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Supporting Information

Intramolecular Interception of the Remote Position of Vinylcarbene Silver Complex Intermediates by C(sp^3)–H Bond Insertion

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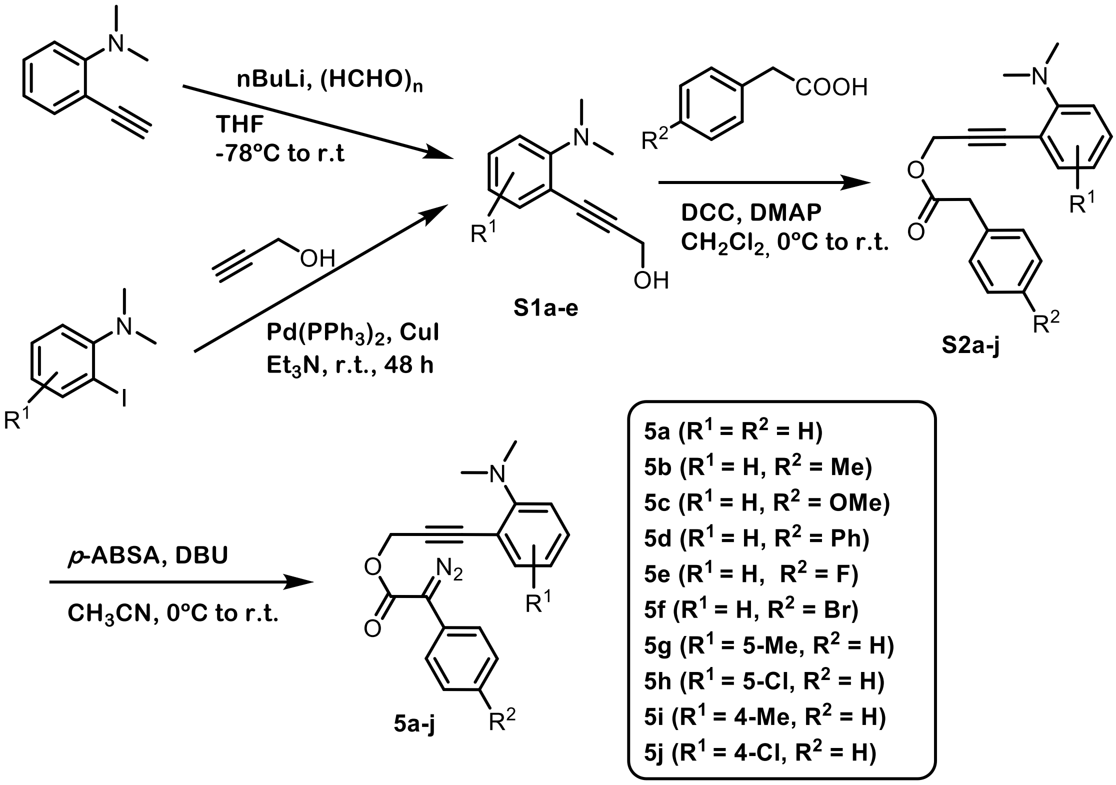
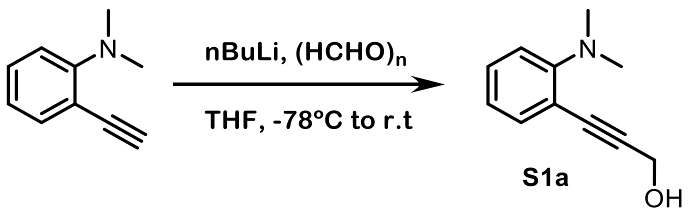
General materials and methods

Unless otherwise noted, materials were obtained from commercial suppliers and used without further purification. Diazo compound **1** was prepared as previously reported in the literature. [1] The identity of dihydroindole derivatives **2** and **3** was confirmed by comparing their spectral data with the reported one. [1] Activated molecular sieves (4Å) were added to commercially available anhydrous chloroform and nitrogen gas was bubbled for 30 minutes to ensure anhydrous and degassed conditions for the reaction solvent. Reaction progress during the preparation of all compounds was monitored using thin layer chromatography on Macherey-Nagel Xtra SIL G/UV254 silica gel plates. Solvents were removed under reduced pressure with a rotary evaporator. Reaction mixtures were chromatographed on silica gel using an automated purification instrument Interchim PuriFlash XS 520 Plus equipped with a quaternary gradient pump (up to 300 ml/min, 20 bar) and an UV-Vis 200-800 nm diode array detector. All ^{1}H and ^{13}C NMR spectra were recorded on a Bruker ASCEND 400 spectrometer equipped with a 5 mm BBFO probe using $CDCl_3$ a deuterated solvent. Chemical shifts for ^{1}H and ^{13}C NMR are reported in ppm (δ) relative to residual solvent signals ($CDCl_3$: 7.26 ppm for ^{1}H, 77,16 ppm for ^{13}C). Coupling constants are given in Hertz (Hz). ^{1}H and ^{13}C NMR signals were assigned based on ^{2}D-NMR HSQC, HMBC, COSY and TOCSY experiments. Electrospray ionization high-resolution mass spectrometry was performed using a Bruker microTOF-Q II instrument operated in the positive ESI (+) ion mode. IR spectra were recorded on an Agilent Cary 630 FT-IR spectrometer equipped with an ATR sampling accessory. The X-ray intensity data were measured on a 'Bruker D8 QUEST ECO' three-circle diffractometer system equipped with a Ceramic x-ray tube (Mo Kα, λ = 0.71076 Å) and a doubly curved silicon crystal Bruker Triumph monochromator. Melting points were measured in a SMP10 apparatus from Stuart without any correction.

S1. General scheme for the synthesis of diazo compounds 5a-j



S2. Experimental procedure for the synthesis of propargyl alcohol (S1a)

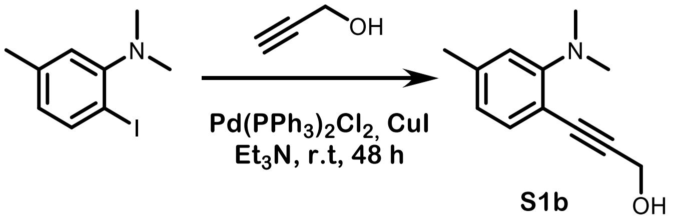


To a stirred solution of ***N,N*-dimethyl-2-ethynylaniline**,[2] (0.89 g, 6.16 mmol) in THF (30 mL) under a nitrogen atmosphere, a 1.6 M solution of nBuLi in hexane (5.0 mL, 8.0 mmol) was added dropwise. The resulting mixture was stirred at -78ºC for 1h and paraformaldehyde (0.55 g, 18.32 mmol) was then added in one portion. After the addition, the reaction mixture was slowly warmed to room temperature and stirred overnight. Upon completion of the reaction (TLC monitoring), the crude was partitioned into water and diethyl ether. The separated aqueous layer was then extracted with diethyl ether (twice) and the combined organic extracts were dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (Hexanes:EtOAc = 9:1 to 7:3) to afford **S1a** as a brown oil (0.85 g, 79 % yield).

MW ($C_{11}H_{13}NO$): 175.23 g/mol; **Rf:** 0.20 (Hexanes/EtOAc 7:3); **^{1}H NMR ($CDCl_3$, 400 MHz):** δ_H 7.38 (dd, *J* = 7.5, 1.7 Hz, 1H), 7.26 (ddd, *J* = 8.5, 7.5, 1.7 Hz, 1H), 6.95 (d, *J* = 8.5 Hz, 1H), 6.91 (td, *J* = 7.5, 1.1 Hz, 1H), 4.55 (s, 2H), 3.36 (broad s, 1H), 2.91 (s, 6H).

^{13}C{H} NMR ($CDCl_3$, 101 MHz):δ_C 154.9, 134.3, 129.4, 121.3, 117.3, 115.5, 93.0, 84.5, 51.6, 43.8. **IR (ATR) ν (cm^{-1}):** 3301, 2919, 1488, 1018, 742; **HRMS (ESI) m/z:** calcd. for $C_{11}H_{13}NONa$ $[M+Na]^+$ 198.0889; Found 198.0893.

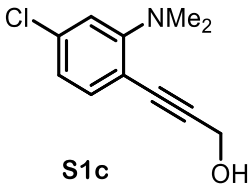
S3. General procedure for the synthesis of propargyl alcohols (S1b-S1e)



S1b

To a 100 mL round-bottom flask containing a mixture of ***N,N*-Dimethyl-2-iodo-5-methylaniline**[3] (1.51 g, 5.78 mmol), CuI (0.04 g, 0.23 mmol), and $Pd(PPh_3)_2Cl_2$ (0.10 g, 0.14 mmol) in triethylamine (40 mL), propargyl alcohol (0.40 mL, 6.87 mmol) was added dropwise under a nitrogen atmosphere. After the addition, the solution was stirred at room temperature for 48h. Upon completion of the reaction (TLC monitoring), the crude was filtered through a Celite pad, rinsed with EtOAc and concentrated under reduced pressure. The crude product was then purified by column chromatography on silica gel (CH_2Cl_2/AcOEt = 98:2) to afford **S1b** as a brown oil (0.52 g, 47 % yield).

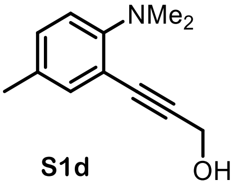
MW ($C_{12}H_{15}NO$): 189.26 g/mol; **Rf:** 0.38 (CH_2Cl_2/EtOAc 8:2); **^{1}H NMR ($CDCl_3$, 400 MHz):** δ_H 7.26 (d, J = 7.7 Hz, 1H,), 6.73 (s, 1H), 6.70 (d, J = 7.7 Hz, 1H), 4.52 (s, 2H), 2.89 (s, 6H), 2.72 (broad s, 1H), 2.32 (s, 3H). **^{13}C{H} NMR ($CDCl_3$, 101 MHz):** δ_C 154.9, 139.7, 134.2, 122.1, 118.1, 112.4, 92.2, 84.8, 51.9, 43.8, 21.9. **IR (ATR) ν (cm^{-1}):** 3297, 2915, 1599, 1498, 1019, 807. **HRMS (ESI) m/z:** calcd. for $C_{12}H_{15}NONa$ $[M+Na]^+$ 212.1046; Found 212.1052.



S1c

Propargyl alcohol **S1c** was obtained from ***N,N*-Dimethyl-2-iodo-5-chloroaniline** [4] (1.18 g, 4.19 mmol) as a brown oil (0.29 g, 33 %) following the same procedure as for **S1b**.

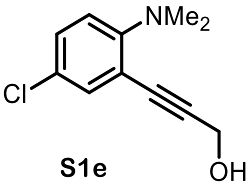
MW ($C_{11}H_{12}ClNO$): 209.67 g/mol; **Rf:** 0.28 (CH_2Cl_2/EtOAc 8:2); **^{1}H NMR ($CDCl_3$, 400 MHz):** δ_H 7.28 (dd, J = 8.2, 1.4 Hz, 1H), 6.86 (d, J = 2.0 Hz, 1H), 6.83 (dd, J = 8.2, 2.0 Hz, 1H), 4.53 (d, J = 5.7 Hz, 2H), 2.92 (s, 6H), 2.04 (broad s, 1H). **^{13}C{H} NMR ($CDCl_3$, 101 MHz):** δ_C 155.9, 135.4, 135.3, 120.8, 117.6, 113.0, 93.4, 84.1, 52.0, 43.5. **IR (ATR) ν (cm^{-1}):** 3290, 2839, 1581, 1452, 1019, 818. **HRMS (ESI) m/z:** calcd. for $C_{11}H_{13}ClNO$ $[M+H]^+$ 210.0680; Found 210.0689.



S1d

Propargyl alcohol **S1d** was obtained from ***N,N*-Dimethyl-2-iodo-4-methylaniline** [5] (2.53 g, 9.69 mmol) as a brown oil (0.85 g, 46%) following the same procedure as for **S1b**.

MW ($C_{12}H_{15}NO$): 189.26 g/mol; **Rf:** 0.25 (CH_2Cl_2/EtOAc 8:2); **^{1}H NMR ($CDCl_3$, 400 MHz):** δ_H 7.21 (d, *J* = 2.2 Hz, 1H), 7.06 (dd, *J* = 8.3, 2.2 Hz, 1H), 6.84 (d, *J* = 8.3 Hz, 1H), 4.53 (s, 2H), 2.87 (s, 6H), 2.24 (s, 3H). **^{13}C{H} NMR ($CDCl_3$, 101 MHz):** δ_C 152.8, 134.8, 130.7, 130.3, 117.3, 115.4, 92.5, 84.8, 51.9, 44.1, 20.4. **IR (ATR) ν (cm^{-1}):** 3309, 2919, 1737, 1497, 1029, 814. **HRMS (ESI) m/z:** calcd. for $C_{12}H_{15}NONa$ $[M+Na]^+$ 212.1046; Found 212.1049.

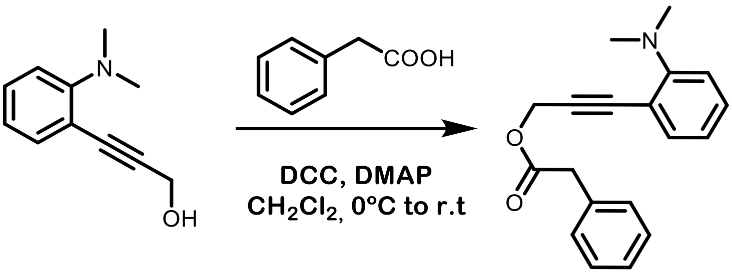


S1e

Propargyl alcohol **S1e** was obtained from ***N,N*-Dimethyl-2-iodo-4-chloroaniline** [5] (2.53 g, 8.99 mmol) as a brown oil (1.09 g, 58%) following the same procedure as for **S1b**.

MW ($C_{11}H_{12}ClNO$): 209.67 g/mol; **Rf:** 0.28 (CH_2Cl_2/EtOAc 8:2); **^{1}H NMR ($CDCl_3$, 400 MHz):** δ_H 7.34 (d, *J* = 2.6 Hz, 1H), 7.18 (dd, *J* = 8.8, 2.6 Hz, 1H), 6.83 (d, *J* = 8.8 Hz, 1H), 4.54 (s, 2H), 2.89 (s, 6H). **^{13}C{H} NMR ($CDCl_3$, 101 Mz):** δ_C 153.7, 133.873, 129.5, 125.6, 118.5, 116.4, 93.7, 83.7, 51.9, 43.7. **IR (ATR) ν (cm^{-1}):** 3294, 2917, 1487, 1022, 812. **HRMS (ESI) m/z:** calcd. for $C_{11}H_{12}ClNONa$ $[M+Na]^+$ 232.0500; Found 232.0507.

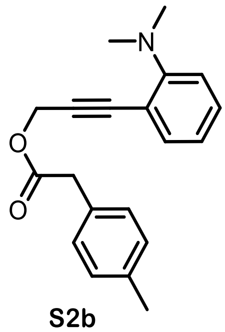
S4. General procedure for the synthesis of propargyl esters (S2a-S2j)



S1a **S2a**

To a 25 mL round-bottom flask containing a mixture of **S1a** (0.22 g, 1.26 mmol), phenylacetic acid (0.17 g, 1.25 mmol), and 4-dimethylaminopyridine (DMAP) (13.9 mg, 0.11 mmol) in dichloromethane (6mL), N,N'-dicyclohexylcarbodiimide (DCC) (0.28 g, 1.36 mmol) was added in batches at 0 ºC. After the addition, the reaction mixture was slowly warmed to room temperature and stirred overnight. Upon completion of the reaction (TLC monitoring), the crude was filtrated through a Celite pad, rinsed with EtOAc and concentrated under reduced pressure. The crude product was then purified by column chromatography on silica gel (Hexanes/EtOAc = 95:05) to afford ester **S2a** as a yellow oil (0.31 g, 86 % yield).

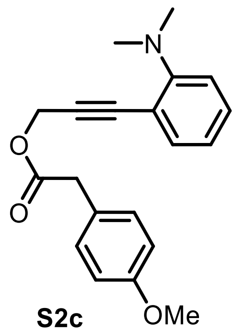
MW ($C_{19}H_{19}NO_2$): 293.37 g/mol; **Rf:** 0.50 (Hexanes/EtOAc 8:2); **^{1}H NMR ($CDCl_3$, 400 MHz):** δ_H 7.40 (dd, J = 7.6, 1.4 Hz, 1H), 7.37 – 7.26 (m, 5H), 7.26 – 7.23 (m, 1H), 6.90 (d, *J* = 8.3 Hz, 1H), 6.86 (td, *J* = 7.6, 1.1 Hz, 1H), 5.00 (s, 2H), 3.70 (s, 2H), 2.90 (s, 6H) **^{13}C{H} NMR ($CDCl_3$, 101 MHz:** δ_C 171.0, 155.3, 134.8, 133.7, 129.8, 129.4, 128.7, 127.3, 120.6, 117.0, 114.2, 88.1, 86.1, 53.7, 43.6, 41.3. **IR (ATR) ν (cm^{-1}):** 2918, 1736, 1491, 1135, 754. **HRMS (ESI) m/z:** calcd. for $C_{19}H_{19}NO_2Na$ $[M+Na]^+$ 316.1308; Found 316.1312.



S2b

Ester **S2b** was obtained from **S1a** (0.35 g, 1.98 mmol) as yellow oil (0.25 g, 41%) following the same procedure as for **S2a**.

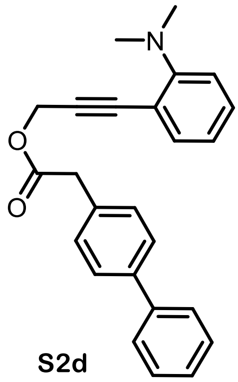
MW ($C_{20}H_{21}NO_2$): 307.39 g/mol; **Rf:** 0.53 (Hexanes/EtOAc 8:2); **^{1}H NMR ($CDCl_3$, 400 MHz):** δ_H 7.38 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.26 – 7.22 (m, 1H (overlapped with chloroform)), 7.19 (d, *J* = 8.2 Hz, 2H), 7.13 (d, *J* = 7.8 Hz, 2H), 6.89 (dd, *J* = 8.2, 1.1 Hz, 1H), 6.85 (dt, *J* = 7.4, 1.1 Hz, 1H), 4.98 (s, 2H), 3.65 (s, 2H), 2.89 (s, 6H), 2.33 (s, 3H). **^{13}C{H} NMR ($CDCl_3$, 101 MHz):** δ_C 171.2, 155.3, 136.9, 134.8, 130.7, 129.8, 129.4, 129.3, 120.5, 117.0, 114.2, 88.2, 86.0, 53.7, 43.6, 40.8, 21.2. **IR (ATR) ν (cm^{-1}):** 2938, 1736, 1490, 1133, 755. **HRMS (ESI) m/z:** calcd. for $C_{20}H_{21}NO_2Na$ $[M+Na]^+$ 330.1465; Found 330.1462.



S2c

Ester **S2c** was obtained from **S1a** (0.19 g, 1.09 mmol) as a yellow oil (0.32 g, 92%) following the same procedure as for **S2a**.

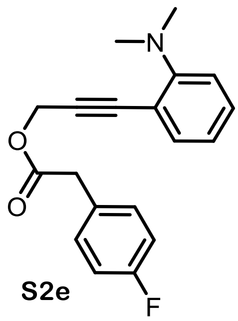
MW ($C_{20}H_{21}NO_3$): 323.39 g/mol; **Rf:** 0.33 (Hexanes/EtOAc 8:2); **^{1}H NMR ($CDCl_3$, 400 MHz):** δ_H 7.38 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.26 – 7.19 (m, 3H), 6.88 (d, *J* = 8.2 Hz, 1H), 6.87 – 6.81 (m, 3H), 4.97 (s, 2H), 3.77 (s, 3H), 3.62 (s, 2H), 2.88 (s, 6H). **^{13}C{H} NMR ($CDCl_3$, 101 MHz):** δ_C 171.3, 158.8, 155.2, 134.7, 130.4, 129.8, 125.8, 120.5, 117.0, 114.1, 88.2, 86.0, 55.3, 53.6, 43.6, 40.3. **IR (ATR) ν (cm^{-1}):** 2936, 1735, 1510, 1243, 1133, 755. **HRMS (ESI) m/z:** calcd. for $C_{20}H_{21}NO_3Na$ $[M+Na]^+$ 346.1414; Found 346.1405.



S2d

Ester **S2d** was obtained from **S1a** (0.26 g, 1.46 mmol) as a yellow oil (0.28 g, 52%) following the same procedure as for S2a.

MW ($C_{25}H_{23}NO_2$): 369.46 g/mol; **Rf:** 0.43 (Hexanes/EtOAc 8:2); **^{1}H NMR ($CDCl_3$, 400 MHz):** δ_H 7.59 – 7.54 (m, 4H), 7.47 – 7.41 (m, 2H), 7.41 – 7.37 (m, 3H), 7.37 – 7.32 (m, 1H), 7.26 – 7.22 (m, 1H), 6.89 (dd, *J* = 8.3, 1.1 Hz, 1H), 6.85 (dt, *J* = 7.4, 1.1 Hz, 1H), 5.01 (s, 2H), 3.74 (s, 2H), 2.89 (s, 6H). **^{13}C{H} NMR ($CDCl_3$, 101 MHz):** δ_C 171.0, 155.3, 140.9, 140.3, 134.8, 132.8, 129.8, 128.9, 127.5, 127.4, 127.2, 120.6, 117.1, 114,1, 88.1, 86.1, 53.8, 43.6, 40.9); **IR (ATR) ν (cm^{-1}):** 2937, 1735, 1487, 1135, 752. **HRMS (ESI) m/z:** calcd. for $C_{25}H_{24}NO_2$ $[M+H]^+$ 370.1802; Found 370.1813

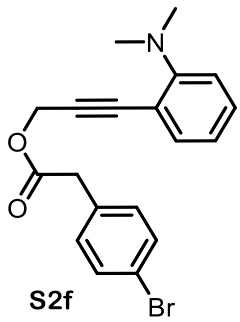


S2e

Ester **S2e** was obtained from **S1a** (0.19 g, 1.09 mmol) as a brown oil (0.30 g, 89%) following the same procedure as for **S2a**.

MW ($C_{19}H_{18}FNO_2$): 311.36 g/mol; **Rf:** 0.3 (Hexanes/EtOAc 8:2); ^{1}**H NMR ($CDCl_3$, 400 MHz):** δ_H 7.38 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.30 – 7.22 (m, 3H (overlapped with chloroform)), 7.05 – 6.97 (m, 2H), 6.90 (dd, *J* = 8.3, 1.1 Hz, 1H), 6.86 (td, *J* = 7.4, 1.1 Hz, 1H), 4.99 (s, 2H), 3.66 (s, 2H), 2.89 (s, 6H). **^{13}C{H} NMR ($CDCl_3$, 101 MHz):** δ_C 170.9, 162.2 (d, $^1J_{C-F}$ = 246.4 Hz), 155.3, 134.8, 131.0

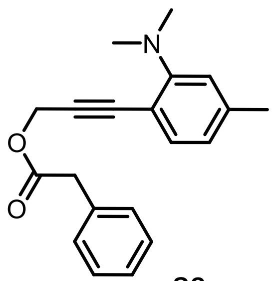
(d, $^3J_{C\text{-}F}$ = 8.1 Hz), 129.9, 129.4 (d, $^4J_{C\text{-}F}$ = 3.3 Hz), 120.6, 117.1, 115.6 (d, $^2J_{C\text{-}F}$ = 21.5 Hz), 114.1, 88.0, 86.2, 53.8, 43.6, 40.3. **^{19}F NMR (CDCl$_3$, 376 MHz): δ_F** -116.51 (s, 1F). **IR (ATR) ν (cm^{-1}):** 2926, 1736, 1134, 1219, 753. **HRMS (ESI) m/z:** calcd. for $C_{19}H_{18}FNO_2Na$ [M+Na]$^+$ 334.1214; Found 334.1222.



S2f

Ester **S2f** was obtained from **S1a** (0.19 g, 1.09 mmol) as a yellow oil (0.36 g, 88%) following the same procedure as for **S2a**.

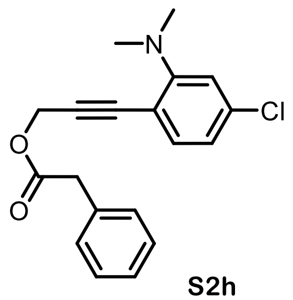
MW ($C_{19}H_{18}BrNO_2$): 372.26 g/mol; **Rf:** 0.33 (Hexanes/EtOAc 8:2); **^{1}H NMR (CDCl$_3$, 400 MHz): δ_H** 7.49 – 7.42 (m, 2H), 7.39 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.30 – 7.22 (m, 1H (overlapped with chloroform)), 7.22 – 7.16 (m, 2H), 6.90 (dd, *J* = 8.3, 1.1 Hz, 1H), 6.86 (td, *J* = 7.4, 1.1 Hz, 1H), 4.99 (s, 2H), 3.64 (s, 2H), 2.89 (s, 6H). **^{13}C{H} NMR (CDCl$_3$, 101 MHz): δ_H** 170.4, 155.2, 134.7, 132.7, 131.8, 131.1, 129.9, 121.4, 120.5, 117.0, 114.0, 87.9, 86.2, 53.8, 43.6, 40.6. **IR (ATR) ν (cm^{-1}):** 2936, 1736, 1487, 1137, 753. **HRMS (ESI) m/z:** calcd. for $C_{19}H_{19}BrNO_2$ [M+H]$^+$ 372.0594-374.0574; Found 372.0597-374.0577.



S2g

Ester **S2g** was obtained from **S1b** (0.21 g, 1.11 mmol) as a yellow oil (0.32 g, 94%) following the same procedure as for **S2a**.

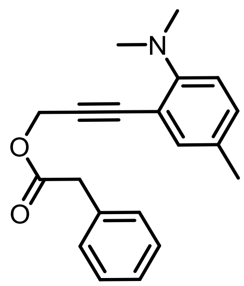
MW ($C_{20}H_{21}NO_2$): 307.39 g/mol; **Rf:** 0.38 (Hexanes/EtOAc 8:2); **^{1}H NMR (CDCl$_3$, 400 MHz): δ_H** 7.36 – 7.25 (m, 6H), 6.70 (s, 1H), 6.69 – 6.66 (m, 1H), 4.98 (s, 2H), 3.69 (s, 2H), 2.88 (s, 6H), 2.32 (s, 3H). **^{13}C{H} NMR (CDCl$_3$, 101 MHz): δ_C** 171.0, 153.1, 135.1, 133.8, 130.6, 130.2, 129.4, 128.7, 127.3, 117.2, 114.5, 87.8, 86.1, 53.8, 43.9, 41.3, 20.3. **IR (ATR) ν (cm^{-1}):** 2969, 1757, 1341, 770. **HRMS (ESI) m/z:** calcd. for $C_{20}H_{21}NO_2Na$ [M+Na]$^+$ 330.1465; Found 330.1467.



S2h

Ester **S2h** was obtained from **S1c** (0.30 g, 1.44 mmol) as a yellow oil (0.36 g, 76%) following the same procedure as for **S2a**.

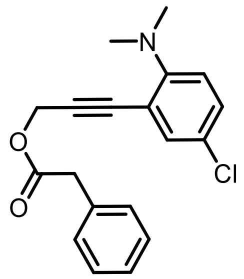
MW ($C_{19}H_{18}ClNO_2$): 327.81 g/mol; **Rf:** 0.60 (Hexanes/EtOAc 8:2); **^{1}H NMR ($CDCl_3$, 400 MHz): δ_H** 7.36 – 7.26 (m, 6H), 6.83 (d, *J* = 2.0 Hz, 1H), 6.80 (dd, *J* = 8.1, 2.0 Hz, 1H), 4.96 (s, 2H), 3.69 (s, 2H), 2.89 (s, 6H). **^{13}C{H} NMR ($CDCl_3$, 101 MHz): δ_C** 171.0, 156.0, 135.7, 135.6, 133.7, 129.4, 128.8, 127.4, 120.3, 117.3, 112.0, 88.9, 85.3, 53.6, 43.3, 41.3. **IR (ATR) ν (cm^{-1}):** 2941, 1736, 1491, 1134. **HRMS (ESI) m/z:** calcd. for $C_{19}H_{18}ClNO_2Na$ $[M+Na]^+$ 350.0918; Found 350.0920.



S2i

Ester **S2i** was obtained from **S1d** (0.31 g, 1.62 mmol) as a brown oil (0.32 g, 64%) following the same procedure as for **S2a**.

MW ($C_{20}H_{21}NO_2$): 307.39 g/mol; **Rf:** 0.42 (Hexanes/EtOAc 8:2); **^{1}H NMR ($CDCl_3$, 400 MHz): δ_H** 7.37 – 7.26 (m, 5H), 7.22 (d, *J* = 2.2 Hz, 1H), 7.06 (dd, *J* = 8.3, 2.2 Hz, 1H), 6.81 (d, *J* = 8.3 Hz, 1H), 4.98 (s, 2H), 3.69 (s, 2H), 2.84 (s, 6H), 2.24 (s, 3H). **^{13}C{H} NMR ($CDCl_3$, 101 MHz): δ_C** 171.0, 153.1, 135.1, 133.8, 130.6, 130.2, 129.4, 128.7, 127.3, 117.2, 114.4, 87.8, 86.1, 53.8, 43.9, 41.3, 20.3. **IR (ATR) ν (cm^{-1}):** 2917, 1736, 1499, 1125. **HRMS (ESI) m/z:** calcd. for $C_{20}H_{21}NO_2Na$ $[M+Na]^+$ 330.1465; Found 330.1466.

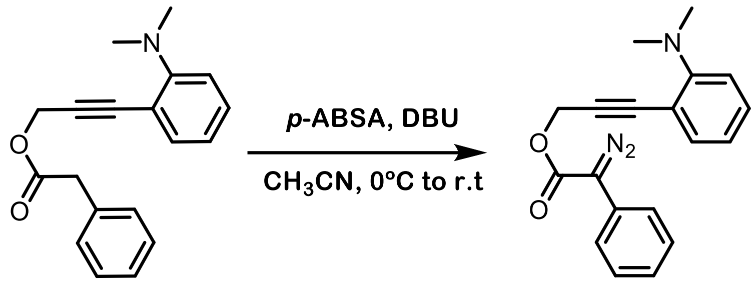


S2j

Ester **S2j** was obtained from **S1e** (0.30 g, 1.44 mmol) as a brown oil (0.27 g, 58%) following the same procedure as for **S2a**.

MW ($C_{19}H_{18}ClNO_2$): 327.81 g/mol; **Rf:** 0.40 (Hexanes/EtOAc 8:2); **^{1}H NMR ($CDCl_3$, 400 MHz):** δ_H 7.36 – 7.26 (m, 6H), 7.18 (dd, *J* = 8.8, 2.6 Hz, 1H), 6.80 (d, *J* = 8.8 Hz, 1H), 4.97 (s, 2H), 3.69 (s, 2H), 2.86 (s, 6H). **^{13}C{H} NMR ($CDCl_3$, 101 MHz):** δ_C 170.9, 153.8, 134.0, 133.7, 129.7, 129.4, 128.8, 127.4, 125.2, 118.2, 115.4, 89.2, 84.8, 53.5, 43.6, 41.3. **IR (ATR) ν (cm^{-1}):** 2940, 1736, 1490, 1127. **HRMS (ESI) m/z:** calcd. for $C_{19}H_{18}ClNO_2Na$ [M+Na]$^+$ 350.0918; Found 350.0930.

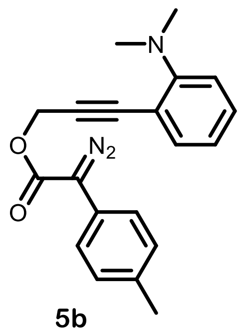
S5. General procedure for the synthesis of diazo compounds (5a-5j)



S2a **5a**

To a 25 mL oven-dried flask containing a mixture of **S2a** (0.21 g, 0.72 mmol) and *p*-acetamidobenzenesulfonyl azide (*p*-ABSA) (0.21 g, 0.87 mmol) in anhydrous CH_3CN (4.5 mL), a solution of 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU) (0.15 mL, 1.00 mmol) in anhydrous CH_3CN (0.9 mL) was added dropwise at 0 ºC. After the addition, the reaction mixture was slowly warmed to room temperature and stirred overnight. Upon completion of the reaction (TLC monitoring), the crude was diluted with Et_2O, and washed with saturated aqueous NH_4Cl, saturated aqueous $NaHCO_3$ and brine. The combined organic extracts were dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (Hexanes: EtOAc: Et_3N= 96:3:1) to afford diazo compound **5a** as an orange oil (0.20 g, 94% yield).

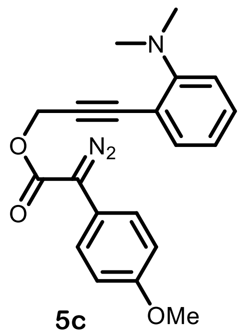
MW ($C_{19}H_{17}N_3O_2$): 319.36 g/mol; **Rf:** 0.63 (Hexanes/EtOAc 8:2); **^{1}H NMR ($CDCl_3$, 400 MHz):** δ_H 7.53 – 7.48 (m, 2H), 7.44 – 7.36 (m, 3H), 7.29 – 7.23 (m, 1H (overlapped with chloroform)), 7.23 – 7.17 (m, 1H), 6.91 (dd, *J* = 8.4, 1.1 Hz, 1H), 6.87 (td, *J* = 7.4, 1.1 Hz, 1H), 5.17 (s, 2H), 2.93 (s, 6H). **^{13}C{H} NMR ($CDCl_3$, 101 MHz):** δ_C 164.6, 155.3, 134.8, 129.9, 129.1, 126.1, 125.4, 124.2, 120.6, 117.1, 114.1 88.2, 86.3, 53.7, 43.7. **IR (ATR) ν (cm^{-1}):** 2925, 2082, 1699, 1238, 1140, 751. **HRMS (ESI) m/z:** calcd. for $C_{19}H_{17}N_3O_2Na$ [M+Na]$^+$ 342.1213; Found 342.1213.



5b

Diazo compound **5b** was obtained from **S2b** (0.18 g, 0.59 mmol) as an orange oil (0.17 g, 86%) following the same procedure as for **5a**.

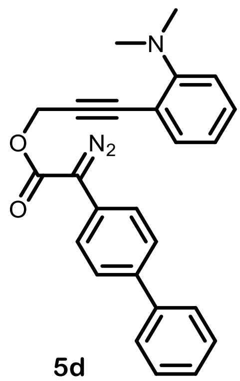
MW ($C_{20}H_{19}N_3O_2$): 333.39 g/mol; **Rf:** 0.64 (Hexanes/EtOAc 8:2); **^{1}H NMR ($CDCl_3$, 400 MHz):** δ_H 7.42 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.38 (d, *J* = 8.2 Hz, 2H), 7.28 – 7.23 (m, 1H (overlapped with chloroform)), 7.21 (d, *J* = 8.2 Hz, 2H), 6.90 (dd, *J* = 8.3, 1.1 Hz, 1H), 6.86 (td, *J* = 7.5, 1.1 Hz, 1H), 5.16 (s, 2H), 2.93 (s, 6H), 2.35 (s, 3H). **^{13}C{H} NMR ($CDCl_3$, 101 MHz):** δ_C 164.9, 155.3, 136.0 134.8, 129.9, 129.8, 124.3, 122.0, 120.6, 117.1, 114.2, 88.3, 86.3, 53.7, 43.7, 21.2. **IR (ATR) ν (cm^{-1}):** 2919, 2082, 1703, 1241, 1139, 756. **HRMS (ESI) m/z:** calcd. for $C_{20}H_{19}N_3O_2Na$ $[M+Na]^+$ 356.1369; Found 356.1367.



5c

Diazo compound **5c** was obtained from **S2c** (0.18 g, 0.56 mmol) as an orange oil (0.17 g, 88%) following the same procedure as for **5a**.

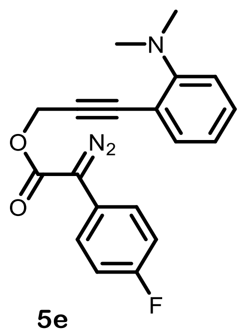
MW ($C_{20}H_{19}N_3O_3$): 349.39 g/mol; **Rf:** 0.45 (Hexanes/EtOAc 8:2; **^{1}H NMR ($CDCl_3$, 400 MHz):** δ_H 7.43 – 7.38 (m, 3H), 7.28 – 7.23 (m, 1H (overlapped with chloroform)), 6.97 – 6.93 (m, 2H), 6.90 (d, *J* = 7.4 Hz, 1H), 6.86 (td, *J* = 7.4, 1.1 Hz, 1H), 5.15 (s, 2H), 3.81 (s, 3H), 2.93 (s, 6H). **^{13}C{H} NMR ($CDCl_3$, 101 MHz):** δ_C 165.0, 158.2, 155.2, 134.7, 129.8, 126.1, 120.5, 117.0, 116.7, 114.7, 114.0, 88.2, 86.1, 55.4, 53.5, 43.6. **IR (ATR) ν (cm^{-1}):** 2920, 2079, 1696, 1239, 1141, 754. **HRMS (ESI) m/z:** calcd. for $C_{20}H_{20}NO_3$ $[M+H-N_2]^+$ 322.1438; Found 322.1449.



5d

Diazo compound **5d** was obtained from **S2d** (0.15 g, 0.41 mol) as an orange solid (0.15 g, 93%) following the same procedure as for **5a**.

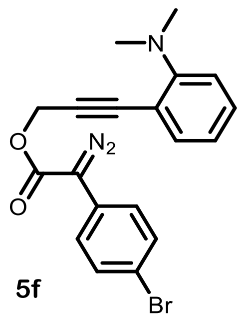
MW ($C_{25}H_{21}N_3O_2$): 395.46 g/mol; **Rf:** 0.53 (Hexanes/EtOAc 8:2); **^{1}H NMR ($CDCl_3$, 400 MHz):** δ_H 7.67 – 7.55 (m, 6H), 7.48 – 7.41 (m, 3H), 7.38 – 7.32 (m, 1H), 7.29 – 7.23 (m,12H, (overlapped with chloroform)), 6.91 (dd, *J* = 8.3, 1.1 Hz, 1H), 6.87 (td, *J* = 7.5, 1.1 Hz, 1H), 5.19 (s, 2H), 2.94 (s, 6H). **^{13}C{H} NMR ($CDCl_3$, 101 MHz):** δ_C 164.6, 155.3, 140.4, 138.9, 134.8, 129.9, 129.0, 127.8, 127.5, 127.0, 124.5, 124.3, 120.6, 117.1, 88.2, 86.4, 53.8, 43.7. **IR (ATR) ν (cm^{-1}):** 2935, 2086, 1704, 1234, 1141, 752. **HRMS (ESI)m/z:** calcd. for $C_{25}H_{21}N_3O_2Na$ [M+Na]$^+$ 418.1526; Found 418.1536.



5e

Diazo compound **5e** was obtained from **S2e** (0.19 g, 0.61 mmol) as an orange solid (0.19 g, 92%) following the same procedure as for **5a**.

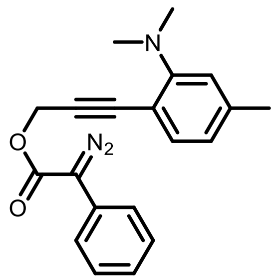
MW ($C_{19}H_{16}FN_3O_2$): 337.35 g/mol; **Rf:** 0.55 (Hexanes/EtOAc 8:2); **^{1}H NMR ($CDCl_3$, 400 MHz):** δ_H 7.49 – 7.43 (m, 2H), 7.41 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.29 – 7.22 (m, 1H (overlapped with chloroform)), 7.14 – 7.06 (m, 2H), 6.91 (dd, *J* = 8.4, 1.1 Hz, 1H), 6.87 (td, *J* = 7.6, 1.1 Hz, 1H), 5.16 (s, 2H), 2.93 (s, 6H). **^{13}C{H} NMR ($CDCl_3$, 101 MHz):** δ_C 164.6, 161.2 (d, $^1J_{C-F}$ = 247.4 Hz), 155.3, 134.8, 129.9, 126.1 (d, $^3J_{C-F}$ = 7.9 Hz), 121.1 (d, $^4J_{C-F}$ = 3.2 Hz), 120.6, 117.1, 116.1 (d, $^2J_{C-F}$ = 22.2 Hz), 114.1, 88.1, 86.4, 53.8, 43.7. **^{19}F NMR (376 MHz, $CDCl_3$):** δ_F -116.96. (s, 1F). **IR (ATR) ν (cm^{-1}):** 2938, 2083, 1742, 1230, 1145, 752. **HRMS (ESI) m/z:** calcd. for $C_{19}H_{16}FN_3O_2Na$ [M+Na]$^+$ 360.1119; Found 360.1119.



5f

Diazo compound **5f** was obtained from **S2f** (0.21 g, 0.56 mmol) as an orange solid (0.22 g, 99%) following the same procedure as for **5a.**

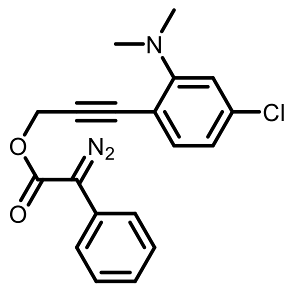
MW ($C_{19}H_{16}BrN_3O_2$): 398.26 g/mol; **Rf:** 0.60 (Hexanes/EtOAc 8:2**^{1}H NMR ($CDCl_3$, 400 MHz):** δ_H 7.53 – 7.48 (m, 2H), 7.41 (dd, *J* = 7.5, 1.7 Hz, 1H), 7.40 – 7.35 (m,1H) 7.29 – 7.23 (m, 1H, overlapped with chloroform), 6.91 (dd, *J* = 8.3, 1.1 Hz, 1H), 6.86 (td, *J* = 7.5, 1.1 Hz, 1H), 5.16 (s, 2H), 2.93 (s, 6H). **^{13}C{H} NMR ($CDCl_3$, 101 MHz):** δ_C 164.2, 155.3, 134.8, 132.2, 130.0, 125.5, 124.6, 120.6, 119.7, 117.1, 114.0, 88.0, 86.5, 53.9, 43.7. **IR (ATR) ν (cm^{-1}):** 2941, 2086, 1703, 1237, 1147, 754. **HRMS (ESI) m/z:** calcd. for $C_{19}H_{16}BrN_3O_2Na$ $[M+Na]^+$ 420.0318-422.0298; Found 420.0321-422.0303.



5g

Diazo compound **5g** was obtained from **S2g** (0.16 g, 0.52 mmol) as an orange solid (0.15 g, 87%) following the same procedure as for **5a**.

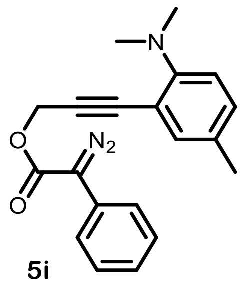
MW ($C_{20}H_{19}N_3O_2$): 333.39 g/mol; **Rf:** 0.63 (Hexanes/EtOAc 8:2); **^{1}H NMR ($CDCl_3$, 400 MHz):** δ_H 7.52 – 7.47 (m, 2H), 7.42 – 7.36 (m, 2H), 7.31 (d, *J* = 7.6 Hz, 1H), 7.20 (td, *J* = 7.2, 1.2 Hz, 1H), 6.71 (s, 1H), 6.69 (d, *J* = 7.6 Hz, 1H), 5.16 (s, 2H), 2.92 (s, 6H), 2.32 (s, 3H). **^{13}C{H} NMR ($CDCl_3$, 101 MHz):** δ_C 164.6, 155.2, 140.2, 134.6, 129.1 126.1, 125.4, 124.2, 121.6, 117.9, 111.2, 87.5, 86.5, 53.8, 43.7, 22.0. **IR (ATR) ν (cm^{-1}):** 2940, 2087, 1699, 1241, 1142, 753. **HRMS (ESI) m/z:** calcd. for $C_{20}H_{19}N_3O_2Na$ $[M+Na]^+$ 356.1369; Found 356.1372.



5h

Diazo compound **5h** was obtained from **S2h** (0.18 g, 0.55 mmol) as an orange solid (0.16 g, 82%) following the same procedure as for **5a**.

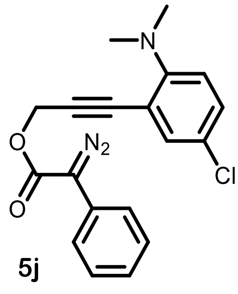
MW ($C_{19}H_{16}ClN_3O_2$): 353.81 g/mol; **Rf:** 0.65 (Hexanes/EtOAc 8:2); **^{1}H NMR ($CDCl_3$, 400 MHz):** δ_H 7.52 – 7.47 (m, 2H), 7.43 – 7.36 (m, 2H), 7.31 (d, *J* = 8.1 Hz, 1H), 7.23 – 7.16 (m, 1H), 6.84 (d, *J* = 2.0 Hz, 1H), 6.82 (dd, *J* = 8.1, 2.0 Hz, 1H), 5.14 (s, 2H), 2.94 (s, 6H). **^{13}C{H} NMR ($CDCl_3$, 101 MHz):** δ_C 164.5, 156.1, 135.7, 129.1, 126.2, 125.3, 124.2, 120.4, 117.4, 111.9, 88.9, 85.5, 53.6, 43.4. **IR (ATR) ν (cm^{-1}):** 2946, 2082, 1737, 1231, 1138, 756. **HRMS (ESI) m/z:** calcd. for $C_{19}H_{16}ClN_3O_2Na$ $[M+Na]^+$ 376.0823; Found 376.0826.



5i

Diazo compound **5i** was obtained from **S2i** (0.21 g, 0.68 mmol) as an orange oil (0.20 g, 88%) following the same procedure as for **5a**.

MW ($C_{20}H_{19}N_3O_2$): 333.39 g/mol; **Rf:** 0.73 (Hexanes/EtOAc 8:2); **^{1}H NMR ($CDCl_3$, 400 MHz):** δ_H 7.53 – 7.47 (m, 2H), 7.43 – 7.35 (m, 2H), 7.25 (d, *J* = 2.3 Hz, 1H), 7.23 – 7.17 (m, 1H), 7.07 (dd, *J* = 8.3, 1.8 Hz, 1H), 6.83 (d, *J* = 8.3 Hz, 1H), 5.16 (s, 2H), 2.88 (s, 6H), 2.25 (s, 3H). **^{13}C{H} NMR ($CDCl_3$, 101 MHz):** δ_C 164.6,153.2, 135.0, 130.7, 130.3, 129.1, 126.1, 125.4, 124.2, 117.2, 114.4, 87.9, 86.3, 53.8, 44.0, 20.3. **IR (ATR) ν (cm^{-1}):** 2938, 2081, 1699, 1238, 1141, 753. **HRMS (ESI) m/z:** calcd.for $C_{20}H_{19}N_3O_2Na$ $[M+Na]^+$ 356.1369; Found 356.1373.

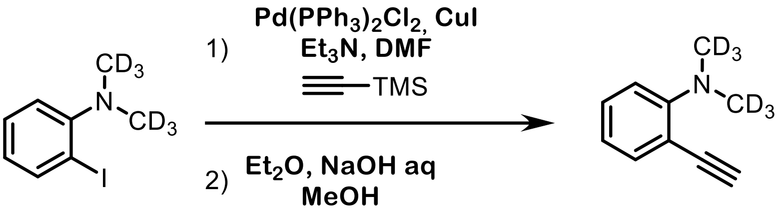


5j

Diazo compound **5j** was obtained from **S2j** (0.17 g, 0.52 mmol) as an orange oil (0.16 g, 87%) following the same procedure as for **5a**.

MW ($C_{19}H_{16}ClN_3O_2$): 353.81 g/mol; **Rf:** 0.70 (Hexanes/EtOAc 8:2); **^{1}H NMR ($CDCl_3$, 400 MHz):** δ_H 7.54 – 7.46 (m, 2H), 7.44 – 7.36 (m, 3H), 7.24 – 7.15 (m, 2H), 6.81 (d, *J* = 8.8 Hz, 1H), 5.15 (s, 2H), 2.91 (s, 6H). **^{13}C{H} NMR ($CDCl_3$, 101 MHz):** δ_C 164.5, 153.9, 134.0, 129.8, 129.1, 126.2, 125.3,125.2, 124.2, 118.3, 115.4, 89.2, 85.0, 53.5, 43.6. **IR (ATR) ν (cm^{-1}):** 2940, 2081, 1698, 1236, 1139, 751. **HRMS (ESI) m/z:** calcd. for $C_{19}H_{16}ClN_3O_2Na$ $[M+Na]^+$ 376.0823; Found 376.0830.

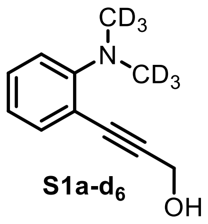
S6. Preparation of 5a-d$_6$



S3-d$_6$

In a 50 mL round-bottom flask containing a mixture of ***N,N*-Dimethyl-*d*$_3$-2-iodoaniline** [6] (1.23 g, 4.86 mmol), CuI (37.1 mg, 0.20 mmol), $Pd(PPh_3)_2Cl_2$ (68.2 mg, 0.10 mmol.), and triethylamine (0.68 mL, 4.88 mmol.) in DMF (12 mL), trimethylsilylacetylene (0.81 mL, 5.86 mmol) was added dropwise under a nitrogen atmosphere. After the addition, the solution was stirred at room temperature overnight. Upon completion of the reaction (TLC monitoring), the crude was diluted with Et_2O, and washed with saturated aqueous NH_4Cl and brine. The organic layer was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude was then dissolved with methanol (19 mL) and Et_2O (19 mL) and a 10% aqueous NaOH solution (11 mL) was added and the mixture was stirred at room temperature overnight. Upon completion of the reaction (TLC monitoring), the organic layer was separated, and the aqueous layer was back-extracted with Et_2O twice. The combined organic extracts were washed with brine, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by column chromatography on silica gel (Hexanes 100%) to afford **S3-d$_6$** as a yellow oil (0.52 g, 71 % yield).

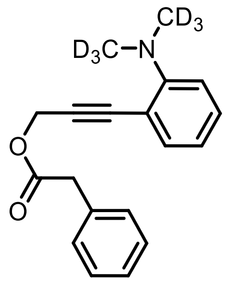
MW ($C_{10}H_5D_6N$): 151.24 g/mol; **Rf:** 0.50 (Hexanes/EtOAc 8:2); **^{1}H NMR ($CDCl_3$, 400 MHz):** δ_H 7.46 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.27 (ddd, *J* = 8.3, 7.3, 1.7 Hz (overlapped with chloroform), 1H), 6.92 (dd, *J* = 8.3, 1.1 Hz, 1H), 6.88 (td, *J* = 7.6, 1.1 Hz, 1H), 3.41 (s, 1H). **^{13}C{H} NMR ($CDCl_3$, 101 MHz):** δ_C 135.0, 129.7, 120.7, 117.1, 114.4, 83.0, 82.3 (carbons bonded to deuterium are not observed in the spectrum with the standard acquisition parameters). **IR (ATR) ν (cm^{-1}):** 3280, 2046, 1482, 749. **HRMS (ESI) m/z:** calcd. for $C_{10}H_6D_6N$ $[M+H]^+$ 152.1341; Found 152.1348.



S1a-d$_6$

Propargyl alcohol **S1a-d$_6$** was obtained from **S3** (0.52 g, 3.44 mmol) as a brown oil (0.51 g, 82%) following the same procedure as for **S1a**.

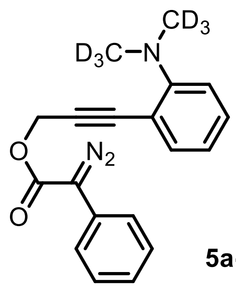
MW ($C_{11}H_7D_6NO$): 181.27 g/mol; **Rf:** 0.25 (Hexanes/EtOAc 7:3); **^{1}H NMR ($CDCl_3$, 400 MHz):** δ_H 7.38 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.27 – 7.22 (m, 1H, (overlapped with chloroform)), 6.93 (d, *J* = 1.1 Hz, 1H), 6.92 (dd, *J* = 8.2, 1.1 Hz, 1H), 4.55 (s, 2H), 2.21 (broad s, 1H). **^{13}C{H} NMR ($CDCl_3$, 101 MHz):** δ_C 155.1, 134.5, 129.6, 121.0, 117.2, 115.1, 92.7, 84.9, 52.0 (carbons bonded to deuterium are not observed in the spectrum with the standard acquisition parameters). **IR (ATR) ν (cm^{-1}):** 3290, 2918, 1590, 1483, 1021, 752. **HRMS (ESI)m/z:** calcd. for $C_{11}H_8D_6NO$ [M+H]$^+$ 182.1447; Found 182.1456.



S2a-d$_6$

Ester **S2a-d$_6$** was obtained from **S1a-d$_6$** (0.39 g, 2.15 mmol) as an orange oil (0.57 g, 88%) following the same procedure as for **S2a.**

MW ($C_{19}H_{13}D_6NO_2$): 299.40 g/mol; **Rf:** 0.55 (Hexanes/EtOAc 8:2); **^{1}H NMR ($CDCl_3$, 400 MHz):** δ_H 7.39 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.34 – 7.26 (m, 6H), 7.25 – 7.23 (m, 1H), 6.91 – 6.82 (m, 2H), 4.99 (s, 2H), 3.70 (s, 2H). **^{13}C{H} NMR ($CDCl_3$, 101 MHz):** δ_C 171.0, 155.3, 134.8, 133.8, 129.8, 129.4, 128.7, 127.3, 120.5, 117.0, 114.1, 88.1, 86.1, 53.8, 41.3 (carbons bonded to deuterium are not observed in the spectrum with the standard acquisition parameters). **IR (ATR) ν (cm^{-1}):** 2918, 1736, 1485, 1131, 751. **HRMS (ESI)m/z:** calcd. for $C_{19}H_{13}D_6NO_2Na$ [M+Na]$^+$ 322.1685; Found 322.1691.



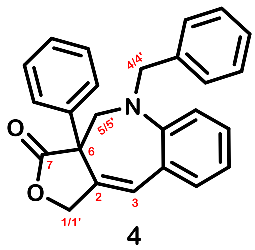
5a-d$_6$

Diazo **5a-d_6** was obtained from **S2a-d_6** (0.32 g, 1.07 mmol) as an orange solid (0.26 g, 75%) following the same procedure as for **5a.**

MW ($C_{19}H_{11}D_6N_3O_2$): 325.40 g/mol; **Rf:** 0.58 (Hexanes/EtOAc 8:2); **^{1}H NMR ($CDCl_3$, 400 MHz):** δ_H 7.54 – 7.45 (m, 2H), 7.45 – 7.34 (m, 3H), 7.31 – 7.23 (m, 2H, (overlapped with chloroform)), 7.23 – 7.17 (m, 1H), 6.89 (dd, *J* = 8.0, 1.1 Hz, 1H), 6.86 (td, *J* = 8.0, 1.1 Hz, 1H), 5.17 (s, 2H). **^{13}C{H} NMR ($CDCl_3$, 101 MHz):** δ_C 164.6, 155.3, 134.8, 129.9, 129.1, 126.1, 125.4, 124.2, 120.5, 117.0, 114.0, 88.1, 86.4, 53.7 (carbons bonded to deuterium are not observed in the spectrum with the standard acquisition parameters). **IR (ATR) ν (cm^{-1}):** 2927, 2085, 1700, 1242, 1143, 748. **HRMS (ESI) m/z:** calcd. for $C_{19}H_{11}D_6N_3O_2Na$ $[M+Na]^+$ 348.1590; Found 348.1589.

S7. Silver catalyzed carbene/alkyne metathesis tandem reaction.

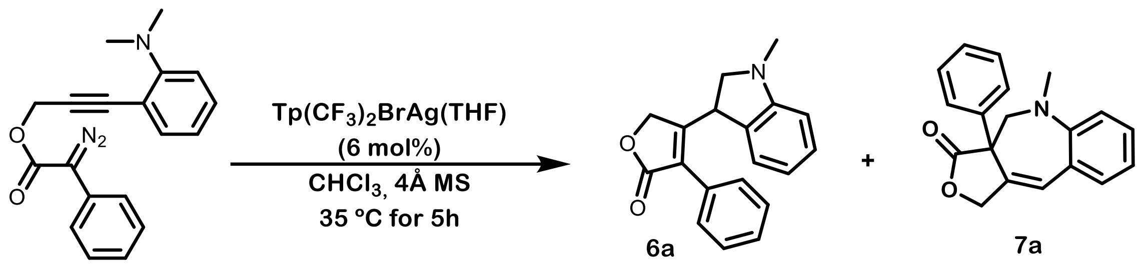
S7.1. NMR Characterization of compound 4



4

MW ($C_{25}H_{21}NO_2$): 367.15 g/mol; **Rf:** 0.53 (Hexanes/EtOAc 8:2)**; ^{1}H NMR ($CDCl_3$, 400 MHz):** δ_H 7.50 – 7.43 (m, 2H, **H_{Ph}**), 7.38 – 7.19 (m, 7H, **H_{Ph}** (overlapped with chloroform), 7.10 – 7.04 (m, 1H, **H_{Ph}**), 6.97 (d, J = 7.0 Hz, 2H, **H_{Ph}**), 6.86 (s, 1H, **H_3**), 6.83 (d, *J* = 7.0 Hz, 1H, **H_{Ph}**), 6.66 (d, *J* = 8.3 Hz, 1H, **H_{Ph}**), 4.93 (dd, *J* = 11.8, 1.8 Hz, 1H, **$H_{1/1'}$**), 4.84 (d, *J* = 11.8 Hz, 1H, **$H_{1/1'}$**), 4.25 (d, *J* = 18.1 Hz, 1H, **$H_{4/4'}$**,), 4.16 (d, *J* = 13.8 Hz, 1H, **$H_{5/5'}$**), 3.40 (d, *J* = 18.1 Hz, 1H, **$H_{4/4'}$**), 3.34 (dd, *J* = 13.8, 1.6 Hz, 1H, **$H_{5/5'}$**).**^{13}C{H} NMR ($CDCl_3$, 101 MHz):** δ_C 175.6 (**C_7**), 148.9 (**C_{Ph}**), 138.3 (**C_{Ph}**), 136.0 (**C_{Ph}**), 134.9 (**C_{Ph}**), 133.7 (**C_2**), 129.5 (**C_3**), 129.2 (**C_{Ph}**), 128.8 (**C_{Ph}**), 128.4 (**C_{Ph}**), 127.7 (**C_{Ph}**), 127.1 (**C_{Ph}**), 126.2 (**C_{Ph}**), 120.9 (**C_{Ph}**), 118.7 (**C_{Ph}**), 116.7 (**C_{Ph}**), 71.0 (**C_1**), 58.6 (**C_4**), 58.4 (**C_6**), 57.0 (**C_5**).

S7.2. Optimization of silver catalyzed carbene/alkyne metathesis tandem reaction[a]

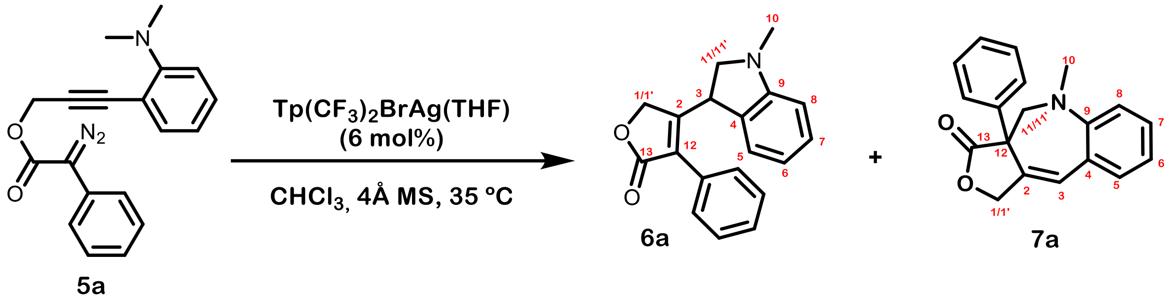


5a 6a 7a

Entry	Deviation from standard conditions[b]	Yield (%) (**6a** / **7a**)
1	none	81 (10 / 71)
2	CH_2Cl_2 as solvent	90 (19 / 71)
3	MS beads[b] instead of powdered MS	84 (19 / 65)
4	45ºC	72 (13 / 59)
5	RT	67 (10 / 57)
6	CH_2Cl_2 as solvent at RT	57 (12 / 45)
7	DCE as solvent at RT	28 (5 / 23)[c,e]
8	Chlorobenzene as solvent at RT	44 (13 / 41)[d,e]
9	Dichlorobenzene as solvent at RT	36 (10 / 26)[e]
10	1,2-DCP as solvent at RT for 17h	NR[e]
11	$[TpBr_3Ag]_2$ as catalyst and CH_2Cl2 as solvent at RT	69 (34 / 35)
12	Tp*BrAg(THF) as catalyst and CH_2Cl_2 as solvent at RT for 24h	NR

[a] Standard conditions: Unless otherwise noted, reactions were carried out with 0.06 mmol of 5a ([5a] = 3.8 mM), at room temperature in 16 mL of $CHCl_3$ for 5h. The yields given are isolated yields. [b] All of the reactions in Table were carried out with 4 Å MS beads except for those shown in entry 1 and 2 that were carried out with powdered 4 Å MS. [c] 26% starting material was recovered. [d] 14% starting material was recovered. [e] Yields and product ratios were determined by NMR using 1,3,5-trimethoxybenzene as internal standard. RT, room temperature; NR, no reaction.

