Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Iron-catalyzed Ene-type Propargylation of Diarylethylenes with Propargyl Alcohols

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Supporting Information

Contents

1. General Information

Chemicals and solvents were purchased from commercial suppliers and used as received. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker ACF300 (300 MHz) spectrometer. Chemical shifts were reported in parts per million (ppm), and the residual solvent peak was used as an internal reference: proton (chloroform δ 7.26), carbon (chloroform δ 77.0) or tetramethylsilane (TMS δ 0.00) was used as a reference. Multiplicity was indicated as follows: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), dd (doublet of doublet), bs (broad singlet). Coupling constants were reported in Hertz (Hz). Low resolution mass spectra were obtained on a Finnigan/MAT LCQ spectrometer in EI mode and API 3000™ in APCI (Heated Nebulizer) mode. All high resolution mass spectra were obtained on a Finnigan/MAT 95XL-T spectrometer. For thin layer chromatography (TLC), Merck pre-coated TLC plates (Merck 60 F254) were used, and compounds were visualized with a UV light at 254 nm. Further visualization was achieved by staining with iodine. Flash chromatography separations were performed on Merck 60 (0.040-0.063 mm) mesh silica gel.

2. Preparation of Starting Materials

Compounds **1a** and **2a** were commercially available. Compounds **1b-1d**[1], **2b-2s**[2] and **2t-2y**[3] were prepared according to literature, respectively.

Reference:

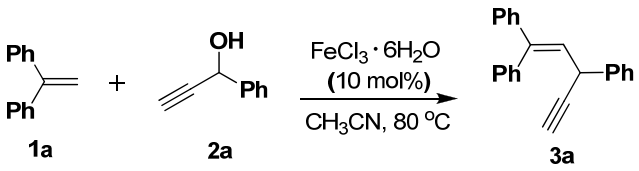
[1] Alberti, Mariza N.; Orfanopoulos, Michael. *Organic Letters*, **2008**, *10(12)*, 2465-2468.

[2] Casey, Charles P.; Dzwiniel, Trevor L.; Kraft, Stefan; Guzei, Ilia A. *Organometallics*, **2003**, *22(19)*, 3915-3920.

[3] Yan, Wuming; Wang, Qiaoyi; Chen, Yunfeng; Petersen, Jeffrey L.; Shi, Xiaodong. O*rganic*

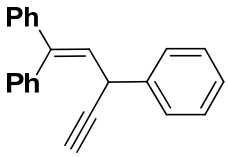
Letters, **2010**, *12(15)*, 3308-3311.

3. Representative Procedure for Iron-catalyzed Reaction

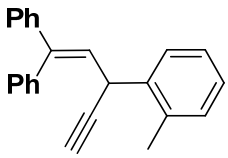


To a solution of **1a** (0.2 mmol) and **2a** (0.24 mmol) in 1 ml acetonitrile, Iron (III) chloride hexahydrate (0.02 mmol) was added. The reaction mixture was stirred at 80°C for 2h. The crude product was purified by column chromatography on silica gel, eluted by hexane to afford the desired product **3a** as oil liquid (77% yield).

4. Analytical Data of the Products

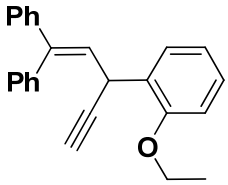


Pent-1-en-4-yne-1,1,3-triyltribenzene (3a): 77% yield; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.46–7.22 (m, 15H), 6.16 (d, *J* = 10.2 Hz, 1H), 4.52 (dd, *J* = 10.2, 2.5 Hz, 1H), 2.40 (d, *J* = 3.0 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 142.09, 141.57, 139.97, 139.04, 129.83, 128.61, 128.51, 128.14, 128.05, 127.60, 127.52, 127.28, 126.95, 84.35, 77.42, 77.00, 76.58, 71.76, 37.04; HRMS (EI) calcd for $C_{23}H_{18}$ $[M+H]^+$ 294.1409. found 294.1407.

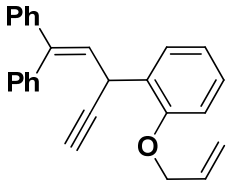


(3-*o*-Tolylpent-1-en-4-yne-1,1-diyl)dibenzene (3b): 72% yield; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.72

(d, *J* = 7.5 Hz, 1H), 7.51–7.12 (m, 14H), 6.14 (d, *J* = 9.9 Hz, 1H), 4.62 (dd, *J* = 9.9, 2.5 Hz, 1H), 2.44 (d, *J* = 2.5 Hz, 1H), 2.03 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 142.30, 141.80, 139.12, 138.61, 135.66, 130.49, 129.91, 128.31, 128.10, 127.67, 127.50, 127.46, 127.28, 127.01, 126.43, 85.11, 77.42, 77.00, 76.58, 71.28, 34.84, 19.05; HRMS (EI) calcd for $C_{24}H_{20}$ $[M+H]^+$ 308.1565, found 308.1578.

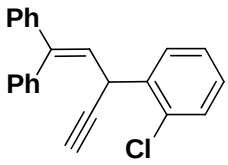


(3-(2-Ethoxyphenyl)pent-1-en-4-yne-1,1-diyl)dibenzene (3c): 74% yield; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.58 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.44–7.15 (m, 12H), 6.97 (td, *J* = 7.5, 0.9 Hz, 1H), 6.81 (d, *J* = 8.1 Hz, 1H), 6.12 (d, *J* = 9.8 Hz, 1H), 4.88 (dd, *J* = 9.8, 2.5 Hz, 1H), 3.92 (m, 3H), 2.31 (d, *J* = 2.6 Hz, 1H), 1.17 (t, *J* = 7.0 Hz, 2H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 155.75, 142.23, 141.84, 139.36, 130.03, 128.98, 128.46, 128.13, 128.07, 128.00, 127.66, 127.29, 127.24, 120.65, 111.70, 85.56, 77.42, 77.00, 76.58, 70.21, 63.66, 31.60, 14.69; HRMS (EI) calcd for $C_{25}H_{22}O$ $[M+H]^+$ 338.1671, found 338.1682.

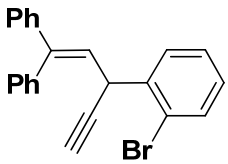


(3-(2-(Allyloxy)phenyl)pent-1-en-4-yne-1,1-diyl)dibenzene (3d): 84% yield; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.60 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.46–7.18 (m, 12H), 7.00 (td, *J* = 7.5, 1.0 Hz, 1H), 6.85–6.78 (m, 1H), 6.16 (d, *J* = 9.9 Hz, 1H), 5.84 (ddt, *J* = 17.3, 10.4, 5.1 Hz, 1H), 5.27–5.11 (m, 2H), 4.90 (dd, *J* = 9.9, 2.5 Hz, 1H), 4.52–4.34 (m, 2H), 2.32 (d, *J* = 2.6 Hz, 1H); ^{13}C NMR (75 MHz,

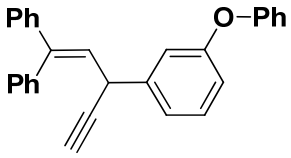
$CDCl_3$): δ = 155.37, 142.14, 141.96, 139.33, 133.27, 130.01, 129.06, 128.49, 128.10, 128.00, 127.84, 127.62, 127.30, 127.26, 120.97, 117.06, 112.10, 85.35, 77.42, 77.00, 76.58, 70.32, 68.89, 31.79; HRMS (EI) calcd for $C_{26}H_{22}O$ $[M+H]^+$ 350.1671, found 350.1683.



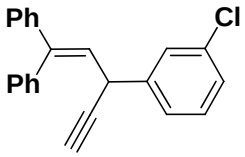
(3-(2-Chlorophenyl)pent-1-en-4-yne-1,1-diyl)dibenzene (3e): 52% yield; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.73 (dd, *J* = 8.1, 1.6 Hz, 1H), 7.46–7.16 (m, 14H), 6.01 (d, *J* = 9.7 Hz, 1H), 4.82 (dd, *J* = 9.7, 2.5 Hz, 1H), 2.41 (d, *J* = 2.6 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ = 143.40, 141.79, 139.06, 138.02, 133.27, 129.91, 129.71, 129.09, 128.34, 128.21, 128.08, 127.69, 127.61, 127.56, 127.18, 126.26, 84.21, 77.42, 77.00, 76.58, 71.65, 35.13; HRMS (EI) calcd for $C_{23}H_{17}Cl$ $[M+H]^+$ 328.1019, found 328.1018.



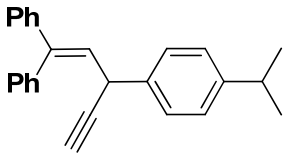
(3-(2-Bromophenyl)pent-1-en-4-yne-1,1-diyl)dibenzene (3f): 73% yield; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.63 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.38 (dd, *J* = 8.0, 1.1 Hz, 1H), 7.33–7.05 (m, 12H), 7.00 (td, *J* = 7.7, 1.6 Hz, 1H), 5.87 (d, *J* = 9.6 Hz, 1H), 4.70 (dd, *J* = 9.6, 2.5 Hz, 1H), 2.30 (d, *J* = 2.5 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 143.54, 141.90, 139.88, 139.10, 133.07, 130.03, 129.30, 128.60, 128.18, 128.08, 127.83, 127.77, 127.63, 127.57, 126.42, 123.50, 84.45, 77.42, 77.00, 76.58, 71.76, 37.54; HRMS (EI) calcd for $C_{23}H_{17}Br$ $[M+H]^+$ 372.0514, found 372.0522.



(3-(3-Phenoxyphenyl)pent-1-en-4-yne-1,1-diyl)dibenzene (3g): 73% yield; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.44–7.19 (m, 13H), 7.15–7.08 (m, 2H), 7.03 (ddd, *J* = 6.4, 3.1, 1.4 Hz, 3H), 6.87 (dd, *J* = 8.1, 1.8 Hz, 1H), 6.13 (d, *J* = 10.2 Hz, 1H), 4.48 (dd, *J* = 10.1, 2.4 Hz, 1H), 2.39 (d, *J* = 2.5 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 157.60, 156.98, 142.46, 141.98, 141.47, 138.93, 129.81, 129.76, 128.52, 128.15, 127.68, 127.61, 127.51, 123.34, 122.01, 119.03, 117.82, 117.10, 83.92, 77.42, 77.00, 76.58, 71.98, 36.89; HRMS (EI) calcd for $C_{29}H_{22}O$ $[M+H]^+$ 386.1671, found 386.1672.

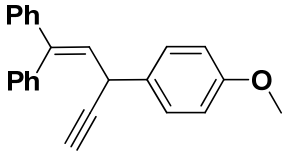


(3-(3-Chlorophenyl)pent-1-en-4-yne-1,1-diyl)dibenzene (3h): 50% yield; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.58–7.06 (m, 15H), 6.11 (d, *J* = 10.1 Hz, 1H), 4.49 (dd, *J* = 10.1, 2.4 Hz, 1H), 2.43 (d, *J* = 2.5 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 142.76, 142.03, 141.32, 138.83, 134.45, 129.81, 129.74, 128.60, 128.20, 127.75, 127.71, 127.52, 127.49, 127.21, 127.19, 125.55, 83.57, 77.42, 77.00, 76.58, 72.33, 36.79; HRMS (EI) calcd for $C_{23}H_{17}Cl$ $[M+H]^+$ 328.1019, found 328.1019.

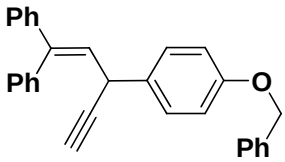


(3-(4-isopropylphenyl)pent-1-en-4-yne-1,1-diyl)dibenzene (3i): 85% yield; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.48–7.18 (m, 15H), 6.18 (d, *J* = 10.2 Hz, 1H), 4.51 (dd, *J* = 10.2, 2.4 Hz, 1H), 3.01–2.81 (m, 1H), 2.39 (d, *J* = 2.5 Hz, 1H), 1.26 (d, *J* = 6.9 Hz, 6H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 147.56,

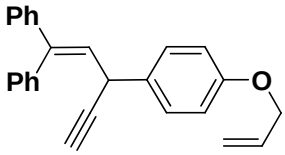
141.87, 141.64, 139.09, 137.26, 129.85, 128.47, 128.22, 128.11, 127.52, 127.46, 127.17, 126.67, 84.61, 77.42, 77.00, 76.58, 71.53, 36.65, 33.71, 23.98; HRMS (EI) calcd for $C_{26}H_{24}$ $[M+H]^+$ 336.1878, found 336.1887.



(3-(4-Methoxyphenyl)pent-1-en-4-yne-1,1-diyl)dibenzene (3j): 85% yield; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.44–7.21 (m, 12H), 6.90–6.83 (m, 2H), 6.13 (d, *J* = 10.2 Hz, 1H), 4.46 (dd, *J* = 10.2, 2.5 Hz, 1H), 3.80 (s, 3H), 2.39 (d, *J* = 2.5 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 158.57, 141.75, 141.64, 139.09, 132.11, 129.84, 128.48, 128.35, 128.28, 128.12, 127.56, 127.52, 114.00, 84.69, 77.42, 77.00, 76.58, 71.53, 55.29, 36.26; HRMS (EI) calcd for $C_{24}H_{20}O$ $[M+H]^+$ 324.1514, found 324.1517.



(3-(4-(Benzyloxy)phenyl)pent-1-en-4-yne-1,1-diyl)dibenzene (3k): 61% yield; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.48–7.23 (m, 18H), 7.00–6.90 (m, 2H), 6.15 (d, *J* = 10.2 Hz, 1H), 5.07 (s, 2H), 4.49 (dd, *J* = 10.1, 2.5 Hz, 1H), 2.40 (d, *J* = 2.5 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 157.79, 141.77, 141.61, 139.06, 137.00, 132.35, 129.83, 128.56, 128.48, 128.30, 128.12, 127.93, 127.56, 127.51, 127.48, 127.43, 114.95, 84.64, 77.42, 77.00, 76.58, 71.57, 70.05, 36.26; HRMS (EI) calcd for $C_{30}H_{24}O$ $[M+H]^+$ 400.1827, found 400.1822.



(3-(4-(Allyloxy)phenyl)pent-1-en-4-yne-1,1-diyl)dibenzene (3l): 76% yield; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.47–7.21 (m, 12H), 6.91–6.84 (m, 2H), 6.13 (d, *J* = 10.1 Hz, 1H), 6.10–5.98 (m, 1H), 5.41 (dd, *J* = 17.3, 1.6 Hz, 1H), 5.29 (dd, *J* = 10.5, 1.4 Hz, 1H), 4.53 (dt, *J* = 5.3, 1.5 Hz, 2H), 4.46 (dd, *J* = 10.2, 2.5 Hz, 1H), 2.39 (d, *J* = 2.5 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 157.60, 141.77, 141.64, 139.08, 133.31, 132.27, 129.84, 128.48, 128.33, 128.26, 128.12, 127.56, 127.52, 127.47, 117.63, 114.85, 84.66, 77.42, 77.00, 76.58, 71.55, 68.87, 36.26; HRMS (EI) calcd for $C_{26}H_{22}O$ $[M+H]^+$ 350.1671, found 350.1681

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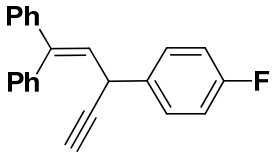
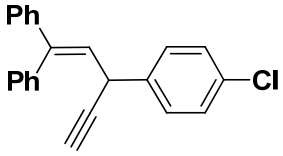
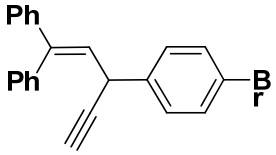


(3-(4-Fluorophenyl)pent-1-en-4-yne-1,1-diyl)dibenzene (3m): 75% yield; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.48–7.20 (m, 12H), 7.05–6.96 (m, 2H), 6.11 (d, *J* = 10.1 Hz, 1H), 4.49 (dd, *J* = 10.1, 2.2 Hz, 1H), 2.41 (d, *J* = 2.5 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 142.26, 141.43, 138.92, 129.77, 128.87, 128.76, 128.56, 128.18, 127.81, 127.69, 127.63, 127.51, 115.52, 115.24, 84.16, 77.42, 77.00, 76.58, 71.98, 36.36; HRMS (EI) calcd for $C_{23}H_{17}F$ $[M+H]^+$ 312.1314, found 312.1329

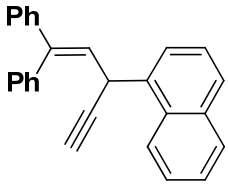


(3-(4-Chlorophenyl)pent-1-en-4-yne-1,1-diyl)dibenzene (3n): 44% yield; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.44–7.16 (m, 14H), 6.07 (d, *J* = 10.1 Hz, 1H), 4.46 (dd, *J* = 10.1, 2.5 Hz, 1H), 2.38 (d, *J* =

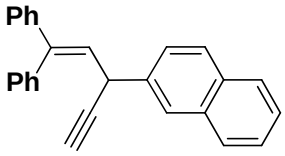
2.5 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 142.53, 141.36, 138.87, 138.53, 132.78, 129.74, 128.70, 128.66, 128.57, 128.18, 127.72, 127.67, 127.51, 127.45, 83.84, 77.42, 77.00, 76.58, 72.15, 36.52; HRMS (EI) calcd for $C_{23}H_{17}Cl$ $[M+H]^+$ 328.1019, found 328.1033.



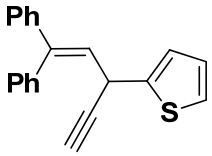
(3-(4-Bromophenyl)pent-1-en-4-yne-1,1-diyl)dibenzene (3o): 78% yield; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.49–7.16 (m, 14H), 6.09 (d, *J* = 10.1 Hz, 1H), 4.47 (dd, *J* = 10.1, 2.4 Hz, 1H), 2.41 (d, *J* = 2.5 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 142.59, 141.36, 139.10, 138.87, 131.67, 129.74, 129.05, 128.58, 128.19, 127.73, 127.68, 127.52, 127.37, 120.89, 83.77, 77.42, 77.00, 76.58, 72.16, 36.60; HRMS (EI) calcd for $C_{23}H_{17}Br$ $[M+H]^+$ 372.0514, found 372.0517.



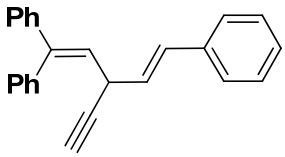
1-(1,1-Diphenylpent-1-en-4-yn-3-yl)naphthalene (3p): 90% yield; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.92–7.84 (m, 2H), 7.81 (d, *J* = 8.2 Hz, 1H), 7.62 (d, *J* = 8.4 Hz, 1H), 7.56–7.42 (m, 7H), 7.37 (ddd, *J* = 8.3, 6.9, 1.3 Hz, 1H), 7.27–7.13 (m, 5H), 6.24 (d, *J* = 9.9 Hz, 1H), 5.18 (dd, *J* = 9.9, 2.4 Hz, 1H), 2.53 (d, *J* = 2.5 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 142.27, 141.79, 139.10, 136.13, 133.93, 130.73, 130.02, 128.71, 128.50, 128.16, 128.05, 127.93, 127.88, 127.73, 127.50, 125.85, 125.60, 125.57, 124.97, 123.61, 84.93, 77.42, 77.00, 76.58, 72.26, 34.84; HRMS (EI) calcd for $C_{27}H_{20}$ $[M+H]^+$ 344.1565, found 344.1565.



2-(1,1-Diphenylpent-1-en-4-yn-3-yl)naphthalene (3q): 79% yield; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.87 (dd, *J* = 7.3, 4.0 Hz, 2H), 7.81 (d, *J* = 8.2 Hz, 1H), 7.61 (d, *J* = 8.5 Hz, 1H), 7.55–7.41 (m, 7H), 7.36 (ddd, *J* = 8.3, 6.9, 1.3 Hz, 1H), 7.27–7.14 (m, 5H), 6.23 (d, *J* = 9.9 Hz, 1H), 5.16 (dd, *J* = 9.9, 2.5 Hz, 1H), 2.52 (d, *J* = 2.5 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 142.28, 141.80, 139.11, 136.14, 133.95, 130.74, 130.03, 128.72, 128.50, 128.17, 128.06, 127.94, 127.88, 127.74, 127.50, 125.85, 125.60, 125.58, 124.97, 123.62, 84.94, 77.42, 77.00, 76.58, 72.25, 34.84; HRMS (EI) calcd for $C_{27}H_{20}$ $[M+H]^+$ 344.1565, found 344.1568.

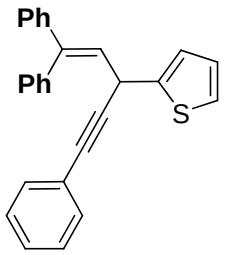


2-(1,1-Diphenylpent-1-en-4-yn-3-yl)thiophene (3r): 73% yield; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.44–7.23 (m, 10H), 7.19 (dd, *J* = 5.1, 1.1 Hz, 1H), 7.01–6.98 (m, 1H), 6.94 (dd, *J* = 5.1, 3.5 Hz, 1H), 6.20 (d, *J* = 10.0 Hz, 1H), 4.71–4.64 (m, 1H), 2.40 (d, *J* = 2.5 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 143.83, 142.62, 141.36, 138.66, 129.73, 128.52, 128.19, 127.73, 127.70, 127.62, 127.08, 126.87, 124.63, 124.57, 83.62, 77.42, 77.00, 76.58, 71.33, 32.79; HRMS (EI): calculated for $C_{21}H_{16}S$ $[M+H]^+$ 300.0973, found 300.0974.

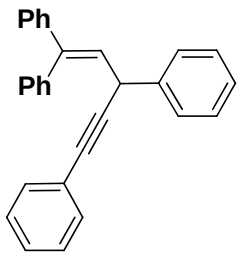


(3-Ethynylpenta-1,4-diene-1,1,5-triyl)tribenzene (3s): 76% yield; ^{1}H NMR (300 MHz, $CDCl_3$): δ =

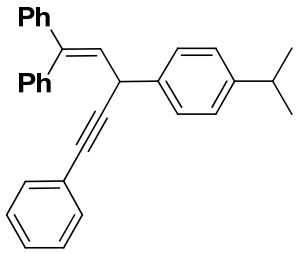
7.53–7.21 (m, 30H), 6.73 (dd, *J* = 15.8, 1.4 Hz, 1H), 6.53 (dd, *J* = 16.0, 6.3 Hz, 1H), 6.26 (dd, *J* = 8.9, 3.8 Hz, 2H), 6.12 (d, *J* = 10.0 Hz, 1H), 5.62 (ddd, *J* = 14.1, 3.8, 2.0 Hz, 1H), 4.33 (dd, *J* = 9.5, 7.0 Hz, 1H), 4.20–4.07 (m, 1H), 2.94 (d, *J* = 2.2 Hz, 1H), 2.45 (d, *J* = 2.4 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 147.60, 145.70, 142.85, 142.75, 142.19, 141.84, 141.58, 139.42, 138.99, 136.86, 130.63, 130.16, 129.67, 129.55, 128.72, 128.51, 128.46, 128.38, 128.16, 128.14, 127.59, 127.56, 127.52, 127.49, 127.42, 127.41, 127.35, 126.71, 126.42, 109.32, 108.07, 83.63, 82.19, 81.76, 77.42, 77.00, 76.58, 71.89, 48.32, 45.81, 34.56; HRMS (EI) calcd for $C_{25}H_{20}$ $[M+H]^+$ 320.1565, found 320.1558.



