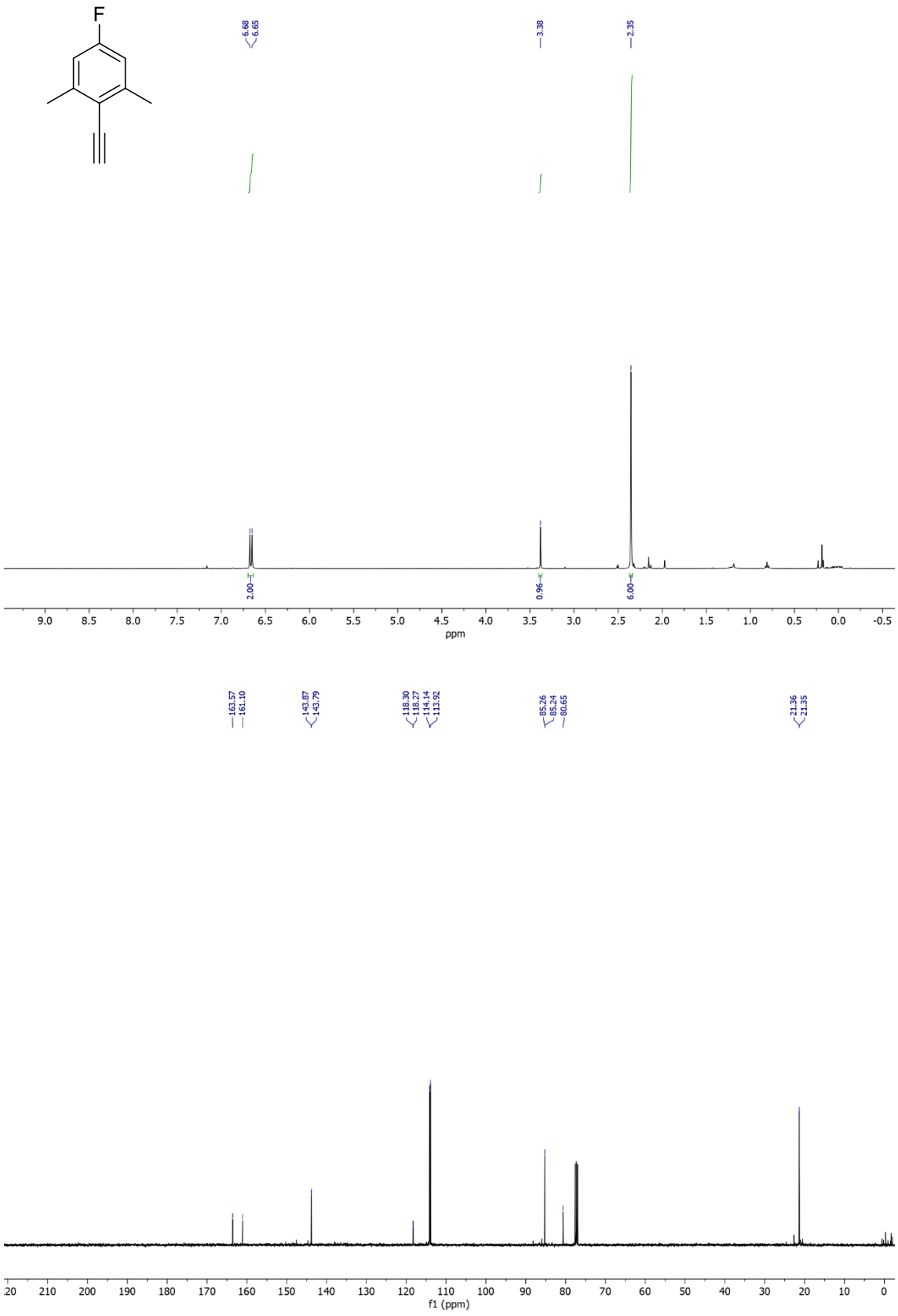


^{1}H-NMR (500 MHz, $CDCl_3$) and ^{13}C-NMR (126 MHz, $CDCl_3$) of compound S3h

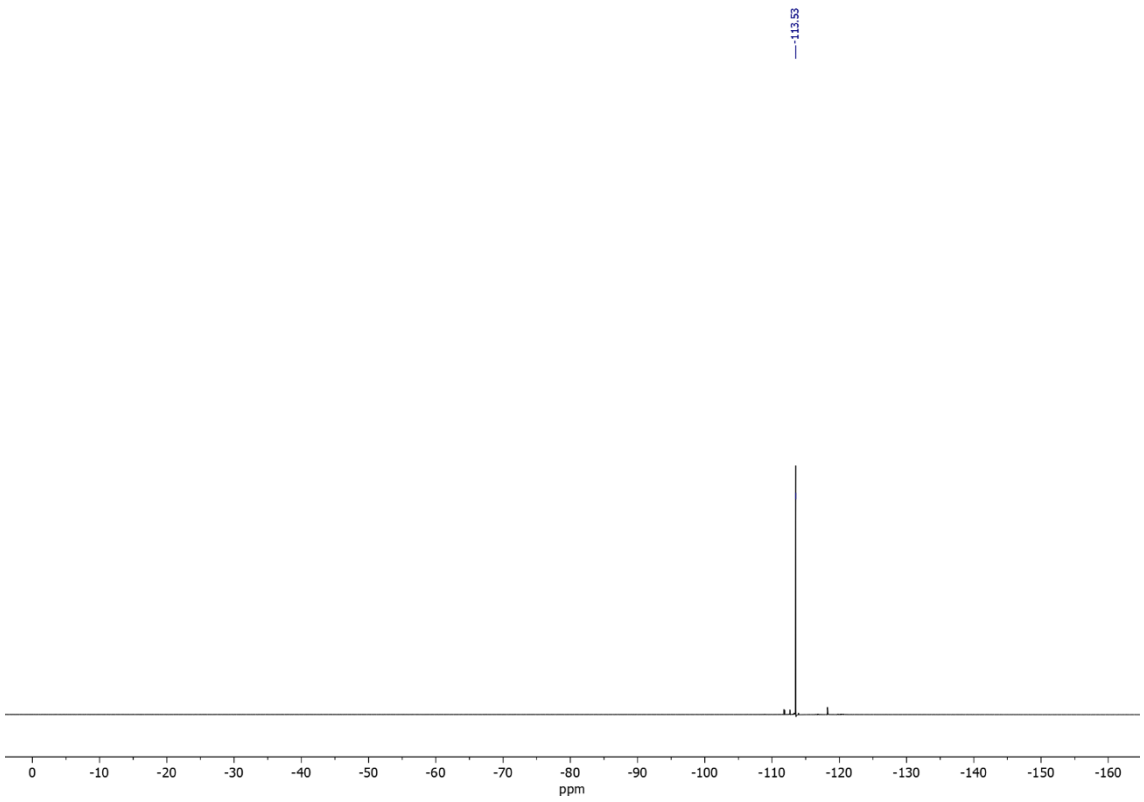




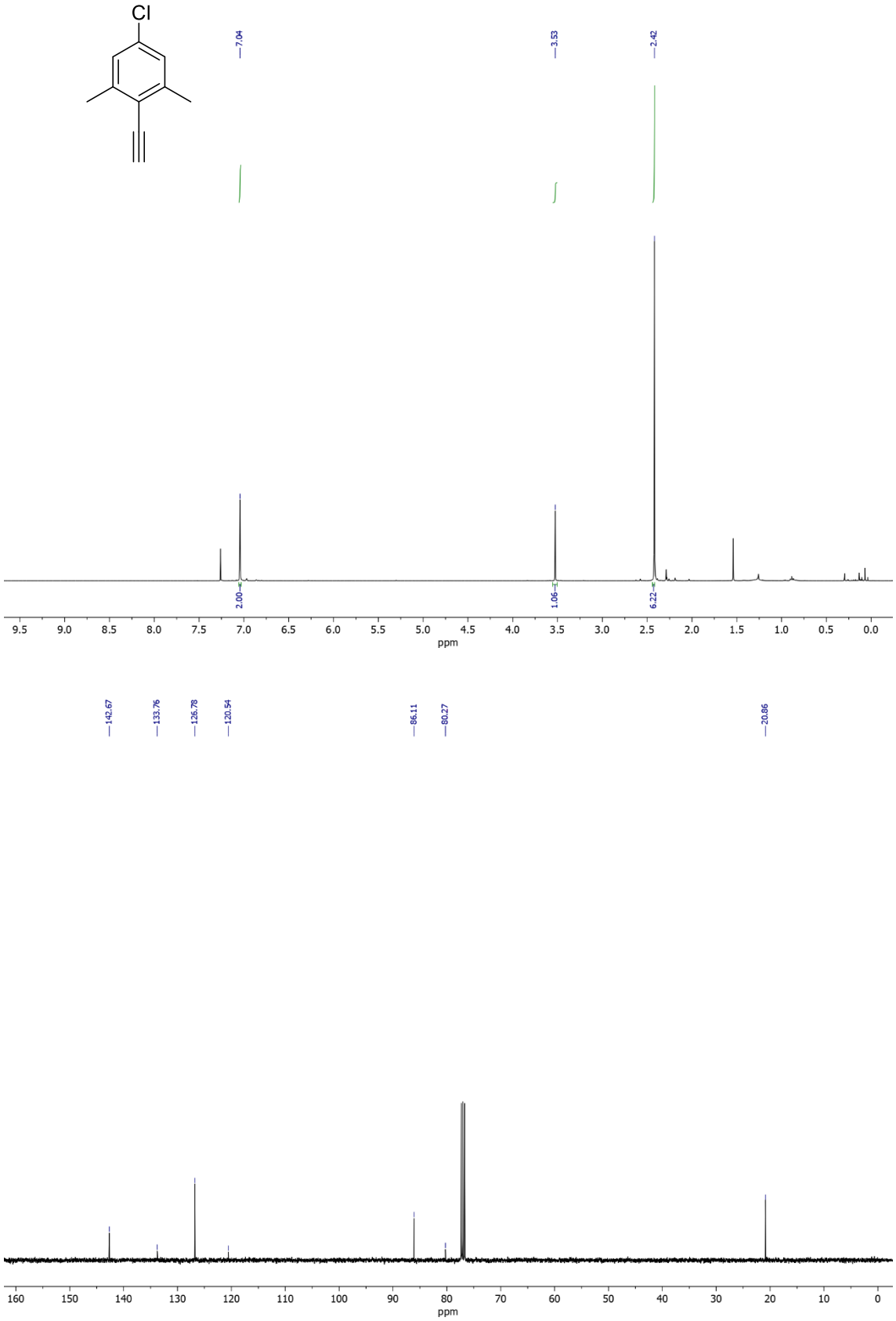
^{1}H-NMR (500 MHz, $CDCl_3$) and ^{13}C-NMR (126 MHz, $CDCl_3$) of compound 6a



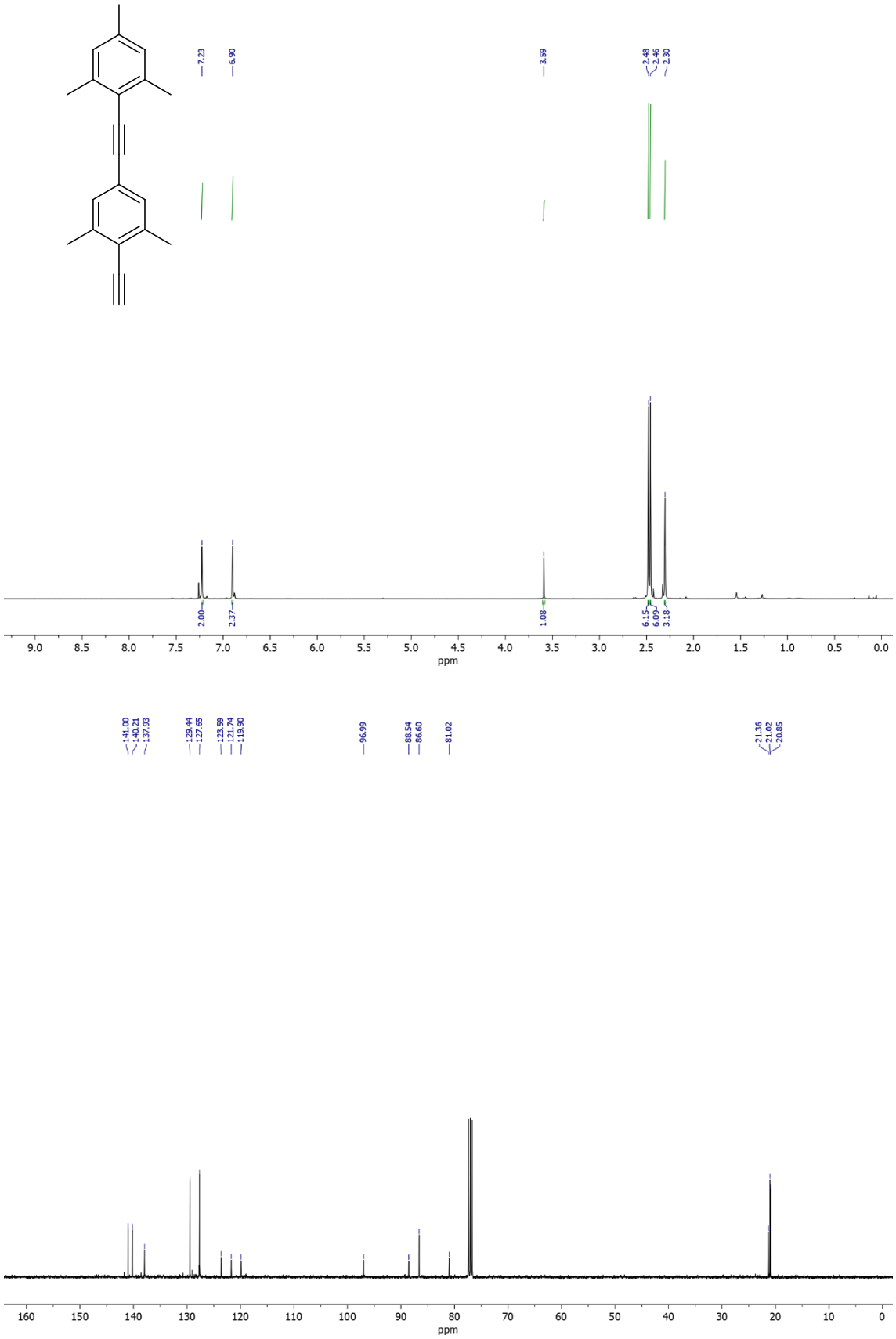
^{19}F-NMR (376 MHz, $CDCl_3$) of compound 6a



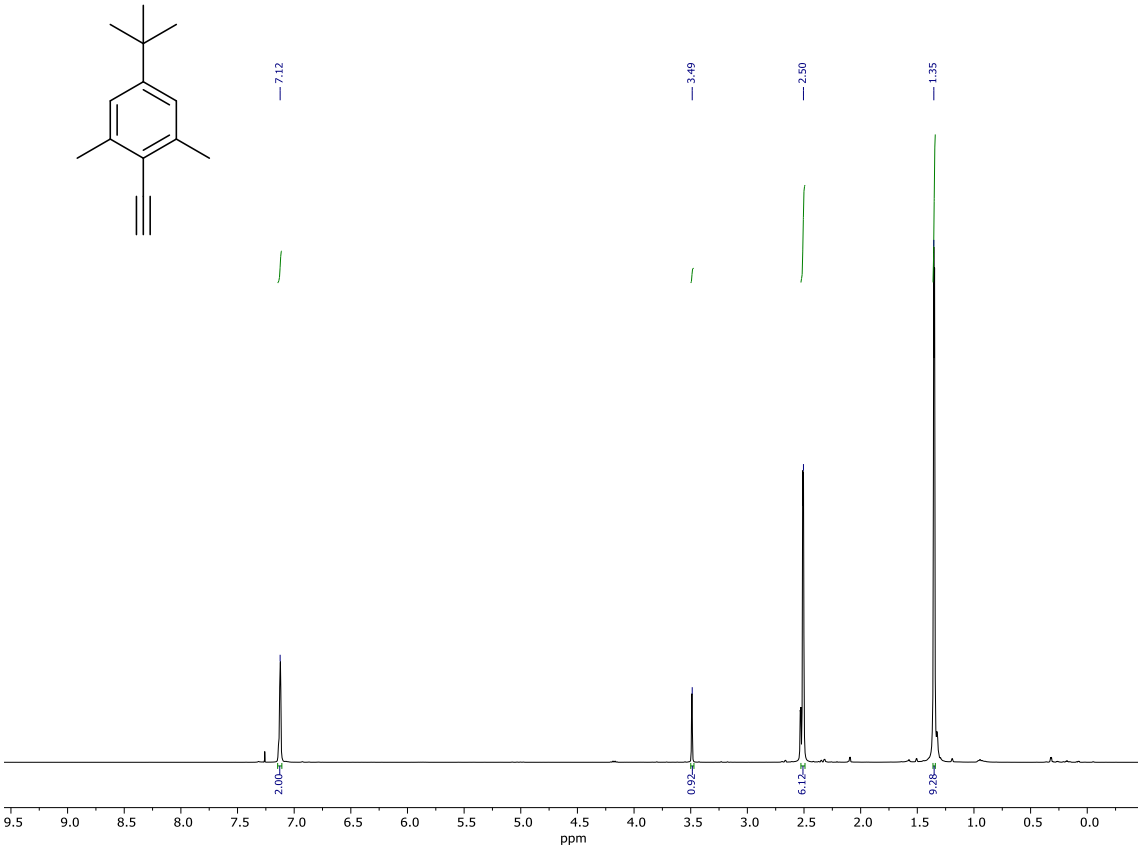
^{1}H-NMR (500 MHz, $CDCl_3$) and ^{13}C-NMR (126 MHz, $CDCl_3$) of compound 6b

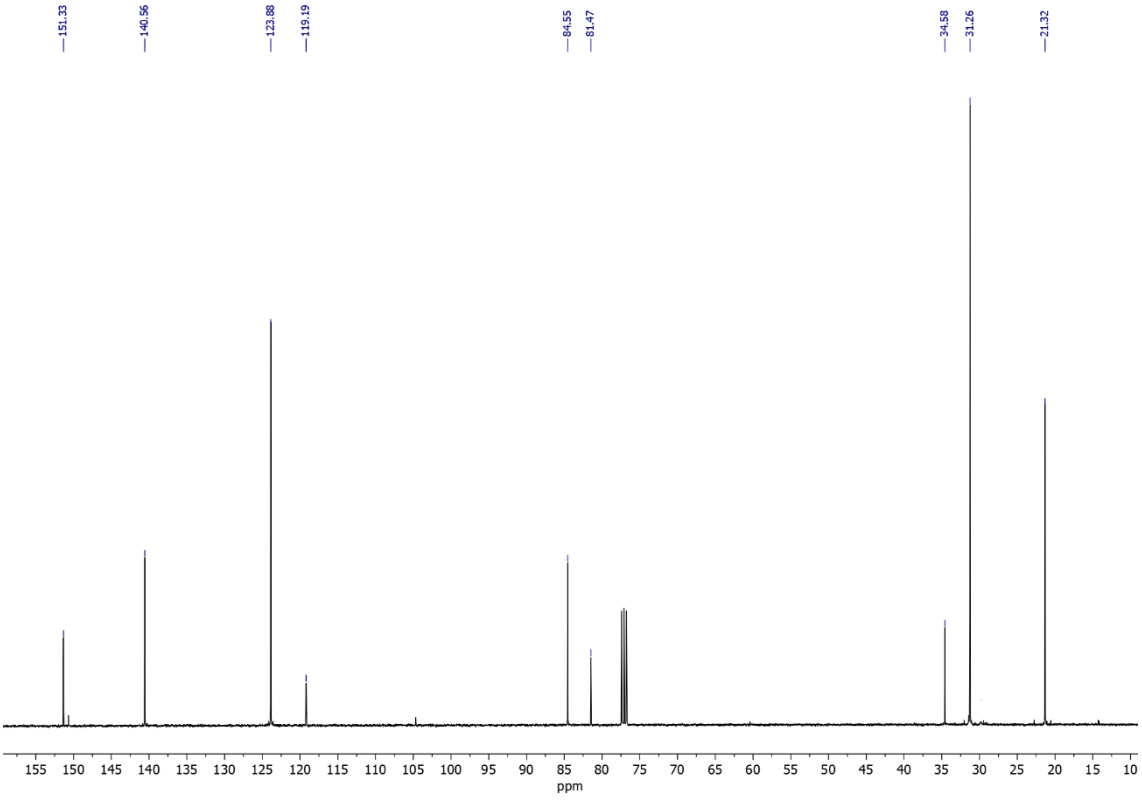


^{1}H-NMR (500 MHz, $CDCl_3$) and ^{13}C-NMR (126 MHz, $CDCl_3$) of compound 6c

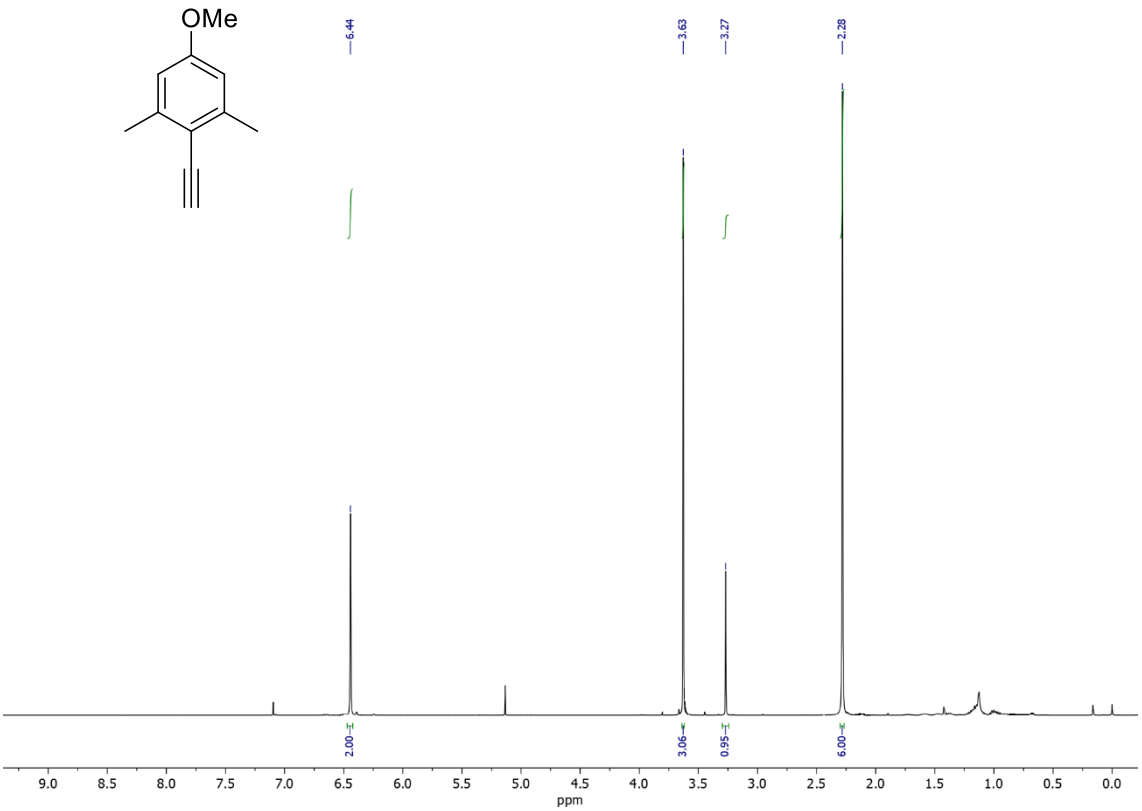


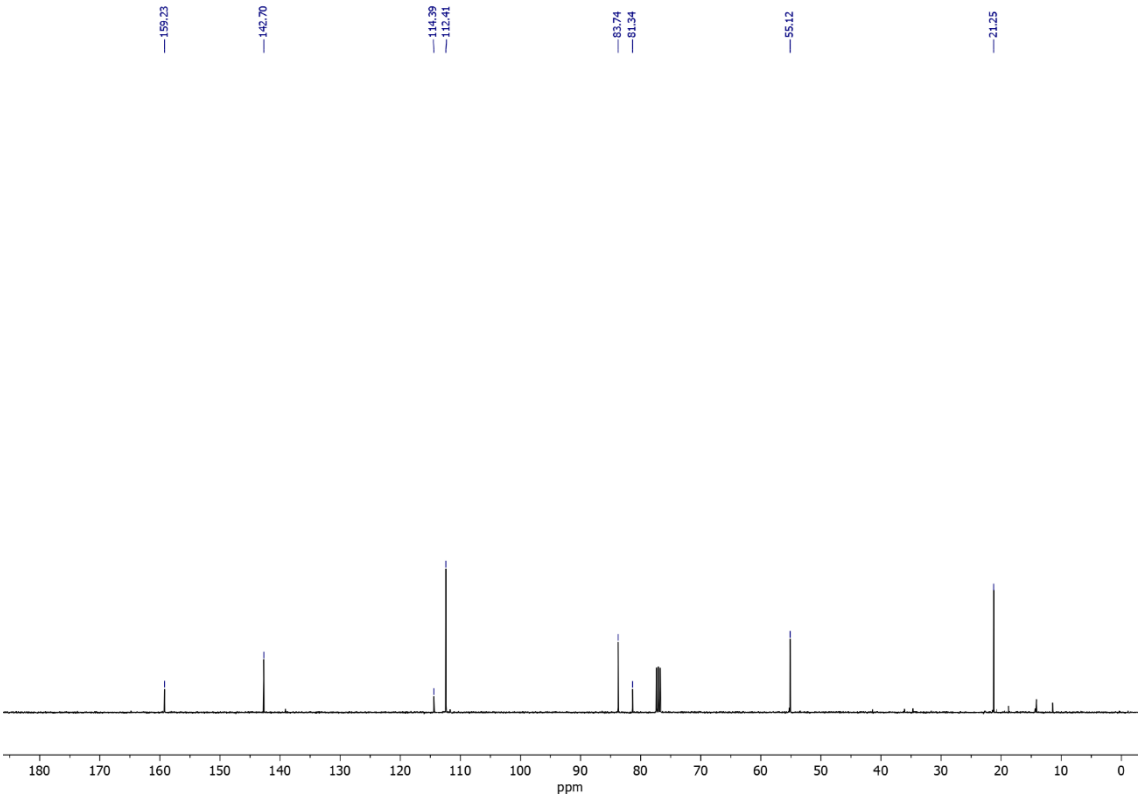
^{1}H-NMR (500 MHz, $CDCl_3$) and ^{13}C-NMR (126 MHz, $CDCl_3$) of compound 6e



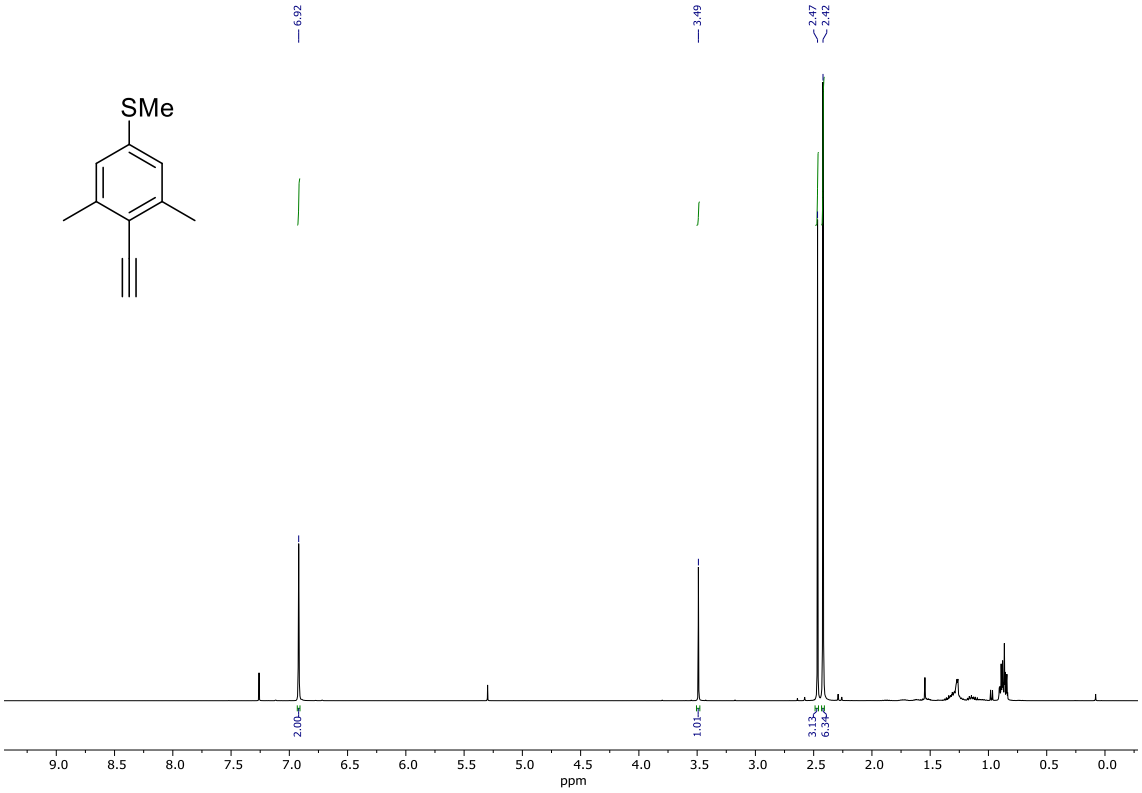


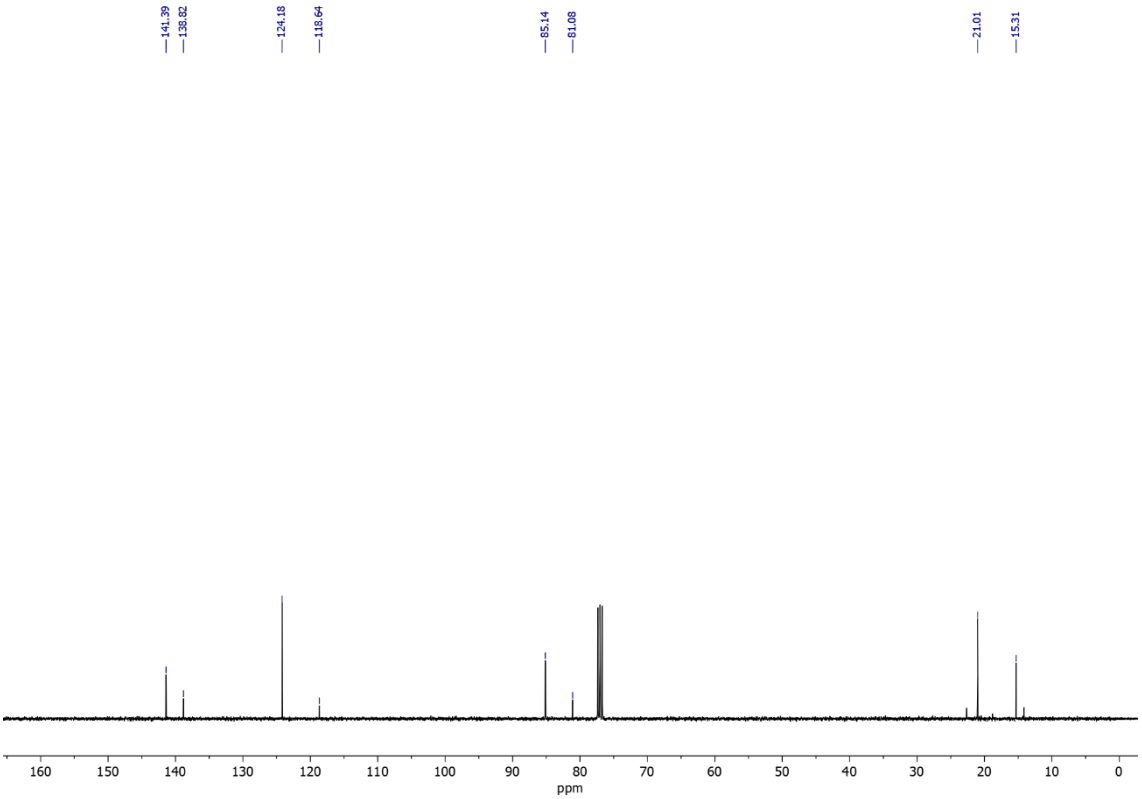
^{1}H-NMR (500 MHz, $CDCl_3$) and ^{13}C-NMR (126 MHz, $CDCl_3$) of compound 6f



