Electronic Supplementary Material (ESI) for Chemical Communications


Supporting Information

# Direct Difunctionalization of Activated Alkynes *via* Domino Oxidative Benzylation/1,4-Aryl Migration/Decarboxylation under Metal-free Conditions

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## I. General considerations

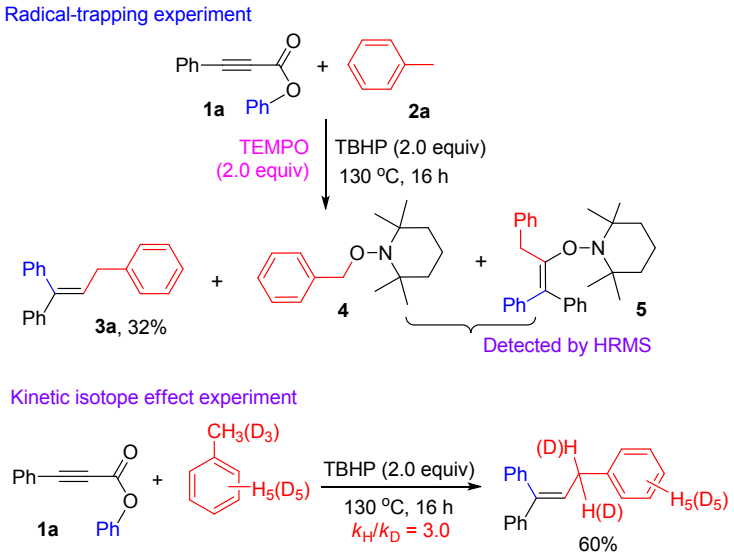
All reactions were carried out under air. $^{1}H$ NMR and $^{13}C$ NMR spectra were measured on a Bruker Avance NMR spectrometer (400 MHz or 100 MHz, respectively) in $CDCl_3$ as solvent and recorded in ppm relative to internal standard tetramethylsilane. $^{1}H$ NMR data are reported as follows: δ, chemical shift; coupling constants (*J* are given in Hertz, Hz) and integration. Abbreviations to denote the multiplicity of a particular signal were s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), and br (broad singlet). High resolution mass spectroscopic data of the products were collected on an Agilent Technologies 6540 UHD Accurate-Mass Q-TOF LC/MS using ESI.

Unless otherwise stated, all reactions were carried out under air atmosphere. The chemicals and solvents were purchased from commercial suppliers either from Aldrich (USA) or Shanghai Chemical Company (China) without further purification. Products were purified by flash chromatography on 100–200 mesh silica gels, $SiO_2$.

## II. General experimental procedure

The Schlenk tube equipped with a stir bar was charged with phenyl 3-phenylpropiolate (**1a**) (0.25 mmol), toluene (4.0 mL), and *tert*-butyl hydroperoxide (2.0 equiv, 70% solution in water) was added by syringe. The reaction mixture was stirred at 130 °C for 16 h. Subsequently the reaction was concentrated under reduced pressure to yield the crude product, which was further purified by flash chromatography on silica gel with petroleum ether to provide the corresponding product.

## III. Machenistic investigation (**Scheme S-1: Control experiments**)




**a. The radical trapping experiments**

Two equivalents of radical scavenger (2,2,6,6-tetramethylpiperidinoxy) was added to the reaction of **1a** with **2a** in the standard conditions, After 16 h, the reaction mixture was cooled to room temperature. The crude reaction mixture was detected by ESI-MS, two adducts of benzenyl and intermediate **IV** vinyl radical with radical scavenger was detected as shown in Figure S1 and Figure S2, and the desired product was obtained with 32% yield by flash chromatography on silica gel with petroleum ether. When four equivalents of radical scavenger (2,2,6,6-tetramethylpiperidinoxy) was used, no desired product was found.

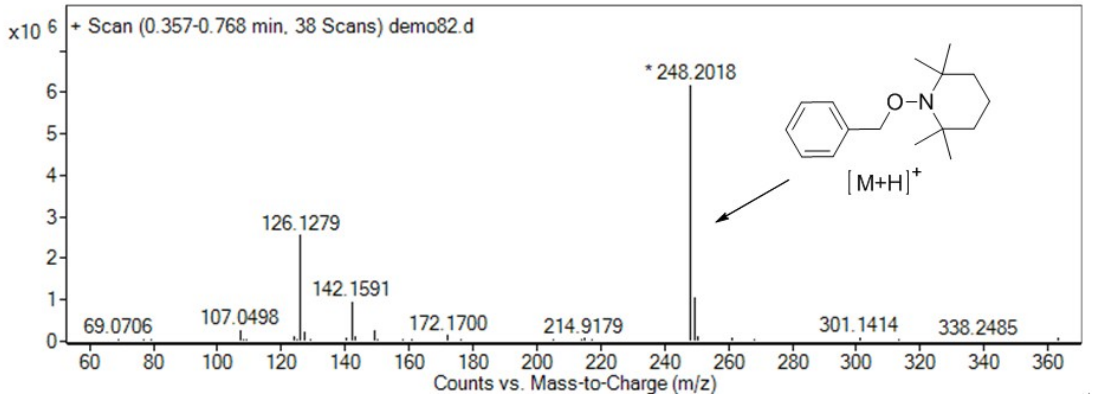



**Figure S1. ESI-MS spectra of TEMPO-$CH_2Ph$ adduct**

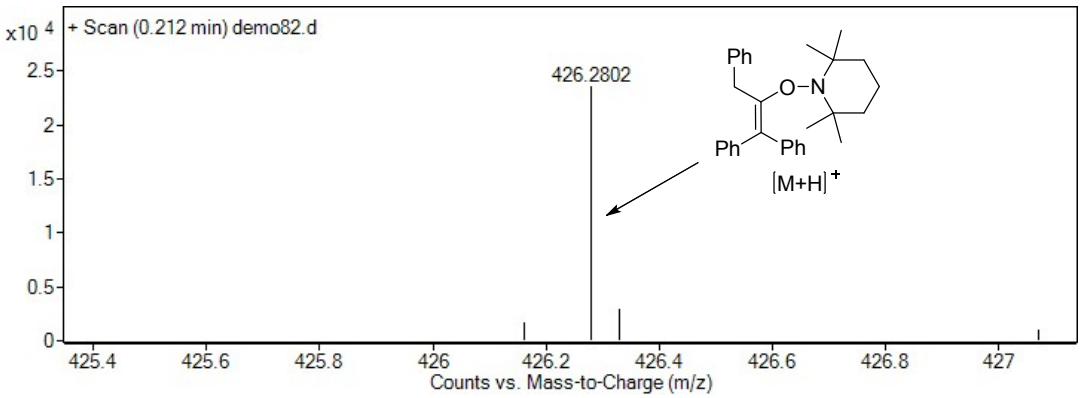
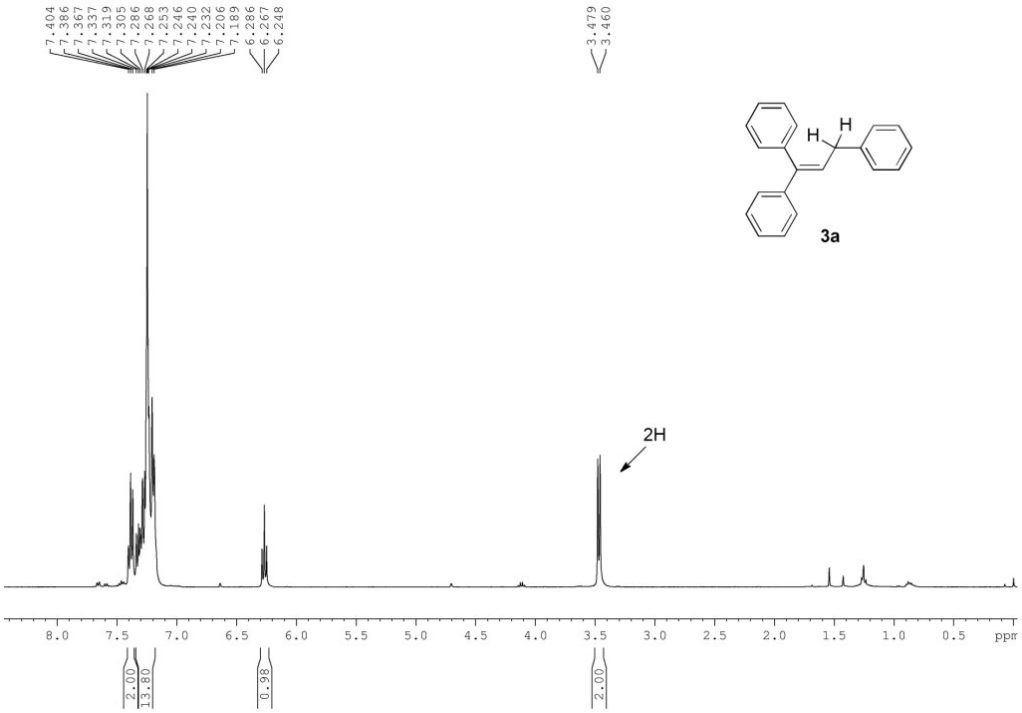



**Figure S2. ESI-MS spectra of TEMPO-intermediate IV vinyl radical adduct**

**b. Isotope labeling experiments**

The Schlenk tube equipped with a stir bar was charged with phenyl 3-phenylpropiolate (**1a**) (0.25 mmol), toluene (**2a**, 2.0 mL), [D8]-toluene ([D]$_8$-**2a**, 2.0 mL) and *tert*-butyl hydroperoxide (2.0 equiv, 70% solution in water) was added by syringe. The reaction mixture was stirred at 130 °C for 16 h. Subsequently, the reaction was concentrated under reduced pressure to yield the crude product, which was further purified by flash chromatography on silica gel with petroleum ether to provide the corresponding product in 60% yield. The ratio of hydrogen to deuterium was determined from the $^1$H NMR (Figure S3).



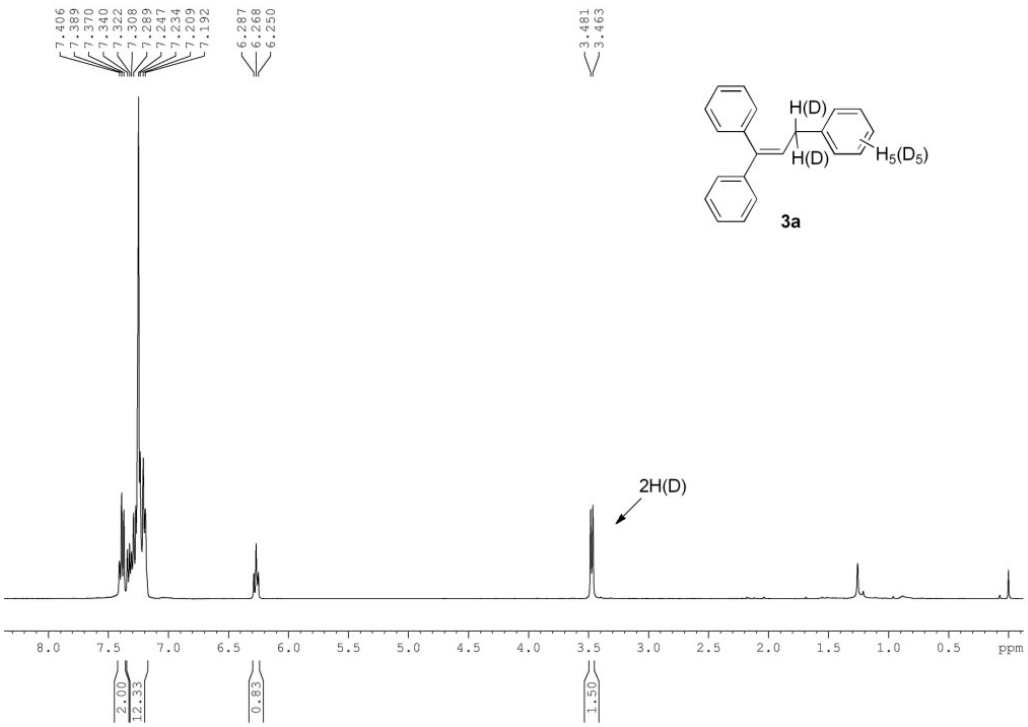
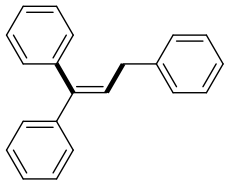


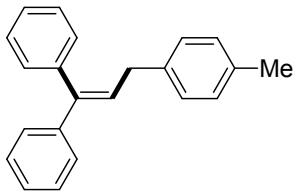

**Figure S3.** $^{1}$H NMR spectrum of **3a** and the mixture of **3a** and **3a-*d***

## IV. Characterization data for the products



**Prop-1-ene-1,1,3-triyltribenzene (3a)**

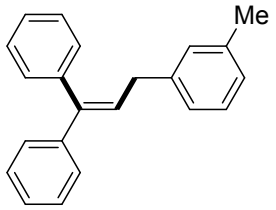
Colorless oil.[1] $^{1}$H NMR (400 MHz, $CDCl_3$) δ: 7.40–7.37 (t, *J* = 7.4 Hz, 2H), 7.34–7.19 (m, 13H), 6.27 (t, *J* = 7.6 Hz, 1H), 3.47 (d, *J* = 7.6 Hz, 2H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ: 142.5, 142.45, 141.0, 139.8, 129.9, 128.5, 128.4, 128.3, 128.1, 127.8, 127.3, 127.1, 127.0, 126.0, 35.9. HRMS (EI) Calcd for $[M]^+$ $C_{21}H_{18}$: 270.1409, Found: 270.1405.




**(3-(*p*-Tolyl)prop-1-ene-1,1-diyl)dibenzene (3b)**

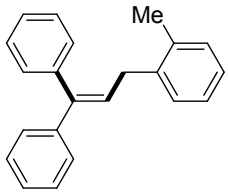
Colorless oil.[1] $^{1}$H NMR (400 MHz, $CDCl_3$) δ: 7.42 (t, *J* = 7.4 Hz, 2H), 7.35 (t, *J* = 7.4

Hz, 1H), 7.29–7.24 (m, 7H), 7.15–7.11 (m, 4H), 6.29 (t, $J$ = 7.6 Hz, 1H), 3.47 (d, $J$ = 7.6 Hz, 2H), 2.36 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ: 142.5, 142.3, 139.9, 137.9, 135.5, 130.0, 129.2, 128.3, 128.27, 128.1, 127.3, 127.1, 127.0, 35.5, 21.0. HRMS (EI) Calcd for $[M]^+$ $C_{22}H_{20}$: 284.1565, Found: 284.1559.



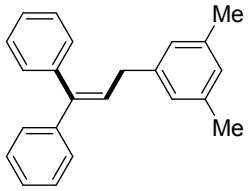

**(3-(*m*-Tolyl)prop-1-ene-1,1-diyl)dibenzene (3c)**

Colorless oil.[1] $^1$H NMR (400 MHz, $CDCl_3$) δ: 7.43 (t, $J$ = 7.2 Hz, 2H), 7.37 (t, $J$ = 7.2 Hz, 1H), 7.30–7.27 (m, 7H), 7.22 (t, $J$ =7.8 Hz, 1H), 7.06–7.04 (m, 3H), 6.31 (t, $J$ = 7.6 Hz, 1H), 3.48 (d, $J$ = 7.6 Hz, 2H), 2.37 (s, 3H).$^{13}$C NMR (100 MHz, $CDCl_3$) δ: 142.5, 142.4, 140.9, 139.9, 138.1, 130.0, 129.2, 128.4, 128.3, 128.1, 127.9, 127.4, 127.1, 127.0, 126.8, 125.4, 35.9, 21.4. HRMS (EI) Calcd for $[M]^+$ $C_{22}H_{20}$: 284.1565, Found: 284.1563.



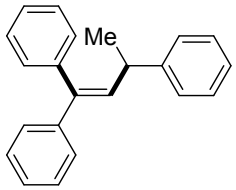

**(3-(*o*-Tolyl)prop-1-ene-1,1-diyl)dibenzene (3d)**

Colorless oil. $^1$H NMR (400 MHz, $CDCl_3$) δ: 7.44 (t, $J$ = 7.2 Hz, 2H), 7.38 (t, $J$ = 7.2 Hz, 1H), 7.31–7.19 (m, 11H), 6.25 (t, $J$ = 7.4 Hz, 1H), 3.49 (d, $J$ = 7.6 Hz, 2H), 2.25 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ: 142.57, 142.55, 139.9, 139.3, 136.3, 130.2, 129.9, 128.7, 128.3, 128.1, 127.4, 127.38, 127.2, 127.1, 126.2, 126.1, 33.8, 19.5. HRMS (EI) Calcd for $[M]^+$ $C_{22}H_{20}$: 284.1565, Found: 284.1560.



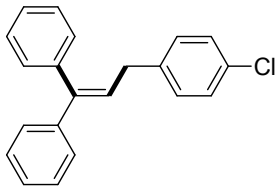

**(3-(3,5-Dimethylphenyl)prop-1-ene-1,1-diyl)dibenzene (3e)**

Colorless oil.[1] $^1$H NMR (400 MHz, $CDCl_3$) δ: 7.42 (t, *J* = 7.4 Hz, 2H), 7.37–7.33 (m, 1H), 7.30–7.23 (m, 7H), 6.88 (s, 1H), 6.85 (s, 2H), 6.30 (t, *J* = 7.6 Hz, 1H), 3.43 (d, *J* = 7.6 Hz, 2H), 2.32 (s, 6H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ: 142.5, 142.2, 140.9, 139.9, 138.0, 130.0, 128.3, 128.1, 128.06, 127.6, 127.3, 127.1, 127.0, 126.2, 35.8, 21.3. HRMS (EI) Calcd for $[M]^+$ $C_{23}H_{22}$: 298.1722, Found: 298.1718.



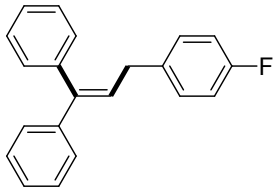

**But-1-ene-1,1,3-triyltribenzene (3f)**

Colorless oil. $^1$H NMR (400 MHz, $CDCl_3$) δ: 7.43 (t, *J* = 7.2 Hz, 2H), 7.39–7.31 (m, 3H), 7.29–7.21 (m, 10H), 6.26 (d, *J* = 10.4 Hz, 1H), 3.68–3.61 (m, 1H), 1.43 (d, *J* = 6.8 Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ: 146.2, 142.4, 140.2, 140.1, 134.2, 129.8, 128.5, 128.3, 128.1, 127.3, 127.1, 127.0, 126.95, 126.0, 39.3, 22.4. HRMS (EI) Calcd for $[M]^+$ $C_{22}H_{20}$: 284.1565, Found: 284.1561.




**(3-(4-Chlorophenyl)prop-1-ene-1,1-diyl)dibenzene (3g)**

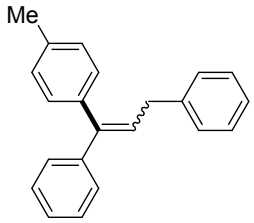
Colorless oil. $^1$H NMR (400 MHz, $CDCl_3$) δ: 7.42 (t, *J* = 7.2 Hz, 2H), 7.37–7.34 (m, 1H), 7.31–7.23 (m, 9H), 7.13 (d, *J* = 8.4 Hz, 2H), 6.24 (t, *J* = 7.6 Hz, 1H), 3.45 (d, *J* = 7.6 Hz, 2H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ: 143.0, 142.2, 139.7, 139.4, 131.8, 129.8, 129.7, 128.6, 128.3, 128.2, 127.3, 127.25, 127.2, 127.0, 35.3. HRMS (EI) Calcd for $[M]^+$ $C_{21}H_{17}Cl$: 304.1019, Found: 304.1015.




**(3-(4-Fluorophenyl)prop-1-ene-1,1-diyl)dibenzene (3h)**

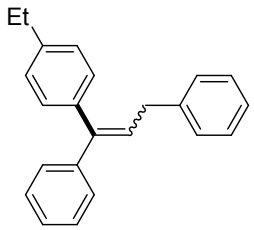
Colorless oil. $^1$H NMR (400 MHz, $CDCl_3$) δ: 7.43 (t, *J* = 7.4 Hz, 2H), 7.39-7.35 (m, 1H), 7.30–7.26 (m, 7H), 7.19–7.16 (m, 2H), 7.01 (t, *J* = 8.2 Hz, 2H), 6.27 (t, *J* = 7.6

Hz, 1H), 3.47 (d, $J$ = 7.6 Hz, 2H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ: 161.4 (d, $J$ = 242.3 Hz), 142.7, 142.3, 139.7, 136.59, 136.55, 129.9, 129.7 (d, $J$ = 7.7 Hz), 128.2 (d, $J$ = 19.0 Hz), 127.48 (d, $J$ = 0.6 Hz), 127.3, 127.23, 127.17, 115.2 (d, $J$ = 21.0 Hz), 35.1. HRMS (EI) Calcd for $[M]^+$ $C_{21}H_{17}F$: 288.1314, Found: 283.1311.



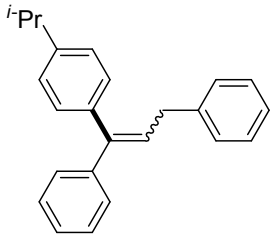

**(1-(*p*-Tolyl)prop-1-ene-1,3-diyl)dibenzene (3i)**

Colorless oil. $^1$H NMR (400 MHz, $CDCl_3$) δ: 7.43 (t, $J$ = 7.2 Hz, 1H), 7.38-7.30 (m, 5H), 7.28-7.24 (m, 5H), 7.21–7.18 (m, 2H), 7.11 (d, $J$ = 8.0 Hz, 1H), 6.29 (t, $J$ = 7.6 Hz, 1H), 3.55–3.50 (m, 2 H), 2.44 (s, 1.6H), 2.37 (s, 1.4H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ: 142.7, 142.5, 142.4, 141.13, 141.11, 140.1, 139.7, 136.9, 136.82, 136.77, 129.94, 129.85, 129.0, 128.8, 128.5, 128.44, 128.43, 128.3, 128.1, 127.6, 127.4, 127.2, 127.1, 127.0, 126.9, 126.0, 36.0, 35.9, 21.3, 21.1. HRMS (EI) Calcd for $[M]^+$ $C_{22}H_{20}$: 284.1565, Found: 284.1568.



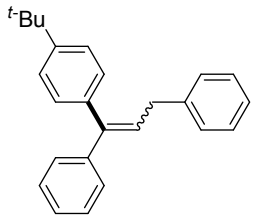

**(1-(4-Ethylphenyl)prop-1-ene-1,3-diyl)dibenzene (3j)**

Colorless oil. $^1$H NMR (400 MHz, $CDCl_3$) δ: 7.42 (t, $J$ = 7.4 Hz, 1H), 7.37-7.18 (m, 12H), 7.12 (d, $J$ = 7.6 Hz, 1H), 6.30–6.25 (m, 1H), 3.53 (d, $J$ = 7.6 Hz, 1.1H), 3.49 (d, $J$ = 7.6 Hz, 0.9H), 2.72 (q, $J$ = 7.6 Hz, 1.1H), 2.65 (q, $J$ = 7.6 Hz, 0.9H), 1.33–1.23 (m, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ: 143.2, 143.1, 142.8, 142.5, 142.4, 141.12, 141.11, 140.0, 139.8, 137.0, 129.93, 129.86, 128.46, 128.45, 128.43, 128.41, 128.3, 128.1, 127.7, 127.61, 127.59, 127.4, 127.2, 127.1, 127.0, 126.9, 126.0, 36.0, 35.9, 28.6, 28.5, 15.5, 15.4. HRMS (EI) Calcd for $[M]^+$ $C_{23}H_{22}$: 298.1722, Found: 298.1748.



