

Supporting Information

Palladium-Catalyzed Hydroarylation of 1,3-diynes with Arylboronic

Acids

Hongtao Shen^a, Xiaoyu Chen^b, Jianhua Qiu^a, Mengqi Chen^a, Bohai Zhang^b, and
Zhiyong Wu^{b,*}

^aTechnology Center, China Tobacco Henan Industrial Co., Ltd., Zhengzhou, 450000, China.

^bCollege of Tobacco Science, Henan Agricultural University, Zhengzhou, 450046, China.

* Correspondence: zhiyongwu@henau.edu.cn (Z.W.); smileyongyong062@163.com.

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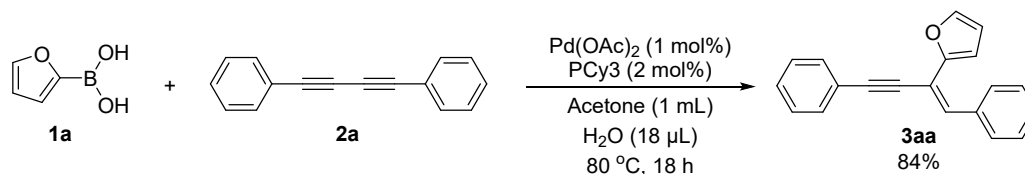
1. General information

All reactions were carried out under air atmosphere in a dried tube. Chemicals were purchased without further purification. Silica gel was purchased from Qing Dao Hai Yang Chemical Industry Co., Ltd., Analytical thin layer chromatography (TLC) was performed on precoated silica gel F₂₅₄ plates. Compounds were visualized by irradiation with UV light (254 nm).

Analytical information: ¹H NMR and ¹³C NMR spectra data were recorded by a BRUKER AVANCE III 400 MHz spectrometer (¹H 400 MHz, ¹³C 100 MHz), using CDCl₃ as the solvent with tetramethylsilane (TMS) as the internal standard at room temperature. ¹H NMR spectral data are given as chemical shifts in ppm followed by multiplicity (s- singlet; d- doublet; t- triplet; q- quartet; m- multiplet), number of protons and coupling constants. ¹³C NMR chemical shifts were expressed in ppm. HRMS data were obtained using AB SCIEX Triple TOF 5600+ high resolution mass spectrometer (USA). The products listed below were determined by ¹H and ¹³C NMR spectra.

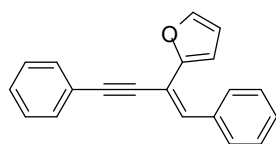
2. General experimental procedures

The preparation of (*Z*)-2-(1,4-diphenylbut-1-en-3-yn-2-yl)furan (**3aa**) is representative for the synthesis of the 23 products.



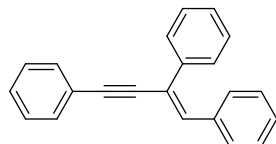
To a 10 mL tube, 2-furanboric acid **1a** (0.25mmol), 1,4-diphenylbutanediyne **2a** (0.25mmol), palladium acetate (0.0025mmol), tricyclohexylphosphine (0.005mmol), H₂O (0.25 mmol) and acetone (1 mL) were added under air atmosphere. The tube was sealed and the resulting solution was heated in 80 °C with vigorous stirring for 18 h. After the reaction, the crude product was purified to obtain the target reaction product **3aa**. In general, the identity and purity of the products were confirmed by ¹H and ¹³C NMR spectroscopy and HRMS.

3. Characterization data of compounds 3aa-3qa, 3bb-3be

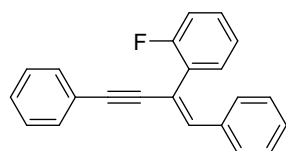


(Z)-2-(1,4-diphenylbut-1-en-3-yn-2-yl)furan (3aa) Purification by column chromatography on silica gel (*R_f* = 0.58, petroleum ether/dichloromethane = 50:1) yielded **3aa** (56.8 mg, 84%) as a brown solid; ¹H NMR (400 MHz, CDCl₃) ppm: 7.99

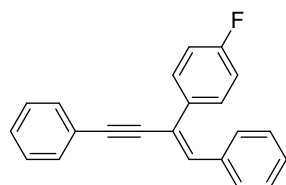
(d, $J = 7.6$ Hz, 2H), 7.61-7.51 (m, 2H), 7.43-7.34 (m, 8H), 6.68 (d, $J = 3.3$ Hz, 1H), 6.47 (dd, $J = 3.3, 1.80$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) ppm: 153.35, 142.52, 136.33, 131.61, 130.66, 129.10, 128.72, 128.53, 128.39, 128.35, 123.08, 111.83, 111.58, 108.73, 95.29, 86.10; HRMS (ESI) calcd. For $\text{C}_{20}\text{H}_{14}\text{O}$ $[\text{M}+\text{H}]^+$: 271.1117, found: 271.1125.



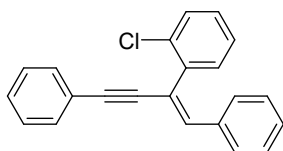
(E)-but-1-en-3-yne-1,2,4-triyltribenzene (3ba): Purification by column chromatography on silica gel ($R_f = 0.56$, petroleum ether/dichloromethane = 50:1) yielded **5a** (56.1 mg, 80%) as a brown solid; ^1H NMR (400 MHz, CDCl_3) ppm: 8.02 (d, $J = 7.4$ Hz, 2H), 7.82-7.77 (m, 2H), 7.57-7.51 (m, 2H), 7.43-7.39 (m, 4H), 7.38-7.29 (m, 5H), 7.22-7.21 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) ppm: 139.60, 136.75, 134.83, 131.61, 129.21, 128.55, 128.51, 128.40, 128.37, 127.98, 126.53, 123.41, 121.73, 97.00, 88.72; HRMS (ESI) calcd. For $\text{C}_{22}\text{H}_{16}$ $[\text{M}+\text{H}]^+$: 281.1325, found: 281.1334. CAS Number: 62677-52-5.



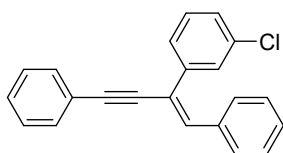
(Z)-(2-(2-fluorophenyl)but-1-en-3-yne-1,4-diyl)dibenzene (3ca) Purification by column chromatography on silica gel ($R_f = 0.54$, petroleum ether/dichloromethane = 40:1) yielded **5b** (64.1 mg, 86%) as a brown solid; ^1H NMR (400 MHz, CDCl_3) ppm: 8.01 (d, $J = 7.4$ Hz, 2H), 7.69 (td, $J = 7.8, 1.7$ Hz, 1H), 7.54-7.08 (m, 12H); ^{13}C NMR (100 MHz, CDCl_3) ppm: 161.15, 158.67, 139.14, 139.07, 136.52, 131.59, 130.58, 130.55, 129.29, 129.26, 129.20, 128.68, 128.57, 128.48, 128.36, 128.11, 127.99, 124.21, 124.18, 123.34, 116.39, 116.21, 116.20, 116.16, 95.91, 88.76; HRMS (ESI) calcd. For $\text{C}_{22}\text{H}_{15}\text{F}$ $[\text{M}+\text{H}]^+$: 299.1231, found: 299.1236.



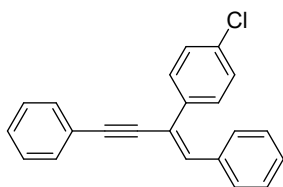
(E)-(2-(4-fluorophenyl)but-1-en-3-yne-1,4-diyl)dibenzene (3da) Purification by column chromatography on silica gel ($R_f = 0.54$, petroleum ether/dichloromethane = 40:1) yielded **5c** (60.4 mg, 81%) as a brown solid; ^1H NMR (400 MHz, CDCl_3) ppm: 8.00 (d, $J = 7.5$ Hz, 2H), 7.78-7.71 (m, 2H), 7.56-7.50 (m, 2H), 7.42-7.29 (m, 6H), 7.14 (s, 1H), 7.11-7.06 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) ppm: 163.90, 161.44, 136.59, 135.69, 135.66, 134.63, 134.61, 131.60, 129.15, 128.68, 128.54, 128.47, 128.40, 128.22, 128.14, 123.23, 120.66, 115.51, 115.30, 97.15, 88.50; HRMS (ESI) calcd. For $\text{C}_{22}\text{H}_{15}\text{F}$ $[\text{M}+\text{H}]^+$: 299.1231, found: 299.1234.



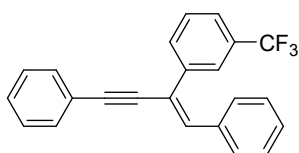
(Z)-2-(2-(2-chlorophenyl)but-1-en-3-yn-1,4-diyl)dibenzene (3ea) Purification by column chromatography on silica gel ($R_f = 0.57$, petroleum ether/dichloromethane = 40:1) yielded **3ea** (30.7 mg, 39%) as a brown solid; $^1\text{H NMR}$ (400 MHz, CDCl_3) ppm: 8.05-8.00 (m, 2H), 7.52-7.40 (m, 6H), 7.36-7.25 (m, 6H), 6.89 (s, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) ppm: 139.72, 139.29, 136.17, 132.82, 131.51, 130.76, 130.16, 129.04, 128.86, 128.72, 128.38, 126.89, 123.40, 119.72, 97.09, 88.56; HRMS (ESI) calcd. For $\text{C}_{22}\text{H}_{15}\text{Cl}$ $[\text{M}+\text{H}]^+$: 315.0936, found:315.0939.



(E)-2-(3-chlorophenyl)but-1-en-3-yn-1,4-diyl)dibenzene (3fa) Purification by column chromatography on silica gel ($R_f = 0.57$, petroleum ether/dichloromethane = 40:1) yielded **3fa** (51.2 mg, 65%) as a brown solid; $^1\text{H NMR}$ (400 MHz, CDCl_3) ppm: 8.01 (d, $J = 7.5$ Hz, 2H), 7.76 (t, $J = 1.7$ Hz, 1H), 7.66 (dt, $J = 7.3, 1.7$ Hz, 1H), 7.57-7.51 (m, 2H), 7.43-7.27 (m, 8H), 7.20 (s, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) ppm: 141.45, 136.34, 135.61, 134.52, 131.64, 129.73, 129.31, 128.75, 128.55, 128.43, 127.92, 126.64, 124.67, 123.12, 120.41, 97.34, 88.08; HRMS (ESI) calcd. For $\text{C}_{22}\text{H}_{15}\text{Cl}$ $[\text{M}+\text{H}]^+$: 315.0936, found:315.0928

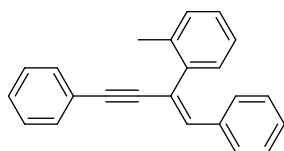


(E)-2-(4-chlorophenyl)but-1-en-3-yn-1,4-diyl)dibenzene (3ga) Purification by column chromatography on silica gel ($R_f = 0.57$, petroleum ether/dichloromethane = 40:1) yielded **3ga** (52.7 mg, 67%) as a brown solid; $^1\text{H NMR}$ (400 MHz, CDCl_3) ppm: 8.00 (d, $J = 7.5$ Hz, 2H), 7.74-7.69 (m, 2H), 7.56-7.51 (m, 2H), 7.43-7.31 (m, 8H), 7.18 (s, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3) ppm: 138.06, 136.46, 134.99, 133.79, 131.61, 129.31, 129.23, 128.73, 128.67, 128.62, 128.55, 128.42, 128.32, 127.97, 127.78, 123.16, 120.56, 97.28, 88.24; HRMS (ESI) calcd. For $\text{C}_{22}\text{H}_{15}\text{Cl}$ $[\text{M}+\text{H}]^+$: 315.0936, found:315.0939.

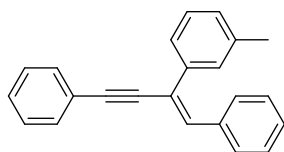


(E)-2-(3-(trifluoromethyl)phenyl)but-1-en-3-yn-1,4-diyl)dibenzene (3ha)

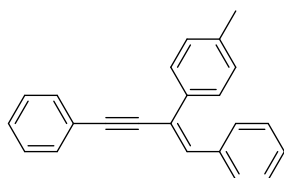
Purification by column chromatography on silica gel ($R_f = 0.60$, petroleum ether/dichloromethane = 40:1) yielded **3ha** (50.5 mg, 58%) as a brown solid; ^1H NMR (400 MHz, CDCl_3) ppm: 7.98 (d, $J = 7.4$ Hz, 2H), 7.73 (d, $J = 7.9$ Hz, 1H), 7.55-7.53 (m, 2H), 7.46-7.40 (m, 5H), 7.36-7.30 (m, 4H), 6.76 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3) ppm: 140.16, 138.76, 138.75, 136.14, 131.78, 131.47, 131.25, 128.98, 128.71, 128.53, 128.40, 128.38, 128.25, 127.79, 126.59, 126.54, 123.29, 119.55, 97.50, 88.71; HRMS (ESI) calcd. For $\text{C}_{23}\text{H}_{15}\text{F}_3$ $[\text{M}+\text{H}]^+$: 349.1199, found:349.1205.



(Z)-2-(o-tolyl)but-1-en-3-yne-1,4-diyl dibenzene (3ia) Purification by column chromatography on silica gel ($R_f = 0.53$, petroleum ether/dichloromethane = 40:1) yielded **3ia** (61.1 mg, 83%) as a brown solid; ^1H NMR (400 MHz, CDCl_3) ppm: 8.00 (d, $J = 7.4$ Hz, 2H), 7.47-7.36(m, 5H), 7.33-7.30 (m, 4H), 7.25-7.23 (m, 3H), 6.77 (s, 1H), 2.52 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) ppm: 140.97, 138.30, 136.66, 136.12, 131.64, 131.50, 130.59, 129.14, 128.94, 128.47, 128.43, 127.96, 127.83, 126.11, 125.84, 123.58, 122.30, 97.49, 89.19, 20.40; HRMS (ESI) calcd. For $\text{C}_{23}\text{H}_{18}$ $[\text{M}+\text{H}]^+$: 295.1482, found:295.1485.

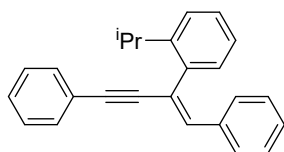


(E)-2-(m-tolyl)but-1-en-3-yne-1,4-diyl dibenzene (3ja) Purification by column chromatography on silica gel ($R_f = 0.53$, petroleum ether/dichloromethane = 40:1) yielded **3ja** (39.0 mg, 53%) as a brown solid; ^1H NMR (400 MHz, CDCl_3) ppm: 8.02 (d, $J = 7.4$ Hz, 2H), 7.62-7.57 (m, 2H), 7.57-7.53 (m, 2H), 7.43-7.29 (m, 7H), 7.21 (s, 1H), 7.15 (d, $J = 7.5$ Hz, 1H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) ppm: 139.60, 138.12, 136.80, 134.73, 131.60, 129.18, 128.77, 128.51, 128.49, 128.44, 128.34, 128.32, 127.20, 123.73, 123.47, 121.81, 96.87, 88.83, 21.62; HRMS (ESI) calcd. For $\text{C}_{23}\text{H}_{18}$ $[\text{M}+\text{H}]^+$: 295.1482, found:295.1482.