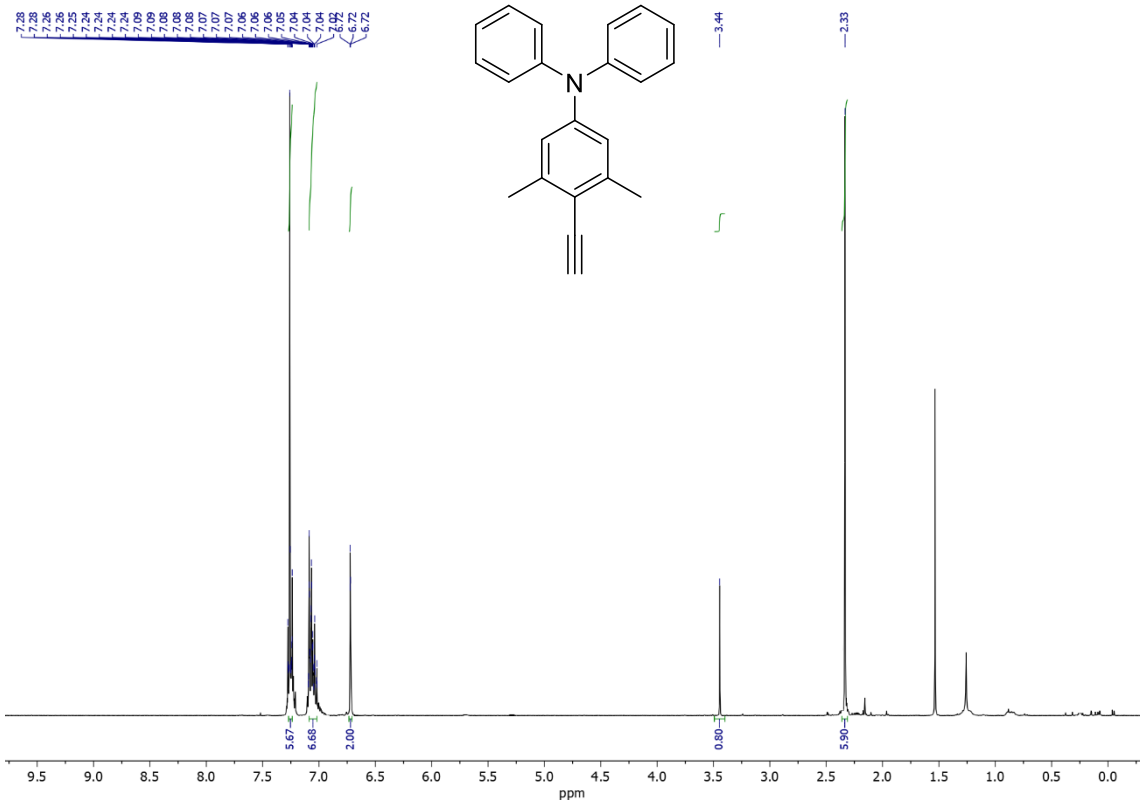


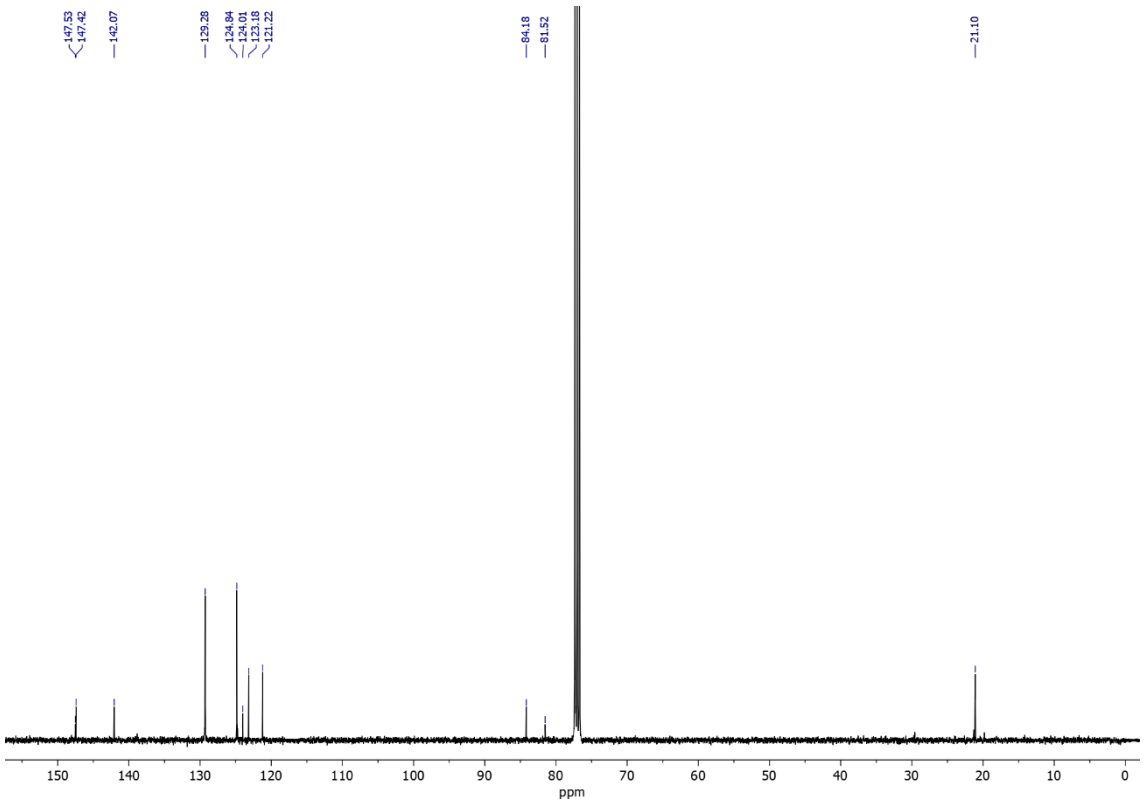
^{1}H-NMR (500 MHz, $CDCl_3$) and ^{13}C-NMR (126 MHz, $CDCl_3$) of compound 6g



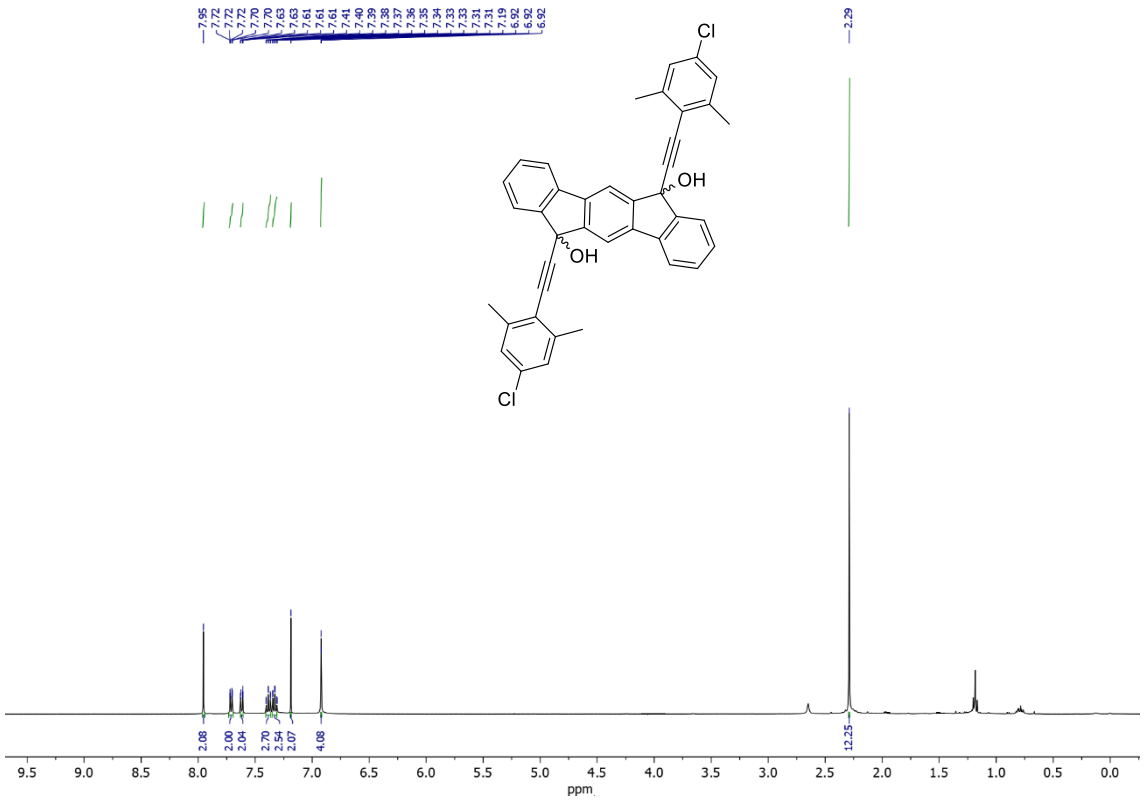


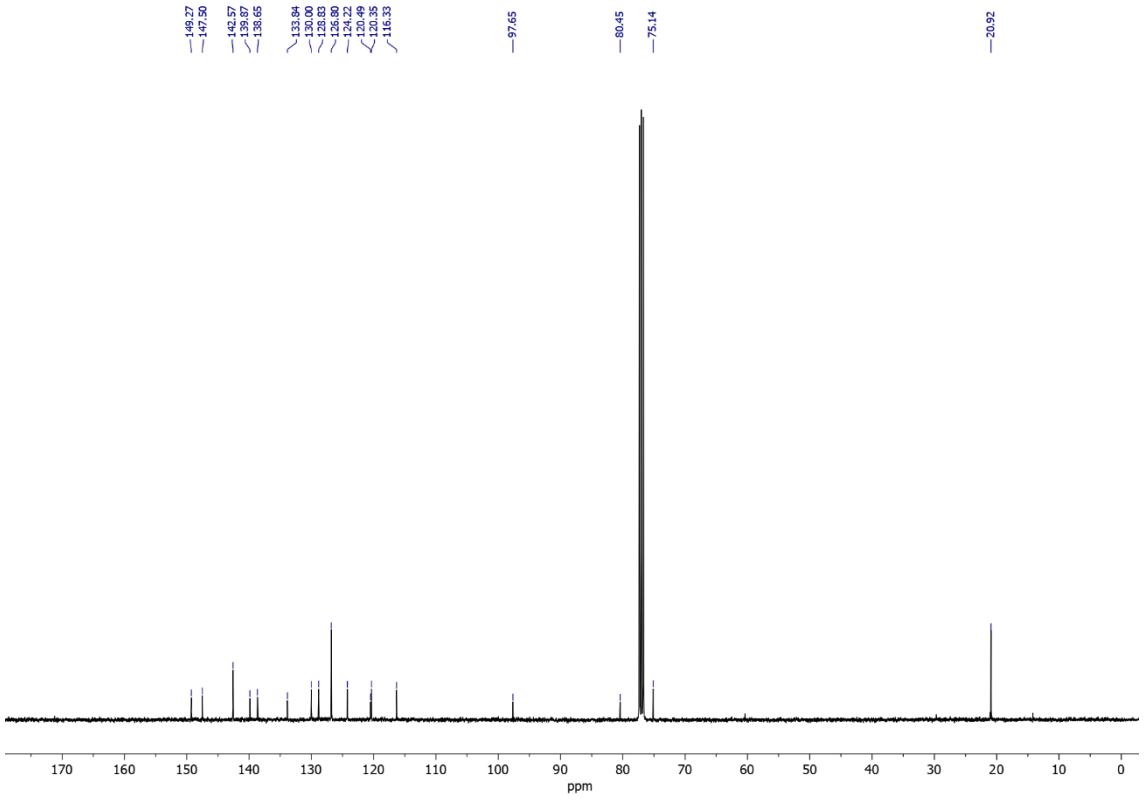
^{1}H-NMR (500 MHz, $CDCl_3$) and ^{13}C-NMR (126 MHz, $CDCl_3$) of compound 6h



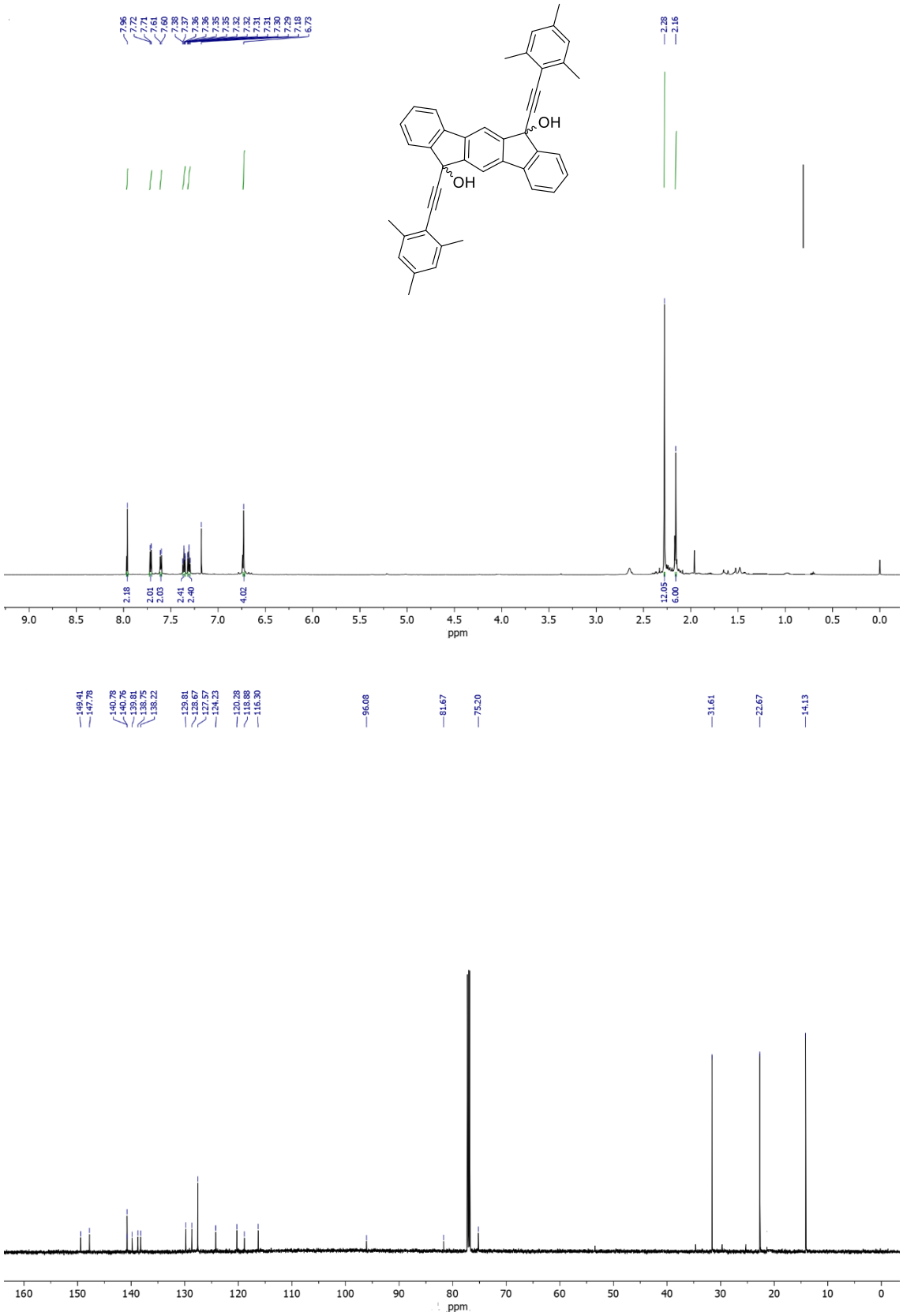


^{1}H-NMR (500 MHz, $CDCl_3$) and ^{13}C-NMR (126 MHz, $CDCl_3$) of compound 7b

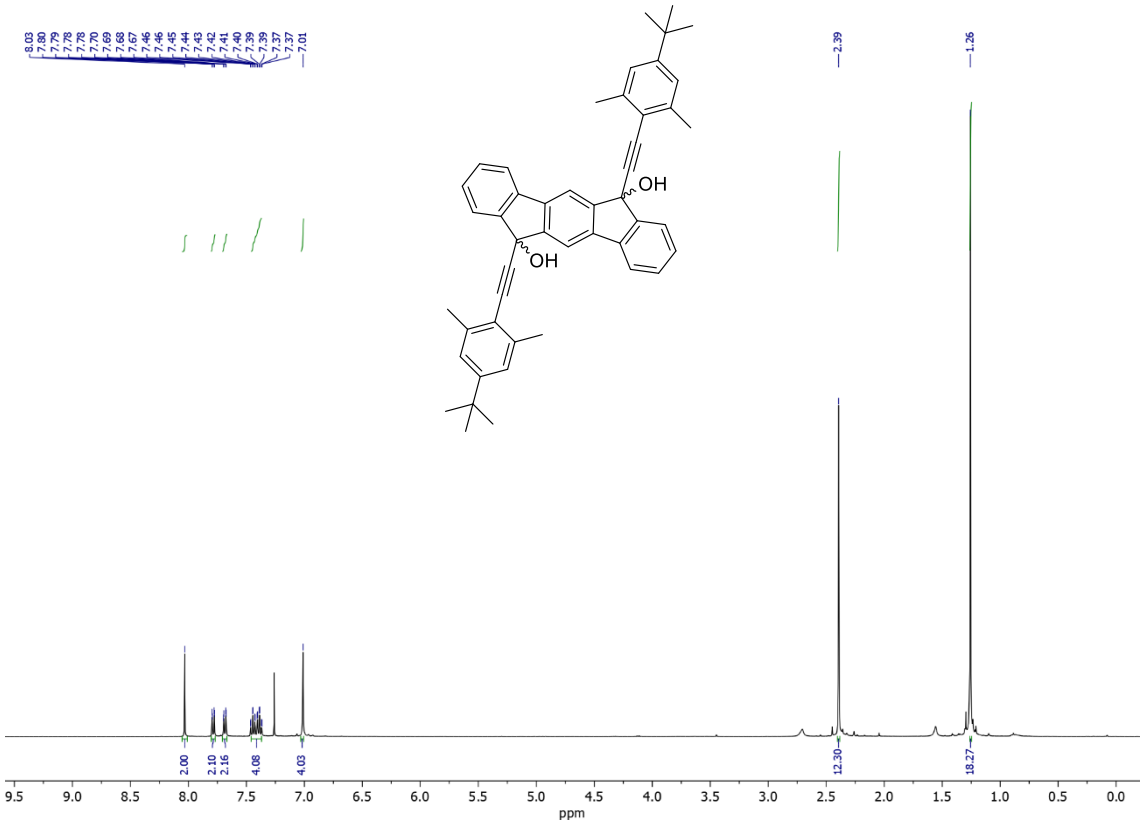


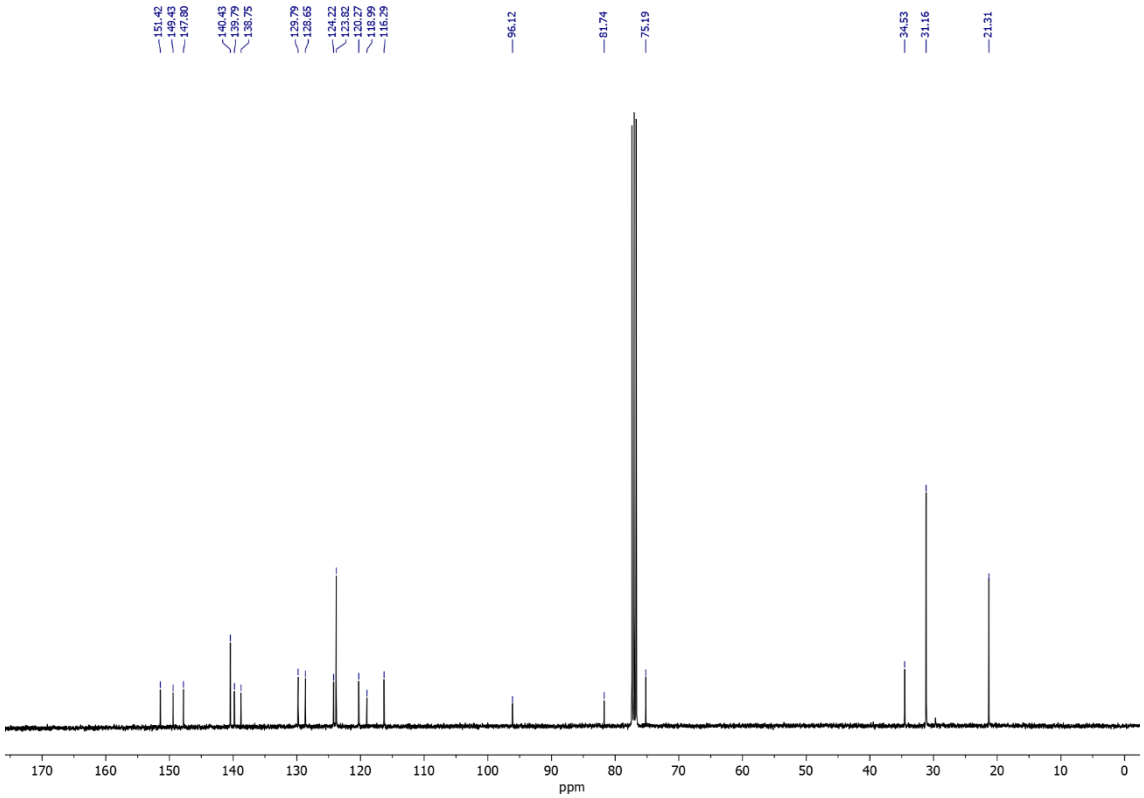


^{1}H-NMR (500 MHz, $CDCl_3$) and ^{13}C-NMR (126 MHz, $CDCl_3$) of compound 7d

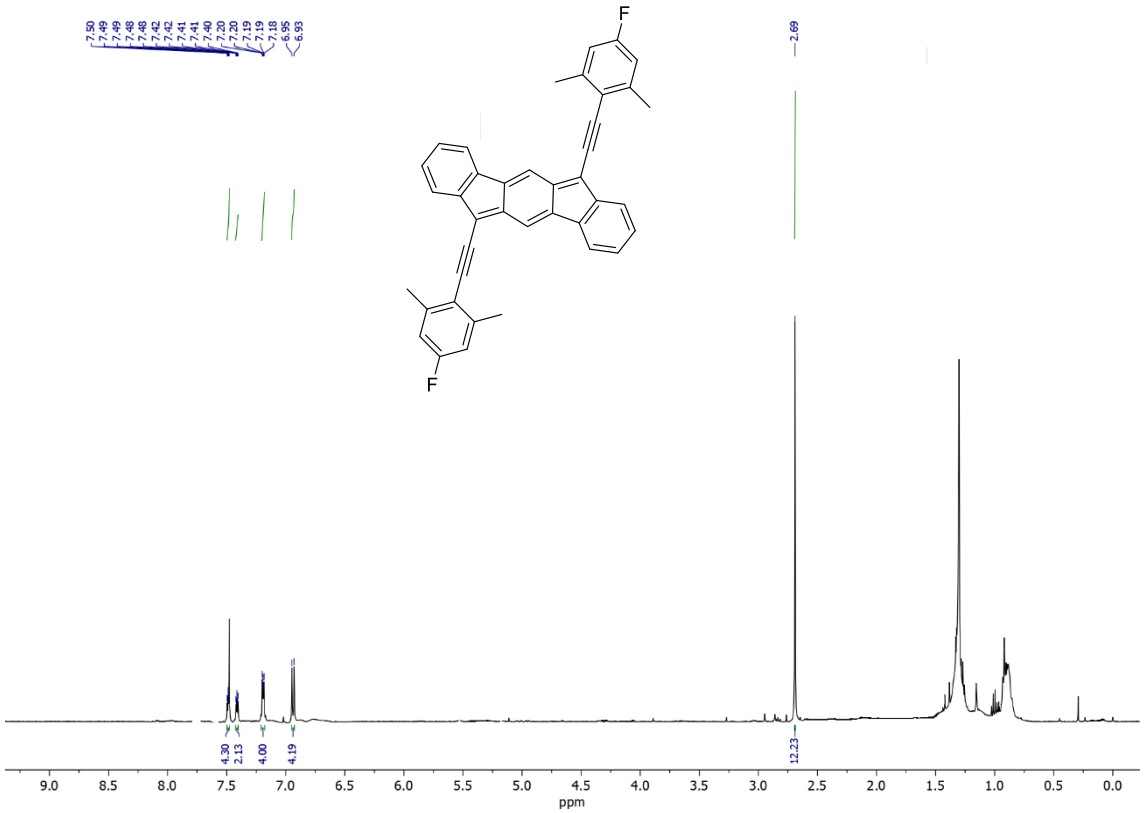


^{1}H-NMR (500 MHz, $CDCl_3$) and ^{13}C-NMR (126 MHz, $CDCl_3$) of compound 7e

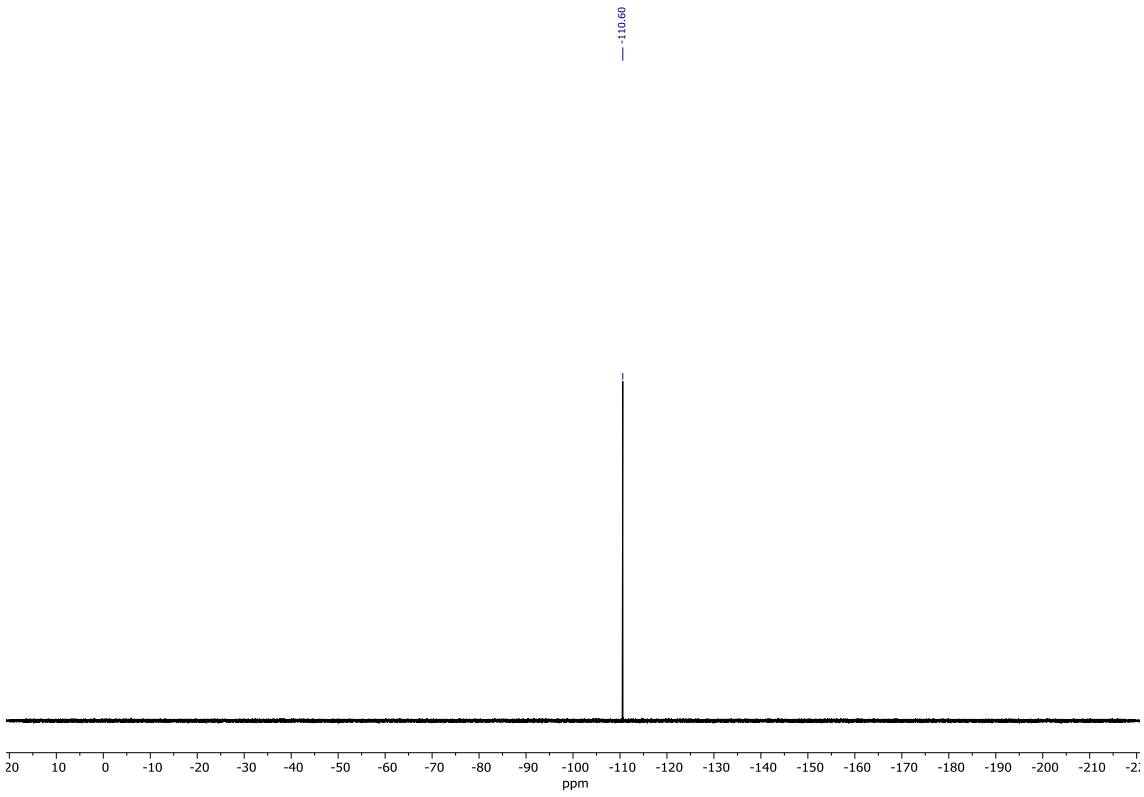




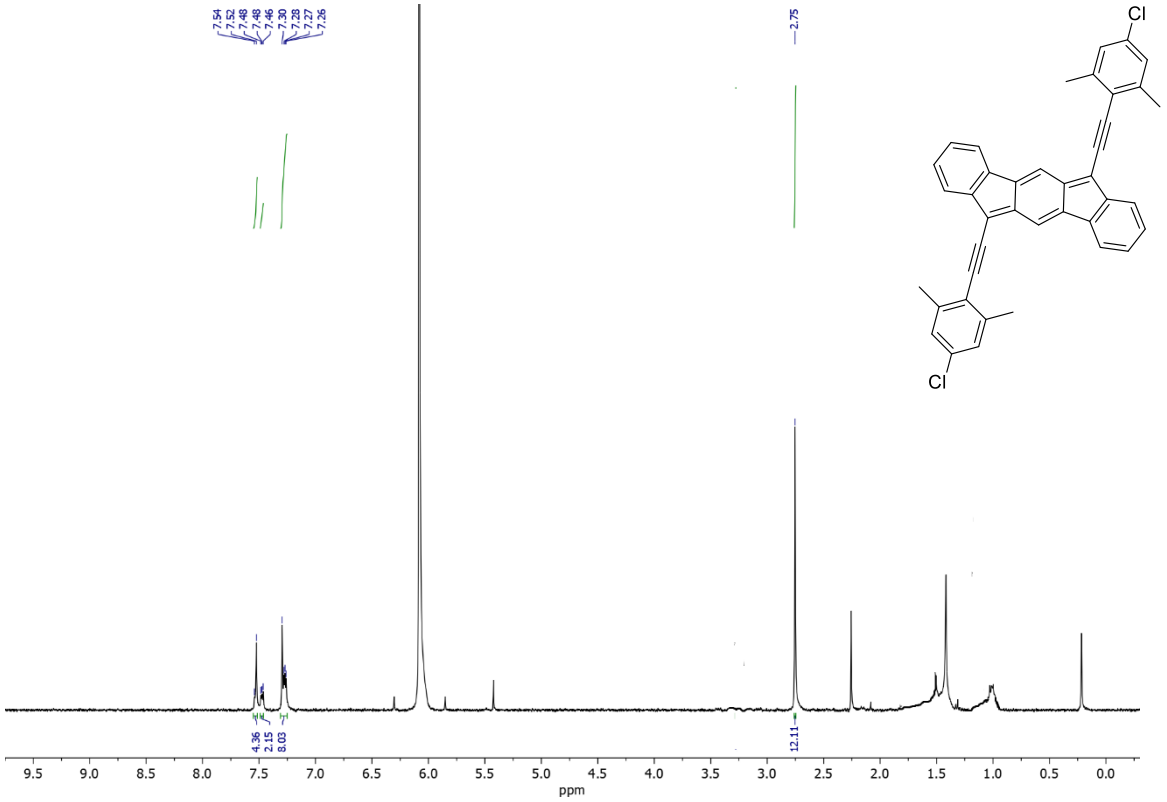
^{1}H-NMR (500 MHz, $CDCl_3$) of compound 4a