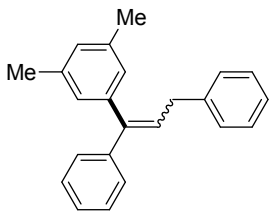

**(1-(4-Isopropylphenyl)prop-1-ene-1,3-diyl)dibenzene (3k)**

Colorless oil. $^{1}$H NMR (400 MHz, $CDCl_3$) δ: 7.43 (t, *J* = 7.2 Hz, 1H), 7.38–7.22 (m, 12H), 7.18 (t, *J* = 8.4 Hz, 1H), 6.32–6.26 (m, 1H), 3.55 (d, *J* = 7.6 Hz, 1H), 3.50 (d, *J* = 7.6 Hz, 1H), 3.02–2.89 (m, 1H), 1.33 (d, *J* = 6.8 Hz, 3H), 1.28 (d, *J* = 6.8 Hz, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ: 147.8, 147.7, 142.8, 142.6, 142.4, 141.2, 141.1, 140.1, 139.9, 137.1, 130.0, 129.9, 128.91, 128.88, 128.6, 128.48, 128.47, 128.4, 128.3, 128.23, 128.15, 128.1, 127.7, 127.6, 127.5, 127.3, 127.2, 127.13, 127.07, 127.0, 126.9, 126.5, 126.4, 126.3, 126.2, 125.97, 125.96, 36.0, 35.9, 33.9, 33.8, 24.0, 23.97. HRMS (EI) Calcd for $[M]^+$ $C_{24}H_{24}$: 312.1878, Found: 312.1875.



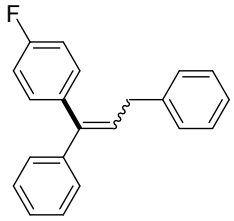

**(1-(4-(*tert*-Butyl)phenyl)prop-1-ene-1,3-diyl)dibenzene (3l)**

Colorless oil. $^{1}$H NMR (400 MHz, $CDCl_3$) δ: 7.44–7.42 (m, 1H), 7.41–7.20 (m, 12H), 6.33–6.25 (m, 1H), 3.54 (d, *J* = 7.6 Hz, 1.1H), 3.49 (d, *J* = 7.6 Hz, 0.9H), 1.39 (s, 4.7H), 1.34 (s, 4.3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ: 150.1, 150.0, 142.8, 142.5, 142.3, 141.2, 141.1, 140.0, 139.4, 136.7, 129.9, 129.6, 128.5, 128.44, 128.42, 128.3, 128.1, 127.6, 127.5, 127.0, 126.96, 126.93, 126.9, 126.0, 125.9, 125.1, 125.0, 36.0, 35.9, 34.6, 34.5, 31.4, 31.3. HRMS (EI) Calcd for $[M]^+$ $C_{25}H_{26}$: 326.2035, Found: 326.2033.



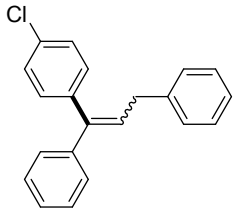
**(1-(3,5-Dimethylphenyl)prop-1-ene-1,3-diyl)dibenzene (3m)**

Colorless oil. $^1$H NMR (400 MHz, $CDCl_3$) δ: 7.43 (t, *J* = 7.4 Hz, 1H), 7.38–7.29 (m, 5H), 7.27–7.23 (m, 4H), 7.00 (s, 1H), 6.91 (s, 1H), 6.90 (s, 1H), 6.27 (t, *J* = 7.4 Hz, 1H), 3.52–3.48 (m, 2H), 2.36 (s, 3H), 2.29 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ: 142.69, 142.67, 142.6, 142.5, 141.2, 141.1, 140.1, 139.7, 137.7, 137.5, 129.9, 128.8, 128.7, 128.46, 128.45, 128.2, 128.1, 127.7, 127.54, 127.51, 127.3, 127.0, 126.9, 126.0, 125.9, 125.3, 36.0, 35.9, 21.4, 21.3. HRMS (EI) Calcd for $[M]^+$ $C_{23}H_{22}$: 298.1722, Found: 298.1719.




**(1-(4-Fluorophenyl)prop-1-ene-1,3-diyl)dibenzene (3n)**

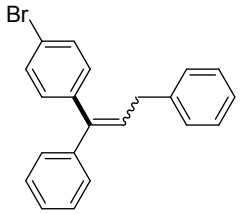
Colorless oil. $^1$H NMR (400 MHz, $CDCl_3$) δ: 7.44 (t, *J* = 7.2 Hz, 1H), 7.39–7.31 (m, 3H), 7.29–7.22 (m, 8H), 7.12 (t, *J* = 8.8 Hz, 1H), 6.98 (t, *J* = 8.8 Hz, 1H), 6.32 (t, *J* = 7.6 Hz, 0.45 H), 6.24 (t, *J* = 7.6 Hz, 0.55 H), 3.50 (d, *J* = 7.6 Hz, 2H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ: 162.2 (d, *J* = 244.8 Hz), 162.1 (d, *J* = 244.6 Hz), 142.32, 142.31, 141.6, 141.5, 140.9, 140.8, 139.68, 139.66, 138.64, 138.61, 135.71, 135.68, 131.55 (d, *J* = 7.9 Hz), 129.9, 128.89 (d, *J* = 7.9 Hz), 128.6, 128.5, 128.40, 128.36, 128.2, 128.1, 127.68, 127.67, 127.31, 127.30, 127.2, 126.10, 126.07, 115.28 (d, *J* = 21.2 Hz), 114.9 (d, *J* = 21.2 Hz), 36.0, 35.9. HRMS (EI) Calcd for $[M]^+$ $C_{21}H_{17}F$: 288.1314, Found: 288.1311.




**(1-(4-Chlorophenyl)prop-1-ene-1,3-diyl)dibenzene (3o)**

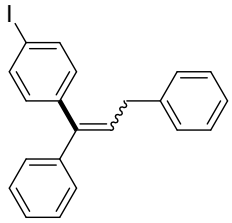
Colorless oil. $^1$H NMR (400 MHz, $CDCl_3$) δ: 7.44 (t, *J* = 7.6 Hz, 2H), 7.38 (t, *J* = 7.8 Hz, 1H), 7.34–7.29 (m, 3H), 7.27–7.20 (m, 8H), 6.35–6.27 (m, 1H), 3.51 (d, *J* = 3.8 Hz, 2H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ: 142.0, 141.5, 141.4, 141.0, 140.7, 140.6, 139.4, 138.3, 133.1, 132.9, 131.3, 129.9, 128.61, 128.59, 128.58, 128.56, 128.5,

128.41, 128.36, 128.33, 128.27, 128.2, 127.4, 127.33, 127.3, 126.14, 126.11, 36.0, 35.9. HRMS (EI) Calcd for $[M]^+$ $C_{21}H_{17}Cl$: 304.1019, Found: 304.1015.



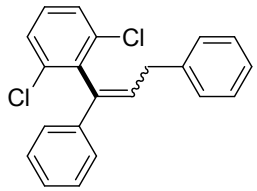

**(1-(4-Bromophenyl)prop-1-ene-1,3-diyl)dibenzene (3p)**

Colorless oil. $^1$H NMR (400 MHz, $CDCl_3$) δ: 7.56 (d, *J* = 7.2 Hz, 1H), 7.45–7.38 (m, 3H), 7.34 (t, *J* = 7.4 Hz, 2H), 7.29–7.21 (m, 6H), 7.16–7.14 (m, 2H), 6.35–6.28 (m, 1H), 3.50 (d, *J* = 7.6 Hz, 2H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ: 142.0, 141.49, 141.46, 141.4, 140.7, 140.6, 139.3, 138.8, 131.7, 131.6, 131.2, 129.9, 129.0, 128.6, 128.5, 128.41, 128.35, 128.3, 128.2, 127.4, 127.3, 126.14, 126.12, 121.3, 121.1, 36.0, 35.9. HRMS (EI) Calcd for $[M]^+$ $C_{21}H_{17}Br$: 348.0514, Found: 348.0521.



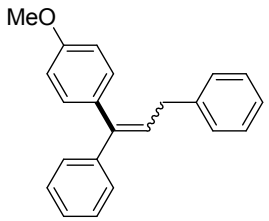

**(1-(4-Iodophenyl)prop-1-ene-1,3-diyl)dibenzene (3q)**

Colorless oil. $^1$H NMR (400 MHz, $CDCl_3$) δ: 7.75 (d, *J* = 8.4 Hz, 1H), 7.60 (d, *J* = 8.4 Hz, 1H), 7.45–7.38 (m, 2H), 7.36–7.20 (m, 8H), 7.03–7.00 (m, 2H), 6.33–6.25 (m, 1H), 3.48 (d, *J* = 7.6 Hz, 2H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ: 142.0, 141.9, 141.6, 141.5, 140.63, 140.59, 139.4, 139.2, 137.5, 137.2, 131.9, 129.9, 129.2, 128.6, 128.54, 128.45, 128.44, 128.39., 128.3, 128.2, 127.4, 127.33, 127.3, 126.13, 126.11, 121.5, 92.9, 92.6, 36.0, 35.9. HRMS (EI) Calcd for $[M]^+$ $C_{21}H_{17}I$: 396.0375, Found: 396.0382.



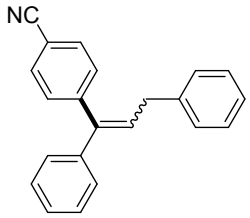

**(1-(2,6-Dichlorophenyl)prop-1-ene-1,3-diyl)dibenzene (3r)**

$^{1}$H NMR (400 MHz, $CDCl_3$) δ: 7.48–7.43 (m, 2H), 7.39–7.27 (m, 11H), 6.55 (t, *J* = 7.2 Hz, 0.73H), 5.94 (t, *J* = 7.5 Hz, 0.27H), 3.81 (d, *J* = 7.5 Hz, 0.53H), 3.35 (d, *J* = 7.2 Hz, 1.47H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ: 141.4, 140.3, 139.9, 138.7, 137.6, 137.4, 137.2, 136.7, 135.6, 135.4, 132.7, 130.6, 129.3, 129.2, 128.7, 128.52, 128.46, 128.44, 128.4, 128.2, 128.1, 128.0, 127.4, 127.3, 126.2, 126.1, 126.0, 36.2, 35.2. HRMS (EI) Calcd for $[M]^+$ $C_{21}H_{16}Cl_2$: 338.0624, Found: 338.0620.



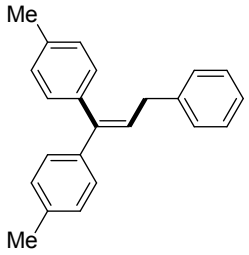

**(1-(4-Methoxyphenyl)prop-1-ene-1,3-diyl)dibenzene (3s)**

$^{1}$H NMR (400 MHz, $CDCl_3$) δ:7.38–7.34 (m, 1H), 7.31–7.15 (m, 10 H), 6.87–6.74 (m, 3H), 6.29–6.24 (m, 1H), 3.73 (s, 1.4 H), 3.70 (s, 1.6 H), 3.46 (t, *J* = 6.8 Hz, 2 H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ: 159.7, 159.6, 144.1, 142.5, 142.2, 141.3, 141.04, 141.0, 139.8, 130.0, 129.4, 129.1, 128.57, 128.5, 128.4, 128.2, 128.0, 127.8, 127.3, 127.24, 127.16, 126.07, 122.5, 120.1, 115.5, 113.5, 112.8, 112.4, 55.2, 36.1, 36.0. HRMS (EI) Calcd for $[M]^+$ $C_{22}H_{20}O$: 300.1509, Found: 300.1505.



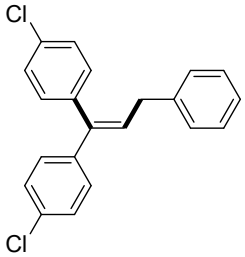

**4-(1,3-Diphenylprop-1-en-1-yl)benzonitrile (3t)**

$^{1}$H NMR (400 MHz, $CDCl_3$) δ: 7.72 (d, *J* = 8.0 Hz, 1H), 7.56 (d, *J* = 8.4 Hz, 1H), 7.47–7.21 (m, 12H), 6.44–6.37 (m, 1H), 3.54–3.47 (m, 2H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ: 146.7, 144.8,141.2, 141.09, 141.06, 140.1, 140.0, 138.4, 132.1, 131.9, 131.1, 130.7, 129.8, 129.2, 128.60, 128.59, 128.57, 128.3, 128.2, 127.71, 127.67, 127.6, 127.3, 126.3, 126.2, 118.9, 118.7, 111.1, 110.4, 36.0, 35.8. HRMS (EI) Calcd for $[M]^+$ $C_{22}H_{17}N$: 295.1356, Found: 295.1359.



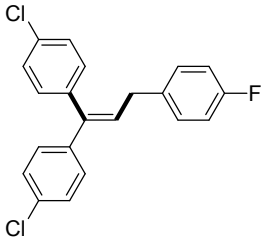

**4,4'-(3-Phenylprop-1-ene-1,1-diyl)bis(methylbenzene) (3u)**

Colorless oil. $^{1}$H NMR (400 MHz, $CDCl_3$) δ: 7.33–7.30 (m, 2H), 7.24–7.21 (m, 5H), 7.19-7.15 (m, 4H), 7.09 (d, *J* = 8.0 Hz, 2H), 6.23 (t, *J* = 7.6 Hz, 1H), 3.50 (d, *J* = 7.6 Hz, 2H), 2.41 (s, 3H), 2.35 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ: 142.3, 141.2, 139.9, 137.0, 136.7, 136.6, 129.8, 128.9, 128.8, 128.42, 128.41, 127.3, 126.7, 125.9, 35.9, 21.2, 21.0. HRMS (EI) Calcd for $[M]^+$ $C_{23}H_{22}$: 298.1722, Found: 298.1720.




**4,4'-(3-Phenylprop-1-ene-1,1-diyl)bis(chlorobenzene) (3v)**

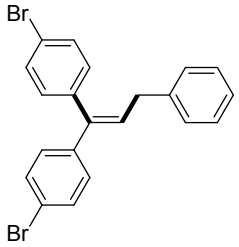
Colorless oil. $^{1}$H NMR (400 MHz, $CDCl_3$) δ: 7.39 (d, *J* = 8.4 Hz, 2H), 7.31 (t, *J* = 7.4 Hz, 2H), 7.25–7.14 (m, 9H), 6.27 (t, *J* = 7.6 Hz, 1H), 3.46 (d, *J* = 8.0 Hz, 2H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ: 140.5, 140.4, 137.8, 133.4, 133.2, 131.2, 128.9, 128.7, 128.61, 128.55, 128.4, 128.3, 126.2, 35.9. HRMS (EI) Calcd for $[M]^+$ $C_{21}H_{16}Cl_2$: 338.0629, Found: 338.0625.




**4,4'-(3-(4-Fluorophenyl)prop-1-ene-1,1-diyl)bis(chlorobenzene) (3w)**

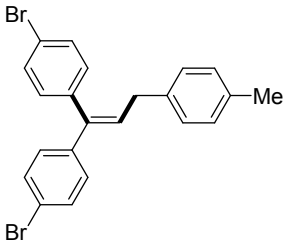
Colorless oil. $^{1}$H NMR (400 MHz, $CDCl_3$) δ: 7.39 (d, *J* = 8.4 Hz, 2H), 7.27–7.16 (m, 2H), 7.14–7.10 (m, 6H), 7.01–6.97 (t, *J* = 8.6 Hz, 2H), 6.22 (t, *J* = 7.6 Hz, 1H), 3.42 (d, *J* = 7.6 Hz, 2H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ: 162.0 (d, *J* = 242.8 Hz), 140.5 (d, *J* = 22.0 Hz), 137.6, 135.96 (d, *J* = 3.3 Hz), 133.5, 133.3, 131.2, 129.64 (d, *J* = 7.8

Hz), 128.8, 128.5, 128.4, 115.37 (d, $J$ = 21.1 Hz), 35.1. HRMS (EI) Calcd for $[M]^+$ $C_{21}H_{15}Cl_2F$: 356.0305, Found: 356.0304.



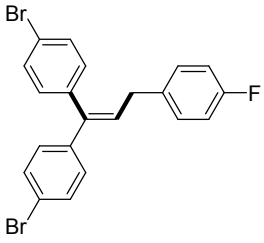

**4,4'-(3-Phenylprop-1-ene-1,1-diyl)bis(bromobenzene) (3x)**

Colorless oil. $^1$H NMR (400 MHz, $CDCl_3$) δ: 7.56 (d, $J$ = 8.4 Hz, 2H), 7.41 (d, $J$ = 8.4 Hz, 2H), 7.33–7.26 (m, 2H), 7.24–7.18 (m, 3H), 7.13–7.10 (m, 4H), 6.30 (t, $J$ = 7.6 Hz, 1H), 3.47 (d, $J$ = 7.6 Hz, 2H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ: 141.8, 140.9, 140.4, 140.3, 138.1, 131.7, 131.6, 131.3, 128.9, 128.6, 128.3, 126.2, 121.5, 121.4, 35.9. HRMS (EI) Calcd for $[M]^+$ $C_{21}H_{16}Br_2$: 425.9619, Found: 426.9617.




**4,4'-(3-(*p*-Tolyl)prop-1-ene-1,1-diyl)bis(bromobenzene) (3y)**

Colorless oil. $^1$H NMR (400 MHz, $CDCl_3$) δ: 7.54 (d, $J$ = 8.0 Hz, 2H), 7.39 (d, $J$ = 8.4 Hz, 2H), 7.14–7.06 (m, 8H), 6.25 (t, $J$ = 7.6 Hz, 1H), 3.41 (d, $J$ = 7.6 Hz, 2H), 2.34 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ: 140.9, 140.2, 138.2, 137.2, 135.8, 131.7, 131.6, 131.3 129.3, 129.2, 128.9, 128.2 121.5, 121.3, 35.5, 21.0. HRMS (EI) Calcd for $[M]^+$ $C_{22}H_{18}Br_2$: 439.9775, Found: 439.9772.




**4,4'-(3-(4-Fluorophenyl)prop-1-ene-1,1-diyl)bis(bromobenzene) (3z)**

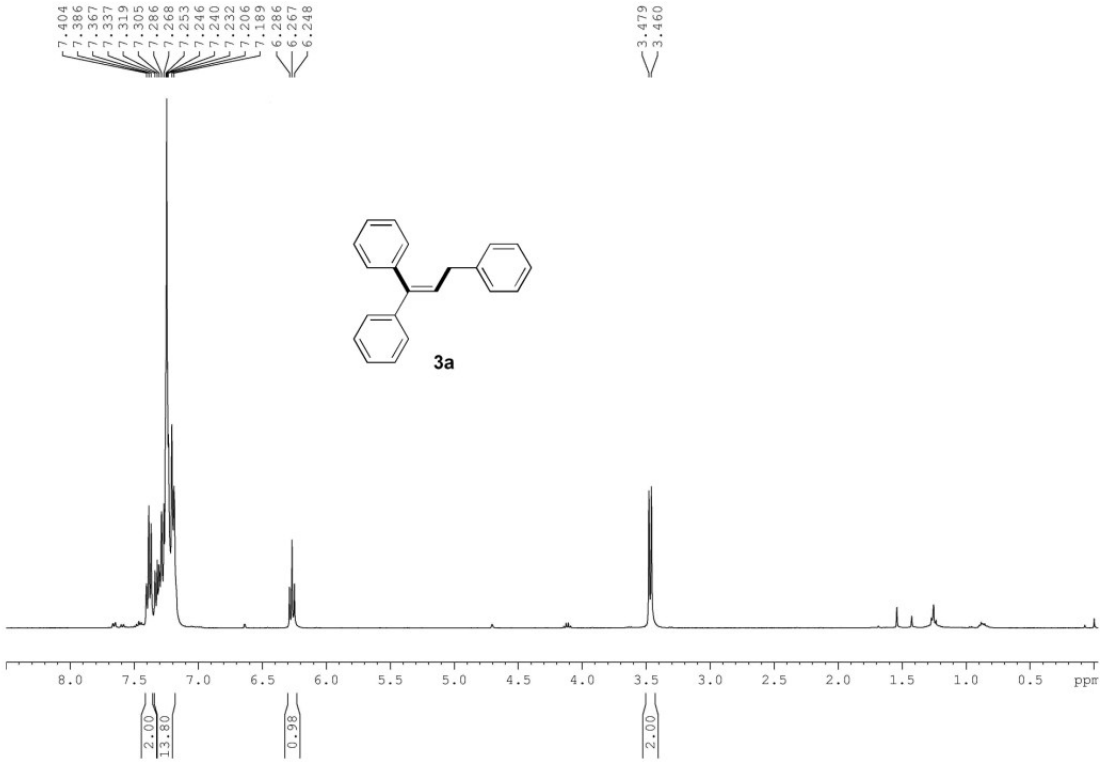
Colorless oil. $^1$H NMR (400 MHz, $CDCl_3$) δ: 7.55 (d, $J$ = 8.0 Hz, 2H), 7.41(d, $J$ = 8.4

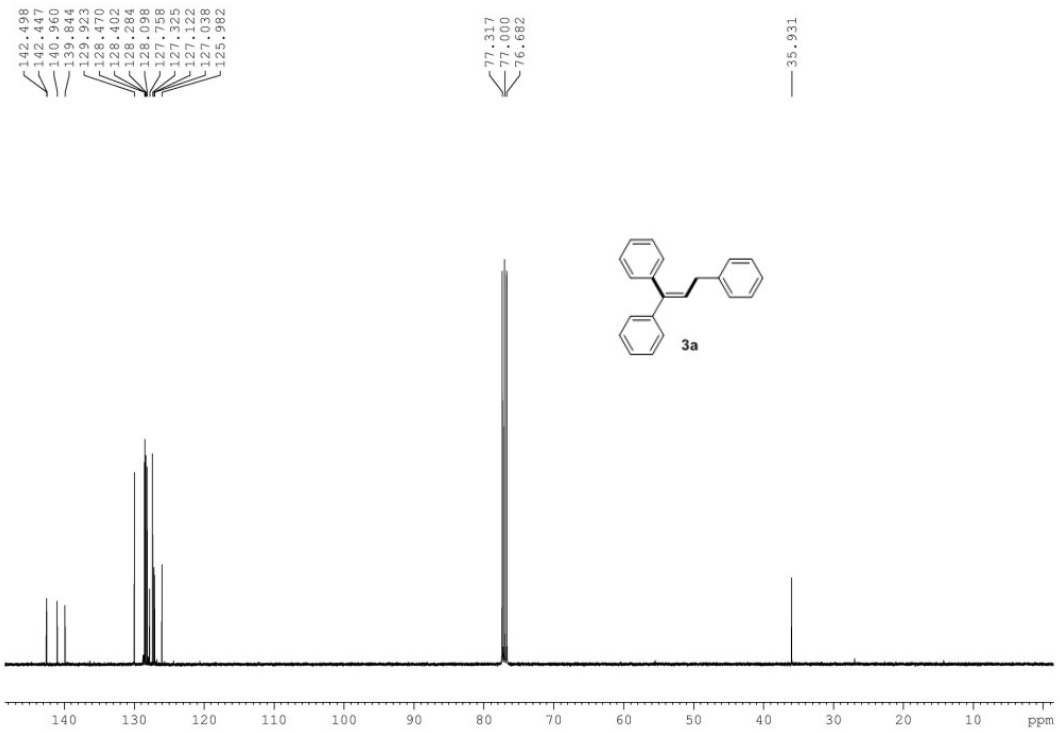
Hz, 2H), 7.14–7.09 (m, 6H), 7.02–6.97 (m, 2H), 6.25 (t, *J* = 7.6 Hz, 1H), 3.43(d, *J* = 7.6 Hz, 2H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ: 161.5 (d, *J* = 242.8 Hz), 140.65 (d, *J* = 9.8 Hz), 138.0, 135.87 (d, *J* = 3.2 Hz), 131.7, 131.5, 131.4, 129.62 (d, *J* = 7.8 Hz), 128.9, 128.6, 121.54 (d, *J* = 17.4 Hz), 115.36 (d, *J* = 21.1 Hz), 35.1. HRMS (EI) Calcd for $[M]^+$ $C_{21}H_{15}Br_2F$: 443.9525, Found: 443.9524.