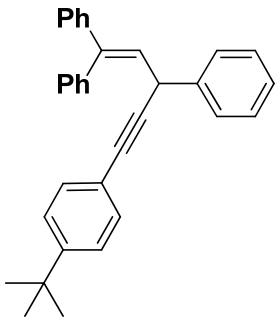
2-(1,1,5-Triphenylpent-1-en-4-yn-3-yl)thiophene (3t): 41% yield; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.39–7.12 (m, 15H), 7.10 (dd, *J* = 5.1, 1.1 Hz, 1H), 6.96–6.92 (m, 1H), 6.85 (dd, *J* = 5.1, 3.5 Hz, 1H), 6.17 (d, *J* = 10.0 Hz, 1H), 4.79 (d, *J* = 9.9 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 144.74, 142.26, 141.53, 138.79, 131.73, 129.84, 128.51, 128.22, 128.19, 128.07, 127.68, 127.64, 127.49, 126.88, 124.52, 124.47, 123.27, 89.08, 83.36, 77.42, 77.00, 76.58, 33.60; HRMS (EI) calcd for $C_{27}H_{20}S$ $[M+H]^+$ 376.1286, found 376.1290.



Pent-1-en-4-yne-1,1,3,5-tetrayltetrabenzene (3u): 81% yield; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.38–7.07 (m, 20H), 6.11 (d, *J* = 10.1 Hz, 1H), 4.61 (d, *J* = 10.1 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 141.72, 140.64, 139.16, 131.70, 129.93, 128.59, 128.50, 128.46, 128.20, 128.14, 127.90, 127.54, 127.46, 127.40, 126.86, 123.58, 89.75, 83.95, 77.42, 77.00, 76.58, 37.85. HRMS (EI) calcd for $C_{29}H_{22}$ $[M+H]^+$ 370.1722, found 370.1729.

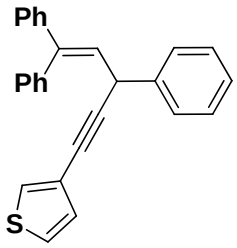


(3-(4-isopropylphenyl)pent-1-en-4-yne-1,1,5-triyl)tribenzene (3v): 60% yield; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.51–7.42 (m, 4H), 7.41–7.36 (m, 5H), 7.34–7.19 (m, 10H), 6.25 (d, *J* = 10.1 Hz, 1H), 4.72 (d, *J* = 10.1 Hz, 1H), 2.92 (hept, *J* = 6.9 Hz, 1H), 1.27 (d, *J* = 6.9 Hz, 6H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 147.47, 141.83, 141.54, 139.25, 137.96, 131.72, 129.97, 128.69, 128.48, 128.19, 128.13, 127.83, 127.55, 127.50, 127.41, 127.32, 126.65, 123.73, 90.06, 83.76, 77.25, 77.00, 76.75, 37.48, 33.74, 24.00; HRMS (EI) calcd for $C_{32}H_{28}$ $[M+H]^+$ 412.2191, found 412.2196.

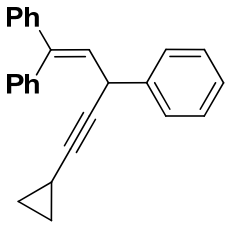


(5-(4-tert-Butylphenyl)pent-1-en-4-yne-1,1,3-triyl)tribenzene (3w): 60% yield; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.45 (dd, *J* = 7.7, 4.5 Hz, 6H), 7.41–7.33 (m, 7H), 7.29–7.23 (m, 6H), 6.25 (d, *J* = 10.1 Hz,

1H), 4.75 (d, *J* = 10.1 Hz, 1H), 1.33 (s, 9H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 151.13, 141.81, 141.60, 140.81, 139.24, 131.43, 129.97, 128.70, 128.56, 128.49, 128.14, 127.56, 127.53, 127.43, 126.81, 125.20, 120.61, 89.02, 84.04, 77.25, 77.00, 76.75, 37.90, 34.70, 31.18. HRMS (EI) calcd for $C_{33}H_{30}$ $[M+H]^+$ 426.2348, found 426.2346.

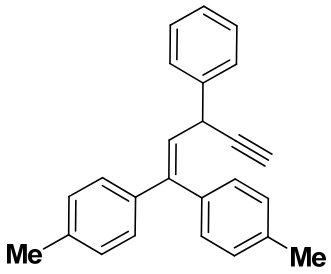


3-(3,5,5-Triphenylpent-4-en-1-ynyl)thiophene (3x): 43% yield; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.49–7.30 (m, 10H), 7.29–7.21 (m, 7H), 7.15 (dd, *J* = 5.0, 1.1 Hz, 1H), 6.22 (d, *J* = 10.1 Hz, 1H), 4.71 (d, *J* = 10.1 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 141.73, 140.61, 139.15, 130.08, 129.93, 128.60, 128.50, 128.39, 128.22, 128.14, 127.54, 127.48, 127.40, 126.87, 125.07, 122.56, 89.26, 78.96, 77.42, 77.00, 76.58, 37.86; HRMS (EI) calcd for $C_{27}H_{20}S$ $[M+H]^+$ 376.1289, found 376.1289.

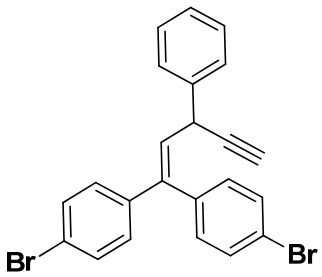


(5-Cyclopropylpent-1-en-4-yne-1,1,3-triyl)tribenzene (3y): 53% yield ; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.41 (t, *J* = 7.4 Hz, 2H), 7.38–7.27 (m, 7H), 7.25–7.20 (m, 6H), 6.10 (d, *J* = 10.2 Hz, 1H), 4.44 (dd, *J* = 10.1, 0.8 Hz, 1H), 1.32 (dddd, *J* = 8.0, 7.0, 5.0, 1.7 Hz, 1H), 0.79–0.74 (m, 2H), 0.72–0.67 (m, 2H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 141.88, 141.23, 140.99, 139.25, 129.93, 129.31, 128.44, 128.40, 128.08, 127.51, 127.41, 127.31, 126.63, 87.10, 77.42, 77.00, 76.58, 75.33, 37.21, 8.26, 0.20; HRMS

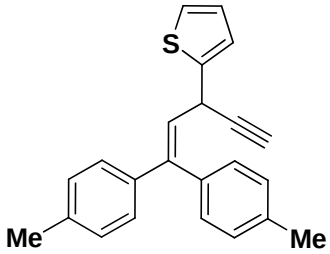
(EI) calcd for $C_{26}H_{22}$ $[M+H]^+$ 334.1727, found 334.1727.



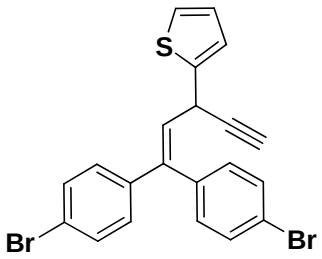
4,4'-(3-Phenylpent-1-en-4-yne-1,1-diyl)bis(methylbenzene) (3z): 98% yield; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.32–7.20 (m, 4H), 7.19–7.09 (m, 5H), 7.08–7.02 (m, 2H), 6.98 (d, *J* = 8.1 Hz, 2H), 6.01 (d, *J* = 10.1 Hz,1H), 4.45 (dd, *J* = 10.1, 2.5 Hz, 1H), 2.32 (s, 3H), 2.31 (d, *J* = 2.5 Hz, 1H), 2.24 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 141.94, 140.21, 139.01, 137.27, 137.19, 136.23, 129.72, 129.14, 128.80, 128.55, 127.45, 127.29, 127.02, 126.85, 84.60, 77.42, 77.00, 76.58, 71.58, 37.02, 21.25, 21.06; HRMS (EI) calcd for $C_{25}H_{22}$ $[M+H]^+$ 322.1722, found 322.1727.



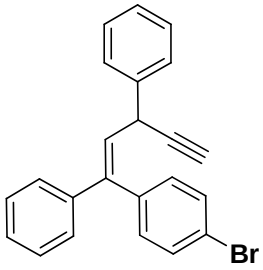
4,4'-(3-Phenylpent-1-en-4-yne-1,1-diyl)bis(bromobenzene) (3a'): 85% yield; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.50–7.43 (m, 2H), 7.31–7.13 (m, 8H), 7.10–7.04 (m, 2H), 6.98–6.91 (m, 2H), 6.03 (d, *J* = 10.2 Hz, 1H), 4.34 (dd, *J* = 10.2, 2.5 Hz, 1H), 2.30 (d, *J* = 2.5 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 140.03, 139.96, 139.43, 137.38, 131.91, 131.47, 131.38, 129.09, 128.76, 127.20, 122.11, 121.91, 83.76, 77.42, 77.00, 76.58, 72.19, 37.13; HRMS (EI) calcd for $C_{23}H_{16}Br_2$ $[M+H]^+$ 451.9619, found 451.9636.



2-(1,1-Dip-tolylpent-1-en-4-yn-3-yl)thiophene (3b'): 73% yield; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.28–7.11 (m, 9H), 7.06 (dd, *J* = 2.9, 1.7 Hz, 1H), 7.00 (dd, *J* = 5.0, 3.5 Hz, 1H), 6.20 (d, *J* = 10.0 Hz, 1H), 4.76 (dd, *J* = 10.0, 1.4 Hz, 1H), 2.45 (d, *J* = 1.7 Hz, 4H), 2.38 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 144.14, 142.49, 138.78, 137.47, 137.34, 135.84, 129.61, 129.15, 128.85, 127.54, 126.82, 126.06, 124.53, 124.48, 83.86, 77.42, 77.00, 76.58, 71.15, 32.78, 21.24, 21.08; HRMS (EI) calcd for $C_{23}H_{20}S$ $[M+H]^+$ 328.1286, found 328.1281.



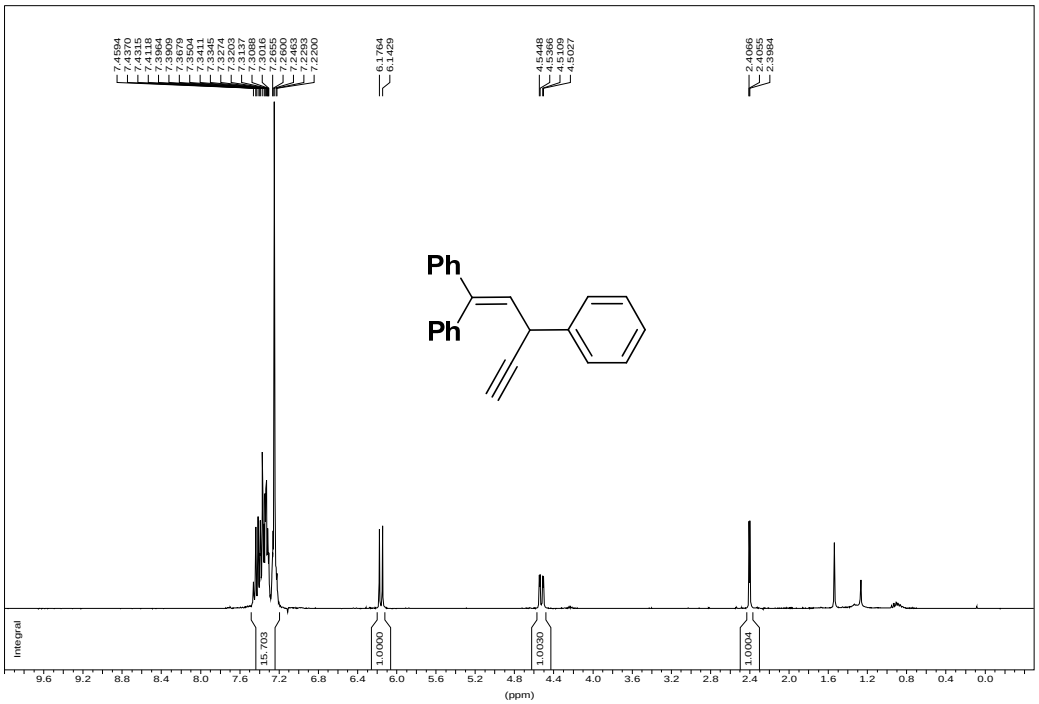
2-(1,1-Bis(4-bromophenyl)pent-1-en-4-yn-3-yl)thiophene (3c'): 57% yield; ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.63–7.57 (m, 2H), 7.48–7.42 (m, 2H), 7.26 (dd, *J* = 5.0, 1.3 Hz, 1H), 7.24–7.19 (m, 2H), 7.17–7.11 (m, 2H), 7.05–6.97 (m, 2H), 6.23 (d, *J* = 10.1 Hz, 1H), 4.66 (ddd, *J* = 10.1, 2.4, 1.0 Hz, 1H), 2.46 (d, *J* = 2.5 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 143.08, 140.48, 139.80, 136.98, 131.93, 131.45, 131.36, 129.18, 128.09, 126.99, 124.85, 124.72, 122.27, 122.13, 83.00, 77.42, 77.00, 76.58, 71.78, 32.79. HRMS (EI) calcd for $C_{21}H_{14}Br_2S$ $[M+H]^+$ 455.9183, found 457.9165.

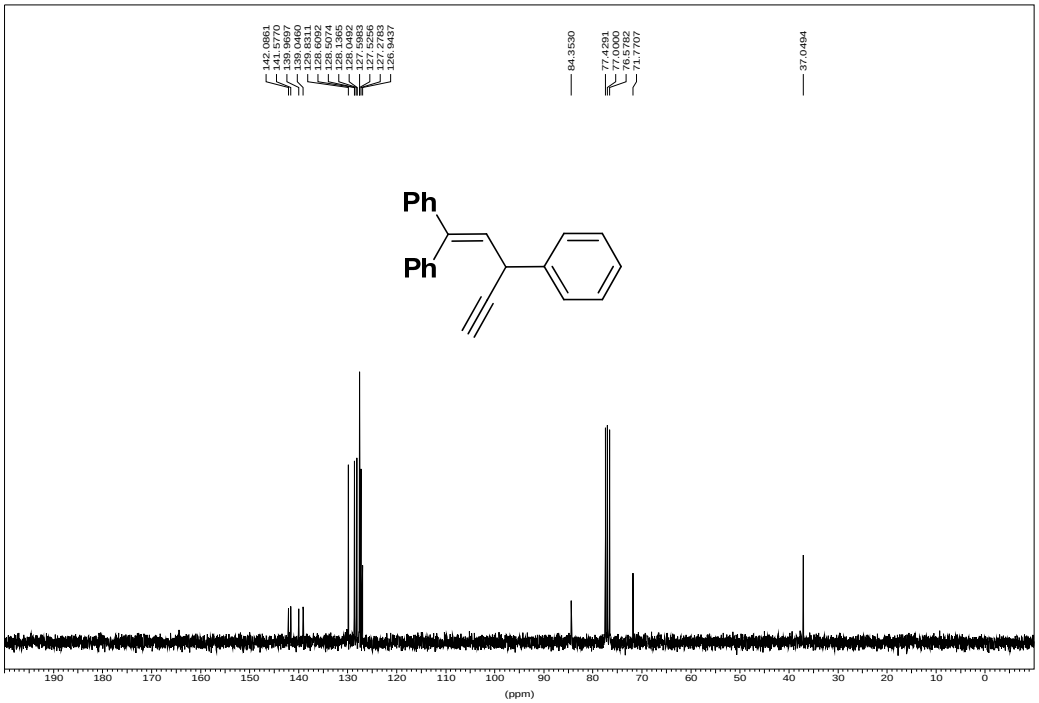


(1-(4-bromophenyl)pent-1-en-4-yne-1,3-diyl)dibenzene (3d'): 75% yield (Z/E~1:1); ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.61–7.55 (m, 1H), 7.49–7.18 (m, 12H), 7.14–7.04 (m, 1H), 6.16 (dd, *J* = 10.1, 9.2 Hz, 1H), 4.58–4.38 (m, 1H), 2.42 (dd, *J* = 2.5, 0.8 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 141.07, 140.99, 140.55, 139.71, 138.48, 137.96, 131.75, 131.56, 131.25, 129.76, 129.14, 128.70, 128.67, 128.66, 128.57, 128.25, 127.85, 127.77, 127.50, 127.25, 127.23, 127.08, 127.05, 121.83, 121.63, 84.07, 84.04, 77.42, 77.00, 76.58, 72.00, 71.94, 37.09. HRMS (EI) calcd for $C_{23}H_{17}Br$ $[M+H]^+$ 372.0514, found 372.0522.

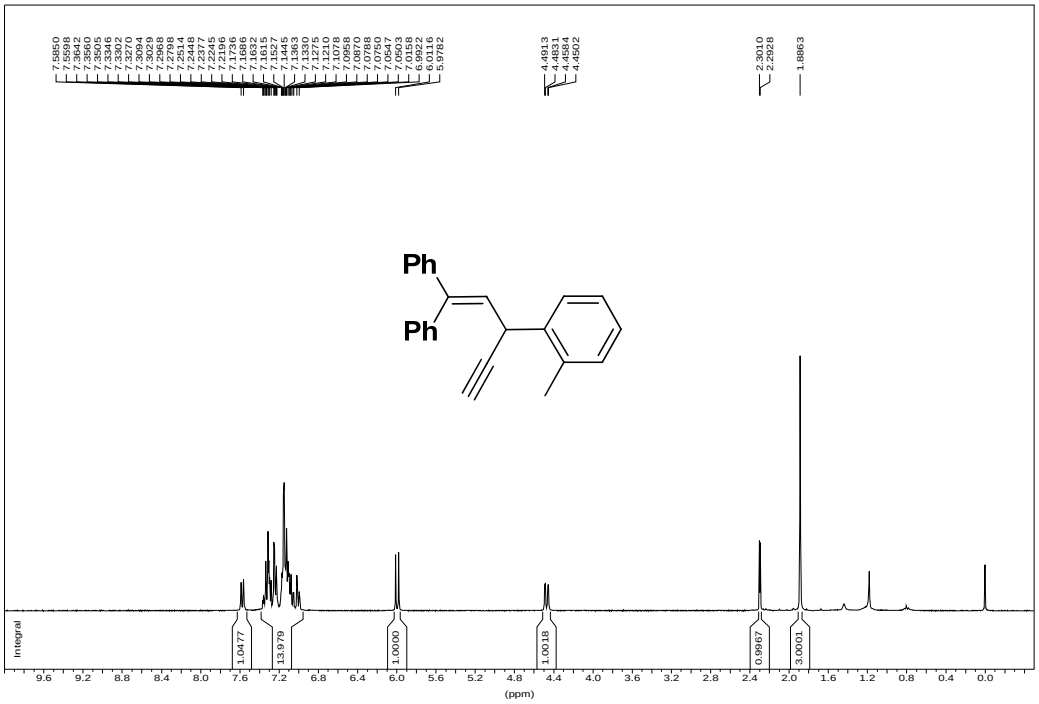
5. NMR Spectra of the Products

Compound **3a**





Compound **3b**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1.0000
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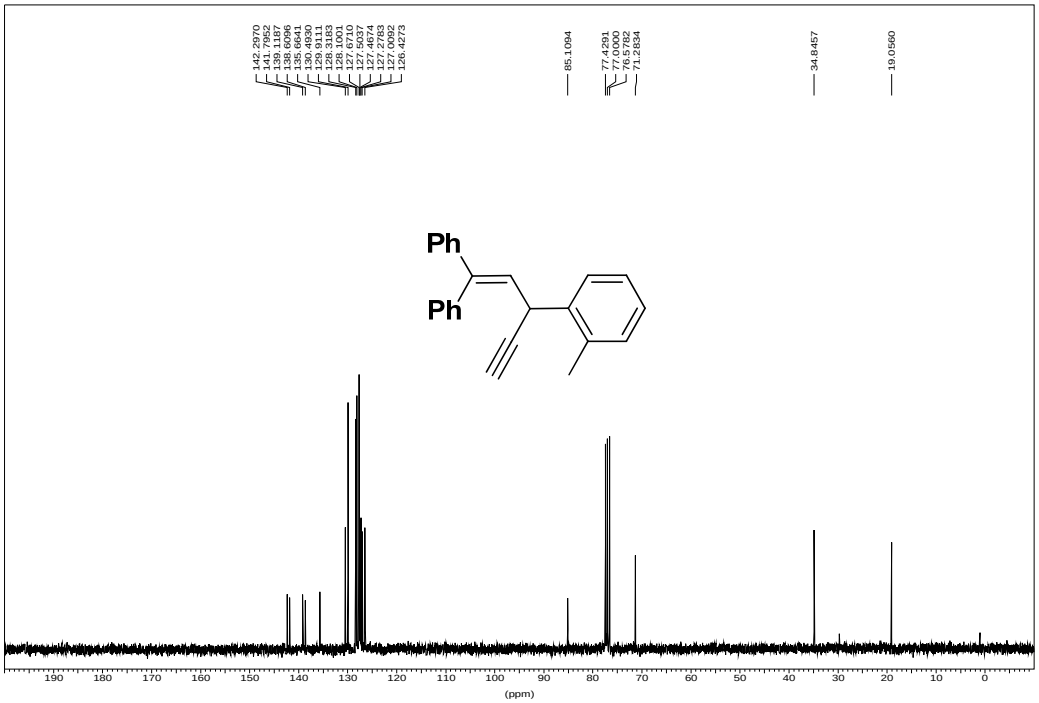
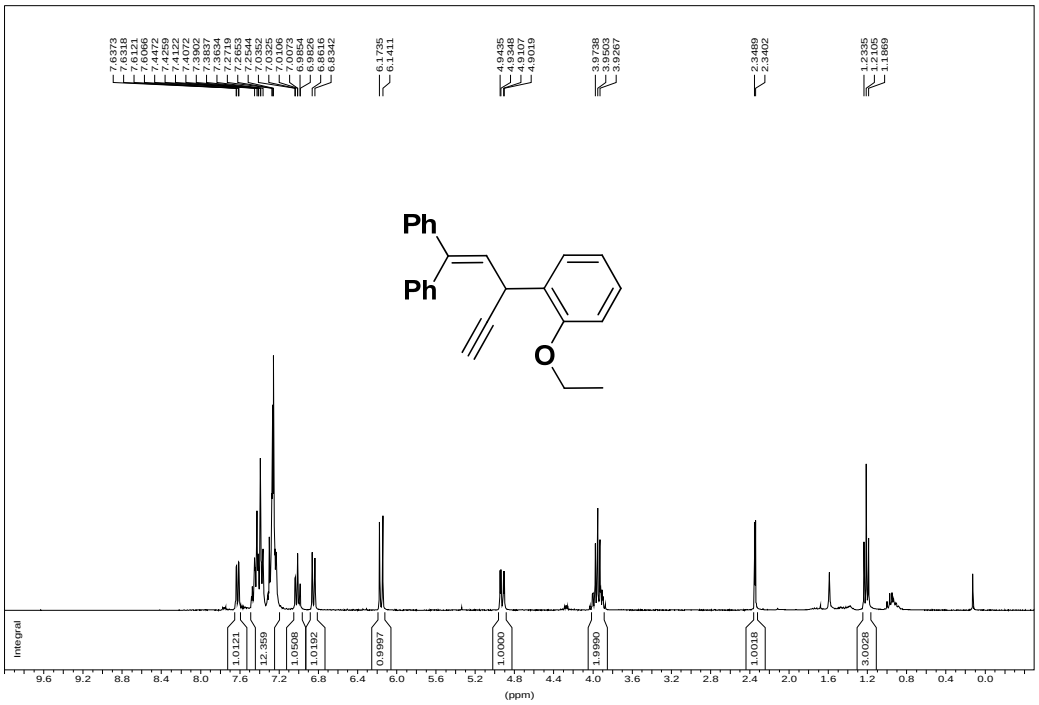
3.0001
(ppm)