S7.3. General procedure for the silver catalyzed carbene/alkyne metathesis tandem reaction

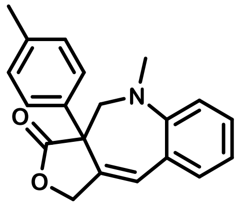


To an oven-dried Schlenk flask containing diazo compound **5a** (18.5 mg, 0.0580 mmol) and 4Å MS (100 mg) in anhydrous chloroform (14.4 mL), a solution of $Tp(CF_3)_2BrAg(THF)$ (3.6 mg, 0.0035 mmol) in chloroform (0.6 mL) was added dropwise under a nitrogen atmosphere. The mixture was then heated to 35ºC and stirred in the dark for 5h. The solvent was then removed under reduced pressure and the crude reaction mixture was purified by column chromatography on silica gel using hexane/EtOAc mixtures as the eluent (96:4 to 75:25). Concentration under reduced pressure afforded compound **7a** (12.0 mg, 71% yield) as a colorless solid, and **6a** (1.7 mg, 10% yield) as a colorless solid.

A mmol scale reaction was carried using the following amounts of materials: diazo compound **5a** (320.5 mg, 1.00 mmol), 4Å MS (1000 mg), anhydrous chloroform (251 mL + 3 mL (for the catalyst addition)) and $Tp(CF_3)_2BrAg(THF)$ (62.2 mg, 0.06 mmol) affording compound **7a** (166.7 mg, 57% yield), and **6a** (28.4 mg, 10 % yield).

7a: MW ($C_{19}H_{17}NO_2$): 291.35 g/mol; **Rf:** 0.53 (Hexanes/EtOAc 8:2). **MP (ºC):** 165. **^{1}H NMR ($CDCl_3$, 400 MHz):** δ_H 7.47 – 7.40 (m, 2H, **H_{Ph}**), 7.34 – 7.27 (m, 3H, **H_{Ph}**), 7.26 (m, 1H, **H5** (overlapped with chloroform)), 7.20 (ddd, *J* = 8.6, 7.4, 1.7 Hz, 1H, **H7**), 6.84 (td, *J* = 7.4, 1.1 Hz, 1H, **H6**), 6.80 (broad s, 1H, **H3**), 6.73 (d, *J* = 7.5 Hz, 1H, **H8**), 4.91 (dd, *J* = 11.3, 1.9 Hz, 1H, **H1/1'**), 4.80 (dd, *J* = 11.3, 1.0 Hz, 1H, **H1/1'**), 3.98 (d, *J* = 13.5 Hz, 1H, **H11/11'**), 3.17 (d, *J* = 13.5 Hz, 1H, **H11/11'**), 2.52 (s, 3H, **H10**). **^{13}C{H} NMR ($CDCl_3$, 101 MHz):** δ_C 175.7 (**C13**), 149.1(**C9**), 136.7 (**C_{Ph}**), 134.8 (**C5**), 133.5 (**C2**), 129.5 (**C3**), 129.0 (**C7**), 128.6 (**C_{Ph}**), 128.1 (**C_{Ph}**), 127.5 (**C_{Ph}**), 121.1 (**C4**), 118.3 (**C6**), 115.2 (**C8**), 71.1 (**C1**), 59.1 (**C11**), 58.3 (**C12**), 42.3 (**C10**). **IR (ATR) ν (cm^{-1}):** 3016, 2858, 1753, 1491, 756. **HRMS (ESI) m/z:** calcd. for $C_{19}H_{17}NO_2Na$ $[M+Na]^+$ 314.1151; Found 314.1149.

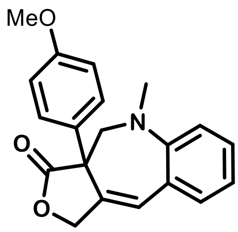
6a: MW ($C_{19}H_{17}NO_2$): 291.35 g/mol; **Rf:** 0.27 (Hexanes/EtOAc 8:2). **MP (ºC):** 139. **^{1}H NMR ($CDCl_3$, 400 MHz):** δ_H 7.56 – 7.39 (m, 5H, **H_{Ph}**), 7.18 (t, *J* = 7.9 Hz, 1H, **H7**), 7.00 (d, *J* = 7.5 Hz, 1H,**H5**), 6.73 (td, *J* = 7.5, 1.0 Hz, 1H, **H6**), 6.57 (d, *J* = 7.9 Hz, 1H, **H8**), 4.88 (d, *J* = 17.8, 1H, **H1/1'**), 4.70 (dd, *J* = 8.8, 6.2 Hz, 1H, **H3**), 4.63 (d, J = 17.9 Hz, 1H, **H1/1'**), 3.58 (t, *J* = 8.8 Hz, 1H, **H11/11'**), 3.30 (dd, *J* = 8.8, 6.2 Hz, 1H, **H11/11'**), 2.79 (s, 3H, **H10**). **^{13}C{H} NMR ($CDCl_3$, 101 MHz):** δ_C 173.3 (**C13**), 161.7 (**C2**), 153.1 (**C9**), 129.8 (**C4**), 129.3 (**C7**), 129.2 (**C_{Ph}**), 129.1 (**C_{Ph}**), 129.0 (**C$_{Ph}$**), 128.9 (**C$_{Ph}$**), 127.7 (**C12**), 124.4 (**C5**), 118.9 (**C6**), 108.3 (**C8**), 69.5 (**C1**), 61.4 (**C11)**, 39.9 (**C3**), 36.0 (**C10**). **IR (ATR) *ν* (cm^{-1}):** 2918, 2853, 1742, 1127, 736. **HRMS (ESI) m/z:** calcd. for $C_{19}H_{17}NO_2Na$ [M+Na]$^+$ 314.1151; Found 314.1157.



7b

Starting from diazo compound **5b (**33.7 mg, 0.10 mmol)**,** compound **7b** was obtained as a yellow oil (17.7 mg, 57 % yield), alongside **6b** (6.7 mg, 22% yield).

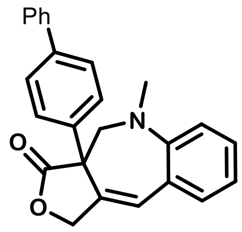
MW ($C_{20}H_{19}NO_2$): 305.38 g/mol; **Rf:** 0.48 (Hexanes/EtOAc 8:2); **^{1}H NMR (CDCl$_3$, 400 MHz): δ_H** 7.31 (*d*, J = 8.4 Hz, 2H), 7.26-7.24 (m, 1H (overlapped with chloroform)), 7.19 (ddd, *J* = 8.8, 7.3, 1.7 Hz, 1H), 7.11 (d, *J* = 8.4 Hz, 2H), 6.83 (td, *J* = 7.3, 1.1 Hz, 1H), 6.77 (broad s, 1H), 6.73 (d, *J* = 8.8 Hz, 1H), 4.90 (dd, *J* = 11.3, 1.9 Hz, 1H), 4.78 (dd, *J* = 11.3, 1.1 Hz, 1H), 3.96 (d, *J* = 13.5 Hz, 1H), 3.15 (d, *J* = 13.5 Hz, 1H), 2.55 (s, 3H), 2.32 (s, 3H). **^{13}C{H} NMR (CDCl$_3$, 101 MHz): δ_C** 175.8, 149.2, 137.9, 134.7, 133.8, 133.7, 129.3, 129.2, 129.0, 127.4, 121.2, 118.2, 115.1, 71.1, 59.0, 58.0, 42.4, 21.2. **IR (ATR) *ν* (cm^{-1}):** 3018, 2876, 1758, 1494, 745. **HRMS (ESI) m/z:** calcd. for $C_{20}H_{19}NO_2Na$ [M+Na]$^+$ 328.1308; Found 328.1313.



7c

Starting from diazo compound **5c** (35.1 mg, 0.10 mmol), compound **7c** was obtained as a yellow oil (13.5 mg, 42 % yield), alongside **6c** (8.9 mg, 28% yield).

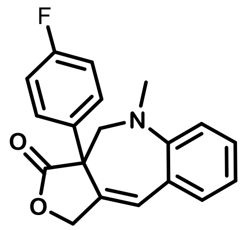
MW ($C_{20}H_{19}NO_3$): 321.38 g/mol; **Rf:** 0.38 (Hexanes/EtOAc 8:2); **^{1}H NMR (400 MHz, CDCl$_3$) δ (ppm):** 7.37 – 7.31 (m, 2H), 7.28 – 7.24 (m, 1H (overlapped with chloroform)), 7.20 (ddd, *J* = 8.6, 7.2, 1.7 Hz, 1H), 6.86 – 6.80 (m, 3H), 6.76 (broad s, 1H), 6.74 (d, *J* = 8.6 Hz, 1H), 4.90 (dd, *J* = 11.3, 1.9 Hz, 1H), 4.78 (d, *J* = 11.3 Hz, 1H), 3.92 (d, *J* = 13.5 Hz, 1H), 3.78 (s, 3H), 3.14 (d, *J* = 13.5 Hz, 1H), 2.56 (s, 3H). **^{13}C{H} NMR (CDCl$_3$, 101 MHz): δ_C** 175.9, 159.5, 149.2, 134.7, 133.9, 129.1, 129.0, 128.8, 128.7, 121.2, 118.2, 115.2, 113.9, 71.1, 59.0, 57.6, 55.4, 42.4. **IR (ATR) *ν* (cm^{-1}):** 3060, 2849, 1756, 1494, 746. **HRMS (ESI) m/z:** calcd. for $C_{20}H_{19}NO_3Na$ [M+Na]$^+$ 344.1257; Found 344.1260.



7d

Starting from diazo compound **5d** (23.8 mg, 0.060 mmol)**,** compound **7d** was obtained as a colorless solid (9.3 mg, 42 % yield), alongside **6d** (7.4 mg, 33% yield).

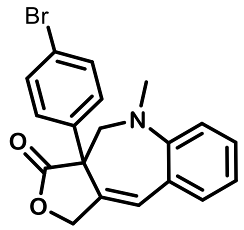
MW ($C_{25}H_{21}NO_2$): 367.45 g/mol; **Rf:** 0.53 (Hexanes/EtOAc 8:2); **MP (ºC):** 99; **^{1}H NMR ($CDCl_3$, 400 MHz):** δ_H 7.60 – 7.48 (m, 6H), 7.47 – 7.40 (m, 2H), 7.38 – 7.32 (m, 1H), 7.29 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.21 (ddd, *J* = 8.4, 7.6, 1.7 Hz, 1H), 6.85 (td, *J* = 7.6, 1.1 Hz, 1H), 6.82 (broad s, 1H), 6.75 (d, *J* = 8.4 Hz, 1H), 4.95 (dd, J = 11.4, 1.9 Hz, 1H), 4.83 (d, J = 11.4 Hz, 1H), 4.03 (d, *J* = 13.6 Hz, 1H), 3.20 (d, *J* = 13.6 Hz, 1H), 2.59 (s, 3H). **^{13}C{H} NMR ($CDCl_3$, 101 MHz):** δ_C 175.7, 149.1, 140.9, 140.4, 135.8, 134.8, 133.5, 129.5, 129.1, 129.0, 128.0, 127.7, 127.2, 127.1, 121.2, 118.3, 115.2, 71.2, 59.0, 58.1, 42.5. **IR (ATR) ν (cm^{-1}):** 3027, 2875, 1721, 1493, 746. **HRMS (ESI) m/z:** calcd. for $C_{25}H_{21}NO_2Na$ $[M+Na]^+$ 390.1465; Found 390.1477.



7e

Starting from diazo compound 5**e** (38.0 mg, 0.11 mmol)**,** compound **7e** was obtained as a colorless solid (10.5 mg, 31 % yield), alongside **6e** (11.5 mg, 34 % yield).

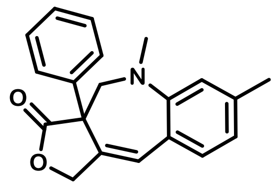
MW ($C_{19}H_{16}FNO_2$): 309.34 g/mol; **Rf:** 0.58 (Hexanes/EtOAc 8:2); **MP (ºC):** 126; **^{1}H NMR ($CDCl_3$, 400 MHz):** δ_H 7.46 – 7.37 (m, 2H), 7.29 – 7.25 (m, 1H, (overlapped with chloroform)), 7.21 (ddd, *J* = 8.4, 7.3, 1.7 Hz, 1H), 7.05 – 6.95 (m, 2H), 6.85 (td, *J* = 7.3, 1.2 Hz, 1H), 6.79 (broad s, 1H), 6.74 (d, *J* = 8.4 Hz, 1H), 4.89 (dd, *J* = 11.4, 1.9 Hz, 1H), 4.81 (d, *J* = 11.4 Hz, 1H), 3.93 (d, *J* = 13.6 Hz, 1H), 3.16 (d, *J* = 13.6 Hz, 1H), 2.55 (s, 3H). **^{13}C{H} NMR ($CDCl_3$, 101 MHz):** δ_C 175.6, 162.7 (d, $^1J_{C-F}$ = 248.4 Hz), 149.0, 134.9, 133.3, 132.5 (d, $^4J_{C-F}$ = 3.2 Hz), 129.6, 129.3, 129.2 (d, $^3J_{C-F}$ = 6.2 Hz), 121.0, 118.5, 115.6, 115.3 (d, $^2J_{C-F}$ = 23.4 Hz), 71.1, 59.0, 57.8, 42.4. **^{19}F NMR ($CDCl_3$, 376 MHz):** δ_F -115.16. (s, 1F). **IR (ATR) ν (cm^{-1}):** 3014, 2851, 1749, 1491, 759. **HRMS (ESI) m/z:** calcd. for $C_{19}H_{16}FNO_2Na$ $[M+Na]^+$ 332.1057; Found 332.1069.



7f

The reaction was run at 55ºC for 24h instead of 35ºC for 5h. Starting from diazo compound **5f** (23.2 mg, 0.058 mmol)**,** compound **7f** was obtained as a colorless solid (5.0 mg, 24 % yield), alongside **6f** (8.1 mg, 38 % yield).

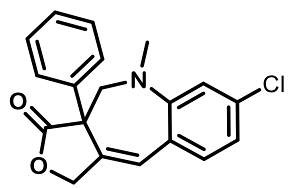
MW ($C_{19}H_{16}BrNO_2$): 370.25 g/mol; **Rf:** 0.61 (Hexanes/EtOAc 8:2); **MP (ºC):** 77; **^{1}H NMR ($CDCl_3$, 400 MHz):** δ_H 7.48 – 7.40 (m, 2H), 7.35 – 7.29 (m, 2H), 7.28 – 7.25 (m, 1H , (overlapped with chloroform)), 7.21 (ddd, *J* = 8.5, 7.3, 1.7 Hz, 1H), 6.85 (td, *J* = 7.3, 1.2 Hz, 1H), 6.80 (s, 1H), 6.75 (d, *J* = 8.5 Hz, 1H), 4.88 (dd, *J* = 11.4, 1.9 Hz, 1H), 4.80 (d, *J* = 11.4 Hz, 1H), 3.94 (d, *J* = 13.6 Hz, 1H), 3.16 (d, *J* = 13.6 Hz, 1H), 2.57 (s, 3H). **^{13}C{H} NMR ($CDCl_3$, 101 MHz):** δ_C 175.3, 149.0, 135.9, 134.9, 132.8, 131.8, 129.9, 129.3, 129.3, 122.5, 121.0, 118.5, 115.2, 71.1, 59.0, 58.0, 42.6. **IR (ATR) ν (cm^{-1}):** 3066, 2880, 1764, 1481, 1003, 753. **HRMS (ESI) m/z:** calcd. for $C_{19}H_{16}BrNO_2Na$ [M+Na]$^+$ 392.0257-394.0237; Found 392.0244-394.0233.



7g

Starting from diazo compound **5g** (19.2 mg, 0.058 mmol), compound **7g** was obtained as a colorless solid (10.6, 60% yield)), alongside **6g** (1.2 mg, 7 % yield).

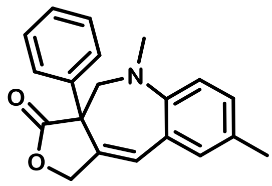
MW ($C_{20}H_{19}NO_2$): 305.38 g/mol; **Rf:** 0.55 (Hexanes/EtOAc 8:2); **MP (ºC):** 110; **^{1}H NMR ($CDCl_3$,400 MHz):** δ_H 7.46 – 7.41 (m, 2H), 7.34 – 7.27 (m, 3H), 7.16 (d, *J* = 7.8 Hz, 1H), 6.77 (s, 1H), 6.66 (dd, *J* = 7.8, 1.6 Hz, 1H), 6.53 (s, 1H), 4.89 (dd, *J* = 11.2, 1.9 Hz, 1H), 4.78 (d, *J* = 11.2 Hz, 1H), 3.96 (d, *J* = 13.5 Hz, 1H), 3.17 (d, *J* = 13.5 Hz, 1H), 2.51 (s, 3H), 2.32 (s, 3H). **^{13}C{H} NMR ($CDCl_3$, 101 MHz):** δ_C 175.8, 149.0, 139.2, 136.8, 134.8, 132.3, 129.2,128.1, 127.6, 119.4, 118.7, 115.7, 71.2, 59.1, 58.3, 42.3, 21.7. **IR (ATR) ν (cm^{-1}):** 3024, 2848, 1757, 1341, 770. **HRMS (ESI) m/z:** calcd. for $C_{20}H_{19}NO_2Na$ [M+Na]$^+$ 328.1308; Found 328.1312.



7h

Starting from diazo compound **5h** (21.0 mg, 0.59 mmol), compound **7h** was obtained as a colorless solid (13.4 mg, 69 % yield), alongside **6h** (2.3 mg, 12 % yield).

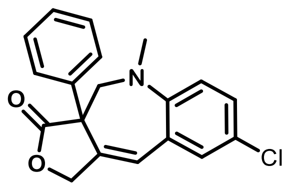
MW ($C_{19}H_{16}ClNO_2$): 325.79 g/mol; **Rf:** 0.55 (Hexanes/EtOAc 8:2); **MP (ºC):** 154; **^{1}H NMR ($CDCl_3$, 400 MHz):** δ_H 7.44 – 7.36 (m, 2H), 7.35 – 7.28 (m, 3H), 7.17 (d, *J* = 8.3 Hz, 1H), 6.80 (dd, *J* = 8.3, 2.1 Hz, 1H), 6.75 (broad s, 1H), 6.68 (d, *J* = 2.1 Hz, 1H), 4.89 (dd, *J* = 11.4, 1.9 Hz, 1H), 4.79 (d, *J* = 11.4 Hz, 1H), 3.98 (d, *J* = 13.6 Hz, 1H), 3.17 (d, *J* = 13.6 Hz, 1H), 2.51 (s, 3H). **^{13}C{H} NMR ($CDCl_3$, 101 MHz):** δ_C 175.4, 149.8, 136.3, 134.9, 133.9, 128.8, 128.4, 128.3, 127.4, 119.7, 118.4, 115.1, 71.0, 59.1, 58.2, 42.5. **IR (ATR) ν (cm^{-1}):** 3030, 2849, 1760, 1491, 702. **HRMS (ESI) m/z:** calcd. for $C_{19}H_{16}ClNO_2Na$ [M+Na]$^+$ 348.0762; Found 348.0769.



7i

Starting from diazo compound **5i** (19.5 mg, 0.059 mmol), compound **7i** was obtained as a colorless solid (11.8 mg, 66 % yield), alongside **6i** (1.7 mg, 10 % yield).

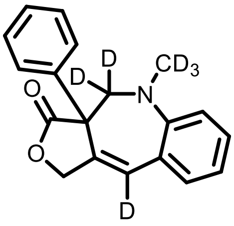
MW ($C_{20}H_{19}NO_2$): 305.38 g/mol; **Rf:** 0.60 (Hexanes/EtOAc 8:2); **MP (ºC):** 158; **^{1}H NMR ($CDCl_3$, 400 MHz):** δ_H 7.47 – 7.40 (m, 2H), 7.34 – 7.27 (m, 3H), 7.07 (d, *J* = 2.2 Hz, 1H), 7.02 (dd, *J* = 8.5, 2.2 Hz, 1H), 6.75 (broad s, 1H), 6.65 (d, *J* = 8.5 Hz, 1H), 4.90 (dd, *J* = 11.4, 1.9 Hz, 1H), 4.78 (d, *J* = 11.4 Hz, 1H), 3.95 (d, *J* = 13.5 Hz, 1H), 3.14 (d, *J* = 13.5 Hz, 1H), 2.50 (s, 3H), 2.30 (s, 3H). **^{13}C{H} NMR ($CDCl_3$,101 MHz):** δ_C 175.7, 147.0, 136.8, 135.0, 133.5, 129.9, 129.4, 128.6, 128.1, 127.5, 127.3, 121.0, 115.2, 71.2, 59.0, 58.4, 42.3, 20.2. **IR (ATR) ν (cm^{-1}):** 3002, 2945, 1738, 1365, 1214. **HRMS (ESI) m/z:** calcd. for $C_{20}H_{19}NO_2Na$ [M+Na]$^+$ 328.1308; Found 328.1315.



7j

Starting from diazo compound **5j** (20.3 mg, 0.057 mmol) compound **7j** was obtained as a colorless solid (10.9 mg, 60 % yield), alongside **6j** (2.0 mg, 11 % yield).

MW ($C_{19}H_{16}ClNO_2$): 325.79 g/mol; **Rf:** 0.54 (Hexanes/EtOAc 8:2); **MP (ºC):** 193**^{1}H NMR ($CDCl_3$, 400 MHz):** δ_H 7.44 – 7.35 (m, 2H), 7.35 – 7.28 (m, 3H), 7.23 (d, *J* = 2.5 Hz, 1H), 7.13 (dd, *J* = 8.9, 2.5 Hz, 1H), 6.70 (broad s, 1H), 6.64 (d, *J* = 8.9 Hz, 1H), 4.91 (dd, *J* = 11.5, 1.9 Hz, 1H), 4.80 (d, *J* = 11.5 Hz, 1H), 3.99 (d, *J* = 13.6 Hz, 1H), 3.13 (d, *J* = 13.6 Hz, 1H), 2.50 (s, 3H). **^{13}C{H} NMR ($CDCl_3$, 101 MHz):** δ_C 175.3, 147.6, 136.3, 135.2, 133.6, 128.7, 128.7, 128.3, 128.2, 127.4, 122.8, 122.3, 116.5, 70.9, 59.0, 58.3, 42.6. **IR (ATR) ν (cm^{-1}):** 3031, 2851, 1742, 1491, 695. **HRMS (ESI) m/z:** calcd. for $C_{19}H_{16}ClNO_2Na$ [M+Na]$^+$ 348.0762; Found 348.0765.

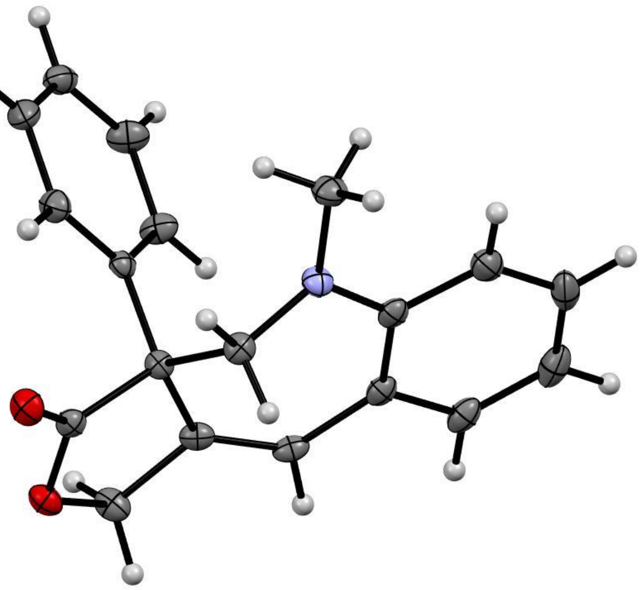


7a-d$_6$

Starting from diazo compound **5a-d6** (19.2 mg, 0.059 mmol) compound **7j** was obtained as a colorless solid (10.6 mg, 60 % yield), alongside **6j** (1.5 mg, 9 % yield).

MW ($C_{19}H_{11}D_6NO_2$): 297.39 g/mol; **Rf:** 0.48 (Hexanes/EtOAc 8:2); **MP (ºC):** 162; **^{1}H NMR (CDCl$_3$, 400 MHz):** δ_H 7.47 – 7.38 (m, 2H), 7.35 – 7.27 (m, 3H), 7.26 (m, 1H (overlapped with chloroform)), 7.20 (ddd, *J* = 8.6, 7.3, 1.7 Hz, 1H), 6.83 (td, *J* = 7.3, 1.2 Hz, 1H), 6.72 (dd, *J* = 8.4, 1.2 Hz, 1H), 4.91 (d, *J* = 11.3 Hz, 1H), 4.80 (d, *J* = 11.3 Hz, 1H). **^{13}C{H} NMR (CDCl$_3$, 101 MHz):** δ_C 175.7, 149.1, 136.7, 134.7, 133.3, 129.0, 128.6, 128.1, 127.5, 121.0, 118.2, 115.1, 71.1, 58.2 (carbons bonded to deuterium are not observed in the spectrum with the standard acquisition parameters). **IR (ATR) ν (cm^{-1}):** 2919, 1752, 1484, 697. **HRMS (ESI) m/z:** calcd. for $C_{19}H_{12}D_6NO_2$ [M+H]$^+$ 298.1709; Found 298.1719.

S8 Crystal structure of compound 7a with probability level of 50 %



Colourless needle-like crystals of **7a** were grown at 2-6 °C upon slow diffusion of pentane into a solution of **7a** in chloroform.

A colorless prism-like specimen of $C_{19}H_{17}NO_2$, approximate dimensions 0.140 mm x 0.260 mm x 0.800 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured on a D8 QUEST ECO three-circle diffractometer system equipped with a Ceramic x-ray tube (Mo Kα, λ = 0.71073 Å) and a doubly curved silicon crystal Bruker Triumph monochromator.A total of 1998 frames were collected. The total exposure time was 16.65 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 56871 reflections to a maximum θ angle of 27.52° (0.77 Å resolution), of which 3353 were independent (average redundancy 16.961, completeness = 99.7%, Rint = 4.32%, Rsig = 1.53%) and 3135 (93.50%) were greater than 2σ(F2). The final cell constants of a = 6.1270(2) Å, b = 22.8523(7) Å, c = 10.9205(3) Å, β = 106.0910(10)°, volume = 1469.14(8) Å3, are based upon the refinement of the XYZ-centroids of 9905 reflections above 20 σ(I) with 6.61° < 2θ < 54.90°. Data were corrected for absorption effects using the Multi-Scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.903. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9350 and 0.9880.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P 1 21/c 1, with Z = 4 for the formula unit, C19H17NO2. The final anisotropic full-matrix least-squares refinement on F2 with 267 variables converged at R1 = 5.40%, for the observed data and wR2 = 11.58% for all data. The goodness-of-fit was 1.261. The largest peak in the final difference electron density synthesis was 0.416 e-/Å3 and the largest hole was -0.231 e-/Å3 with an RMS deviation of 0.049 e-/Å3. On the basis of the final model, the calculated density was 1.317 g/cm3 and F(000), 616 e-.

Sample and crystal data for AD838

Identification code	AD838
Chemical formula	$C_{19}H_{17}NO_2$
Formula weight	291.33 g/mol
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal size	0.140 x 0.260 x 0.800 mm
Crystal habit	colorless prism
Crystal system	monoclinic
Space group	P 1 21/c 1
Unit cell dimensions	a = 6.1270(2) Å α = 90°
	b = 22.8523(7) Å β = 106.0910(10)°
	c = 10.9205(3) Å γ = 90°
Volume	1469.14(8) Å3
Z	4
Density (calculated)	1.317 g/cm3
Absorption coefficient	0.085 mm-1
F(000)	616

Data collection and structure refinement for AD838

Diffractometer	D8 QUEST ECO three-circle diffractometer
Radiation source	Ceramic x-ray tube (Mo Kα, λ = 0.71073 Å)
Theta range for data collection	3.31 to 27.52°
Index ranges	-7<=h<=7, -29<=k<=29, -14<=l<=14
Reflections collected	56871
Independent reflections	3353 [R(int) = 0.0432]
Coverage of independent reflections	99.7%
Absorption correction	Multi-Scan
Max. and min. transmission	0.9880 and 0.9350
Structure solution technique	direct methods
Structure solution program	SHELXT 2014/5 (Sheldrick, 2014)
Refinement method	Full-matrix least-squares on F2
Refinement program	SHELXL-2017/1 (Sheldrick, 2017)
Function minimized	Σ w(Fo2 - Fc2)2
Data / restraints / parameters	3353 / 0 / 267
Goodness-of-fit on F2	1.261

Final R indices	3135 data; I>2σ(I)	R1 = 0.0540, wR2 = 0.1145
	all data	R1 = 0.0574, wR2 = 0.1158
Weighting scheme	w=1/[σ2(Fo2)+(0.0148P)2+1.6317P]	
	where P=(Fo2+2Fc2)/3	
Largest diff. peak and hole	0.416 and -0.231 eÅ-3	
R.M.S. deviation from mean	0.049 eÅ-3	

Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for 7a

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x/a	y/b	z/c	U(eq)
O1	0.3528(2)	0.31854(6)	0.99095(12)	0.0188(3)
O3	0.0529(2)	0.36260(6)	0.02741(13)	0.0212(3)
C2	0.2524(3)	0.35138(7)	0.06265(17)	0.0155(3)
C4	0.4232(3)	0.37001(7)	0.18736(16)	0.0138(3)
C5	0.3256(3)	0.35748(8)	0.30101(17)	0.0162(3)
N6	0.4652(3)	0.38190(7)	0.41873(14)	0.0174(3)
C7	0.6650(3)	0.35509(7)	0.48705(17)	0.0167(3)
C9	0.9395(3)	0.33919(9)	0.69437(19)	0.0252(4)
C8	0.7394(3)	0.36320(8)	0.62008(18)	0.0221(4)
C10	0.0736(3)	0.30502(9)	0.6390(2)	0.0254(4)
C11	0.0022(3)	0.29559(8)	0.50957(19)	0.0205(4)
C12	0.8020(3)	0.32004(7)	0.42956(17)	0.0166(4)
C13	0.7629(3)	0.30694(7)	0.29358(18)	0.0168(4)
C14	0.6163(3)	0.32934(7)	0.19098(17)	0.0154(3)
C15	0.5935(3)	0.30988(9)	0.05696(18)	0.0196(4)
C16	0.4784(3)	0.43520(7)	0.18104(16)	0.0141(3)
C17	0.3069(3)	0.47596(8)	0.13305(18)	0.0201(4)
C18	0.3585(4)	0.53502(9)	0.13035(19)	0.0232(4)
C19	0.5810(3)	0.55414(8)	0.17660(18)	0.0218(4)
C20	0.7514(3)	0.51402(8)	0.2254(2)	0.0239(4)
C21	0.7002(3)	0.45483(8)	0.22770(19)	0.0202(4)
C22	0.3553(3)	0.42485(9)	0.48026(19)	0.0221(4)

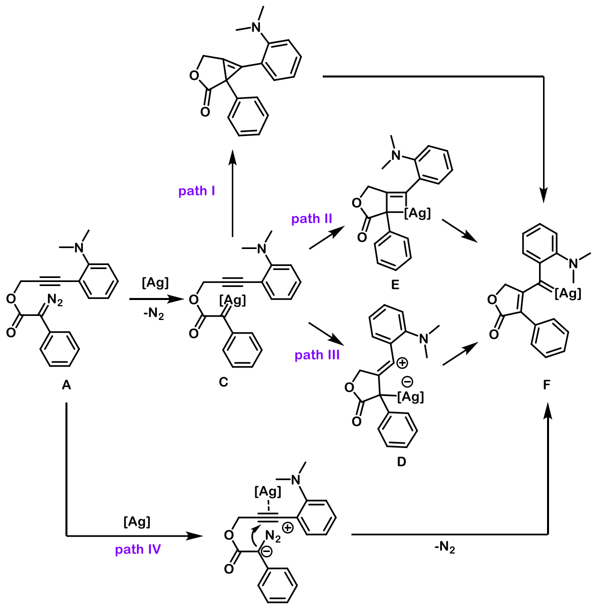
S9 Computational Details

All DFT static calculations were performed with the Gaussian 16 software package.[7] Geometry optimizations were performed without symmetry constraints and with analytical frequency calculations for the characterization of the located stationary points. These frequencies were used to calculate unscaled zero-point energies (ZPEs) as well as thermal corrections and entropy effects at 298 K. For this calculations, we used the BP86 functional of Becke and Perdew,[8],[9],[10] together with the Grimme D3 correction term to the electronic energy.[11] The electronic configuration of the molecular systems was described with the double-ζ basis set with polarization of Ahlrichs for main-group atoms (Def2SVP keyword in Gaussian),[12] whereas for silver atoms the small-core quasi-relativistic Stuttgart/Dresden effective core potential, with an associated valence basis set (standard SDD keywords in Gaussian16) were employed.[13],[14],[15] Energies were obtained by single-point calculations on the optimized geometries with the B3LYP functional,[16],[17] with the Grimme D3 correction term, coupled with the Def2TZVP basis set.[18] Solvent corrections were considered using the universal solvation model SMD of Cramer and Truhlar,[19] using chloroform as the solvent. The reported free energies in this work include energies obtained at the B3LYP-D3/Def2TZVP~sdd level of theory (with solvent corrections included) corrected with zero-point energies, thermal corrections and entropy effects evaluated at 298 K, achieved at the BP86-D3/Def2SVP~sdd level.

S10 Mechanism discussion

S10.1. Formation of vinylcarbene species F

Given the different mechanistic proposals based on literature precedents to obtain the vinylcarbene species **F** from the initial diazo species **A** (Scheme S1), the energy profiles for all the possibilities were studied in detail (Figure S1).



Scheme S1. Plausible mechanistic pathways for the formation of vinylcarbene species **F** from diazo species **A**, based on literature precedents.

Paths **I**, **II** and **III** share the first step of the transformation (already discussed and depicted in Scheme 4 and Figure 1 in the manuscript). Coordination of the silver complex to the carbenic carbon of the diazo species is a mildly endergonic step (3.7 kcal/mol) that is followed by extrusion of nitrogen through transition state **TS-BC** with an overall energy barrier of 11.9 kcal/mol with respect to **A** leading to the silver carbene **C** (-18.9 kcal/mol). On the other hand, path **IV** consists of the coordination of the silver catalyst to the triple bond of diazo species **A** to form intermediate **B1** with a relative energy of -3.2 kcal/mol with respect to isolated reactants. Then, the formation of the C-C bond takes place through transition state **TS-B1C1** with a kinetic cost of 15.9 kcal/mol from the previous minimum (see **Figure S1**). Therefore, given that the barrier to overcome **TS-B1C1** is 4.0 kcal/mol higher in energy than that for **TS-BC**, path **IV** can be discarded.

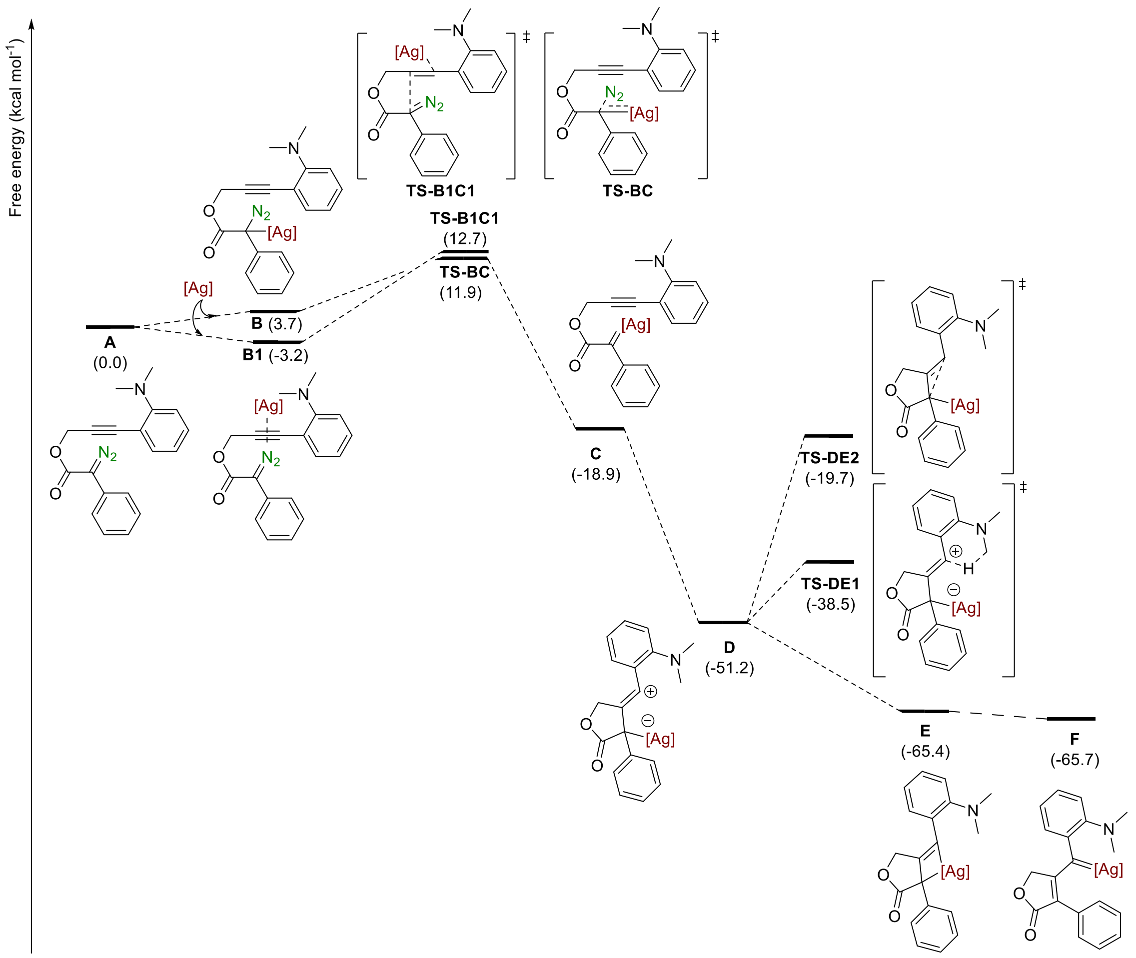


Figure S1. Gibbs energy profile (in kcal/mol) of the studied pathways for the formation of the vinylcarbene species ([Ag] = $Tp^{(CF3)2,Br}Ag$).

Once the carbene species **C** is generated, plausible pathways **I**, **II** and **III** (Scheme S1) are considered. As described in the manuscript, following path **III** silver carbene species **C** is transformed to ylide species **D** in a barrierless process. Ylide species **D** subsequently cyclizes to silver η^3-vinylcarbene **E**, that is the intermediate postulated in pathway **II**. At this point, pathway **I** which leads to the formation of the the ring-fused cyclopropene was considered. The formation of this intermediate from **C** could not be located. However, its formation from ylide intermediate **D** was located and found to have a kinetic cost of 31.5 kcal/mol overcoming **TS-DE2**. Given the barrierless character of the evolution from ylide intermediate **D** to the vinylcarbene species **F**, all the described paths were discarded based on kinetic barriers (Figure S1), and the overall formation of silver η^1-vinylcarbene **F** is postulated based on DFT calculations to proceed through a new pathway that combines previously postulated paths **II** and **III**.

Moreover, the possibility of a H-shift through **TS-DE1** to the carbocation of the ylide intermediate was also considered, showing an energy barrier of 12.7 kcal/mol from **D**. Again, given the barrierless character of the evolution from ylide intermediate **D** to the vinylcarbene species **F**, the possibility of a H-shift was discarded based on kinetic barriers (Figure S1).

S10.2. Kinetic barriers towards vinylogous and carbenic products

Due to the short difference between the kinetic barriers that lead to the vinylogous and carbenic products,[20],[21],[22] a benchmark study was carried out. In all cases, the kinetic cost to obtain the vinylogous product is lower than the one to obtain the carbenic product. The $\Delta\Delta G^{\ddagger}$ values are in the 0.4 – 5.8 kcal/mol range as shown in Table S1.

Table S1. Benchmark study of the selectivity step for the formation of the vinylogous **7a** and carbenic **7a** products. Energies reported in kcal/mol.

Level of theory for the solvent single point calculations[a]	$\Delta G^{\ddagger}$ vinylogous (kcal/mol)	$\Delta G^{\ddagger}$ carbenic (kcal/mol)	$\Delta\Delta G^{\ddagger}$ (kcal/mol)
B3LYP/6-31G**	8.0	10.2	2.2
B3LYP/Def2SVP	7.5	9.5	2.0
B3LYP/Def2TZVP	10.5	10.9	0.4
B3LYP/Def2TZVP-PCM	10.1	10.6	0.4
BP86/6-31G**	6.2	9.3	3.1
BP86/Def2SVP	5.6	8.7	3.0
BP86/Def2TZVP	8.3	10.1	1.8
M06/6-31G**	5.9	11.6	5.6
M06/Def2SVP	5.0	10.8	5.8
M06/Def2TZVP	7.8	12.1	4.3
PBE/6-31G**	5.0	8.3	3.3
PBE/Def2SVP	4.4	7.6	3.2
PBE/Def2TZVP	7.1	9.2	2.1

[a]All optimizations were carried out at the BP86-D3/Def2SVP-SDD level of theory. Single point solvent calculations were carried out in the indicated levels of theory using the SMD solvation model in chloroform unless noted.

As a further test to confirm the accuracy of the chosen level of theory, the structure of **G**, **TS-GH** and **TS-GI** were optimized for substrates **5a** to **5f** of the manuscript. By means of transition state theory (TST) the vinylogous/carbenic product ratio was calculated and compared to the experimental results as shown in Table S2. For substrates **5a** to **5d** the DFT calculation predict that the vinylogous product is favored over the carbenic one as experimentally observed, for **5e** both products are predicted to be formed in a 1:1 ratio and were observed to be formed in 0.9:1 ratio, and finally for **5f** the carbenic product (**6f**) is computed to be favored over the vinylogous one (**7f**) as observed experimentally.

Table S2. Energy barrier difference (in kcal/mol) for the formation of the vinylogous and carbenic products calculated at the B3LYP-D3/Def2TZVP-SDD-SMD($CHCl_3$)//BP86-D3/Def2SVP-SDD level of theory.

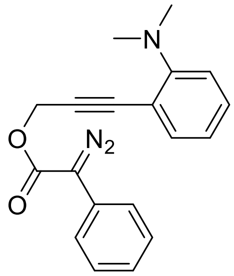
Species	$\Delta\Delta G^{\ddagger}$ (kcal/mol) vinylogous/carbenic ratio	Experimental vinylogous/carbenic ratio
7a	0.4 (2:1)	71%/10% (7.1:1)
7b	0.9 (4.6:1)	57%/22% (2.6:1)
7c	1.4 (10.6:1)	42%/28% (1.5:1)
7d	1.3 (9.0:1)	42%/33% (1.3:1)
7e	0.0 (1:1)	30%/33% (0.9:1)
7f	-1.2 (0.1:1)	23%/38% (0.6:1)

S10.3. Steric hindrance towards vinylogous and carbenic products

Table S3. Percentage buried volume (%V_{Bur}) around the vinylogous and carbenic carbon atoms in the common minima **G** and their respective transition states **TS-GH** and **TS-GI** (with a radius of 3.5 Å).

		Vinylogous	Carbenic
G	With Hydrogens	88.4	96.3
	Without Hydrogens	86.9	94.9
TS-GH	With Hydrogens	92.5	
	Without Hydrogens	90.6	
TS-GI	With Hydrogens		95.8
	Without Hydrogens		94.5

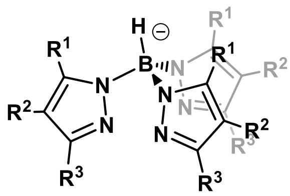
S11 XYZ Coordinates



41

A SCF Done: -1048.14032018 A.U.

C	-1.492006	-1.066830	-0.818456
C	-2.857448	-0.711982	-0.652870
C	-3.652199	-1.297404	0.340585
C	-3.122367	-2.269845	1.211189
C	-1.772156	-2.620406	1.093407
C	-0.939305	-2.023385	0.113600
H	-3.306304	0.025887	-1.332340
H	-4.710502	-1.001814	0.423893
H	-3.752561	-2.737334	1.982781
H	-1.319348	-3.342308	1.790517
C	0.471117	-2.210744	0.157899
C	1.701449	-2.226676	0.171701
C	3.111895	-1.859886	0.191333
H	3.511043	-1.862916	1.232690
H	3.735215	-2.568495	-0.394748
C	2.459017	0.463517	-0.497563
C	1.653862	0.790739	0.697743
C	0.452333	1.666851	0.662149
C	0.469924	2.884950	-0.055411
C	-0.726252	1.276242	1.338402
C	-0.677125	3.693546	-0.090033
H	1.380465	3.177156	-0.595953
C	-1.868802	2.089858	1.298028
H	-0.760890	0.308857	1.863791
C	-1.848291	3.302453	0.585404
H	-0.654978	4.640149	-0.652983
H	-2.785624	1.758753	1.809631
H	-2.745892	3.939902	0.551579
O	3.371624	-0.566511	-0.440013
O	2.376760	1.113891	-1.527616
N	1.973210	0.253468	1.857568
N	2.261749	-0.213435	2.868881
C	0.184546	-1.227757	-2.656692
H	1.191628	-0.762840	-2.718362
H	0.298302	-2.264398	-2.295781
H	-0.247015	-1.268879	-3.686165
C	-1.073855	0.833095	-2.331676
H	-1.768418	0.747203	-3.205237
H	-1.545318	1.464246	-1.555382
H	-0.152878	1.354563	-2.664717
N	-0.692106	-0.455002	-1.778539



Tp^x

	R^3	R^2	R^1
Tp$^{(CF3)2,Br}$	CF_3	Br	CF_3

45

TpCF3BrAg SCF Done: -10590.3609159 A.U.

Ag	-0.000321	-0.000219	-2.243122
N	0.111417	1.795079	-0.751518
N	0.383281	1.424890	0.517694
N	1.498804	-0.994361	-0.751358
N	1.041989	-1.044926	0.517750
N	-1.610978	-0.801473	-0.751285
N	-1.426378	-0.380445	0.517780
B	-0.000402	-0.000124	1.043779
C	0.583934	3.037701	-0.925021
C	1.176679	3.508280	0.275112
C	1.036196	2.436063	1.175036
C	2.339330	-2.024407	-0.924644

	C 2.450641 -2.772901 0.275553 C 1.591633 -2.115646 1.175217 C -2.923366 -1.013806 -0.924738 C -3.627317 -0.735326 0.275244 C -2.628574 -0.320374 1.175039 H -0.000212 0.000031 2.244752 C 0.408284 3.738342 -2.249249 F -0.582424 4.655784 -2.202540 F 1.539047 4.365975 -2.630671 F 0.084469 2.841238 -3.230758 C 1.520313 2.277151 2.598571 F 0.495352 2.128056 3.468463 F 2.314045 1.178448 2.706631 F 2.242227 3.344567 2.989411 C -3.441770 -1.517015 -2.248893 F -4.552574 -0.854254 -2.629476 F -2.503831 -1.346088 -3.230792 F -3.737541 -2.834520 -2.202658 C -2.733188 0.179106 2.598285 F -2.178485 1.415848 2.705827 F -4.018643 0.270957 2.988782 F -2.091876 -0.633623 3.468703 C 3.034119 -2.222292 -2.248832 F 4.322911 -1.819406 -2.202978 F 3.015745 -3.515800 -2.628879 F 2.416877 -1.496023 -3.231002 C 1.212044 -2.455518 2.598741 F -0.136312 -2.593241 2.707038 F 1.775277 -3.614654 2.989297 F 1.595820 -1.493502 3.468609 Br 3.542544 -4.277560 0.547032 Br 1.934951 5.205748 0.546238 Br -5.476471 -0.927459 0.546446
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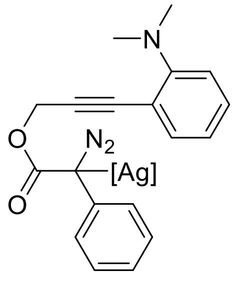	86 B SCF Done: -11638.5377222 A.U. C 7.631388 0.137612 -0.604987 C 8.885248 -0.313715 -0.107243 C 8.969043 -1.171200 0.997061 C 7.807027 -1.625076 1.650553 C 6.559851 -1.176774 1.202271 C 6.447351 -0.280079 0.105933 H 9.811171 -0.014383 -0.618433 H 9.961256 -1.506941 1.339190 H 7.875555 -2.306783 2.511783 H 5.634641 -1.474222 1.717138 C 5.160515 0.247585 -0.201745 C 4.029125 0.664641 -0.435022 C 2.698480 1.091419 -0.821247 H 1.917359 0.407046 -0.415852 H 2.454587 2.107883 -0.449819 C 1.946628 0.399871 -3.130349 C 1.241126 -0.857787 -2.594797 C 1.838625 -1.865668 -1.622983 C 3.233610 -2.068628 -1.594260

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	H	4.883103	-3.113398	-0.649943
	H	0.894692	-4.219217	0.687095
	H	3.386844	-4.503150	0.820710
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	F	-2.460288	-1.167205	-3.847318
	F	-1.857866	-2.916571	-2.683351
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	C	-5.428522	0.293532	0.914098
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	F	-2.028303	-3.730745	3.007097
	F	-3.347071	-2.159513	2.258542
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	C	-0.053201	3.720915	-1.716772
	F	-0.620045	4.871745	-2.132808
	F	1.259622	3.971091	-1.478953
	F	-0.122727	2.830662	-2.741335
	C	-2.132519	3.018211	2.970464
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	F	-1.799560	4.203486	3.517370
	F	-3.478715	2.893858	3.038877
	Br	-0.529807	5.654790	1.114998
	Br	-6.333770	-1.611422	-1.986352
	Br	1.035489	-3.458187	3.548006
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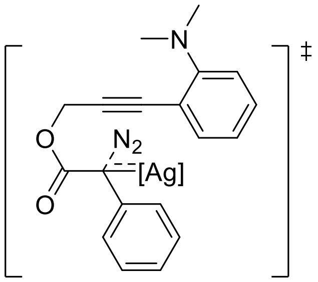
	C	6.515790	0.811568	-2.733649

	H 6.988147 0.739965 -3.739511 H 5.949816 -0.124169 -2.569590 H 5.784196 1.648828 -2.746547 C 8.716928 1.730029 -2.141019 H 9.429184 1.140467 -2.771592 H 8.382237 2.602115 -2.740219 H 9.269459 2.122859 -1.264096
	86 TS-BC SCF Done: -11638.5236538 A.U. C 7.019519 0.009207 -0.940668 C 8.211946 -0.751139 -0.850107 C 8.818608 -1.016591 0.388020 C 8.260768 -0.524720 1.581538 C 7.071902 0.214954 1.525552 C 6.429132 0.475962 0.291727 H 8.688463 -1.123729 -1.767934 H 9.751064 -1.602843 0.414734 H 8.740912 -0.728282 2.550688 H 6.589481 0.571894 2.448057 C 5.126351 1.048578 0.260498 C 3.961790 1.409204 0.110764 C 2.611756 1.673365 -0.358407 H 1.873070 0.950255 0.061831 H 2.245581 2.686308 -0.097353 C 2.442465 0.513151 -2.550380 C 1.733038 -0.637077 -1.865464 C 2.463290 -1.551118 -0.969744 C 3.883263 -1.578940 -0.963365 C 1.750160 -2.452123 -0.129561 C 4.571571 -2.444103 -0.102267 H 4.455053 -0.900790 -1.618002 C 2.442150 -3.344707 0.692851 H 0.647344 -2.447040 -0.141562 C 3.851656 -3.328942 0.720091 H 5.672159 -2.421839 -0.077145 H 1.884667 -4.042529 1.333774 H 4.391068 -4.014721 1.392472 O 2.621876 1.642442 -1.818816 O 2.747424 0.527270 -3.732405 Ag -0.254148 -0.143133 -1.347197 N -2.287823 -1.036214 -0.912611 N -3.079378 -0.447943 0.001863 N -1.297897 1.800341 -0.573065 N -1.948753 1.741549 0.606361 N -0.037887 0.334595 1.885719 N -1.176296 -0.374197 1.722808 B -2.442478 0.376847 1.164263 C -3.072055 -1.718379 -1.762822 C -4.434577 -1.550737 -1.403293 C -4.393817 -0.721671 -0.264427 C -0.937923 3.079503 -0.769047 C -1.348699 3.876956 0.329857 C -1.990996 2.974673 1.195300 C 0.799345 -0.430437 2.598955 C 0.199982 -1.678770 2.911822 C -1.076734 -1.605438 2.330343 H -3.261766 0.549754 2.032300 C -2.401823 -2.436380 -2.906467 F -1.892944 -1.541178 -3.806374

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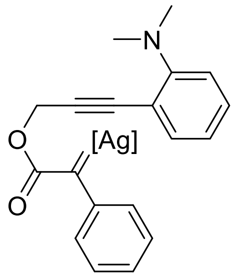 	84 C SCF Done: -11529.1021015 A.U. C 6.940076 0.131867 -1.075060 C 8.072658 -0.720830 -1.030326 C 8.559754 -1.224084 0.185996 C 7.939222 -0.890164 1.403872 C 6.809049 -0.062422 1.389648 C 6.286931 0.442800 0.174619 H 8.595278 -0.976743 -1.963024 H 9.449024 -1.874544 0.180036 H 8.325369 -1.283587 2.356316 H 6.274570 0.173667 2.322017 C 5.024846 1.100616 0.151027 C 3.900068 1.573009 0.004541 C 2.564314 1.950946 -0.424723 H 1.787780 1.267439 0.002261 H 2.274708 2.979754 -0.133035 C 2.307938 0.759778 -2.503258 C 1.675132 -0.362771 -1.792094 C 2.462750 -1.456097 -1.324861 C 3.895761 -1.434255 -1.397055 C 1.824849 -2.590234 -0.717875 C 4.649628 -2.464165 -0.833439

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H	6.683601	-1.240273	-3.342768
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H	6.809512	2.453019	-3.192516

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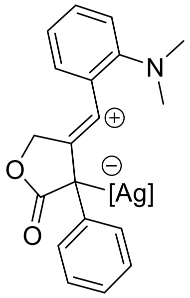	84 D SCF Done: -11529.1604944 A.U. C 5.279947 0.256560 -0.623821 C 5.830831 1.291404 0.203400 C 5.055865 2.353321 0.648507 C 3.674187 2.473636 0.326659 C 3.112590 1.523998 -0.494838 C 3.885394 0.437379 -1.070358 H 6.879451 1.246886 0.520161 H 5.527118 3.113445 1.292307 H 3.074586 3.303783 0.726169 H 2.055336 1.571796 -0.781415 C 3.289776 -0.289722 -2.076896 C 2.206089 -0.362252 -2.871592 C 2.077749 0.544750 -4.112727 H 1.816509 1.578556 -3.803994 H 3.021207 0.570880 -4.696874 C 0.470462 -1.122834 -4.280394 C 1.089217 -1.294517 -2.927913 C 1.073167 -2.591778 -2.194707 C 0.283767 -3.692540 -2.618195 C 1.880085 -2.760027 -1.043123 C 0.333765 -4.909283 -1.921128 H -0.367528 -3.572997 -3.493950 C 1.947579 -3.985498 -0.367071 H 2.438640 -1.901426 -0.643861 C 1.168933 -5.071702 -0.800093 H -0.290870 -5.748482 -2.267157 H 2.598195 -4.076805 0.514709 H 1.202063 -6.029996 -0.258670 O 1.038949 -0.010394 -4.902034 O -0.391086 -1.771293 -4.835728 Ag -0.350814 -0.176263 -1.648685 N -2.279748 -0.529184 -0.495690 N -2.475039 0.127481 0.663546 N -0.517149 1.878795 -0.476561 N -0.587972 1.793798 0.865581 N 1.100239 -0.252874 1.596938 N -0.203206 -0.599710 1.637360 B -1.265440 0.555225 1.539375 C -3.481976 -0.773162 -1.039785 C -4.504430 -0.233851 -0.215158 C -3.813001 0.340993 0.868173 C 0.003829 3.081076 -0.776005 C 0.310704 3.789336 0.412711 C -0.079476 2.920222 1.448217 C 1.793316 -1.295757 2.078994 C 0.922952 -2.362137 2.436094 C -0.358932 -1.874398 2.139321 H -1.651931 0.862939 2.641461 C -3.519169 -1.442042 -2.394397 F -4.756319 -1.851771 -2.728785 F -3.088464 -0.576000 -3.355653 F -2.692404 -2.514070 -2.423301 C -4.315460 1.152301 2.041079 F -4.075112 0.554825 3.230255

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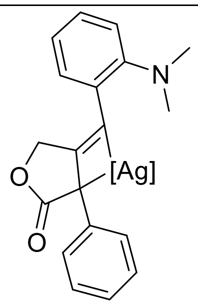	84 E SCF Done: -11529.1899227 A.U. C 5.341075 1.420955 -0.545956 C 6.044472 2.373866 -1.344038 C 5.364588 3.193009 -2.244177 C 3.956041 3.118213 -2.393952 C 3.263508 2.153321 -1.682745 C 3.926545 1.185290 -0.849337 H 7.121951 2.529446 -1.199946 H 5.936414 3.943709 -2.813321 H 3.420585 3.791500 -3.078528 H 2.178637 2.038292 -1.809000 C 3.197073 -0.006926 -0.552197 C 3.839862 -1.275655 -0.415348 C 4.998828 -1.698962 -1.316479 H 4.760778 -1.517538 -2.386709 H 5.941328 -1.162875 -1.075880 C 4.323528 -3.546805 -0.114707 C 3.480541 -2.397266 0.329858 C 2.383820 -2.527545 1.275438 C 1.658751 -3.749533 1.360940 C 1.924145 -1.417093 2.036337 C 0.471307 -3.819223 2.097338 H 2.012692 -4.619247 0.794218 C 0.759172 -1.515528 2.813418 H 2.520110 -0.496208 2.075286 C 0.008482 -2.700516 2.819661 H -0.107389 -4.756091 2.099629 H 0.441816 -0.657176 3.420962

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	Ag	1.079306	-0.049004	-0.541711
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	N	-0.160788	1.269755	1.174335
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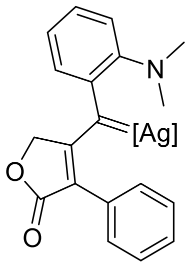
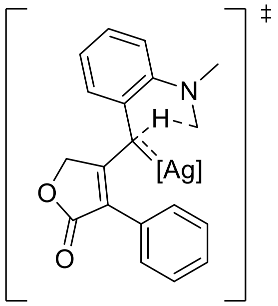
	N	-0.668422	-1.663564	-0.491057
	N	-1.899458	-1.325047	-0.048463
	B	-2.248654	0.142682	0.335864
	C	-1.022928	1.865042	-2.649862
	C	-2.161331	2.688869	-2.442772
	C	-2.784906	2.136357	-1.311235
	C	0.306142	1.856339	2.286843
	C	-0.598847	1.666737	3.364389
	C	-1.655102	0.927643	2.803437
	C	-0.744936	-2.910753	-0.977194
	C	-2.065968	-3.413556	-0.837114
	C	-2.781433	-2.363471	-0.242191
	H	-3.395193	0.193640	0.687185
	C	0.037138	1.983553	-3.712272
	F	-0.496946	2.047149	-4.950230
	F	0.780771	3.117602	-3.536439
	F	0.895000	0.934303	-3.678897
	C	-4.015382	2.571222	-0.553197
	F	-4.993736	1.636794	-0.594020
	F	-3.716689	2.790987	0.757909
	F	-4.519083	3.717283	-1.052085
	C	0.371355	-3.564344	-1.755017
	F	0.019735	-3.676699	-3.060620
	F	1.520814	-2.846885	-1.710277
	F	0.643972	-4.811407	-1.303943
	C	-4.263050	-2.248112	0.038801
	F	-4.832307	-1.312949	-0.766770
	F	-4.892158	-3.418733	-0.190971
	F	-4.520342	-1.894185	1.319126
	C	1.645107	2.536862	2.303246
	F	1.600078	3.728311	2.933791
	F	2.576114	1.773316	2.966247
	F	2.121174	2.739150	1.054005
	C	-2.874786	0.324110	3.456488
	F	-2.870897	-1.028419	3.283849
	F	-2.886037	0.561546	4.783673
	F	-4.031644	0.797730	2.945648
	Br	-0.353092	2.254016	5.134578
	Br	-2.670546	4.162857	-3.494182
	Br	-2.648024	-5.127479	-1.350056
	C	5.290583	0.291302	1.679385
	H	5.231207	-0.819340	1.708561
	H	5.837128	0.641620	2.580487
	H	4.263399	0.694376	1.719958
	C	7.436903	0.790524	0.583688
	H	7.756731	-0.048811	1.230933
	H	7.899177	0.642385	-0.412037
	H	7.826204	1.737834	1.022630
	N	5.978839	0.783153	0.489571

