Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Palladium-catalyzed Allylic Allenylation of Homoallyl Alcohols with Propargylic Carbonates

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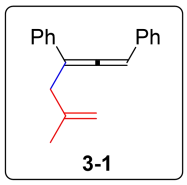
1. General remarks

The desired product was purified by flash column chromatography, silica gel (200~300 mesh). ^{1}H NMR spectra and ^{13}C NMR spectra were recorded on 400 MHz in $CDCl_3$ and TMS as internal standard. All products were further characterized by HRMS (high resolution mass spectra). Copies of their ^{1}H NMR and ^{13}C NMR spectra are provided. For propargylic carbonates[1] and homoallyl alcohols[2] was prepared based on reported procedures. All reactions were heated by oil bath. All solvents were dried and distilled according to standard procedures. Commercially available reagents and solvents were used without further purification.

2. General procedure for the preparation of the products 3

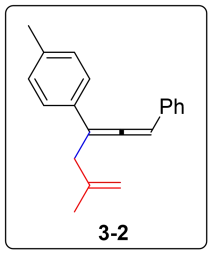
An oven-dried Schlenk tube under a nitrogen atmosphere was charged propargylic carbonates **1** (0.3 mmol, 1.0 equiv), homoallyl alcohols **2** (0.6 mmol, 2.0 equiv), $Pd(OAc)_2$ (5 mol %), $P[3,5\text{-}(CF_3)_2C_6H_3)]_3$ (10 mol%), Cs_2CO_3 (0.6 mmol, 2.0 equiv), solvent (2.0 mL). The mixture was stirred at 35 °C for 30 mins and then stirred at 90 °C for 20 h. The resulting mixture was cooled to room temperature and filtered through Celite eluting with EtOAc. The volatiles were evaporated under reduced pressure and the residue was purified by silica gel flash chromatography to afford the desired products **3**.

3. Spectral data of compound 3



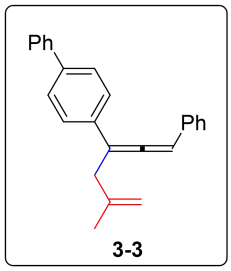
3-1

(5-Methylhexa-1,2,5-triene-1,3-diyl)dibenzene: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.39-7.36(m, 2H), 7.28-7.20(m, 6H), 7.14-7.10(m, 2H), 6.44(t, *J*=2.0Hz, 1H), 4.81(d, *J*=19.6Hz, 2H), 3.27-3.18(m, 2H), 1.72(s, 3H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 207.5, 142.8, 135.7, 134.3, 128.7, 128.4, 127.1, 127.0, 126.9, 126.3, 112.7, 107.3, 97.1, 39.5, 22.5; HRMS(APCI) m/z: $[M+H]^+$ calcd for $C_{19}H_{19}$ 247.1481; found 247.1487.



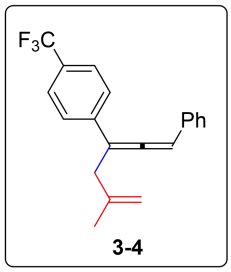
3-2

1-Methyl-4-(5-methyl-1-phenylhexa-1,2,5-trien-3-yl)benzene: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.27-7.20(m, 6H), 7.13-7.09(m, 1H), 7.02(d, *J*=8.0Hz, 2H), 6.42(s, 1H), 4.79(d, *J*=20.0Hz, 2H), 3.25-3.16(m, 2H), 2.23(s, 3H), 1.71(s, 3H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 207.2, 142.9, 136.8, 134.5, 132.7, 129.1, 128.7, 127.0, 126.9, 126.2, 112.6, 107.1, 97.0, 39.5, 22.5, 21.1; HRMS(APCI) m/z: $[M+H]^+$ calcd for $C_{20}H_{21}$ 261.1638; found 261.1634.



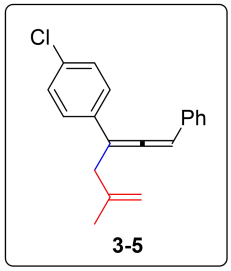
3-3

4-(5-Methyl-1-phenylhexa-1,2,5-trien-3-yl)-1,1'-biphenyl: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.59-7.56(m, 2H), 7.53-7.51(m, 4H), 7.41(t, *J*=7.6Hz, 2H), 7.38-7.35(m, 2H), 7.33-7.29(m, 3H), 7.23-7.19(m, 1H), 6.56-6.55(m, 1H), 4.92(d, *J*=22.4Hz, 2H), 3.38-3.29(m, 2H), 1.83(s, 3H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 207.7, 142.8, 140.7, 139.8, 134.7, 134.2, 128.8, 128.7, 127.2, 127.1, 126.9, 126.7, 112.7, 107.0, 97.2, 39.5, 22.6; HRMS(APCI) m/z: $[M+H]^+$ calcd for $C_{25}H_{23}$ 323.1794; found 323.1797.



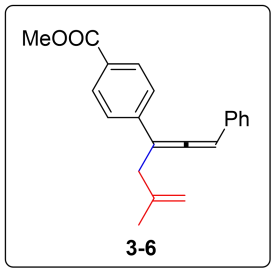
3-4

1-(5-Methyl-1-phenylhexa-1,2,5-trien-3-yl)-4-(trifluoromethyl)benzene: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.54(s, 4H), 7.34-7.30(m, 4H), 7.26-7.23(m, 1H), 6.58(s, 1H), 4.89(d, *J*=7.6Hz, 2H), 3.36-3.27(m, 2H), 1.81(s, 3H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 208.1, 142.3, 139.6, 133.6, 129.0, 128.8, 128.7, 127.4, 127.0, 126.4, 125.2(m), 113.0, 106.5, 97.6, 39.4, 22.5; HRMS(APCI) m/z: $[M+H]^+$ calcd for $C_{20}H_{18}F_3$ 315.1355; found 315.1352.



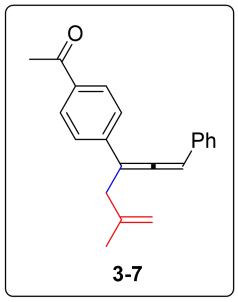
3-5

1-Chloro-4-(5-methyl-1-phenylhexa-1,2,5-trien-3-yl)benzene: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.38-7.36(m, 2H), 7.33-7.29(m, 4H), 7.26-7.22(m, 3H), 6.53-6.52(m, 1H), 4.88(d, *J*=9.6Hz, 2H), 3.32-3.23(m, 2H), 1.79(s, 3H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 207.4, 142.5, 134.2, 133.9, 132.7, 128.8, 128.5, 127.5, 127.3, 126.9, 112.9, 106.5, 97.4, 39.5, 22.5; HRMS(APCI) m/z: $[M+H]^+$ calcd for $C_{19}H_{18}Cl$ 281.1092; found 281.1090.



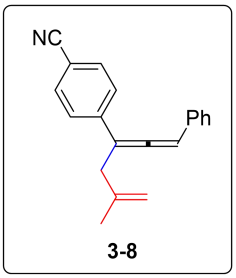
3-6

Methyl 4-(5-methyl-1-phenylhexa-1,2,5-trien-3-yl)benzoate: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.96(dd, *J*=2.0Hz, 6.8Hz, 2H), 7.50(d, *J*=8.4Hz, 2H), 7.35-7.30(m, 4H), 7.25-7.23(m, 1H), 6.58(t, *J*=2.0Hz, 1H), 4.88(d, *J*=10.0Hz, 2H), 3.89(s, 3H), 3.36-3.27(m, 2H), 1.80(s, 3H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 208.4, 166.9, 142.4, 140.6, 133.6, 129.7, 128.8, 128.5, 127.4, 127.0, 126.1, 112.9, 106.9, 97.5, 52.0, 39.3, 22.5; HRMS(APCI) m/z: $[M+H]^+$ calcd for $C_{21}H_{21}O_2$ 305.1536; found 305.1530.



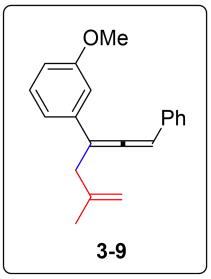
3-7

1-(4-(5-Methyl-1-phenylhexa-1,2,5-trien-3-yl)phenyl)ethan-1-one: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.90-7.88(m, 2H), 7.53(dd, *J*=1.6Hz, 6.8Hz, 2H), 7.35-7.30(m, 4H), 7.26-7.22(m, 1H), 6.59-6.58(m, 1H), 4.89(d, *J*=8.8Hz, 2H), 3.37-3.28(m, 2H), 2.57(s, 3H), 1.81(s, 3H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 208.6, 197.5, 142.4, 140.8, 135.5, 133.5, 128.8, 128.5, 127.4, 127.0, 126.3, 112.9, 106.9, 97.5, 39.3, 26.5, 22.5; HRMS(APCI) m/z: $[M+H]^+$ calcd for $C_{21}H_{21}O$ 289.1587; found 289.1586.



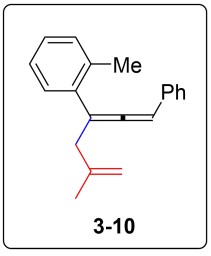
3-8

4-(5-Methyl-1-phenylhexa-1,2,5-trien-3-yl)benzonitrile: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.51-7-44(m, 4H), 7.28-7.24(m, 4H), 7.19-7.16(m, 1H), 6.54-6.53(m, 1H), 4.81(d, *J*=0.8Hz, 2H), 3.27-3.18(m, 2H), 1.73(s, 3H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 208.6, 142.1, 140.8, 133.1, 132.2, 128.9, 127.6, 127.0, 126.8, 119.0, 113.1, 110.2, 106.5, 97.9, 39.2, 22.5; HRMS(ESI) m/z: $[M+Na]^+$ calcd for $C_{20}H_{17}NNa$ 294.1253; found 294.1251.



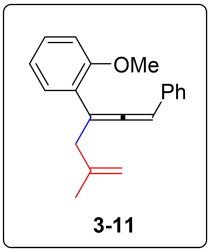
3-9

1-Methoxy-3-(5-methyl-1-phenylhexa-1,2,5-trien-3-yl)benzene: ^{1}H NMR(400MHz, $CDCl_3$) δ: 7.28-7.23(m, 4H), 7.18-7.13(m, 2H), 6.99(d, *J*=7.6Hz, 1H), 6.95-6.94(m, 1H), 6.69(dd, *J*=2.4Hz, 8.0Hz, 1H), 6.45-6.44(m, 1H), 4.82(d, *J*=19.2Hz, 2H), 3.70(s, 3H), 3.27-3.18(m, 2H), 1.73(s, 3H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 207.5, 159.7, 142.9, 137.3, 134.2, 129.3, 128.7, 127.1, 126.9, 118.9, 112.7, 112.2, 112.1, 107.2, 97.1, 55.2, 39.6, 22.5; HRMS(APCI) m/z: $[M+H]^+$ calcd for $C_{20}H_{21}O$ 277.1587; found 277.1584.



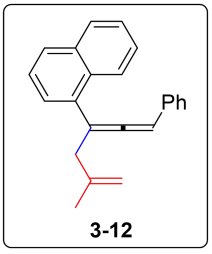
3-10

1-Methyl-2-(5-methyl-1-phenylhexa-1,2,5-trien-3-yl)benzene: ^{1}H NMR(400MHz, $CDCl_3$) δ: 7.26-7.20(m, 5H), 7.13-7.07(m, 4H), 6.20-6.18(m, 1H), 4.71-4.70(m, 2H), 3.19-3.07(m, 2H), 2.31(s, 3H), 1.72(s, 3H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 205.2, 142.6, 136.6, 136.0, 134.7, 130.6, 128.5, 128.0, 127.0, 126.9, 126.8, 125.7, 113.0, 106.4, 94.8, 43.2, 22.3, 20.8; HRMS(APCI) m/z: $[M+H]^+$ calcd for $C_{20}H_{21}$ 261.1638; found 261.1641.



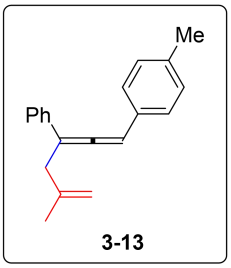
3-11

1-Methoxy-2-(5-methyl-1-phenylhexa-1,2,5-trien-3-yl)benzene: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.42-7.39(m, 2H), 7.32-7.27(m, 3H), 7.23-7.18(m, 2H), 6.92-6.86(m, 2H), 6.26(t, *J*=2.4Hz, 1H), 4.76(d, *J*=15.2Hz, 2H), 3.78(s, 3H), 3.36-3.21(m, 2H), 1.77(s, 3H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 207.0, 156.8, 143.2, 135.1, 129.5, 128.5, 128.4, 126.9, 126.6, 126.0, 120.5, 112.4, 111.1, 104.7, 93.9, 55.5, 41.9, 22.3; HRMS(APCI) m/z: $[M+H]^+$ calcd for $C_{20}H_{21}O$ 277.1587; found 277.1584.



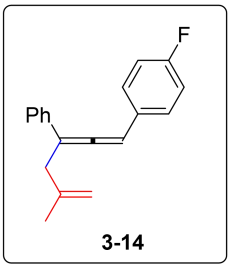
3-12

1-(5-Methyl-1-phenylhexa-1,2,5-trien-3-yl)naphthalene: ^{1}H NMR(400MHz, $CDCl_3$) δ: 7.83(s, 1H), 7.80-7.75(m, 2H), 7.71(d, *J*=8.4Hz, 1H), 7.63-7.60(m, 1H), 7.44-7.41(m, 2H), 7.39-7.37(m ,2H), 7.33-7.30(m, 2H), 7.24-7.20(m, 1H), 6.60-6.59(m, 1H), 4.93(d, *J*=33.2Hz, 2H), 3.47-3.38(m, 2H), 1.84(s, 3H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 208.1, 142.8, 134.2, 133.5, 133.0, 132.5, 128.7, 128.1, 127.9, 127.5, 127.1, 127.0, 126.1, 125.8, 125.3, 124.2, 112.8, 107.6, 97.4, 39.5, 22.6; HRMS(APCI) m/z: $[M+H]^+$ calcd for $C_{23}H_{21}$ 297.1638; found 297.1635.



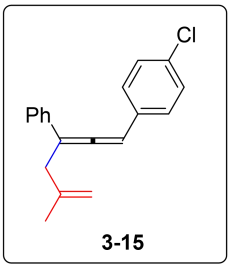
3-13

1-Methyl-4-(5-methyl-3-phenylhexa-1,2,5-trien-1-yl)benzene: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.46-7.44(m, 2H), 7.31-7.19(m, 5H), 7.11(d, *J*=7.6Hz, 2H), 6.51-6.49(m, 1H), 4.88(d, *J*=19.6Hz, 2H), 3.34-3.25(m, 2H), 2.32(s, 3H), 1.80(s, 3H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 207.2, 142.9, 136.9, 135.9, 131.2, 129.4, 128.4, 126.9, 126.8, 126.2, 112.6, 107.1, 96.9, 39.5, 22.5, 21.2; HRMS(APCI) m/z: $[M+H]^+$ calcd for $C_{20}H_{21}$ 261.1638; found 261.1640.



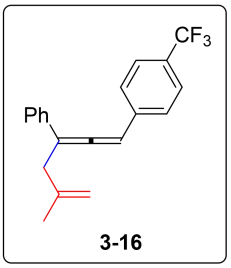
3-14

1-Fluoro-4-(5-methyl-3-phenylhexa-1,2,5-trien-1-yl)benzene: ^{1}H NMR(400MHz, $CDCl_3$) δ: 7.45-7.43(m, 2H), 7.33-7.28(m, 4H), 7.24-7.22(m, 1H), 7.02-6.97(m, 2H), 6.50-6.49(m, 1H), 4.88(d, *J*=14.0Hz, 2H), 3.34-3.25(m, 2H), 1.80(s, 3H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 207.2(d, *J*=2.0Hz), 161.9(d, *J*=245Hz), 142.8, 135.6, 130.3(d, *J*=3.0Hz), 128.4, 128.3(d, *J*=8.0Hz), 127.1, 126.2, 115.6(d, *J*=22.0Hz), 112.7, 107.6, 96.2, 39.5, 22.5; HRMS(APCI) m/z: $[M+H]^+$ calcd for $C_{19}H_{18}F$ 265.1387; found 265.1384.



3-15

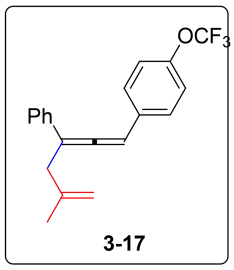
1-Chloro-4-(5-methyl-3-phenylhexa-1,2,5-trien-1-yl)benzene: ^{1}H NMR(400MHz, $CDCl_3$) δ: 7.45-7.42(m, 2H), 7.32-7.29(m, 2H), 7.26(s, 4H), 7.23-7.21(m, 1H), 6.48(t, *J*=2.4Hz, 1H), 4.88(d, *J*=13.2Hz, 2H), 3.34-3.25(m, 2H), 1.79(s, 3H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 207.5, 142.7, 135.4, 132.8, 132.6, 128.8, 128.5, 128.0, 127.2, 126.2, 112.8, 107.8, 96.3, 39.4, 22.5; HRMS(APCI) m/z: $[M+H]^+$ calcd for $C_{19}H_{18}Cl$ 281.1092; found 281.1091.



3-16

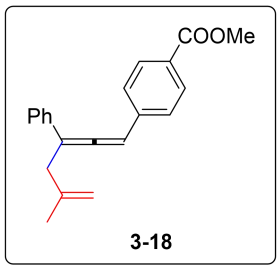
1-(5-Methyl-3-phenylhexa-1,2,5-trien-1-yl)-4-(trifluoromethyl)benzene: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.55(d, *J*=8.0Hz, 2H), 7.45-7.42(m, 4H), 7.34-7.30(m, 2H), 7.25-7.21(m, 1H), 6.55-6.54(m, 1H), 4.89(d, *J*=13.2Hz, 2H), 3.36-3.27(m, 2H), 1.80(s, 3H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 208.4, 142.5, 138.3, 135.1, 128.9(d, *J*=32.0Hz), 128.5, 127.4, 126.9, 126.3, 125.6(m), 122.9, 112.9, 108.1, 96.4, 39.3, 22.5; HRMS(APCI) m/z: $[M+H]^+$ calcd for $C_{20}H_{18}F_3$ 315.1355;

found 315.1358.



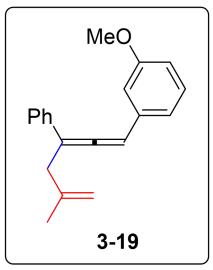
3-17

1-(5-Methyl-3-phenylhexa-1,2,5-trien-1-yl)-4-(trifluoromethoxy)benzene: ^{1}H NMR(400MHz, $CDCl_3$) δ: 7.37-7.35(m, 2H), 7.27-7.21(m, 4H), 7.15-7.14(m, 1H), 7.06(d, *J*=8.0Hz, 2H), 6.43-6.42(m, 1H), 4.80(d, *J*=13.2Hz, 2H), 3.27-3.18(m, 2H), 1.72(s, 3H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 207.6, 148.1, 142.7, 135.3, 133.2, 128.5, 128.0, 127.3, 126.3, 121.3, 112.8, 107.9, 96.0, 39.4, 22.5; HRMS(APCI) m/z: $[M+H]^+$ calcd for $C_{20}H_{18}F_3O$ 331.1304; found 331.1305.



3-18

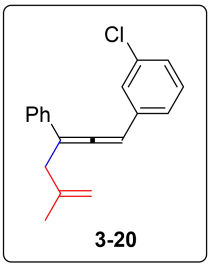
Methyl 4-(5-methyl-3-phenylhexa-1,2,5-trien-1-yl)benzoate: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.98(d, *J*=8.0Hz, 2H), 7.44(d, *J*=7.6Hz, 2H), 7.39(d, *J*=8.4Hz, 2H), 7.32(t, *J*=7.6Hz, 2H), 7.24(d, *J*=7.2Hz, 1H), 6.56(t, *J*=2.0Hz, 1H), 4.89(d, *J*=15.2Hz, 2H), 3.90(s, 3H), 3.36-3.27(m, 2H), 1.80(s, 3H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 208.7, 166.9, 142.5, 139.3, 135.1, 130.0, 128.6, 128.5, 127.3, 126.7, 126.3, 112.9, 107.9, 96.7, 52.0, 39.3, 22.5; HRMS(APCI) m/z: $[M+H]^+$ calcd for $C_{21}H_{21}O_2$ 305.1536; found 305.1524.



3-19

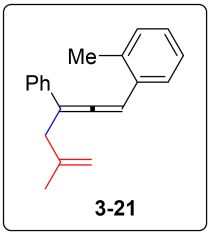
1-Methoxy-3-(5-methyl-3-phenylhexa-1,2,5-trien-1-yl)benzene: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.46-7.44(m, 2H), 7.32-7.28(m, 2H), 7.24-7.21(m, 2H), 6.94(d, *J*=7.6Hz, 1H), 6.91-6.90(m, 1H), 6.78-6.76(m, 1H), 6.50-6.49(m, 1H), 4.89(d, *J*=19.6Hz, 2H), 3.77(s, 3H), 3.35-3.26(m, 2H), 1.81(s, 3H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 207.5, 159.9, 142.9, 135.8, 135.7, 129.7, 128.4, 127.1,

126.3, 119.6, 112.9, 112.7, 111.9, 107.4, 97.1, 55.2, 39.5, 22.5; HRMS(APCI) m/z: $[M+H]^+$ calcd for $C_{20}H_{21}O$ 277.1587; found 277.1589.



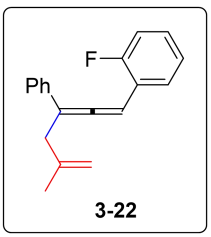
3-20

1-chloro-3-(5-methyl-3-phenylhexa-1,2,5-trien-1-yl)benzene: ^{1}H NMR(400MHz, $CDCl_3$) δ: 7.44(d, *J*=7.2Hz, 2H), 7.33-7.29(m, 3H), 7.24-7.16(m, 4H), 6.46(t, *J*=2.0Hz, 1H), 4.89(d, *J*=13.2Hz, 2H), 3.35-3.26(m, 2H), 1.80(s, 3H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 207.7, 142.6, 136.4, 135.3, 134.6, 129.9, 128.5, 127.3, 127.1, 126.7, 126.3, 125.0, 112.9, 107.9, 96.3, 39.4, 22.5; HRMS(APCI) m/z: $[M+H]^+$ calcd for $C_{19}H_{18}Cl$ 281.1092; found 281.1090.



3-21

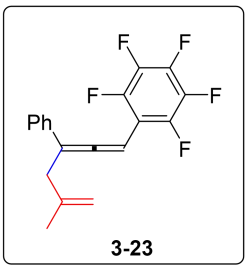
1-methyl-2-(5-methyl-3-phenylhexa-1,2,5-trien-1-yl)benzene: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.37(d, *J*=7.6Hz, 2H), 7.33-7.31(m, 1H), 7.24-7.20(m, 2H), 7.13-7.09(m, 1H), 7.06-7.02(m, 3H), 6.63(t, *J*=2.0Hz, 1H), 4.79(d, *J*=16.4Hz, 2H), 3.22(t, *J*=17.2, 2H), 2.32(s, 3H), 1.72(s, 3H); ^{13}C NMR(100MHz, CDCl3) δ: 208.0, 142.8, 135.9, 135.2, 132.5, 130.6, 128.4, 127.4, 126.9, 126.8, 126.2, 126.1, 112.6, 106.3, 94.4, 39.5, 22.5, 19.9; HRMS(APCI) m/z: $[M+H]^+$ calcd for $C_{20}H_{21}$ 261.1638; found 261.1636.



3-22

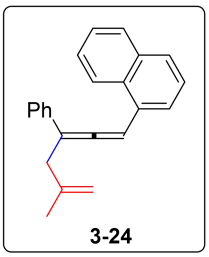
1-Fluoro-2-(5-methyl-3-phenylhexa-1,2,5-trien-1-yl)benzene: ^{1}H NMR(400MHz, $CDCl_3$) δ: 7.46-7.44(m, 2H), 7.43-7.38(m, 1H), 7.32-7.29(m, 2H), 7.23-7.13(m, 2H), 7.07-7.03(m, 2H), 6.75-6.74(m, 1H), 4.88(d, *J*=16.4Hz, 2H), 3.35-3.26(m, 2H), 1.80(s, 3H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 208.0(d, *J*=20.0Hz), 159.8(d, *J*=248.0Hz), 142.7, 135.5, 128.5, 128.4, 128.2(d,

J=4.0Hz), 127.1, 126.3, 124.1(d, *J*=40.0Hz), 121.9(d, *J*=12.0Hz), 115.7(d, *J*=22.0Hz), 112.8, 107.4, 89.6(d, *J*=7.0Hz), 39.4, 22.5; HRMS(APCI) m/z: $[M+H]^+$ calcd for $C_{19}H_{18}F$ 265.1387; found 265.1388.



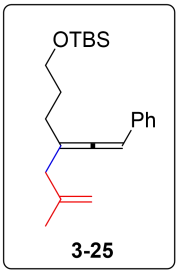
3-23

1,2,3,4,5-Pentafluoro-6-(5-methyl-3-phenylhexa-1,2,5-trien-1-yl)benzene: ^1H NMR(400MHz, $CDCl_3$) δ: 7.44-7.41(m, 2H), 7.35-7.31(m, 2H), 7.26-7.22(m, 1H), 6.53(s, 1H), 4.86(s, 2H), 3.33-3.24(m, 2H), 1.78(s, 3H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 210.2(d, *J*=2.0Hz), 144.12(dm, *J*=250.0Hz), 142.1, 139.72(dm, *J*=252.0Hz), 137.7(dm, *J*=249.0Hz), 134.8, 128.5, 127.5, 126.6, 113.1, 109.72(m), 106.9, 81.8(d, *J*=3.0Hz), 39.4, 22.3; HRMS(APCI) m/z: $[M+H]^+$ calcd for $C_{19}H_{14}F_5$ 337.1010; found 337.1012.



3-24

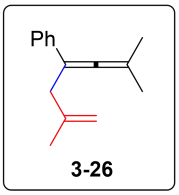
1-(5-Methyl-3-phenylhexa-1,2,5-trien-1-yl)naphthalene: ^1H NMR(400MHz, $CDCl_3$) δ: 7.69-7.63(m, 4H), 7.44-7.40(m, 3H), 7.34(t, *J*=6.8Hz, 2H), 7.23(t, *J*=7.6Hz, 2H), 7.15-7.12(m, 1H), 6.61(s, 1H), 4.82(d, *J*=24.4Hz, 2H), 3.30-3.22(m, 2H), 1.74(s, 3H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 208.0, 142.8, 135.7, 133.7, 132.7, 131.8, 128.5, 128.3, 127.7, 127.1, 126.3, 126.2, 125.7, 125.6, 124.7, 112.8, 107.5, 97.5, 39.5, 22.6; HRMS(APCI) m/z: $[M+H]^+$ calcd for $C_{23}H_{21}$ 297.1638; found 297.1640.



3-25

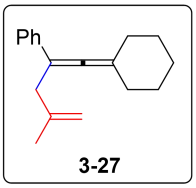
Tert-butyldimethyl((6-methyl-4-(2-phenylvinylidene)hept-6-en-1-yl)oxy)silane: ^1H NMR

(400MHz, $CDCl_3$) δ: 7.28-7.27(m, 4H), 7.19-7.15(m, 1H), 6.13(t, *J*=2.4Hz, 1H), 4.81(s, 2H), 3.62(t, *J*=6.4Hz, 2H), 2.83(s, 2H), 2.17-2.07(m, 2H), 1.75(s, 3H), 1.71-1.67(m, 2H), 0.87(s, 9H), 0.01(s, 6H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 202.9, 142.9, 135.7, 128.5, 126.5, 126.4, 112.5, 105.8, 95.0, 62.7, 42.6, 30.8, 27.9, 25.9, 22.0, 18.3, -5.3; HRMS(APCI) m/z: $[M+H]^+$ calcd for $C_{22}H_{35}OSi$ 343.2452; found 343.2458.



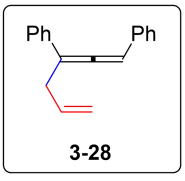
3-26

(2,6-Dimethylhepta-1,4,5-trien-4-yl)benzene: ^1H NMR (400MHz, $CDCl_3$) δ: 7.36(dd, *J*=1.2Hz, 8.4Hz, 2H), 7.29-7.25(m, 2H), 7.17-7.12(m, 1H), 4.82(dd, *J*=0.8Hz, 9.6Hz, 2H), 3.12(s, 2H), 1.80(s, 6H), 1.77(s, 3H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 203.0, 143.7, 138.0, 131.6, 128.1, 126.1, 111.8, 100.8, 97.4, 39.8, 22.3, 20.2.



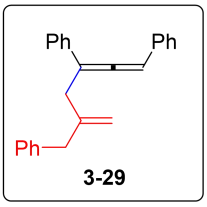
3-27

(1-Cyclohexylidene-4-methylpenta-1,4-dien-2-yl)benzene: ^1H NMR(400MHz, $CDCl_3$) δ: 7.33-7.31(m, 2H), 7.23-7.18(m, 2H), 7.08(t, *J*=7.2Hz, 1H), 4.75(d, *J*=6.4Hz, 2H), 3.06(s, 2H), 2.16-2.10(m, 4H), 1.70(s, 3H), 1.61-1.56(m, 4H), 1.53-1.48(m, 2H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 199.3, 143.7, 138.1, 128.1, 126.0, 111.9, 105.0, 100.7, 39.9, 31.4, 27.8, 26.2, 22.3; HRMS(APCI) m/z: $[M+H]^+$ calcd for $C_{18}H_{23}$ 239.1794; found 239.1790.



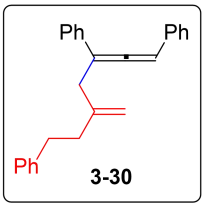
3-28

Hexa-1,2,5-triene-1,3-diyldibenzene: ^1H NMR (400MHz, $CDCl_3$) δ: 7.46-7.44(m, 2H), 7.33-7.28(m, 6H), 7.23-7.19(m, 2H), 6.54(t, *J*=2.8Hz, 1H), 6.04-5.94(m, 1H), 5.20(dd, *J*=1.6Hz, 16.8Hz, 1H), 5.09-5.06(m, 1H), 3.36-3.33(m, 2H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 206.9, 135.6, 135.5, 134.3, 128.7, 128.5, 127.1, 126.8, 126.1, 116.5, 108.2, 98.0, 34.8; HRMS(APCI) m/z: $[M+H]^+$ calcd for $C_{18}H_{17}$ 233.1325; found 233.1324.



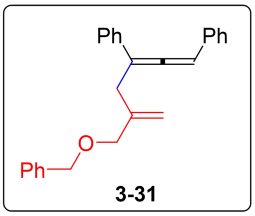
3-29

(5-Methylenehexa-1,2-diene-1,3,6-triyl)tribenzene: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.38-7.33(m, 4H), 7.31-7.23(m, 6H), 7.21-7.14(m, 5H), 6.52-6.51(m, 1H), 5.03(s, 1H), 4.86(s, 1H), 3.41(s, 2H), 3.25(s, 2H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 207.6, 145.9, 139.3, 135.6, 134.2, 129.1, 128.7, 128.4, 128.3, 127.1, 127.0, 126.9, 126.2, 126.1, 113.9, 107.3, 97.4, 42.8, 37.0; HRMS(APCI) m/z: $[M+H]^+$ calcd for $C_{25}H_{33}$ 323.1794; found 323.1792.



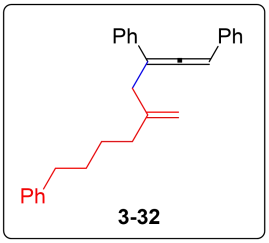
3-30

(5-Methylenehepta-1,2-diene-1,3,7-triyl)tribenzene: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.45-7.43(m, 2H), 7.32-7.20(m, 11H), 7.10-7.08(m, 2H), 6.53-6.52(m, 1H), 4.95(d, *J*=30.0Hz, 2H), 3.40-3.31(m, 2H), 2.79-2.74(m, 2H), 2.43-2.39(m, 2H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 207.5, 146.1, 141.9, 135.6, 134.2, 128.7, 128.4, 128.3, 128.2, 127.1, 127.0, 126.9, 126.3, 125.7, 112.2, 107.3, 97.2, 38.3, 37.4, 34.1; HRMS(APCI) m/z: $[M+H]^+$ calcd for $C_{26}H_{25}$ 337.1951; found 337.1952.



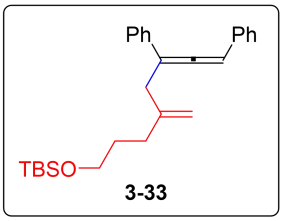
3-31

(5-((Benzyloxy)methyl)hexa-1,2,5-triene-1,3-diyl)dibenzene: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.39-7.36(m, 2H), 7.25-7.18(m, 11H), 7.14-7.10(m, 2H), 6.42-6.41(m, 1H), 5.08(d, *J*=16.8Hz, 2H), 4.37(dd, *J*=12.0Hz, 14.8Hz, 2H), 3.95(t, *J*=13.6Hz, 2H), 3.37-3.27(m, 2H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 207.4, 143.0, 138.3, 135.5, 134.1, 128.7, 128.4, 128.3, 127.6, 127.5, 127.1, 127.0, 126.9, 126.2, 114.5, 107.1, 97.5, 72.8, 72.0, 34.6; HRMS(APCI) m/z: $[M+H]^+$ calcd for $C_{26}H_{25}O$ 353.1900; found 353.1895.