## V. Reference

1. H. Gu and C. Wang, *Org. Biomol. Chem*., 2015, **13**, 5880.

## VI. $^1$H and $^{13}$C NMR spectra of the products

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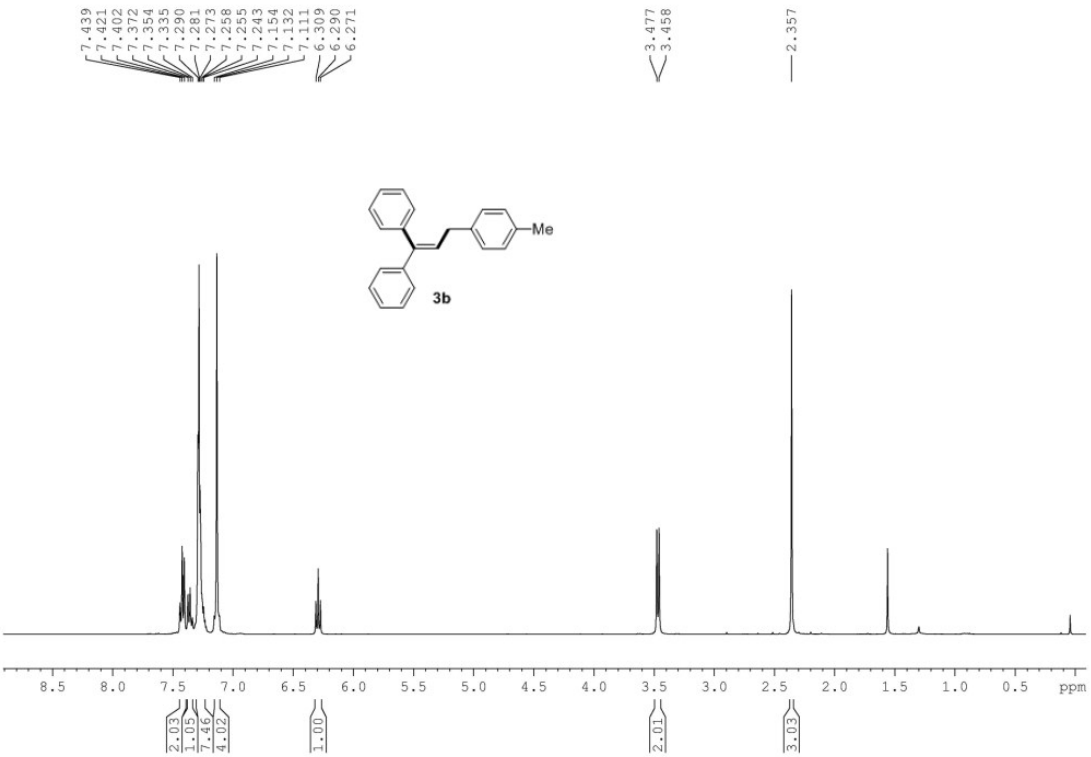
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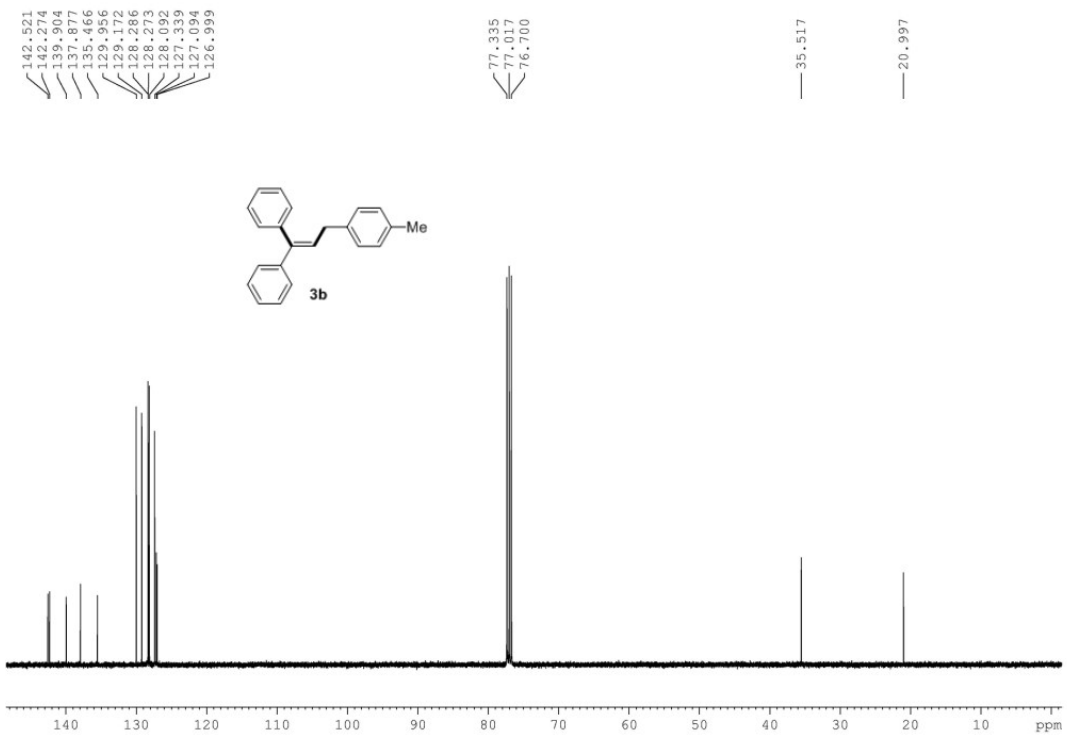
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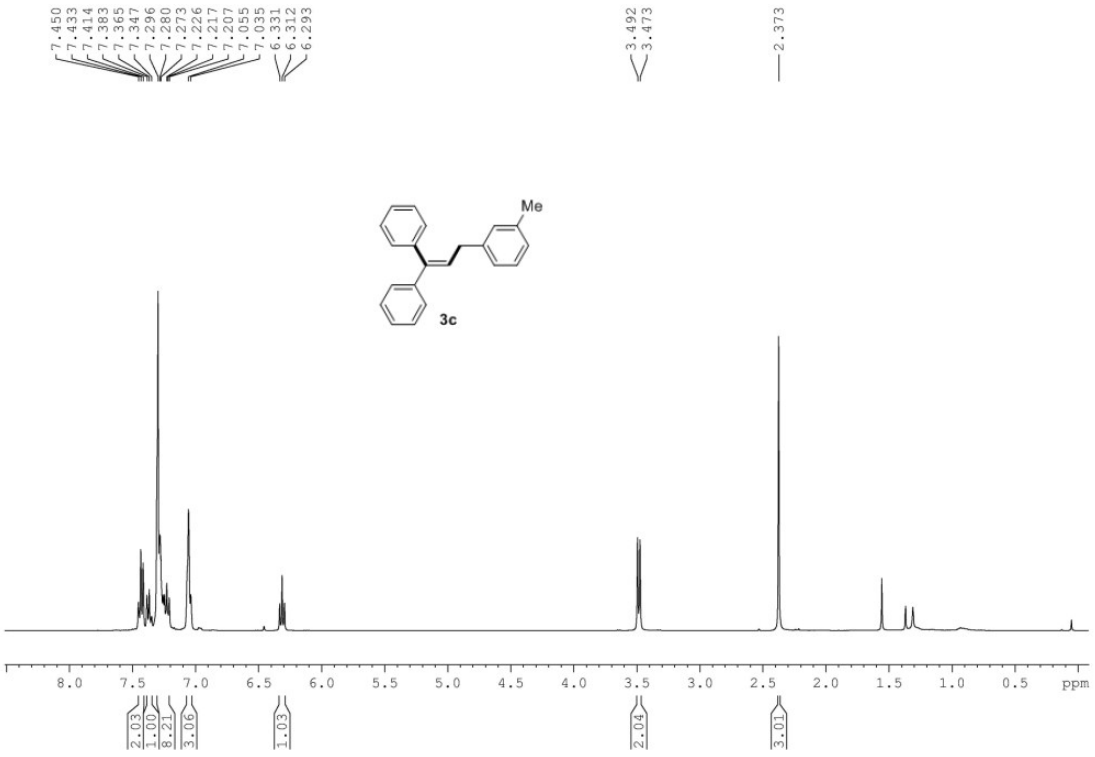
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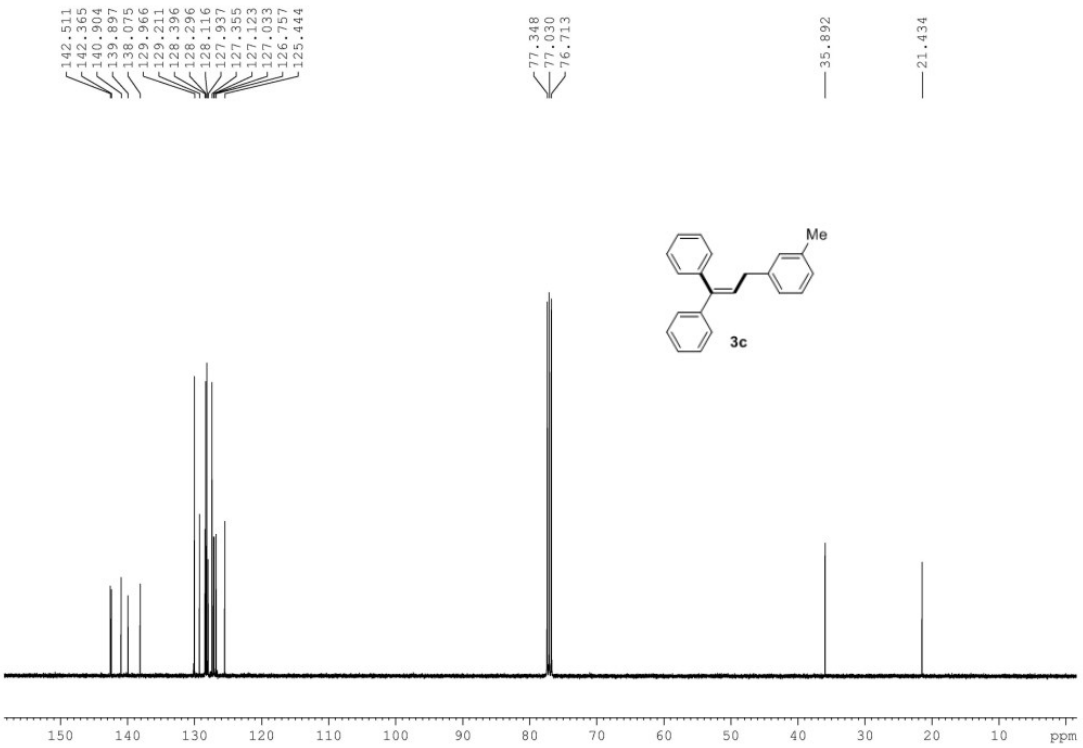
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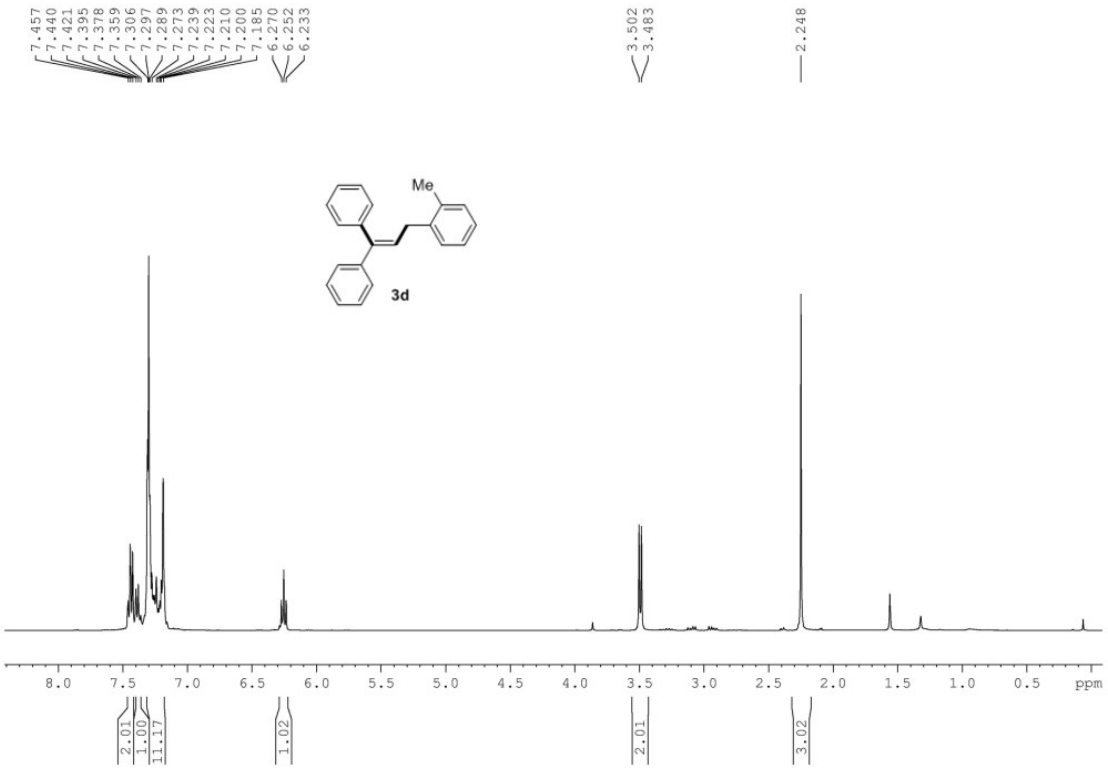
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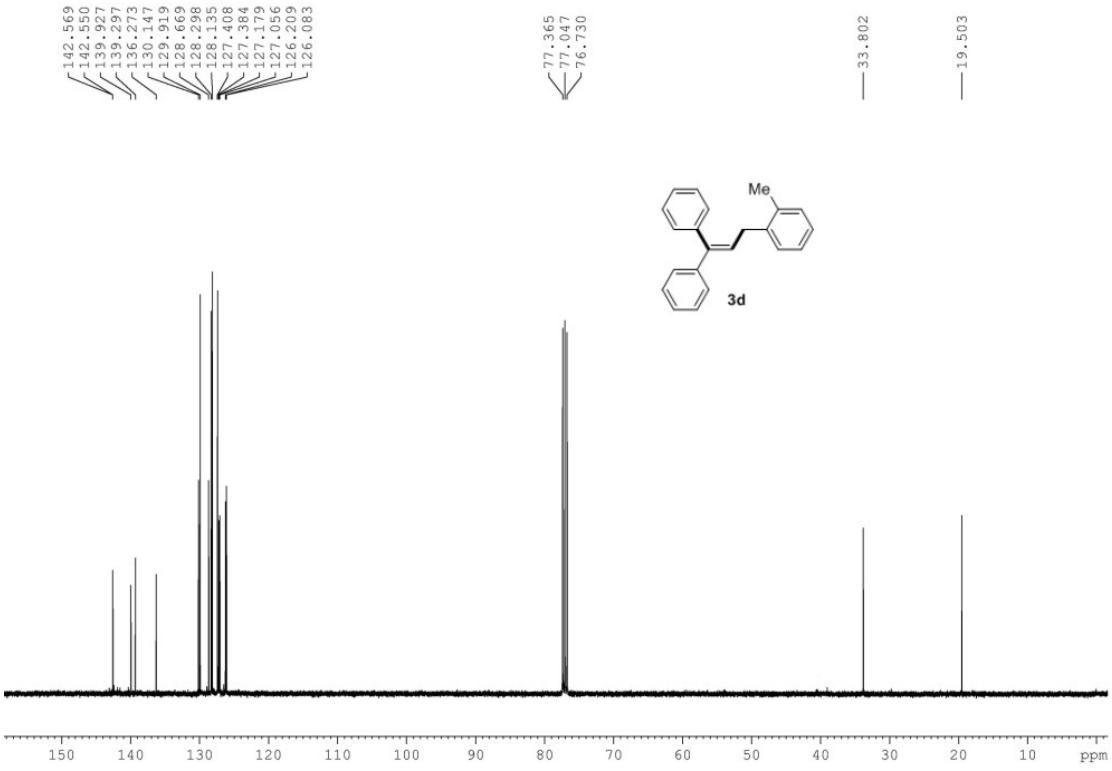
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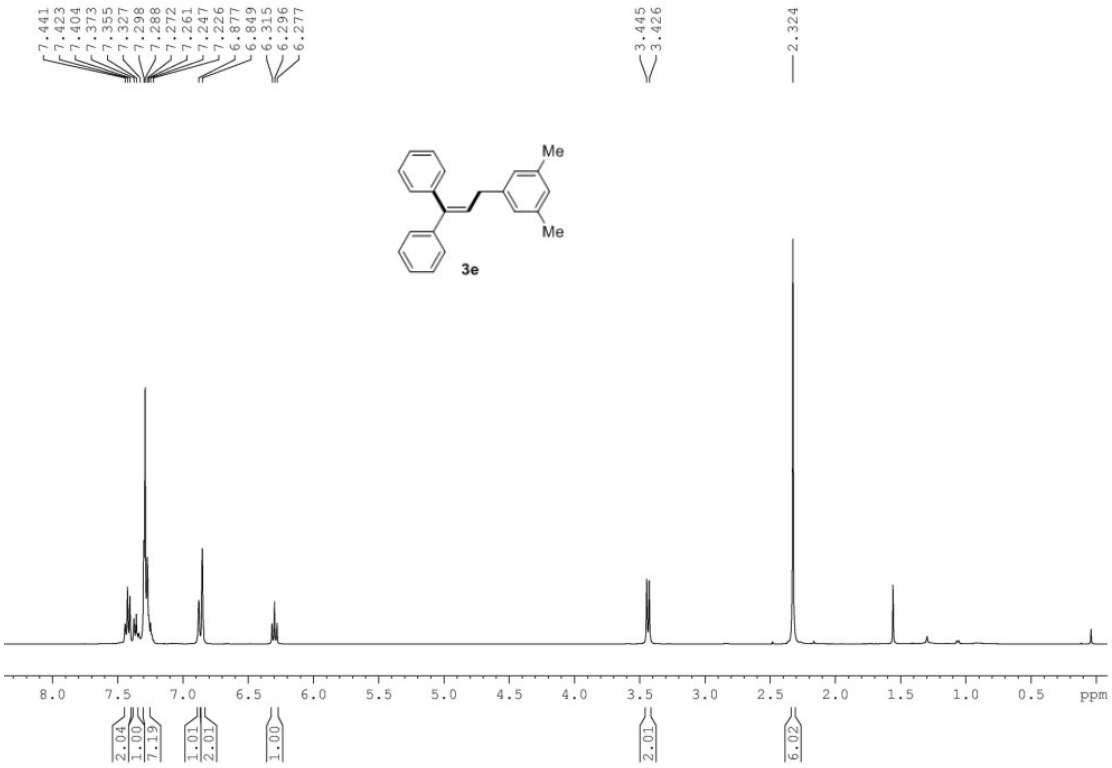
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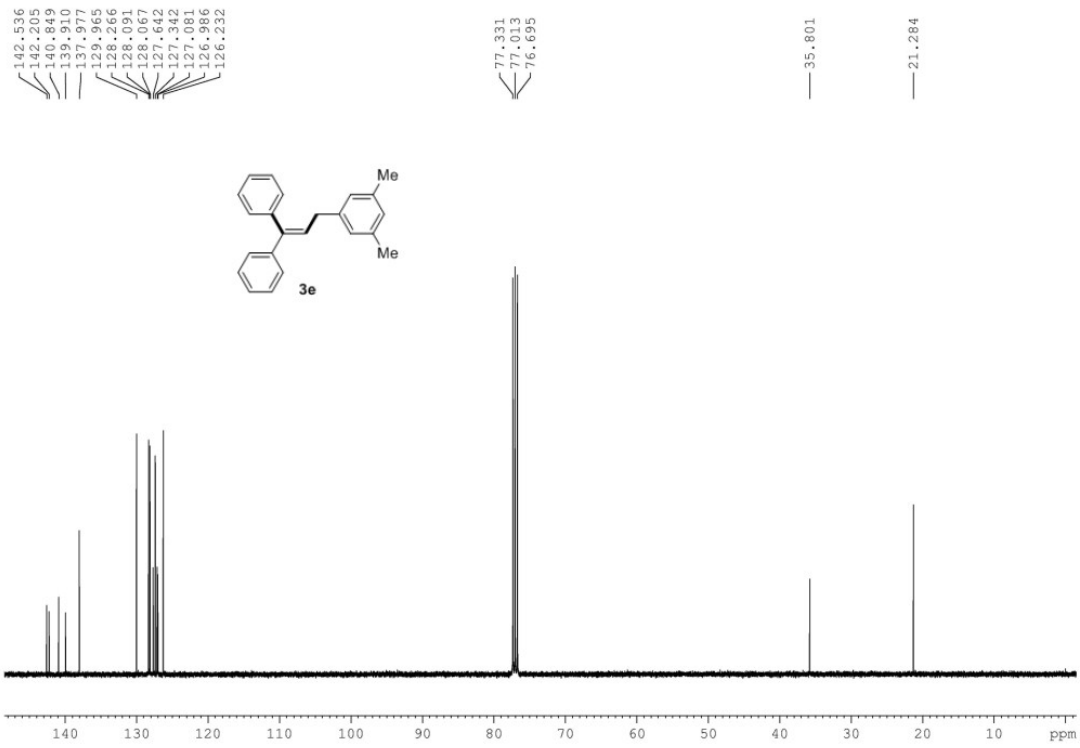
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30
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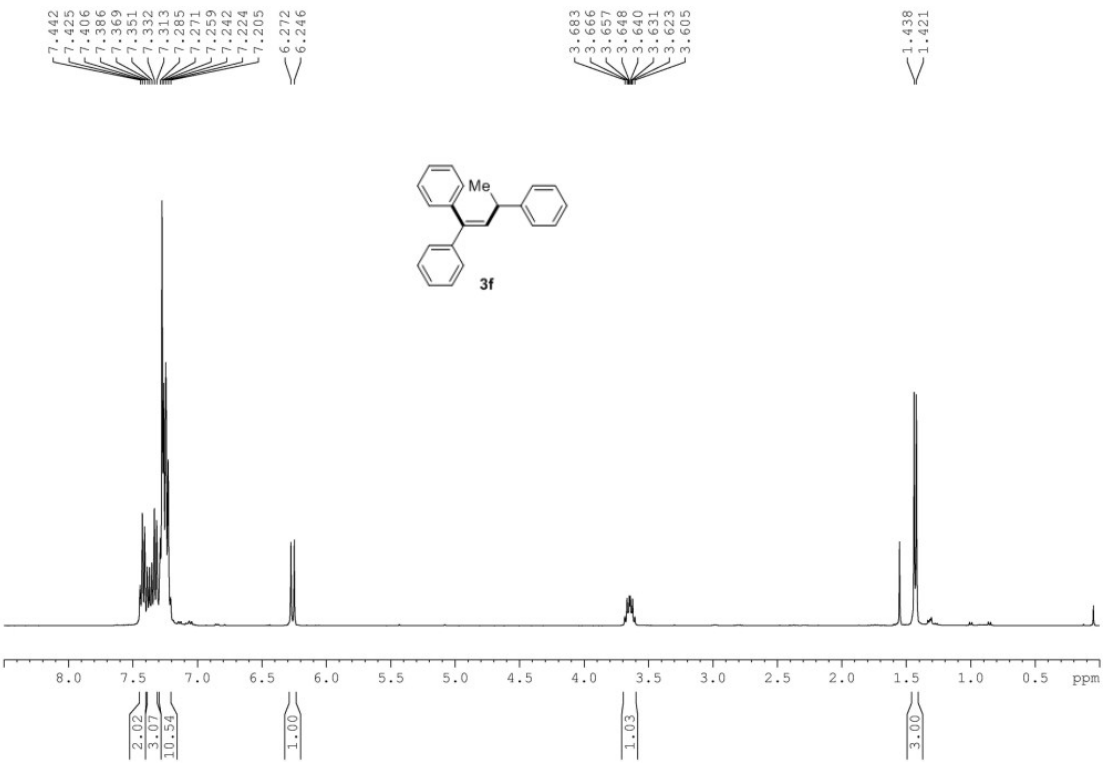
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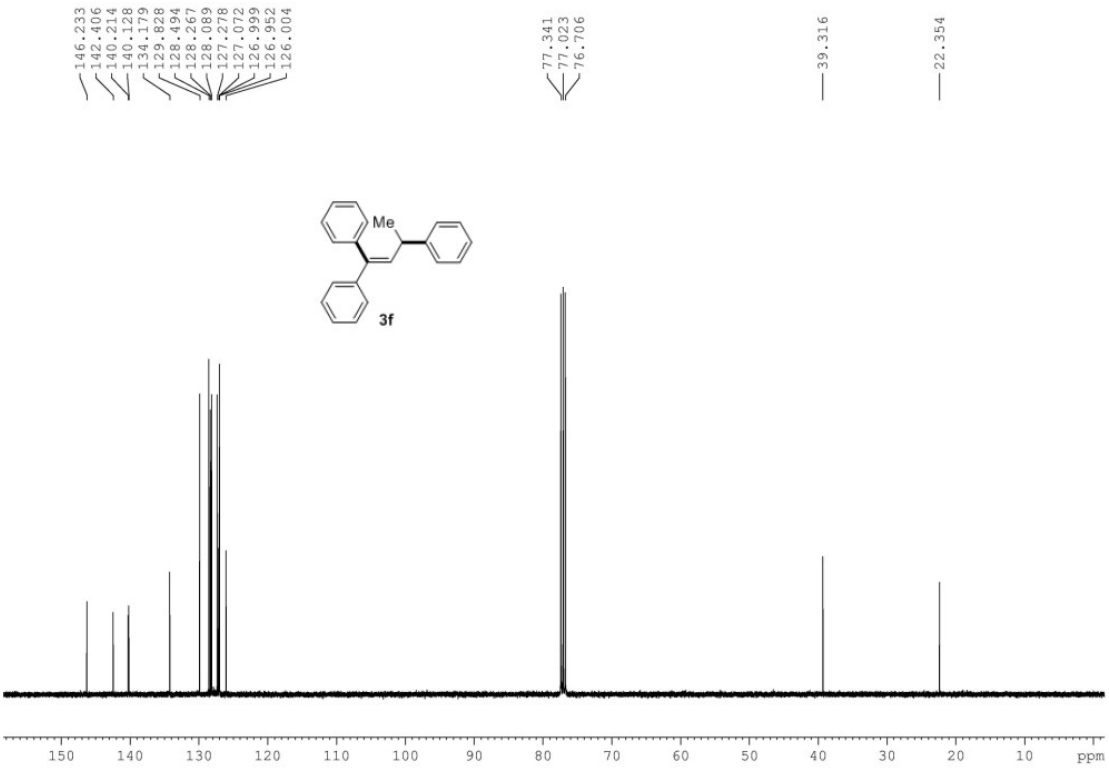
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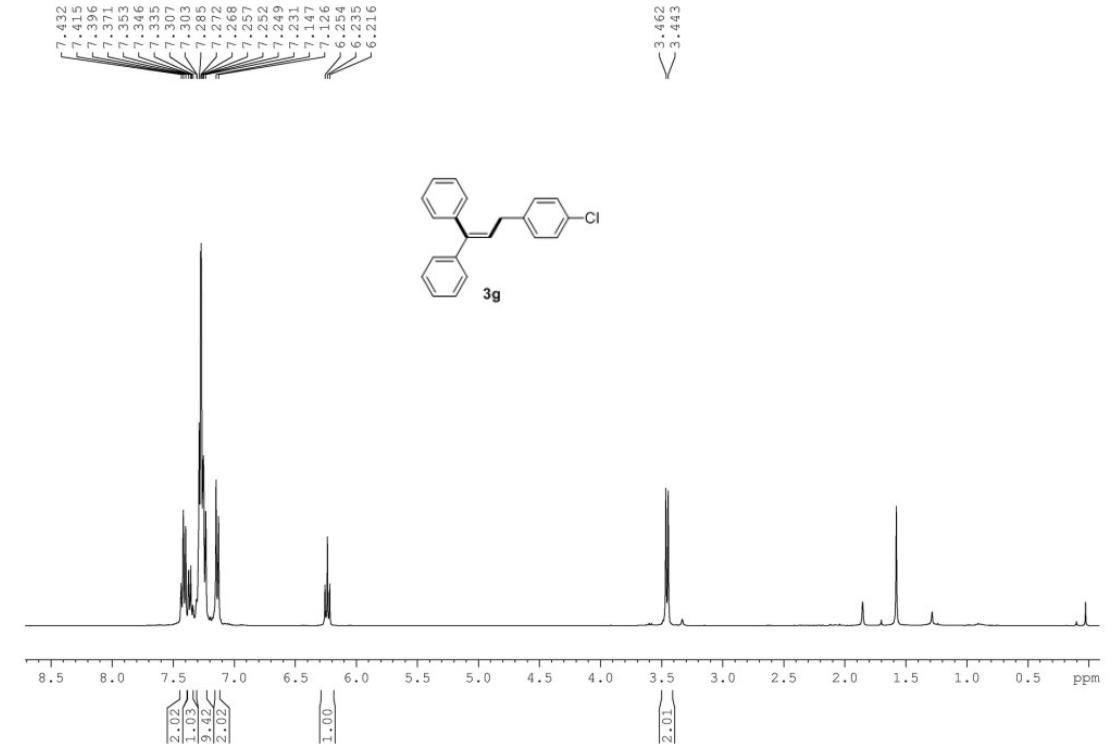
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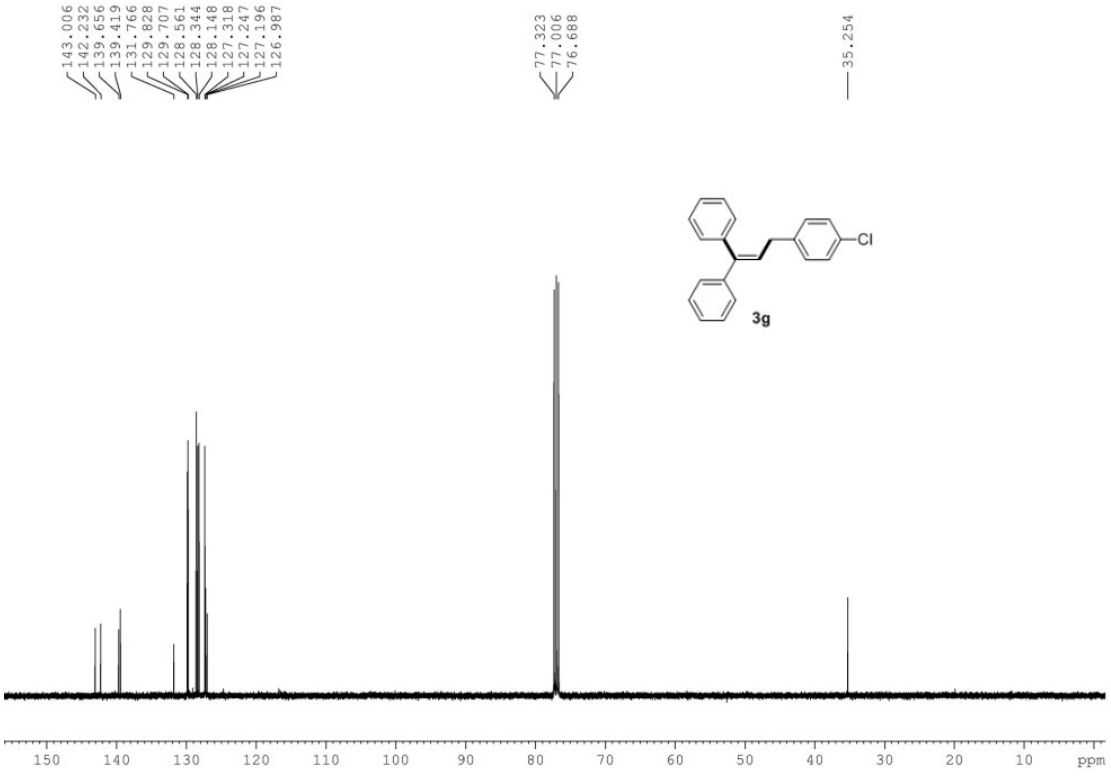
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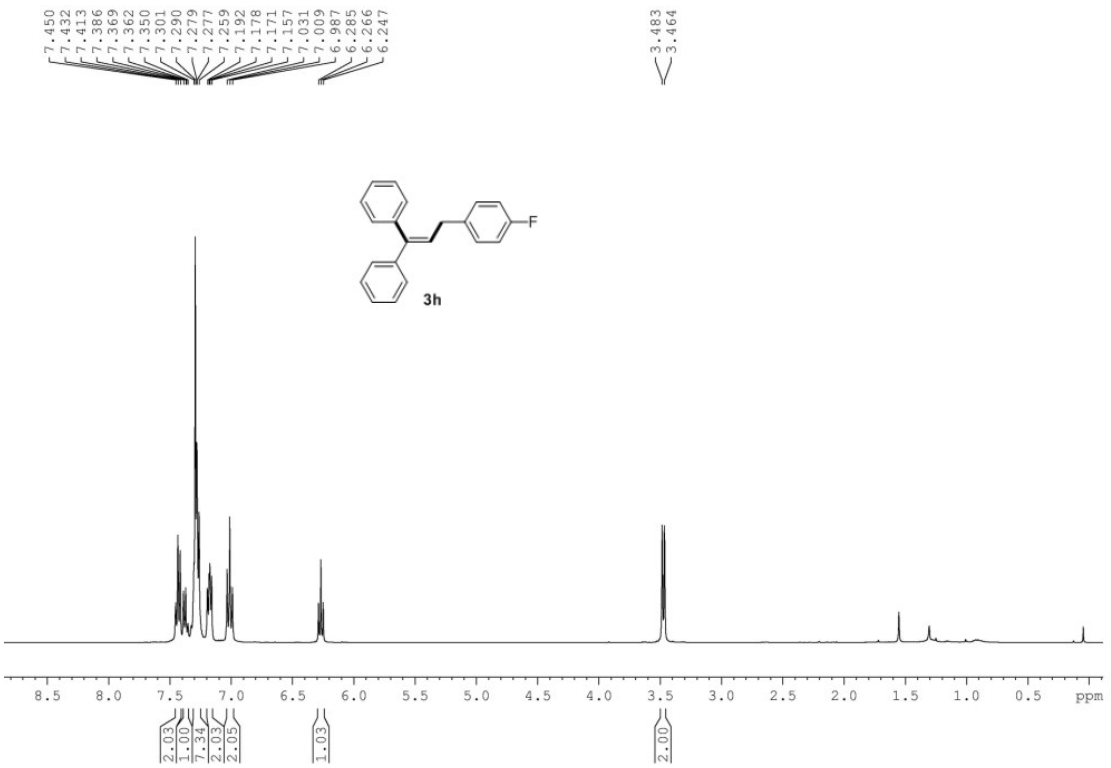
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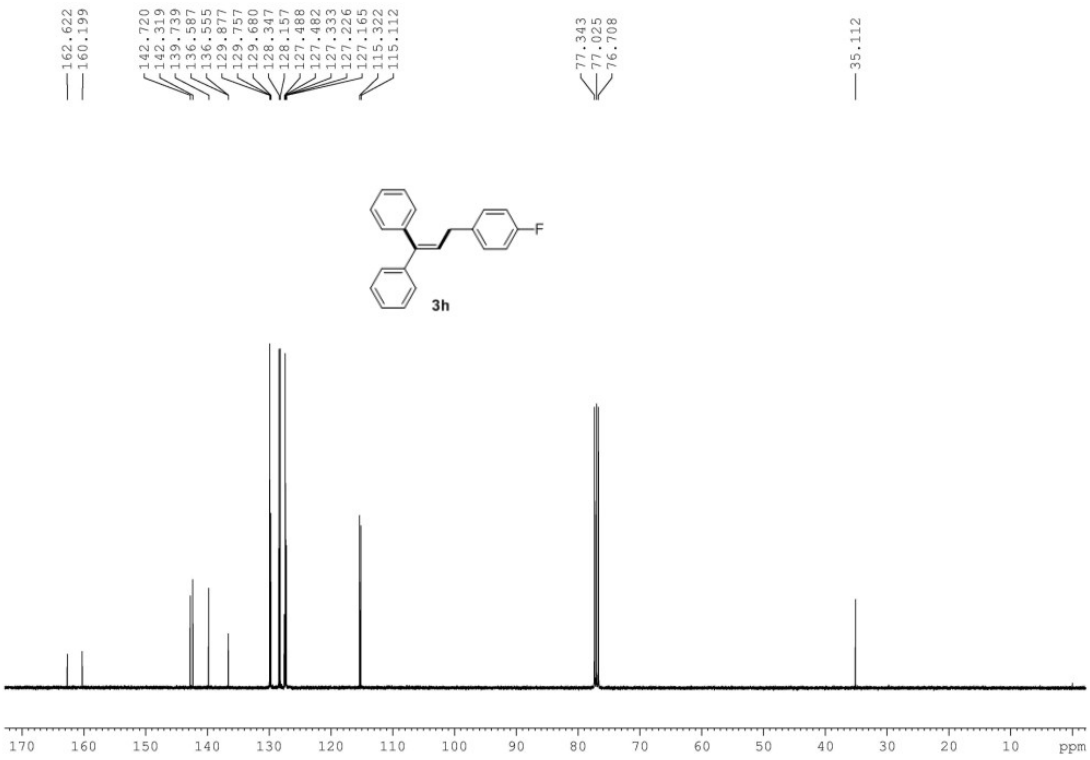