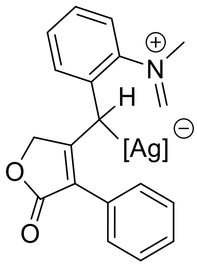


84
F SCF Done: -11529.1922169 A.U.

C	4.792619	0.580515	-0.033289
C	5.676376	-0.536443	-0.110791
C	5.206602	-1.777775	-0.538332
C	3.850236	-1.973652	-0.904622
C	2.947853	-0.945929	-0.704663
C	3.349262	0.311592	-0.123700
H	6.753821	-0.405953	0.058555
H	5.924257	-2.607170	-0.644987
H	3.512028	-2.940377	-1.303373
H	1.882439	-1.082578	-0.944140
C	2.356125	1.095926	0.512793
C	2.612229	2.044248	1.552108
C	3.458628	1.715243	2.775712
H	3.084613	0.798319	3.278127
H	4.528760	1.558238	2.521981
C	2.544630	3.815825	3.068513
C	2.076239	3.315536	1.742017
C	1.172627	4.031747	0.853617
C	0.369754	5.108502	1.326139
C	0.998809	3.611293	-0.497494
C	-0.586796	5.695475	0.491587
H	0.499645	5.452544	2.361240
C	0.021312	4.191498	-1.321329
H	1.675800	2.865243	-0.933188
C	-0.777155	5.233986	-0.827722
H	-1.211395	6.515178	0.880312
H	-0.095390	3.833737	-2.355978
H	-1.540518	5.697349	-1.472428
O	3.335637	2.834146	3.648688
O	2.320212	4.864510	3.635865
Ag	0.296513	0.715413	0.440005
N	0.097810	-1.857526	1.042959
N	-0.423659	-2.440274	-0.053670
N	0.089687	-0.733767	-2.198936
N	-1.213243	-0.823462	-1.879222
N	-1.856122	0.318589	0.658400
N	-2.366868	-0.892498	0.349141
B	-1.673071	-1.793401	-0.727822
C	1.141701	-2.602169	1.430363
C	1.311026	-3.709068	0.557946
C	0.287493	-3.561200	-0.395463
C	0.207292	0.244594	-3.112752
C	-1.058135	0.827906	-3.381417
C	-1.954543	0.095077	-2.584594
C	-2.662406	0.883336	1.575966
C	-3.728547	0.002257	1.888716
C	-3.490537	-1.131375	1.086721
H	-2.435320	-2.641270	-1.127261
C	1.972293	-2.181465	2.613127
F	2.040827	-3.150152	3.552927
F	3.254250	-1.886839	2.249832
F	1.463097	-1.064482	3.195878
C	-0.095987	-4.433780	-1.562647
F	-1.118487	-5.265581	-1.246742
F	-0.494652	-3.692430	-2.626499
F	0.949160	-5.193470	-1.960790
C	-2.321652	2.271976	2.064530
F	-3.216294	2.738516	2.951416

	F -1.094252 2.286405 2.666948 F -2.259374 3.138153 1.024746 C -4.213903 -2.459354 1.012877 F -3.331343 -3.483236 1.162249 F -5.132019 -2.567242 1.993024 F -4.848021 -2.637907 -0.167305 C 1.563428 0.635453 -3.631991 F 1.513002 1.053017 -4.914052 F 2.096961 1.674499 -2.901769 F 2.443956 -0.384911 -3.555243 C -3.440659 0.287548 -2.417081 F -3.726755 1.161526 -1.411117 F -3.999074 0.775986 -3.543288 F -4.062585 -0.877724 -2.117798 Br -1.432905 2.282055 -4.518970 Br 2.626562 -5.047733 0.698418 Br -5.150386 0.304329 3.080633 C 4.612873 3.026002 -0.463097 H 4.227187 3.706129 0.326436 H 5.339162 3.584510 -1.091632 H 3.765730 2.716159 -1.100103 C 6.655913 2.085001 0.535879 H 6.729490 3.112145 0.943219 H 6.936394 1.380327 1.342663 H 7.386670 1.986494 -0.299339 N 5.282258 1.852430 0.095903
	84 TS-FG SCF Done: -11529.1676287 A.U. C -3.716551 -2.945368 -0.125062 C -3.910546 -4.345093 -0.113623 C -2.947248 -5.195299 -0.665467 C -1.752425 -4.661144 -1.185072 C -1.545719 -3.278110 -1.185562 C -2.545027 -2.377005 -0.746550 H -4.820162 -4.765385 0.338857 H -3.115647 -6.282994 -0.663272 H -0.973655 -5.321791 -1.594267 H -0.611418 -2.863760 -1.583141 C -2.373256 -0.923403 -0.903513 C -2.969884 -0.292578 -2.070772 C -2.966627 -1.044816 -3.390159 H -1.946473 -1.357894 -3.700007 H -3.593464 -1.964469 -3.309122 C -3.949760 1.005745 -3.729657 C -3.597806 0.928302 -2.274244 C -3.931782 1.996419 -1.319341 C -4.976212 2.917943 -1.610359 C -3.246653 2.144602 -0.082325 C -5.327213 3.917311 -0.693075 H -5.498308 2.845549 -2.573699 C -3.596605 3.151939 0.827700 H -2.395789 1.491654 0.162795 C -4.646273 4.038180 0.532877 H -6.142216 4.615559 -0.941839 H -3.029084 3.246825 1.765253 H -4.925807 4.826474 1.249748 O -3.512597 -0.155244 -4.351478 O -4.505375 1.881532 -4.358097 Ag -0.490482 0.013541 -0.780142

	N 1.753951 -0.864572 -1.049647 N 2.565504 -0.752618 0.020467 N 0.725780 -1.711313 1.707046 N 0.894588 -0.381013 1.842774 N 0.822787 1.777440 -0.295001 N 1.868013 1.625486 0.547050 B 2.187356 0.231117 1.172623 C 2.262962 -1.819833 -1.840136 C 3.434974 -2.369102 -1.257221 C 3.590385 -1.657694 -0.055033 C -0.415101 -2.031526 2.328925 C -1.015462 -0.876171 2.894749 C -0.127377 0.169342 2.585467 C 0.833077 3.041108 -0.742174 C 1.917476 3.750086 -0.161948 C 2.563298 2.803886 0.651857 H 3.093371 0.333405 1.960642 C 1.612006 -2.181442 -3.148735 F 2.466783 -2.067426 -4.184460 F 1.153763 -3.463250 -3.137175 F 0.539579 -1.377540 -3.404994 C 4.623347 -1.790702 1.040061 F 5.357965 -0.659787 1.170310 F 4.036402 -2.035767 2.238365 F 5.472916 -2.806086 0.784297 C -0.221584 3.555576 -1.694627 F 0.332163 4.301787 -2.673507 F -0.889097 2.529231 -2.290369 F -1.133897 4.320676 -1.054094 C 3.846376 2.918126 1.446232 F 4.794479 2.093287 0.933247 F 4.330488 4.175298 1.404091 F 3.678689 2.588552 2.747982 C -0.811491 -3.477321 2.462387 F -0.527980 -3.952944 3.700496 F -2.156809 -3.642196 2.282874 F -0.180380 -4.256132 1.564234 C -0.204730 1.624459 2.963335 F -0.727060 2.397685 1.962266 F -0.987975 1.810296 4.045330 F 1.020969 2.124455 3.246257 Br -2.670199 -0.775464 3.796868 Br 4.494123 -3.736127 -1.994655 Br 2.324870 5.563496 -0.441425 C -4.470570 -0.733240 0.415681 H -3.220725 -0.480560 0.128521 H -4.889544 -0.381086 -0.548508 H -4.751845 -0.105802 1.279664 C -5.133346 -2.617353 1.881921 H -5.382427 -1.769049 2.546348 H -6.078539 -3.149688 1.639273 H -4.446889 -3.305066 2.410934 N -4.510111 -2.097281 0.662853



84
G SCF Done: -11529.1966545 A.U.

C	-3.694051	-2.949224	-0.577513
C	-3.978095	-4.319366	-0.513581
C	-2.918785	-5.230601	-0.679679
C	-1.610719	-4.758634	-0.884626
C	-1.348597	-3.378357	-0.926541
C	-2.387424	-2.446752	-0.776867
H	-5.008254	-4.666718	-0.339131
H	-3.118952	-6.312330	-0.639876
H	-0.778203	-5.468805	-1.001142
H	-0.322523	-3.007017	-1.045915
C	-2.249877	-0.942377	-0.749076
C	-2.884633	-0.253521	-1.842074
C	-2.767146	-0.711644	-3.285846
H	-1.755056	-0.504610	-3.695618
H	-2.948624	-1.805218	-3.399279
C	-4.385399	0.935437	-3.198386
C	-3.862035	0.761023	-1.815060
C	-4.290385	1.586639	-0.675904
C	-5.613655	2.101274	-0.616149
C	-3.411654	1.870737	0.399657
C	-6.047094	2.830106	0.501061
H	-6.287813	1.942220	-1.471023
C	-3.846340	2.612665	1.508729
H	-2.361256	1.549343	0.353598
C	-5.169703	3.081202	1.573498
H	-7.078511	3.216472	0.530026
H	-3.139529	2.825861	2.324141
H	-5.512198	3.655972	2.448471
O	-3.742609	0.023891	-4.028988
O	-5.269603	1.655254	-3.615695
Ag	-0.335184	0.000596	-0.949905
N	1.911110	-1.010627	-0.942647
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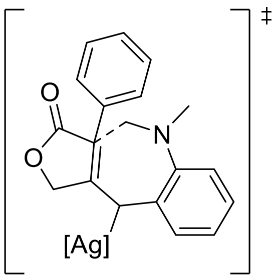
B	2.240323	0.375592	1.124071
C	2.396206	-2.116597	-1.522633
C	3.478292	-2.637594	-0.764767
C	3.602783	-1.749617	0.317333
C	-0.555439	-1.574689	2.412888
C	-1.073047	-0.327931	2.851482
C	-0.108265	0.612665	2.450557
C	1.030426	2.941115	-1.198151
C	2.132865	3.687647	-0.705596
C	2.742058	2.833267	0.234670
H	3.096876	0.573008	1.948957
C	1.819377	-2.640511	-2.811712
F	2.732832	-2.641521	-3.806091
F	1.373758	-3.917216	-2.667763
F	0.760378	-1.888764	-3.223491
C	4.537874	-1.765674	1.503483
F	5.330795	-0.666990	1.526398
F	3.845720	-1.791928	2.670919
F	5.338284	-2.850521	1.477365
C	-0.055654	3.259264	-2.198553
F	0.181589	4.395909	-2.871524

	F -0.172837 2.247082 -3.111371 F -1.264379 3.368766 -1.588516 C 4.021560 2.999816 1.026172 F 4.913241 2.034024 0.684904 F 4.595781 4.193395 0.778185 F 3.817994 2.913332 2.361021 C -1.114120 -2.952377 2.647825 F -1.124019 -3.260459 3.967685 F -2.413555 -3.041959 2.221136 F -0.408057 -3.898822 2.002132 C -0.086052 2.103022 2.658069 F -0.523834 2.788923 1.560862 F -0.885030 2.465932 3.686819 F 1.164436 2.545865 2.926985 Br -2.713536 -0.044687 3.737187 Br 4.481592 -4.171138 -1.185869 Br 2.628137 5.432570 -1.200803 C -5.283662 -1.315833 -1.384388 H -2.575647 -0.548716 0.235241 H -5.119832 -1.703589 -2.399445 H -6.067715 -0.568370 -1.198514 C -5.069128 -1.604990 1.032375 H -5.601236 -0.635635 1.061344 H -5.693425 -2.407244 1.478376 H -4.134812 -1.526068 1.617584 N -4.748945 -1.956667 -0.362797
	84 TS-GH SCF Done: -11529.1927656 A.U. C -3.881573 -2.985210 -0.693101 C -4.379910 -4.294404 -0.767291 C -3.473669 -5.361293 -0.923303 C -2.090863 -5.114470 -0.996655 C -1.594362 -3.800490 -0.907846 C -2.488127 -2.734352 -0.752171 H -5.465298 -4.471463 -0.709081 H -3.852929 -6.392943 -0.989402 H -1.387918 -5.953248 -1.117088 H -0.514855 -3.602096 -0.938358 C -2.202090 -1.269504 -0.610971 C -2.579746 -0.447222 -1.699256 C -2.431684 -0.866144 -3.159756 H -1.382756 -0.831150 -3.517129 H -2.799655 -1.906667 -3.321753 C -3.903570 0.923638 -3.109822 C -3.679159 0.509803 -1.675989 C -4.016000 1.472102 -0.588270 C -5.256382 2.158770 -0.634687 C -3.148307 1.732034 0.494569 C -5.621163 3.053082 0.381666 H -5.921409 2.014237 -1.498574 C -3.512576 2.634059 1.507937 H -2.154812 1.260800 0.536220 C -4.753308 3.289171 1.463190 H -6.587625 3.578291 0.321741 H -2.817663 2.828528 2.336185 H -5.037351 3.991873 2.262287 O -3.212670 0.052039 -3.929665 O -4.624998 1.784396 -3.560421 Ag -0.335170 -0.232518 -0.897715

	N	1.856553	-1.112645	-0.832436
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	N	0.905634	0.013377	1.841295
	N	0.833621	1.658379	-0.657859
	N	1.901372	1.686648	0.165015
	B	2.220152	0.462814	1.093481
	C	2.383642	-2.226494	-1.360524
	C	3.538448	-2.615287	-0.633255
	C	3.659893	-1.640637	0.372463
	C	-0.545592	-1.436776	2.520830
	C	-1.011547	-0.177067	2.981090
	C	-0.038640	0.736592	2.537832
	C	0.786496	2.818902	-1.328179
	C	1.865934	3.648213	-0.925457
	C	2.565946	2.877552	0.023481
	H	3.103529	0.755786	1.858406
	C	1.784723	-2.886969	-2.574974
	F	2.651710	-2.906419	-3.608765
	F	1.430190	-4.170349	-2.313141
	F	0.660823	-2.235472	-2.993641
	C	4.654456	-1.512241	1.504061
	F	5.377899	-0.372044	1.404870
	F	4.021498	-1.491943	2.704532
	F	5.516050	-2.548511	1.511581
	C	-0.361626	3.061048	-2.281693
	F	-0.098105	4.047498	-3.153083
	F	-0.627319	1.927997	-3.005801
	F	-1.498364	3.371047	-1.615369
	C	3.890233	3.141637	0.710241
	F	4.791845	2.188805	0.356827
	F	4.394585	4.337128	0.347904
	F	3.792214	3.130498	2.058046
	C	-1.171548	-2.792340	2.717369
	F	-1.196552	-3.143844	4.024744
	F	-2.469794	-2.796483	2.285071
	F	-0.512050	-3.749711	2.036605
	C	0.049480	2.226132	2.731208
	F	-0.335602	2.917022	1.617504
	F	-0.745538	2.637703	3.743247
	F	1.316393	2.610999	3.010918
	Br	-2.609248	0.132383	3.927823
	Br	4.622719	-4.104485	-1.003661
	Br	2.229014	5.393294	-1.521878
	C	-5.011217	-0.953314	-1.522983
	H	-2.525200	-0.884605	0.374861
	H	-4.962753	-1.401586	-2.531107
	H	-5.892464	-0.308867	-1.364414
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	H	-5.812045	-0.635466	0.877465
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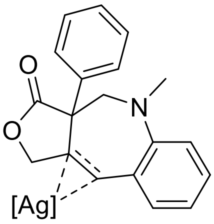

84

H-Ag SCF Done: -11529.1963386 A.U.

C	-4.594083	-2.262447	-0.675549
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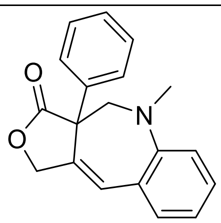
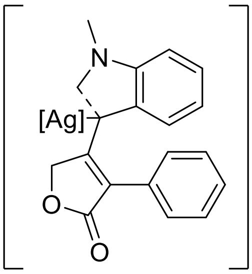
	39 H SCF Done: -938.827237545 A.U. C 2.051926 0.364636 0.550485 C 3.172123 1.217145 0.768283 C 4.417849 0.968838 0.185015 C 4.603017 -0.155889 -0.640798 C 3.510042 -0.988754 -0.888636 C 2.213319 -0.756251 -0.349270 H 3.069195 2.075563 1.446239 H 5.257538 1.650113 0.396308 H 5.582857 -0.370415 -1.093485 H 3.634944 -1.854084 -1.560573 C 1.157034 -1.644818 -0.845555 C -0.186897 -1.643004 -0.647905 C -1.154711 -2.653306 -1.212778 H -1.666766 -2.291447 -2.134661 H -0.701262 -3.643837 -1.422616 C -2.071536 -1.818592 0.743101 C -0.975698 -0.812750 0.322909 C -1.614738 0.451988 -0.277185 C -2.786238 1.011234 0.278147 C -0.952591 1.139401 -1.315559 C -3.282502 2.236325 -0.199280 H -3.303626 0.485948 1.095549 C -1.448816 2.366530 -1.788145 H -0.034063 0.712152 -1.746252 C -2.614900 2.919827 -1.231406 H -4.198693 2.660402 0.241819 H -0.918079 2.893085 -2.597385 H -3.004590 3.881095 -1.602334 O -2.163574 -2.818384 -0.181030 O -2.770967 -1.773177 1.731233 C -0.086929 -0.402729 1.536106

	H 0.450370 -1.302693 1.904243 H 1.535110 -2.427550 -1.528952 H -0.749801 -0.053881 2.352157 C 0.570455 1.988669 1.687052 H -0.525902 2.115591 1.777162 H 1.031966 2.199678 2.681615 H 0.926651 2.748710 0.962387 N 0.852748 0.646152 1.197095
 ‡	84 TS-GI SCF Done: -11529.1813808 A.U. C -3.957144 -2.942176 -0.495271 C -4.194089 -4.320345 -0.595347 C -3.169310 -5.168662 -1.053004 C -1.913079 -4.635410 -1.373787 C -1.681656 -3.251824 -1.256361 C -2.693856 -2.367334 -0.850959 H -5.177140 -4.731407 -0.321018 H -3.355727 -6.249825 -1.142281 H -1.095132 -5.289234 -1.711193 H -0.686499 -2.848453 -1.482016 C -2.537005 -0.882559 -0.758407 C -2.625310 -0.045003 -1.938972 C -2.531290 -0.660294 -3.330748 H -1.555932 -1.145584 -3.544924 H -3.317555 -1.444798 -3.455574 C -3.116178 1.555860 -3.562853 C -3.079748 1.270484 -2.104429 C -3.556310 2.206257 -1.086115 C -4.450876 3.259445 -1.432176 C -3.194290 2.078615 0.282140 C -4.981376 4.102066 -0.448102 H -4.714210 3.405720 -2.488494 C -3.723059 2.929368 1.264572 H -2.430208 1.352144 0.585625 C -4.631452 3.938832 0.907527 H -5.677031 4.903931 -0.743169 H -3.401564 2.806235 2.310038 H -5.050613 4.607790 1.675767 O -2.747816 0.400618 -4.249367 O -3.414843 2.567691 -4.163827 Ag -0.367978 -0.039687 -1.013631 N 1.770535 -1.074367 -0.912460 N 2.492437 -0.891310 0.212105 N 0.422049 -1.625359 1.719695 N 0.668872 -0.303598 1.811764 N 0.956427 1.715703 -0.438286 N 1.889323 1.563727 0.525023 B 2.059298 0.192835 1.251333 C 2.304633 -2.115221 -1.567819 C 3.396155 -2.650039 -0.836085 C 3.479279 -1.836154 0.306804 C -0.791085 -1.839544 2.241145 C -1.362049 -0.618724 2.692269 C -0.377101 0.351289 2.424077 C 1.074479 2.951554 -0.942002 C 2.114074 3.648426 -0.271430 C 2.620122 2.718639 0.655551 H 2.883100 0.292329 2.124541 C 1.746797 -2.582316 -2.886315

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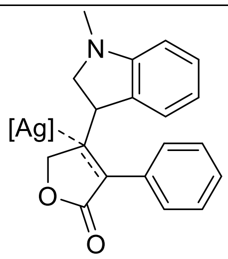	84 I-Ag SCF Done: -11529.2518398 A.U. C 5.077005 -0.127698 1.024683 C 5.905446 -1.233226 0.761329 C 5.448971 -2.196008 -0.163726 C 4.218328 -2.051305 -0.826648 C 3.384812 -0.947574 -0.541768 C 3.811769 -0.009895 0.397065 H 6.893717 -1.334962 1.233712 H 6.089241 -3.063527 -0.390035 H 3.905088 -2.794457 -1.574734 H 2.440384 -0.784470 -1.080778 C 3.151634 1.273041 0.888496 C 2.180128 1.094952 2.040756 C 2.590735 0.322168 3.281034 H 2.641072 -0.774107 3.129404 H 3.601151 0.655806 3.612507 C 0.777219 1.638916 3.855034 C 1.092392 1.919118 2.393411 C 0.523233 3.114996 1.719960 C -0.860932 3.385509 1.849342 C 1.326096 4.010045 0.974045 C -1.428818 4.503145 1.223327 H -1.491197 2.709127 2.441022

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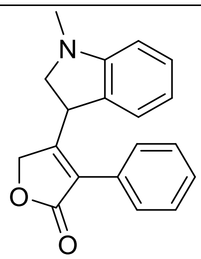
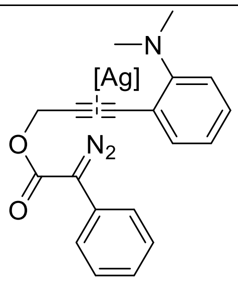
	39 I SCF Done: -938.829644473 A.U. C 3.010124 -0.441438 -0.246800 C 4.096565 -0.948273 0.491824 C 3.862672 -1.360073 1.821019 C 2.591228 -1.256697 2.413141 C 1.508021 -0.736010 1.667524 C 1.726656 -0.339863 0.348812 H 5.104486 -1.013658 0.055657 H 4.704853 -1.756191 2.410847 H 2.440885 -1.569572 3.457518 H 0.509280 -0.626029 2.121192 C 0.759909 0.203257 -0.704266 C -0.288768 1.112911 -0.145049 C 0.019355 2.506753 0.341292 H 0.776724 2.495545 1.159036 H 0.409953 3.168811 -0.465213 C -2.217153 2.102911 0.675057 C -1.608665 0.857620 0.094038 C -2.399613 -0.363905 -0.141729 C -3.748491 -0.265428 -0.566647 C -1.846360 -1.653923 0.059714 C -4.504078 -1.421697 -0.813224 H -4.199637 0.728883 -0.692163 C -2.607343 -2.806998 -0.187621 H -0.821635 -1.758156 0.447294 C -3.937116 -2.695868 -0.631067 H -5.549263 -1.325856 -1.147774 H -2.160299 -3.799712 -0.020055 H -4.534584 -3.601361 -0.822437 O -1.210980 3.041129 0.826002 O -3.365551 2.337814 0.980784 C 1.755124 0.825760 -1.726103 H 0.254394 -0.660179 -1.193602 H 1.964757 1.900037 -1.480153 H 1.378747 0.785322 -2.768915 C 4.169574 0.407306 -2.272642 H 3.925236 0.606641 -3.335713 H 4.652128 1.323737 -1.846097 H 4.912481 -0.415830 -2.250717 N 2.970557 0.018280 -1.563805
	86 B1 SCF Done: -11642.9068337 A.U. C -4.267259 0.174576 -1.565348 C -4.959566 -0.999737 -1.978460 C -4.430097 -2.275139 -1.777418 C -3.185143 -2.456490 -1.138964 C -2.504454 -1.335363 -0.669749 C -3.028582 -0.023761 -0.844222 H -5.913915 -0.897770 -2.512254 H -4.990496 -3.148658 -2.146831 H -2.759979 -3.461304 -1.001478 H -1.553859 -1.451379 -0.128270 C -2.384171 1.074022 -0.204690 C -2.017807 2.124895 0.389081 C -2.207589 3.305593 1.254897

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	C	1.447001	-1.821093	3.235210
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	H	3.630786	-1.498279	-0.336060
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	F	5.853649	-0.243230	-0.429131
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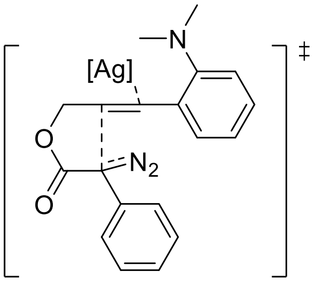

86

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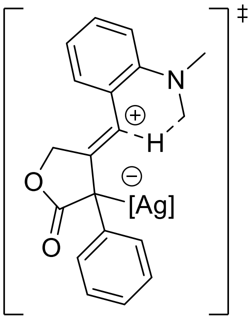	84 TS-DE1 SCF Done: -11533.3767973 A.U. C -5.239092 0.303079 0.809102 C -5.890104 1.303795 0.032034 C -5.284010 2.531073 -0.202882 C -3.974713 2.803152 0.293682 C -3.318677 1.852209 1.047041 C -3.941644 0.604148 1.422669 H -6.885973 1.101158 -0.386841 H -5.812214 3.290820 -0.799315 H -3.481531 3.762044 0.071218 H -2.307727 2.043486 1.424730 C -3.290824 -0.284546 2.272202 C -2.070959 -0.297410 2.928273 C -1.819435 0.719464 4.057284 H -1.609894 1.740293 3.677578 H -2.702902 0.771099 4.728718

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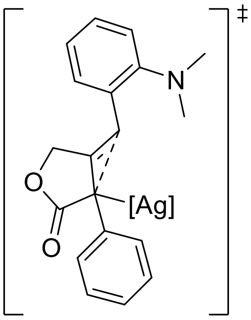 	84 TS-DE2 SCF Done: -11529.1257329 A.U. C 5.685917 -0.959281 -0.794845 C 6.223188 -2.260431 -0.655492 C 6.229668 -2.913956 0.584290 C 5.693942 -2.289014 1.730391 C 5.117278 -1.023026 1.627046 C 5.072332 -0.351321 0.368393 H 6.673134 -2.753404 -1.529218 H 6.676665 -3.917405 0.662140 H 5.703920 -2.804237 2.702851 H 4.636900 -0.552457 2.494391 C 4.231640 0.756373 0.183507 C 3.149676 1.496074 0.013283 C 2.881077 2.913776 -0.367855 H 1.823578 3.216900 -0.215227 H 3.563806 3.642584 0.106353 C 3.126406 1.581166 -2.315702 C 2.954268 0.637988 -1.179062 C 2.449125 -0.738092 -1.269713 C 2.343528 -1.412585 -2.535071 C 2.264544 -1.529202 -0.080756 C 2.107870 -2.795835 -2.585262 H 2.504028 -0.828581 -3.452513 C 2.036988 -2.909913 -0.158536 H 2.365853 -1.050815 0.901872 C 1.969971 -3.552696 -1.406997 H 2.027214 -3.287139 -3.566948 H 1.913557 -3.480094 0.774103 H 1.791805 -4.636676 -1.463309 O 3.152390 2.875128 -1.808811 O 3.188206 1.377823 -3.515811 Ag 0.185737 -0.219066 -1.243151 N -1.794701 -1.311894 -0.843703 N -2.609945 -0.846891 0.124225 N -1.171882 1.629563 -0.846169 N -1.958475 1.620383 0.250352 N 0.051643 1.072965 1.915199 N -0.747566 0.002605 1.721062 B -2.154294 0.307473 1.069106 C -2.450180 -2.271778 -1.510784 C -3.742081 -2.456011 -0.950898 C -3.811131 -1.511839 0.089092 C -1.091260 2.898148 -1.274505 C -1.834412 3.751793 -0.419960 C -2.369124 2.890733 0.553713 C 1.075490 0.668060 2.676491 C 0.946147 -0.710787 2.998147 C -0.250084 -1.104476 2.372624 H -2.988389 0.473388 1.922809

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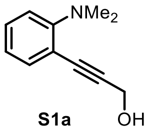
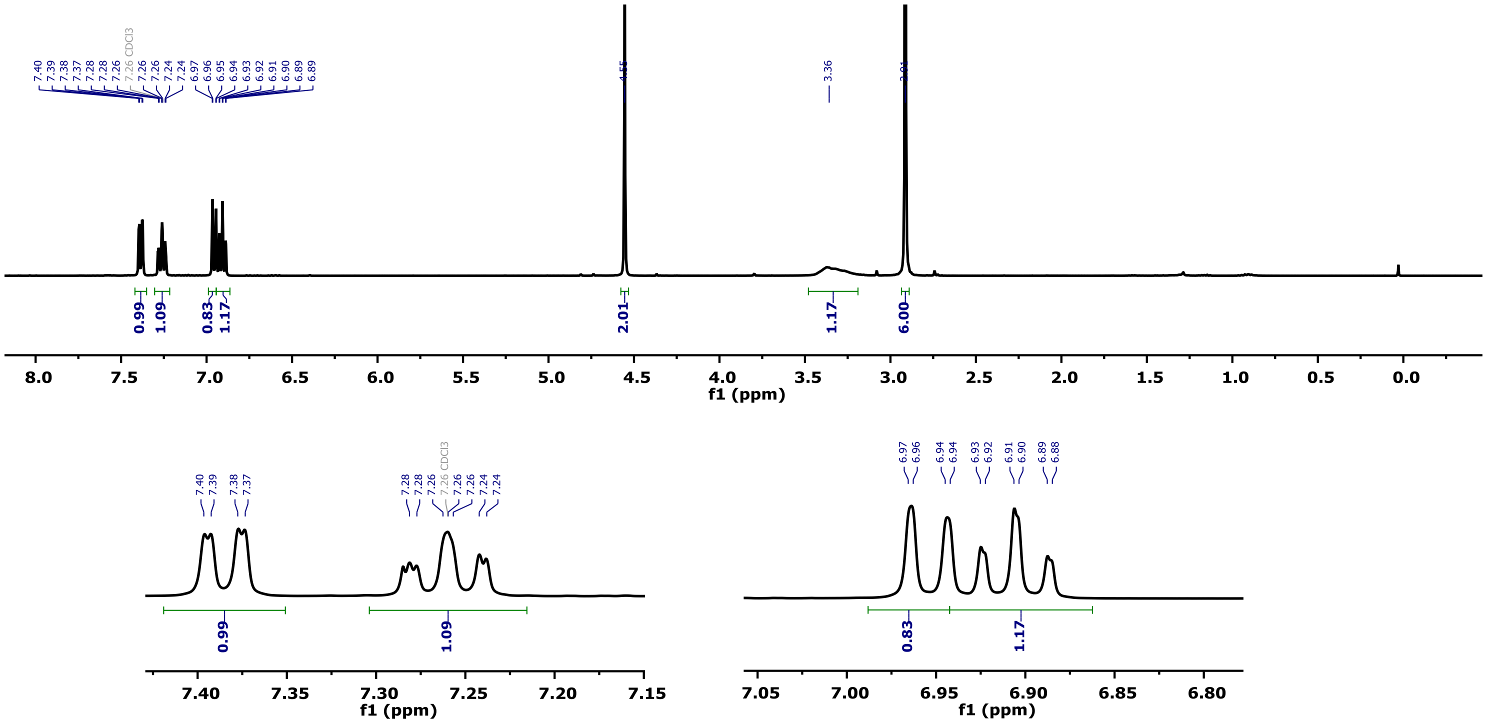
S13 NMR SPECTRA

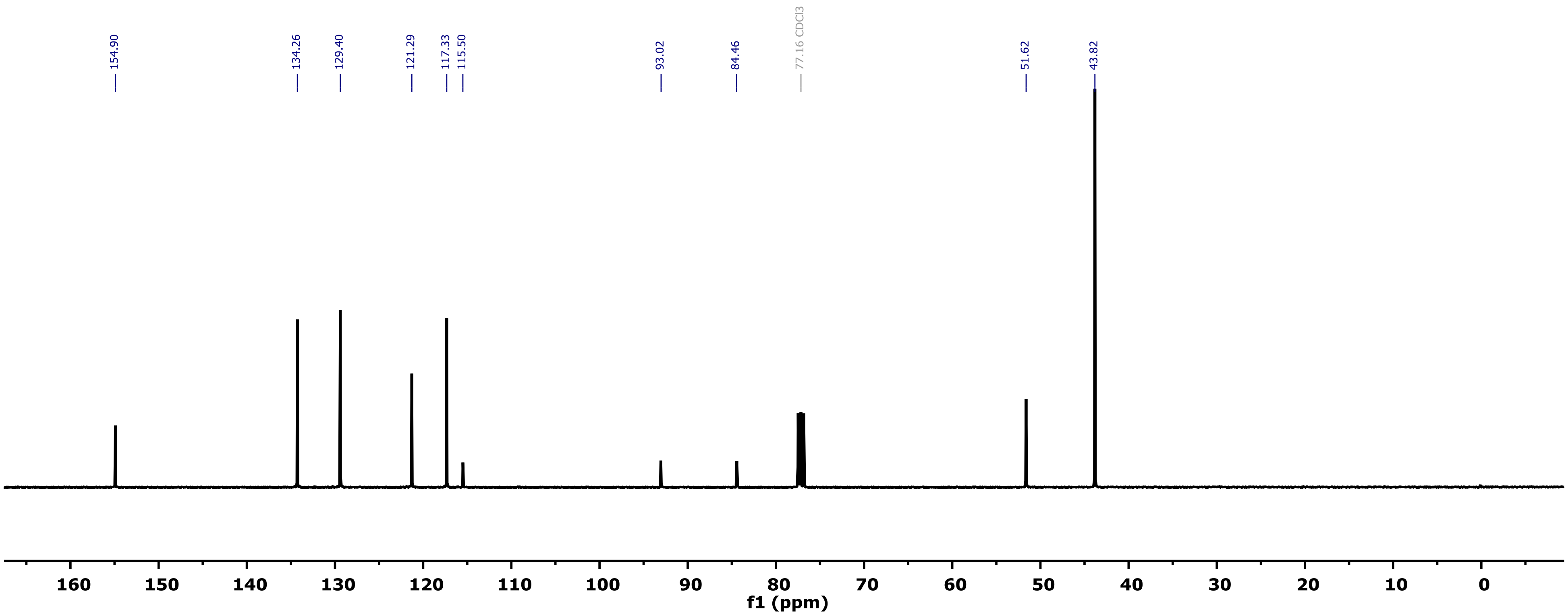


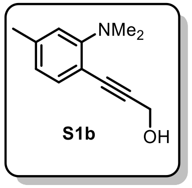
S1a

^{1}H NMR (400 MHz, $CDCl_3$)



$^{13}C\{H\}$ NMR ($CDCl_3$, 101 MHz)





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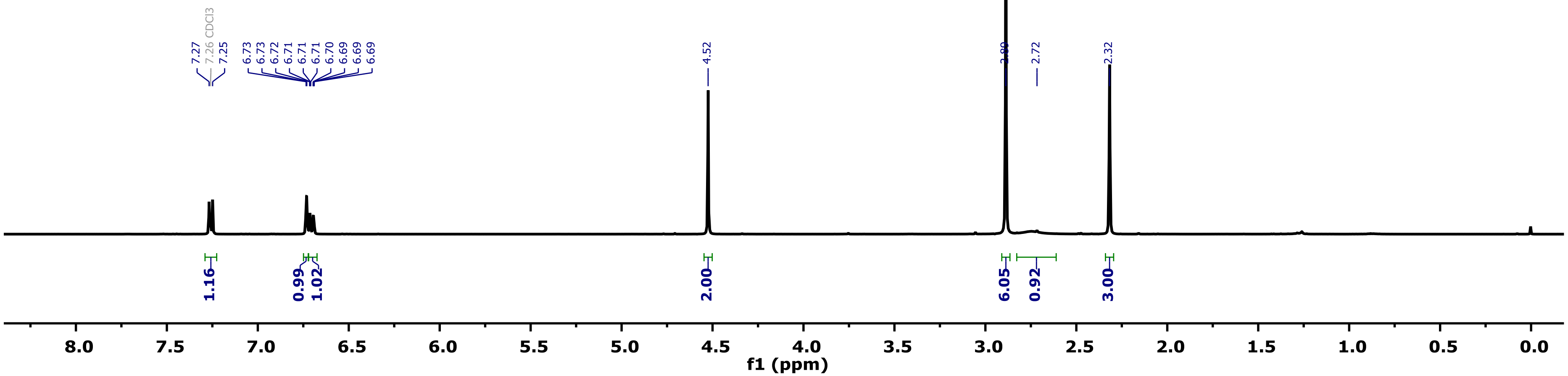

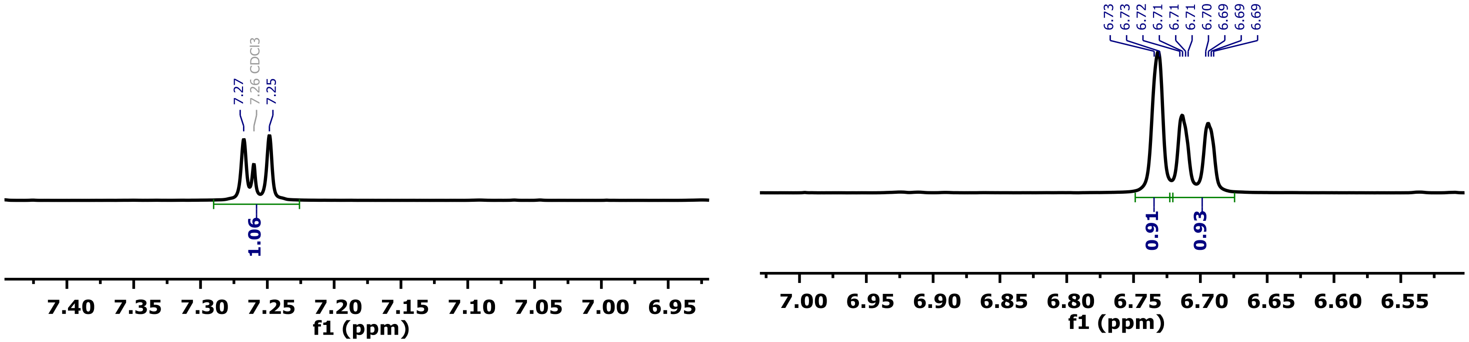

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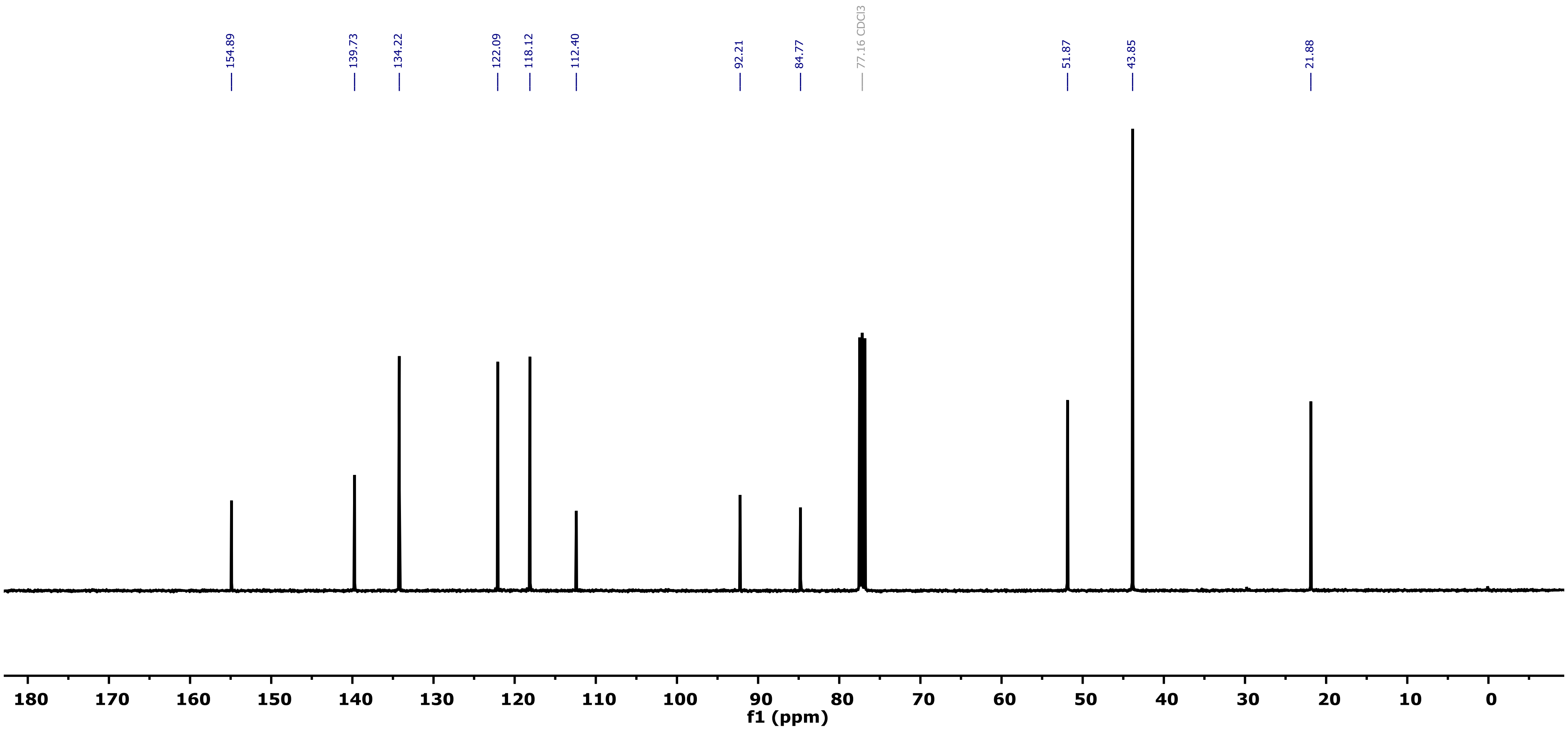

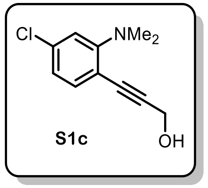

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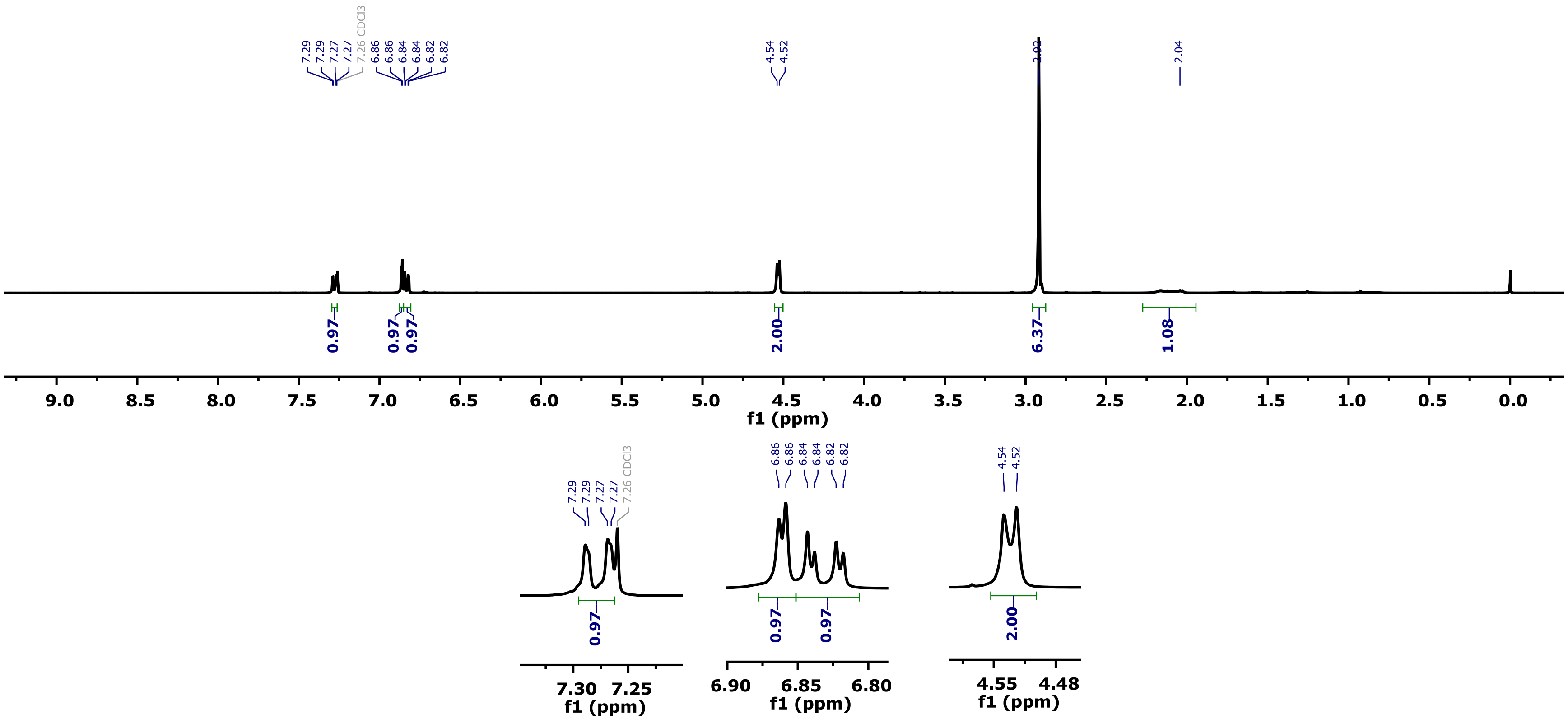

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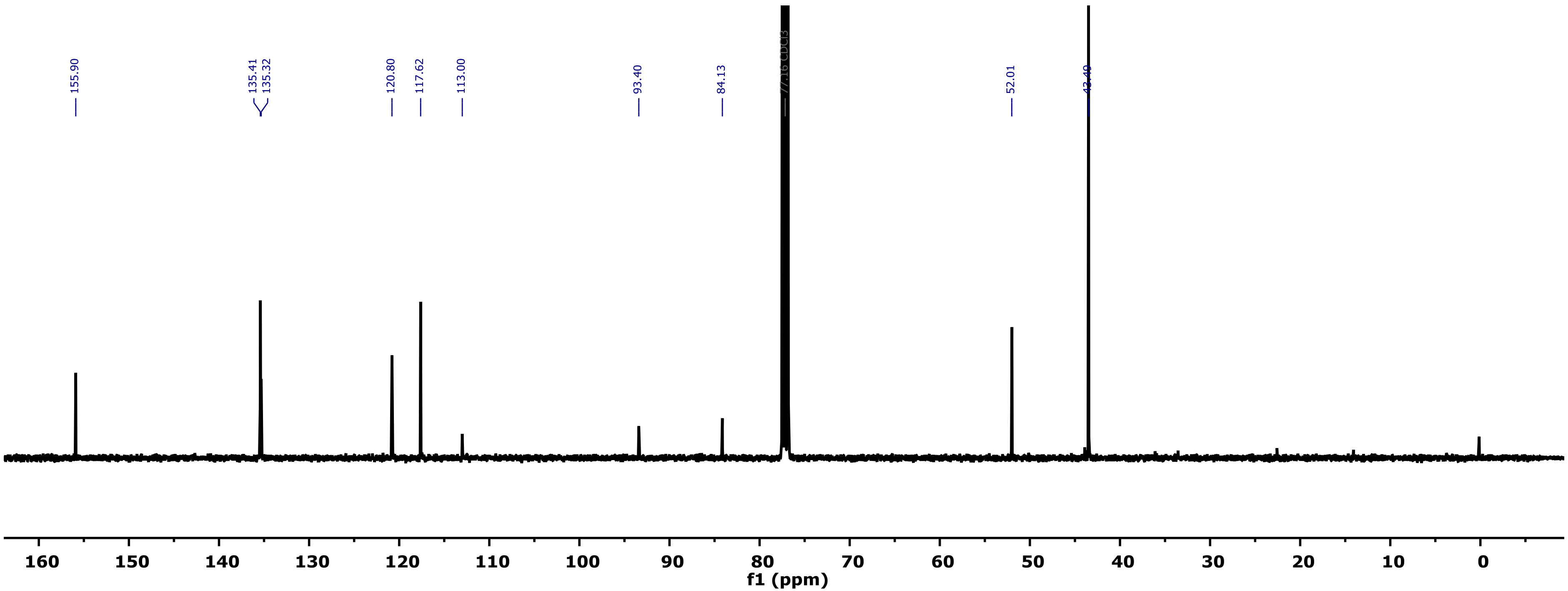
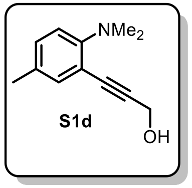
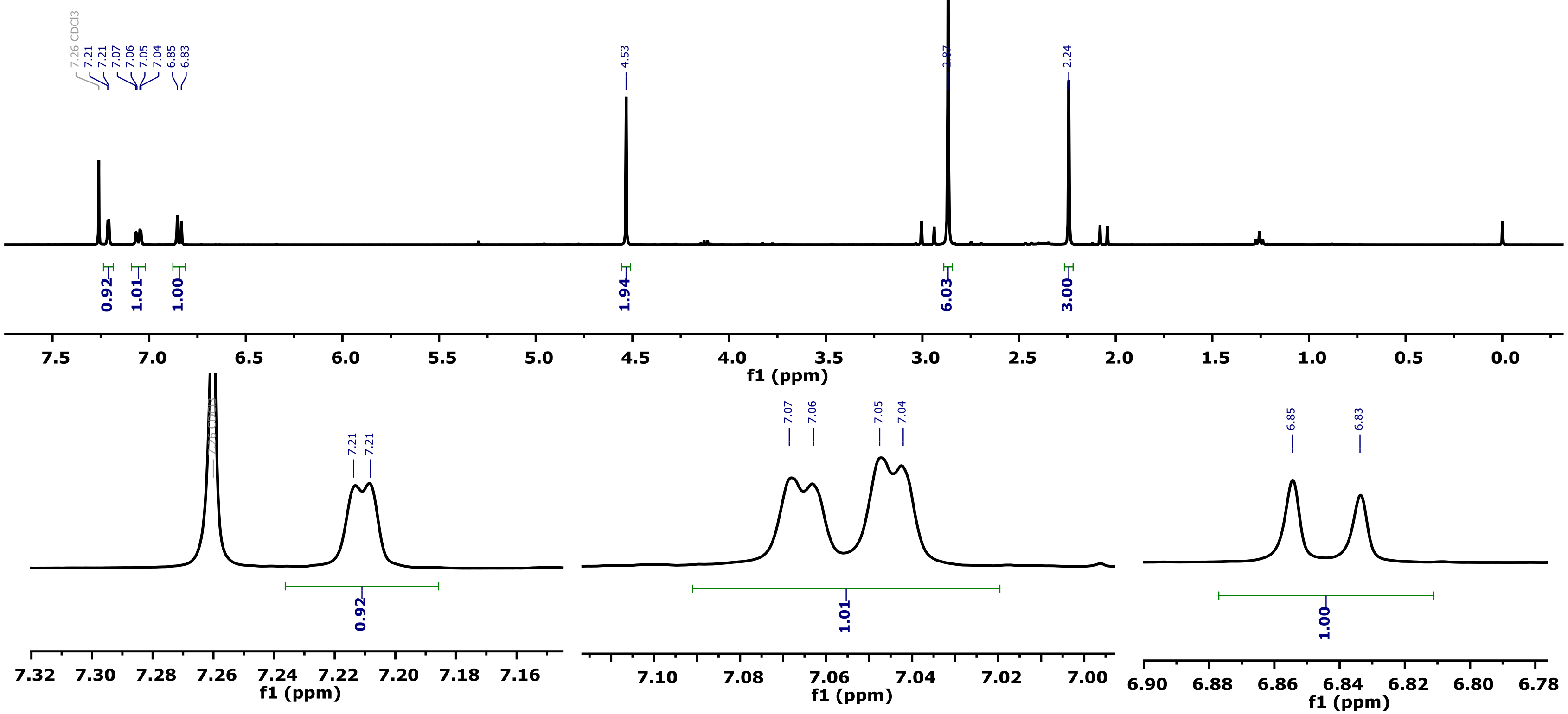


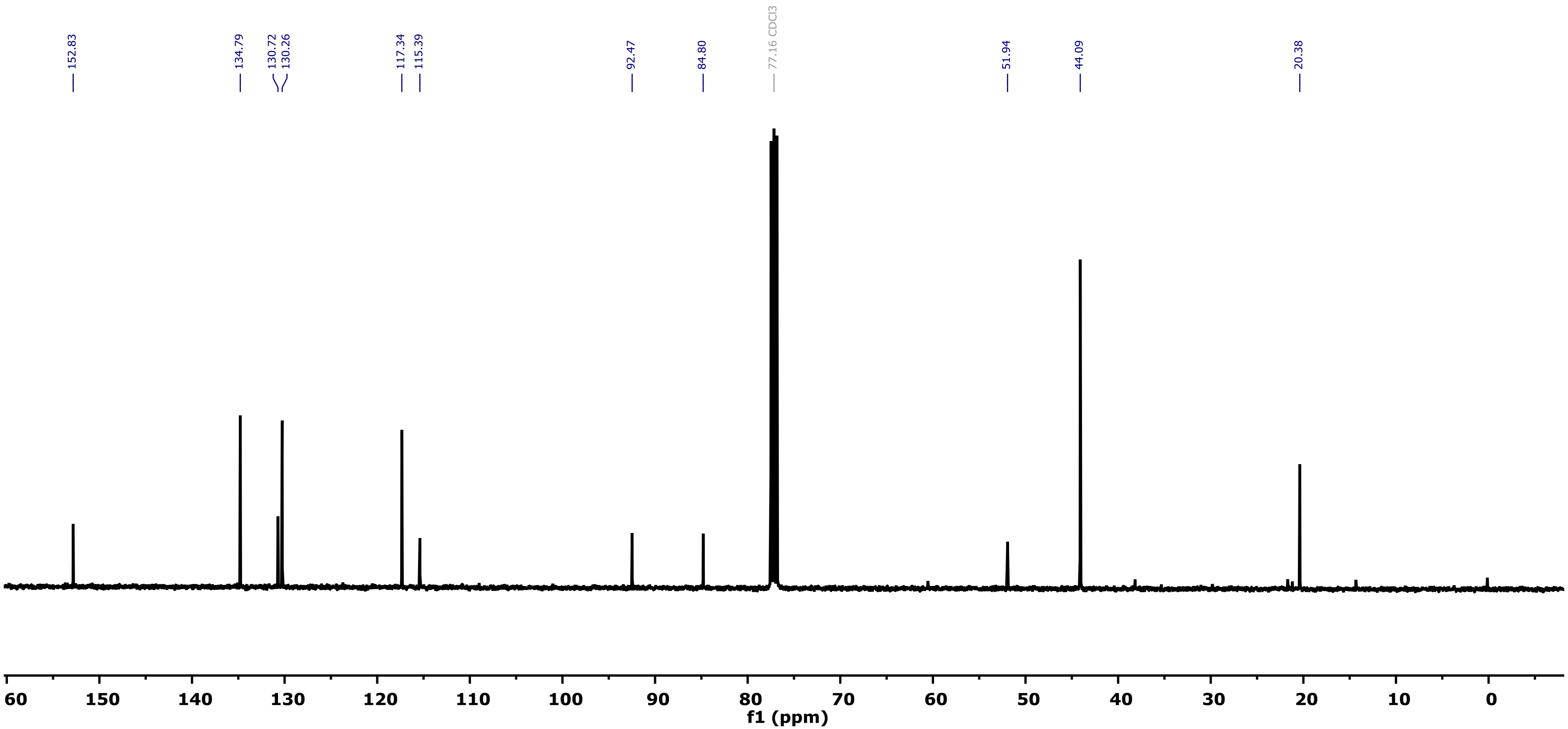


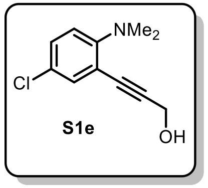
S1d

^{1}H NMR (400 MHz, CDCl$_3$)



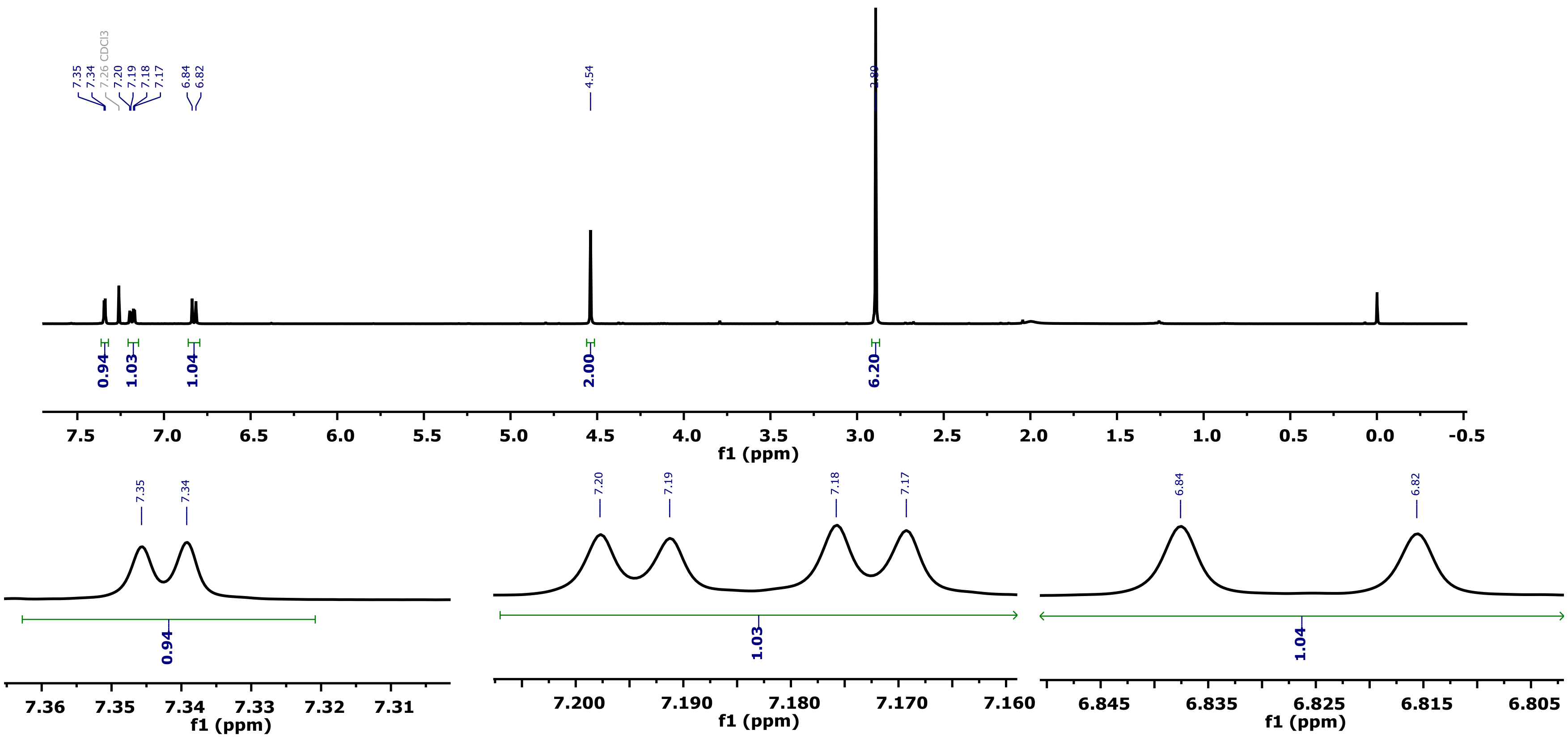
$^{13}C\{H\}$ NMR ($CDCl_3$, 101 MHz)

