

Supporting Information
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Electronic Supporting Information

Synthesis of Internal Alkynes *via* an Effective Tandem

Elimination-Hydrodebromination-Cross Coupling of

gem-Dibromoalkenes with Halobenzenes

Yuan Ji^a

Ning Zhong^a

Zinan Kang^a

Guobing Yan*^b

Ming Zhao*^a

^a School of Chemical Engineering, China University of Mining and Technology, No1 Daxue Road, Xuzhou 221116, People's Republic of China

Fax: +86-516-83591059; E-mail: ming815zhao@aliyun.com

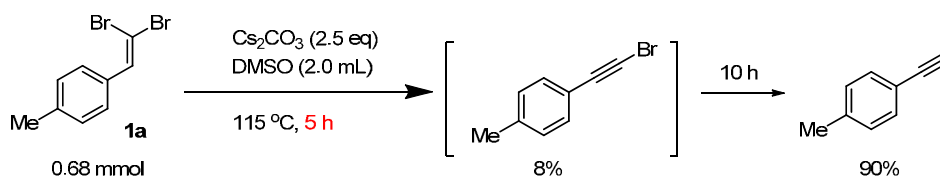
^b Department of Chemistry, Lishui University, Lishui 323000, People's Republic of China

Fax: +86-578-2271-458; E-mail: gbyan@lsu.edu.cn

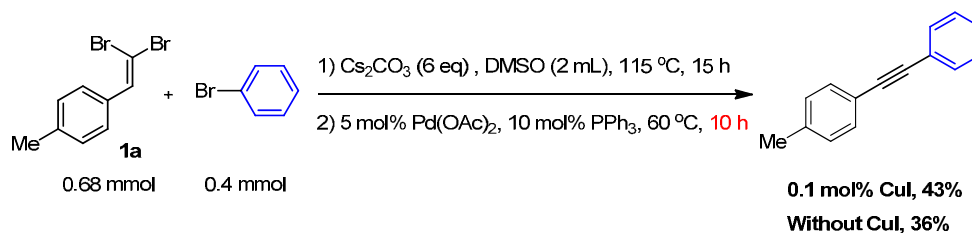
Experimental

General experimental

Chemicals and reagents were purchased from commercial suppliers and used without special instructions. Pd/C (5 wt%), Pd(acac)₂ and Pd(OAc)₂ were purchased from Alfa Aesar. *gem*-Dibromoalkenes were prepared using typical Corey-Fuchs reaction conditions. For product purification, flash column chromatography was performed using silica gel (300-400 mesh). Analytical thin-layer chromatography was performed using glass plates pre-coated with 200-300 mesh silica gel impregnated with a fluorescent indicator (254 nm). NMR spectra were recorded in CDCl₃ on a Varian Inova-400 NMR spectrometer (400 MHz) with TMS as an internal reference. HRMS were measured on a Waters EI-TOF-MS at the Department of Chemistry, Zhejiang University, Zhejiang, China.



Scheme S1. Elimination-dehalogenation reaction of *gem*-dibromoalkene **1a**.



Scheme S2. Investigation of the effect of CuI in the coupling reaction of **1a** and bromobenzene.

Synthesis of *gem*-dibromoalkene **1a**

To a solution of PPh_3 (5.246 g, 20 mmol) in CH_2Cl_2 (15 mL) at 0°C was added CBr_4 (3.316 g, 10 mmol). The reaction mixture was stirred for 10 min before aldehyde **1a** (0.601 g, 5 mmol) was added. The reaction was stirred at room temperature for 1 h. After removal of solvent, hexane (30 mL) was added and filtered through Celite. The filtrate was concentrated under reduced pressure. The crude product was purified by flash column chromatography to afford *gem*-dibromoalkene **1a** as a yellow oil (1.325 g, 96%).

General procedure for Pd-catalyzed cross coupling reaction between *gem*-dibromoalkene and iodobenzene

A mixture of *gem*-dibromoalkene **1** (0.68 mmol), Cs_2CO_3 (2.4 mmol) and DMSO (2 mL) was stirred at 115°C for 15 h. After **1** was completely consumed, iodobenzene (0.4 mmol) and Pd/C (5 mol%) were added and the reaction was deaerated with nitrogen gas and stirred at 80°C for 25 h. After finished, the reaction was cooled down to room temperature and diluted with ethyl acetate and water for extraction. The combined organic phase from three time extraction was dried over anhydrous MgSO_4 . After removal of the solvent, the residue was subjected to column chromatography on silica gel to obtain alkyne **3** in high purity.

General procedure for Pd-catalyzed cross coupling between *gem*-dibromoalkene and bromobenzene or *p*-chloronitrobenzene

A mixture of *gem*-dibromoalkene **1** (0.68 mmol), Cs_2CO_3 (2.4 mmol) and DMSO (2 mL) was stirred at 115°C for 15 h. After **1** was completely consumed, bromobenzene **4** or *p*-chloronitrobenzene (0.4 mmol), $\text{Pd}(\text{OAc})_2$ (5 mol%) and PPh_3 (10 mol%) were added, and the reaction was deaerated with nitrogen gas and stirred at 60°C or 80°C for 25 h. After finished, the reaction was cooled down to room temperature and diluted with ethyl acetate and water for extraction. The combined organic phase from three time extraction was dried over anhydrous MgSO_4 . After removal of the solvent, the residue was subjected to column chromatography on silica gel to obtain alkyne **3** in high purity.

Product characterization

1-methyl-4-(phenylethynyl)benzene (3a)^{1,2}: ^1H NMR (400 MHz, CDCl_3) δ 7.58 – 7.51 (m, 2H), 7.49 – 7.43 (m, 2H), 7.40 – 7.31 (m, 3H), 7.19 (d, $J = 7.9$ Hz, 2H), 2.40 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 138.4, 131.6, 131.5, 129.1, 128.3, 128.1, 123.5, 120.2, 89.6, 88.7, 21.5.

1-methyl-3-(phenylethynyl)benzene (3b)¹: ^1H NMR (400 MHz, CDCl_3) δ 7.59 – 7.44 (m, 2H), 7.40 – 7.25 (m, 5H), 7.23 – 7.16 (m, 1H), 7.12 (t, $J = 8.2$ Hz, 1H), 2.31 (d, $J = 9.9$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 138.1, 132.2, 131.7, 129.2, 128.7, 128.4, 128.3, 128.2, 123.4, 123.1, 89.6, 89.1, 21.3.

1-methyl-2-(phenylethynyl)benzene (3c)²: ^1H NMR (400 MHz, CDCl_3) δ 7.60 – 7.39 (m, 3H), 7.38 – 7.26 (m, 3H), 7.24 – 7.09 (m, 3H), 2.49 (d, $J = 11.1$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 140.1, 131.8, 131.4, 129.4, 128.3, 128.2, 128.1, 125.5, 123.5, 123.0, 93.3, 88.3, 20.7.

1-(tert-butyl)-4-(phenylethynyl)benzene (3d)²: ^1H NMR (400 MHz, CDCl_3) δ 7.55 – 7.40 (m, 4H), 7.39 – 7.20 (m, 5H), 1.35 – 1.27 (m, 9H). ^{13}C NMR (101 MHz, CDCl_3) δ 151.6, 131.7, 131.4, 128.4, 128.1, 125.4, 123.6, 120.3, 89.6, 88.8, 34.8, 31.3.

1,2-diphenylethyne (3e)^{1,2}: ^1H NMR (400 MHz, CDCl_3): δ 7.60 (dt, $J = 5.1, 3.8$ Hz, 4H), 7.44 – 7.35 (m, 6H). ^{13}C NMR (101 MHz, CDCl_3) δ 131.6, 128.3, 128.2, 123.3, 89.4.

1-(phenylethynyl)naphthalene (3f)²: ^1H NMR (400 MHz, CDCl_3) δ 8.45 (d, $J = 8.3$ Hz, 1H), 7.87 – 7.71 (m, 3H), 7.68 – 7.28 (m, 8H). ^{13}C NMR (101 MHz, CDCl_3) δ 133.2, 133.2, 131.6, 130.3, 128.7, 128.4, 128.3, 128.3, 126.7, 126.4, 126.2, 125.2, 123.4, 120.8, 94.3, 87.5.

1-methoxy-4-(phenylethynyl)benzene (3g)¹: ^1H NMR (400 MHz, CDCl_3) δ 7.58 – 7.48 (m, 2H), 7.48 – 7.38 (m, 2H), 7.37 – 7.23 (m, 3H), 6.90 – 6.79 (m, 2H), 3.79 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 159.5, 132.9, 131.4, 128.5, 127.9, 123.4, 115.2, 113.8, 89.3, 88.2, 55.1.

1-methoxy-3-(phenylethynyl)benzene (3h)^{1,2}: ¹H NMR (400 MHz, CDCl₃) δ 7.62 – 7.42 (m, 2H), 7.38 – 7.27 (m, 3H), 7.27 – 7.19 (m, 1H), 7.13 (d, *J* = 7.6 Hz, 1H), 7.06 (d, *J* = 1.7 Hz, 1H), 6.88 (dd, *J* = 8.3, 2.6 Hz, 1H), 3.79 (s, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 159.2, 131.5, 129.3, 128.2, 128.2, 124.1, 124.0, 123.0, 116.2, 114.8, 89.2, 89.1, 55.1.

1-methoxy-2-(phenylethynyl)benzene (3i)¹: ¹H NMR (400 MHz, CDCl₃) δ 7.69 – 7.60 (m, 2H), 7.56 (dt, *J* = 8.7, 4.4 Hz, 1H), 7.46 – 7.25 (m, 4H), 7.04 – 6.89 (m, 2H), 3.94 (d, *J* = 7.1 Hz, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 159.9, 133.5, 131.6, 129.7, 128.2, 128.0, 123.5, 120.4, 112.4, 110.6, 93.4, 85.7, 55.7.

1-chloro-4-(phenylethynyl)benzene (3j)³: ¹H NMR (400 MHz, CDCl₃) δ 7.62 – 7.53 (m, 2H), 7.53 – 7.44 (m, 2H), 7.44 – 7.30 (m, 5H). ¹³C NMR (101 MHz, CDCl₃) δ 134.1, 132.7, 131.5, 128.6, 128.4, 128.3, 122.8, 121.7, 90.2, 88.1.

1-chloro-3-(phenylethynyl)benzene (3k)³: ¹H NMR (400 MHz, CDCl₃) δ 7.60 – 7.46 (m, 3H), 7.38 (t, *J* = 6.1 Hz, 1H), 7.36 – 7.18 (m, 5H). ¹³C NMR (101 MHz, CDCl₃) δ 134.1, 131.6, 131.4, 129.6, 129.5, 128.5, 128.4, 128.3, 124.9, 122.7, 90.5, 87.8.

1-chloro-2-(phenylethynyl)benzene (3l)¹: ¹H NMR (400 MHz, CDCl₃) δ 7.67 – 7.46 (m, 3H), 7.46 – 7.39 (m, 1H), 7.39 – 7.29 (m, 3H), 7.29 – 7.16 (m, 2H). ¹³C NMR (101 MHz, CDCl₃) δ 135.8, 133.1, 131.6, 129.2, 129.1, 128.5, 128.3, 126.3, 123.1, 122.8, 94.4, 86.1.

1,2-dichloro-4-(phenylethynyl)benzene (3m): ¹H NMR (400 MHz, CDCl₃) δ 7.60 (t, *J* = 5.6 Hz, 1H), 7.54 – 7.48 (m, 2H), 7.43 – 7.27 (m, 5H). ¹³C NMR (101 MHz, CDCl₃) δ 133.1, 132.5, 132.5, 131.6, 130.6, 130.3, 128.7, 128.3, 123.2, 122.4, 91.2, 86.9. HRMS (EI): calcd. for C₁₄H₈Cl₂ [M]⁺ 246.0003, found 246.0012.

1-bromo-4-(phenylethynyl)benzene (3n)³: ¹H NMR (400 MHz, CDCl₃) δ 7.55 – 7.49 (m, 2H), 7.46 (t, *J* = 8.3 Hz, 2H), 7.40 – 7.29 (m, 5H). ¹³C NMR (101 MHz, CDCl₃) δ 133.0, 131.6, 131.6, 128.5, 128.4, 122.9, 122.5, 122.3, 90.5, 88.3.

1-fluoro-4-(phenylethynyl)benzene (3o)¹: ¹H NMR (400 MHz, CDCl₃) δ 7.59 – 7.40 (m, 4H), 7.39 – 7.25 (m, 3H), 7.03 (t, *J* = 8.7 Hz, 2H). ¹³C NMR (101 MHz, CDCl₃) δ 162.6 (*J*_{CF} = 249.2 Hz), 133.5 (*J*_{CF} = 7.6 Hz), 131.6, 128.4, 128.4, 123.2, 119.4 (*J*_{CF} = 3.0 Hz), 115.7 (*J*_{CF} = 22.7 Hz), 89.1, 88.4.

3-(phenylethynyl)pyridine (3p)¹: ¹H NMR (400 MHz, CDCl₃) δ 8.86 – 8.65 (m, 1H), 8.54 (dd, *J* = 4.8, 1.0 Hz, 1H), 7.80 (d, *J* = 7.9 Hz, 1H), 7.55 (dd, *J* = 6.6, 3.0 Hz, 2H), 7.39 – 7.32 (m, 3H), 7.27 (dd, *J* = 7.9, 4.9 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 152.4, 148.7, 138.6, 131.9, 129.0, 128.6, 123.2, 122.7, 120.6, 92.8, 86.1.

2-(phenylethynyl)furan (3q)⁴: ¹H NMR (400 MHz, CDCl₃) δ 7.55 (dt, *J* = 6.2, 3.2 Hz, 2H), 7.47 – 7.42 (m, 1H), 7.39 – 7.34 (m, 3H), 6.68 (d, *J* = 3.4 Hz, 1H), 6.45 (dd, *J* = 3.1, 1.9 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 143.6, 137.2, 131.4, 128.7, 128.4, 122.3, 115.2, 111.1, 93.2, 79.4.

1-nitro-4-(phenylethynyl)benzene (3r)^{1,2}: ¹H NMR (400 MHz, CDCl₃) δ 8.23 (d, *J* = 8.7 Hz, 2H), 7.67 (d, *J* = 8.7 Hz, 2H), 7.57 (dd, *J* = 6.5, 3.0 Hz, 2H), 7.43 – 7.35 (m, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 147.0, 132.3, 131.9, 130.3, 129.3, 128.6, 123.7, 122.1, 94.7, 87.6.

but-1-yne-1,4-diylidibenzene (3s)²: ¹H NMR (400 MHz, CDCl₃) δ 7.41 – 7.33 (m, 2H), 7.33 – 7.14 (m, 8H), 2.91 (t, *J* = 7.5 Hz, 2H), 2.68 (t, *J* = 7.5 Hz, 2H). ¹³C NMR (101 MHz, CDCl₃) δ 140.8, 131.6, 128.6, 128.4, 128.2, 127.7, 126.4, 123.9, 89.5, 81.4, 35.2, 21.7.

1-methoxy-4-(p-tolyethynyl)benzene (3t)¹: ¹H NMR (400 MHz, CDCl₃) δ 7.49 – 7.42 (m, 2H), 7.38 (dd, *J* = 16.6, 7.2 Hz, 2H), 7.12 (d, *J* = 8.1 Hz, 2H), 6.84 (t, *J* = 7.8 Hz, 2H), 3.81 (d, *J* = 13.0 Hz, 3H), 2.36 – 2.30 (m, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 159.4, 137.9, 132.9, 131.2, 129.0, 120.4, 115.5, 113.9, 88.6, 88.1, 55.2, 21.4.

methyl 4-(p-tolyethynyl)benzoate (3u)⁵: ¹H NMR (400 MHz, CDCl₃) δ 8.11 – 7.89 (m, 2H), 7.66 – 7.32 (m, 4H), 7.26 – 7.03 (m, 2H), 3.89 (s, 3H), 2.32 (d, *J* = 23.0 Hz, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 166.7, 139.2, 131.8, 131.6, 129.7, 129.4, 129.4, 128.4, 119.8, 92.8, 88.2, 52.4, 21.7.

1,2-bis(4-methoxyphenyl)ethyne (3v)⁶: ¹H NMR (400 MHz, CDCl₃) δ 7.47 (dd, *J* = 18.0, 8.5 Hz, 4H), 6.85 (t, *J* = 7.7 Hz, 4H), 3.81 (s, 6H). ¹³C NMR (101 MHz, CDCl₃) δ 159.3, 132.8, 115.6, 113.8, 87.8, 55.2.

methyl 4-((4-methoxyphenyl)ethynyl)benzoate (3w)⁷: ¹H NMR (400 MHz, CDCl₃) δ 8.00 (d, *J* = 8.3 Hz, 2H), 7.56 (d, *J* = 8.2 Hz, 2H), 7.47 (dd, *J* = 11.6, 6.4 Hz, 2H), 6.89 (t, *J* = 8.0 Hz, 2H), 3.92 (s, 3H), 3.84 – 3.80 (m, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 166.6, 160.0, 133.3, 131.3, 129.5, 129.1, 128.4, 114.8, 114.1, 92.6, 87.5, 55.3, 52.2.

1-chloro-4-((4-methoxyphenyl)ethynyl)benzene (3x): ¹H NMR (400 MHz, CDCl₃) δ 7.50 – 7.36 (m, 4H), 7.32 – 7.25 (m, 2H), 6.92 – 6.77 (m, 2H), 3.83 – 3.69 (m, 3H). ¹³C NMR (101 MHz, CDCl₃) δ 160.0, 133.2, 132.8, 131.8, 128.8, 128.5, 122.3, 114.2, 90.5, 87.2, 55.5. HRMS (EI): calcd. for C₁₅H₁₁OCl [M]⁺ 242.0498, found 242.0506.

methyl 4-((4-chlorophenyl)ethynyl)benzoate (3y): ^1H NMR (400 MHz, CDCl_3) δ 8.10 – 7.96 (m, 2H), 7.61 – 7.50 (m, 2H), 7.44 (t, $J = 13.1$ Hz, 2H), 7.36 – 7.27 (m, 2H), 3.98 – 3.83 (m, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 166.6, 134.9, 133.0, 131.6, 129.8, 129.7, 128.9, 127.7, 121.3, 91.2, 89.6, 52.3. HRMS (EI): calcd. for $\text{C}_{16}\text{H}_{11}\text{O}_2\text{Cl}$ $[\text{M}]^+$ 270.0448, found 270.0459.

1-fluoro-4-((4-methoxyphenyl)ethynyl)benzene (3z): ^1H NMR (400 MHz, CDCl_3) δ 7.53 – 7.35 (m, 4H), 7.06 – 6.95 (m, 2H), 6.85 (d, $J = 8.5$ Hz, 2H), 3.81 (d, $J = 14.4$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 162.3 ($J_{\text{CF}} = 249.2$ Hz), 159.7, 133.3 ($J_{\text{CF}} = 7.6$ Hz), 133.0, 119.7 ($J_{\text{CF}} = 3.0$ Hz), 115.7, 115.4 ($J_{\text{CF}} = 22.7$ Hz), 114.1, 89.1, 87.0, 55.3. HRMS (EI): calcd. for $\text{C}_{15}\text{H}_{11}\text{OF}$ $[\text{M}]^+$ 226.0794, found 226.0800.

methyl 4-((4-fluorophenyl)ethynyl)benzoate (3za): ^1H NMR (400 MHz, CDCl_3) δ 8.01 (d, $J = 8.2$ Hz, 2H), 7.64 – 7.41 (m, 4H), 7.05 (t, $J = 8.6$ Hz, 2H), 3.90 (d, $J = 12.0$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 166.5, 162.8 ($J_{\text{CF}} = 250.7$ Hz), 133.7 ($J_{\text{CF}} = 9.01$ Hz), 131.5, 129.6, 128.4, 127.8, 118.8 ($J_{\text{CF}} = 3.0$ Hz), 115.8 ($J_{\text{CF}} = 22.7$ Hz), 91.3, 88.4, 52.2. HRMS (EI): calcd. for $\text{C}_{16}\text{H}_{11}\text{O}_2\text{F}$ $[\text{M}]^+$ 254.0743, found 254.0750.

(E)-but-1-en-3-yne-1,4-diyl dibenzene (3zb): 8 : ^1H NMR (400 MHz, CDCl_3) δ 7.47 (dd, $J = 7.2, 2.2$ Hz, 2H), 7.42 (d, $J = 7.4$ Hz, 2H), 7.38 – 7.27 (m, 6H), 7.04 (d, $J = 16.3$ Hz, 1H), 6.39 (d, $J = 16.2$ Hz, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 141.3, 136.4, 131.6, 128.8, 128.7, 128.4, 128.2, 126.3, 123.4, 108.2, 91.8, 88.9.

1-methyl-4-((4-nitrophenyl)ethynyl)benzene (3zc): 9 : ^1H NMR (400 MHz, CDCl_3) δ 8.24 – 8.20 (m, 2H), 7.67 – 7.63 (m, 2H), 7.46 (d, $J = 8.4$ Hz, 2H), 7.20 (d, $J = 8.4$ Hz, 2H), 2.39 (d, $J = 4.2$ Hz, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ 146.8, 139.7, 132.2, 131.8, 130.5, 129.3, 123.6, 119.0, 95.1, 87.1, 21.6.