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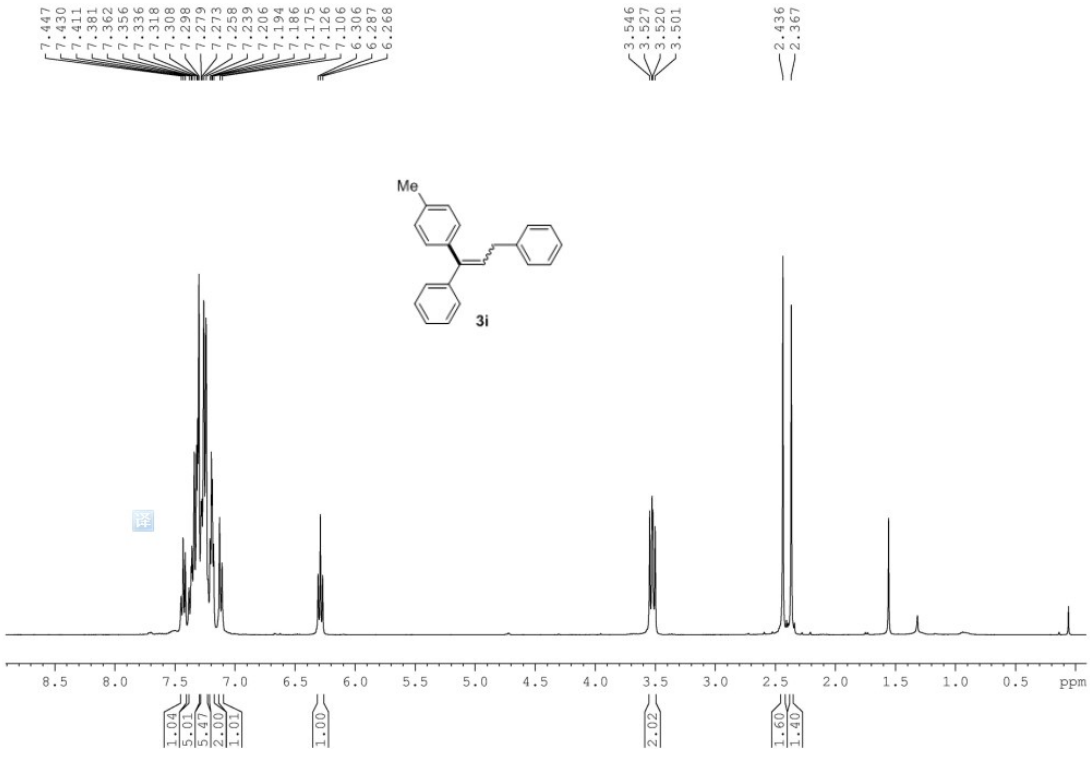
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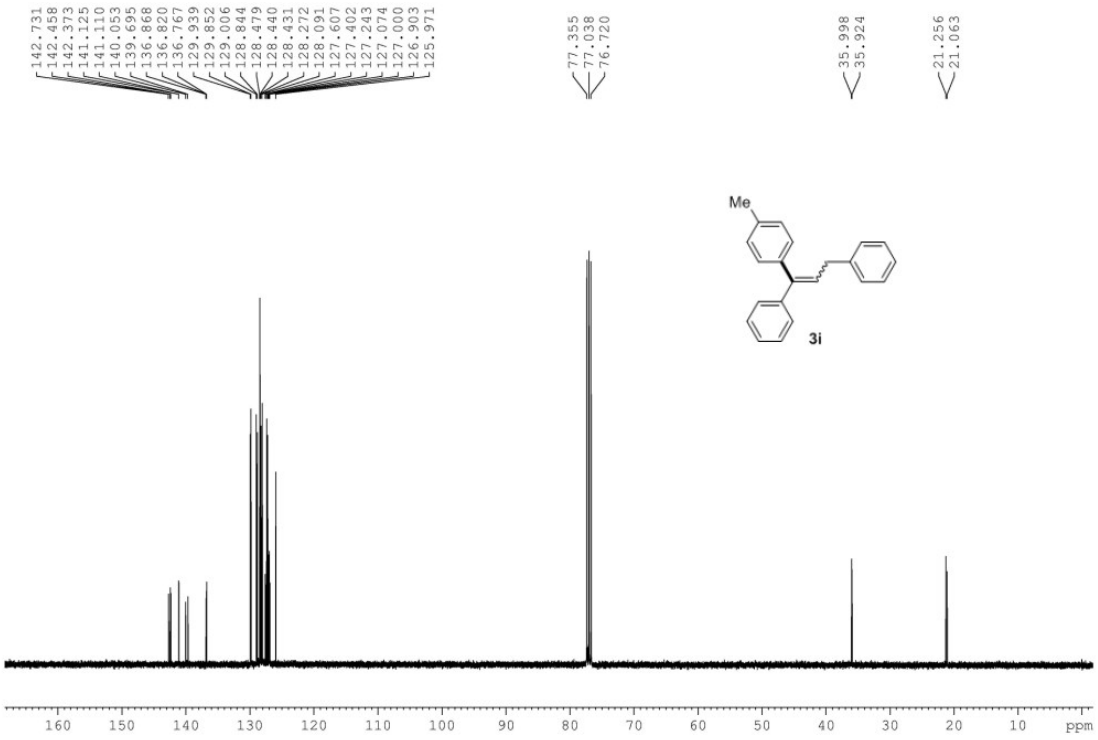
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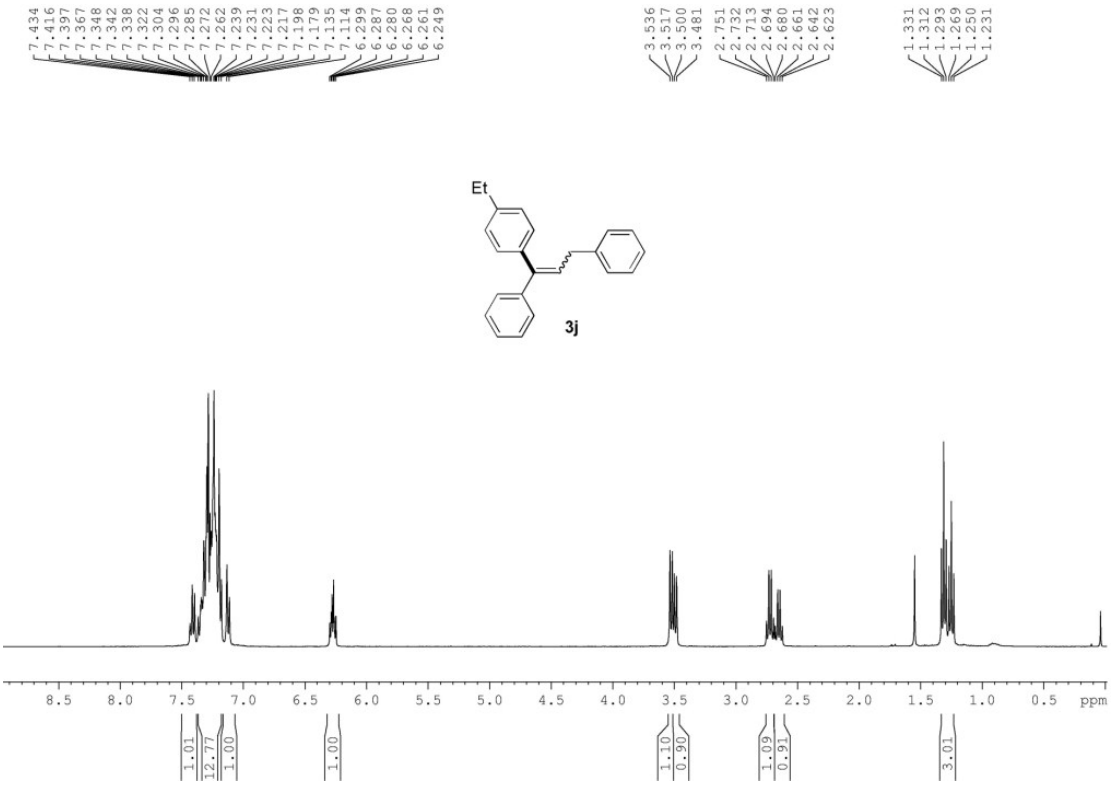
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4.0
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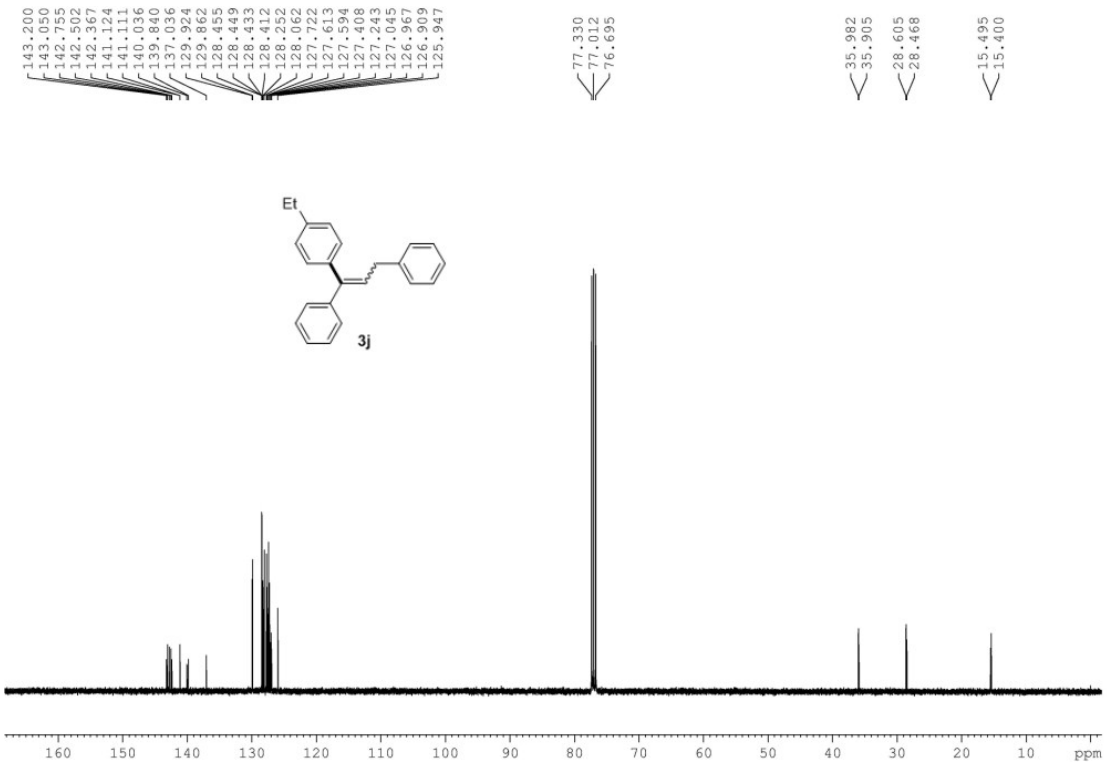
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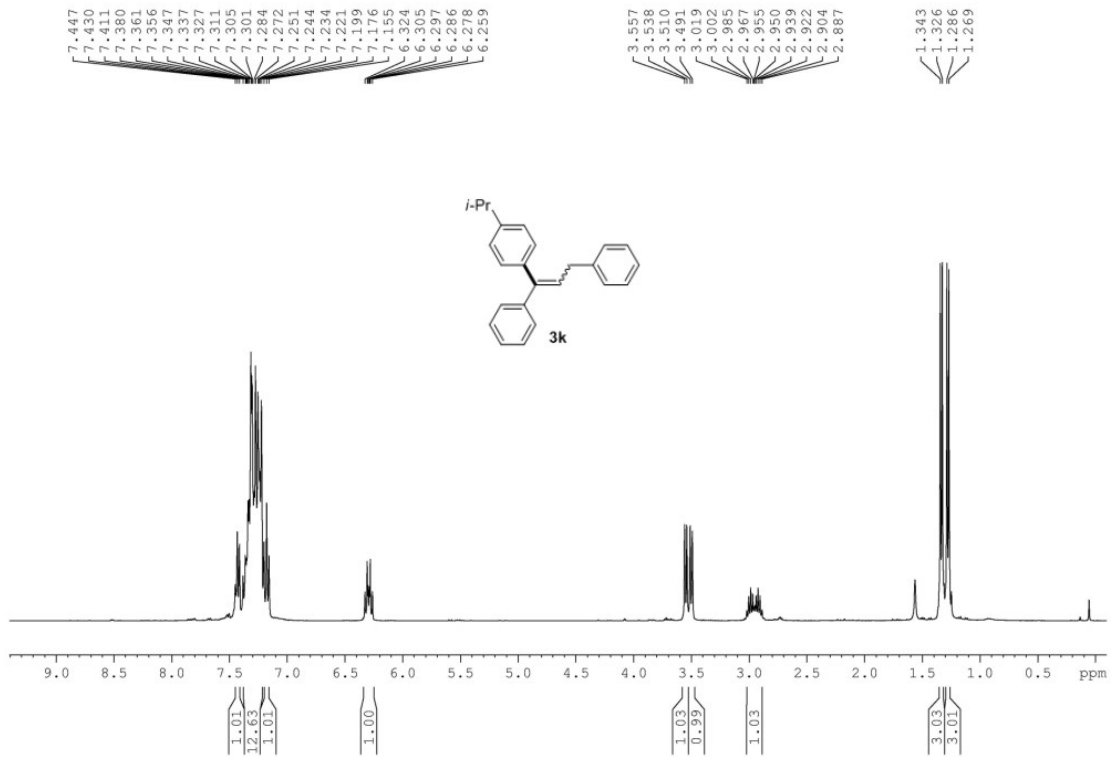
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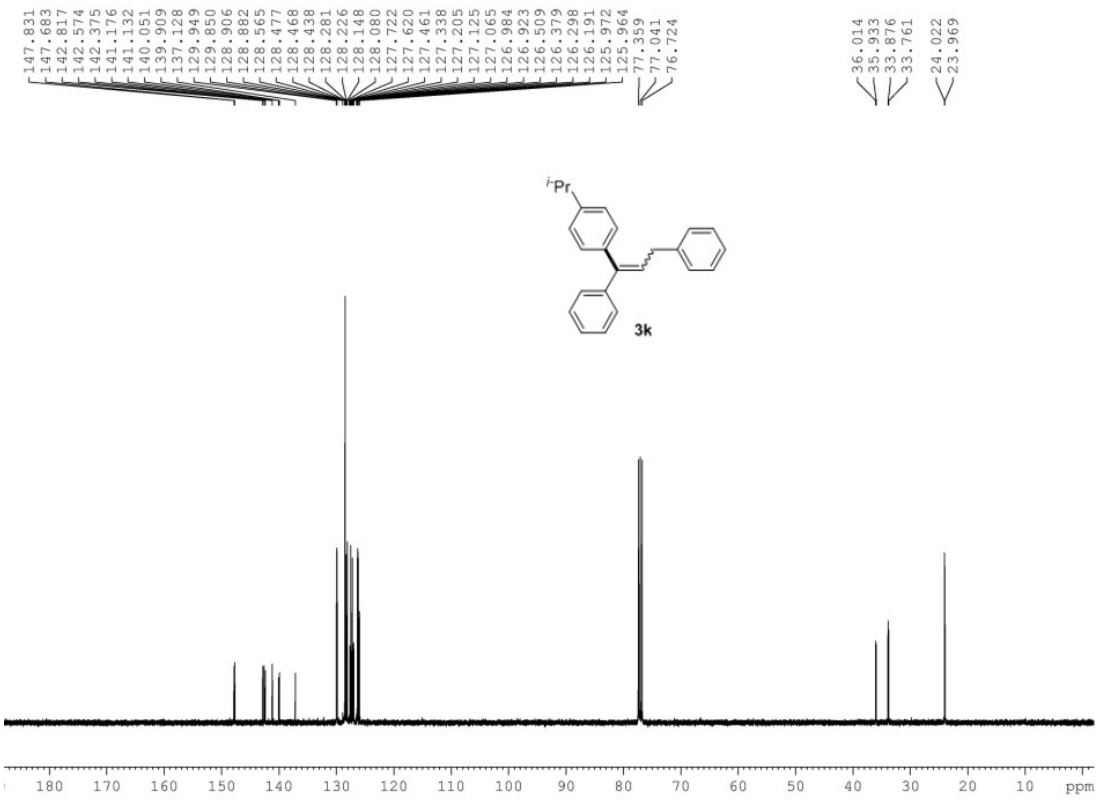
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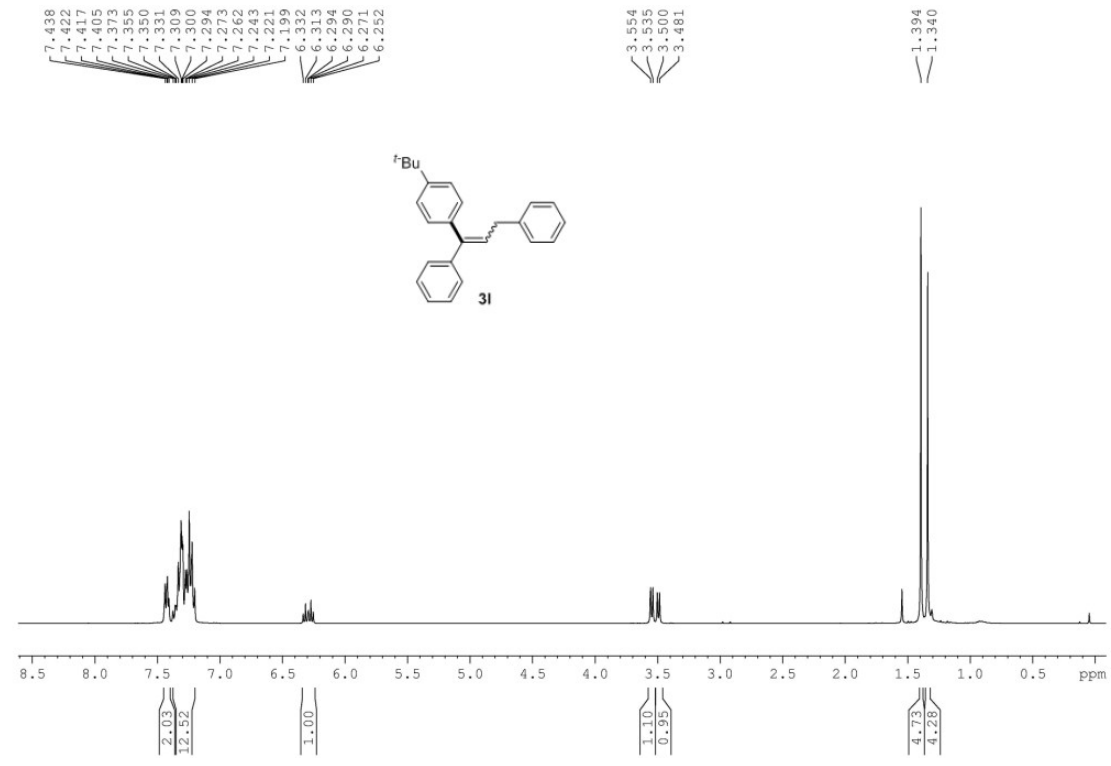
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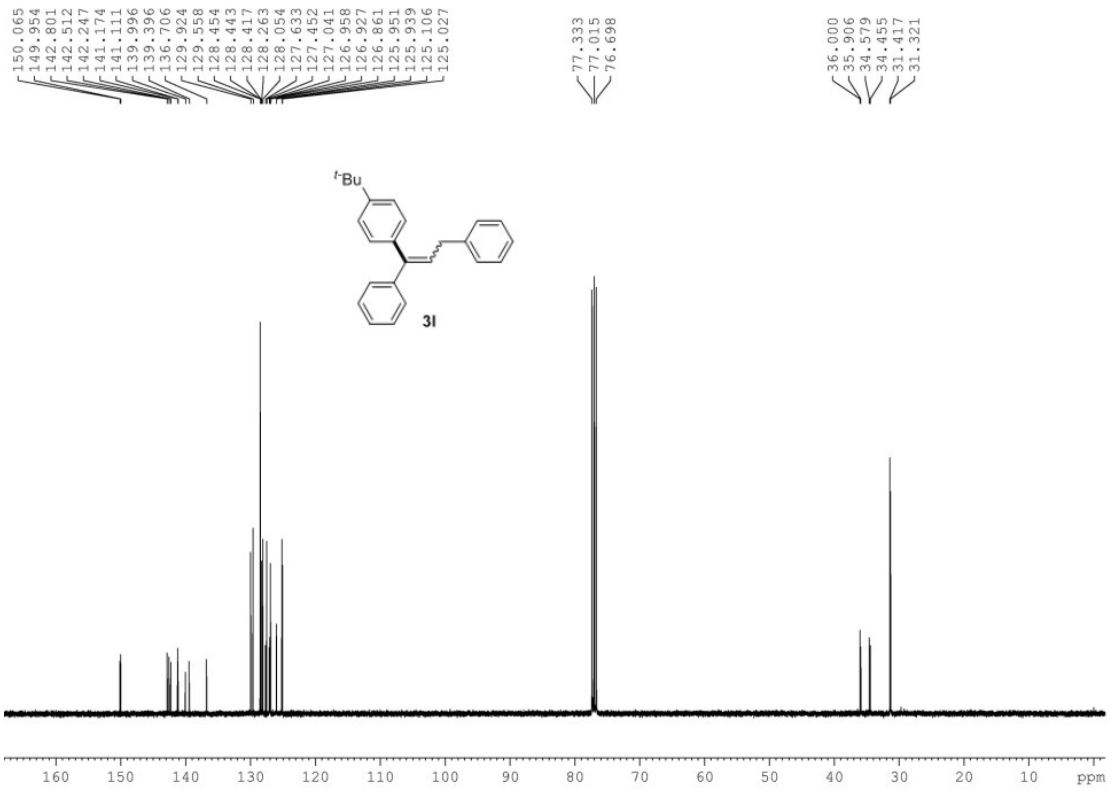
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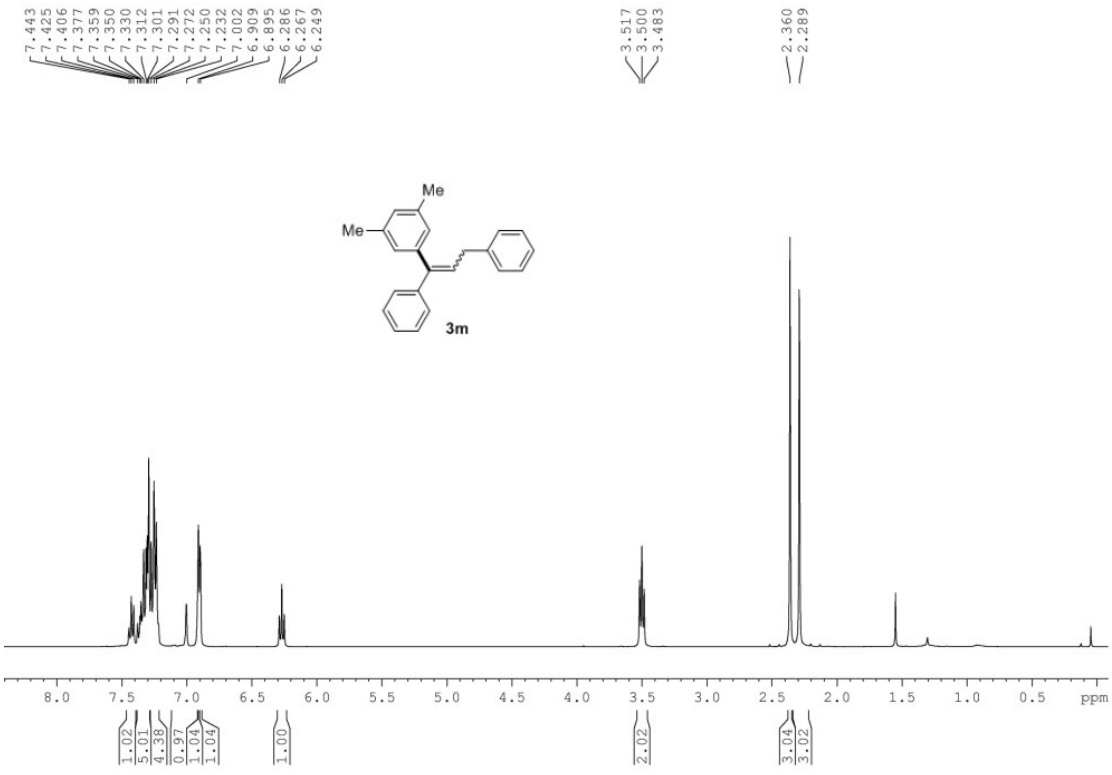
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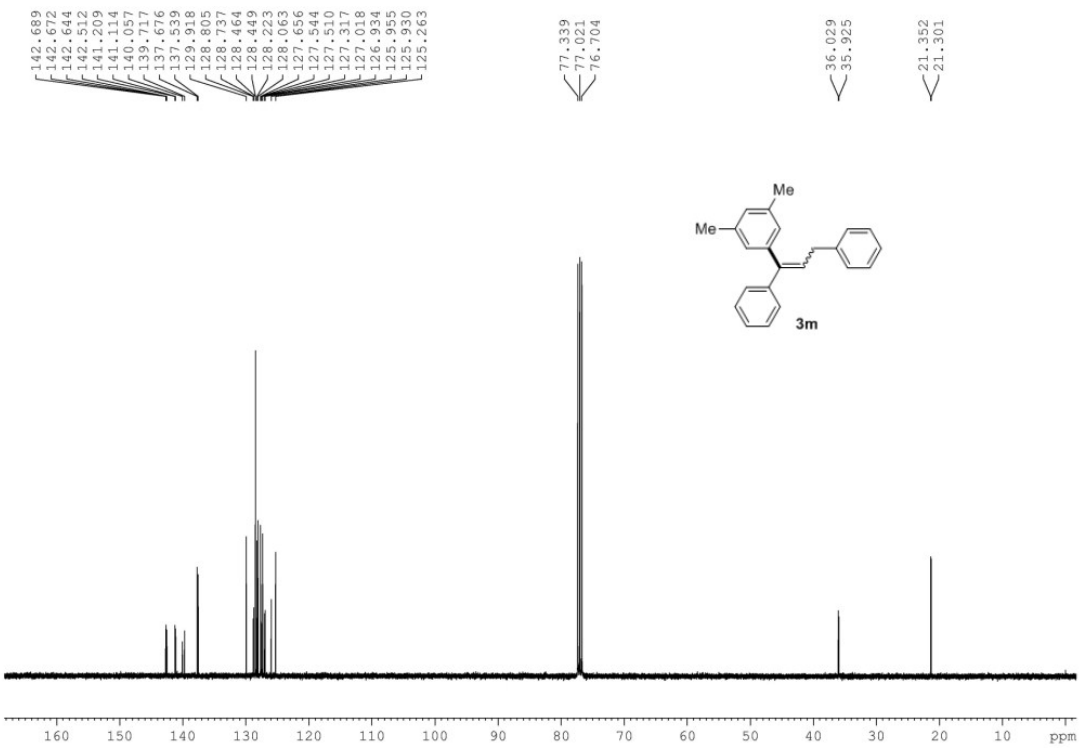
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77.021
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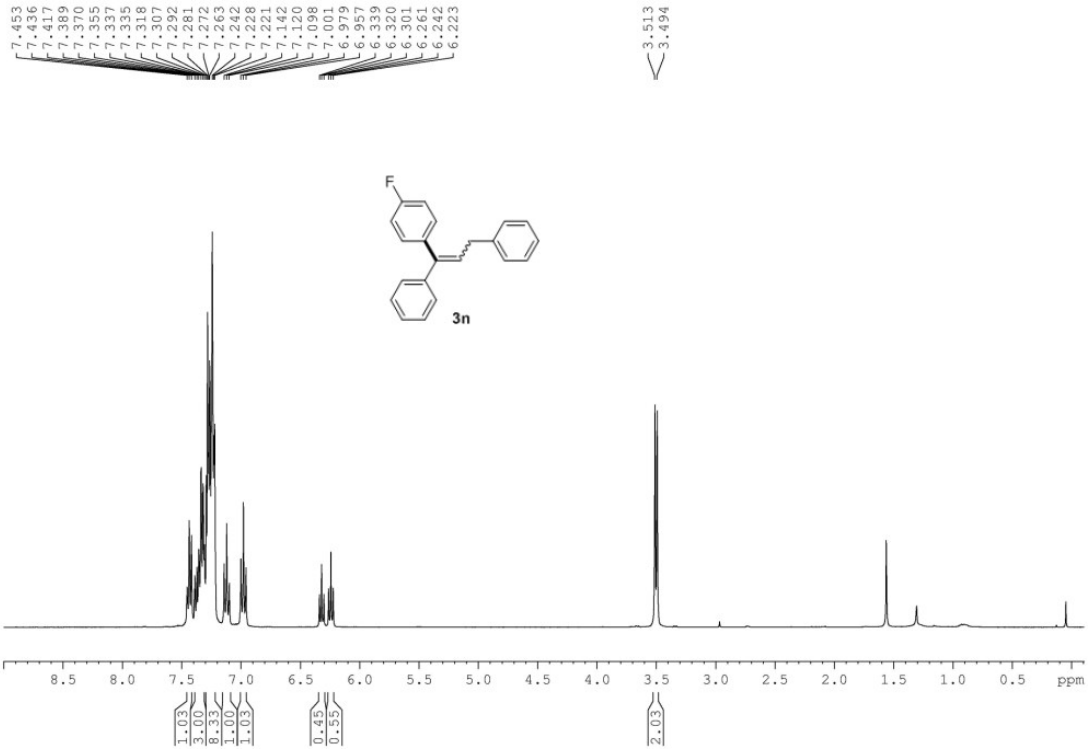
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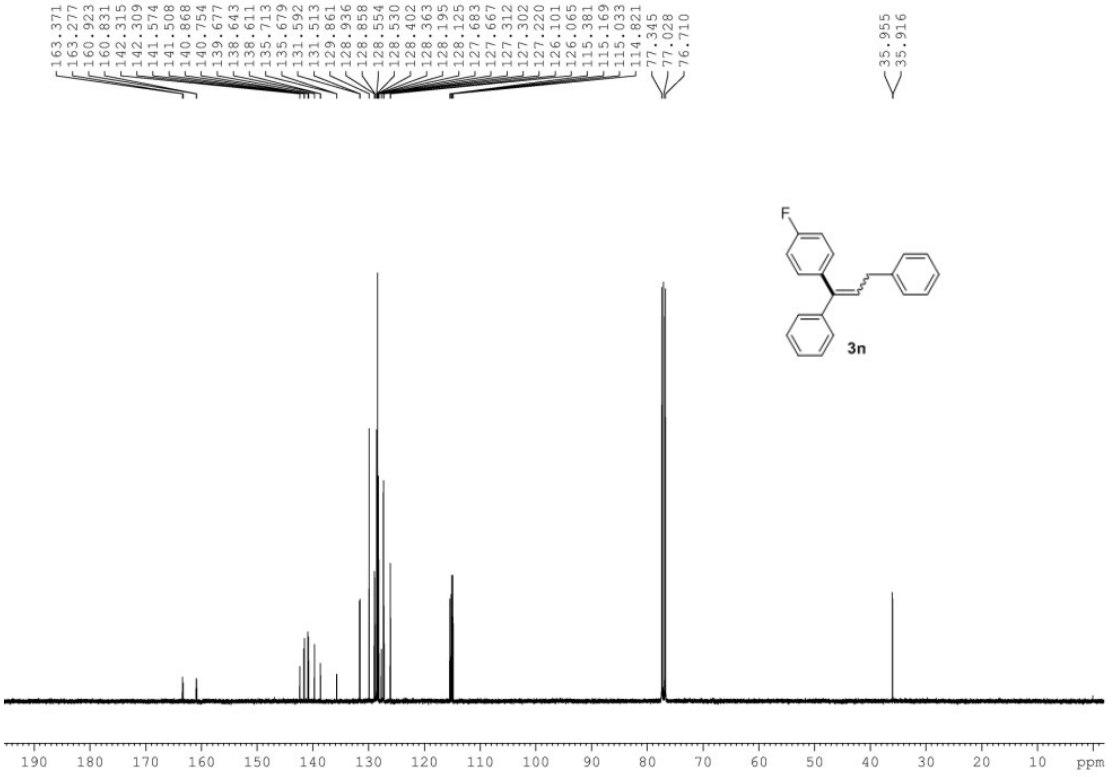
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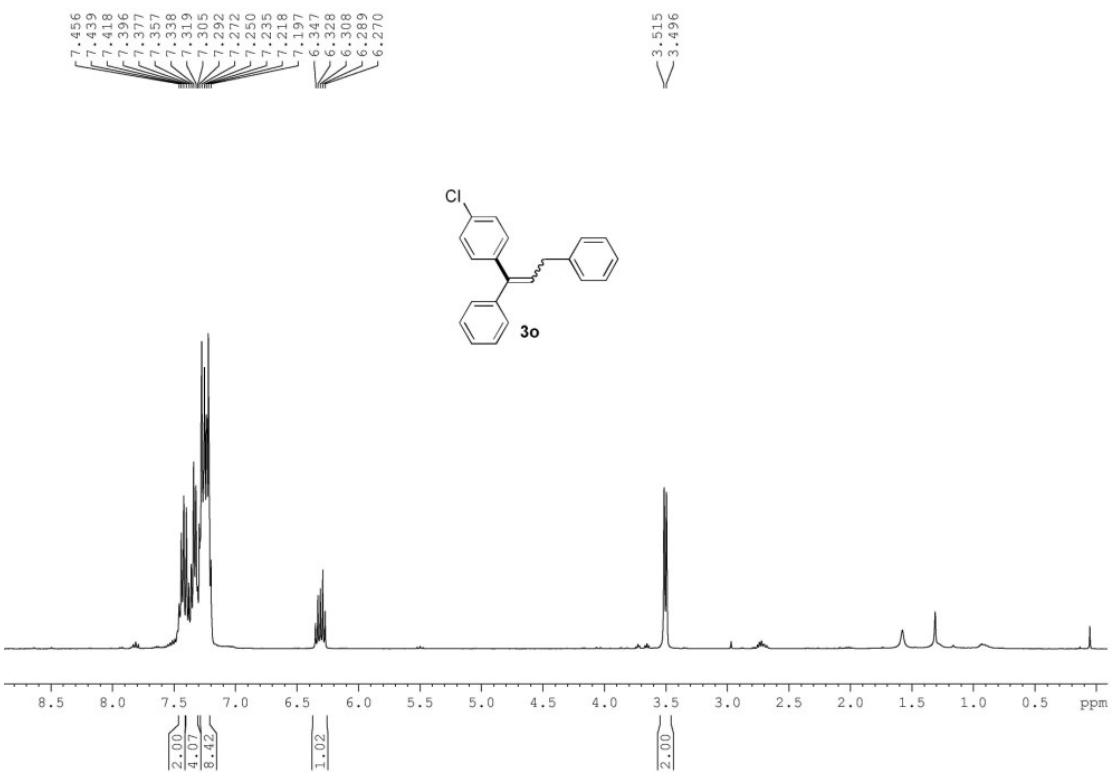
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6.308
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Cl
3o