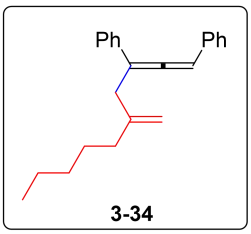
3-32

(5-Methylenenona-1,2-diene-1,3,9-triyl)tribenzene: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.38-7.35(m, 2H), 7.27-7.19(m, 6H), 7.17-7.07(m, 5H), 7.04(d, *J*=8.4Hz, 2H), 6.41(s, 1H), 4.82(d, *J*=36.0Hz, 2H), 3.26-3.17(m, 2H), 2.49-2.46(m, 2H), 2.07-2.03(m, 2H), 1.52-1.41(m, 4H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 207.6, 146.5, 142.6, 135.8, 134.3, 128.7, 128.4, 128.3, 128.2, 127.1, 127.0, 126.9, 126.3, 125.6, 111.8, 107.4, 97.1, 38.0, 35.8, 35.7, 31.1, 27.2; HRMS(APCI) m/z: $[M+H]^+$ calcd for $C_{28}H_{29}$ 365.2264; found 365.2267.



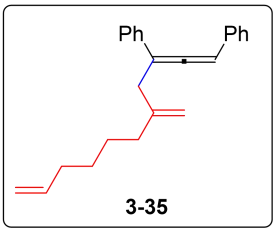
3-33

Tert-butyldimethyl((4-methylene-6,8-diphenylocta-6,7-dien-1-yl)oxy)silane: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.44(d, *J*=7.6Hz, 2H), 7.34-7.28(m, 6H), 7.22-7.20(d, *J*=7.2Hz, 2H), 6.51(s, 1H), 4.91(d, *J*=30.4Hz, 2H), 3.59-3.55(m, 2H), 3.32(t, *J*=17.2Hz, 2H), 2.17-2.13(m, 2H), 1.70-1.67(m, 2H), 0.88(s, 9H), 0.02(s, 6H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 207.6, 146.3, 135.8, 134.3, 128.7, 128.4, 127.1, 127.0, 126.9, 126.3, 111.7, 107.4, 97.1, 62.8, 38.1, 32.1, 30.9, 26.0, 18.3, -5.3; HRMS(APCI) m/z: $[M+H]^+$ calcd for $C_{27}H_{37}OSi$ 405.2608; found 405.2604.

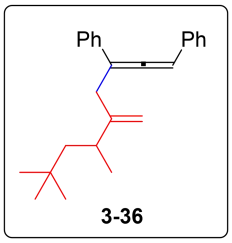


3-34

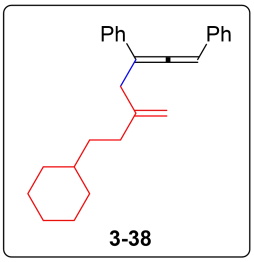
(5-Methylenedeca-1,2-diene-1,3-diyl)dibenzene: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.38-7.36(m, 2H), 7.27-7.19(m, 6H), 7.13-7.09(m, 2H), 6.43-6.42(m, 1H), 4.81(d, *J*=30.0Hz, 2H), 3.28-3.19(m, 2H), 2.01(t, *J*=7.6Hz, 2H), 1.38-1.34(m, 2H), 1.19-1.13(m, 4H), 0.77(t, *J*=6.8Hz, 3H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 207.6, 146.8, 135.7, 134.3, 128.6, 128.4, 127.1, 127.0, 126.9, 126.3, 111.5, 107.3, 97.1, 38.0, 35.9, 31.6, 27.3, 22.5, 14.1; HRMS(APCI) m/z: $[M+H]^+$ calcd for $C_{23}H_{27}$ 303.2107; found 303.2111.



(5-Methyleneundeca-1,2,10-triene-1,3-diyl)dibenzene: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.44(d, *J*=7.2Hz, 2H), 7.33-7.28(m, 6H), 7.22-7.19(m, 2H), 6.51(s, 1H), 5.80-5.73(m, 1H), 4.99-4.86(m, 4H), 3.36-3.27(m, 2H), 2.12-2.09(m, 2H), 2.03-1.98(m, 2H), 1.49-1.43(m, 2H), 1.39-1.33(m, 2H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 207.6, 146.6, 138.9, 135.8, 134.3, 128.7, 128.4, 127.1, 127.0, 126.9, 126.3, 114.3, 111.7, 107.4, 97.1, 38.0, 35.7, 33.6, 28.6, 27.1; HRMS(APCI) m/z: $[M+H]^+$ calcd for $C_{24}H_{27}$ 315.2107; found 315.2106.

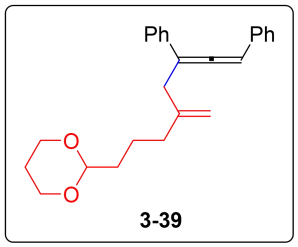


(6,8,8-Trimethyl-5-methylenenona-1,2-diene-1,3-diyl)dibenzene: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.45(d, *J*=7.6Hz, 2H), 7.35-7.28(m, 6H), 7.22-7.20(m, 2H), 6.50(s, 1H), 4.90-4.87(m, 2H), 3.37-3.26(m, 2H), 2.37-2.32(m, 1H), 1.58-1.52(m, 1H), 1.21-1.17(m, 1H), 1.08(dd, *J*=6.8Hz, 20.0Hz, 3H), 0.89-0.87(m, 9H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 207.9, 153.2, 136.0, 134.4, 128.7, 128.4, 127.0, 126.9, 126.4, 126.3, 110.1, 107.7, 97.1, 49.8, 36.4, 36.2, 36.0, 31.2, 30.0, 22.9, 22.6; HRMS(APCI) m/z: $[M+H]^+$ calcd for $C_{25}H_{31}$ 331.2420; found 331.2429.



(7-Cyclohexyl-5-methylenehepta-1,2-diene-1,3-diyl)dibenzene: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.37(d, *J*=8.0Hz, 2H), 7.27-7.19(m, 6H), 7.13-7.10(m, 2H), 6.42(s, 1H), 4.81(d, *J*=29.6Hz, 2H), 3.23(dd, *J*=16.0Hz, 21.6Hz, 2H), 2.02(dd, *J*=6.0Hz, 10.0Hz, 2H), 1.61-1.53(m, 5H), 1.28-1.22(m, 2H), 1.10-1.04(m, 4H), 0.80-0.72(m, 2H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 207.6, 147.2, 135.8, 134.4, 128.7, 128.4, 127.1, 127.0, 126.9, 126.3, 111.3, 107.4, 97.1, 38.2, 37.5, 35.4, 33.3, 33.2,

26.7, 26.4; HRMS(APCI) m/z: $[M+H]^+$ calcd for $C_{26}H_{31}$ 343.2420; found 343.2419.



3-39

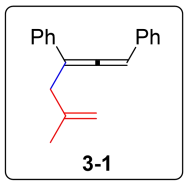
2-(4-Methylene-6,8-diphenylocta-6,7-dien-1-yl)-1,3-dioxane: ^{1}H NMR (400MHz, $CDCl_3$) δ: 7.44(d, *J*=7.2Hz, 2H), 7.33-7.29(m, 6H), 7.22-7.18(m, 2H), 6.51(s, 1H), 4.91(d, *J*=30.4Hz, 2H), 4.46-4.44(m, 1H), 4.08-4.04(m, 2H), 3.73-3.67(m, 2H), 3.31(dd, *J*=16.0Hz, 21.2Hz, 2H), 2.11-2.04(m, 3H), 1.60-1.56(m, 4H), 1.31-1.27(m, 1H); ^{13}C NMR(100MHz, $CDCl_3$) δ: 207.6, 146.2, 135.7, 134.3, 128.7, 128.4, 127.0, 126.9, 126.8, 126.3, 112.0, 107.3, 102.1, 97.1, 66.8, 37.9, 35.6, 34.8, 25.8, 22.0; HRMS(APCI) m/z: $[M+H]^+$ calcd for $C_{25}H_{29}O_2$ 361.2162; found 361.2147.

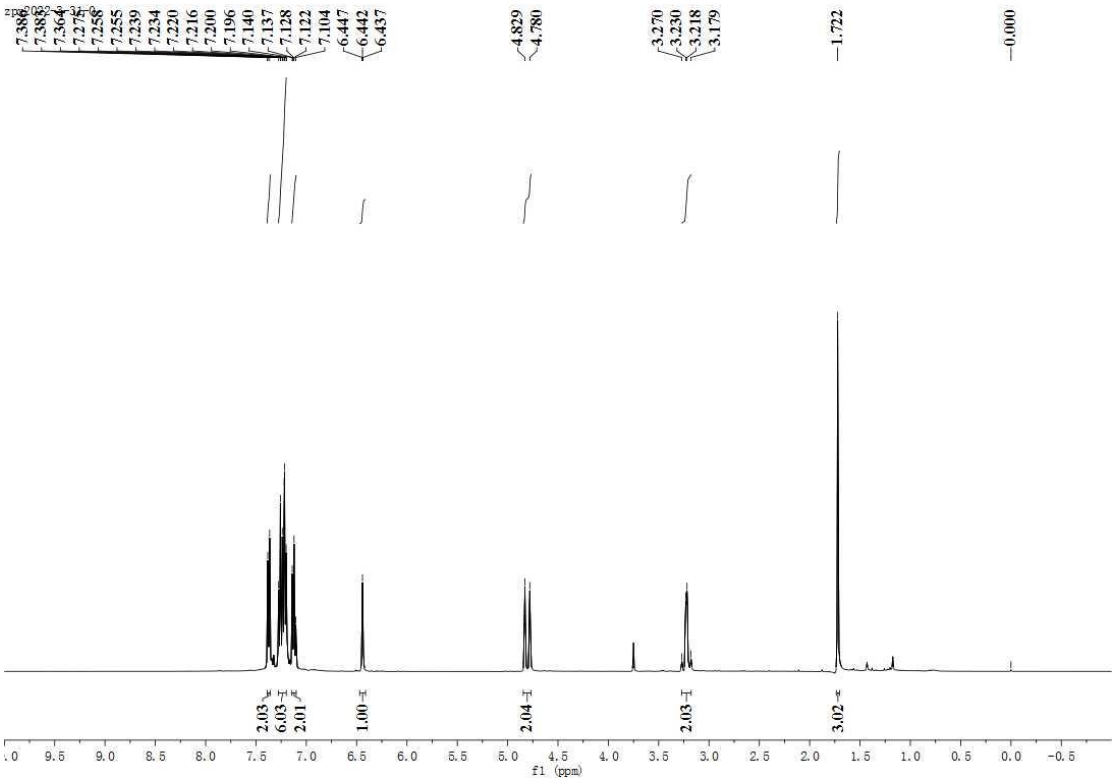
4. References

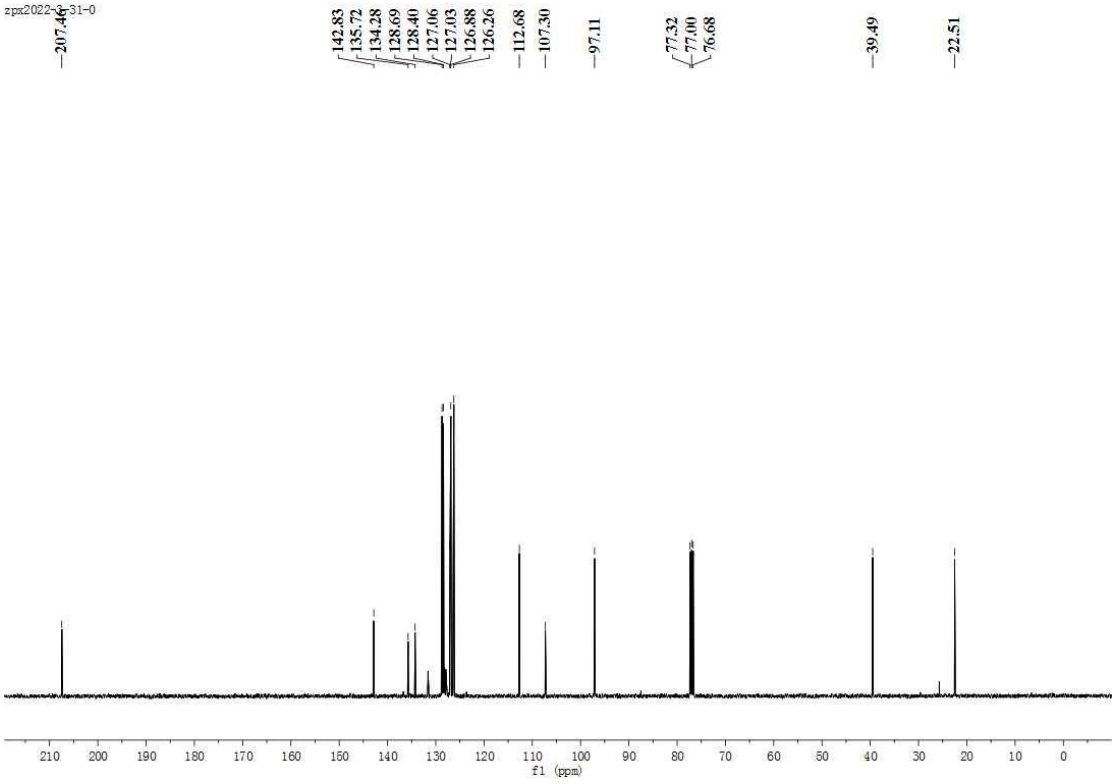
1. (a) Z. Zhou, G. Liu, Y. Chen and X. Lu, Cascade Synthesis of 3-Alkylidene Dihydrobenzofuran Derivatives via Rhodium(III)-Catalyzed Redox-Neutral C-H Functionalization/Cyclization, *Org. Lett*, 2015, **17**, 5874; (b) A. E. Nibbs, T. D. Montgomery, Y. Zhu and V. H. Rawal, Access to Spirocyclized Oxindoles and Indolenines via Palladium-Catalyzed Cascade Reactions of Propargyl Carbonates with 2-Oxotryptamines and Tryptamines, *J. Org. Chem*, 2015, **80**, 4928.

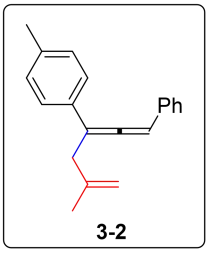
2. (a) M. Iwasaki, S. Hayashi, K. Hirano, H. Yorimitsu and K. Oshima, $Pd(OAc)_2/P(^cC_6H_{11})_3$-Catalyzed Allylation of Aryl Halides with Homoallyl Alcohols via Retro-Allylation, *J. Am. Chem. Soc*, 2007, **129**, 4463; (b) A. Arribas, M. Calvelo, D. F. Fernández, C. A. B. Rodrigues, J. L. Mascareñas and F. López, Highly Enantioselective Iridium(I)-Catalyzed Hydrocarbonation of Alkenes: A Versatile Approach to Heterocyclic Systems Bearing Quaternary Stereocenters, *Angew. Chem., Int. Ed*, 2021, **60**, 19297.

5. ^{1}H, ^{13}C spectra for compound 3

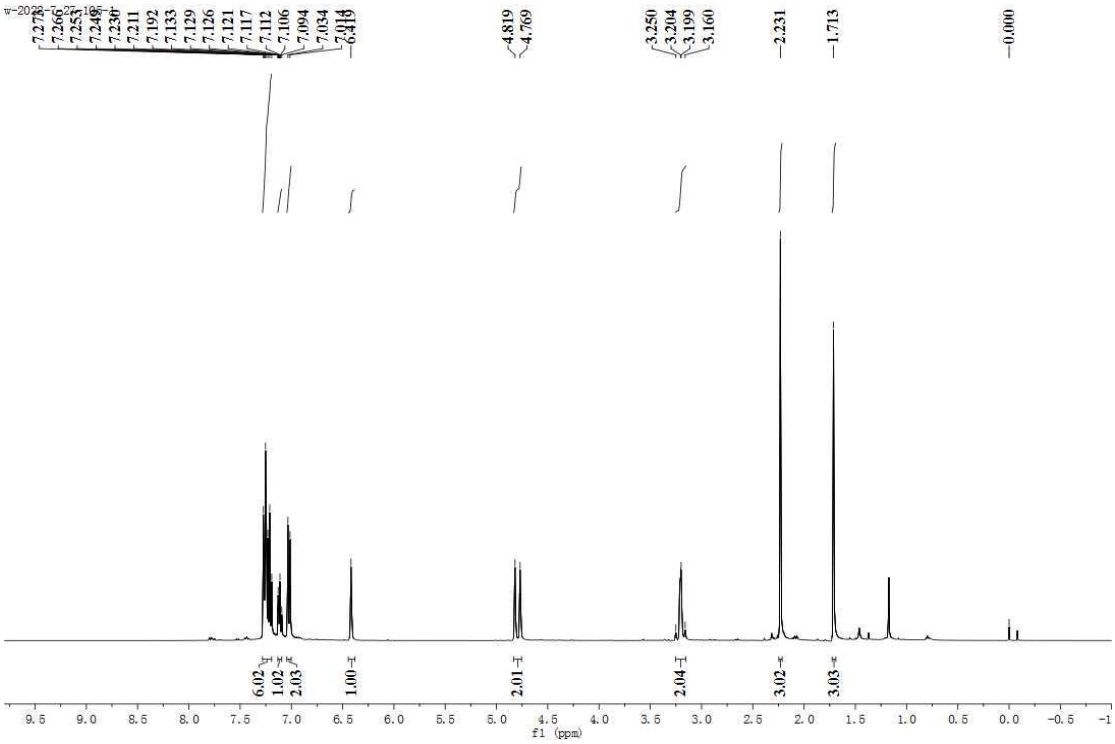







Ph

3-2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7.253
7.248
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7.211
7.192
7.133
7.129
7.126
7.121
7.117
7.112
7.106
7.094
7.034
7.014
6.419
4.819
4.769
3.250
3.204
3.199
3.160
2.231
1.713
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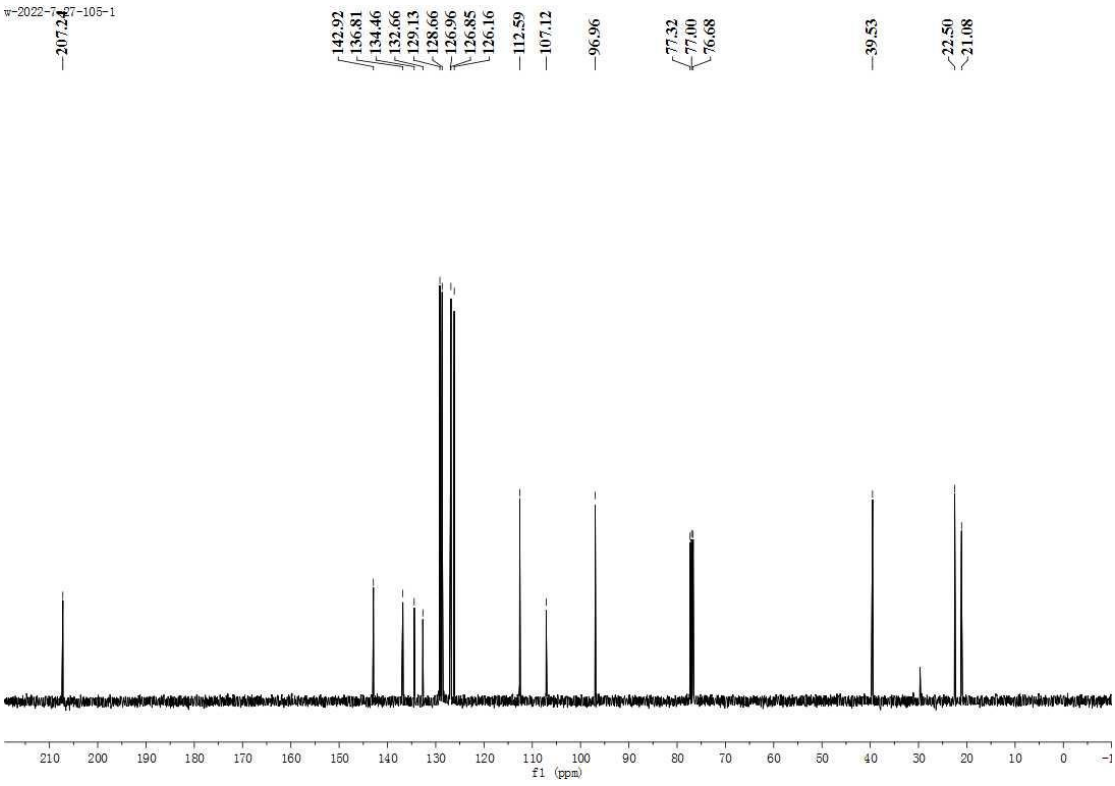
6.02
1.02
2.03
1.00
2.01
2.04
3.02
3.03
f1 (ppm)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132.66
129.13
128.66
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126.16
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107.12
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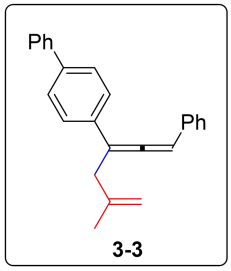
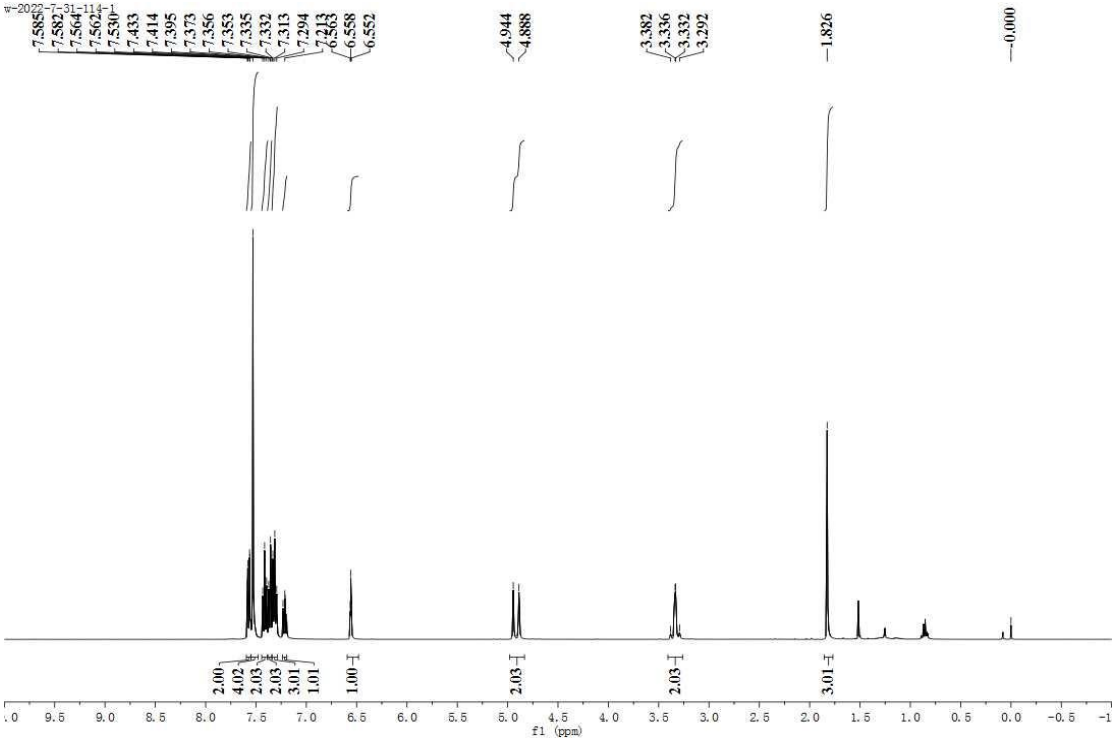
76.68
39.53
22.50
21.08
f1 (ppm)


Ph
Ph

3-3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7.530
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7.395
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7.356
7.353
7.335
7.332
7.313
7.294
7.213
6.563
6.558
6.552
4.944
4.888
3.382
3.336
3.332
3.292
1.826
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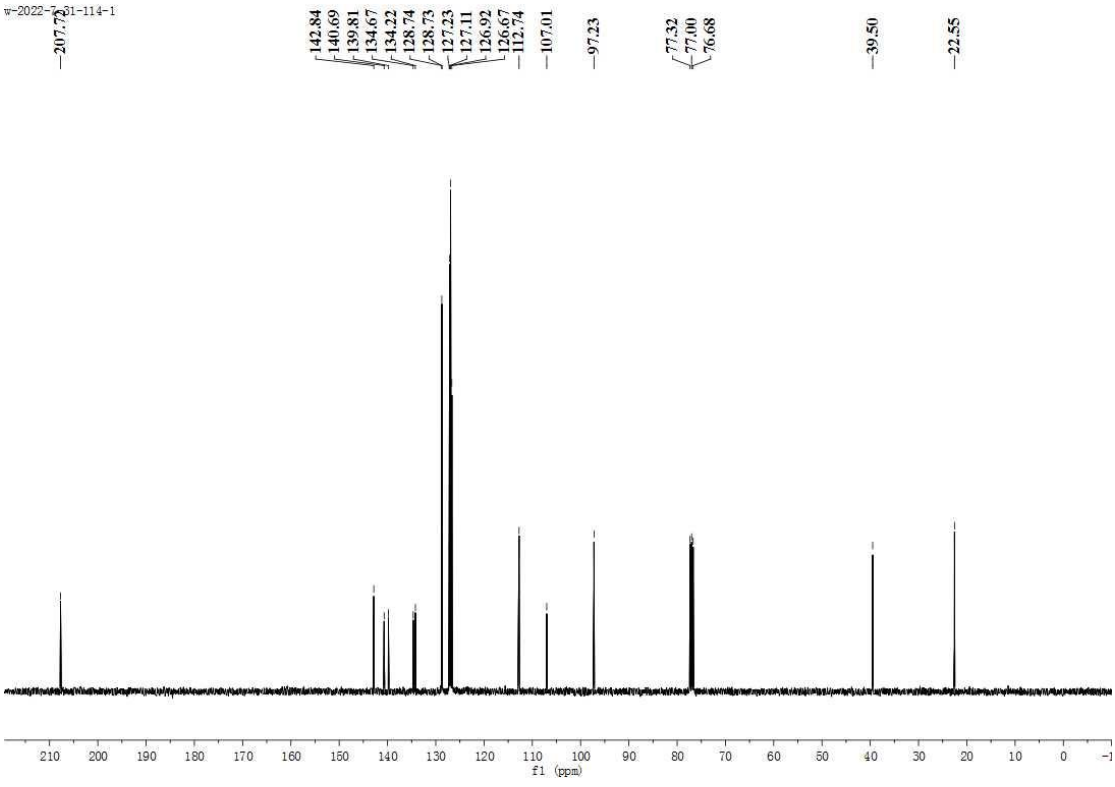
2.03
3.01
1.01
1.00
2.03
2.03
3.01
f1 (ppm)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112.74
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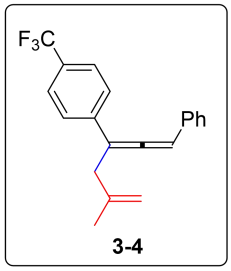
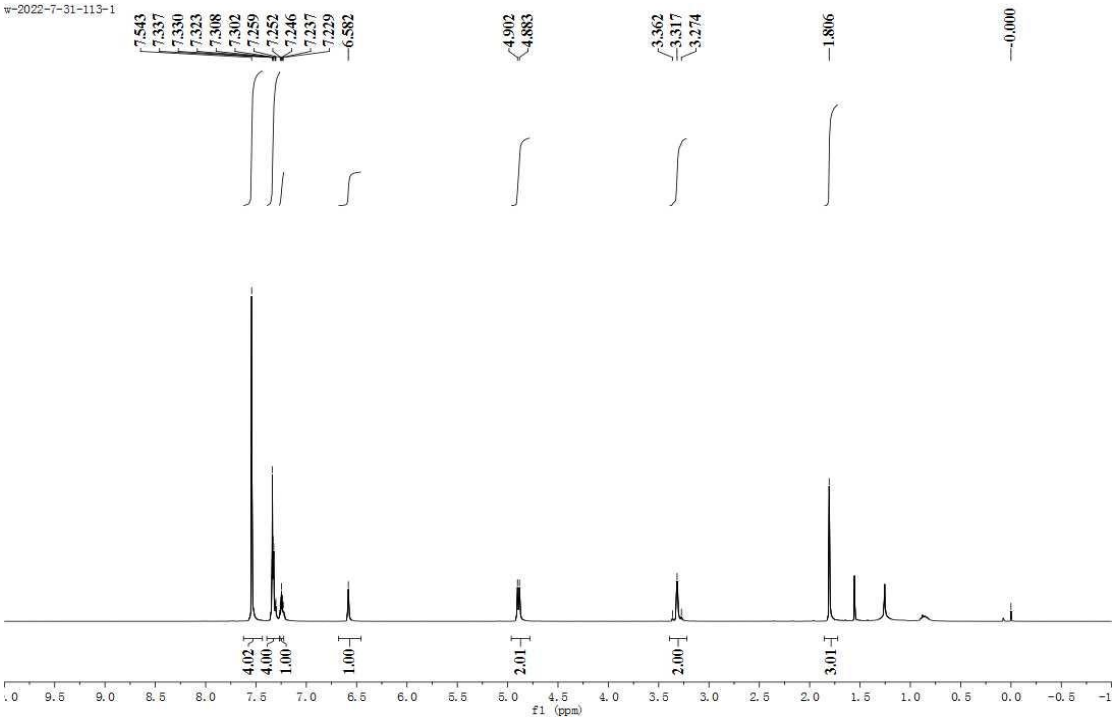
77.00
76.68
39.50
22.55
f1 (ppm)


F3C
Ph

3-4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7.237
7.229
6.582
4.902
4.883
3.362
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3.274
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4.00
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1.00
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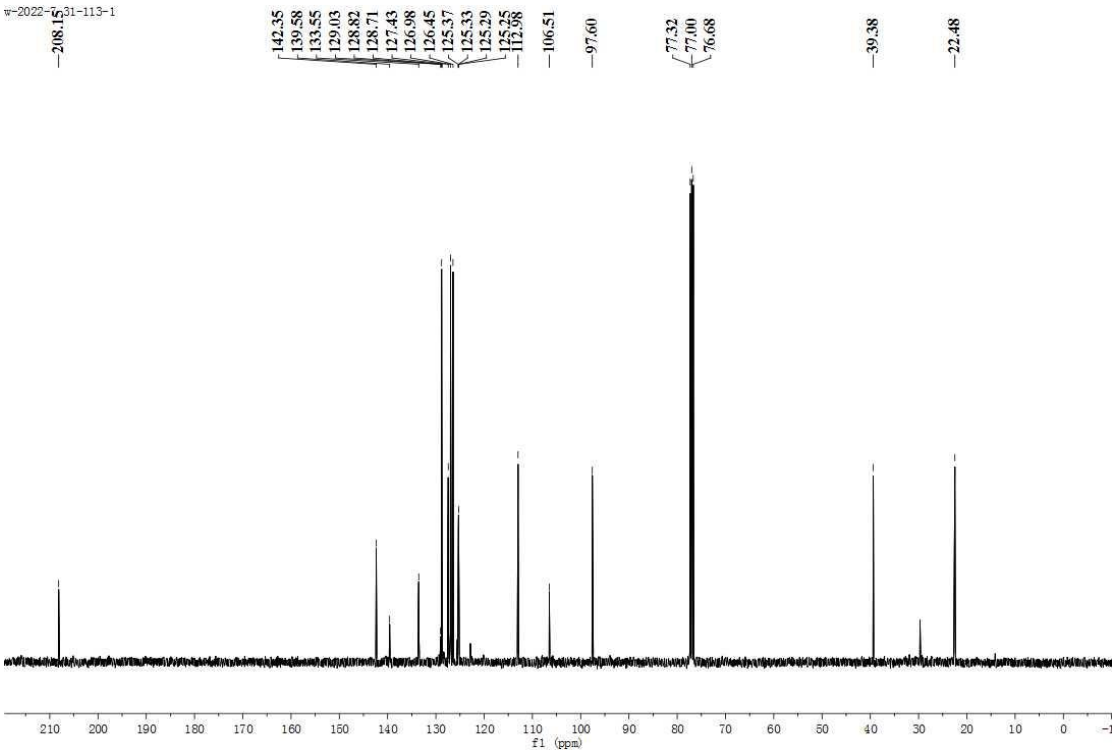
2.00
3.01
f1 (ppm)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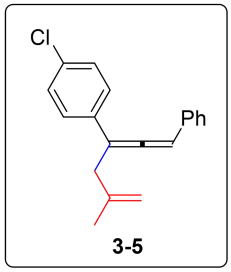
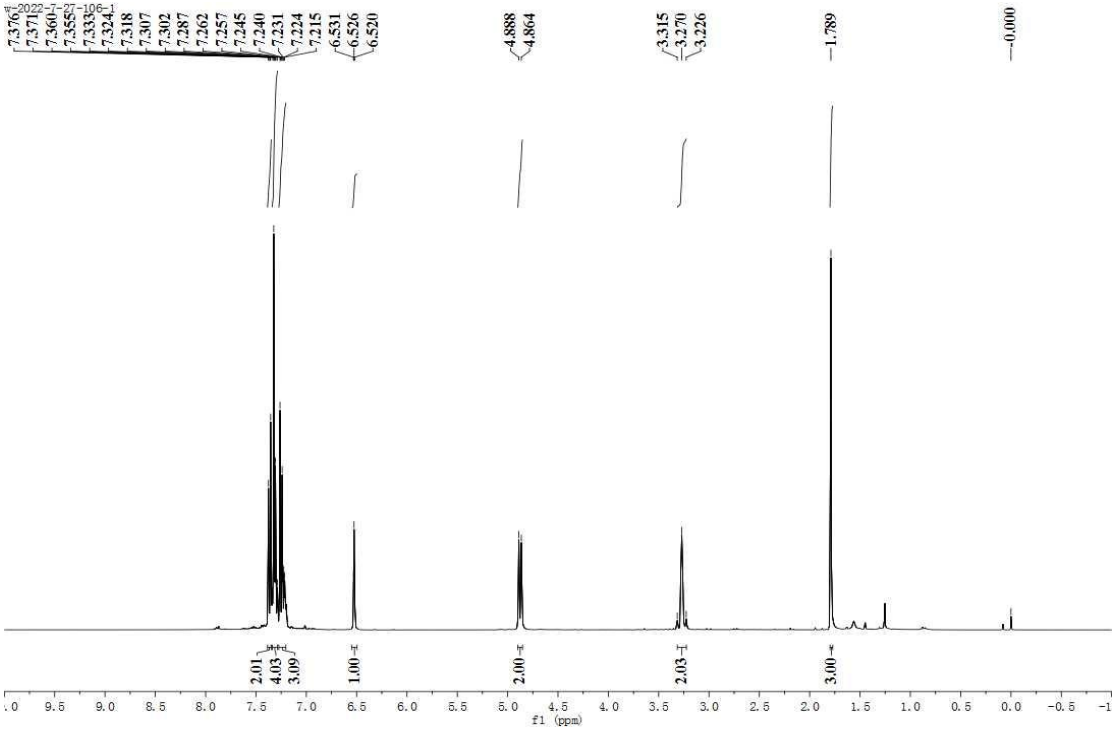
f1 (ppm)


