SUPPORTING INFORMATION
for the article entitled

Synthesis of Multi-Substituted Pyrroles Using Enamides and Alkynes Catalyzed by $Pd(OAc)_2$ with Molecular Oxygen as Oxidant

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Supporting information

Table of contents

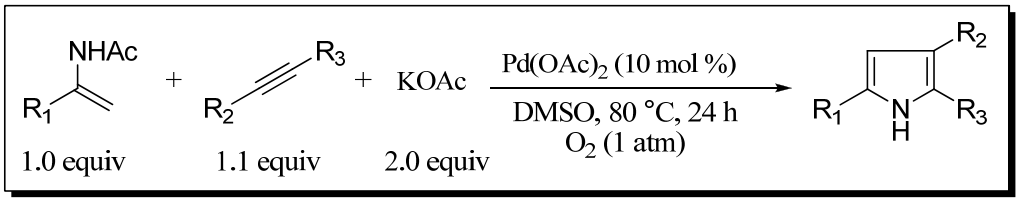
1. General experimental details.
2. General experimental procedure for the reaction.
3. Experimental characterization data for compounds.
4. Copies of product NMR spectra.

1. General experimental details

All commercially obtained reagents were used as received without further purification. The starting material enamides and diarylsubstituted alkynes were synthetized according to the reported reference. All catalytic reactions were run under 1 atm O_2 atmosphere without precaution taken to exclude moisture. ^1H, ^{13}C and ^{19}F NMR spectra were recorded on a 400 MHz NMR spectrometer. ^1H NMR chemical shifts were determined relative to the signal of DMSO-d_6 at δ 2.54 ppm or to the signal of the residual solvent peak: H_2O in DMSO-d_6: δ 3.33. ^{13}C NMR chemical shifts were determined relative to DMSO-d_6 at δ 39.54. ^{19}F NMR chemical shifts were determined relative to $CFCl_3$ at δ 0.0. Datas for ^1H, ^{13}C and ^{19}F NMR were recorded as follows: chemical shift (δ, ppm), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet, q = quartet). Coupling constants are reported in hertz (Hz). High-resolution mass datas were recorded on a high-resolution mass spectrometer in the ESI mode

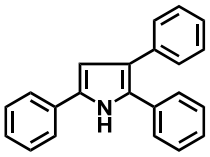
2. General experimental procedure for the reaction

Representative experimental procedures for synthesis of pyrroles.



A 10 mL dried round bottom flask was charged sequentially with a stirring bar, $Pd(OAc)_2$ (10 mol %, 0.04 mmol), enamide (1.0 equiv, 0.40 mmol), alkyne (1.1 equiv, 0.44 mmol), potassium acetate (2.0 equiv, 0.80 mmol) and anhydrous DMSO (4 mL). The reaction mixture was stirred at 80 ℃ under 1 atm of oxygen (balloon pressure) for 24 h. After cooling down, the mixture was diluted with ethyl acetate, filtered and washed with water twice and the solution of saturated sodium chloride once. The organic layer was dried with anhydrous Na_2SO_4, filtered and concentrated to afford the crude product which was then directly applied to a flash column chromatography (EtOAc/Petroleum Ether mixtures). Finally, the yields of all reactions are isolated yields.

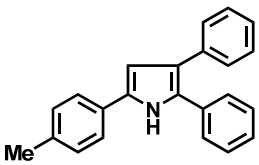
3. Experimental characterization data for compounds



3a

2,3,5-triphenyl-1*H*-pyrrole

This compound was prepared by the general procedure described above. Yield = 67%. ^{1}H NMR (400 MHz, DMSO-d_6) δ = 11.41 (s, 1H), 7.83 (dd, J_1 = 7.2 Hz, J_2 = 1.2 Hz, 2H), 7.46-7.36 (m, 6H), 7.35-7.28 (m, 5H), 7.25-7.18 (m, 2H), 6.79 (d, J = 2.8 Hz, 1H) ppm;
^{13}C NMR (100 MHz, DMSO-d_6) δ = 136.59, 132.88, 132.29, 131.94, 129.35, 128.57, 128.25, 128.09, 127.89, 126.62, 125.85, 125.55, 123.90, 122.63, 108.01 ppm.
HRMS (ESI) m/z calculated for $C_{22}H_{18}N$ $[M+H]^+$: 296.1439, found 296.1450.