Ph
Ph
(ppm)

Compound **3c**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7.4072
7.3902
7.3837
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7.2653
7.2544
7.2352
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7.0106
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6.9954
6.9826
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6.8342
6.1735
6.1411
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4.9019
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2.3402
1.2335
1.2195
1.1869
Ph
Ph
O
Integral
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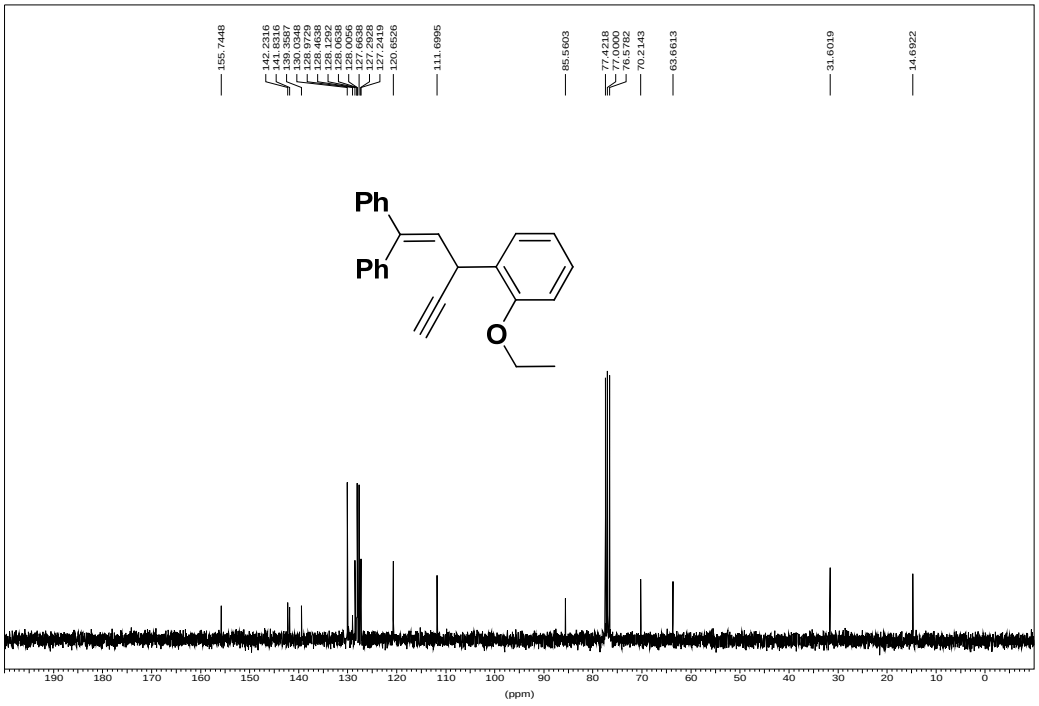
1.0508
1.0192
0.9997
1.0000
1.9990
1.0018
3.0028
(ppm)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127.2419
120.6526
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77.0000
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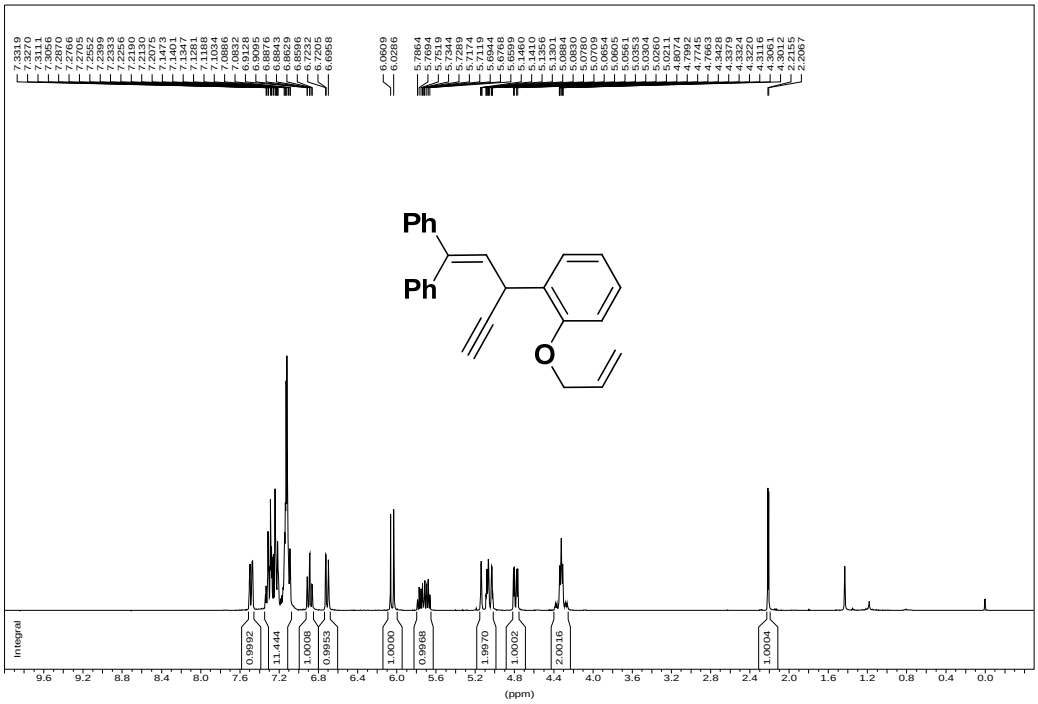
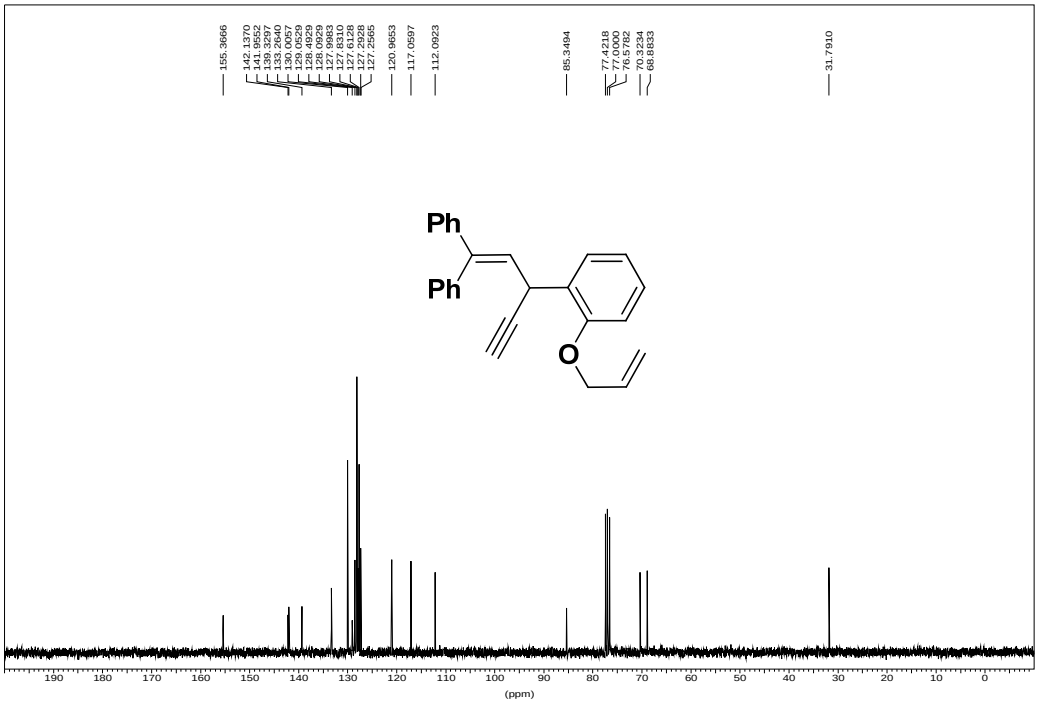
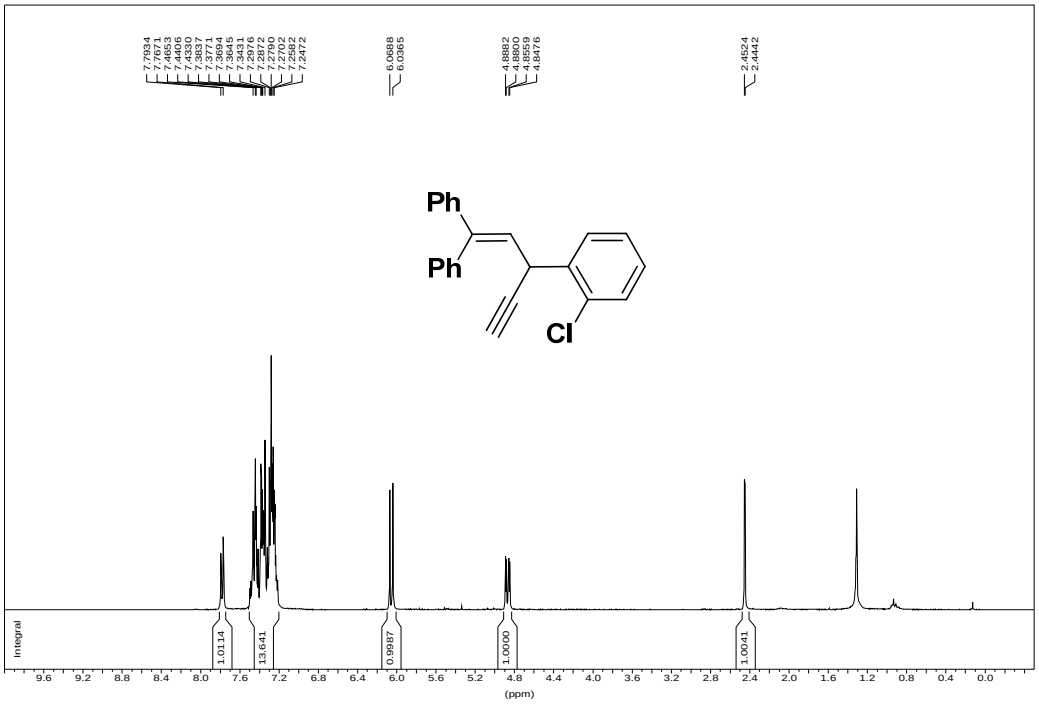
70.2143
63.6613
31.6019
14.6922
Ph
Ph
O
(ppm)

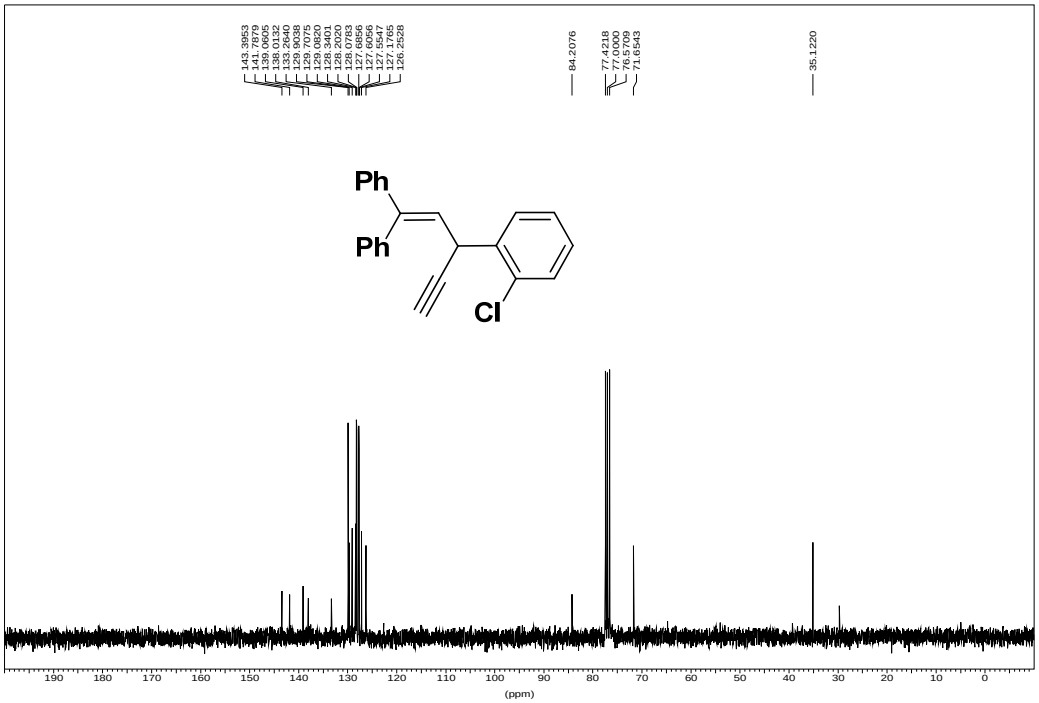
Compound **3d**


Ph
Ph
O
Integral
0.9992
11.444
1.0008
0.9953
1.0000
0.9968
1.9970
1.0002
2.0016
1.0004
(ppm)

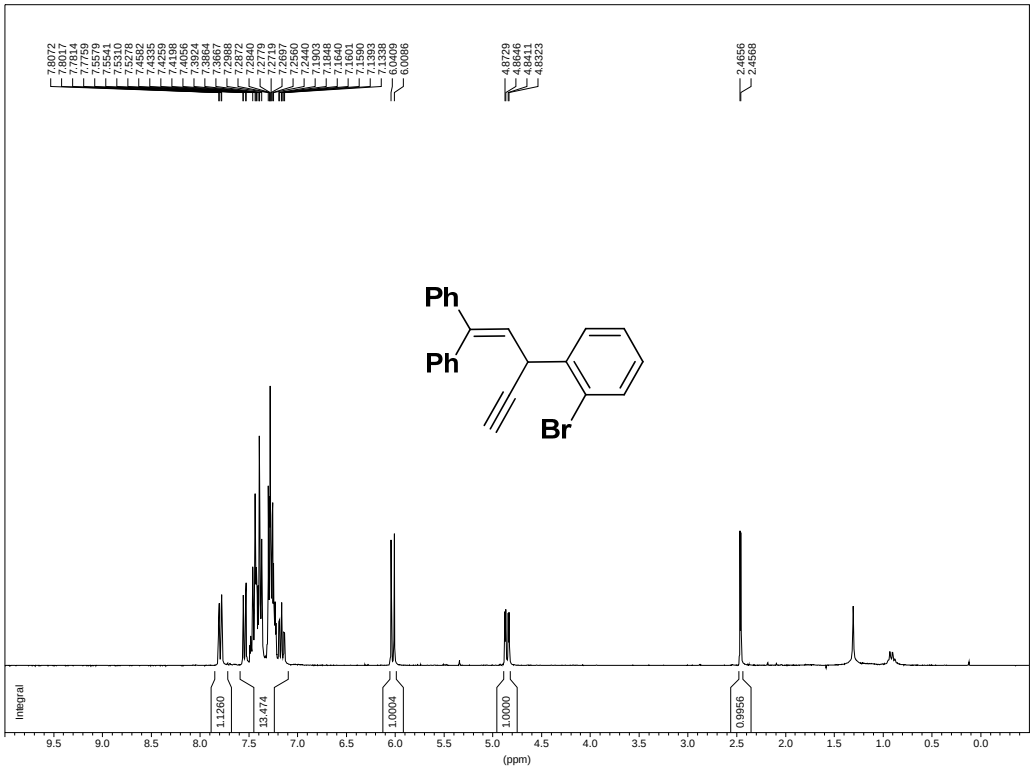

Ph
Ph
O
155.3666
142.1370
141.9552
139.3297
133.2640
130.0057
129.0598
128.4929
128.0929
127.8983
127.4110
127.6128
127.2928
127.2565
120.9653
117.0597
112.0923
85.3494
77.4218
77.0000
76.5782
70.3234
68.8833
31.7910
(ppm)

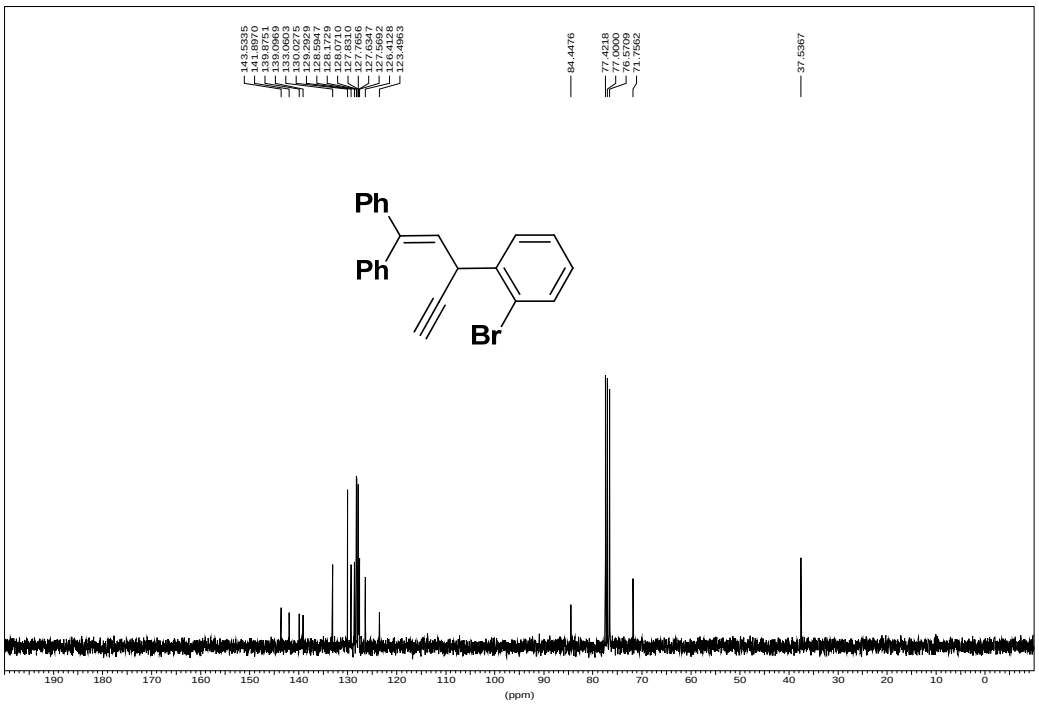
Compound **3e**


7.7934
7.7671
7.4653
7.4406
7.4239
7.3837
7.3771
7.3694
7.3645
7.3431
7.2976
7.2872
7.2760
7.2702
7.2582
7.2472
6.0688
6.0365
4.8882
4.8800
4.8559
4.8476
2.4524
2.4442
Ph
Ph
Cl
Integral
1.0114
13.641
0.9987
1.0000
1.0041
(ppm)

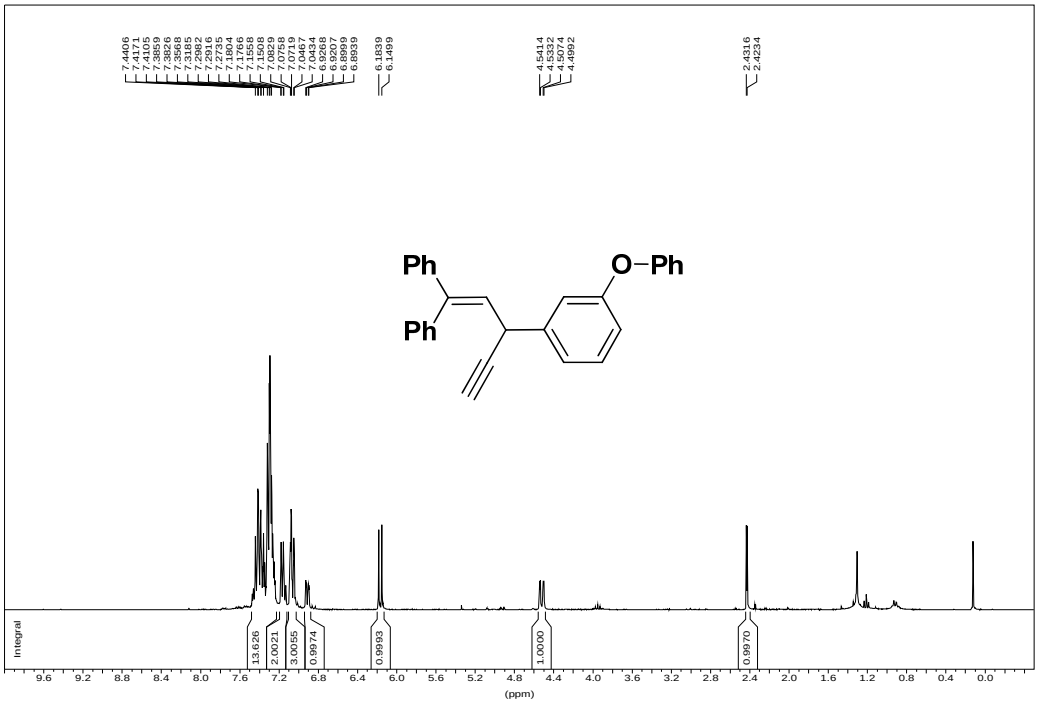

143.3953
141.7879
139.0605
138.0132
133.2644
129.9038
129.7075
129.0820
128.3401
128.2020
128.0783
127.6856
127.6585
127.5547
127.1765
126.2528
84.2076
77.4218
77.0000
76.5709
71.6543
35.1220
Ph
Ph
Cl
(ppm)

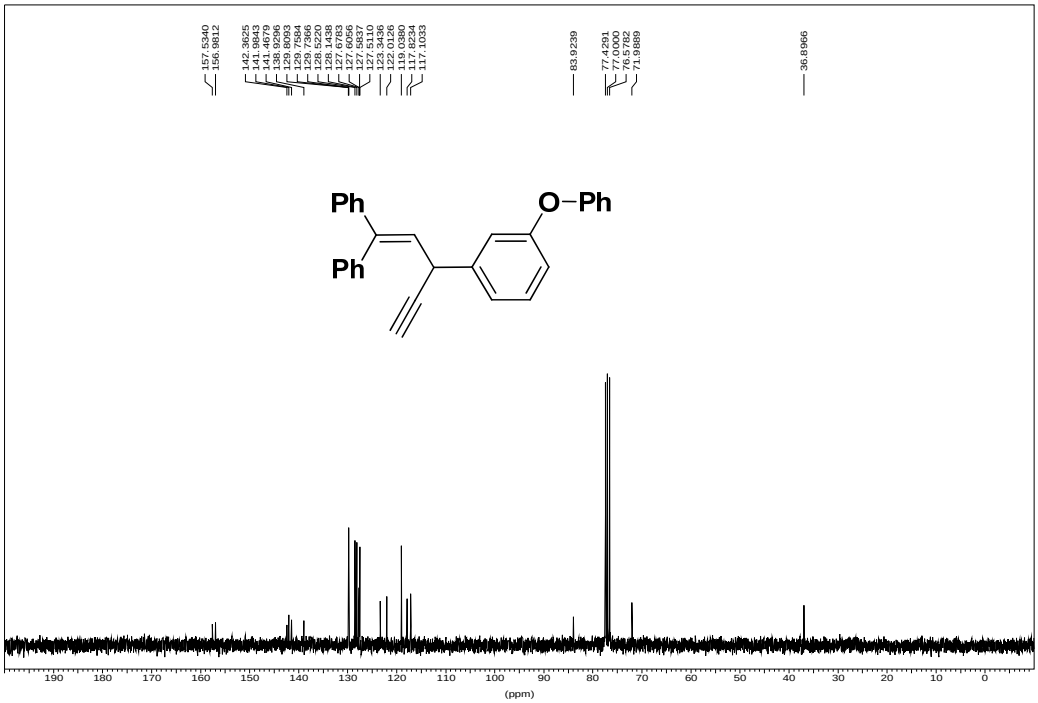
Compound **3f**


7.8072
7.8017
7.7814
7.7759
7.5579
7.5541
7.5310
7.5278
7.4582
7.4335
7.4259
7.4198
7.4056
7.3924
7.3864
7.3667
7.3098
7.2872
7.2840
7.2779
7.2719
7.2697
7.2560
7.2440
7.1903
7.1846
7.1640
7.1601
7.1590
7.1393
7.1338
6.0409
6.0086
4.8729
4.8646
4.8411
4.8323
2.4656
2.4568
Ph
Ph
Br
Integral
1.1260
13.474
1.0004
1.0000
0.9956
(ppm)