Cl
Ph

3-5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7.257
7.245
7.240
7.231
7.224
7.215
6.531
6.526
6.520
4.888
4.864
3.315
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4.03
3.09
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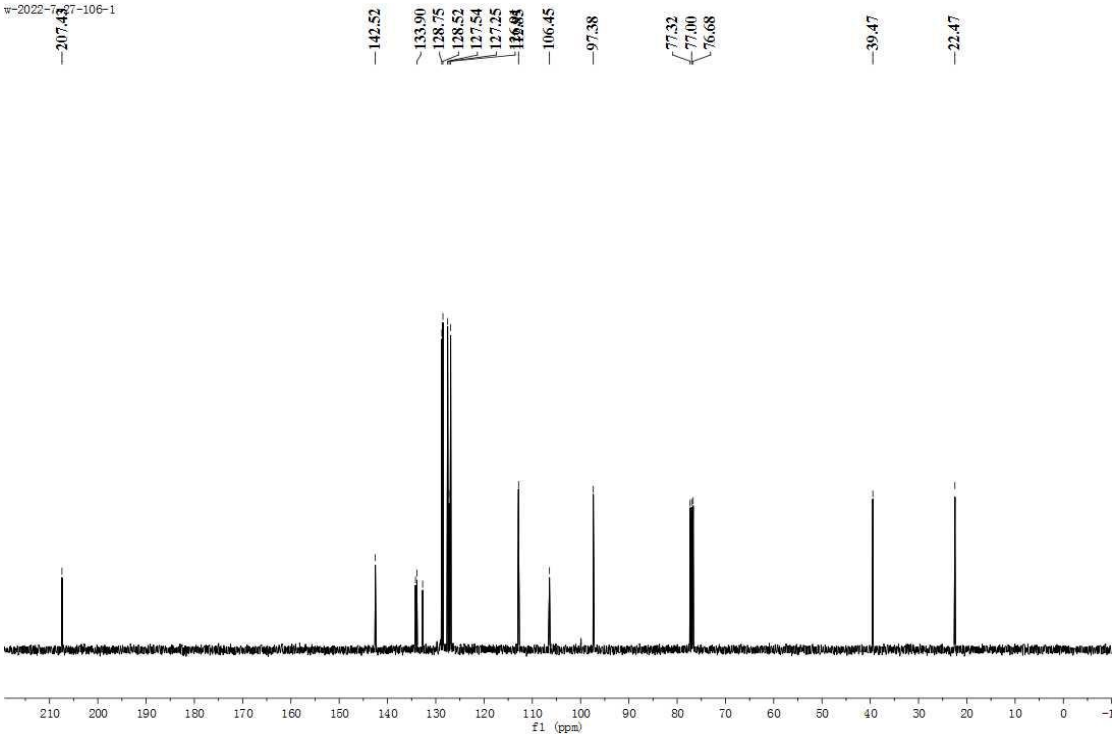
2.00
2.03
3.00
f1 (ppm)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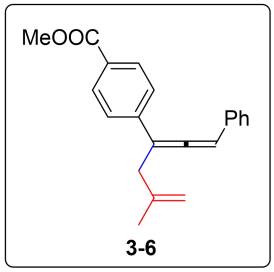
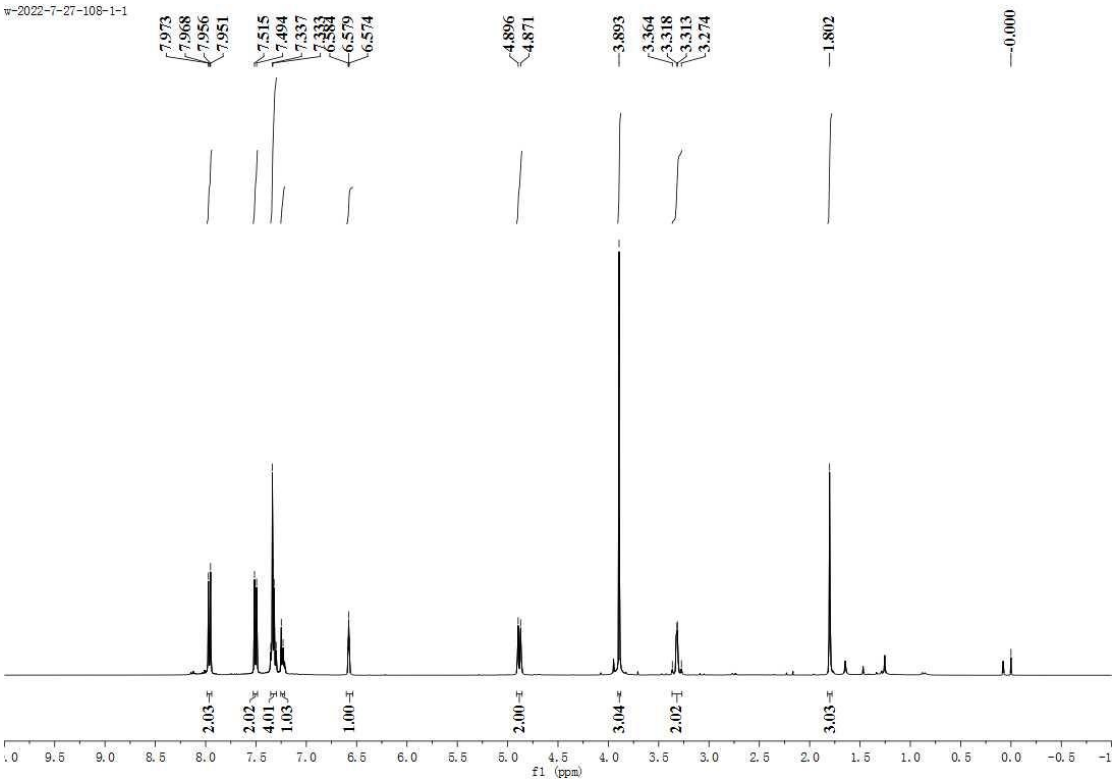

MeOOC
Ph

3-6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3.274
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4.01
1.03
1.00
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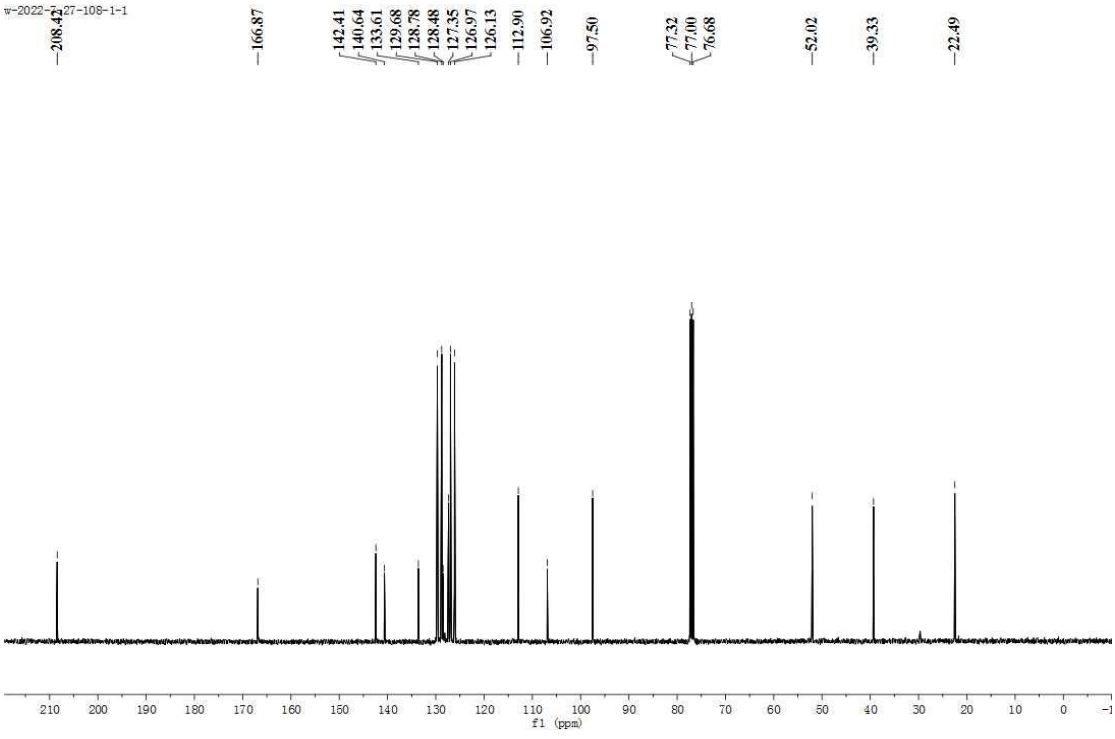
2.02
3.03
f1 (ppm)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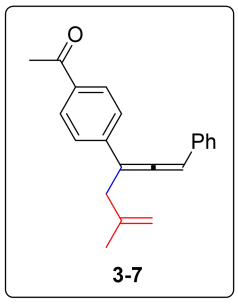
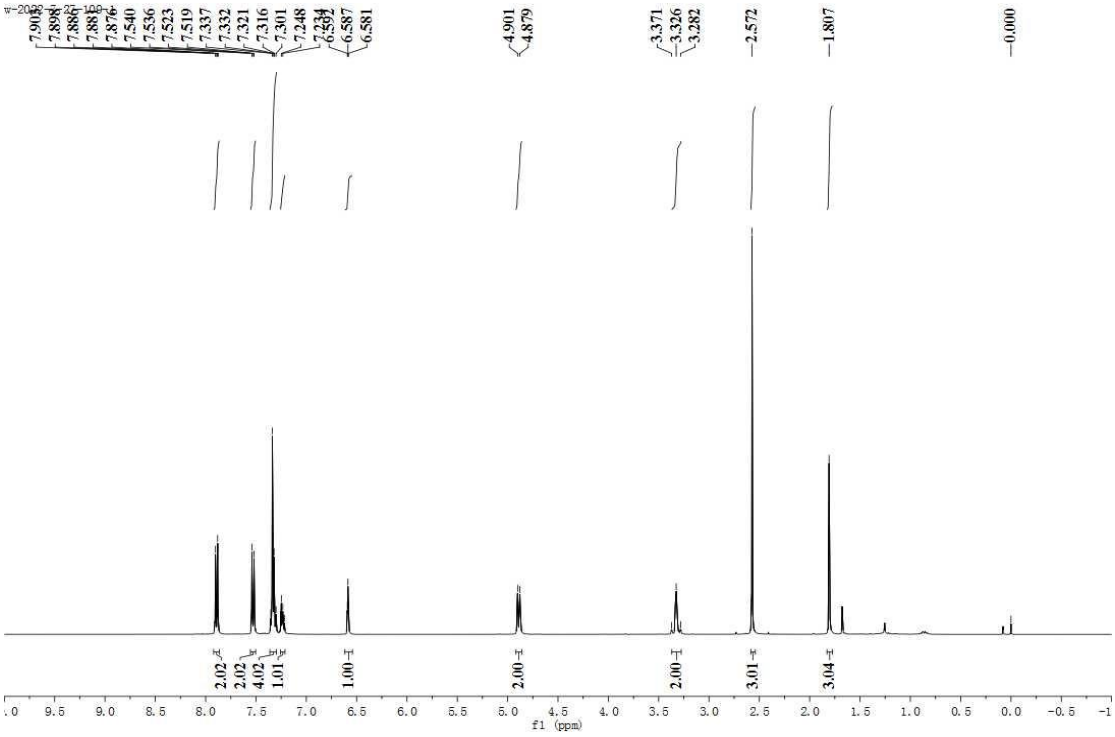
22.49
f1 (ppm)


O
Ph

3-7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7.316
7.301
7.248
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6.581
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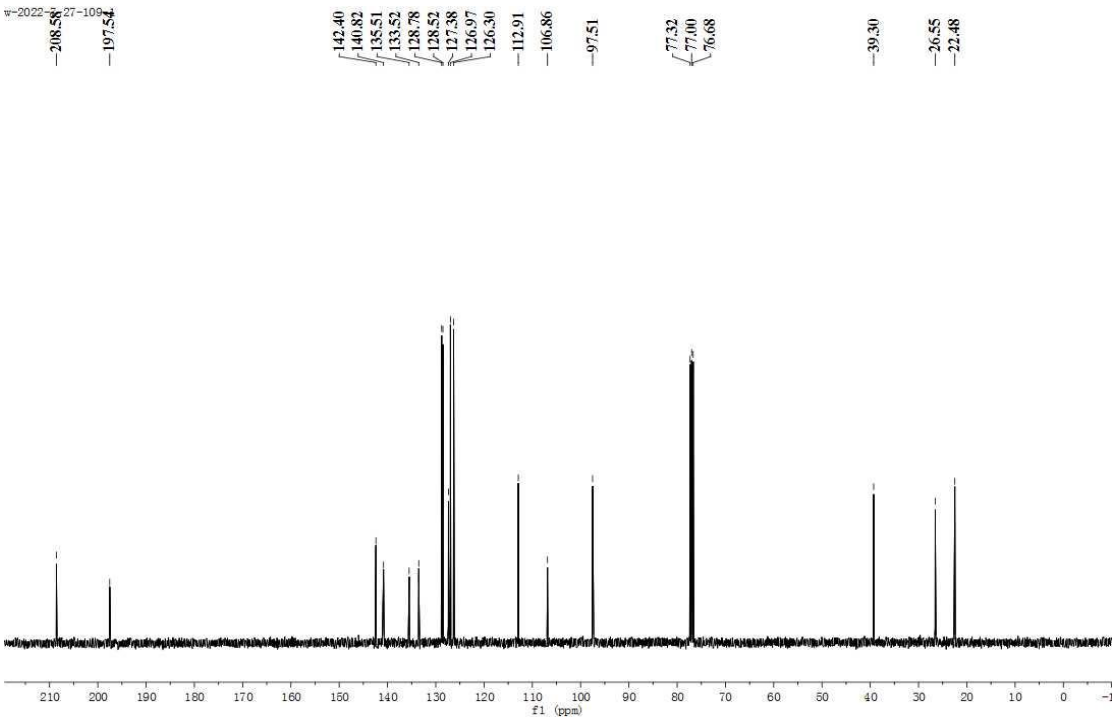
f1 (ppm)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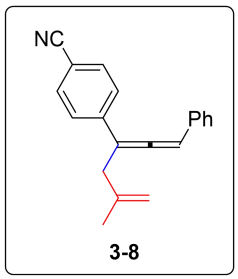
f1 (ppm)


NC
Ph

3-8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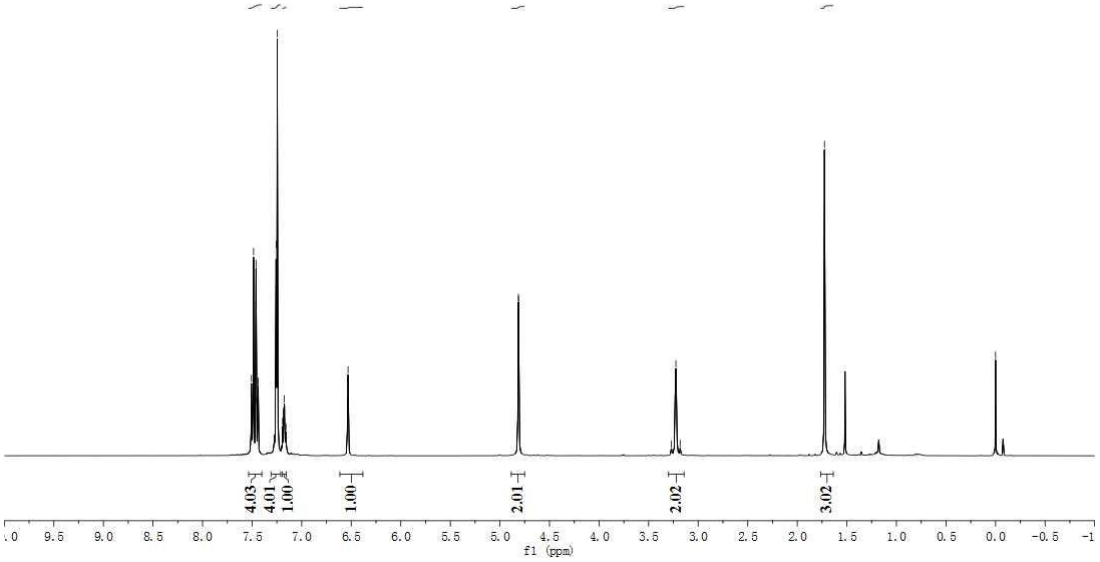
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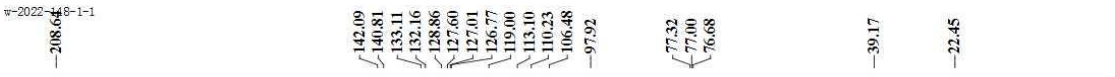
f1 (ppm)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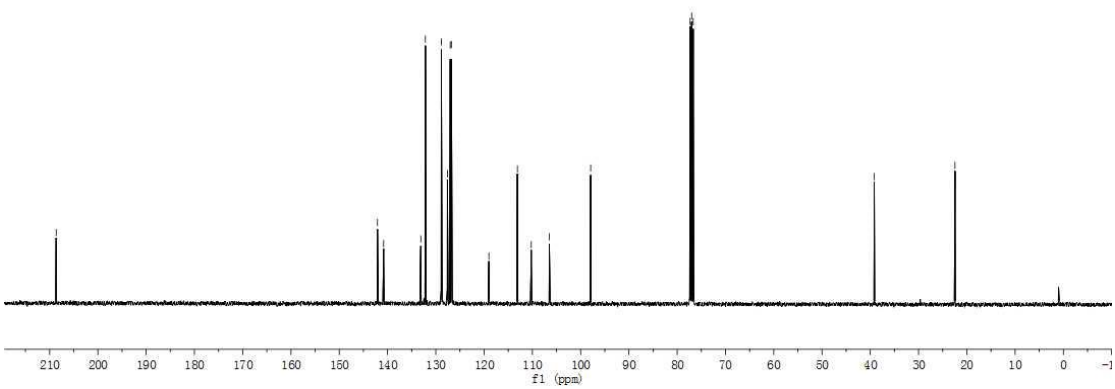
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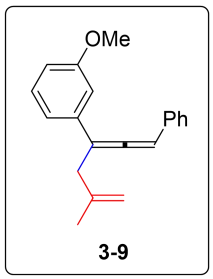
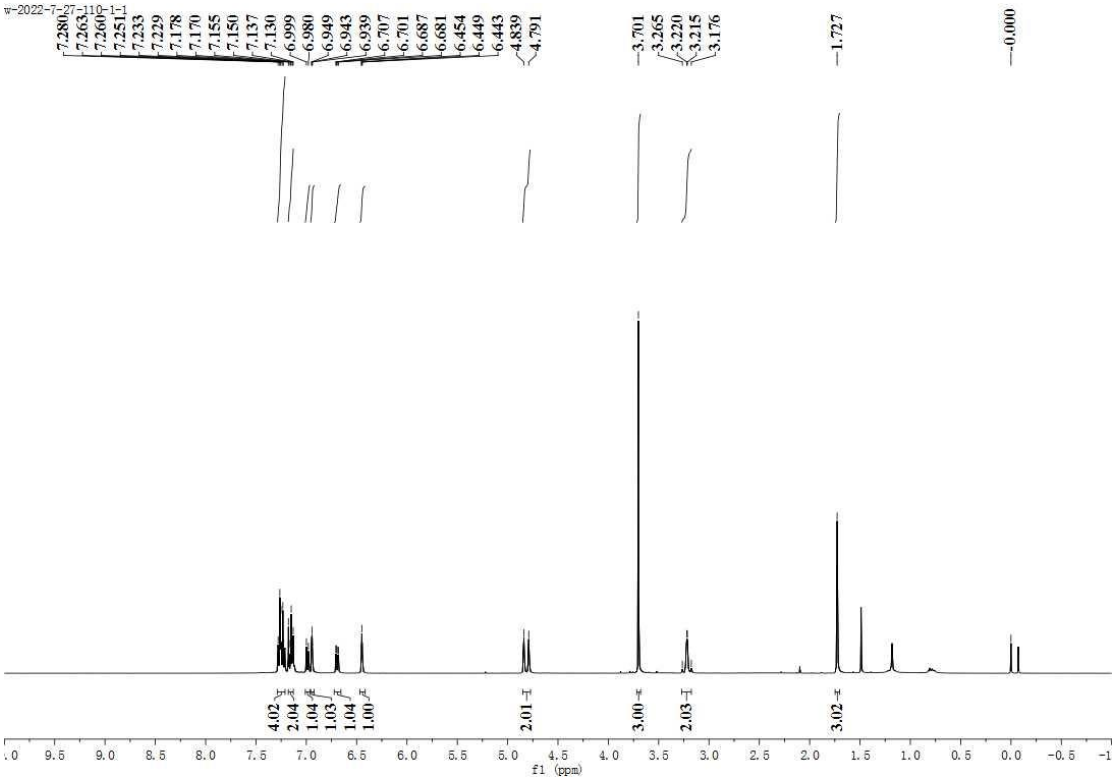

OMe
Ph

3-9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6.687
6.681
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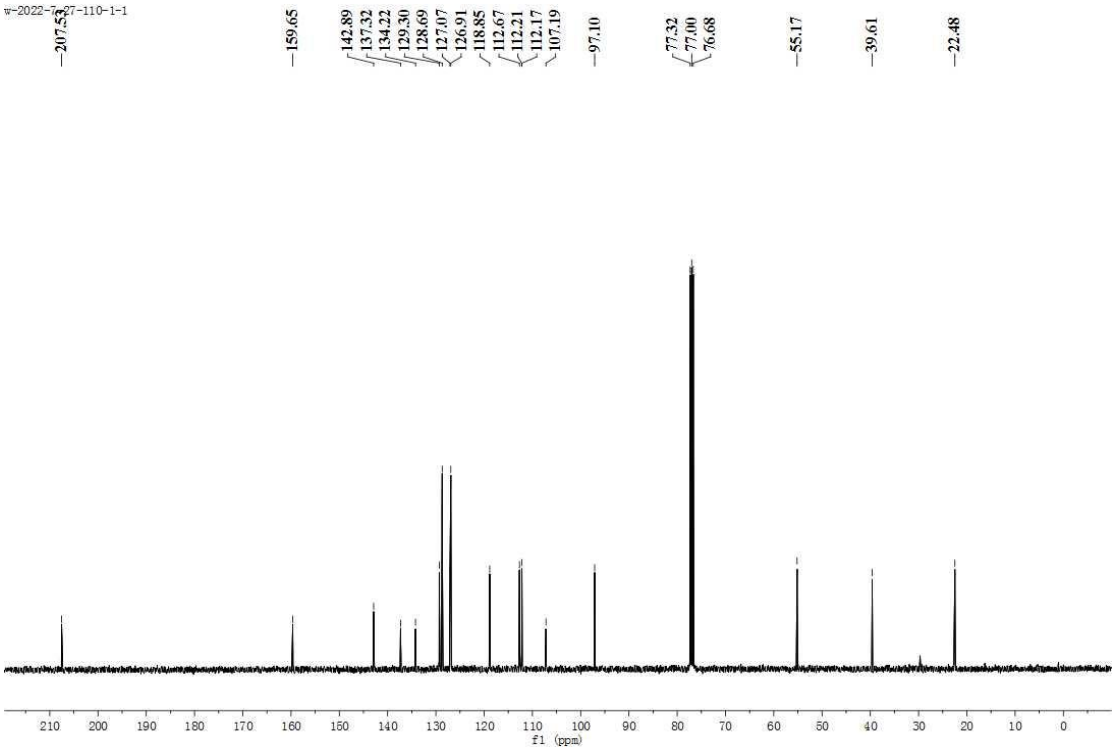
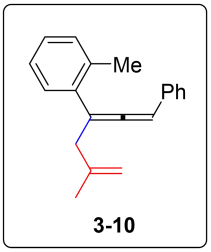
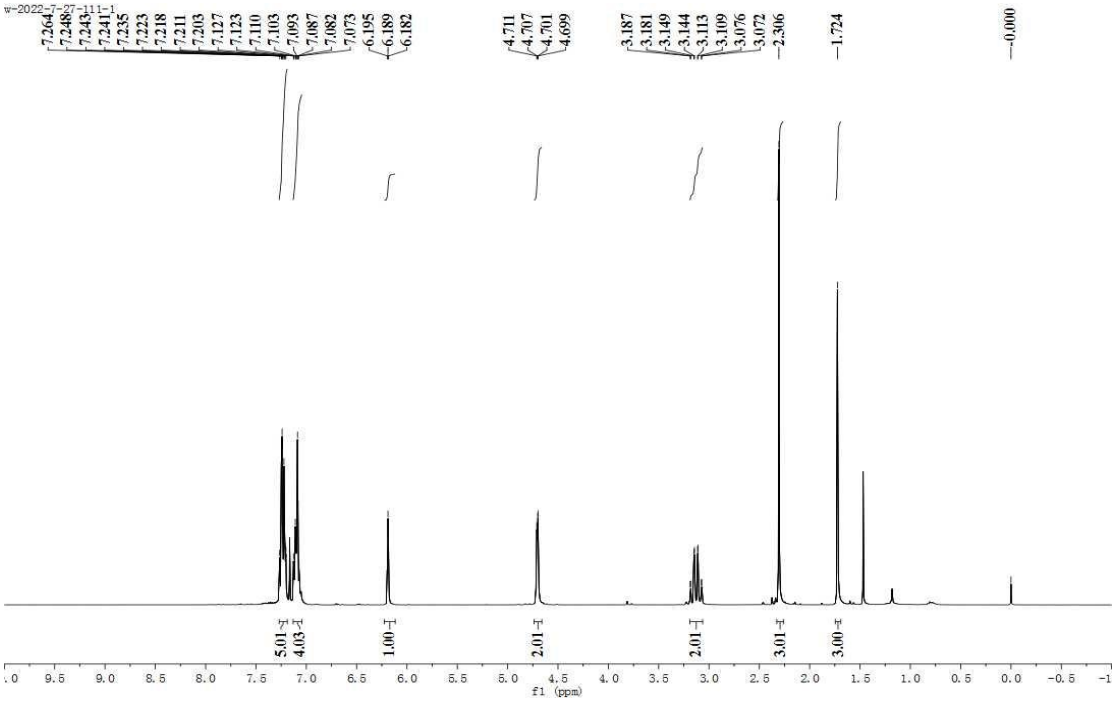
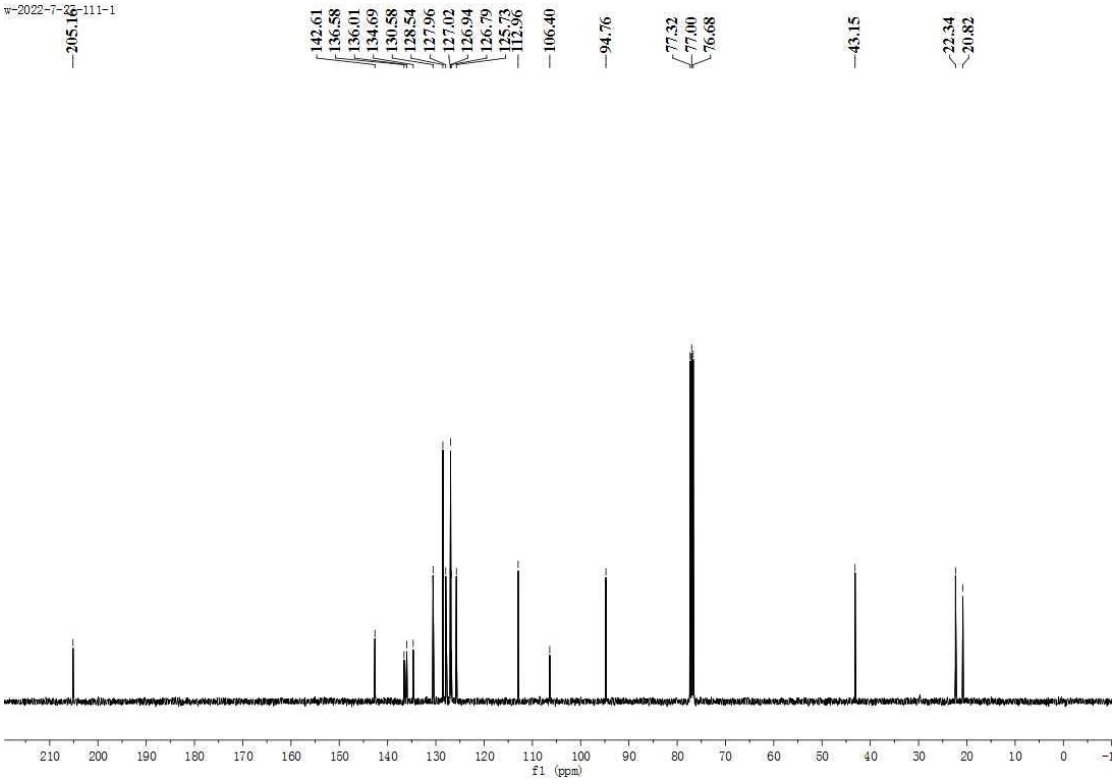
1.03
1.04
1.00
2.01
3.00
2.03
3.02
f1 (ppm)

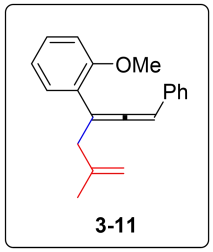

w-2022-7-27-110-1-1
207.53
159.65
142.89
137.32
134.22
129.30
128.69
127.07
126.91
118.85
112.67
112.21
112.17
107.19
97.10
77.32
77.00
76.68
55.17
39.61
22.48
f1 (ppm)