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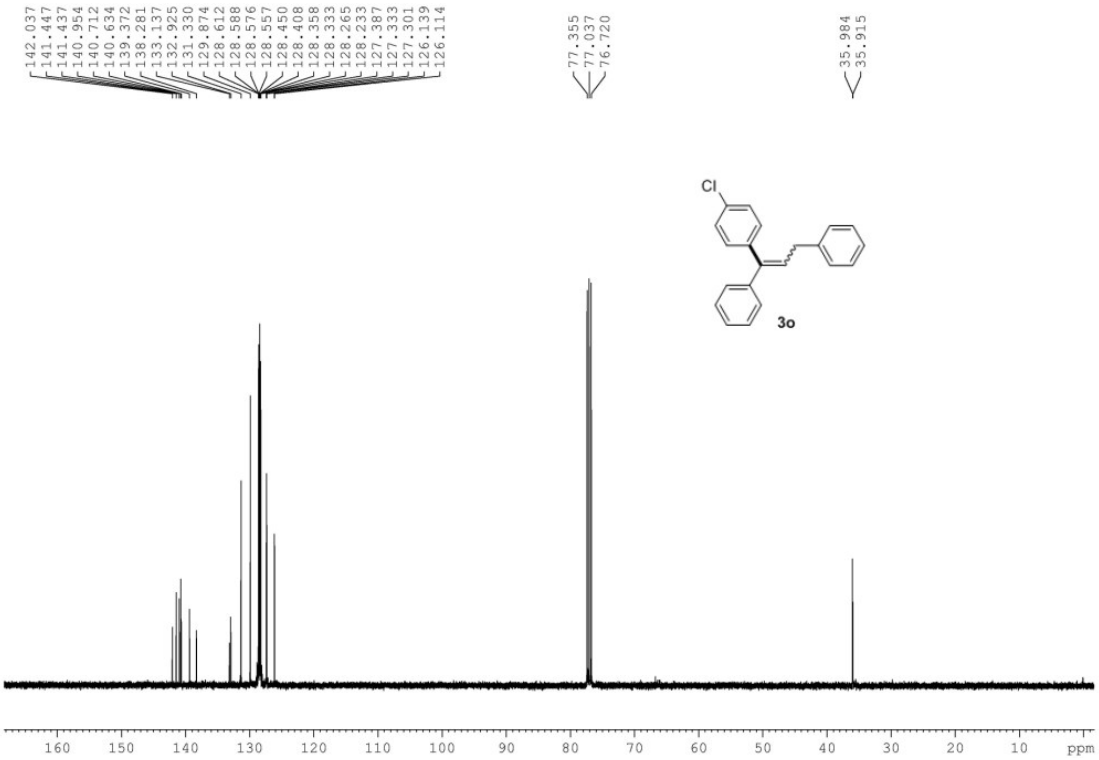
1.02
2.00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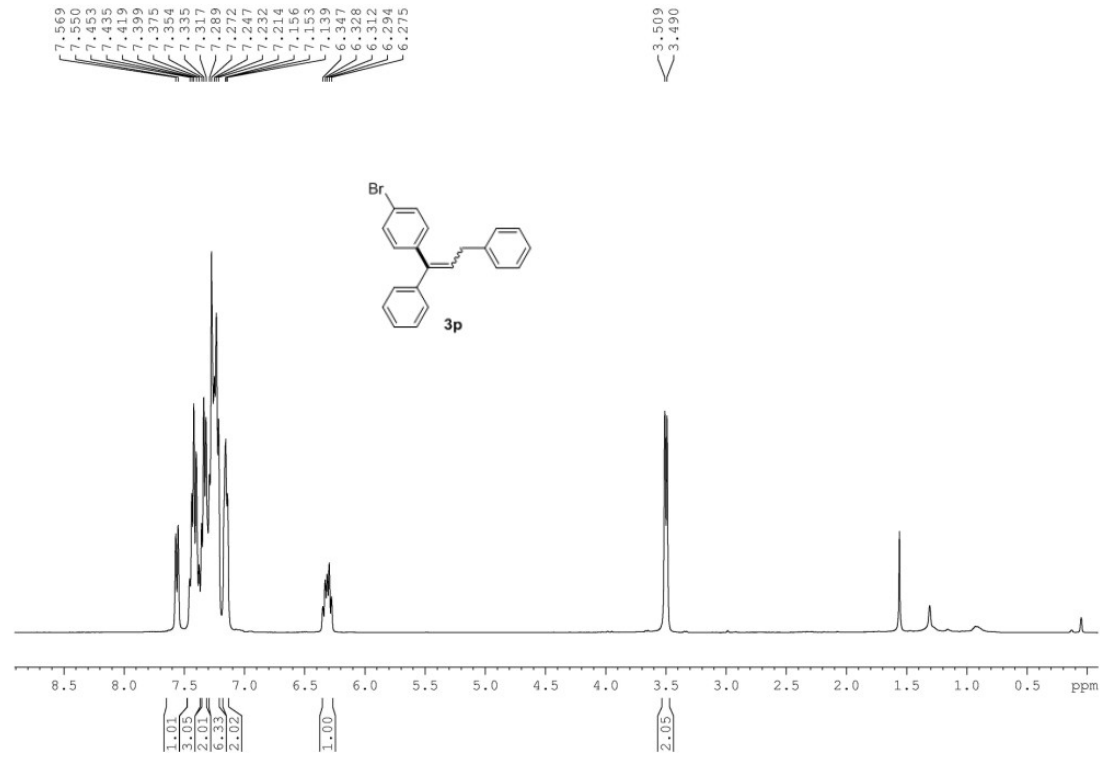
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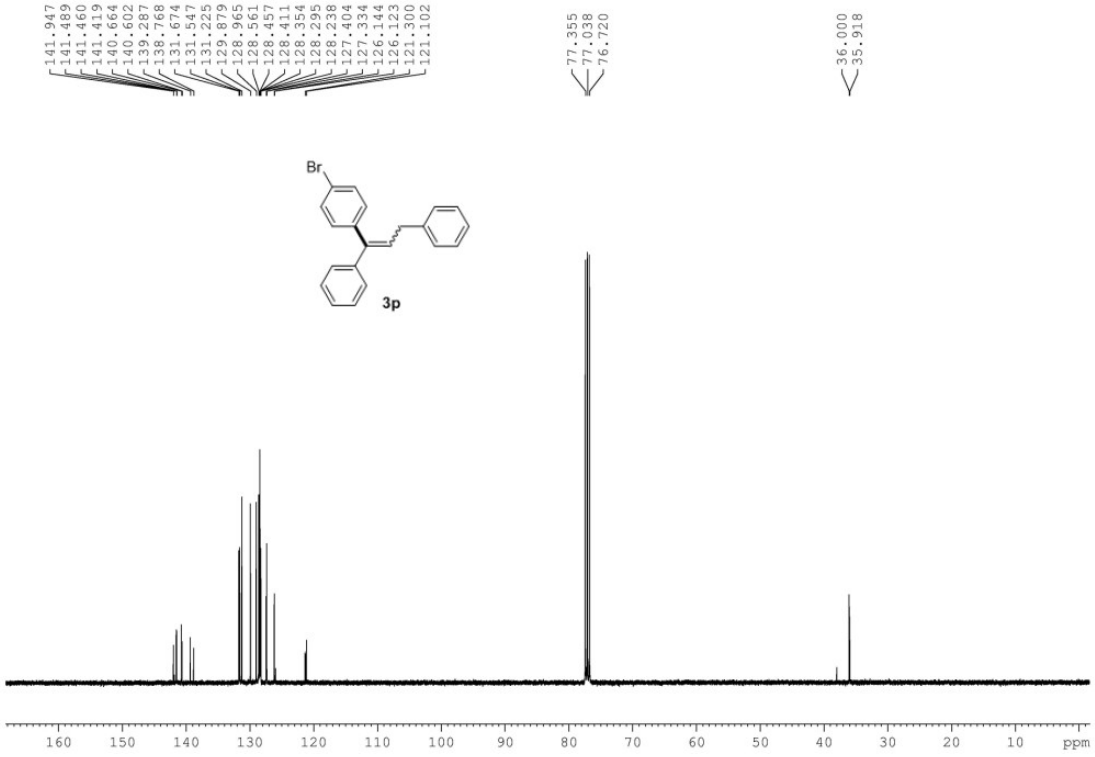
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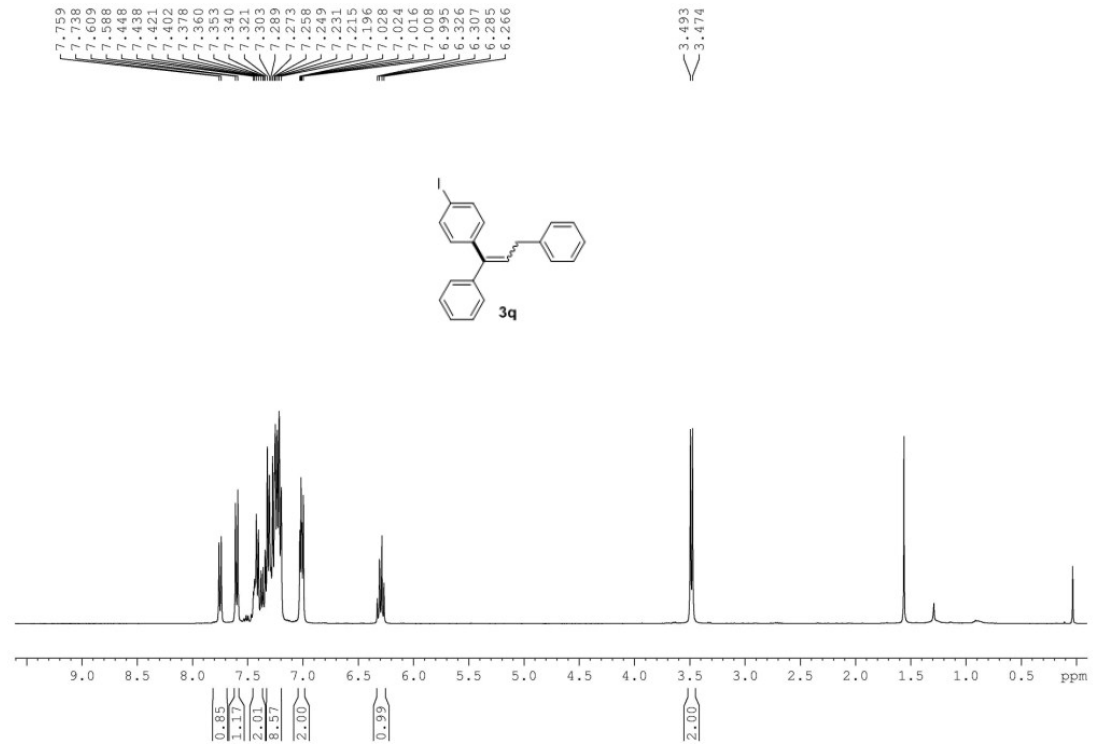
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7.008
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6.307
6.285
6.266
3.493
3.474
I
3q
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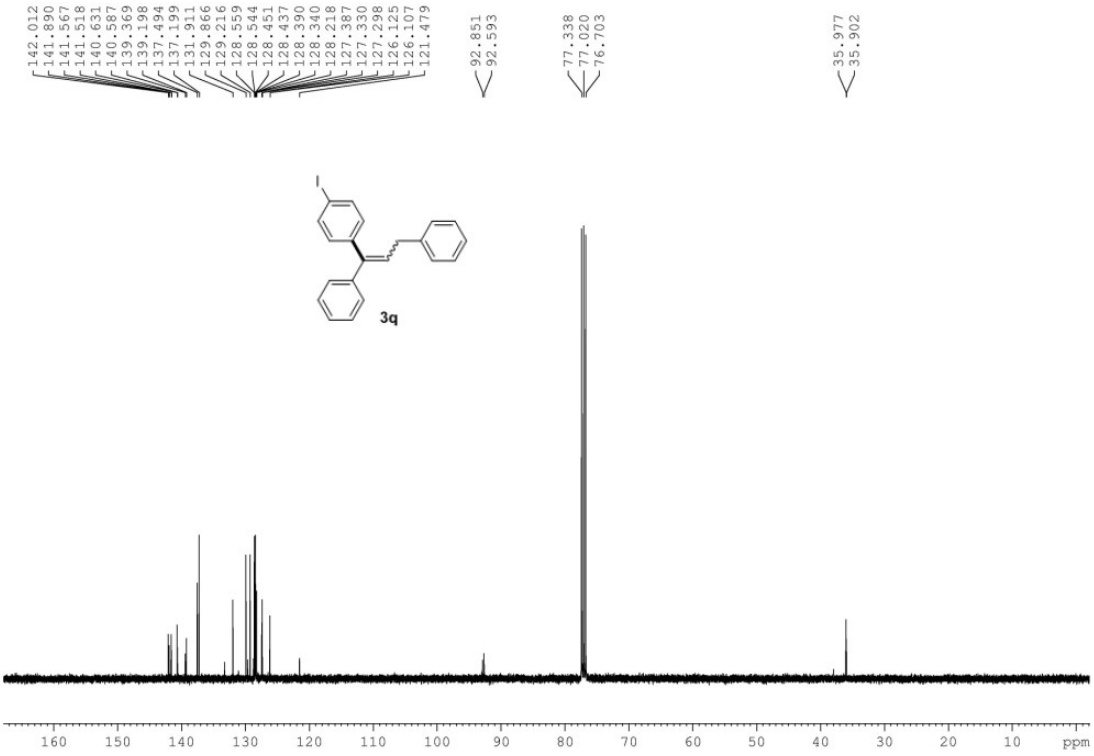
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126.107
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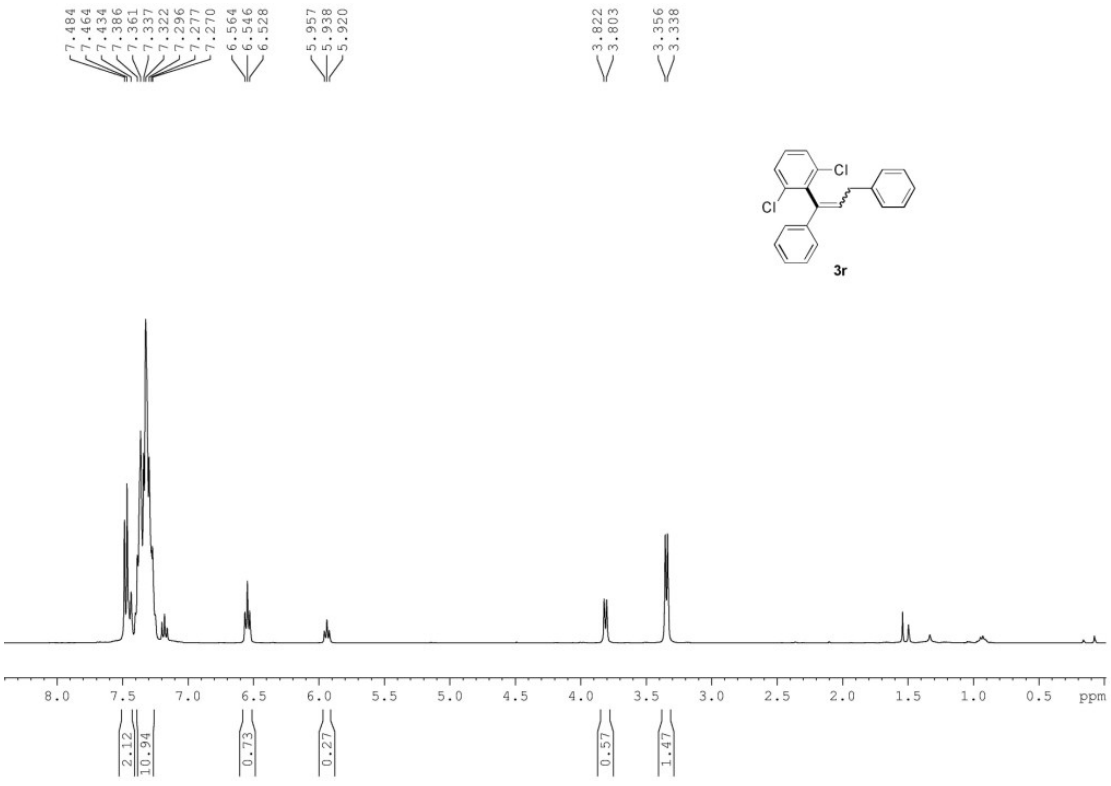
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3.356
3.338
Cl
Cl
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6.0
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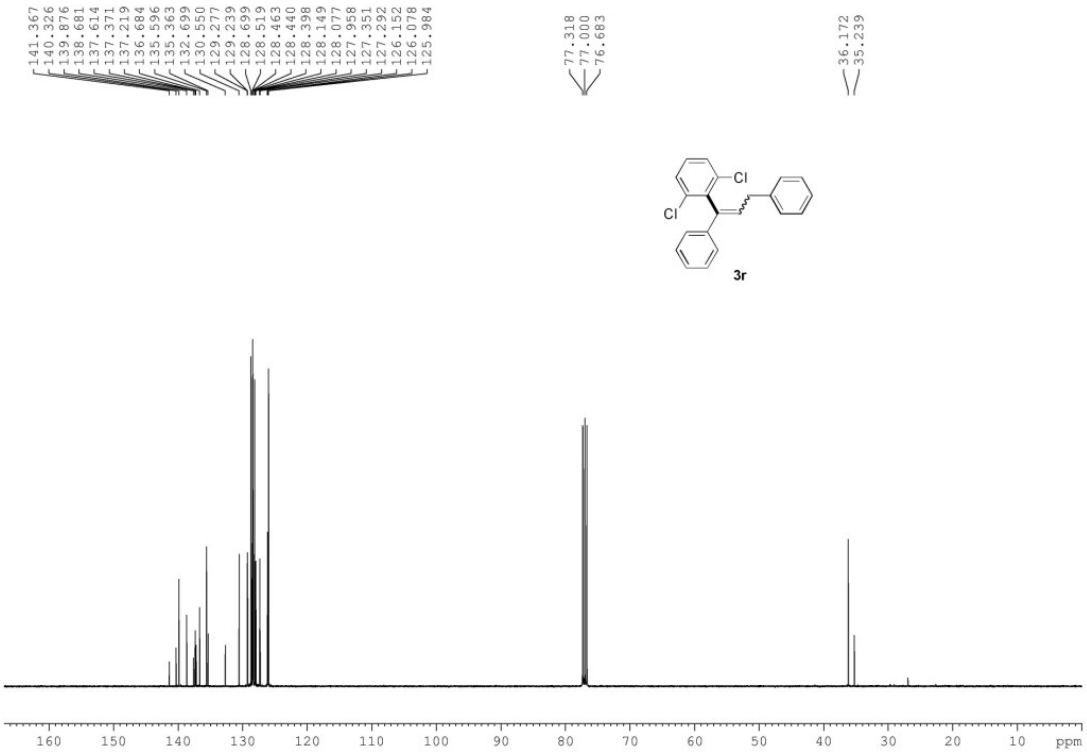
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127.292
126.152
126.078
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35.239
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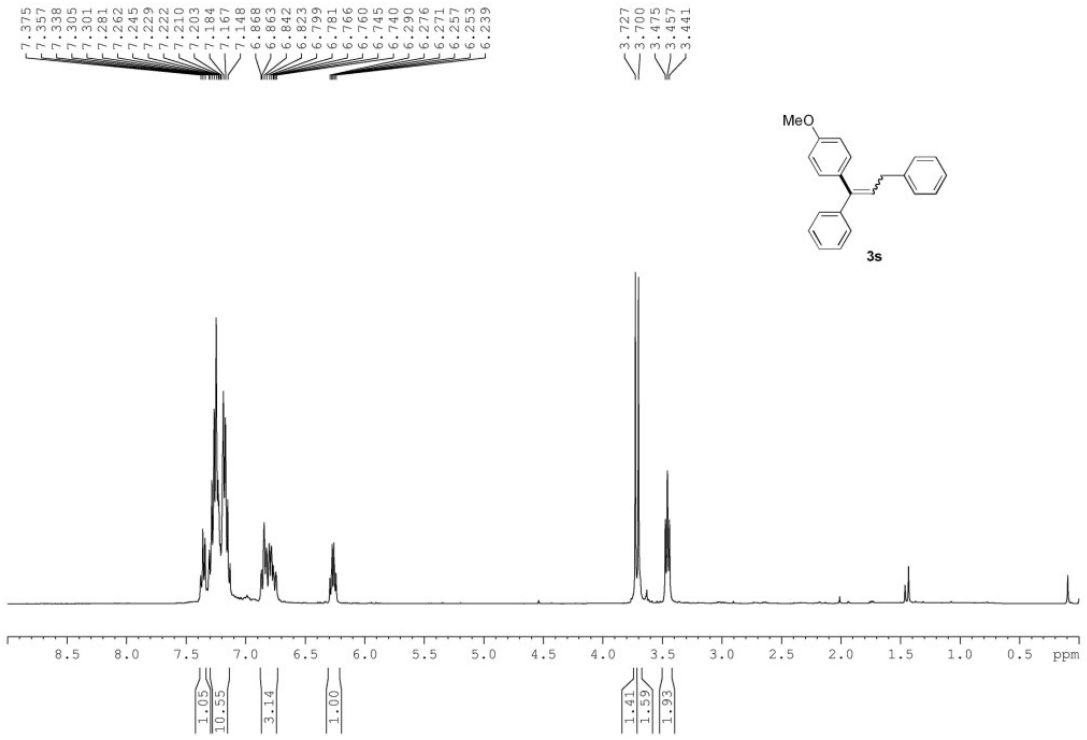
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7.167
7.148
6.868
6.863
6.842
6.823
6.799
6.781
6.766
6.760
6.745
6.740
6.290
6.276
6.271
6.257
6.253
6.239
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3.700
3.475
3.457
3.441
MeO
3s
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7.0