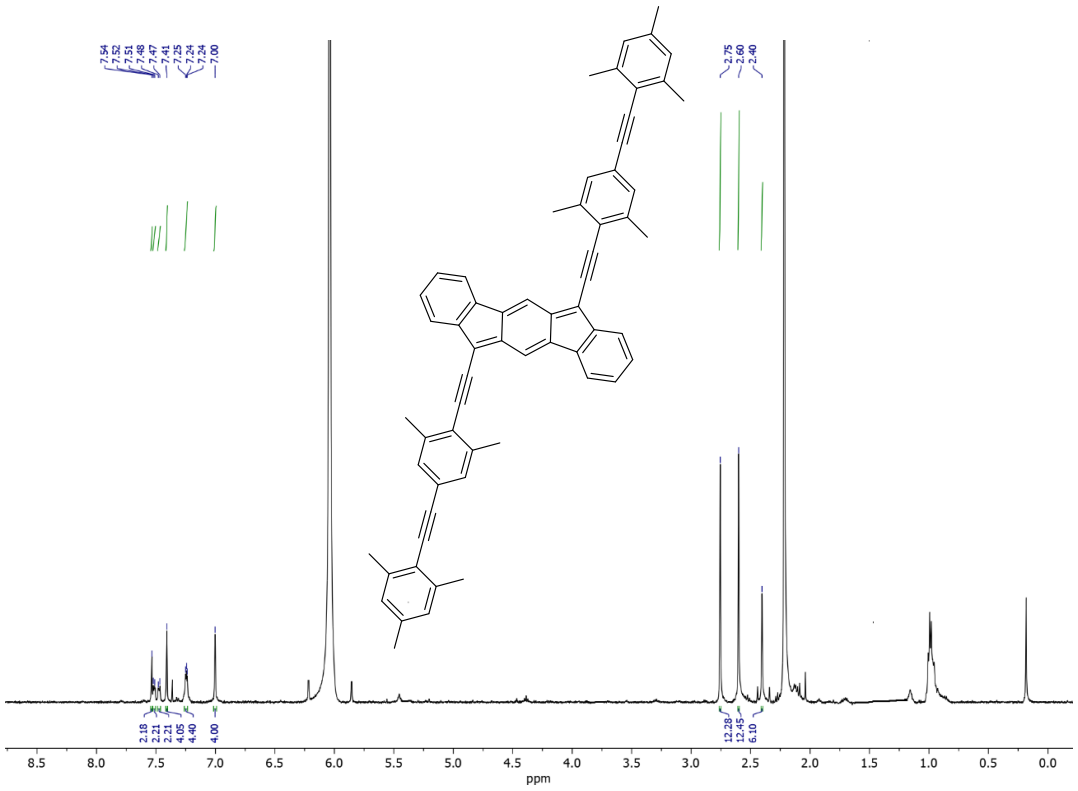
^{9}F-NMR (376 MHz, $CDCl_3$) of compound 4a



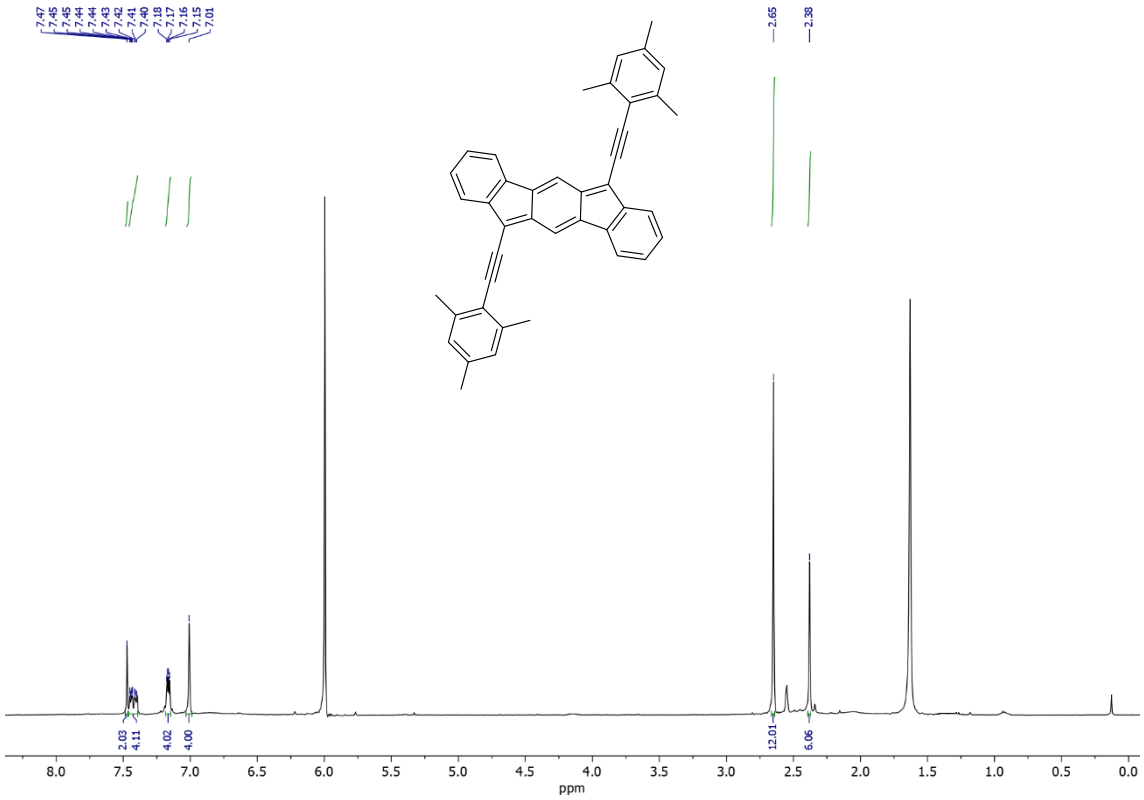
^{1}H-NMR (500 MHz, $C_2D_2Cl_4$) of compound 4b



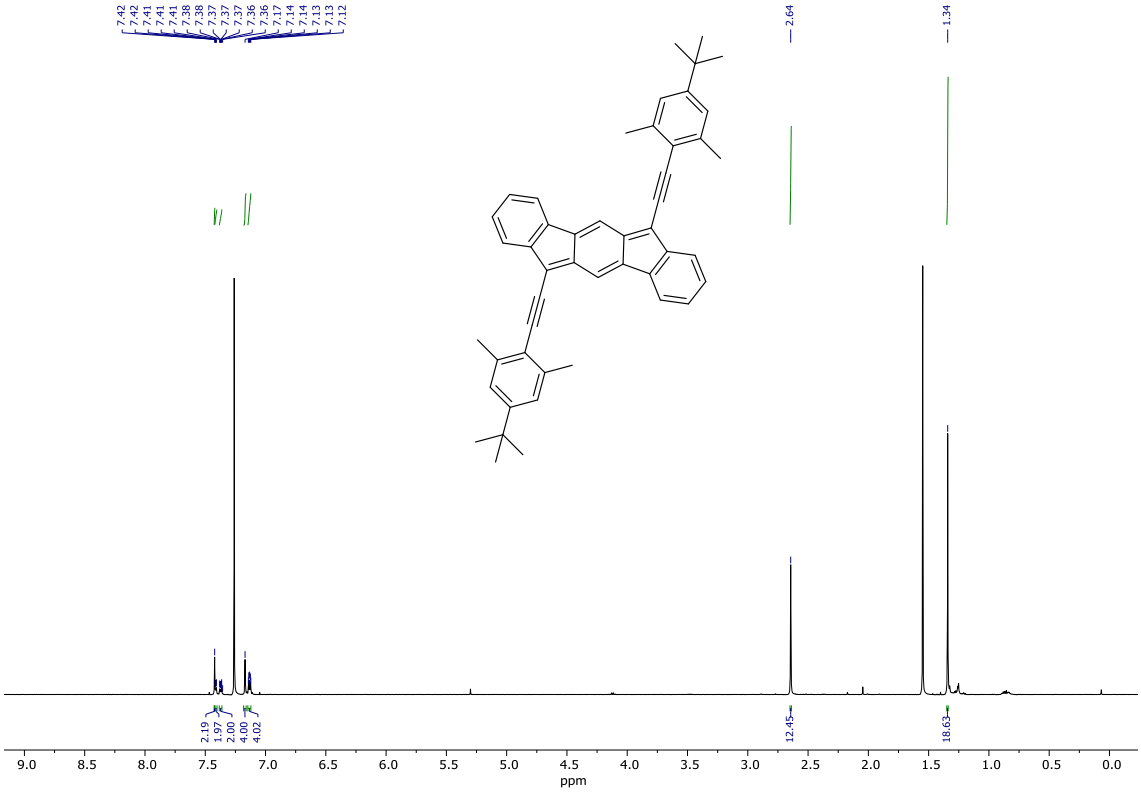
^{1}H-NMR (500 MHz, $C_2D_2Cl_4$, 375 K) of compound 4c

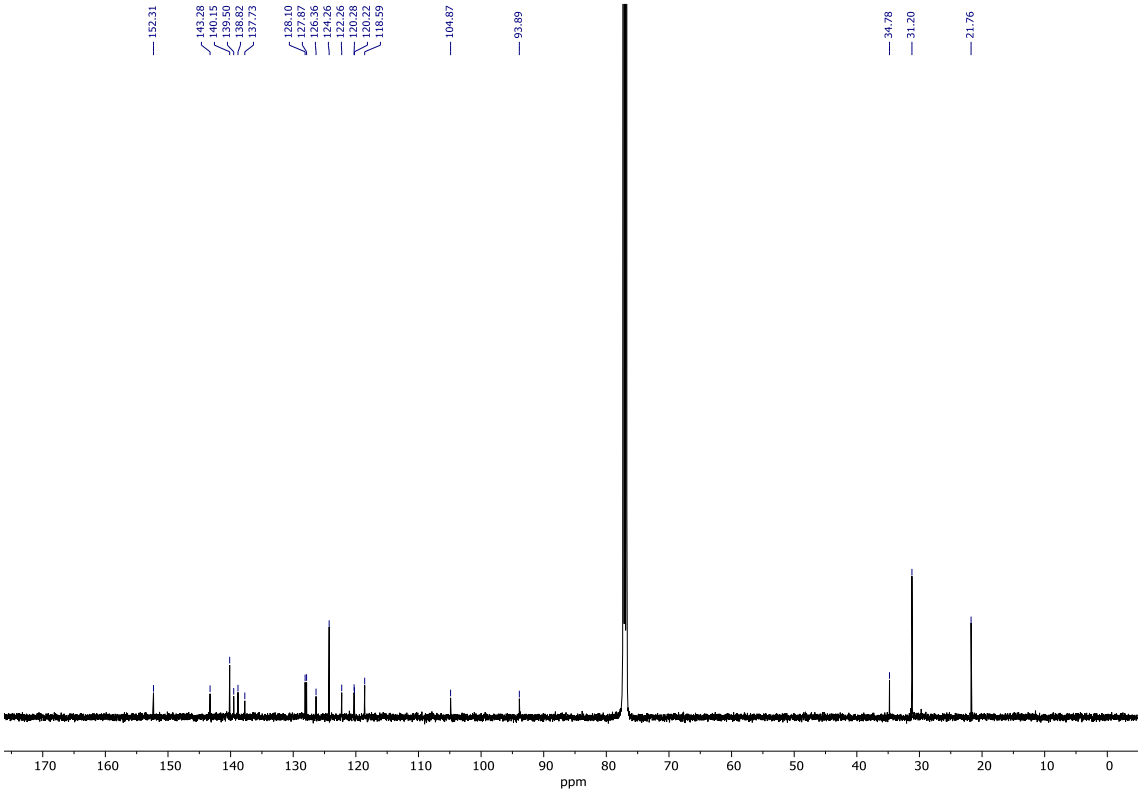


^{1}H-NMR (500 MHz, $C_2D_2Cl_4$, 375 K) of compound 4d

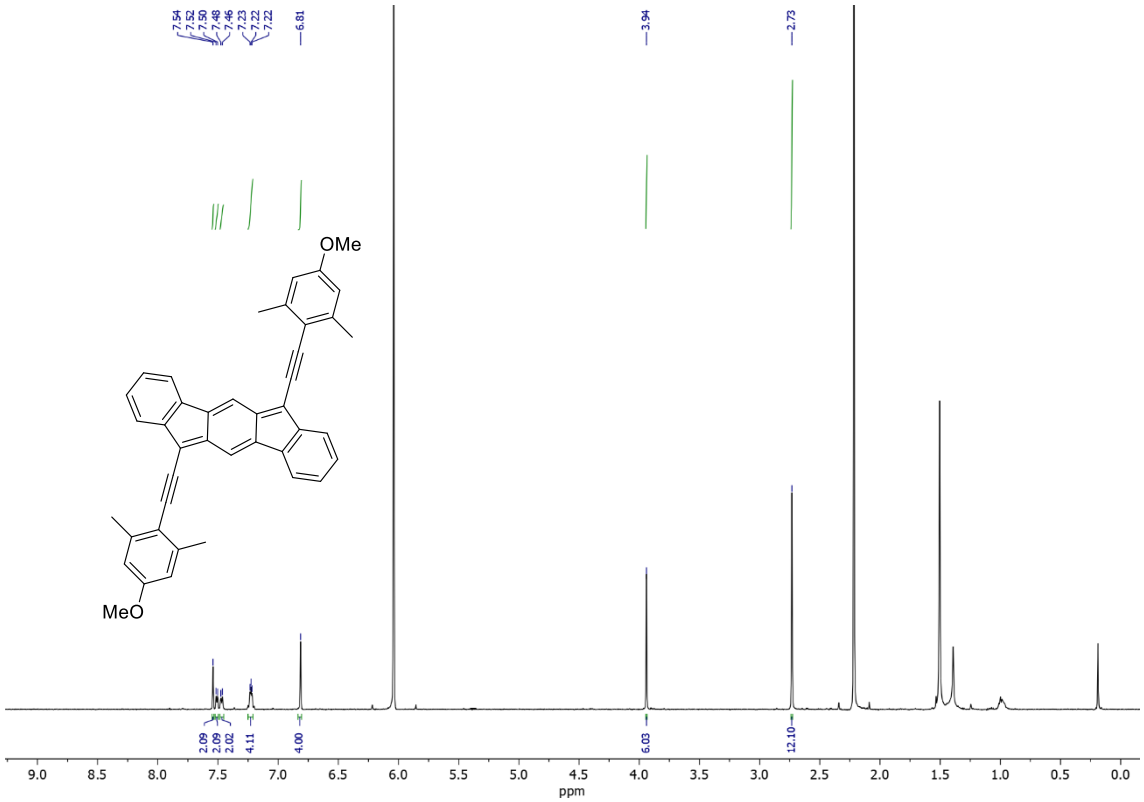


^{1}H-NMR (500 MHz, $CDCl_3$) and ^{13}C-NMR (126 MHz, $CDCl_3$) of compound 4e

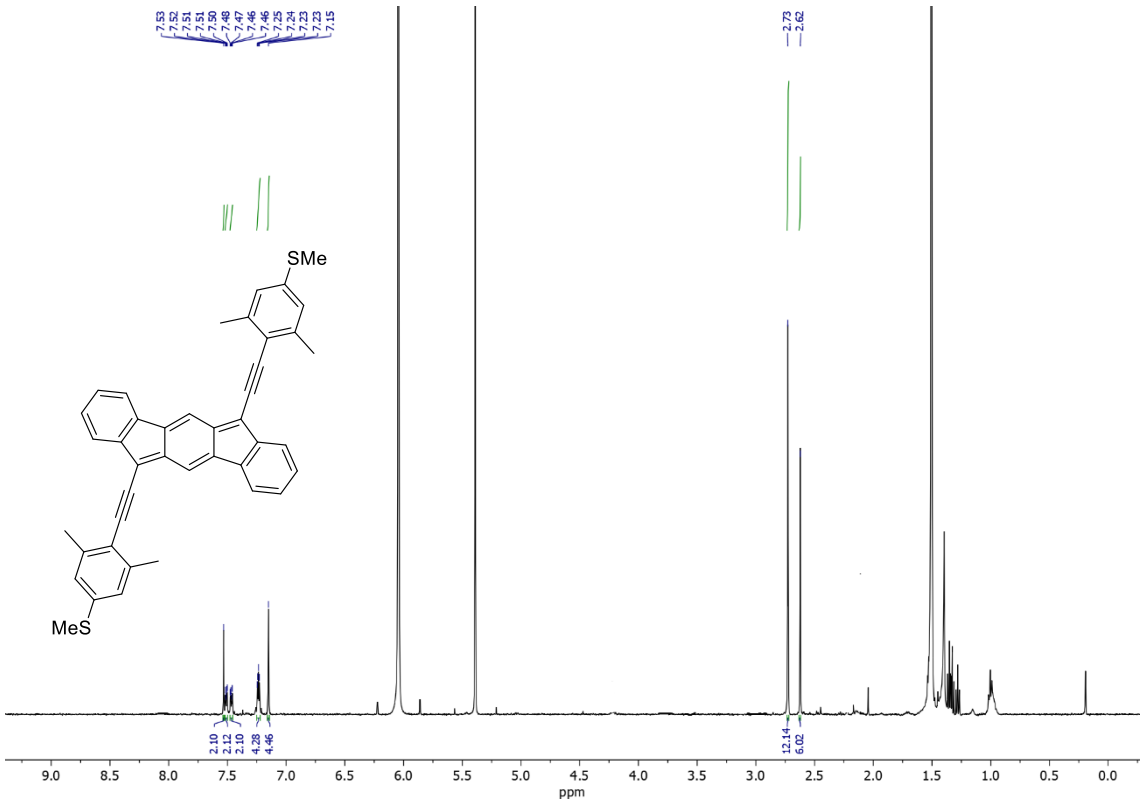




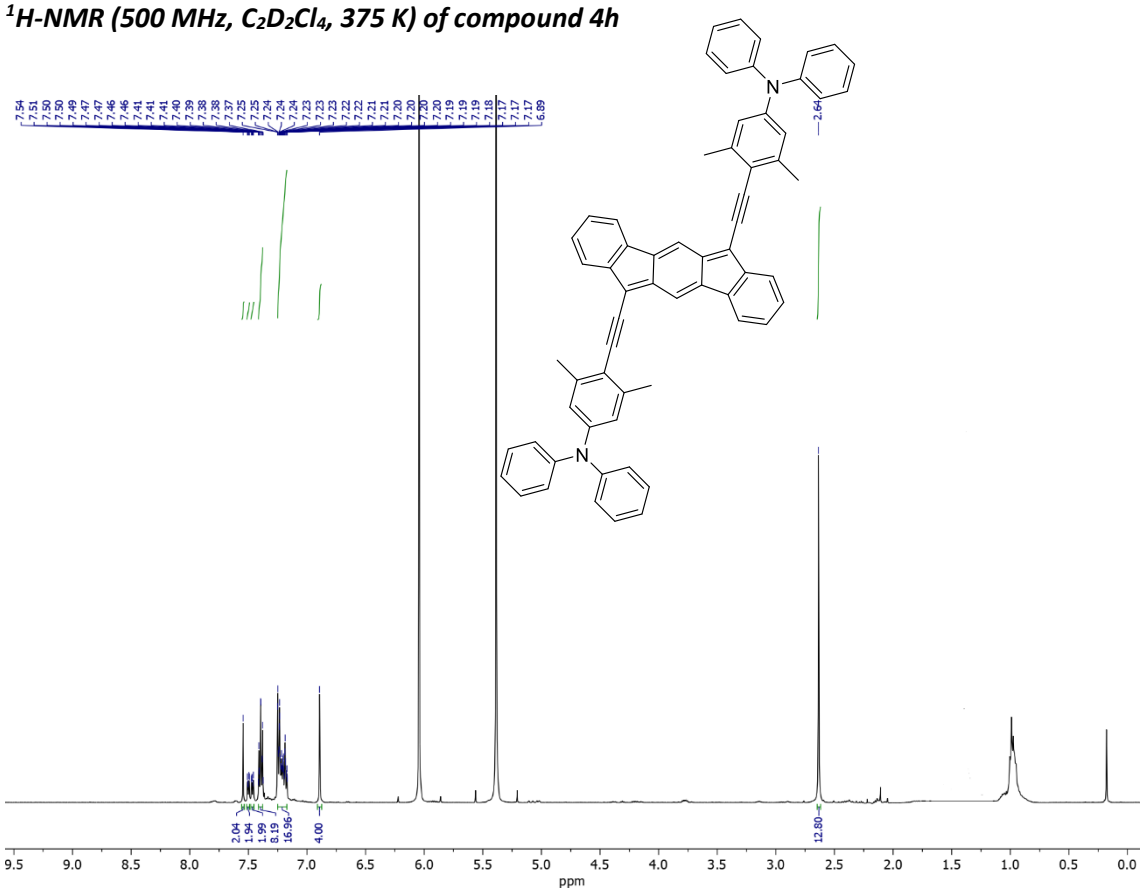
^{1}H-NMR (500 MHz, $C_2D_2Cl_4$, 375 K) of compound 4f



^{1}H-NMR (500 MHz, $C_2D_2Cl_4$, 375 K) of compound 4g



^{1}H-NMR (500 MHz, $C_2D_2Cl_4$, 375 K) of compound 4h



4. High-resolution mass spectra. Isotopic distribution

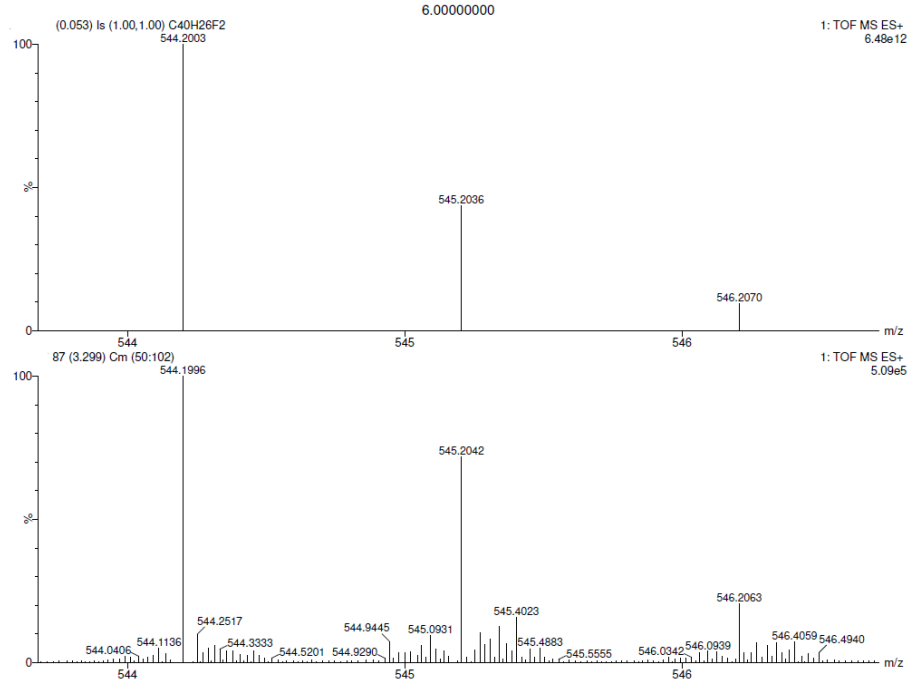


Figure S1. HRMS (ESI) isotopic distribution of the $[M]^+$ peak of compound **4a**. Top: Calculated. Bottom: Experimental.

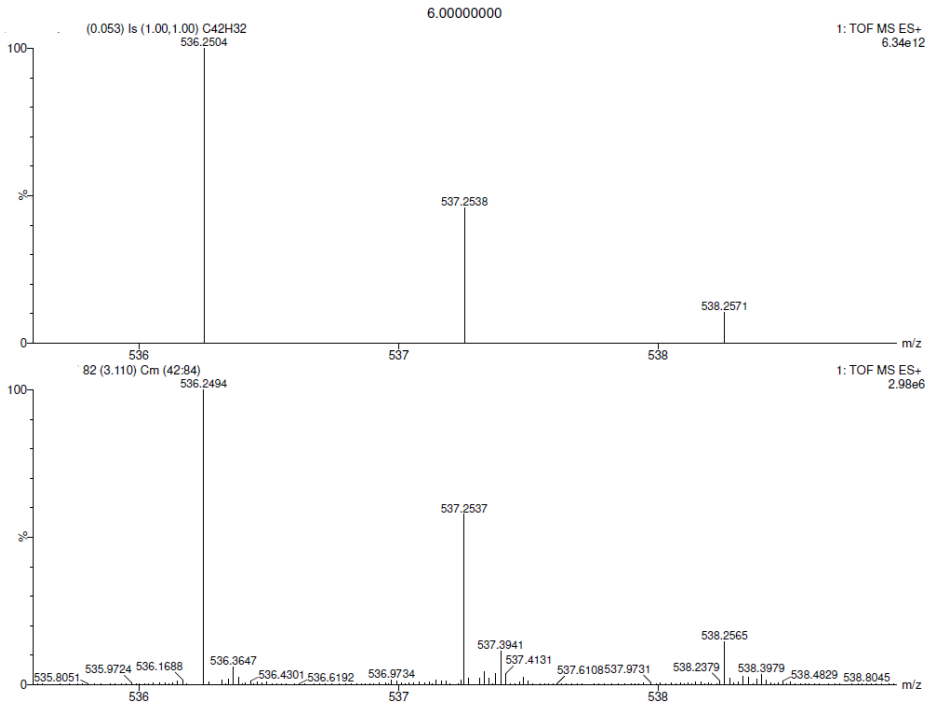


Figure S2. HRMS (ESI) isotopic distribution of the $[M]^+$ peak of compound **4d**. Top: Calculated. Bottom: Experimental.

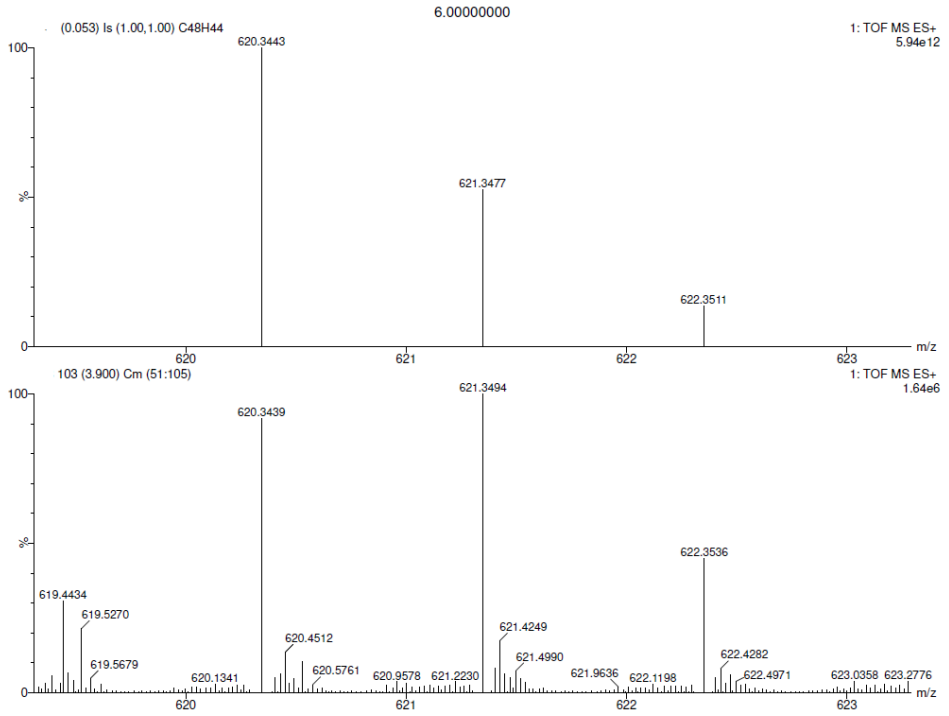


Figure S3. HRMS (ESI) isotopic distribution of the $[M]^+$ peak of compound **4e**. Top: Calculated. Bottom: Experimental.

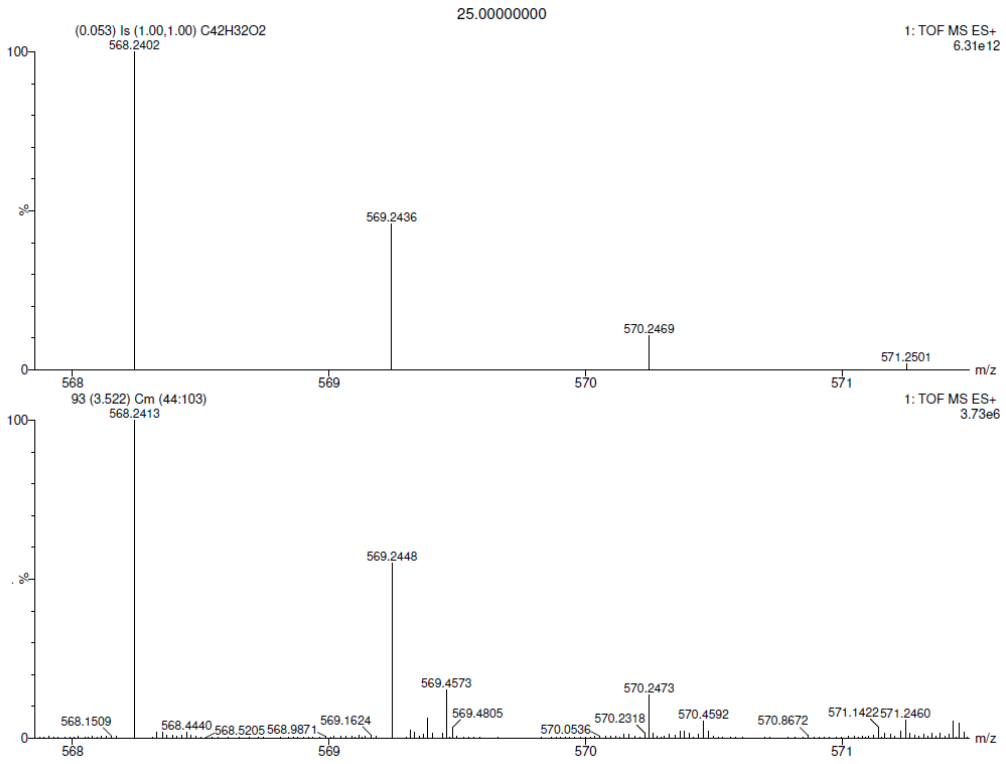


Figure S4. HRMS (ESI) isotopic distribution of the $[M]^+$ peak of compound **4f**. Top: Calculated. Bottom: Experimental.