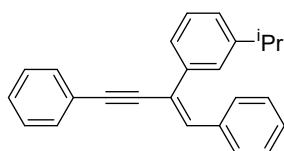


(E)-2-(p-tolyl)but-1-en-3-yne-1,4-diyl dibenzene (3ka) Purification by column chromatography on silica gel ($R_f = 0.53$, petroleum ether/dichloromethane = 40:1) yielded **3ka** (47.1 mg, 64%) as a brown solid; ^1H NMR (400 MHz, CDCl_3) ppm: 8.01 (d, $J = 7.5$ Hz, 2H), 7.69 (d, $J = 8.2$ Hz, 2H), 7.55-7.53 (m, 2H), 7.42-7.28 (m, 6H), 7.22 (d, $J = 7.5$ Hz, 2H), 7.19 (s, 1H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) ppm:

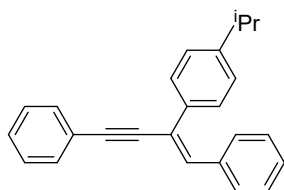
137.90, 136.88, 136.78, 134.03, 131.61, 131.40, 129.26, 129.15, 128.50, 128.34, 128.24, 127.97, 127.82, 126.41, 123.49, 121.62, 96.86, 88.87, 29.77, 21.23; HRMS (ESI) calcd. For C₂₃H₁₈ [M+H]⁺: 295.1482, found:295.1486.



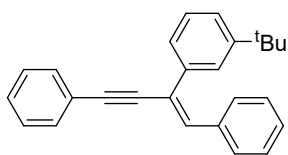
(Z)-2-(2-isopropylphenyl)but-1-en-3-yn-1,4-diyl dibenzene (3la) Purification by column chromatography on silica gel ($R_f = 0.55$, petroleum ether/dichloromethane = 40:1) yielded **3la** (58.1 mg, 72%) as a brown solid; ¹H NMR (400 MHz, CDCl₃) ppm: 8.01 (d, $J = 7.5$ Hz, 2H), 7.45-7.29 (m, 11H), 7.22-7.18(m, 1H), 6.75 (s, 1H), 3.60 (m, 1H), 1.28 (d, $J = 6.8$ Hz, 6H); ¹³C NMR (100 MHz, CDCl₃) ppm: 147.04, 140.10, 138.21, 136.65, 131.44, 129.32, 128.89, 128.45, 128.42, 128.24, 125.87, 123.58, 122.26, 97.64, 89.67, 29.92, 24.29; HRMS (ESI) calcd. For C₂₅H₂₂ [M+H]⁺: 323.1795, found:323.1802.



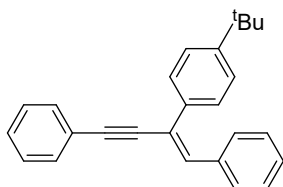
(E)-2-(3-isopropylphenyl)but-1-en-3-yn-1,4-diyl dibenzene (3ma) Purification by column chromatography on silica gel ($R_f = 0.55$, petroleum ether/dichloromethane = 40:1) yielded **3ma** (37.1 mg, 46%) as a brown solid; ¹H NMR (400 MHz, CDCl₃) ppm: 8.03 (d, $J = 7.5$ Hz, 2H), 7.66 (s, 1H), 7.61 (d, $J = 7.8$ Hz, 1H), 7.56-7.53 (m, 2H), 7.44-7.21 (m, 9H), 2.98 (m, 1H), 1.31 (d, $J = 6.9$ Hz, 6H); ¹³C NMR (100 MHz, CDCl₃) ppm: 149.14, 139.61, 136.83, 134.65, 131.57, 129.17, 128.49, 128.33, 128.29, 126.14, 124.77, 124.11, 123.49, 122.03, 96.89, 88.93, 34.29, 24.09; HRMS (ESI) calcd. For C₂₅H₂₂ [M+H]⁺: 323.1795, found:323.1803.



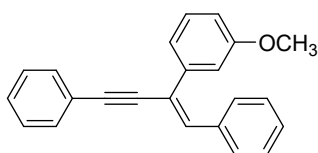
(E)-2-(4-isopropylphenyl)but-1-en-3-yn-1,4-diyl dibenzene (3na) Purification by column chromatography on silica gel ($R_f = 0.55$, petroleum ether/dichloromethane = 40:1) yielded **3na** (50.0 mg, 62%) as a brown solid; ¹H NMR (400 MHz, CDCl₃) ppm: 8.01 (d, $J = 7.4$ Hz, 2H), 7.76-7.69 (m, 2H), 7.54 (dt, $J = 4.7, 3.0$ Hz, 2H), 7.41 (dd, $J = 10.5, 4.8$ Hz, 2H), 7.38-7.33 (m, 3H), 7.33-7.29 (m, 1H), 7.28 (d, $J = 8.2$ Hz, 2H), 7.19 (s, 1H), 3.02-2.88 (m, 1H), 1.28 (t, $J = 5.1$ Hz, 6H); ¹³C NMR (100 MHz, CDCl₃) ppm: 148.89, 137.18, 136.88, 134.13, 131.60, 129.14, 128.48, 128.33, 128.22, 126.63, 126.50, 123.49, 121.64, 96.82, 88.89, 33.91, 24.01; HRMS (ESI) calcd. For C₂₅H₂₂ [M+H]⁺: 323.1805, found:323.1809.



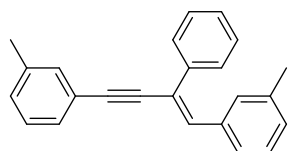
(E)-2-(3-(tert-butyl)phenyl)but-1-en-3-yne-1,4-diyl dibenzene (30a) Purification by column chromatography on silica gel ($R_f = 0.58$, petroleum ether/dichloromethane = 20:1) yielded **30a** (69.8 mg, 83%) as a brown solid; ^1H NMR (400 MHz, CDCl_3) ppm: 8.03 (d, $J = 7.4$ Hz, 2H), 7.85-7.84 (m, 1H), 7.60 (dt, $J = 7.1, 1.7$ Hz, 1H), 7.56-7.51 (m, 2H), 7.41-7.20 (m, 8H), 7.20 (s, 1H), 1.39 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) ppm: 151.40, 139.37, 136.88, 134.65, 131.58, 129.21, 128.55, 128.37, 128.33, 128.28, 125.14, 123.82, 123.68, 123.54, 122.30, 96.98, 89.06, 34.92, 31.48; HRMS (ESI) calcd. For $\text{C}_{26}\text{H}_{24}$ $[\text{M}+\text{H}]^+$: 337.1951, found:337.1945.



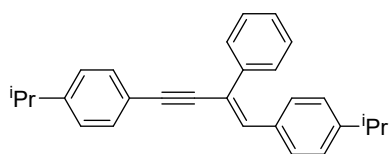
(E)-2-(4-(tert-butyl)phenyl)but-1-en-3-yne-1,4-diyl dibenzene (3pa) Purification by column chromatography on silica gel ($R_f = 0.58$, petroleum ether/dichloromethane = 40:1) yielded **3pa** (54.7 mg, 65%) as a brown solid; ^1H NMR (400 MHz, CDCl_3) ppm: 8.01 (d, $J = 7.5$ Hz, 2H), 7.75-7.71 (m, 2H), 7.56-7.53 (m, 2H), 7.45-7.25 (m, 8H), 7.20 (d, $J = 4.2$ Hz, 1H), 1.35 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) ppm: 151.14, 136.89, 136.78, 134.18, 131.61, 129.16, 128.49, 128.35, 128.25, 126.24, 125.51, 123.51, 121.55, 96.86, 88.89, 34.66, 31.38; HRMS (ESI) calcd. For $\text{C}_{26}\text{H}_{24}$ $[\text{M}+\text{H}]^+$: 337.1951, found:337.1954.



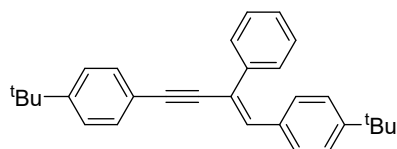
(E)-2-(3-methoxyphenyl)but-1-en-3-yne-1,4-diyl dibenzene (3qa) Purification by column chromatography on silica gel ($R_f = 0.59$, petroleum ether/dichloromethane = 20:1) yielded **3qa** (67.5 mg, 87%) as a brown solid; ^1H NMR (400 MHz, CDCl_3) ppm: 8.01 (d, $J = 7.4$ Hz, 2H), 7.55-7.53 (m, 2H), 7.42-7.29 (m, 9H), 7.22 (s, 1H), 6.88 (ddd, $J = 8.0, 2.5, 0.9$ Hz, 1H) 3.85 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) ppm: 159.80, 141.12, 136.68, 135.01, 131.61, 129.52, 129.27, 128.60, 128.53, 128.47, 128.39, 123.40, 121.58, 118.99, 113.42, 112.48, 97.00, 88.71, 55.38; HRMS (ESI) calcd. For $\text{C}_{23}\text{H}_{18}\text{O}$ $[\text{M}+\text{H}]^+$: 311.1431, found:311.1429.



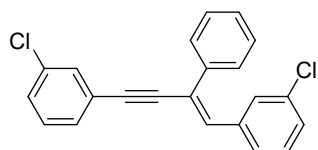
(E)-3,3'-(2-phenylbut-1-en-3-yne-1,4-diyl)bis(methylbenzene) (3bb) Purification by column chromatography on silica gel ($R_f = 0.51$, petroleum ether/dichloromethane = 40:1) yielded **3bb** (44.0 mg, 57%) as a brown solid; ^1H NMR (400 MHz, CDCl_3) ppm: 7.91 (d, $J = 0.3$ Hz, 1H), 7.80-7.78 (m, 3H), 7.43-7.22 (m, 7H), 7.19 (s, 1H), 7.15 (t, $J = 7.9$ Hz, 2H), 2.40 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) ppm: 139.71, 138.18, 137.77, 136.72, 134.83, 132.16, 129.79, 129.43, 129.19, 128.65, 128.52, 128.40, 128.26, 127.88, 126.51, 123.30, 121.54, 97.25, 88.57, 21.61, 21.30; HRMS (ESI) calcd. For $\text{C}_{24}\text{H}_{20}$ $[\text{M}+\text{H}]^+$: 309.1638, found:309.1638.



(E)-4,4'-(2-phenylbut-1-en-3-yne-1,4-diyl)bis(isopropylbenzene) (3bc) Purification by column chromatography on silica gel ($R_f = 0.61$, petroleum ether/dichloromethane = 40:1) yielded **3bc** (63.8 mg, 70%) as a light yellow solid; ^1H NMR (400 MHz, CDCl_3) ppm: 7.98 (d, $J = 8.3$ Hz, 2H), 7.82-7.75 (m, 2H), 7.53-7.46 (m, 2H), 7.43-7.36 (m, 2H), 7.32-7.21 (5H), 7.18 (s, 1H), 2.97-2.89 (m, 2H), 1.28 (d, $J = 5.6$ Hz, 3H), 1.26 (d, $J = 5.5$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) ppm: 149.58, 149.38, 139.93, 134.47, 134.44, 131.62, 129.27, 128.49, 127.74, 126.66, 126.49, 126.47, 120.88, 120.80, 97.32, 88.29, 34.19, 34.11, 23.95, 23.87.



(E)-4,4'-(2-phenylbut-1-en-3-yne-1,4-diyl)bis(tert-butylbenzene) (3bd) Purification by column chromatography on silica gel ($R_f = 0.62$, petroleum ether/dichloromethane = 40:1) yielded **3bd** (84.4 mg, 86%) as a light yellow solid; ^1H NMR (400 MHz, CDCl_3) ppm: 8.00 (d, $J = 8.4$ Hz, 2H), 7.80-7.78 (m, 2H), 7.53-7.48 (m, 2H), 7.45-7.38 (m, 7H), 7.33-7.28 (m, 2H), 7.18 (s, 1H), 1.35 (s, 9H), 1.34 (s, 9H); ^{13}C NMR (100 MHz, CDCl_3) ppm: 151.81, 151.60, 139.93, 134.30, 134.03, 131.34, 128.99, 128.47, 127.73, 126.49, 125.51, 125.32, 120.84, 120.54, 97.31, 88.32, 34.89, 34.82, 31.41, 31.31, 31.23.

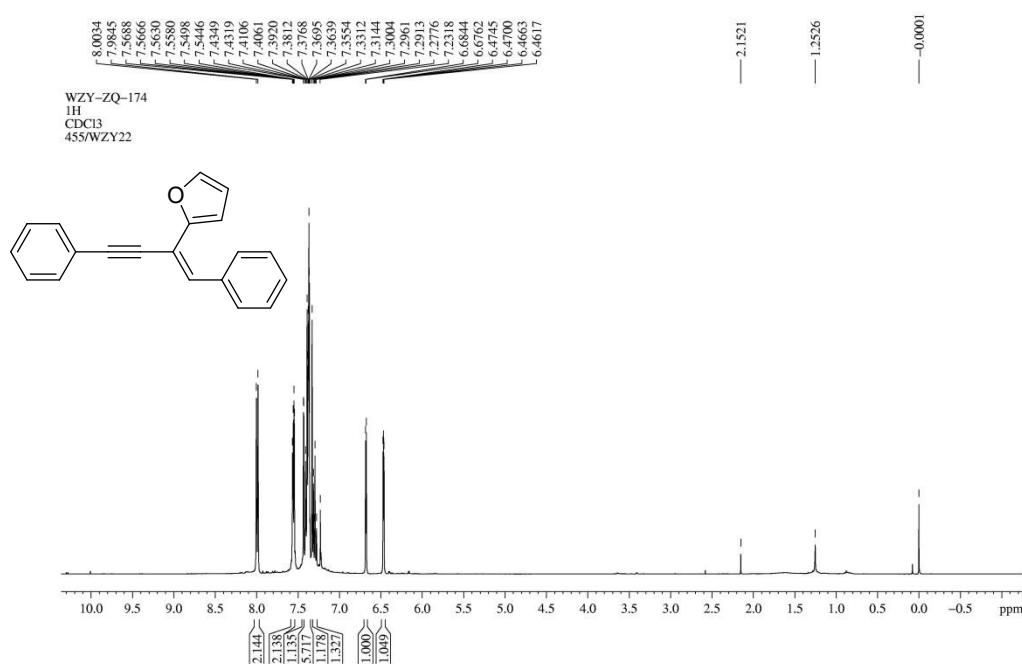


(E)-3,3'-(2-phenylbut-1-en-3-yne-1,4-diyl)bis(chlorobenzene) (3be) Purification by column chromatography on silica gel ($R_f = 0.59$, petroleum ether/dichloromethane =

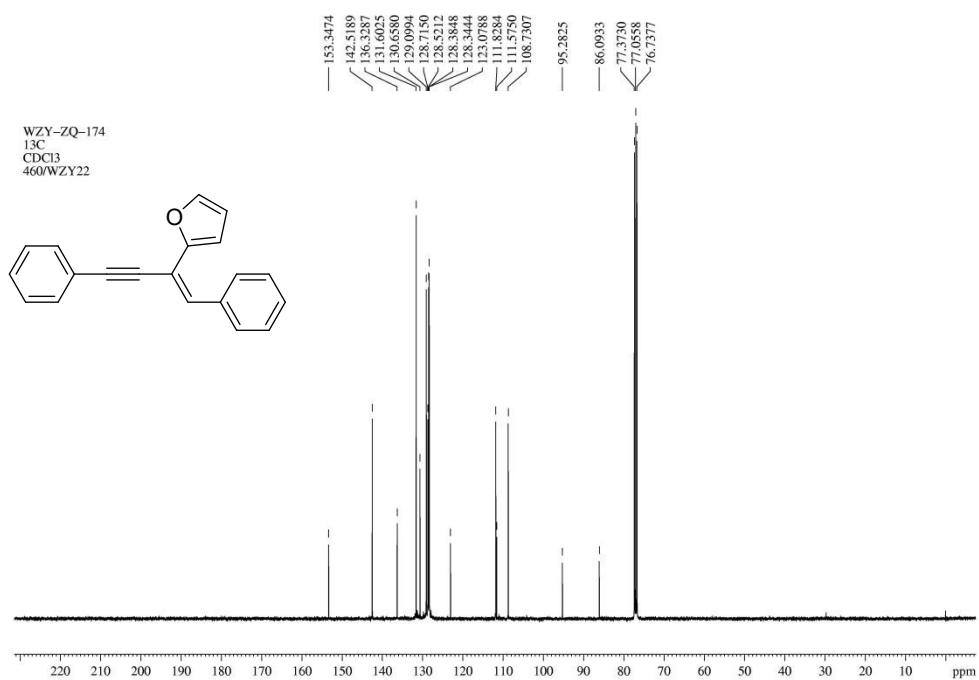
40:1) yielded **3be** (62.0 mg, 71%) as a light yellow solid; ^1H NMR (400 MHz, CDCl_3) ppm: 8.19 (s, 1H), 7.78-7.71 (m, 2H), 7.67 (d, $J = 7.2$ Hz, 1H), 7.55 (d, $J = 1.7$ Hz, 1H), 7.47-7.38 (m, 3H), 7.38-7.27 (m, 6H), 7.15 (s, 1H); ^{13}C NMR (100 MHz, CDCl_3) ppm: 138.79, 138.29, 134.44, 134.29, 133.66, 131.47, 129.79, 129.78, 129.59, 129.04, 128.68, 128.58, 128.54, 128.42, 128.38, 127.69, 126.50, 124.70, 122.86, 96.25, 89.35; HRMS (ESI) calcd. For $\text{C}_{22}\text{H}_{14}\text{Cl}_2$ $[\text{M}+\text{H}]^+$: 349.0546, found:349.0548.