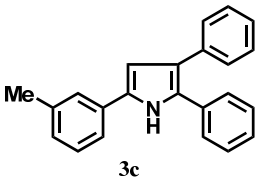


3b

2,3-diphenyl-5-*p*-tolyl-1*H*-pyrrole

This compound was prepared by the general procedure described above. Yield = 65%. ^{1}H NMR (400 MHz, DMSO-d_6) δ = 11.36 (s, 1H), 7.74 (d, J = 8 Hz, 2H), 7.46 (dd, J_1 = 8.4 Hz, J_2 = 1.2

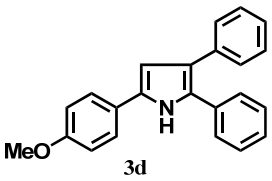
Hz, 2H), 7.39-7.28 (m, 7H), 7.24-7.20 (m, 3H), 6.74 (d, J = 2.4 Hz, 1H), 2.35 (s, 3H) ppm;
^{13}C NMR (100 MHz, DMSO-d_6) δ = 136.72, 135.02, 132.99, 132.16, 129.62, 129.18, 128.96, 128.26, 128.24, 128.06, 127.92, 126.52, 125.52, 123.92, 122.58, 107.50, 20.71 ppm.
HRMS (ESI) m/z calculated for $C_{23}H_{20}N[M+H]^+$: 310.1596, found 310.1590.



3c

2,3-diphenyl-5-*m*-tolyl-1*H*-pyrrole

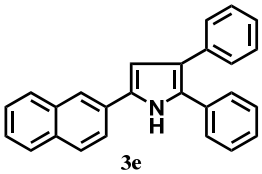
This compound was prepared by the general procedure described above. Yield = 66%. ^{1}H NMR (400 MHz, DMSO-d_6) δ = 11.38 (d, J = 1.2 Hz, 1H), 7.69 (s, 1H), 7.63 (d, J = 8 Hz, 1H), 7.47-7.44 (m, 2H), 7.40-7.28 (m, 8H), 7.23-7.19 (m, 1H), 7.05 (d, J = 8 Hz), 6.77 (d, J = 2.8 Hz, 1H), 2.39 (s, 3H) ppm;
^{13}C NMR(100 MHz, DMSO-d_6) δ = 137.60, 136.64, 132.93, 132.21, 132.08, 129.23, 128.48, 128.26, 128.24, 128.09, 127.90, 126.59, 125.54, 124.50, 122.58, 121.15, 107.93, 21.14 ppm.
HRMS (ESI) m/z calculated for $C_{23}H_{20}N$ $[M+H]^+$: 310.1596, found 310.1582.



3d

5-(4-methoxyphenyl)-2,3-diphenyl-1*H*-pyrrole

This compound was prepared by the general procedure described above. Yield = 65%. ^{1}H NMR (400 MHz, DMSO-d_6) δ = 11.27 (s, 1H) 7.75 (d, J = 8.4 Hz, 2H), 7.43 (d, J = 7.6 Hz, 2H), 7.39-7.26 (m, 7H), 7.22-7.19 (m, 1H), 7.00 (d, J = 8.4 Hz, 2H), 6.65 (d, J = 2.4 Hz, 1H), 3.82 (s, 3H) ppm;
^{13}C NMR (100 MHz, DMSO-d_6) δ = 157.72, 136.77, 133.04, 132.05, 128.49, 128.22, 127.94, 127.88, 126.40, 125.46, 125.31, 125.18, 122.46, 114.06, 106.87, 55.08 ppm.
HRMS (ESI) m/z calculated for $C_{23}H_{20}NO$ $[M+Na]^+$: 348.1364, found 348.1366.



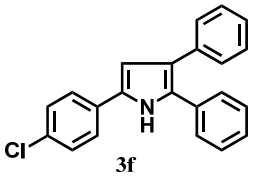
3e

5-(naphthalen-2-yl)-2,3-diphenyl-1*H*-pyrrole

This compound was prepared by the general procedure described above. Yield = 74%. ^{1}H NMR (400 MHz, DMSO-d_6) δ = 11.59 (s, 1H), 8.37 (s, 1H), 8.01 (dd, J_1 = 8.6 Hz, J_2 = 1.7 Hz, 1H), 7.96-7.88 (m, 3H) 7.57-7.53 (m, 1H), 7.50-7.46 (m, 3H), 7.43-7.38 (m, 2H), 7.36-7.31 (m, 5H), 7.25-7.21 (m, 2H), 6.97(d, J = 2.8 Hz, 1H) ppm;
^{13}C NMR (100 MHz, DMSO-d_6) δ = 135.56, 133.46, 132.87, 131.91, 131.57, 129.90, 129.77,

128.32, 128.16, 128.06, 127.94, 127.60, 127.52, 126.77, 126.45, 125.65, 125.24, 123.39, 122.87, 121.03, 108.89 ppm.