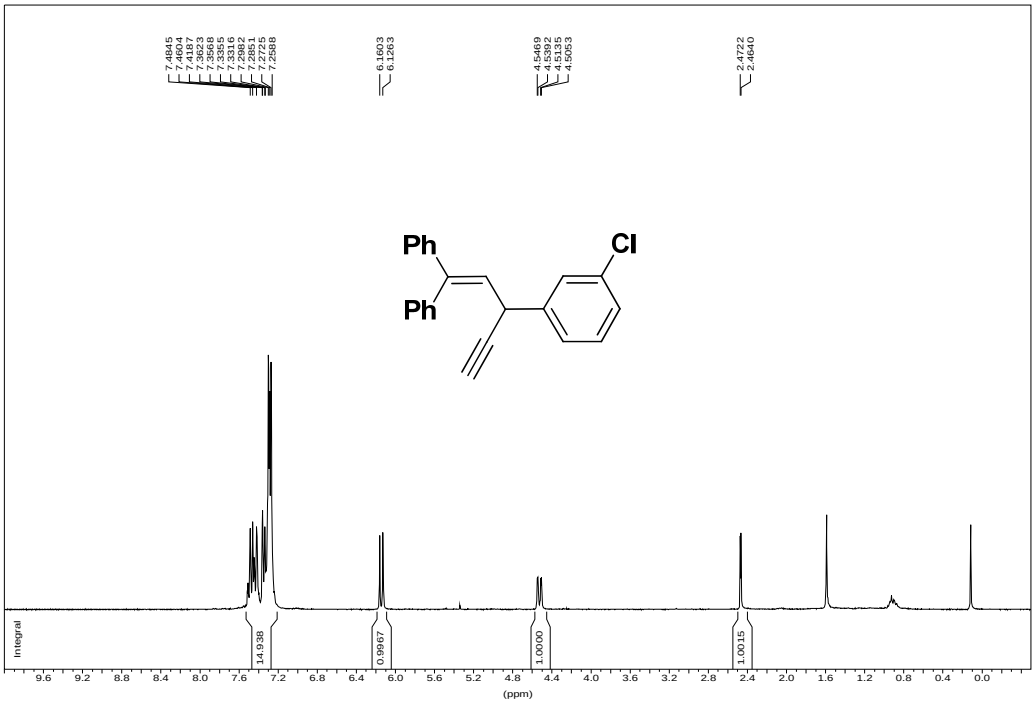

143.5335
141.8970
139.8751
139.0969
138.6662
130.0275
129.2929
128.5947
128.1729
128.0710
127.8310
127.7656
127.6547
127.5692
126.4128
123.4963
84.4476
77.4218
77.0000
76.5709
71.7562
37.5367
Ph
Ph
Br
(ppm)

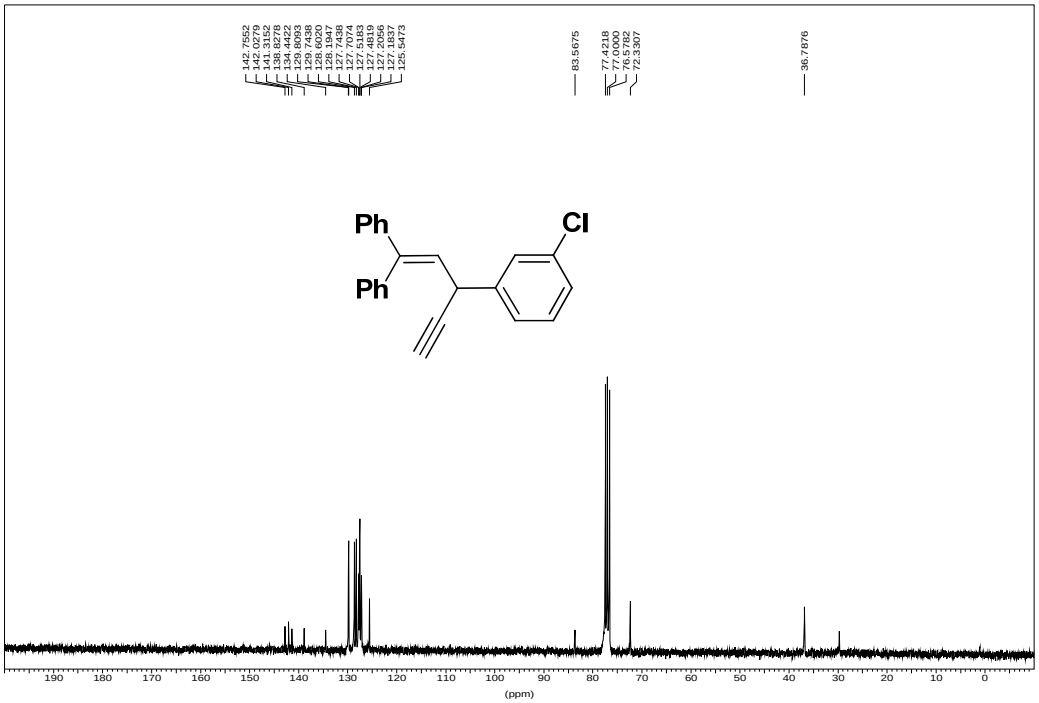
Compound **3g**


7.4406
7.4171
7.4125
7.3859
7.3826
7.3568
7.3185
7.2982
7.2916
7.2735
7.1984
7.1766
7.1558
7.1508
7.1269
7.0758
7.0719
7.0487
7.0464
6.9288
6.9207
6.8999
6.8959
6.1839
6.1499
4.5414
4.5322
4.5074
4.4992
2.4316
2.4234
Ph
Ph
O−Ph
Integral
13.626
2.0021
3.0055
0.9974
0.9993
1.0000
0.9970
(ppm)

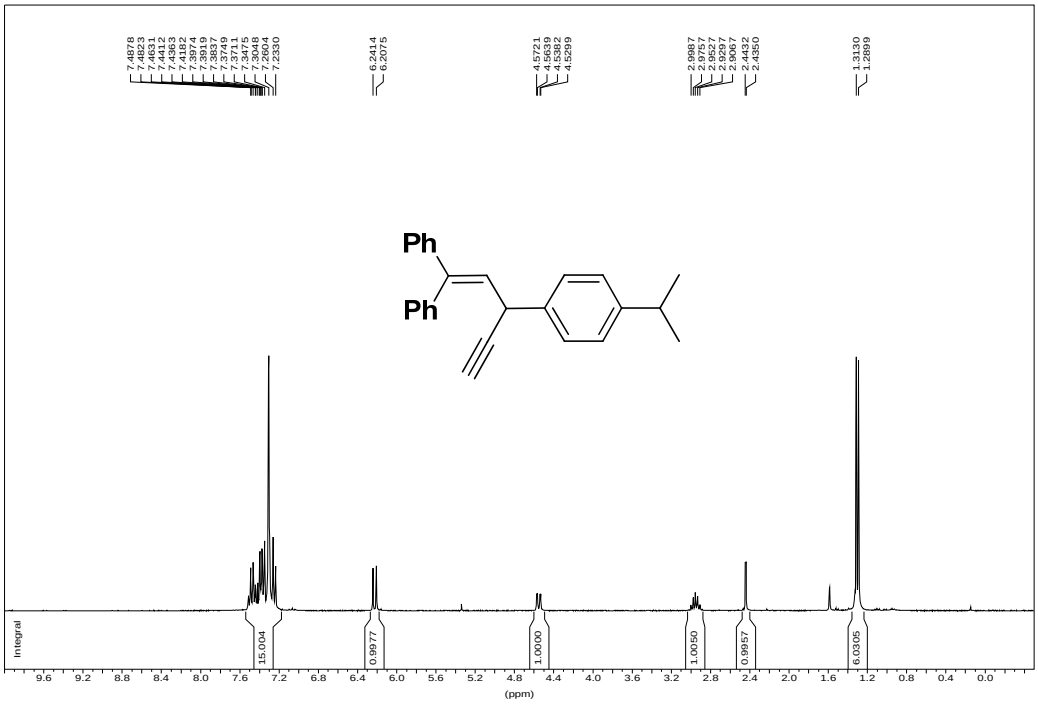

157.5340
156.9612
142.3625
141.9843
141.4679
138.9296
129.9693
129.7584
128.7366
128.5220
128.1498
127.6783
127.6056
127.5837
127.5117
123.3436
122.0126
119.0380
117.8234
117.1033
83.9239
77.4291
77.0000
76.5782
71.9889
36.8966
Ph
Ph
O−Ph
(ppm)

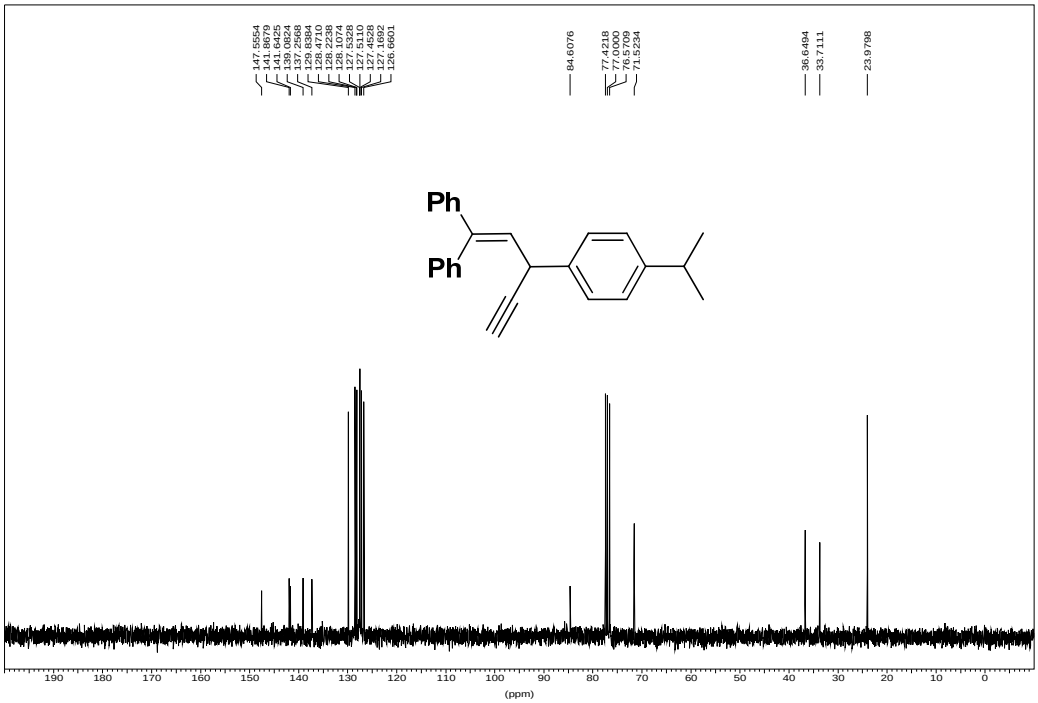
Compound **3h**


7.4845
7.4604
7.4137
7.3963
7.3568
7.3355
7.3316
7.2882
7.2851
7.2725
7.2588
6.1603
6.1263
4.5469
4.5392
4.5135
4.5053
2.4722
2.4640
Ph
Ph
Cl
Integral
14.938
0.9967
1.0000
1.0015
(ppm)

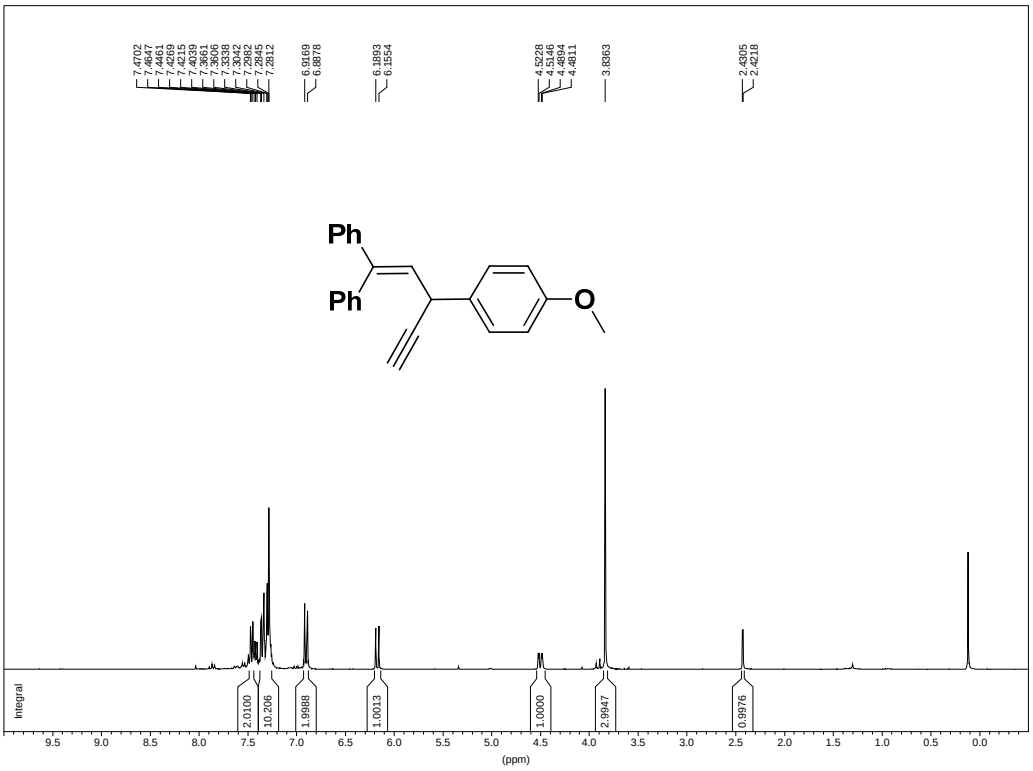

142.7552
142.0770
141.3152
138.8278
134.4432
134.1962
129.7438
128.6020
128.1447
127.7438
127.7074
127.5183
127.4810
127.2056
127.1837
126.5473
83.5675
77.4218
77.0000
76.5782
72.3307
36.7876
Ph
Ph
Cl
(ppm)

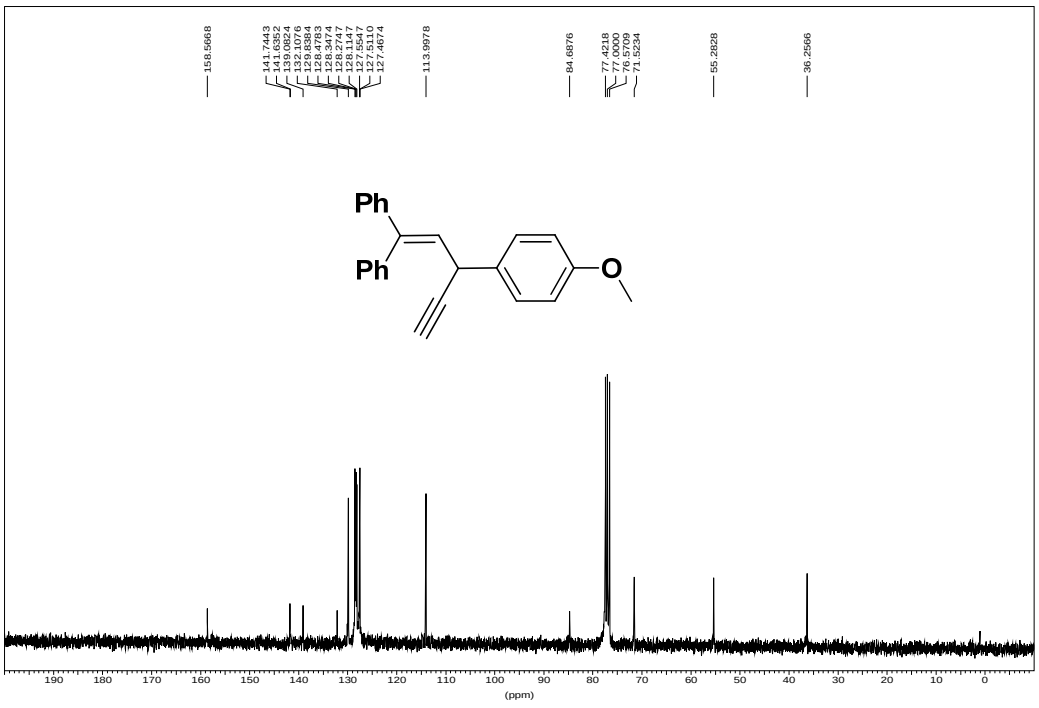
Compound **3i**



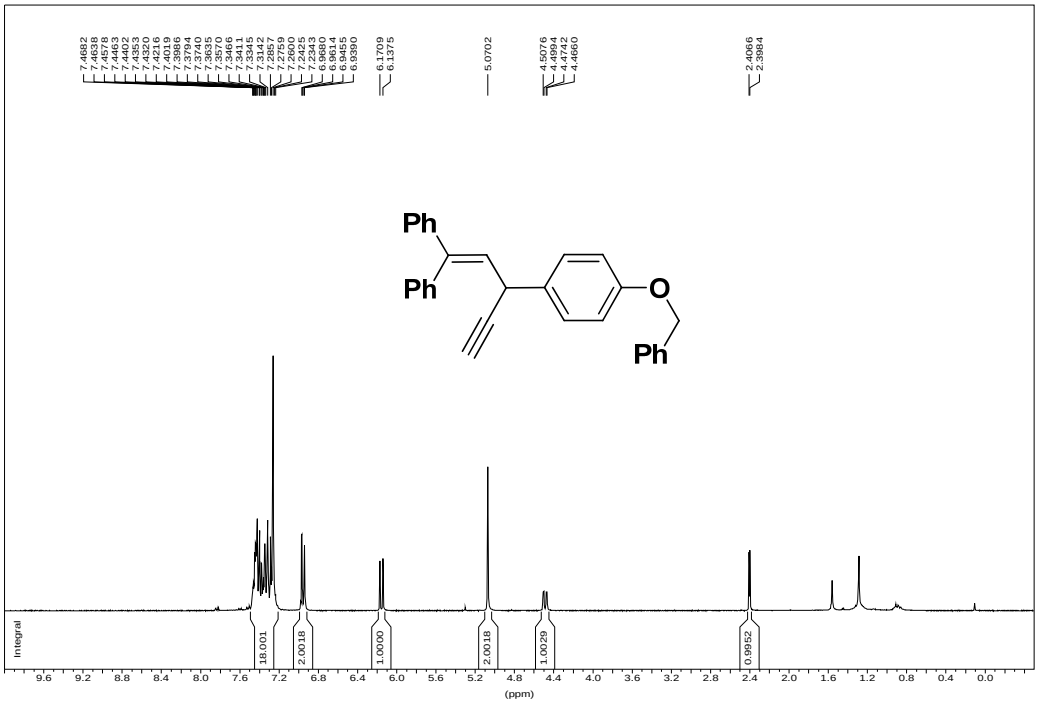


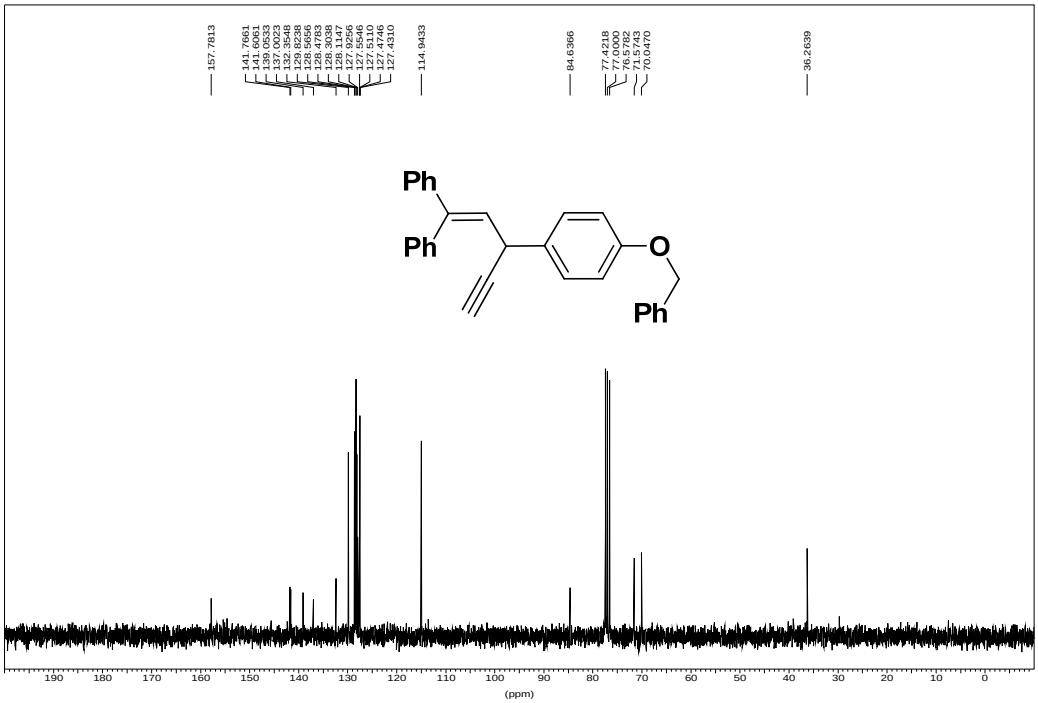
Compound **3j**


7.4702
7.4647
7.4461
7.4409
7.4215
7.4039
7.3866
7.3696
7.3338
7.3042
7.2982
7.2845
7.2812
6.9169
6.8878
6.1893
6.1554
4.5228
4.5146
4.4964
4.4811
3.8363
2.4305
2.4218
Ph
Ph
O
Integral
2.0100
10.206
1.9988
1.0013
1.0000
2.9947
0.9976
(ppm)