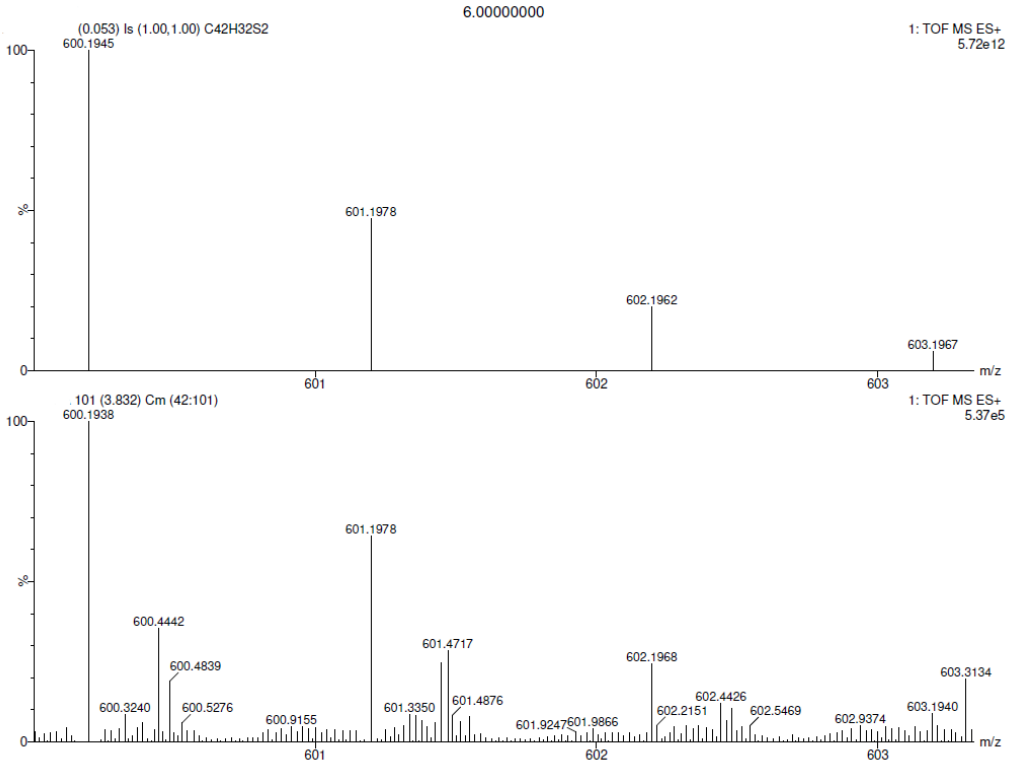


Figure S5. HRMS (ESI) isotopic distribution of the $[M]^+$ peak of compound **4g**. Top: Calculated. Bottom: Experimental.

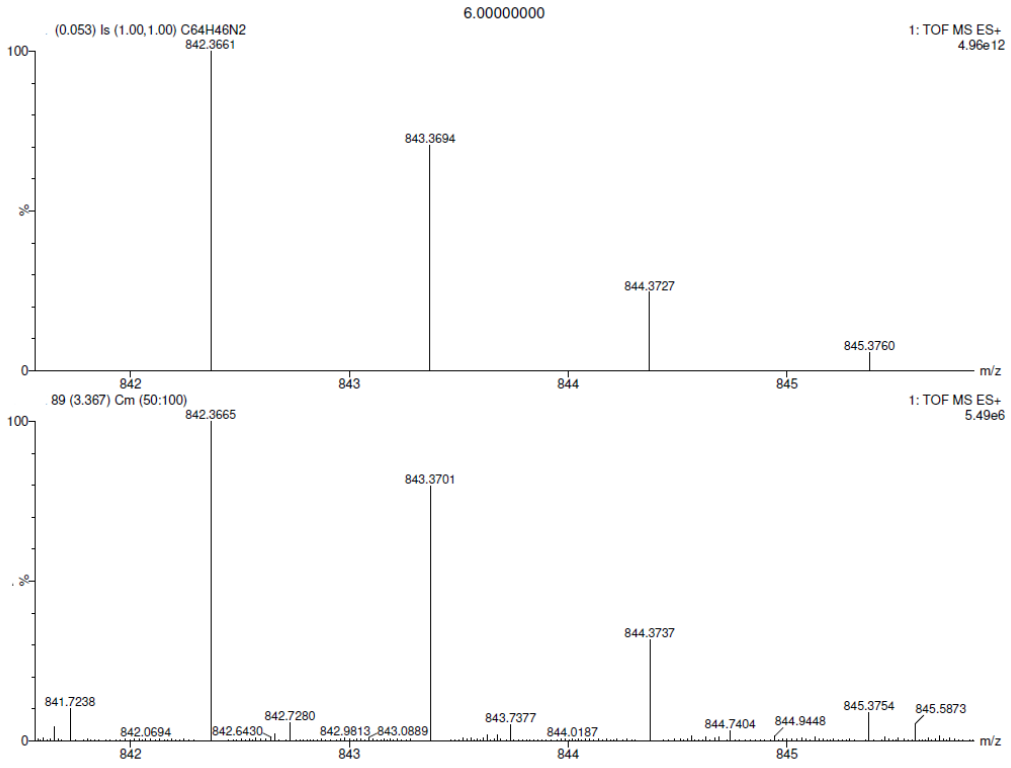


Figure S6. HRMS (ESI) isotopic distribution of the $[M]^+$ peak of compound **4h**. Top: Calculated. Bottom: Experimental.

5. Single crystal X-Ray diffraction

Single crystals of compound **4e** were obtained by slow evaporation of a solution of the compound in a mixture of hexane/DCM (1:1) with a few drops of acetonitrile. These crystals displayed enough quality for their analysis by X-ray diffraction. The diffraction measurements were carried out with a Bruker D8 Venture diffractometer with a Mo radiation source and equipped with a PHOTON III detector. The structure was solved using SHELXT[S2] and refined by means of the full-matrix least-squares against F^2 procedure, using SHELX 2018[S3] and the WinGX32[S4] interface. C–H hydrogen atoms were placed in idealized positions (U_{eg}(H) = 1.2U_{eg}(C) or U_{eg}(H) = 1.5U_{eg}(C)) and were allowed to ride on their parent atoms.

X-ray diffraction measurement and refinement data for 4e: Chemical formula, $C_{48}H_{44}$; *Mr*, 620.83; crystal size [mm^3], 0.390 x 0.031 x 0.026; temperature, 100(2) K; wavelength [Å], 0.71073 (Mo Kα), crystal system, monoclinic; space group, *C*2/*c*; *a* [Å], 32.5657(16); *b* [Å], 5.9071(3); *c* [Å], 22.2300(12); α [°], 90; β [°], 124.048(2); γ [°], 90; *V* [$Å^3$], 3543.3(3); *Z*, 4; ρ_{calcd} [Mg m^{-3}], 1.164; μ [mm^{-1}], 0.065; F(000), 1328; ϑ range [°], 2.211 to 23.286; *hkl* ranges, -36/36, -5/6, -24/24; reflections collected, 24232; independent reflections, 2562; R_{int}, 0.0613; completeness to ϑ = 23.286°, 99.9%; absorption correction, numerical; refinement method; full-matrix least-squares on F^2; Final *R* indices [$I>2\sigma(I)$], R_1 = 0.0537, wR_2 = 0.1397; *R* indices (all data), R_1 = 0.0688, wR_2 = 0.1545; goodness-of-fit on F^2, 1.037.

CCDC-2177496 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via https://www.ccdc.cam.ac.uk/structures/

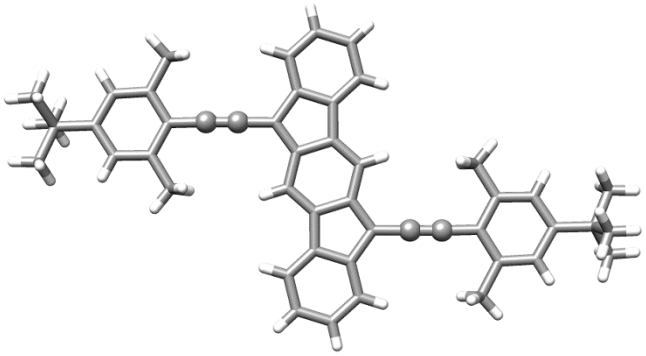


Figure S7. X-Ray structure of compound **4e**.

5.1. Bond lengths comparison

In Table S1 we show experimental C–C bond distances found in our compound **4e** and in the related indeno[1,2-*b*]fluorene **2b**[S5] and **3a**[S6] reported previously in literature. In our compound **4e**, the *p*-quinodimethane (*p*-QDM) central unit present longer double bonds and shorter single bonds. See computational details section (Section 9) for further comparison with theoretical values.

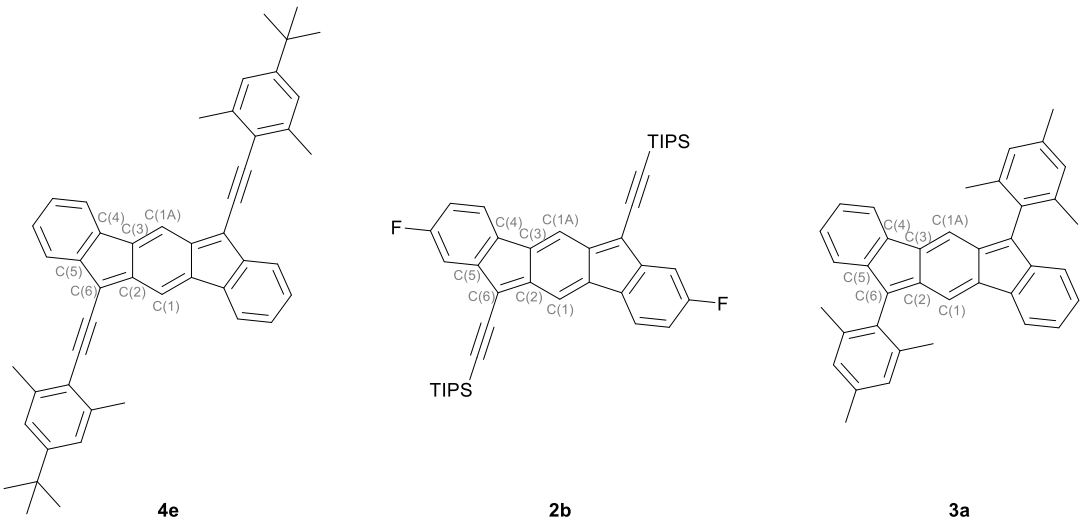


Table S1. Bond lengths of *p*-QDM unit in **4e**, **2b** and **3a**[a]

Bond	**4e**	**2b**[b]	**3a**[c]
C1A–C3	1.361	1.350	1.356
C1–C2	1.418	1.434	1.433
C2–C3	1.451	1.453	1.467
C2–C6	1.397	1.383	1.380

[a] Distances in Å. [b] Data taken from ref S5. [c] Data taken from ref S6

6. UV-Vis spectra

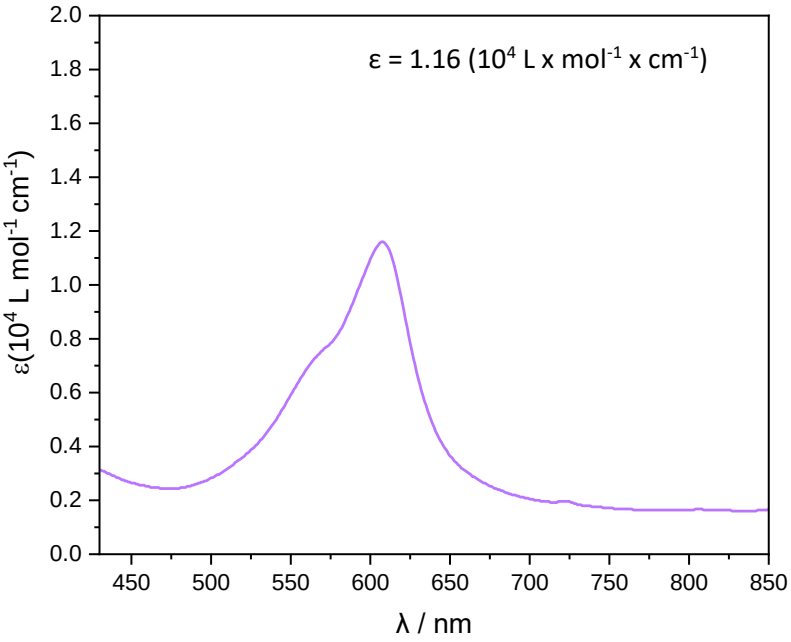


Figure S8. UV-Vis spectra of **4a** in DCM.

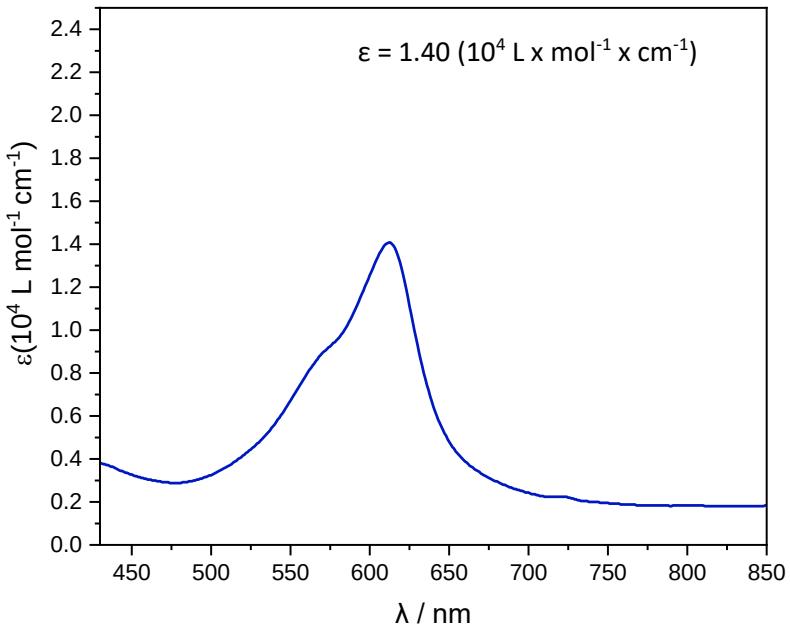


Figure S9. UV-Vis spectra of **4b** in DCM.

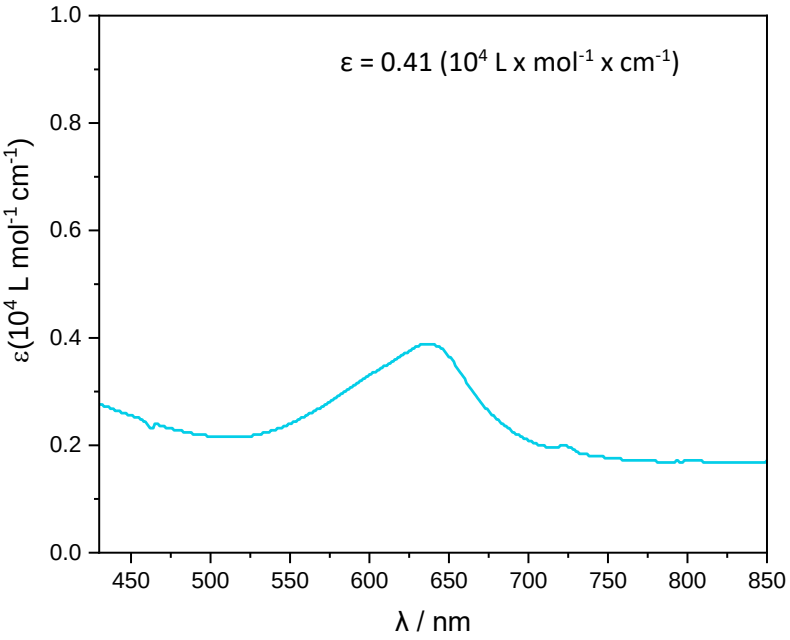


Figure S10. UV-Vis spectra of **4c** in DCM.

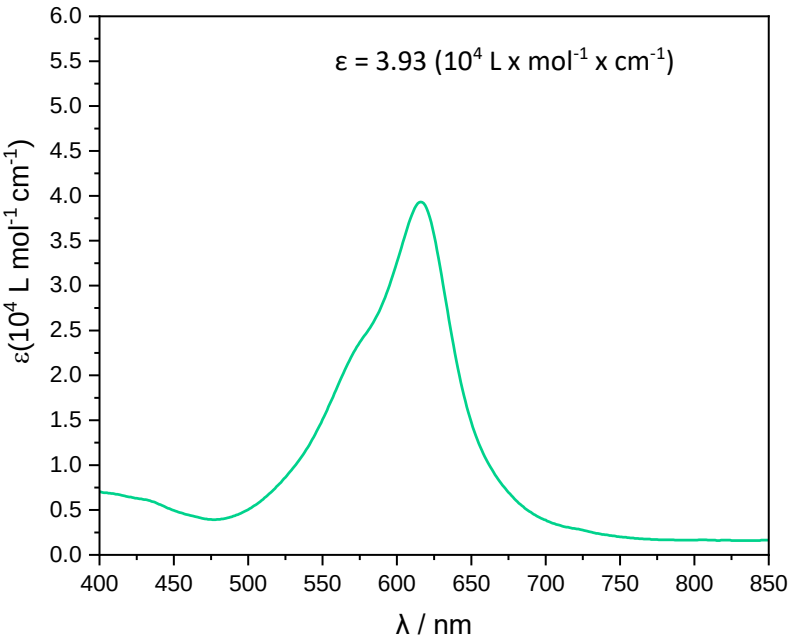


Figure S11. UV-Vis spectra of **4d** in DCM.

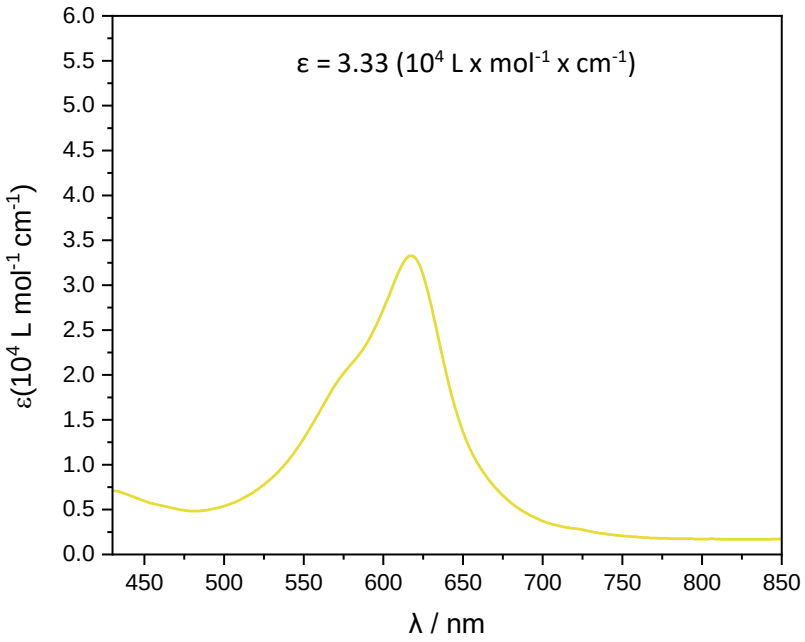


Figure S12. UV-Vis spectra of **4e** in DCM.

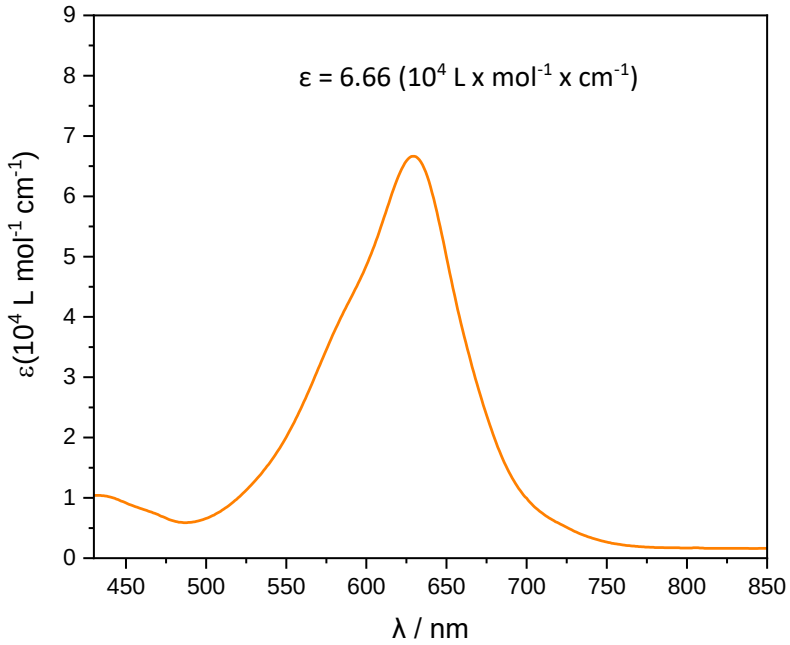


Figure S13. UV-Vis spectra of **4f** in DCM.

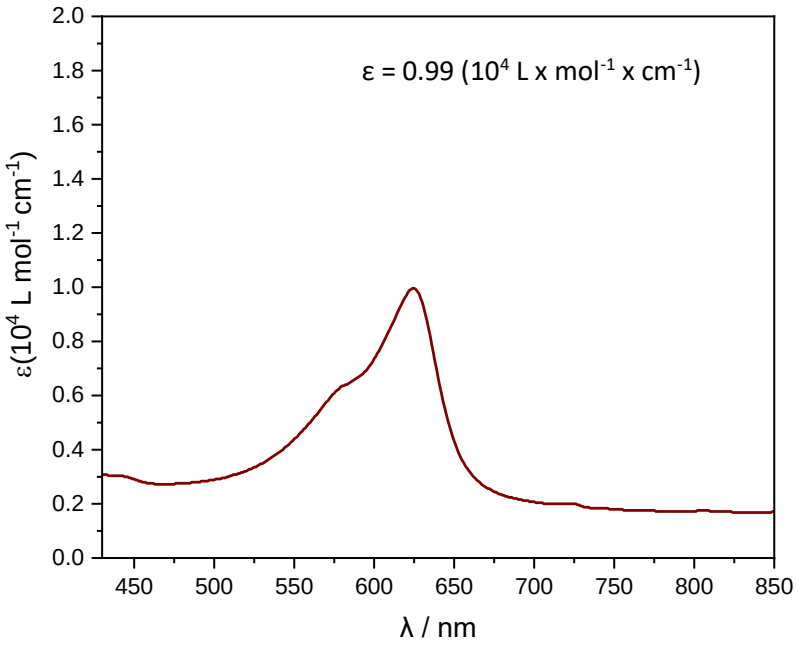


Figure S14. UV-Vis spectra of **4g** in DCM.

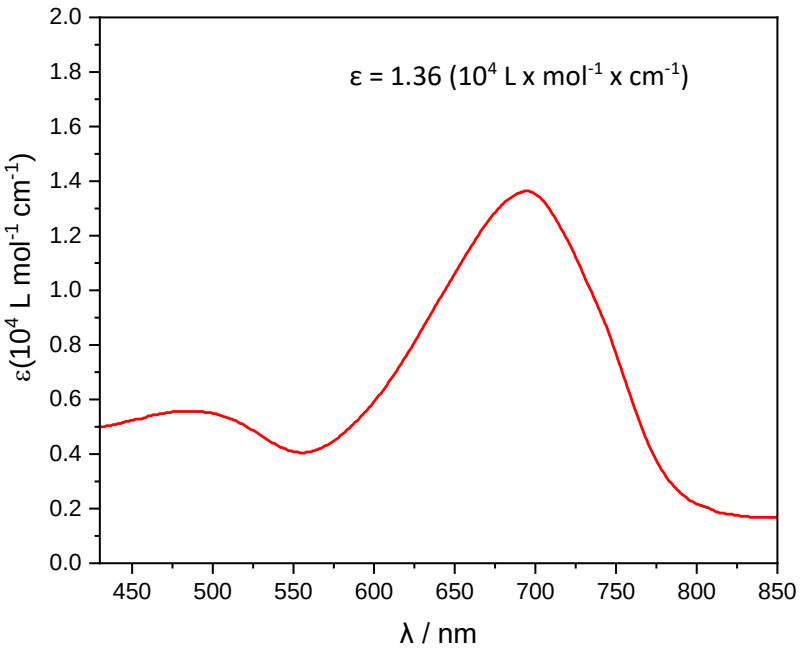


Figure S15. UV-Vis spectra of **4h** in DCM.

6.1. UV-Vis spectra. Stability check of representative compounds

We measured the UV-Vis absorption spectra of molecule **4d** after 2h, 24 h and 72 h not observing any significant diference in its absorption profile (Figure S16). Compund **4e** was checked after 112 days and, again, no significant decomposition was observed.

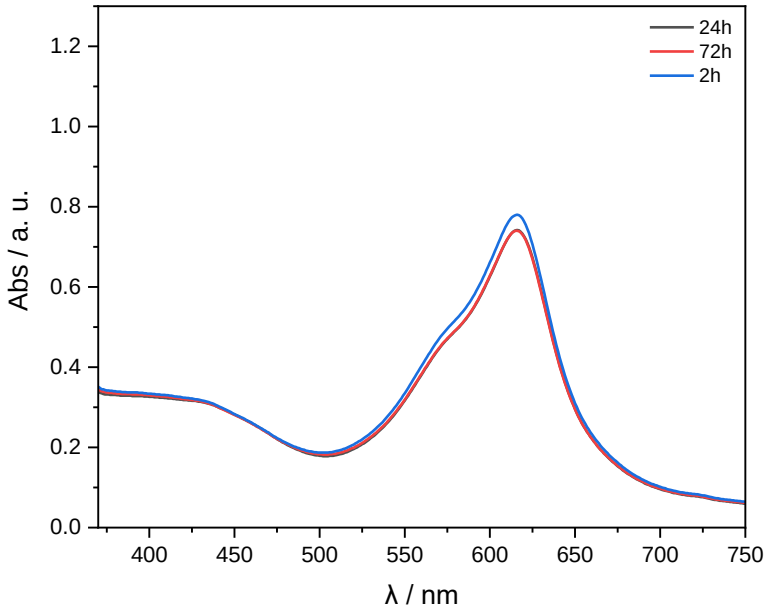


Figure S16. UV-Vis spectra of **4d** in DCM at the same concentration at different times.

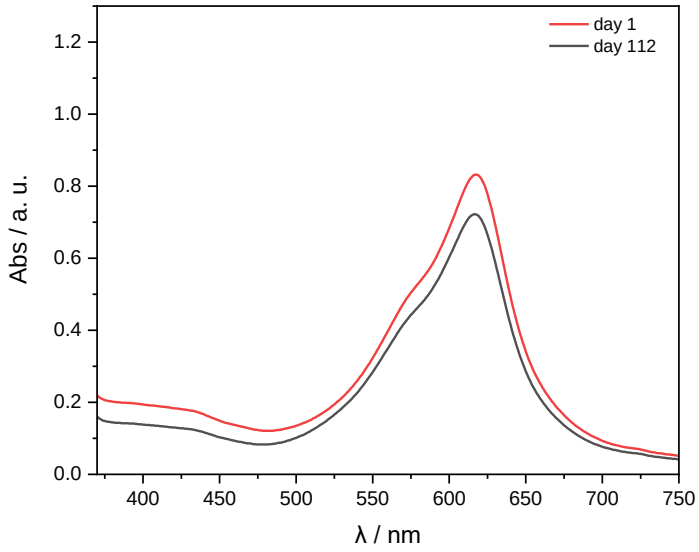


Figure S17. UV-Vis spectra of **4e** in DCM at the same concentration just after preparation (day 1) and after 112 days.

7. Voltammograms

Cyclic Voltammetry (CV) and Square Wave Voltammetry (SWV) were carried out on a PGSTAT2014 potentiostat/galvanostat (Metrohm Autolab B. V.) with a three-electrode cell under Ar atmosphere at 25 °C. A Pt-wire counterelectrode, an Ag wire quasireference electrode and a glassy carbon disk working electrode were used. CH_2Cl_2 was used as solvent to prepare a 0.1 M solution of tetra-*n*-butylammonium hexafluorophosphate ($TBAPF_6$) which was used as work solution. A concentration of 1.5mM of the corresponding **4** was used. The scan rate was 0.05 V/s. Potential values are referred to the ferrocenium/ferrocene ($FeCp_2^+/FeCp_2$) system, Fc added as an internal reference after each measurement. The quality of the voltammograms is probably due to insolubility of the samples.[S7]

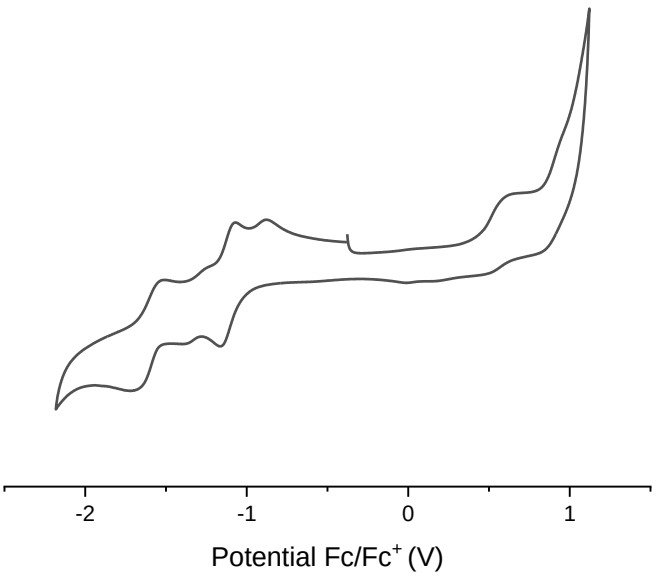


Figure S18. Cyclic voltammetry of **4a**.

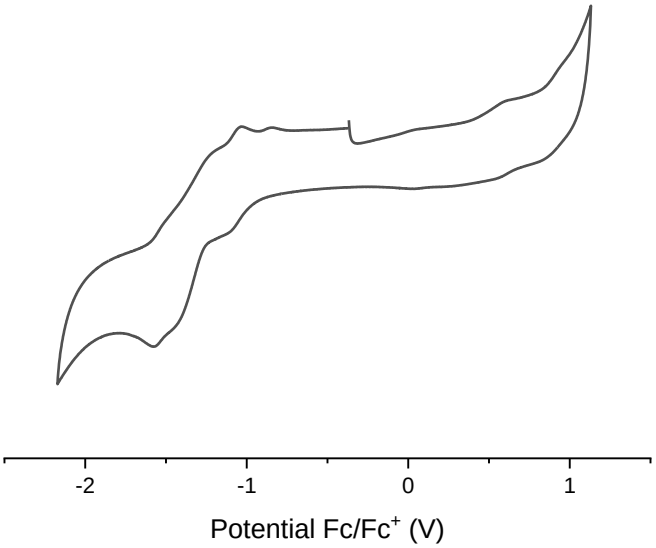


Figure S19. Cyclic voltammetry of **4b**.

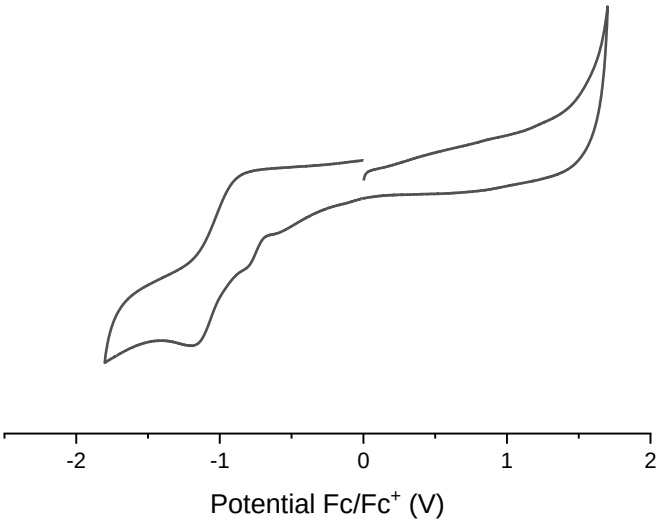


Figure S20. Cyclic voltammetry of **4c**.

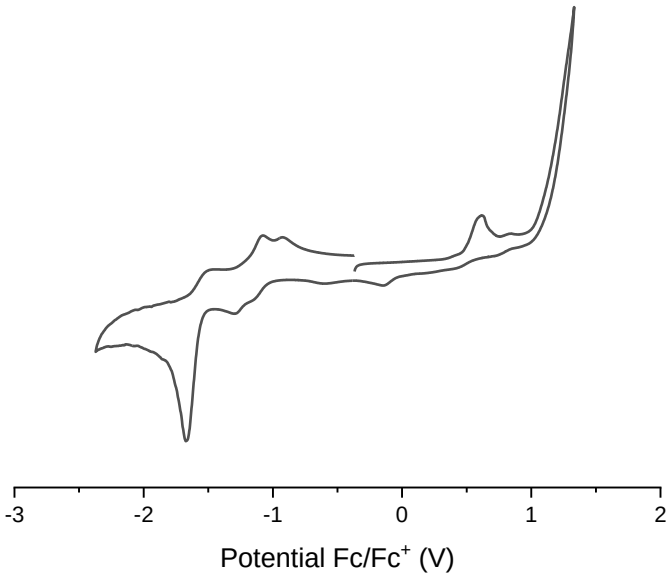


Figure S21. Cyclic voltammetry of **4d**.