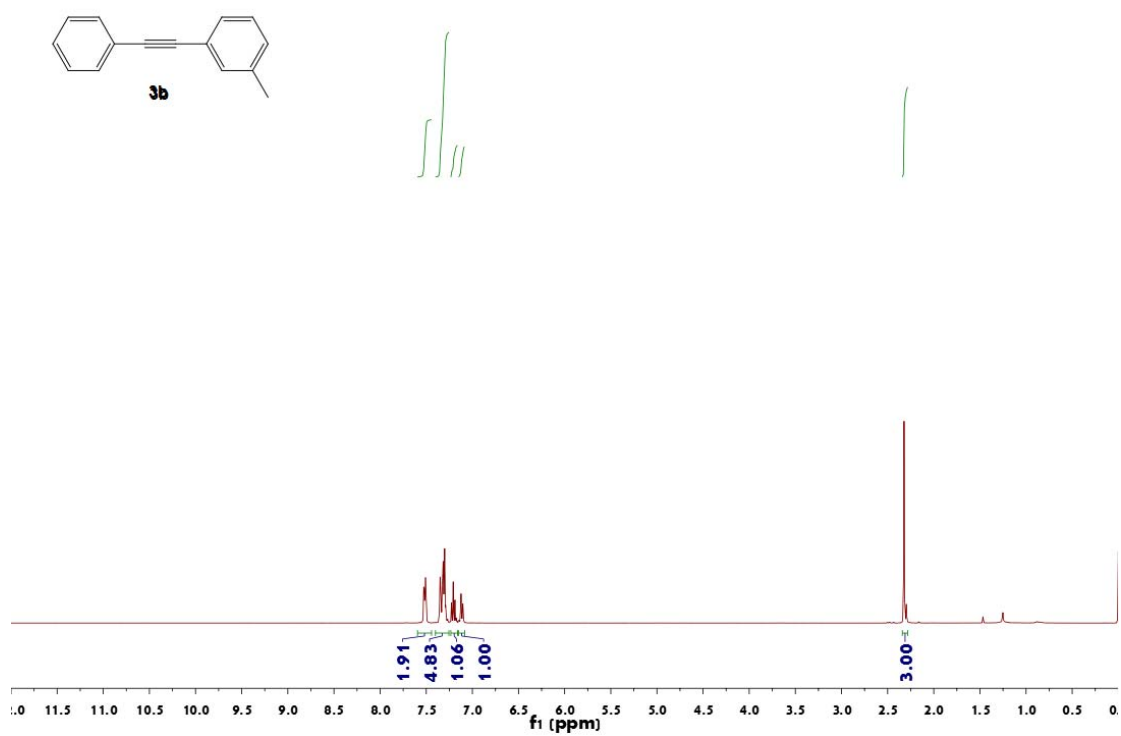
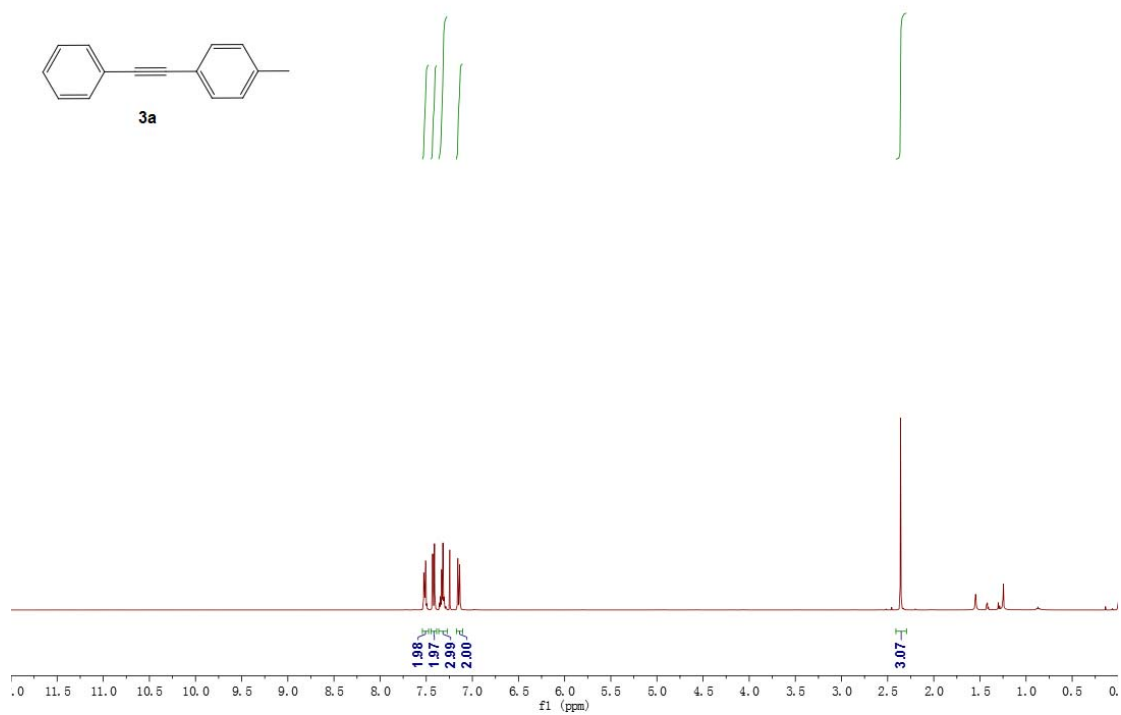
1-methoxy-4-((4-nitrophenyl)ethynyl)benzene (3zd): 7 : ^1H NMR (400 MHz, CDCl_3) δ 8.19 (d, $J = 8.4$ Hz, 2H), 7.62 (d, $J = 8.4$ Hz, 2H), 7.49 (d, $J = 8.4$ Hz, 2H), 6.90 (d, $J = 8.4$ Hz, 2H), 3.84 (s, 3H). ^{13}C NMR (101 MHz, CDCl_3) δ : 159.1, 145.4, 132.1, 130.7, 129.4, 122.3, 112.9, 112.8, 93.8, 85.3, 54.1.

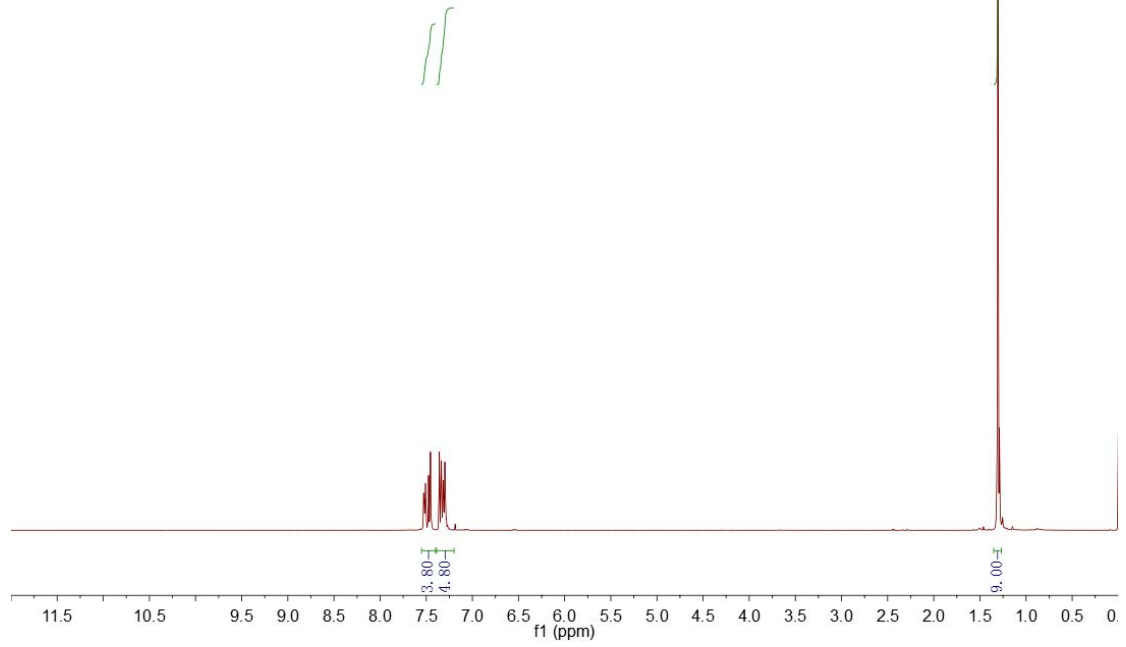
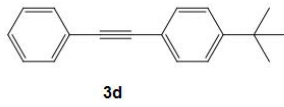
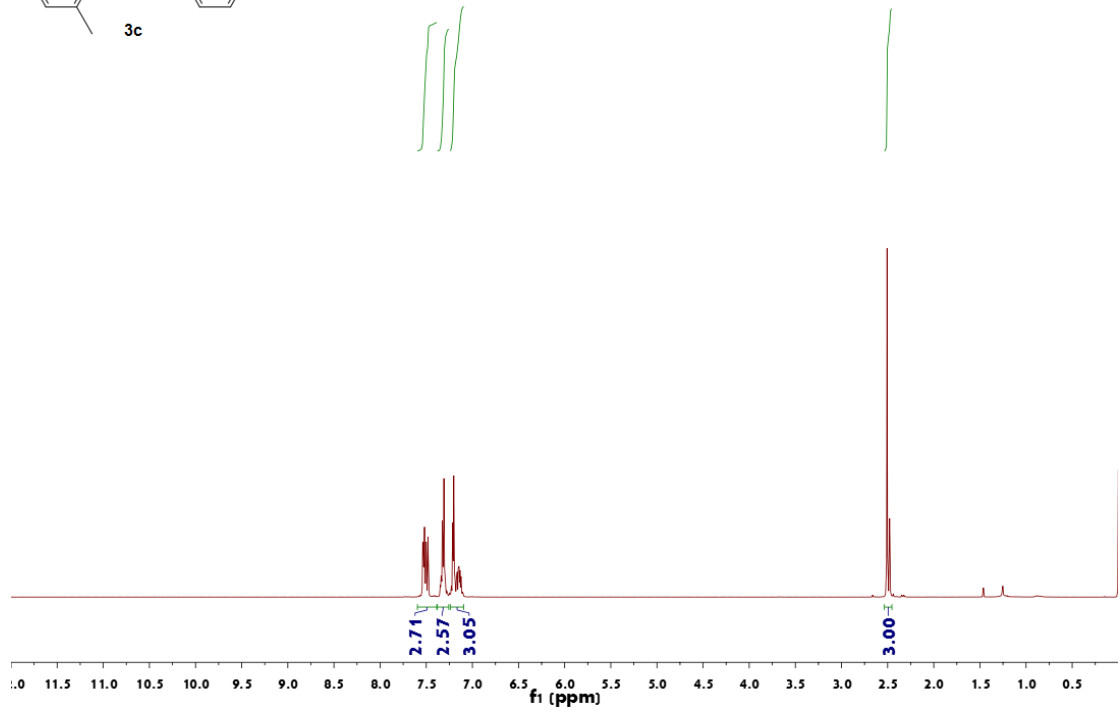
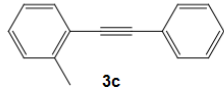
1-chloro-4-((4-nitrophenyl)ethynyl)benzene (3ze): ^1H NMR (400 MHz, CDCl_3) δ 8.22 (d, $J = 8.4$ Hz, 2H), 7.65 (d, $J = 8.4$ Hz, 2H), 7.48 (d, $J = 8.4$ Hz, 2H), 7.36 (d, $J = 8.4$ Hz, 2H). ^{13}C NMR (101 MHz, CDCl_3) δ 147.1, 135.4, 133.0, 132.3, 129.8, 128.9, 123.7, 120.6, 93.4, 88.4. HRMS (EI): calcd. for $\text{C}_{14}\text{H}_8\text{ClNO}_2$ $[\text{M}]^+$ 257.0244, found 257.0251.

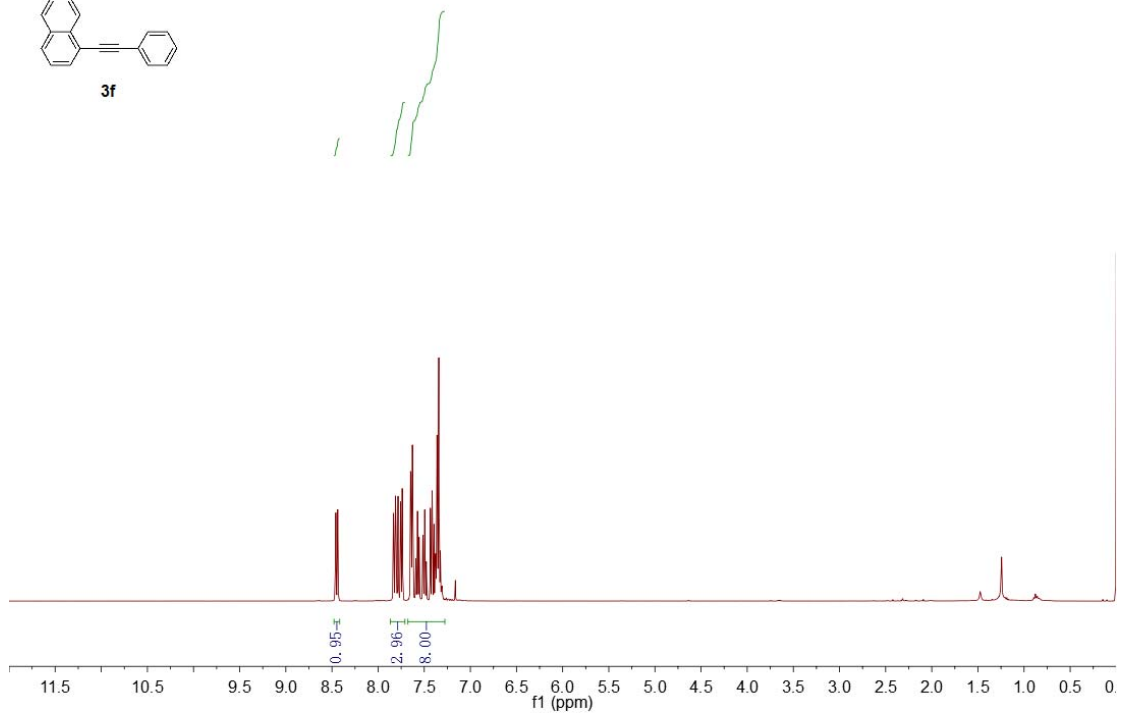
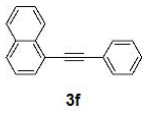
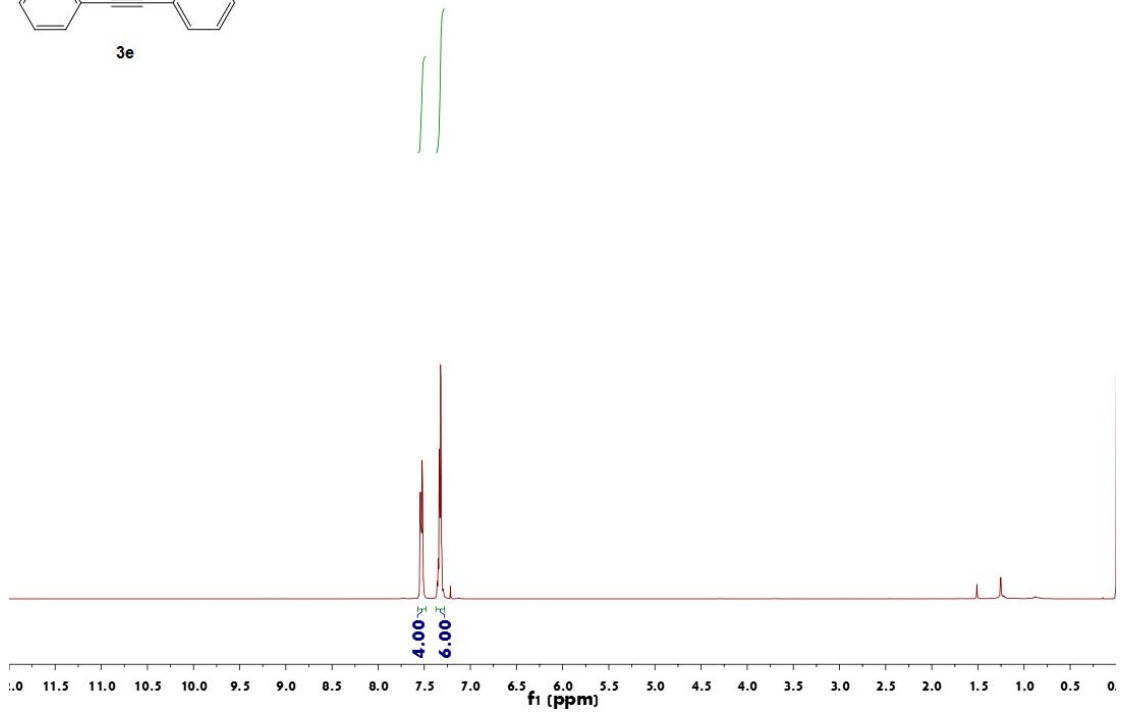
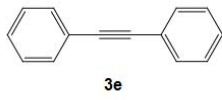
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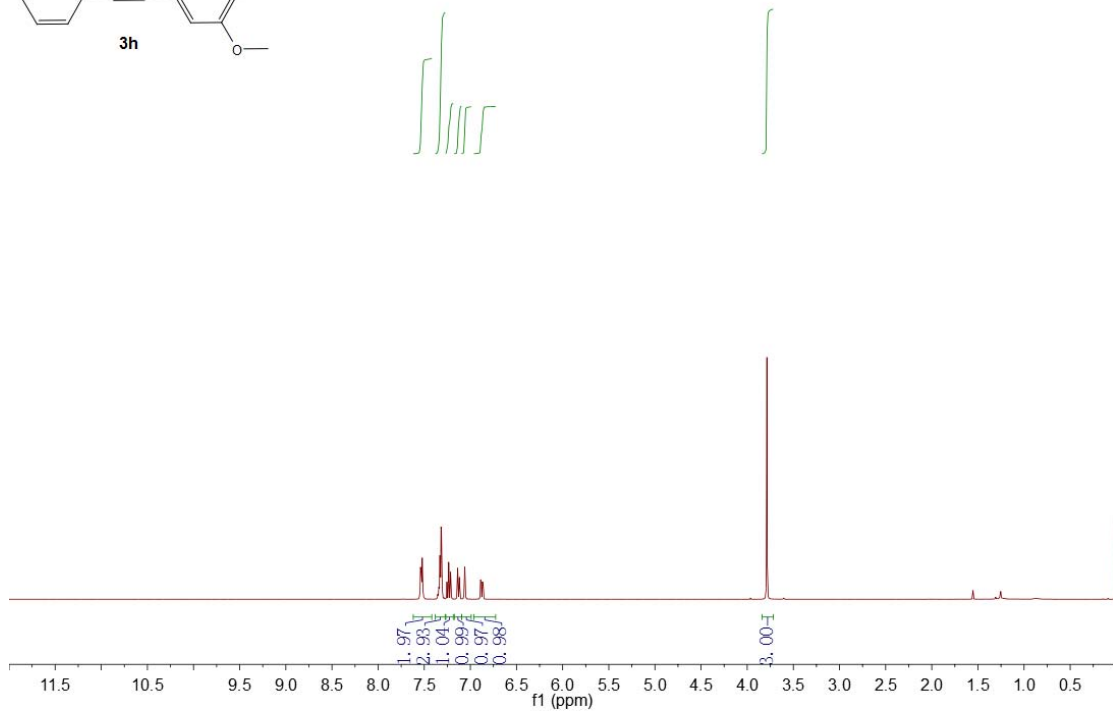
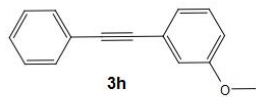
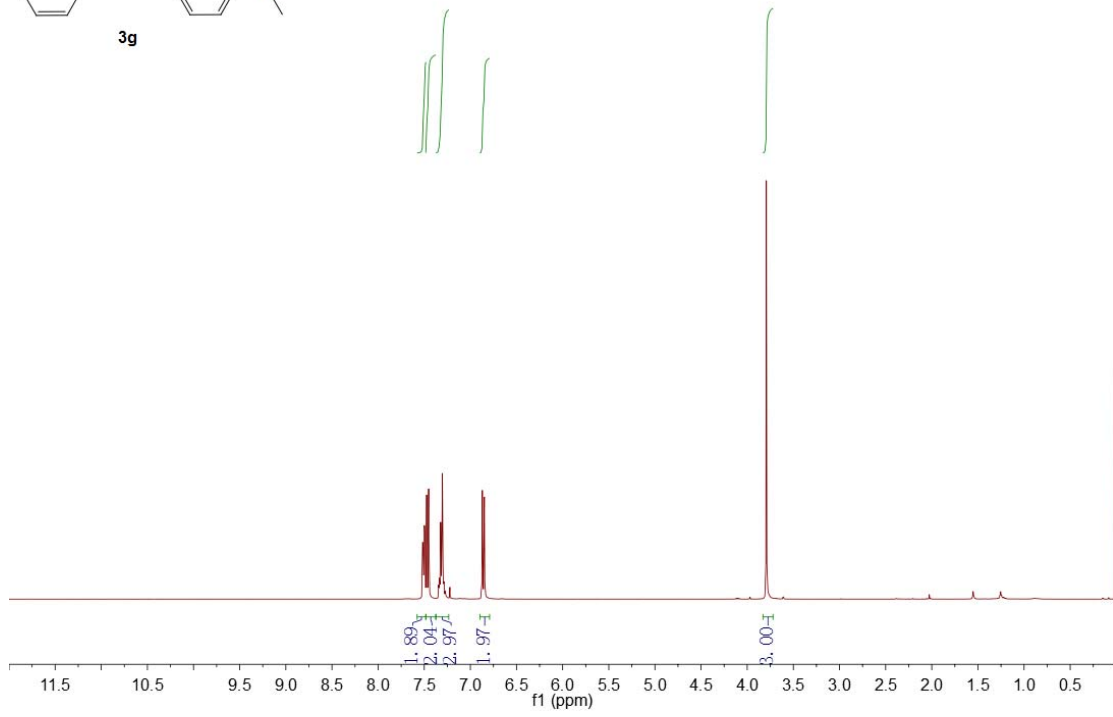
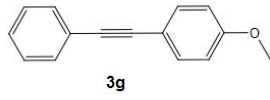
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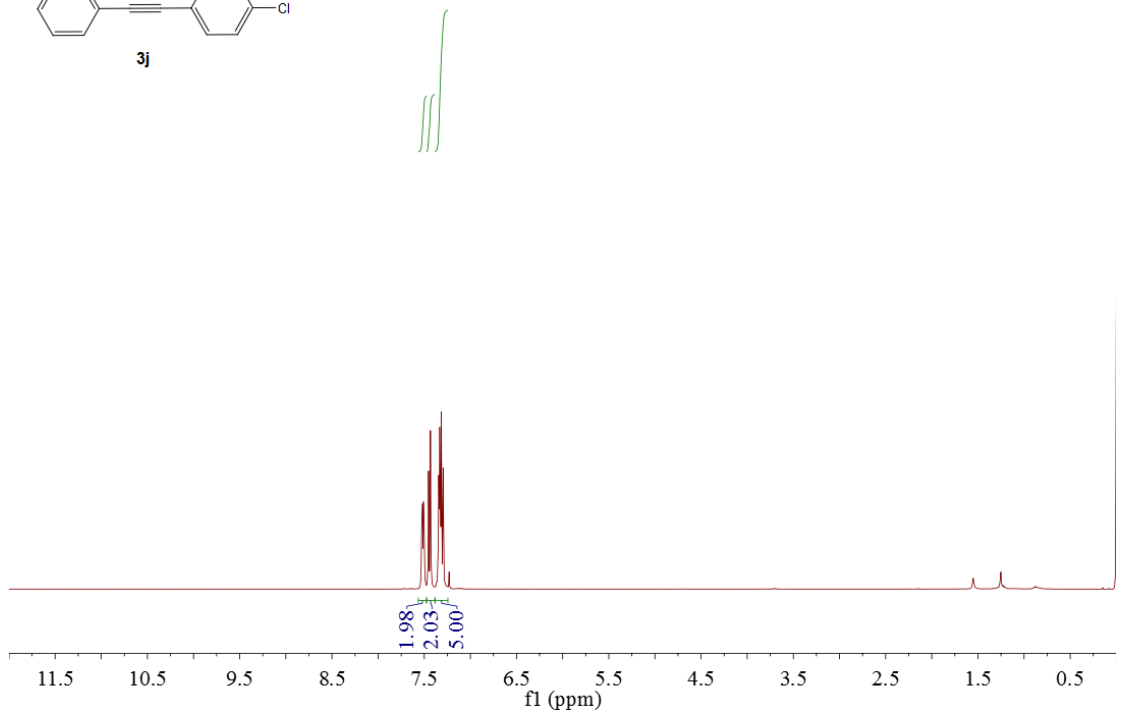
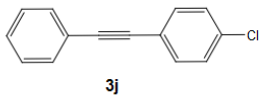
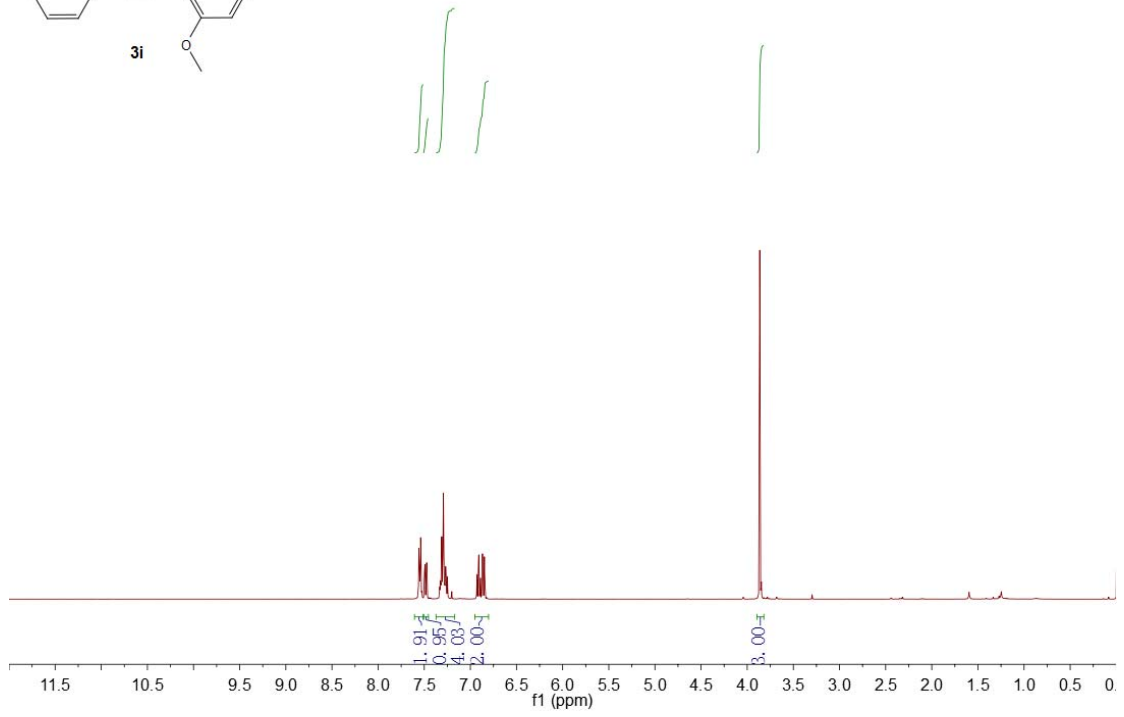
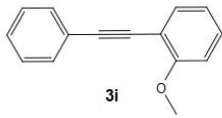
¹H-NMR Spectra