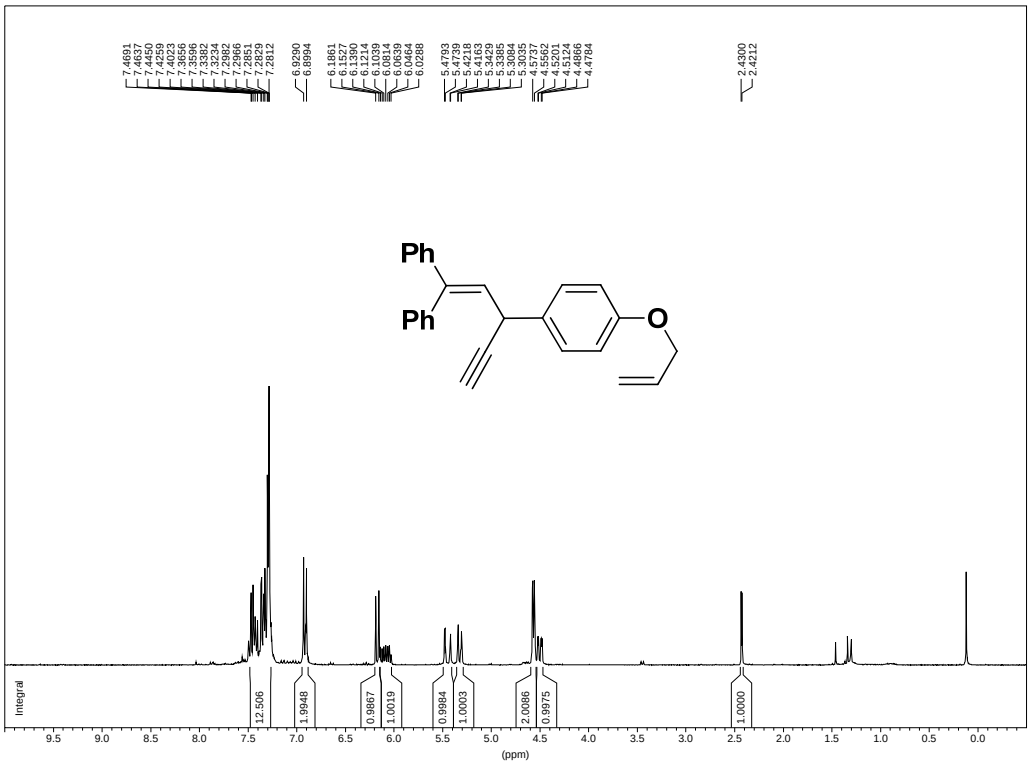

158.5668
141.7443
141.6352
139.0024
133.1070
129.8384
128.4783
128.3477
128.2747
128.1147
127.8547
127.5110
127.4674
113.9978
84.6876
77.4218
77.0000
76.5709
71.5234
55.2828
36.2566
Ph
Ph
O
(ppm)

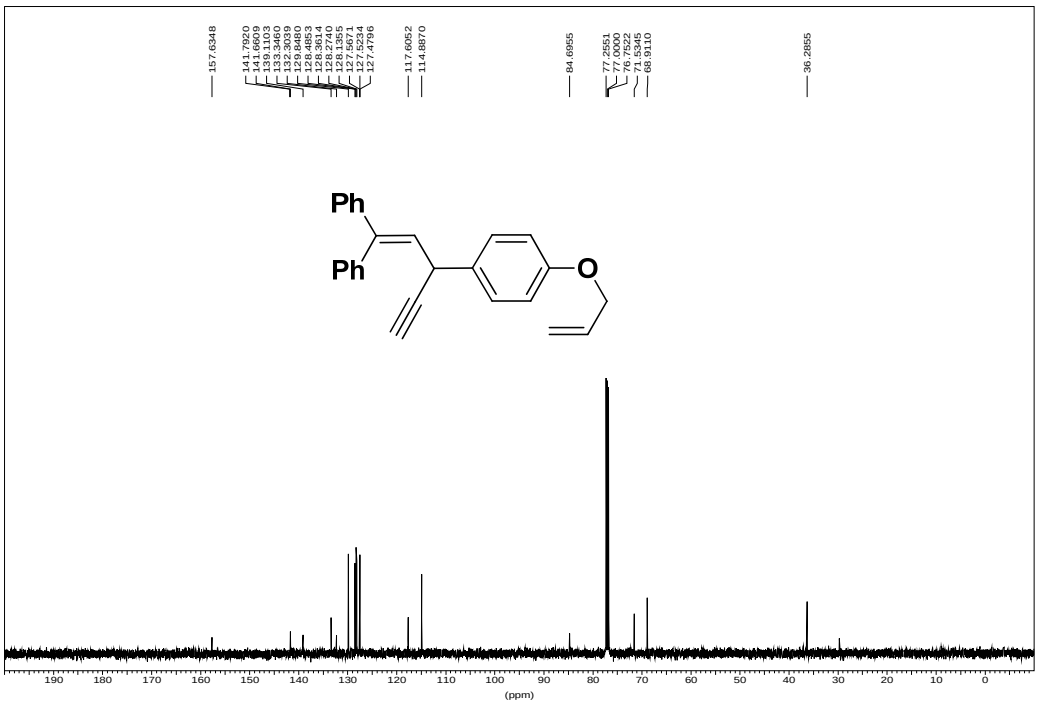
Compound **3k**


7.4682
7.4638
7.4578
7.4463
7.4402
7.4353
7.4321
7.4216
7.4019
7.3986
7.3794
7.3740
7.3635
7.3570
7.3466
7.3411
7.3345
7.3142
7.2957
7.2759
7.2600
7.2425
7.2243
6.9680
6.9614
6.9495
6.8990
6.1709
6.1375
5.0702
4.5076
4.4994
4.4742
4.4660
2.4066
2.3984
Ph
Ph
O
Ph
Integral
18.001
2.0018
1.0000
2.0018
1.0029
0.9952
9.6 9.2 8.8 8.4 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8 0.4 0.0
(ppm)

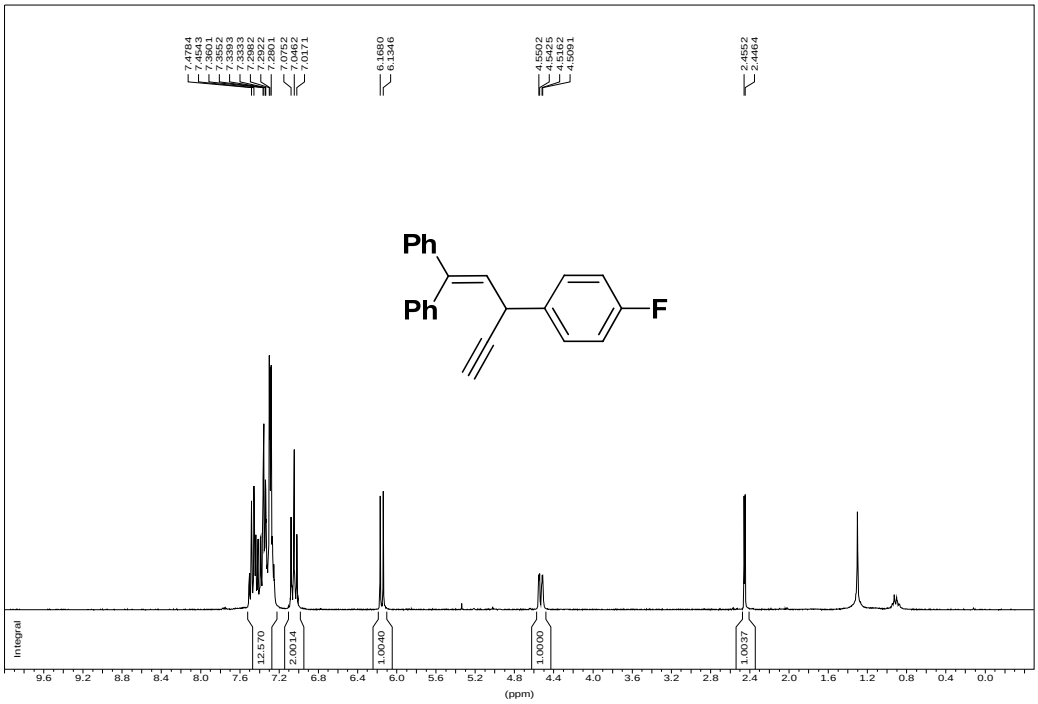

157.7813
141.7661
141.6561
139.0533
137.0023
132.3944
130.8248
128.5656
128.4783
128.3989
128.1147
127.9256
127.5546
127.5110
127.4746
127.4310
114.9433
84.6366
77.4218
77.0000
76.5782
71.7743
70.0470
36.2639
Ph
Ph
O
Ph
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

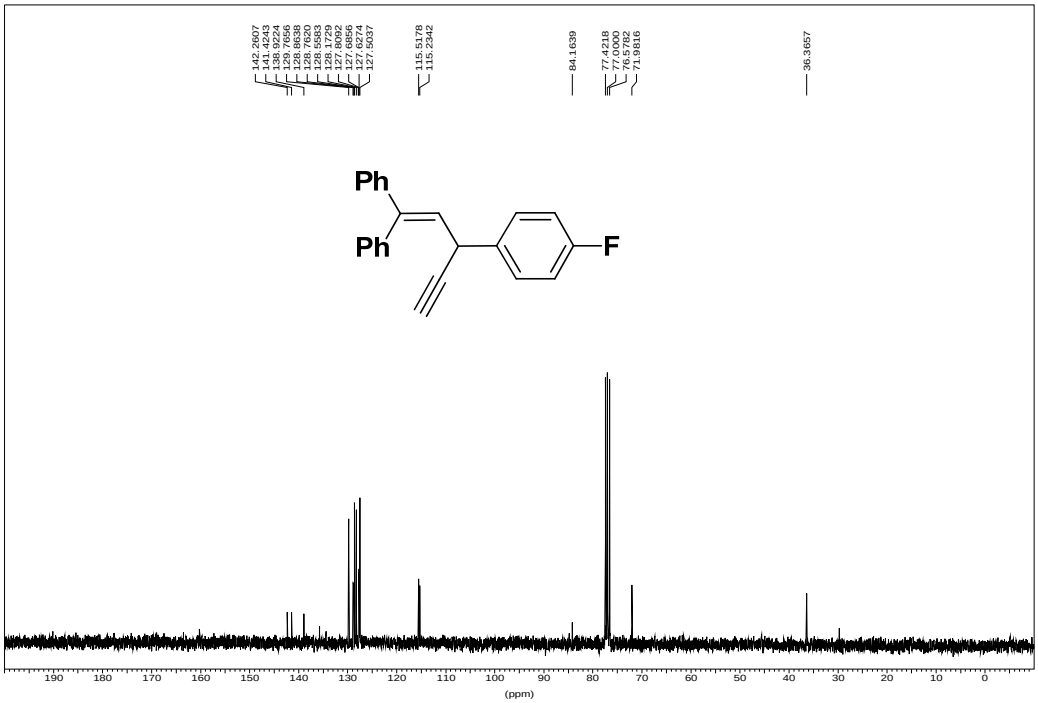
Compound **3l**


7.4691
7.4637
7.4450
7.4259
7.4093
7.3656
7.3596
7.3382
7.3294
7.2982
7.2966
7.2851
7.2829
7.2812
6.9290
6.8994
6.1861
6.1527
6.1390
6.1214
6.1039
6.0814
6.0639
6.0464
6.0288
5.4793
5.4739
5.4218
5.4153
5.3429
5.3385
5.3084
5.2995
5.2737
4.5562
4.5201
4.5124
4.4966
4.4784
2.4300
2.4212
Ph
Ph
O
Integral
12.506
1.9948
0.9887
1.0019
0.9984
1.0003
2.0086
0.9975
1.0000
(ppm)


157.6348
141.7920
141.6669
139.1103
133.3460
132.3439
128.4853
128.3614
128.2274
128.1740
127.5671
127.5234
127.4796
117.6052
114.8870
84.6955
77.2551
77.0000
76.7522
71.8345
69.9110
36.2855
Ph
Ph
O
(ppm)

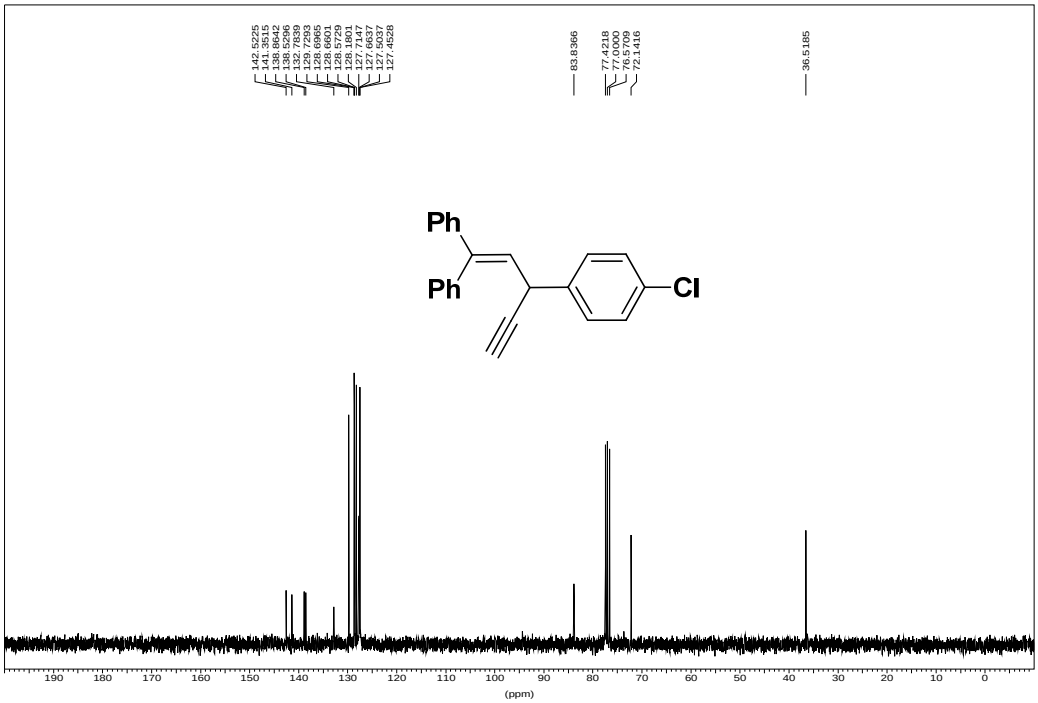
Compound **3m**


7.4784
7.4543
7.3601
7.3552
7.3383
7.3333
7.2982
7.2922
7.2901
7.0752
7.0462
7.0171
6.1680
6.1346
4.5502
4.5425
4.5162
4.5091
2.4552
2.4464
Ph
Ph
F
Integral
12.570
2.0014
1.0040
1.0000
1.0037
(ppm)

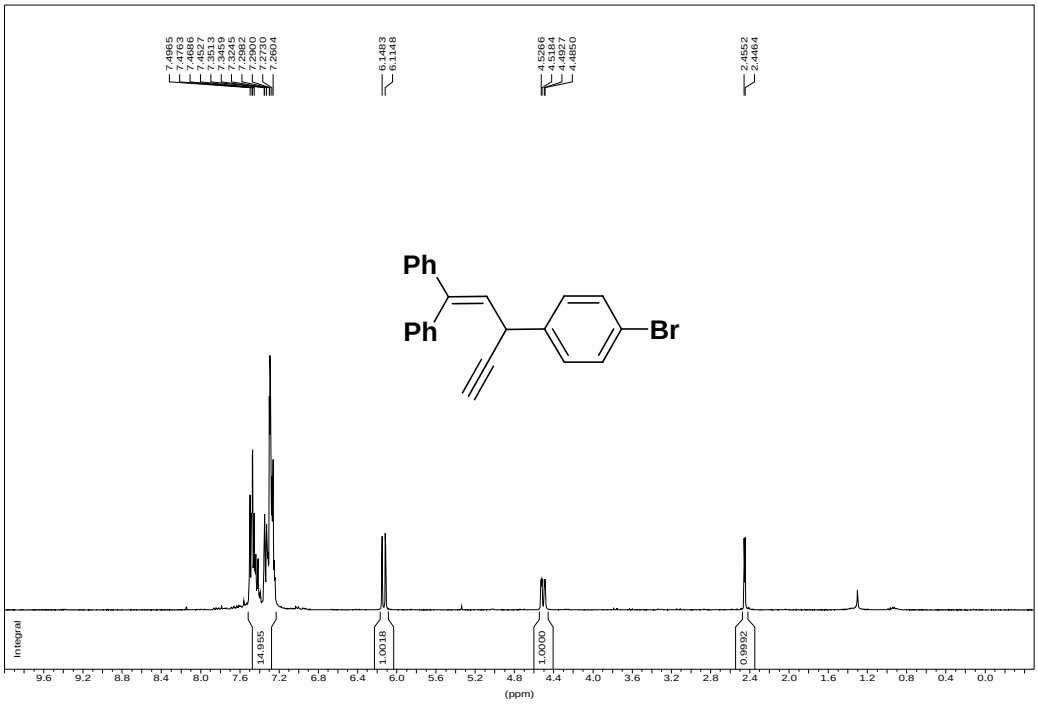

142.2607
141.4243
138.9224
138.7966
128.8638
128.7620
128.5583
128.1729
127.8092
127.6856
127.6274
127.5837
115.5178
115.2342
84.1639
77.4218
77.0000
76.5782
71.9816
36.3657
Ph
Ph
F
(ppm)

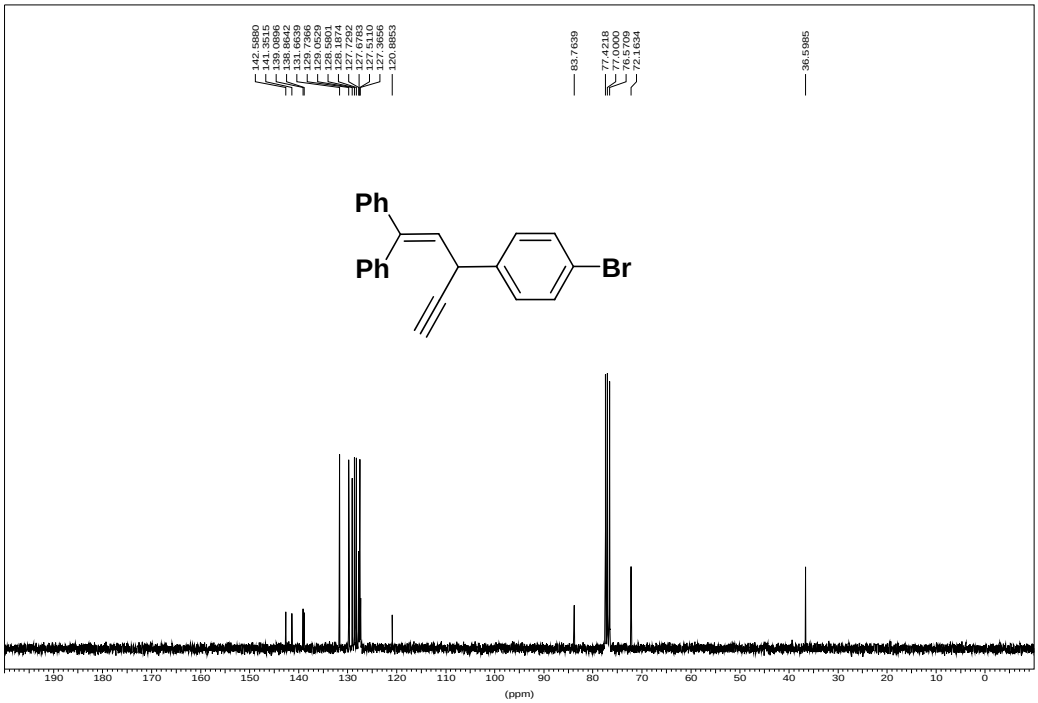
Compound **3n**


7.4549
7.4488
7.4308
7.4251
7.4138
7.3908
7.3360
7.3305
7.3201
7.3097
7.2948
7.2845
7.2752
7.2735
7.2609
7.2582
7.2554
7.2428
6.1351
6.1017
4.5271
4.5159
4.4937
4.4850
2.4327
2.4245
Ph
Ph
Cl
Integral
3.0398
11.600
1.0000
0.9985
1.0006
(ppm)

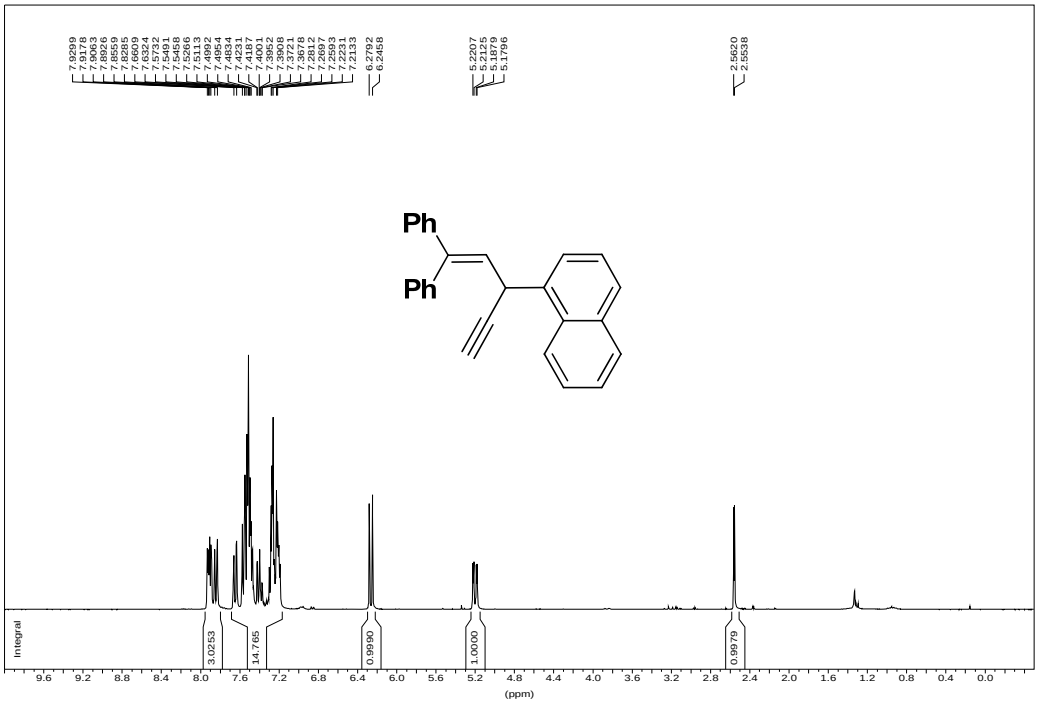

142.5225
141.3515
138.8642
138.5799
132.7839
129.7293
128.6965
128.6601
128.5729
128.1801
127.7147
127.6657
127.5037
127.4528
83.8366
77.4218
77.0000
76.5709
72.1416
36.5185
Ph
Ph
Cl
(ppm)

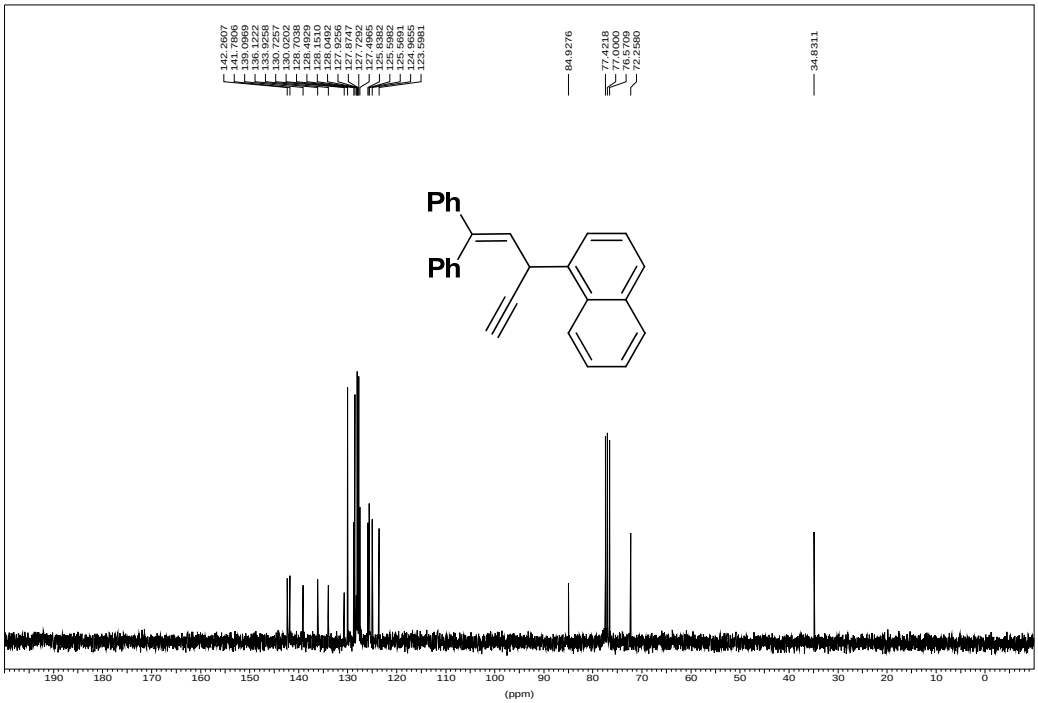
Compound **3o**


7.4965
7.4763
7.4686
7.4627
7.3513
7.3459
7.3245
7.2982
7.2900
7.2730
7.2604
6.1483
6.1148
4.5266
4.5154
4.4927
4.4850
2.4552
2.4464
Ph
Ph
Br
Integral
14.9955
1.0018
1.0000
0.9992
(ppm)