4. ^1H NMR, ^{13}C NMR spectra for **3aa-3qa**, **3bb-3be**

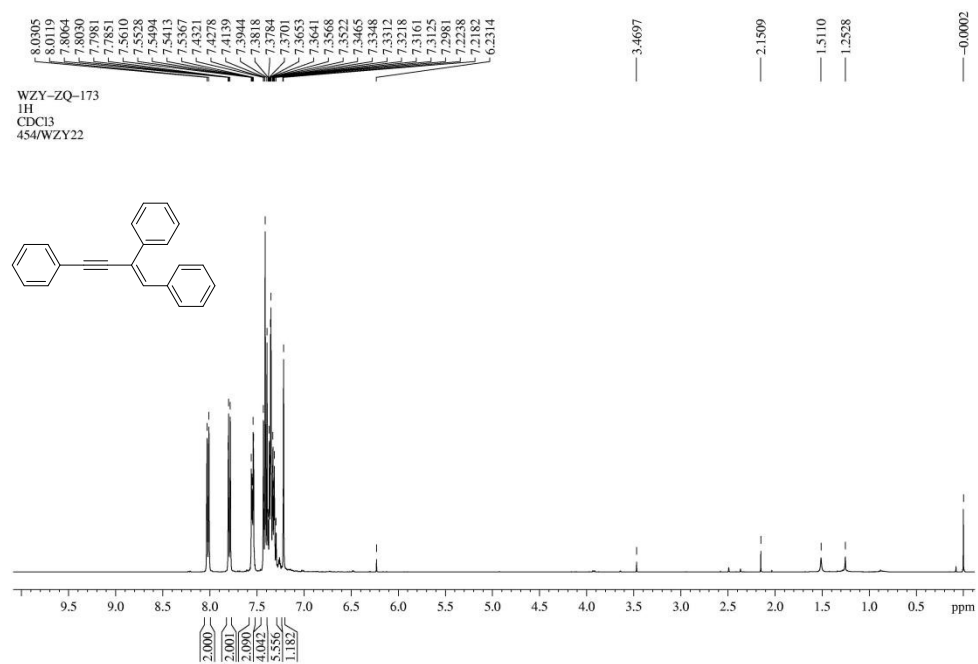
^1H NMR spectrum of compound **3aa**



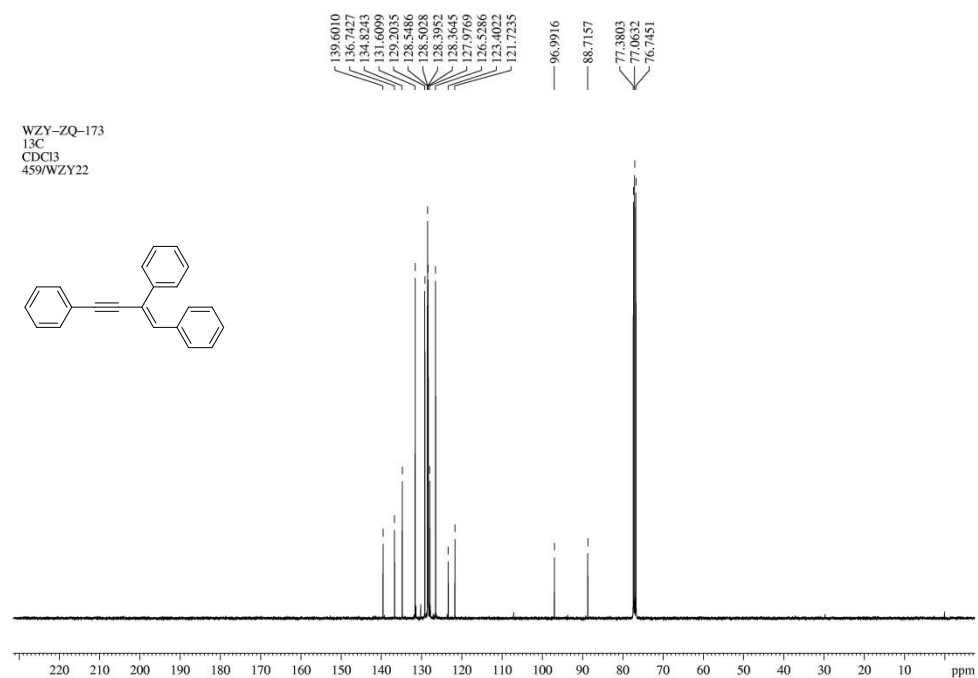
^{13}C NMR spectrum of compound **3aa**



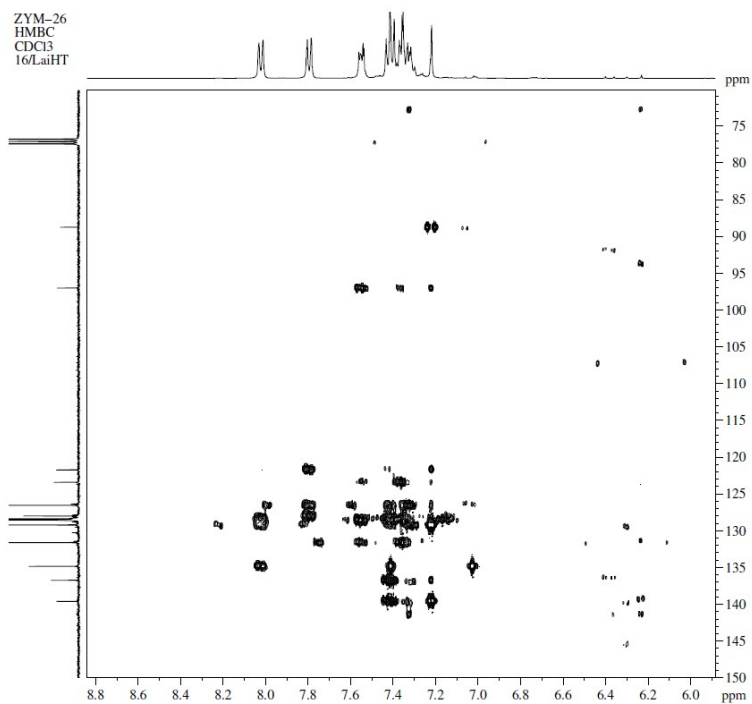
¹H NMR spectrum of compound **3ba**



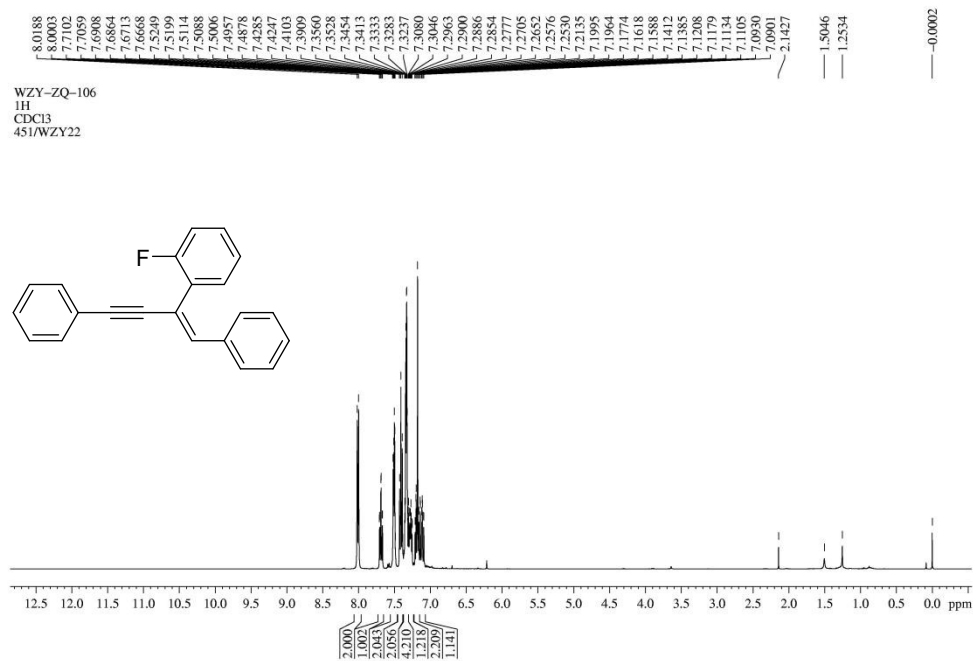
¹³C NMR spectrum of compound **3ba**



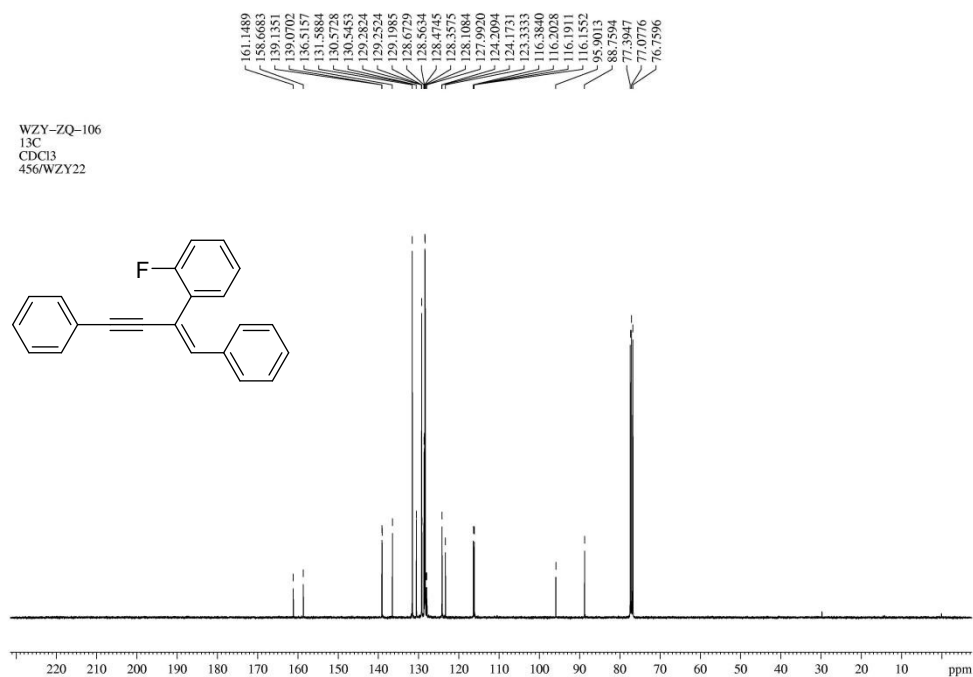
HMBC NMR spectrum of compound **3ba**



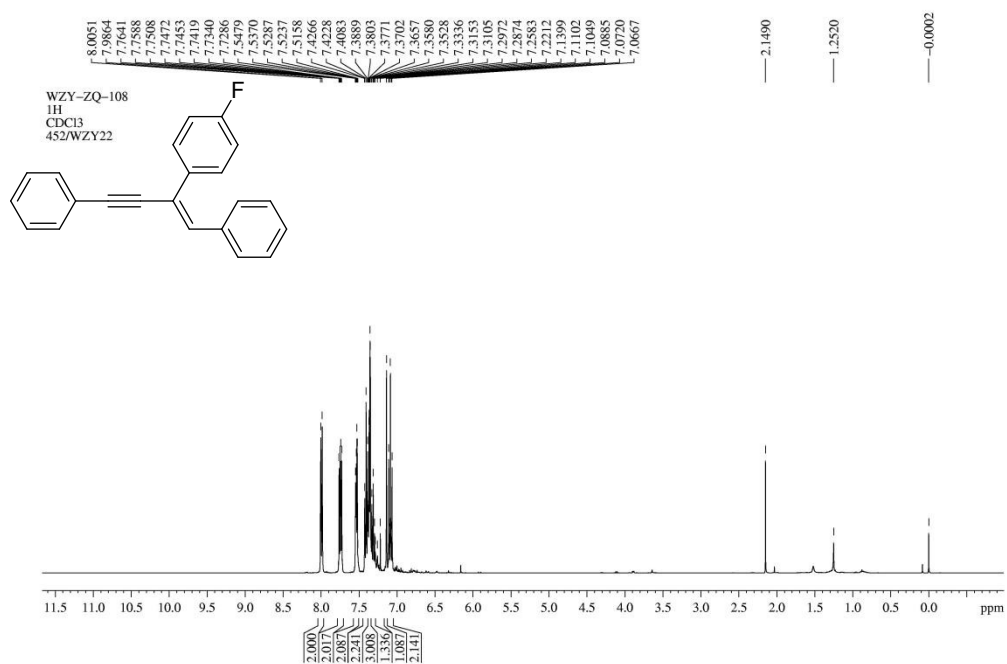
¹H NMR spectrum of compound **3ca**



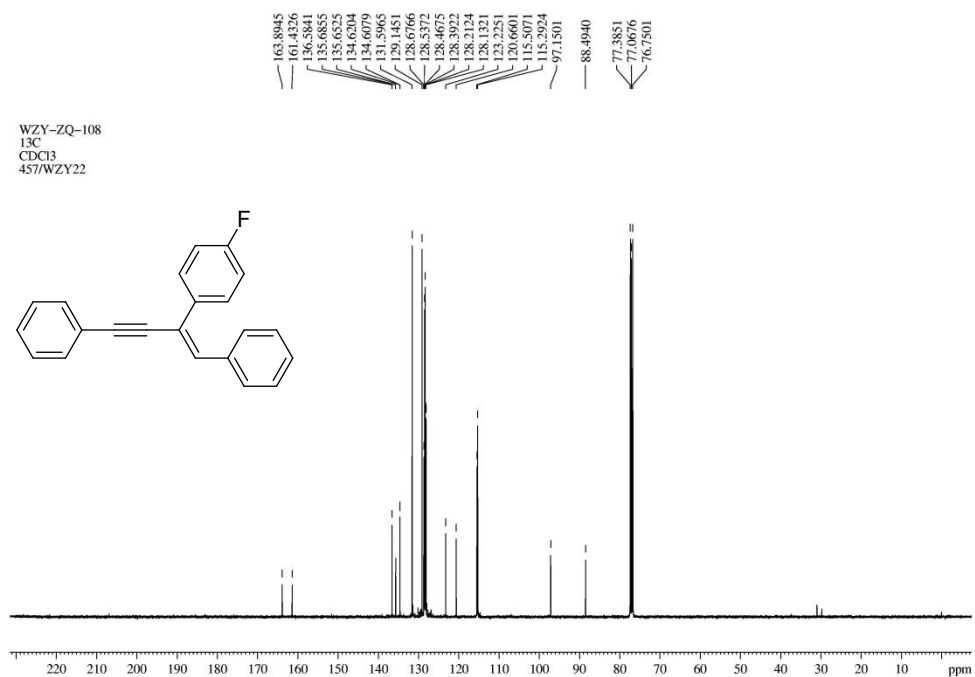
¹³C NMR spectrum of compound **3ca**



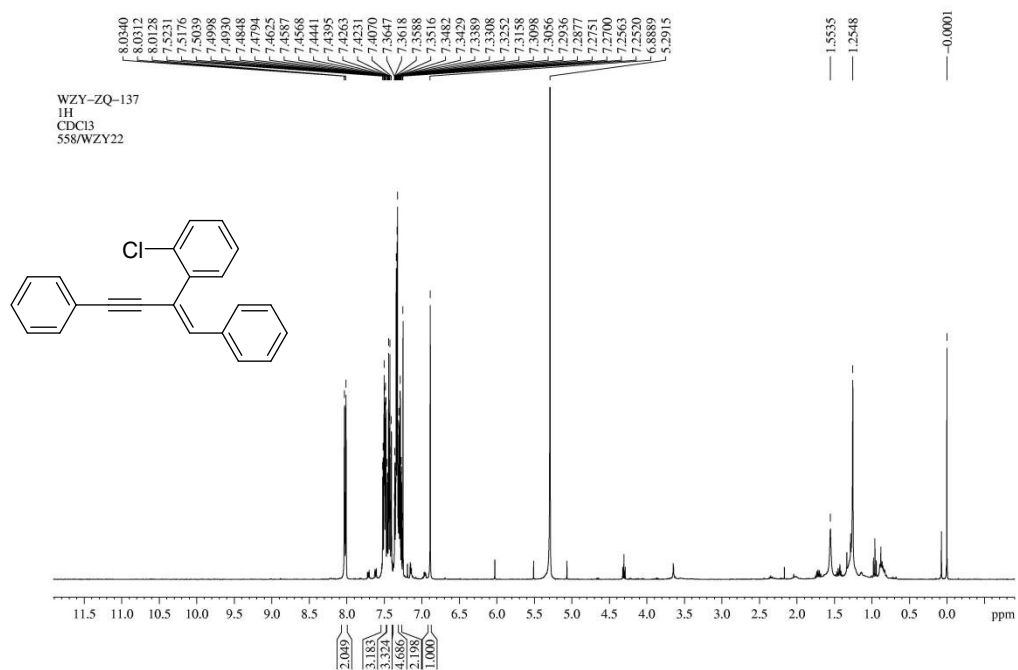
¹H NMR spectrum of compound **3da**



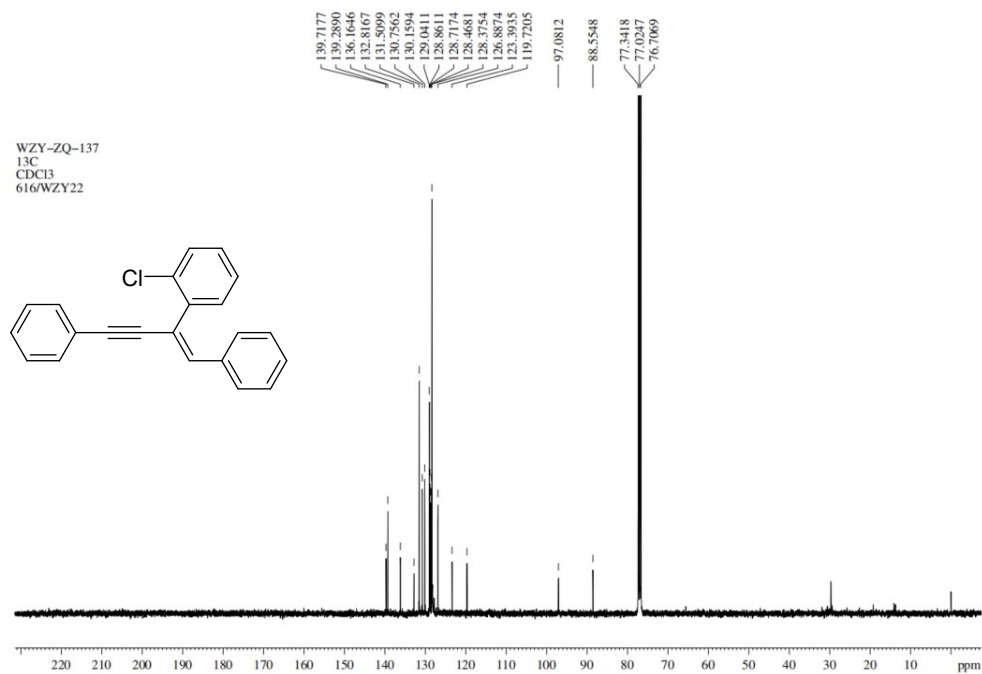
¹³C NMR spectrum of compound **3da**



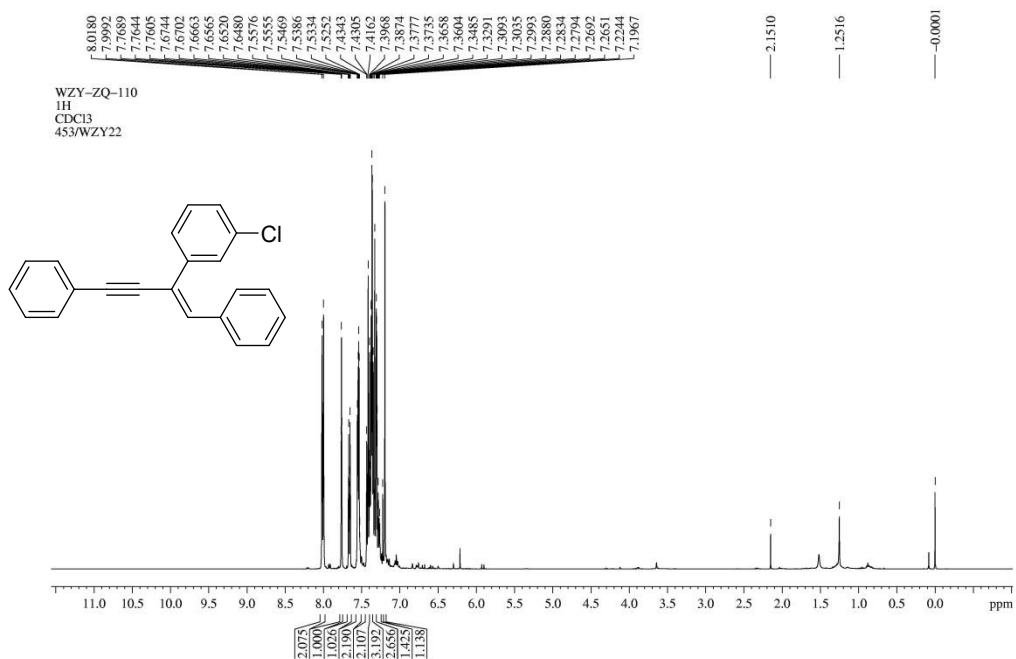
¹H NMR spectrum of compound **3ea**



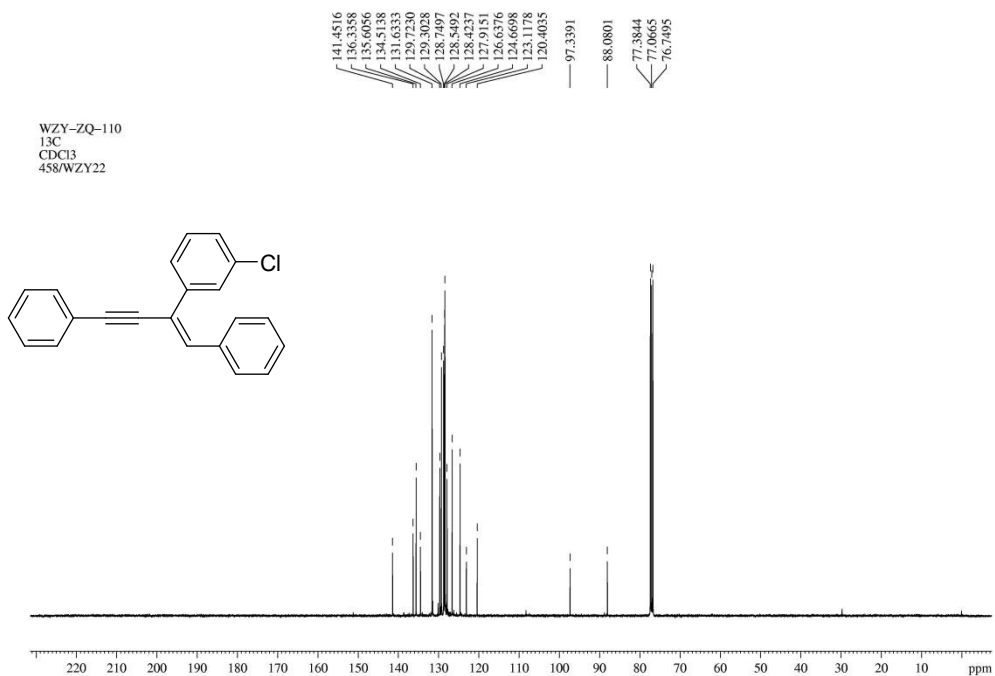
¹³C NMR spectrum of compound **3ea**



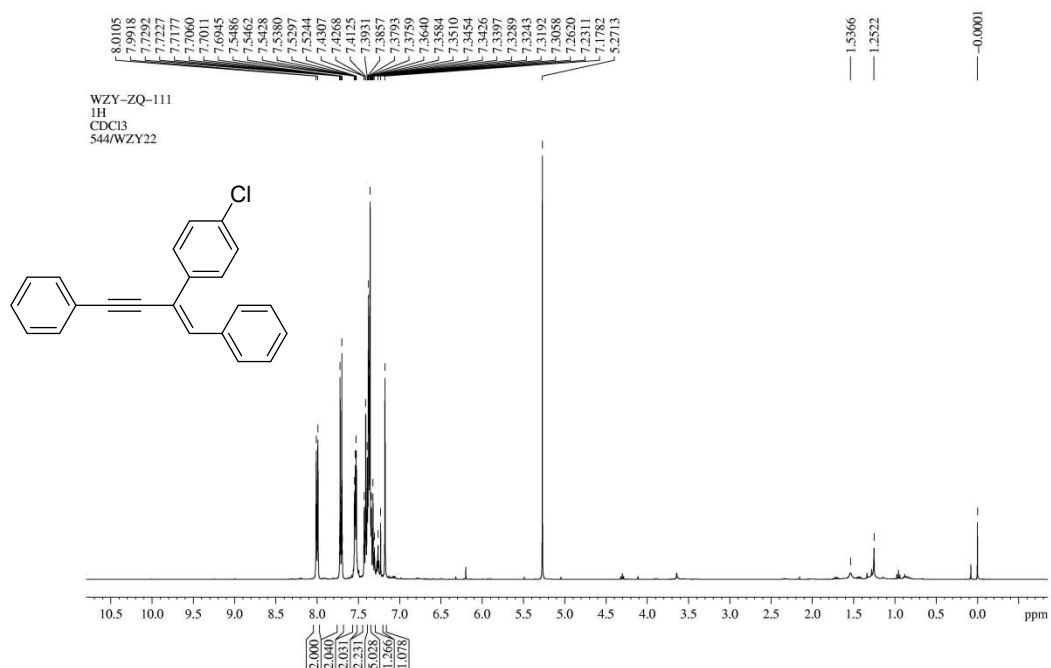
¹H NMR spectrum of compound **3fa**



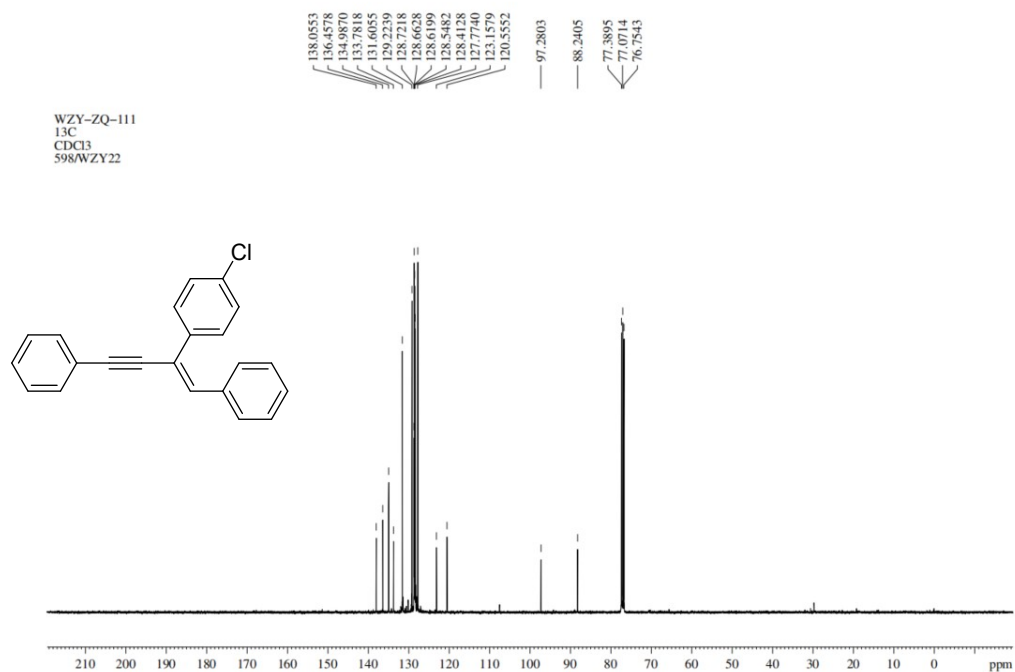
¹³C NMR spectrum of compound **3fa**



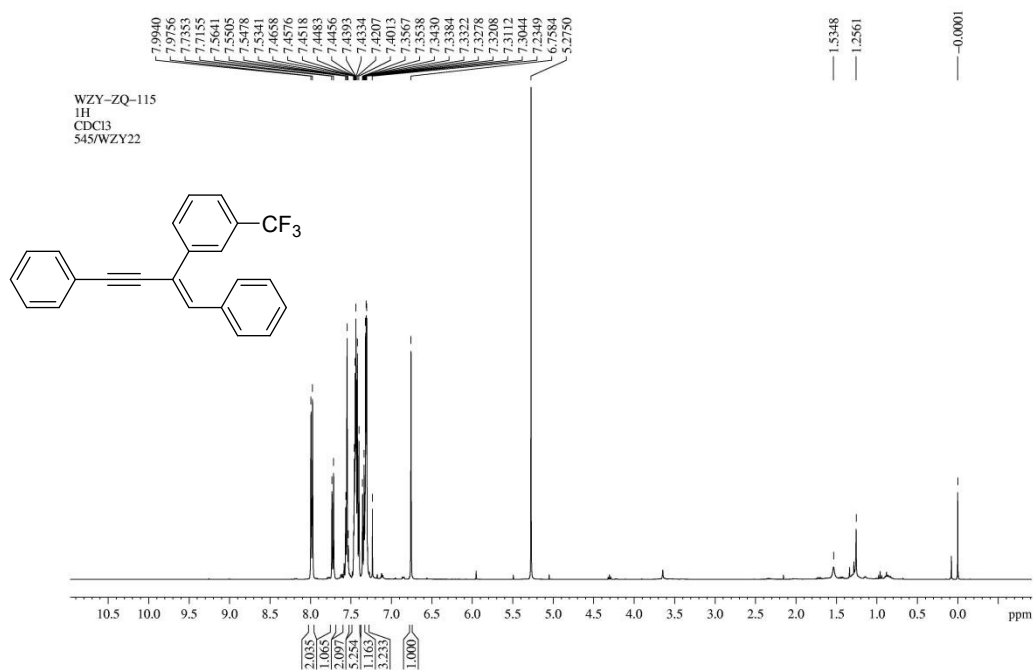
¹H NMR spectrum of compound **3ga**



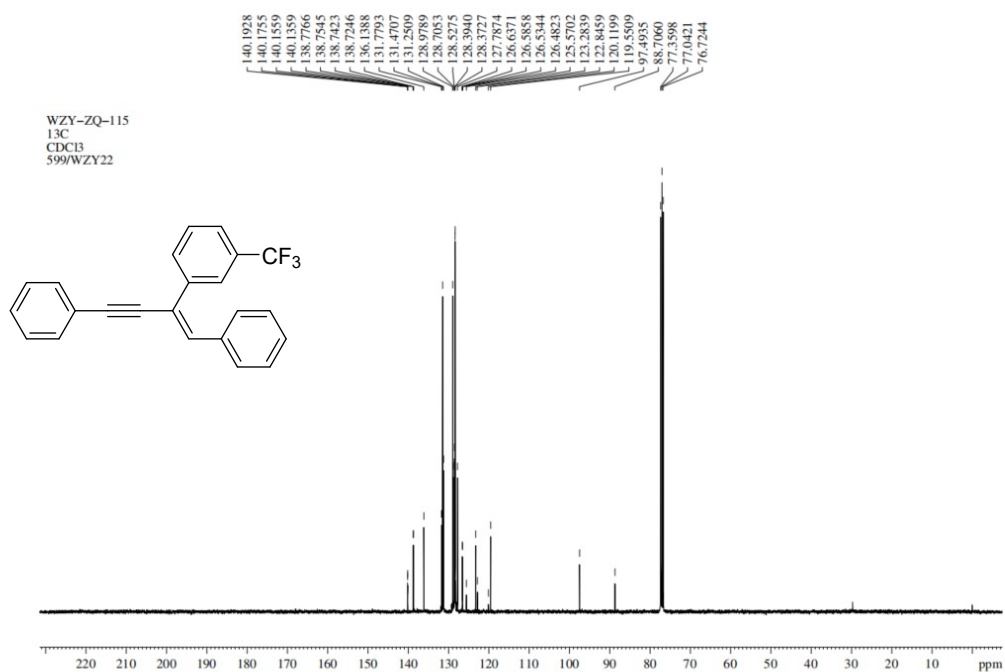
¹³C NMR spectrum of compound **3ga**



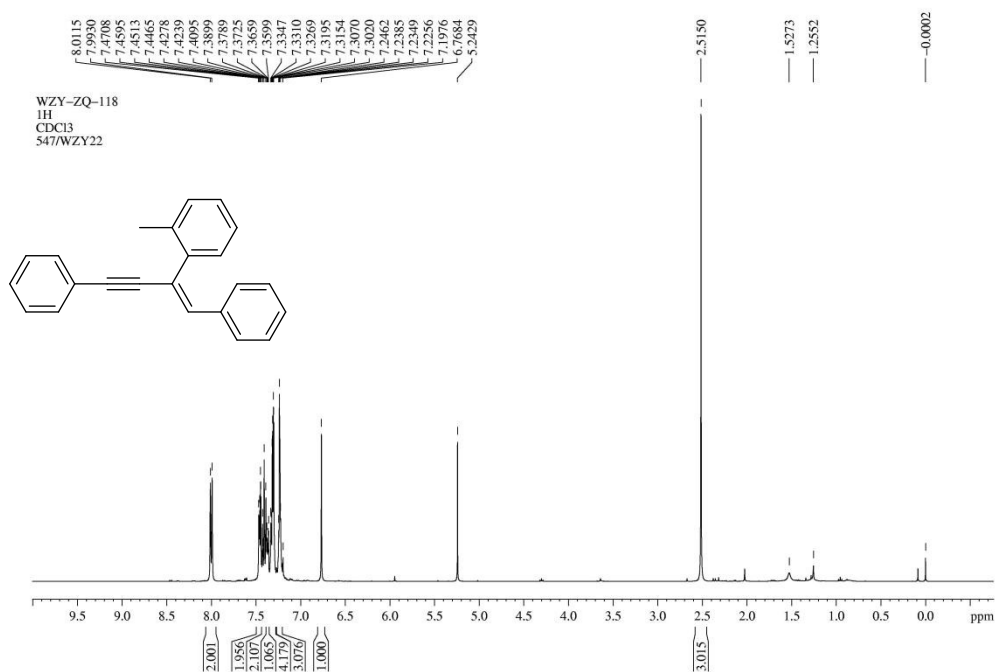
¹H NMR spectrum of compound **3ha**



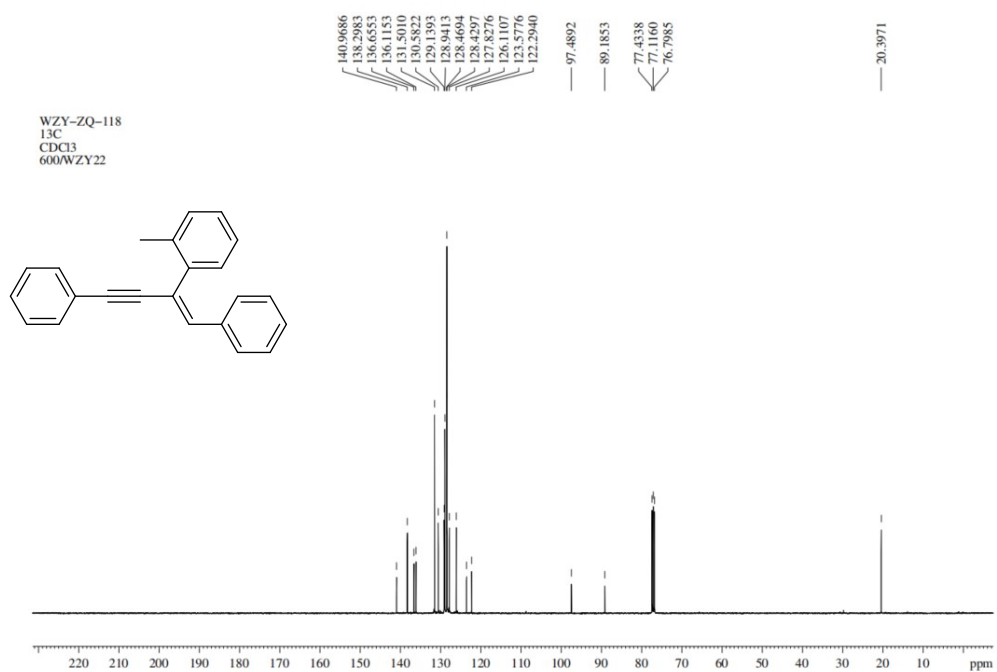
¹³C NMR spectrum of compound **3ha**



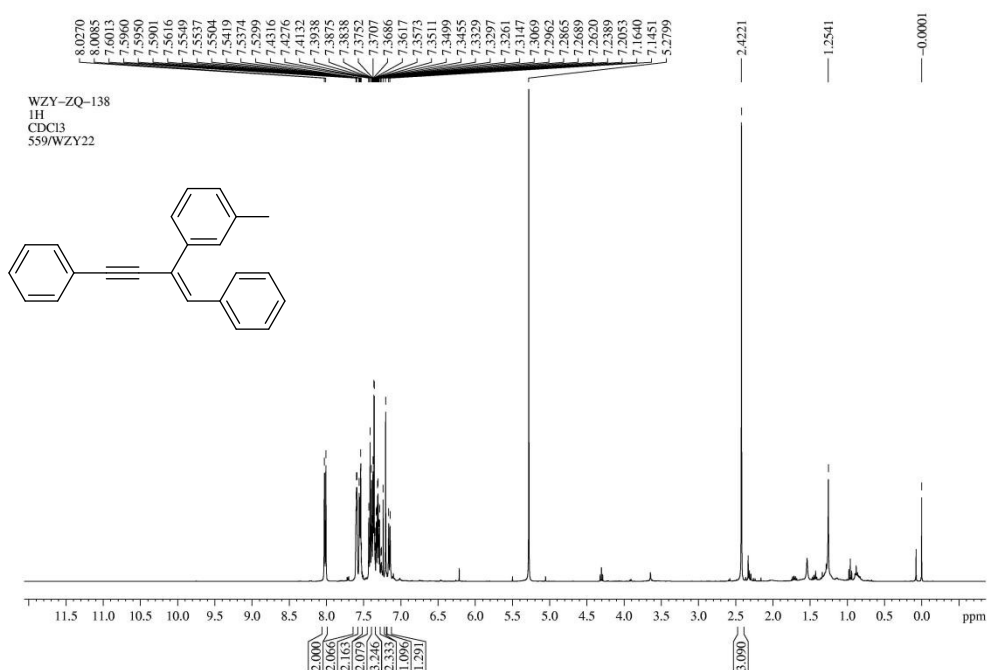