Me
Ph

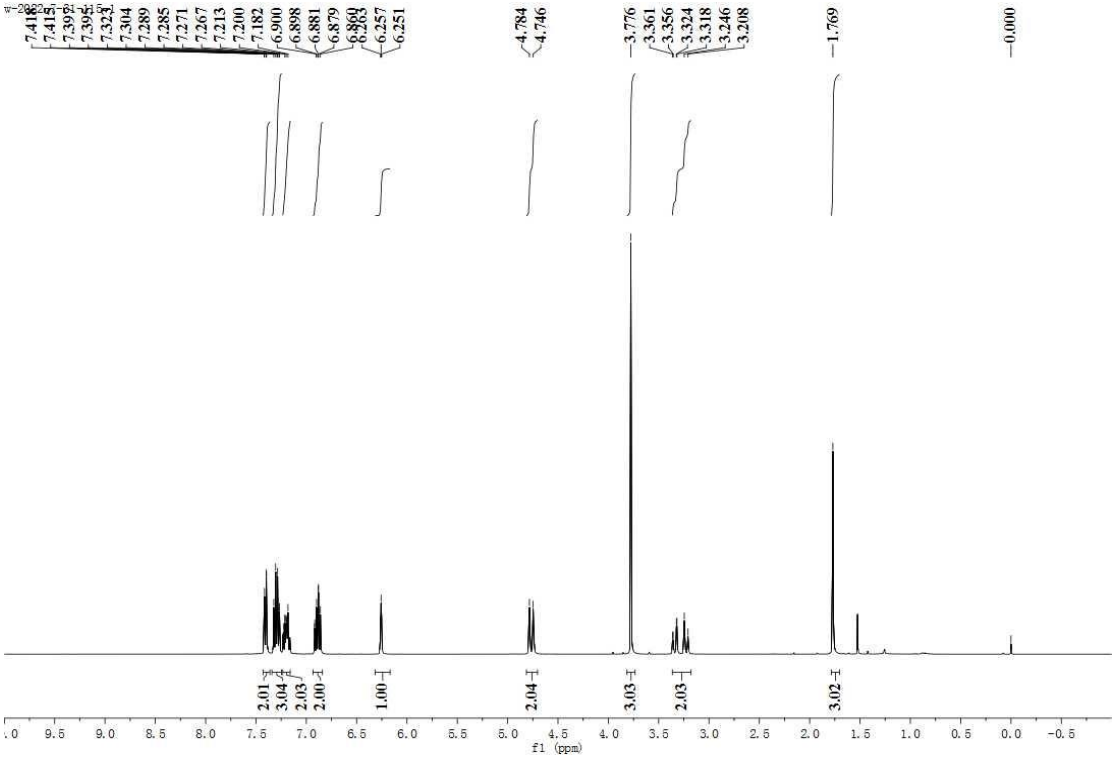
3-10

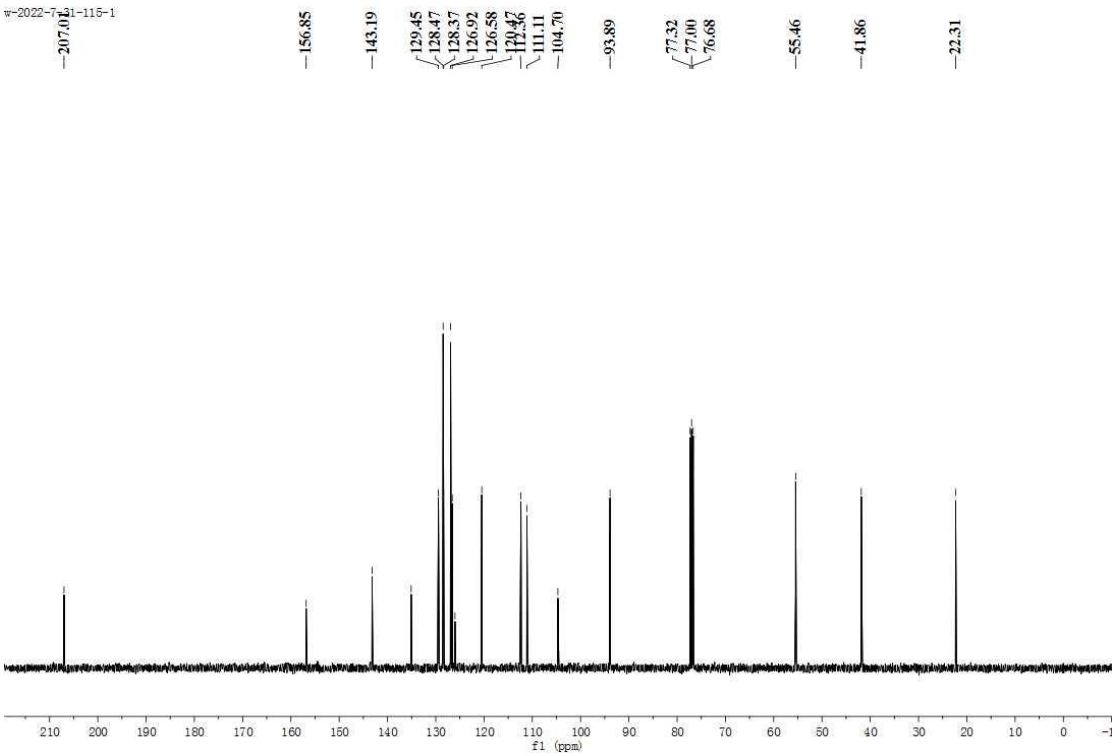

w-2022-7-27-111-1
7.264
7.248
7.243
7.241
7.235
7.223
7.218
7.211
7.203
7.127
7.123
7.110
7.103
7.093
7.087
7.082
7.073
6.195
6.189
6.182
4.711
4.707
4.701
4.699
3.187
3.181
3.149
3.144
3.113
3.109
3.076
3.072
2.306
1.724
0.000
5.01
4.03
1.00
2.01
2.01
3.01
3.00
f1 (ppm)

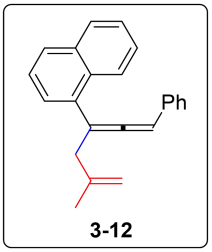

w-2022-7-27-111-1
205.16
142.61
136.58
136.01
134.69
130.58
128.54
127.96
127.02
126.94
126.79
125.73
112.96
106.40
94.76
77.32
77.00
76.68
43.15
22.34
20.82
f1 (ppm)


OMe
Ph

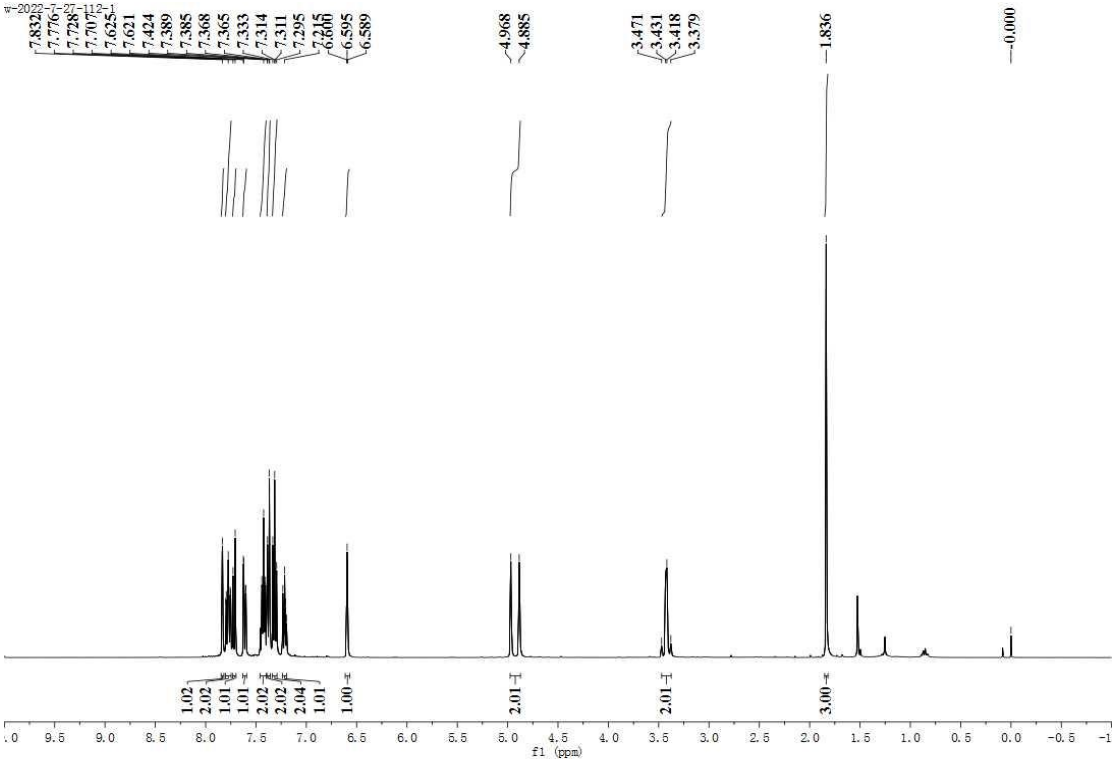
3-11

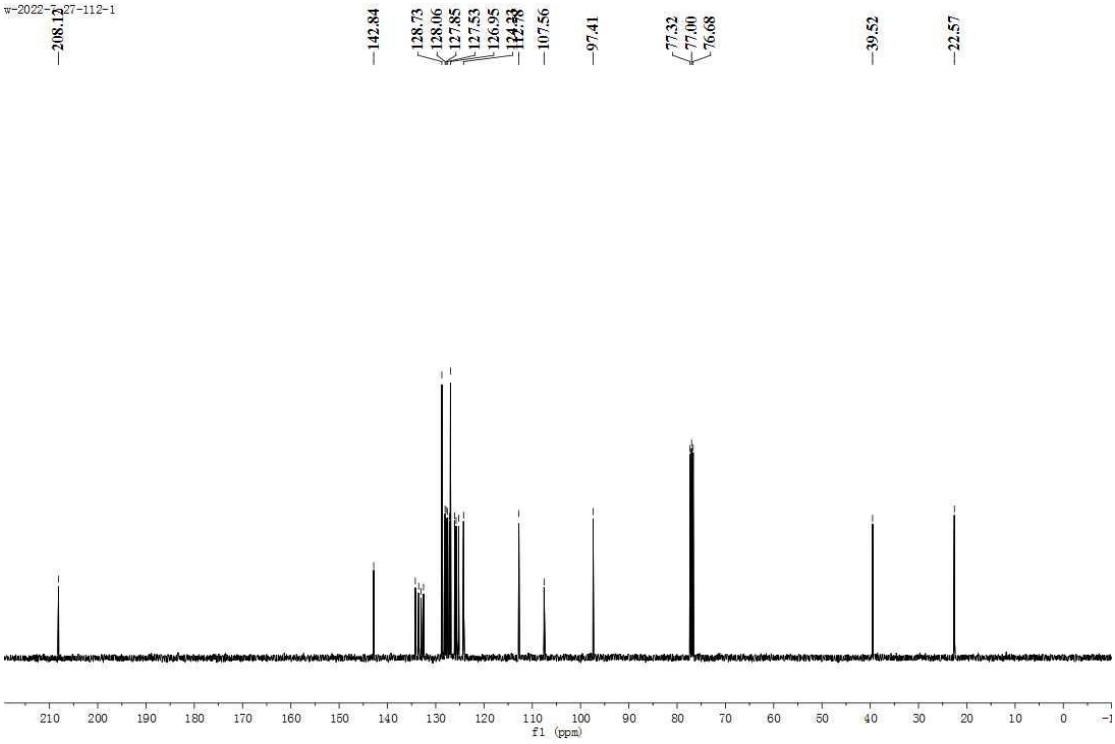

7.415
7.399
7.323
7.304
7.289
7.285
7.271
7.267
7.213
7.200
7.182
6.900
6.898
6.881
6.879
6.257
6.251
4.784
4.746
3.776
3.361
3.356
3.324
3.318
3.246
3.208
1.769
0.000
2.01
3.04
2.03
2.00
1.00
2.04
3.03
2.03
3.02
f1 (ppm)

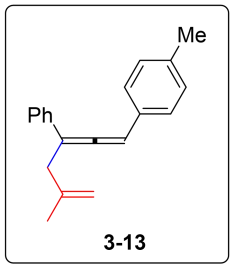

207.01
156.85
143.19
129.45
128.47
128.37
126.92
126.58
120.47
112.36
111.11
104.70
93.89
77.32
77.00
76.68
55.46
41.86
22.31
f1 (ppm)


Ph

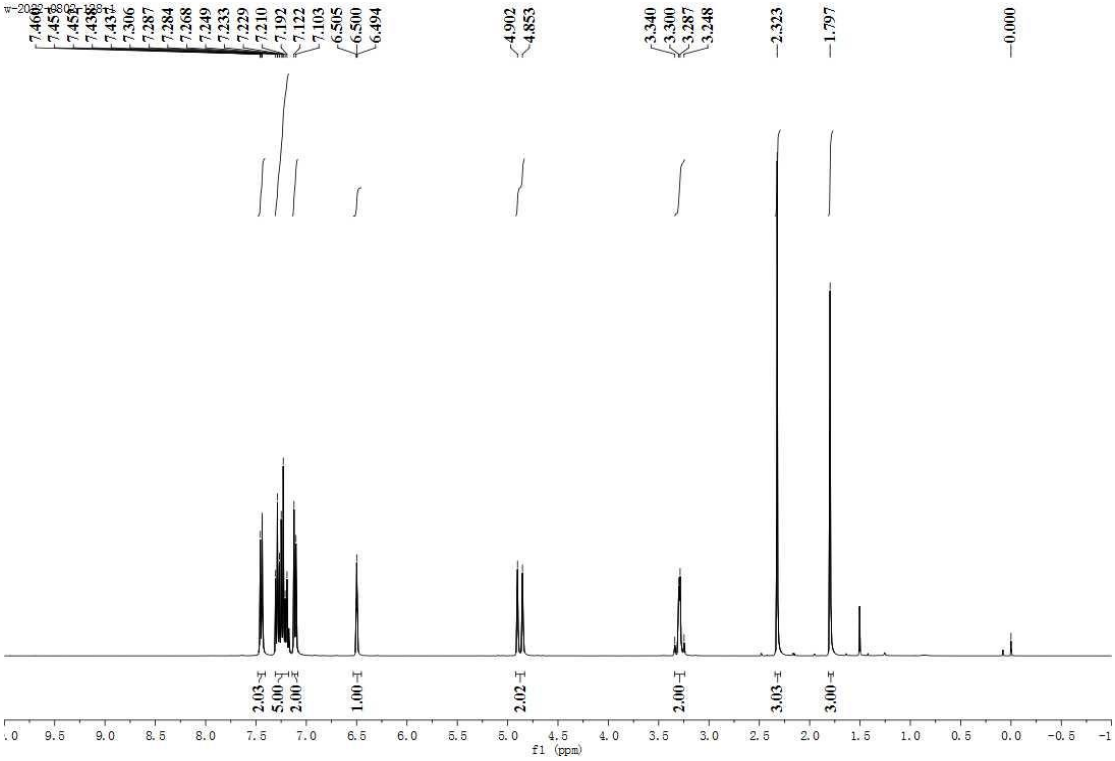
3-12

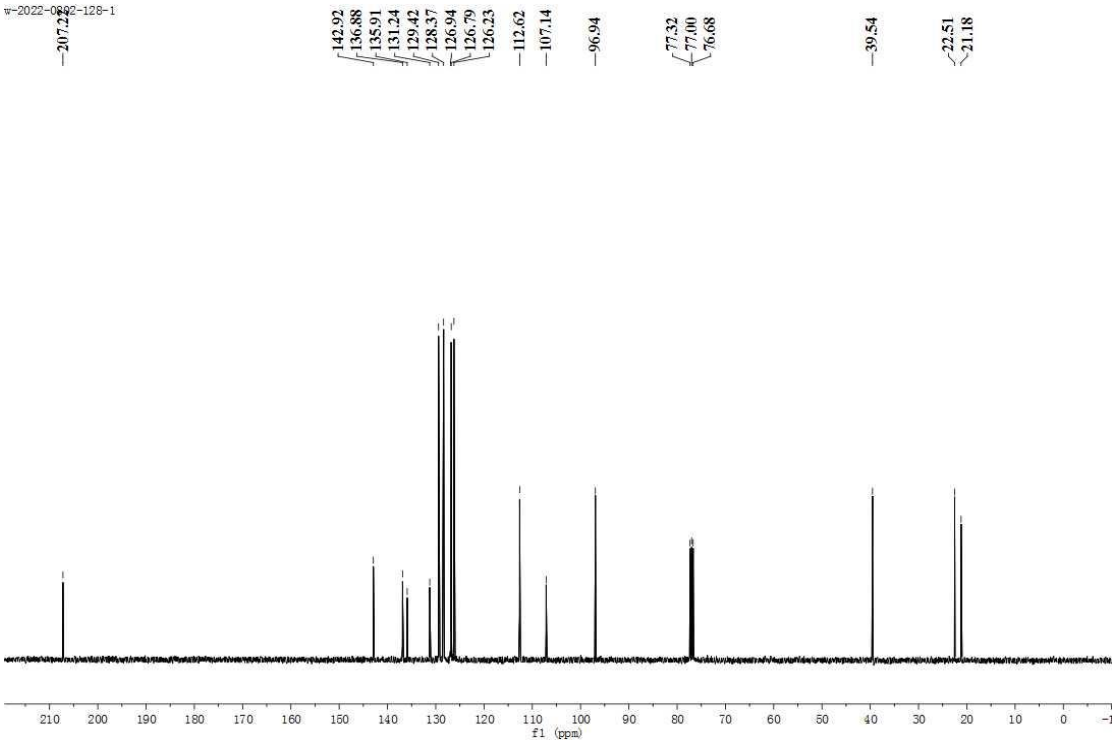

7.832
7.776
7.728
7.707
7.621
7.424
7.389
7.385
7.368
7.365
7.333
7.314
7.311
7.295
7.215
6.600
6.595
6.589
4.968
4.885
3.471
3.431
3.418
3.379
1.836
0.000
1.02
2.02
1.01
1.01
2.02
2.02
2.04
1.01
1.00
2.01
2.01
3.00
f1 (ppm)

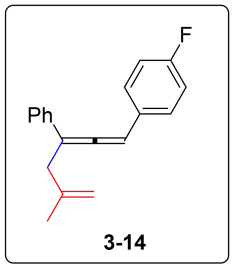

208.12
142.84
128.73
128.06
127.85
127.53
126.95
107.56
97.41
77.32
77.00
76.68
39.52
22.57
f1 (ppm)


Me
Ph

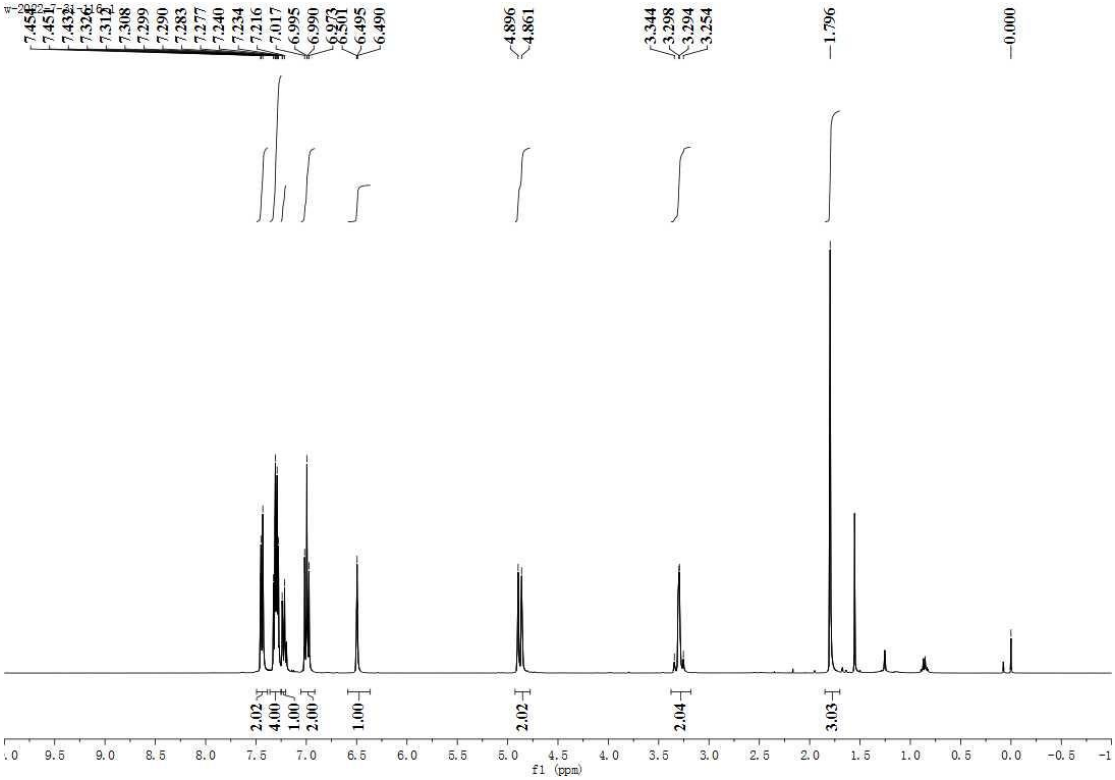
3-13

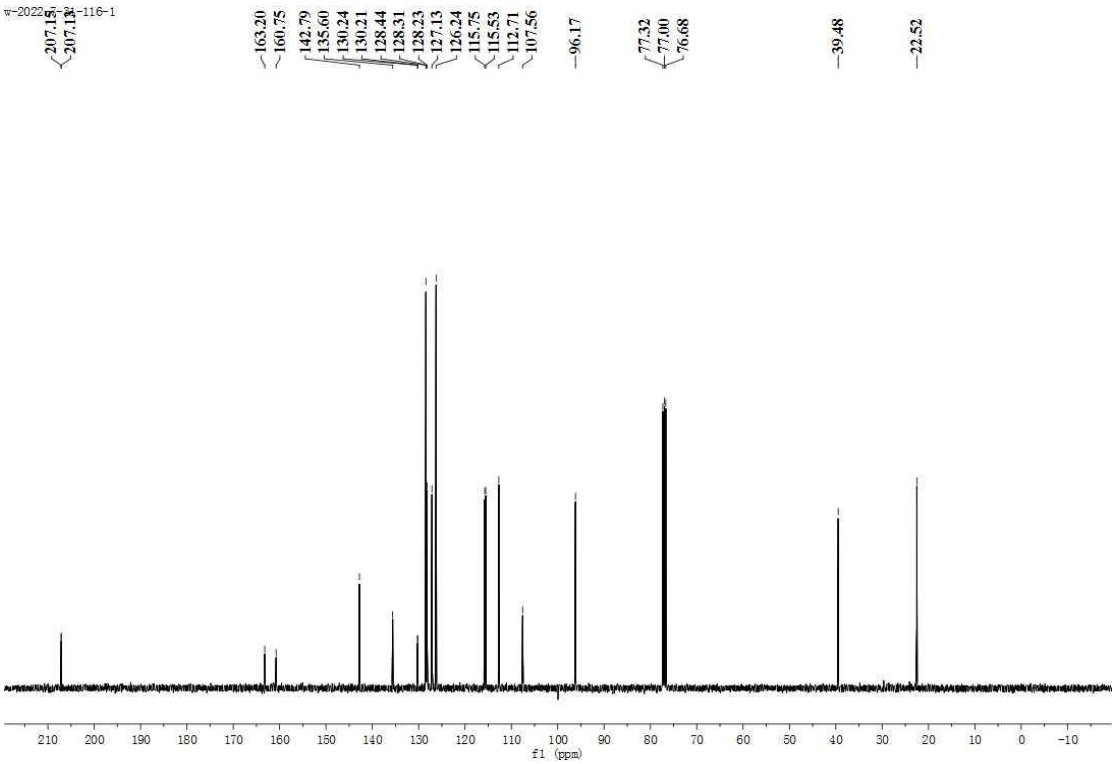

7.460
7.451
7.438
7.437
7.306
7.287
7.284
7.268
7.249
7.233
7.229
7.210
7.192
7.122
7.103
6.505
6.500
6.494
4.902
4.853
3.340
3.300
3.287
3.248
2.323
1.797
0.000
2.03
5.00
2.00
1.00
2.02
2.00
3.03
3.00
f1 (ppm)

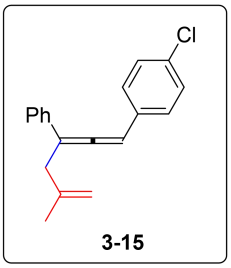

207.22
142.92
136.88
135.91
131.24
129.42
128.37
126.94
126.79
126.23
112.62
107.14
96.94
77.32
77.00
76.68
39.54
22.51
21.18
f1 (ppm)


F
Ph

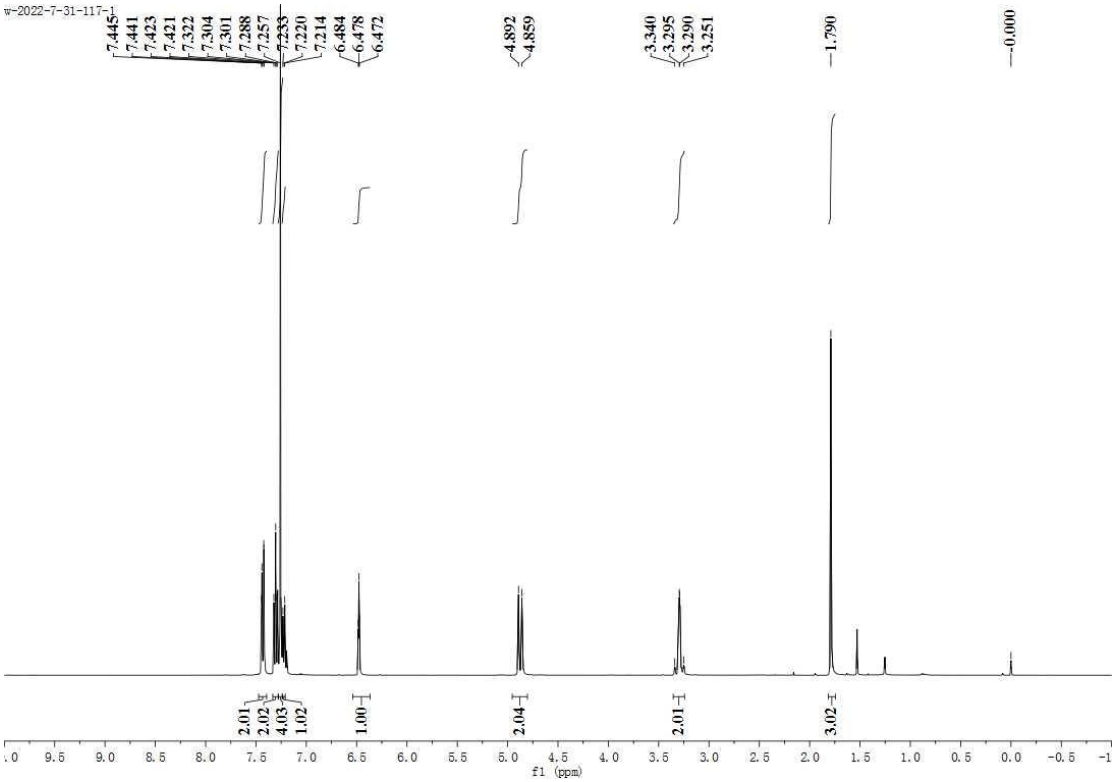
3-14

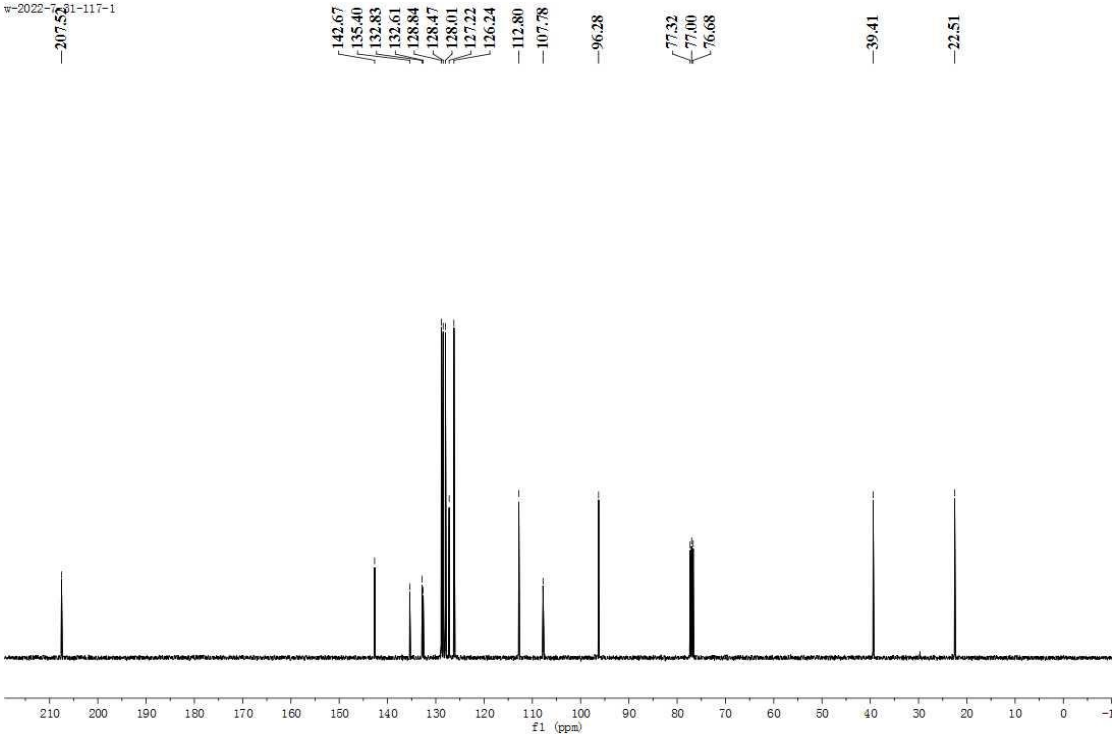

7.451
7.437
7.326
7.312
7.308
7.299
7.290
7.283
7.277
7.240
7.234
7.216
7.017
6.995
6.990
6.973
6.501
6.495
6.490
4.896
4.861
3.344
3.298
3.294
3.254
1.796
0.000
2.02
4.00
1.00
2.00
1.00
2.02
2.04
3.03
f1 (ppm)

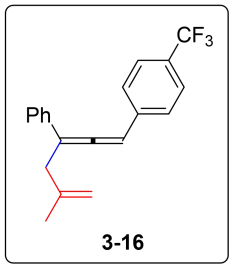

207.15
207.13
163.20
160.75
142.79
135.60
130.24
130.21
128.44
128.31
128.23
127.13
126.24
115.75
115.53
112.71
107.56
96.17
77.32
77.00
76.68
39.48
22.52
f1 (ppm)


Cl
Ph

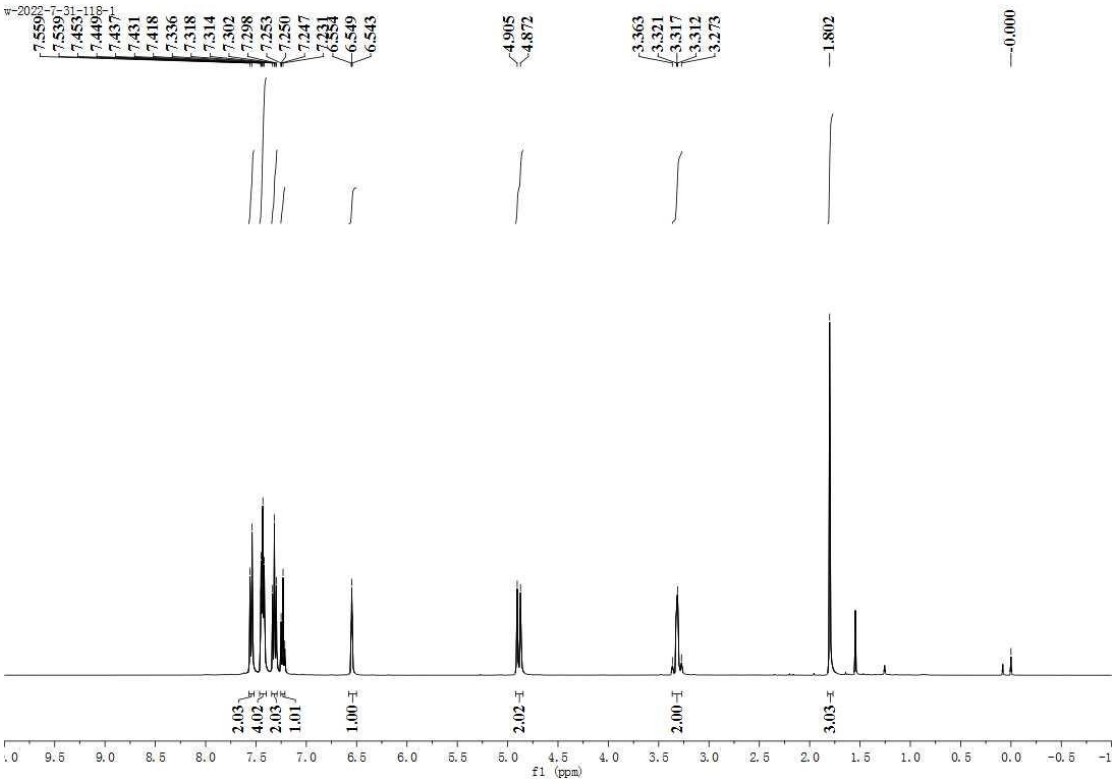
3-15


w-2022-7-31-117-1
7.445
7.441
7.423
7.421
7.322
7.304
7.301
7.288
7.257
7.233
7.220
7.214
6.484
6.478
6.472
4.892
4.859
3.340
3.295
3.290
3.251
1.790
0.000
2.01
2.02
4.03
1.02
1.00
2.04
2.01
3.02
f1 (ppm)


w-2022-7-31-117-1
207.52
142.67
135.40
132.83
132.61
128.84
128.47
128.01
127.22
126.24
112.80
107.78
96.28
77.32
77.00
76.68
39.41
22.51
f1 (ppm)