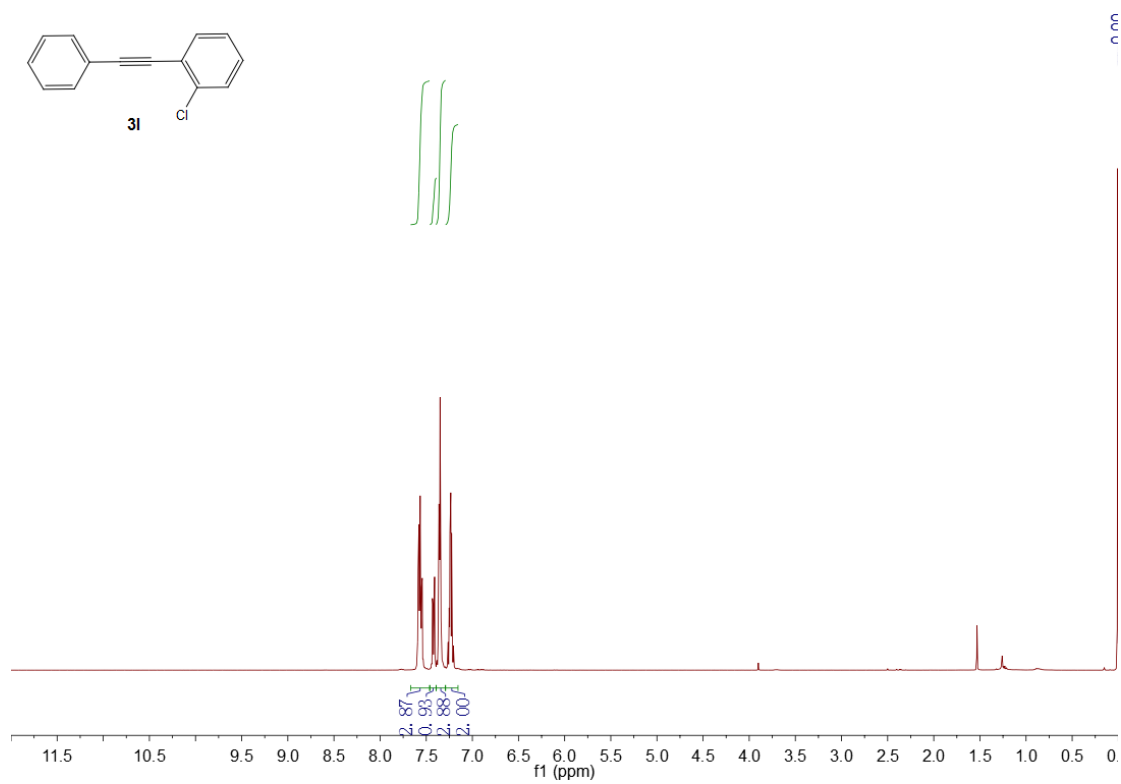
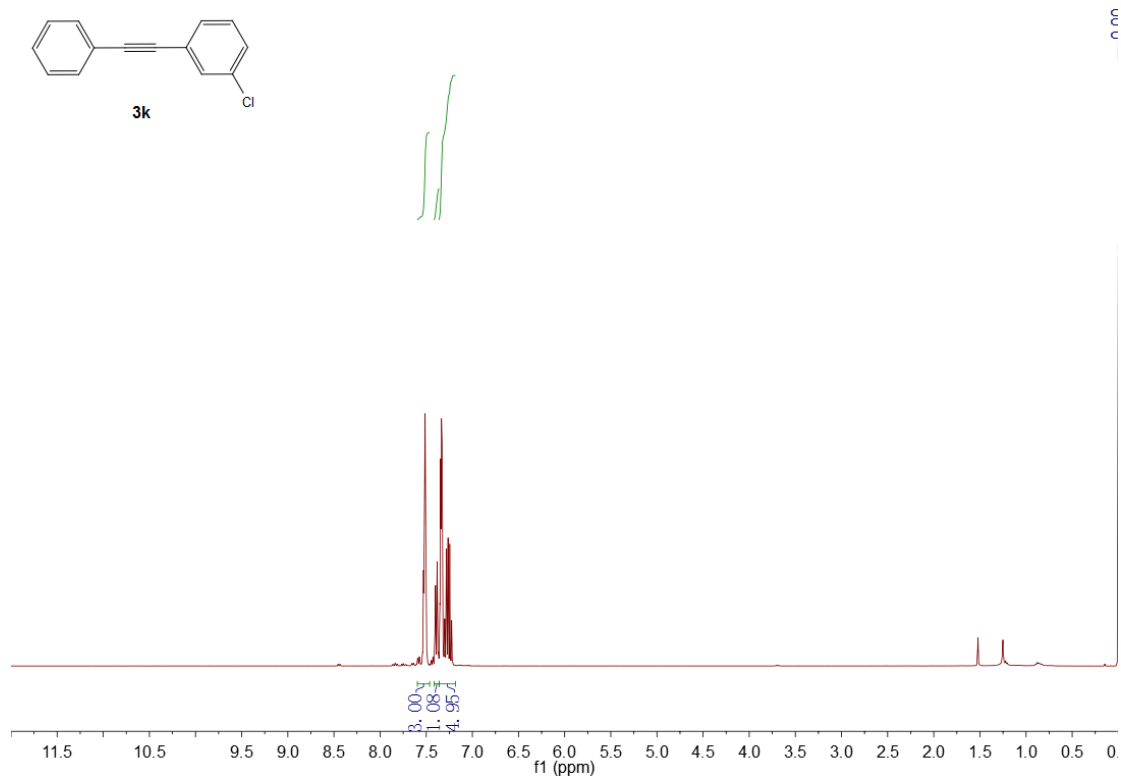


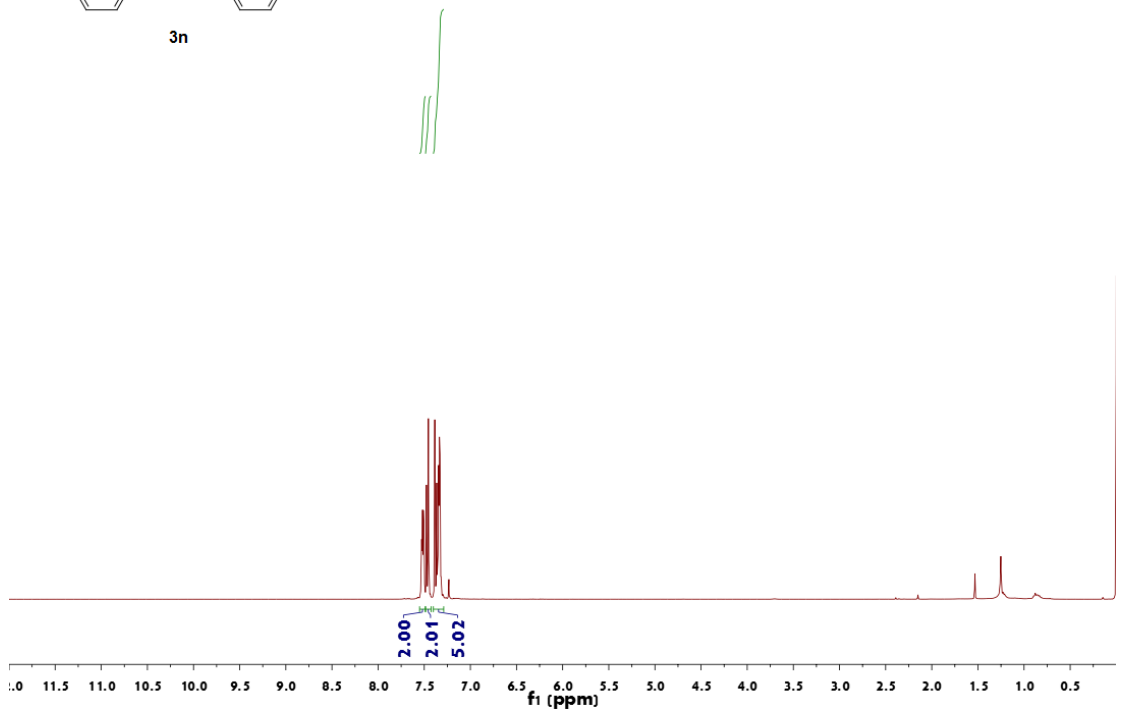
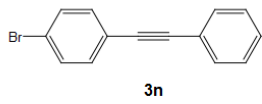
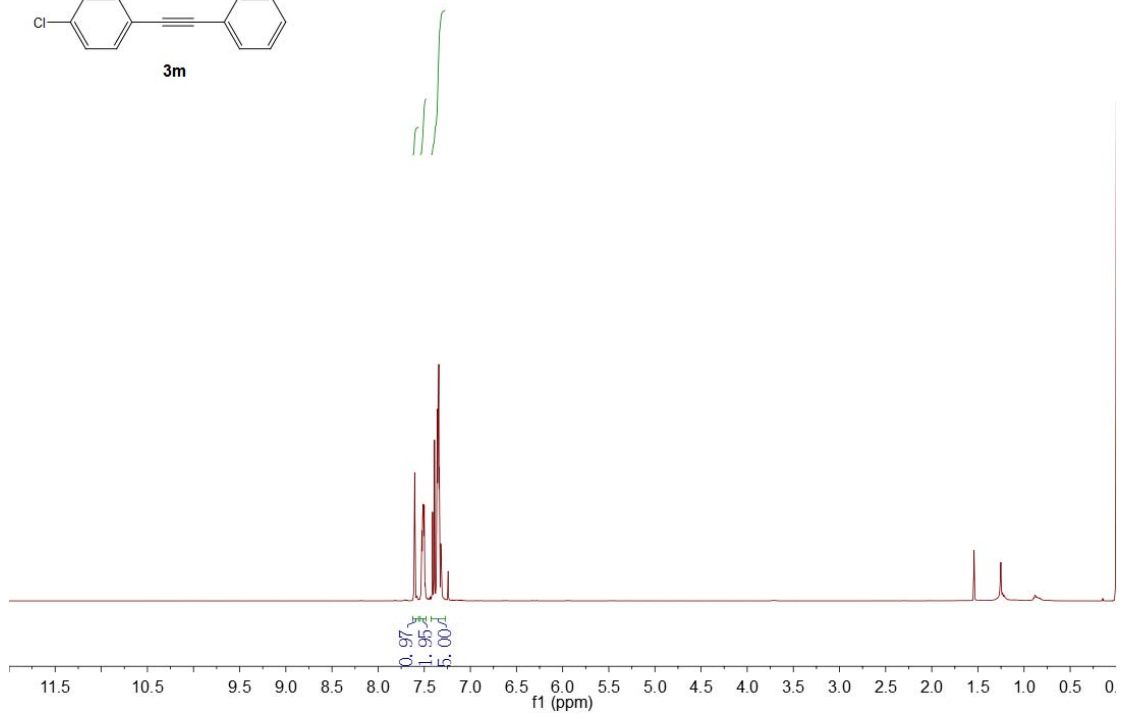
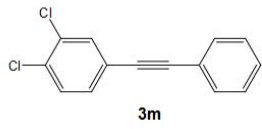


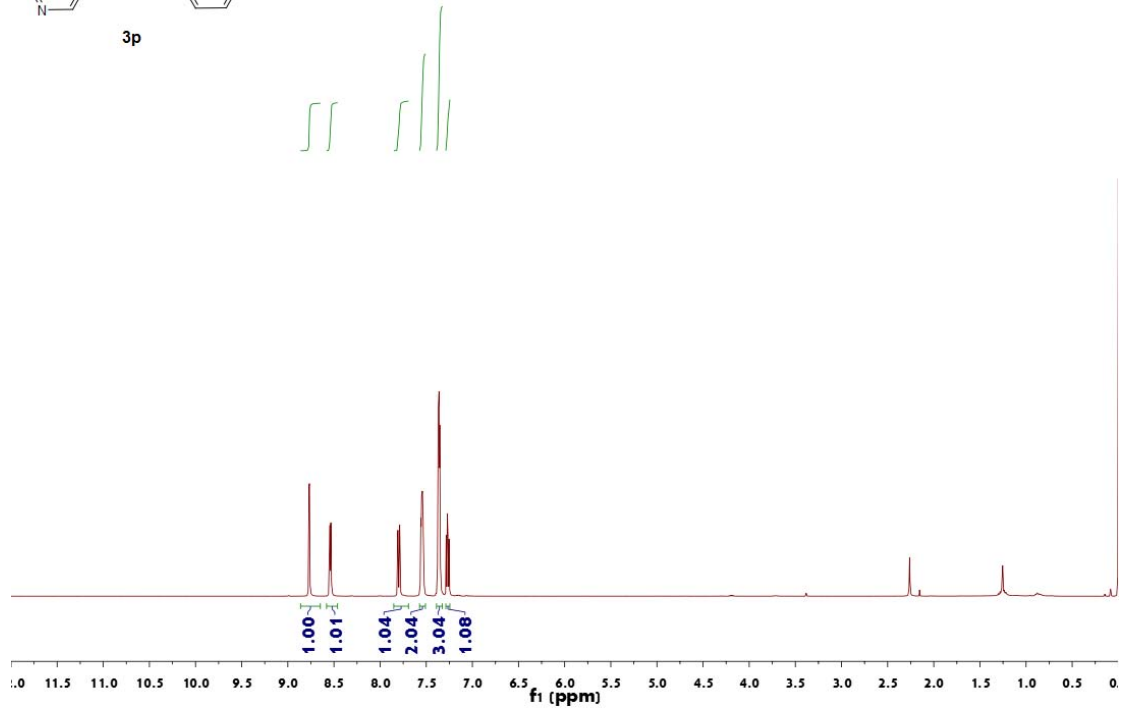
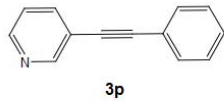
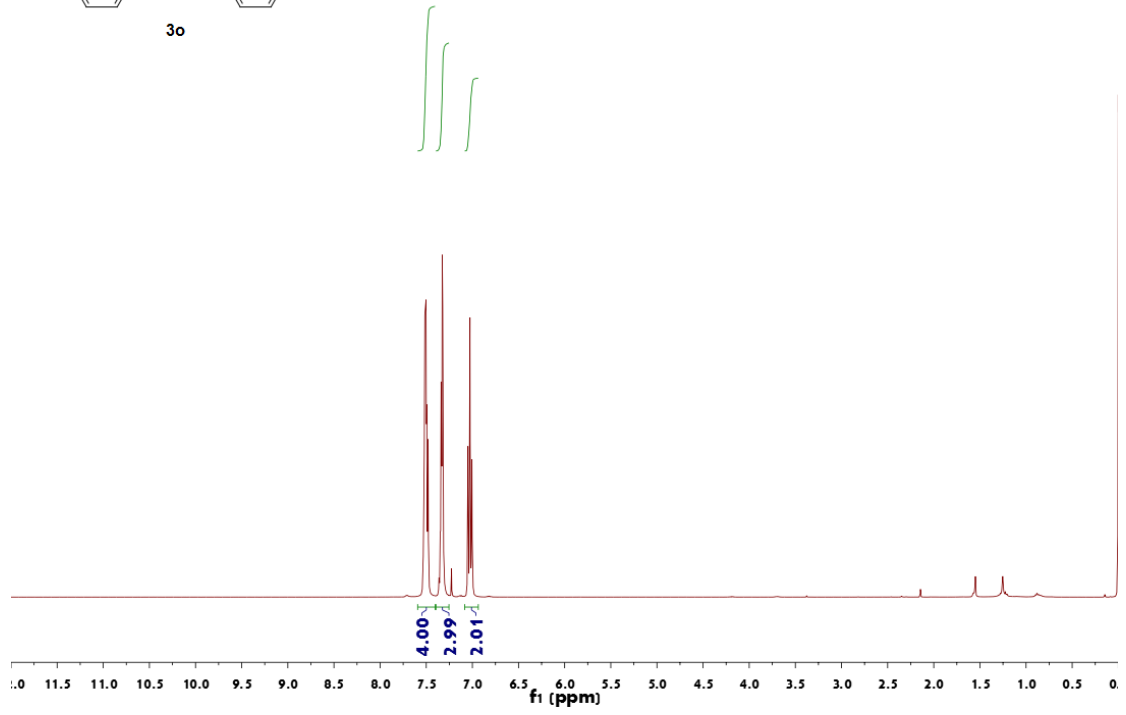
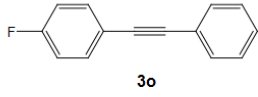


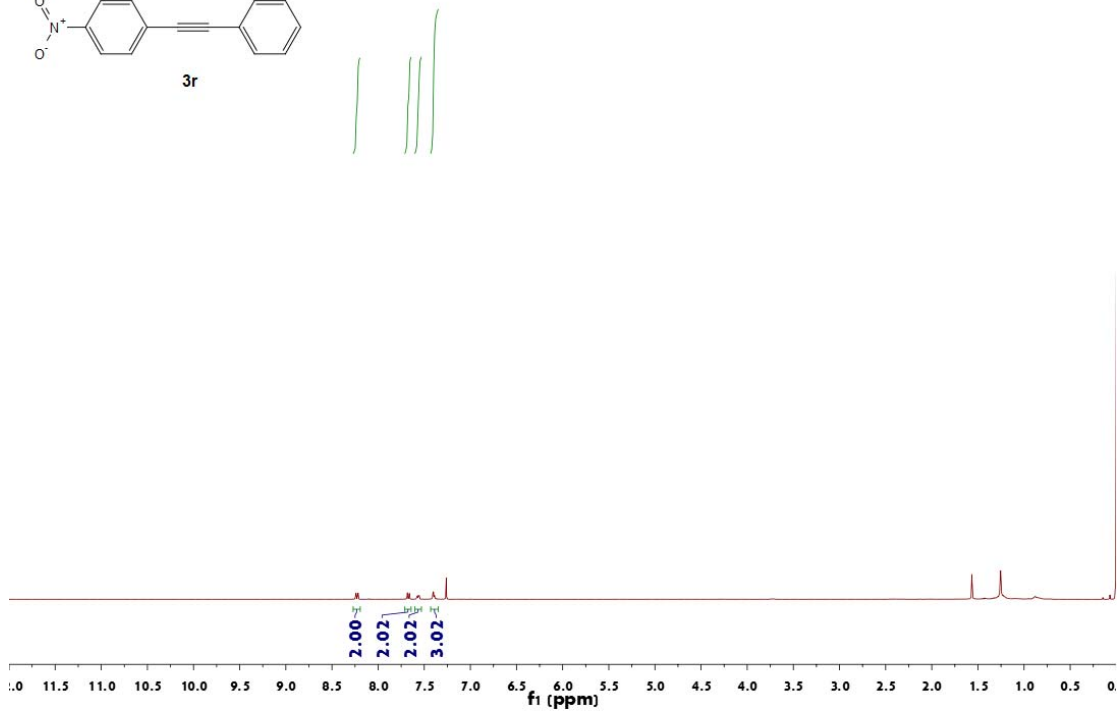
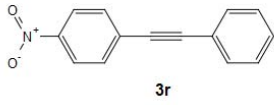
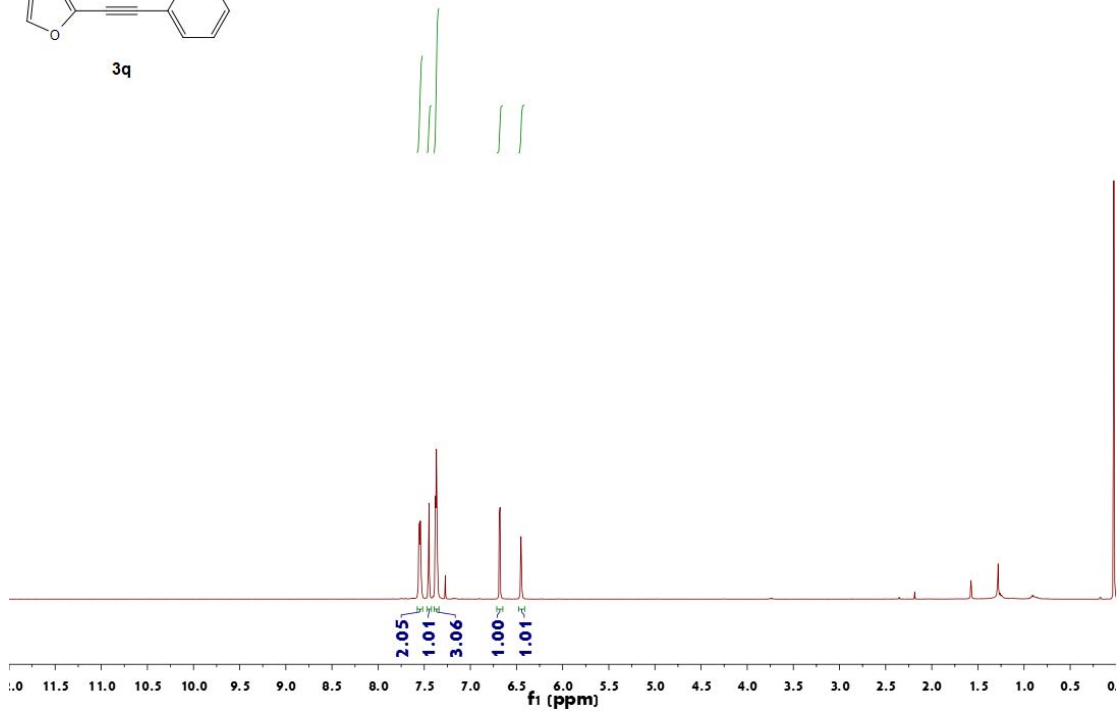
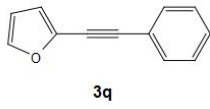