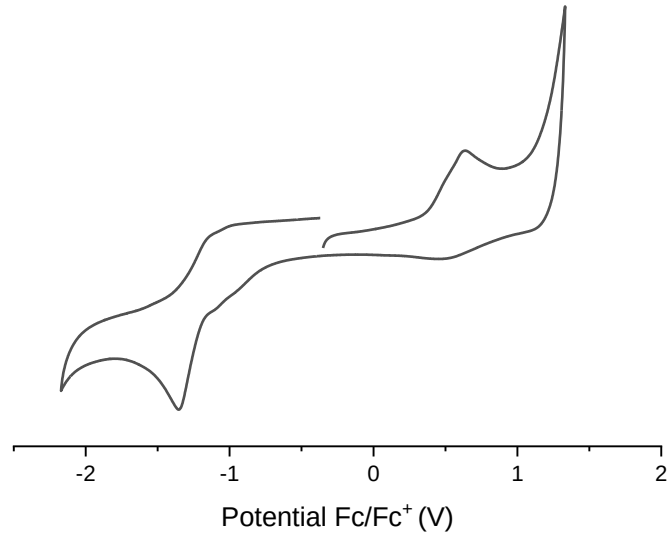


Figure S22. Cyclic voltammetry of **4e**.

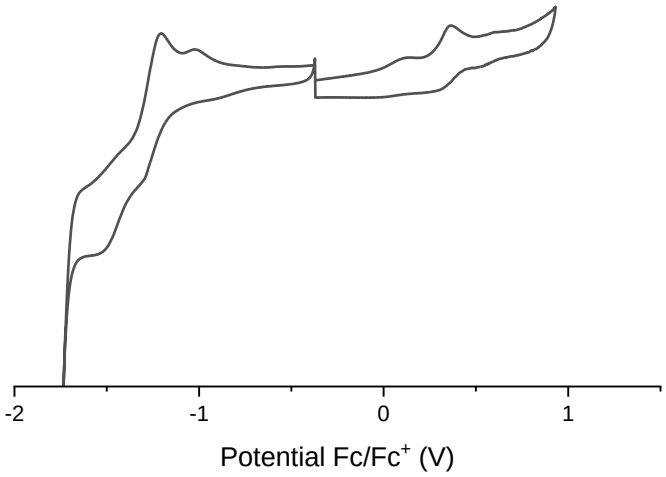


Figure S23. Cyclic voltammetry of **4f**.

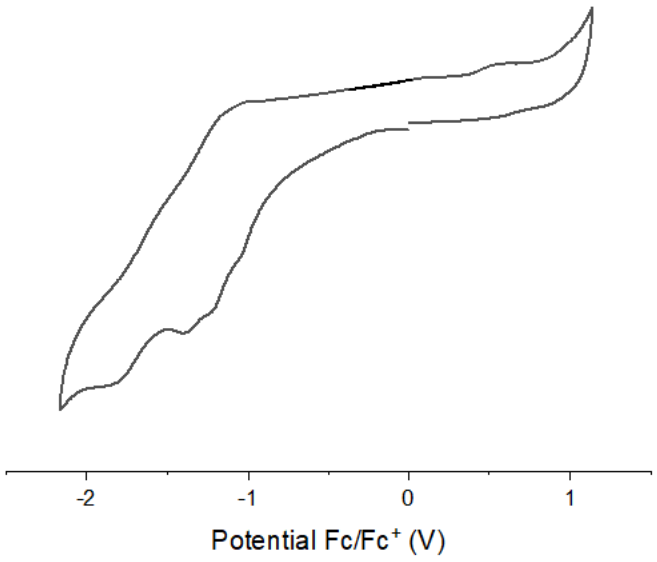


Figure S24. Cyclic voltammetry of **4g**.

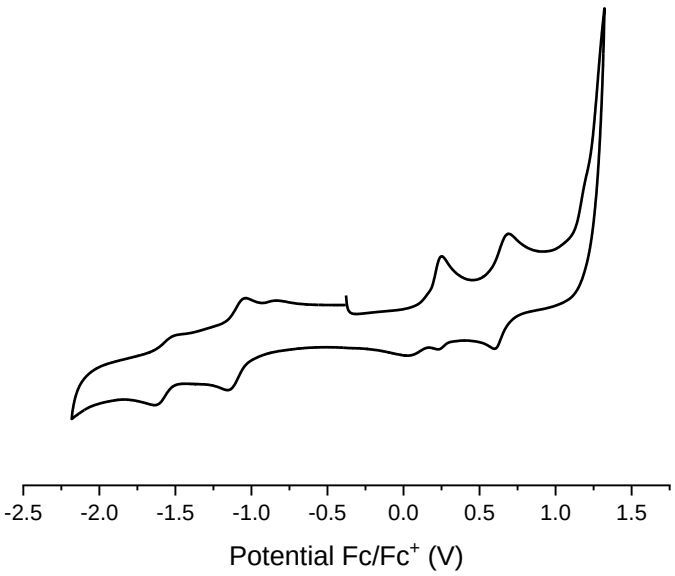


Figure S25. Cyclic voltammetry of **4h**.

8. Electron Spin Resonance (ESR) spectrum

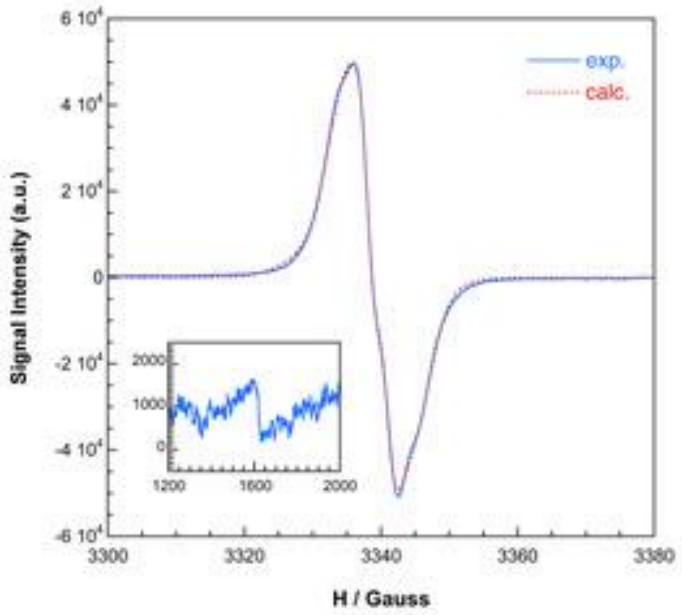


Figure S26. EPR spectrum of powder **4d** measured at room temperature (inset: EPR signal in the Δms= ±2 region). Parameters for calculated spectrum: g_x=2.0031; g_y=2.0029; g_z=2.0043; D= 6.4 Gauss; E= 1.4 Gauss.

9. Computational details

Molecule optimized geometries, absorption spectra, frontier molecular orbitals energies, diradical character (*y*), spin densities, singlet-triplet energy gaps, and Nucleus-Independent Chemical Shifts (NICS) were performed using the Gaussian 16 package.[S8] Absorption spectra, and topologies of the frontier molecular orbitals and spin density distributions have been extracted using Gaussview 6.0 graphical interface program.[S9] Transport calculations were carried out by using the SIESTA, TranSIESTA and Tbtrans codes.[S10] Cartesian coordinates of the optimized molecular and single-molecule junction structures are shown in section 11.

9.1. Molecule optimized geometries

Molecular geometries were first optimized using the B3LYP method with the 6-31G(d) basis set. Then a single point energy calculation was performed at B3LYP/6-311+G(d,p) level of theory to extract the energies of the frontier molecular orbitals and the HOMO-LUMO gap presented at Table 1 in the main text, with the sole aim to make a consistent comparison with the extracted values for compounds **2a** (X = H) and **3a** (Ar = Mes) from ref 3 in main text (ref S6 in this ESI document).

Optimized geometries were also obtained at B3LYP/6-311+G(d,p) level of theory. In this case, absolute energy values reported for the frontier molecular orbitals and the HOMO-LUMO gaps differ from those presented in Table 1 in 0.2 eV at most, see Table S2, without contravene the trend found in the first approximation.

In no case, symmetry constraints were imposed, and all the optimized structures were verified as a stationary point, by harmonic vibrational frequency calculation (no imaginary frequencies) at the same level of theory as in optimizations.

Table S2. Frontier Molecular Orbitals and H-L gap energies (eV)

Compound	E_{HOMO}	E_{LUMO}	E_{gap}
4a	–5.19	–3.46	1.73
4b	–5.24	–3.52	1.72
4c	–4.99	–3.40	1.59
4d	–4.98	–3.27	1.71
4e	–4.98	–3.27	1.71
4f	–4.84	–3.17	1.67
4g	–4.90	–3.26	1.64
4h	–4.72	–3.16	1.56

Table S3. Bond lengths of *p*-QDM unit

	Computational[b]			Experimental (Section 5)		
Bond	**4d(4e)**	**2b**	**3a**	**4e**	**2b**[c]	**3a**[d]
C1A–C3	1.367	1.364	1.361	1.361	1.350	1.356
C1–C2	1.423	1.427	1.435	1.418	1.434	1.433
C2–C3	1.453	1.457	1.466	1.451	1.453	1.467
C2–C6	1.402	1.395	1.381	1.397	1.383	1.380

[a] Distances in Å. [b] B3LYP/6-311+G(d,p). [c] Data taken from ref S5. [d] Data taken from ref S6.

9.2. Absorption spectra

The absorption spectra have been simulated by using the time-dependent DFT approach (TD-DFT) as implemented in the Gaussian16 software. Hybrid, B3LYP and CAM-B3LYP (long-range corrected version of B3YP) functionals were employed with the 6-311+G(d,p) basis set. Solvent effects (CH_2Cl_2) have been considered by using the conductor-like polarized continuum model (C-PCM).[S11] The bathochromic shift of the absorption maxima experimentally observed is suitably reproduced, and it is well interpreted as a function of the HOMO-LUMO gap energies.

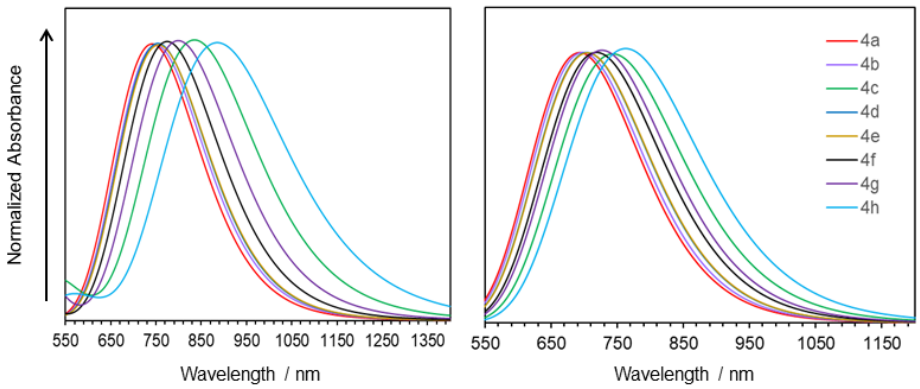


Figure S27: TD-DFT normalized absorption Spectra in CH_2Cl_2 solution computed at the B3LYP (left) and CAM-B3LYP (right)/ 6-311+G(d,p) level of theory.

Table S4. Comparison of the wavelength of the absorption maxima (nm)

Compound	λ_{max} [a]	λ_{max} [b]	λ_{max} [c]
4a	608	741	694
4b	611	750	698
4c	637	835	743
4d	616	754	704
4e	616	456	705
4f	630	775	719
4g	636	799	727
4h	694	885	763

[a] Experimental. [b] B3LYP/6-311+G(d,p) [c] CAM-B3LYP/6-311+G(d,p)

9.3.Topologies of the frontier molecular orbitals

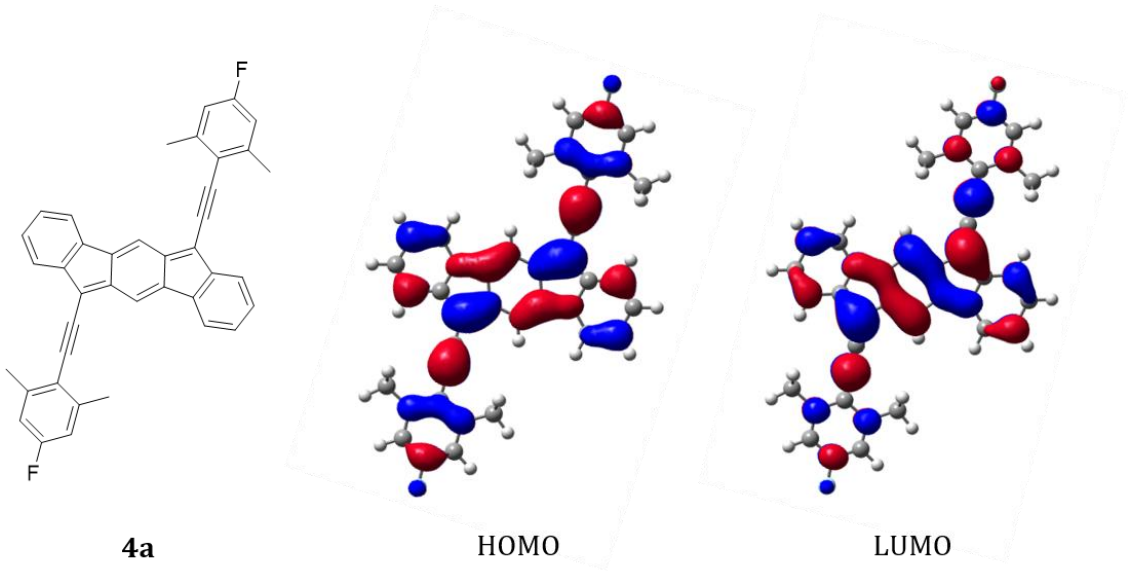


Figure S28. HOMO and LUMO plots for compound **4a**.

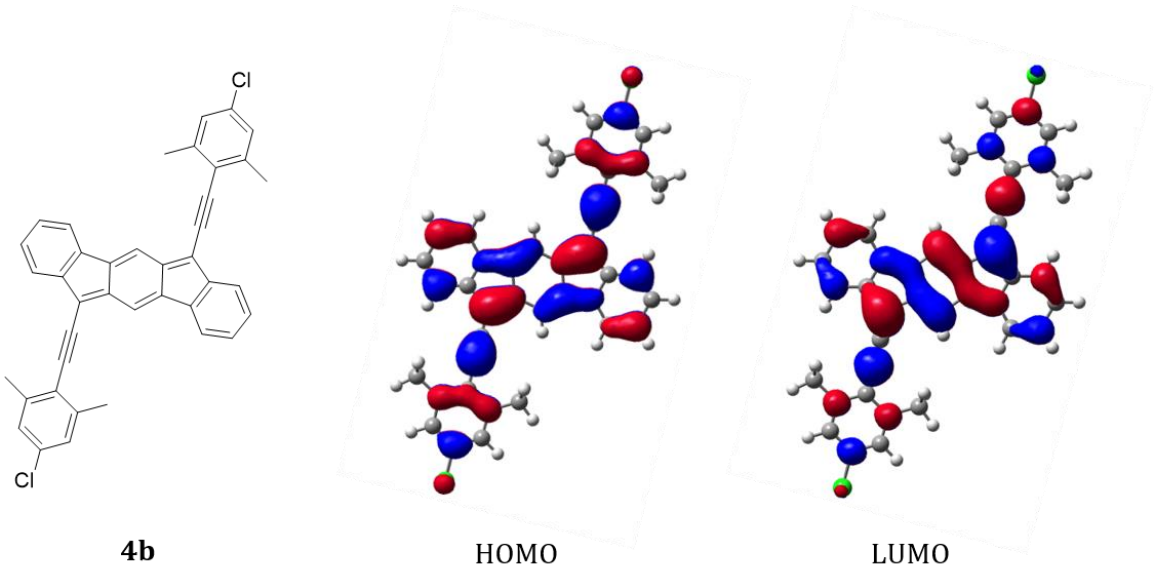


Figure S29. HOMO and LUMO plots for compound **4b**.

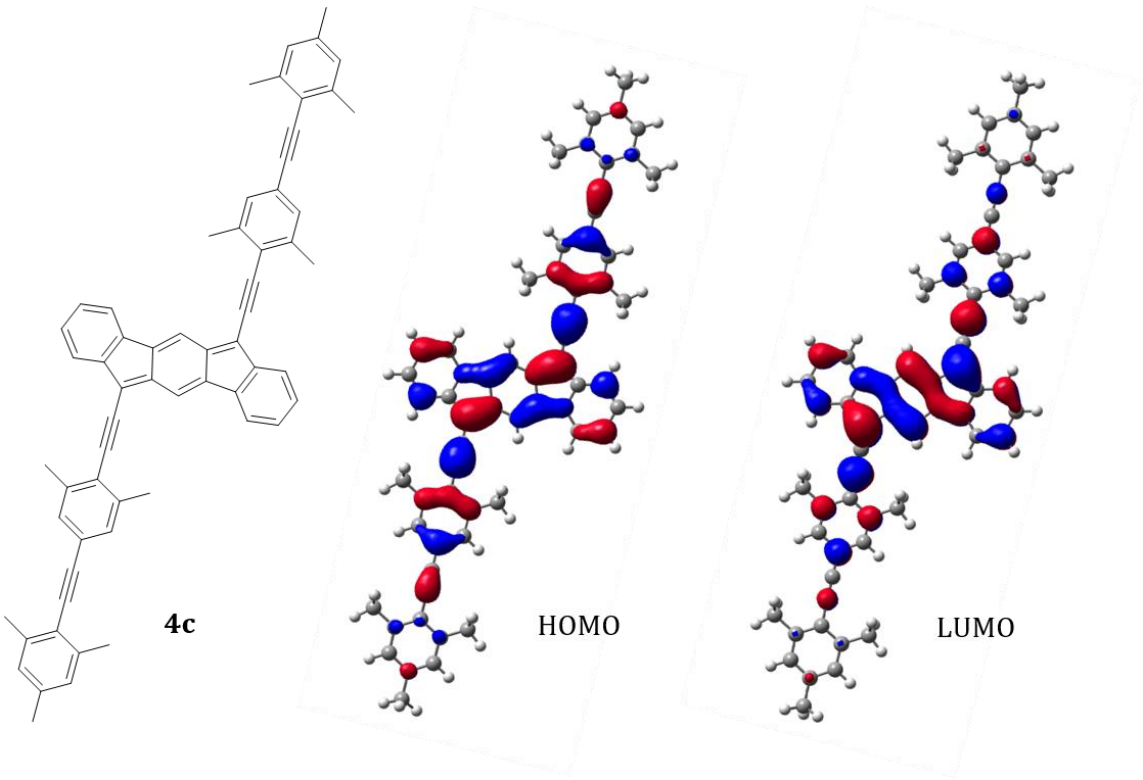


Figure S30. HOMO and LUMO plots for compound **4c**.

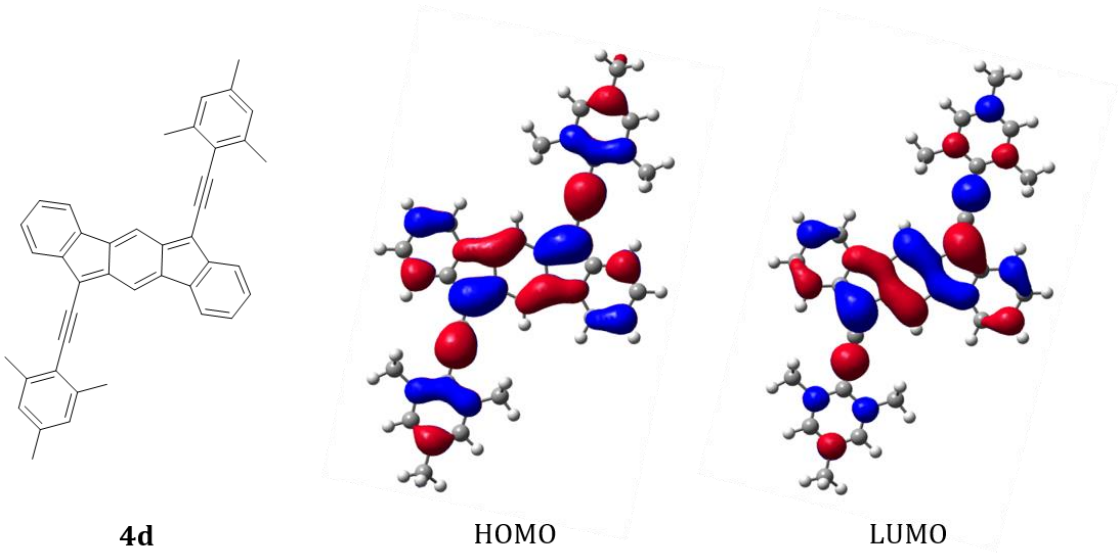


Figure S31. HOMO and LUMO plots for compound **4d**.

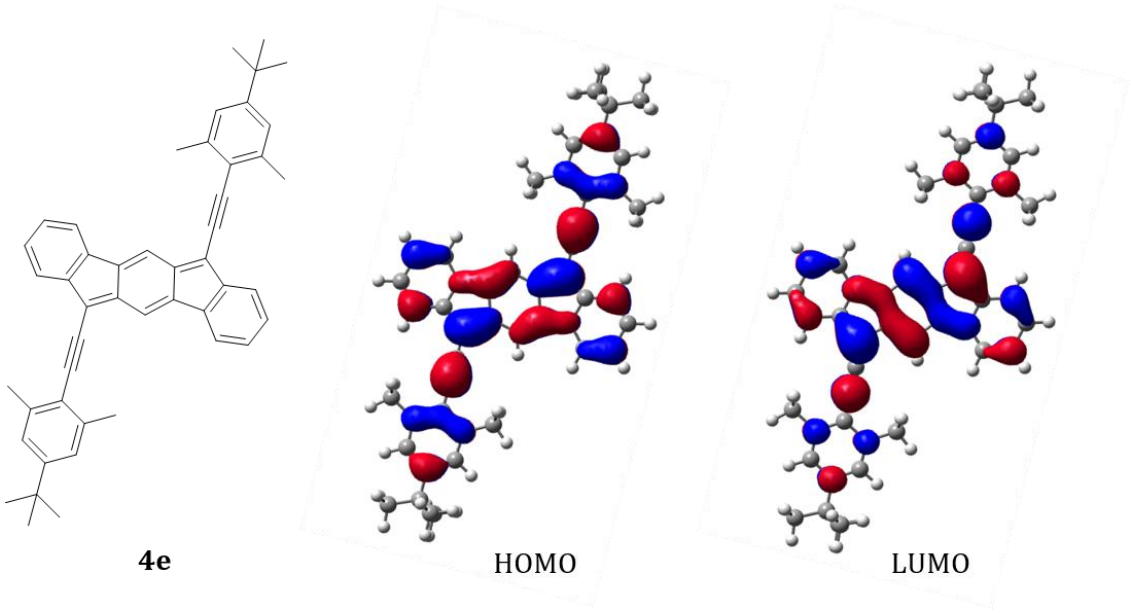


Figure S32. HOMO and LUMO plots for compound **4e**.

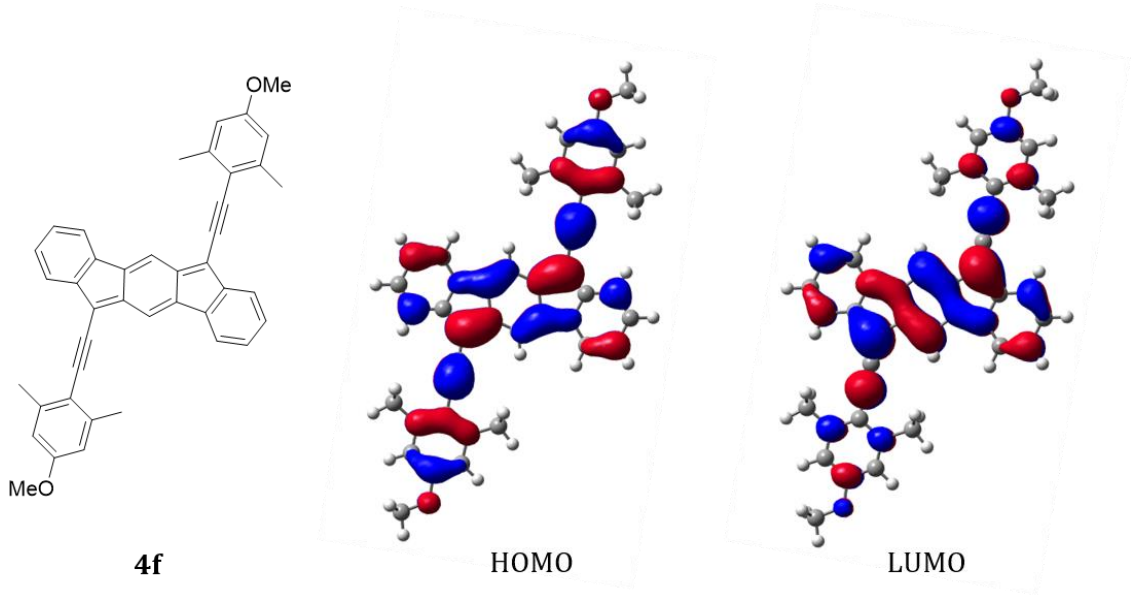


Figure S33. HOMO and LUMO plots for compound **4f**.

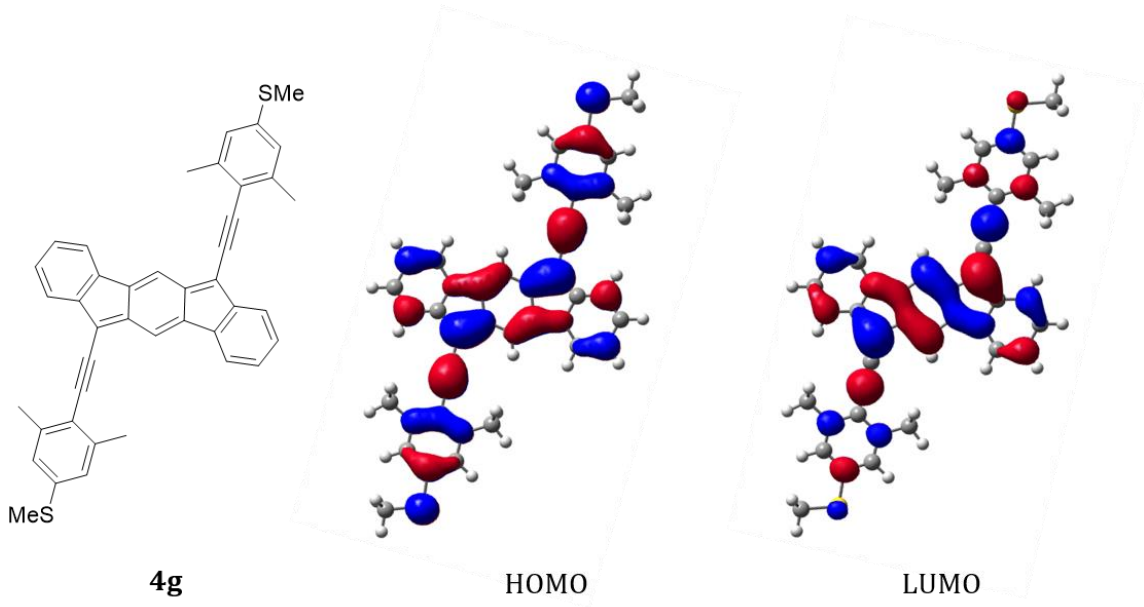


Figure S34. HOMO and LUMO plots for compound **4g**.

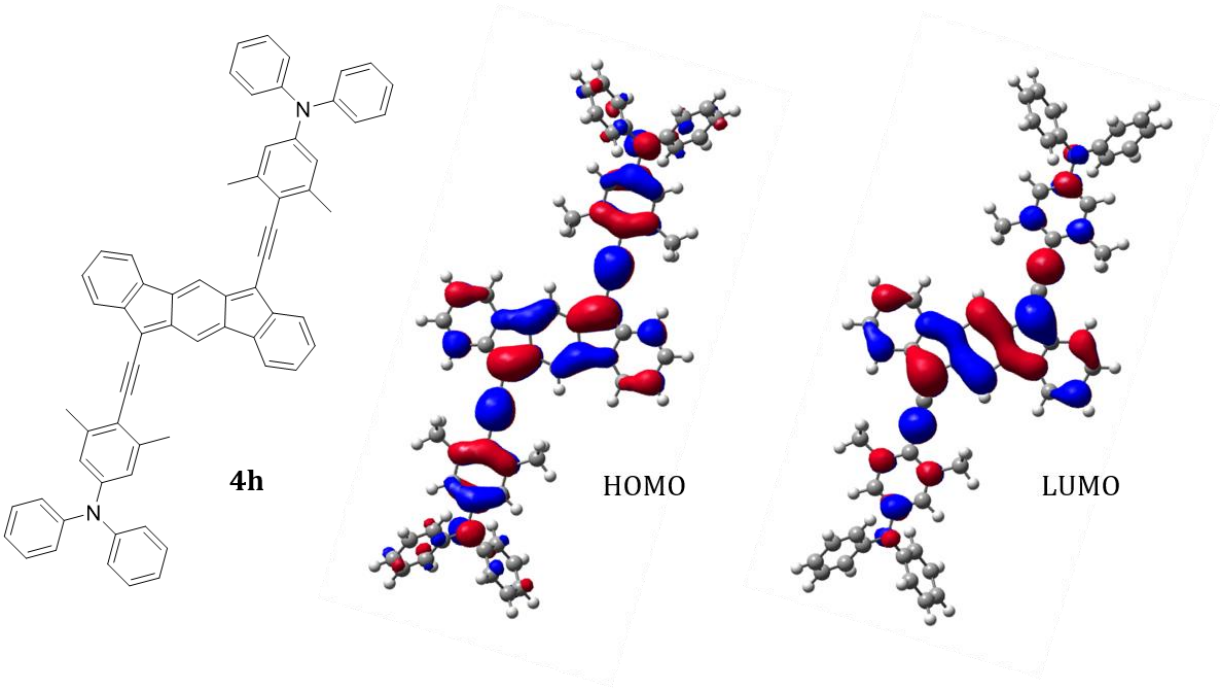


Figure S35. HOMO and LUMO plots for compound **4h**.

9.4. Singlet-triplet energy gap (ΔE_{ST})

Adiabatic singlet-triplet energy gaps have been computed as the energy difference between the ground singlet, and lowest-lying triplet (T) states for compounds **2a**, **3a**, **4e** and **4d**. In the studied cases, the singlet (closed-shell, S) and singlet diradical (open-shell, SD) states are isoenergetic, thus, the singlet-triplet energy gap is the same between S/SD and the T state. For this purpose, the geometries of the open-shell states: SD and T, were optimized at spin-unrestricted UB3LYP/6-311+G** level of theory. Broken Symmetry (BS) DFT method was employed on SD geometry optimizations.