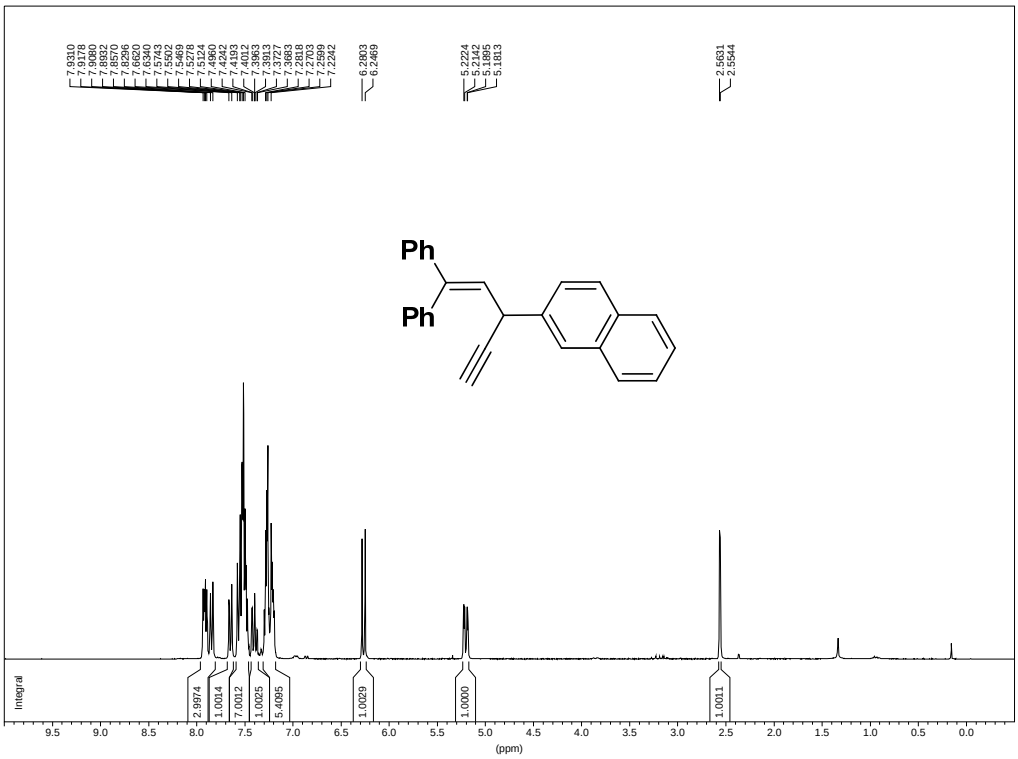

142.5880
141.3515
139.0896
138.8842
131.6539
129.7366
129.0529
128.5691
128.1874
127.7292
127.6783
127.5110
127.3656
120.8853
83.7639
77.4218
77.0000
76.5709
72.1634
36.5985
Ph
Ph
Br
(ppm)

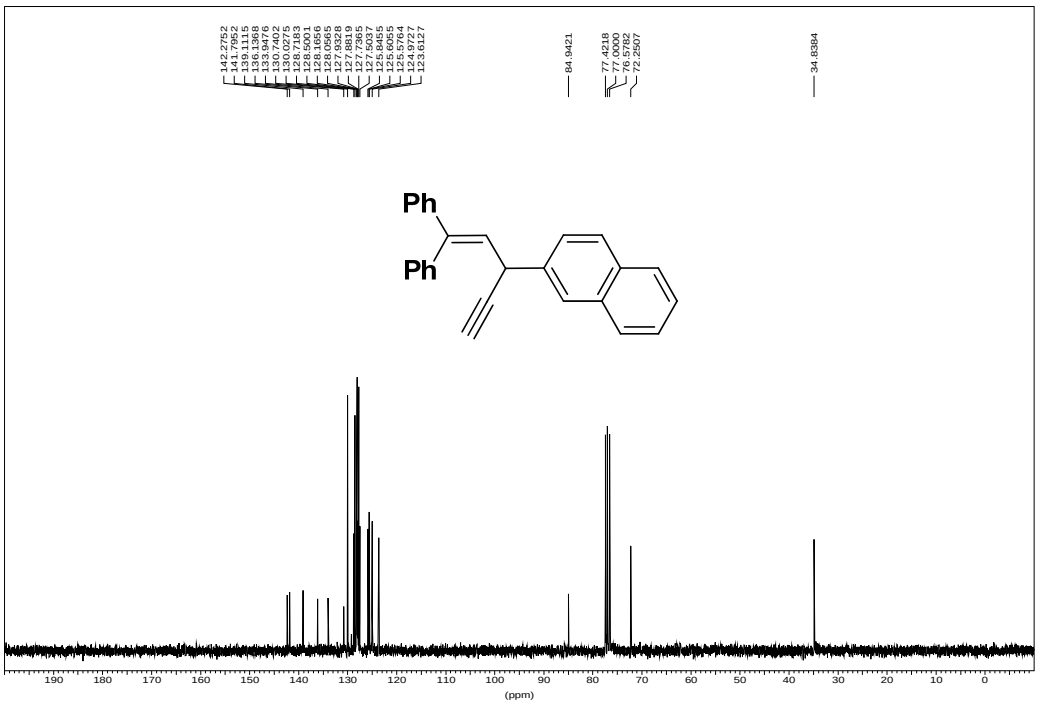
Compound **3p**


7.9299
7.9178
7.9063
7.8926
7.8859
7.8285
7.6609
7.6524
7.5732
7.5491
7.5458
7.5266
7.5113
7.4992
7.4954
7.4844
7.4231
7.4187
7.4091
7.4052
7.3908
7.3721
7.3618
7.3517
7.2697
7.2593
7.2231
7.2133
6.2792
6.2458
5.2207
5.2175
5.1879
5.1796
2.5620
2.5538
Ph
Ph
Integral
3.0253
14.7765
0.9990
1.0000
0.9979
(ppm)

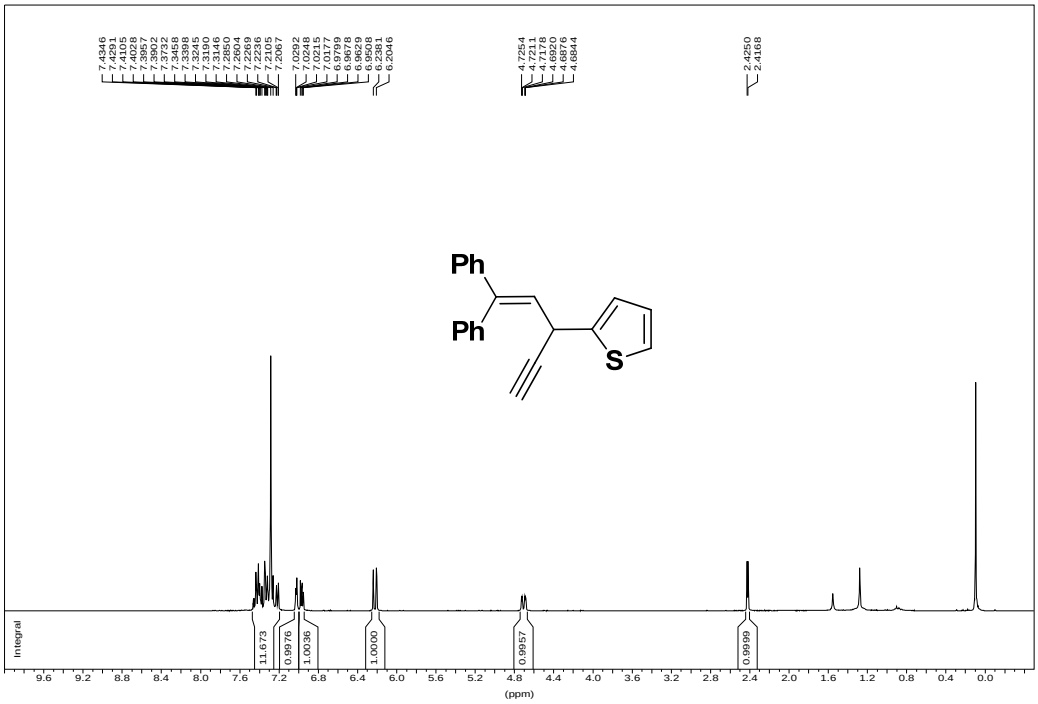

142.2607
141.7806
141.0999
138.1222
133.9258
130.7257
130.0037
128.7038
128.4929
128.1510
128.0067
127.9256
127.8747
127.7292
127.4966
126.8382
125.5982
125.5691
124.9655
123.5981
84.9276
77.4218
77.0000
76.5709
72.2580
34.8311
Ph
Ph
(ppm)

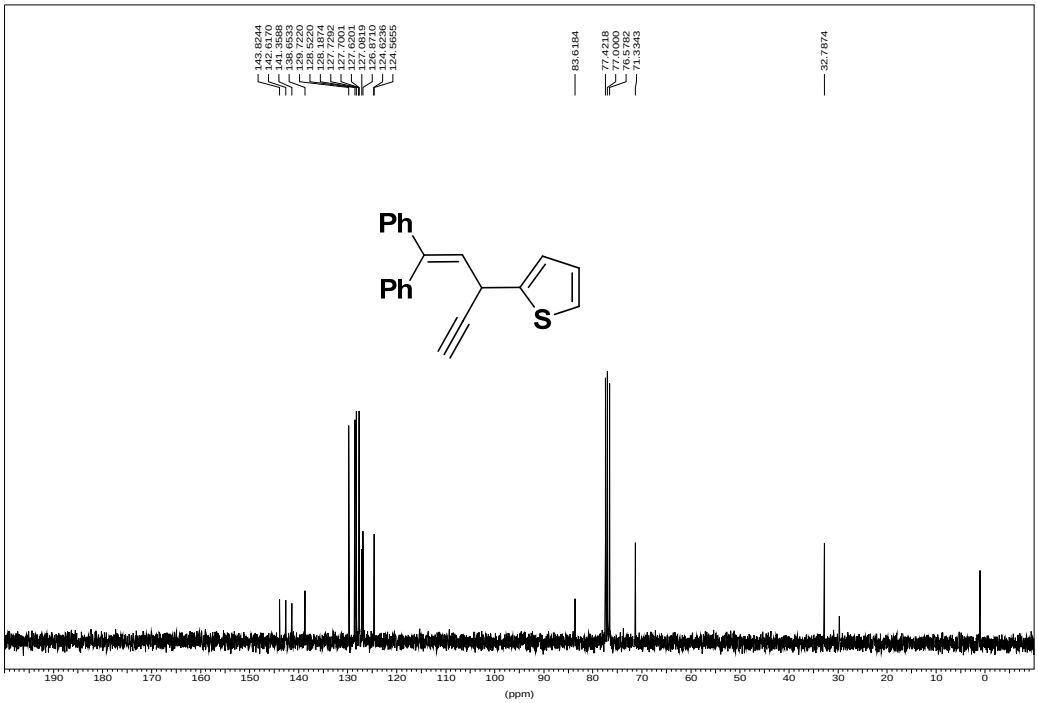
Compound **3q**


7.9310
7.9178
7.9080
7.8932
7.8570
7.8296
7.6620
7.6340
7.5743
7.5502
7.5469
7.5278
7.5224
7.4960
7.4242
7.4193
7.4012
7.3868
7.3913
7.3727
7.3683
7.2818
7.2703
7.2599
7.2242
6.2803
6.2469
5.2224
5.2142
5.1895
5.1813
2.5631
2.5544
Ph
Ph
Integral
2.9974
1.0014
7.0012
1.0025
5.4095
1.0029
1.0000
1.0011
(ppm)

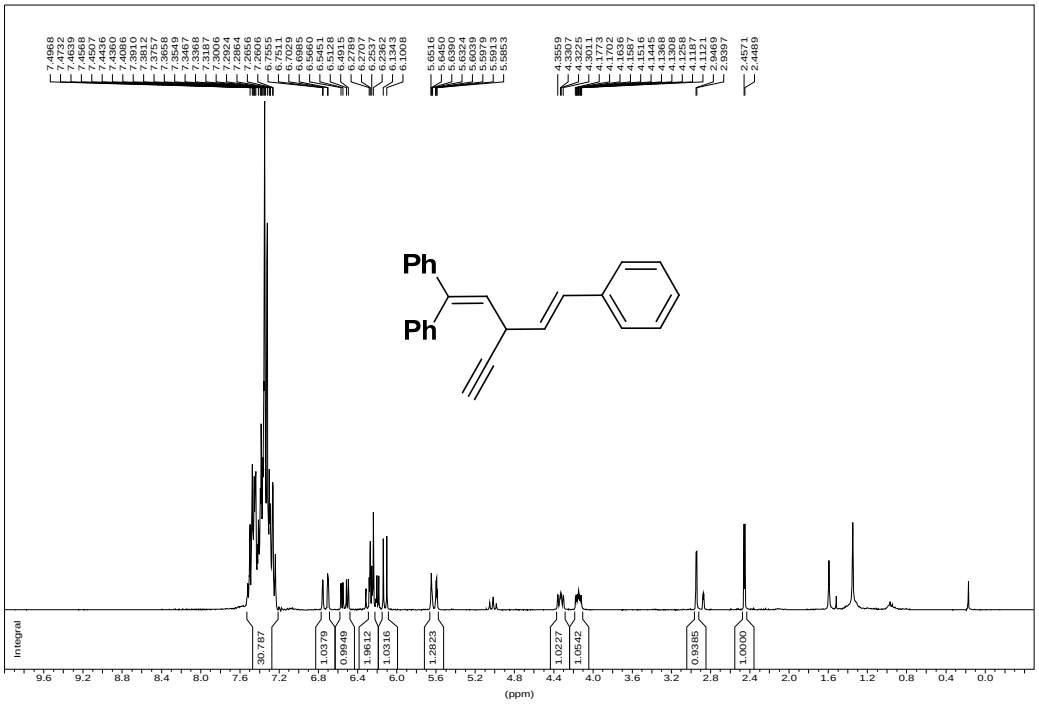

142.2752
141.7952
138.1111
138.1368
133.9476
130.7402
130.0777
128.7183
128.5001
128.1656
128.0966
127.9328
127.8819
127.7385
127.5937
126.8455
126.6055
125.5764
124.3477
123.6127
84.9421
77.4218
77.0000
76.5782
72.2507
34.8384
Ph
Ph
(ppm)

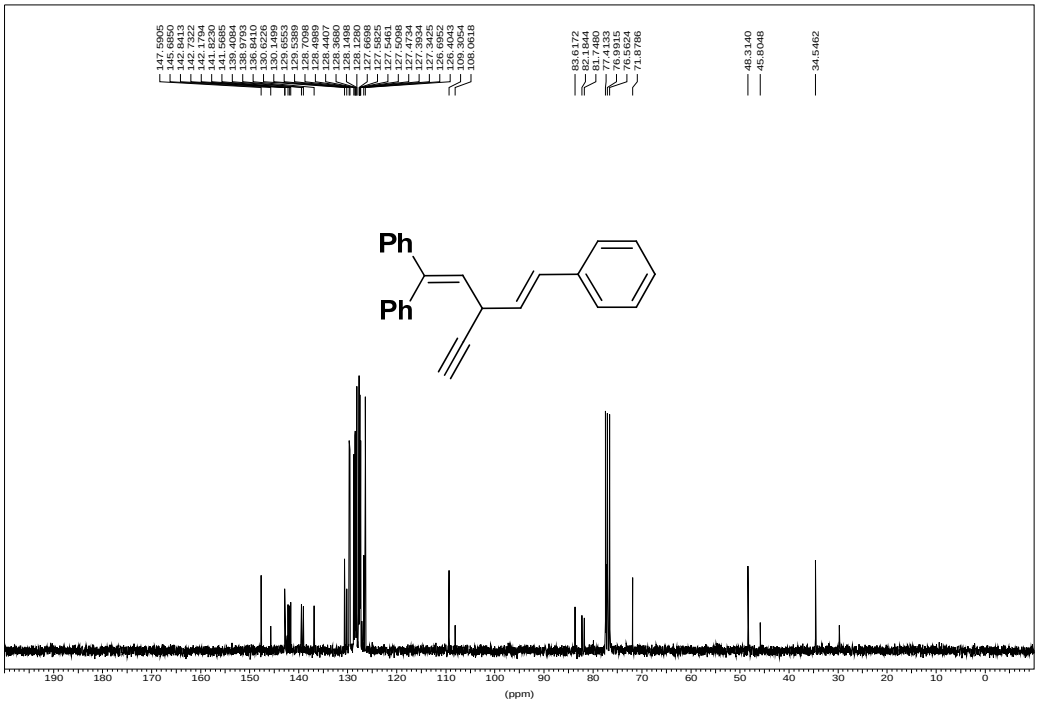
Compound **3r**


7.4346
7.4291
7.4105
7.4029
7.3967
7.3902
7.3732
7.3498
7.3458
7.3245
7.3190
7.3146
7.2850
7.2604
7.2269
7.2226
7.2105
7.2067
7.0292
7.0248
7.0215
7.0177
6.9799
6.9678
6.9629
6.9568
6.2381
6.2046
4.7254
4.7211
4.7178
4.6870
4.6837
4.6844
2.4250
2.4168
Ph
Ph
S
Integral
11.673
0.9976
1.0036
1.0000
0.9957
0.9999
(ppm)


143.8244
142.6170
141.3588
138.6533
137.7220
128.5220
128.1874
127.7292
127.7001
127.6201
127.0819
126.8710
126.6636
124.5655
83.6184
77.4218
77.0000
76.5782
71.3343
32.7874
Ph
Ph
S
(ppm)

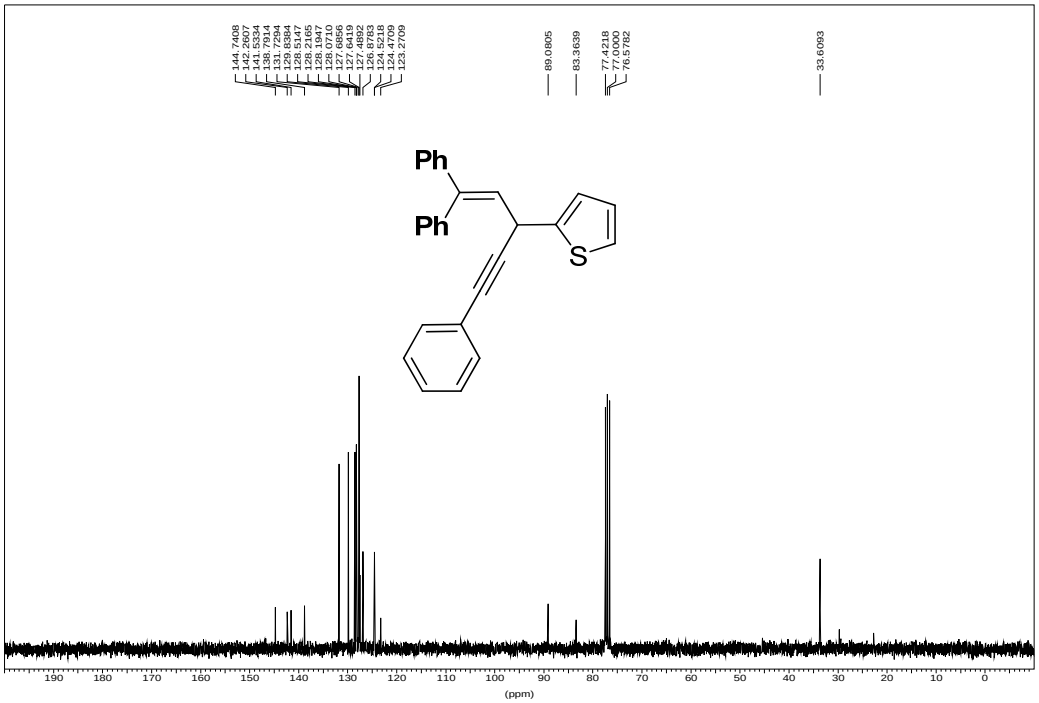
Compound **3s**


Ph
Ph
Integral
30.787
1.0379
0.9949
1.9612
1.0316
1.2823
1.0227
1.0542
0.9385
1.0000
(ppm)

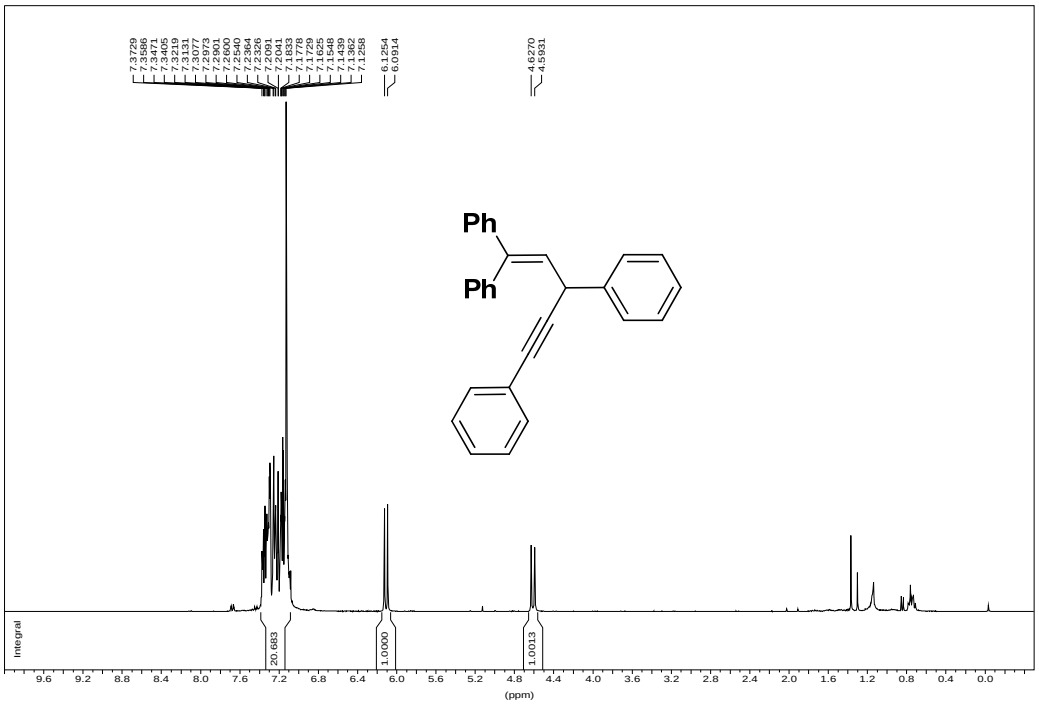

Ph
Ph
(ppm)