¹H NMR spectrum of compound **3ia**



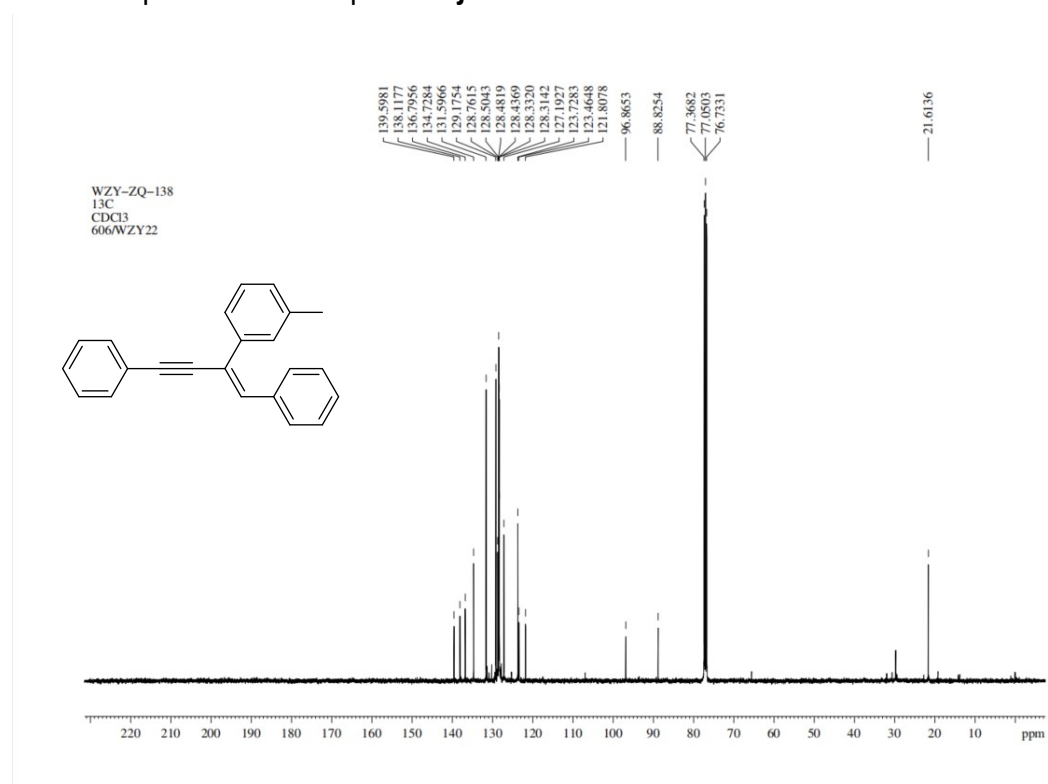
¹³C NMR spectrum of compound **3ia**



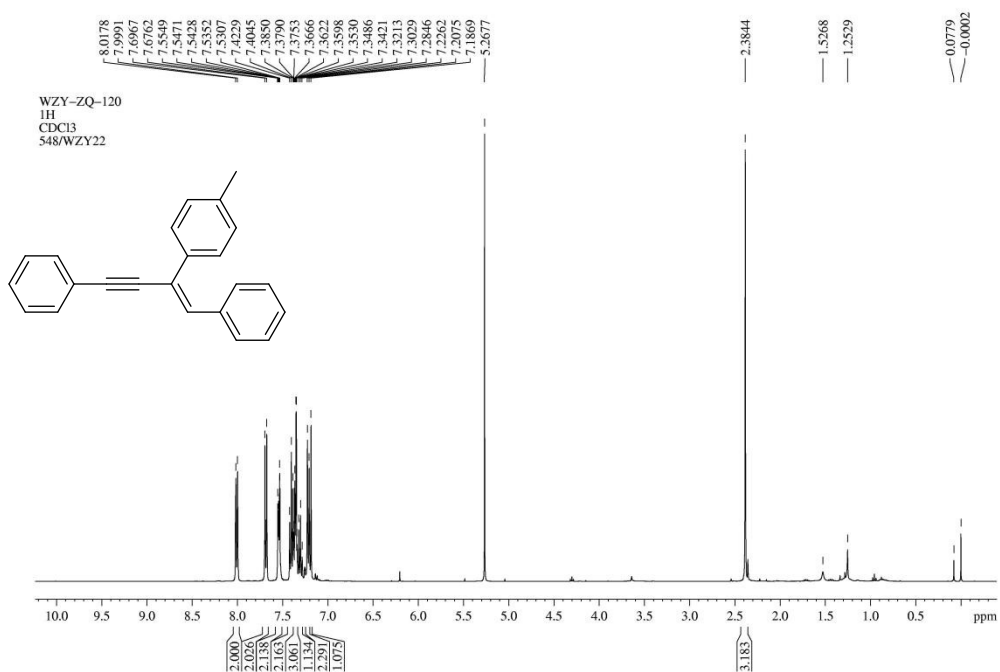
¹H NMR spectrum of compound **3ja**



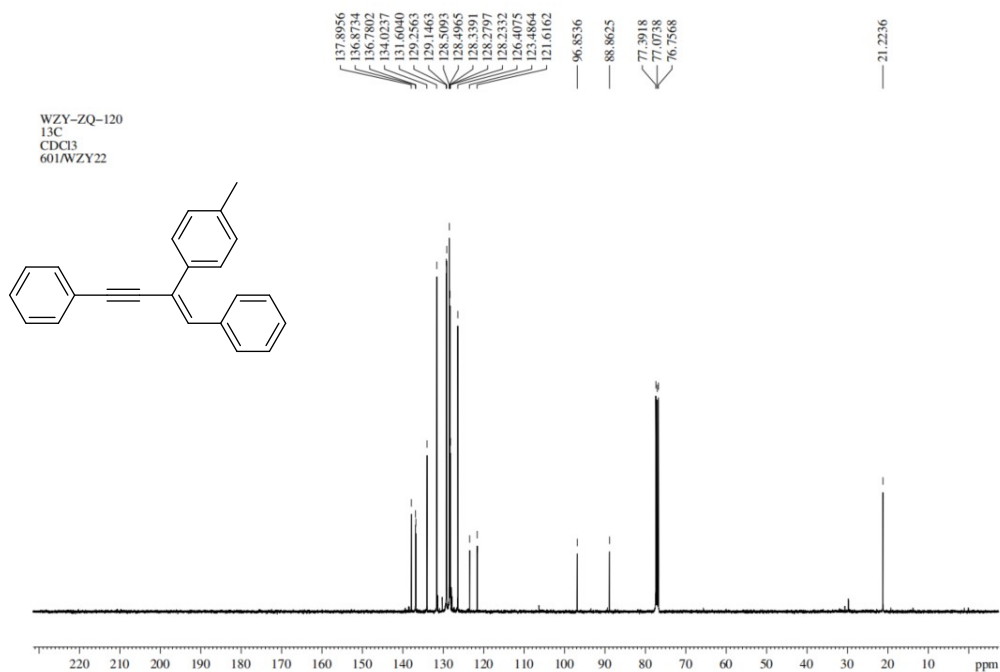
¹³C NMR spectrum of compound **3ja**



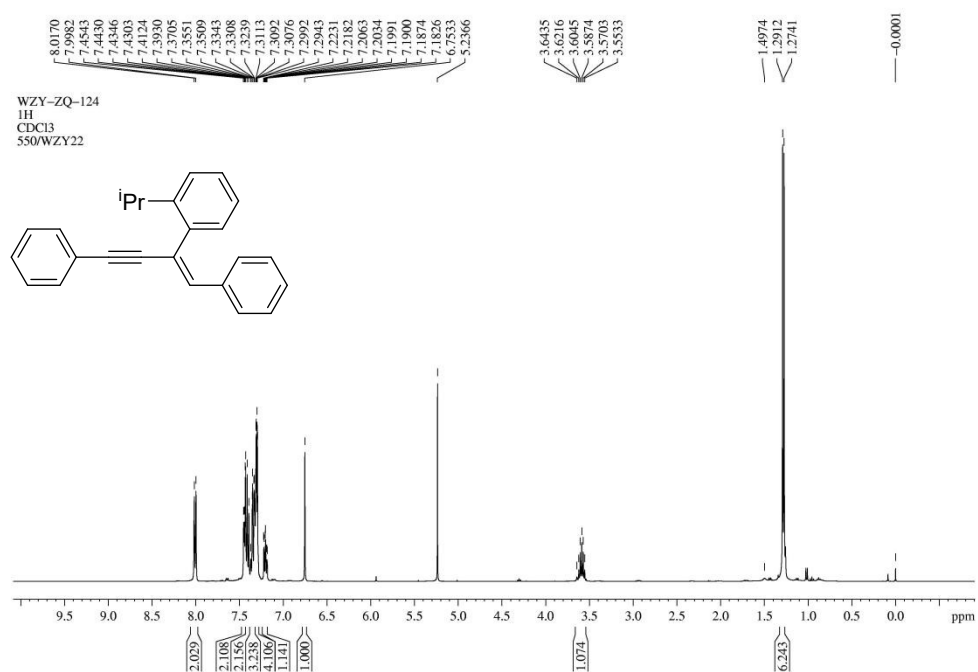
¹H NMR spectrum of compound **3ka**



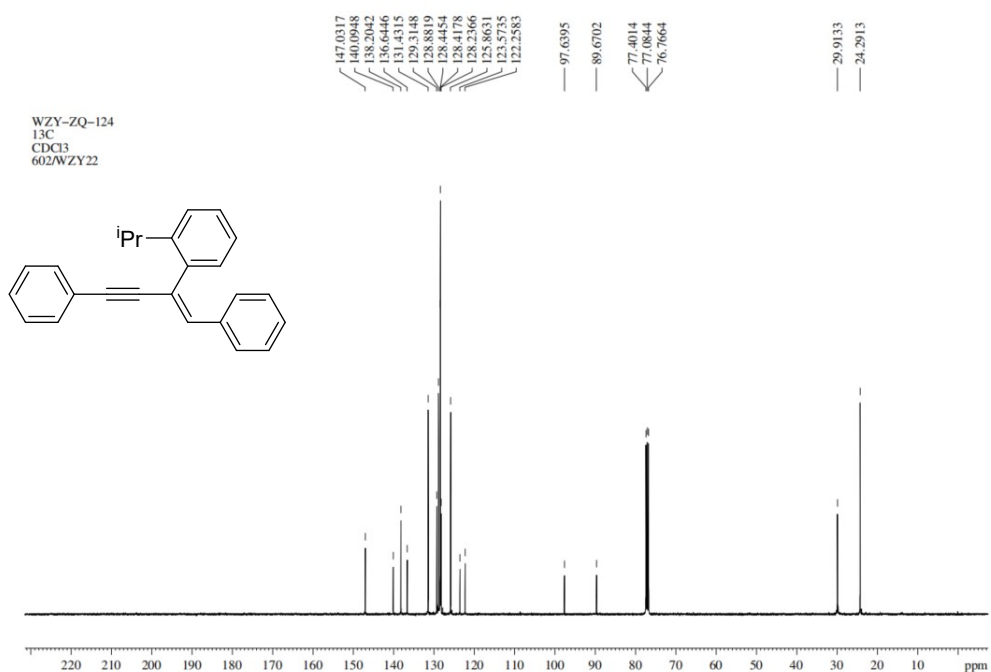
¹³C NMR spectrum of compound **3ka**



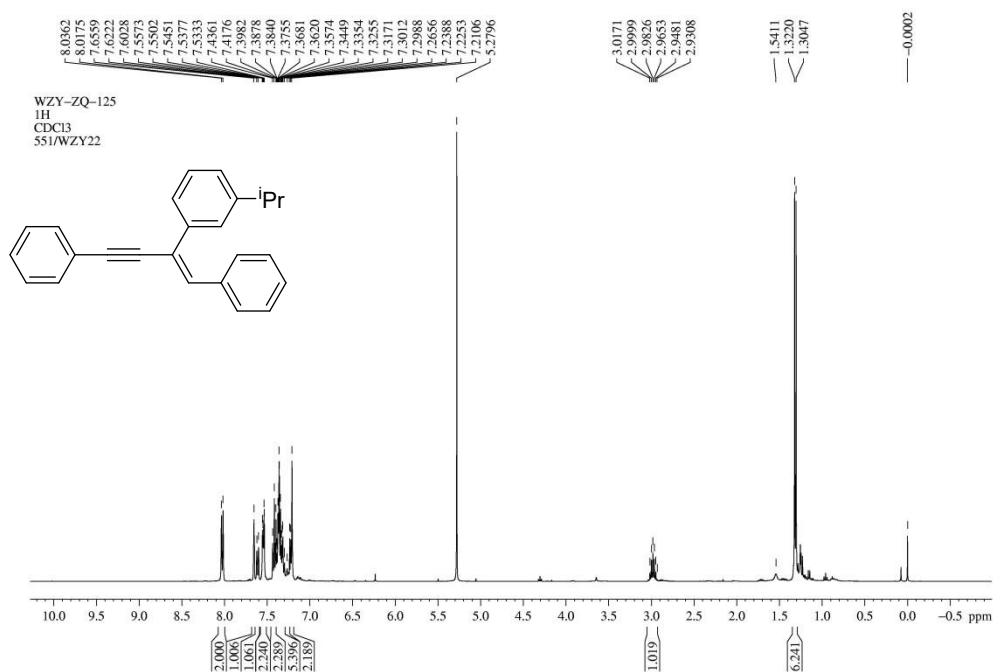
¹H NMR spectrum of compound **3la**



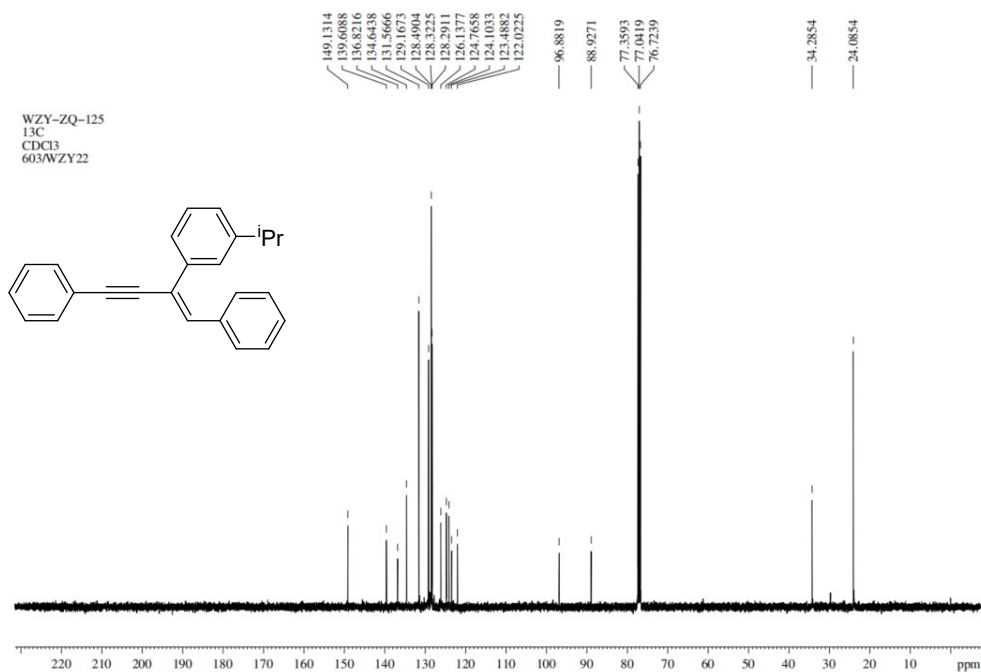
¹³C NMR spectrum of compound **3la**



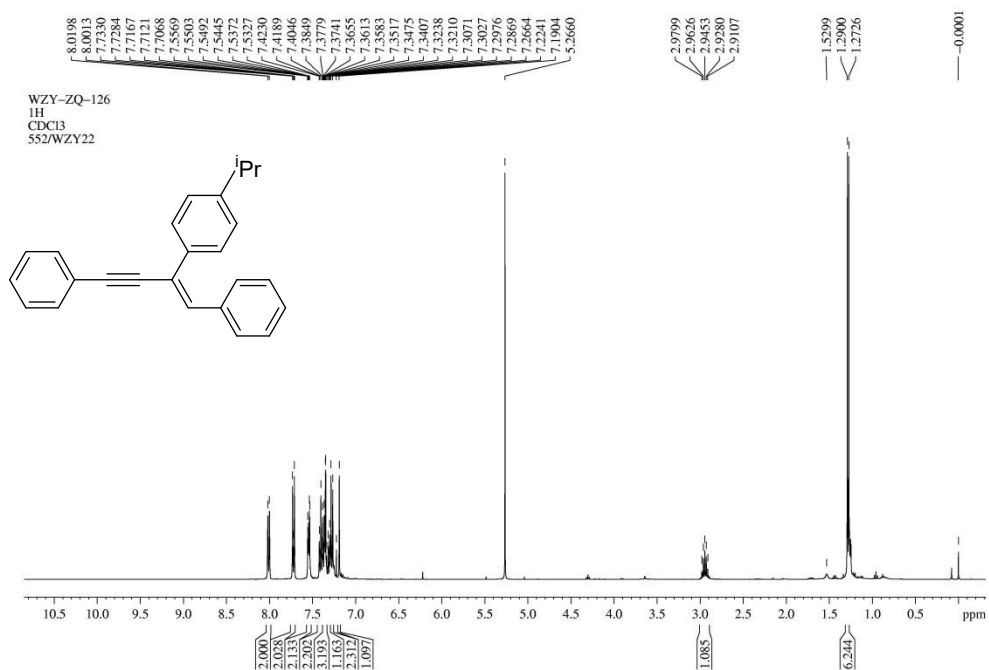
¹H NMR spectrum of compound **3ma**



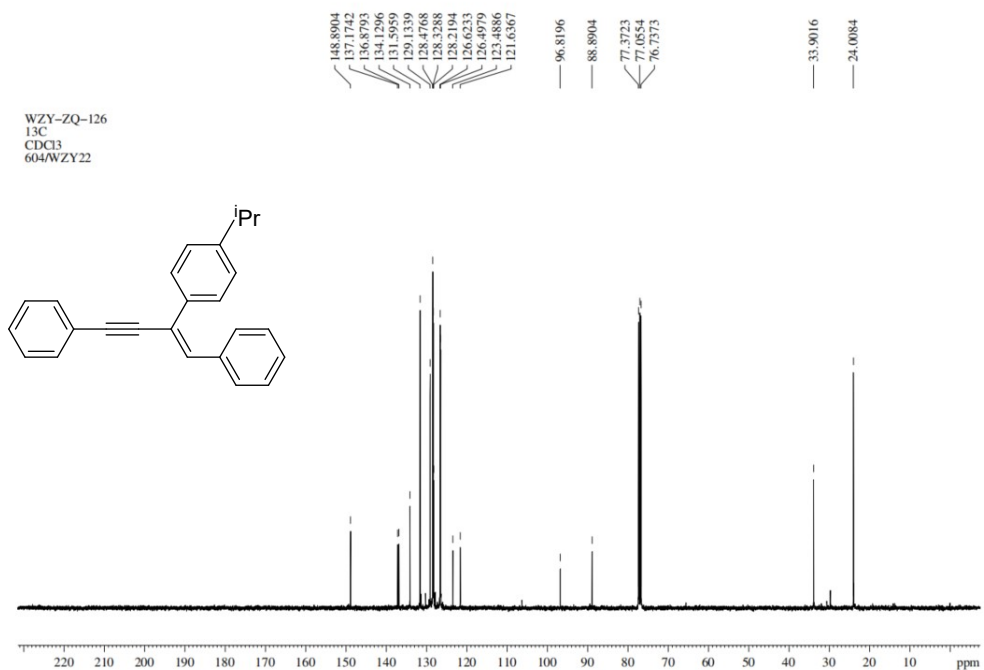
¹³C NMR spectrum of compound **3ma**



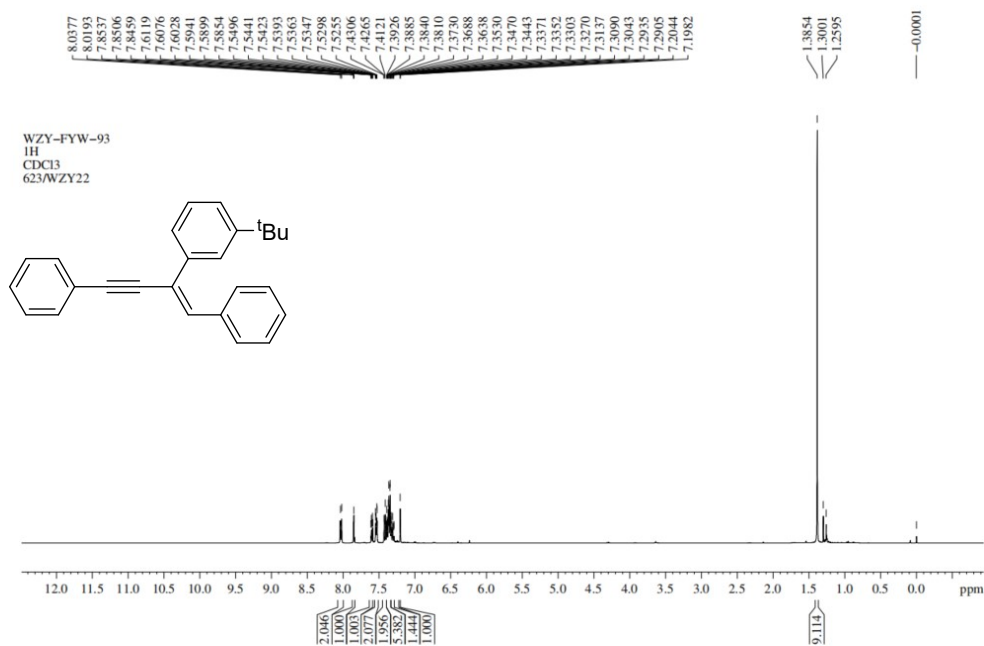
¹H NMR spectrum of compound **3na**



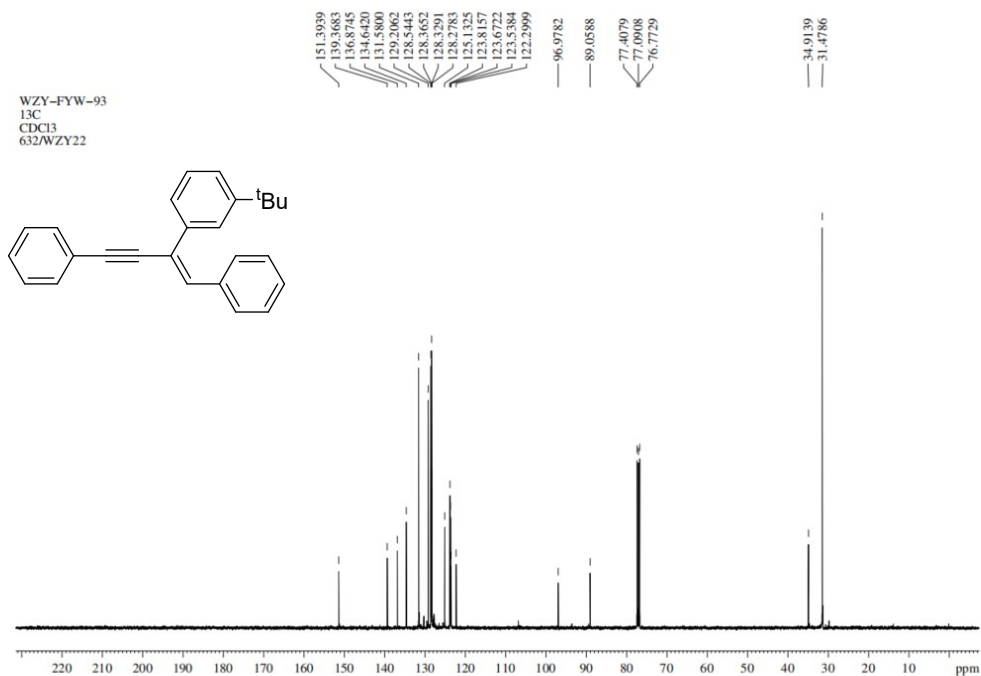
¹³C NMR spectrum of compound **3na**



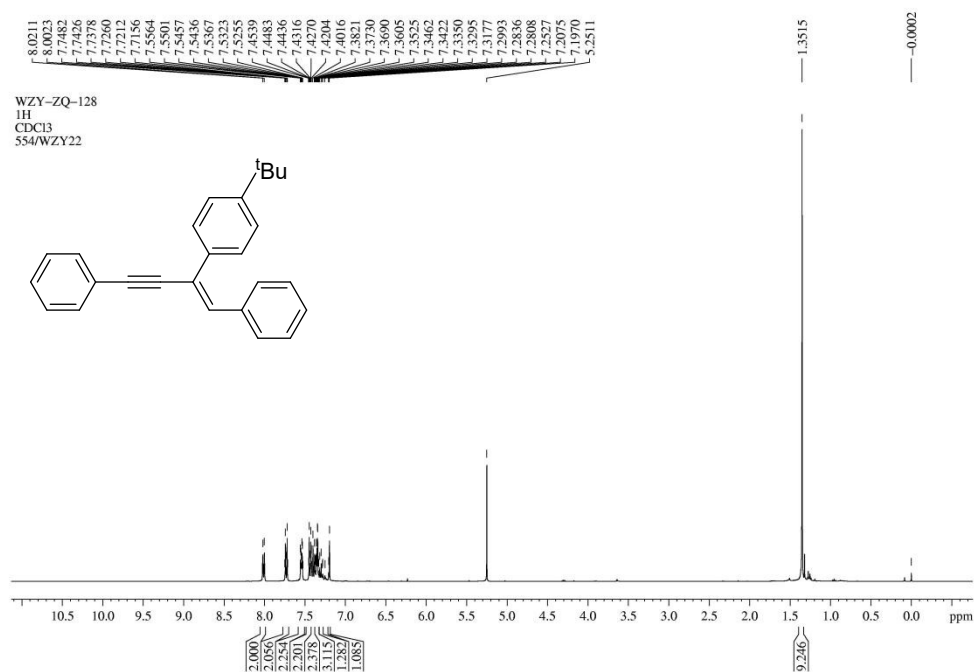
¹H NMR spectrum of compound **30a**



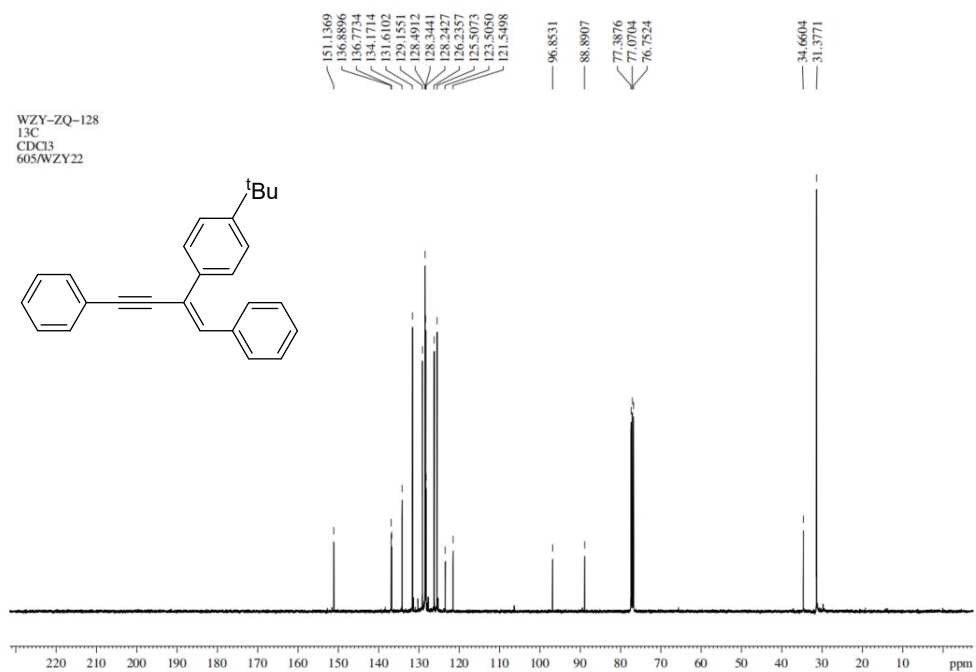
¹³C NMR spectrum of compound **30a**



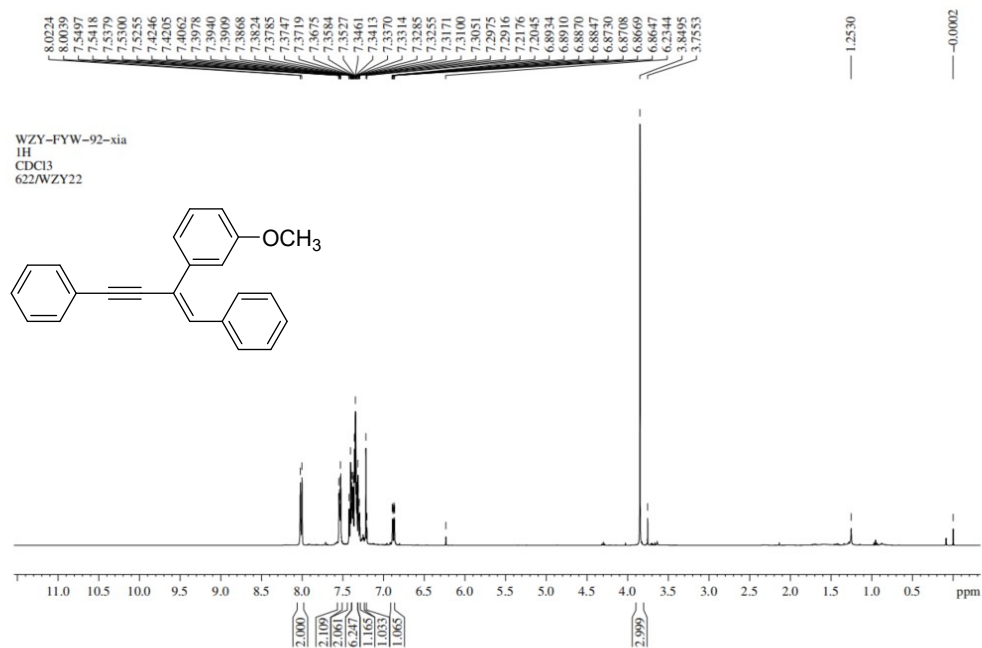
¹H NMR spectrum of compound **3pa**



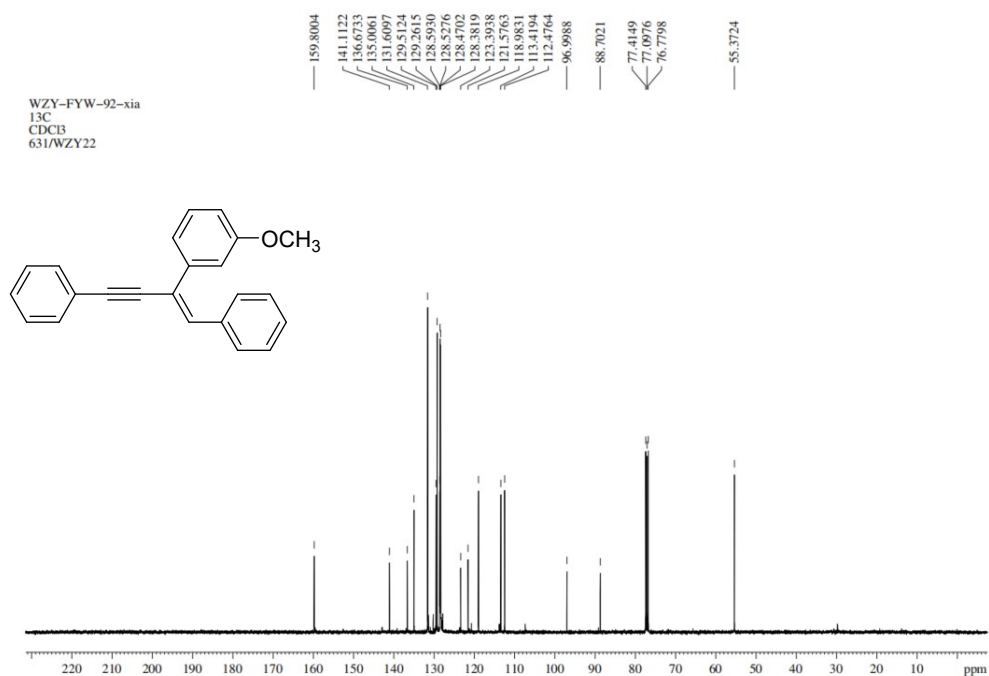
¹³C NMR spectrum of compound **3pa**



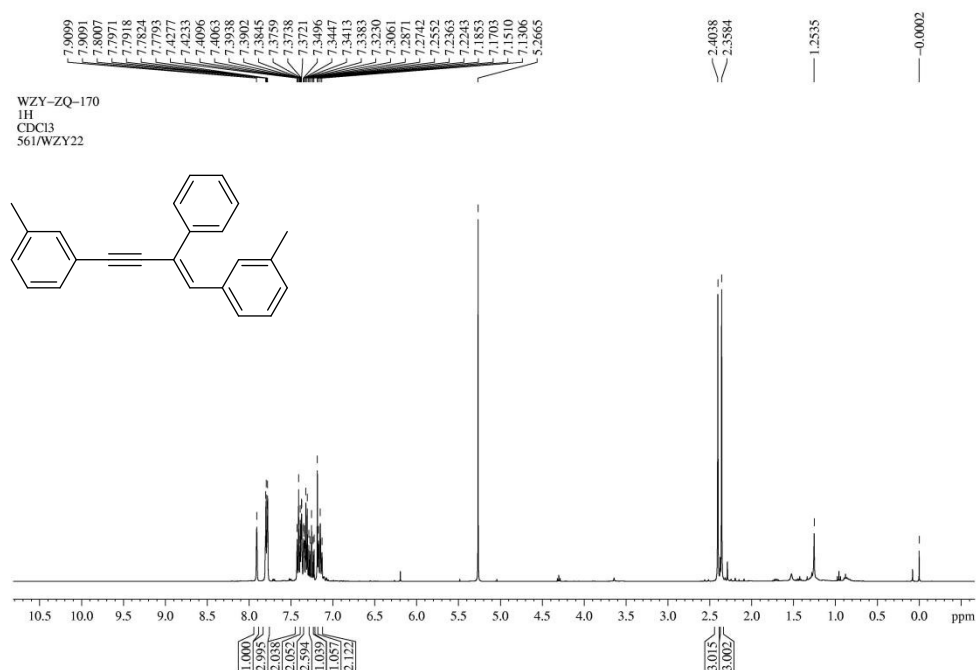
¹H NMR spectrum of compound **3qa**



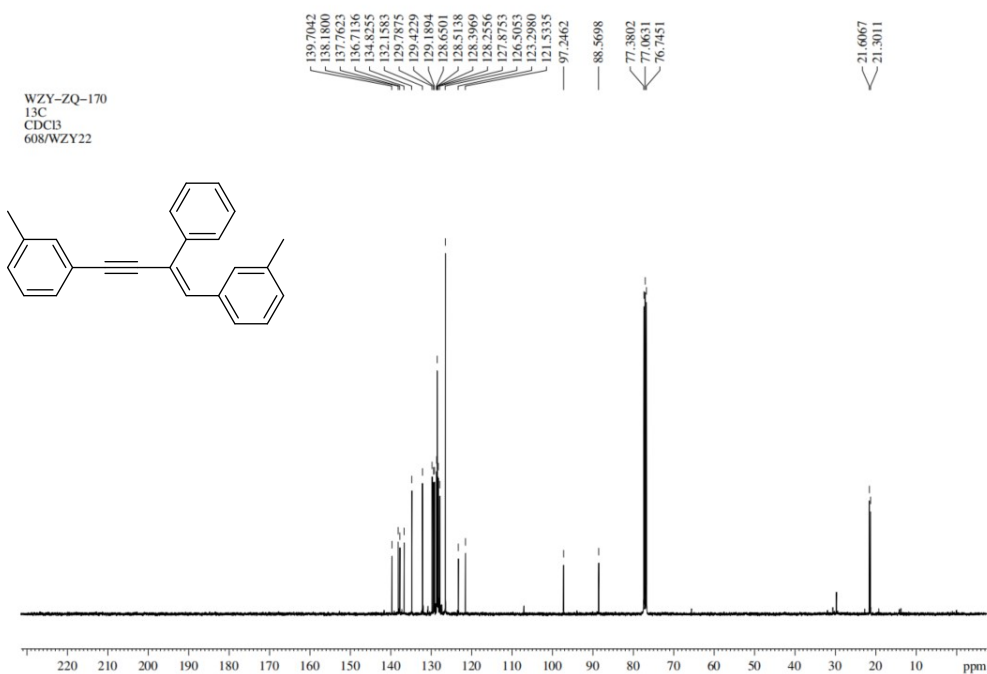
¹³C NMR spectrum of compound **3qa**



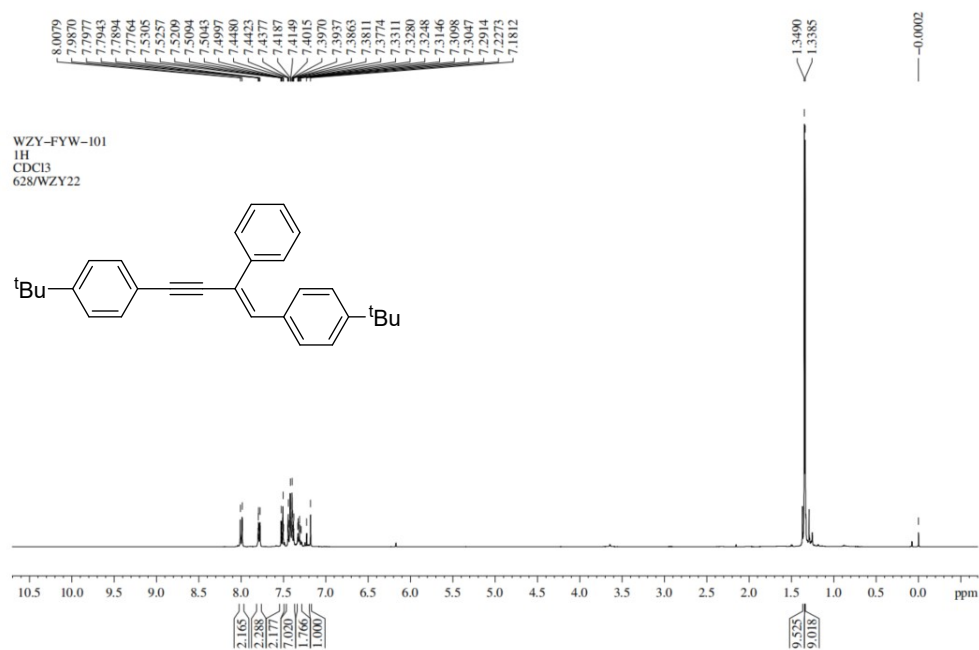
¹H NMR spectrum of compound **3bb**