6.5
6.0
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5.0
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4.0
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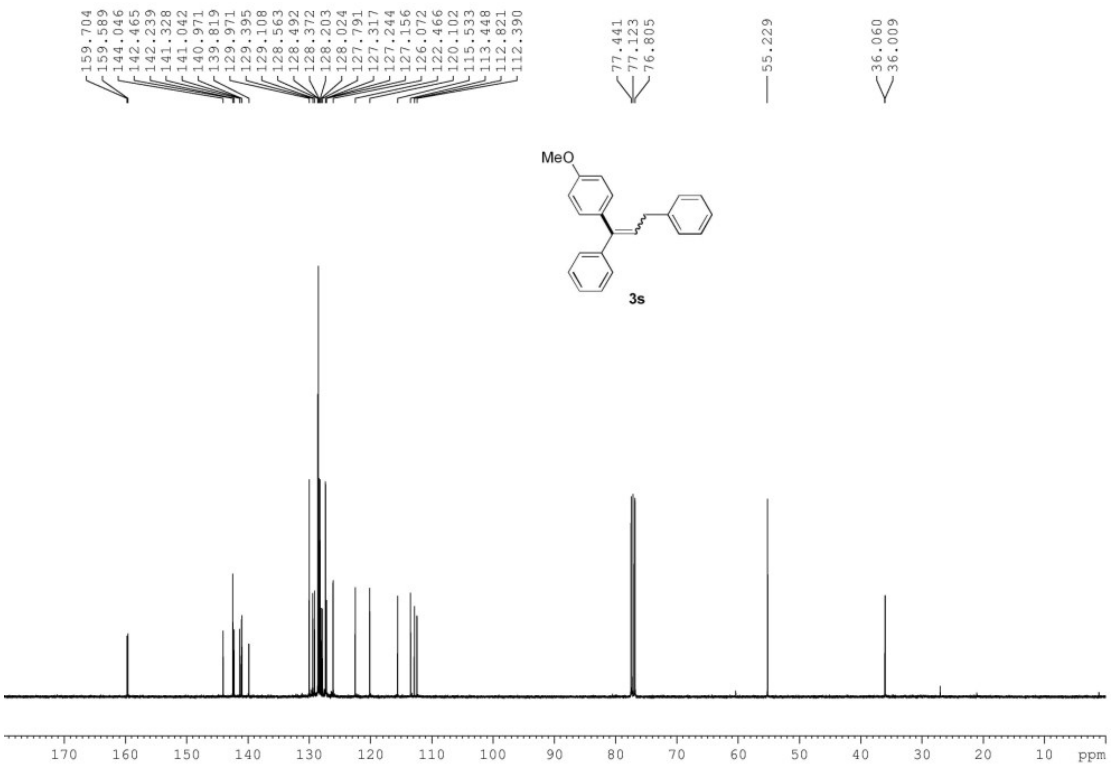
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128.563
128.492
128.372
128.203
128.024
127.791
127.317
127.244
127.156
126.072
122.466
120.102
115.533
113.448
112.821
112.390
77.441
77.123
76.805
55.229
36.060
36.009
MeO
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150
140
130
120
110
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30
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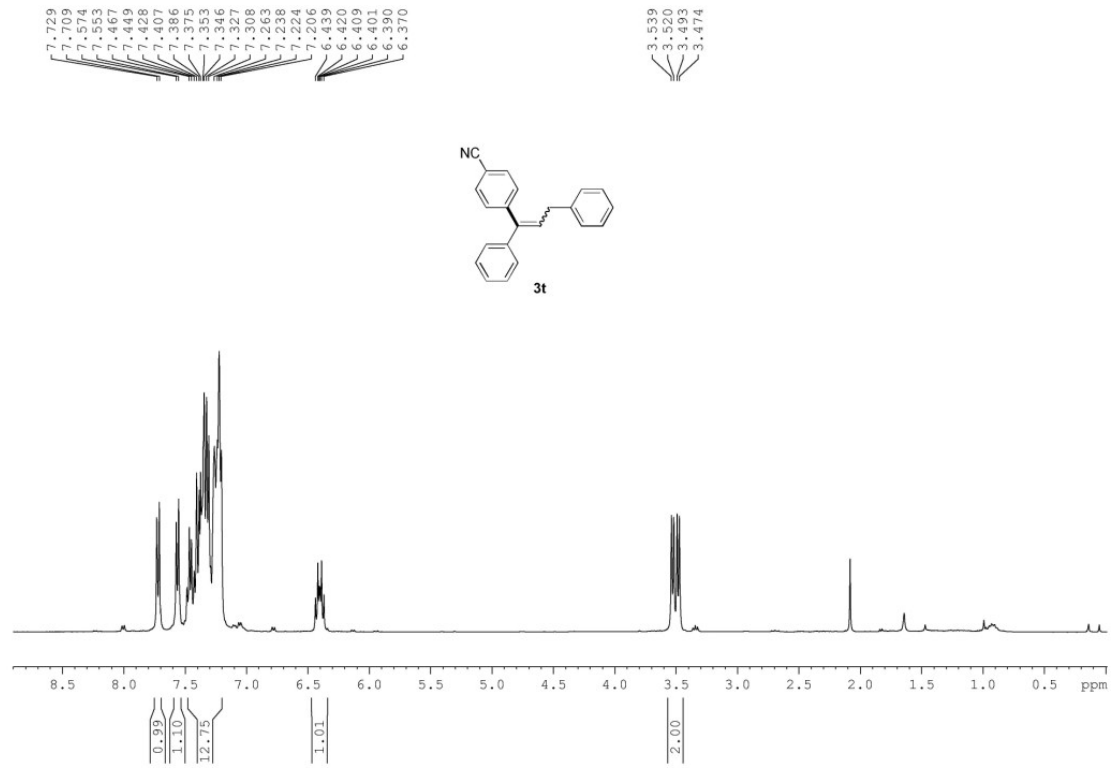
ppm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7.238
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7.206
6.439
6.420
6.409
6.401
6.390
6.370
3.539
3.520
3.493
3.474
NC
3t
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7.5
7.0
6.5
6.0
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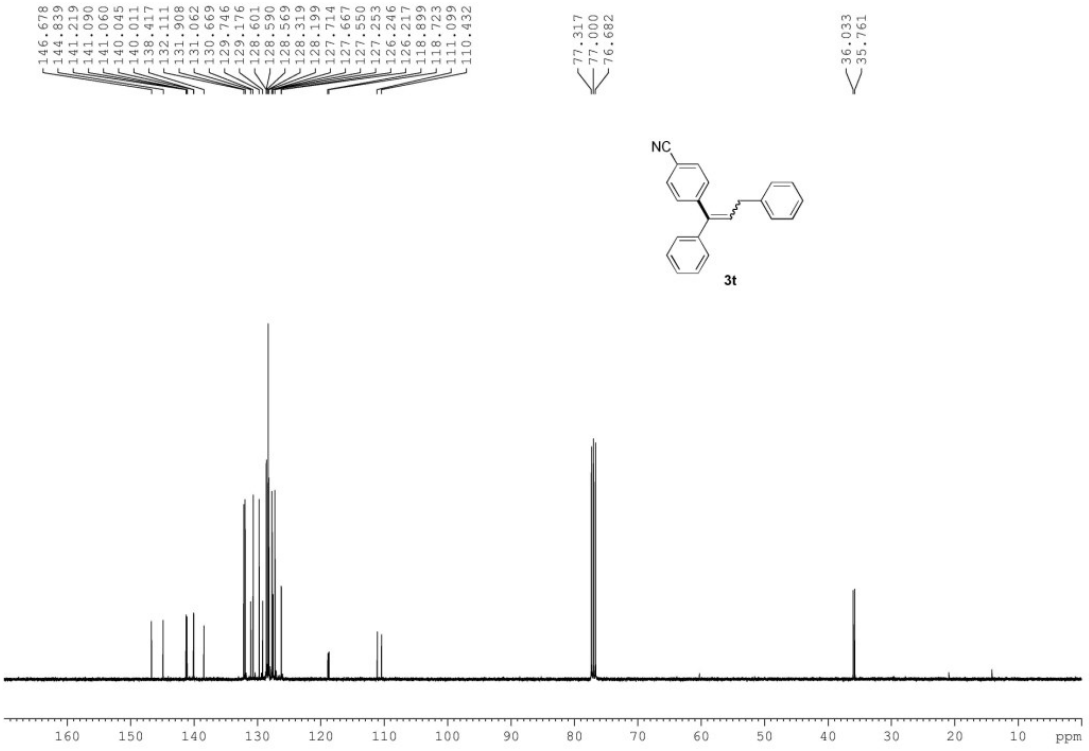
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128.590
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128.319
128.199
127.714
127.667
127.550
127.253
126.246
126.217
118.899
118.723
111.099
110.432
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77.000
76.682
36.033
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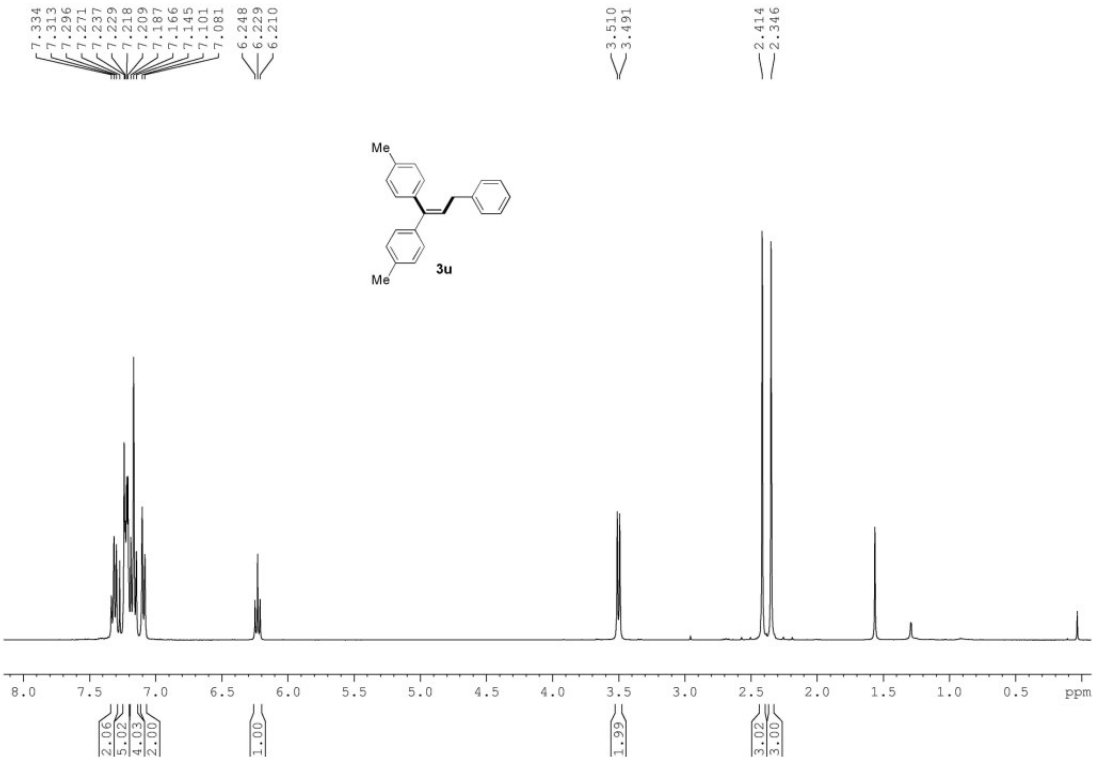
10
ppm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7.166
7.145
7.101