HRMS (ESI) m/z calculated for $C_{26}H_{20}N$ $[M+H]^+$: 346.1596, found 346.1599.



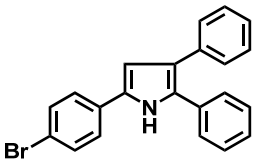
3f

5-(4-chlorophenyl)-2,3-diphenyl-1*H*-pyrrole

This compound was prepared by the general procedure described above. Yield = 50%. ^{1}H NMR (400 MHz, DMSO-d_6) δ = 11.49 (s, 1H), 7.86 (d, J = 8.4 Hz, 2H), 7.48-7.44 (m, 4H), 7.40-7.36 (m, 2H), 7.34-7.28 (m, 5H), 7.24-7.19 (m, 1H), 6.84 (d, J = 2.8 Hz, 1H) ppm;

^{13}C NMR (100 MHz, DMSO-d_6) δ = 136.43, 132.76, 131.22, 130.75, 130.11, 129.86, 128.58, 128.29, 128.13, 127.93, 126.79, 125.66, 125.50, 122.84, 108.65 ppm.

HRMS (ESI) m/z calculated for $C_{22}H_{17}NCl$ $[M+H]^+$: 330.1050, found 330.1047.



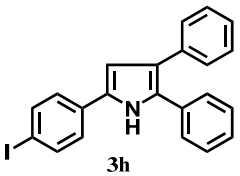
3g

5-(4-bromophenyl)-2,3-diphenyl-1*H*-pyrrole

This compound was prepared by the general procedure described above. Yield = 56%. ^{1}H NMR (400 MHz, DMSO-d_6) δ = 11.50 (s, 1H), 7.80 (d, J = 8.8 Hz, 2H), 7.60 (d, J = 8.4 Hz, 2H), 7.45-7.43 (m, 2H), 7.40-7.37 (m, 2H), 7.32-7.28 (m, 5H), 7.23-7.19 (m, 1H), 6.86 (d, J = 2.8 Hz, 1H) ppm;

^{13}C NMR (100 MHz, DMSO-d_6) δ = 136.41, 132.74, 131.55, 131.46, 130.75, 129.92, 128.31, 128.13, 127.92, 126.82, 125.83, 125.68, 122.85, 118.52, 108.70 ppm.

HRMS (ESI) m/z calculated for $C_{22}H_{17}NBr$ $[M+H]^+$: 374.0544, found 374.0543.



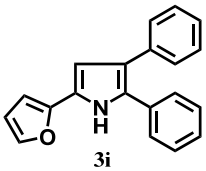
3h

5-(4-iodophenyl)-2,3-diphenyl-1*H*-pyrrole

This compound was prepared by the general procedure described above. Yield = 39%. ^{1}H NMR (400 MHz, DMSO-d_6) δ = 11.49 (s, 1H), 7.76 (d, J = 8.4 Hz, 2H), 7.65 (d, J = 8.4 Hz), 7.43 (d, J = 7.6 Hz, 2H), 7.38 (t, J = 7.2 Hz, 2H), 7.32-7.28 (m, 5H), 7.23-7.20 (m, 1H), 6.85 (d, J = 2.4 Hz, 1H) ppm;

^{13}C NMR (100 MHz, DMSO-d_6) δ = 137.27, 136.41, 132.73, 131.85, 130.88, 129.94, 128.30, 128.14, 127.92, 126.81, 125.98, 125.67, 122.84, 108.66, 90.91 ppm.

HRMS (ESI) m/z calculated for $C_{22}H_{17}NI$ $[M+H]^+$: 422.0406, found 422.0406.