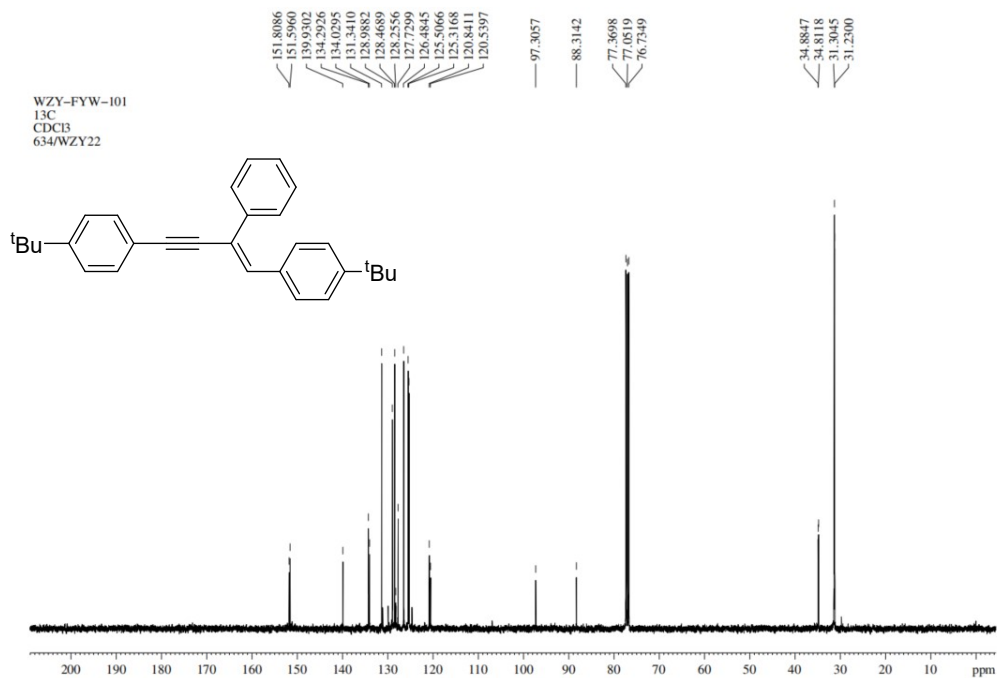
¹³C NMR spectrum of compound **3bb**



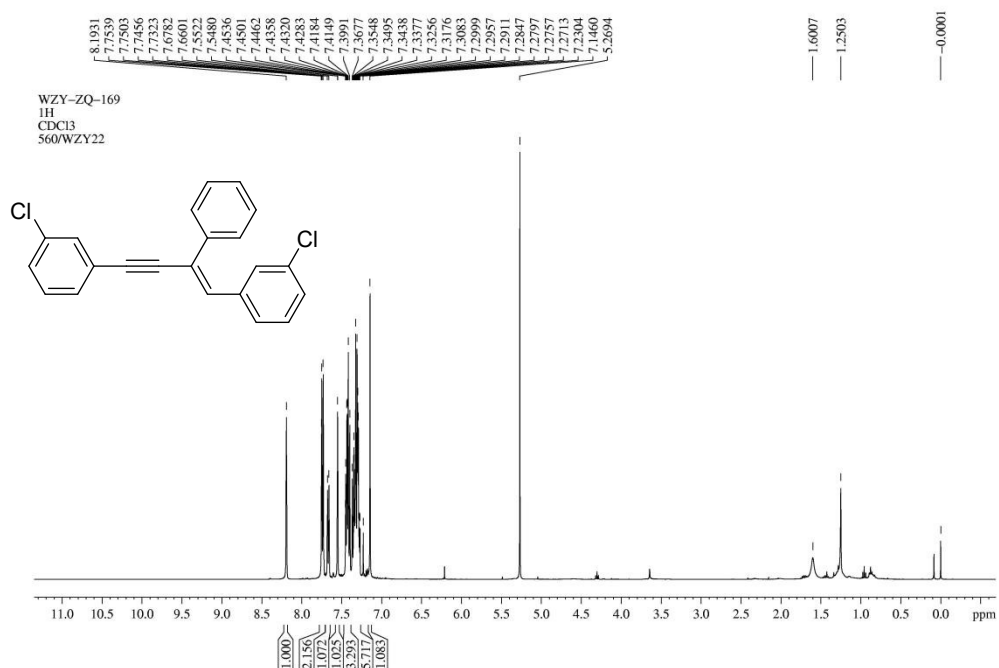
¹H NMR spectrum of compound **3bd**



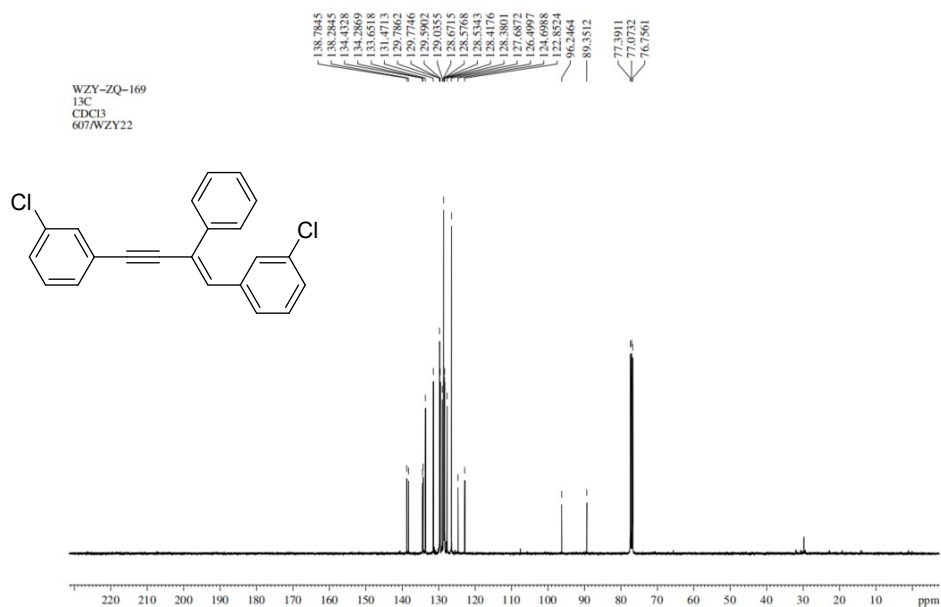
¹³C NMR spectrum of compound **3bd**



¹H NMR spectrum of compound **3be**



¹³C NMR spectrum of compound **3be**



5. DFT Studies on the Plausible Reaction Mechanism

All theoretical calculations were performed using the GFN2-xTB methodology.^[1] The SMD implicit solvation model was employed to replicate the solvent environment. The structures of reactants, intermediates and products were optimized, and the harmonic frequencies were computed to verify that the optimized structures resided at local minima on the potential surface.

Table S1. The Gibbs free energy of reactants, intermediates, and product.

Species	Gibbs free energy (Hartree)
Pd(OAc) ₂	-32.45542084
PCy ₃	-57.54048182
A	-147.6266519
H ₂ O	-5.078597137
B	-134.1793709
2	-39.08468631
C	-173.2529863
1	-25.77460565
F	-24.43825213
D	-174.6111935
3	-54.92873863
E	-119.7219795
HOAc	-14.43933338

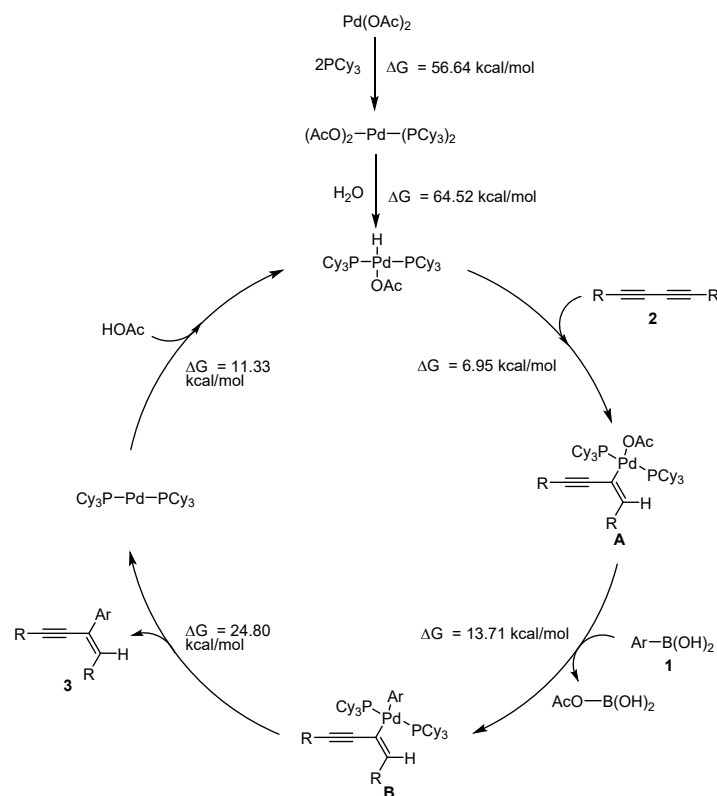


Figure S1. Plausible Reaction Mechanism.

Cartesian coordinates

Pd(OAc) ₂			
Pd	0.00069444940056	-0.00167625284018	-0.20208160921225
O	1.54524974775314		0.39388673671607
1.03434245814641			
C	2.35520083199105		0.12926614503322
0.09673665385131			
O	-1.83761806921236		0.20735300239023
0.60249797967283			
C	-2.35345113392364	-0.13262320811309	-0.50368672614651