9.5. Diradical character

The open-shell character (diradical character y) has been determined within the single determinant UDFT scheme, where is defined as the occupation number of the LUNO (lowest unoccupied natural orbital) of the unrestricted wave function, n_{LUNO}:[S12]

$$y = n_{LUNO} = 2 - n_{HONO}$$

which range from 0 (molecule with a close-shell structure) to 1 (a pure open-shell (diradical) structure).

The long-range corrected[S13] unrestricted density functional theory (DFT) method, with the Lee-Yang-Parr correlation functional (LC-BLYP) and the 6-311+G** basis set were used. The range separation parameter, μ, was set in 0.33 $bohr^{-1}$.

Table S5. Singlet-Triplet energy gap (kcal/mol) and Diradical character (*y*)

Compound	ΔE_{ST}	*y*
2a	12.22	0.30
3a	18.24	0.09
4d	10.70	0.36
4e	10.70	0.36

9.6. Spin Density Distribution

In order to evaluate the stability of the target molecules (**4a-h**) in terms of the 2,4,6-substitution in the phenyl acetylene fragments, two model molecules were considered (**D4** and **D26** shown in Figure S36). In them, only the methyl group substitution in the 4- position (para-), or in the 2,6- positions (ortho-) in the arene group is contemplated.

Geometries were optimized in their SD state following the methodology already described. The estimation of the spin density distribution in the two model compounds, and their comparison with that for the target system, **4d** is shown in Figure S37.

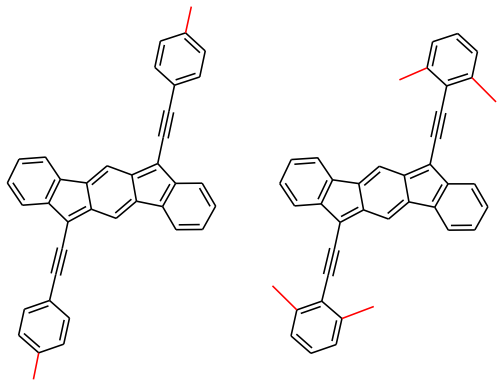
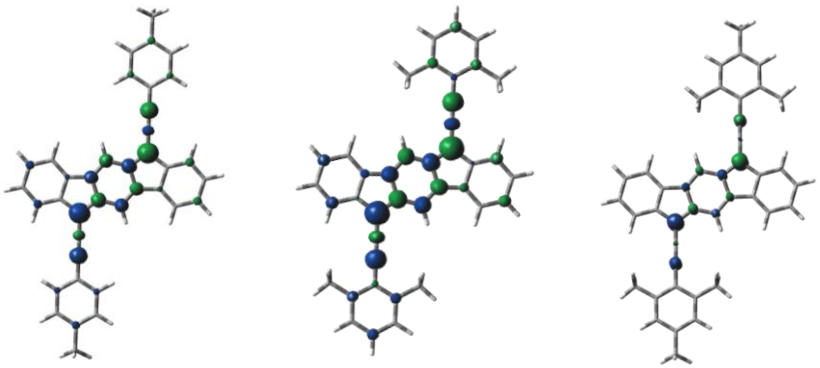


Figure S36. Chemical structures of model molecules: **D4** and **D26.**



D4 **D26** **4d**

Figure S37. Spin Density distributions for **D4**, **D26** and **4d** compounds, calculated at the UB3LYP/6-311+G** level. Blue and green surfaces depict the α and β electronic spin density, respectively. A 4e-08 isovalue was employed.

As can be seen, when the methyl substituent is attached to ortho- and para- positions of the arene (**4d**), the spin density is mitigated at most carbon centers, leaving the radical (reactive) sites shielded by substitution. Conversely, systems bearing 2,6-dimethylphenylacetylene (**D26**) and 4-methylphenyl acetylene (**D4**), results in the delocalization of the spin density over a larger number of atoms, most of them non protected, what can be the cause of the unsuccessful synthesis.

9.7.Transport calculations

The junction optimized geometry were carried out using the Perdew-Burke-Ernzerhof (PBE) functional withing the Generalized Gradient Approximation (GGA),[S14] as implemented in the SIESTA package.[S10] The valence electrons were described using a single-ζ plus polarization basis set for Au atoms, and double-ζζ plus polarization basis set for the molecule atoms, whereas Troullier− Martins pseudopotentials are used for the description of the core electrons.

Electrodes were build by six layers of 49 gold atoms in a 7x7 unit cell of the Au (111) surface. In addition, a pyramidal-shaped tip was modeled, attaching the sulfur atom of the molecular anchoring groups to the last gold atom of the tip (see Figure S38 left). During the geometry relaxation, the first four gold layers of the bottom electrode were kept at bulk values, while the outer four layers of the top electrode were only allowed to relax along the transport direction (z) as rigid body. The three coodinates of the molecule, the tips and the two inner gold layers were allowed to fully relax. Thus, the molecule geometry at the junction, the molecule-gold contact and the junction length were optimized at the same time, obtaining a S-

to-S vertical distance of 2.12 nm, in consonance with the 2.08 nm value estimated experimentally. For that purpose, large vacuumm along the z-axis, a 3x3x1 k-grid sampling of the transverse Brillouin zone, and a cutoff energy of 300.00Ry for real-space integrations were used, minimizing the forces until down 0.04 eV/angstroms.

On the optimized junction were simulated the transport properties by means of the TranSIESTA package,[S10b] by using the double-ζζ basis set for gold atoms, double-ζζ plus polarization basis set for the molecule atoms, and the same parameters (functional, kmesh, mesh cutoff, etc.) as in the optimization. Landauer zero-bias transmission function was calculated by increasing the k-grid sampling to 8x8x1 by using the post-processing TBTrans tool.[S10c] These parameters were thoroughly tested to warrant the convergence of the transmission spectrum.

Within the Landauer formalism, zero-bias conductance can be approximated as the transmission probability at the Fermi level, $G/G_0 = T(E_F)$. We have employed the zero bias self-energy corrected DFT(DFT+Σ) method, as in previous works,[S15,S16] to overcome the deficiencies of the standard DFT method on the conductance overestimation. The DFT+Σ zero-bias transmission probability function is shown in Figure S36. We have calculated a value for the most probable conductance in the end-to-end single molecule junction, in good agreement with the experimental value : $\log (G/G_0)_{DFT+\Sigma} = -3.27$ vs. $\log (G/G_0)_{exp.} = -3.60$.

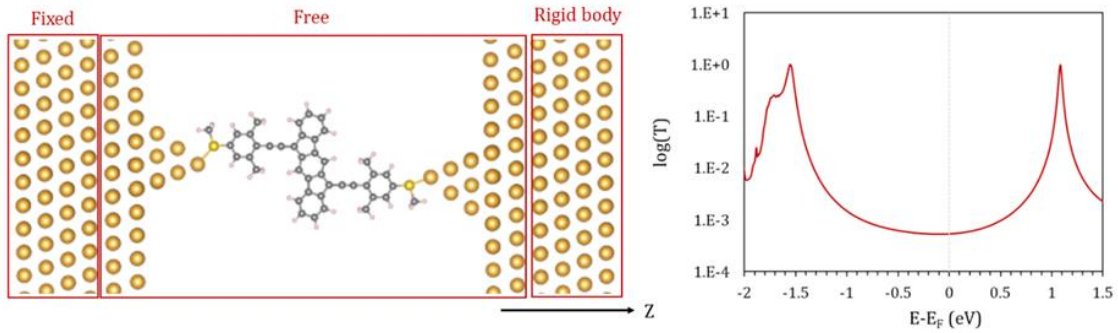


Figure S38. Left: Single-molecule junction for compound **4g**.; Right: DFT+Σ -zero-bias transmission as a function of the energy for the single-molecule junction of molecule **4g** in its end-to-end configuration.

9.8. Nucleus-independent chemical shift

Nucleus-independent chemical shift (NICS) calculations were carried out as an aromaticity index at the center of mass of all fused rings on the **4g** molecule in its junction geometry, and

on **2a**, **3a**, **4e** and **4d** compounds in the their three states: SCS, SOS and T. Out of plane-axial π contributions were considered (zz). The gauge-independent atomic orbital (GIAO) approach,[S17] on the (U)BLYP functional together with the 6-311+G** basis set were employed within the Gaussian16 suite. For open-shell states, the long-range corrected method[S13] with the range separating parameter μ, of 0.33 $bohr^{-1}$ were used.

NICS index quantifies diatropicity/paratropicity of the induced ring current by the effective magnetic shielding, associated with an aromatic/antiaromatic character. The more positive value of NICS, the more anti-aromatic ring nature. Significant negative values reflects an aromatic ring character, meanwhile values around zero characterice non-aromatic rings. NICS values were evaluated at 1 Å above and below the central fused core, NICS(1)zz. Results are shown in Figure S40 y Table S6.

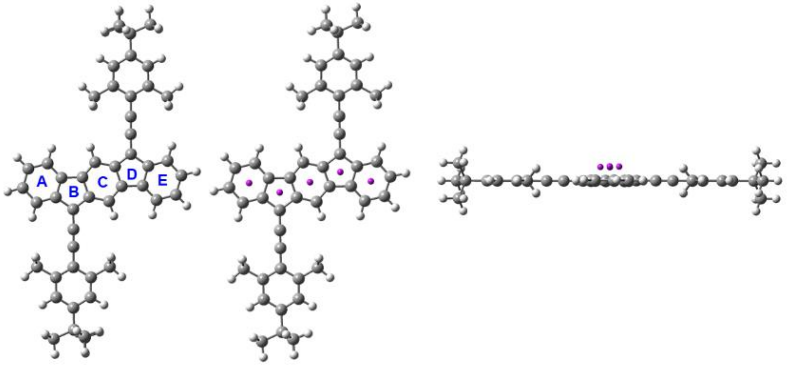


Figure S39. Depiction of probe atom (Bq) at 1 Å above of the centre of mass of each fused core rings, for NICS (1)zz calculations. **4e** molecule is shown as example.

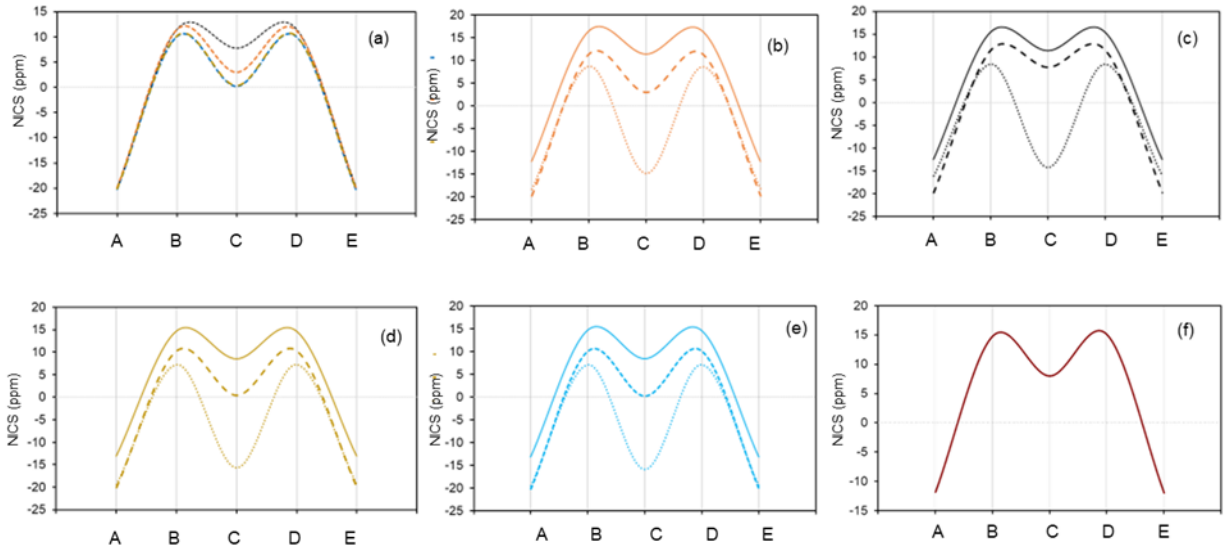


Figure S40. Magnetic Shielding Tensor Components -σzz [ppm] 1 Å above the centre of each ring: (a) at the SD state of **2a** (orange), **3a** (black), **4e** and **4d** (blue); (b) **2a**, (c) **3a** (d) **4e** and (e) **4d** in the gas phase, and (f) **4g** in the junction geometry, at S (continuous line), SD (dashed line) and T (dotted line). Numerical values in Table S6.

Table S6. Magnetic Shielding Tensor Components -σzz [ppm] 1 Å above the centre of each ring: for **2a**, **3a**, **4e** and **4d** compounds in S, SD and T states, and **4g** in the junction geometry. Corresponding graph: Figure S36.

	NICS (1)zz [ppm]				
Compound	A	B	C	D	E
2a (S)	-12.190	16.450	11.373	16.291	-12.211
2a (SD)	-19.816	11.429	2.984	11.283	-19.802
2a (T)	-18.332	8.738	-14.847	8.622	-18.293
3a (S)	-12.541	15.380	11.293	15.380	-12.541
3a (SD)	-19.846	11.531	7.732	11.531	-19.846
3a (T)	-16.140	8.462	-14.286	8.462	-16.140
4d (S)	-13.124	14.647	8.393	14.560	-13.124
4d (SD)	-20.158	10.087	0.230	10.092	-20.158
4d (T)	-19.537	7.076	-15.903	7.076	-19.534
4e (S)	-13.069	14.647	8.514	14.647	-13.069
4e (SD)	-20.066	10.213	0.368	10.213	-20.066
4e (T)	-19.398	7.251	-15.664	7.251	-19.398
4g	-11.769	14.760	7.980	15.028	-11.918

10.STM-BJ experiments and analysis

Sample preparation. Before the preparation of the samples, the substrates were cleaned with EtOH and flame-annealed. Later, they were immersed in a 10^{-3} M solution of the compound **4g** in CH_2Cl_2 for 15 minutes and dried with nitrogen gas. We used freshly cut gold wires (Goodfellow) as tip and commercial gold on quartz samples (Arrandee) as substrates.

Single-Molecule Conductivity Studies. Single-molecule conductance (G) experiments were carried out using the scanning tunneling microscope break-junction (STM-BJ) technique. For these experiments, we used a home-built STM operating in air and room temperature. A constant 0.16 V bias voltage was applied between the electrodes along the experiments. A made-in-house linear current-to-voltage (*I*-*V*) converter with two stages of amplification was used for obtaining the current-distance (*I*-*z*) traces. We used gains of 10^8 V/A and 4.4×10^9 V/A, which allowed us to explore a range in conductance *G*=*I*/*V* of 8 orders of magnitude between 10 G_0 and 10^{-7} G_0. A protection resistor of 2×10^6 Ω was placed in-series with the STM circuit. Several rounds of thousands of conductance-distance (*G*-*z*) traces were collected while pulling the STM tip for this compound, changing to new tips, substrates or even different product batches in order to ensure the reproducibility of results.

10.1 Data analysis

G-z pulling traces were aligned so that $G(z=0) = 0.5\ G_0$ (just after each gold contact is broken), and those traces presenting plateaus were separated from the ones without plateaus using an automatized program as previously described.[S18] The criterion for considering a trace containing plateau was that, at any conductance below 0.5 G_0, a displacement Δ*z* larger than 0.1 nm is needed to produce a change in conductance of $\Delta\log(G/G_0) = 0.1$. This process gave rise to a rate of success (percentage of traces containing plateaus) of 18%.

1D *G* and 2D *G*-*z* histograms were constructed with the separated groups of traces (see Figure 5 in the main text) and normalized as previously reported.[S18] The plateau length in each G-z trace displaying plateau was calculated as the variation of *z* (Δ*z*) that took place in the trace for G to change from 0.5 G_0 to 10^5 G_0 (a value below the conductance peak in 1D histogram). A probability (*p*) distribution was then calculated using the length of all the detected plateaus (Figure 5c inset in the main text).

10.2. Current *vs.* voltage curves

Current vs voltage (*I*-*V*) curves were recorded by pausing the separation between the STM tip and substrate at various positions along the conductance plateaus and sweeping the bias voltage between +1 V and –1 V. Two voltage ramps (increasing and decreasing voltage) were recorded at each position. For convenience, we then represented conductance vs voltage (*G*-*V*) curves, where the conductance was simply obtained as *G=I/V* (therefore flat *G*-*V* curves correspond to linear *I*-*V* curves). Figure S41a shows an example of a *G*-*z* trace for which *G*-*V* curves were recorded at 6 positions marked with circles along its conductance plateau. Those *G*-*V* curves are displayed in Figure S41b, while Figure S41c shows a 2D *G*-*V* histogram of 1100 *G*-*V* curves recorded along 200 similar conductance plateaus. Asymmetry in the *G*-*V* curves can come from variations in the molecule-electrode coupling at both sides of the molecular junction. To have a proper assessment of global asymmetry in the curves, each *G*-*V* curve was flipped if necessary to ensure that the arm of higher conductance is oriented to positive voltages, before generating the histogram. As expected, no significant asymmetry was observed for **4g** curves, as better seen in the averaged *G*-*V* curve depicted as a thick black line on top of the 2D histogram of Figure S41c.

For comparison, Figure S41d shows the equivalent results for related compound dibenzopentalene (DBP), which have been already separately reported.[S19] The figure shows that, while the *G*-*V* curves for DBP are generally flat in the studied voltage range, for **4g** they present a conductance increase outside the (–0.6 V, + 0.6 V) interval. This increase suggests that the closest level of **4g** is placed at a closer energy to the gold Fermi energy than that of DBP (see main text for further discussion).

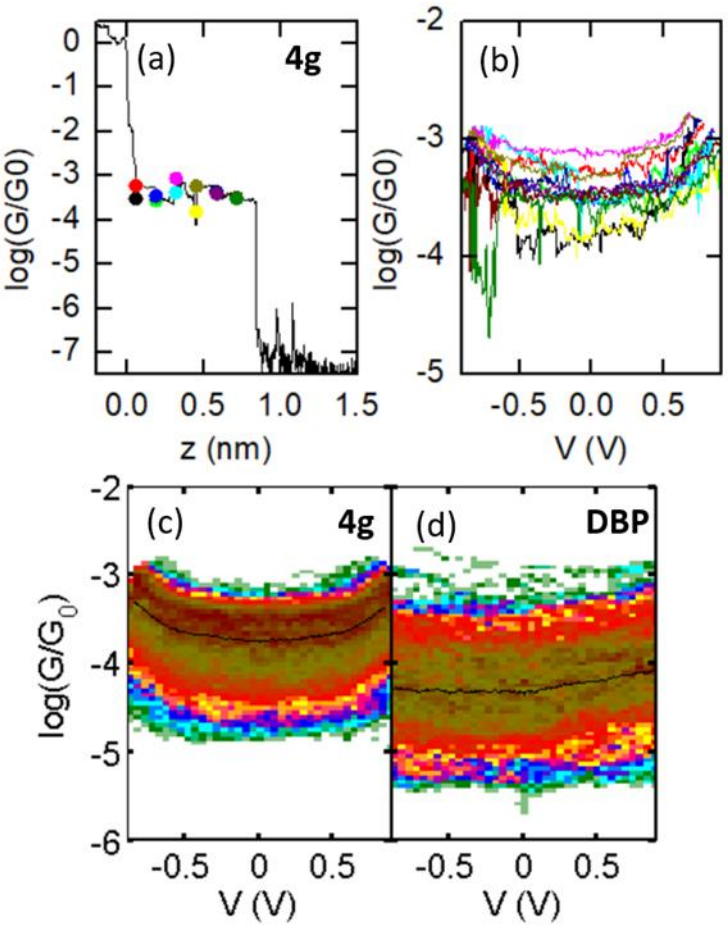


Figure S41. Conductance vs Voltage curves for **4g**. (a) Example of a *G-z* trace displaying a conductance plateau. Along the process of separating the electrodes from each other, their position was held still at several positions indicated by coloured circles. (b) *G-V* curves recorded at the positions indicated by the circles in part (a). Each *G-V* curve in (b) and its correspondent point in (a) have the same colour. (c) 2D histogram of 1100 *G-V* curves for **4g**. The thick black line corresponds to the global *G-V* average. (d) Equivalent 2D histogram and averaged curve for *G-V* curves recorded for DBP.

11. Cartesian coordinates of the optimized geometries in the gas phase

2a S

Si	0.44196	6.67694	0.00000
C	2.35228	6.54684	0.00000
C	-0.14504	7.48916	1.63337
H	2.72010	7.58228	0.00000
C	-0.14504	7.48916	-1.63337
C	-0.23113	4.95273	0.00000
H	0.26837	6.81880	2.39941
C	-0.66505	3.81192	0.00000
C	-1.18699	2.50915	0.00000
C	-0.46351	1.31586	0.00000
C	-2.61580	2.17644	0.00000
C	0.94532	1.09249	0.00000
C	-1.39514	0.19617	0.00000
C	-3.74026	2.99674	0.00000
C	-2.74661	0.76332	0.00000
C	1.39514	-0.19617	0.00000
H	1.62444	1.93828	0.00000
C	-0.94532	-1.09249	0.00000
C	-5.00320	2.39955	0.00000
H	-3.63673	4.07591	0.00000
C	-4.00702	0.17988	0.00000
C	2.74661	-0.76332	0.00000
C	0.46351	-1.31586	0.00000
H	-1.62444	-1.93828	0.00000
C	-5.13504	1.00818	0.00000
H	-5.89114	3.02146	0.00000
H	-4.12401	-0.89838	0.00000
C	4.00702	-0.17988	0.00000
C	2.61580	-2.17644	0.00000
C	1.18699	-2.50915	0.00000
H	-6.12420	0.56448	0.00000
C	5.13504	-1.00818	0.00000
H	4.12401	0.89838	0.00000
C	3.74026	-2.99674	0.00000
C	0.66505	-3.81192	0.00000
C	5.00320	-2.39955	0.00000
H	6.12420	-0.56448	0.00000
H	3.63673	-4.07591	0.00000
C	0.23113	-4.95273	0.00000
H	5.89114	-3.02146	0.00000
Si	-0.44196	-6.67694	0.00000
C	0.14504	-7.48916	1.63337
C	-2.35228	-6.54684	0.00000
C	0.14504	-7.48916	-1.63337
H	0.26837	6.81880	-2.39941
H	-2.72010	-7.58228	0.00000
C	-0.45014	-8.88920	1.88035
H	-0.05666	-9.62532	1.17324
H	-0.19482	-9.24155	2.88616
H	-1.54065	-8.90205	1.79835
C	-0.45014	-8.88920	-1.88035
H	-0.19482	-9.24155	-2.88616
H	-0.05666	-9.62532	-1.17324
H	-1.54065	-8.90205	-1.79835
C	-2.89854	-5.85983	1.26613
H	-3.99334	-5.81670	1.23977
H	-2.61549	-6.38675	2.18116
H	-2.53189	-4.83190	1.35040
C	-2.89854	-5.85983	-1.26613
H	-2.61549	-6.38675	-2.18116
H	-3.99334	-5.81670	-1.23977
H	-2.53189	-4.83190	-1.35040
C	1.67216	-7.50081	1.83024
H	2.11147	-6.51136	1.68070
H	1.92409	-7.82479	2.84649
H	2.16297	-8.19339	1.14076
C	1.67216	-7.50081	-1.83024
H	2.16297	-8.19339	-1.14076
H	1.92409	-7.82479	-2.84649
H	2.11147	-6.51136	-1.68070
H	-0.26837	-6.81880	-2.39941
H	-0.26837	-6.81880	2.39941
C	2.89854	5.85983	1.26613
H	3.99334	5.81670	1.23977
H	2.61549	6.38675	2.18116
H	2.53189	4.83190	1.35040
C	2.89854	5.85983	-1.26613
H	2.61549	6.38675	-2.18116
H	3.99334	5.81670	-1.23977
H	2.53189	4.83190	-1.35040
C	0.45014	8.88920	1.88035
H	0.05666	9.62532	1.17324
H	0.19482	9.24155	2.88616
H	1.54065	8.90205	1.79835
C	0.45014	8.88920	-1.88035
H	0.19482	9.24155	-2.88616
H	0.05666	9.62532	-1.17324
H	1.54065	8.90205	-1.79835
C	-1.67216	7.50081	-1.83024
H	-1.92409	7.82479	-2.84649
H	-2.11147	6.51136	-1.68070
H	-2.16297	8.19339	-1.14076
C	-1.67216	7.50081	1.83024
H	-1.92409	7.82479	2.84649
H	-2.16297	8.19339	1.14076
H	-2.11147	6.51136	1.68070

2a SD

Si	-6.68174	0.30351	-0.09335
C	-7.28199	0.23507	-1.91120
C	-6.59118	2.12811	0.48293
C	-7.33750	-1.20179	-2.46403
C	-6.45141	1.13846	-2.84262
H	-8.30902	0.62605	-1.89685
C	-7.72827	-0.89459	0.97356
C	-4.94682	-0.33954	-0.05520
H	-5.88712	2.57300	-0.23408
H	-7.70933	-1.20343	-3.49491
H	-6.34400	-1.66086	-2.47454
H	-7.99692	-1.84853	-1.87905
H	-6.83878	1.09529	-3.86685
H	-5.40529	0.81844	-2.87496
H	-6.46910	2.18649	-2.53176
H	-7.57845	-1.86014	0.47075
C	-3.79962	-0.75580	-0.03856
C	-2.48731	-1.25222	-0.01660
C	-1.30944	-0.50391	-0.01681
C	-2.12515	-2.67342	0.01096
C	-1.11675	0.90923	-0.03805
C	-0.17064	-1.41154	0.01149
C	-2.92229	-3.81435	0.02146
C	-0.70965	-2.77453	0.02821
C	0.16197	1.38655	-0.03083
H	-1.97732	1.56927	-0.05933
C	1.10814	-0.93421	0.01880
C	-2.29910	-5.06437	0.04923
H	-4.00328	-3.73259	0.00842
C	-0.10046	-4.02237	0.05590
C	0.70058	2.74965	-0.04592
C	1.30088	0.47901	-0.00189
H	1.96872	-1.59425	0.04017
C	-0.90537	-5.16719	0.06627
H	-2.90239	-5.96503	0.05777
H	0.97995	-4.11687	0.06945
C	0.09104	3.99733	-0.07356
C	2.11600	2.64889	-0.02578
C	2.47853	1.22769	0.00093
H	-0.44142	-6.14679	0.08787
C	0.89563	5.14239	-0.08111
H	-0.98936	4.09151	-0.08912
C	2.91283	3.79006	-0.03317
C	3.79151	0.73330	0.02727
C	2.28935	5.03993	-0.06110
H	0.43146	6.12188	-0.10270
H	3.99380	3.70865	-0.01742
C	4.94049	0.32218	0.04898
H	2.89241	5.94076	-0.06731
Si	6.68083	-0.30503	0.10193
C	7.13280	-0.59069	1.94155
C	6.67993	-1.98105	-0.82576
C	7.78023	1.08770	-0.61909
C	7.10447	0.70963	2.76721
C	6.25580	-1.66924	2.60563
H	8.16803	-0.95964	1.93698
H	5.93512	-2.56575	-0.26802
H	7.56627	1.93434	0.04802
H	7.38989	0.51178	3.80662
H	6.10186	1.14826	2.78127
H	7.79265	1.46523	2.37893
H	6.55884	-1.82431	3.64730
H	5.20209	-1.37337	2.61268
H	6.32710	-2.63529	2.09860
C	7.39765	1.53374	-2.04265
H	6.33115	1.75559	-2.13109
H	7.94992	2.43851	-2.32146
H	7.64081	0.76764	-2.78407
C	-5.98588	2.32525	1.88525
H	-5.03593	1.79727	2.00145
H	-5.80144	3.38853	2.07712
H	-6.66146	1.97029	2.66846
C	-7.23046	-1.06396	2.42111
H	-7.76566	-1.88233	2.91622
H	-6.16257	-1.29240	2.46382
H	-7.40228	-0.16191	3.01492
C	6.18716	-1.90408	-2.28282
H	6.04902	-2.91065	-2.69399
H	5.23298	-1.37770	-2.36679
H	6.90824	-1.39094	-2.92515
C	-7.92295	2.89207	0.34950
H	-7.77737	3.95678	0.56455
H	-8.34985	2.81826	-0.65460
H	-8.67231	2.52223	1.05549
C	-9.23951	-0.59376	0.94528
H	-9.79796	-1.38741	1.45445
H	-9.47315	0.34299	1.45981
H	-9.63394	-0.51952	-0.07210
C	8.01689	-2.74271	-0.73909
H	8.36552	-2.86229	0.29055
H	7.91480	-3.74624	-1.16753
H	8.80746	-2.23439	-1.29888
C	9.29125	0.80017	-0.52280
H	9.58894	-0.01589	-1.18784
H	9.86922	1.68281	-0.81924
H	9.60366	0.53179	0.49035

2a T

Si	-6.683686	0.290218	-0.089647
C	-7.285982	0.233985	-1.907787
C	-6.573979	2.112159	0.491842
C	-7.357151	-1.200238	-2.465549
C	-6.447197	1.132116	-2.836852
H	-8.308898	0.635549	-1.890641
C	-7.743528	-0.900302	0.973123
C	-4.957251	-0.371963	-0.052827
H	-5.865033	2.551763	-0.223582
H	-7.730559	-1.194299	-3.495848
H	-6.368524	-1.669641	-2.479302
H	-8.022325	-1.842248	-1.881902
H	-6.836725	1.097291	-3.86058
H	-5.404593	0.801143	-2.872397
H	-6.453033	2.178996	-2.521746
H	-7.60534	-1.865297	0.46599
C	-3.812124	-0.813584	-0.036151
C	-2.517004	-1.303742	-0.014756
C	-1.292786	-0.502432	-0.018879
C	-2.117117	-2.693472	0.016187
C	-1.126116	0.883876	-0.044616
C	-0.177057	-1.386171	0.010476
C	-2.881832	-3.863825	0.03132
C	-0.693626	-2.758247	0.031916
C	0.174859	1.380277	-0.040445
H	-1.98737	1.542413	-0.067079
C	1.123925	-0.889762	0.01494
C	-2.226375	-5.093558	0.0619
H	-3.96474	-3.811961	0.019427
C	-0.054018	-3.989772	0.062482
C	0.691386	2.752371	-0.061348
C	1.290581	0.49656	-0.010271
H	1.985212	-1.548258	0.037616
C	-0.828035	-5.15687	0.077351
H	-2.803718	-6.010931	0.073901
H	1.028445	-4.056406	0.074836
C	0.051743	3.983857	-0.092774
C	2.114844	2.687672	-0.043164
C	2.514755	1.297955	-0.011617
H	-0.337057	-6.123191	0.101184
C	0.825709	5.151003	-0.106199
H	-1.0307	4.050419	-0.106836
C	2.879505	3.858082	-0.056621
C	3.809809	0.808003	0.016818
C	2.224022	5.087775	-0.088241
H	0.334716	6.117298	-0.130775
H	3.962388	3.806313	-0.0426
C	4.954963	0.366837	0.041605
H	2.801327	6.005188	-0.099064
Si	6.680461	-0.295873	0.104075
C	7.16476	-0.468943	1.950085
C	6.622416	-2.030439	-0.706756
C	7.796526	1.018622	-0.729836
C	7.189698	0.884523	2.685443
C	6.275245	-1.475437	2.704302
H	8.189565	-0.866003	1.94885
H	5.884345	-2.561134	-0.08927
H	7.605832	1.916175	-0.12518
H	7.496394	0.749993	3.728908
H	6.198932	1.349469	2.69346
H	7.886254	1.593623	2.230164
H	6.598362	-1.568539	3.74732
H	5.230035	-1.150963	2.713835
H	6.309408	-2.474934	2.26255
C	7.404162	1.364677	-2.178316
H	6.340677	1.599036	-2.271313
H	7.968525	2.236058	-2.529779
H	7.624938	0.541341	-2.863341
C	-5.967231	2.298757	1.894979
H	-5.02191	1.762183	2.009407
H	-5.773386	3.359665	2.090659
H	-6.646075	1.947034	2.676838
C	-7.246451	-1.081667	2.419442
H	-7.791557	-1.895066	2.911944
H	-6.181519	-1.323991	2.460095
H	-7.405871	-0.17986	3.017074
C	6.08821	-2.043389	-2.151169
H	5.920321	-3.072815	-2.487991
H	5.141417	-1.505372	-2.244346
H	6.798847	-1.589588	-2.847476
C	-7.897656	2.890424	0.360345
H	-7.740888	3.952822	0.578941
H	-8.325	2.824487	-0.644116
H	-8.65114	2.526249	1.064882
C	-9.251131	-0.581636	0.947463
H	-9.818428	-1.371124	1.45332
H	-9.473397	0.355313	1.466641
H	-9.645444	-0.497979	-0.069226
C	7.947772	-2.810497	-0.60633
H	8.324755	-2.867509	0.4187
H	7.815402	-3.838377	-0.962692
H	8.730085	-2.3565	-1.221681
C	9.303298	0.710983	-0.629147
H	9.578551	-0.157684	-1.23452
H	9.892855	1.558327	-0.997175
H	9.623518	0.513284	0.397694