7.081
6.248
6.229
6.210
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3.491
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2.346
Me
Me
3u
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6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
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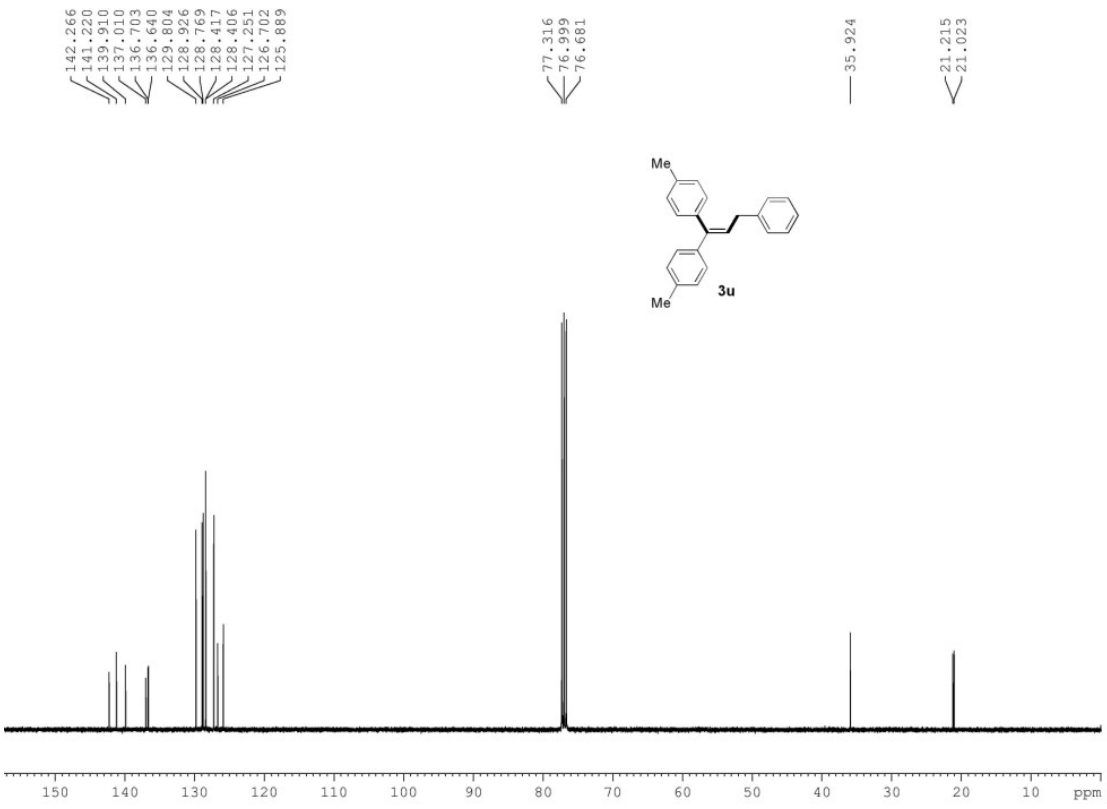
1.00
1.99
3.02
3.00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127.251
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76.999
76.681
35.924
21.215
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Me
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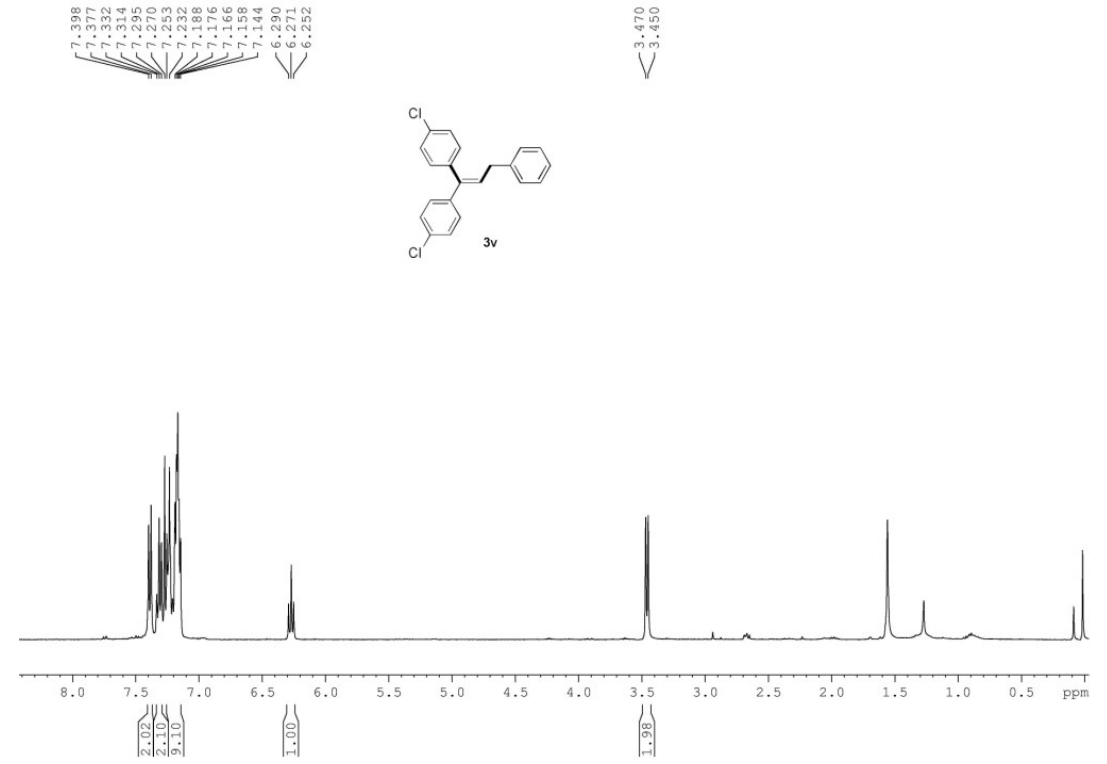
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7.232
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7.144
6.290
6.271
6.252
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3.450
Cl
Cl
3v
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7.0
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6.0
5.5
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4.0
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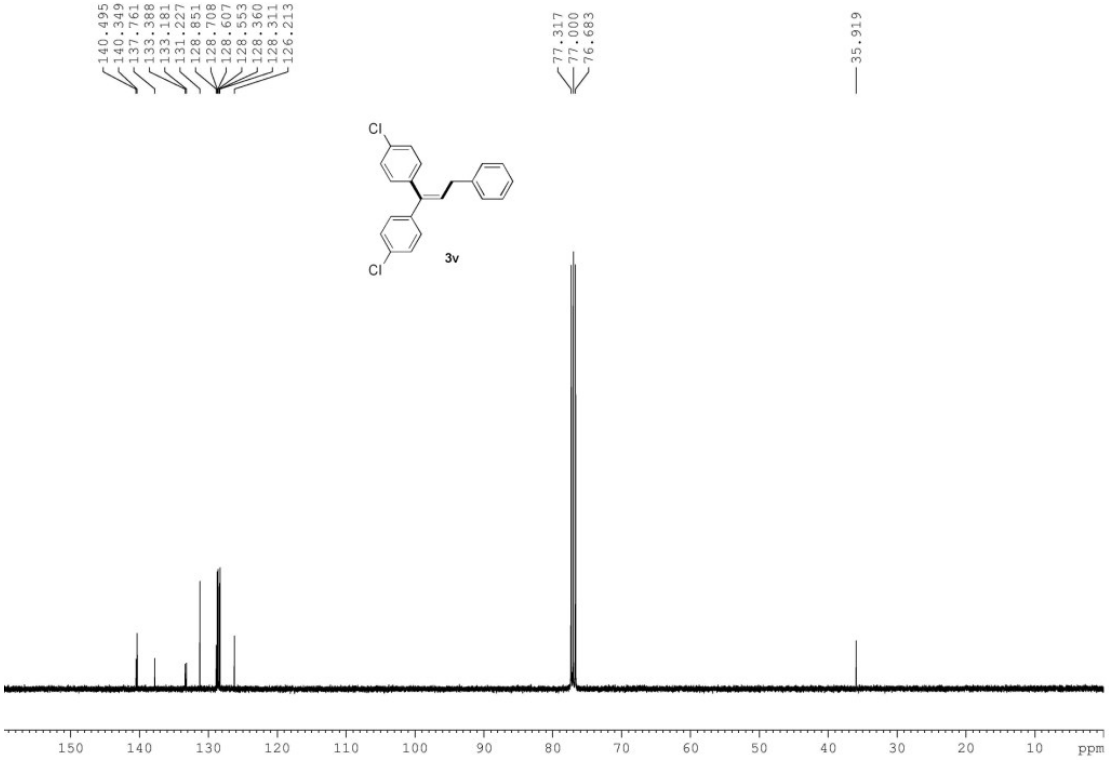
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128.311
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76.683
35.919
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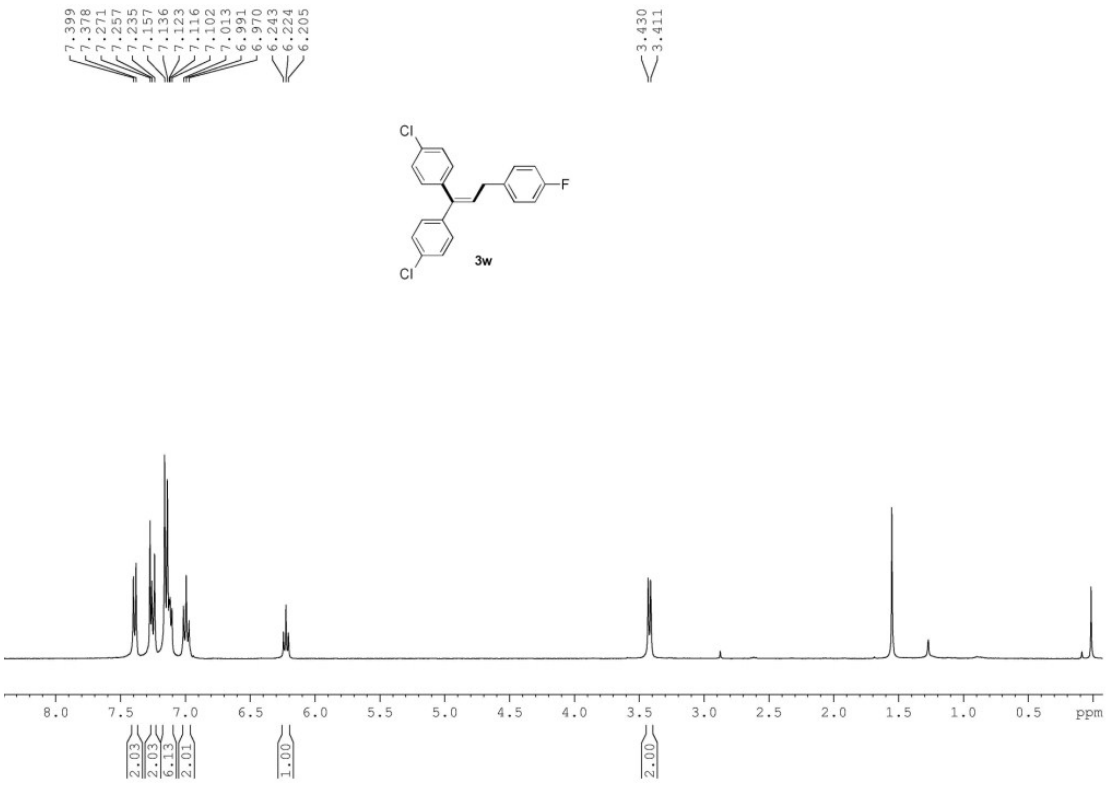
10
ppm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6.243
6.224
6.205
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3.411