O	1.83851405376288	-0.21031608047921	-
1.00801229392786			
O	-1.54311587219430	-0.39570515538224	-1.43999161003034
C	3.83425666975275		0.22016511727011
0.28353174623146			
H	4.11630817915220		-0.29266197259960
1.20017048541032			
H	4.34069063222791	-0.21034638607512	-
0.57507227728889			
H	4.11194830445707		1.26774326037716
0.38906126280736			
C	-3.83290035754402	-0.22294042642183	-0.68843870808665
H	-4.30342073356343	0.67405823793620	-
0.29273432085787			
H	-4.06557826056285	-0.35284452840154	-1.74109056743083
H	-4.20678920144790	-1.07336385431528	-0.12026695311414
PCy ₃			
P	-0.85144067100460	-0.39627150689087	-1.26052149519221
C	-1.79169576452964	1.07675965146066	-
0.55304657702870			
C	-2.05352020747798		1.20423116495985
0.94519249629980			
C	-1.18540638853885	2.36867615861030	-
1.10166970192833			
H	-2.77119963741254	0.94532242639221	-
1.04097785485345			
C	-2.98424292236856		2.38977597437588
1.20500125736803			
H	-1.12132558338494		1.36430065666054
1.48514545722145			
H	-2.52369726657300		0.29708189698417
1.32669803457691			
C	-2.10938525538843	3.55315107042526	-

0.83286541029582				
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H	-1.01398336907026		2.26381761026714	-
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C	-2.38163072824902		3.68246805108478	
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H	-3.16433806784123		2.48485288674011	
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H	-3.94714792667333		2.20946300473684	
0.71966853191053				