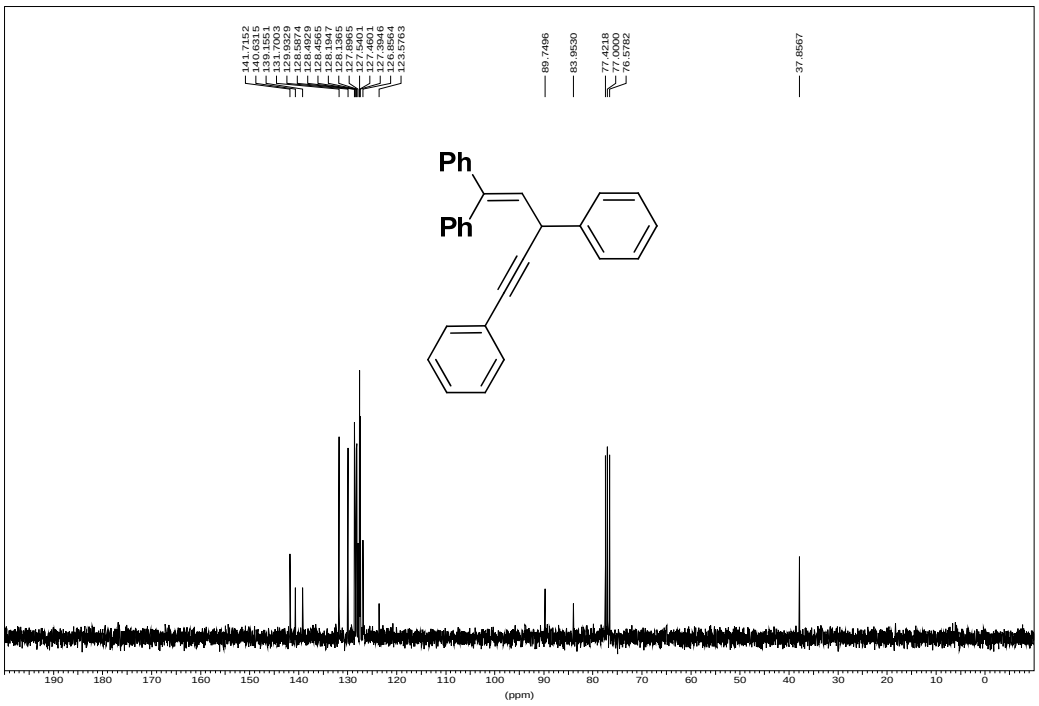
Compound **3t**


7.5458
7.5415
7.5338
7.5256
7.4686
7.4324
7.3760
7.3639
7.3541
7.3453
7.2923
7.2785
7.2653
7.2615
7.1174
7.1059
7.0413
7.0292
7.0123
7.0128
6.3619
6.3285
4.9797
4.9775
4.9468
4.9441
Ph
Ph
S
Integral
16.633
0.9970
1.0036
0.9956
1.0000
(ppm)

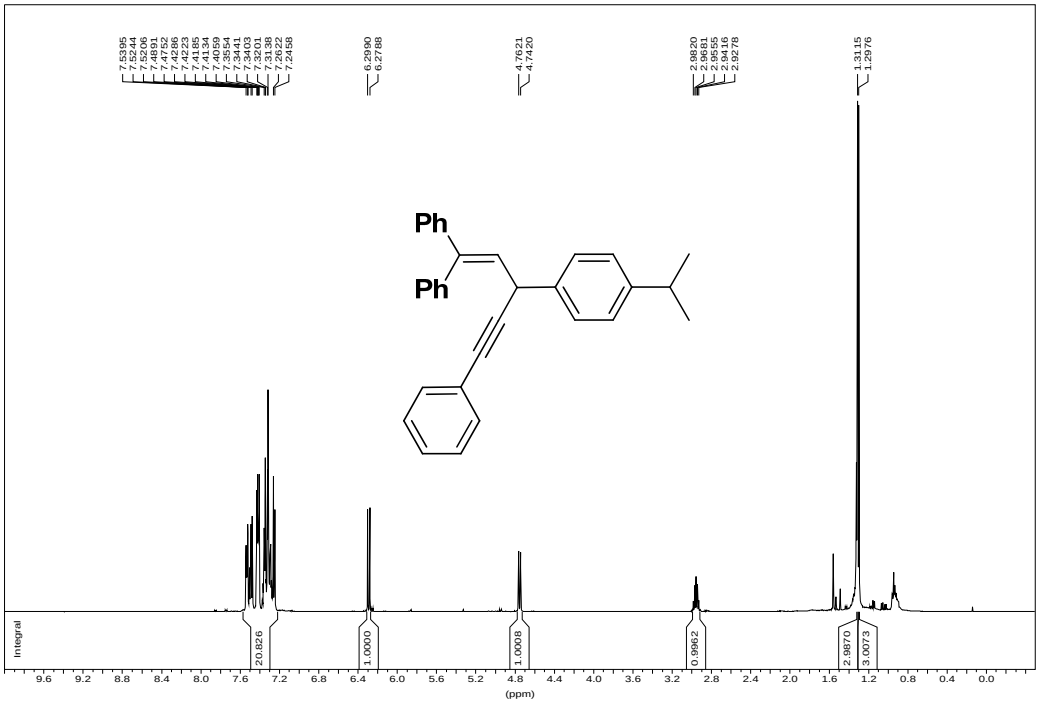

144.7408
142.2607
141.5564
138.7914
131.7294
129.8394
129.5417
128.2165
128.1947
128.0770
127.6656
127.6419
127.4882
126.5972
124.5218
124.4709
123.2709
89.0805
83.3639
77.4218
77.0000
76.5782
33.6093
Ph
Ph
S
(ppm)

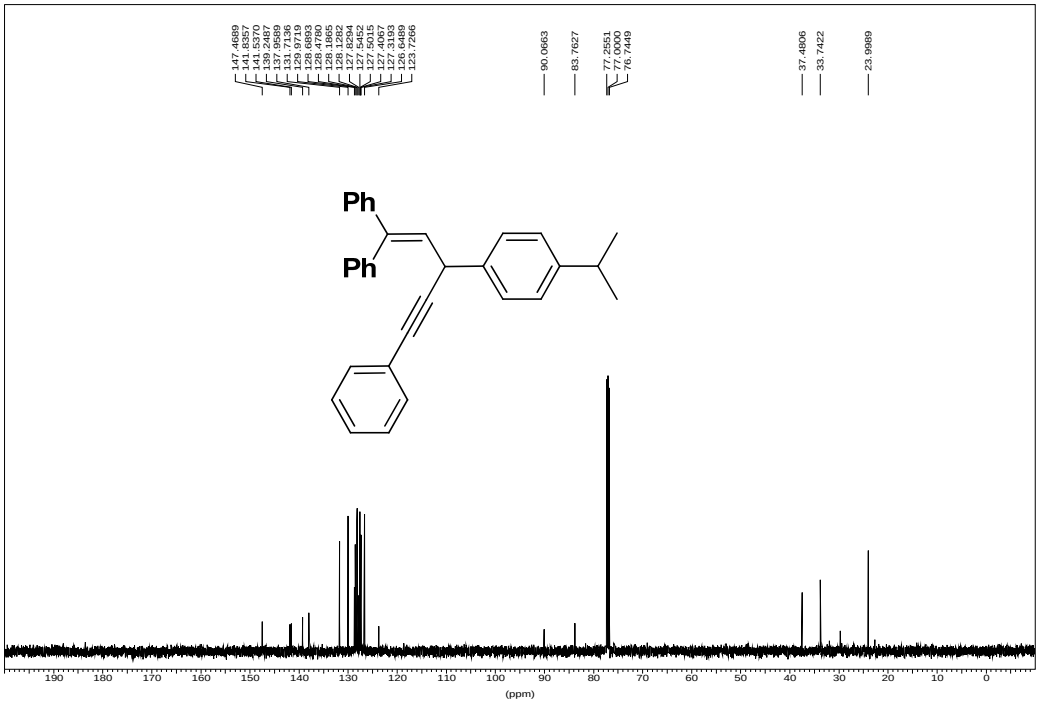
Compound **3u**


7.3729
7.3568
7.3471
7.3405
7.3219
7.3131
7.3077
7.2973
7.2901
7.2900
7.2540
7.2364
7.2236
7.2091
7.2041
7.1833
7.1778
7.1729
7.1625
7.1548
7.1439
7.1362
7.1258
6.1254
6.0914
4.6270
4.5931
Ph
Ph
Integral
20.683
1.0000
1.0013
9.6 9.2 8.8 8.4 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.4 4.0 3.6 3.2 2.8 2.4 2.0 1.6 1.2 0.8 0.4 0.0
(ppm)


141.7152
140.6515
139.1551
131.7003
128.9329
128.8974
128.4929
128.4565
128.1344
128.1365
127.8965
127.5401
127.4491
127.3946
126.8564
123.5763
89.7496
83.9530
77.4218
77.0000
76.5782
37.8567
Ph
Ph
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

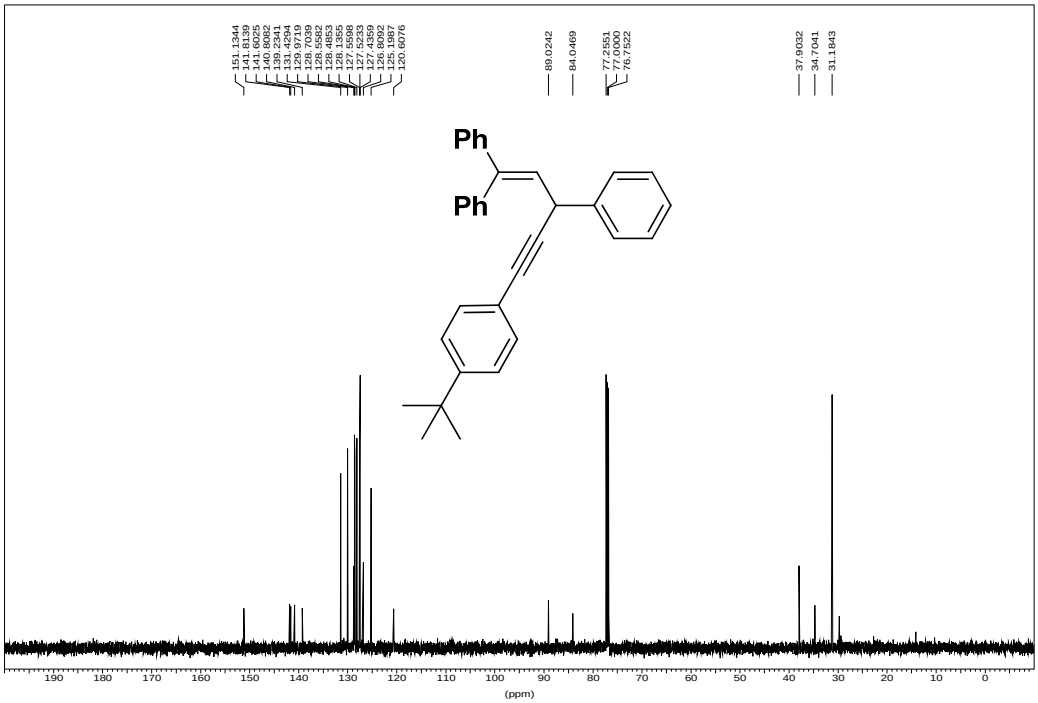
Compound **3v**


7.5395
7.5214
7.5046
7.4891
7.4752
7.4586
7.4223
7.4185
7.4134
7.4049
7.3954
7.3441
7.3403
7.3201
7.3138
7.2622
7.2458
6.2990
6.2788
4.7621
4.7420
2.9820
2.9681
2.9555
2.9416
2.9278
1.3115
1.2976
Ph
Ph
Integral
20.826
1.0000
1.0008
0.9962
2.9870
3.0073
(ppm)

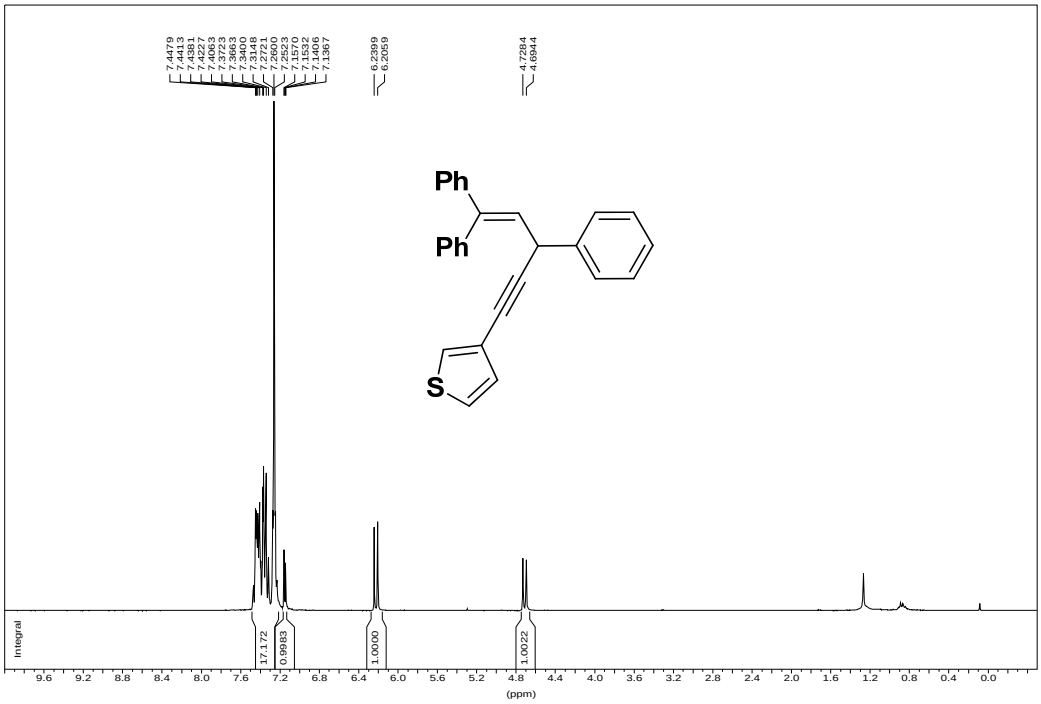

147.4689
141.8357
141.5707
139.2487
137.9589
137.7736
130.9710
128.6893
128.4780
128.1965
128.1382
127.8294
127.5452
127.5015
127.4067
127.3193
126.6489
123.7266
90.0663
83.7627
77.2551
77.0000
76.7449
37.4806
33.7422
23.9989
Ph
Ph
(ppm)

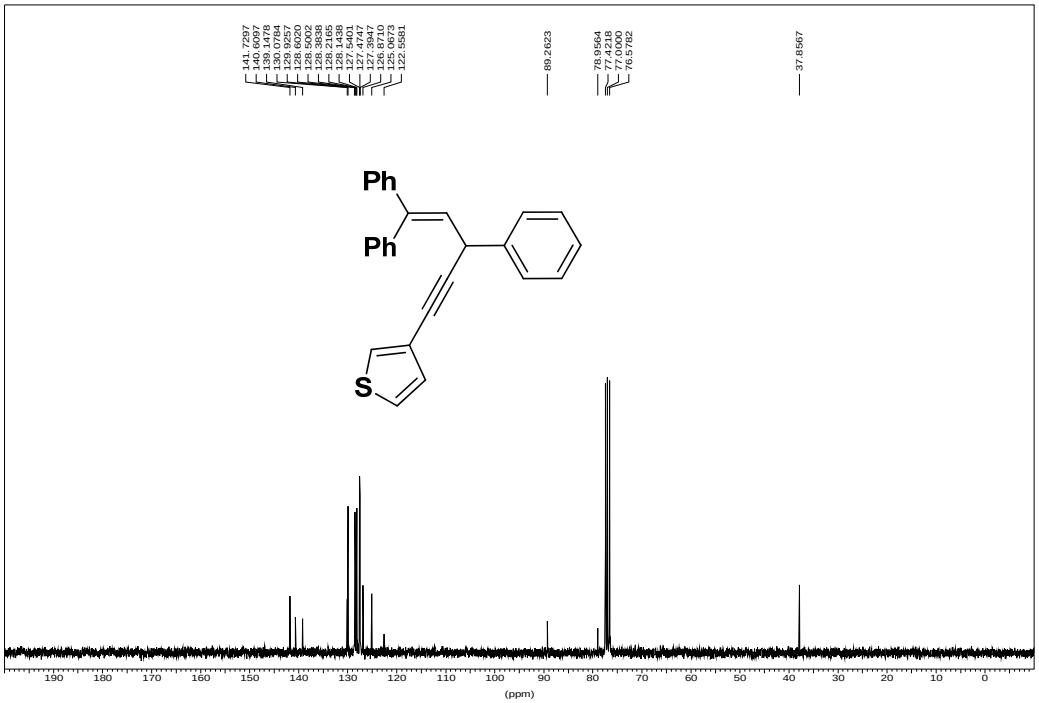
Compound **3w**


7.5030
7.4967
7.4878
7.4500
7.4449
7.4097
7.3971
7.3933
7.3838
7.3239
6.3053
6.2851
4.8050
4.7848
1.3809
Ph
Ph
Integral
20.085
1.0000
0.9997
8.9983
(ppm)

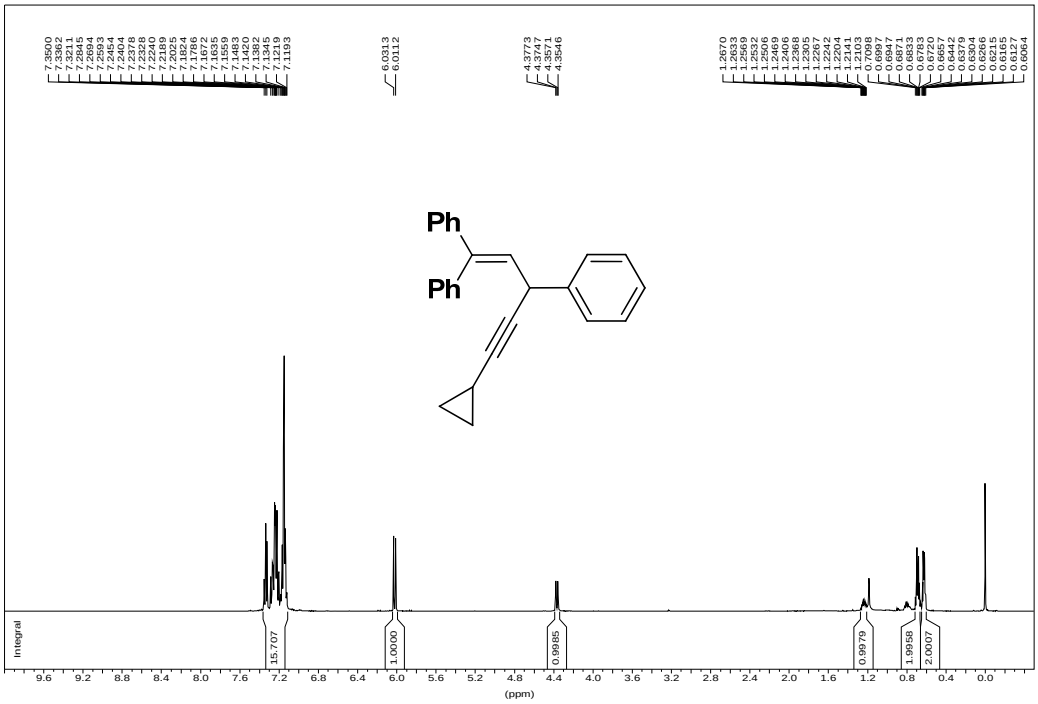

151.1344
141.8139
141.6055
140.8082
139.2341
131.4294
129.9110
128.7039
128.5582
128.4453
128.1355
127.5598
127.5233
127.4556
126.8092
126.1987
120.6076
89.0242
84.0469
77.2551
77.0000
76.7522
37.9032
34.7041
31.1843
Ph
Ph
(ppm)

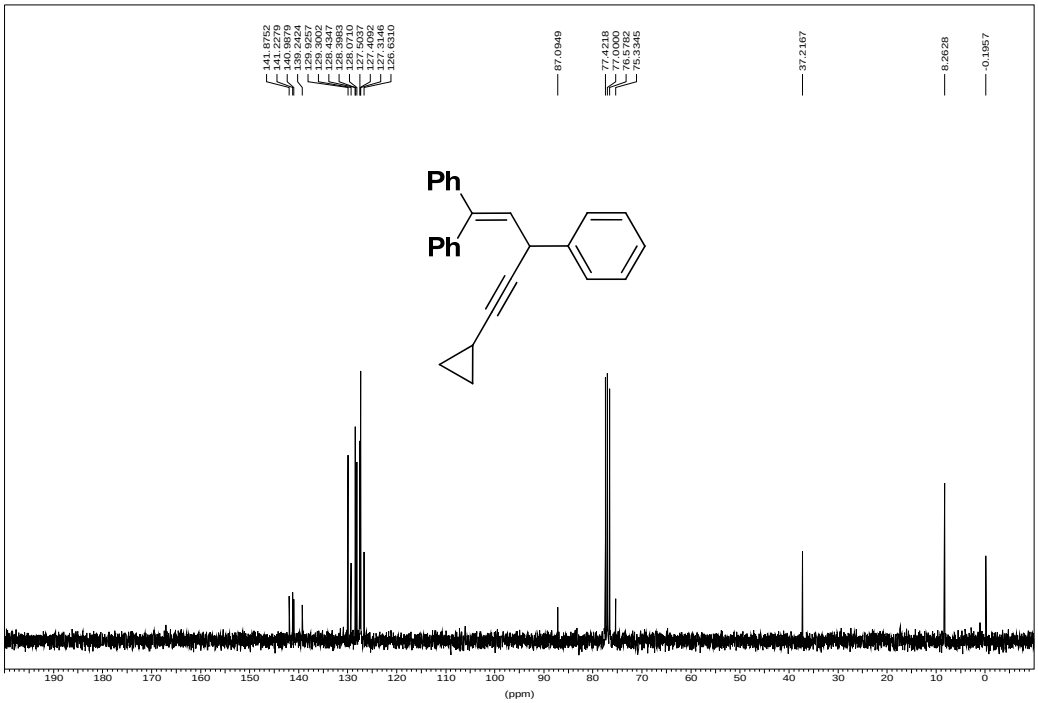
Compound **3x**


7.4479
7.4413
7.4381
7.4227
7.4063
7.3723
7.3663
7.3400
7.3148
7.2721
7.2600
7.2523
7.1570
7.1532
7.1406
7.1367
6.2399
6.2059
4.7284
4.6944
Ph
Ph
S
Integral
17.172
0.9983
1.0000
1.0022
(ppm)