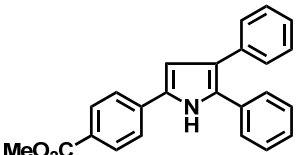
3i

5-(furan-2-yl)-2,3-diphenyl-1*H*-pyrrole

This compound was prepared by the general procedure described above. Yield = 29%. ^{1}H NMR (400 MHz, DMSO-d_6) δ = 11.55 (s, 1H), 7.67 (dd, J_1 = 1.6 Hz, J_2 = 0.8 Hz, 1H), 7.43-7.35 (m, 4H), 7.32-7.28 (m, 5H), 7.23-7.19 (m, 1H), 6.76 (dd, J_1 = 3.6 Hz, J_2 = 0.8 Hz, 1H), 6.59 (d, J_1 = 3.6 Hz, J_2 = 3.0 Hz, 2H) ppm;

^{13}C NMR(100 MHz, DMSO-d_6) δ = 148.23, 141.81, 136.81, 133.12, 129.47, 129.08, 129.06, 128.57, 128.43, 127.52, 126.53, 124.79, 122.92, 112.31, 107.82, 103.96 ppm.

HRMS (ESI) m/z calculated for $C_{20}H_{16}NO$ $[M+H]^+$: 286.1232, found 286.1219.



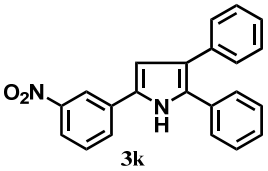
3j

methyl 4-(4,5-diphenyl-1*H*-pyrrol-2-yl)benzoate

This compound was prepared by the general procedure described above. Yield = 59%. ^{1}H NMR (400 MHz, DMSO-d_6) δ = 11.67 (d, J = 2 Hz, 1H), 8.02-7.96 (m, 4H), 7.49-7.46 (m, 2H), 7.42-7.37 (m, 2H), 7.36-7.29 (m, 5H), 7.23 (tt, J_1 = 6.8 Hz, J_2 = 1.6 Hz, 1H), 7.00 (d, J = 2.4 Hz, 1H), 3.89 (s, 3H);

^{13}C NMR (100 MHz, DMSO-d_6) δ = 166.11, 136.73, 136.25, 132.59, 131.10, 130.77, 129.73, 128.36, 128.31, 127.98, 127.07, 126.29, 125.81, 123.58, 123.30, 110.20, 51.94 ppm.

HRMS (ESI) m/z calculated for $C_{24}H_{20}NO_2$ $[M+H]^+$: 354.1494, found 354.1494.



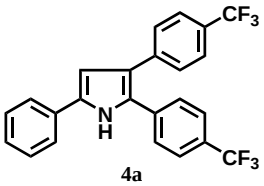
3k

5-(3-nitrophenyl)-2,3-diphenyl-1*H*-pyrrole

This compound was prepared by the general procedure described above, but the reaction time was extended to 36 h. Yield = 47%. ^{1}H NMR (400 MHz, DMSO-d_6) δ = 11.80 (s, 1H), 8.76 (t, J = 2 Hz, 1H), 8.26 (dq, J_1 = 8 Hz, J_2 = 1.6 Hz, 1H), 8.05 (ddd, J_1 = 8 Hz, J_2 = 2.4 Hz, J_3 = 0.8 Hz, 1H), 7.69 (t, J = 8 Hz, 1H), 7.48-7.45 (m, 2H), 7.43-7.39 (m, 2H), 7.36-7.30 (m, 5H), 7.25-7.20 (m, 1H), 7.07 (d, J = 2.8 Hz, 1H) ppm;

^{13}C NMR (100 MHz, DMSO-d_6) δ = 148.62, 136.16, 134.02, 132.54, 130.86, 130.12, 130.08, 129.65, 128.38, 128.36, 128.29, 127.95, 127.11, 125.83, 123.08, 120.11, 117.74, 110.02 ppm.

HRMS (ESI) m/z calculated for $C_{22}H_{17}N_2O_2$ $[M+H]^+$: 341.1290, found 341.1291.