H	-1.65600270923720		4.47254269234282	-
1.21186463517896				
H	-3.05433670264068		3.40383908171391	-
1.36122942780498				
H	-3.06173612588924		4.51743568247251	
0.84865638313529				
H	-1.44483742044238		3.89230131284852	
1.18539211335669				
C	-1.66071681135050	-1.83371056154181	-0.34187705205865	
C	-1.56799936582703	-3.04792657660114	-1.27207323270378	
C	-1.14271164447803		-2.21919316630677	
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H	-2.71812610743817	-1.55046989660753	-0.25890490755444	
C	-2.35730037700927	-4.23000324149492	-0.71849447657981	
H	-0.51897743580559	-3.33265401234842	-1.38838167660608	
H	-1.94767367300656	-2.77856926249694	-2.26081394859781	
C	-1.95249193187103		-3.38898780398710	
1.60042066900120				
H	-0.09631415026581		-2.52107727393284	
0.97332508822819				
H	-1.21036244559792		-1.37782444760046	
1.73106944695853				
C	-1.86008134281179		-4.59806075674803	
0.67561993480177				
H	-2.26161067066526	-5.08753602168030	-1.38896318650439	
H	-3.41595313187967	-3.96344358726278	-0.66543445964478	
H	-1.57957579463421		-3.64980422938961	
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H	-2.45063453854499		-5.42424519546959	
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H	-0.82023703885463		-4.92842249383312	

0.61429328872662				
C	0.91406052816751	-0.38977502482511	-	
0.59097190141401				
C	1.80820228209735	0.22987903842483	-	
1.67012387922322				
C	1.23213448212845	0.25024208475830		
0.75655348119244				