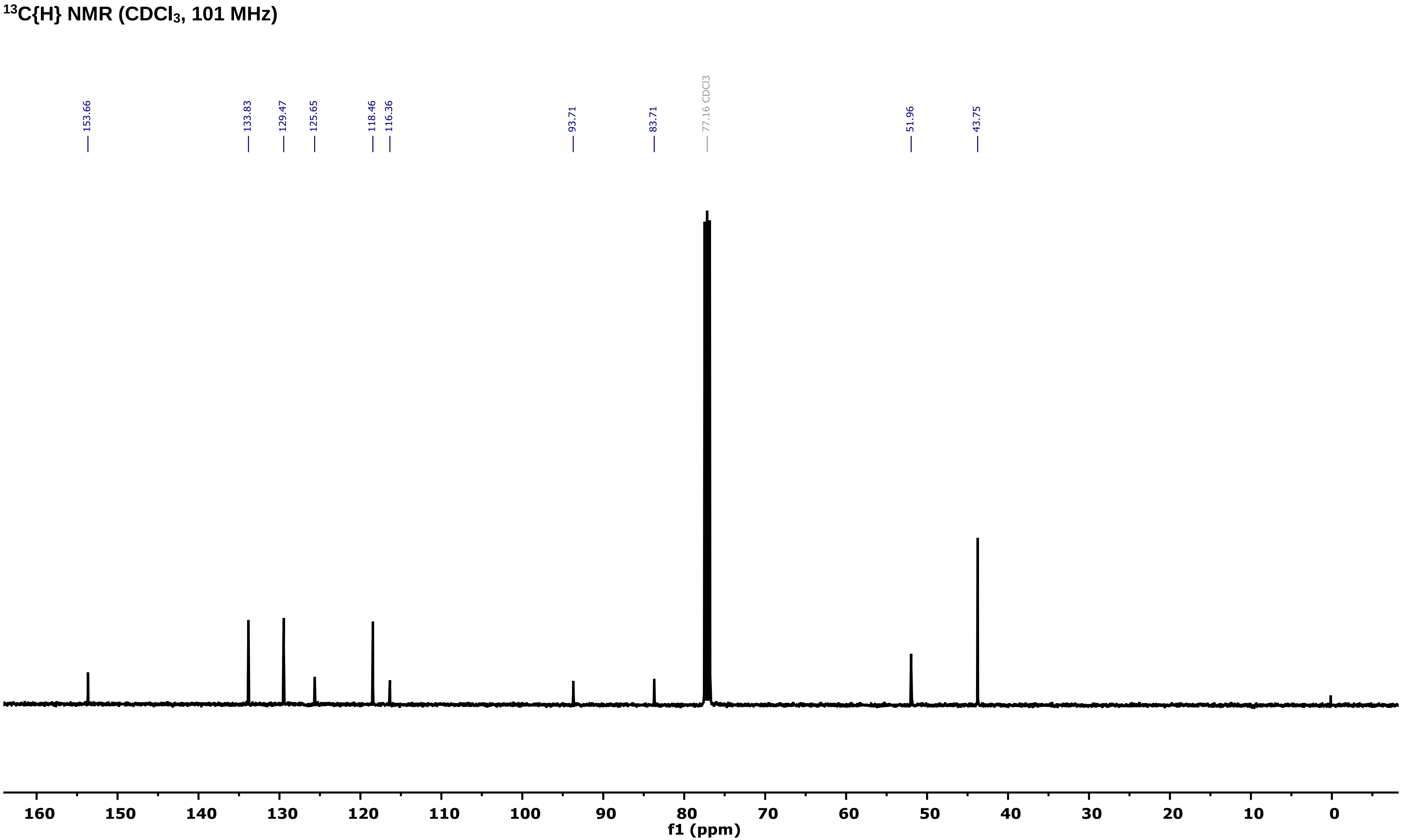




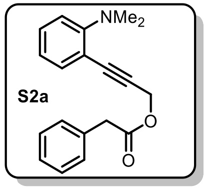
S1e

[1]H NMR (400 MHz, $CDCl_3$)

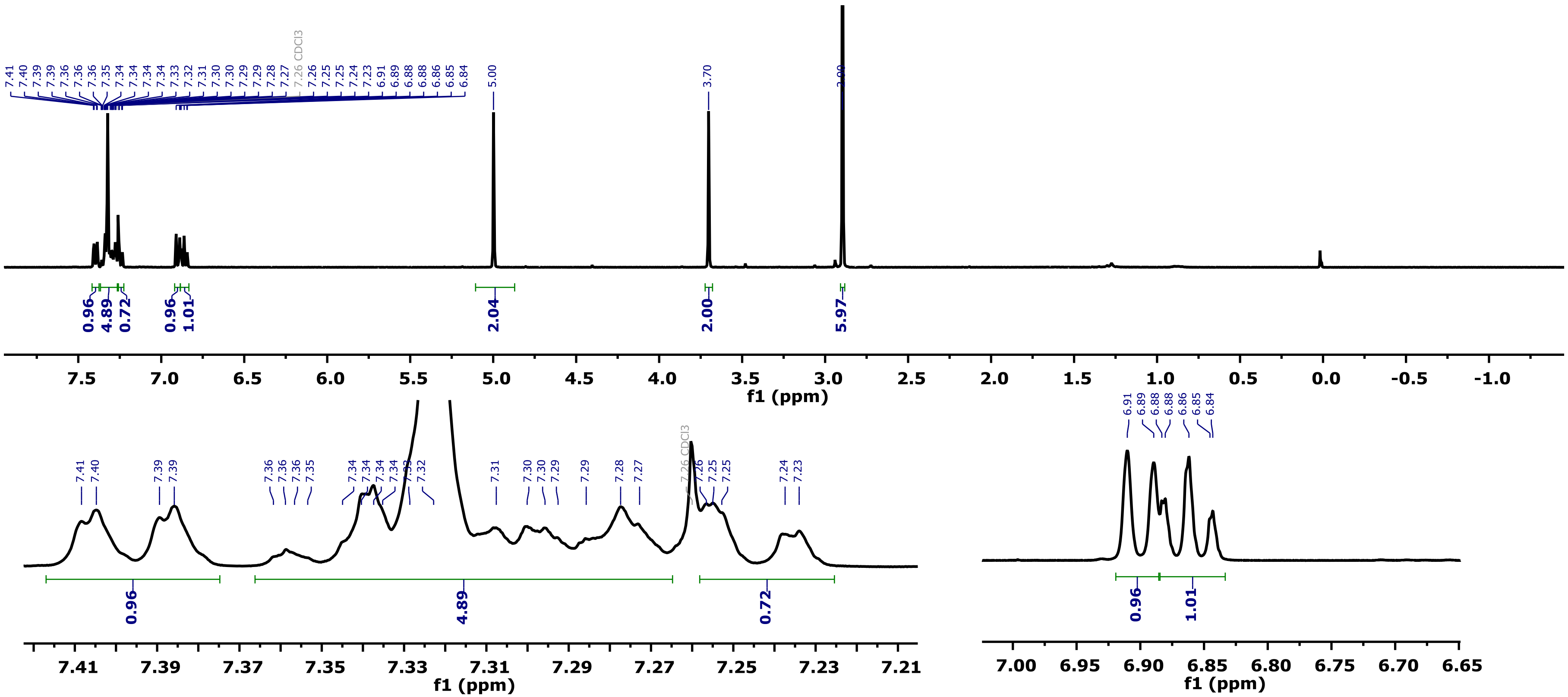




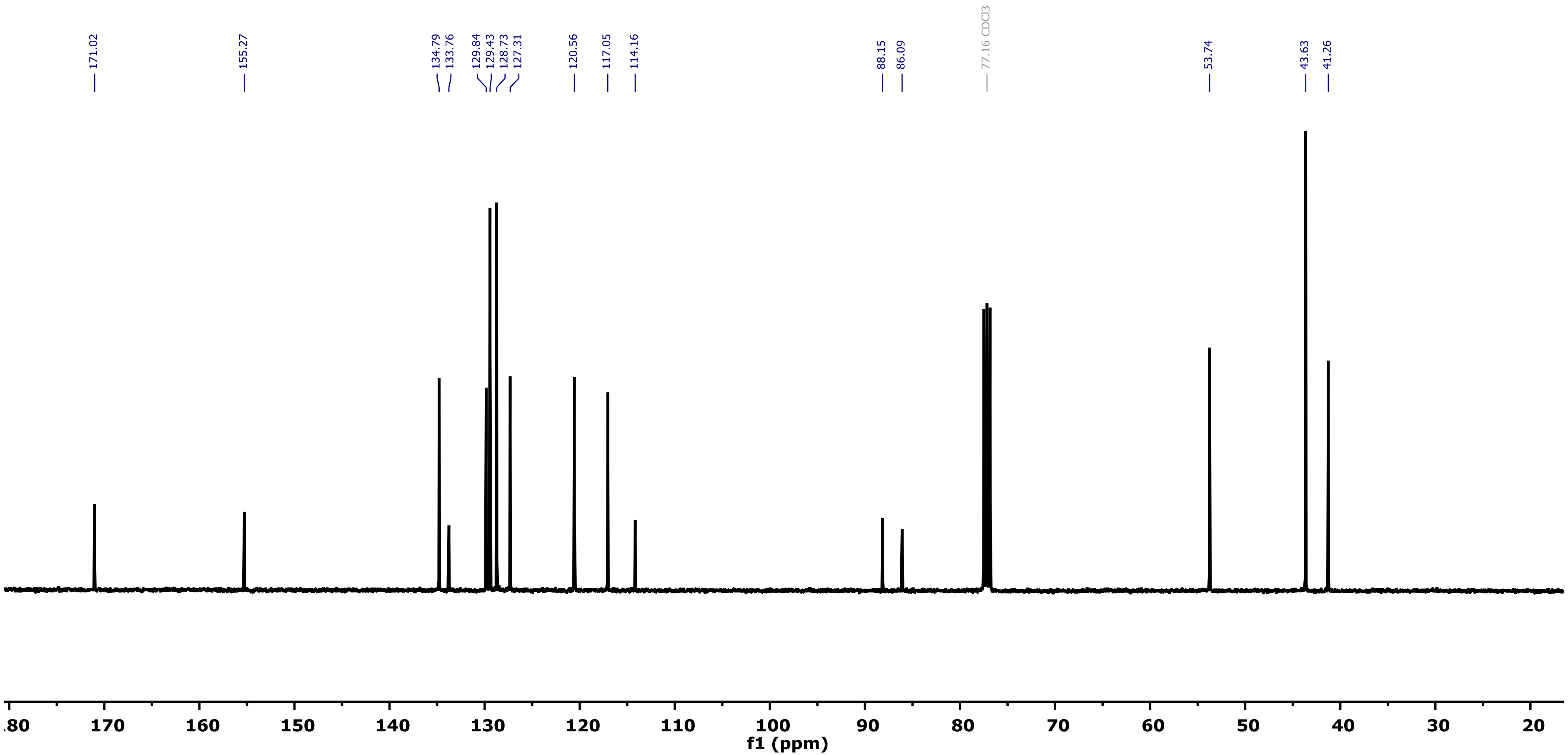
$^{13}C\{H\}$ NMR ($CDCl_3$, 101 MHz)
153.66
133.83
129.47
125.65
118.46
116.36
93.71
83.71
77.16 CDCl3
51.96
43.75
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

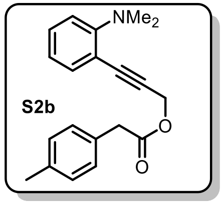


^{1}H NMR (400 MHz, $CDCl_3$)

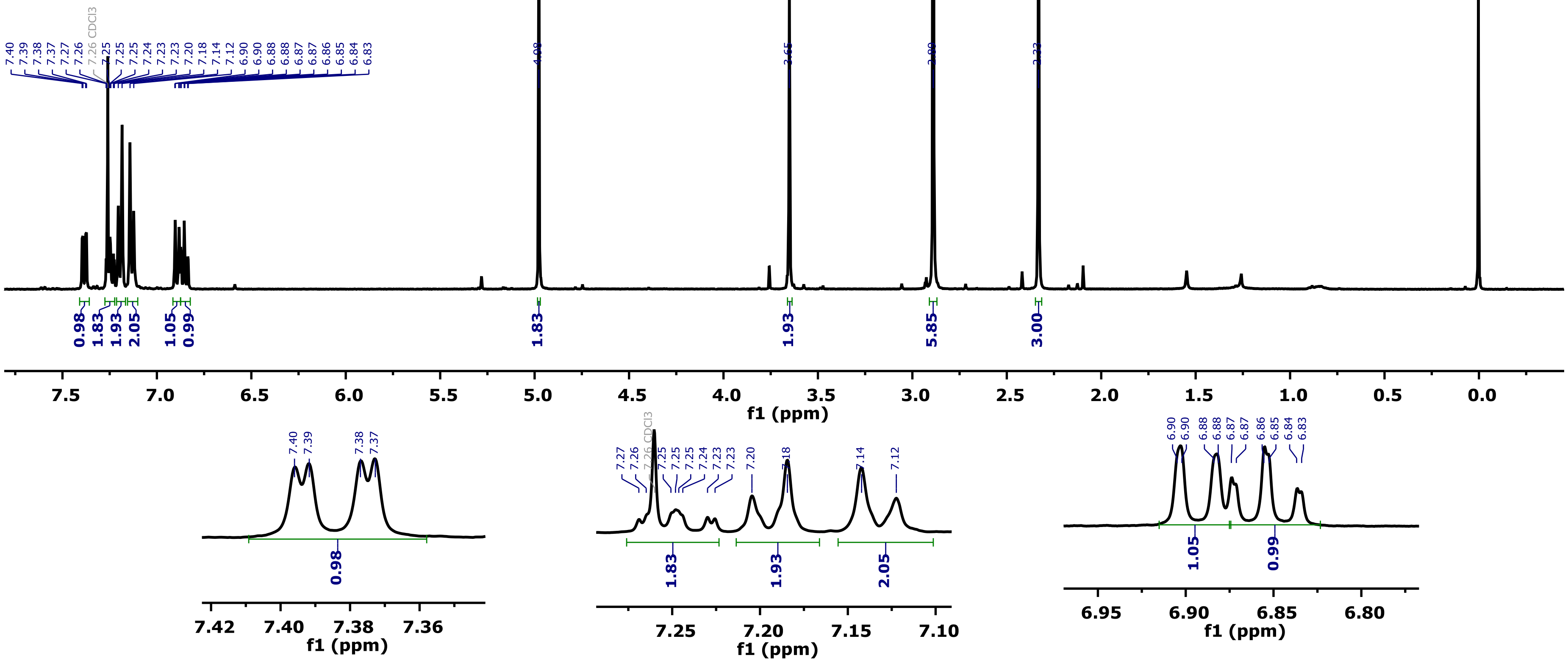


$^{13}C\{H\}$ NMR ($CDCl_3$, 101 MHz)

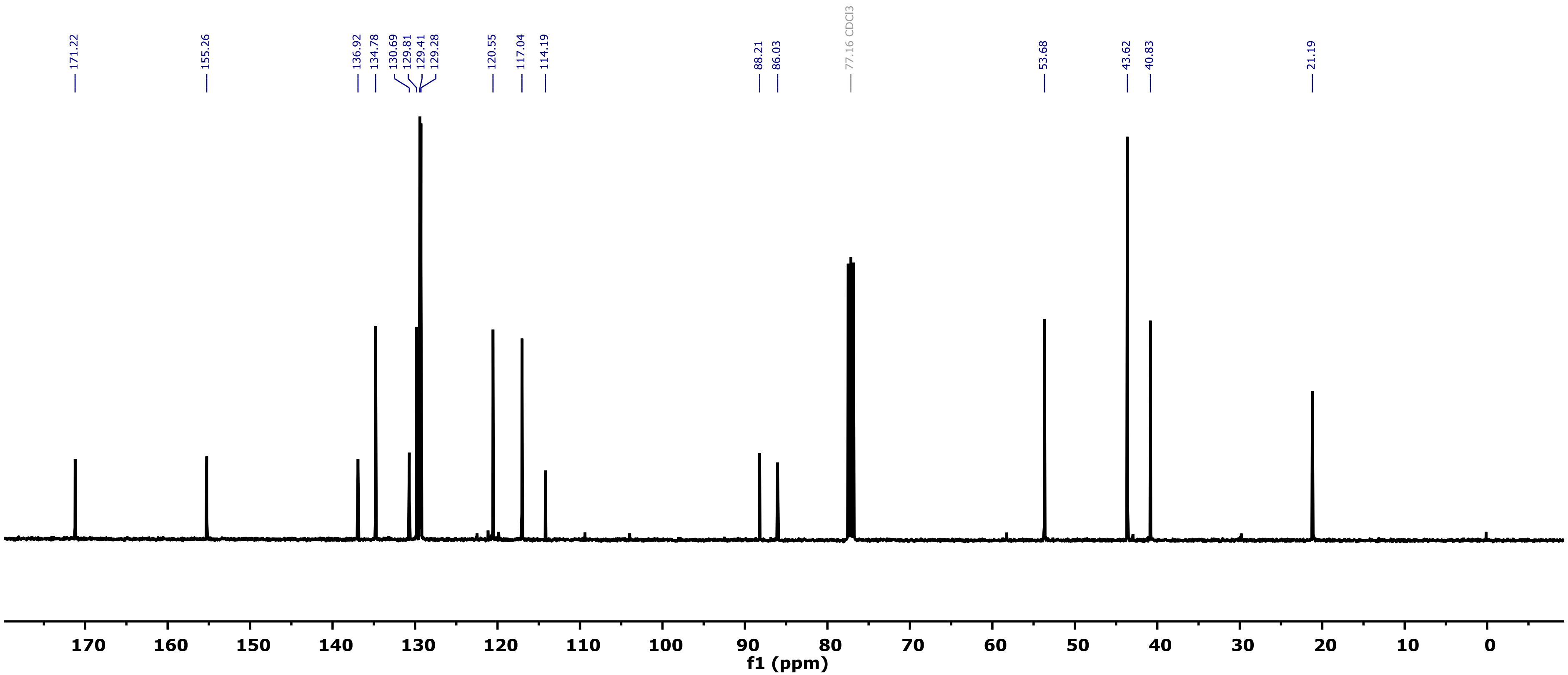


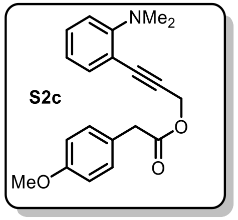


^{1}H NMR (400 MHz, $CDCl_3$)



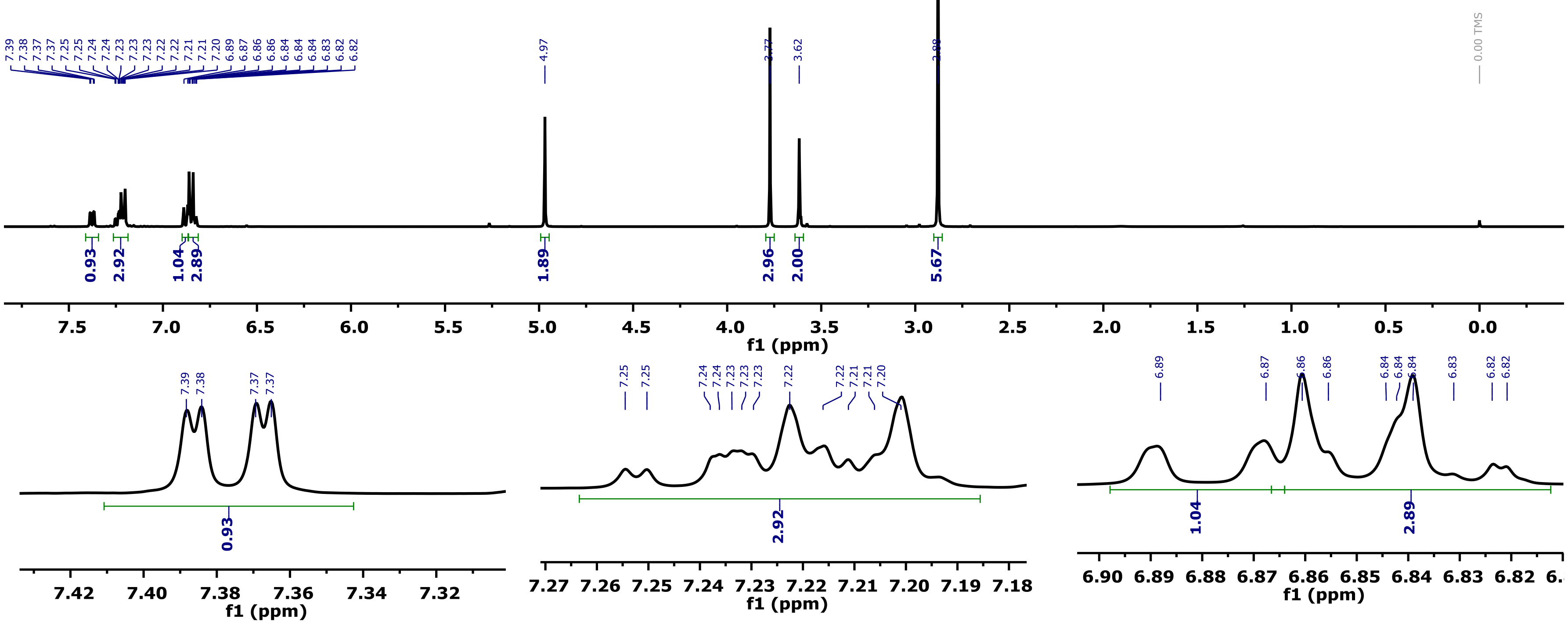
$^{13}C\{H\}$ NMR ($CDCl_3$, 101 MHz)



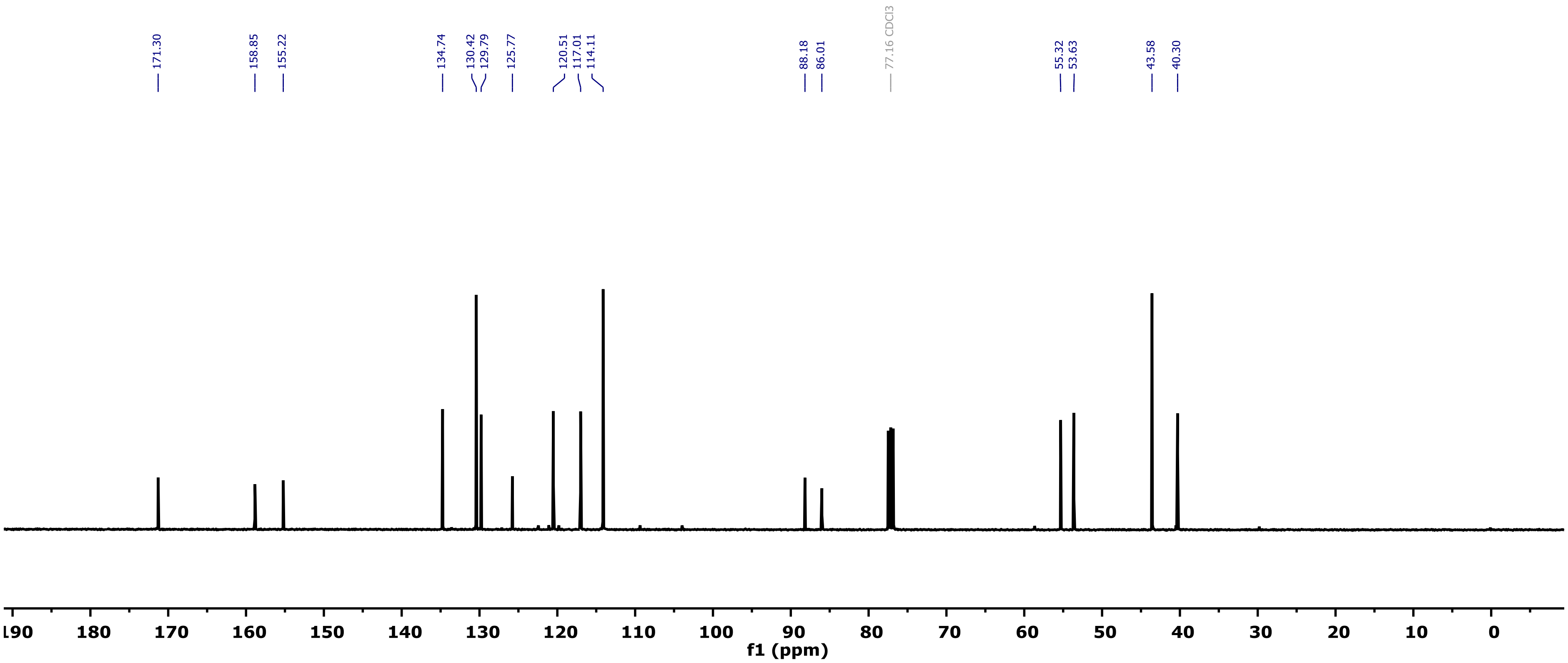


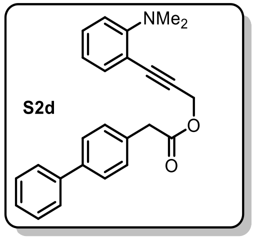
S2c

[1]H NMR (400 MHz, CDCl$_3$)



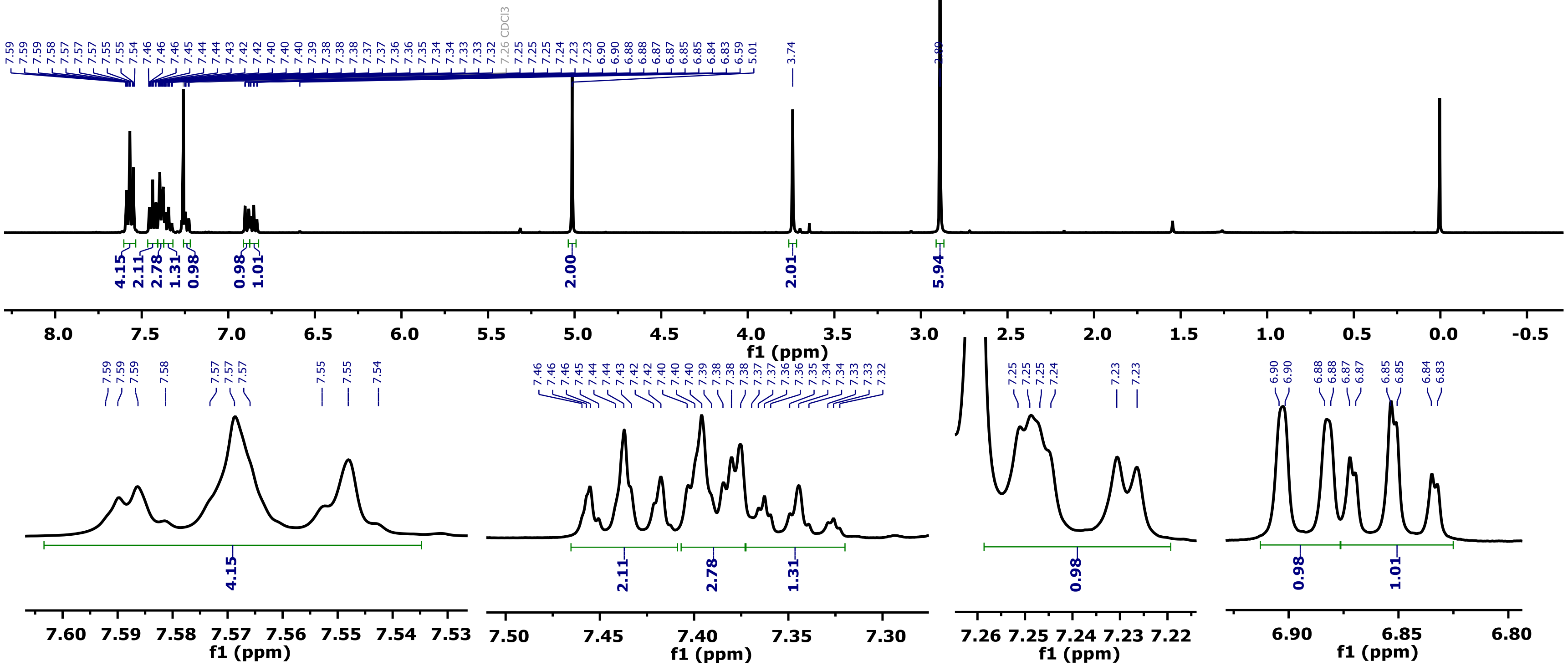
$^{13}C\{H\}$ NMR ($CDCl_3$, 101 MHz)



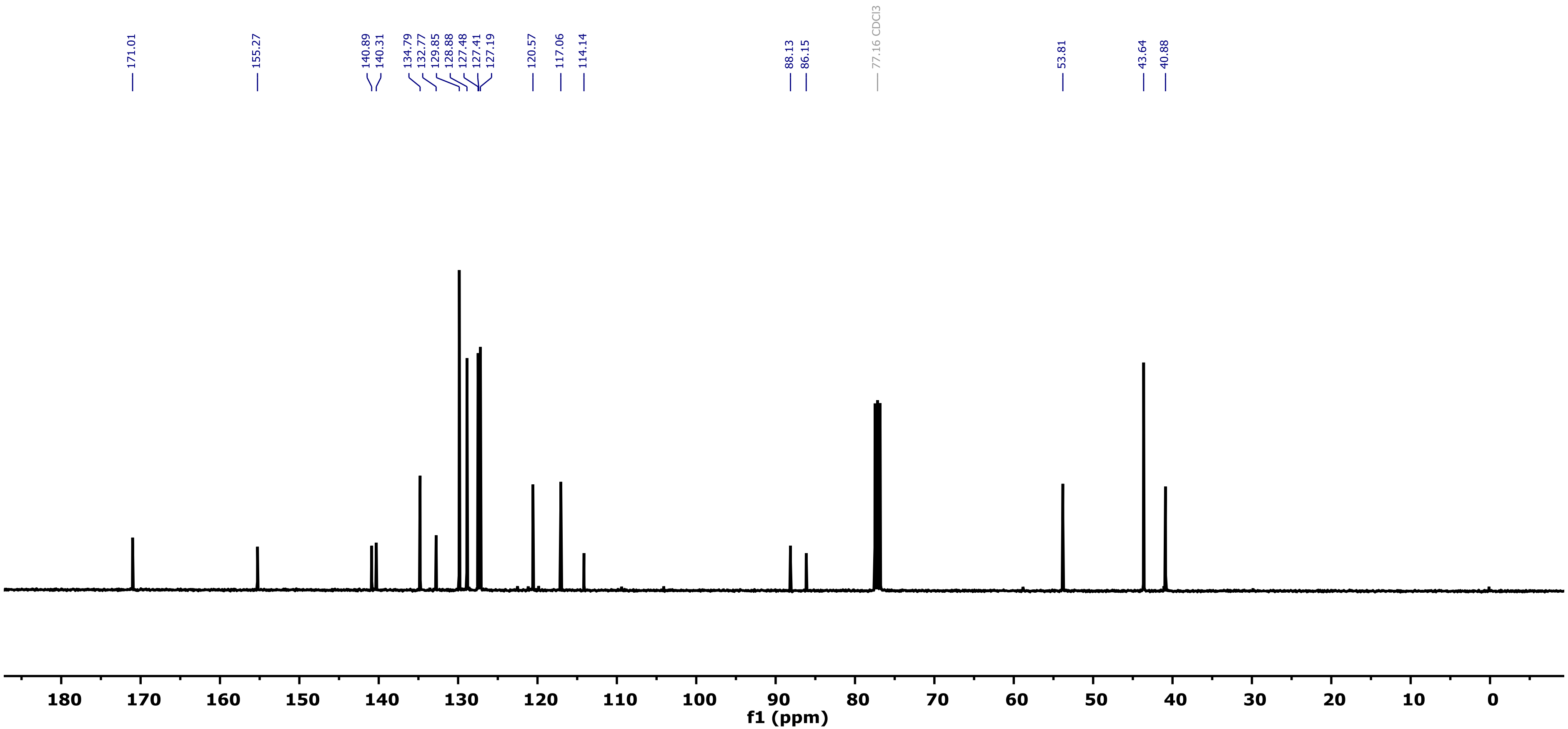


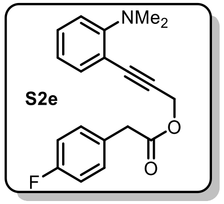
S2d

[1]H NMR (400 MHz, $CDCl_3$)

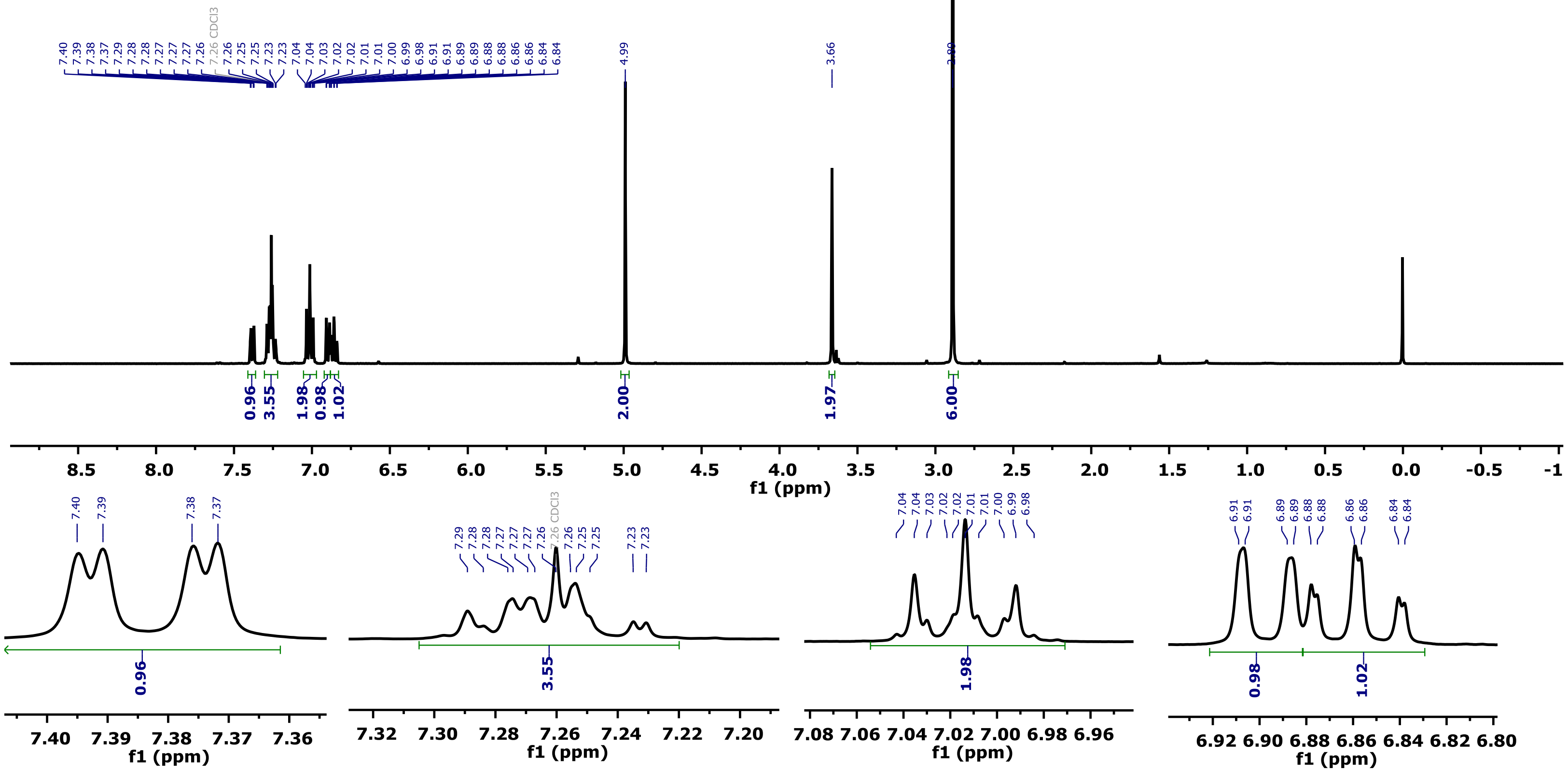


$^{13}C\{H\}$ NMR ($CDCl_3$, 101 MHz)

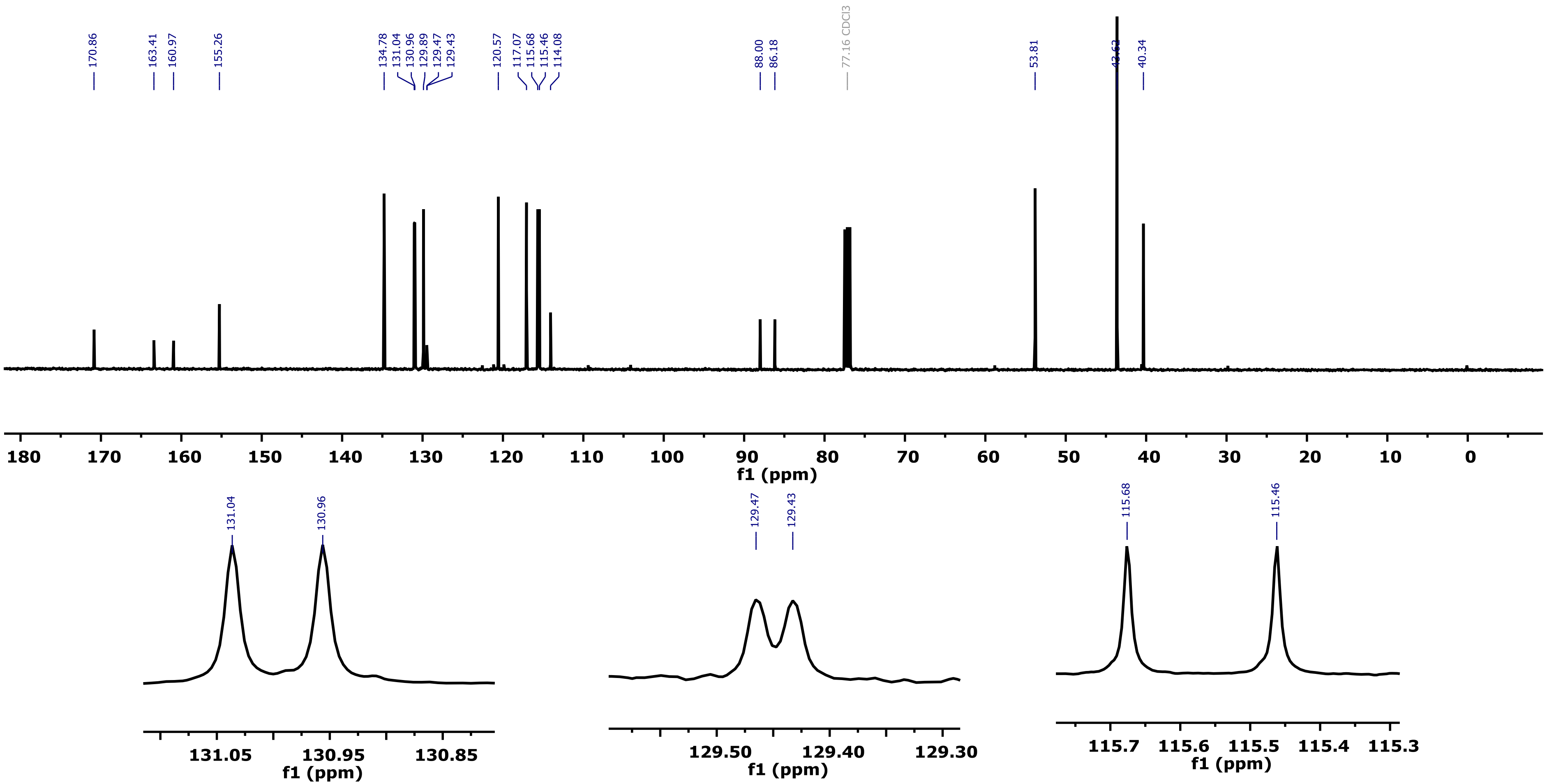




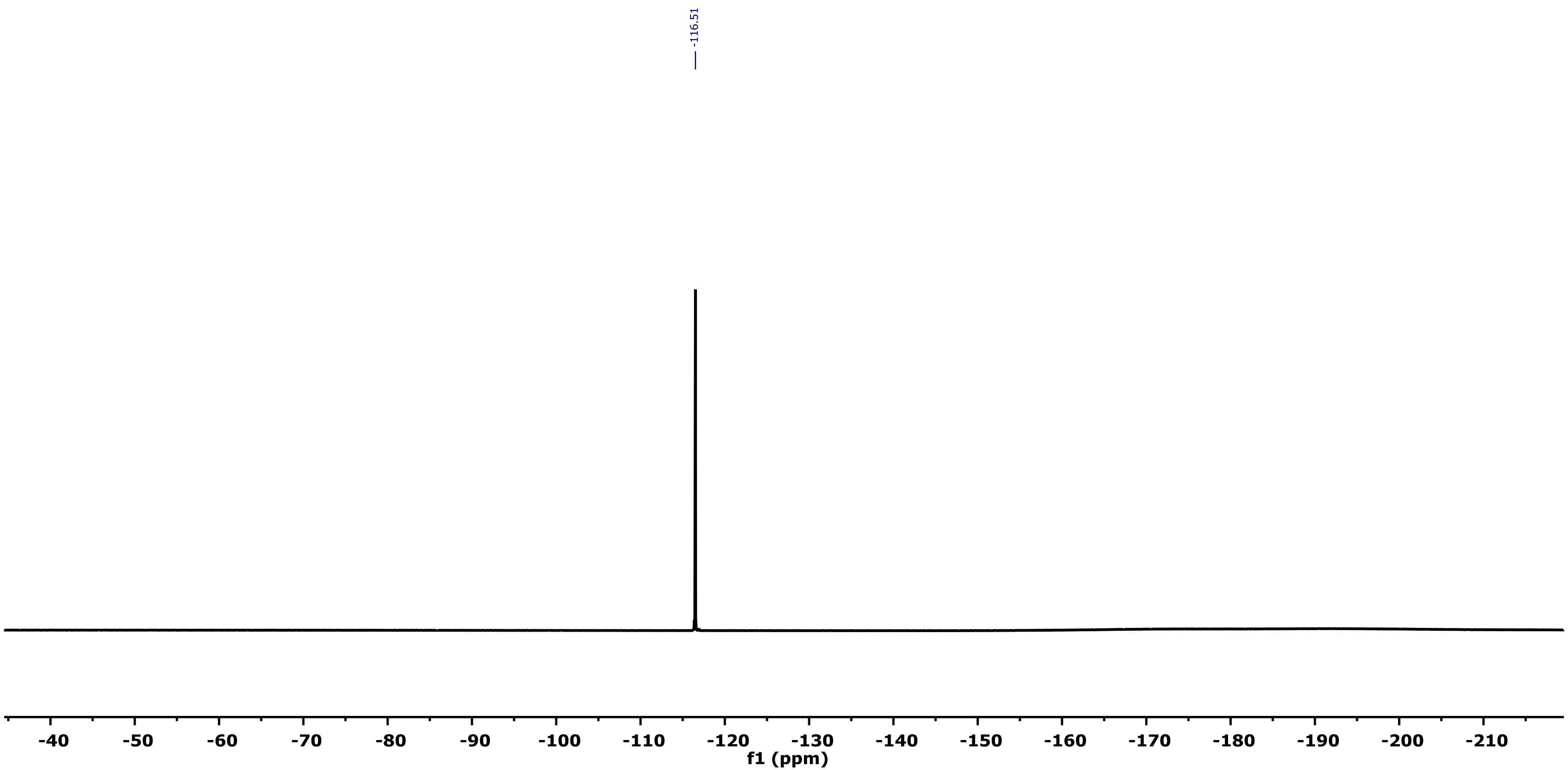
^{1}H NMR (400 MHz, $CDCl_3$)

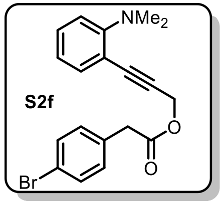


$^{13}C\{H\}$ NMR ($CDCl_3$, 101 MHz)

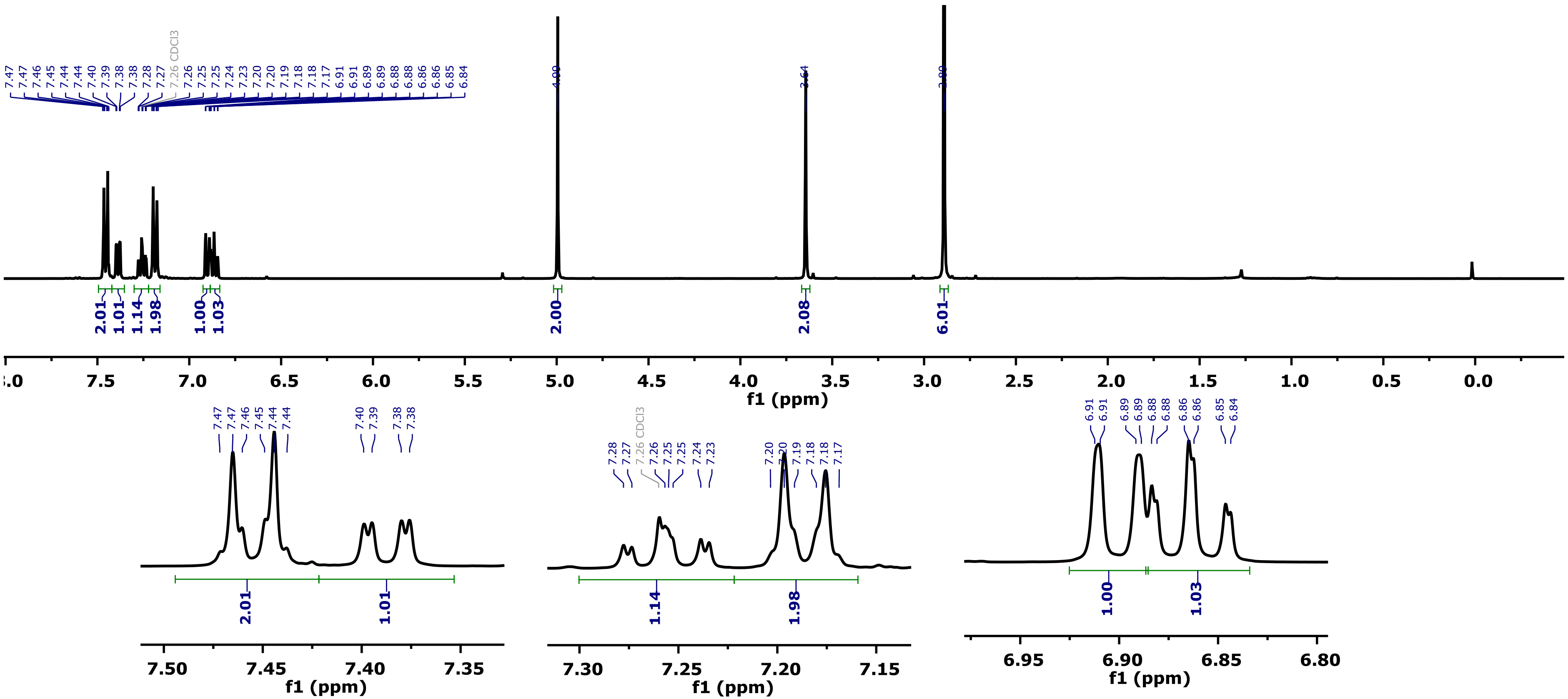


^{19}F NMR ($CDCl_3$, 376 MHz):

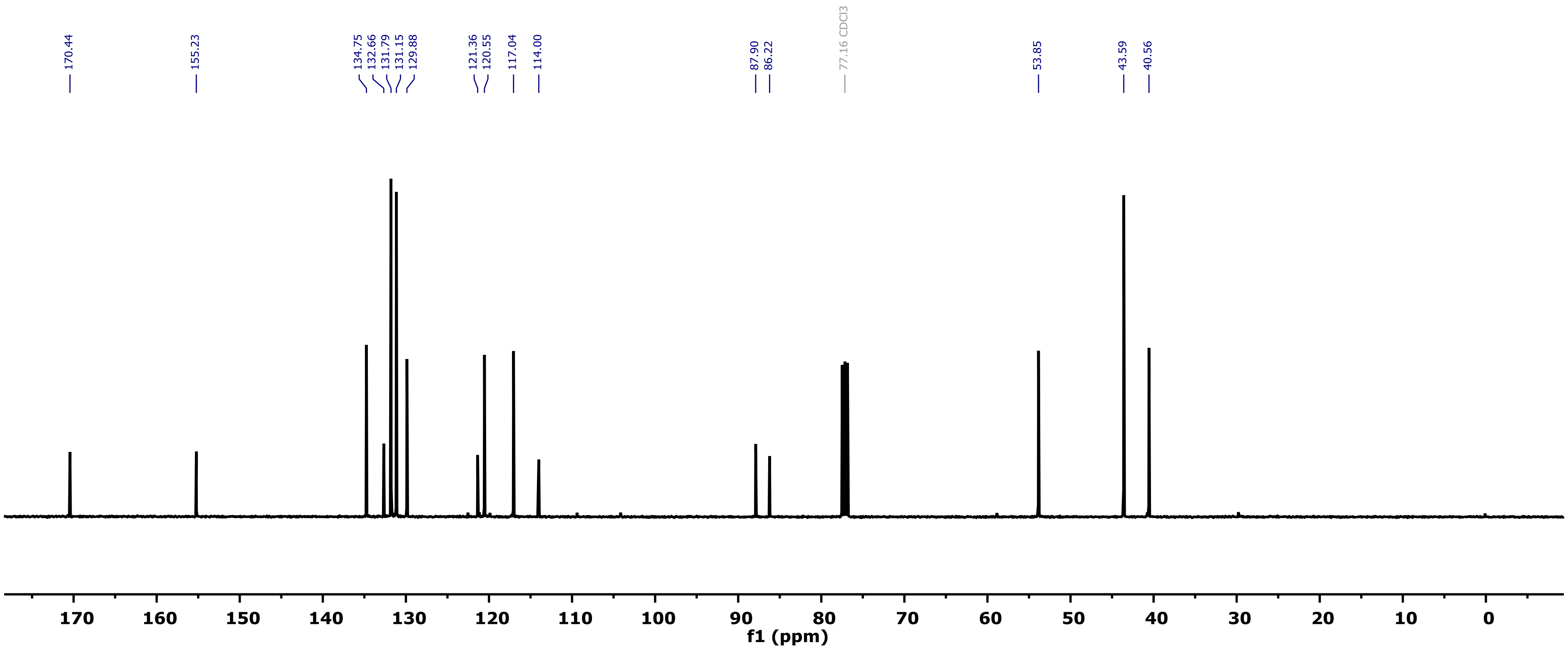


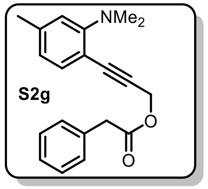


^{1}H NMR (400 MHz, $CDCl_3$)



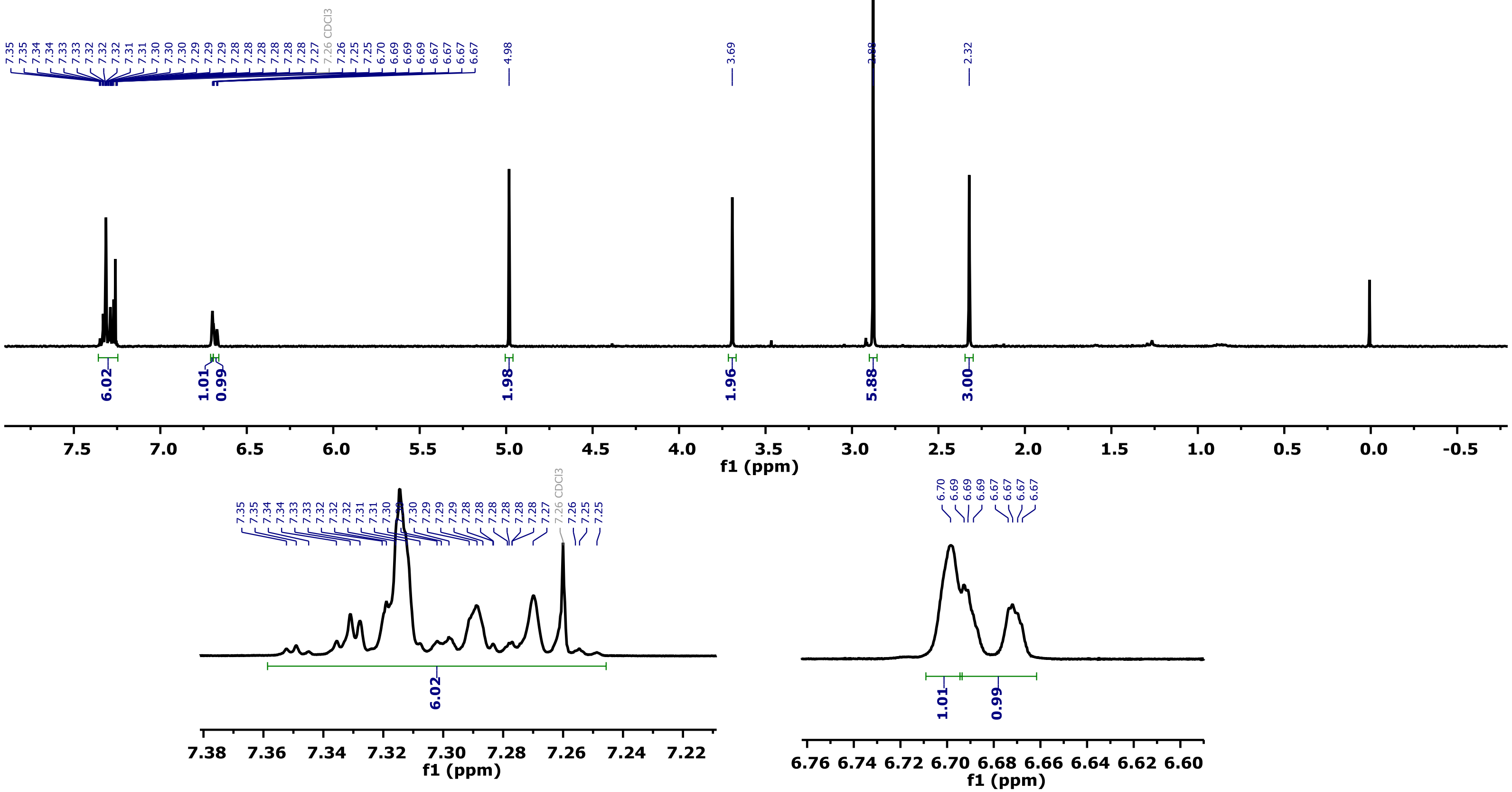
$^{13}C\{H\}$ NMR ($CDCl_3$, 101 MHz)



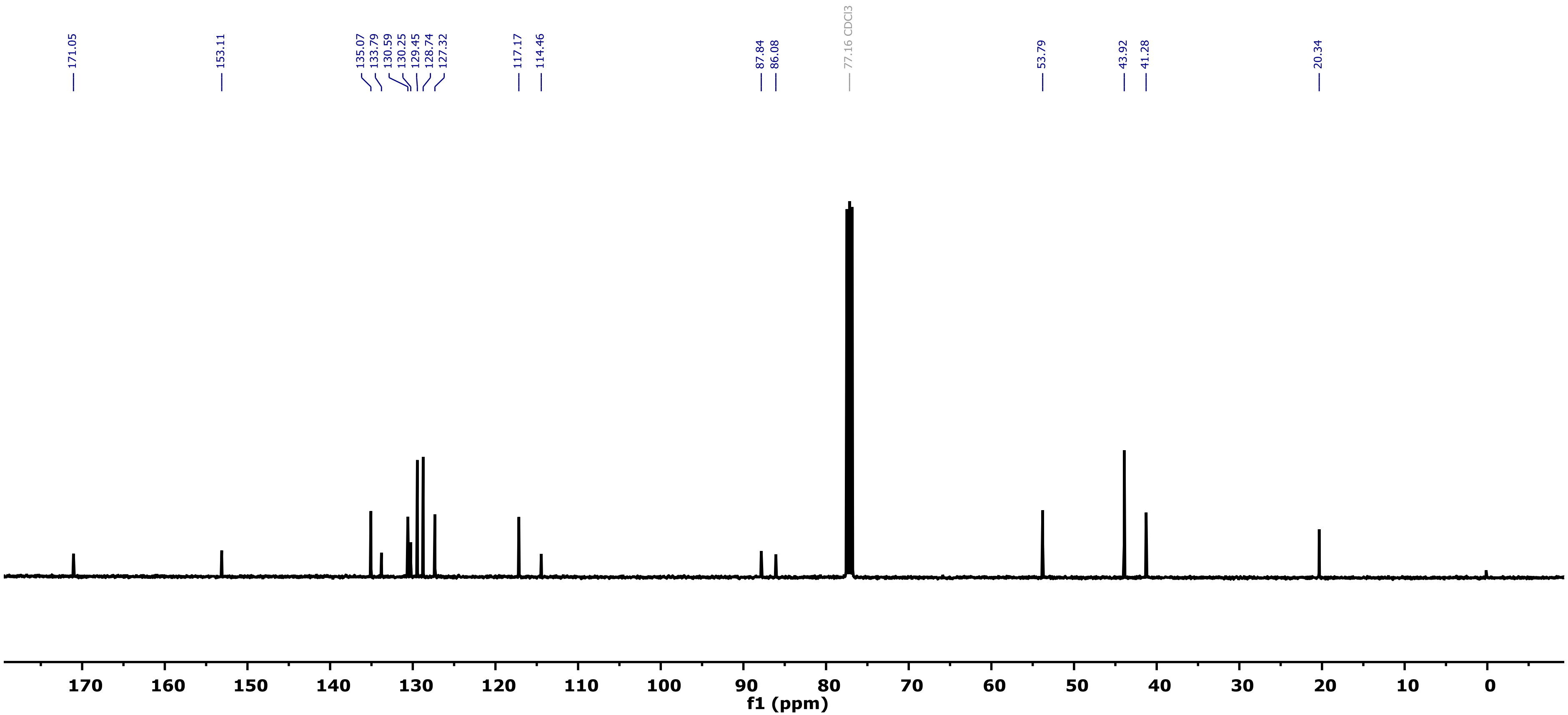


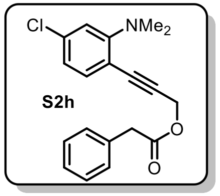
S2g

^{1}H NMR (400 MHz, $CDCl_3$)



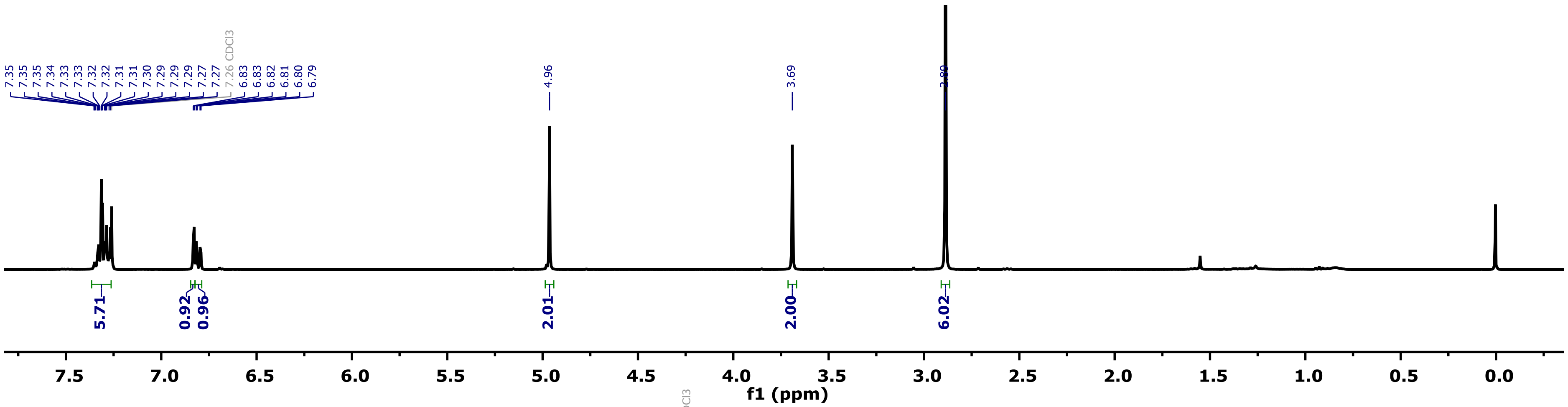
$^{13}C\{H\}$ NMR ($CDCl_3$, 101 MHz)

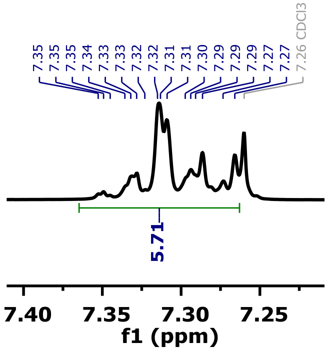


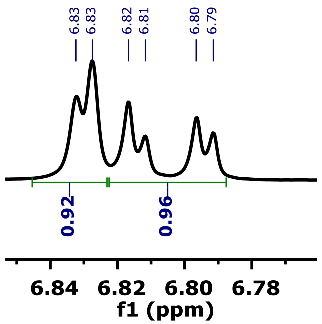


S2h

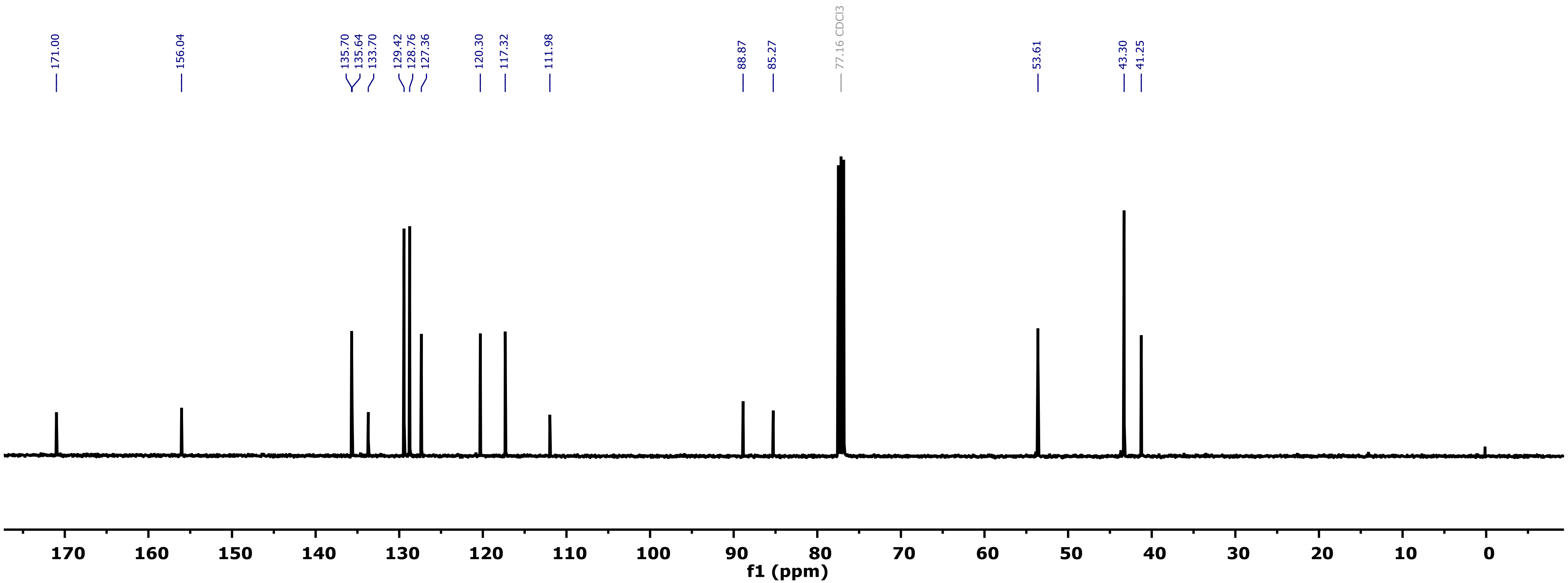
^{1}H NMR (400 MHz, $CDCl_3$)