4a

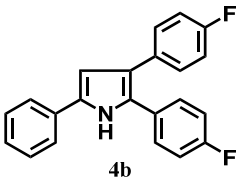
5-phenyl-2,3-bis(4-(trifluoromethyl)phenyl)-1*H*-pyrrole

This compound was prepared by the general procedure described above. Yield = 71%. ^{1}H NMR (400 MHz, DMSO-d_6) δ = 11.77 (d, J = 2.0 Hz, 1H), 7.87 (dd, J_1 = 7.2, J_2 = 1.1 Hz, 2H), 7.77 (d, J = 8.4 Hz, 2H), 7.69 (d, J = 8 Hz, 2H), 7.65 (d, J = 8 Hz, 2Hz), 7.54 (d, J = 8 Hz, 2H), 7.46 (t, J = 7.6 Hz, 2H), 7.28 (t, J = 7.6 Hz, 1H), 6.92 (d, J = 2.8 Hz, 1H);

^{13}C NMR (100 MHz, DMSO-d_6) δ = 140.50, 136.36, 133.62, 131.84, 128.73, 128.62, 128.53, 127.04 (q, J = 31.5 Hz), 126.54, 126.50, 126.18, 125.86, 125.73, 125.41 (t, J = 3.6 Hz), 124.33, 123.10 (d, J = 13 Hz), 122.64, 108.66.

^{19}F NMR (376 MHz, DMSO-d_6): δ = -61.04 (s, 3F), -61.17 (s, 3F) ppm.

HRMS (ESI) m/z calculated for $C_{24}H_{16}F_6N$ $[M+H]^+$: 432.1187, found 432.1189.



4b

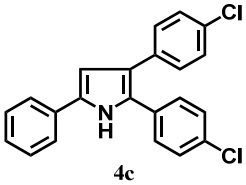
2,3-bis(4-fluorophenyl)-5-phenyl-1*H*-pyrrole

This compound was prepared by the general procedure described above. Yield = 53%. ^{1}H NMR (400 MHz, DMSO-d_6) δ = 11.45 (s, 1H), 7.82 (dd, J_1 = 7.2 Hz, J_2 = 1.2 Hz, 2H), 7.47-7.39 (m, 4H), 7.34-7.30 (m, 2H), 7.27-7.22 (m, 3H), 7.16 (tt, J_1 = 8.8 Hz, J_2 = 2.0 Hz, 2H), 6.78 (d, J = 2.8 Hz, 1H) ppm;

^{13}C NMR (100 MHz, DMSO-d_6) δ = 162.10 (J = 56 Hz), 159.68 (J = 54 Hz), 132.87 (J = 3 Hz), 132.24, 131.99, 130.15 (J = 8 Hz), 129.69 (J = 8 Hz), 129.23 (J = 3 Hz), 128.67, 128.35, 126.01, 123.96, 121.64, 115.38 (J = 11 Hz), 115.17 (J = 11 Hz), 107.95 ppm;

^{19}F NMR (376 MHz, DMSO-d_6): δ = -115.43 (s, 1F), -117.39 (s, 1F) ppm.

HRMS (ESI) m/z calculated for $C_{22}H_{16}F_2N$ $[M+H]^+$: 332.1251, found 332.1251.



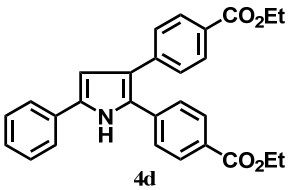
4c

2,3-bis(4-chlorophenyl)-5-phenyl-1*H*-pyrrole

This compound was prepared by the general procedure described above. Yield = 72%. ^{1}H NMR (400 MHz, DMSO-d_6) δ = 11.56 (s, 1H), 7.83 (d, J = 7.6 Hz, 2H), 7.48-7.37 (m, 8H), 7.34-7.32 (m, 2H), 7.25 (t, J = 7.6 Hz, 1H), 6.81 (d, J = 2.8 Hz, 1H) ppm;

^{13}C NMR (100 MHz, DMSO-d_6) δ = 135.25, 132.62, 132.06, 131.39, 131.36, 130.36, 129.75, 129.62, 128.64, 128.43, 128.29, 126.16, 124.08, 121.87, 108.12 ppm.

HRMS (ESI) m/z calculated for $C_{22}H_{16}Cl_2N$ $[M+H]^+$: 364.0660, found 364.0668.