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1.75160449443404				
H	1.58198017456683	-0.22569928296656	-	
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C	2.70476379523780	0.02716822024089		
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H	1.04598833313713	1.32409570559761		
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H	0.61135691159567	-0.17180747436554		
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C	3.60764980815720	0.62827181611370		
0.03013807298927				
H	3.90703140310344	0.48534531182446	-	
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4.09852746340273				
H	-1.64184053273309		0.57609340925163	-
4.22883652892408				
H	-3.25182042230222		2.06874690764441	-
5.37016986383012				
H	-3.46932824690496		2.99549388357253	-
3.88346343951770				
HOAc				
C	-3.69090819598027	-0.44257248214004	-0.18324021679256	
O	-2.65556821317915	-0.34010608253837	-0.79900594145764	
O		-4.33360431331276	0.60393050222270	
0.32028189062168				
H		-3.88742179499790	1.45055121621369	
0.13588940071534				
C		-4.41058173223543	-1.73211056993930	
0.09391312540058				
H		-5.05313658877277	-1.61513626751036	
0.96090153199804				
H	-5.02356758190431	-1.97561970786184	-0.77216937511541	
H		-3.69208476856091	-2.53288925891903	
0.24205458412540				

6. References

[1] Bannwarth, C.; Caldeweyher, E.; Ehlert, S.; Hansen, A.; Pracht, P.; Seibert, J.; Spicher, S. Grimme, S. Extended tight-binding quantum chemistry methods. *WIREs Comput. Mol. Sci.* **2021**, *11*, e1493.