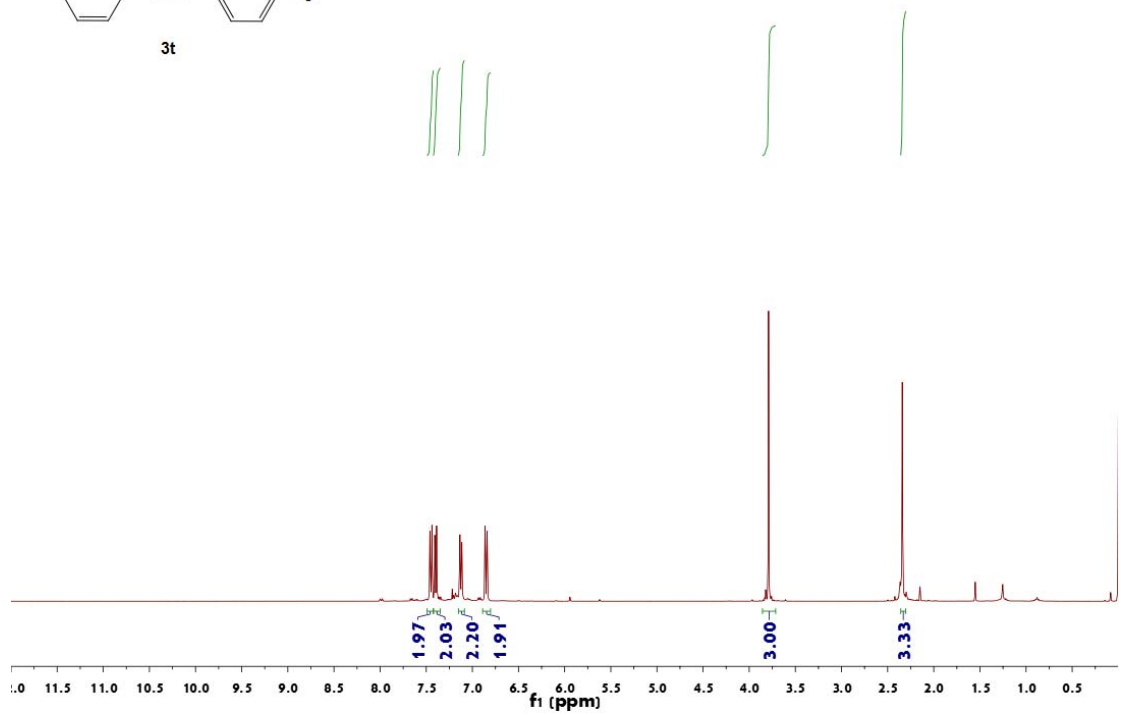
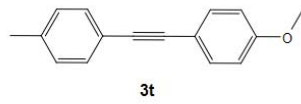
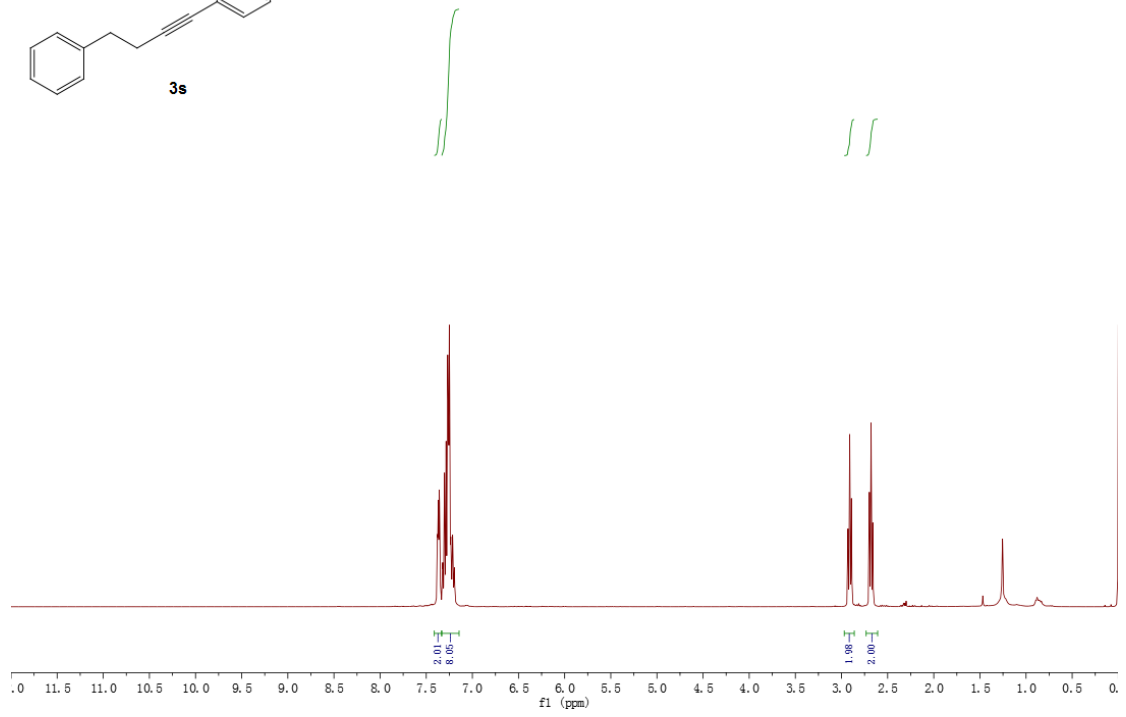
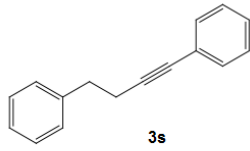


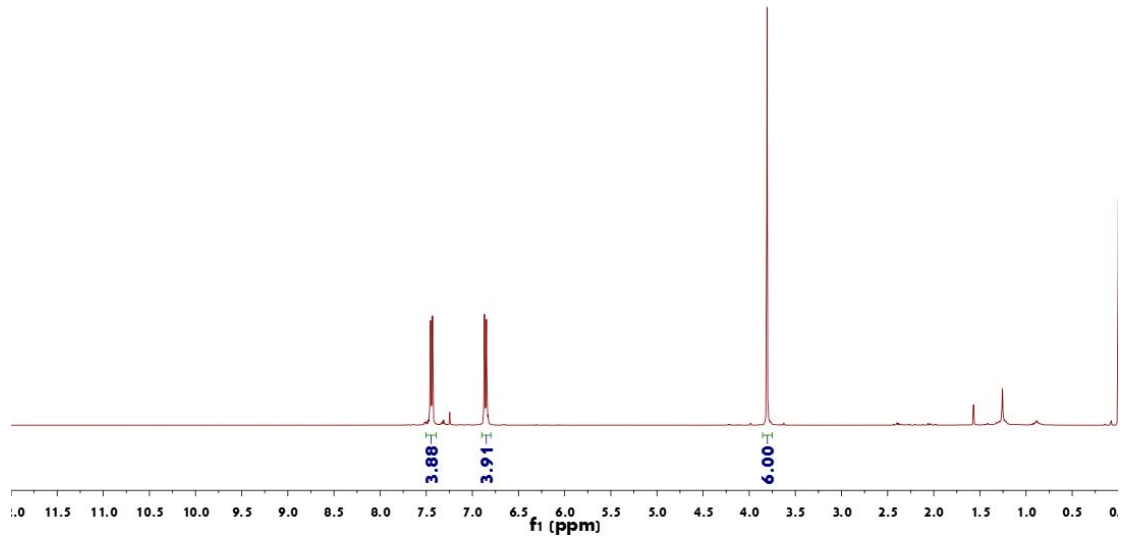
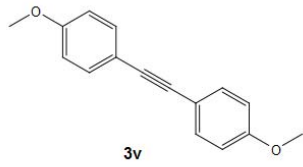
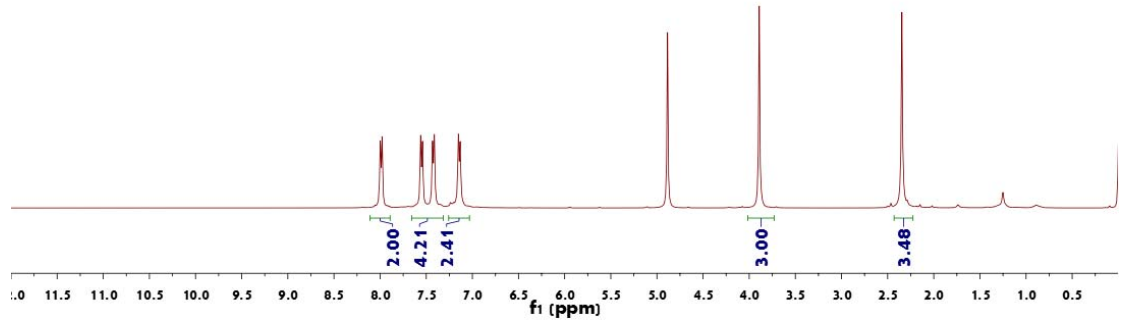
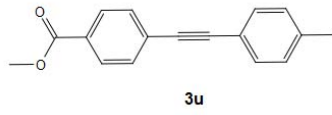


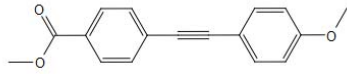




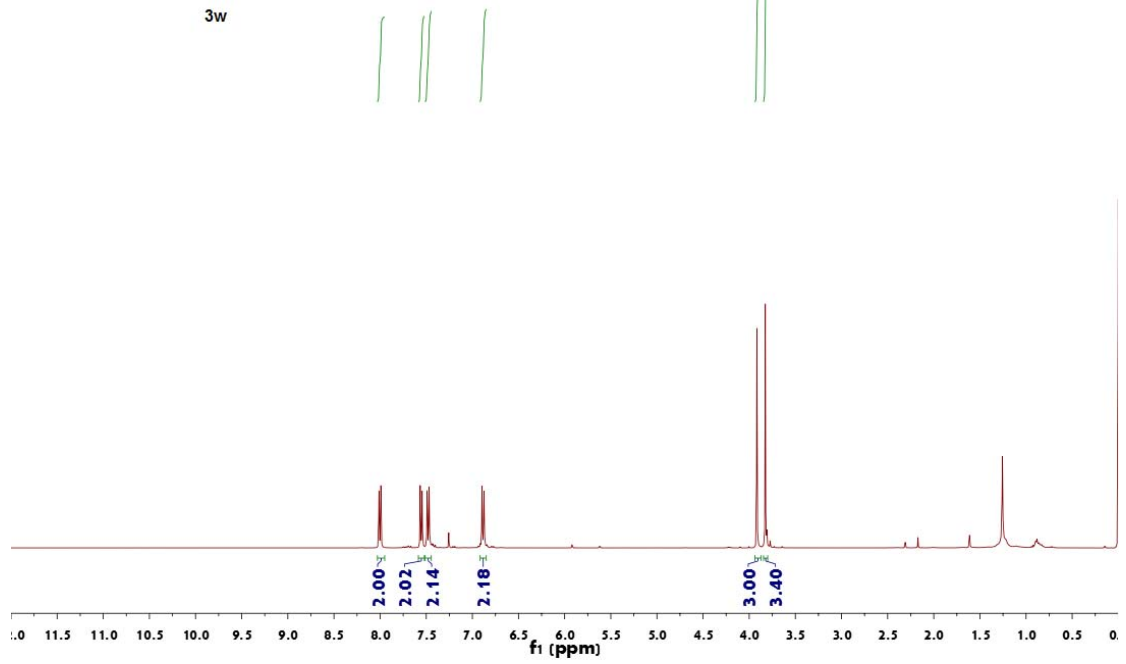




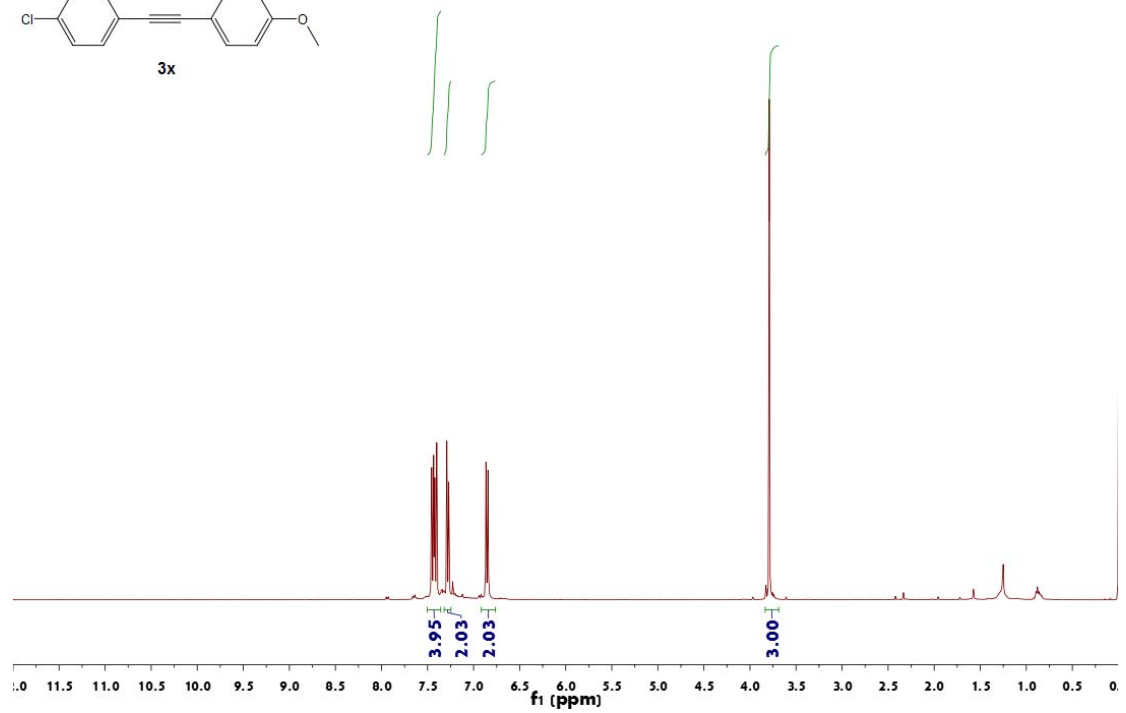


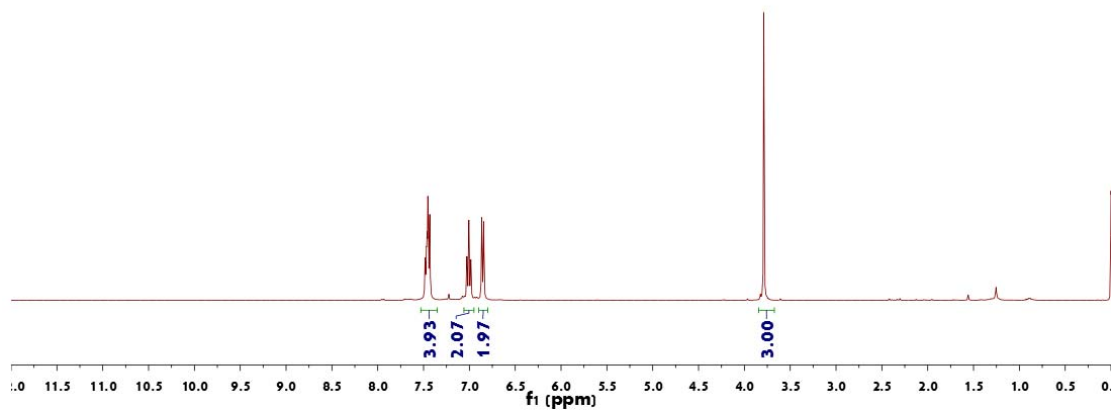
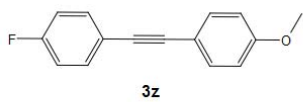
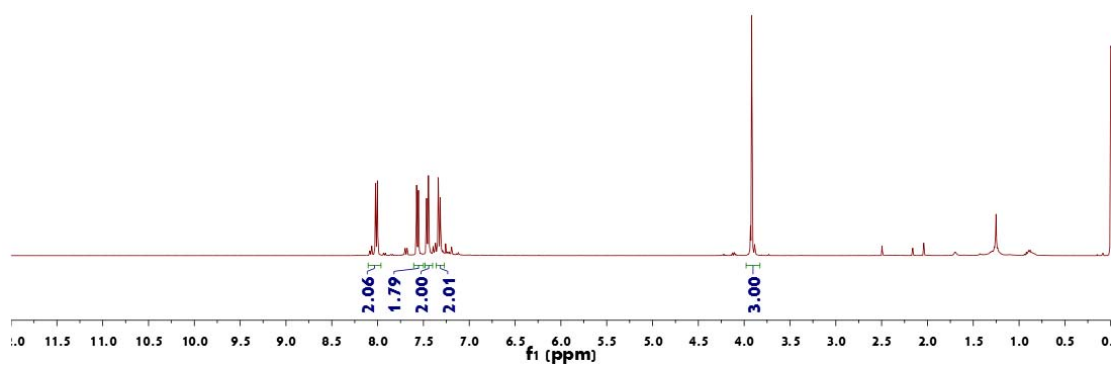
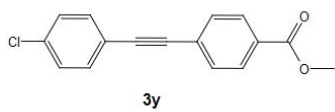


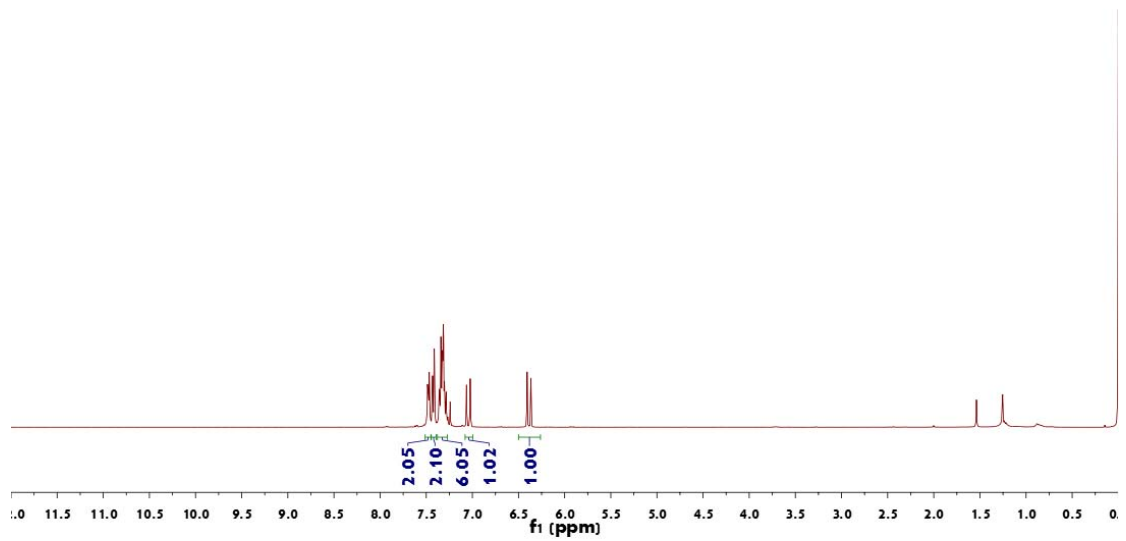
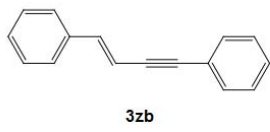
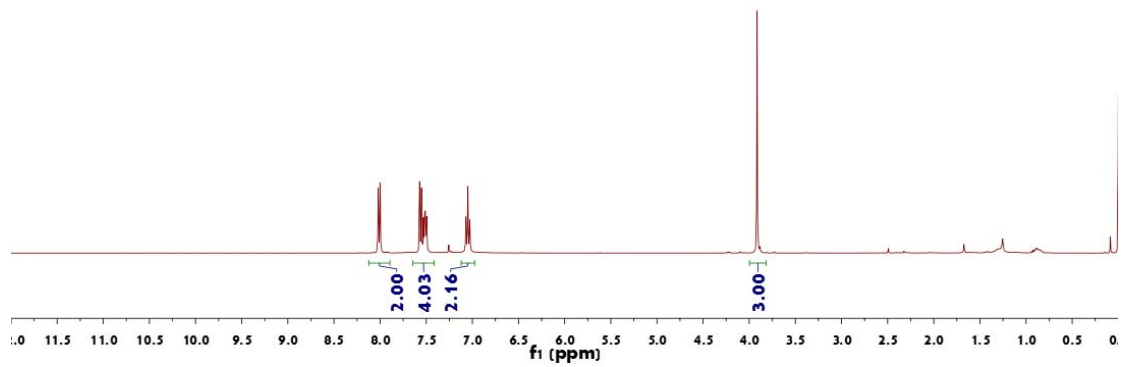
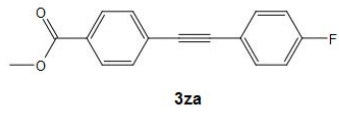
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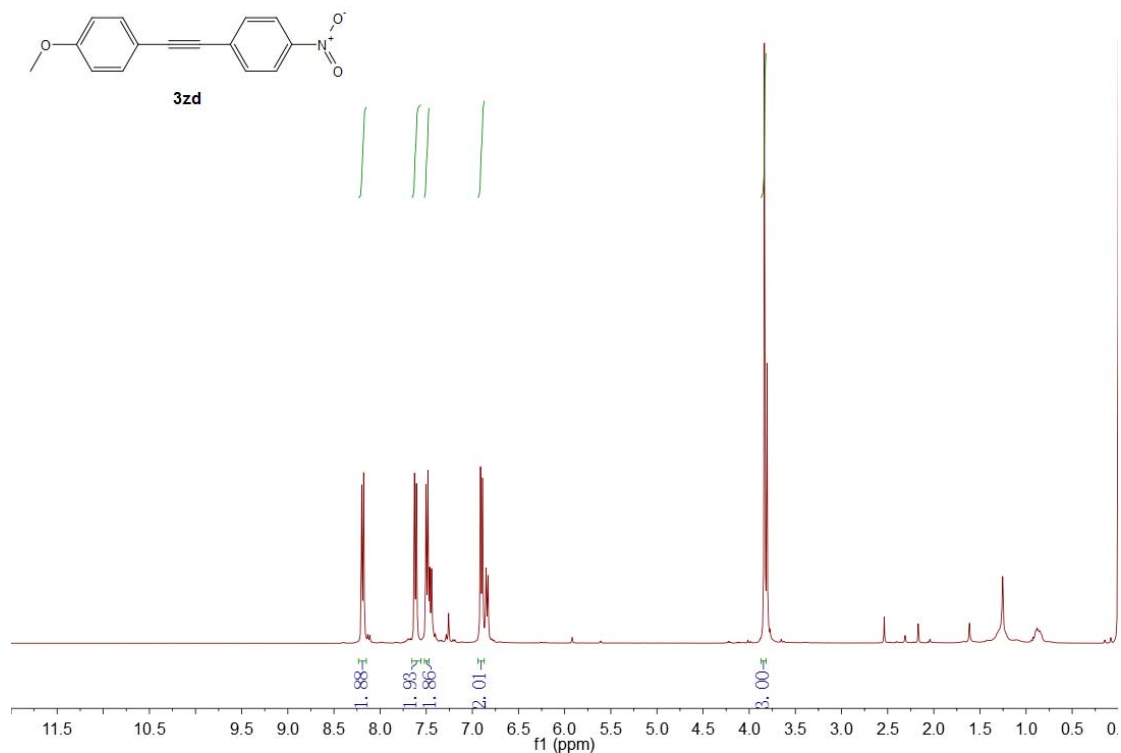
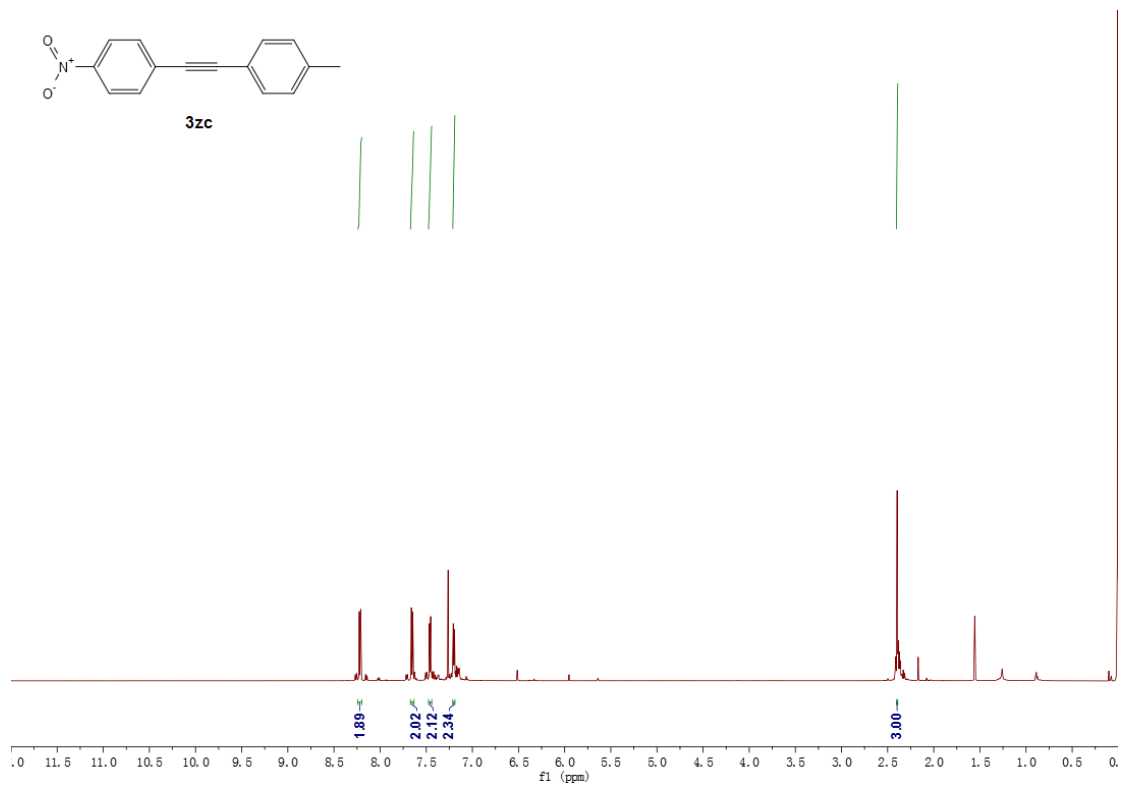