CF3
Ph

3-16


w-2022-7-31-118-1
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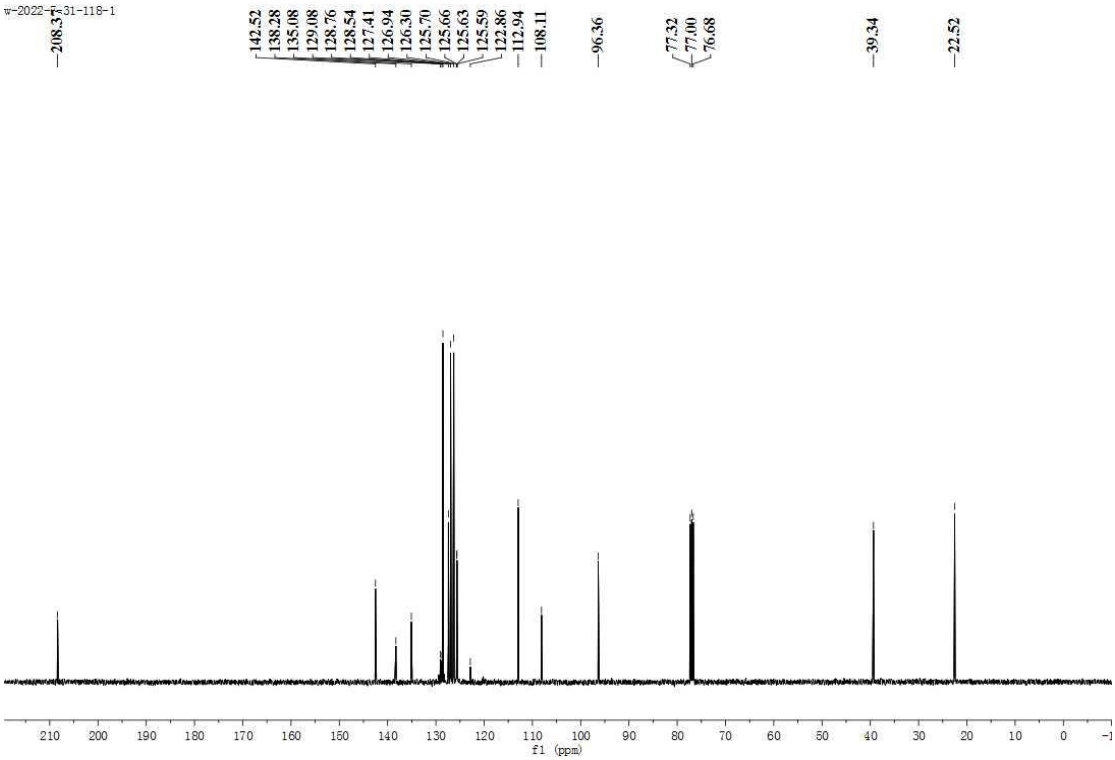
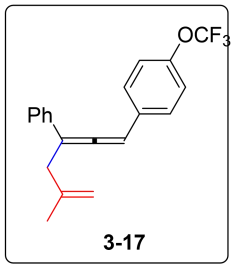
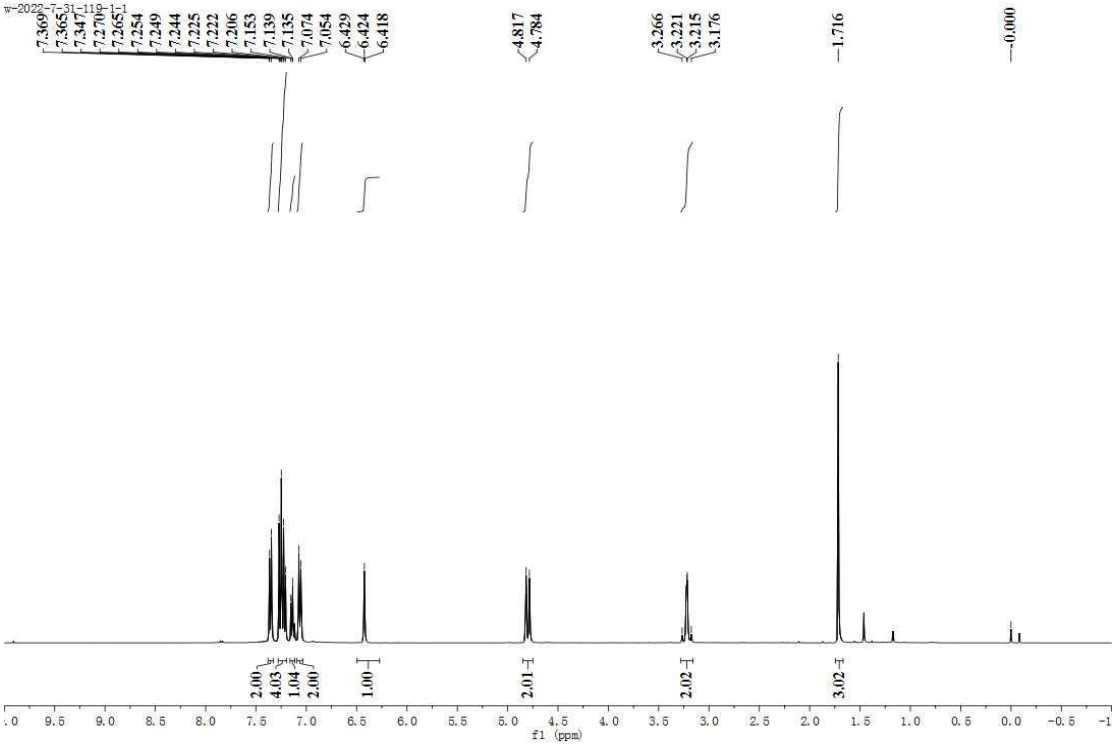
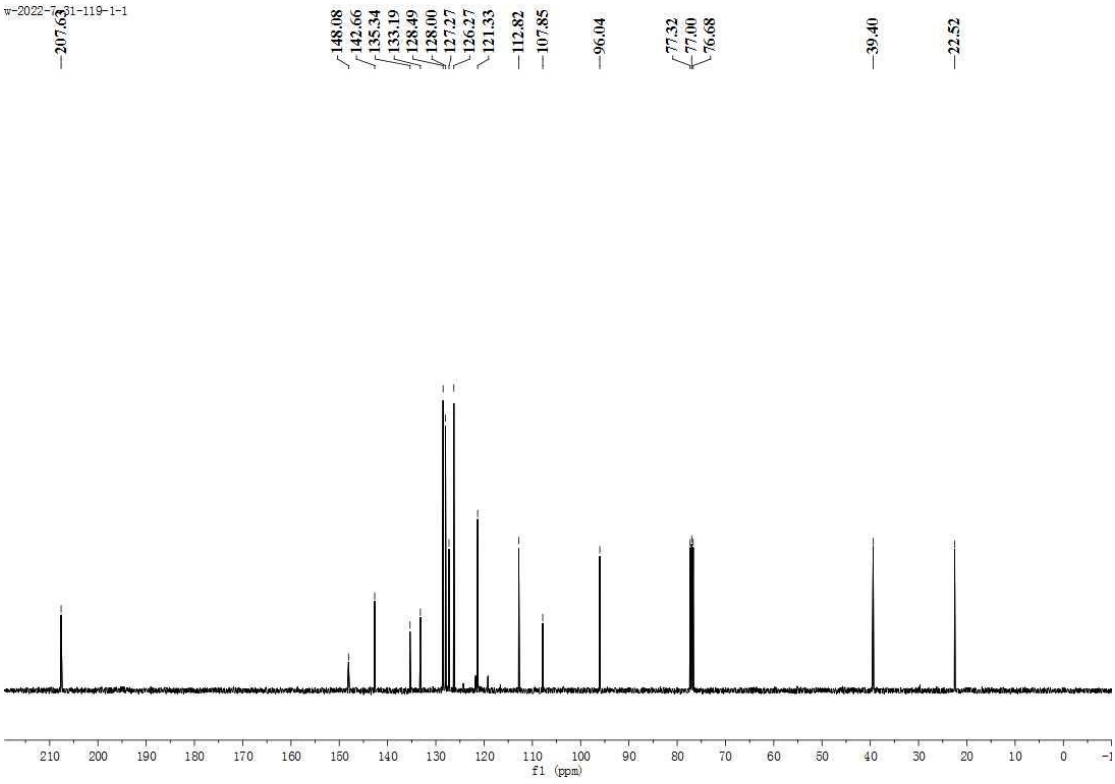
7.539
7.453
7.449
7.437
7.431
7.418
7.336
7.318
7.314
7.302
7.298
7.253
7.250
7.247
7.231
6.554
6.549
6.543
4.905
4.872
3.363
3.321
3.317
3.312
3.273
1.802
0.000
2.03
4.02
2.03
1.01
1.00
2.02
2.00
3.03
f1 (ppm)


w-2022-7-31-118-1
208.31
142.52
138.28
135.08
129.08
128.76
128.54
127.41
126.94
126.30
125.70
125.66
125.63
125.59
122.86
112.94
108.11
96.36
77.32
77.00
76.68
39.34
22.52
f1 (ppm)


OCF3
Ph

3-17


7.369
7.365
7.347
7.270
7.265
7.254
7.249
7.244
7.225
7.222
7.206
7.153
7.139
7.135
7.074
7.054
6.429
6.424
6.418
4.817
4.784
3.266
3.221
3.215
3.176
1.716
0.000
2.00
4.03
1.04
2.00
1.00
2.01
2.02
3.02
f1 (ppm)


207.63
148.08
142.66
135.34
133.19
128.49
128.00
127.27
126.27
121.33
112.82
107.85
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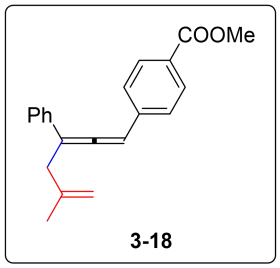
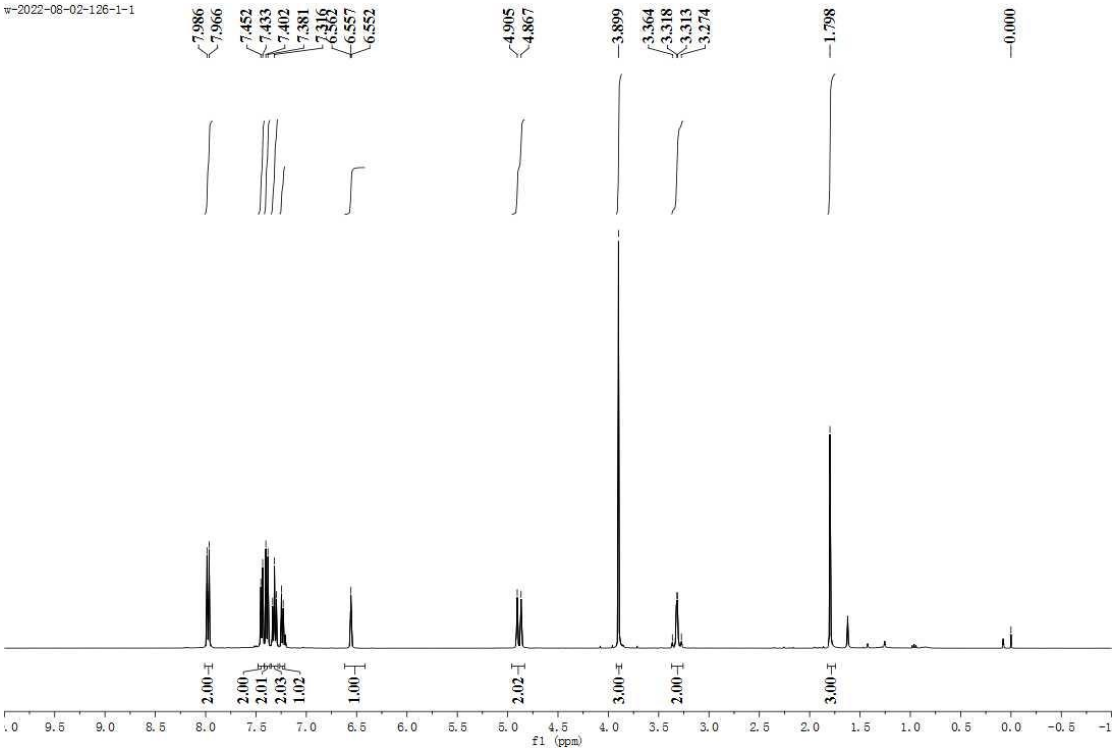
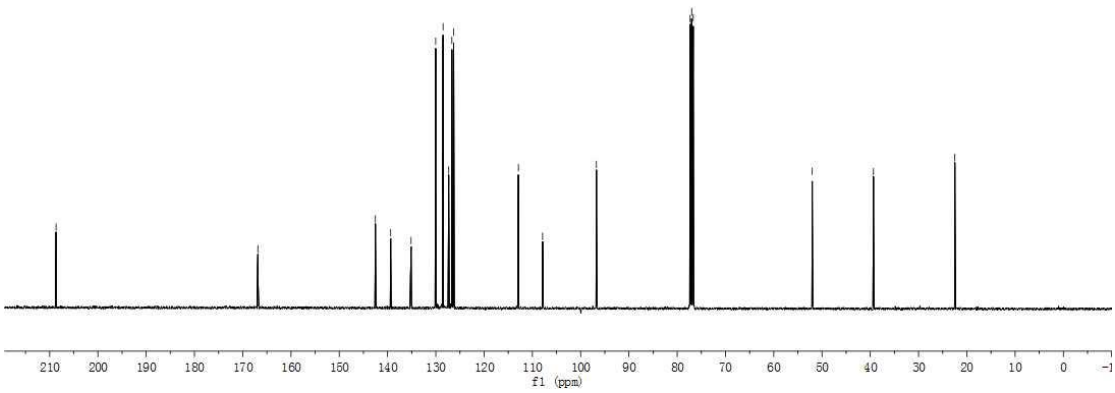
77.00
76.68
39.40
22.52
f1 (ppm)

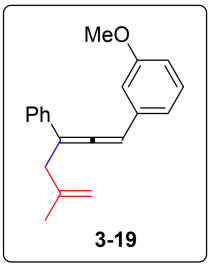

COOMe
Ph

3-18

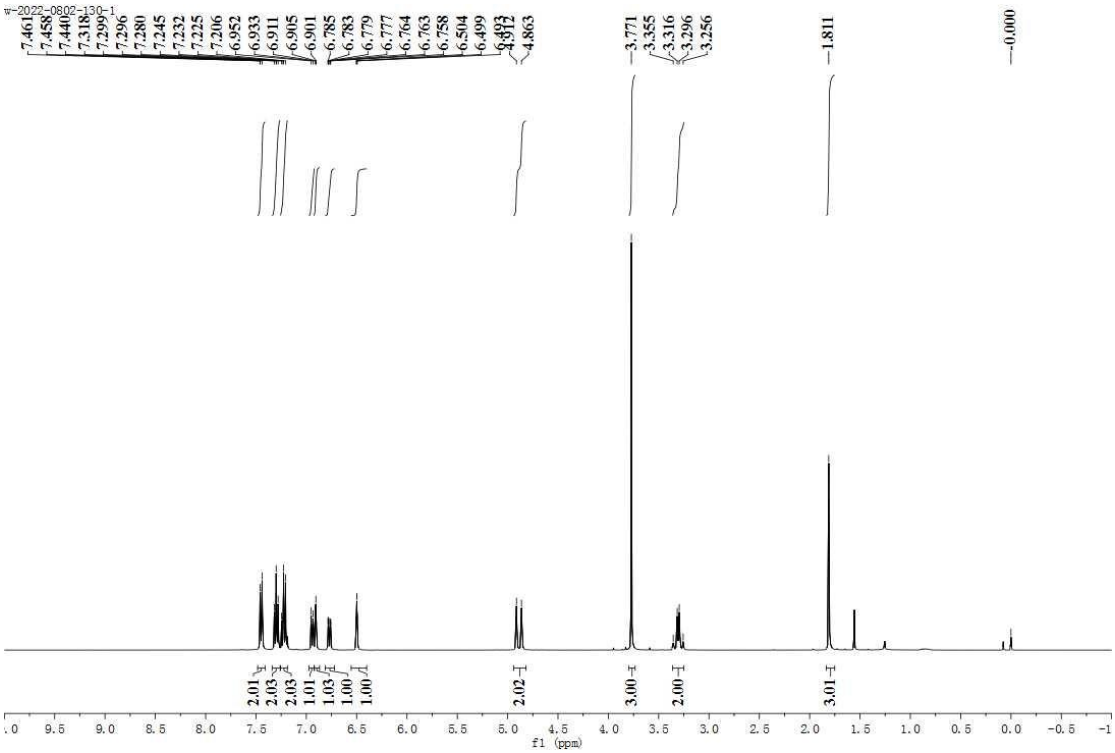

w-2022-08-02-126-1-1
7.986
7.966
7.452
7.433
7.402
7.381
7.316
6.562
6.557
6.552
4.905
4.867
3.899
3.364
3.318
3.313
3.274
1.798
0.000
2.00
2.00
2.01
2.03
1.02
1.00
2.02
3.00
2.00
3.00
f1 (ppm)

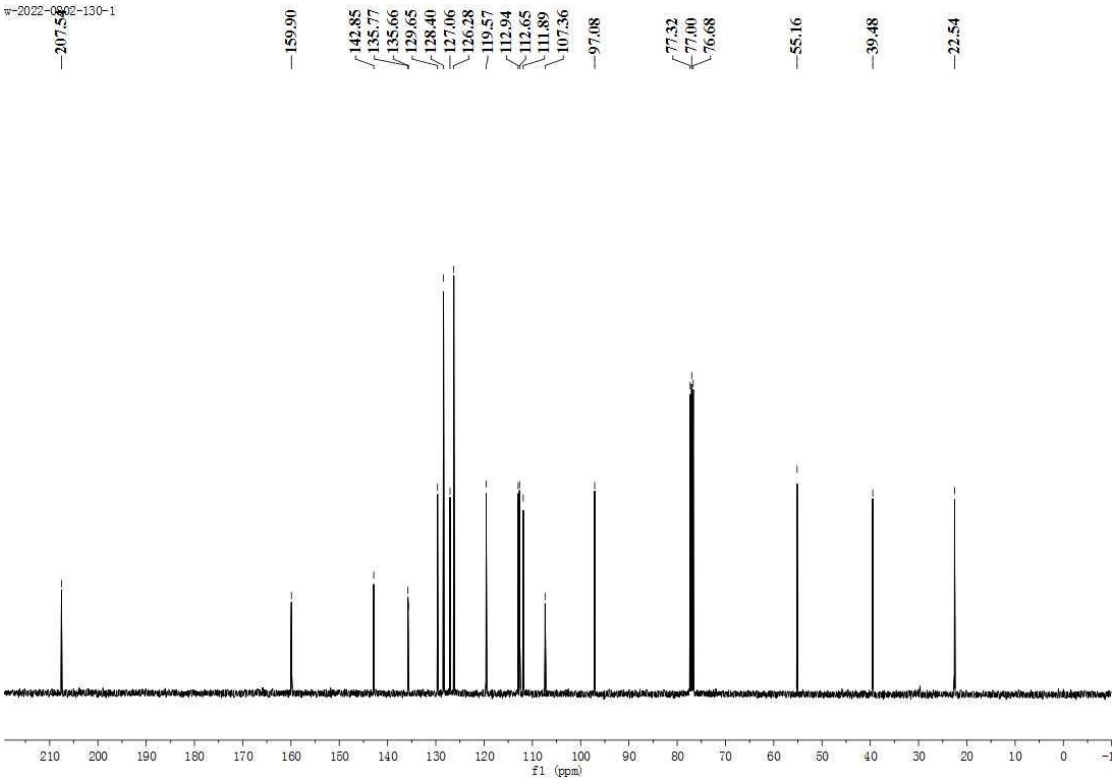

w-2022-08-02-126-1-1
208.68
166.86
142.52
139.35
135.12
130.03
128.55
128.50
127.33
126.68
126.30
112.89
107.88
96.73
77.32
77.00
76.68
52.02
39.35
22.48

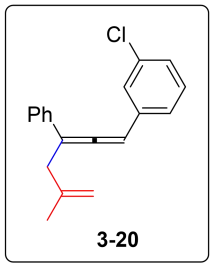

f1 (ppm)


MeO
Ph

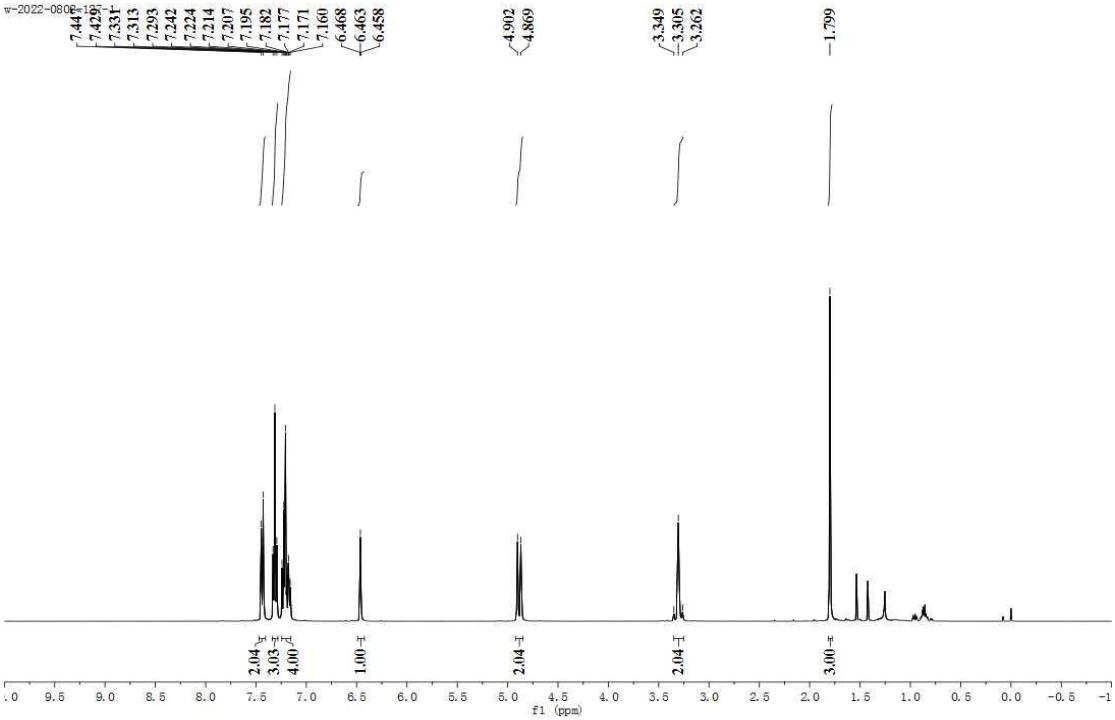
3-19

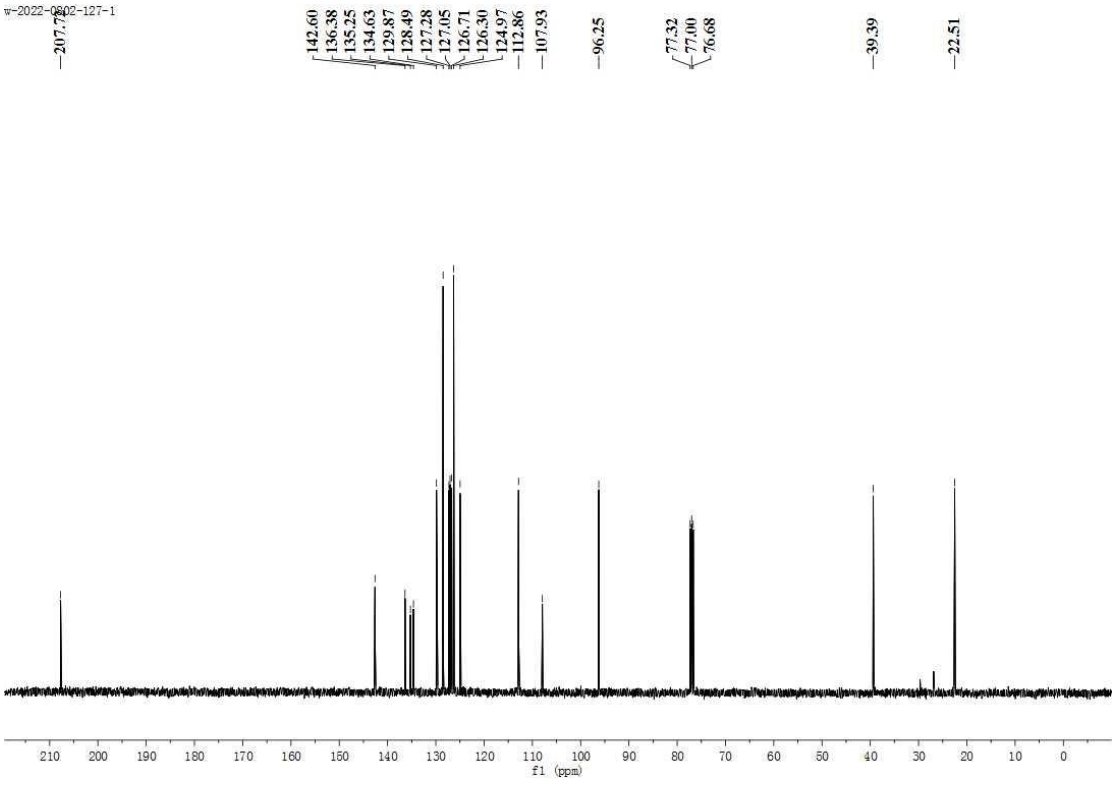

w-2022-0802-130-1
7.461
7.458
7.440
7.318
7.299
7.296
7.280
7.245
7.232
7.225
7.206
6.952
6.933
6.911
6.905
6.901
6.785
6.783
6.779
6.777
6.764
6.763
6.758
6.504
6.499
6.493
4.912
4.863
3.771
3.355
3.316
3.296
3.256
1.811
0.000
2.01
2.03
2.03
1.01
1.03
1.00
1.00
2.02
3.00
2.00
3.01
f1 (ppm)

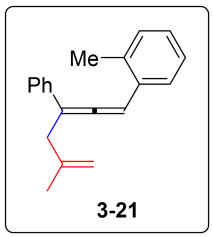

w-2022-0802-130-1
207.58
159.90
142.85
135.77
135.66
129.65
128.40
127.06
126.28
119.57
112.94
112.65
111.89
107.36
97.08
77.32
77.00
76.68
55.16
39.48
22.54
f1 (ppm)


Cl
Ph

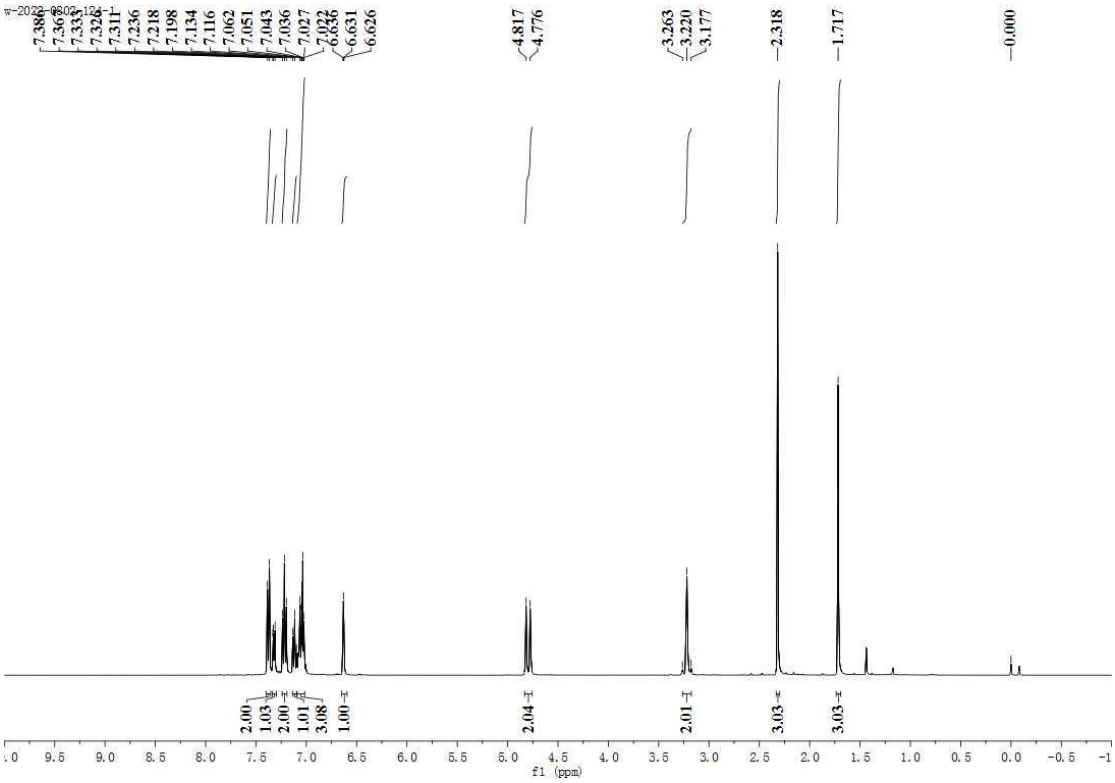
3-20

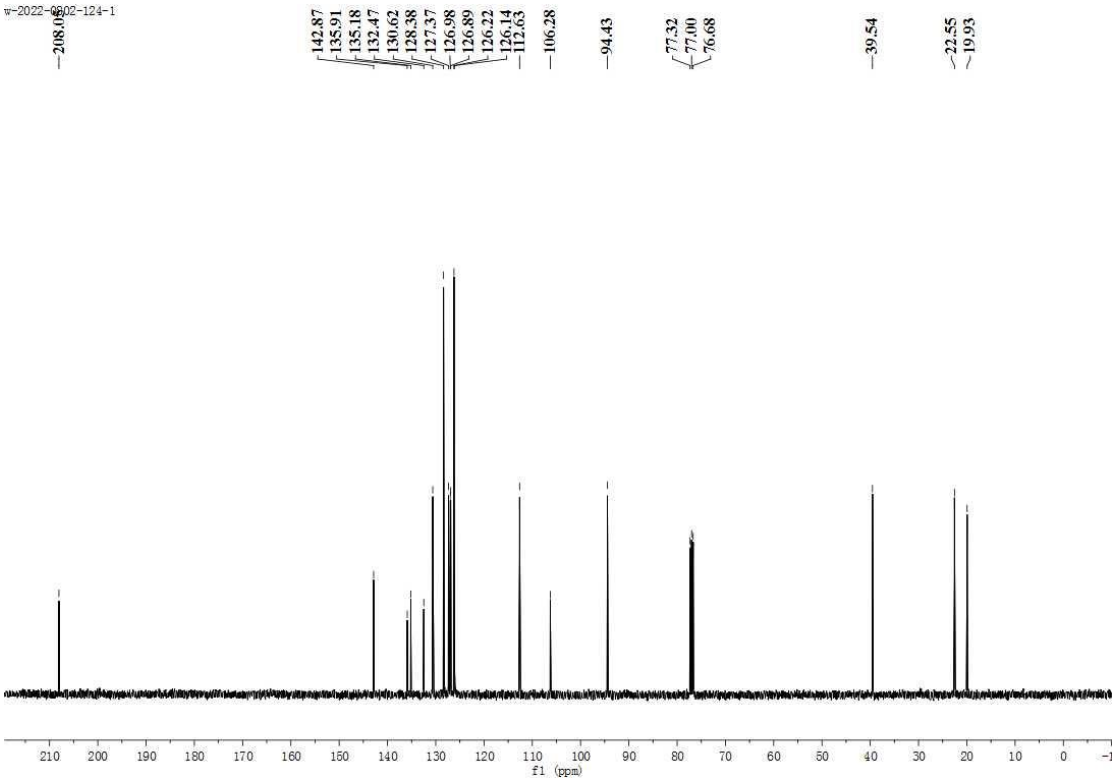

7.443
7.429
7.331
7.313
7.293
7.242
7.224
7.214
7.207
7.195
7.182
7.177
7.171
7.160
6.468
6.463
6.458
4.902
4.869
3.349
3.305
3.262
1.799
2.04
3.03
4.00
1.00
2.04
2.04
3.00
f1 (ppm)

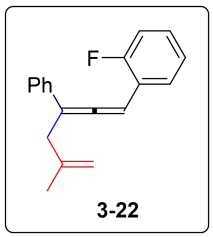

207.77
142.60
136.38
135.25
134.63
129.87
128.49
127.28
127.05
126.71
126.30
124.97
112.86
107.93
96.25
77.32
77.00
76.68
39.39
22.51
f1 (ppm)