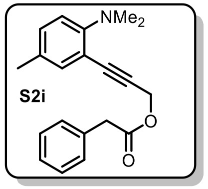






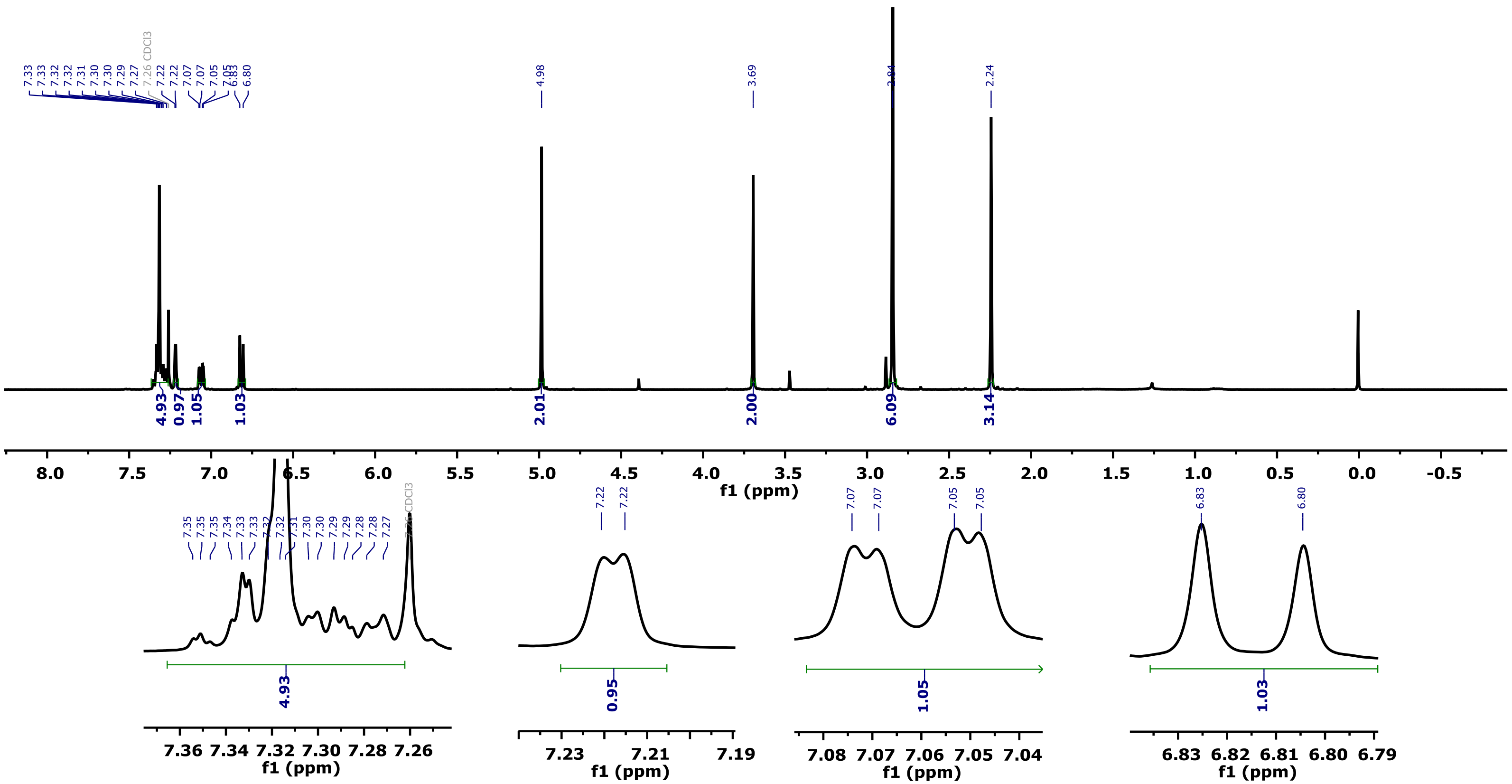
$^{13}C\{H\}$ NMR ($CDCl_3$, 101 MHz)



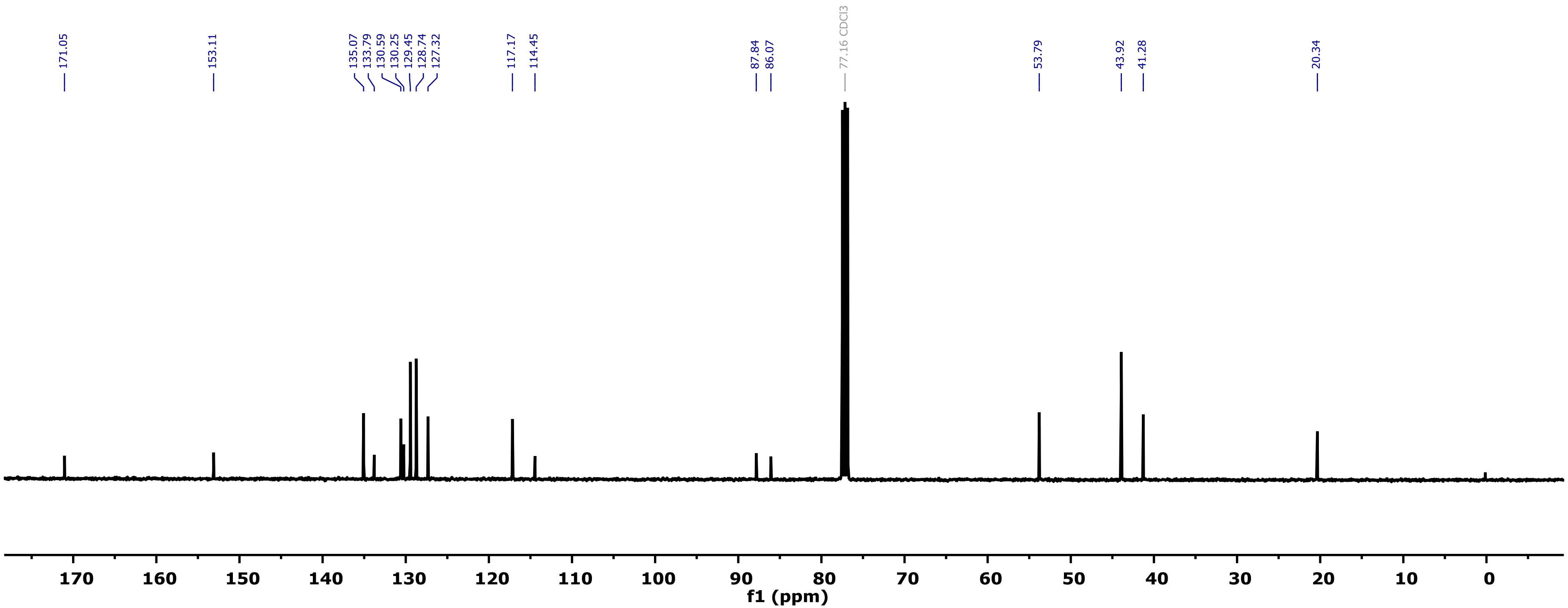


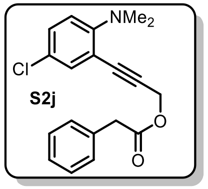
S2i

^{1}H NMR (400 MHz, $CDCl_3$)

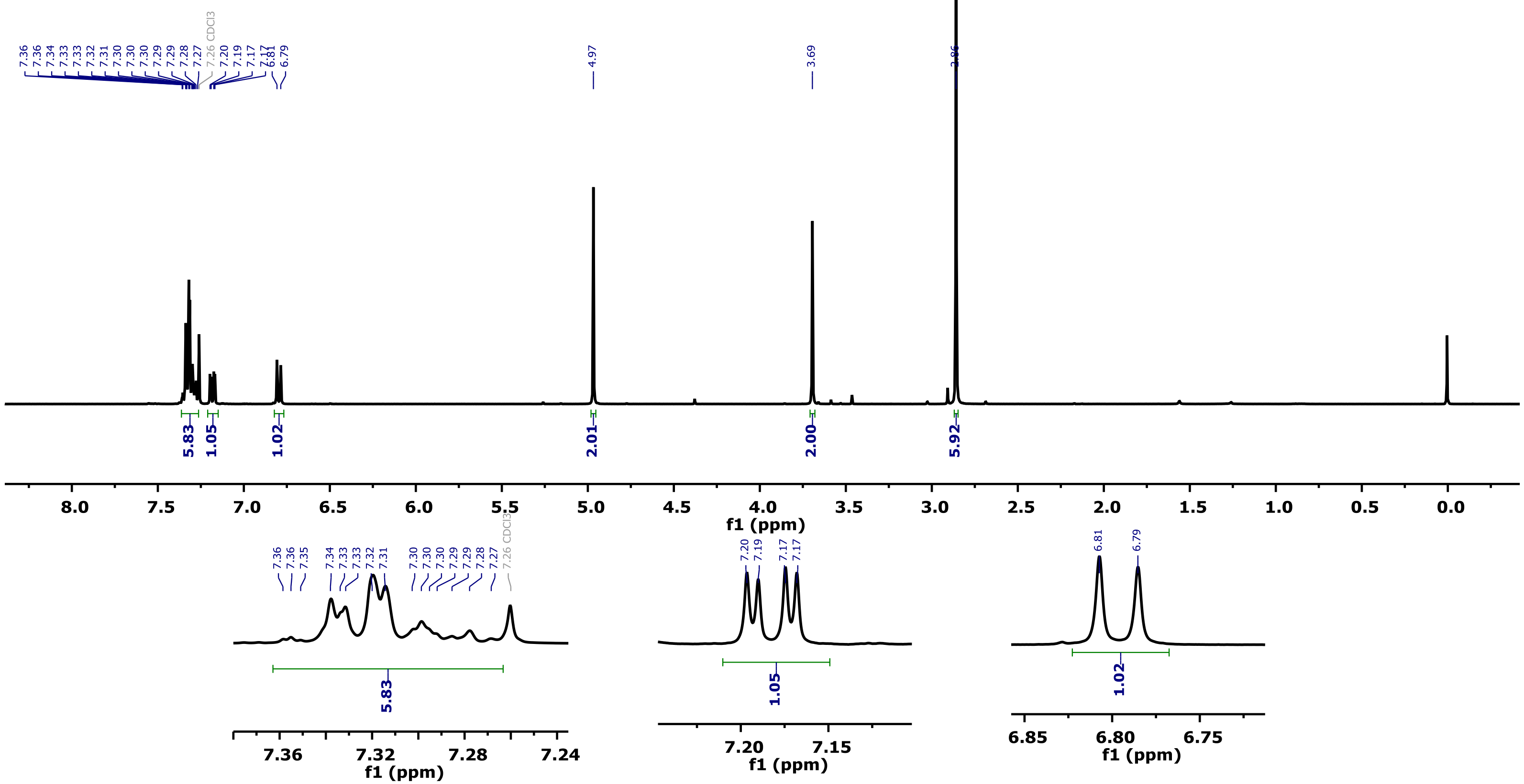


$^{13}C\{H\}$ NMR ($CDCl_3$, 101 MHz)

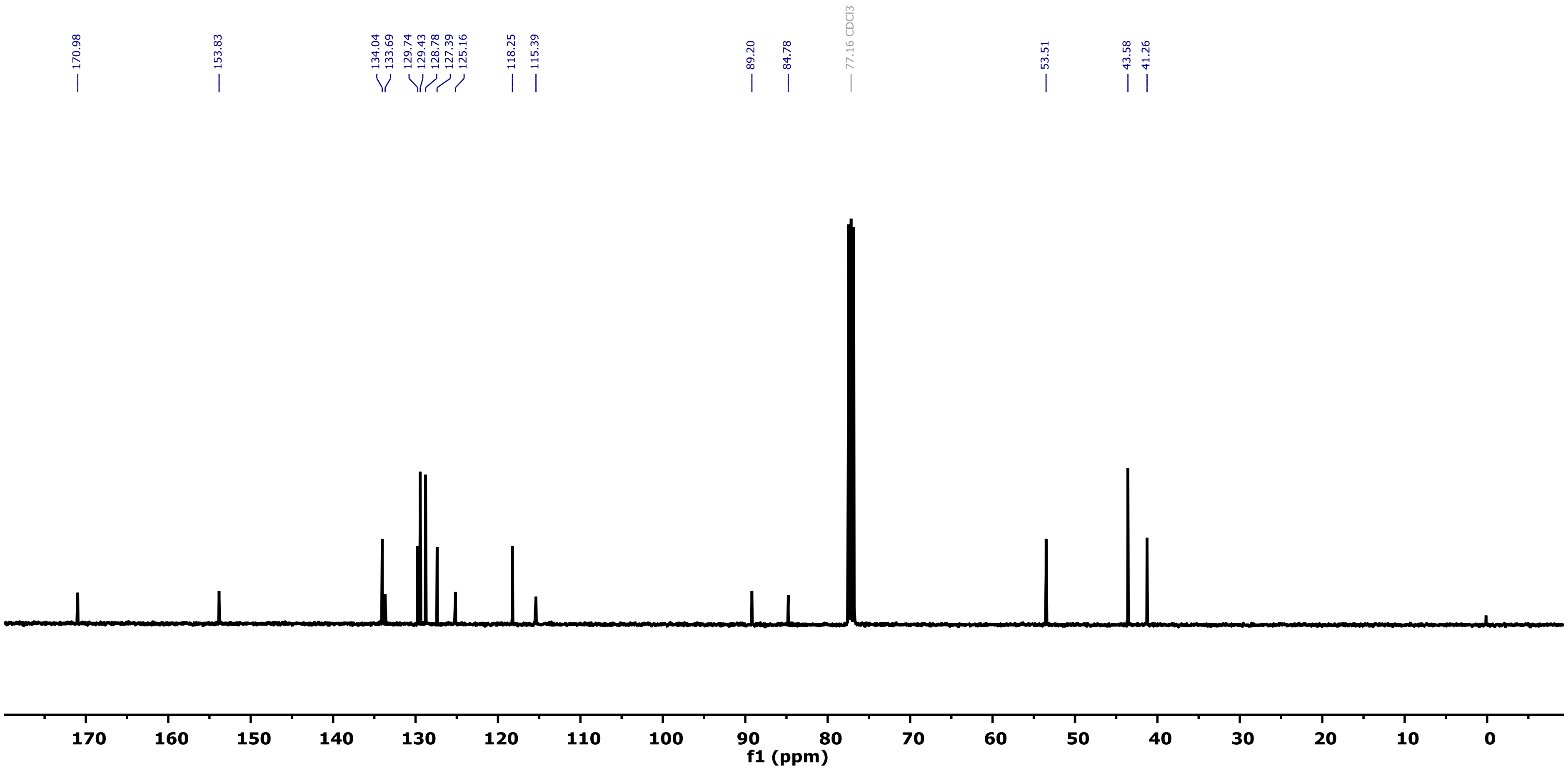


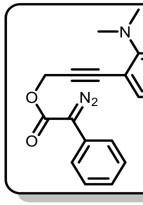


^{1}H NMR (400 MHz, $CDCl_3$)



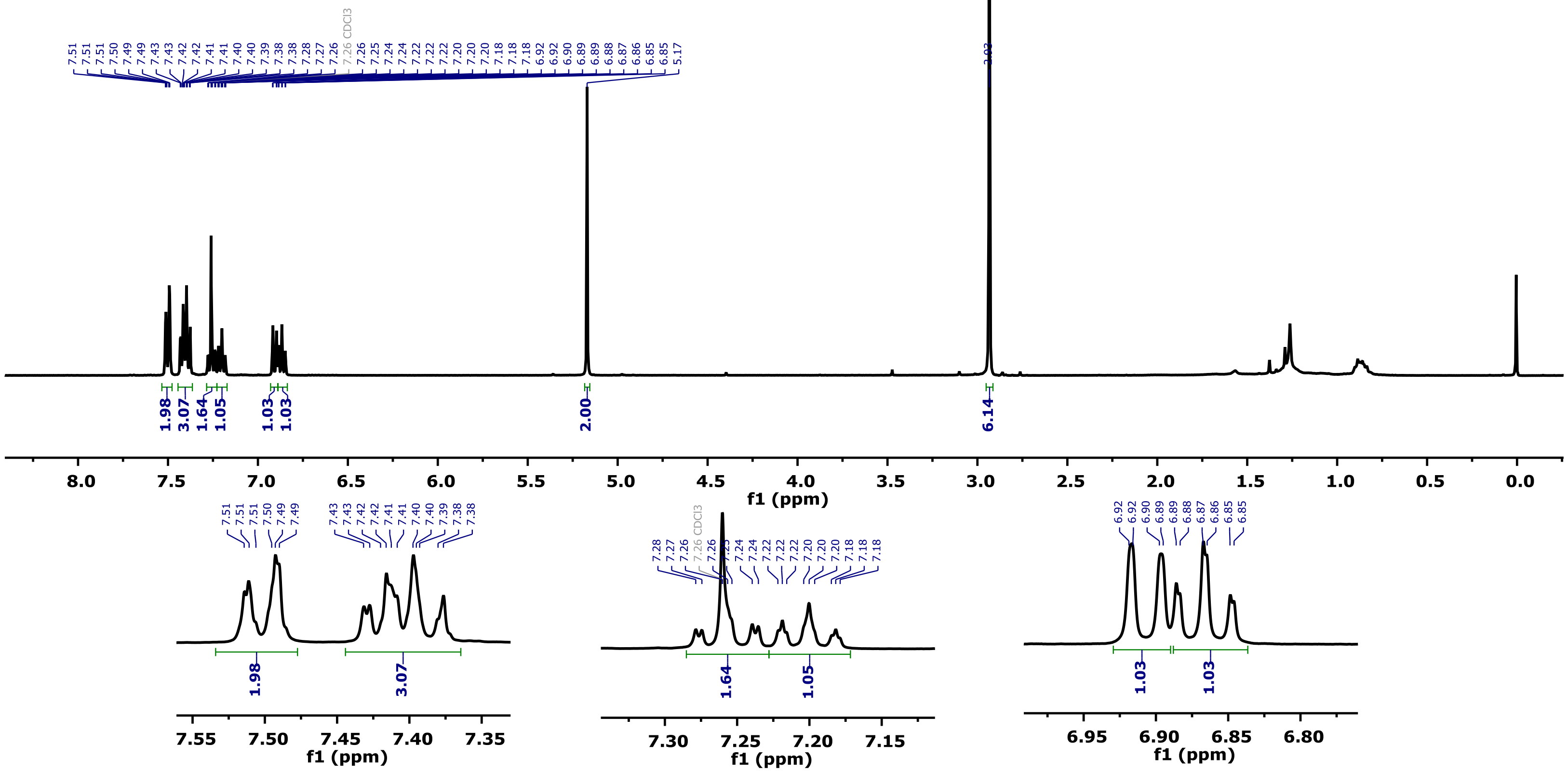
$^{13}C\{H\}$ NMR ($CDCl_3$, 101 MHz)



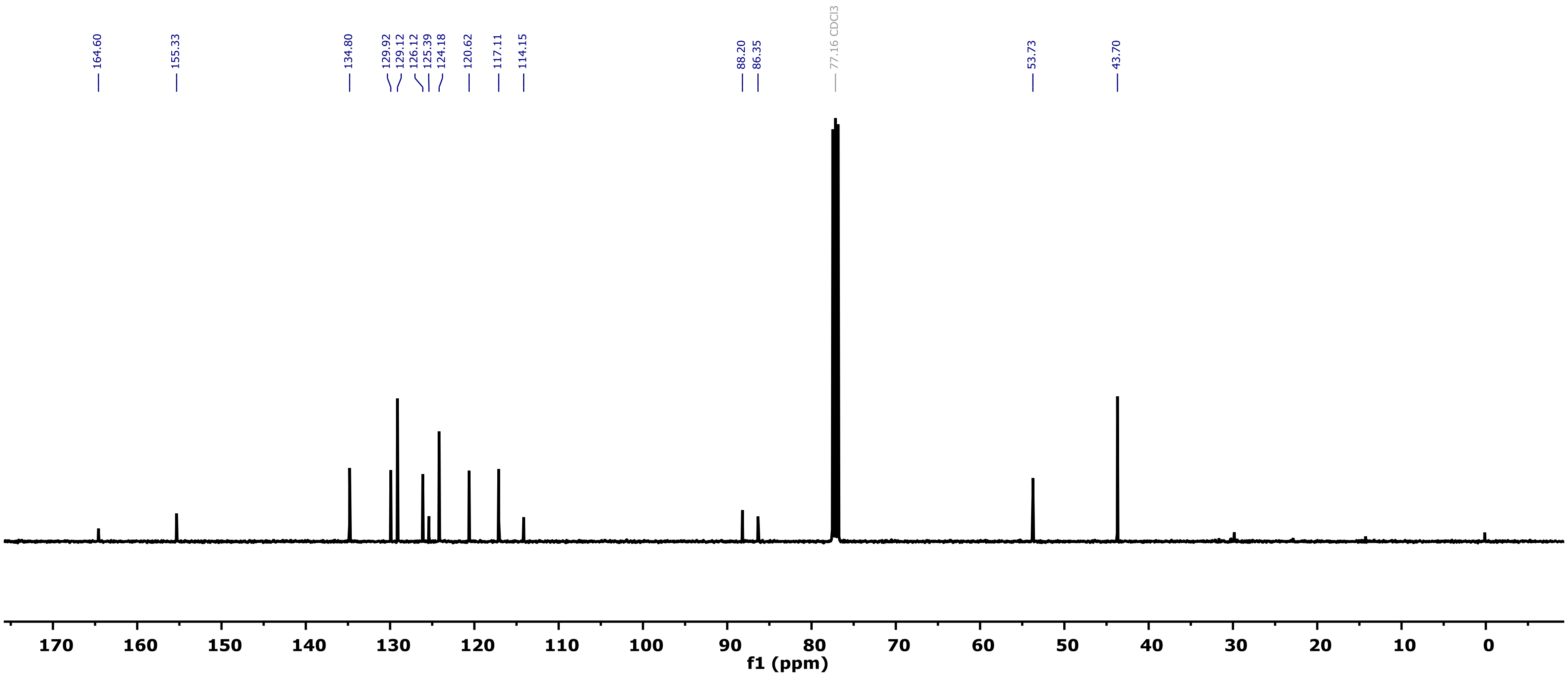


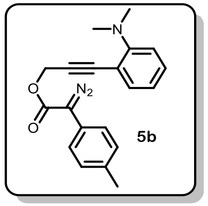
5a

[1]H NMR (400 MHz, CDCl$_3$)

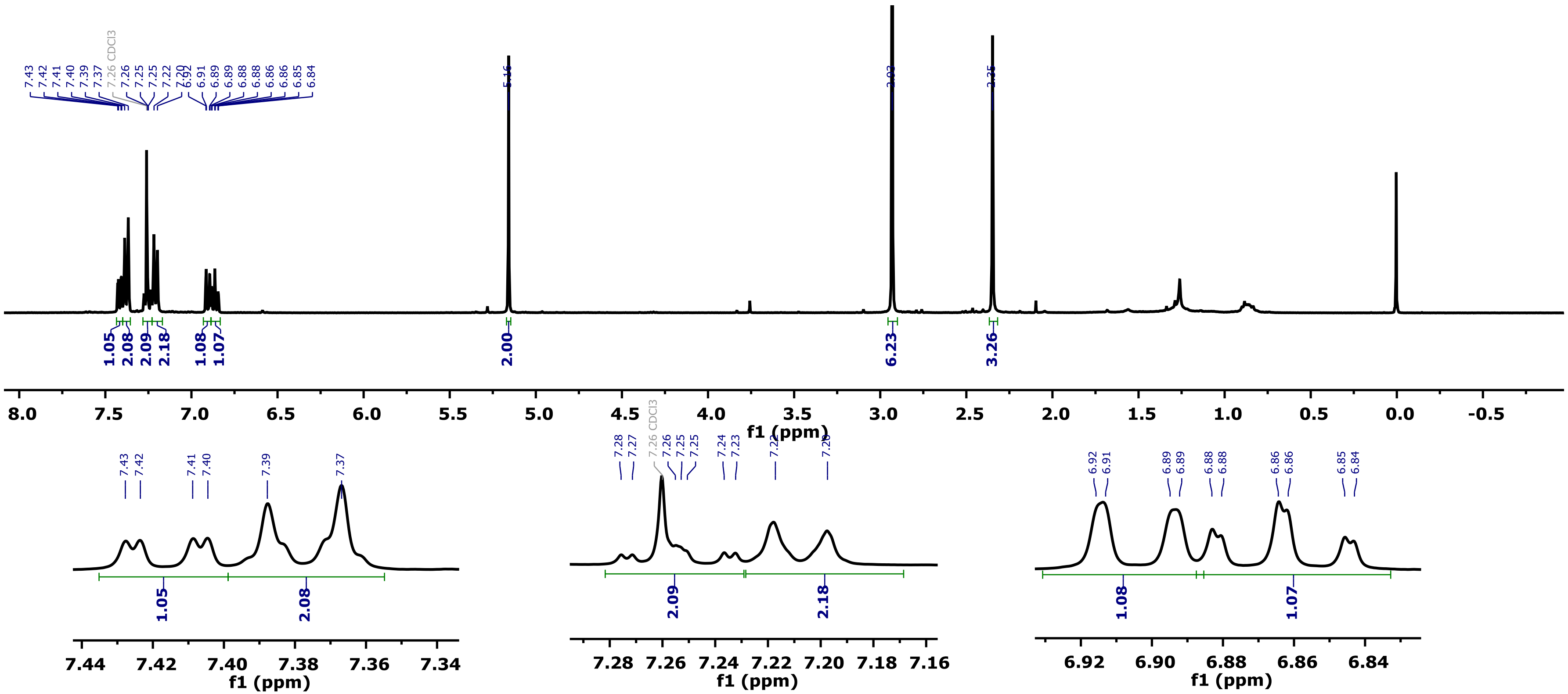


$^{13}C\{H\}$ NMR ($CDCl_3$, 101 MHz)

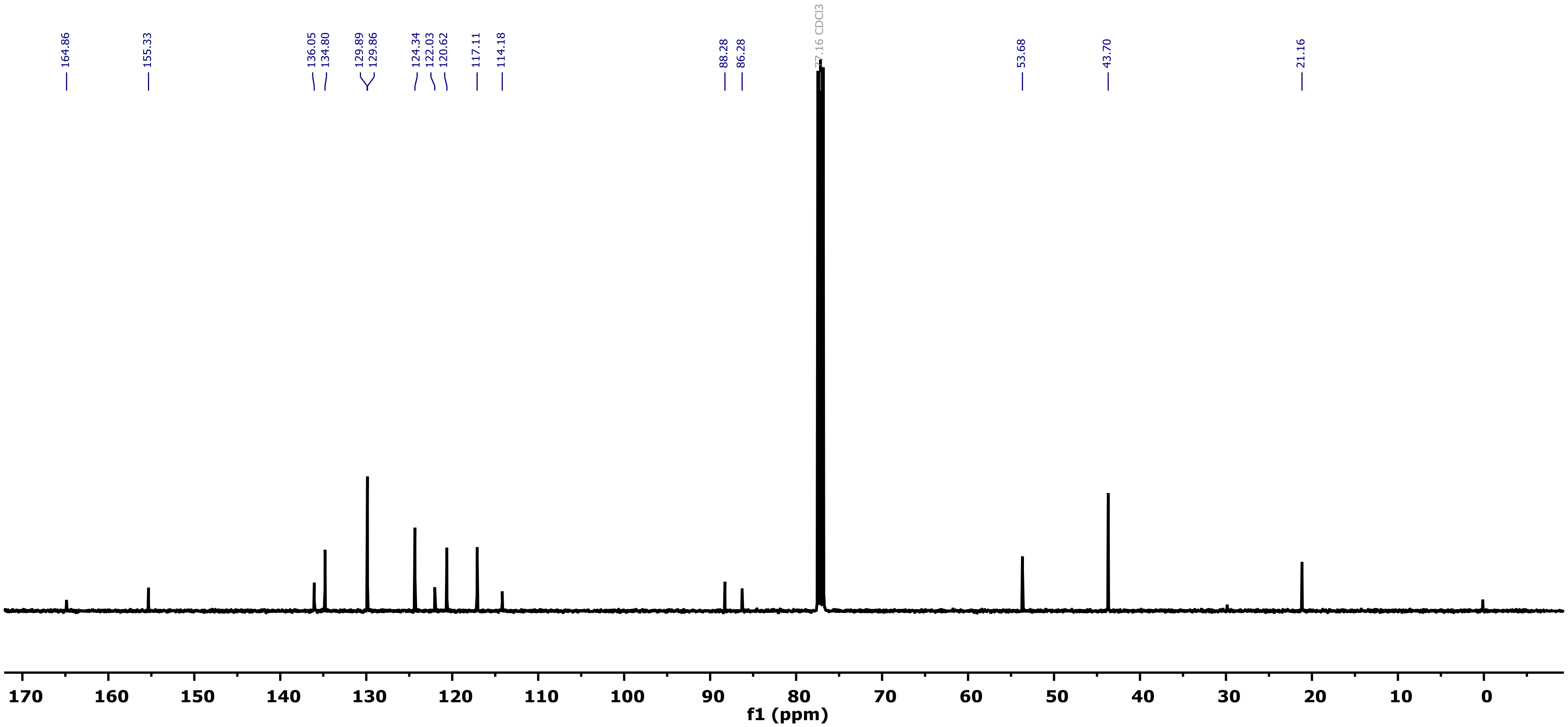


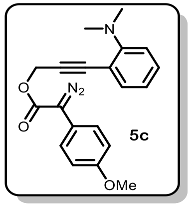


[1]H NMR (400 MHz, CDCl3)

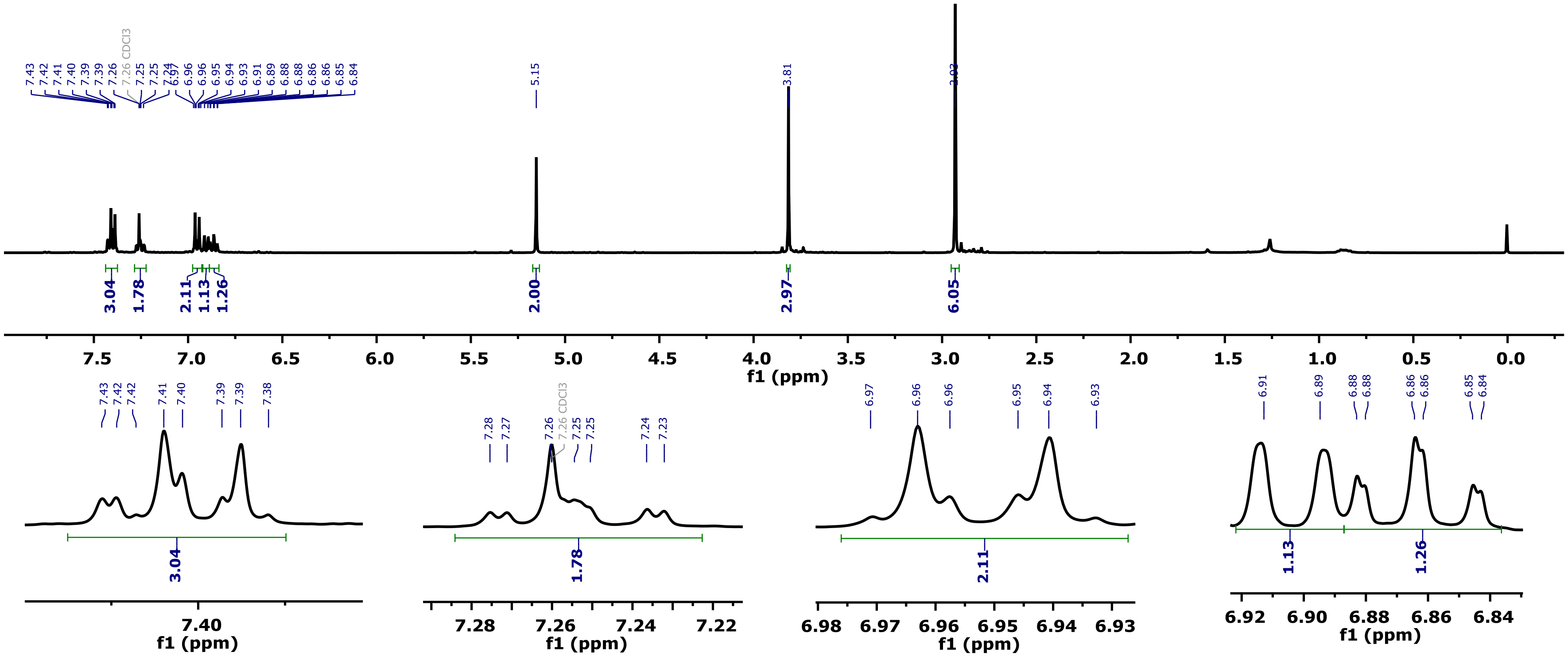


$^{13}C\{H\}$ NMR ($CDCl_3$, 101 MHz)

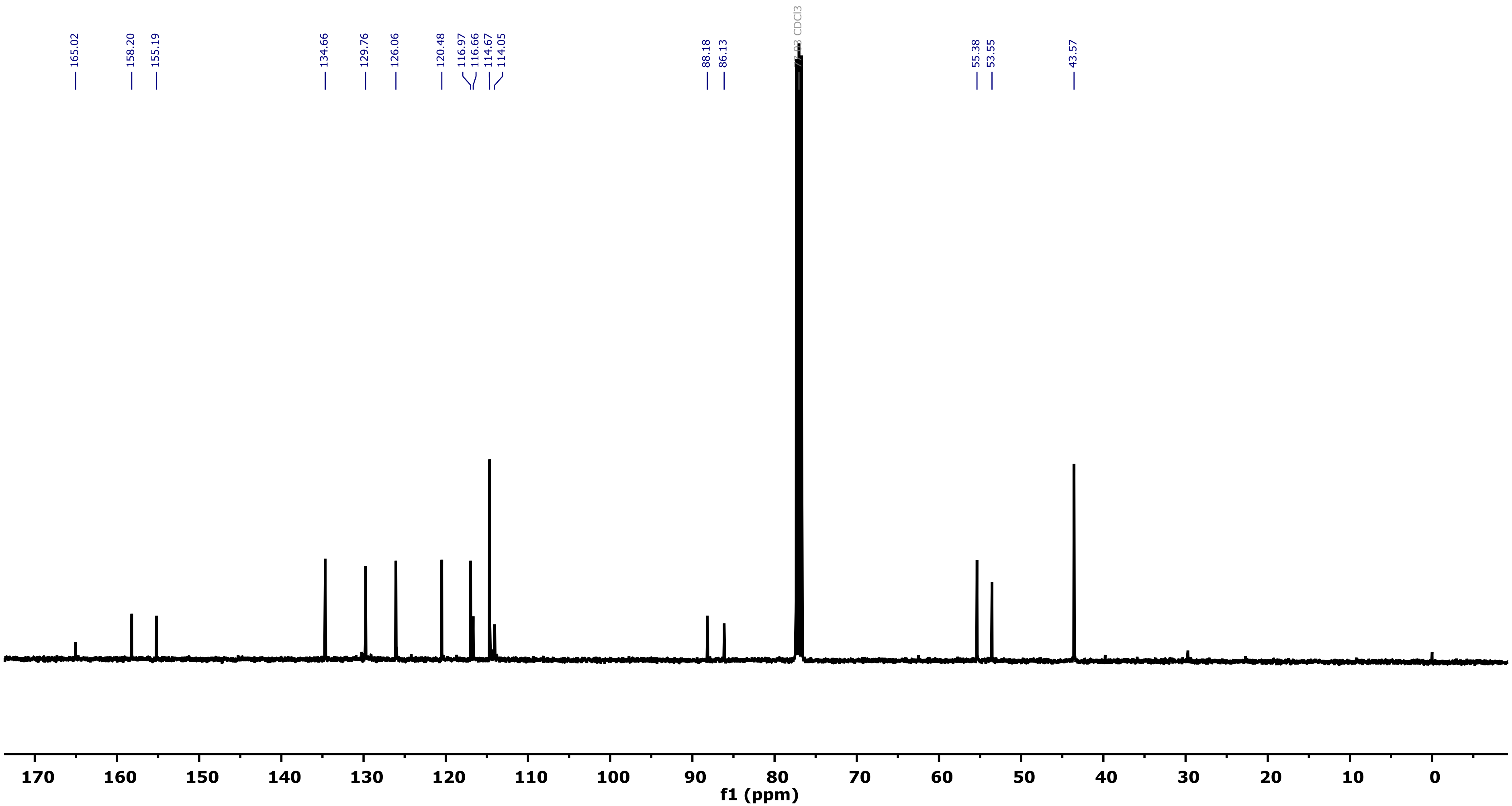


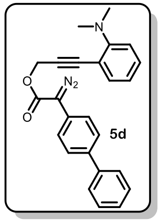


^{1}H NMR (400 MHz, $CDCl_3$)

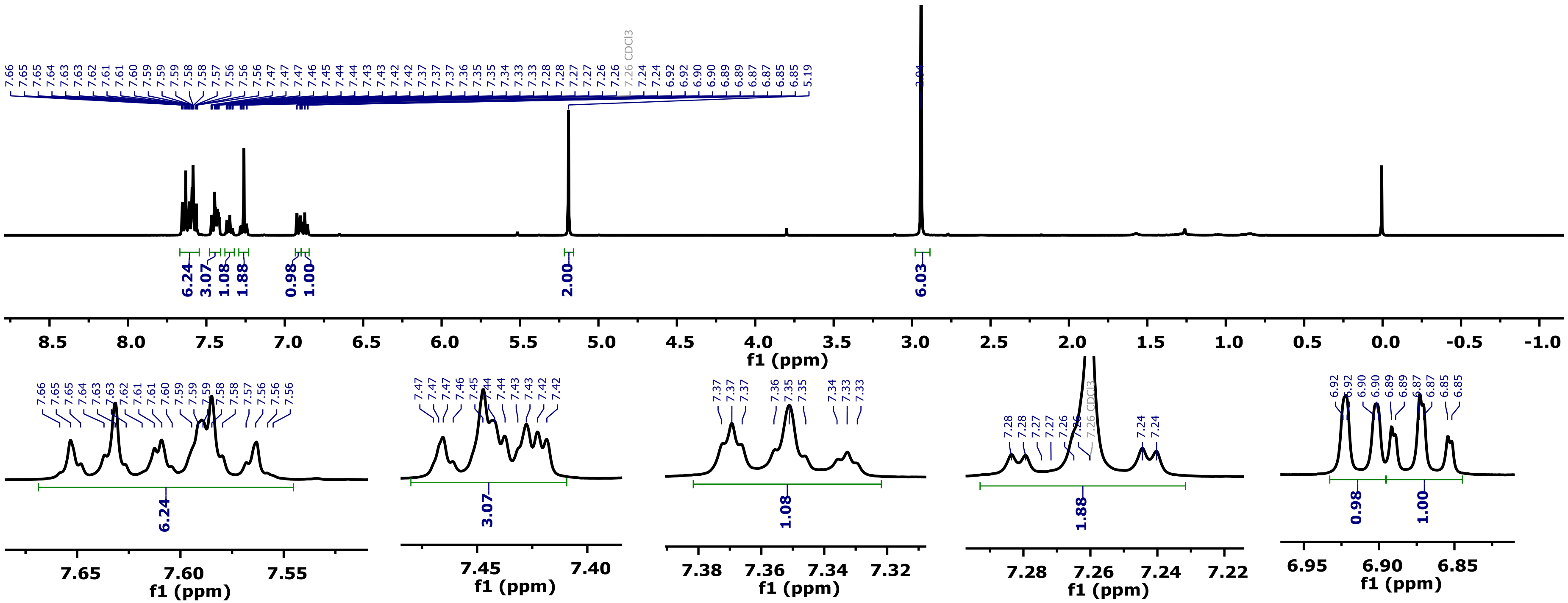


$^{13}C\{H\}$ NMR ($CDCl_3$, 101 MHz)

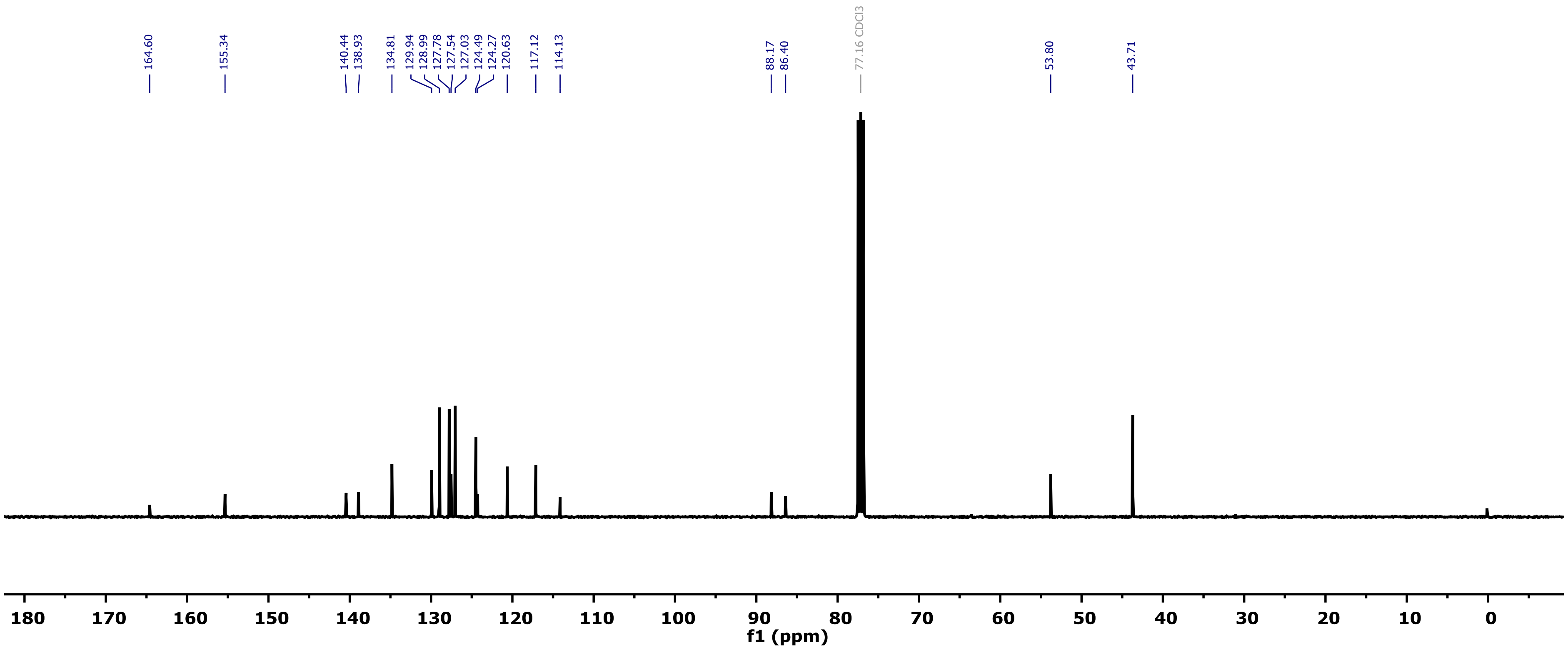


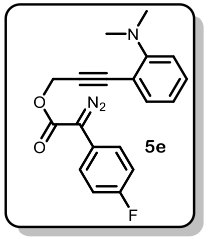


^{1}H NMR (400 MHz, $CDCl_3$)



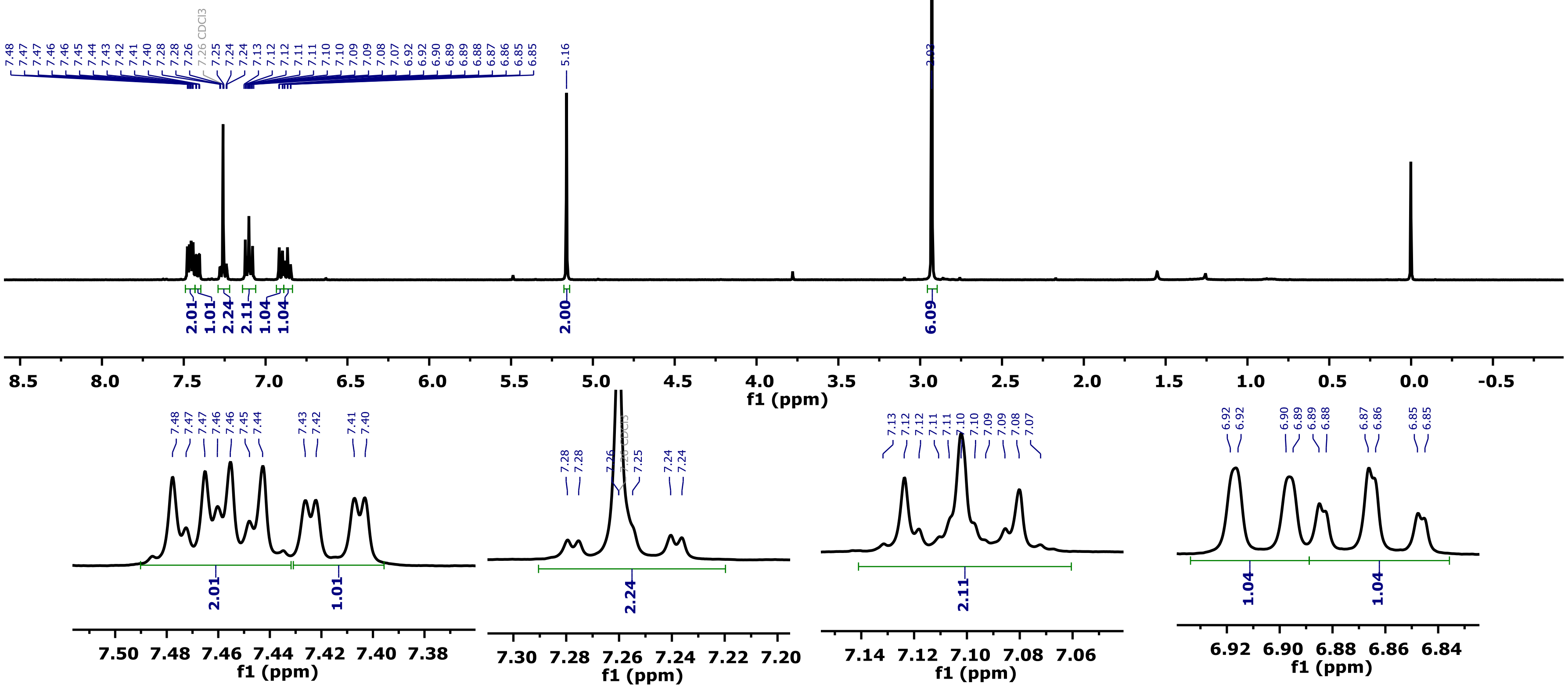
$^{13}C\{H\}$ NMR ($CDCl_3$, 101 MHz)



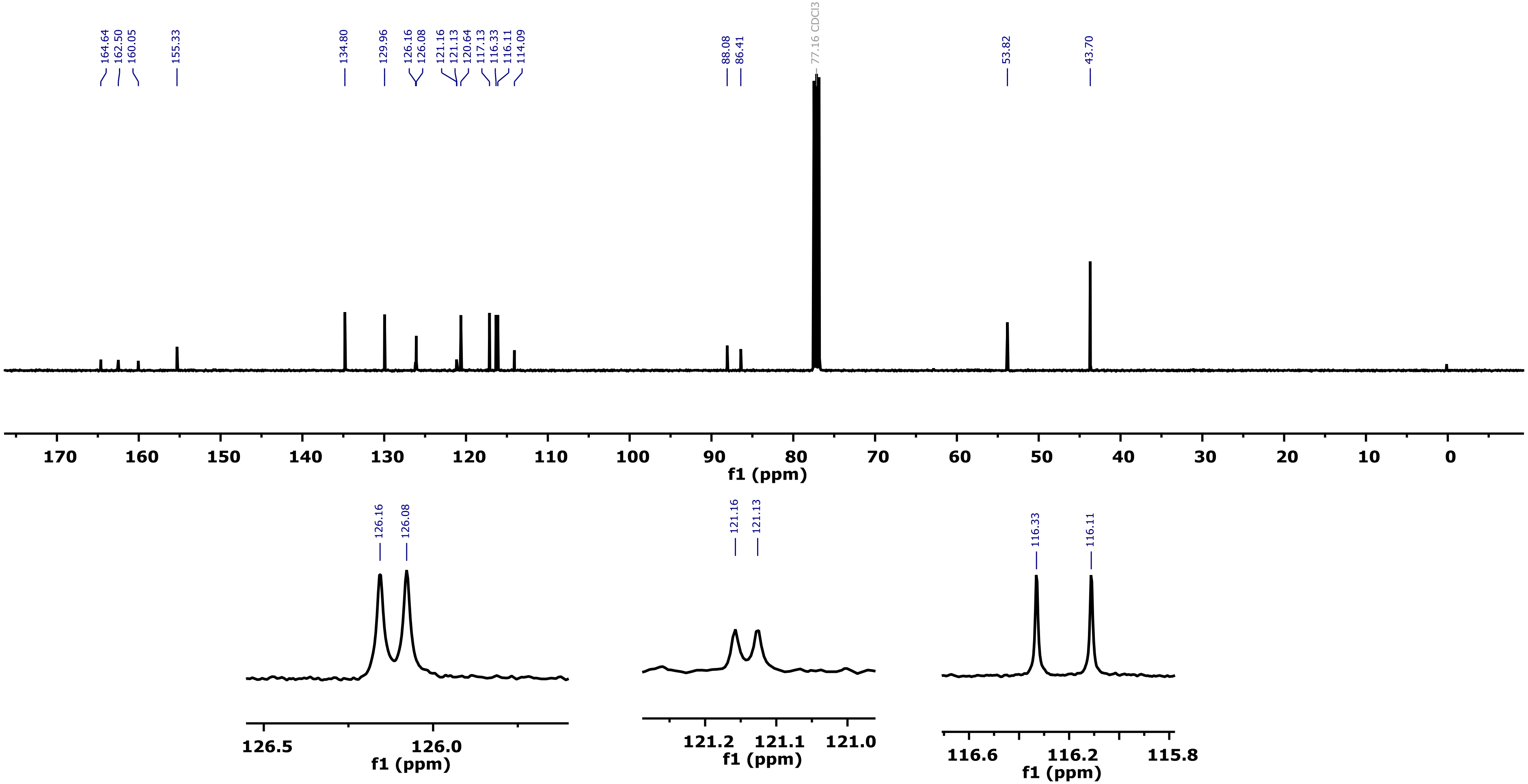


5e

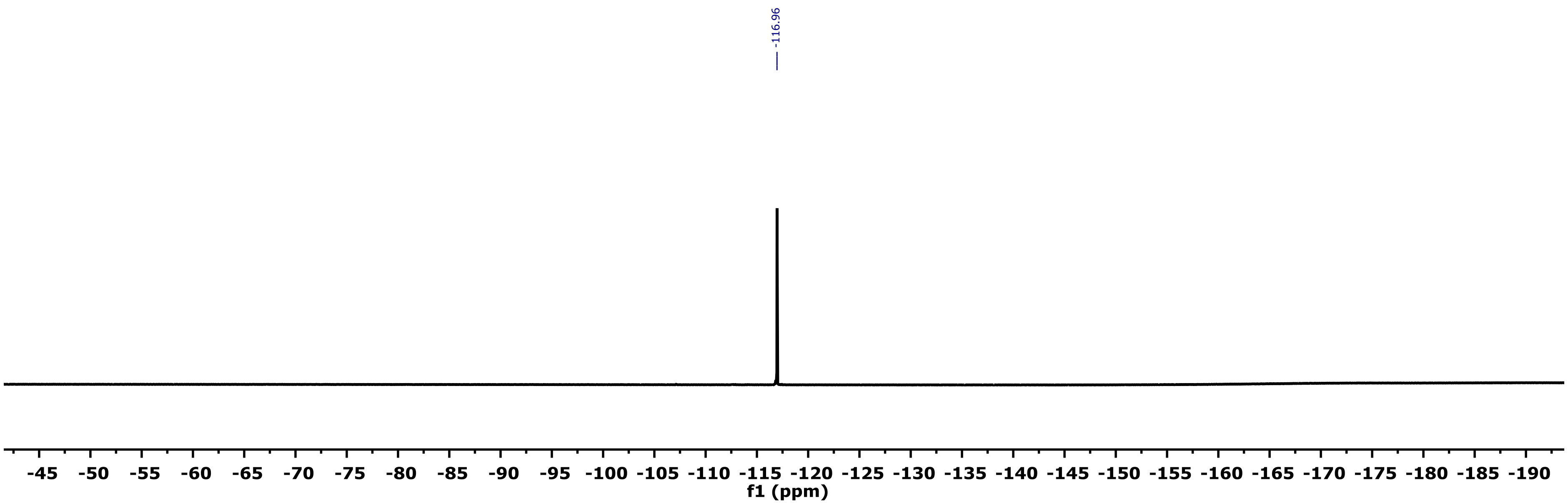
^{1}H NMR (400 MHz, $CDCl_3$)

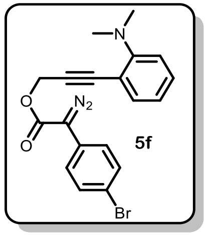


$^{13}C\{H\}$ NMR ($CDCl_3$, 101 MHz)

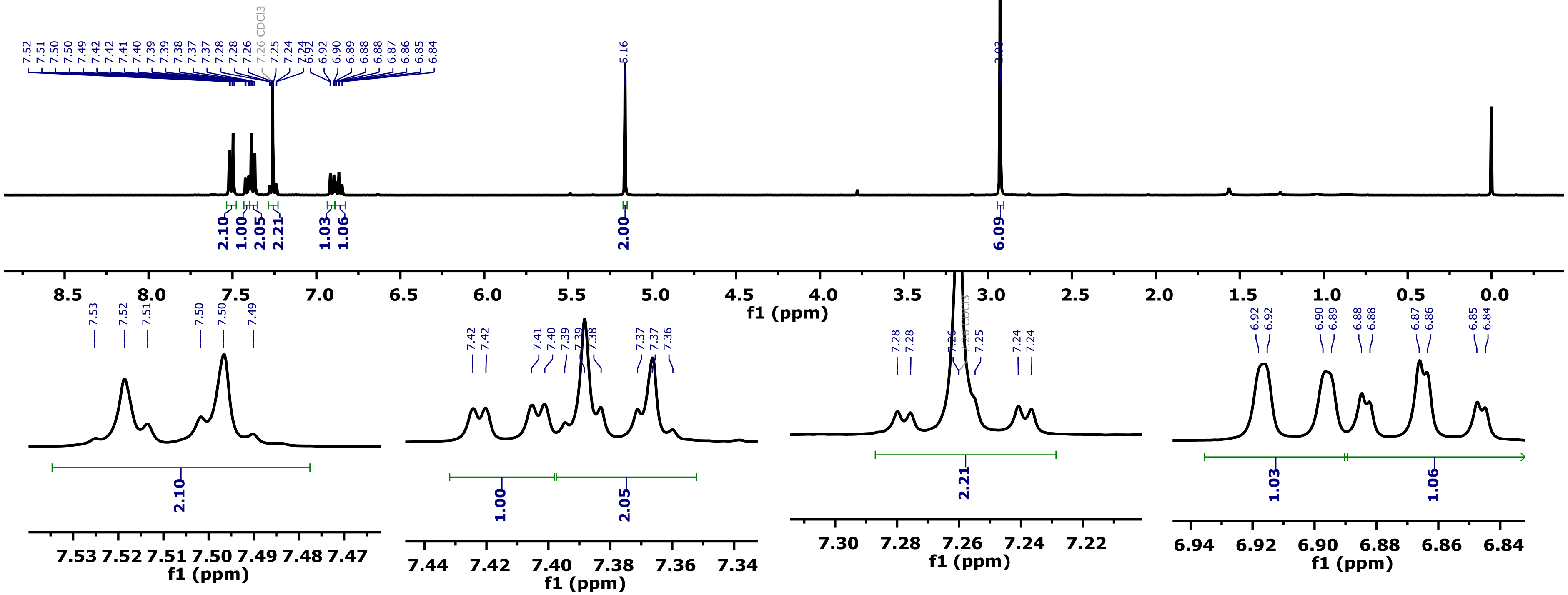


^{19}F NMR ($CDCl_3$, 376 MHz):

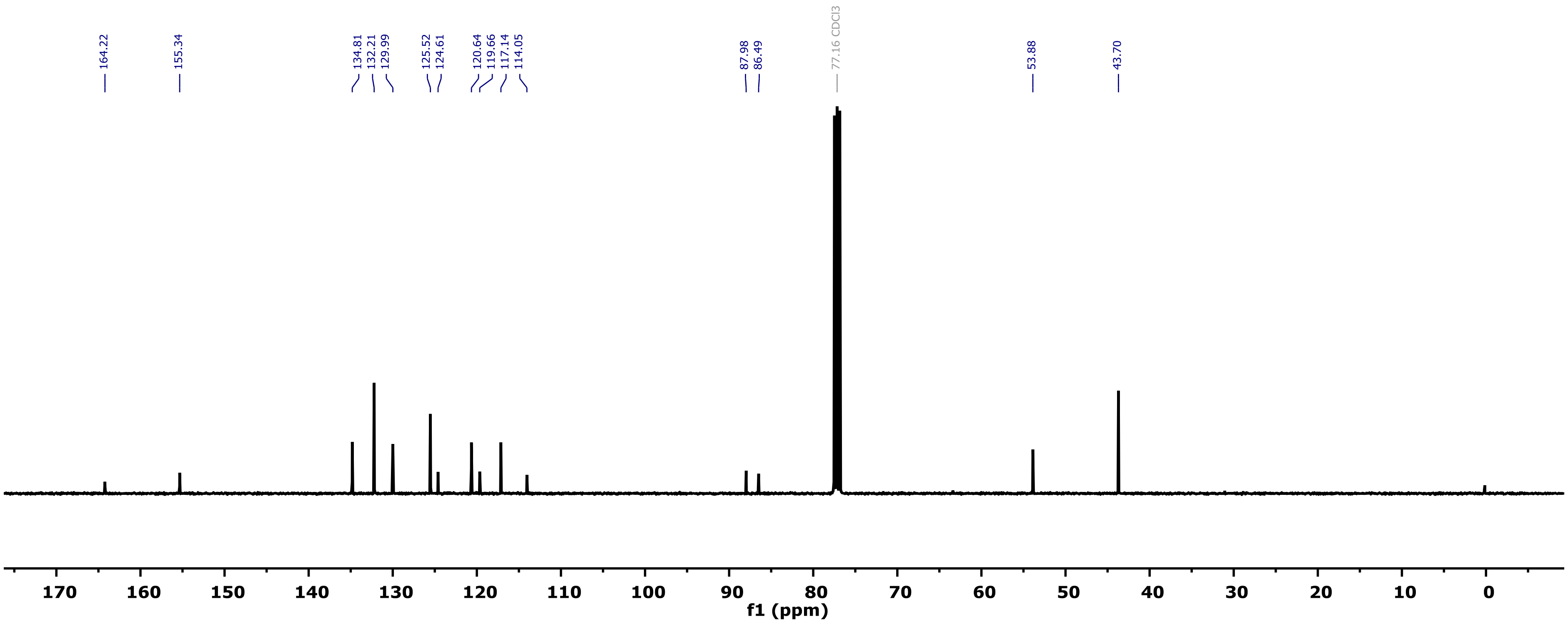


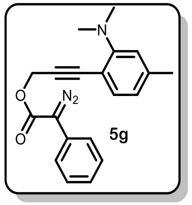


^{1}H NMR (400 MHz, $CDCl_3$)