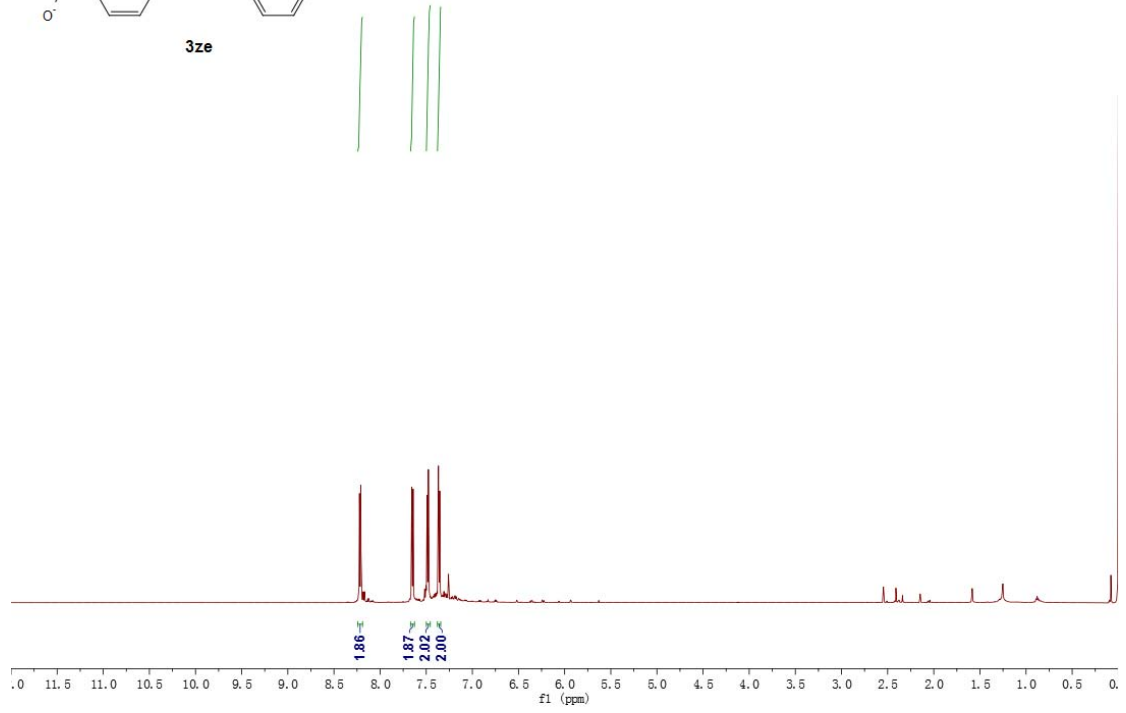
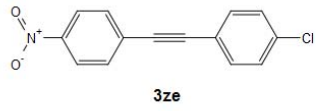
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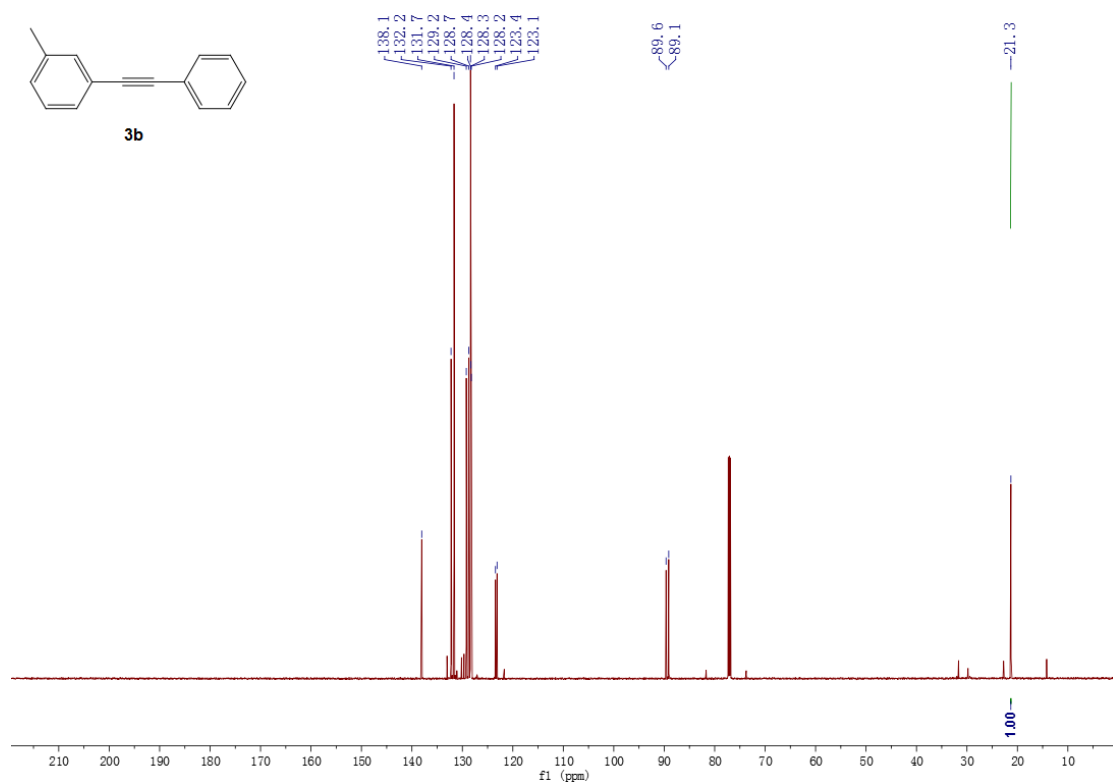
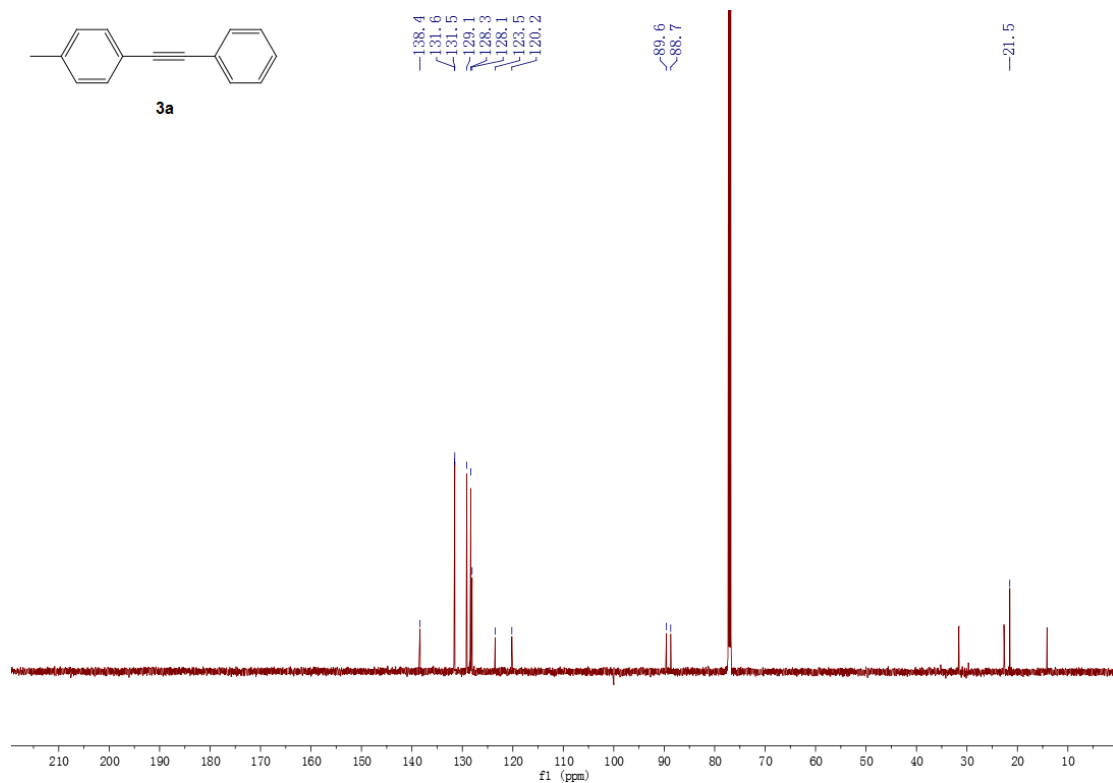


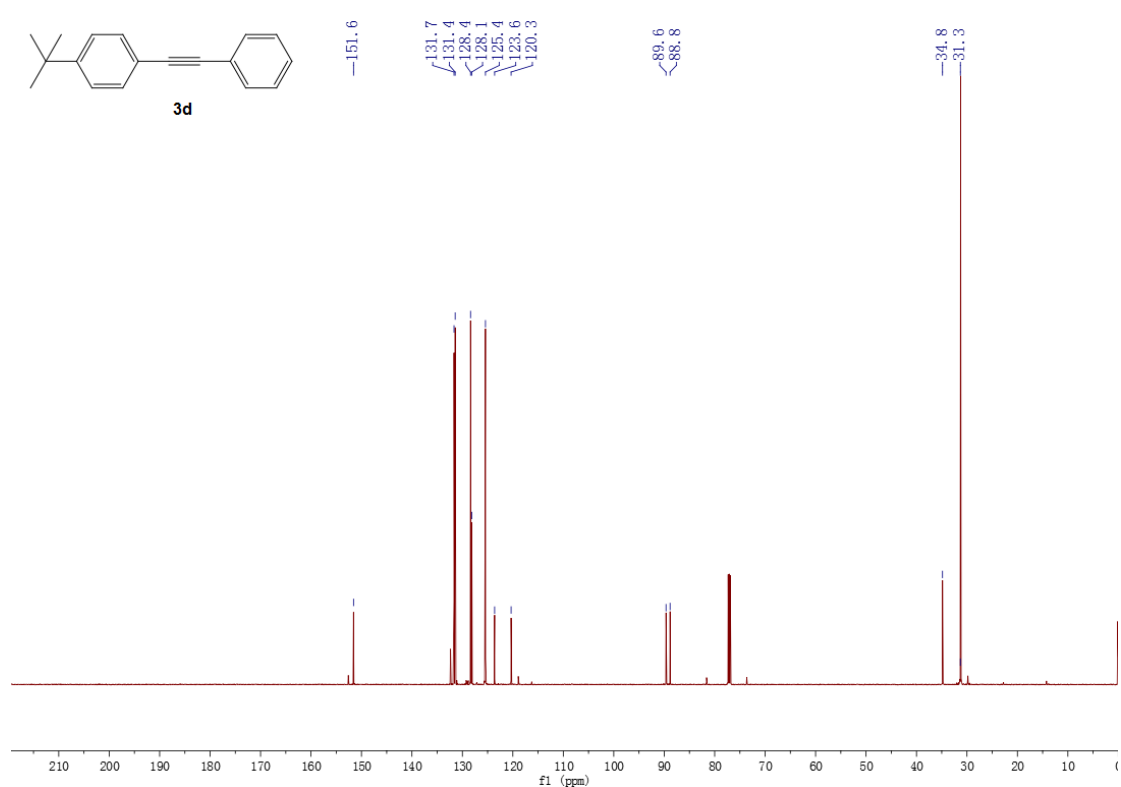
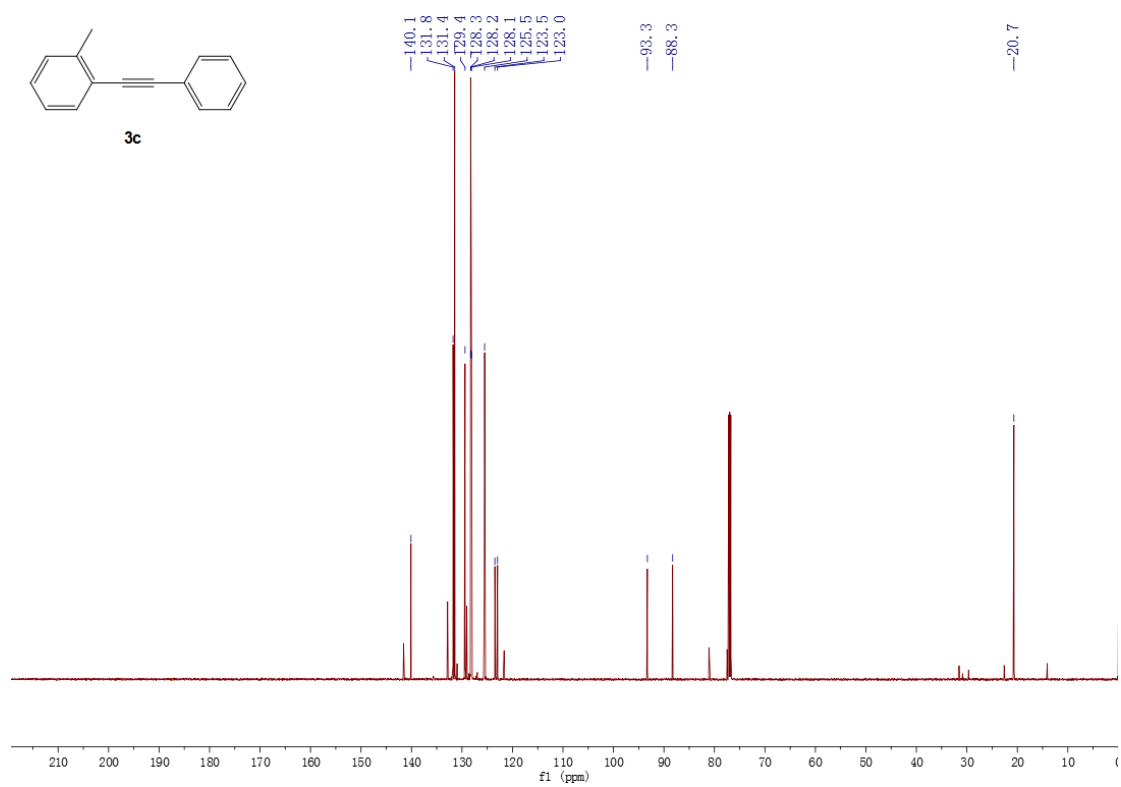






¹³C-NMR Spectra



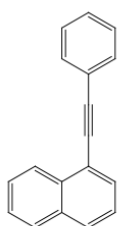
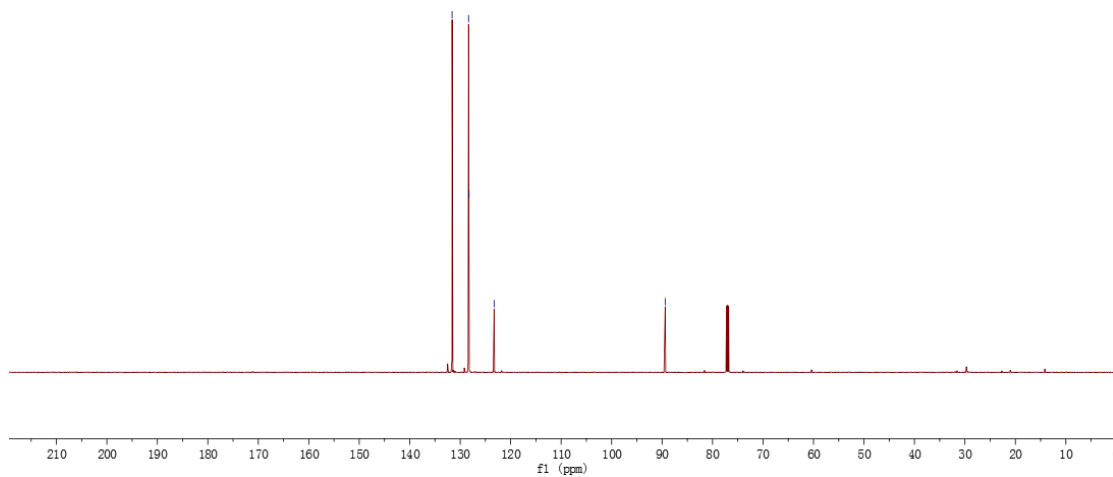