Me
Ph

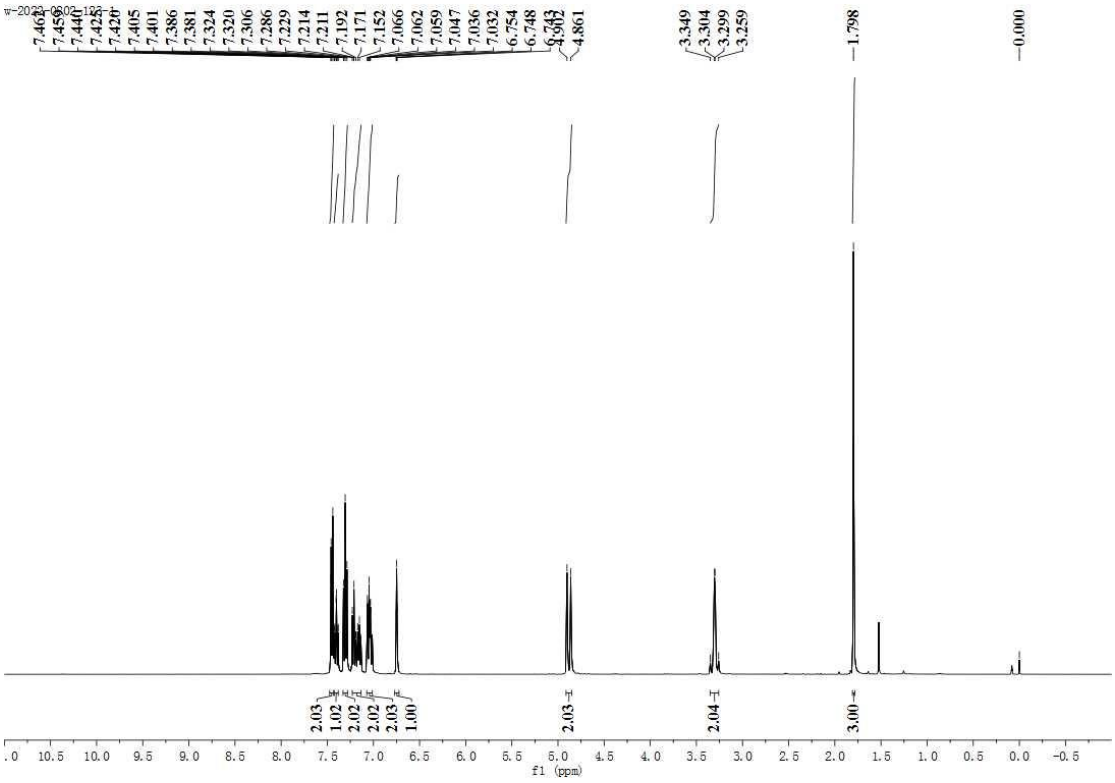
3-21

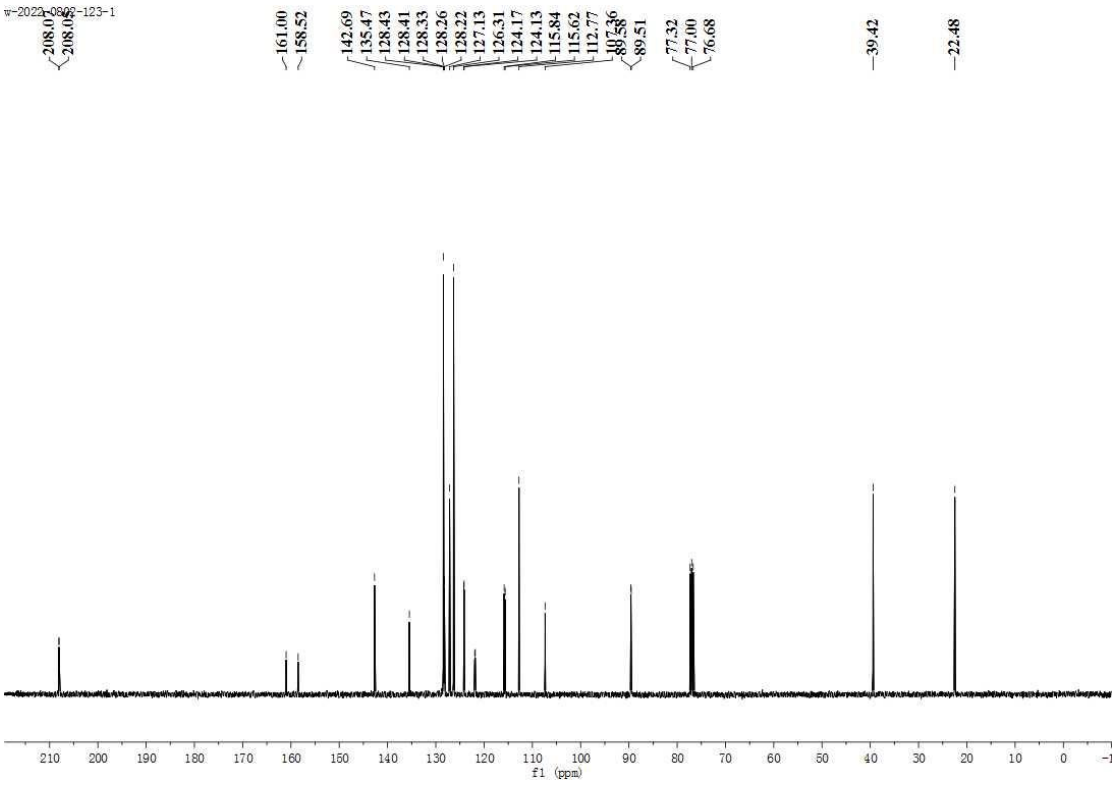

7.386
7.367
7.333
7.324
7.311
7.236
7.218
7.198
7.134
7.116
7.062
7.051
7.043
7.036
7.027
7.022
6.636
6.631
6.626
4.817
4.776
3.263
3.220
3.177
2.318
1.717
0.000
2.00
1.03
2.00
1.01
3.08
1.00
2.04
2.01
3.03
3.03
f1 (ppm)

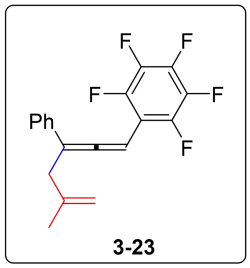

208.07
142.87
135.91
135.18
132.47
130.62
128.38
127.37
126.98
126.89
126.22
126.14
112.63
106.28
94.43
77.32
77.00
76.68
39.54
22.55
19.93
f1 (ppm)


F
Ph

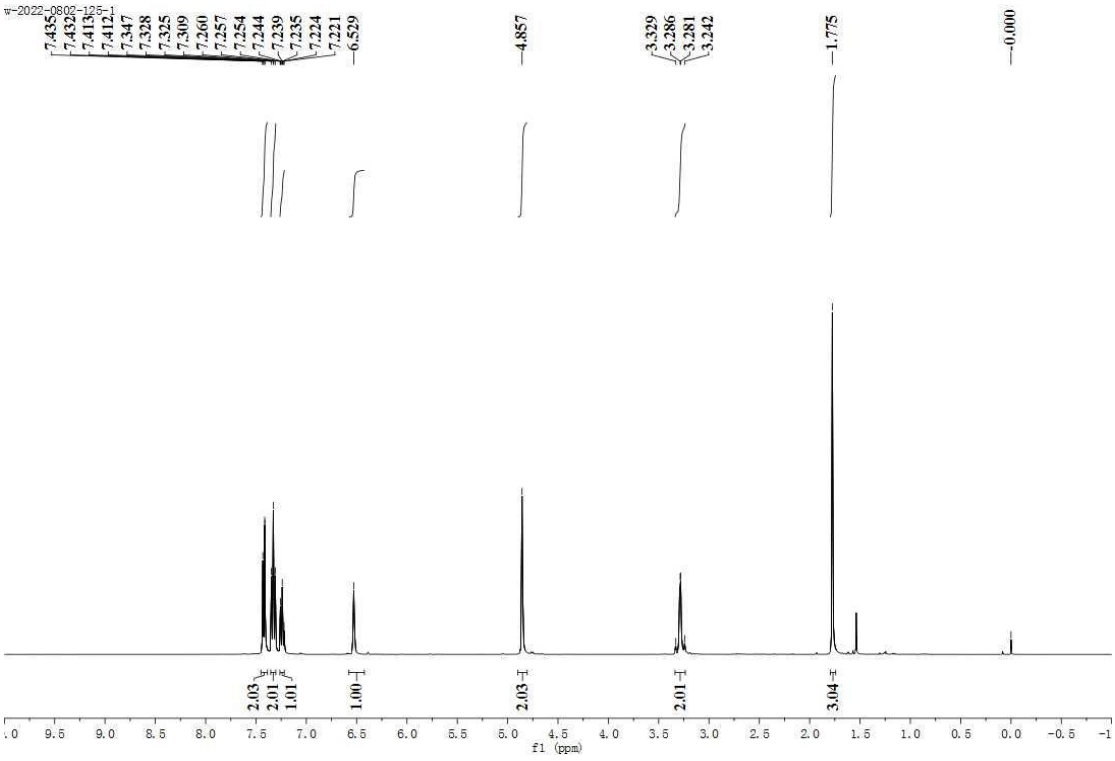
3-22

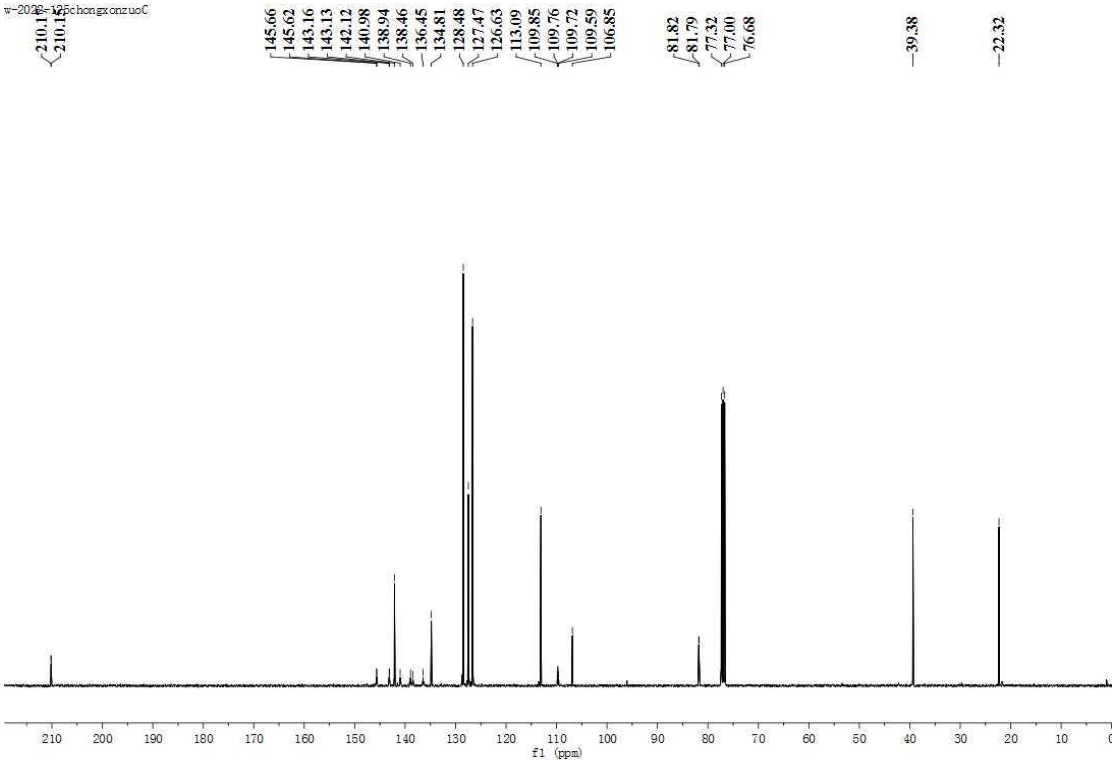

7.463
7.458
7.440
7.425
7.420
7.405
7.401
7.386
7.381
7.324
7.320
7.306
7.286
7.229
7.214
7.211
7.192
7.171
7.152
7.066
7.062
7.059
7.047
7.036
7.032
6.754
6.748
4.861
3.349
3.304
3.299
3.259
1.798
0.000
2.03
1.02
2.02
2.02
2.03
1.00
2.03
2.04
3.00
f1 (ppm)

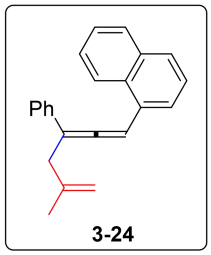

208.01
208.05
161.00
158.52
142.69
135.47
128.43
128.41
128.33
128.26
128.22
127.13
126.31
124.17
124.13
115.84
115.62
112.77
89.58
89.51
77.32
77.00
76.68
39.42
22.48
f1 (ppm)


F
F
F
F
Ph
F

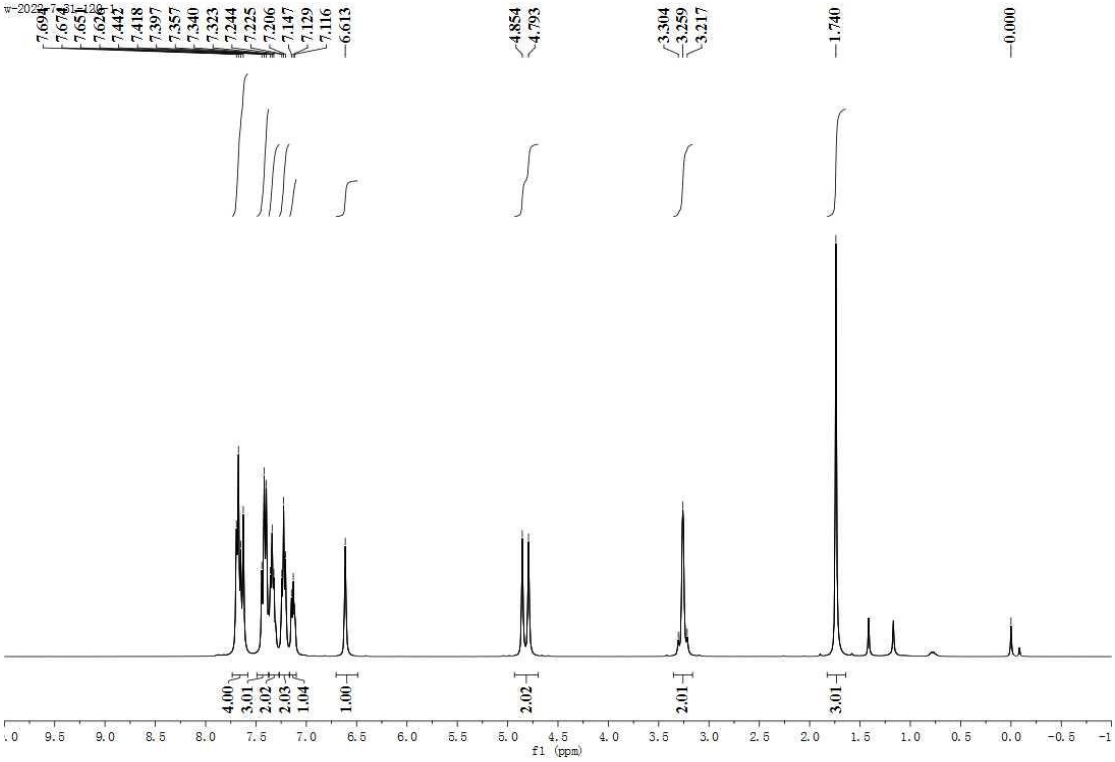
3-23

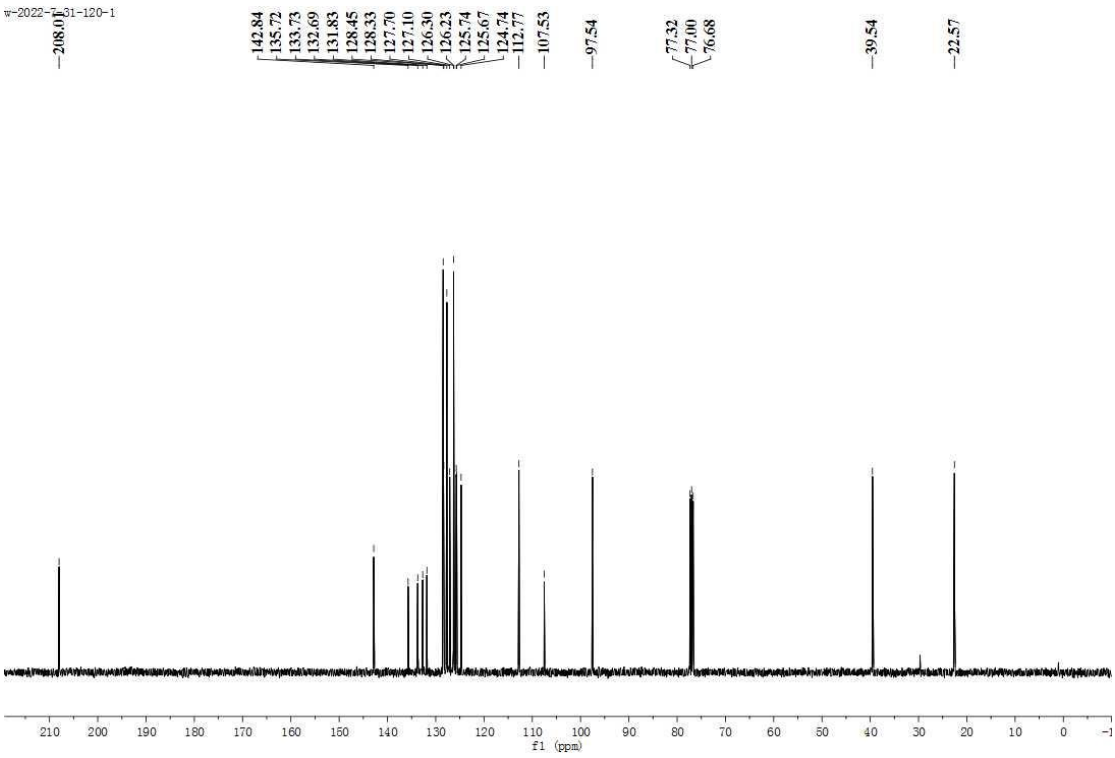

w-2022-0802-125-1
7.435
7.432
7.413
7.412
7.347
7.328
7.325
7.309
7.260
7.257
7.254
7.244
7.239
7.235
7.224
7.221
6.529
4.857
3.329
3.286
3.281
3.242
1.775
0.000
2.03
2.01
1.01
1.00
2.03
2.01
3.04
f1 (ppm)

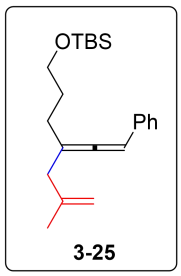

210.11
210.15
145.66
145.62
143.16
143.13
142.12
140.98
138.94
138.46
136.45
134.81
128.48
127.47
126.63
113.09
109.85
109.76
109.72
109.59
106.85
81.82
81.79
77.32
77.00
76.68
39.38
22.32
f1 (ppm)


Ph

3-24

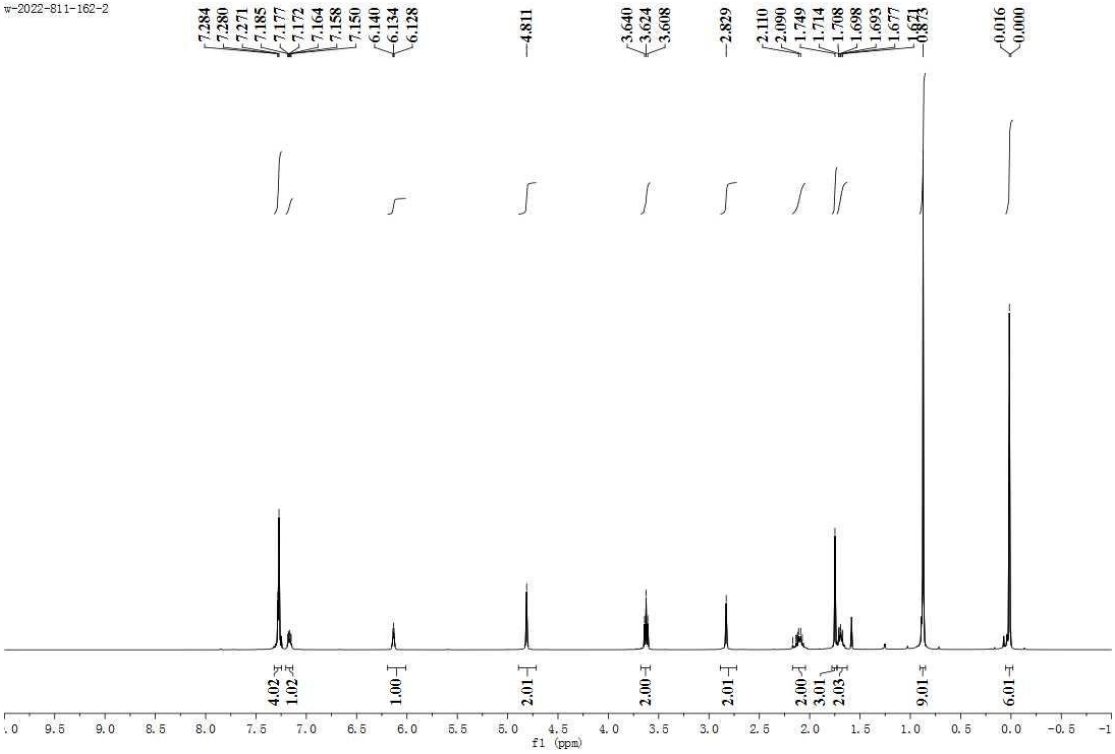

7.694
7.678
7.651
7.624
7.442
7.418
7.397
7.357
7.340
7.323
7.244
7.225
7.206
7.147
7.129
7.116
6.613
4.854
4.793
3.304
3.259
3.217
1.740
0.000
4.00
3.01
2.02
2.03
1.04
1.00
2.02
2.01
3.01
f1 (ppm)


208.01
142.84
135.72
133.73
132.69
131.83
128.45
128.33
127.70
127.10
126.30
126.23
125.74
125.67
124.74
112.77
107.53
97.54
77.32
77.00
76.68
39.54
22.57
f1 (ppm)

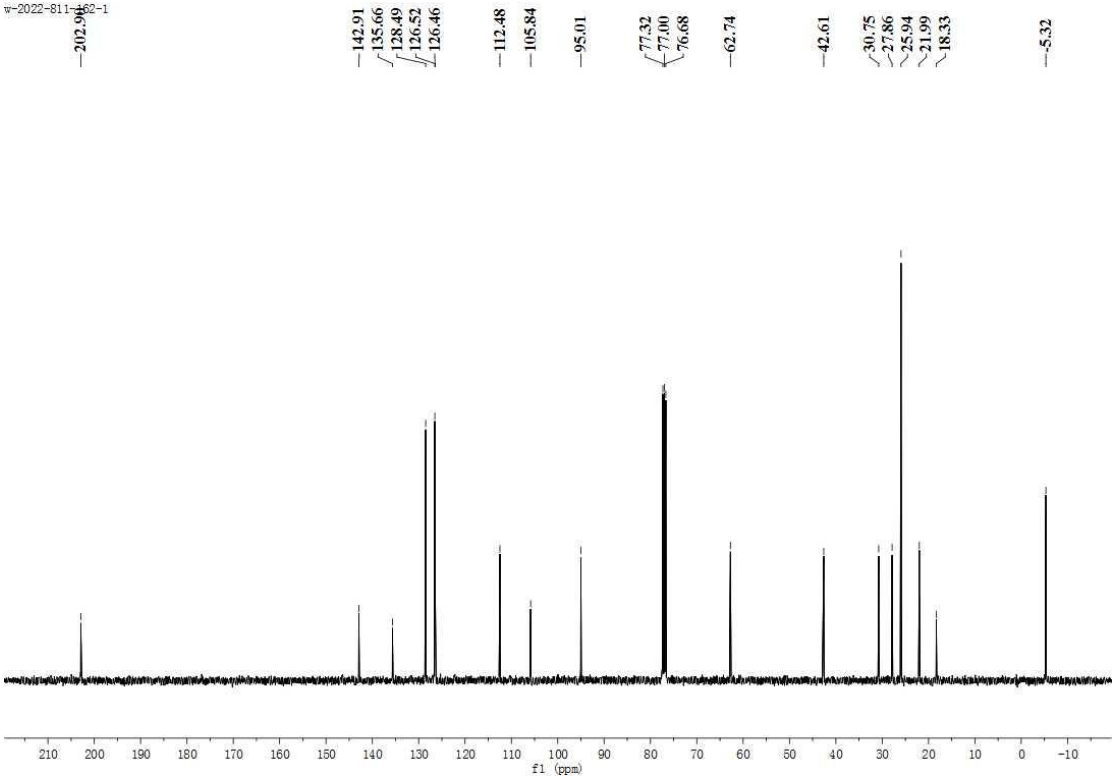


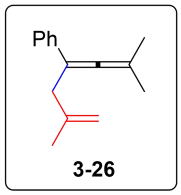
3-25

w-2022-811-162-2

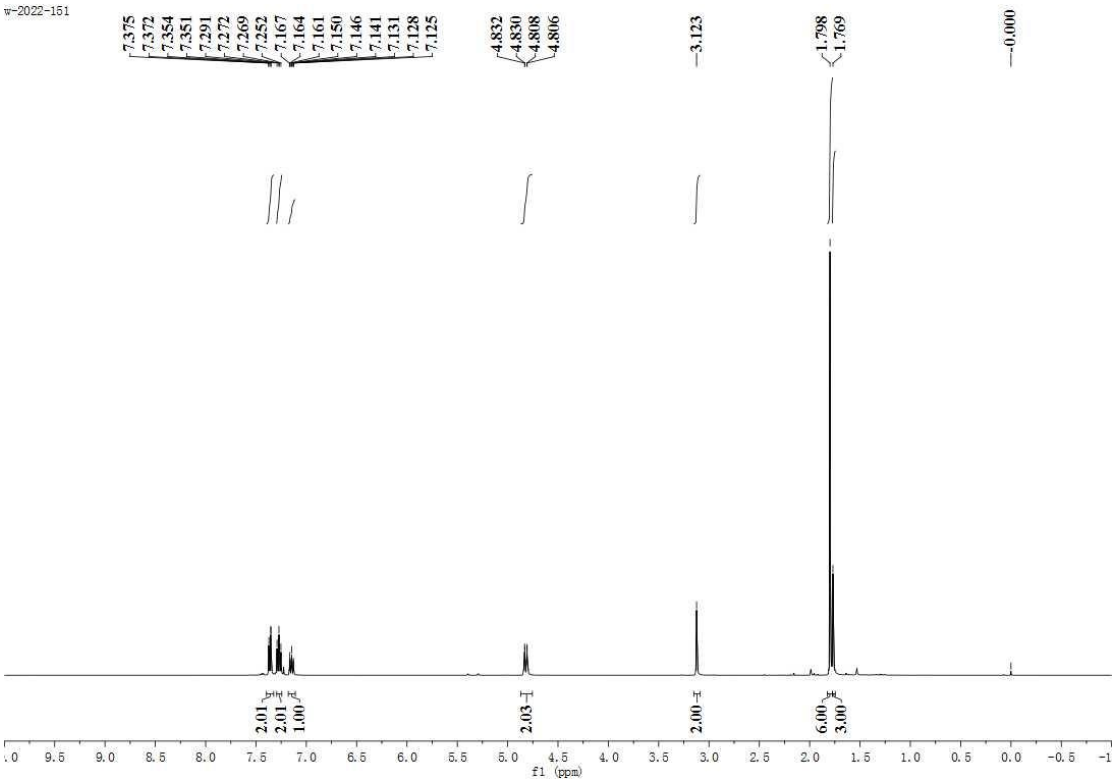


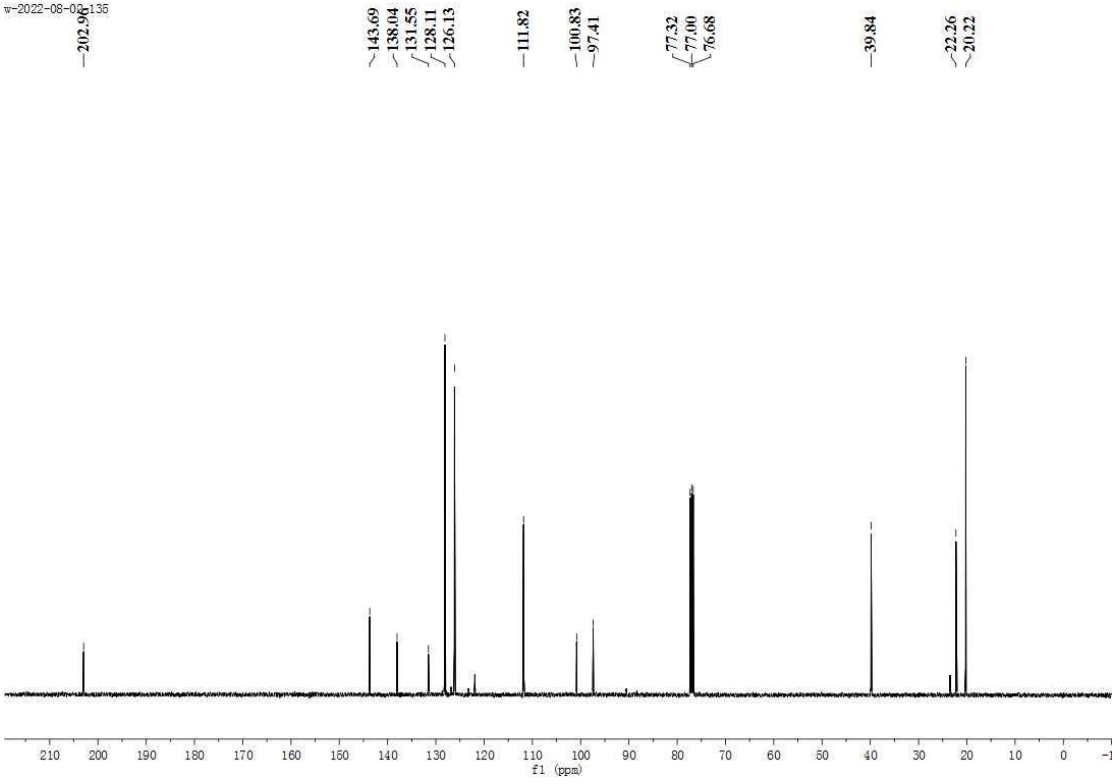
w-2022-811-162-1

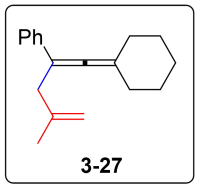



Ph

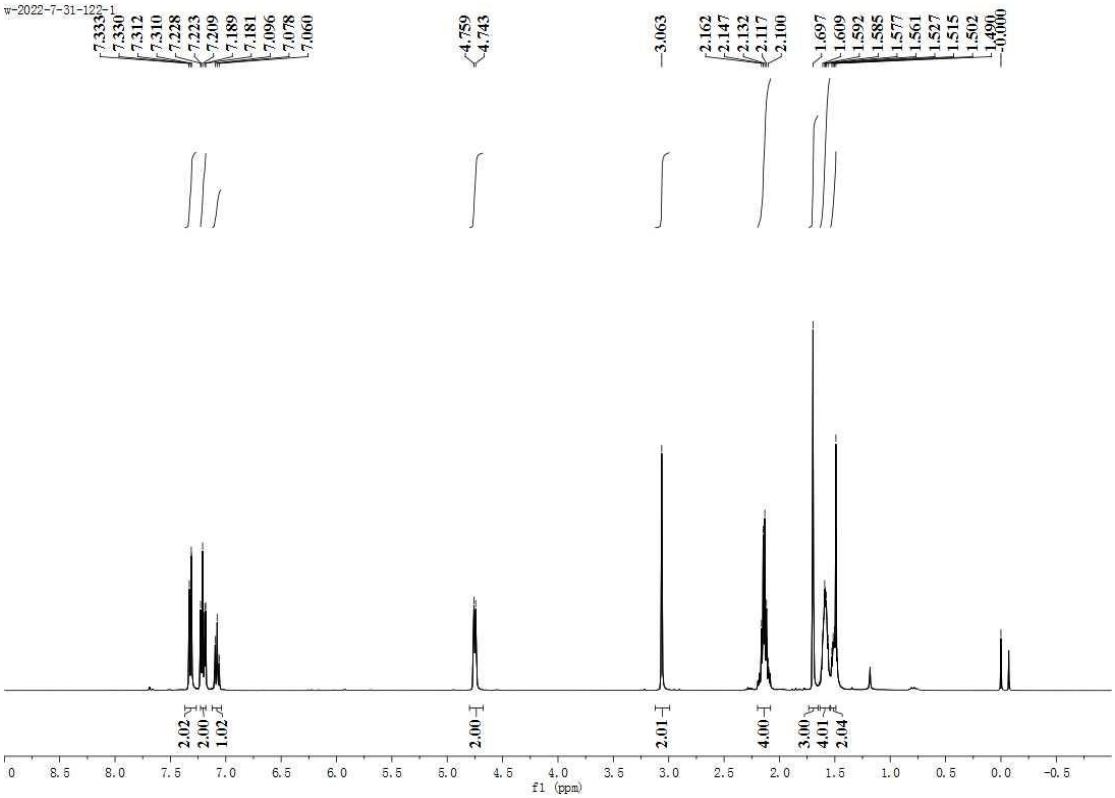
3-26

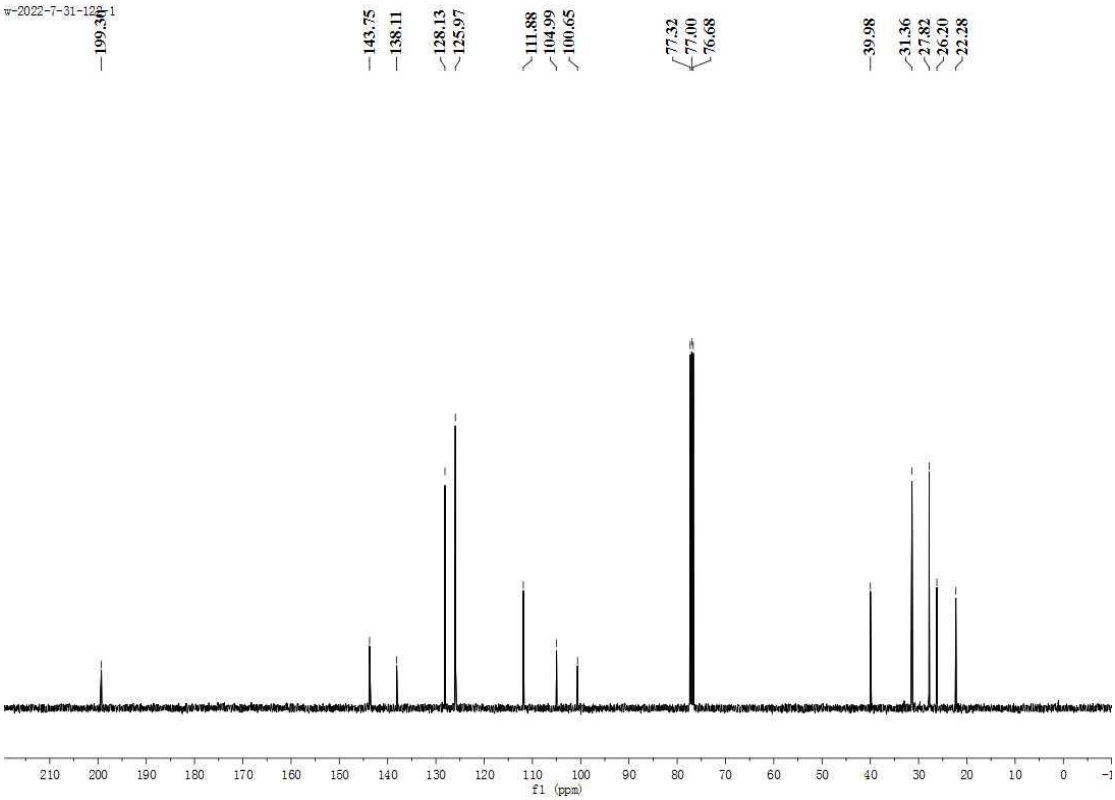

w-2022-151
7.375
7.372
7.354
7.351
7.291
7.272
7.269
7.252
7.167
7.164
7.161
7.150
7.146
7.141
7.131
7.128
7.125
4.832
4.830
4.808
4.806
3.123
1.798
1.769
0.000
2.01
2.01
1.00
2.03
2.00
6.00
3.00
f1 (ppm)