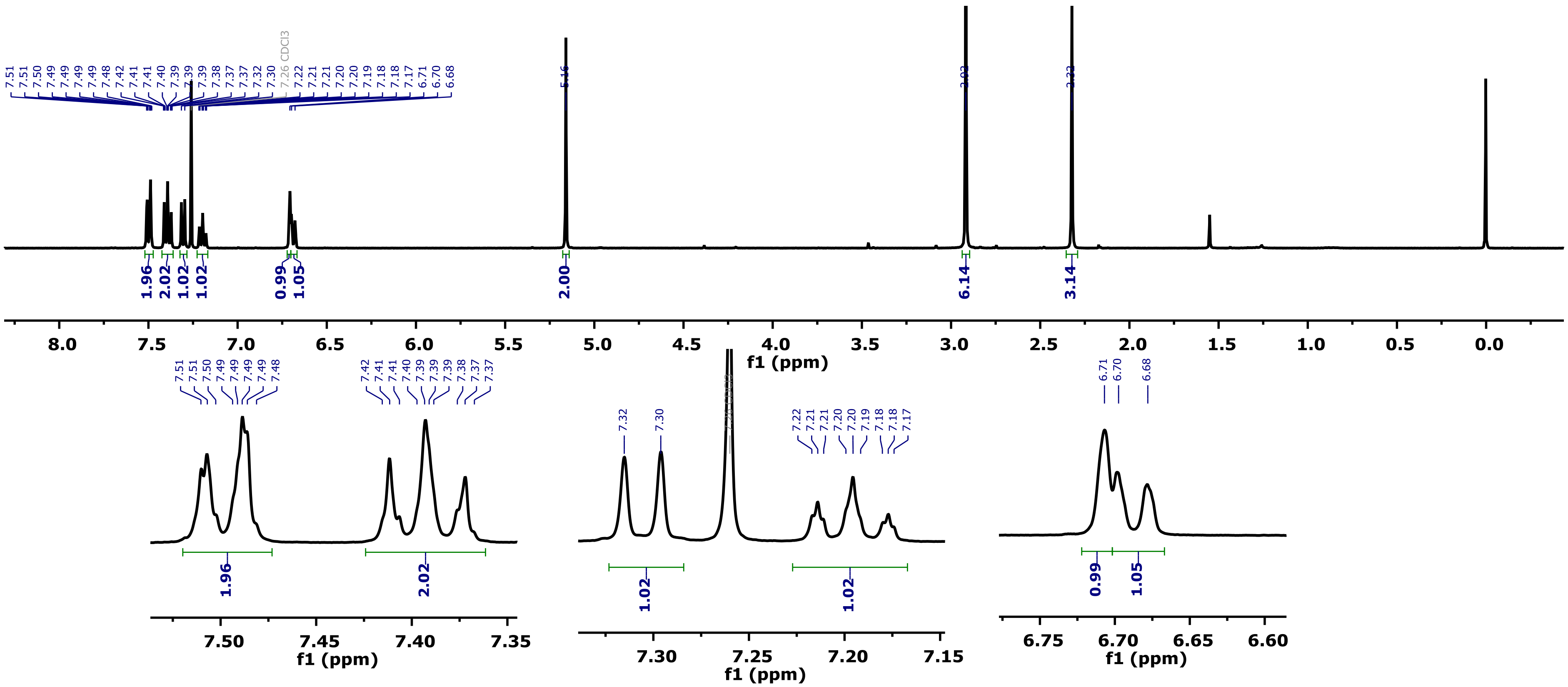


$^{13}C\{H\}$ NMR ($CDCl_3$, 101 MHz)

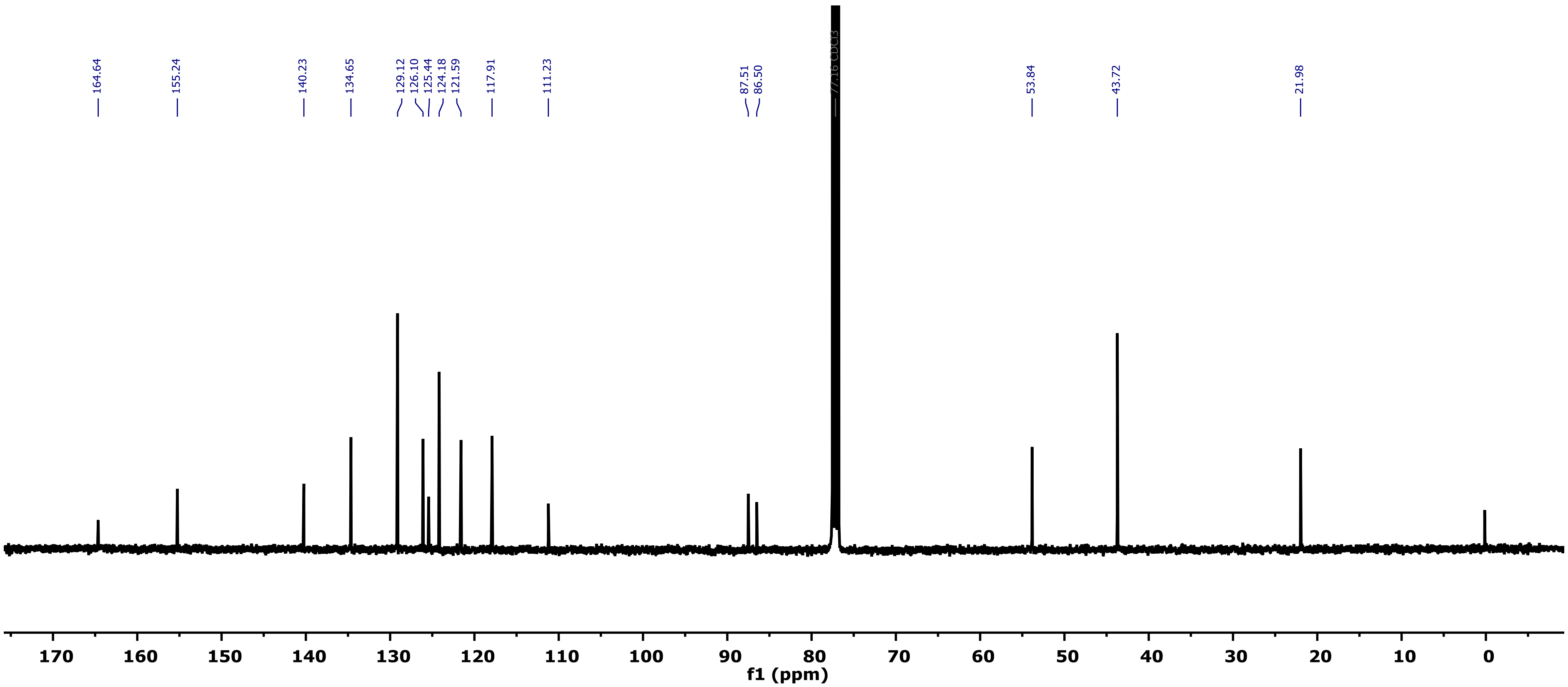


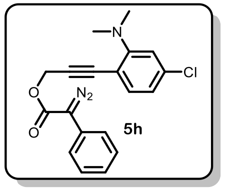


^1H NMR (400 MHz, $CDCl_3$)

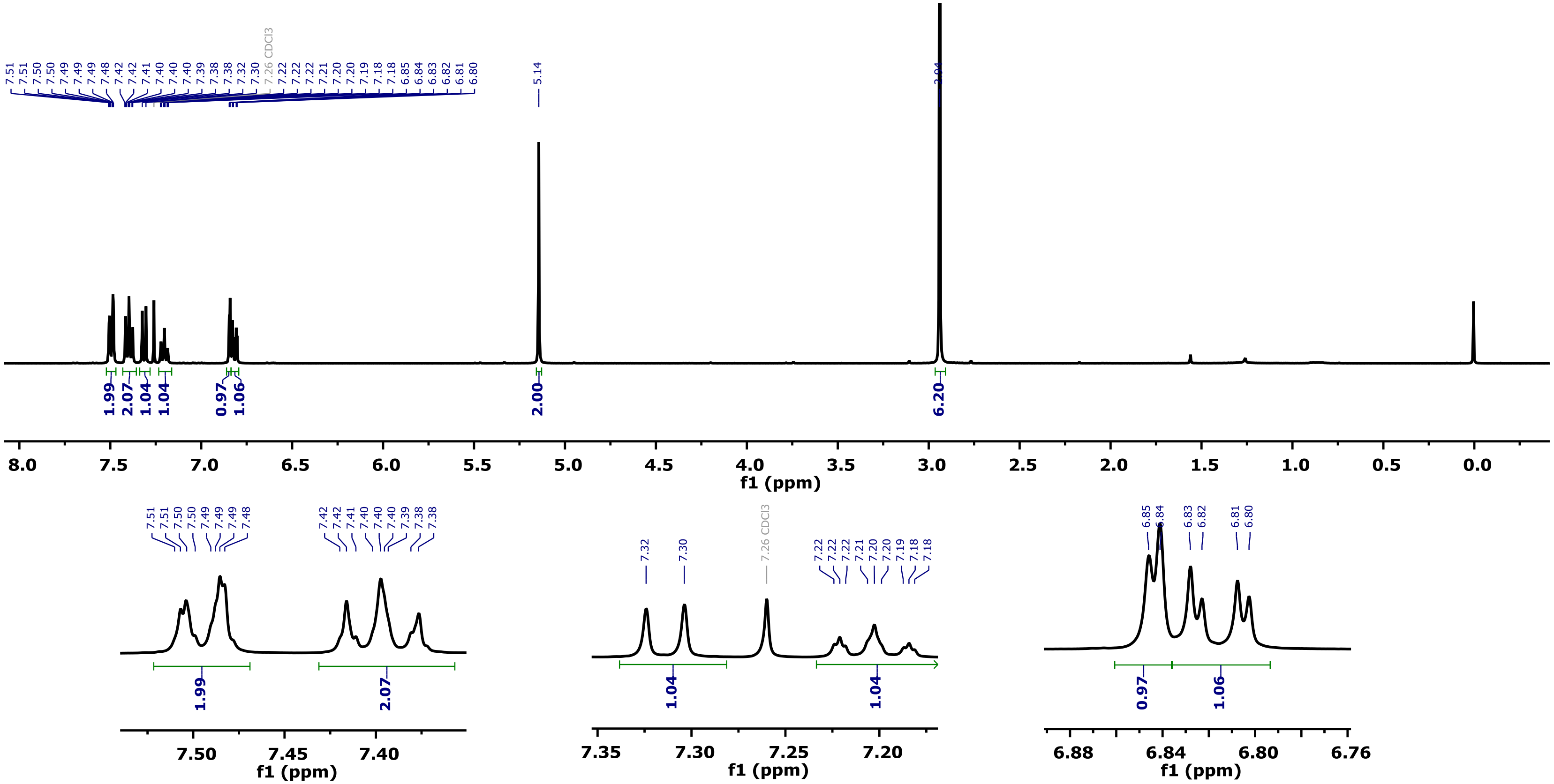


$^{13}C\{H\}$ NMR ($CDCl_3$, 101 MHz)

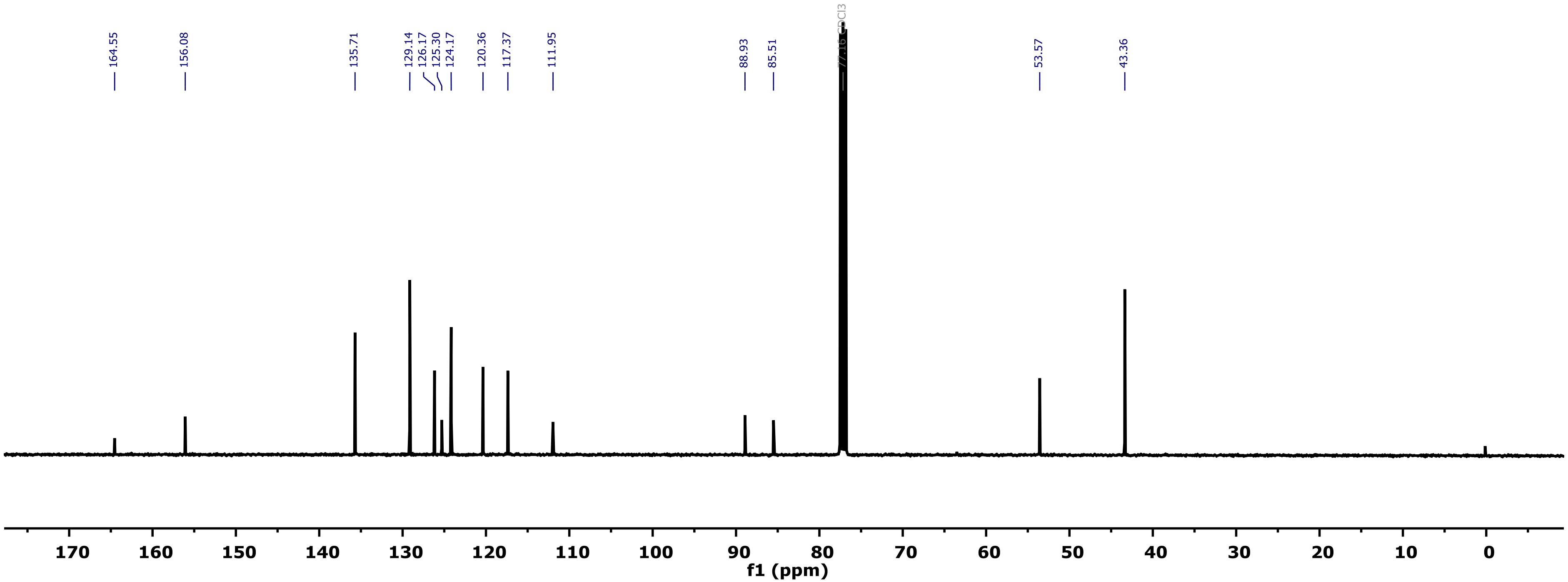


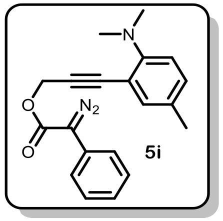


^{1}H NMR (400 MHz, $CDCl_3$)

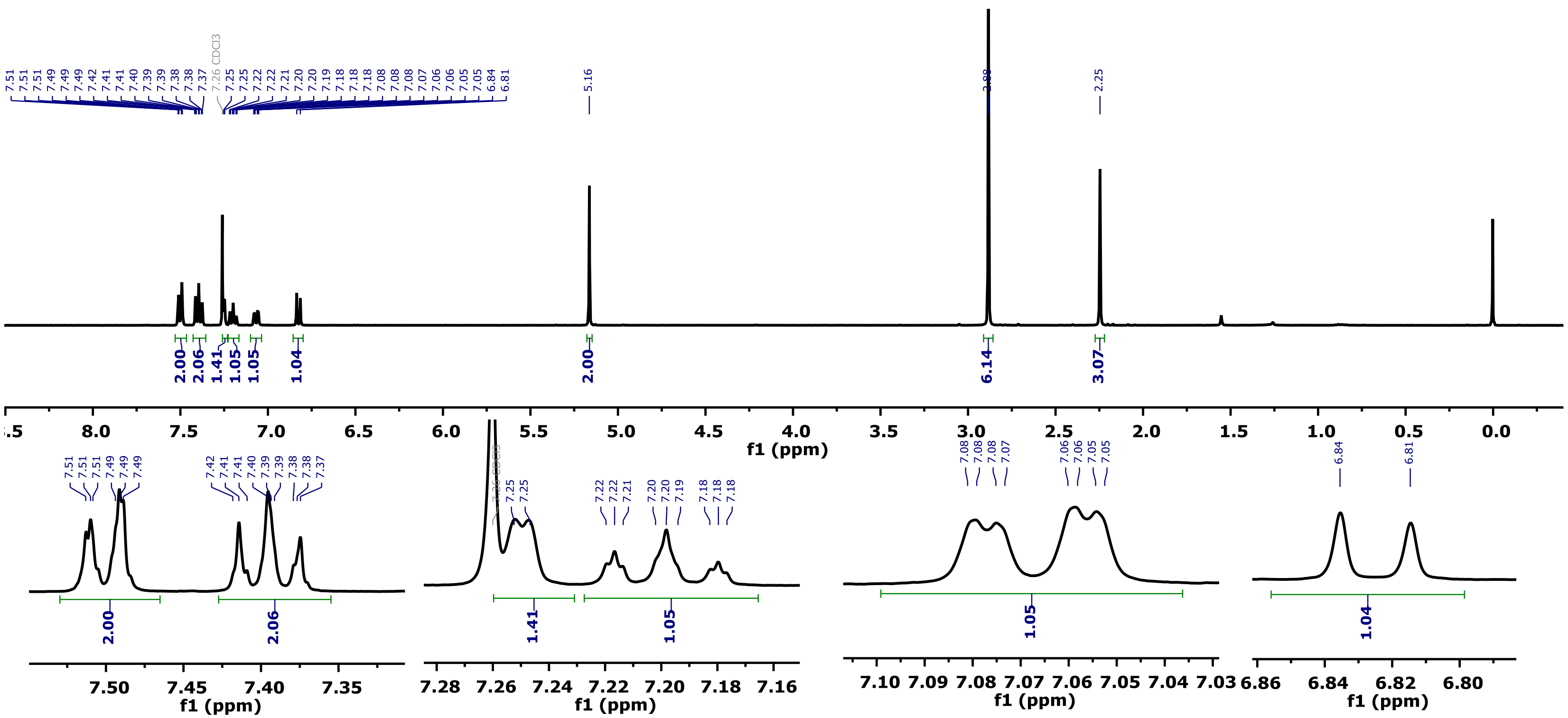


$^{13}C\{H\}$ NMR ($CDCl_3$, 101 MHz)

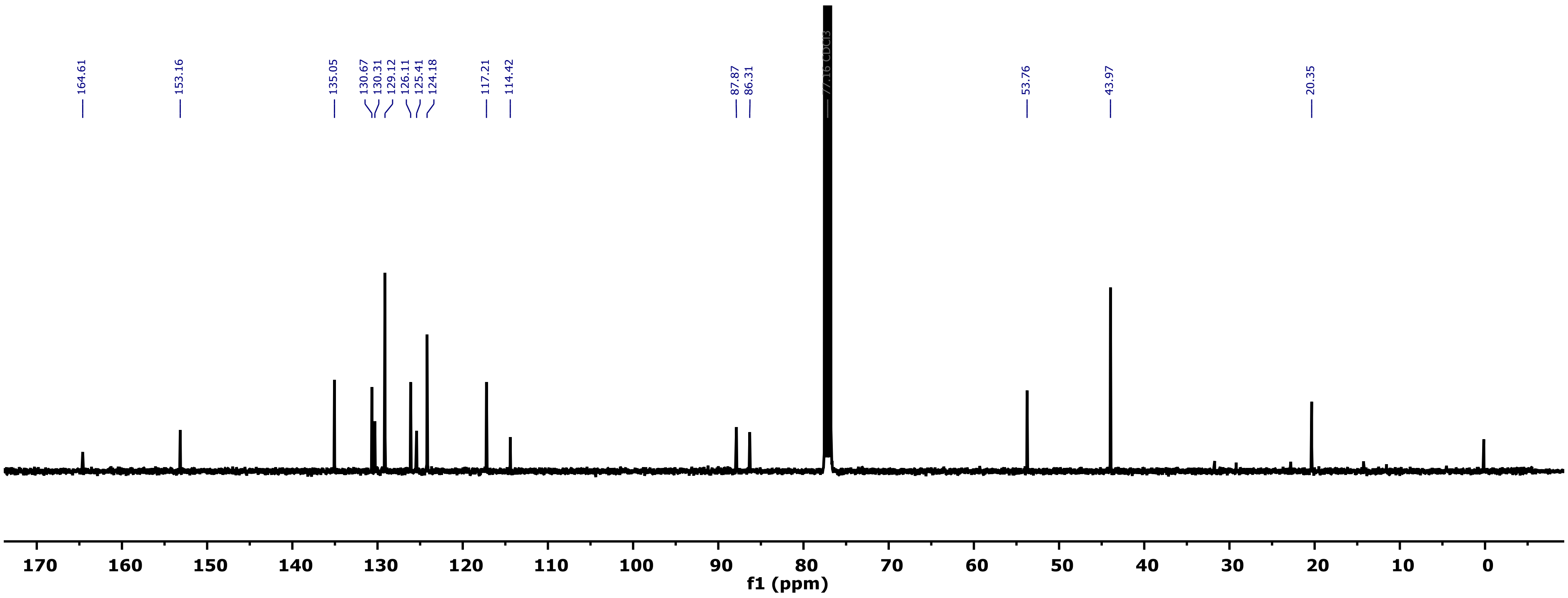


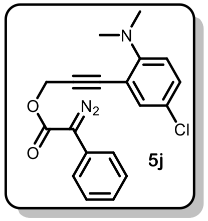


[1]H NMR (400 MHz, $CDCl_3$)

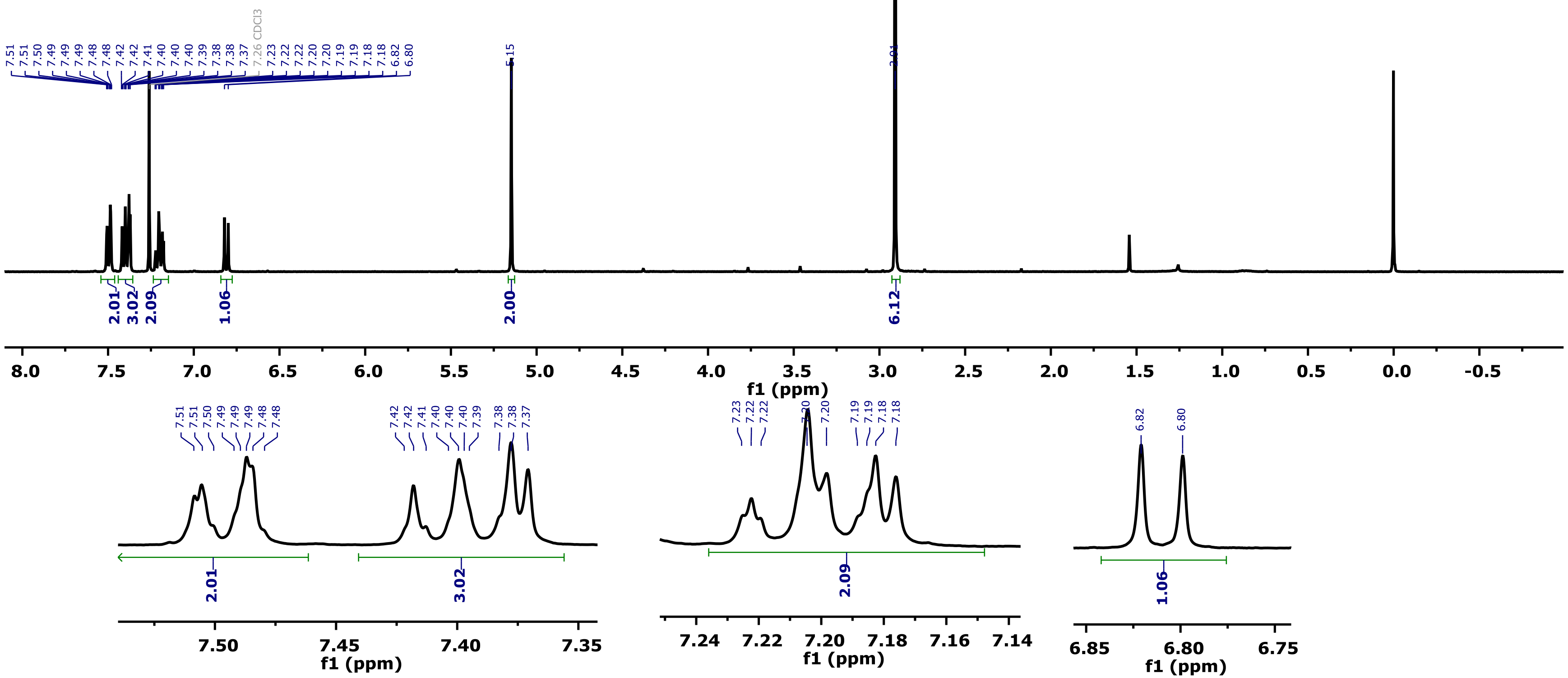


^{13}C{H} NMR (CDCl$_3$, 101 MHz)

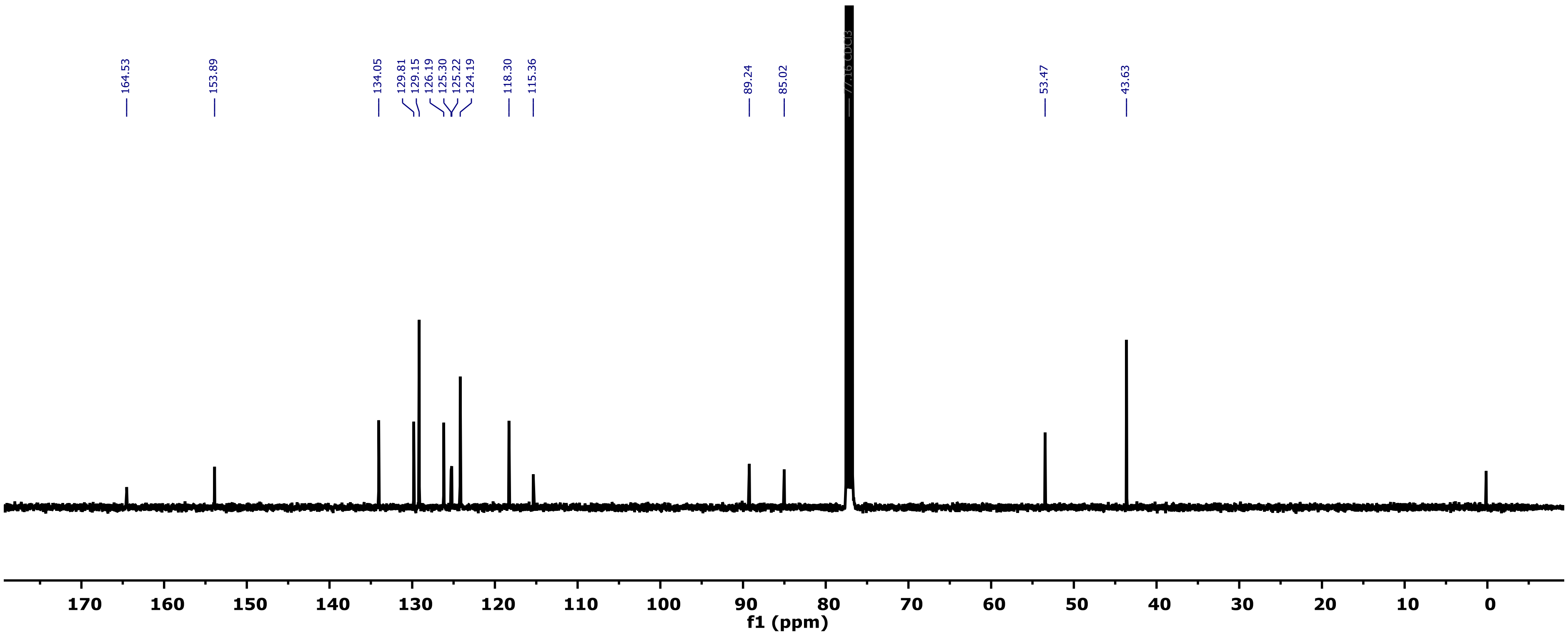


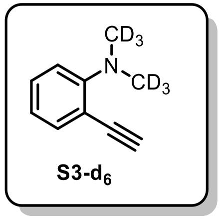


[1]H NMR (400 MHz, $CDCl_3$)



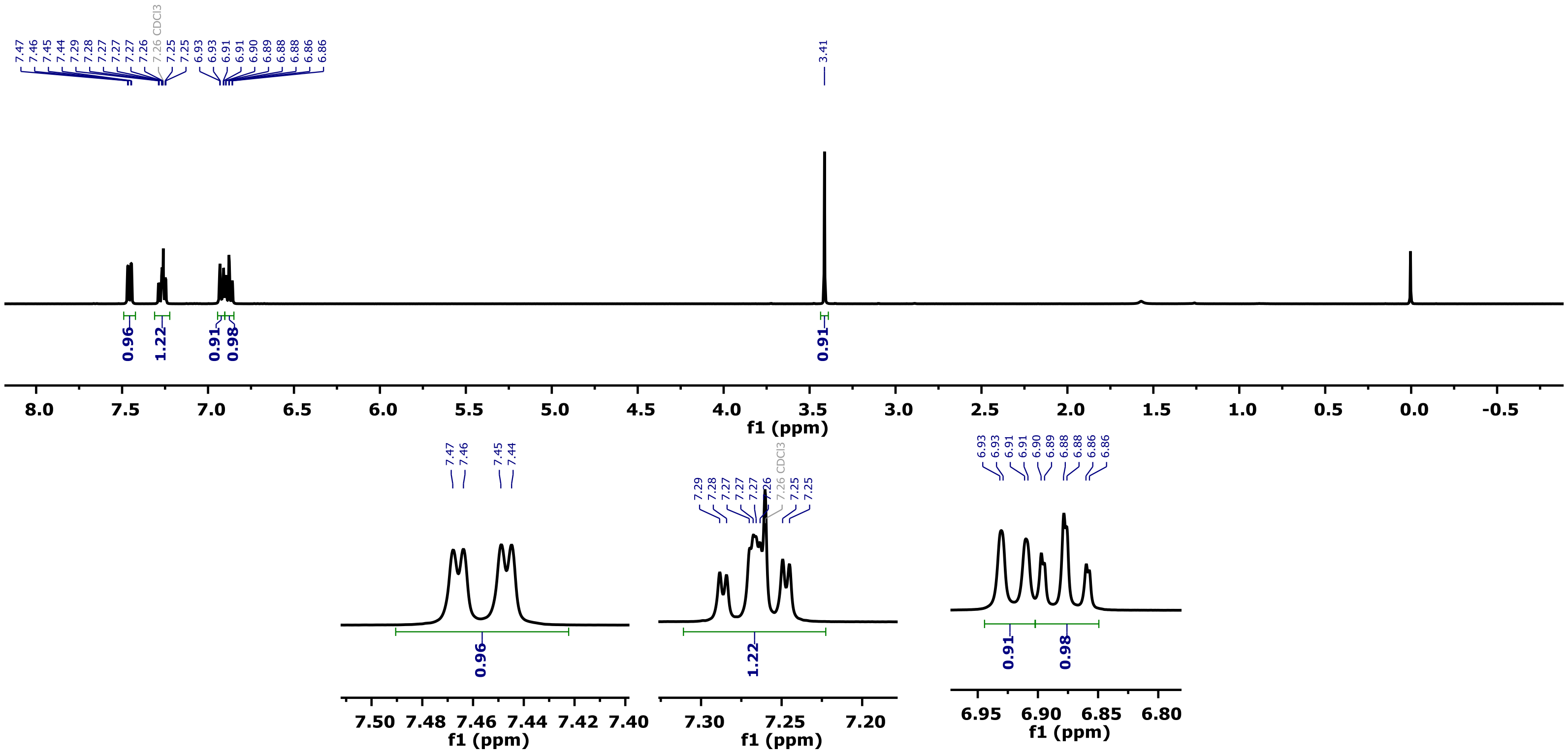
$^{13}C\{H\}$ NMR ($CDCl_3$, 101 MHz)



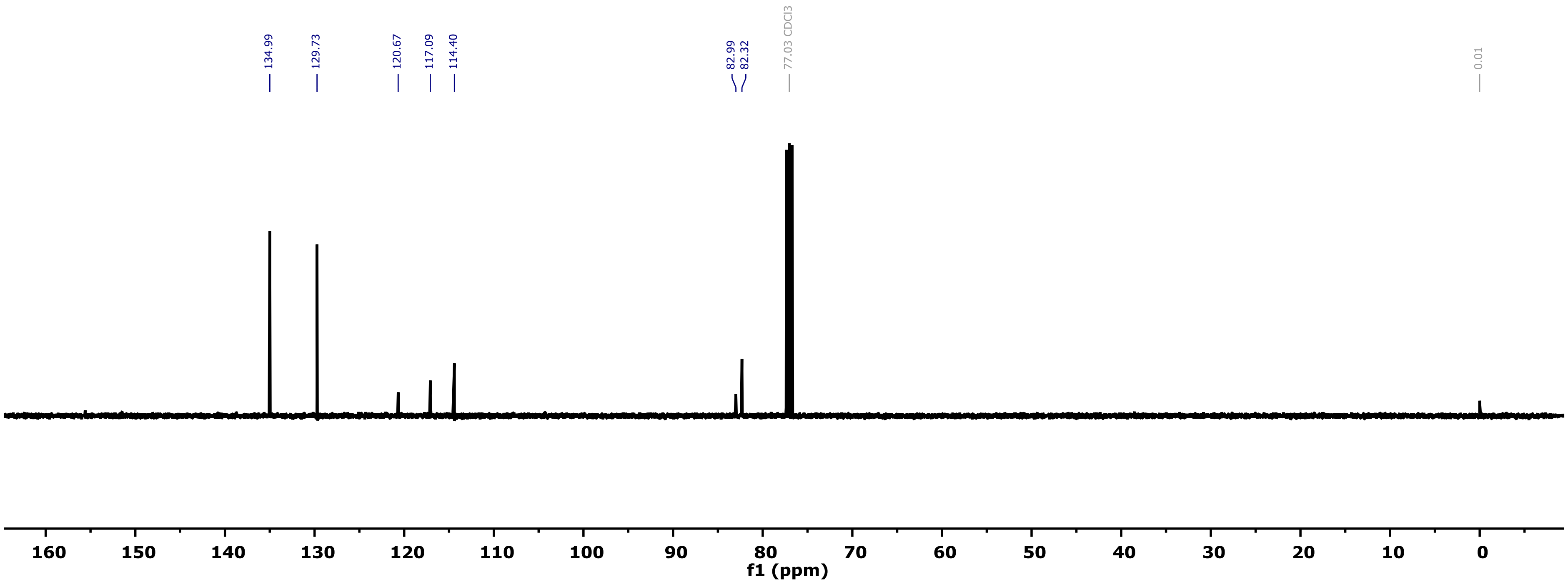


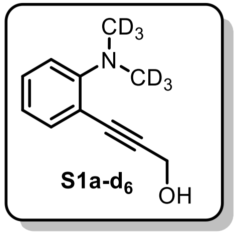
S3-d$_6$

^{1}H NMR (400 MHz, $CDCl_3$)



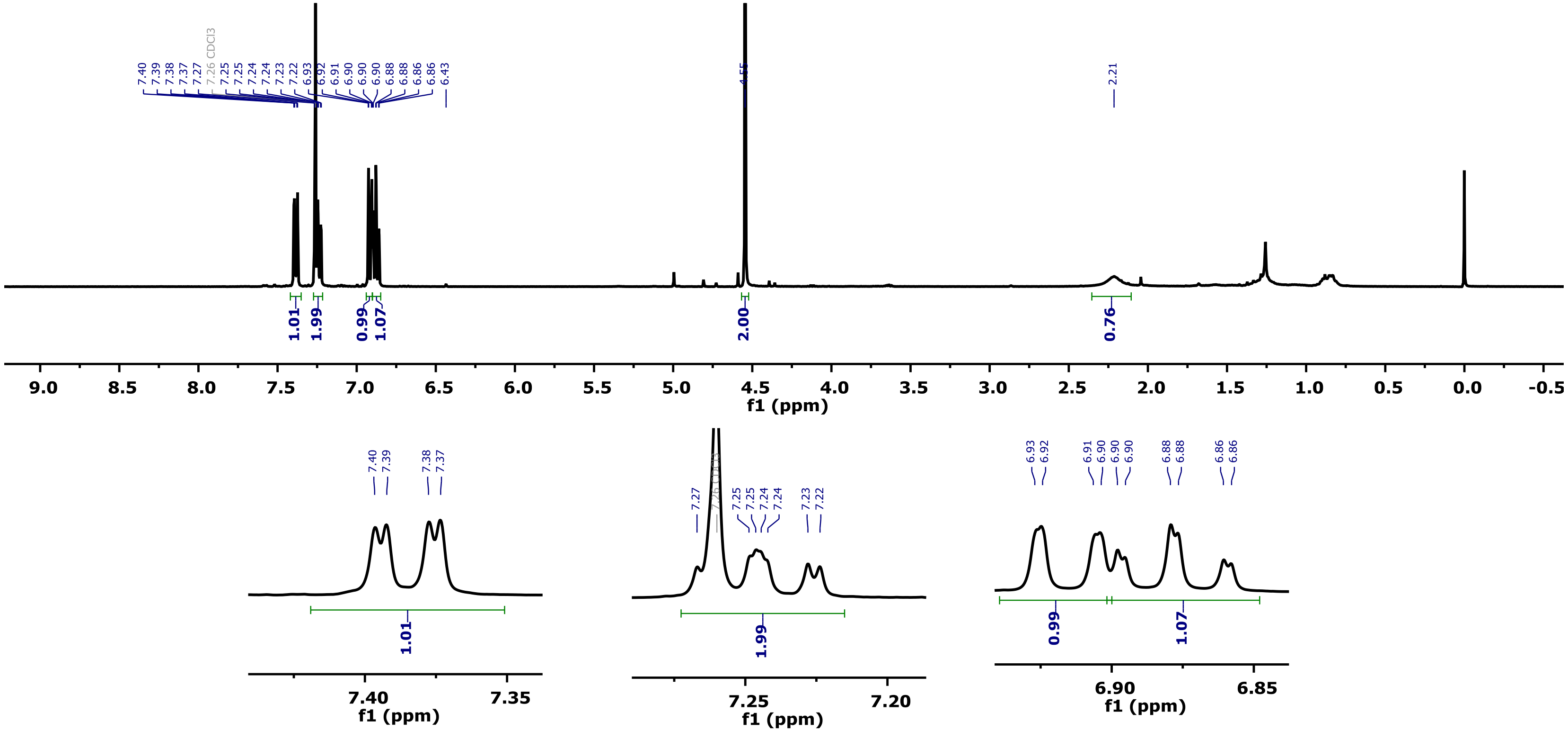
$^{13}C\{H\}$ NMR ($CDCl_3$, 101 MHz)



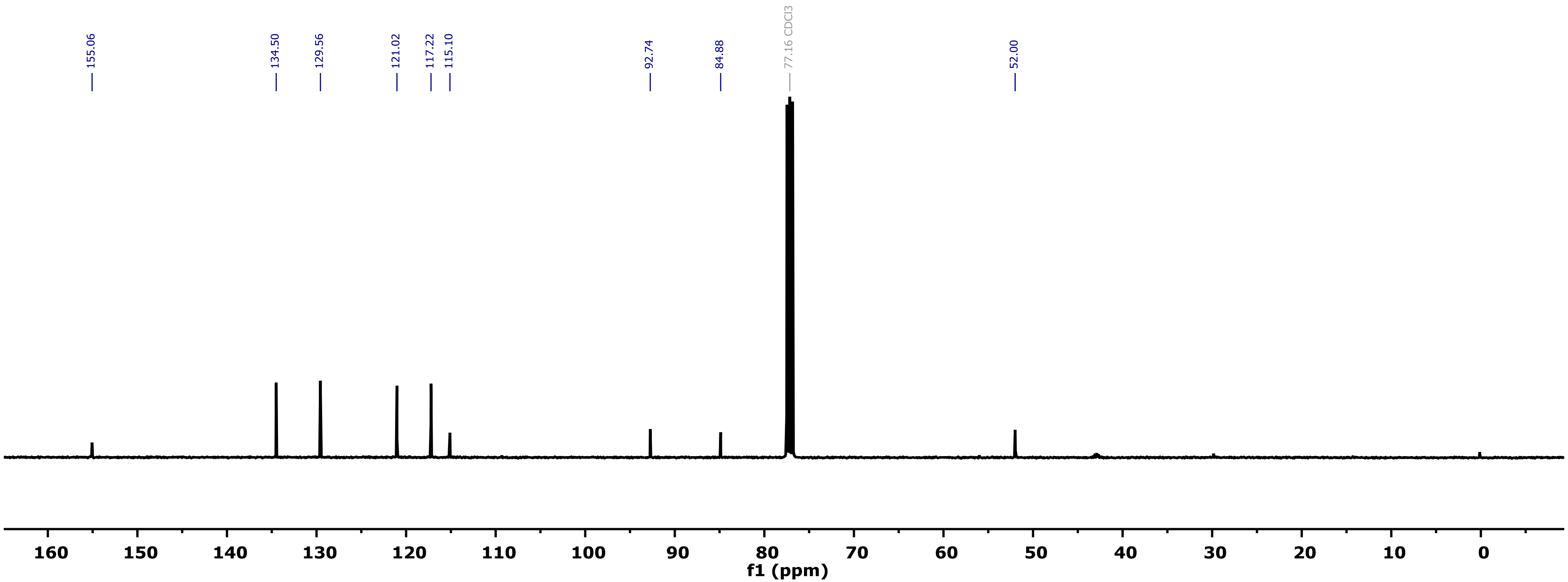


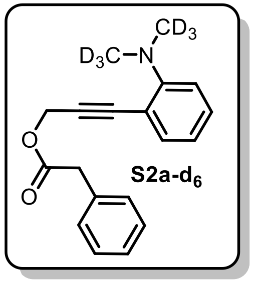
S1a-d$_6$

^{1}H NMR (400 MHz, $CDCl_3$)

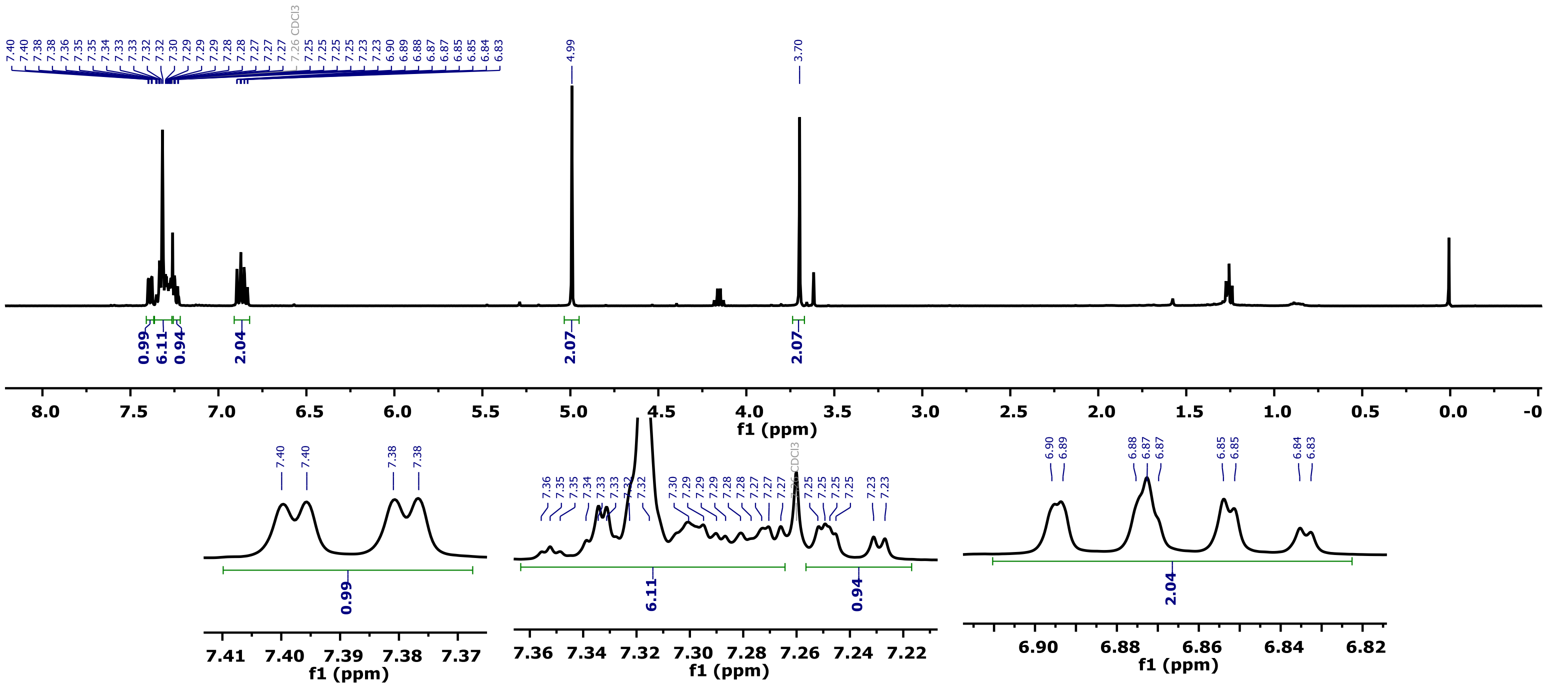


$^{13}C\{H\}$ NMR ($CDCl_3$, 101 MHz)

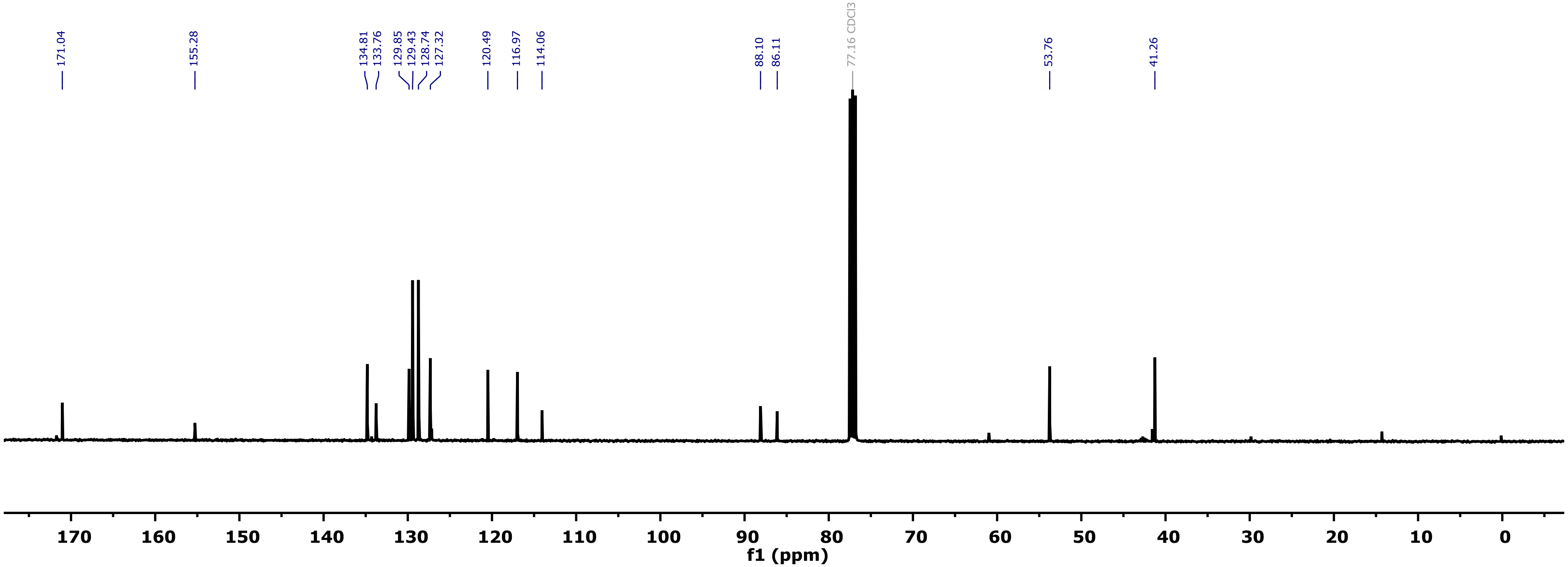


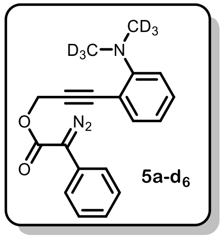


^{1}H NMR (400 MHz, $CDCl_3$)



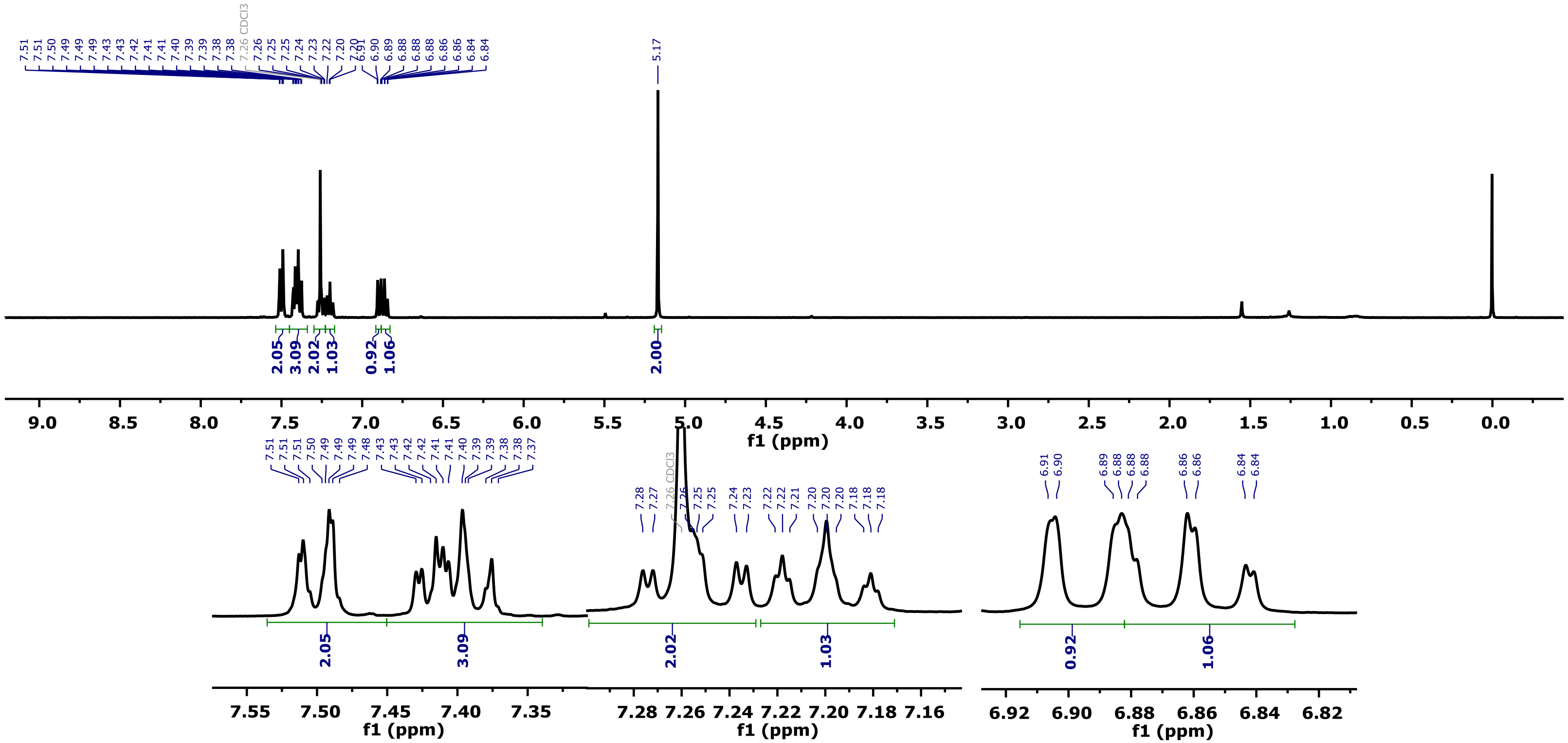
$^{13}C\{H\}$ NMR ($CDCl_3$, 101 MHz)



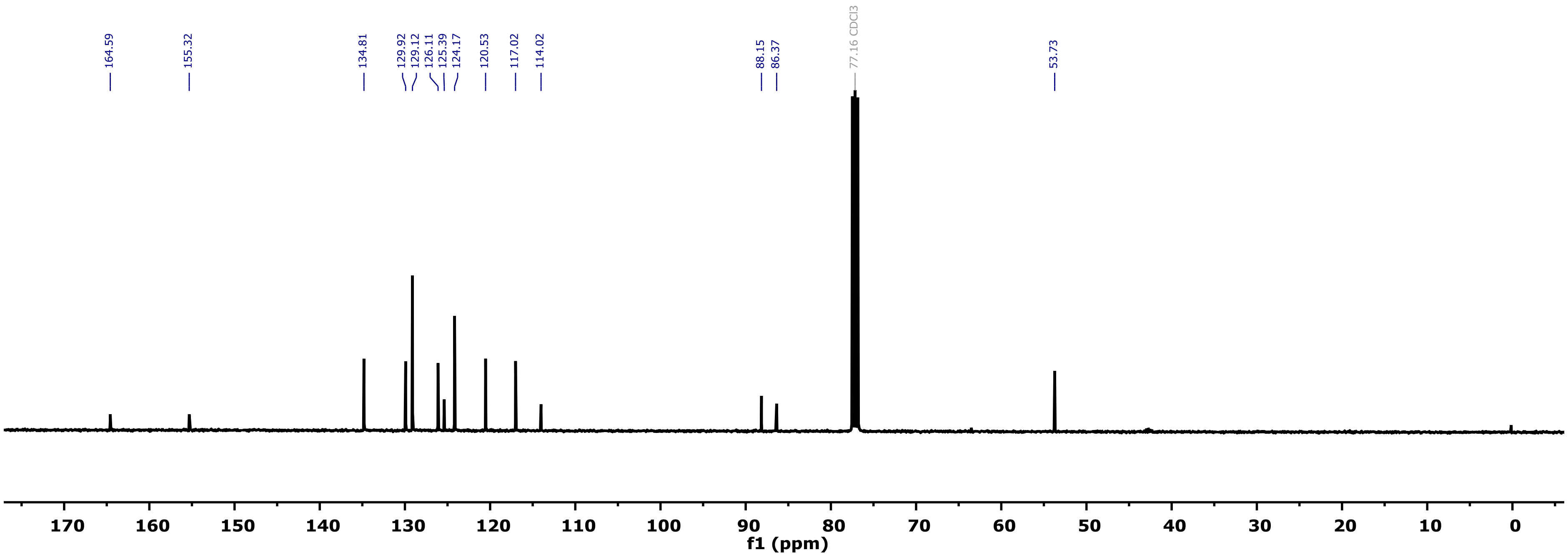


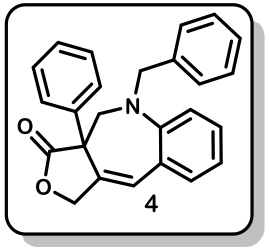
5a-d6

^{1}H NMR (400 MHz, $CDCl_3$)



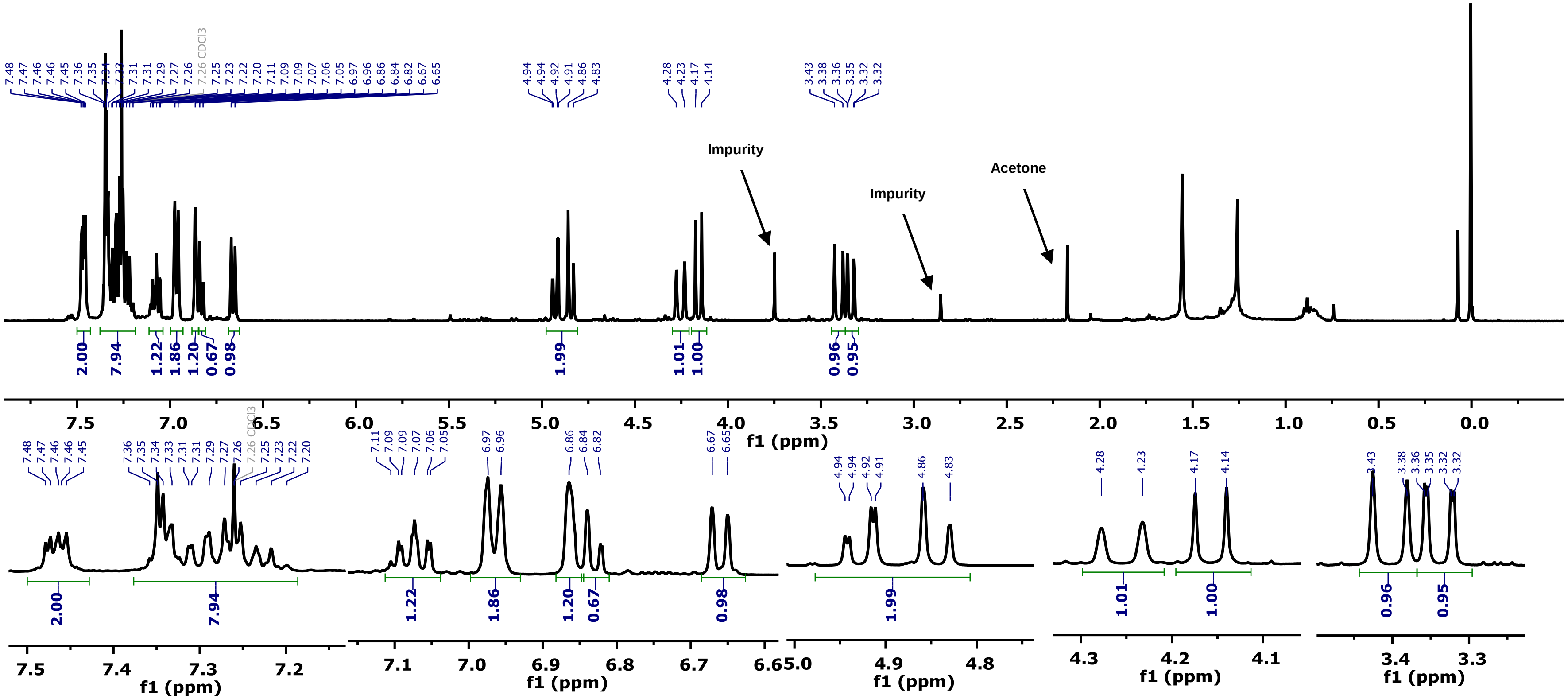
$^{13}C\{H\}$ NMR ($CDCl_3$, 101 MHz)



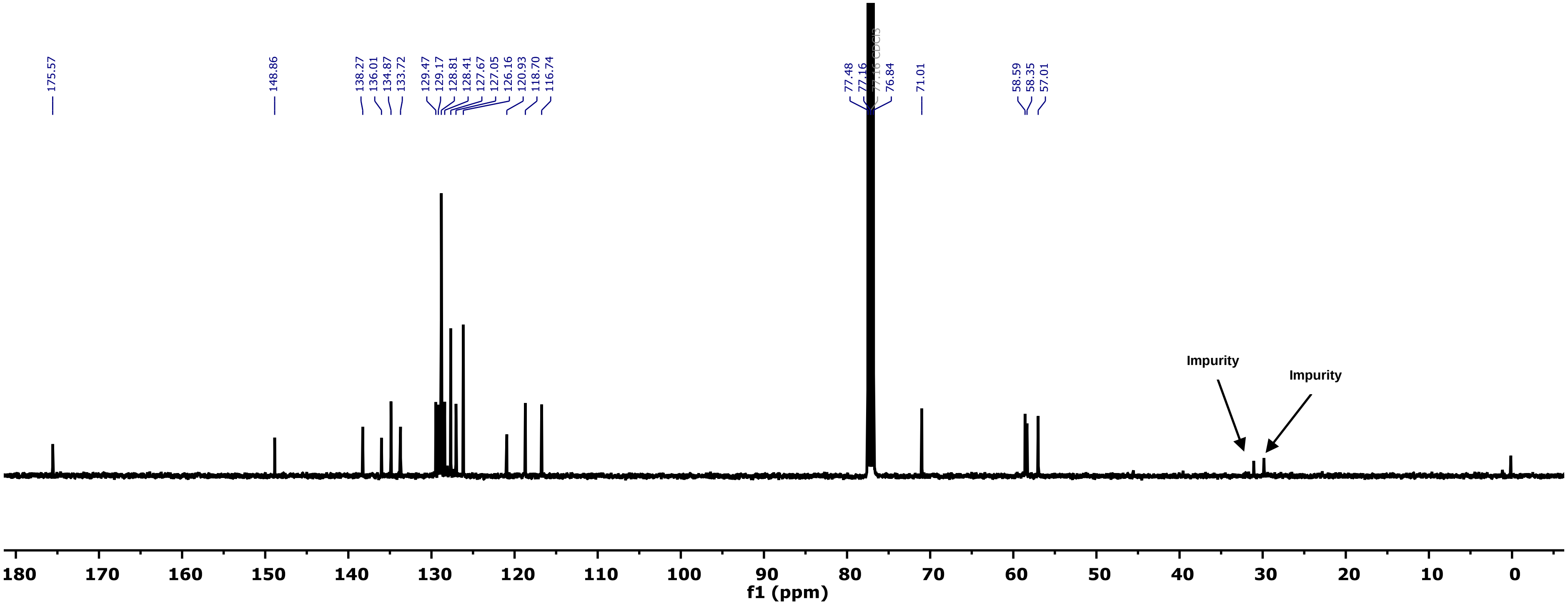


4

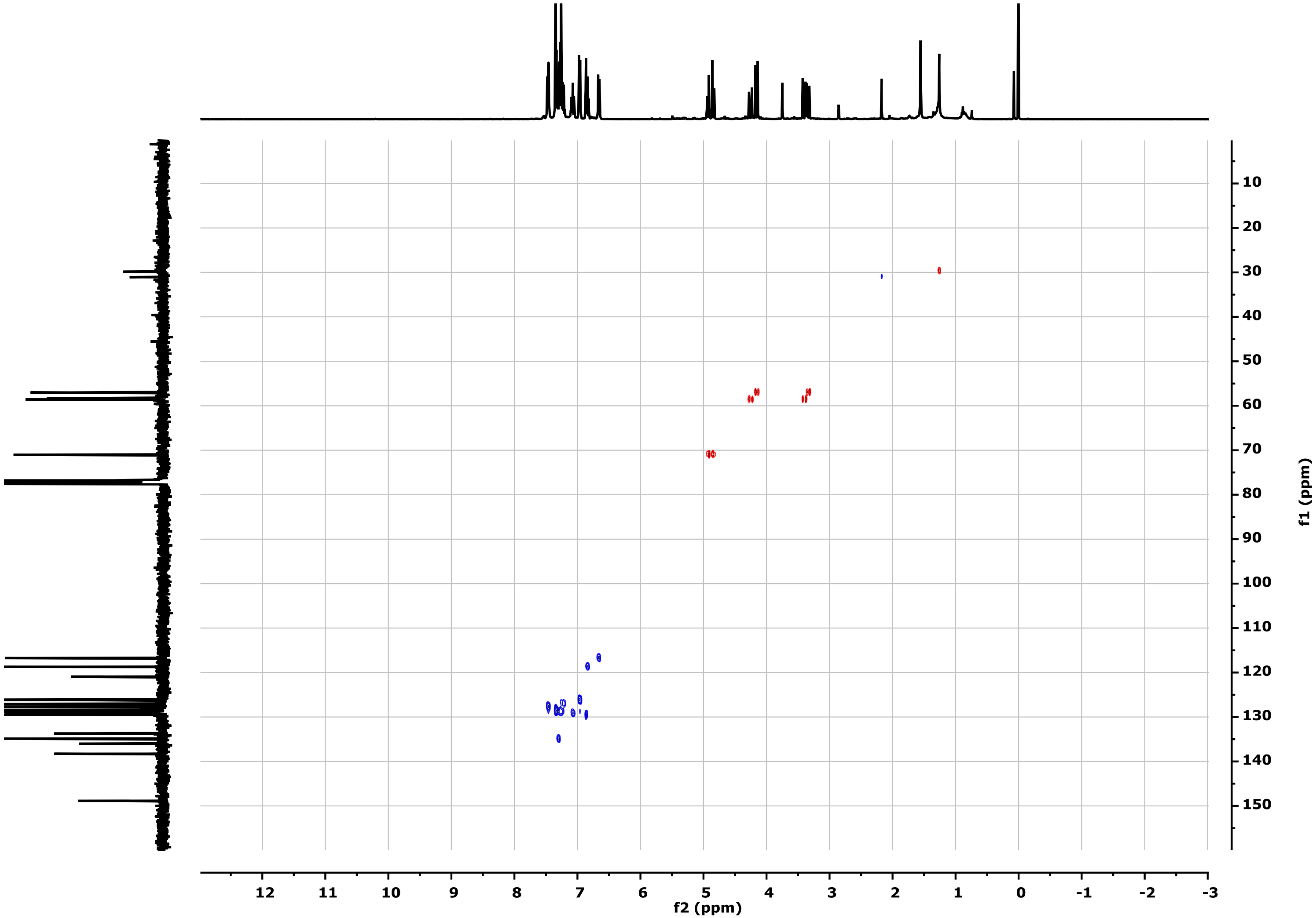
^{1}H NMR (400 MHz, $CDCl_3$)