3a S

C	-1.38234	-0.23752	0.00000
C	-0.42323	-1.34614	0.00000
C	0.91835	-1.11998	0.00000
C	1.38234	0.23752	0.00000
C	0.42323	1.34614	0.00000
C	-0.91835	1.11998	0.00000
H	1.63757	-1.93292	0.00000
H	-1.63757	1.93292	0.00000
C	2.66857	0.74018	0.00000
C	2.58310	2.20163	0.00000
C	3.58510	3.17057	0.00000
C	3.21619	4.51862	0.00000
C	1.86913	4.89064	0.00000
C	0.85723	3.92276	0.00000
C	1.21253	2.58084	0.00000
H	4.63107	2.88361	0.00000
H	1.60399	5.94191	0.00000
H	-0.18446	4.22577	0.00000
C	-1.21253	-2.58084	0.00000
C	-2.66857	-0.74018	0.00000
C	-2.58310	-2.20163	0.00000
C	-0.85723	-3.92276	0.00000
C	-3.58509	-3.17057	0.00000
C	-1.86913	-4.89064	0.00000
C	-3.21619	-4.51862	0.00000
H	0.18446	-4.22577	0.00000
H	-1.60399	-5.94191	0.00000
H	-4.63107	-2.88361	0.00000
C	3.93510	-0.03489	0.00000
C	4.54241	-0.39326	-1.22007
C	4.54242	-0.39326	1.22007
C	5.74198	-1.10890	-1.19644
C	5.74198	-1.10890	1.19644
C	6.35714	-1.47988	0.00000
H	6.20805	-1.37947	-2.13952
H	6.20805	-1.37946	2.13951
C	3.91577	-0.01609	2.54271
C	3.91576	-0.01610	-2.54271
C	7.63689	-2.28132	0.00000
H	2.94099	-0.49499	-2.67437
H	3.75049	1.06250	-2.61593
H	4.55473	-0.31844	-3.37455
H	4.55474	-0.31844	3.37455
H	3.75050	1.06251	2.61593
H	2.94100	-0.49498	2.67438
H	7.42627	-3.35659	0.00001
H	8.24152	-2.06748	-0.88458
H	8.24154	-2.06746	0.88456
C	-3.93510	0.03489	0.00000
C	-4.54241	0.39326	-1.22007
C	-4.54242	0.39326	1.22007
C	-5.74198	1.10890	-1.19644
C	-5.74199	1.10890	1.19644
C	-6.35714	1.47988	0.00000
H	-6.20805	1.37947	-2.13952
H	-6.20806	1.37946	2.13951
C	-3.91576	0.01610	-2.54271
C	-3.91577	0.01609	2.54271
C	-7.63689	2.28132	0.00000
H	-8.24154	2.06745	0.88456
H	-7.42627	3.35659	0.00002
H	-8.24152	2.06749	-0.88458
H	-3.75050	-1.06251	2.61593
H	-2.94100	0.49498	2.67438
H	-4.55474	0.31843	3.37455
H	-3.75049	-1.06250	-2.61593
H	-4.55473	0.31844	-3.37455
H	-2.94099	0.49499	-2.67437
H	-3.98295	-5.28521	0.00000
H	3.98295	5.28521	0.00000

3a SD

C	1.38234	0.23752	0.00000
C	0.42323	1.34614	0.00000
C	-0.91835	1.11998	0.00000
C	-1.38234	-0.23752	0.00000
C	-0.42323	-1.34614	0.00000
C	0.91835	-1.11998	0.00000
H	-1.63757	1.93292	0.00000
H	1.63757	-1.93292	0.00000
C	-2.66857	-0.74018	0.00000
C	-2.58310	-2.20163	0.00000
C	-3.58509	-3.17057	0.00000
C	-3.21619	-4.51862	0.00000
C	-1.86913	-4.89064	0.00000
C	-0.85723	-3.92276	0.00000
C	-1.21253	-2.58084	0.00000
H	-4.63107	-2.88361	0.00000
H	-1.60399	-5.94191	0.00000
H	0.18446	-4.22576	0.00000
C	1.21253	2.58084	0.00000
C	2.66857	0.74018	0.00000
C	2.58310	2.20163	0.00000
C	0.85723	3.92276	0.00000
C	3.58509	3.17057	0.00000
C	1.86913	4.89064	0.00000
C	3.21619	4.51862	0.00000
H	-0.18446	4.22576	0.00000
H	1.60398	5.94191	0.00000
H	4.63107	2.88361	0.00000
C	-3.93510	0.03489	0.00000
C	-4.54241	0.39326	-1.22007
C	-4.54241	0.39326	1.22007
C	-5.74198	1.10890	-1.19644
C	-5.74198	1.10890	1.19644
C	-6.35714	1.47988	0.00000
H	-6.20805	1.37946	-2.13952
H	-6.20805	1.37946	2.13951
C	-3.91576	0.01609	2.54271
C	-3.91576	0.01609	-2.54271
C	-7.63689	2.28132	0.00000
H	-2.94100	0.49498	-2.67437
H	-3.75049	-1.06251	-2.61593
H	-4.55473	0.31843	-3.37455
H	-4.55474	0.31844	3.37455
H	-3.75049	-1.06250	2.61593
H	-2.94100	0.49499	2.67437
H	-7.42627	3.35659	-0.00002
H	-8.24154	2.06746	-0.88457
H	-8.24153	2.06748	0.88457
C	3.93510	-0.03489	0.00000
C	4.54242	-0.39325	-1.22007
C	4.54241	-0.39326	1.22007
C	5.74198	-1.10889	-1.19644
C	5.74198	-1.10890	1.19644
C	6.35714	-1.47988	0.00000
H	6.20805	-1.37946	-2.13952
H	6.20805	-1.37947	2.13951
C	3.91577	-0.01608	-2.54271
C	3.91576	-0.01610	2.54271
C	7.63689	-2.28132	0.00000
H	8.24153	-2.06748	0.88457
H	7.42627	-3.35659	-0.00002
H	8.24154	-2.06746	-0.88457
H	3.75048	1.06250	2.61593
H	2.94100	-0.49500	2.67438
H	4.55474	-0.31844	3.37455
H	3.75050	1.06251	-2.61593
H	4.55474	-0.31843	-3.37455
H	2.94100	-0.49498	-2.67438
H	3.98295	5.28521	0.00000
H	-3.98295	-5.28521	0.00000

3a T

C	-1.36978	0.24115	0.01701
C	-0.43989	1.32365	0.01226
C	0.93300	1.08852	0.01047
C	1.36978	-0.24115	0.01701
C	0.43989	-1.32365	0.01226
C	-0.93300	-1.08852	0.01047
H	1.64868	1.90384	-0.00092
H	-1.64868	-1.90384	-0.00092
C	2.72259	-0.78470	0.00474
C	2.60430	-2.21000	-0.00631
C	3.58695	-3.21334	-0.00592
C	3.18945	-4.54807	-0.00739
C	1.83062	-4.89006	-0.00539
C	0.83773	-3.89930	0.00044
C	1.21621	-2.56614	0.00057
H	4.63905	-2.94976	-0.00145
H	1.54233	-5.93519	-0.00584
H	-0.20941	-4.18292	0.00636
C	-1.21621	2.56613	0.00056
C	-2.72259	0.78470	0.00474
C	-2.60430	2.21000	-0.00631
C	-0.83773	3.89930	0.00044
C	-3.58694	3.21334	-0.00592
C	-1.83062	4.89006	-0.00539
C	-3.18945	4.54807	-0.00740
H	0.20941	4.18292	0.00636
H	-1.54232	5.93519	-0.00584
H	-4.63905	2.94976	-0.00146
C	3.97534	0.00283	0.00121
C	4.46046	0.56399	1.20109
C	4.68830	0.19405	-1.20061
C	5.64577	1.30207	1.17585
C	5.86741	0.94260	-1.17941
C	6.36341	1.50712	-0.00352
H	6.01980	1.72233	2.10504
H	6.41015	1.08923	-2.10883
C	4.18876	-0.38558	-2.50418
C	3.73175	0.35365	2.50835
C	7.62312	2.33949	-0.01190
H	2.72798	0.78768	2.48542
H	3.61129	-0.71075	2.72997
H	4.27792	0.81193	3.33501
H	4.80371	-0.04589	-3.33977
H	4.20974	-1.47923	-2.49366
H	3.15430	-0.09085	-2.70190
H	7.39401	3.39584	-0.19145
H	8.14832	2.27775	0.94423
H	8.30965	2.01645	-0.79808
C	-3.97534	-0.00283	0.00121
C	-4.46046	-0.56399	1.20109
C	-4.68829	-0.19405	-1.20062
C	-5.64577	-1.30207	1.17585
C	-5.86741	-0.94260	-1.17941
C	-6.36341	-1.50712	-0.00352
H	-6.01980	-1.72232	2.10504
H	-6.41015	-1.08924	-2.10883
C	-3.73176	-0.35364	2.50835
C	-4.18876	0.38557	-2.50418
C	-7.62312	-2.33948	-0.01190
H	-8.30965	-2.01644	-0.79808
H	-7.39401	-3.39584	-0.19145
H	-8.14832	-2.27775	0.94423
H	-4.20973	1.47922	-2.49367
H	-3.15430	0.09084	-2.70190
H	-4.80370	0.04588	-3.33977
H	-3.61131	0.71076	2.72997
H	-4.27792	-0.81193	3.33501
H	-2.72798	-0.78766	2.48542
H	-3.93763	5.33266	-0.00815
H	3.93763	-5.33266	-0.00815

4a S

C	-1.30477	0.49559	0.00001
C	-0.16455	1.39700	0.00001
C	1.11485	0.91504	0.00001
C	1.30477	-0.49559	-0.00001
C	0.16455	-1.39700	-0.00001
C	-1.11485	-0.91504	-0.00001
H	1.97498	1.57584	0.00001
H	-1.97498	-1.57584	-0.00001
C	2.48460	-1.25139	-0.00001
C	2.11161	-2.67059	-0.00002
C	2.89919	-3.81859	-0.00003
C	2.26771	-5.06434	-0.00004
C	0.87297	-5.15751	-0.00004
C	0.07736	-4.00683	-0.00003
C	0.69548	-2.76256	-0.00002
H	3.98076	-3.74643	-0.00003
H	0.40195	-6.13396	-0.00005
H	-1.00380	-4.09350	-0.00003
C	-0.69548	2.76256	0.00002
C	-2.48460	1.25139	0.00001
C	-2.11161	2.67059	0.00002
C	-0.07736	4.00683	0.00003
C	-2.89919	3.81859	0.00003
C	-0.87297	5.15751	0.00004
C	-2.26771	5.06434	0.00004
H	1.00380	4.09350	0.00003
H	-0.40195	6.13396	0.00005
H	-3.98076	3.74643	0.00003
H	-2.86465	5.96927	0.00005
H	2.86465	-5.96927	-0.00005
C	-3.79420	0.76649	0.00001
C	-4.94231	0.36091	0.00001
C	-6.27568	-0.11582	0.00001
C	-6.52526	-1.51343	-0.00001
C	-7.35437	0.80730	0.00001
C	-7.84210	-1.96622	-0.00001
C	-8.65997	0.32290	0.00001
C	-8.87619	-1.04499	0.00000
H	-8.07066	-3.02492	-0.00002
H	-9.50765	0.99710	0.00002
C	-7.09707	2.29102	0.00002
H	-6.51821	2.58866	0.87928
H	-6.51821	2.58868	-0.87923
H	-8.03356	2.85050	0.00003
C	-5.38604	-2.49849	-0.00001
H	-4.75002	-2.36208	-0.87959
H	-4.75002	-2.36209	0.87956
H	-5.75646	-3.52458	-0.00002
C	3.79420	-0.76649	-0.00001
C	4.94231	-0.36091	-0.00001
C	6.27568	0.11582	-0.00001
C	7.35437	-0.80730	-0.00001
C	6.52526	1.51343	0.00001
C	8.65997	-0.32290	-0.00001
C	7.84210	1.96622	0.00001
C	8.87619	1.04499	0.00000
H	9.50765	-0.99710	-0.00002
H	8.07066	3.02492	0.00002
C	5.38604	2.49849	0.00001
H	4.75002	2.36209	-0.87956
H	4.75002	2.36208	0.87959
H	5.75646	3.52458	0.00002
C	7.09707	-2.29102	-0.00002
H	6.51821	-2.58868	0.87923
H	6.51821	-2.58866	-0.87928
H	8.03356	-2.85050	-0.00003
F	10.15148	1.50071	0.00000
F	-10.15148	-1.50071	0.00000

4b S

C	1.28559	0.54258	0.00000
C	0.11365	1.40217	0.00000
C	-1.14739	0.87404	0.00000
C	-1.28559	-0.54258	0.00000
C	-0.11365	-1.40217	0.00000
C	1.14739	-0.87404	0.00000
H	-2.03105	1.50299	0.00000
H	2.03105	-1.50299	0.00000
C	-2.43724	-1.34082	0.00000
C	-2.01324	-2.74569	0.00000
C	-2.75881	-3.92131	0.00000
C	-2.08253	-5.14336	0.00000
C	-0.68541	-5.18589	0.00000
C	0.06807	-4.00712	0.00000
C	-0.59480	-2.78620	0.00000
H	-3.84229	-3.88846	0.00000
H	-0.17931	-6.14460	0.00000
H	1.15164	-4.05464	0.00000
C	0.59480	2.78620	0.00000
C	2.43724	1.34082	0.00000
C	2.01324	2.74569	0.00000
C	-0.06807	4.00712	0.00000
C	2.75881	3.92131	0.00000
C	0.68541	5.18589	0.00000
C	2.08253	5.14336	0.00000
H	-1.15164	4.05464	0.00000
H	0.17931	6.14460	0.00000
H	3.84229	3.88846	0.00000
H	2.64627	6.06931	0.00000
H	-2.64627	-6.06931	0.00000
C	3.76317	0.90319	0.00000
C	4.92534	0.53971	0.00000
C	6.27488	0.11213	0.00000
C	6.57693	-1.27423	0.00000
C	7.31954	1.07235	0.00000
C	7.90963	-1.67737	0.00000
C	8.64151	0.63513	0.00000
C	8.92350	-0.72615	0.00000
H	8.15921	-2.73096	0.00000
H	9.45176	1.35334	0.00000
C	7.01023	2.54633	0.00000
H	6.42163	2.82374	-0.87946
H	6.42163	2.82374	0.87946
H	7.92661	3.13820	0.00000
C	5.47597	-2.30218	0.00000
H	4.83536	-2.19057	0.87979
H	4.83536	-2.19057	-0.87979
H	5.88549	-3.31332	0.00000
C	-3.76317	-0.90319	0.00000
C	-4.92534	-0.53971	0.00000
C	-6.27488	-0.11213	0.00000
C	-7.31954	-1.07235	0.00000
C	-6.57693	1.27423	0.00000
C	-8.64151	-0.63513	0.00000
C	-7.90963	1.67737	0.00000
C	-8.92350	0.72615	0.00000
H	-9.45176	-1.35334	0.00000
H	-8.15921	2.73096	0.00000
C	-5.47597	2.30218	0.00000
H	-4.83536	2.19057	0.87979
H	-4.83536	2.19057	-0.87979
H	-5.88549	3.31332	0.00000
C	-7.01023	-2.54633	0.00000
H	-6.42163	-2.82374	-0.87946
H	-6.42163	-2.82374	0.87946
H	-7.92661	-3.13820	0.00000
Cl	-10.59852	1.25635	0.00000
Cl	10.59852	-1.25635	0.00000

4c S

C	1.20490	-0.70384	-0.00002
C	-0.06729	-1.40442	0.00040
C	-1.25052	-0.71773	0.00042
C	-1.20490	0.70384	0.00002
C	0.06729	1.40442	-0.00040
C	1.25052	0.71773	-0.00042
H	-2.20785	-1.22763	0.00073
H	2.20785	1.22763	-0.00073
C	-2.24567	1.64512	-0.00005
C	-1.64243	2.98283	-0.00052
C	-2.22894	4.24551	-0.00076
C	-1.39983	5.36938	-0.00122
C	-0.00880	5.23021	-0.00143
C	0.58519	3.96372	-0.00119
C	-0.23062	2.83893	-0.00074
H	-3.30758	4.35325	-0.00059
H	0.61750	6.11516	-0.00179
H	1.66575	3.86988	-0.00137
C	0.23062	-2.83893	0.00074
C	2.24567	-1.64512	0.00005
C	1.64243	-2.98283	0.00052
C	-0.58519	-3.96372	0.00120
C	2.22894	-4.24551	0.00076
C	0.00880	-5.23021	0.00143
C	1.39983	-5.36938	0.00122
H	-1.66575	-3.86988	0.00137
H	-0.61750	-6.11516	0.00179
H	3.30758	-4.35325	0.00059
H	1.83866	-6.36071	0.00141
H	-1.83866	6.36071	-0.00141
C	3.61495	-1.38268	-0.00024
C	4.81512	-1.16956	-0.00046
C	6.20463	-0.91630	-0.00072
C	6.68168	0.42253	-0.00102
C	7.12341	-2.00066	-0.00067
C	8.05011	0.65019	-0.00126
C	8.48418	-1.73051	-0.00093
C	8.97388	-0.41133	-0.00123
H	8.42224	1.66793	-0.00151
H	9.19154	-2.55143	-0.00091
C	6.62851	-3.42354	-0.00035
H	6.00969	-3.62515	0.87913
H	6.00942	-3.62544	-0.87957
H	7.46308	-4.12637	-0.00037
C	5.71665	1.57955	-0.00107
H	5.06661	1.54991	-0.88065
H	5.06684	1.55019	0.87869
H	6.25003	2.53140	-0.00129
C	-3.61495	1.38268	0.00024
C	-4.81512	1.16957	0.00046
C	-6.20463	0.91630	0.00072
C	-7.12341	2.00066	0.00067
C	-6.68168	-0.42253	0.00102
C	-8.48418	1.73051	0.00093
C	-8.05011	-0.65019	0.00126
C	-8.97388	0.41133	0.00123
H	-9.19154	2.55143	0.00092
H	-8.42224	-1.66793	0.00151
C	-5.71665	-1.57955	0.00107
H	-5.06684	-1.55019	-0.87869
H	-5.06661	-1.54991	0.88065
H	-6.25003	-2.53140	0.00129
C	-6.62851	3.42354	0.00035
H	-6.00942	3.62544	0.87958
H	-6.00969	3.62515	-0.87913
H	-7.46308	4.12637	0.00037
C	-10.36953	0.15661	0.00153
C	10.36953	-0.15661	-0.00153
C	11.56306	0.06176	-0.00212
C	-11.56306	-0.06176	0.00212
C	12.96077	0.31823	-0.00173
C	13.43491	1.65259	-0.00399
C	13.87808	-0.76060	-0.00416
C	14.80958	1.87705	-0.00651
C	15.24278	-0.48189	-0.00669
C	15.73182	0.82718	-0.00477
H	15.17186	2.90069	-0.01176
H	15.94518	-1.30998	-0.01210
C	-12.96077	-0.31823	0.00173
C	-13.87808	0.76060	0.00416
C	-13.43491	-1.65259	0.00399
C	-15.24278	0.48189	0.00669
C	-14.80958	-1.87705	0.00651
C	-15.73182	-0.82718	0.00477
H	-15.94518	1.30998	0.01210
H	-15.17186	-2.90069	0.01176
C	13.38804	-2.18579	-0.00817
H	12.76839	-2.39327	0.86939
H	12.76927	-2.38894	-0.88739
H	14.22517	-2.88601	-0.00940
C	12.47043	2.81065	-0.00782
H	11.81984	2.78077	-0.88703
H	11.81751	2.78426	0.86975
H	13.00411	3.76264	-0.00893
C	17.21542	1.09958	0.02752
H	17.57832	1.16435	1.05954
H	17.77818	0.30413	-0.46661
H	17.45854	2.04475	-0.46351
C	-17.21542	-1.09958	-0.02752
H	-17.57832	-1.16435	-1.05954
H	-17.45854	-2.04475	0.46351
H	-17.77818	-0.30413	0.46660
C	-12.47043	-2.81065	0.00782
H	-11.81751	-2.78426	-0.86975
H	-11.81984	-2.78078	0.88703
H	-13.00411	-3.76264	0.00893
C	-13.38804	2.18579	0.00817
H	-12.76927	2.38894	0.88739
H	-12.76839	2.39327	-0.86939
H	-14.22517	2.88601	0.00940

4d S

C	1.30276	0.50144	0.00050
C	0.15846	1.39736	-0.00079
C	-1.11911	0.90976	-0.00129
C	-1.30276	-0.50144	-0.00050
C	-0.15846	-1.39736	0.00079
C	1.11911	-0.90976	0.00129
H	-1.98240	1.56649	-0.00229
H	1.98240	-1.56649	0.00228
C	-2.47991	-1.26234	-0.00079
C	-2.09983	-2.67962	0.00035
C	-2.88216	-3.83134	0.00057
C	-2.24501	-5.07416	0.00180
C	-0.84969	-5.16106	0.00278
C	-0.05936	-4.00682	0.00255
C	-0.68315	-2.76519	0.00132
H	-3.96406	-3.76353	-0.00021
H	-0.37420	-6.13541	0.00374
H	1.02224	-4.08830	0.00333
C	0.68315	2.76519	-0.00132
C	2.47991	1.26234	0.00079
C	2.09983	2.67962	-0.00035
C	0.05936	4.00682	-0.00255
C	2.88216	3.83135	-0.00057
C	0.84968	5.16106	-0.00278
C	2.24501	5.07416	-0.00180
H	-1.02224	4.08830	-0.00333
H	0.37420	6.13541	-0.00375
H	3.96406	3.76353	0.00021
H	2.83789	5.98184	-0.00199
H	-2.83789	-5.98184	0.00199
C	3.79140	0.78379	0.00181
C	4.94162	0.38302	0.00277
C	6.27656	-0.08850	0.00274
C	6.53675	-1.48291	0.00505
C	7.35446	0.83354	0.00531
C	7.85839	-1.91936	0.00767
C	8.65719	0.34336	0.00797
C	8.93434	-1.02681	0.00598
H	8.05606	-2.98701	0.01290
H	9.48131	1.05030	0.01343
C	10.35619	-1.52882	-0.02661
H	10.70243	-1.65241	-1.05905
H	11.03768	-0.83022	0.46430
H	10.44844	-2.49932	0.46646
C	7.09549	2.31760	0.00922
H	6.51763	2.61981	-0.86945
H	6.51658	2.61534	0.88874
H	8.03256	2.87689	0.01110
C	5.40354	-2.47579	0.00874
H	4.76643	-2.34449	0.88863
H	4.76434	-2.34816	-0.87015
H	5.78227	-3.49925	0.01034
C	-3.79140	-0.78379	-0.00181
C	-4.94162	-0.38302	-0.00277
C	-6.27656	0.08850	-0.00274
C	-7.35446	-0.83354	-0.00531
C	-6.53675	1.48291	-0.00505
C	-8.65719	-0.34336	-0.00797
C	-7.85839	1.91936	-0.00767
C	-8.93434	1.02681	-0.00598
H	-9.48131	-1.05030	-0.01342
H	-8.05606	2.98701	-0.01290
C	-5.40354	2.47579	-0.00875
H	-4.76435	2.34817	0.87015
H	-4.76642	2.34449	-0.88863
H	-5.78227	3.49925	-0.01035
C	-7.09549	-2.31760	-0.00921
H	-6.51659	-2.61534	-0.88874
H	-6.51762	-2.61980	0.86945
H	-8.03256	-2.87689	-0.01109
C	-10.35619	1.52882	0.02662
H	-11.03768	0.83022	-0.46430
H	-10.70244	1.65240	1.05906
H	-10.44844	2.49933	-0.46644

4d SD

C	1.30276	-0.50144	-0.00050
C	0.15846	-1.39736	0.00079
C	-1.11911	-0.90976	0.00129
C	-1.30276	0.50144	0.00050
C	-0.15846	1.39736	-0.00080
C	1.11911	0.90976	-0.00130
H	-1.98241	-1.56649	0.00229
H	1.98240	1.56649	-0.00230
C	-2.47991	1.26234	0.00078
C	-2.09983	2.67962	-0.00036
C	-2.88216	3.83135	-0.00059
C	-2.24501	5.07416	-0.00183
C	-0.84968	5.16106	-0.00281
C	-0.05936	4.00682	-0.00257
C	-0.68315	2.76519	-0.00133
H	-3.96405	3.76353	0.00019
H	-0.37419	6.13542	-0.00378
H	1.02224	4.08830	-0.00335
C	0.68315	-2.76519	0.00133
C	2.47991	-1.26234	-0.00079
C	2.09983	-2.67962	0.00036
C	0.05936	-4.00682	0.00256
C	2.88216	-3.83135	0.00059
C	0.84968	-5.16106	0.00280
C	2.24501	-5.07416	0.00182
H	-1.02224	-4.08830	0.00334
H	0.37419	-6.13541	0.00377
H	3.96405	-3.76353	-0.00020
H	2.83789	-5.98184	0.00202
H	-2.83789	5.98184	-0.00202
C	3.79140	-0.78379	-0.00181
C	4.94162	-0.38303	-0.00277
C	6.27656	0.08850	-0.00274
C	6.53675	1.48291	-0.00506
C	7.35446	-0.83354	-0.00529
C	7.85839	1.91936	-0.00768
C	8.65719	-0.34336	-0.00795
C	8.93434	1.02681	-0.00597
H	8.05606	2.98700	-0.01292
H	9.48131	-1.05030	-0.01340
C	10.35619	1.52882	0.02662
H	10.70242	1.65244	1.05906
H	11.03769	0.83021	-0.46426
H	10.44844	2.49931	-0.46648
C	7.09549	-2.31760	-0.00918
H	6.51762	-2.61980	0.86949
H	6.51659	-2.61535	-0.88870
H	8.03256	-2.87689	-0.01105
C	5.40354	2.47578	-0.00878
H	4.76643	2.34448	-0.88866
H	4.76434	2.34817	0.87012
H	5.78227	3.49925	-0.01038
C	-3.79140	0.78380	0.00181
C	-4.94163	0.38303	0.00277
C	-6.27656	-0.08850	0.00274
C	-7.35446	0.83354	0.00530
C	-6.53675	-1.48291	0.00507
	-8.65719	0.34336	0.00796

C			
C	-7.85839	-1.91936	0.00768
C	-8.93434	-1.02681	0.00598
H	-9.48131	1.05030	0.01341
H	-8.05606	-2.98701	0.01293
C	-5.40354	-2.47578	0.00877
H	-4.76434	-2.34817	-0.87012
H	-4.76642	-2.34448	0.88866
H	-5.78227	-3.49925	0.01038
C	-7.09550	2.31760	0.00919
H	-6.51659	2.61535	0.88870
H	-6.51763	2.61980	-0.86948
H	-8.03256	2.87689	0.01106
C	-10.35619	-1.52883	-0.02661
H	-11.03768	-0.83022	0.46430
H	-10.70243	-1.65243	-1.05905
H	-10.44844	-2.49932	0.46648

4d T

C	-1.29069	0.50800	-0.00052
C	-0.16771	1.38398	0.00084
C	1.12982	0.87938	0.00138
C	1.29069	-0.50800	0.00052
C	0.16771	-1.38398	-0.00085
C	-1.12982	-0.87938	-0.00138
H	1.99367	1.53478	0.00245
H	-1.99367	-1.53478	-0.00245
C	2.50970	-1.31660	0.00080
C	2.09565	-2.70708	-0.00042
C	2.84791	-3.88453	-0.00071
C	2.18158	-5.10897	-0.00205
C	0.78259	-5.16050	-0.00308
C	0.02108	-3.98650	-0.00279
C	0.67283	-2.75965	-0.00144
H	3.93131	-3.84420	0.00010
H	0.28283	-6.12266	-0.00413
H	-1.06214	-4.04224	-0.00361
C	-0.67283	2.75965	0.00144
C	-2.50971	1.31661	-0.00081
C	-2.09565	2.70708	0.00041
C	-0.02108	3.98651	0.00278
C	-2.84791	3.88453	0.00071
C	-0.78259	5.16050	0.00307
C	-2.18158	5.10897	0.00204
H	1.06214	4.04224	0.00360
H	-0.28284	6.12266	0.00412
H	-3.93131	3.84420	-0.00011
H	-2.75110	6.03144	0.00229
H	2.75110	-6.03144	-0.00230
C	-3.80193	0.84215	-0.00183
C	-4.95162	0.41682	-0.00282
C	-6.27411	-0.06885	-0.00286
C	-6.51917	-1.46944	-0.00515
C	-7.36703	0.84075	-0.00547
C	-7.83451	-1.92067	-0.00770
C	-8.66190	0.33368	-0.00807
C	-8.92211	-1.04084	-0.00606
H	-8.01973	-2.99055	-0.01281
H	-9.49531	1.02966	-0.01348
C	-10.33726	-1.56028	0.02703
H	-10.68183	-1.68766	1.05969
H	-11.02757	-0.87039	-0.46391
H	-10.41762	-2.53220	-0.46535
C	-7.12621	2.32750	-0.00949
H	-6.55167	2.63689	0.86888
H	-6.55094	2.63234	-0.88900
H	-8.07007	2.87521	-0.01122
C	-5.37356	-2.44718	-0.00885
H	-4.73796	-2.30739	-0.88862
H	-4.73580	-2.31102	0.86990
H	-5.73891	-3.47549	-0.01044
C	3.80193	-0.84215	0.00183
C	4.95162	-0.41682	0.00283
C	6.27411	0.06885	0.00286
C	7.36703	-0.84076	0.00546
C	6.51917	1.46943	0.00516
	8.66190	-0.33368	0.00807
C			
C	7.83451	1.92067	0.00772
C	8.92211	1.04083	0.00606
H	9.49531	-1.02967	0.01347
H	8.01974	2.99055	0.01283
C	5.37357	2.44718	0.00887
H	4.73580	2.31102	-0.86989
H	4.73796	2.30739	0.88863
H	5.73892	3.47549	0.01046
C	7.12620	-2.32750	0.00948
H	6.55093	-2.63234	0.88899
H	6.55166	-2.63689	-0.86890
H	8.07006	-2.87521	0.01121
C	10.33726	1.56028	-0.02702
H	11.02757	0.87038	0.46391
H	10.68183	1.68767	-1.05968
H	10.41763	2.53218	0.46538