Cl
F
Cl
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6.0
5.5
5.0
4.5
4.0
3.5
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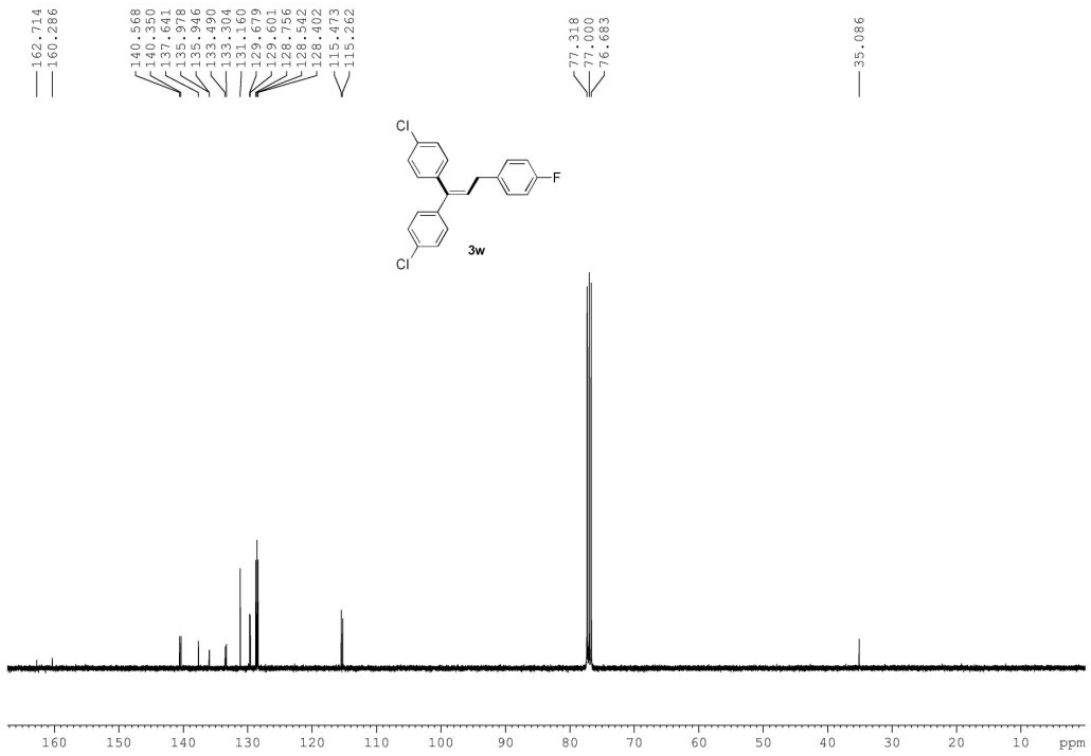
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115.262
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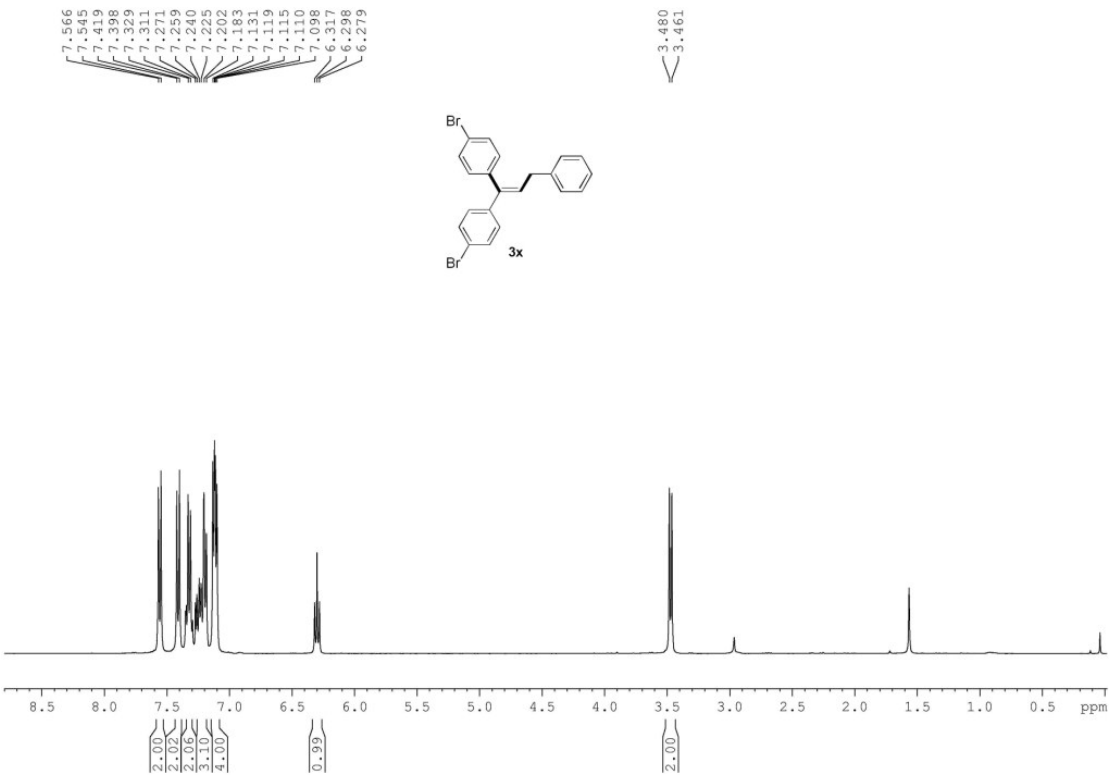
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7.131
7.119
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7.110
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6.298
6.279
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Br
Br
3x
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6.0
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5.0
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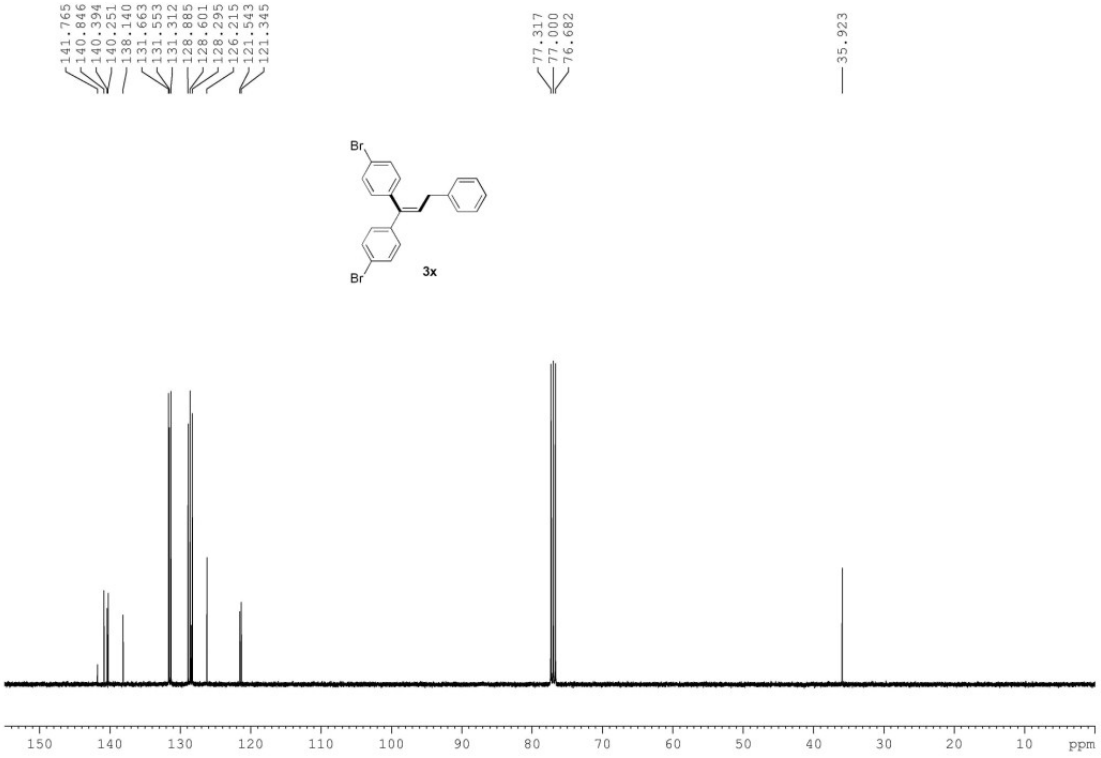
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76.682
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30
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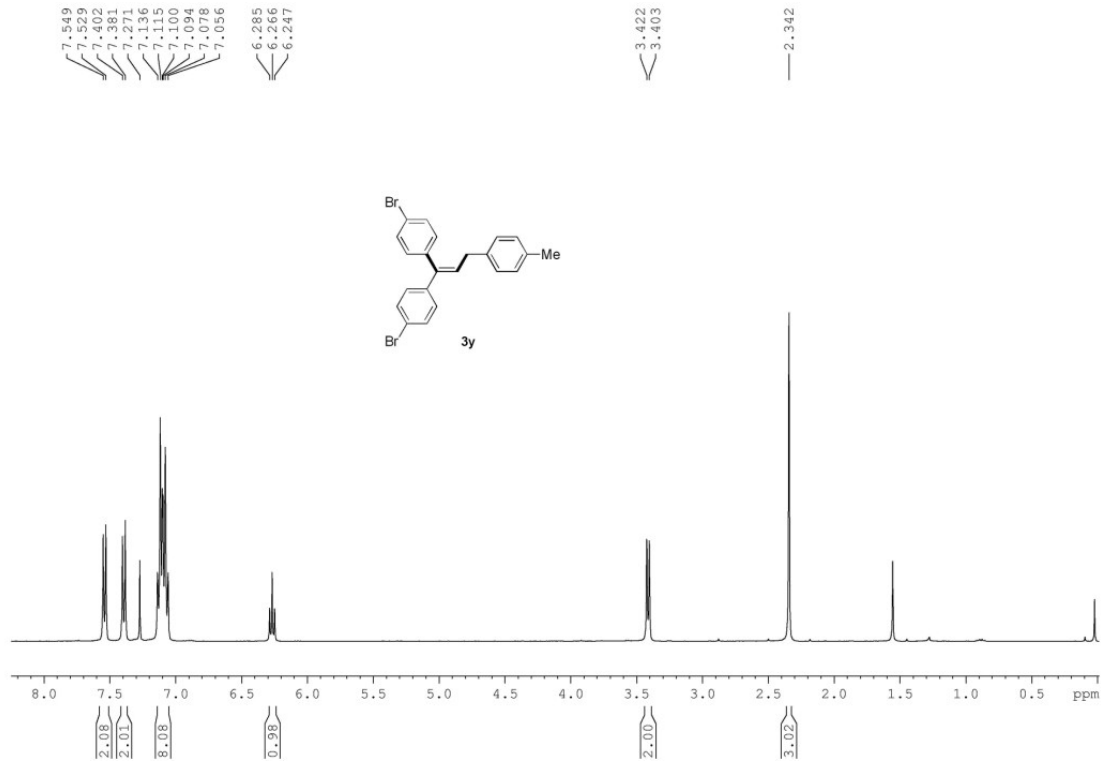
10
ppm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Me
Br
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6.0
5.5
5.0
4.5
4.0
3.5
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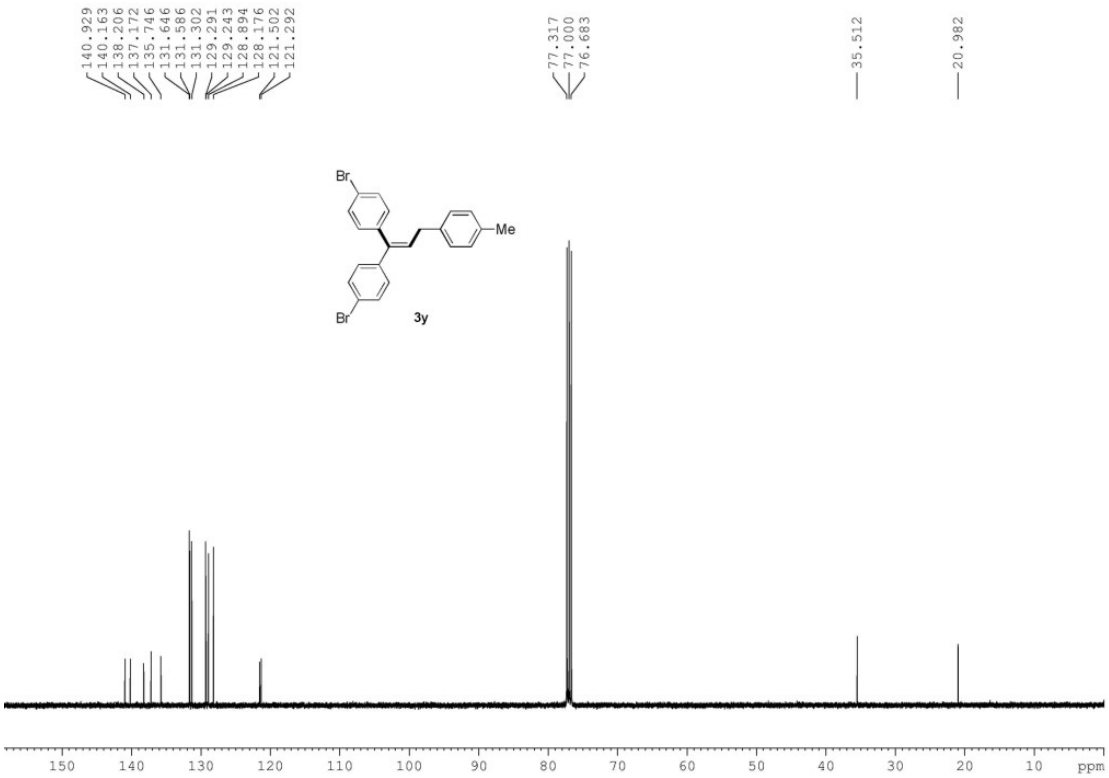
3.02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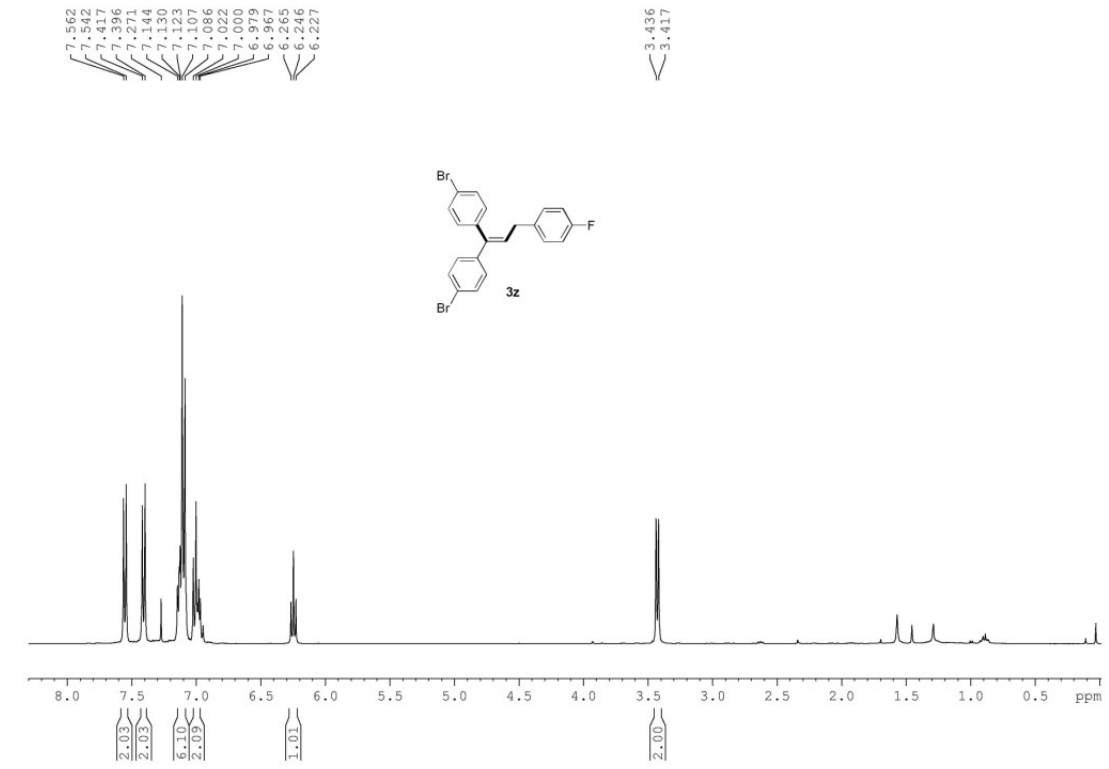
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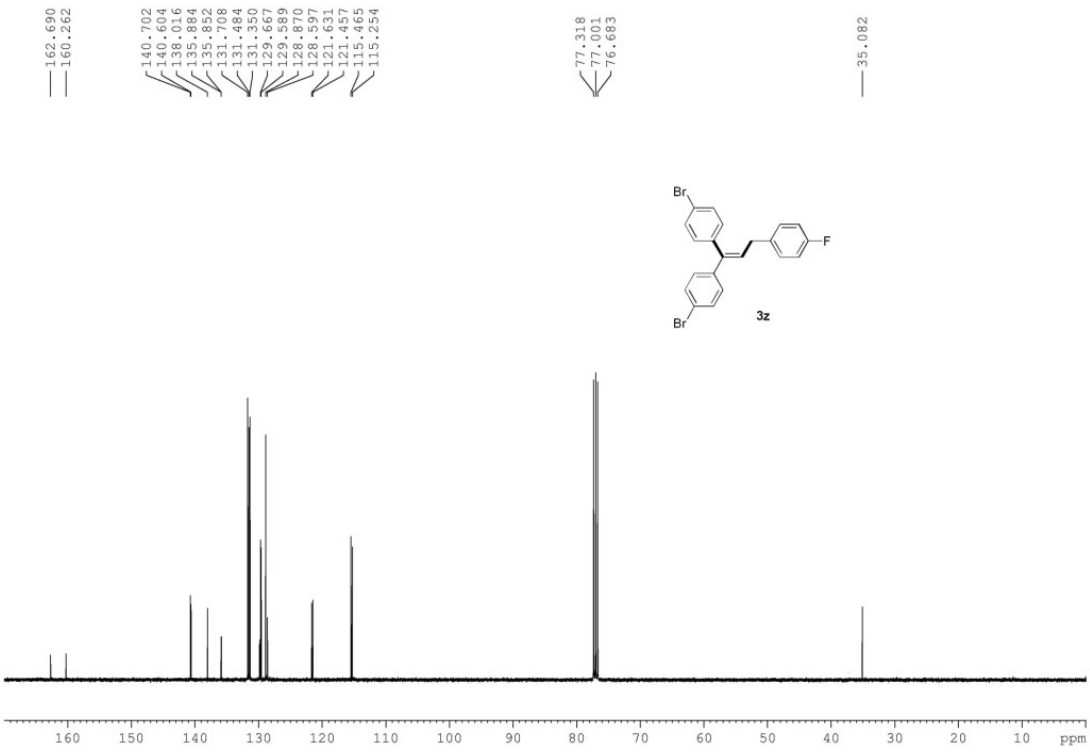
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20
10
ppm