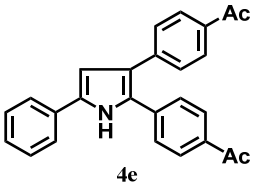
4d

diethyl 4,4'-(5-phenyl-1*H*-pyrrole-2,3-diyl)dibenzoate

This compound was prepared by the general procedure described above. Yield = 78%. ^{1}H NMR (400 MHz, DMSO-d_6) δ = 11.72 (s, 1H), 7.96 (dt, J_1 = 8.8 Hz, J_2 = 1.6 Hz, 2H), 7.92 (dt, J_1 = 8.4 Hz, J_2 = 1.6 Hz, 2H), 7.86 (dd, J_1 = 7.6 Hz, J_2 = 0.8 Hz, 2H), 7.58 (dt, J_1 = 8.8 Hz, J_2 = 2 Hz, 2H), 7.48-7.43 (m, 4H), 7.29 (tt, J_1 = 7.6 Hz, J_2 =1,2 Hz, 1H), 6.92 (d, J = 2.8 Hz, 1H), 4.35 (q, J_1 = 7.2 Hz, J_2 = 4.8 Hz, 4H), 1.36 (t, J = 7.0 Hz, 6H) ppm;

^{13}C NMR(100 MHz, DMSO-d_6) δ = 165.62, 165.49, 141.25, 136.93, 133.61, 131.80, 129.40, 129.26, 129.03, 128.69, 128.07, 127.82, 127.17, 126.48, 124.31, 123.15, 108.67, 60.66, 60.52, 14.19 ppm.

HRMS (ESI) m/z calculated for $C_{28}H_{26}O_4N$ $[M+H]^+$: 440.1862, found 440.1863.



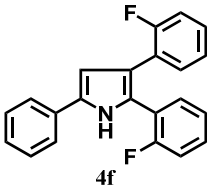
4e

1,1'-(4,4'-(5-phenyl-1*H*-pyrrole-2,3-diyl)bis(4,1-phenylene))diethanone

This compound was prepared by the general procedure described above. Yield = 75%. ^{1}H NMR (400 MHz, DMSO-d_6) δ = 11.74 (d, J = 1.6 Hz, 1H), 7.98 (d, J = 8.4 Hz, 2H), 7.93 (d, J = 8.4 Hz, 2H), 7.88 (d, J = 7.6 Hz, 2H), 7.59 (d, J = 8.4 Hz, 2H), 7.49-7.43 (m, 4H), 7.29 (t, J = 7.2 Hz, 1H), 6.93 (d, J = 2.4 Hz, 1H), 2.62 (s, 3H), 2.60 (s, 3H) ppm;

^{13}C NMR (100 MHz, DMSO-d_6) δ = 197.21, 197.19, 141.31, 136.92, 134.85, 134.34, 133.68, 131.81, 129.14, 128.69, 128.57, 128.41, 128.02, 127.94, 126.50, 124.35, 123.29, 108.79, 26.63, 26.57 ppm.

HRMS (ESI) m/z calculated for $C_{26}H_{22}O_2N$ $[M+H]^+$: 380.1651, found 380.1651.



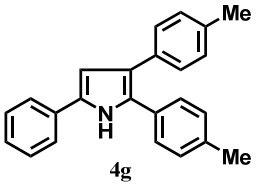
4f

2,3-bis(2-fluorophenyl)-5-phenyl-1*H*-pyrrole

This compound was prepared by the general procedure described above. Yield = 34%. ^{1}H NMR (400 MHz, DMSO-d_6) δ = 11.71 (s, 1H), 7.82 (d, J = 7.2 Hz, 2H), 7.45-7.37 (m, 4H), 7.30-7.10 (m, 7H), 6.84 (d, J = 0.8 Hz, 1H) ppm;

^{13}C NMR (100 MHz, DMSO-d_6) δ = 160.34 (d, J = 7.7 Hz), 157.90 (d, J = 6.1 Hz), 132.40, 132.14, 131.27 (d, J = 3 Hz), 130.66 (d, J = 4 Hz), 129.25 (d, J = 8 Hz), 128.71, 127.79 (d, J = 8 Hz), 126.10, 124.50, 124.22 (d, J = 3 Hz), 124.13 (d, J = 3 Hz), 124.07, 123.91, 121.10 (d, J =

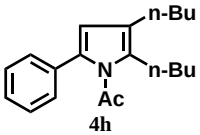
15 Hz), 117.87, 115.78 (d, J = 16 Hz), 115.56 (d, J = 16 Hz);
^{19}F NMR(376 MHz, $CDCl_3$-d): δ = -114.79 (s, 1F), -116.21 (s, 1F) ppm.
HRMS (ESI) m/z calculated for $C_{22}H_{16}F_2N$ $[M+H]^+$: 332.1251, found 332.1259.