4e S

C	-1.26208	-0.59652	0.00000
C	-0.05452	-1.40522	-0.00001
C	1.18345	-0.82442	-0.00001
C	1.26208	0.59652	0.00000
C	0.05452	1.40522	0.00002
C	-1.18345	0.82442	0.00002
H	2.09300	-1.41546	-0.00002
H	-2.09300	1.41546	0.00003
C	2.37959	1.44253	0.00001
C	1.89555	2.82779	0.00002
C	2.59040	4.03431	0.00003
C	1.86288	5.22649	0.00005
C	0.46495	5.20976	0.00006
C	-0.23767	4.00012	0.00005
C	0.47644	2.80816	0.00003
H	3.67435	4.04684	0.00003
H	-0.08143	6.14620	0.00007
H	-1.32233	4.00117	0.00005
C	-0.47644	-2.80816	-0.00003
C	-2.37959	-1.44253	0.00000
C	-1.89555	-2.82778	-0.00002
C	0.23768	-4.00012	-0.00005
C	-2.59040	-4.03431	-0.00003
C	-0.46495	-5.20975	-0.00006
C	-1.86288	-5.22649	-0.00005
H	1.32234	-4.00117	-0.00005
H	0.08143	-6.14620	-0.00007
H	-3.67435	-4.04683	-0.00003
H	-2.38686	-6.17561	-0.00006
H	2.38686	6.17561	0.00006
C	-3.72303	-1.06272	0.00001
C	-4.90001	-0.74914	0.00002
C	-6.26671	-0.37980	0.00002
C	-6.63496	0.99057	0.00005
C	-7.27264	-1.37476	0.00001
C	-7.98394	1.32340	0.00005
C	-8.61177	-0.98474	0.00002
C	-9.00166	0.35780	0.00004
H	-8.24433	2.37601	0.00007
H	-9.36099	-1.76566	0.00001
C	-6.90674	-2.83656	-0.00001
H	-6.30810	-3.09418	-0.87906
H	-6.30810	-3.09421	0.87903
H	-7.80048	-3.46283	-0.00002
C	-5.58095	2.06760	0.00006
H	-4.93467	1.98757	0.87944
H	-4.93467	1.98760	-0.87932
H	-6.03658	3.05931	0.00008
C	3.72303	1.06272	-0.00001
C	4.90001	0.74914	-0.00001
C	6.26671	0.37980	-0.00002
C	7.27264	1.37476	-0.00002
C	6.63496	-0.99057	-0.00004
C	8.61177	0.98474	-0.00003
C	7.98393	-1.32340	-0.00005
C	9.00166	-0.35780	-0.00004
H	9.36099	1.76566	-0.00003
H	8.24433	-2.37601	-0.00006
C	5.58095	-2.06760	-0.00004
H	4.93467	-1.98759	0.87934
H	4.93467	-1.98758	-0.87942
H	6.03658	-3.05931	-0.00006
C	6.90674	2.83656	0.00000
H	6.30809	3.09420	-0.87904
H	6.30811	3.09419	0.87905
H	7.80048	3.46283	-0.00001
C	10.47532	-0.79833	-0.00005
C	-10.47532	0.79833	0.00005
C	10.75760	-1.64736	-1.26224
H	11.80356	-1.96917	-1.27508
H	10.13295	-2.54260	-1.29872
H	10.56825	-1.06993	-2.17128
C	11.44665	0.39636	-0.00005
H	11.32127	1.02409	-0.88647
H	11.32127	1.02407	0.88639
H	12.47658	0.02944	-0.00005
C	10.75762	-1.64739	1.26212
H	10.56827	-1.06997	2.17117
H	10.13296	-2.54263	1.29858
H	11.80357	-1.96919	1.27494
C	-10.75761	1.64740	-1.26212
H	-11.80357	1.96920	-1.27493
H	-10.13296	2.54264	-1.29857
H	-10.56827	1.06999	-2.17117
C	-11.44666	-0.39636	0.00003
H	-11.32127	-1.02406	-0.88642
H	-11.32127	-1.02410	0.88644
H	-12.47659	-0.02945	0.00003
C	-10.75761	1.64735	1.26225
H	-11.80357	1.96915	1.27508
H	-10.56826	1.06990	2.17128
H	-10.13296	2.54259	1.29873

4e SD

C	-1.26208	0.59652	0.00000
C	-0.05452	1.40522	0.00000
C	1.18345	0.82442	0.00000
C	1.26208	-0.59652	0.00000
C	0.05452	-1.40522	0.00000
C	-1.18345	-0.82442	0.00000
H	2.09300	1.41546	0.00000
H	-2.09300	-1.41546	0.00000
C	2.37959	-1.44253	0.00000
C	1.89555	-2.82778	-0.00001
C	2.59041	-4.03431	-0.00001
C	1.86288	-5.22649	-0.00001
C	0.46495	-5.20976	-0.00001
C	-0.23767	-4.00012	-0.00001
C	0.47644	-2.80816	-0.00001
H	3.67435	-4.04683	-0.00001
H	-0.08143	-6.14620	-0.00001
H	-1.32233	-4.00117	-0.00001
C	-0.47644	2.80816	0.00001
C	-2.37959	1.44253	0.00000
C	-1.89555	2.82778	0.00000
C	0.23767	4.00012	0.00001
C	-2.59041	4.03431	0.00001
C	-0.46495	5.20976	0.00001
C	-1.86288	5.22649	0.00001
H	1.32233	4.00117	0.00001
H	0.08143	6.14620	0.00001
H	-3.67435	4.04683	0.00001
H	-2.38686	6.17561	0.00001
H	2.38686	-6.17561	-0.00001
C	-3.72303	1.06272	0.00000
C	-4.90001	0.74914	0.00000
C	-6.26671	0.37980	0.00000
C	-6.63496	-0.99057	-0.00001
C	-7.27264	1.37476	0.00000
C	-7.98393	-1.32340	-0.00001
C	-8.61177	0.98474	0.00000
C	-9.00166	-0.35780	-0.00001
H	-8.24432	-2.37601	-0.00001
H	-9.36099	1.76566	0.00000
C	-6.90674	2.83656	0.00000
H	-6.30810	3.09420	0.87905
H	-6.30810	3.09420	-0.87904
H	-7.80048	3.46283	0.00000
C	-5.58095	-2.06760	-0.00001
H	-4.93467	-1.98758	-0.87938
H	-4.93467	-1.98759	0.87937
H	-6.03657	-3.05931	-0.00001
C	3.72303	-1.06272	0.00000
C	4.90001	-0.74914	0.00000
C	6.26671	-0.37980	0.00000
C	7.27264	-1.37476	0.00000
C	6.63496	0.99057	0.00001
C	8.61177	-0.98474	0.00000
C	7.98393	1.32340	0.00001
C	9.00166	0.35780	0.00001
H	9.36099	-1.76566	0.00000
H	8.24432	2.37601	0.00001
C	5.58095	2.06760	0.00001
H	4.93467	1.98759	-0.87937
H	4.93467	1.98758	0.87938
H	6.03657	3.05931	0.00001
C	6.90674	-2.83656	0.00000
H	6.30810	-3.09420	0.87904
H	6.30810	-3.09420	-0.87905
H	7.80048	-3.46283	0.00000
C	10.47532	0.79833	0.00001
C	-10.47532	-0.79833	-0.00001
C	10.75761	1.64737	1.26219
H	11.80356	1.96918	1.27502
H	10.13295	2.54261	1.29867
H	10.56827	1.06994	2.17124
C	11.44665	-0.39636	0.00001
H	11.32127	-1.02408	0.88644
H	11.32127	-1.02408	-0.88643
H	12.47658	-0.02945	0.00001
C	10.75761	1.64738	-1.26217
H	10.56827	1.06995	-2.17122
H	10.13295	2.54261	-1.29864
H	11.80357	1.96919	-1.27499
C	-10.75761	-1.64738	1.26217
H	-11.80356	-1.96919	1.27499
H	-10.13295	-2.54262	1.29864
H	-10.56827	-1.06995	2.17122
C	-11.44665	0.39636	-0.00001
H	-11.32127	1.02408	0.88643
H	-11.32127	1.02408	-0.88644
H	-12.47658	0.02945	-0.00001
C	-10.75761	-1.64737	-1.26219
H	-11.80356	-1.96918	-1.27502
H	-10.56827	-1.06994	-2.17124
H	-10.13295	-2.54261	-1.29867

4e T

C	-1.24855	0.60430	0.00000
C	-0.06239	1.39265	0.00000
C	1.19322	0.79129	0.00000
C	1.24856	-0.60430	0.00000
C	0.06239	-1.39265	0.00000
C	-1.19322	-0.79129	0.00000
H	2.10420	1.37946	0.00001
H	-2.10420	-1.37946	-0.00001
C	2.40277	-1.50300	0.00000
C	1.88449	-2.85809	-0.00001
C	2.54529	-4.08920	-0.00001
C	1.78800	-5.25958	-0.00001
C	0.38912	-5.20487	-0.00001
C	-0.28117	-3.97651	-0.00001
C	0.46179	-2.80264	-0.00001
H	3.62864	-4.13109	-0.00001
H	-0.18216	-6.12637	-0.00002
H	-1.36549	-3.94986	-0.00001
C	-0.46179	2.80264	0.00001
C	-2.40277	1.50300	0.00000
C	-1.88449	2.85810	0.00001
C	0.28117	3.97651	0.00001
C	-2.54529	4.08920	0.00001
C	-0.38912	5.20487	0.00001
C	-1.78800	5.25958	0.00001
H	1.36549	3.94986	0.00001
H	0.18216	6.12637	0.00002
H	-3.62864	4.13109	0.00001
H	-2.28591	6.22259	0.00002
H	2.28591	-6.22259	-0.00001
C	-3.72738	1.12821	0.00000
C	-4.90631	0.79239	0.00000
C	-6.26240	0.41041	0.00000
C	-6.61845	-0.96656	-0.00001
C	-7.28248	1.39585	0.00000
C	-7.96285	-1.31225	-0.00001
C	-8.61585	0.99071	0.00000
C	-8.99157	-0.35679	-0.00001
H	-8.21278	-2.36739	-0.00001
H	-9.37396	1.76302	0.00000
C	-6.93201	2.86105	0.00000
H	-6.33590	3.12511	0.87890
H	-6.33590	3.12511	-0.87889
H	-7.83235	3.47778	0.00001
C	-5.55278	-2.03137	-0.00001
H	-4.90718	-1.94387	-0.87926
H	-4.90718	-1.94388	0.87924
H	-5.99720	-3.02814	-0.00001
C	3.72738	-1.12821	0.00000
C	4.90631	-0.79239	0.00000
C	6.26240	-0.41041	0.00000
C	7.28248	-1.39585	0.00000
C	6.61845	0.96656	0.00001
C	8.61585	-0.99071	0.00000
C	7.96285	1.31225	0.00001
C	8.99158	0.35679	0.00001
H	9.37396	-1.76302	0.00000
H	8.21278	2.36739	0.00001
C	5.55278	2.03137	0.00001
H	4.90718	1.94388	-0.87924
H	4.90718	1.94387	0.87926
H	5.99720	3.02814	0.00001
C	6.93200	-2.86105	0.00000
H	6.33590	-3.12511	0.87889
H	6.33590	-3.12511	-0.87890
H	7.83234	-3.47778	0.00000
C	10.46000	0.81324	0.00001
C	-10.46000	-0.81325	-0.00001
C	10.73288	1.66550	1.26223
H	11.77516	1.99900	1.27476
H	10.09827	2.55370	1.29883
H	10.55029	1.08599	2.17132
C	11.44446	-0.37065	0.00000
H	11.32604	-0.99969	0.88645
H	11.32604	-0.99969	-0.88644
H	12.47025	0.00765	0.00001
C	10.73288	1.66551	-1.26221
H	10.55029	1.08600	-2.17131
H	10.09827	2.55371	-1.29881
H	11.77516	1.99901	-1.27474
C	-10.73288	-1.66551	1.26221
H	-11.77516	-1.99901	1.27474
H	-10.09827	-2.55371	1.29881
H	-10.55029	-1.08600	2.17131
C	-11.44446	0.37064	0.00000
H	-11.32604	0.99969	0.88644
H	-11.32604	0.99969	-0.88645
H	-12.47025	-0.00766	0.00000
C	-10.73288	-1.66550	-1.26223
H	-11.77516	-1.99900	-1.27476
H	-10.55029	-1.08599	-2.17132
H	-10.09827	-2.55370	-1.29884

4f S

C	-1.29808	-0.51482	0.00000
C	-0.14461	-1.39834	0.00000
C	1.12835	-0.89758	0.00000
C	1.29808	0.51482	0.00000
C	0.14461	1.39834	0.00000
C	-1.12835	0.89758	0.00000
H	1.99790	-1.54606	0.00000
H	-1.99790	1.54606	0.00000
C	2.46807	1.28830	0.00000
C	2.07223	2.70111	0.00000
C	2.84156	3.86180	0.00000
C	2.19104	5.09752	0.00000
C	0.79466	5.16922	0.00000
C	0.01732	4.00642	0.00000
C	0.65451	2.77137	0.00000
H	3.92418	3.80595	0.00000
H	0.30850	6.13833	0.00000
H	-1.06514	4.07594	0.00000
C	-0.65450	-2.77137	0.00000
C	-2.46807	-1.28830	0.00000
C	-2.07223	-2.70111	0.00000
C	-0.01731	-4.00642	0.00000
C	-2.84156	-3.86181	0.00000
C	-0.79466	-5.16922	0.00000
C	-2.19104	-5.09752	0.00000
H	1.06514	-4.07594	0.00000
H	-0.30850	-6.13833	0.00000
H	-3.92418	-3.80596	0.00000
H	-2.77394	-6.01170	0.00000
H	2.77394	6.01170	0.00000
C	-3.78419	-0.82502	0.00000
C	-4.93912	-0.43616	0.00000
C	-6.27695	0.02129	0.00000
C	-6.55416	1.41741	0.00000
C	-7.34538	-0.90724	0.00000
C	-7.87118	1.84560	0.00000
C	-8.66073	-0.44350	0.00000
C	-8.92823	0.92750	0.00000
H	-8.10956	2.90268	0.00000
H	-9.46668	-1.16515	0.00000
C	-7.07181	-2.38896	0.00000
H	-6.48937	-2.68104	-0.87886
H	-6.48937	-2.68104	0.87886
H	-8.00165	-2.96024	0.00000
C	-5.42970	2.41982	0.00000
H	-4.79116	2.29306	0.87930
H	-4.79116	2.29306	-0.87930
H	-5.81612	3.44012	0.00000
C	3.78419	0.82502	0.00000
C	4.93912	0.43616	0.00000
C	6.27694	-0.02130	0.00000
C	7.34538	0.90724	0.00000
C	6.55416	-1.41741	0.00000
C	8.66072	0.44350	0.00000
C	7.87118	-1.84560	0.00000
C	8.92823	-0.92750	0.00000
H	9.46668	1.16515	0.00000
H	8.10956	-2.90268	0.00000
C	5.42970	-2.41983	0.00000
H	4.79116	-2.29306	0.87930
H	4.79116	-2.29306	-0.87930
H	5.81612	-3.44013	0.00000
C	7.07181	2.38896	0.00000
H	6.48937	2.68104	-0.87886
H	6.48937	2.68104	0.87886
H	8.00165	2.96024	0.00000
O	10.17717	-1.46772	0.00000
O	-10.17717	1.46773	0.00000
C	11.30324	-0.59821	0.00000
H	11.31946	0.03295	0.89465
H	12.17744	-1.24688	0.00000
H	11.31946	0.03295	-0.89465
C	-11.30325	0.59822	0.00000
H	-12.17744	1.24688	0.00000
H	-11.31946	-0.03295	-0.89465
H	-11.31946	-0.03295	0.89465

4g S

C	1.28761	-0.53951	0.00000
C	0.11782	-1.40095	0.00000
C	-1.14533	-0.87583	0.00000
C	-1.28761	0.53951	0.00000
C	-0.11782	1.40095	0.00000
C	1.14533	0.87582	0.00000
H	-2.02719	-1.50744	0.00000
H	2.02719	1.50744	0.00000
C	-2.44267	1.33552	0.00000
C	-2.02011	2.74063	0.00000
C	-2.76718	3.91567	0.00000
C	-2.09304	5.13870	0.00000
C	-0.69563	5.18358	0.00000
C	0.05939	4.00611	0.00000
C	-0.60142	2.78362	0.00000
H	-3.85065	3.88069	0.00000
H	-0.19100	6.14317	0.00000
H	1.14295	4.05498	0.00000
C	0.60142	-2.78362	0.00000
C	2.44267	-1.33553	0.00000
C	2.02011	-2.74064	0.00000
C	-0.05939	-4.00611	0.00000
C	2.76718	-3.91567	0.00000
C	0.69563	-5.18359	0.00000
C	2.09304	-5.13870	0.00000
H	-1.14295	-4.05498	0.00000
H	0.19100	-6.14317	0.00000
H	3.85065	-3.88069	0.00000
H	2.65830	-6.06385	0.00000
H	-2.65830	6.06385	0.00000
C	3.76688	-0.89705	0.00000
C	4.92938	-0.53121	0.00000
C	6.27577	-0.10112	0.00000
C	6.58125	1.28741	0.00000
C	7.32593	-1.05220	0.00000
C	7.90915	1.68732	0.00000
C	8.64758	-0.61189	0.00000
C	8.95426	0.75177	0.00000
H	8.14166	2.74706	0.00000
H	9.43537	-1.35372	0.00000
C	7.02253	-2.52793	0.00000
H	6.43468	-2.80848	0.87905
H	6.43468	-2.80848	-0.87905
H	7.94103	-3.11727	0.00000
C	5.47850	2.31365	0.00000
H	4.83752	2.20101	-0.87947
H	4.83752	2.20101	0.87948
H	5.88629	3.32569	0.00000
C	-3.76688	0.89705	0.00000
C	-4.92938	0.53121	0.00000
C	-6.27577	0.10112	0.00000
C	-7.32593	1.05220	0.00000
C	-6.58125	-1.28741	0.00000
C	-8.64758	0.61189	0.00000
C	-7.90915	-1.68732	0.00000
C	-8.95426	-0.75177	0.00000
H	-9.43537	1.35372	0.00000
H	-8.14167	-2.74706	-0.00001
C	-5.47850	-2.31365	0.00000
H	-4.83753	-2.20101	-0.87948
H	-4.83753	-2.20101	0.87947
H	-5.88629	-3.32569	-0.00001
C	-7.02253	2.52793	0.00000
H	-6.43468	2.80848	0.87906
H	-6.43468	2.80848	-0.87905
H	-7.94103	3.11727	0.00000
S	-10.60266	-1.41194	0.00000
S	10.60266	1.41194	0.00000
C	-11.66728	0.06472	0.00000
H	-12.68816	-0.31815	0.00000
H	-11.51624	0.66712	0.89640
H	-11.51624	0.66712	-0.89640
C	11.66728	-0.06471	0.00000
H	12.68816	0.31815	-0.00001
H	11.51625	-0.66712	0.89640
H	11.51624	-0.66712	-0.89641

4h S

C	-1.23115	-0.64280	-0.14479
C	0.01454	-1.37298	-0.29983
C	1.22293	-0.74624	-0.15861
C	1.23115	0.64279	0.14481
C	-0.01454	1.37297	0.29985
C	-1.22293	0.74623	0.15863
H	2.16037	-1.28017	-0.27184
H	-2.16037	1.28016	0.27185
C	2.30675	1.52363	0.34092
C	1.75214	2.85101	0.62885
C	2.38382	4.06306	0.89587
C	1.59646	5.19034	1.13930
C	0.20093	5.10520	1.11569
C	-0.43845	3.89042	0.84806
C	0.33561	2.76206	0.60438
H	3.46575	4.12895	0.91407
H	-0.39270	5.99201	1.30732
H	-1.52177	3.83783	0.83271
C	-0.33561	-2.76207	-0.60437
C	-2.30675	-1.52364	-0.34091
C	-1.75214	-2.85102	-0.62883
C	0.43845	-3.89043	-0.84805
C	-2.38382	-4.06307	-0.89586
C	-0.20093	-5.10521	-1.11568
C	-1.59646	-5.19035	-1.13929
H	1.52177	-3.83784	-0.83269
H	0.39270	-5.99202	-1.30731
H	-3.46575	-4.12896	-0.91406
H	-2.07122	-6.14226	-1.34898
H	2.07122	6.14225	1.34899
C	-3.66564	-1.21954	-0.27911
C	-4.85801	-0.96925	-0.22853
C	-6.23718	-0.67365	-0.16859
C	-6.67381	0.64582	0.12508
C	-7.19797	-1.69369	-0.40160
C	-8.03384	0.91651	0.18291
C	-8.54947	-1.38324	-0.34202
C	-8.99082	-0.08351	-0.04944
H	-8.36392	1.92072	0.41885
H	-9.27965	-2.16023	-0.53218
C	-6.75781	-3.09706	-0.72875
H	-6.13638	-3.11528	-1.62900
H	-6.15512	-3.51814	0.08171
H	-7.61748	-3.74914	-0.89102
C	-5.67296	1.74076	0.38963
H	-5.02567	1.48696	1.23434
H	-5.02141	1.89387	-0.47608
H	-6.17460	2.68389	0.61199
C	3.66564	1.21952	0.27912
C	4.85801	0.96924	0.22855
C	6.23718	0.67365	0.16860
C	7.19796	1.69369	0.40161
C	6.67381	-0.64583	-0.12508
C	8.54946	1.38324	0.34203
C	8.03384	-0.91651	-0.18292
C	8.99082	0.08351	0.04944
H	9.27965	2.16023	0.53219
H	8.36393	-1.92072	-0.41886
C	5.67296	-1.74077	-0.38962
H	5.02144	-1.89389	0.47610
H	5.02566	-1.48696	-1.23432
H	6.17461	-2.68389	-0.61201
C	6.75781	3.09705	0.72876
H	6.15512	3.51814	-0.08170
H	6.13636	3.11527	1.62901
H	7.61748	3.74913	0.89105
N	-10.36963	0.21257	0.00956
N	10.36964	-0.21257	-0.00957
C	11.29358	0.74682	-0.51449
C	12.50024	0.98804	0.15501
C	11.01392	1.45346	-1.69169
C	13.40848	1.91512	-0.34818
H	12.72186	0.44575	1.06626
C	11.92068	2.38946	-2.17995
H	10.08607	1.26567	-2.21837
C	13.12375	2.62418	-1.51454
H	14.33777	2.09158	0.18200
H	11.69072	2.92723	-3.09305
H	13.83050	3.34924	-1.90084
C	10.85648	-1.47454	0.43735
C	10.40963	-2.02187	1.64731
C	11.79785	-2.17979	-0.32345
C	10.88901	-3.25515	2.07855
H	9.68766	-1.47761	2.24406
C	12.28357	-3.40572	0.12238
H	12.14645	-1.76241	-1.26041
C	11.83013	-3.95307	1.32199
H	10.53476	-3.66498	3.01790
H	13.01116	-3.94021	-0.47823
H	12.20608	-4.91033	1.66370
C	-11.29358	-0.74681	0.51448
C	-11.01393	-1.45345	1.69168
C	-12.50024	-0.98803	-0.15502
C	-11.92070	-2.38944	2.17994
H	-10.08609	-1.26565	2.21837
C	-13.40849	-1.91510	0.34816
H	-12.72186	-0.44574	-1.06628
C	-13.12376	-2.62416	1.51452
H	-11.69074	-2.92721	3.09304
H	-14.33777	-2.09156	-0.18203
H	-13.83052	-3.34921	1.90082
C	-10.85647	1.47455	-0.43736
C	-10.40961	2.02187	-1.64732
C	-11.79784	2.17980	0.32343
C	-10.88899	3.25515	-2.07857
H	-9.68764	1.47761	-2.24407
C	-12.28355	3.40573	-0.12241
H	-12.14645	1.76243	1.26039
C	-11.83011	3.95308	-1.32202
H	-10.53474	3.66498	-3.01792
H	-13.01115	3.94022	0.47820
H	-12.20606	4.91033	-1.66373

4g in the single molecule junction

Au	10.071704	7.490954	14.412931
Au	12.975201	7.342853	14.388597
Au	15.860428	7.498899	14.434585
Au	11.409401	10.099534	14.382198
Au	14.558466	10.09801	14.386016
Au	12.978031	12.518487	14.440558
Au	11.470234	8.334836	16.583545
Au	14.441401	8.353153	16.614242
Au	12.998548	10.89604	16.651782
Au	12.910387	9.262744	18.805702
C	12.478365	8.748004	30.01006
C	12.090529	8.428091	31.381851
C	12.83835	8.89486	32.466356
C	13.989049	9.703209	32.192941
C	14.369753	10.022672	30.817639
C	13.625357	9.554615	29.734008
H	12.565847	8.650472	33.512361
H	13.898404	9.793987	28.686619
C	14.929323	10.324893	33.082575
C	15.925161	11.033222	32.255625
C	17.057648	11.792522	32.625289
C	17.836572	12.384798	31.604731
C	17.493081	12.217548	30.239442
C	16.365484	11.45008	29.861782
C	15.579932	10.856769	30.871869
H	17.325664	11.916237	33.691624
H	18.11472	12.694479	29.458498
H	16.109223	11.321777	28.792532
C	10.880671	7.589253	31.308727
C	11.55552	8.123764	29.109028
C	10.553132	7.412185	29.918712
C	10.080085	6.989043	32.30202
C	9.431161	6.647771	29.528307
C	8.96071	6.218144	31.904602
C	8.637732	6.050637	30.53452
H	10.317825	7.113735	33.377021
H	8.328231	5.738694	32.674777
H	9.181875	6.524073	28.455739
H	7.756187	5.445157	30.252011
H	18.725706	12.986331	31.873172
C	11.61457	8.134526	27.702307
C	11.673747	8.09785	26.450649
C	11.755657	8.01495	25.030356
C	12.845597	8.646902	24.332484
C	10.755477	7.280733	24.302855
C	12.932224	8.509906	22.932262
C	10.871053	7.168907	22.902826
C	11.962285	7.76051	22.21551
H	13.762586	8.995165	22.382436
H	10.108689	6.586275	22.354786
C	9.615384	6.612805	25.037907
H	10.001846	5.865761	25.771753
H	9.022418	7.357314	25.619588
H	8.931922	6.089825	24.332524
C	13.876366	9.434635	25.108614
H	13.394505	10.260299	25.683425
H	14.390667	8.783588	25.855057
H	14.645151	9.873906	24.43562
C	14.928944	10.335779	34.492313
C	14.992692	10.440377	35.741236
C	15.031289	10.611931	37.156809
C	16.114409	11.342531	37.761017
C	13.972933	10.080233	37.977851
C	16.101325	11.568558	39.154321
C	13.987563	10.333371	39.36311
C	15.029811	11.096738	39.955405
H	16.929583	12.148039	39.600823
H	13.170974	9.937646	39.998924
C	12.858078	9.283427	37.341408
H	12.309198	9.901038	36.591547
H	13.263713	8.402089	36.791575
H	12.131229	8.922832	38.101777
C	17.234201	11.88861	36.90422
H	17.725883	11.074515	36.321483
H	16.841832	12.62397	36.1615
H	18.007603	12.396734	37.522249
S	14.809212	11.559623	41.671543
S	12.266638	7.443397	20.479477
C	16.427357	12.249589	42.158589
H	16.364862	12.364184	43.266471
H	17.255985	11.549654	41.91613
H	16.585639	13.242078	41.682245
C	10.598945	7.083044	19.822884
H	10.715084	7.104000	18.708395
H	10.256936	6.074556	20.142791
H	9.876865	7.871848	20.12559
Au	14.511371	9.917573	43.614245
Au	14.454982	8.294211	45.78954
Au	12.986168	10.820259	45.819998
Au	15.950353	10.858672	45.82804
Au	14.434559	6.650242	47.993339
Au	12.864678	9.067584	48.047489
Au	16.007505	9.077906	48.055456
Au	11.548915	11.650111	48.001267
Au	14.438907	11.824698	48.044469
Au	17.339285	11.673755	48.022226

12.References

S1 S. Merlet, M. Birau and Z. Y. Wang, *Org. Lett.*, 2002, **13**, 2157.

S2 G. M. Sheldrick, *Acta Cryst.*, 2015, **A71**, 3.

S3 (a) G. M. Sheldrick, *Acta Cryst.*, 2008, **A64**, 112; (b) G. M. Sheldrick, *Acta Cryst.*, 2015, **C71**, 3.

S4 L. J. Farrugia, *J. Appl. Cryst.*, 2012, **45**, 849.

S5 D. T. Chase, A. G. Fix, B. D. Rose, C. D. Weber, S. Nobusue, C. E. Stockwell, L. N. Zakharov, M. C. Lonergan and M. M. Haley, *Angew. Chem. Int. Ed.*, 2011, **50**, 11103.

S6 D. T. Chase, A. G. Fix, S. J. Kang, B. D. Rose, C. D. Weber, Y. Zhong, L. N. Zakharov, M. C. Lonergan, C. Nuckolls and M. M. Haley, *J. Am. Chem. Soc.*, 2012, **134**, 10349.

S7 H. Ueda and S. Yoshimoto, *Chem. Rec.*, 2021, **21**, 2411.

S8 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.

S9 GaussView, Version 6, R. Dennington, T. A. Keith, J. M. Millam, Semichem Inc., Shawnee Mission, KS, 2016.

S10 (a) J. M. Soler, E. Artacho, J. D. Gale, A. Garcia, J. Junquera, P. Ordejon and D. Sanchez-Portal, *J. Phys.: Condens. Matter.*, 2002, **14**, 2745; (b) M. Brandbyge, J.-L. Mozos, P. Ordejón, J. Taylor and K. Stokbro, *Phys. Rev. B* 2002, **65**, 165401; (c) N. Papior, N. Lorente, T. Frederiksen, A. García and M. Brandbyge, *Comput. Phys. Commun.*, 2017, **212**, 8.

S11 (a) V. Barone and M. Cossi, *J. Phys. Chem. A*, 1998, **102**, 1995; (b) M. Cosi, N. Rega, G. Scalmani and V. Barone, *J. Comput. Chem.,* 2003, **24**, 669.

S12 M. Nakano, *Top. Curr. Chem.*, 2017, **375**, 47.

S13 (a) Y. Kawashima and K. Hirao, *J. Phys. Chem. A*, 2017, **121**, 2035; (b) H. Iikura, T, Tsuneda, T. Yanai and K. Hirao, *J. Chem. Phys.*, 2001, **115**, 3540.

S14 (a) J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.*, 1996, **77**, 3865; (b) J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.*, 1997, **78**, 1396; (c) Y. Zhang and W. Yang, *Phys. Rev. Lett.*, 1998, **80**, 890.

S15 L. Palomino-Ruiz, S. Rodríguez-González, J. G. Fallaque, I. R. Márquez, N. Agraït, C. Díaz, E. Leary, J. M. Cuerva, A. G. Campaña, F. Martín, A. Millán and M. T. González, *Angew. Chem. Int. Ed.,* 2021, **60**, 6609.

S16 J. G. Fallaque, S. Rodríguez-González, C. Díaz and F. Martín, *Nanoscale* 2022, **14**, 464.

S17 K. Wolinski, J. F. Hinton and P. Pulay, *J. Am. Chem. Soc.*, 1990, **112**, 8251.

S18 C. R. Arroyo, E. Leary, A. Castellanos-Gomez, G. Rubio Bollinger, M. T. González and N. Agrait, *J. Am. Chem. Soc.*, 2011, **133**, 14313.

S19 M. Schmidt, D. Wassy, M. Hermann, M. T. González, N. Agraït, L. A. Zotti, B. Esser and E. Leary, *Chem. Commun.*, 2021, **57**, 745.