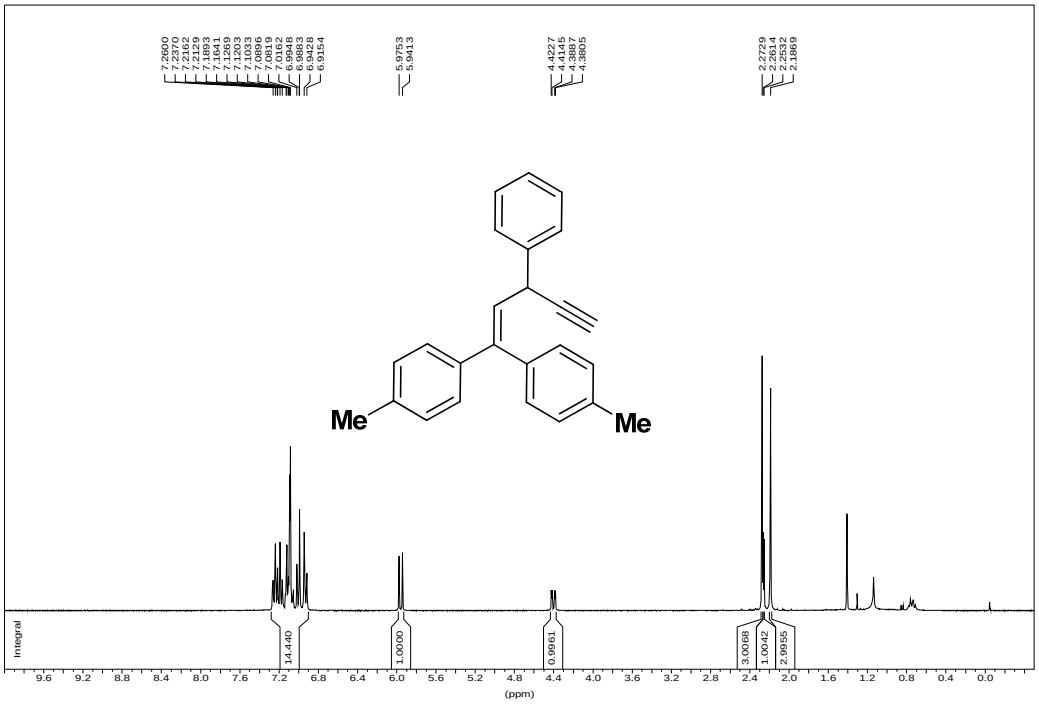

141.7237
140.6297
139.1478
130.0784
129.9557
129.6620
128.5002
128.3838
128.2165
128.1498
127.5401
127.4747
127.2841
126.8710
126.0673
122.5581
89.2623
78.9564
77.2418
77.0000
76.5782
37.8567
Ph
Ph
S
(ppm)

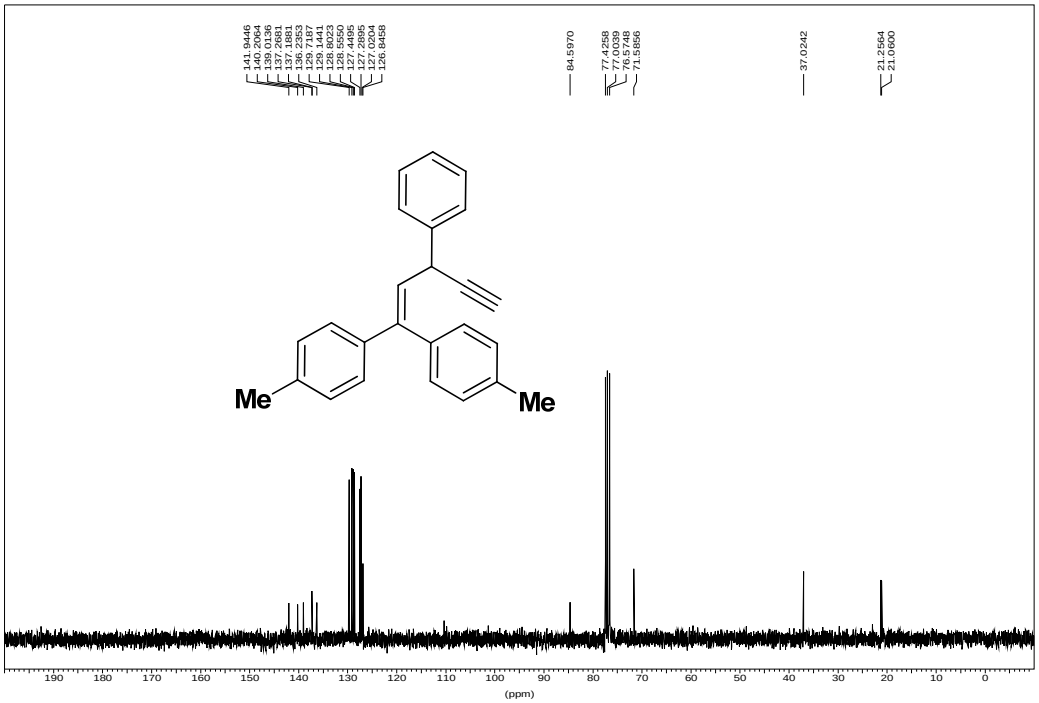
Compound **3y**


Ph
Ph
Integral
15.707
1.0000
0.9985
0.9979
1.9958
2.0007
(ppm)

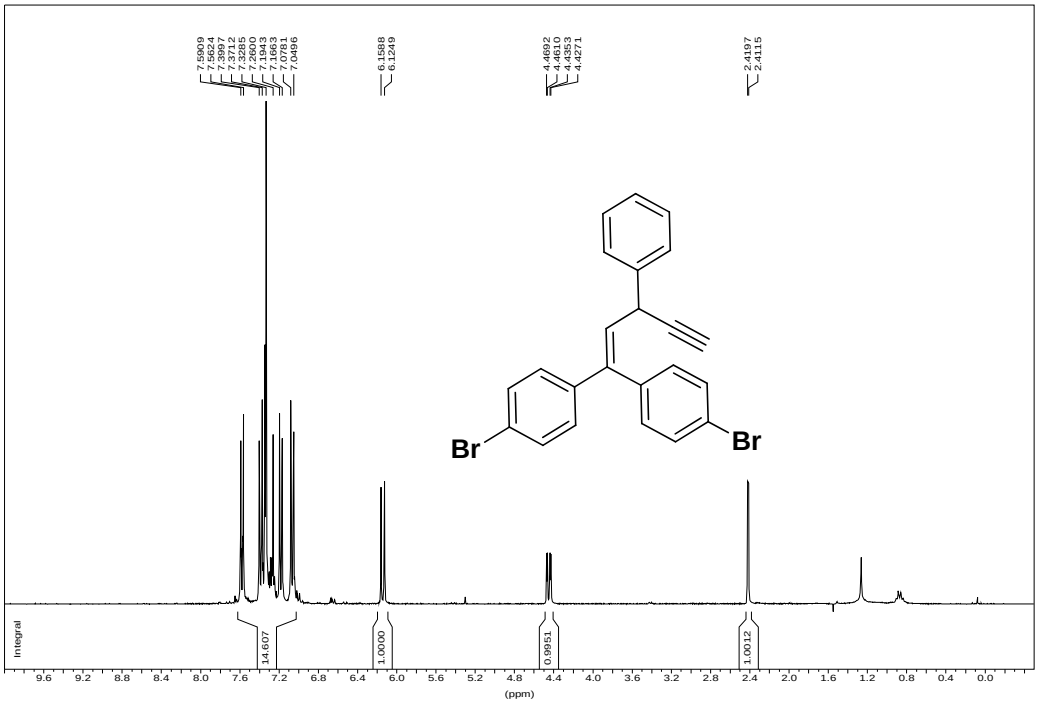

Ph
Ph
87.0949
77.4218
77.0000
76.5782
75.3345
37.2167
8.2628
-0.1957
(ppm)

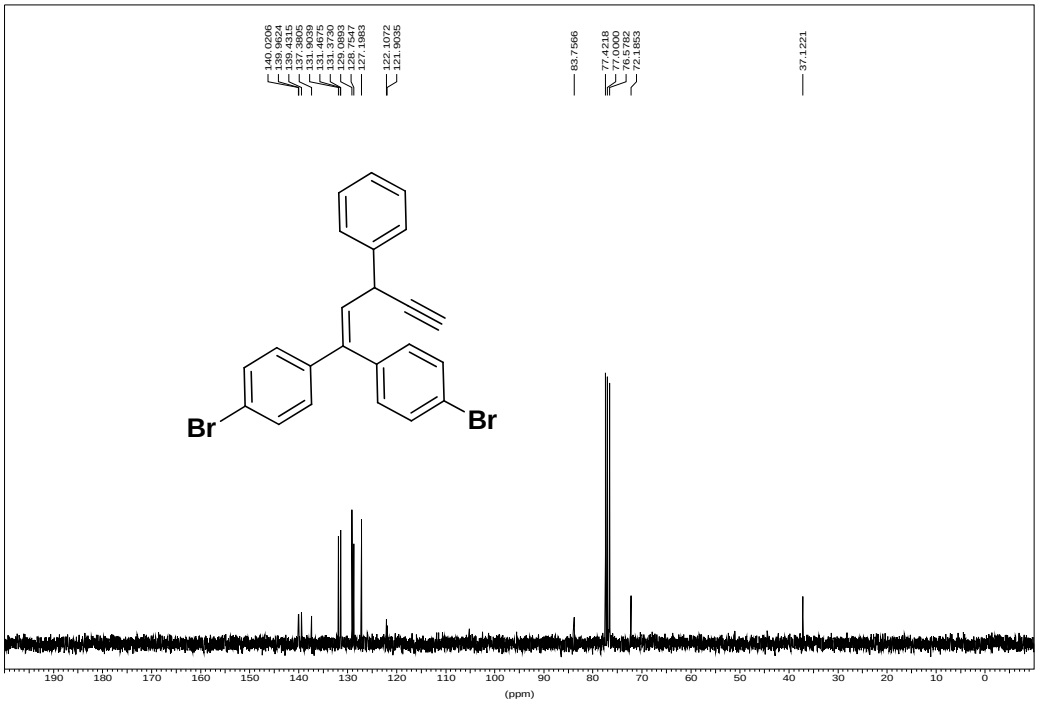
Compound **3z**


7.2600
7.2370
7.2162
7.2129
7.1893
7.1641
7.1269
7.1203
7.1033
7.0896
7.0819
7.0162
6.9948
6.9853
6.9428
6.9154
5.9753
5.9413
4.4227
4.4145
4.3887
4.3805
2.2779
2.2614
2.2532
2.1869
Me
Me
Integral
14.440
1.0000
0.9961
3.0068
1.0042
2.9955
(ppm)

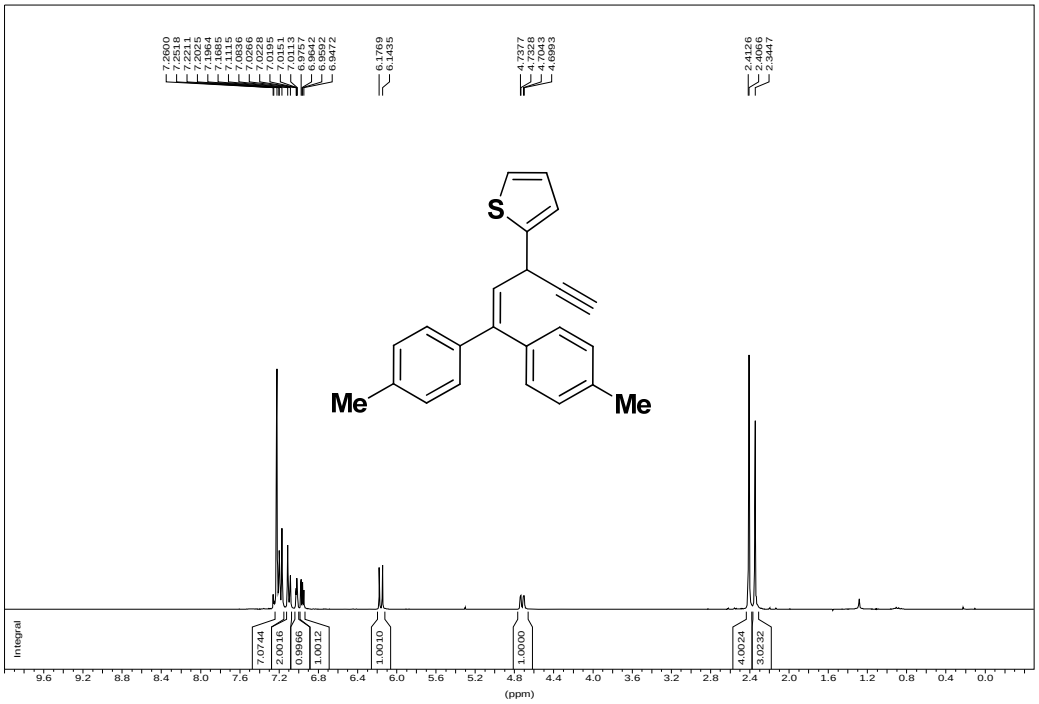

141.9446
140.2664
139.0136
137.2681
137.1881
136.2253
129.7187
128.1441
128.8023
128.5560
127.4495
127.2895
127.0204
126.8458
84.5970
77.4258
77.0039
76.5748
71.5856
37.0242
21.2564
21.0600
Me
Me
(ppm)

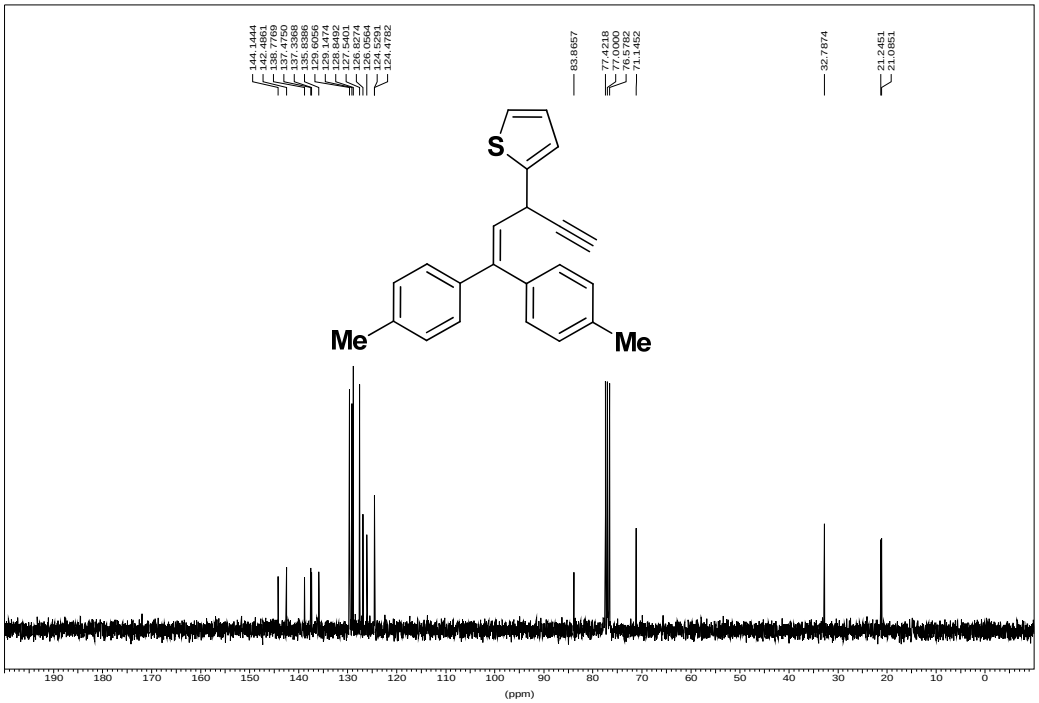
Compound **3a'**


7.5909
7.5624
7.3997
7.3712
7.3485
7.2600
7.1943
7.1683
7.0701
7.0496
6.1588
6.1249
4.4692
4.4610
4.4353
4.4271
2.4197
2.4115
Br
Br
Integral
14.607
1.0000
0.9951
1.0012
(ppm)

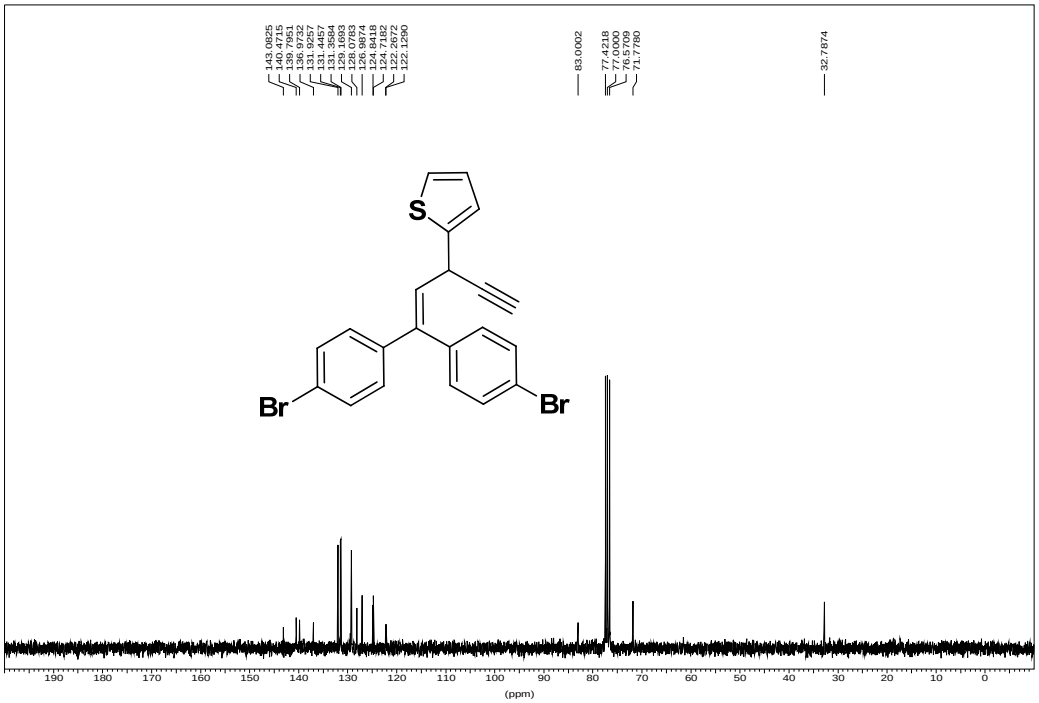

140.0206
139.9624
139.4315
132.2695
131.9039
131.4675
131.3730
129.0983
128.7547
127.1983
122.1072
121.9035
83.7566
77.4218
77.0000
76.5782
72.1853
37.1221
Br
Br
(ppm)

Compound **3b'**

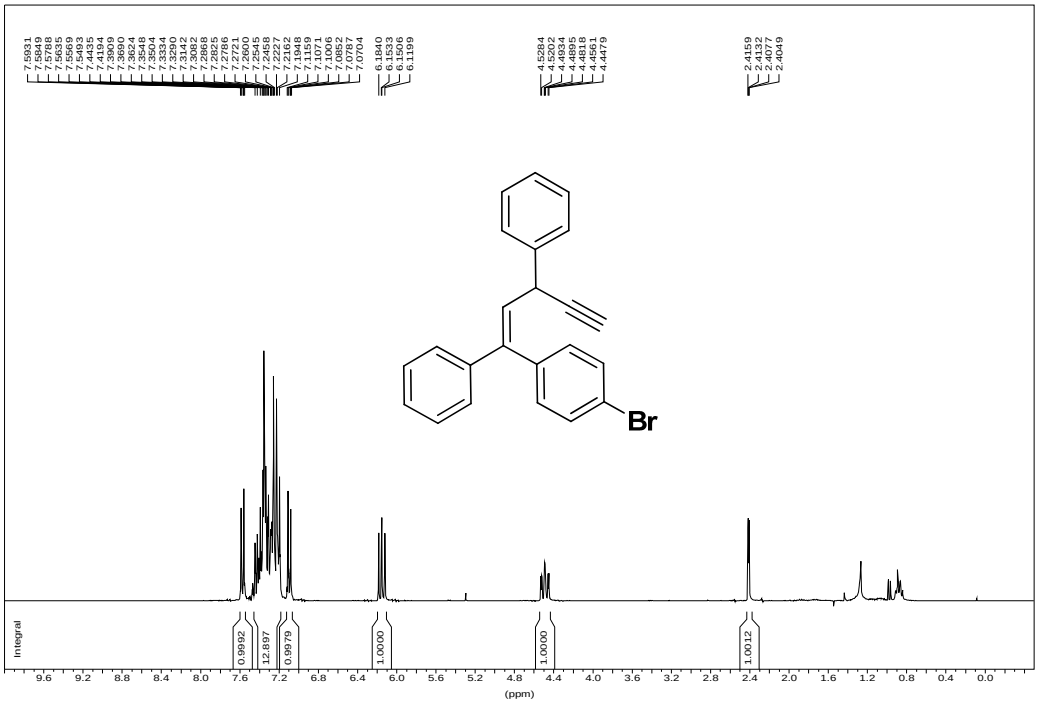

7.2600
7.2518
7.2211
7.2025
7.1964
7.1685
7.1115
7.0836
7.0266
7.0228
7.0105
7.0151
7.0113
6.9757
6.9642
6.9592
6.9472
6.1769
6.1435
4.7377
4.7328
4.7043
4.6993
2.4126
2.4066
2.3447
S
Me
Me
Integral
7.0744
2.0016
0.9986
1.0012
1.0010
1.0000
4.0024
3.0232
(ppm)

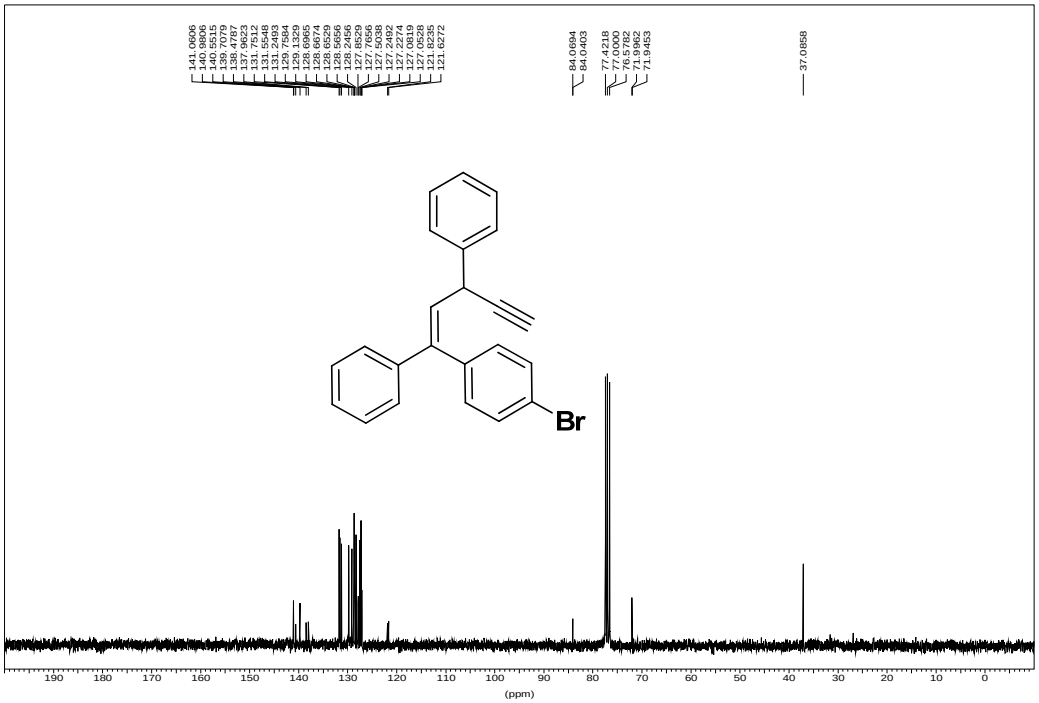

144.1444
142.4861
138.7769
137.4750
137.3368
136.8386
129.6956
129.1474
128.8492
127.5401
126.9774
126.0564
124.5291
124.4782
83.8657
77.4218
77.0000
76.5782
71.1452
32.7874
21.2451
21.0851
S
Me
Me
(ppm)

Compound **3c'**



Compound **3d'**


Br
Integral
0.9992
12.897
0.9979
1.0000
1.0000
1.0012
(ppm)


Br
84.0694
84.0403
77.4218
77.0000
76.5782
71.9453
37.0858
(ppm)