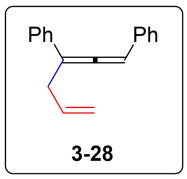

w-2022-08-03-136
202.96
143.69
138.04
131.55
128.11
126.13
111.82
100.83
97.41
77.32
77.00
76.68
39.84
22.26
20.22
f1 (ppm)


Ph

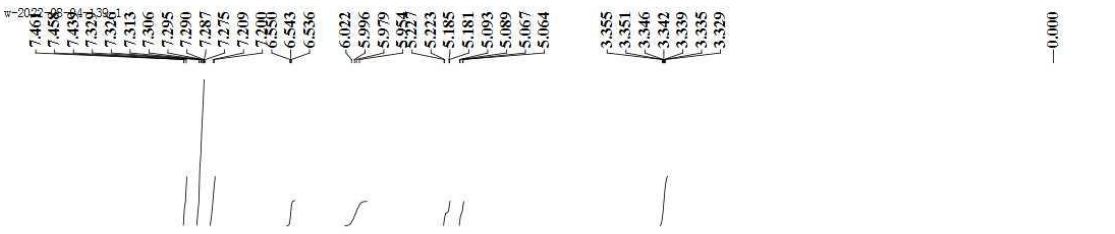
3-27

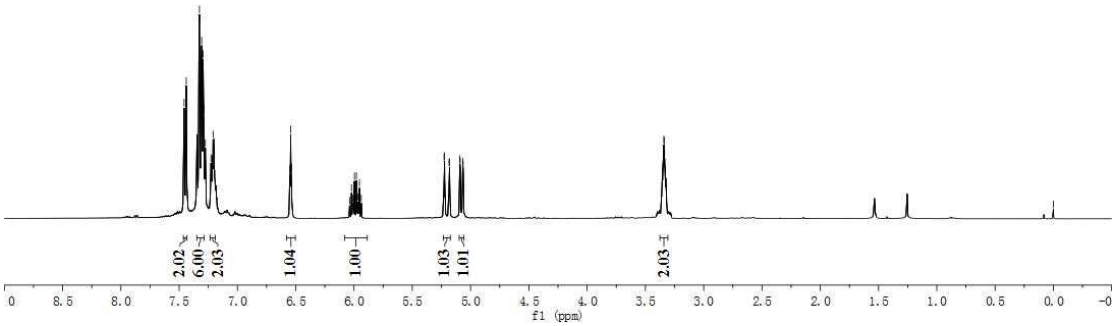

w-2022-7-31-122-1
7.333
7.330
7.312
7.310
7.228
7.223
7.209
7.189
7.181
7.096
7.078
7.060
4.759
4.743
3.063
2.162
2.147
2.132
2.117
2.100
1.697
1.609
1.592
1.585
1.577
1.561
1.527
1.515
1.502
1.490
-0.000
2.02
2.00
1.02
2.00
2.01
4.00
3.00
4.01
2.04
f1 (ppm)

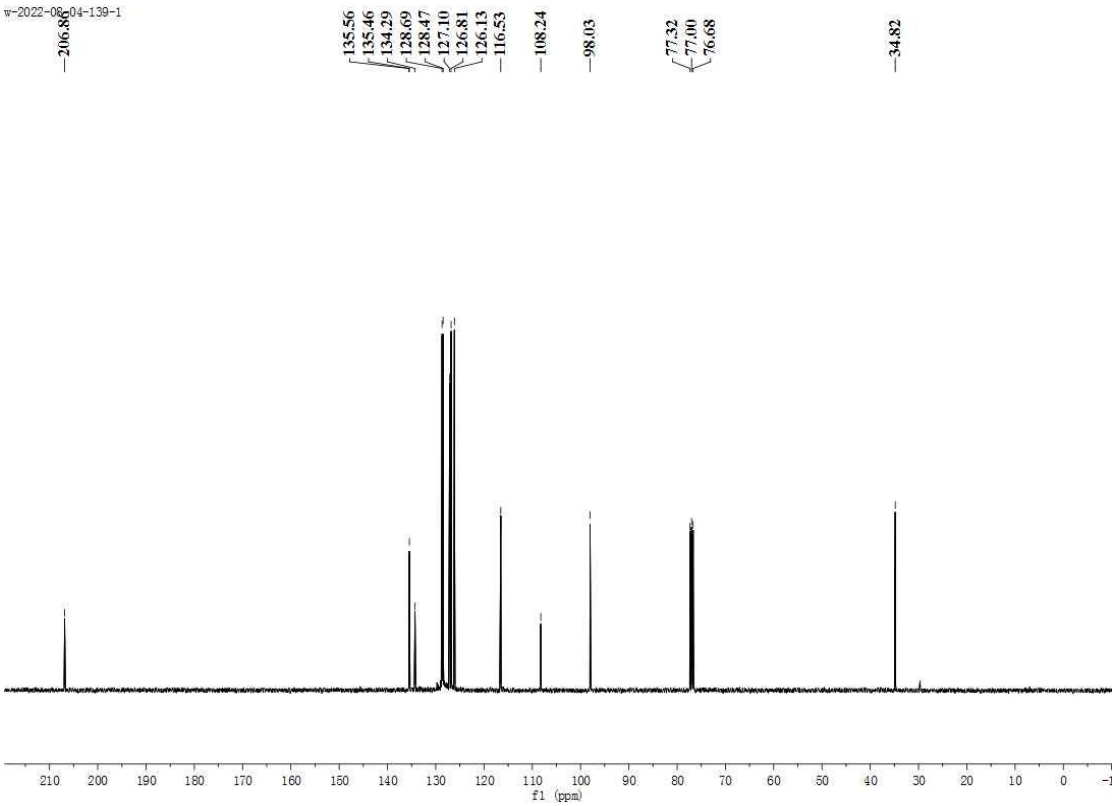

w-2022-7-31-122-1
199.36
143.75
138.11
128.13
125.97
111.88
104.99
100.65
77.32
77.00
76.68
39.98
31.36
27.82
26.20
22.28
f1 (ppm)

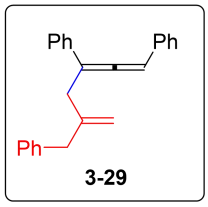

Ph
Ph

3-28

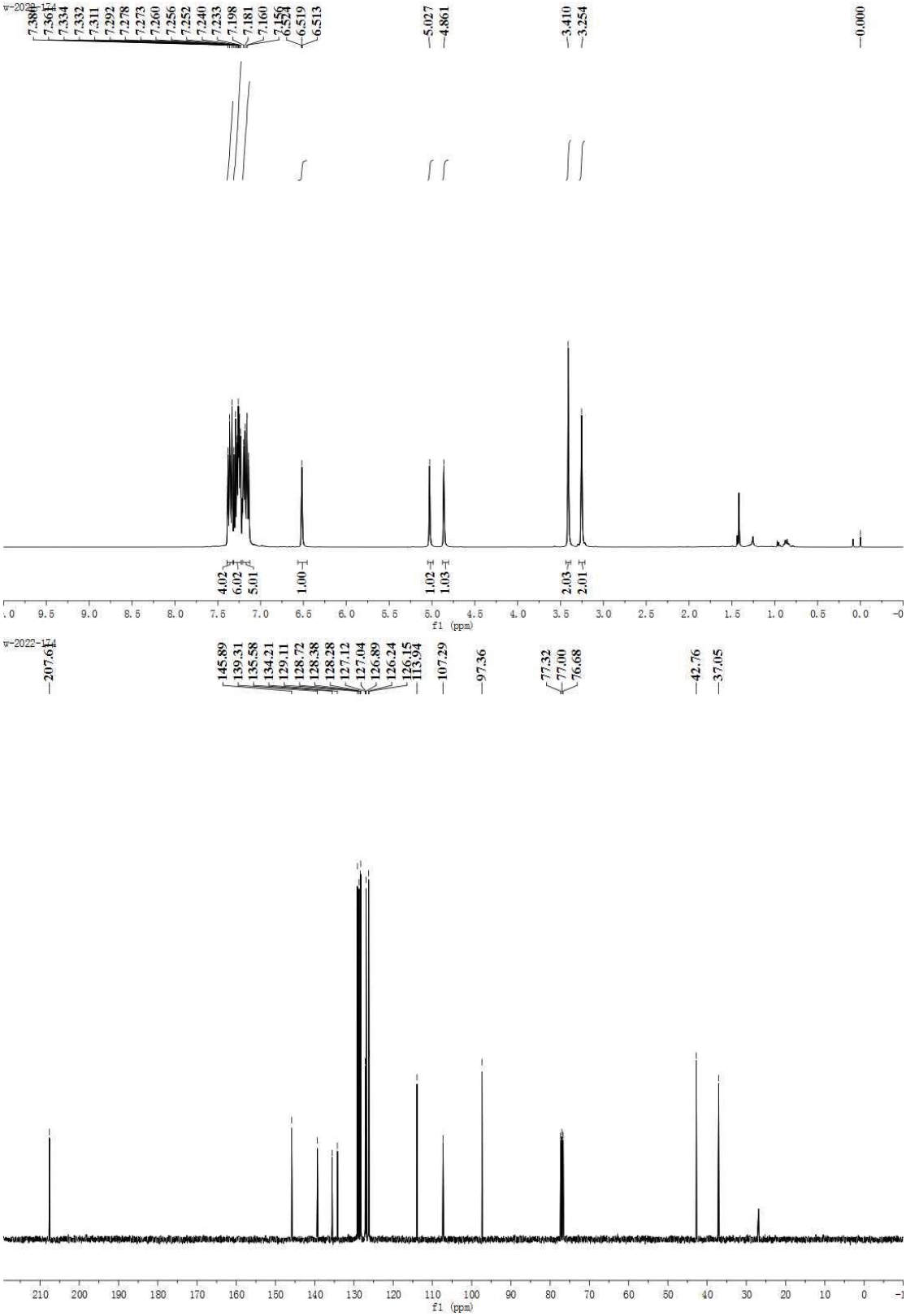

7.461
7.450
7.436
7.329
7.322
7.313
7.306
7.295
7.290
7.287
7.275
7.209
6.543
6.536
6.022
5.996
5.979
5.954
5.227
5.223
5.185
5.181
5.093
5.089
5.067
5.064
3.355
3.351
3.346
3.342
3.339
3.335
3.329
0.000


2.02
6.00
2.03
1.04
1.00
1.03
1.01
2.03
f1 (ppm)


w-2022-08-04-139-1
206.86
135.56
135.46
134.29
128.69
128.47
127.10
126.81
126.13
116.53
108.24
98.03
77.32
77.00
76.68
34.82
f1 (ppm)


Ph
Ph
Ph

3-29


w-2022-174
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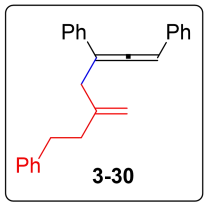
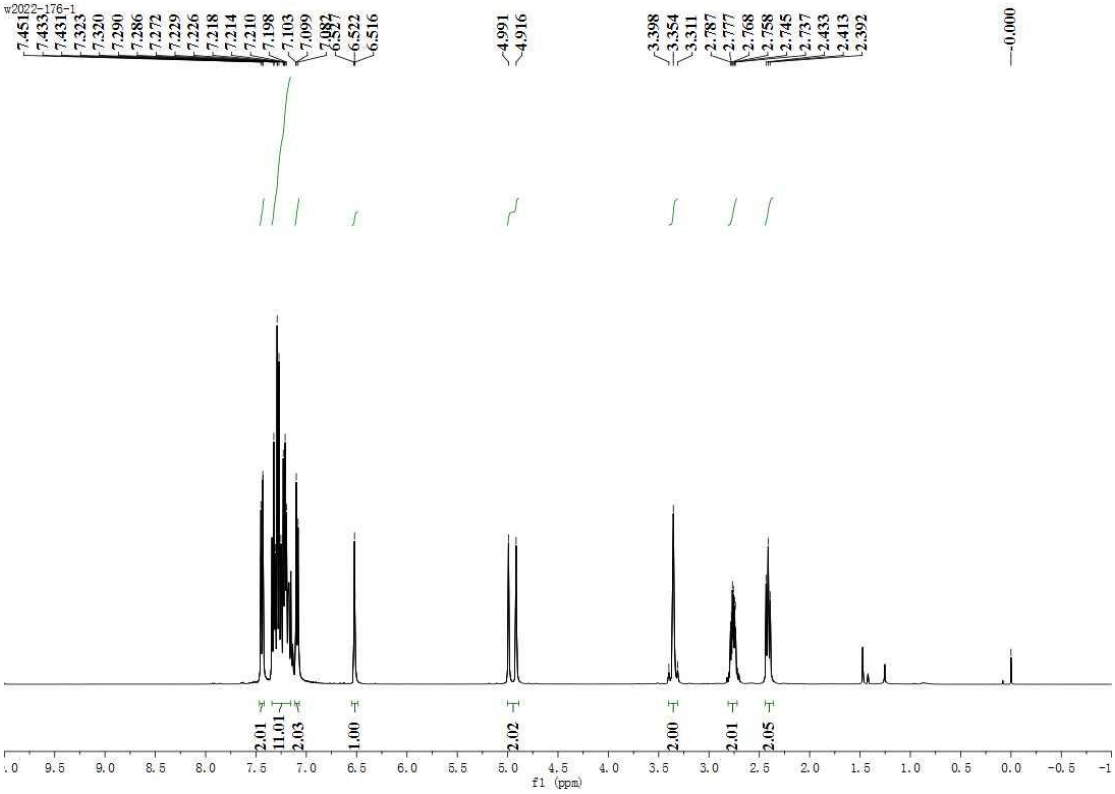
7.361
7.334
7.332
7.311
7.292
7.278
7.273
7.260
7.256
7.252
7.240
7.233
7.198
7.181
7.160
6.524
6.519
6.513
5.027
4.861
3.410
3.254
0.000
4.02
6.02
5.01
1.00
1.02
1.03
2.03
2.01
f1 (ppm)
w-2022-174
207.61
145.89
139.31
135.58
134.21
129.11
128.72
128.38
128.28
127.12
127.04
126.89
126.24
126.15
113.94
107.29
97.36
77.32
77.00
76.68
42.76
37.05
f1 (ppm)


Ph
Ph
Ph

3-30


w2022-176-1
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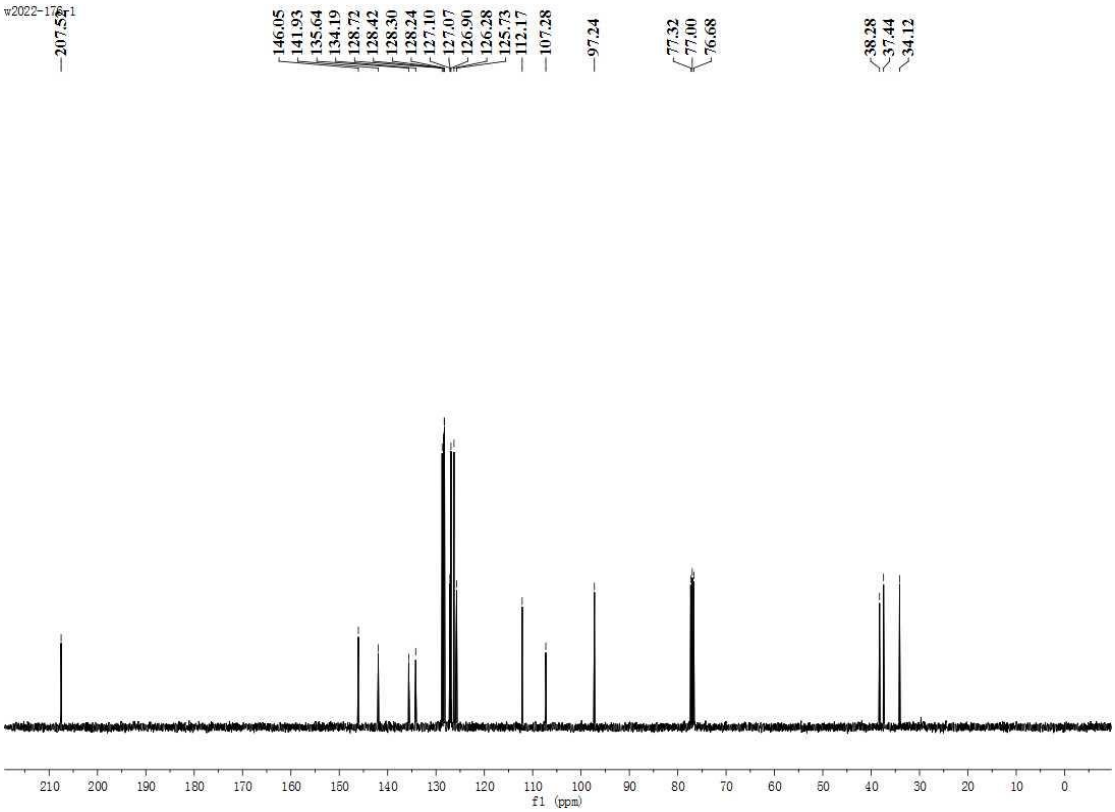
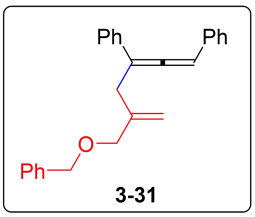
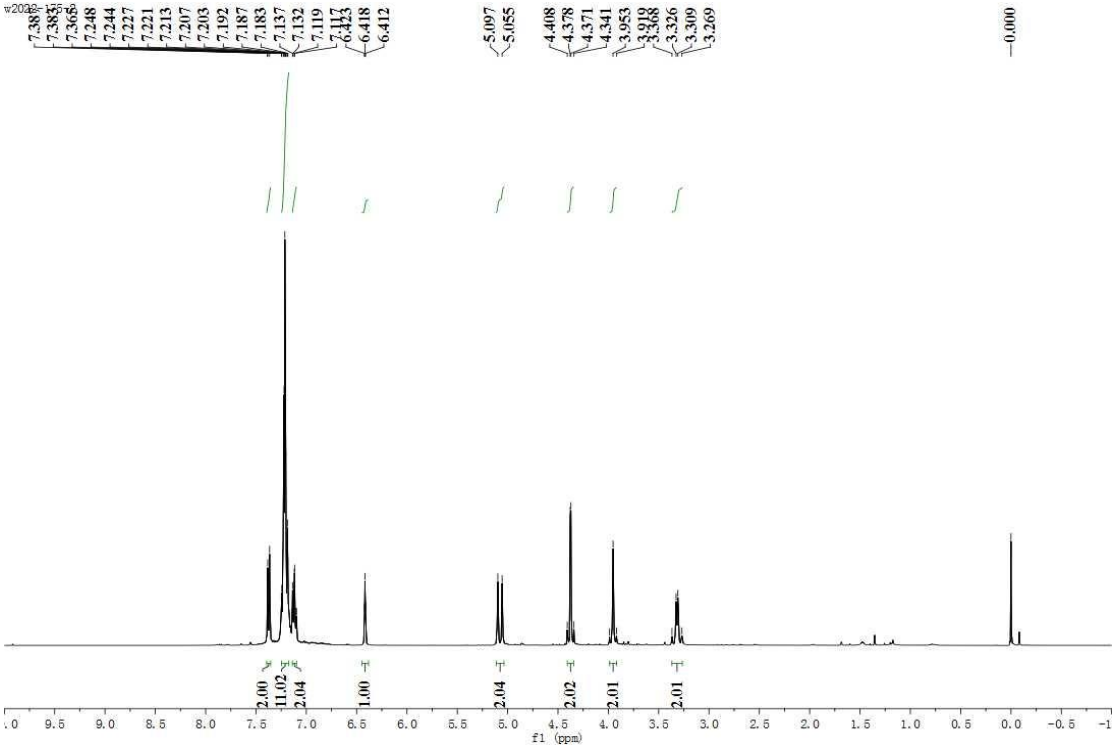
7.431
7.323
7.320
7.290
7.286
7.272
7.229
7.226
7.218
7.214
7.210
7.198
7.103
7.099
6.522
6.516
4.991
4.916
3.398
3.354
3.311
2.787
2.777
2.768
2.758
2.745
2.737
2.433
2.413
2.392
0.000
2.01
11.01
2.03
1.00
2.02
2.00
2.01
2.05
f1 (ppm)


w2022-176-1
207.52
146.05
141.93
135.64
134.19
128.72
128.42
128.30
128.24
127.10
127.07
126.90
126.28
125.73
112.17
107.28
97.24
77.32
77.00
76.68
38.28
37.44
34.12
f1 (ppm)


Ph
Ph
O
Ph

3-31


7.388
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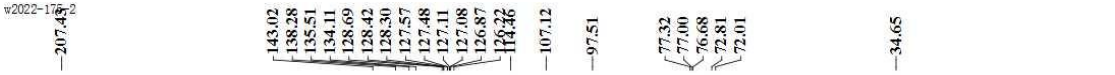
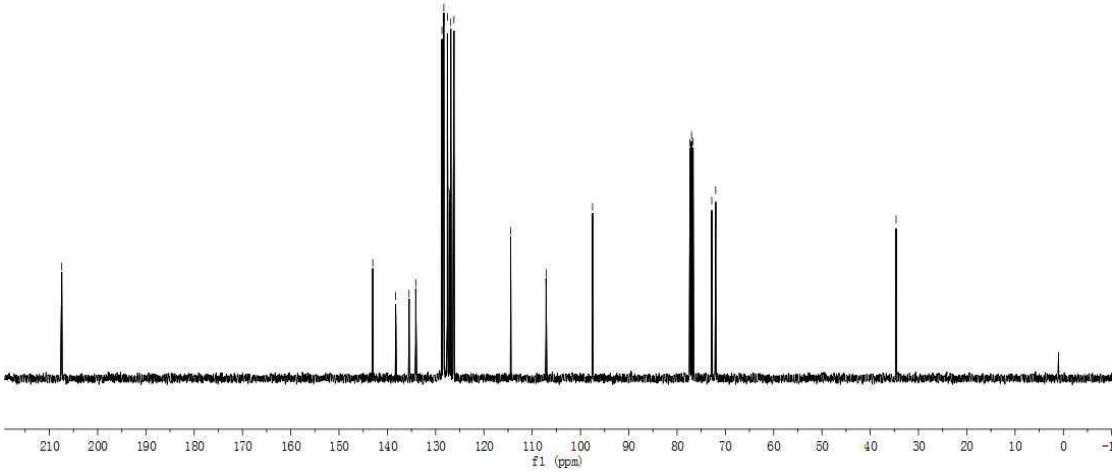
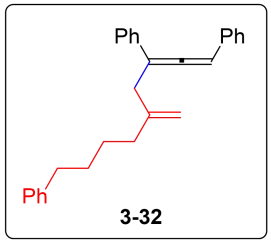
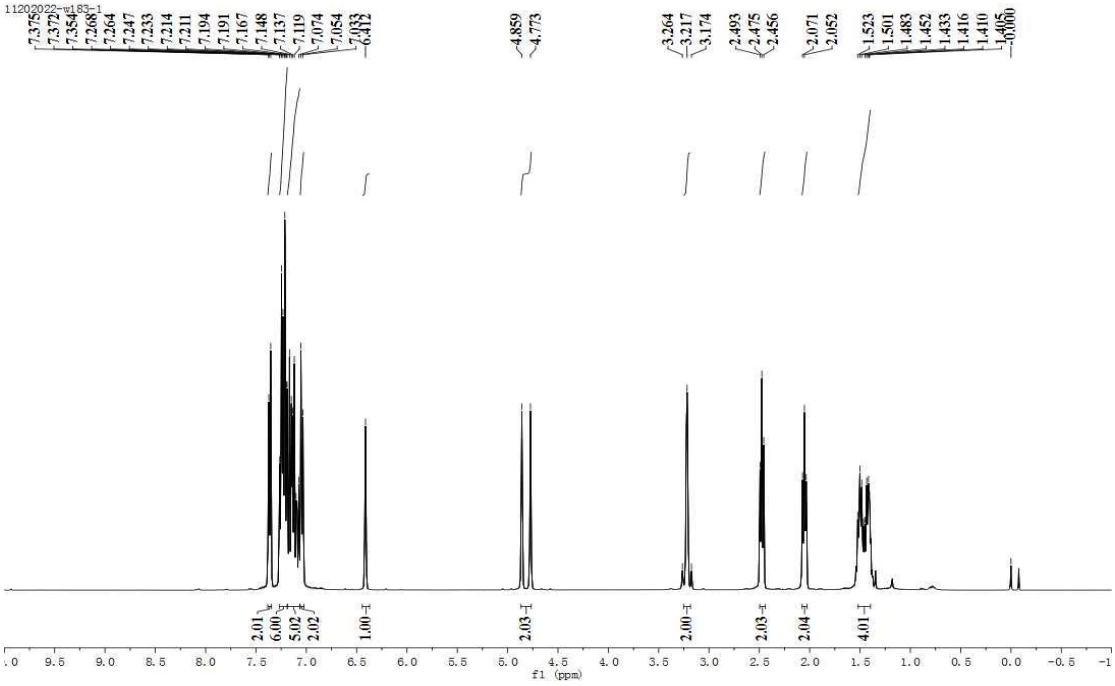
7.365
7.248
7.244
7.227
7.221
7.213
7.207
7.203
7.192
7.187
7.183
7.137
7.132
7.119
7.117
6.423
6.418
6.412
5.097
5.055
4.408
4.378
4.371
4.341
3.953
3.919
3.368
3.326
3.309
3.269
0.000
2.00
11.02
2.04
1.00
2.04
2.02
2.01
2.01
f1 (ppm)

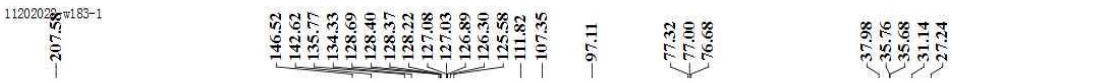

w2022-175-2
207.43
143.02
138.28
135.51
134.11
128.69
128.42
128.30
127.57
127.48
127.11
127.08
126.87
126.22
114.46
107.12
97.51
77.32
77.00
76.68
72.81
72.01
34.65

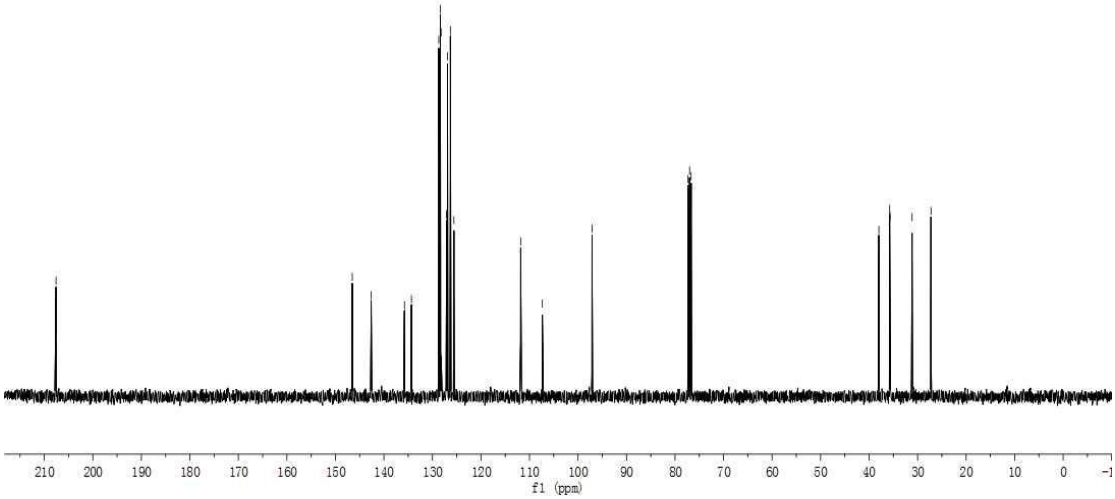

f1 (ppm)