3e

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128.3
128.2
123.3

89.4

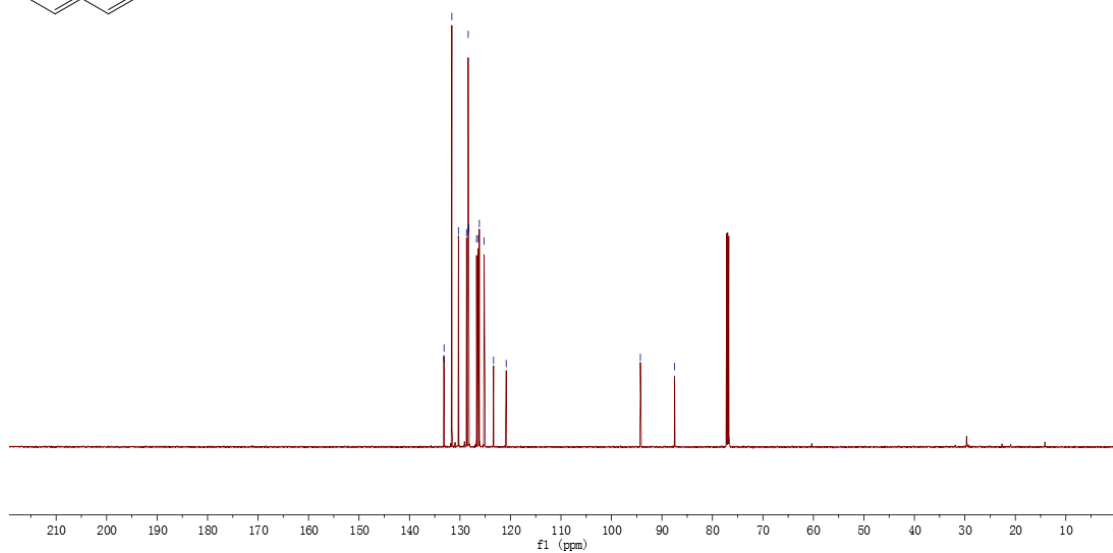


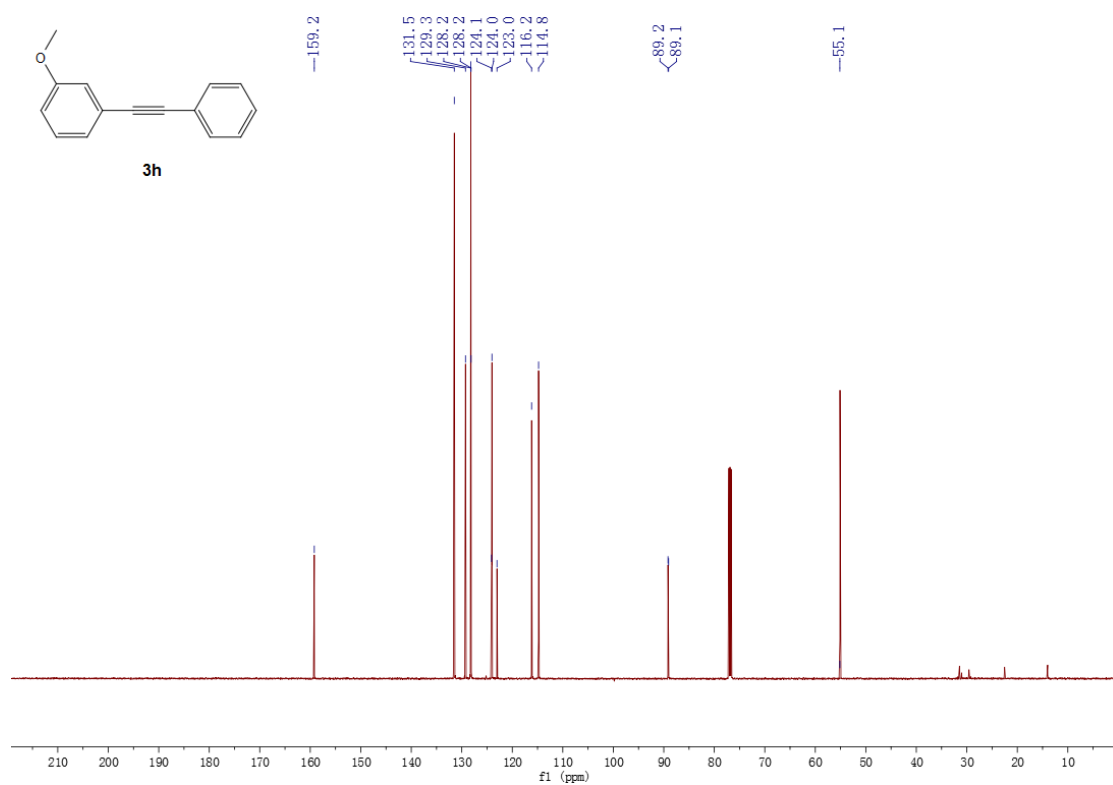
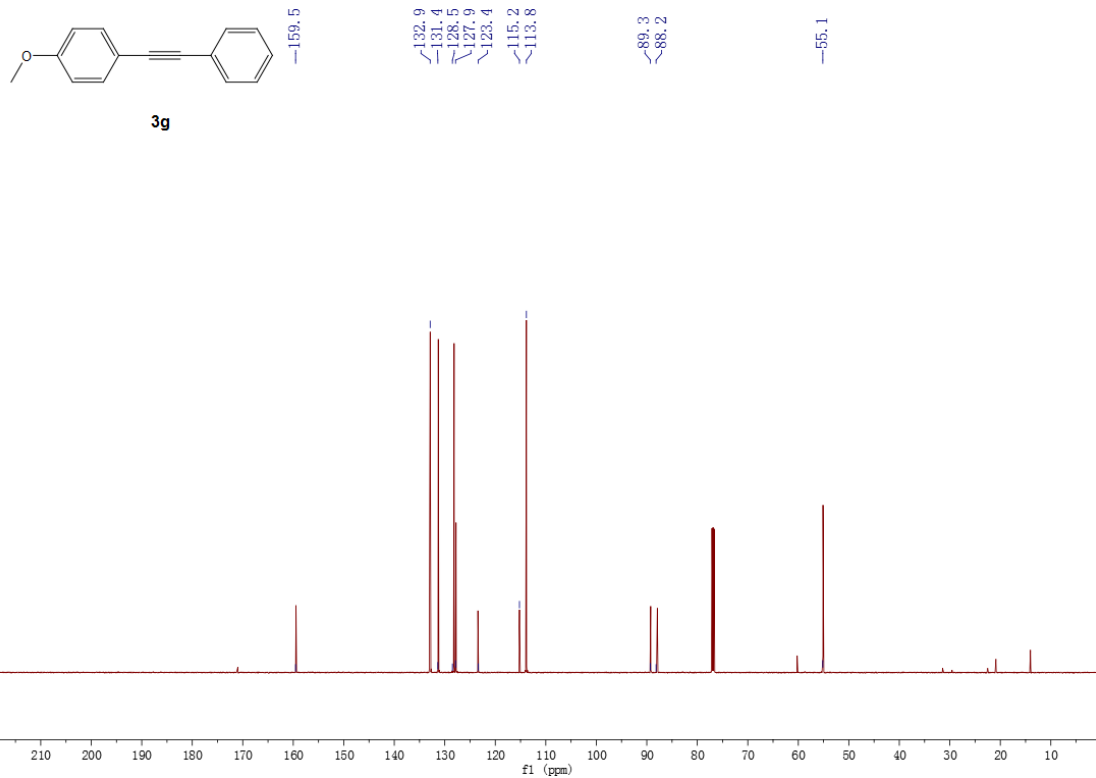
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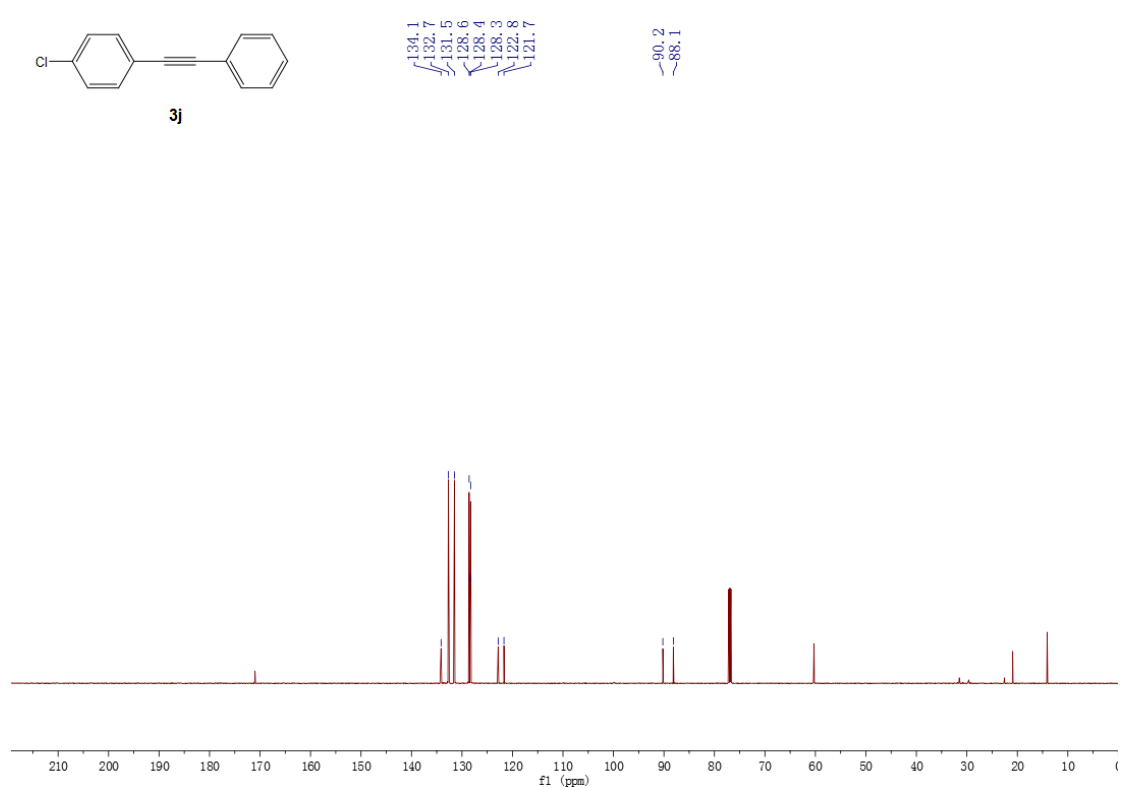
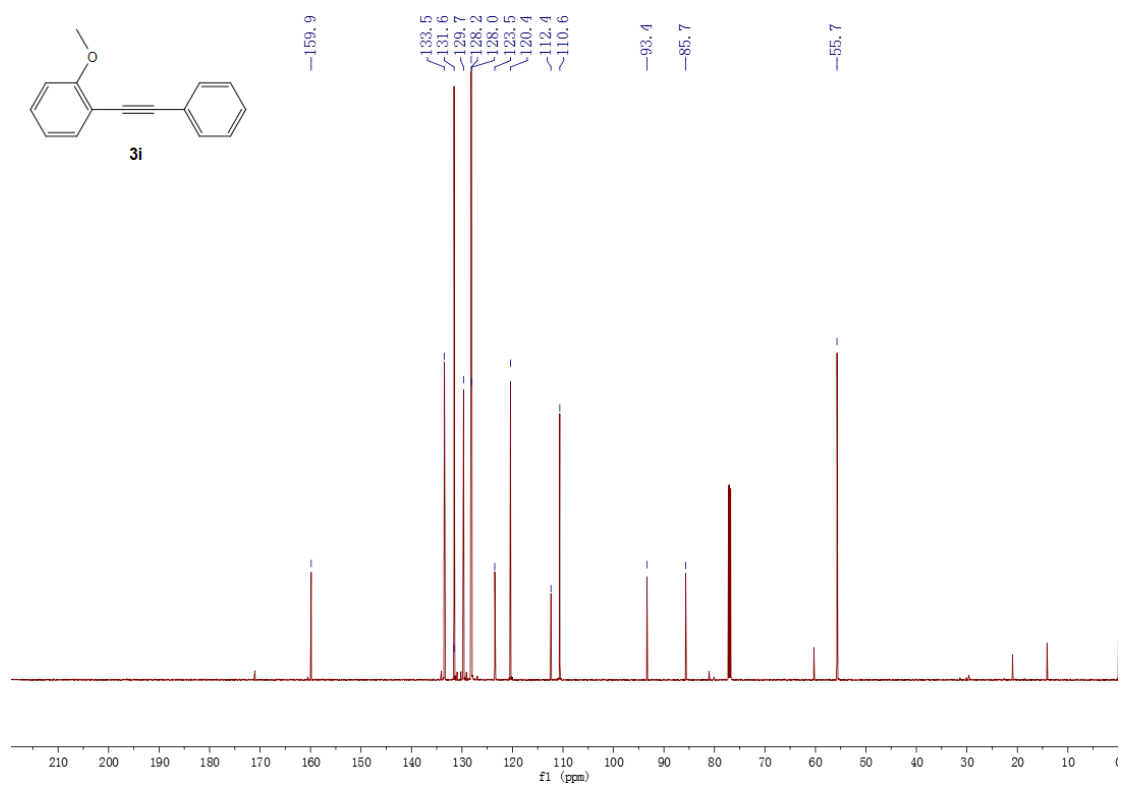
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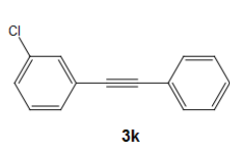
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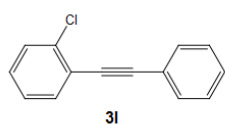
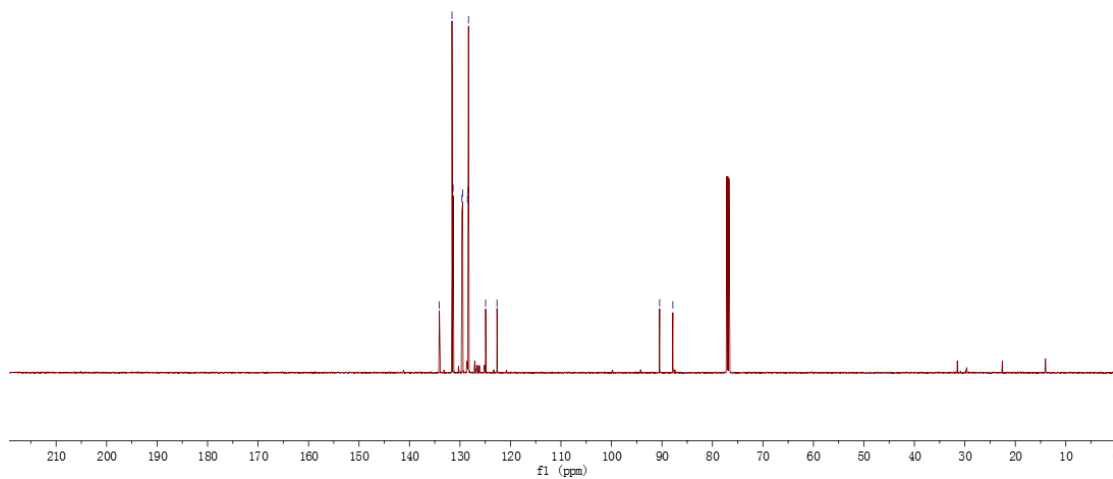






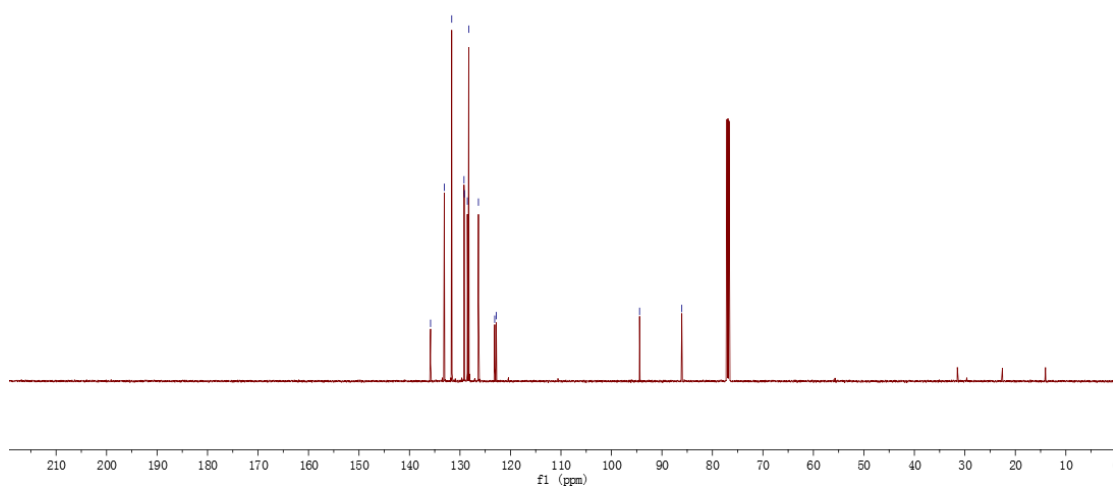
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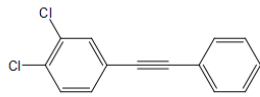
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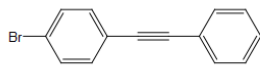
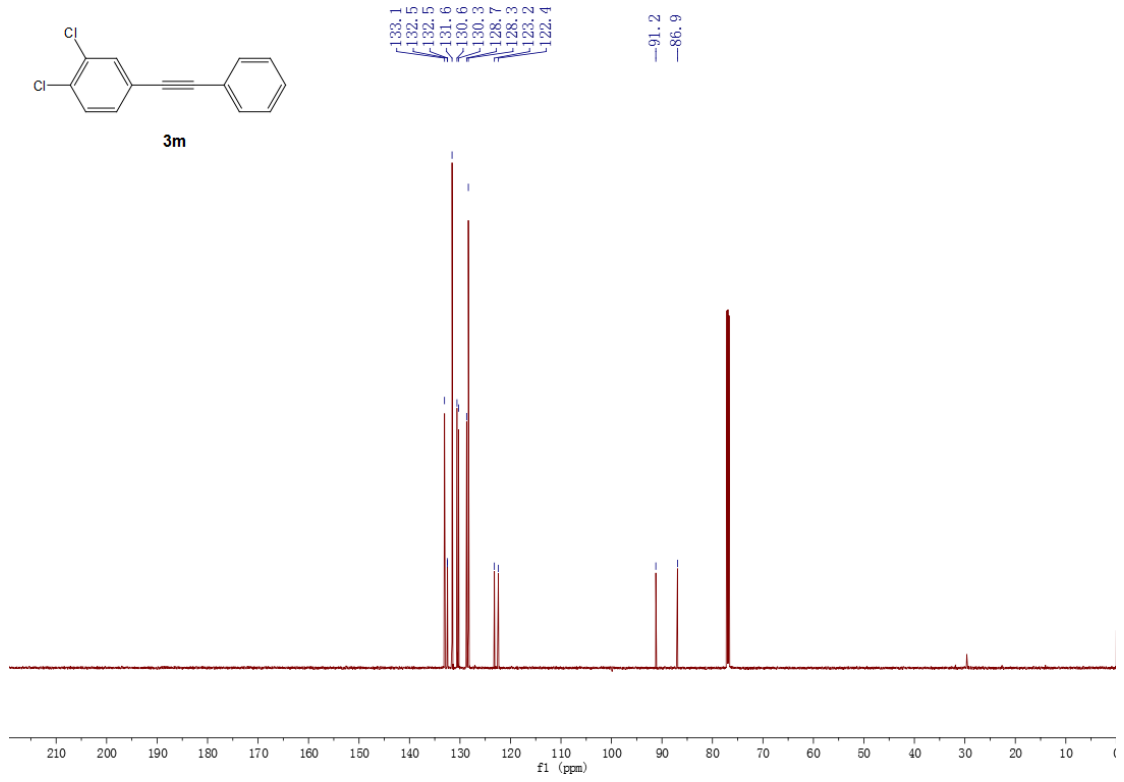
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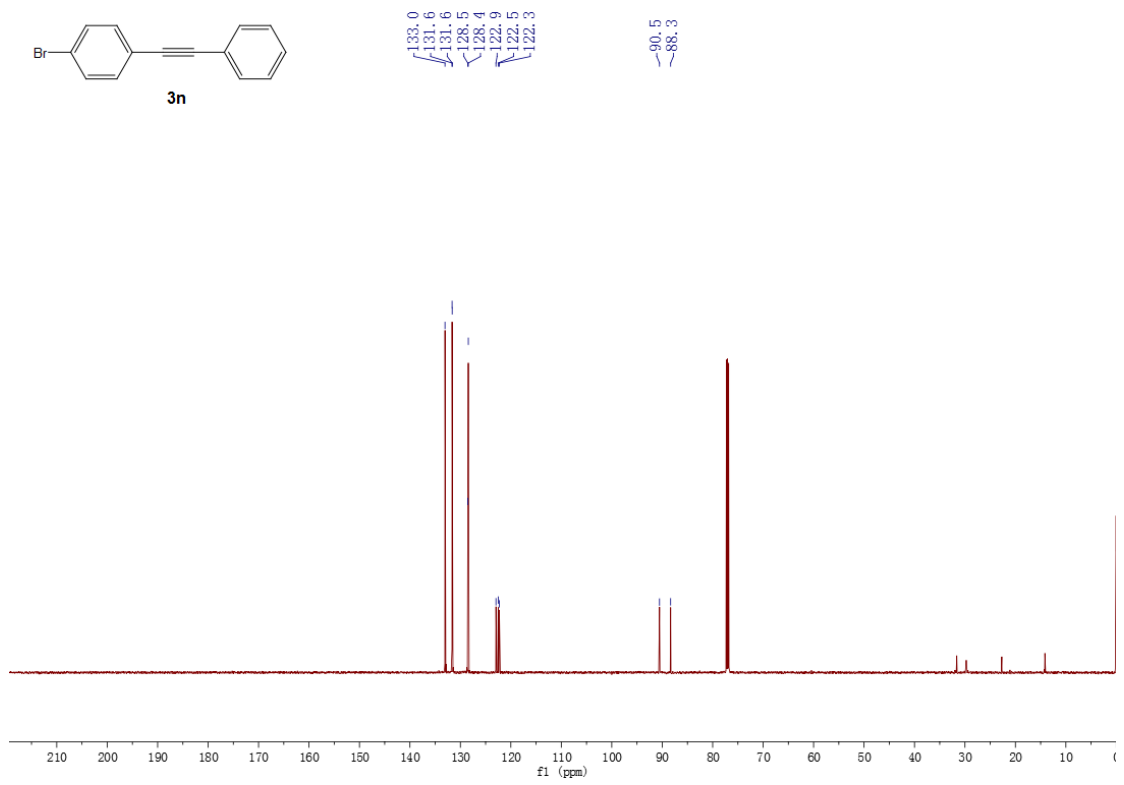


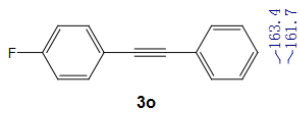


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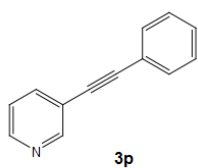
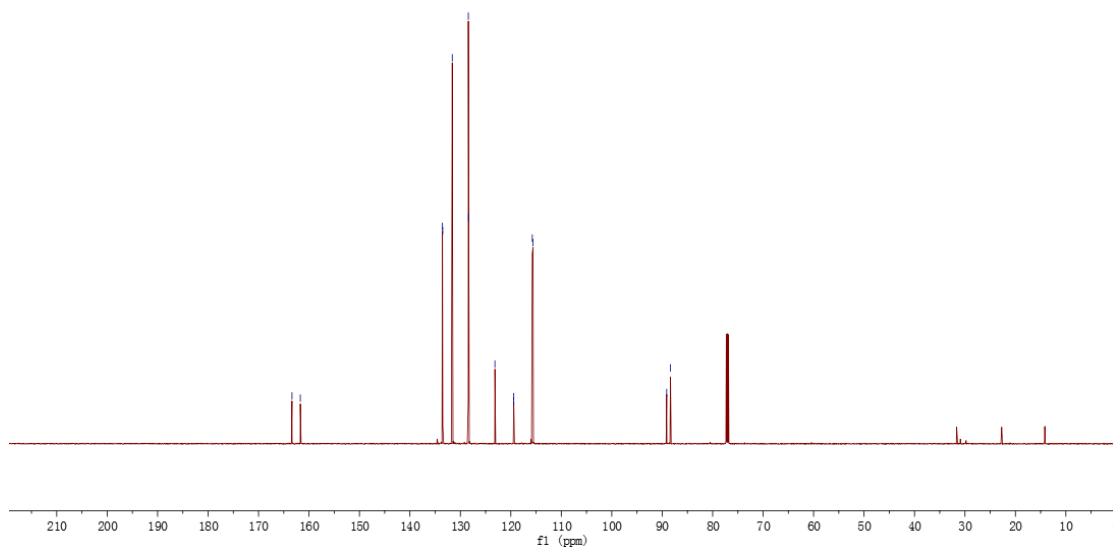


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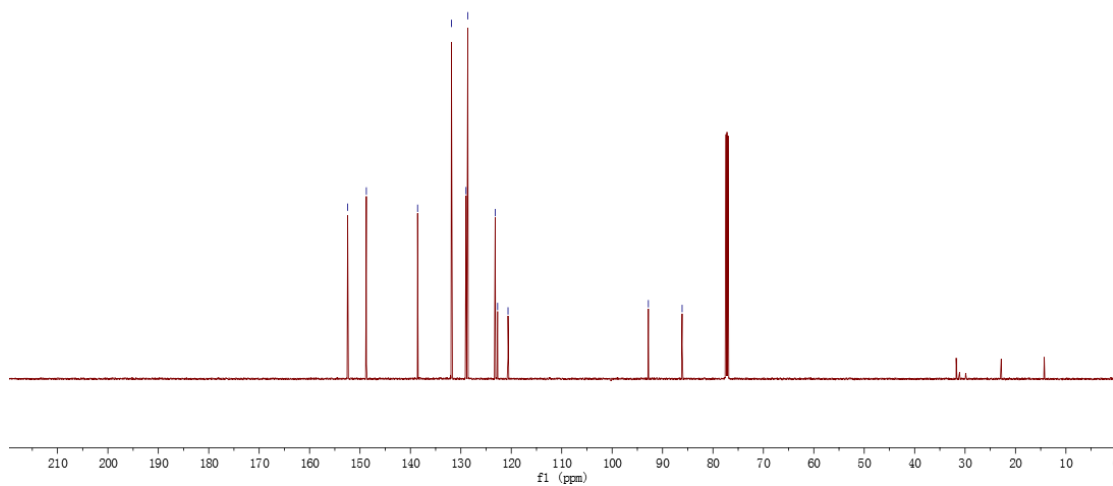


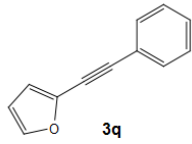


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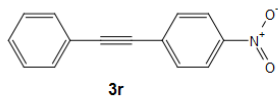
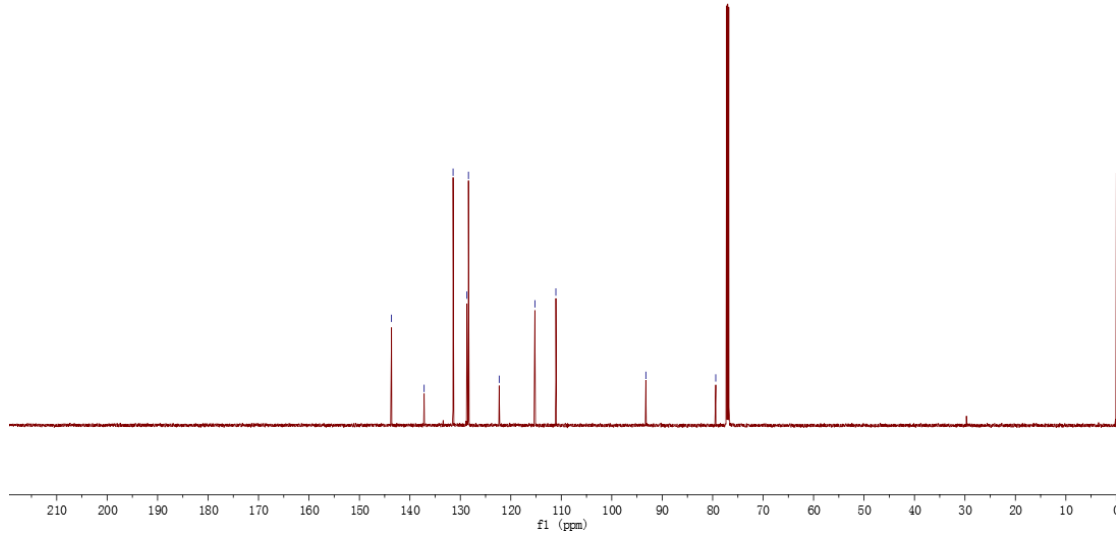