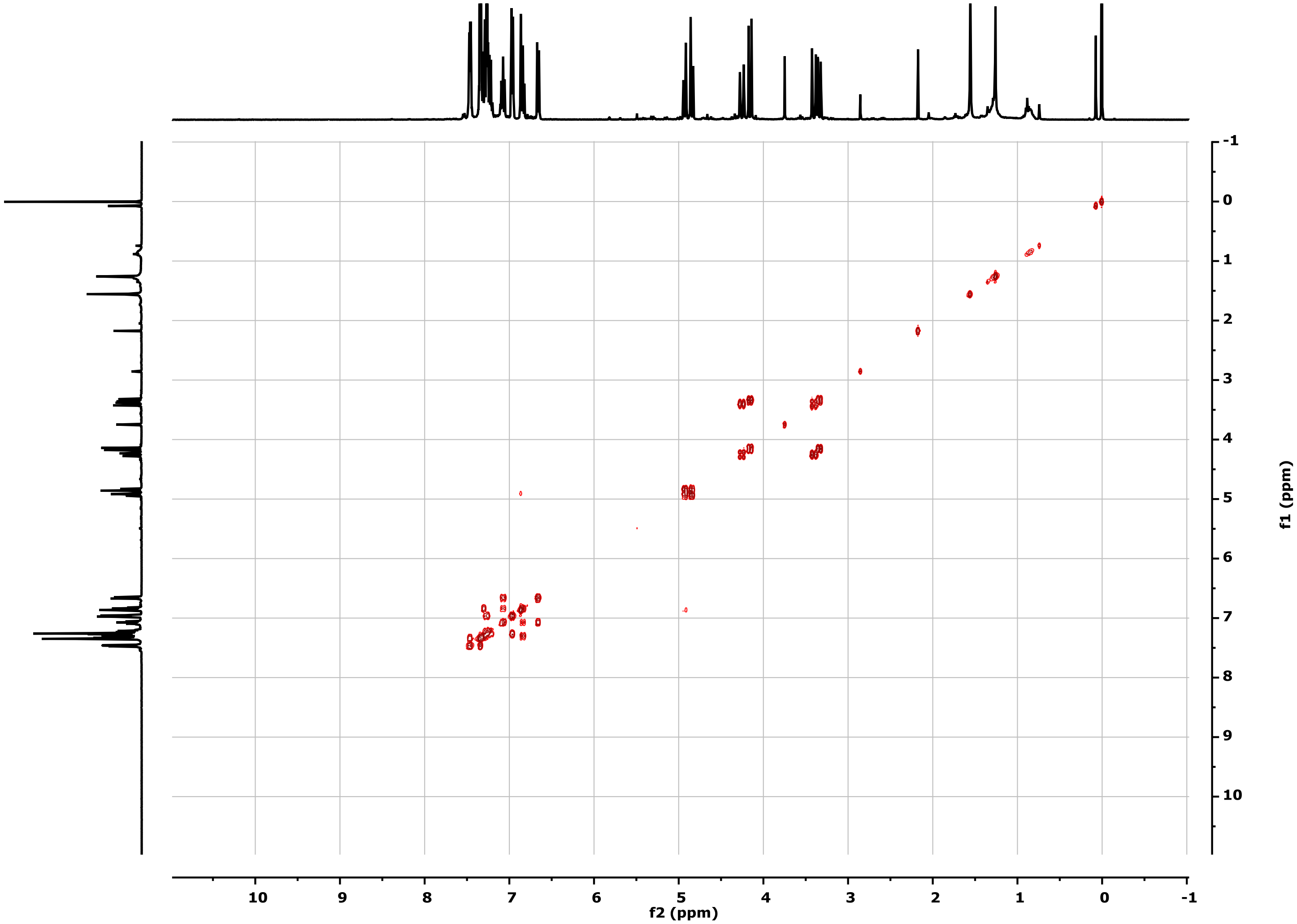
$^{13}C\{H\}$ NMR ($CDCl_3$, 101 MHz)



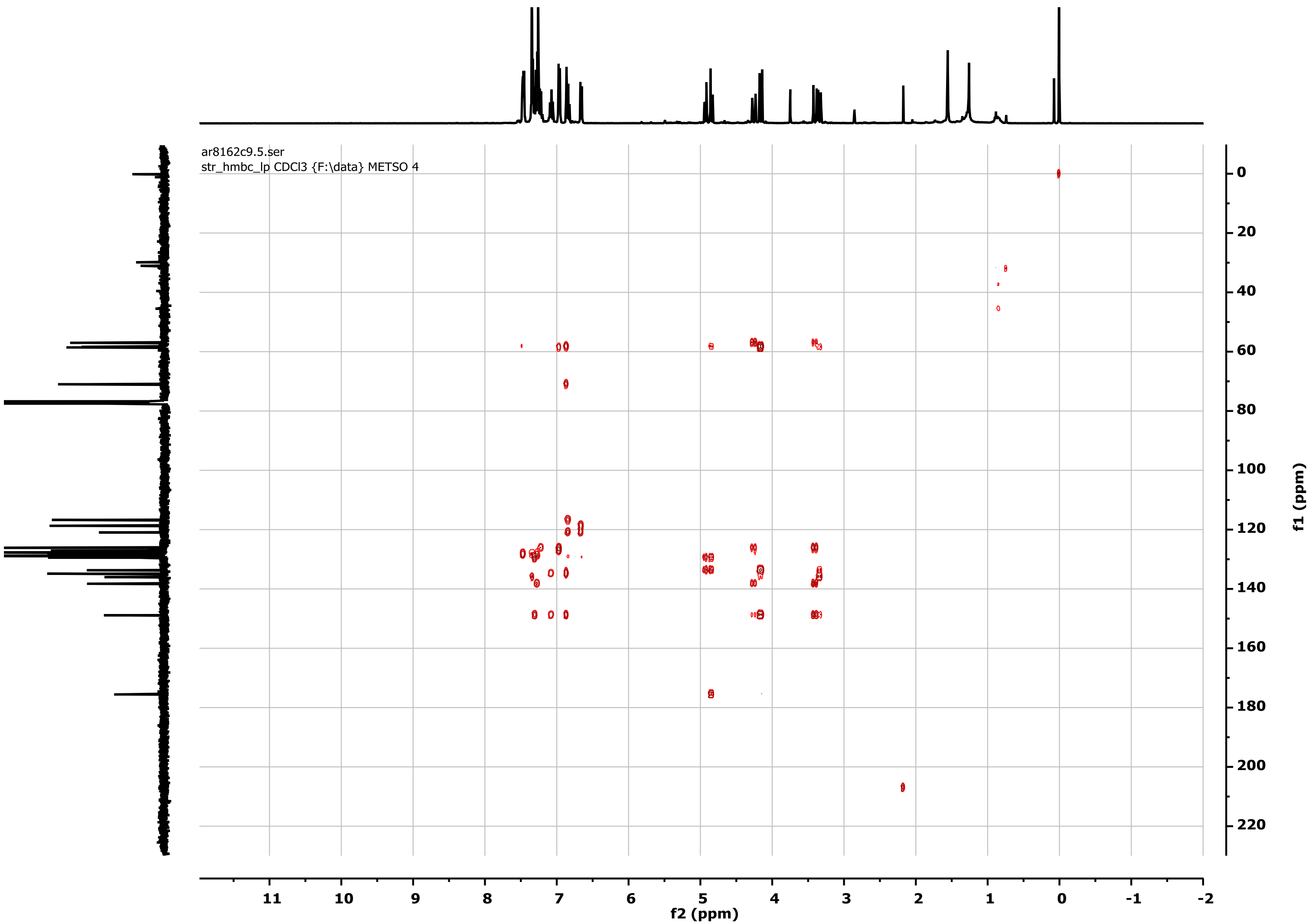
2D NMR HSQC ($CDCl_3$)

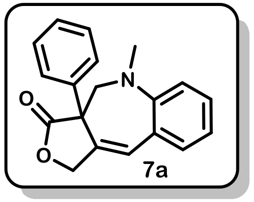


2D NMR COSY ($CDCl_3$)

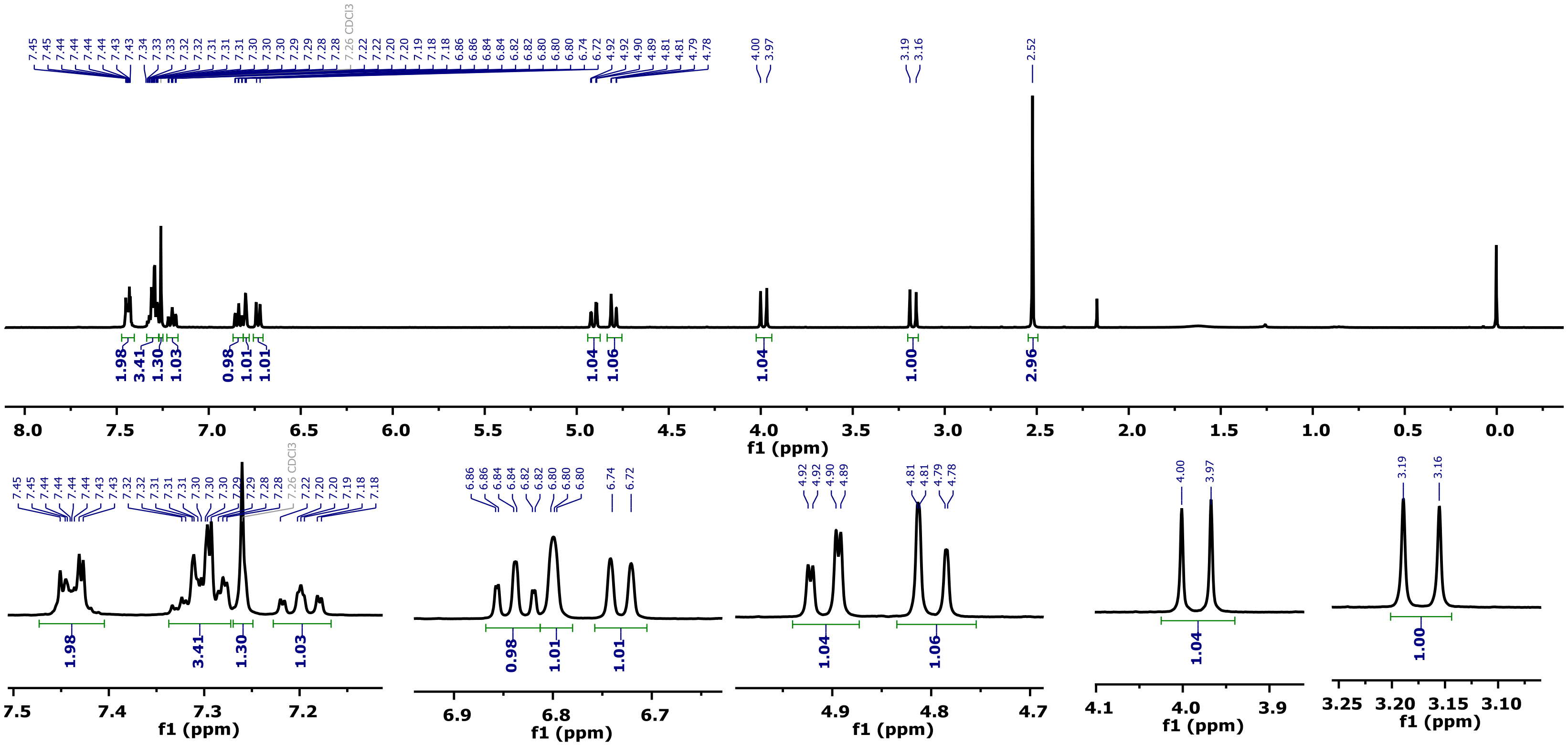


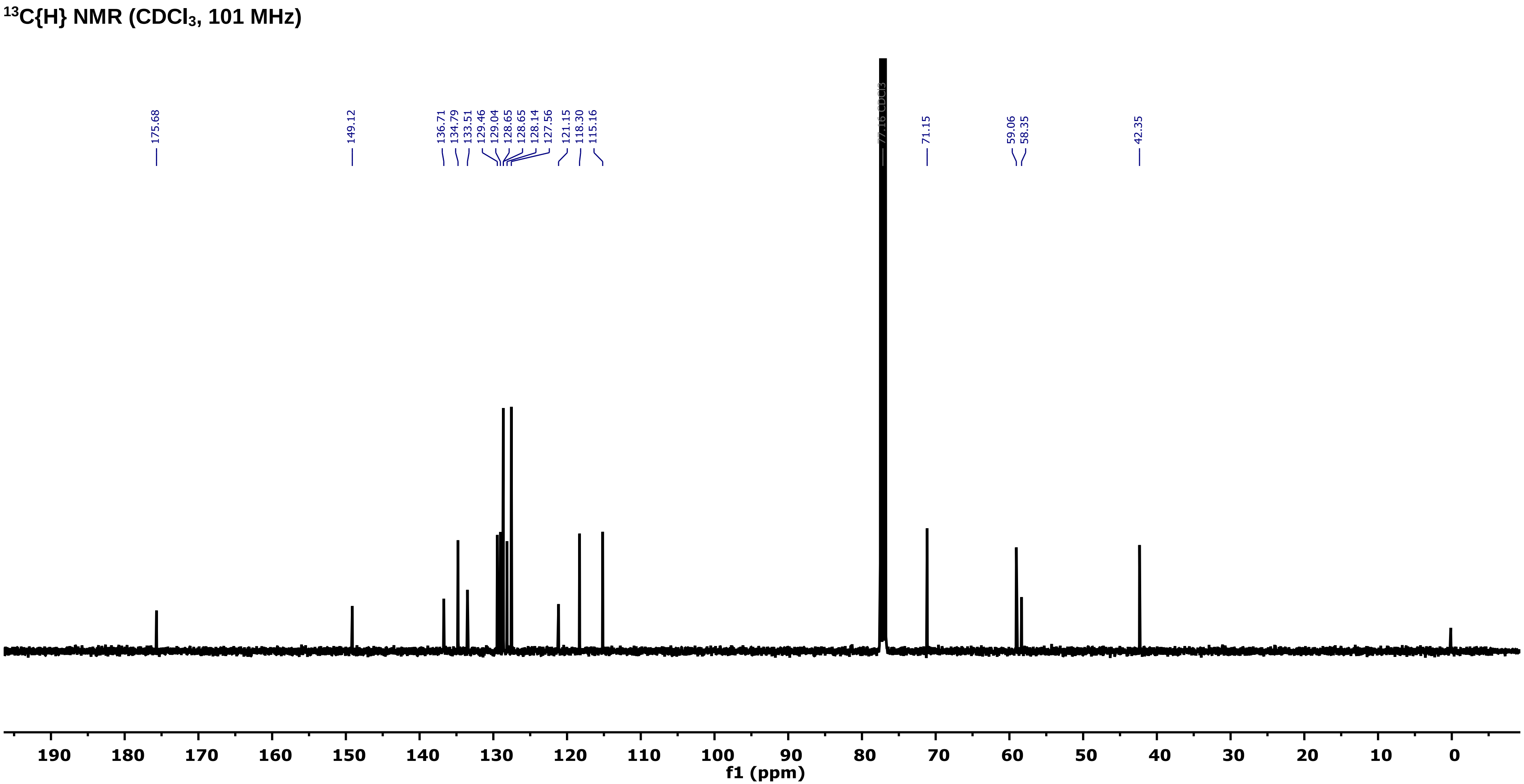
2D NMR HMBC ($CDCl_3$)



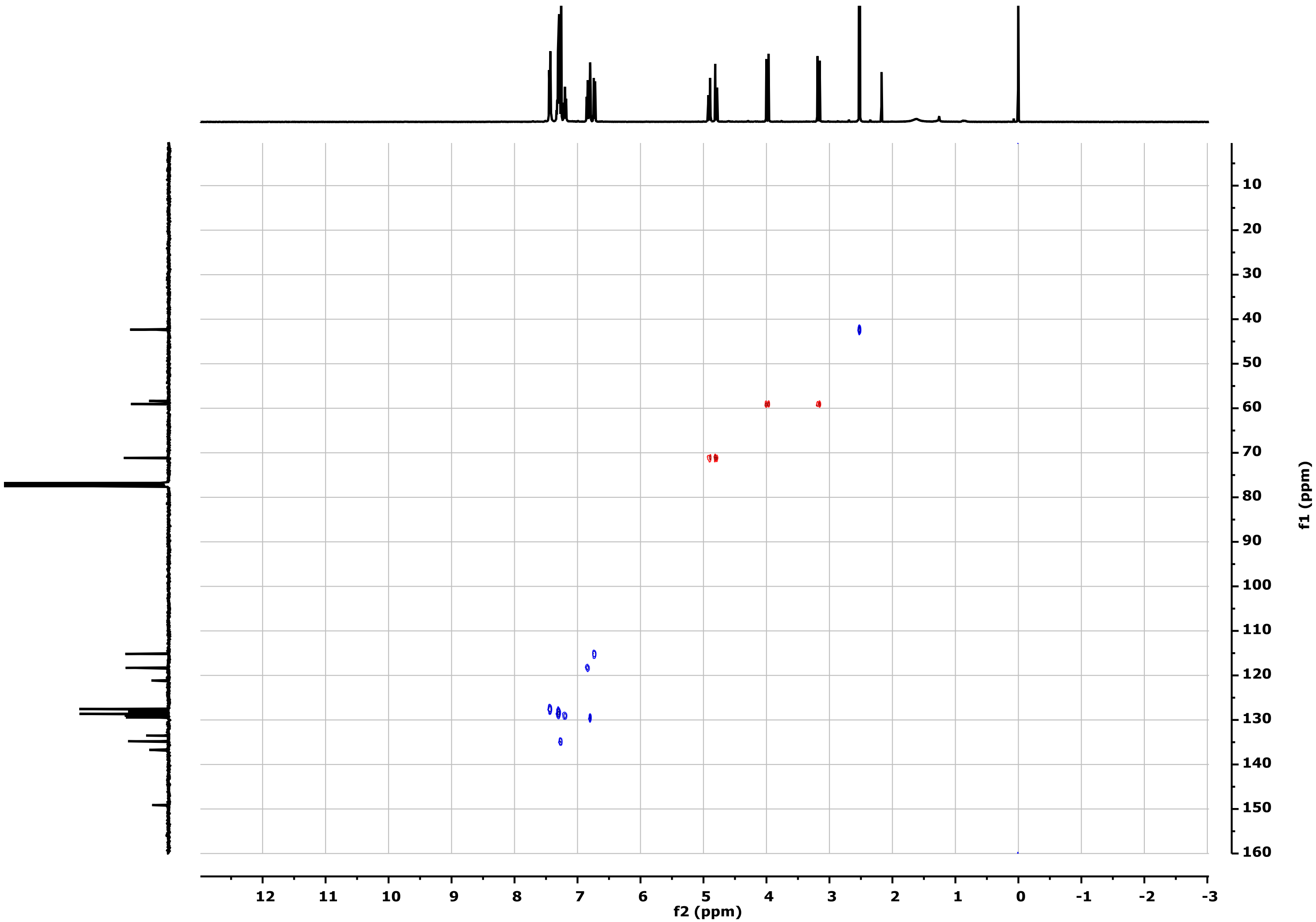


^1H NMR (400 MHz, $CDCl_3$)

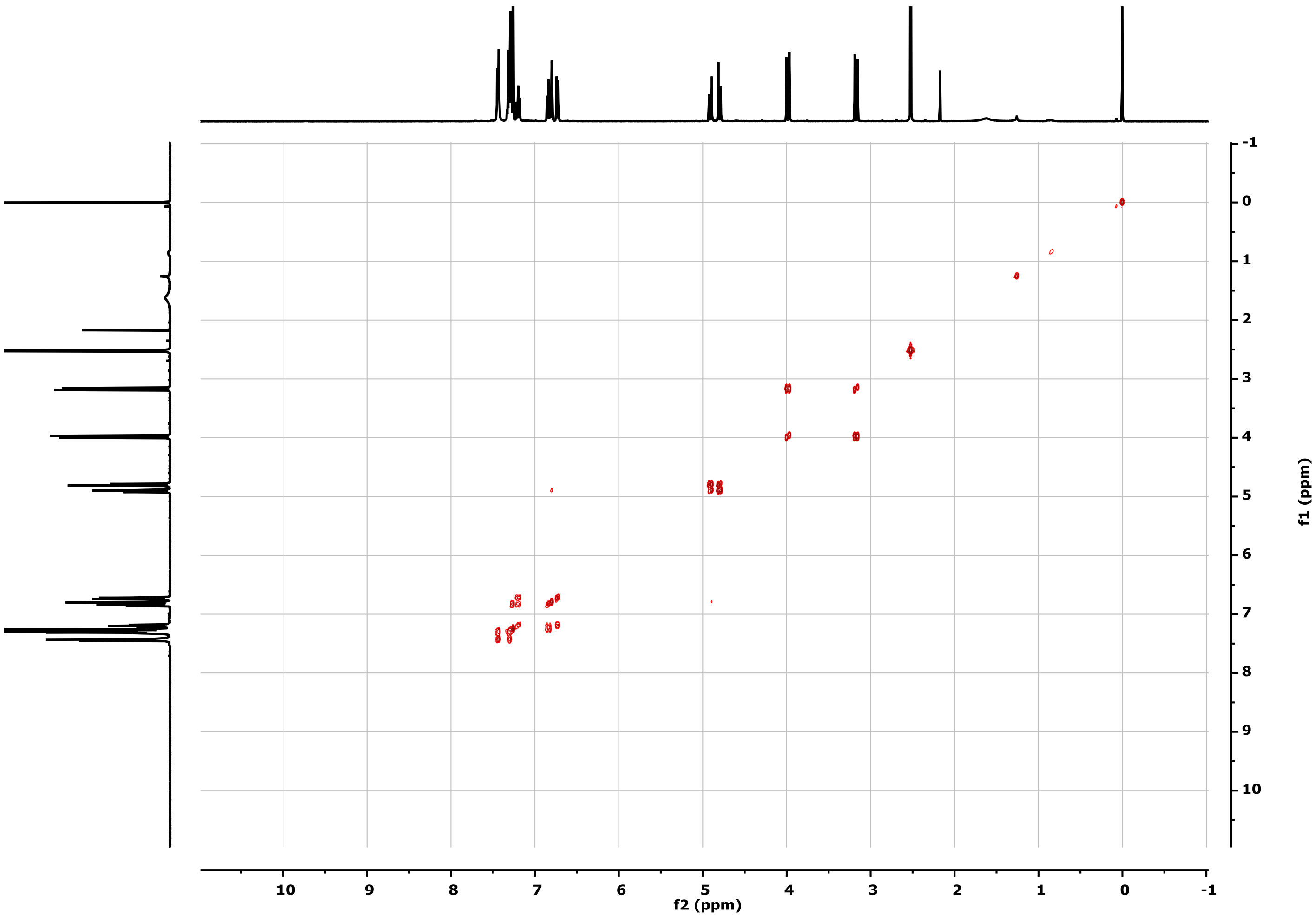



13C{H} NMR (CDCl3, 101 MHz)
175.68
149.12
136.71
134.79
133.51
129.46
129.04
128.65
128.65
128.14
127.56
121.15
118.30
115.16
77.16 CDCl3
71.15
59.06
58.35
42.35
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

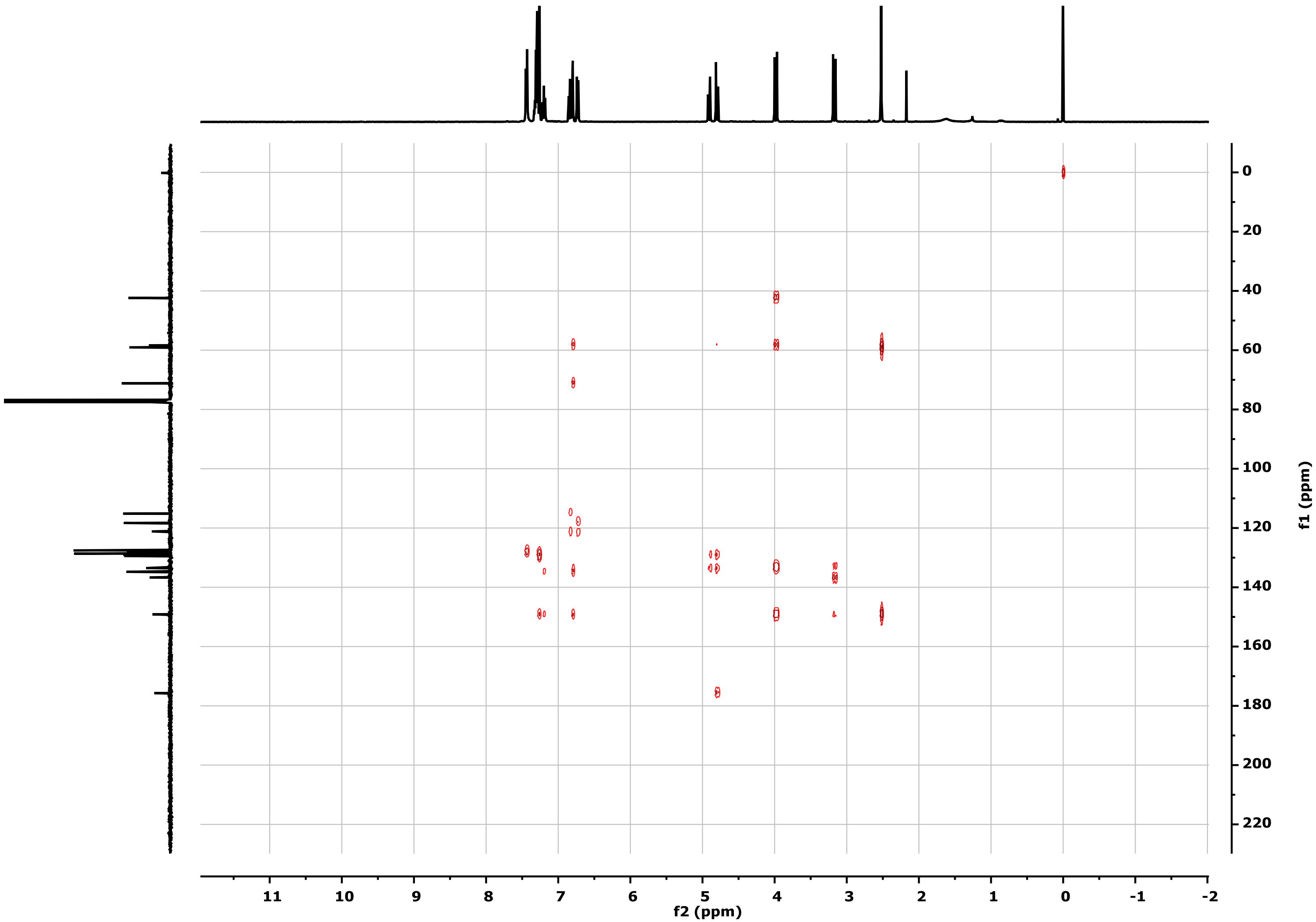
2D NMR HSQC ($CDCl_3$)

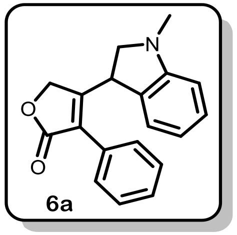


2D NMR COSY ($CDCl_3$)

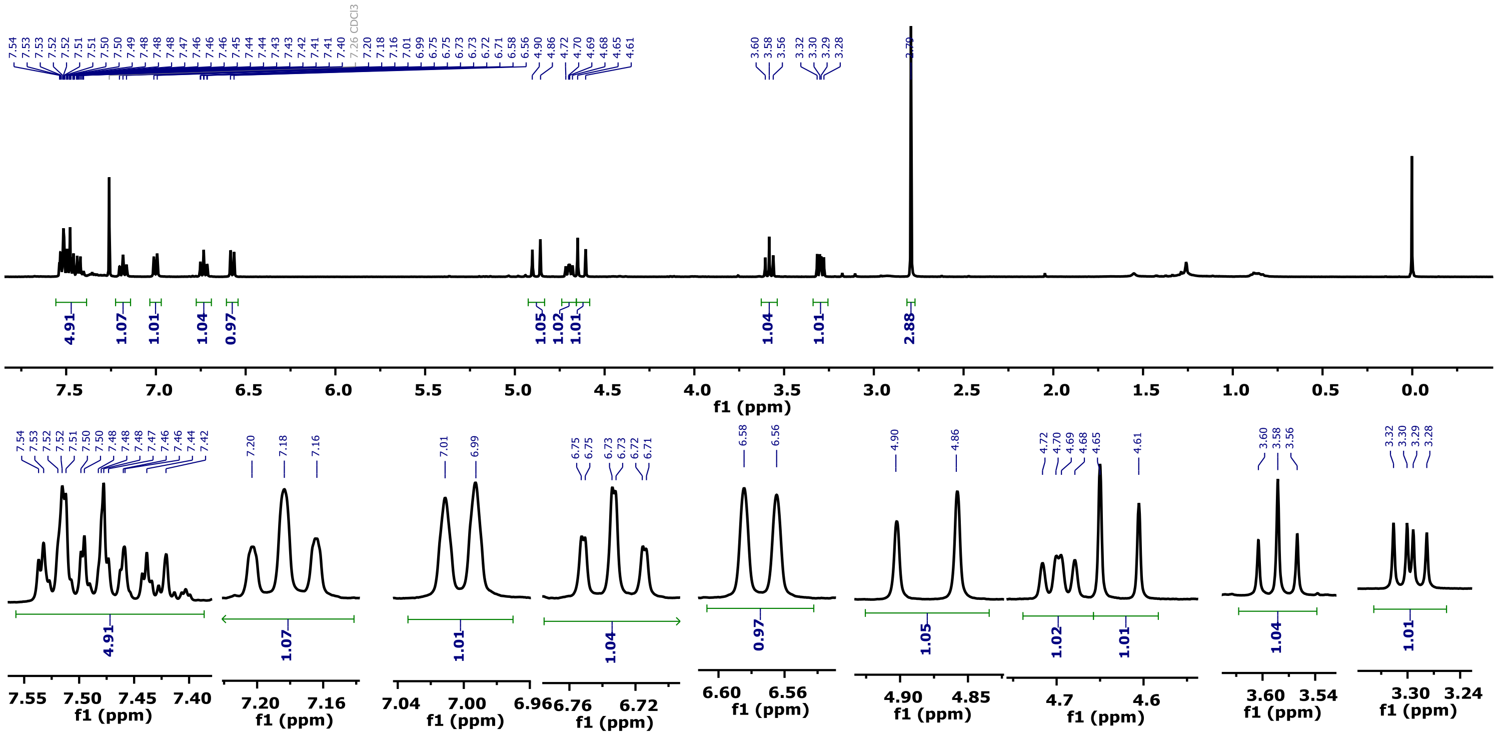


2D NMR HMBC ($CDCl_3$)

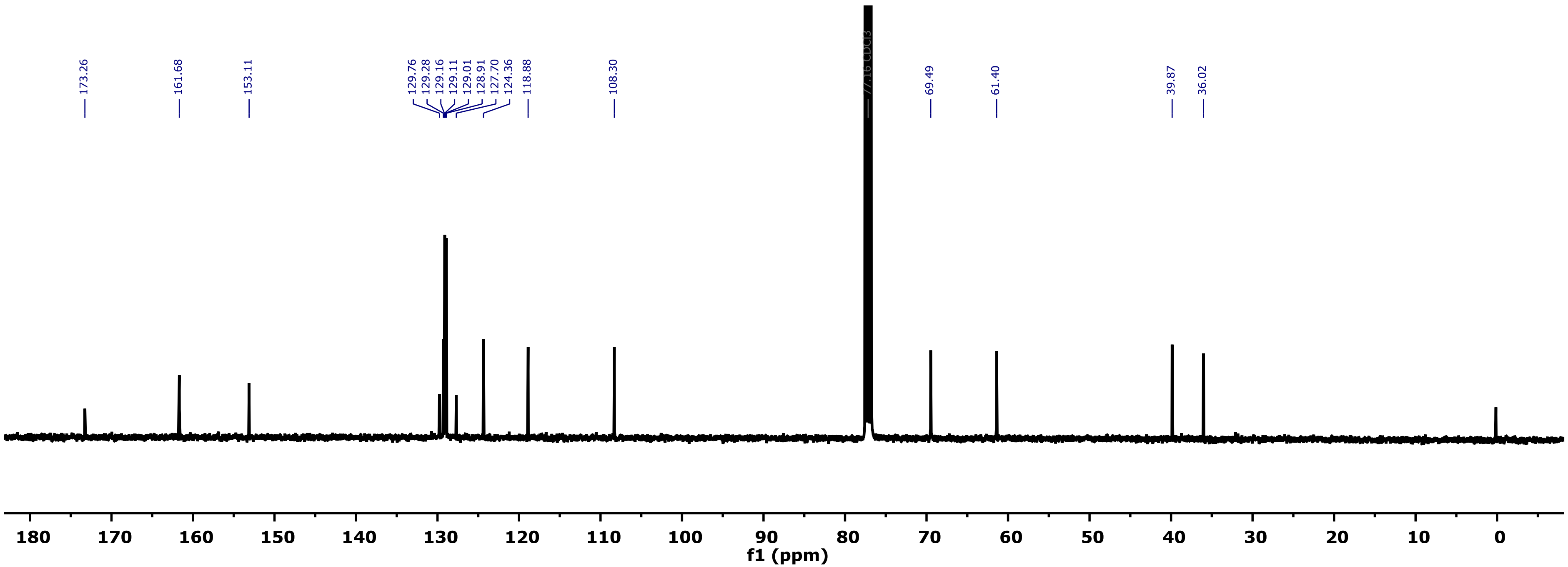



6a

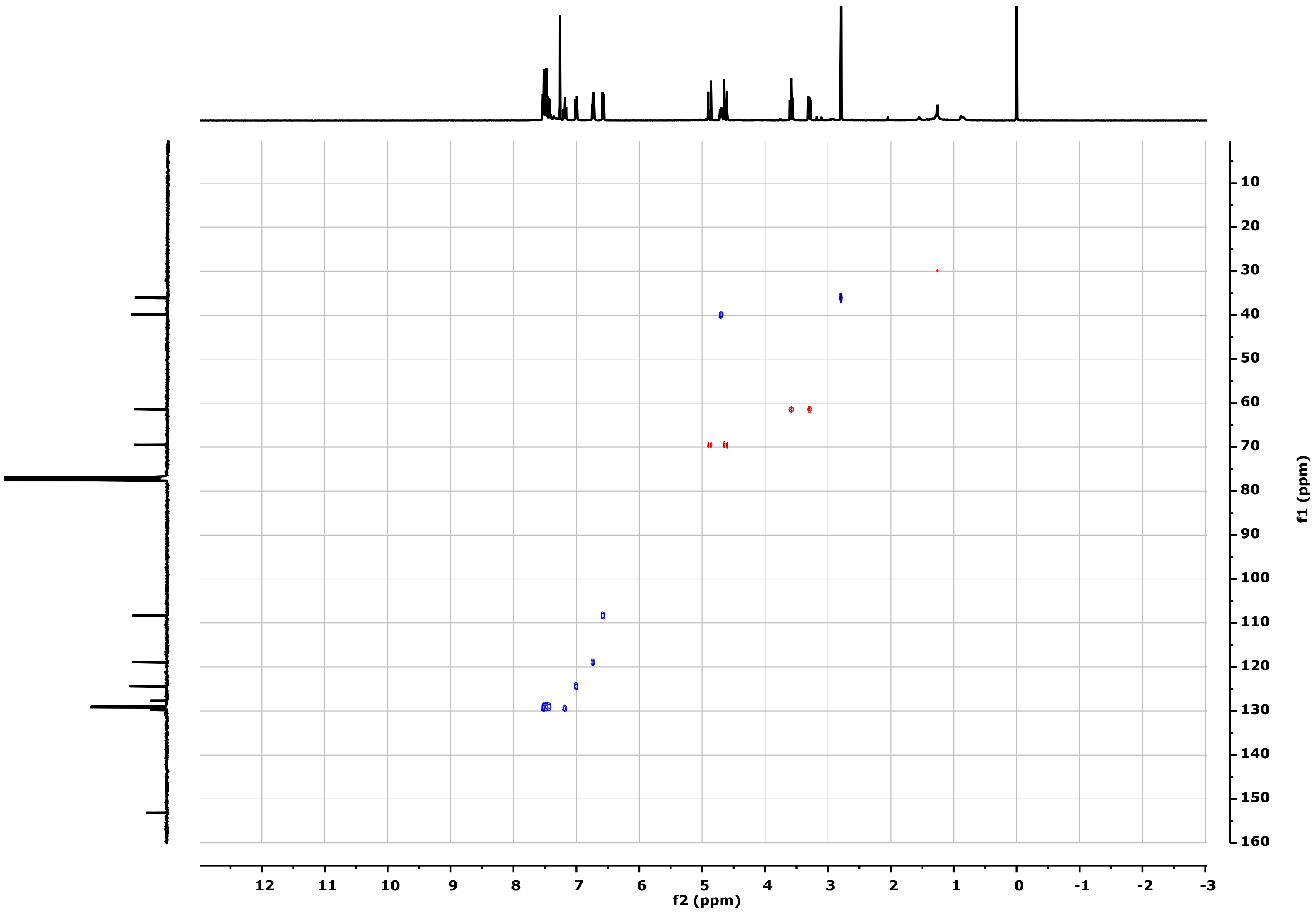
^{1}H NMR (400 MHz, CDCl$_3$)



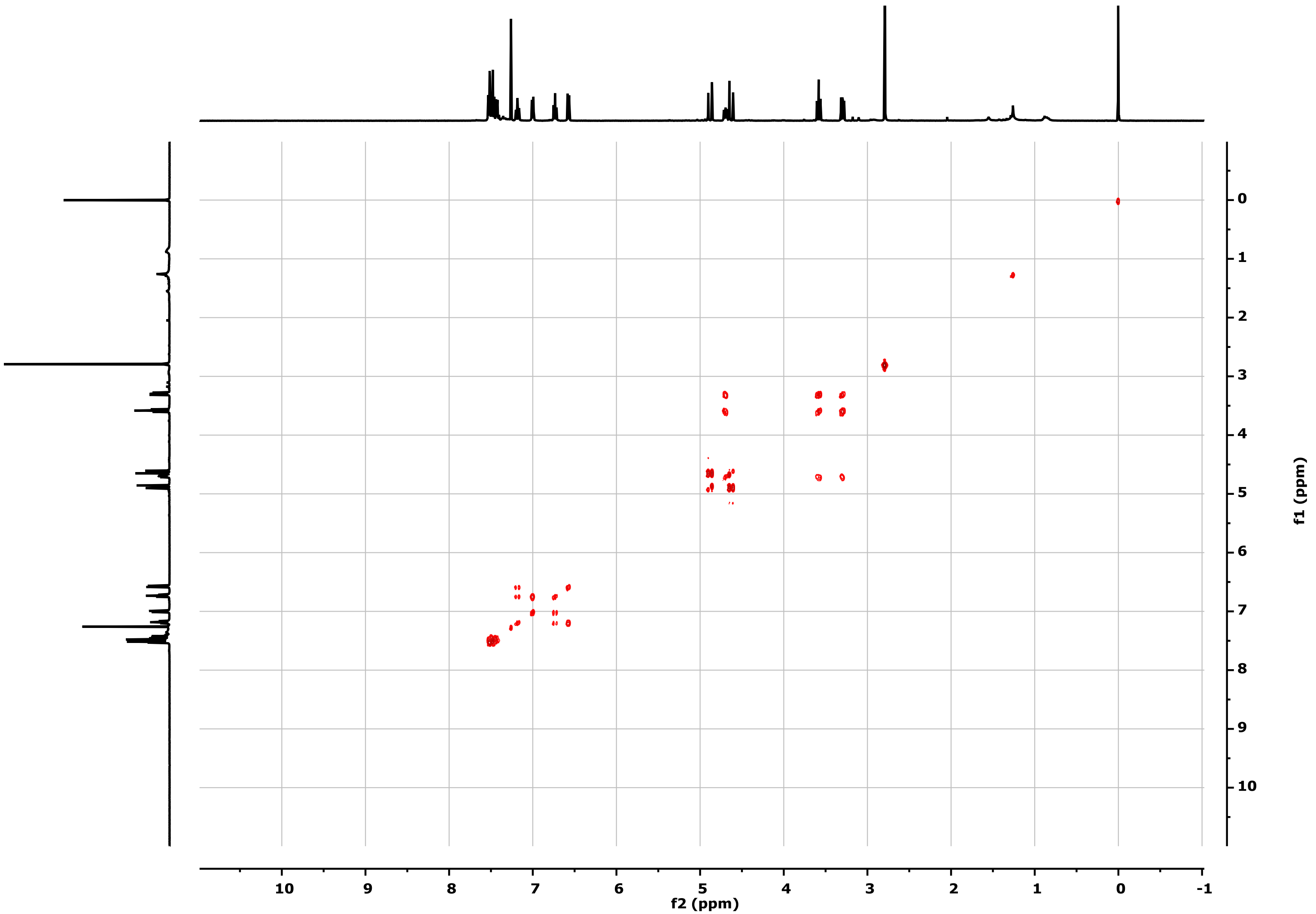
$^{13}C\{H\}$ NMR ($CDCl_3$, 101 MHz)



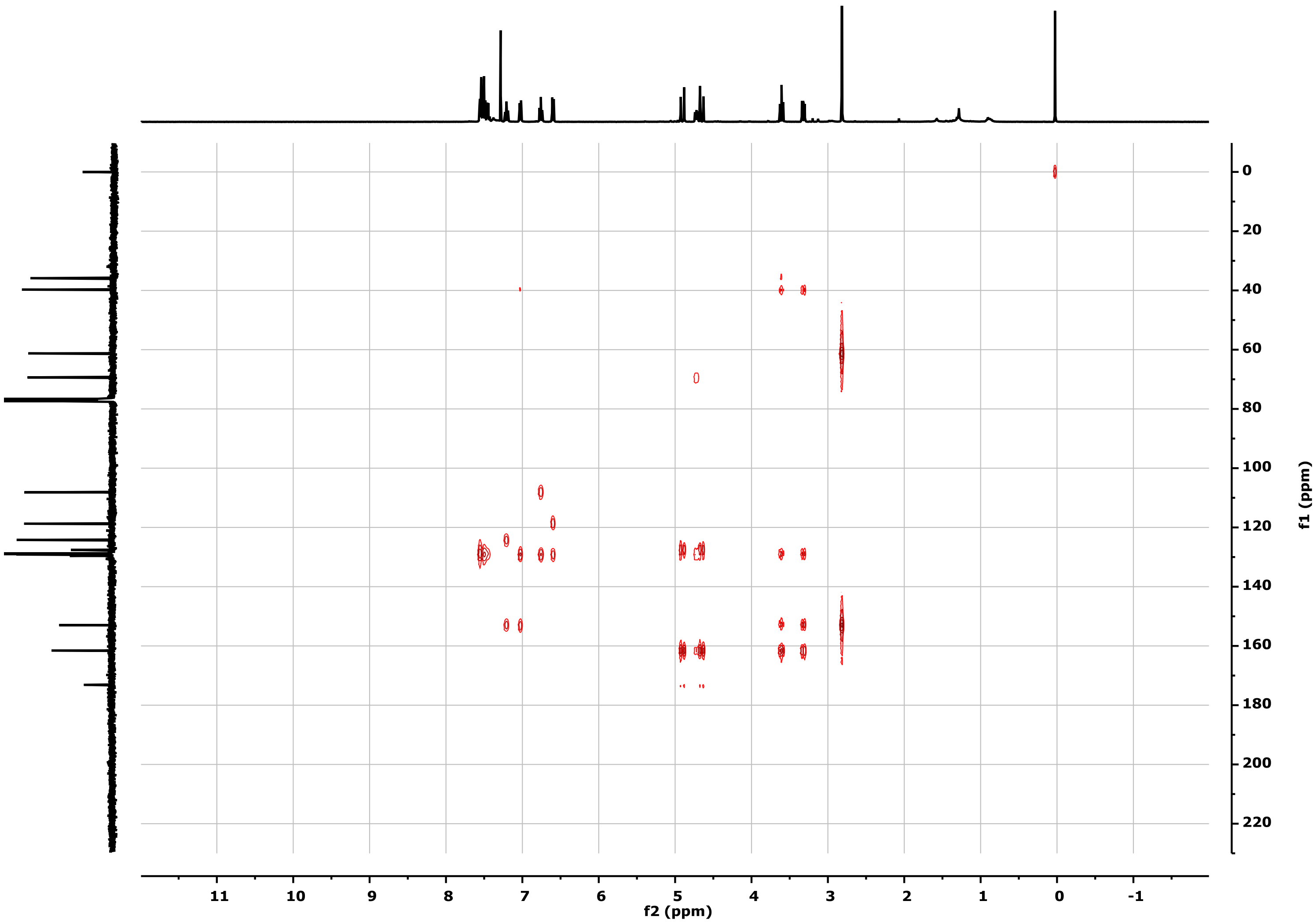
2D NMR HSQC ($CDCl_3$)

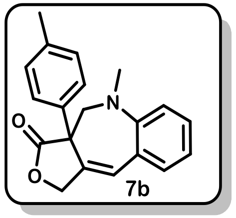


2D NMR COSY ($CDCl_3$)

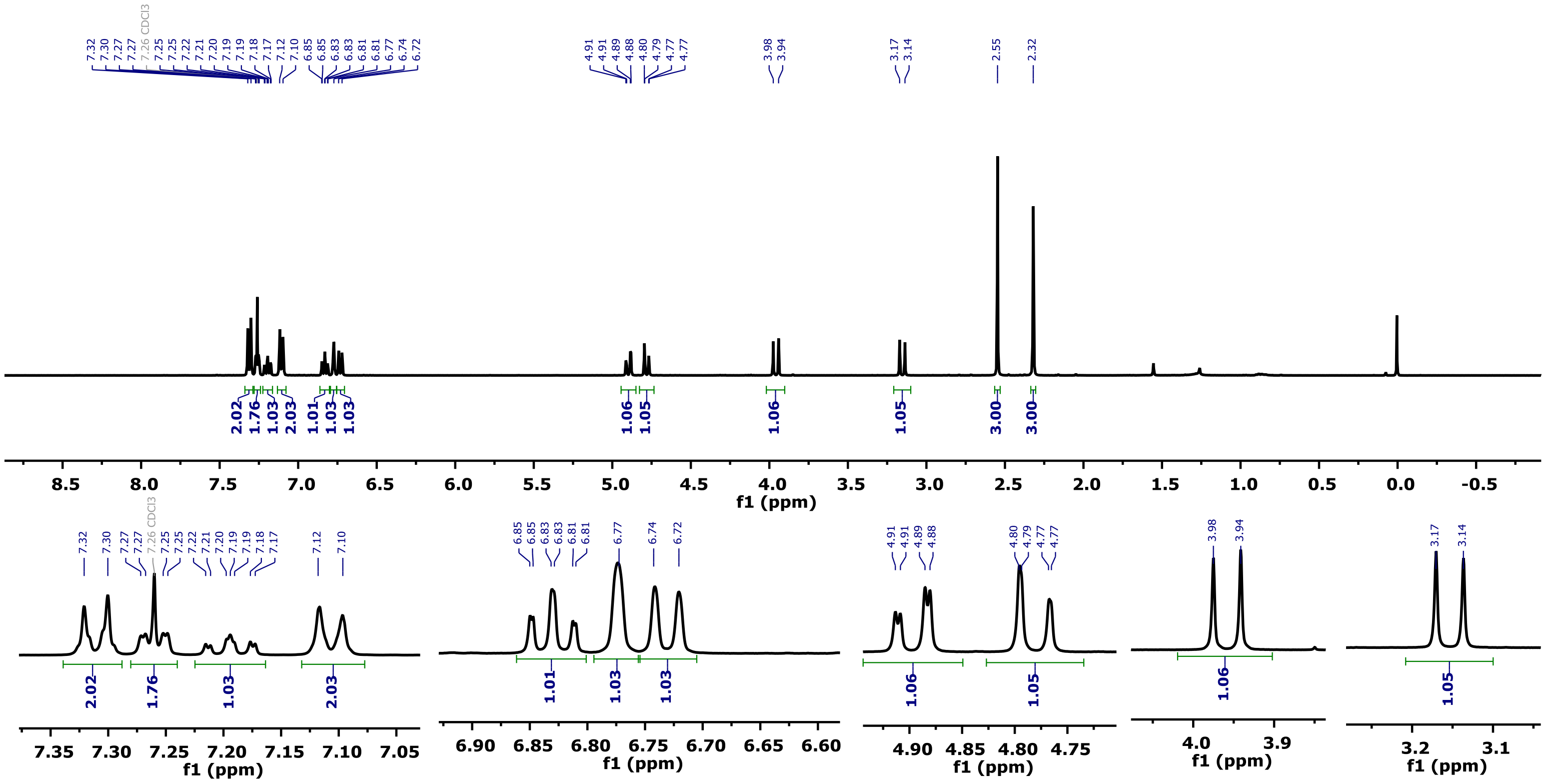


2D NMR HMBC ($CDCl_3$)

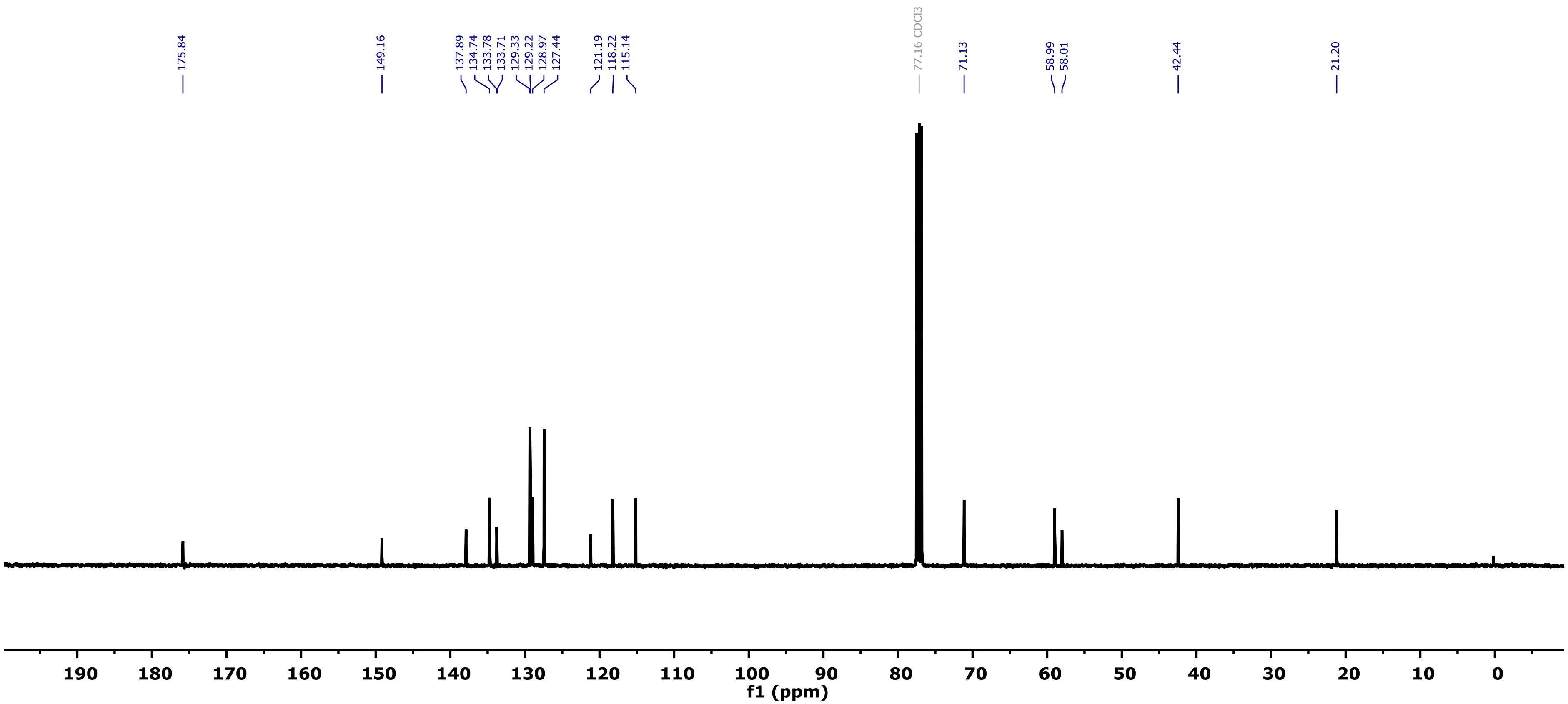


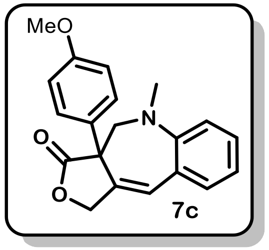


[1]H NMR (400 MHz, $CDCl_3$)



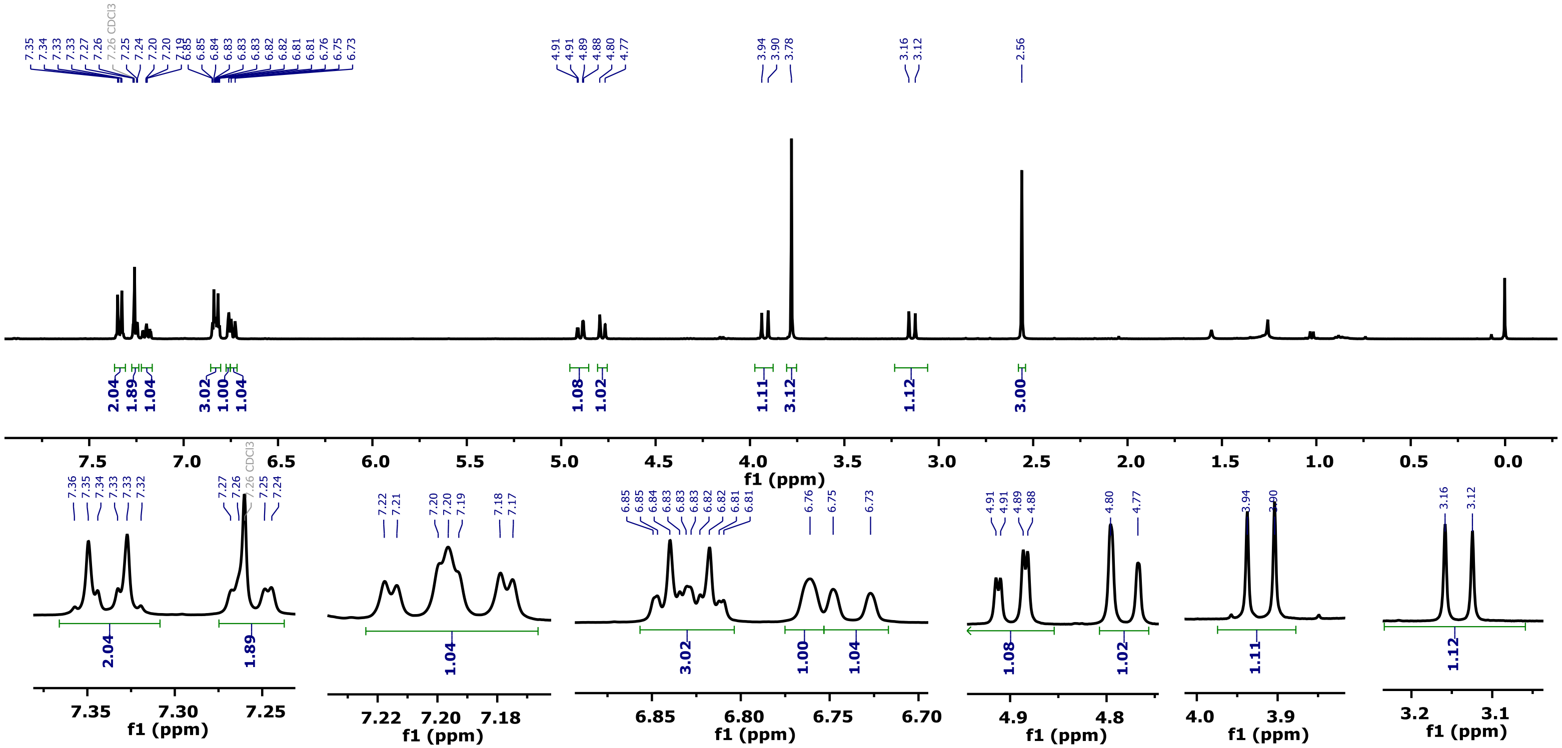
$^{13}C\{H\}$ NMR ($CDCl_3$, 101 MHz)