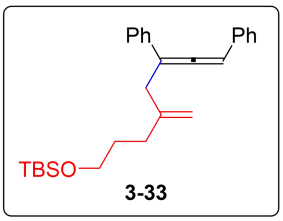


3-32

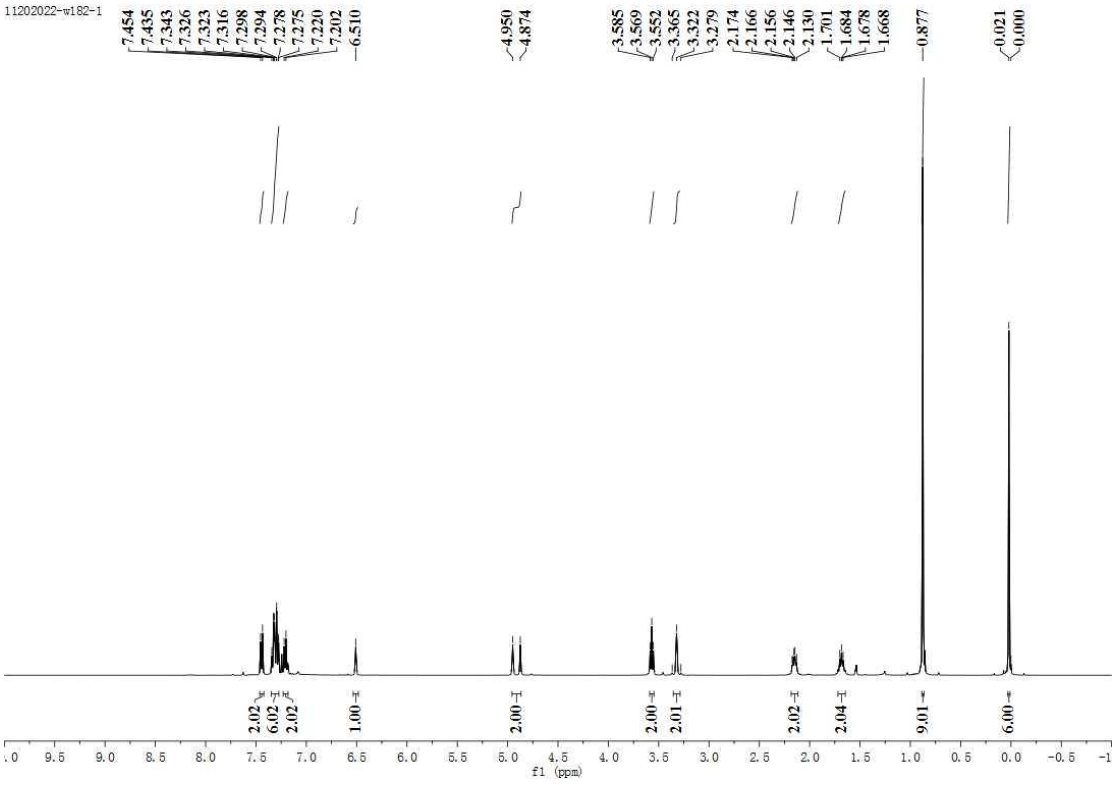


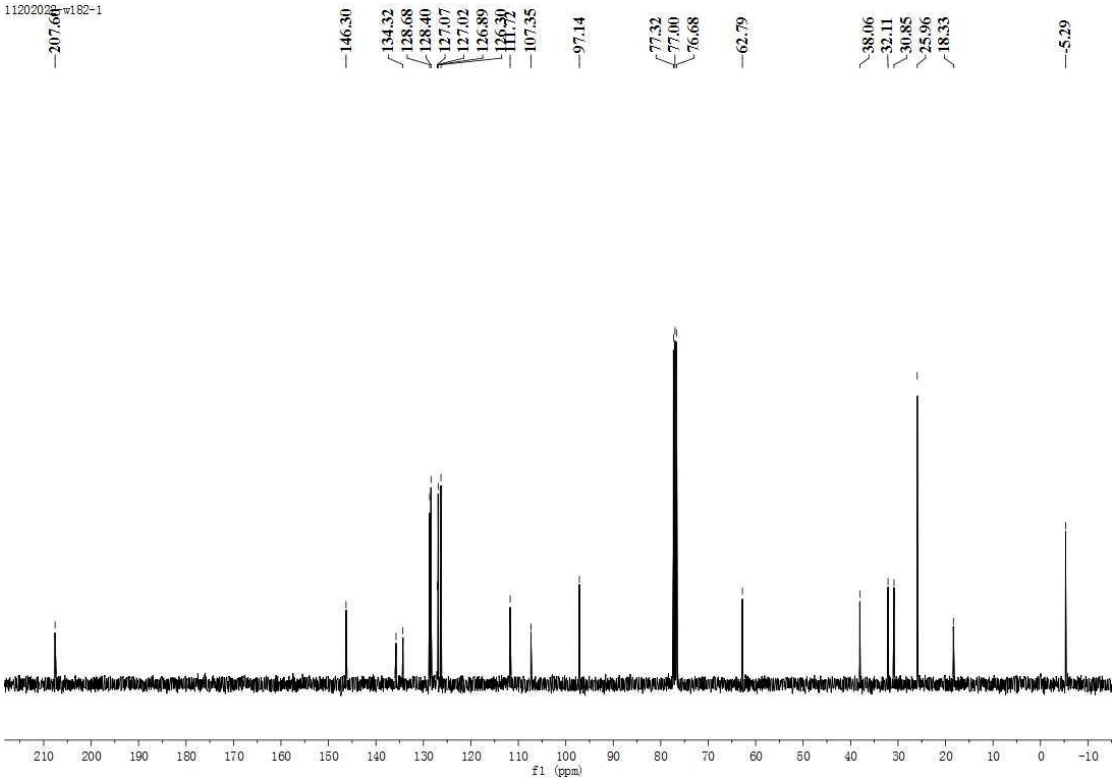


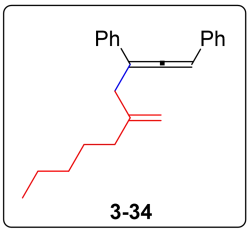



Ph
Ph
TBSO

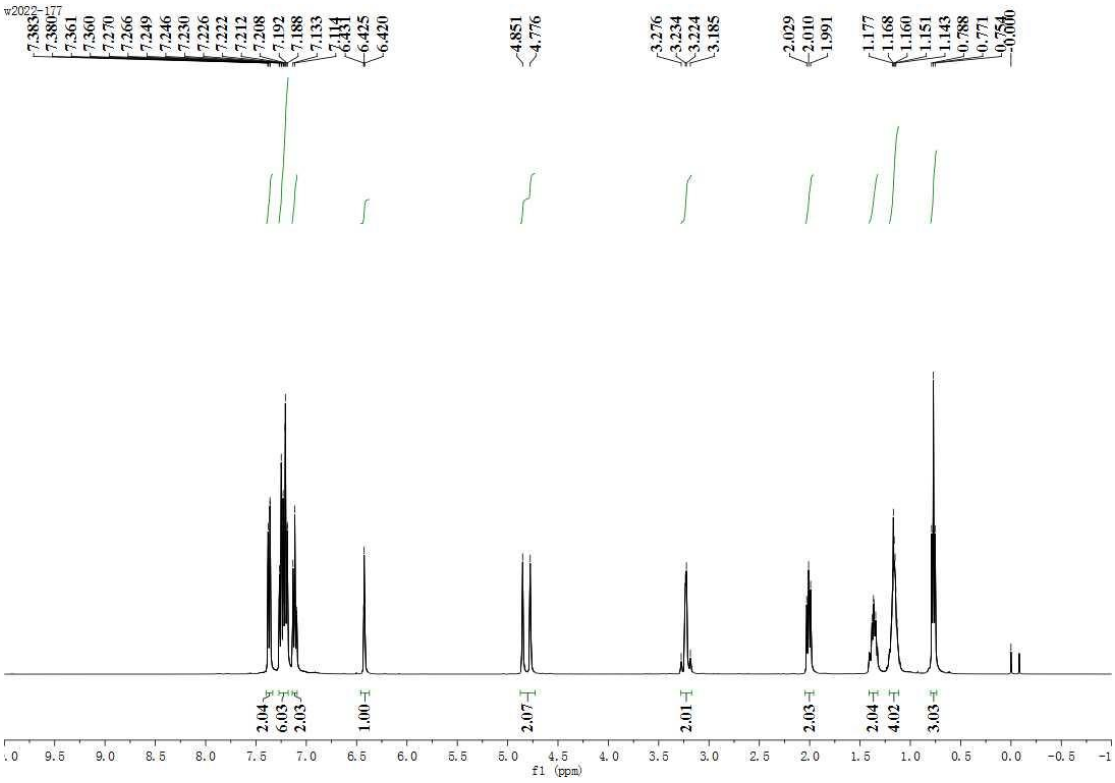
3-33

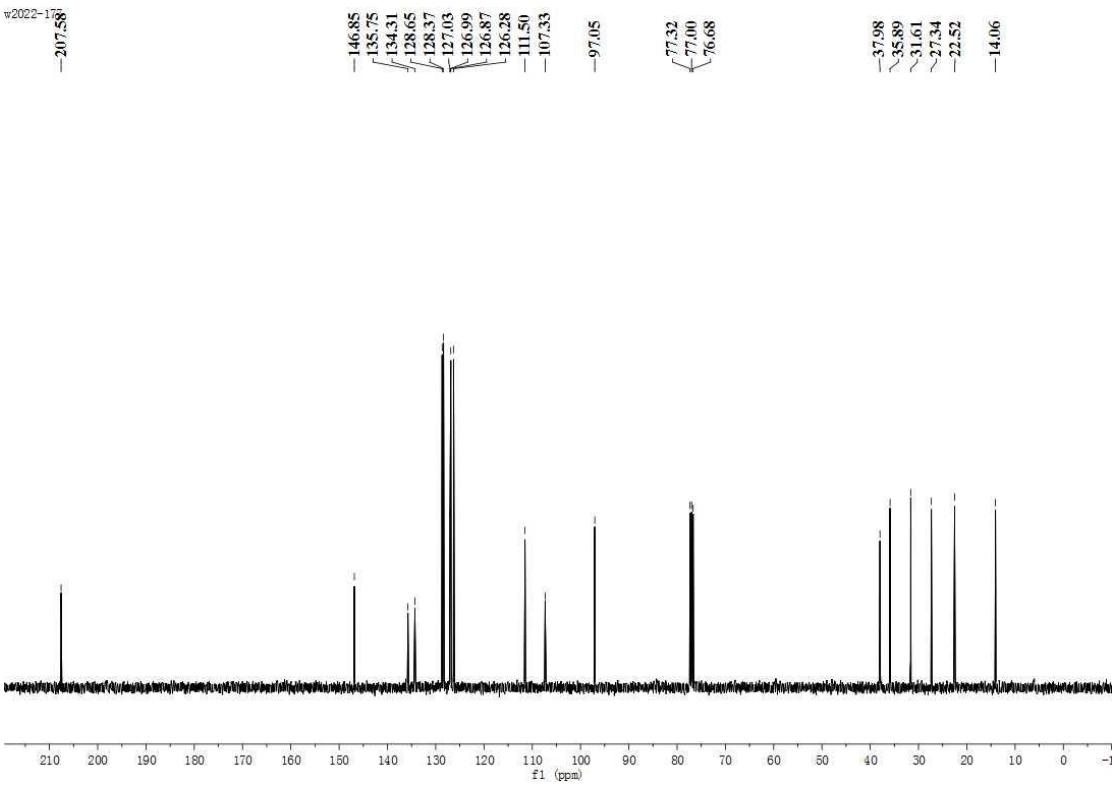

11202022-w182-1
7.454
7.435
7.343
7.326
7.323
7.316
7.298
7.294
7.278
7.275
7.220
7.202
6.510
4.950
4.874
3.585
3.569
3.552
3.365
3.322
3.279
2.174
2.166
2.156
2.146
2.130
1.701
1.684
1.678
1.668
0.877
0.021
0.000
2.02
6.02
2.02
1.00
2.00
2.00
2.01
2.02
2.04
9.01
6.00
f1 (ppm)

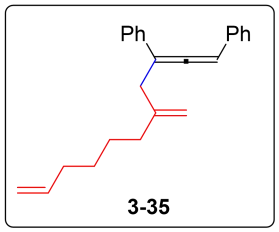

11202022-w182-1
207.66
146.30
134.32
128.68
128.40
127.07
127.02
126.89
126.30
117.72
107.35
97.14
77.32
77.00
76.68
62.79
38.06
32.11
30.85
25.96
18.33
-5.29
f1 (ppm)


Ph
Ph

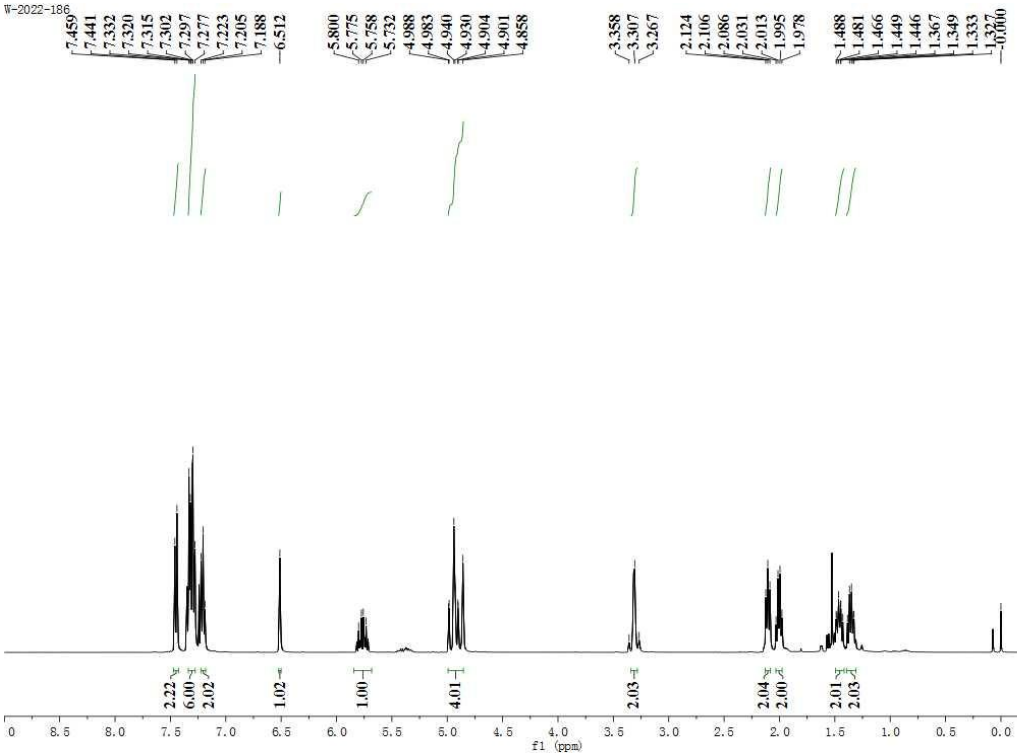
3-34

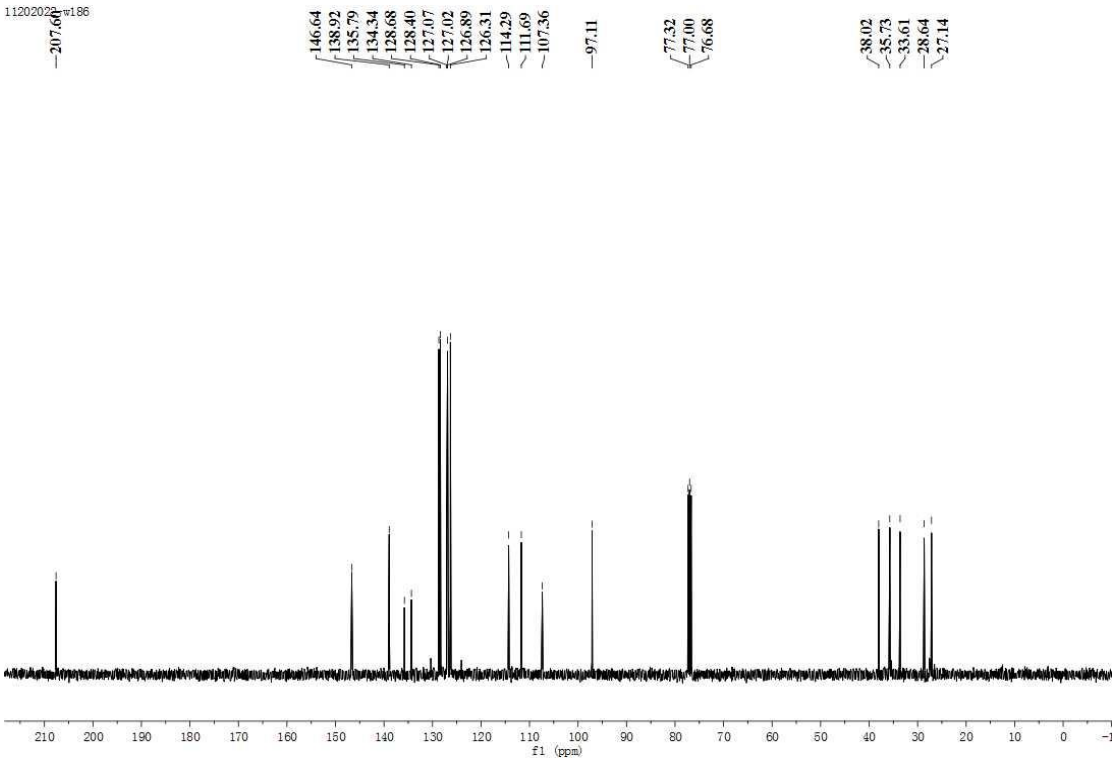

w2022-177
7.383
7.380
7.361
7.360
7.270
7.266
7.249
7.246
7.230
7.226
7.222
7.212
7.208
7.192
7.188
7.133
7.114
6.431
6.425
6.420
4.851
4.776
3.276
3.234
3.224
3.185
2.029
2.010
1.991
1.177
1.168
1.160
1.151
1.143
0.788
0.771
0.754
0.000
2.04
6.03
2.03
1.00
2.07
2.01
2.03
2.04
4.02
3.03
f1 (ppm)

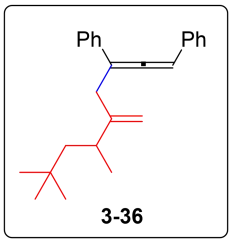

w2022-177
207.58
146.85
135.75
134.31
128.65
128.37
127.03
126.99
126.87
126.28
111.50
107.33
97.05
77.32
77.00
76.68
37.98
35.89
31.61
27.34
22.52
14.06
f1 (ppm)


Ph
Ph

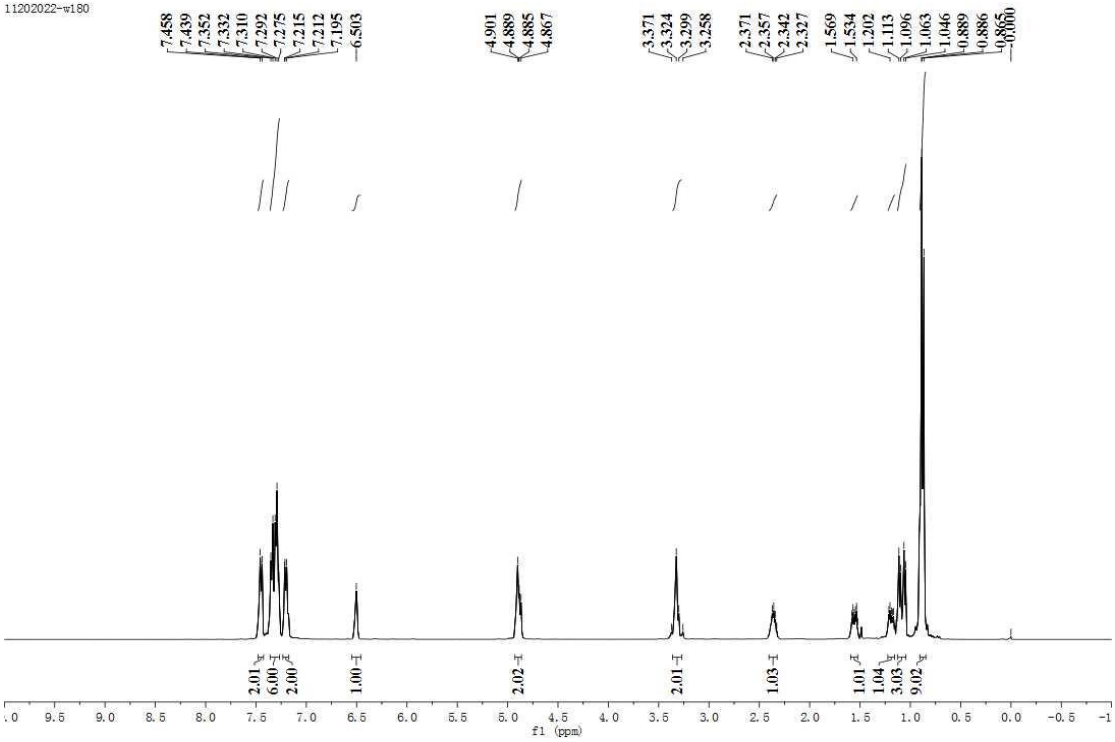
3-35

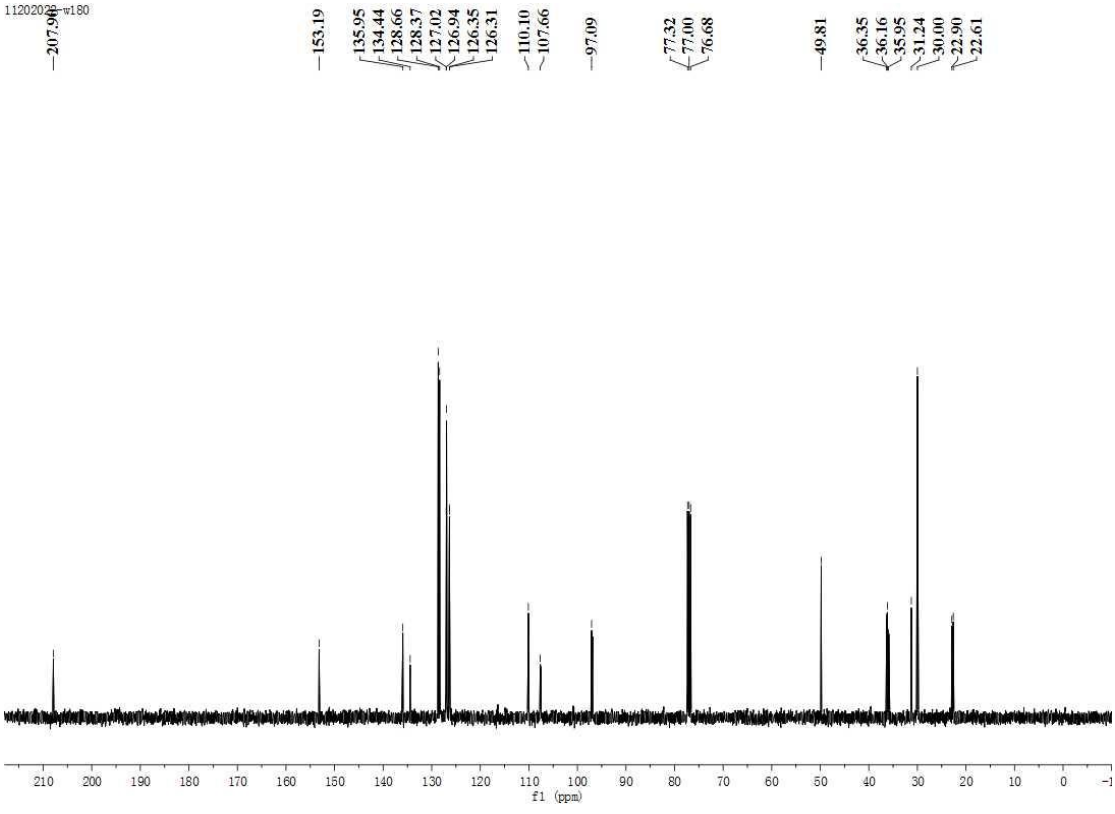

W-2022-186
7.459
7.441
7.332
7.320
7.315
7.302
7.297
7.277
7.223
7.205
7.188
6.512
5.800
5.775
5.758
5.732
4.988
4.983
4.940
4.930
4.904
4.901
4.858
3.358
3.307
3.267
2.124
2.106
2.086
2.031
2.013
1.995
1.978
1.488
1.481
1.466
1.449
1.446
1.367
1.349
1.333
1.327
0.000
2.22
6.00
2.02
1.02
1.00
4.01
2.03
2.04
2.00
2.01
2.03
f1 (ppm)

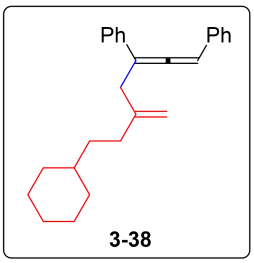

207.66
146.64
138.92
135.79
134.34
128.68
128.40
127.07
127.02
126.89
126.31
114.29
111.69
107.36
97.11
77.32
77.00
76.68
38.02
35.73
33.61
28.64
27.14
f1 (ppm)


Ph
Ph

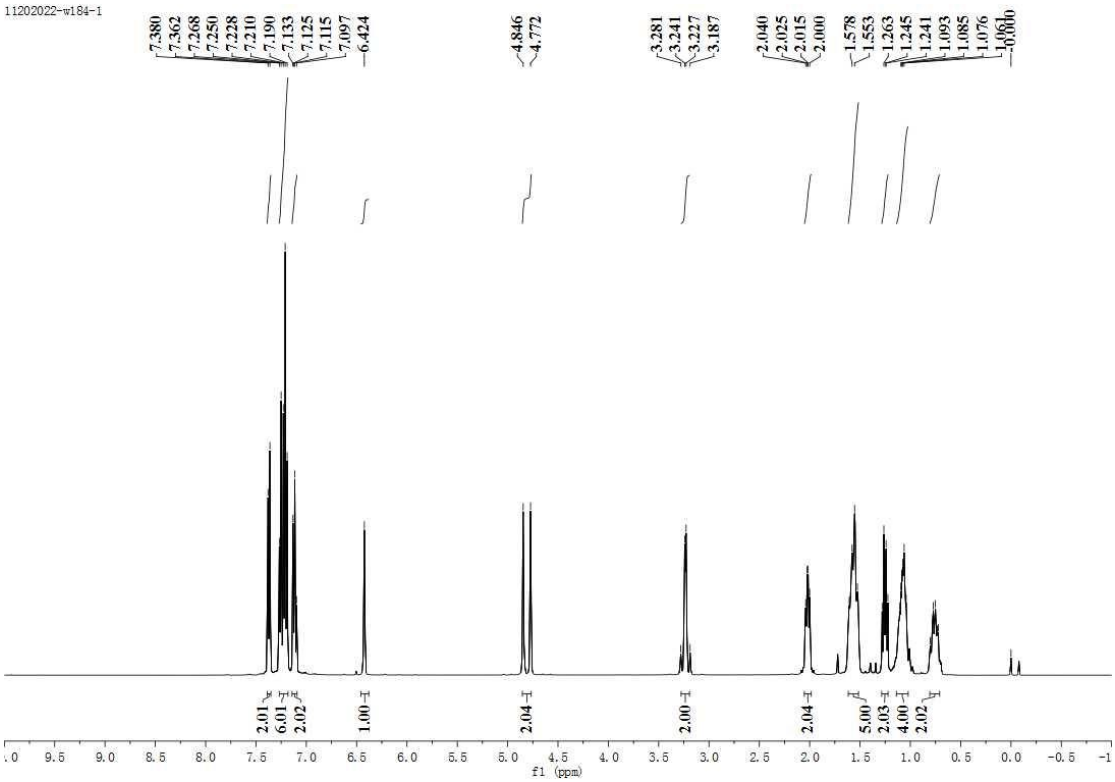
3-36

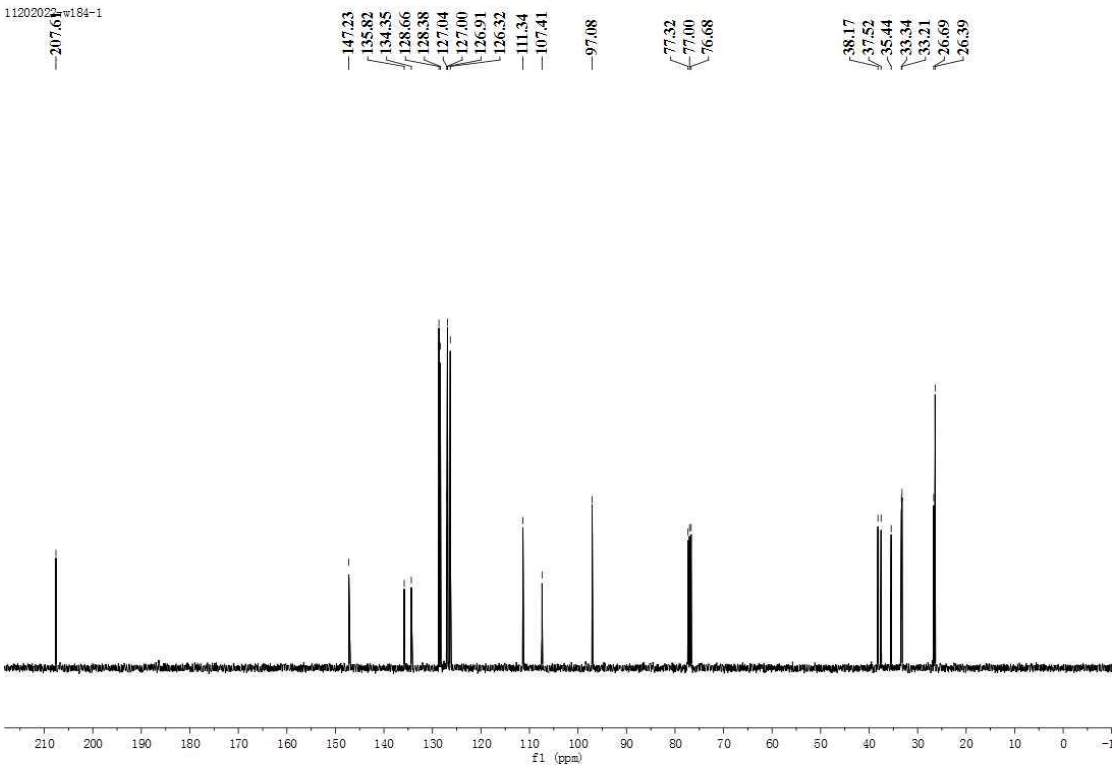

11202022-w180
7.458
7.439
7.352
7.332
7.310
7.292
7.275
7.215
7.212
7.195
6.503
4.901
4.889
4.885
4.867
3.371
3.324
3.299
3.258
2.371
2.357
2.342
2.327
1.569
1.534
1.202
1.113
1.096
1.063
1.046
0.889
0.886
0.000
2.01
6.00
2.00
1.00
2.02
2.01
1.03
1.01
1.04
3.03
9.02
f1 (ppm)

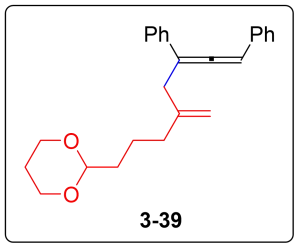

11202022-w180
207.98
153.19
135.95
134.44
128.66
128.37
127.02
126.94
126.35
126.31
110.10
107.66
97.09
77.32
77.00
76.68
49.81
36.35
36.16
35.95
31.24
30.00
22.90
22.61
f1 (ppm)


Ph
Ph

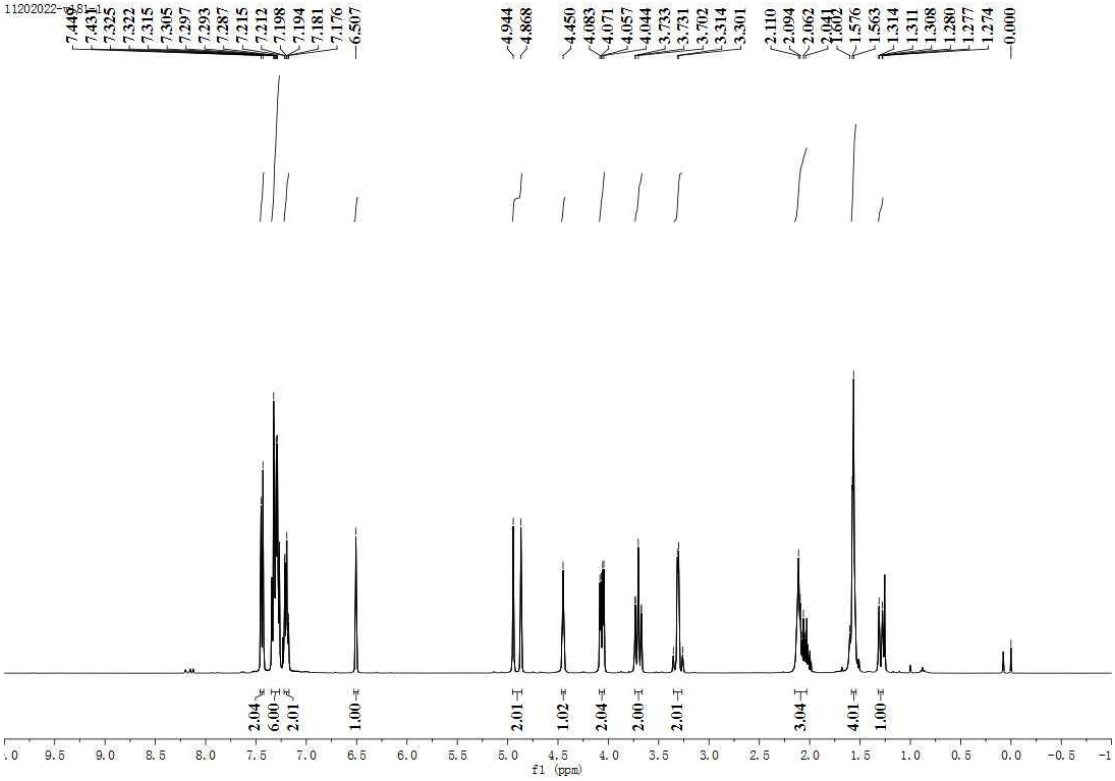
3-38

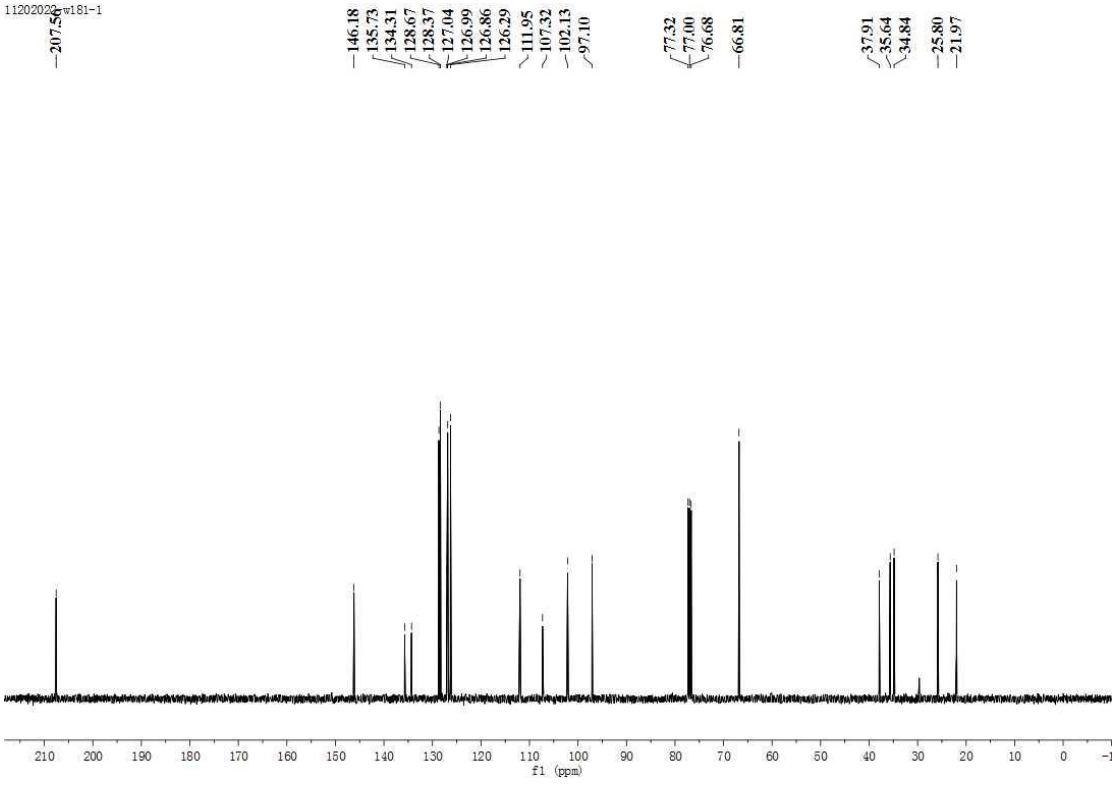

11202022-w184-1
7.380
7.362
7.268
7.250
7.228
7.210
7.190
7.133
7.125
7.115
7.097
6.424
4.846
4.772
3.281
3.241
3.227
3.187
2.040
2.025
2.015
2.000
1.578
1.553
1.263
1.245
1.241
1.093
1.085
1.076
1.061
0.000
2.01
6.01
2.02
1.00
2.04
2.00
2.04
5.00
2.03
4.00
2.02
f1 (ppm)


11202022-w184-1
207.61
147.23
135.82
134.35
128.66
128.38
127.04
127.00
126.91
126.32
111.34
107.41
97.08
77.32
77.00
76.68
38.17
37.52
35.44
33.34
33.21
26.69
26.39
f1 (ppm)


Ph
Ph
O
O

3-39


11202022-w181
7.446
7.431
7.325
7.322
7.315
7.305
7.297
7.293
7.287
7.215
7.212
7.198
7.194
7.181
7.176
6.507
4.944
4.868
4.450
4.083
4.071
4.057
4.044
3.733
3.731
3.702
3.314
3.301
2.110
2.094
2.062
2.041
1.601
1.576
1.563
1.314
1.311
1.308
1.280
1.277
1.274
0.000
2.04
6.00
2.01
1.00
2.01
1.02
2.04
2.00
2.01
3.04
4.01
1.00
f1 (ppm)


11202022-w181-1
207.56
146.18
135.73
134.31
128.67
128.37
127.04
126.99
126.86
126.29
111.95
107.32
102.13
97.10
77.32
77.00
76.68
66.81
37.91
35.64
34.84
25.80
21.97
f1 (ppm)