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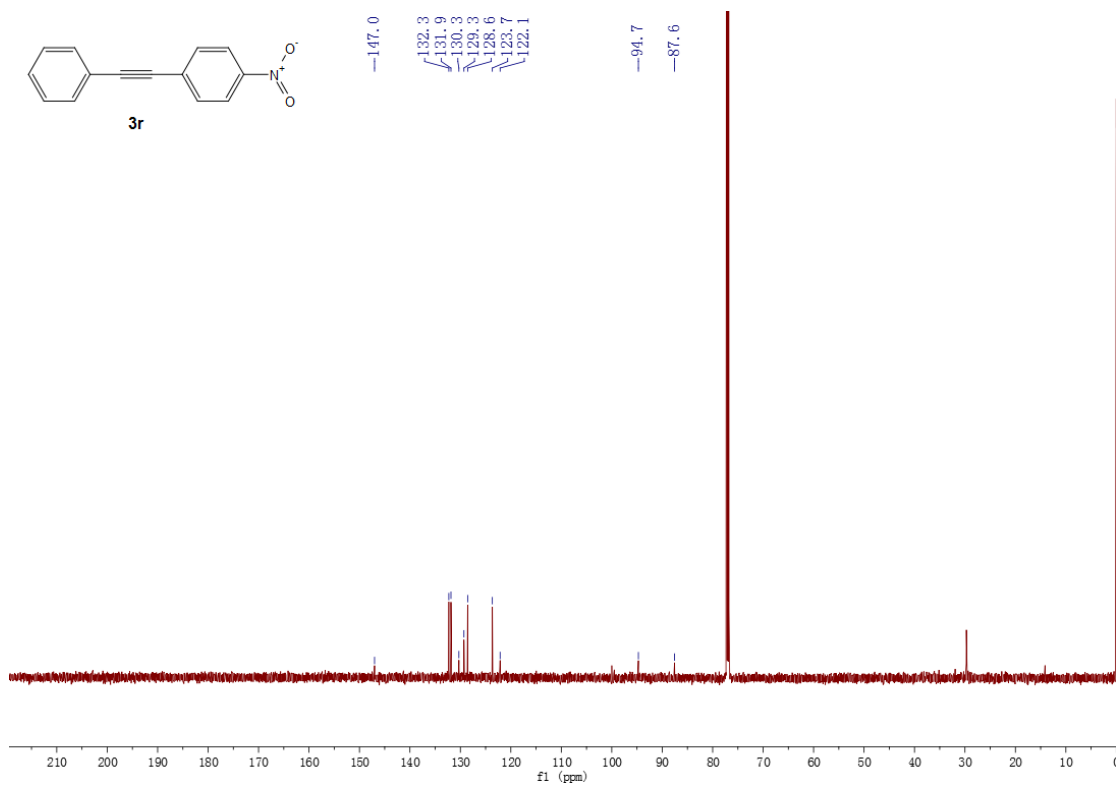


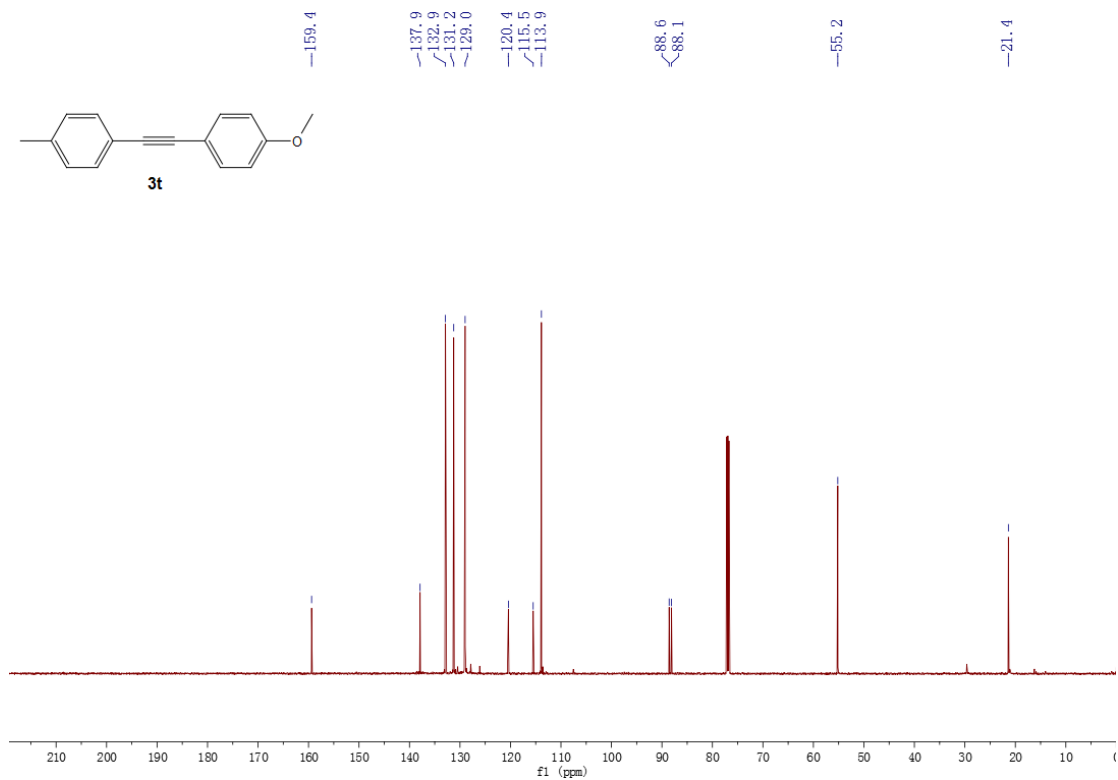
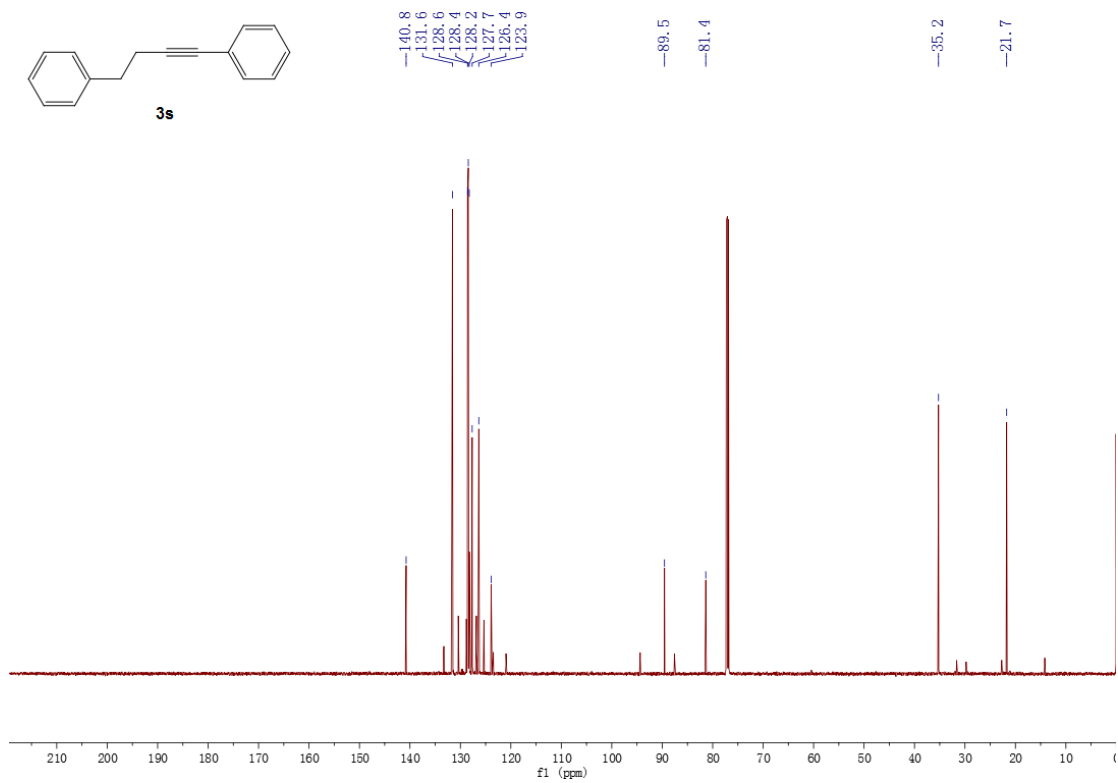
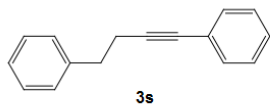


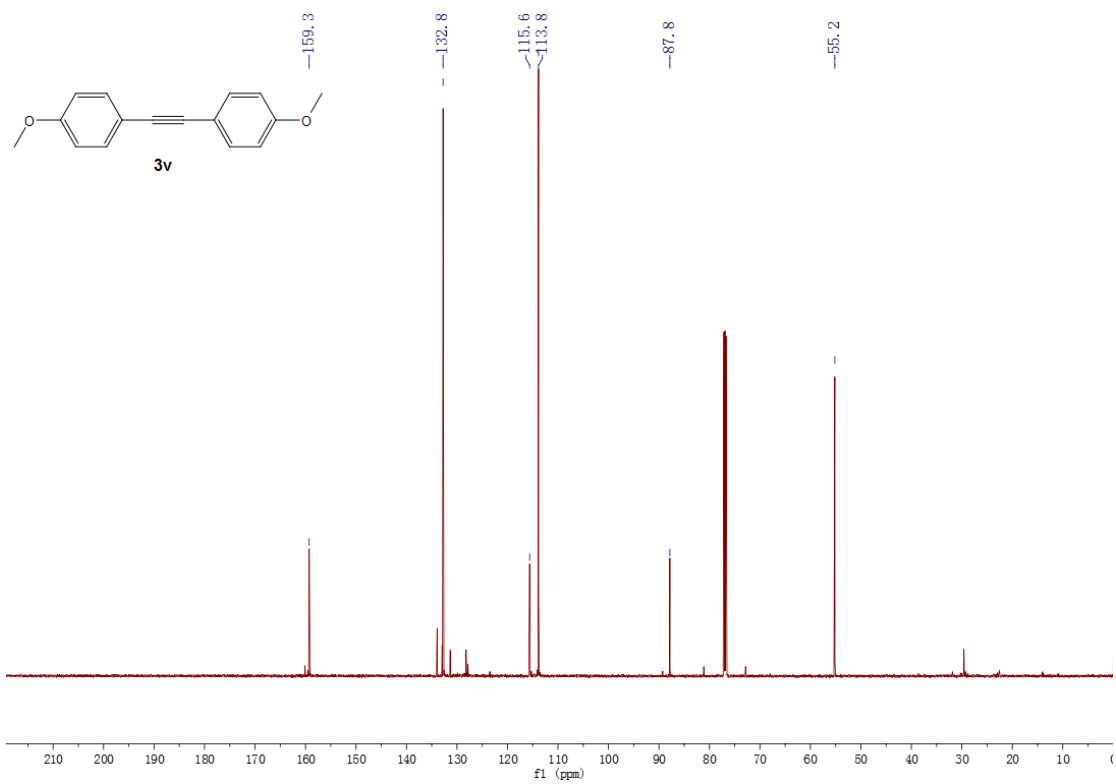
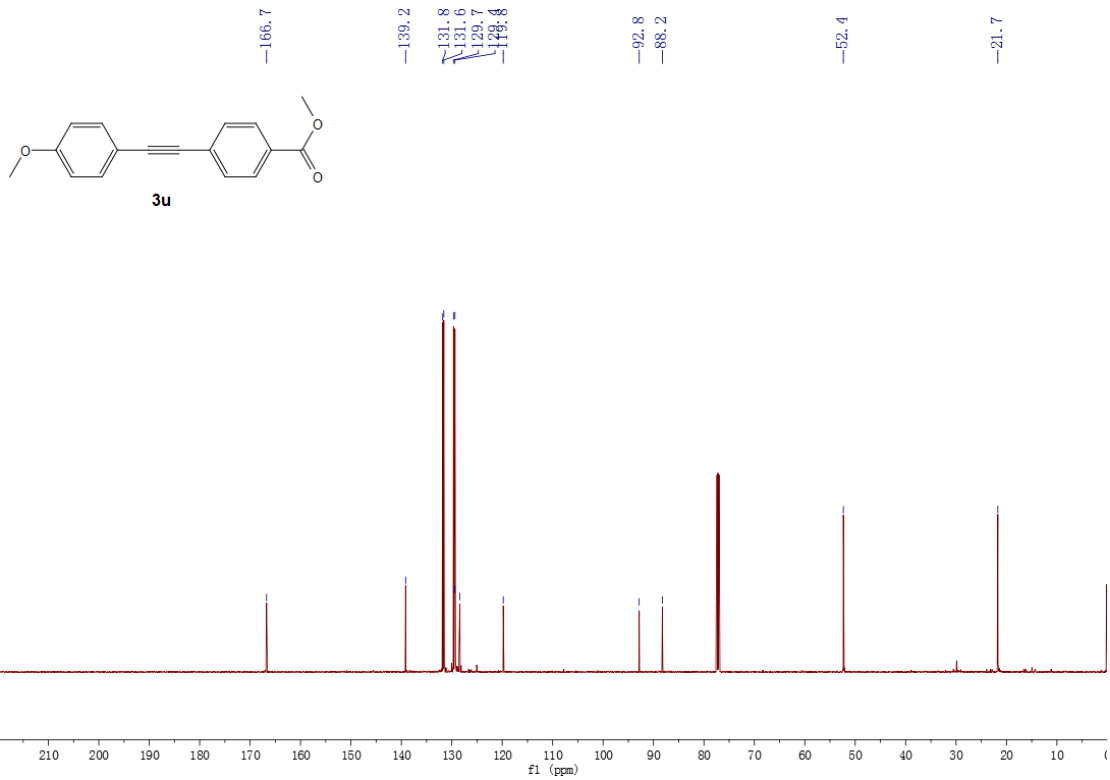
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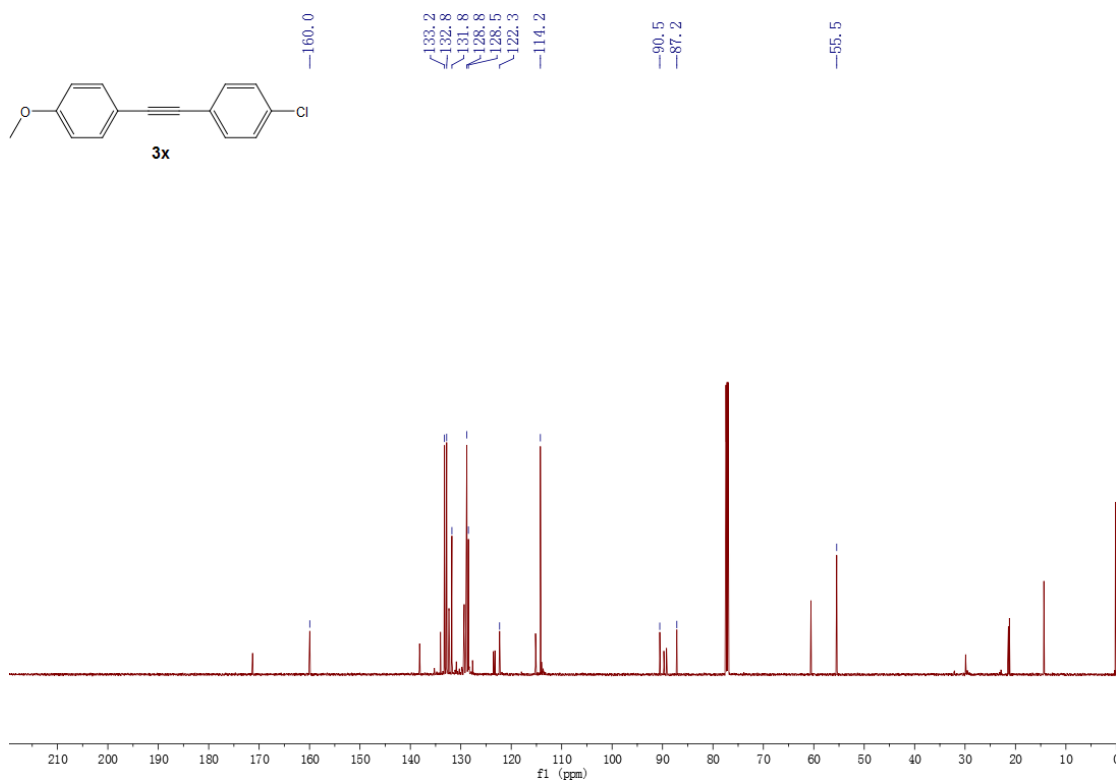
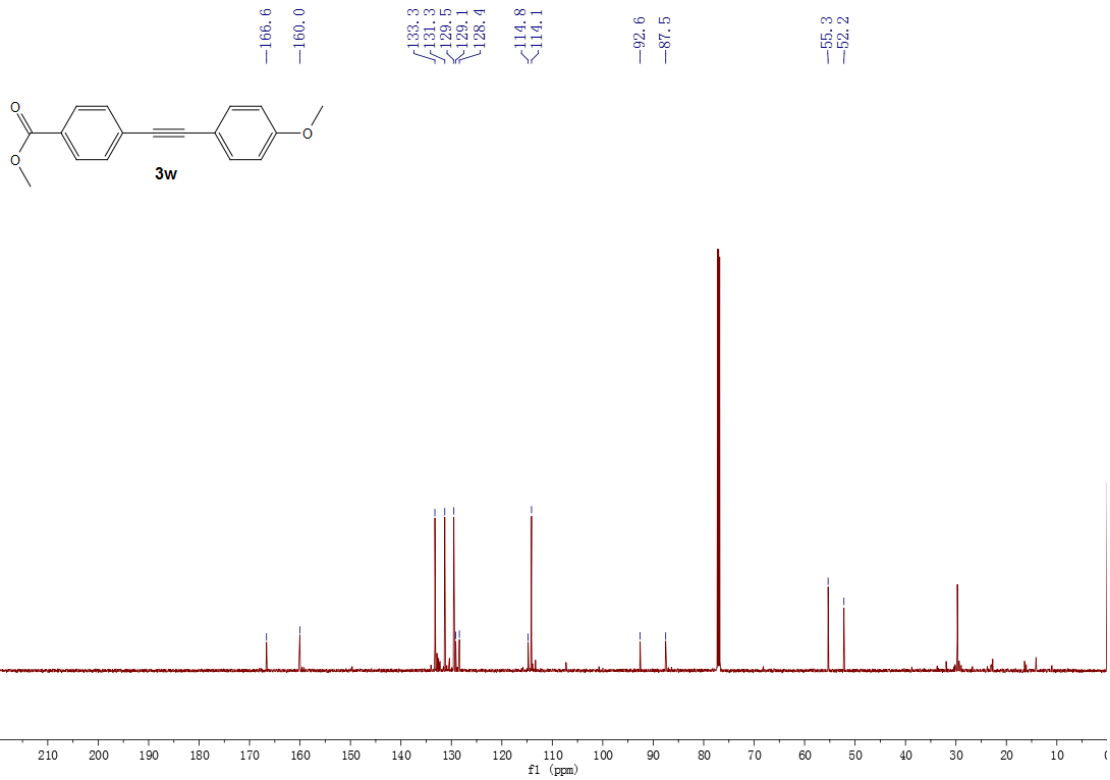