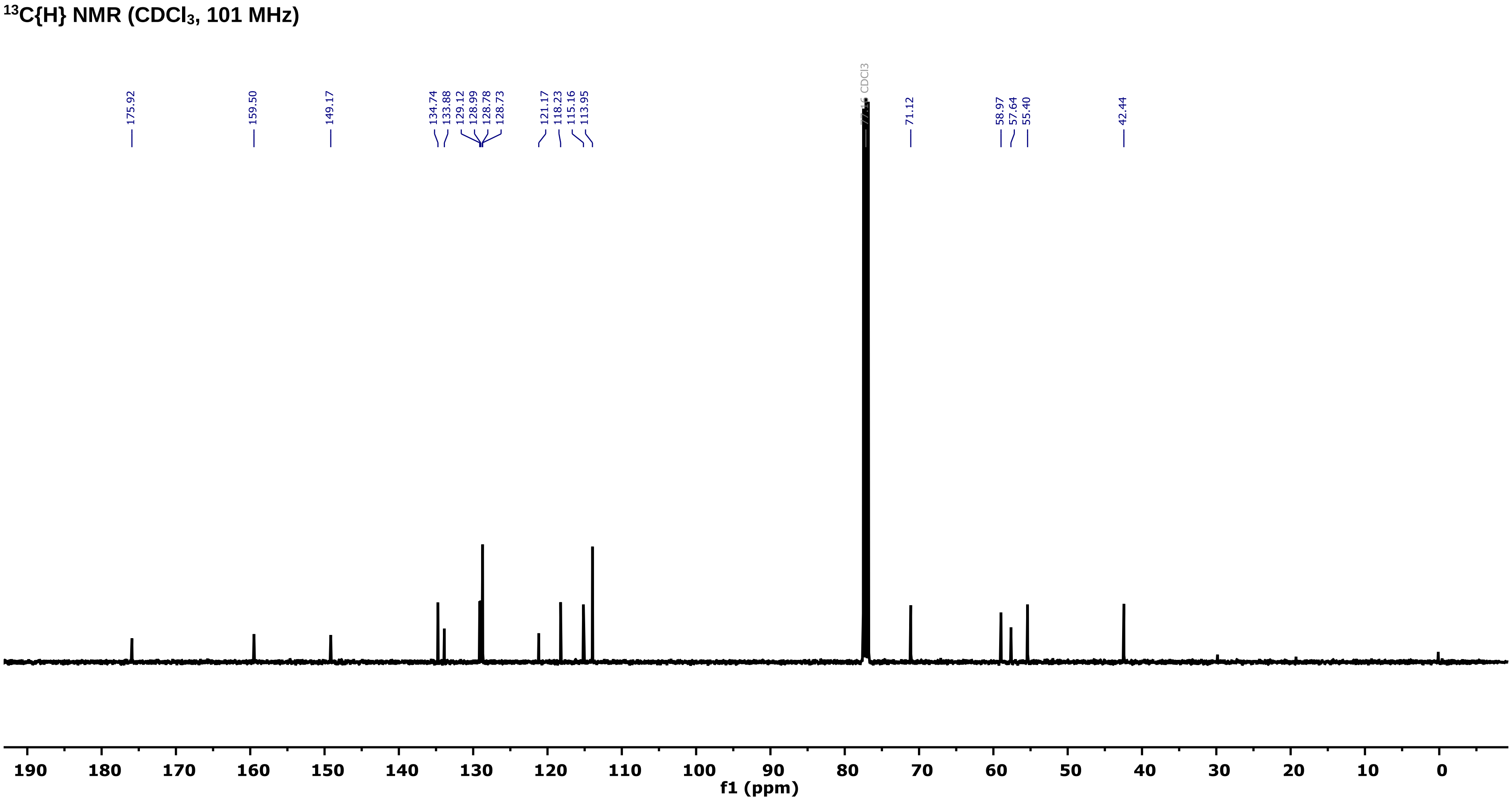




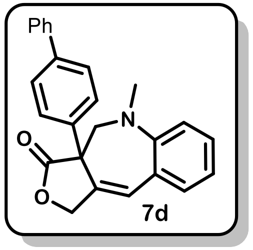
7c

^{1}H NMR (400 MHz, $CDCl_3$)



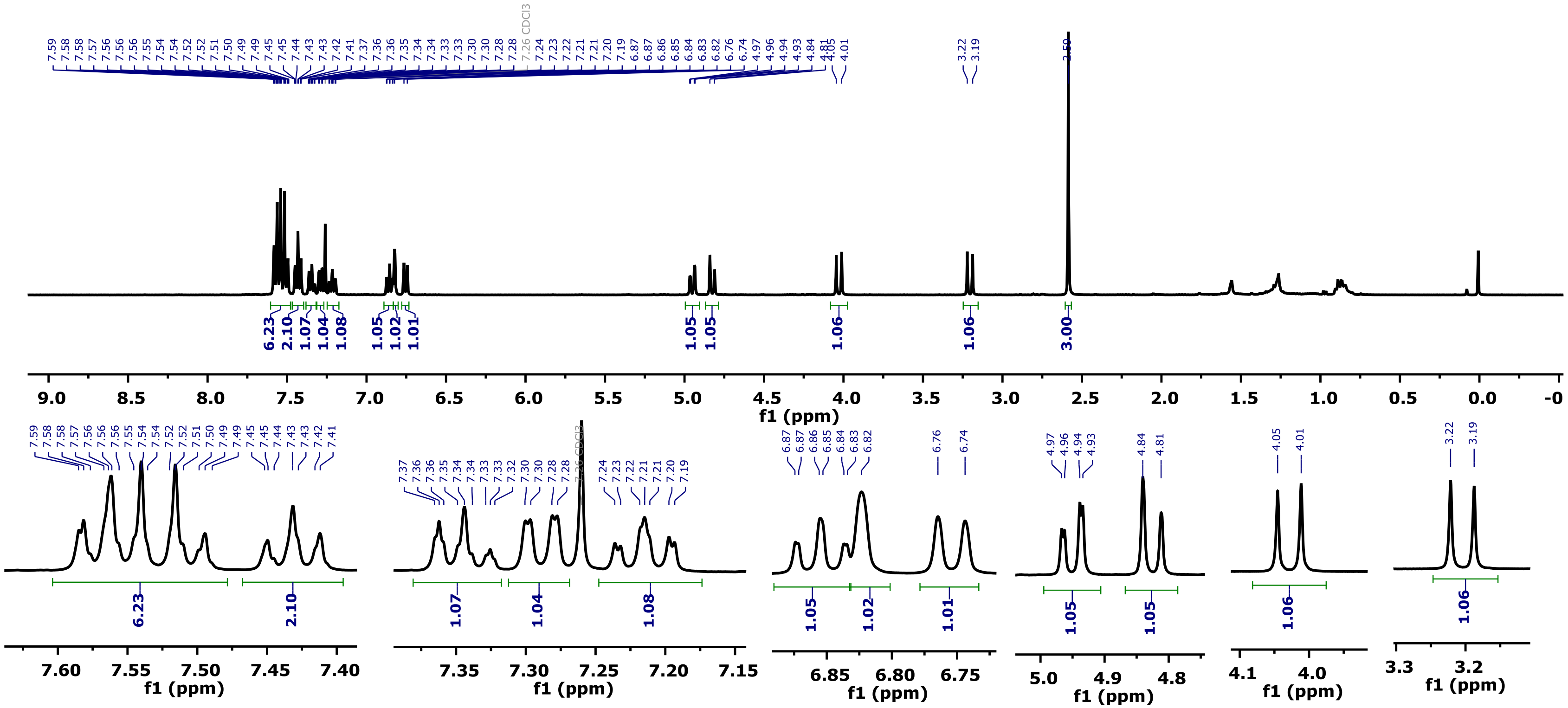


$^{13}C\{H\}$ NMR ($CDCl_3$, 101 MHz)
175.92
159.50
149.17
134.74
133.88
129.12
128.99
128.78
128.73
121.17
118.23
115.16
113.95
CDCl3
71.12
58.97
57.64
55.40
42.44
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

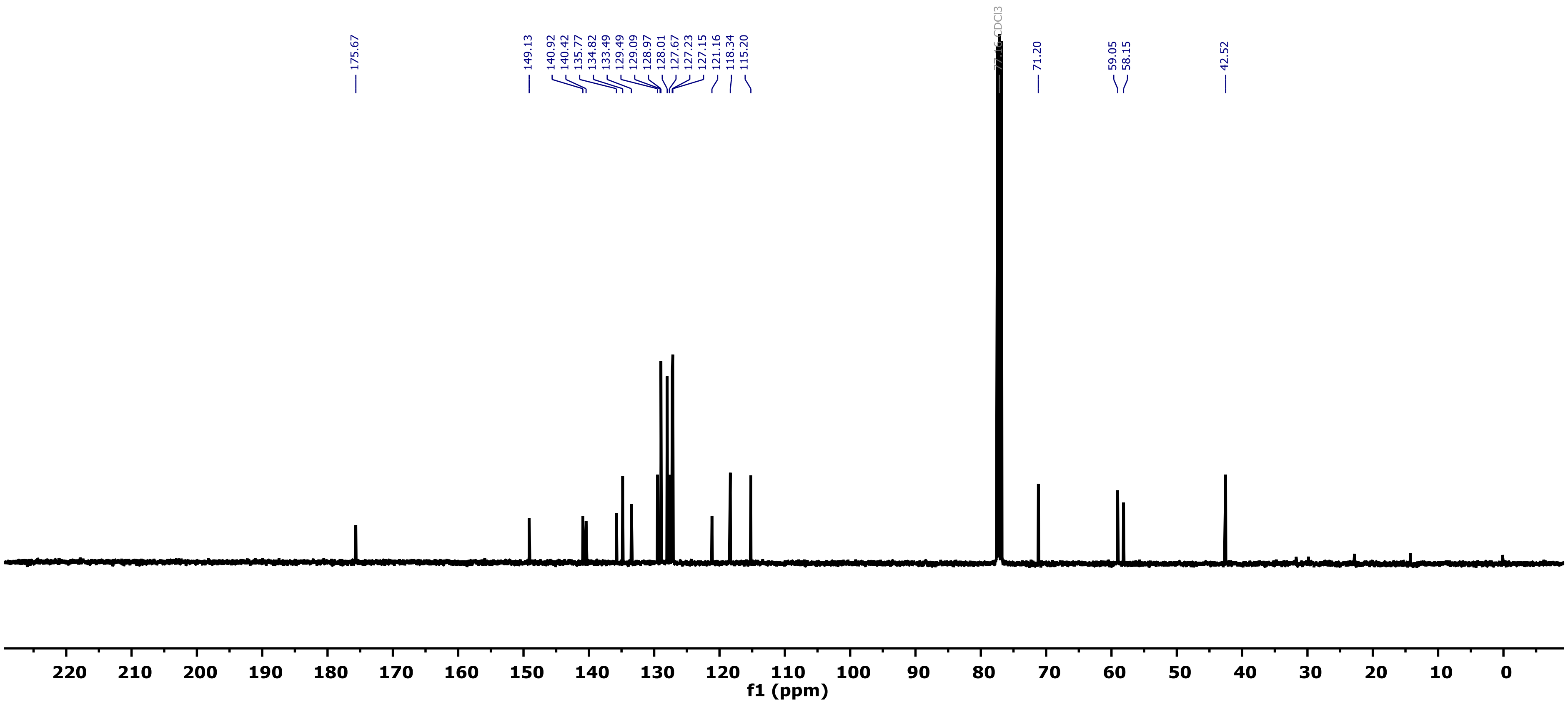


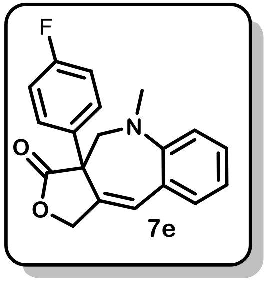
7d

^{1}H NMR (400 MHz, $CDCl_3$)



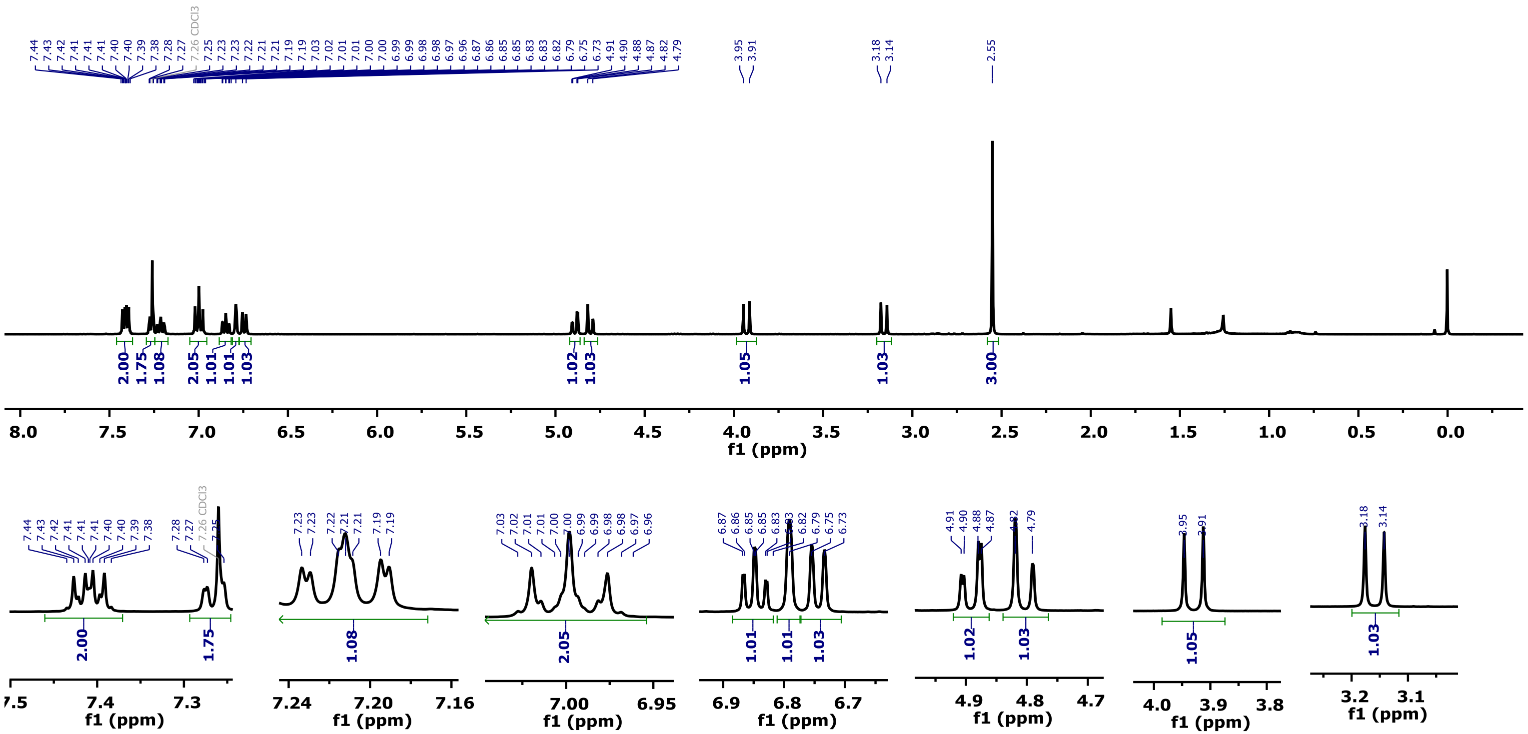
$^{13}C\{H\}$ NMR ($CDCl_3$, 101 MHz)



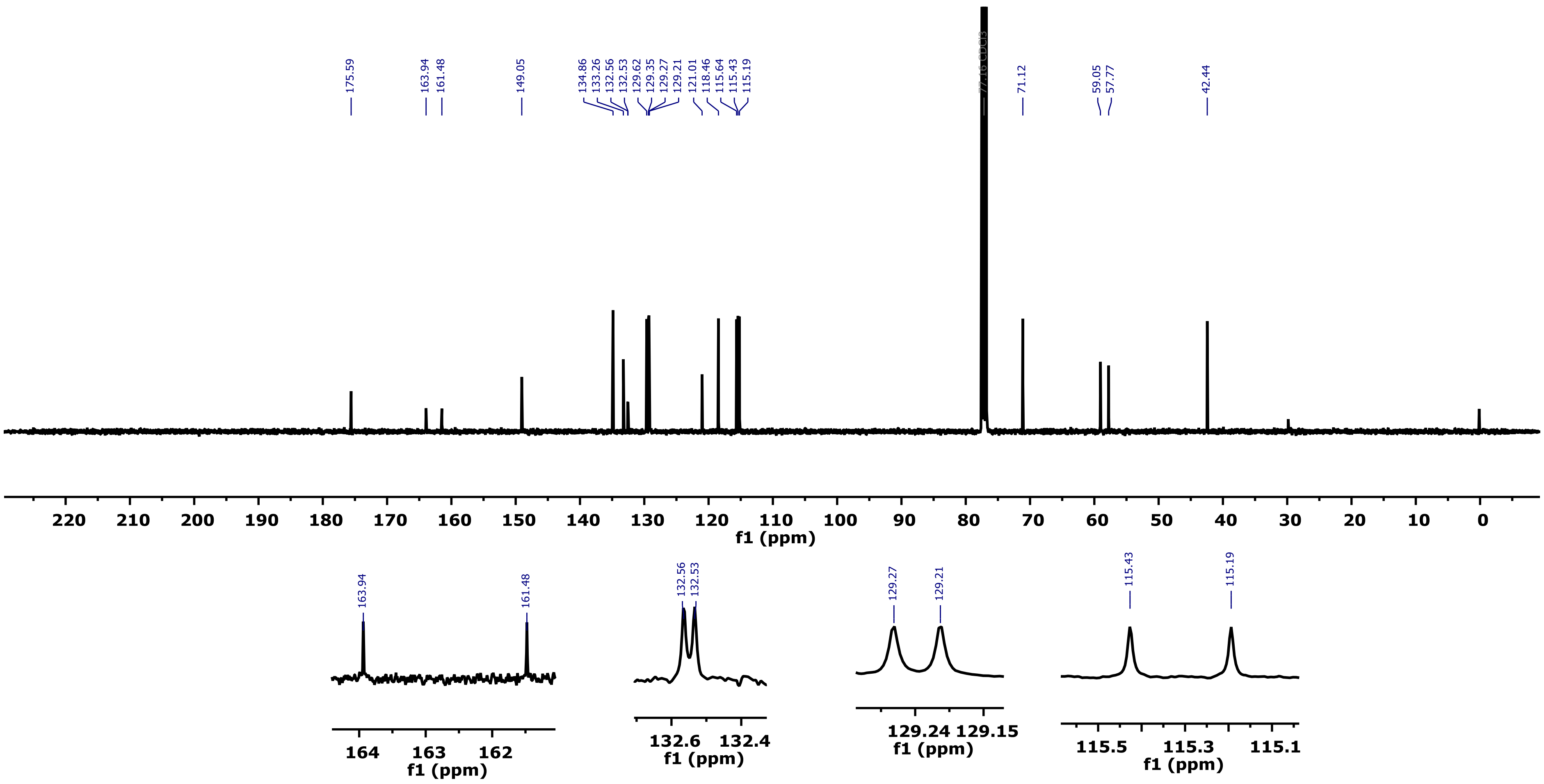


7e

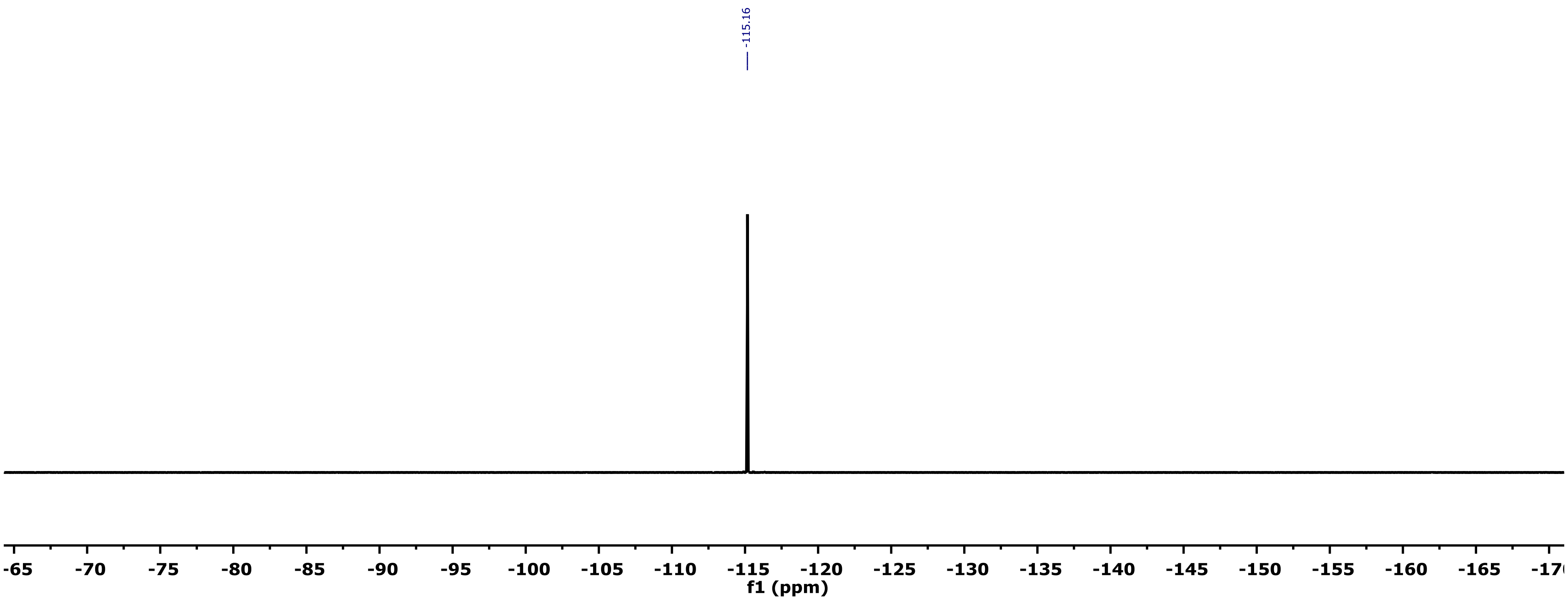
[1]H NMR (400 MHz, $CDCl_3$)

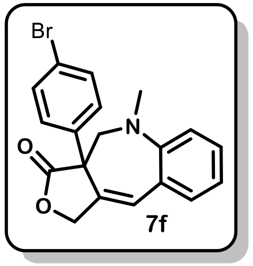


$^{13}C\{H\}$ NMR ($CDCl_3$, 101 MHz)



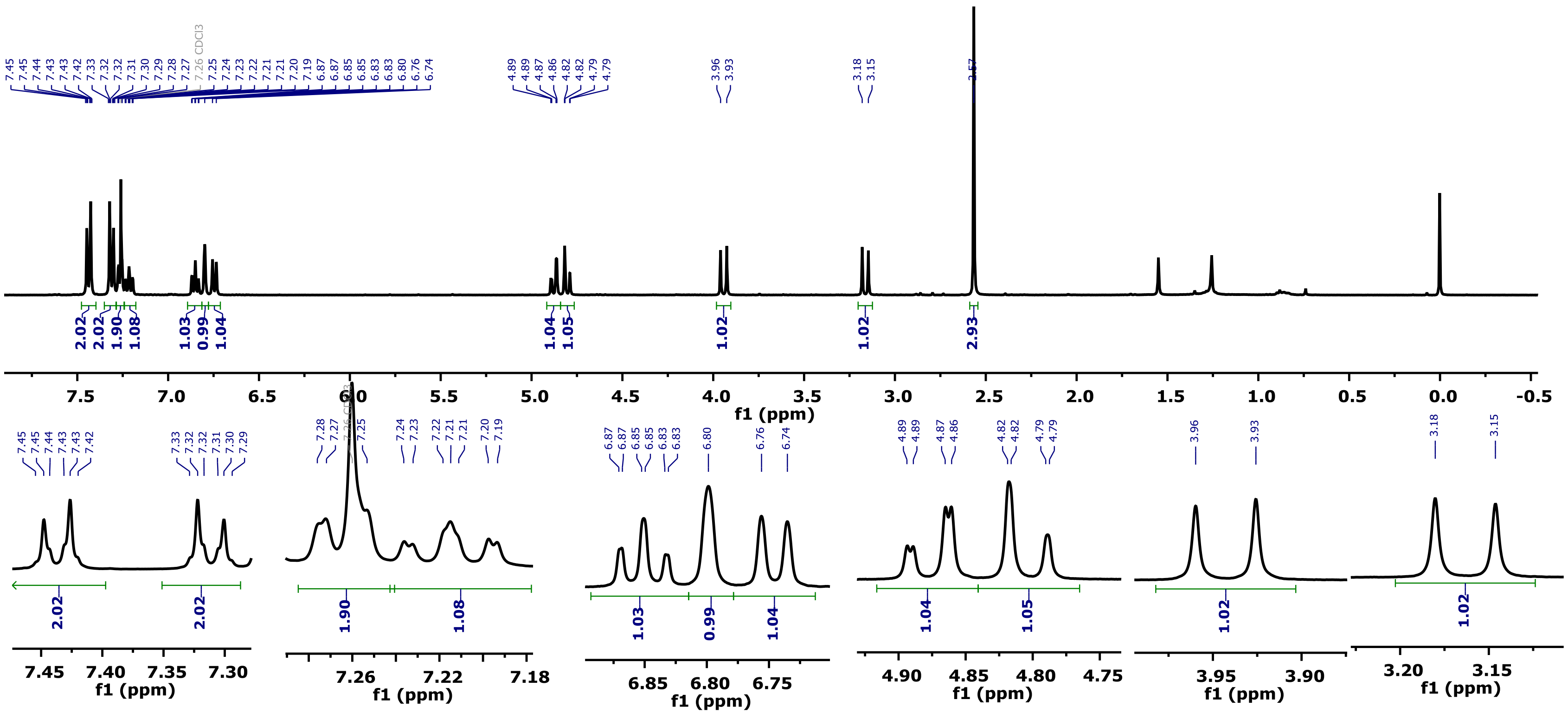
^{19}F NMR ($CDCl_3$, 376 MHz):



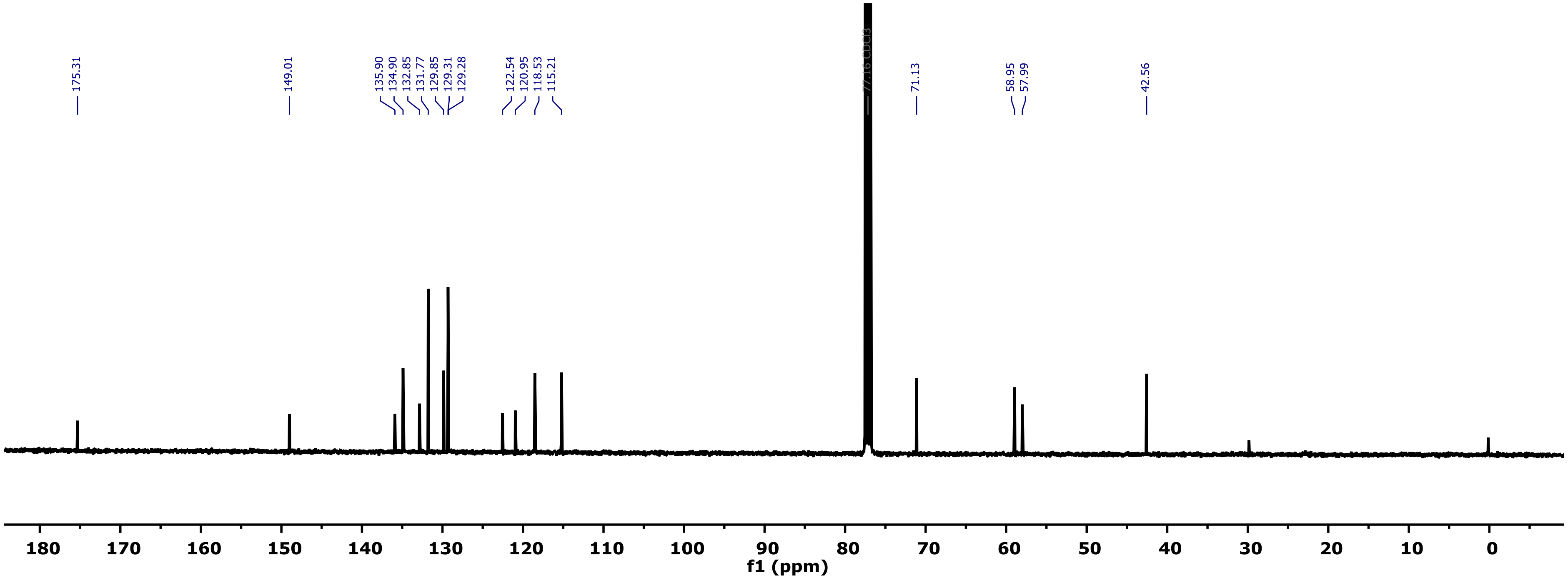


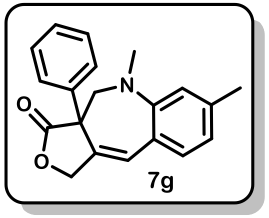
7f

^{1}H NMR (400 MHz, CDCl$_3$)



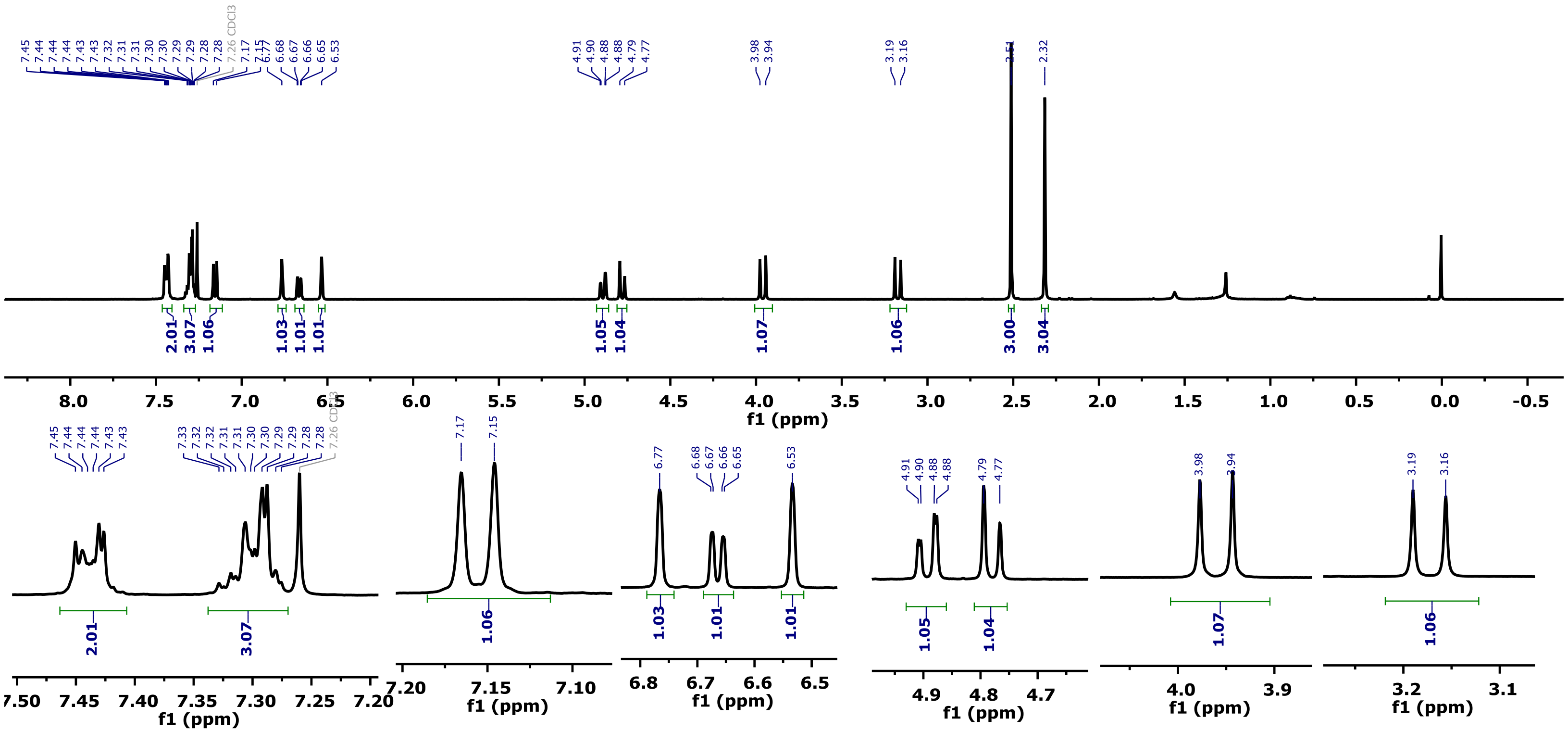
$^{13}C\{H\}$ NMR ($CDCl_3$, 101 MHz)



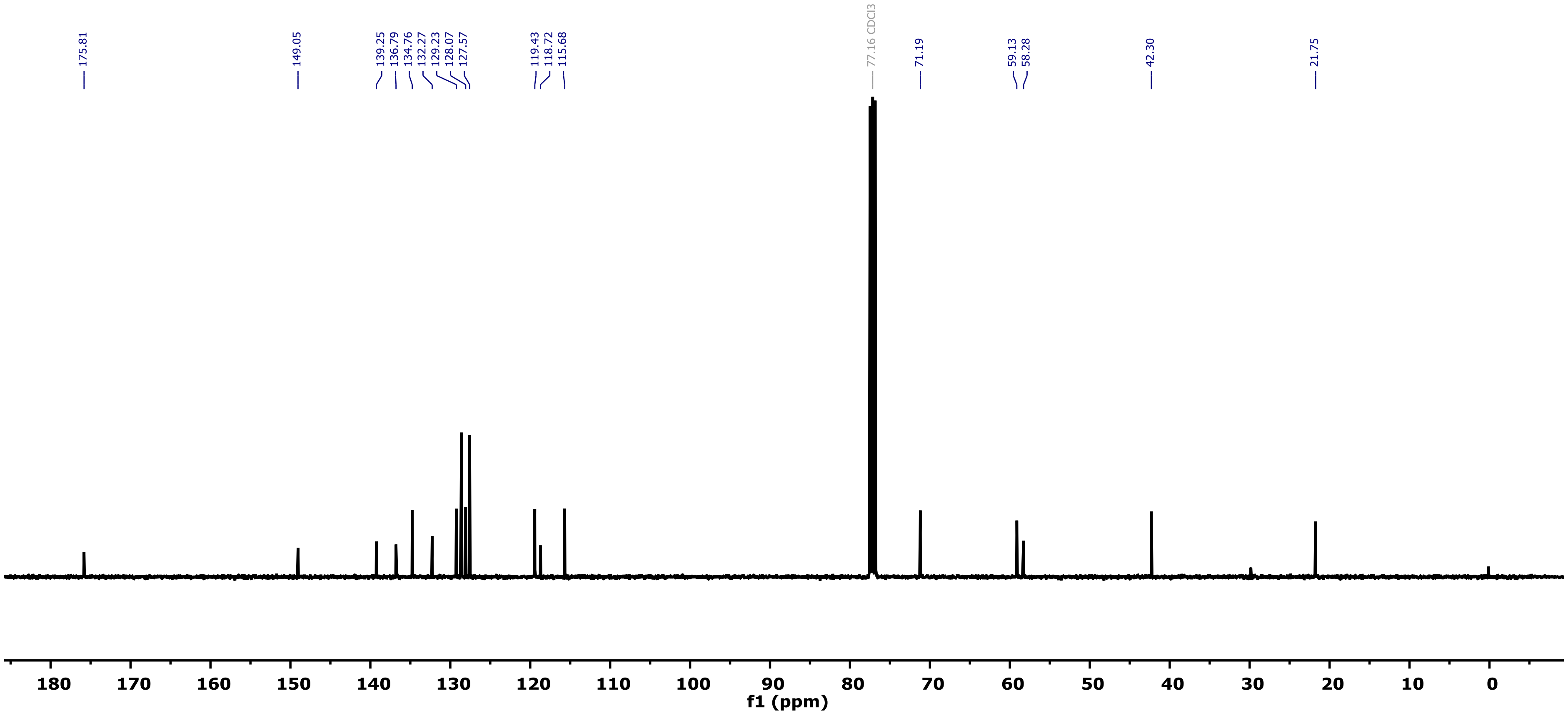


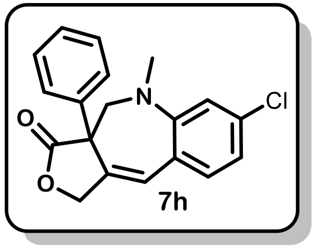
7g

^{1}H NMR (400 MHz, $CDCl_3$)



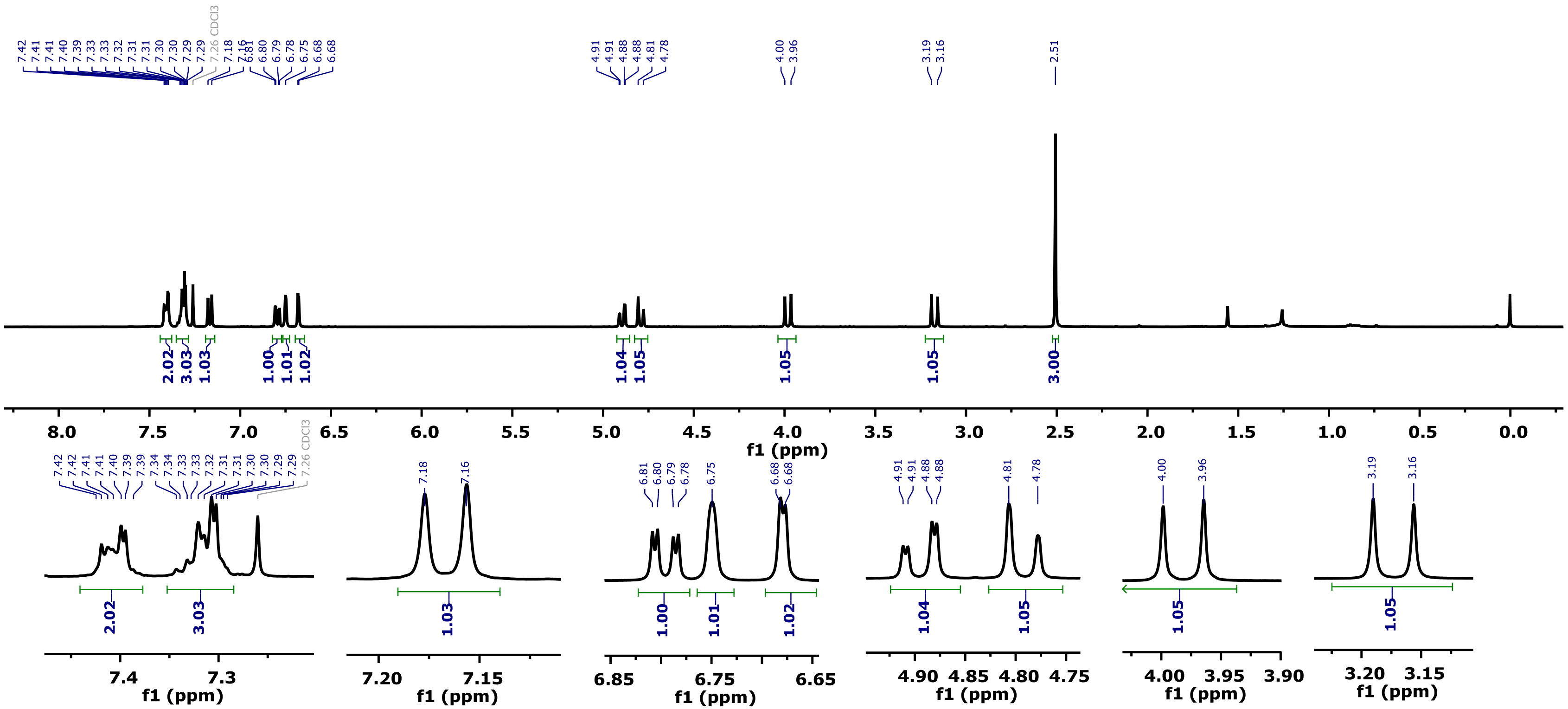
$^{13}C\{H\}$ NMR ($CDCl_3$, 101 MHz)



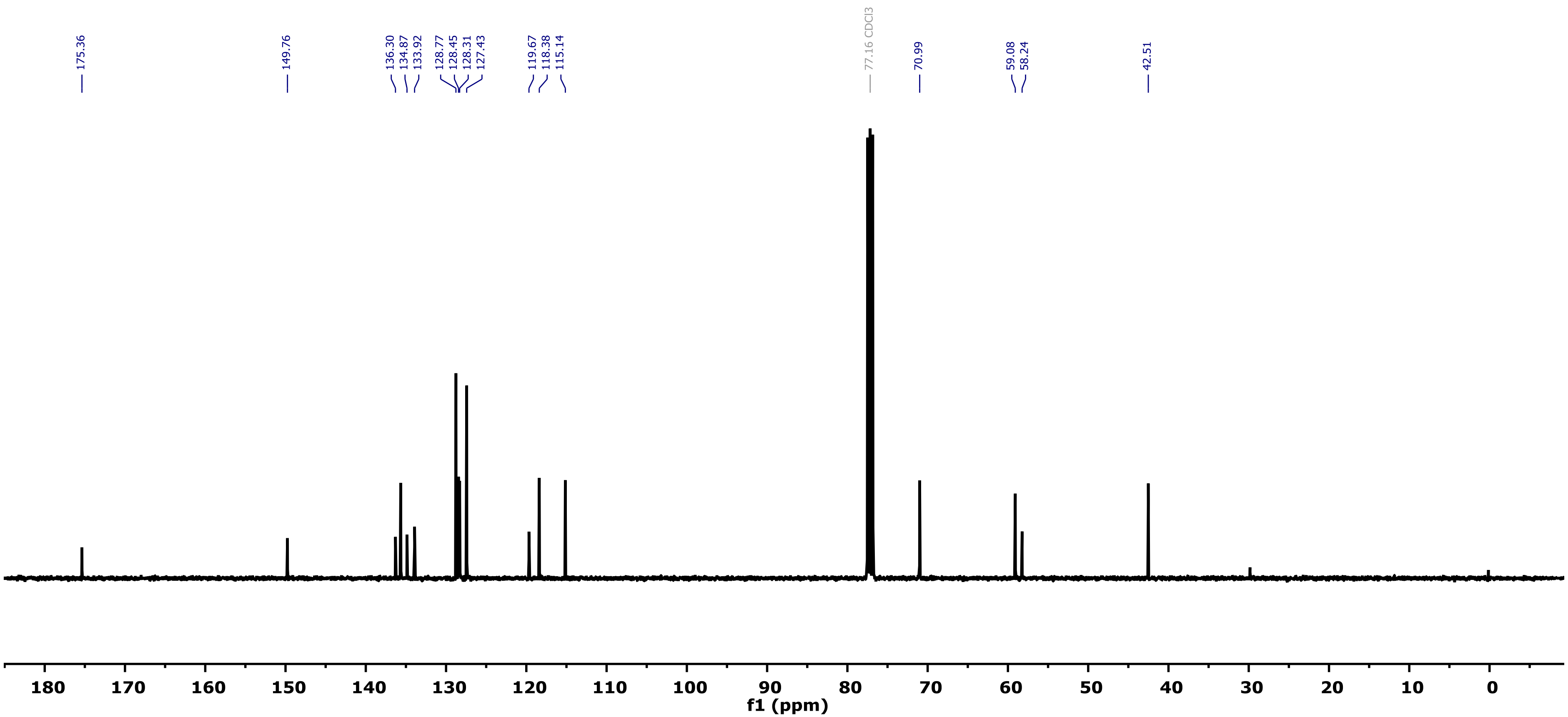


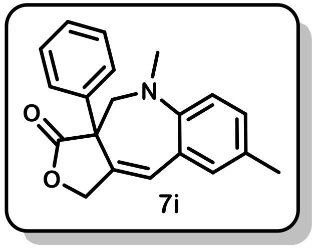
7h

^{1}H NMR (400 MHz, $CDCl_3$)



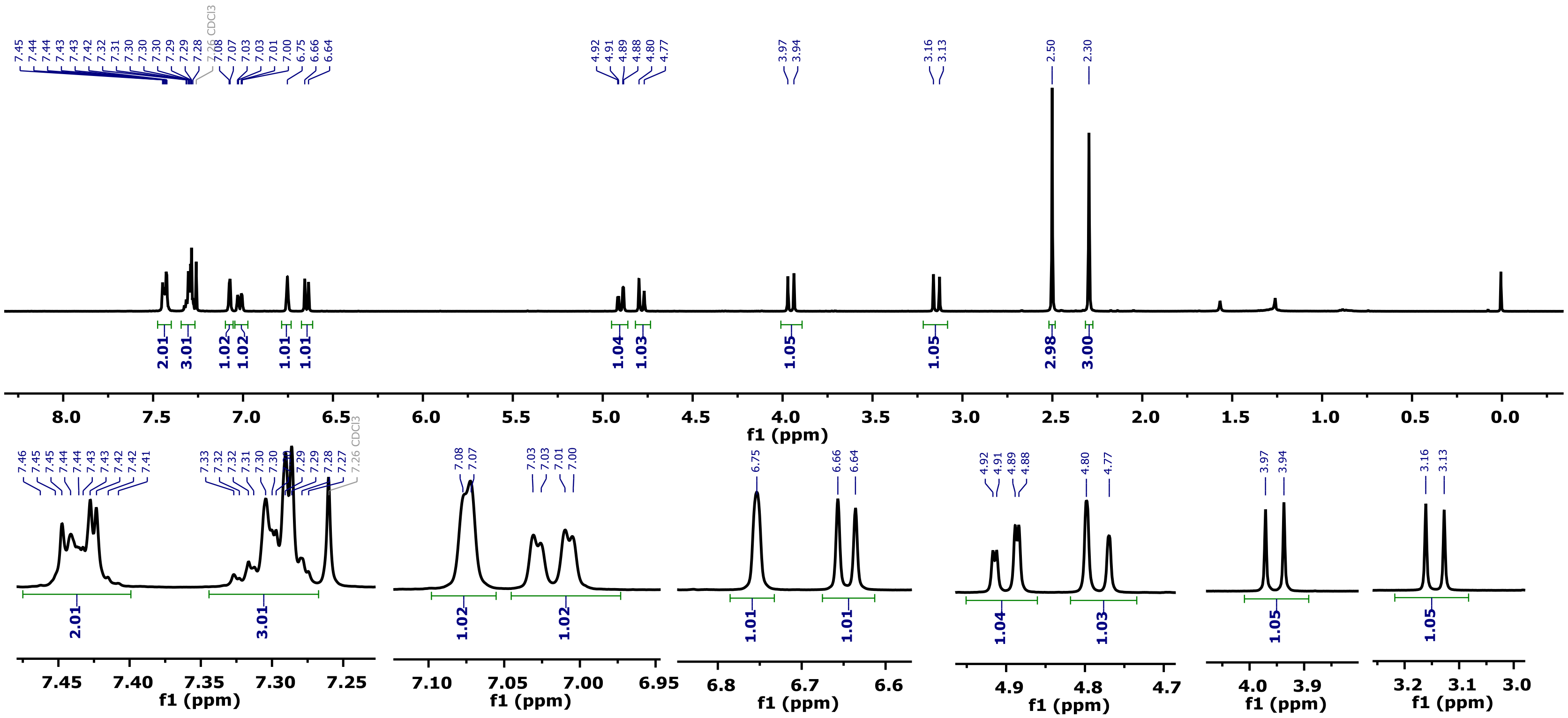
$^{13}C\{H\}$ NMR ($CDCl_3$, 101 MHz)



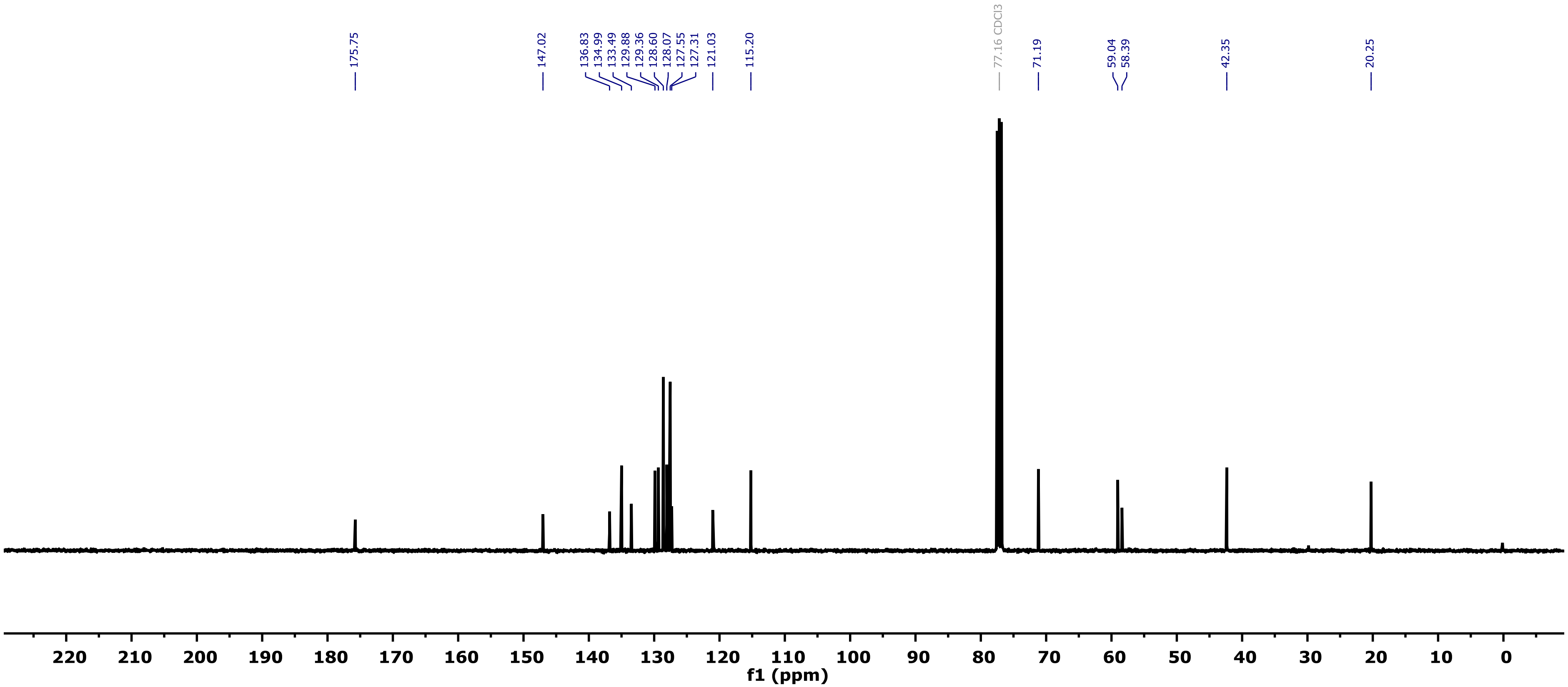


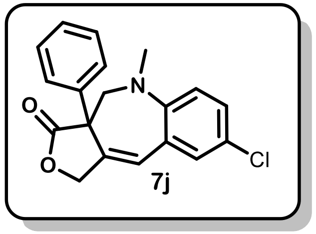
7i

^{1}H NMR (400 MHz, $CDCl_3$)

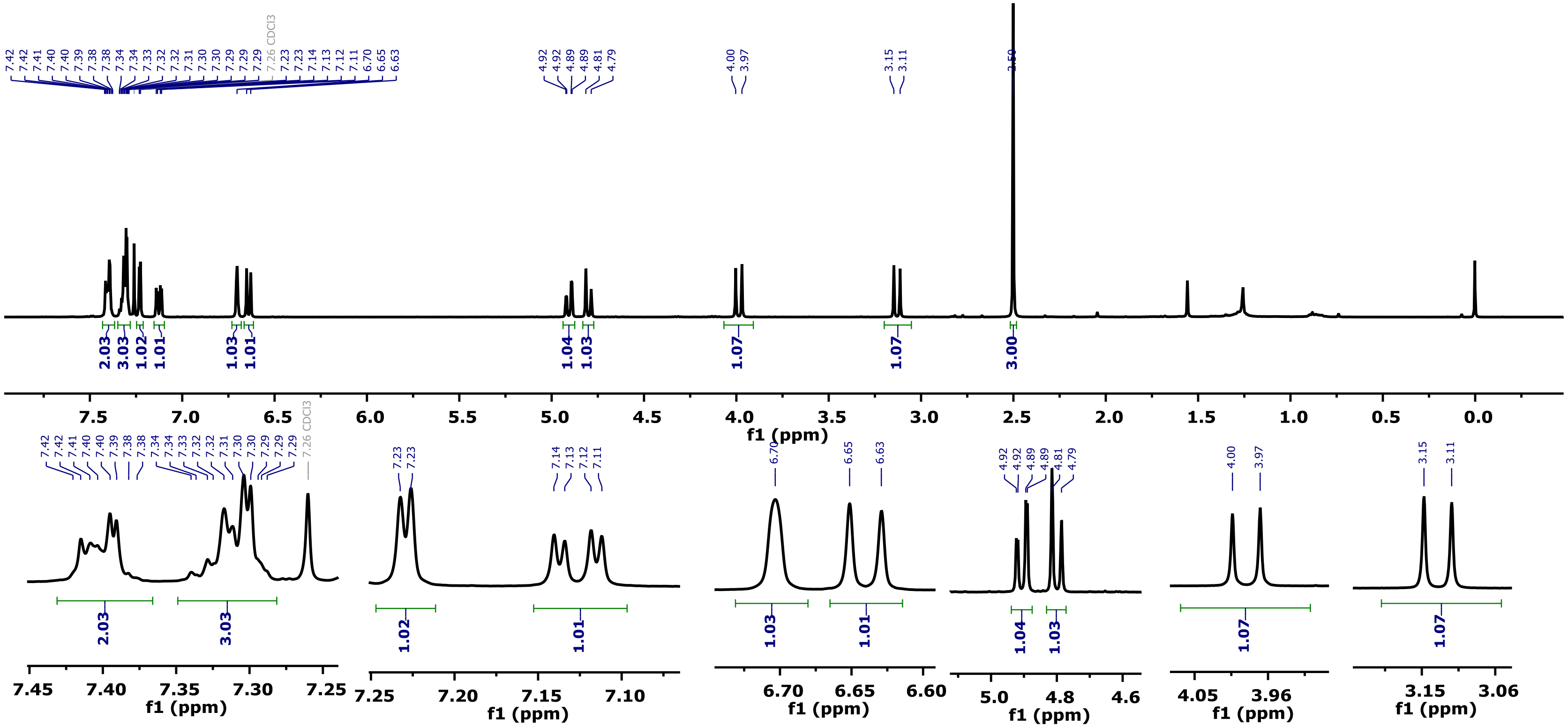


$^{13}C\{H\}$ NMR ($CDCl_3$, 101 MHz)

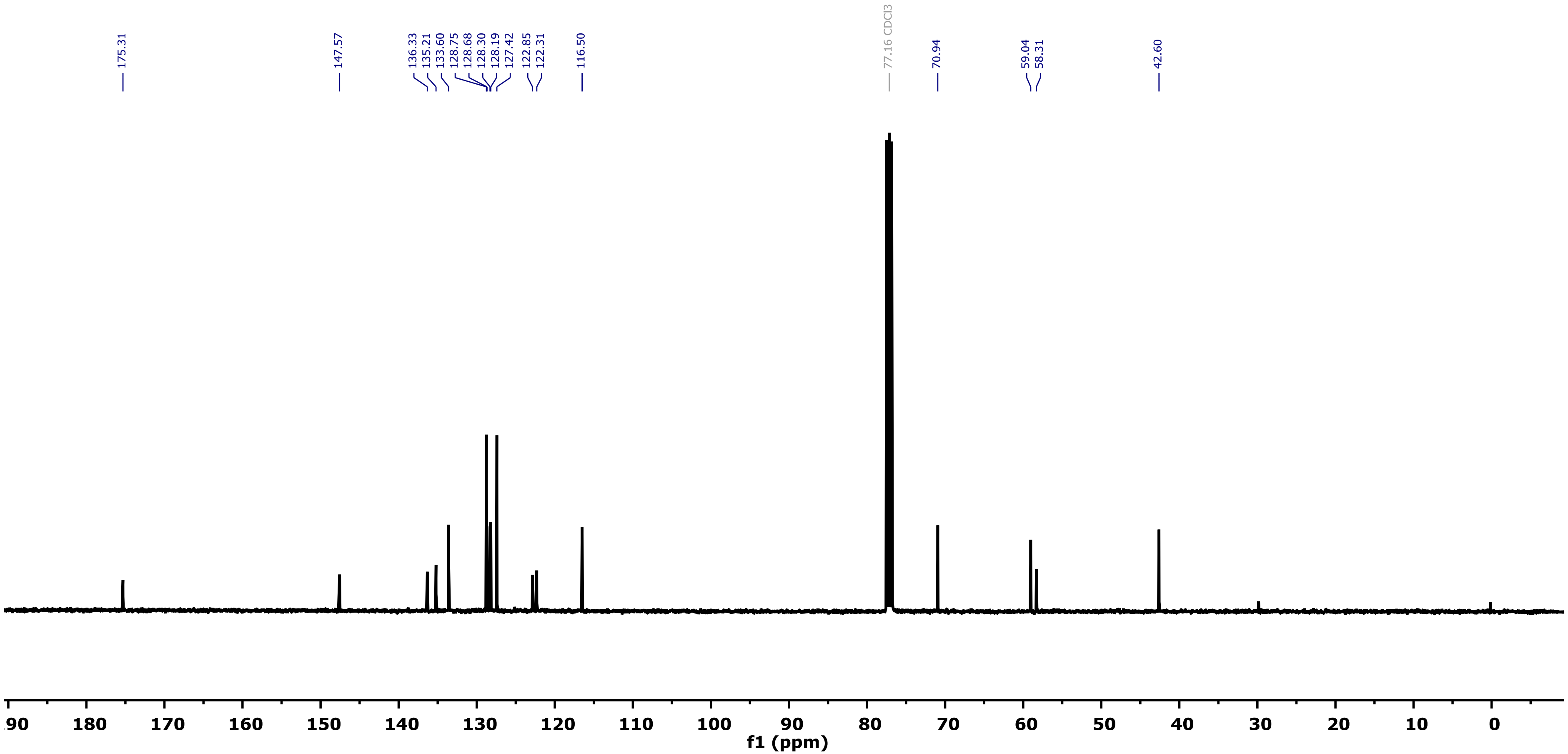


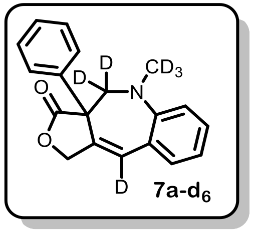


^{1}H NMR (400 MHz, $CDCl_3$)

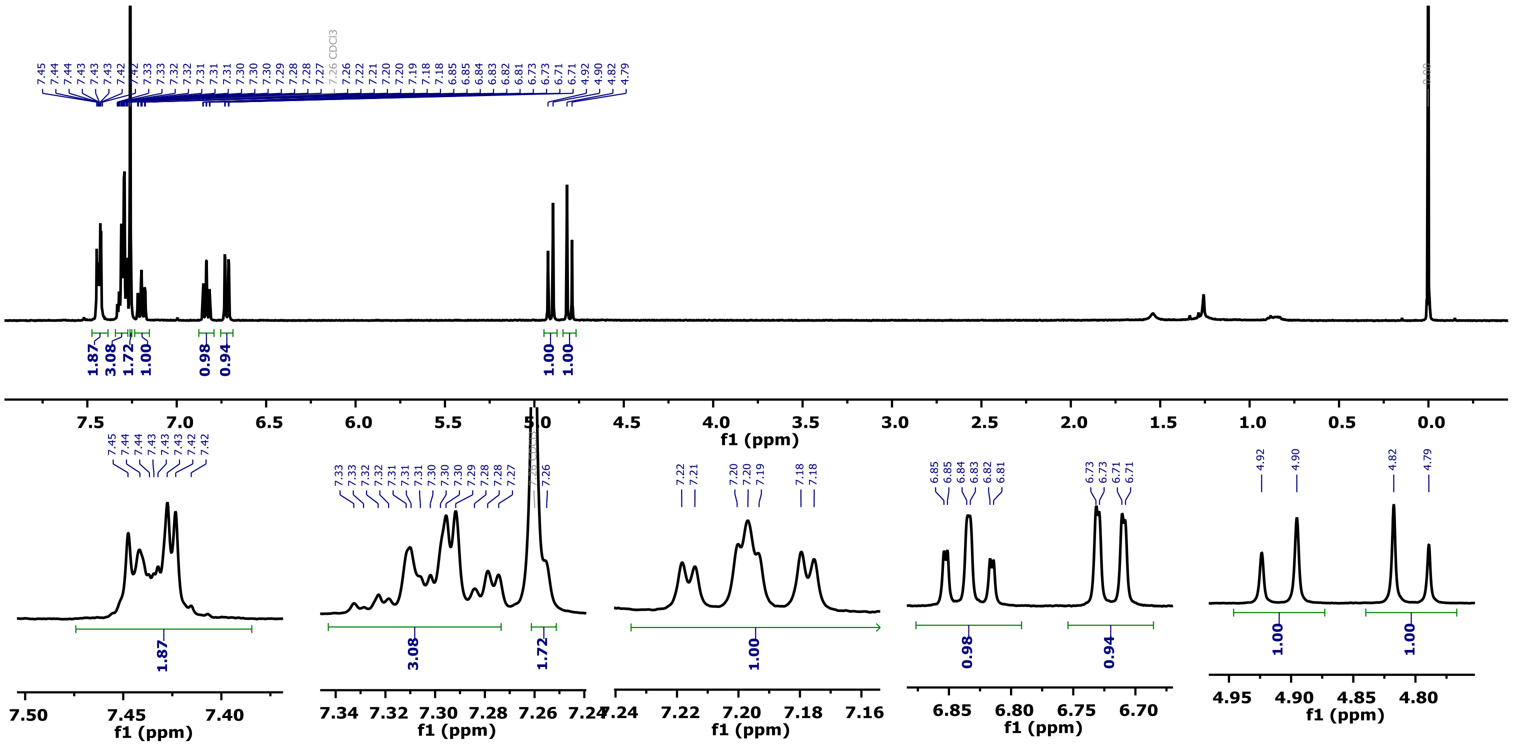


$^{13}C\{H\}$ NMR ($CDCl_3$, 101 MHz)





^{1}H NMR (400 MHz, $CDCl_3$)



^{13}C{H} NMR ($CDCl_3$, 101 MHz)