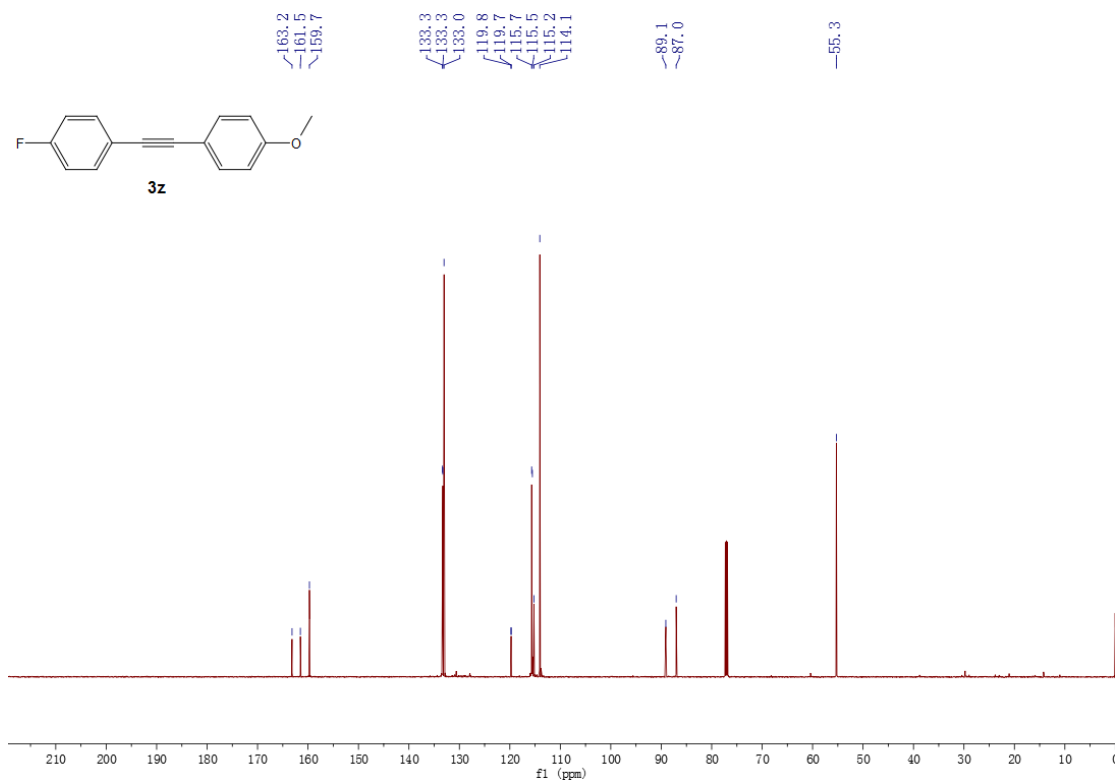
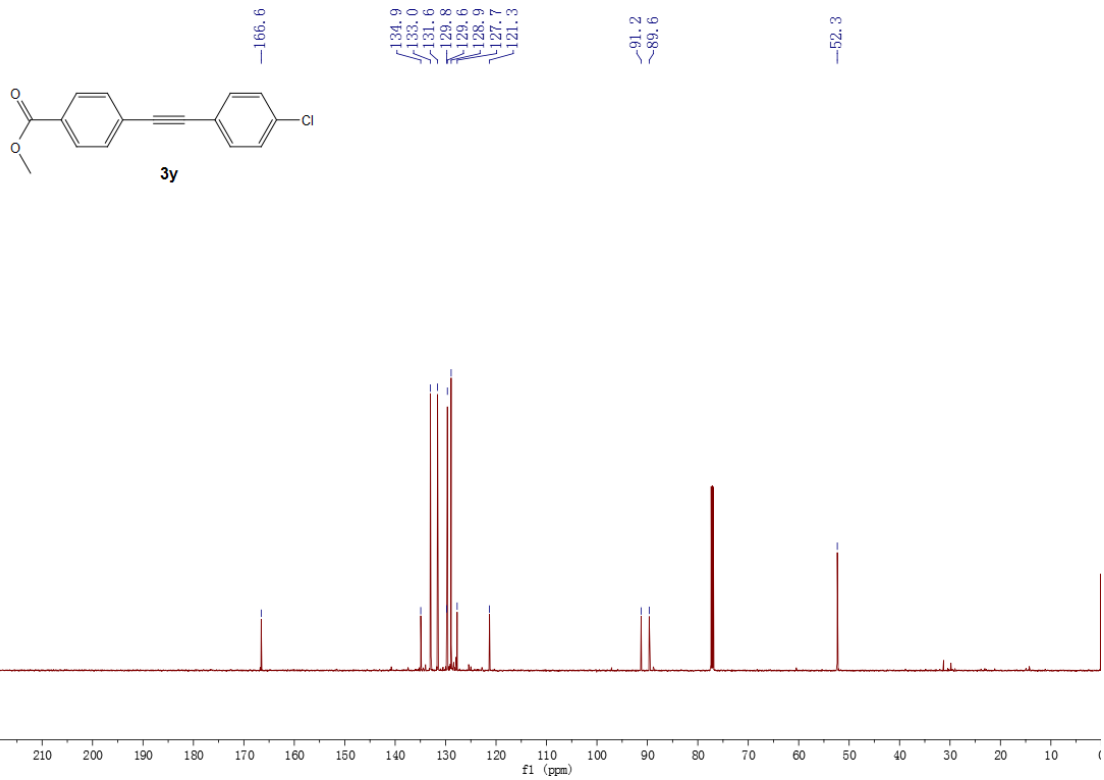
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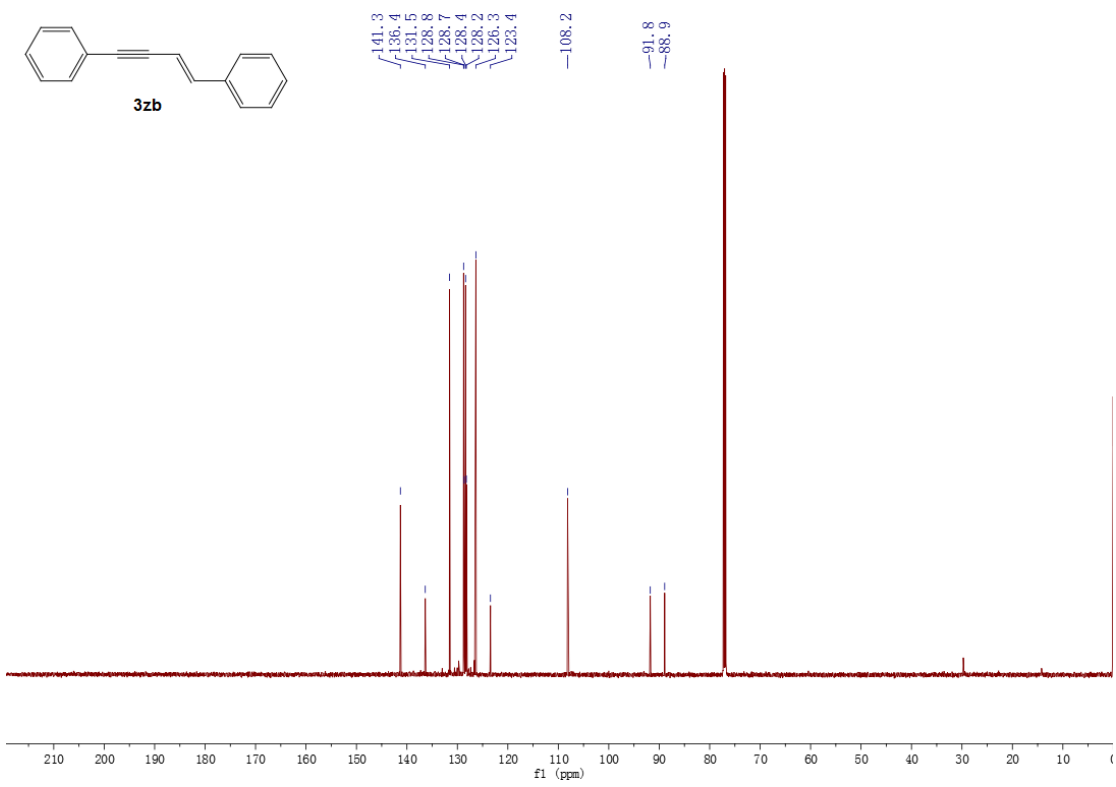
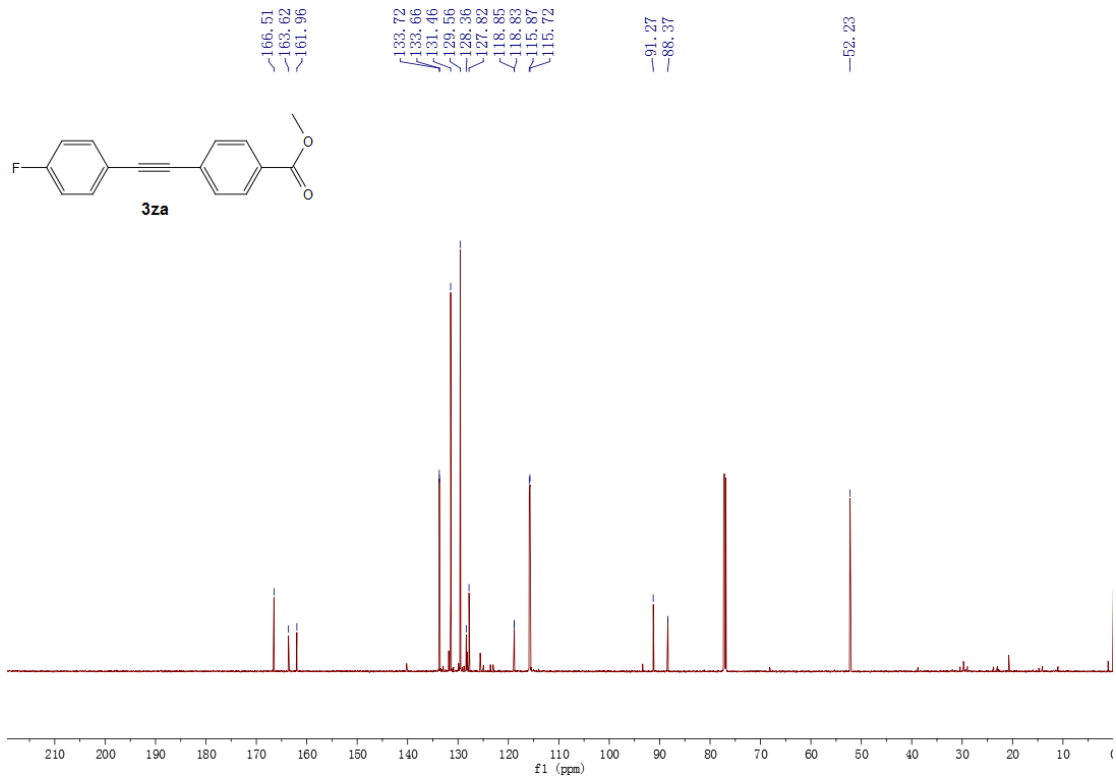


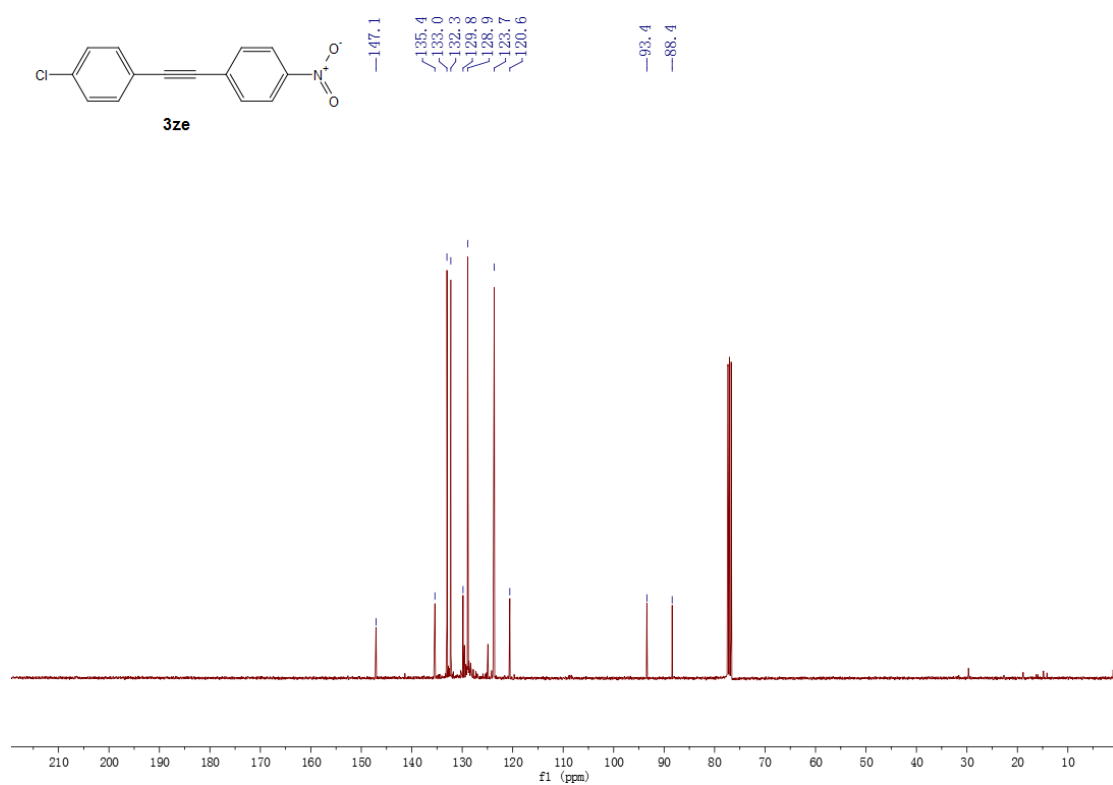
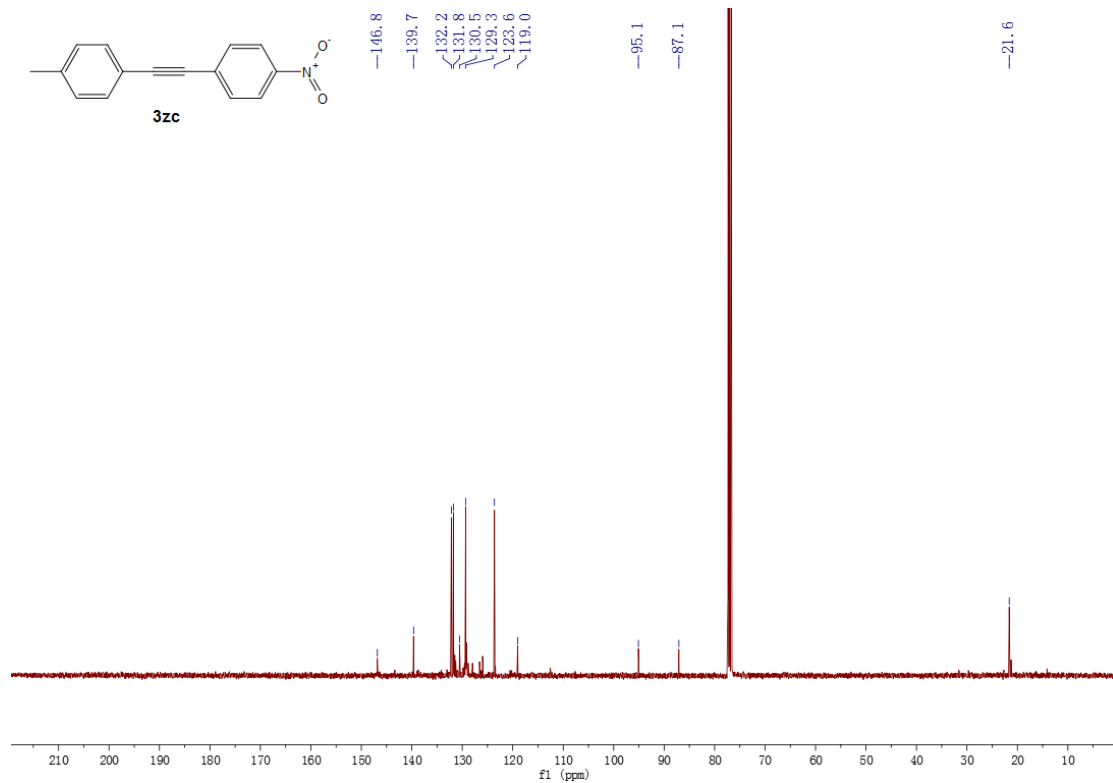












Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions

3 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

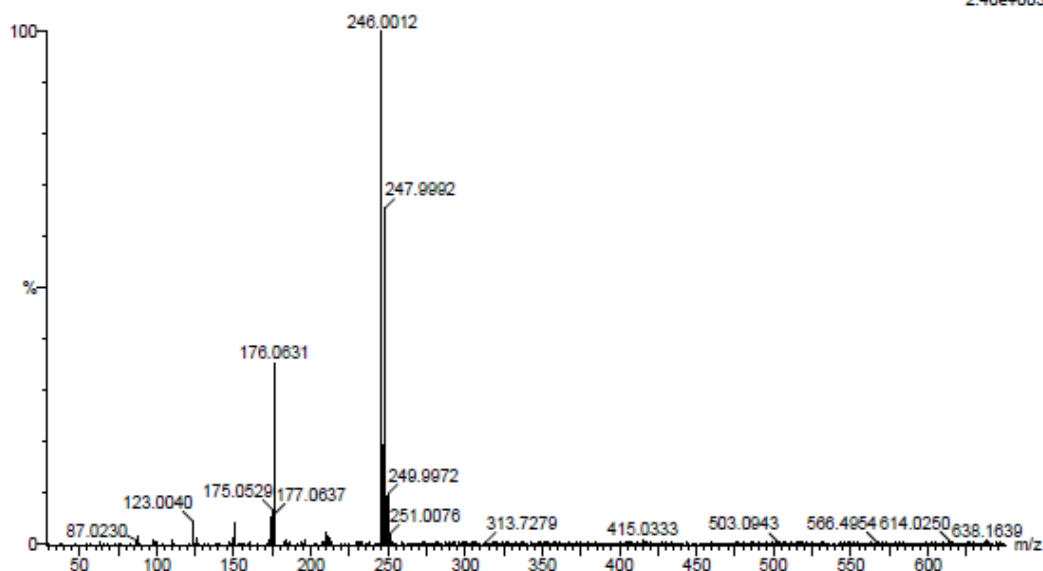
Elements Used:

C: 0-17 H: 0-12 Cl: 0-3

default file

HR-XC-A 1839 (12.317) Cm (1837:1839-(1822:1829+1861:1866))

TOF MS EI+
2.40e+003



Minimum:

Maximum: 5.0 10.0 -1.5

50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
246.0012	246.0003	0.9	3.7	10.0	6.8	C14 H8 C12

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions

21 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

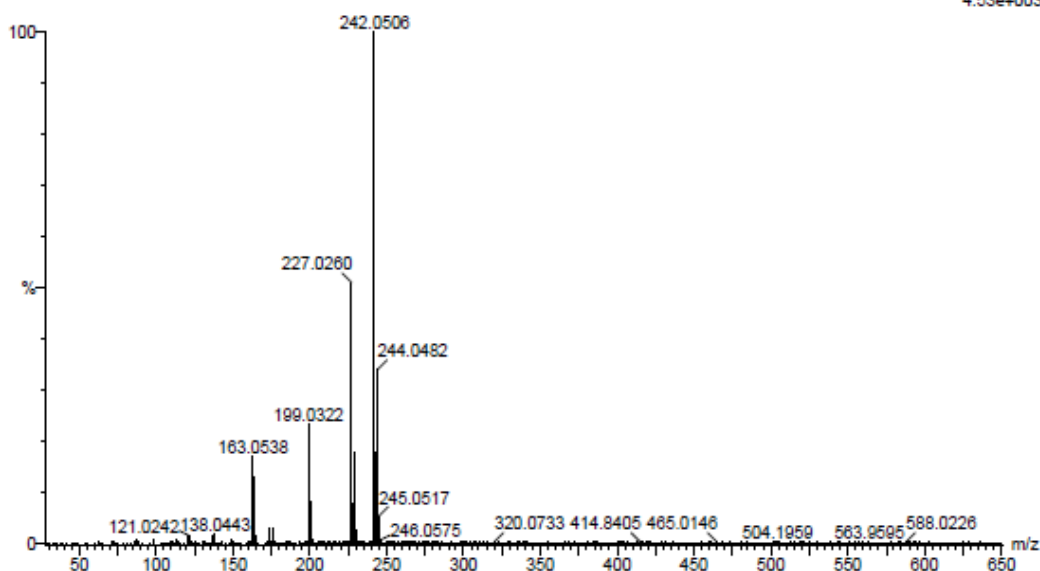
Elements Used:

C: 0-18 H: 0-15 O: 0-3 Cl: 0-3

default file

HR-XC-B1 1938 (12.816) Cm (1938:1944-(1948:1957+1923:1929))

TOF MS EI+
4.53e+003



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
242.0506	242.0498	0.8	3.3	10.0	1.2	C15 H11 O Cl

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions

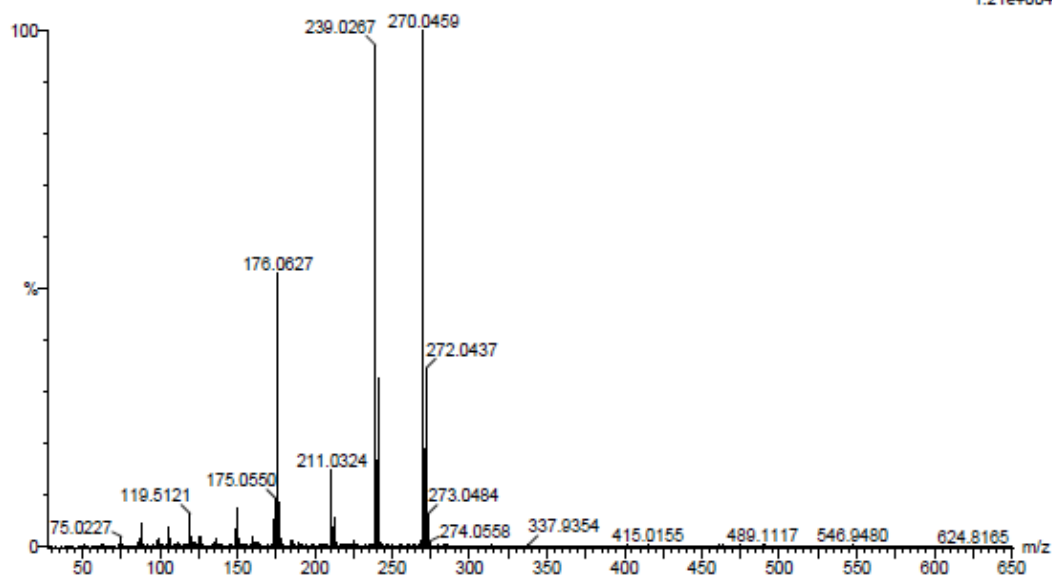
17 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-18 H: 0-15 O: 0-3 Cl: 0-3

default file

HR-XC-3 2087 (13.566) Cm (2087:2096-(2124:2130+2062:2071))

TOF MS EI+
1.21e+004

Minimum:

Maximum: 5.0 10.0 -1.5

Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
270.0459	270.0448	1.1	4.1	11.0	2.8	C16 H11 O2 Cl

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions

8 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

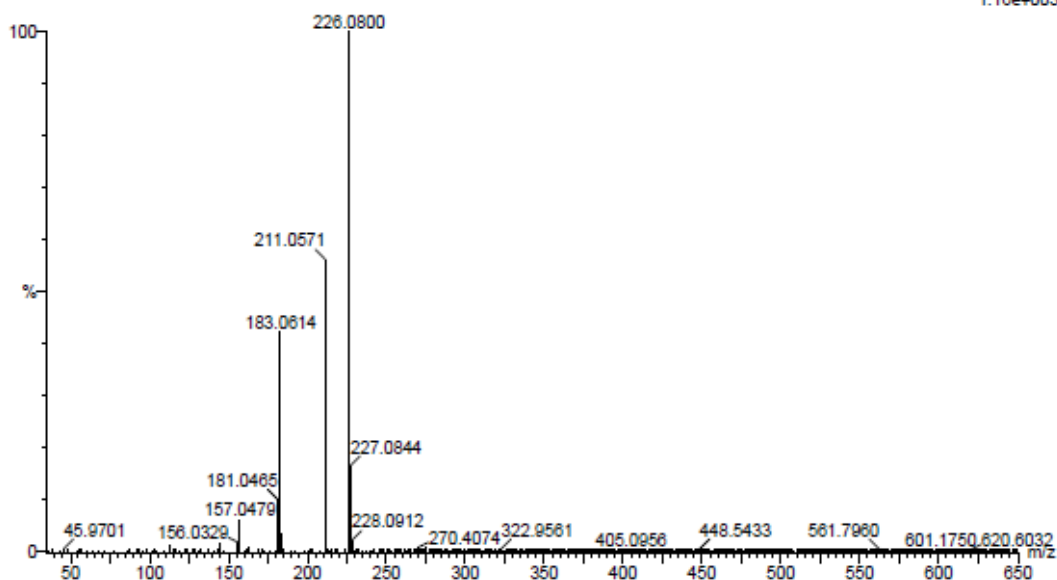
Elements Used:

C: 0-17 H: 0-12 O: 0-3 F: 0-1

default file

HR-XC-A 1722 (11.728) Cm (1722:1726-(1728:1737+1701:1711))

TOF MS EI+
1.16e+003



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
226.0800	226.0794	0.6	2.7	10.0	0.8	C15 H11 O F

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
 Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions

8 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

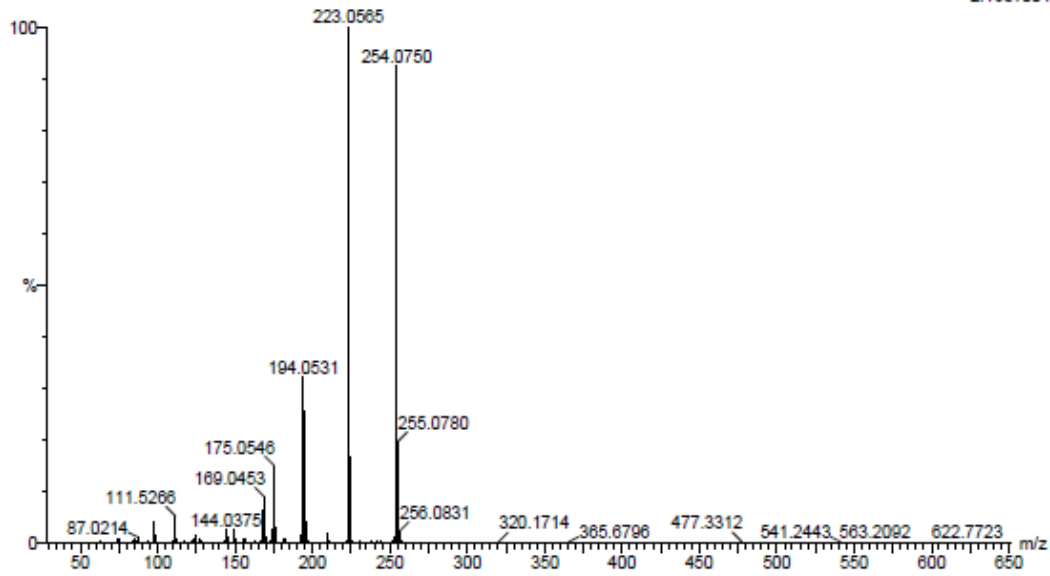
Elements Used:

C: 0-18 H: 0-15 O: 0-3 F: 0-1

default file

HR-XC-B1 1876 (12.504) Cm (1873:1881-(1856:1867+1896:1908))

TOF MS EI+
 2.16e+04



Minimum: -1.5
 Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
254.0750	254.0743	0.7	2.8	11.0	39.7	C16 H11 O2 F