4g

5-phenyl-2,3-di*p*-tolyl-1*H*-pyrrole

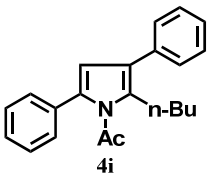
This compound was prepared by the general procedure described above. Yield = 54%. ^{1}H NMR (400 MHz, DMSO-d_6) δ = 11.32 (s, 1H), 7.82 (d, J = 7.6 Hz, 2H), 7.41 (t, J = 7.2 Hz, 2H), 7.35 (d, J = 7.6 Hz, 2H), 7.24-7.17 (m, 5H), 7.11 (d, J = 7.6 Hz, 2H), 6.74 (s, 1H), 2.35 (s, 3H), 2.32 (s, 3H) ppm;
^{13}C NMR (100 MHz, DMSO-d_6) δ = 135.76, 134.45, 133.79, 132.44, 131.61, 130.17, 129.25, 128.88, 128.84, 128.57, 127.95, 127.79, 125.72, 123.86, 122.28, 107.93, 20.77, 20.68 ppm.
HRMS (ESI) m/z calculated for $C_{24}H_{22}N$ $[M+Na]^+$: 346.1572, found 346.1573.



4h

1-(2,3-dibutyl-5-phenyl-1*H*-pyrrol-1-yl)ethanone

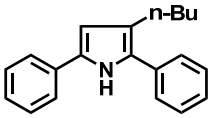
This compound was prepared by the general procedure described above. Yield = 23%. ^{1}H NMR (400 MHz, DMSO-d_6) δ = 7.44 (t, J = 7.2 Hz, 2H), 7.36-7.30 (m, 3H), 6.21 (s, 1H), 2.71 (t, J = 7.6 Hz, 2H), 2.38 (t, J = 7.2 Hz, 2H), 1.57-1.43 (m, 4H), 1.42-1.31 (m, 4H), 0.95-0.90 (m, 6H) ppm;
^{13}C NMR (100 MHz, DMSO-d_6) δ = 172.98, 133.97, 132.53, 132.38, 128.77, 127.46, 127.10, 12.82, 114.38, 32.59, 32.42, 28.30, 24.70, 22.08, 22.03, 13.83, 13.76 ppm.
HRMS (ESI) m/z calculated for $C_{20}H_{28}NO$ $[M+H]^+$: 298.2171, found 298.2171.



4i

1-(2-butyl-3,5-diphenyl-1*H*-pyrrol-1-yl)ethanone

This compound was prepared by the general procedure described above. Yield = 12%. ^{1}H NMR (400 MHz, DMSO-d_6) δ = 7.51-7.47 (m, 2H), 7.45-7.40 (m, 3H), 7.37-7.31 (m, 5H), 6.35 (s, 1H), 2.31 (t, J = 7.2 Hz, 2H), 1.54-1.46 (m, 2H), 1.32-1.22 (m, 2H), 0.83 (t, J = 7.2 Hz, 3H) ppm;
^{13}C NMR (100 MHz, DMSO-d_6) δ = 172.21, 133.89, 133.41, 132.74, 130.88, 129.93, 128.36, 128.03, 127.61, 127.10, 125.13, 113.76, 32.26, 28.16, 24.83, 21.89, 13.69 ppm.
HRMS (ESI) m/z calculated for $C_{22}H_{24}NO$ $[M+H]^+$: 318.1858, found 318.1858.



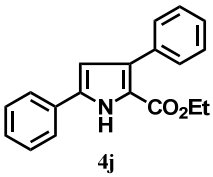
4i′

3-butyl-2,5-diphenyl-1*H*-pyrrole

This compound was prepared by the general procedure described above. Yield = 26%. ^{1}H NMR (400 MHz, DMSO-d_6) δ = 11.04 (s, 1H), 7.76 (d, J = 7.6 Hz, 2H), 7.55 (dd, J_1 = 8 Hz, J_2 = 1.2 Hz, 2H), 7.47 (t, J = 7.6 Hz, 2H), 7.38 (t, J = 8 Hz, 2H), 7.29 (t, J = 7.2 Hz, 1H), 7.18 (t, J = 7.6 Hz, 1H), 6.54 (d, J = 2.8 Hz, 1H), 2.60 (t, J = 6.4 Hz, 2H), 1.66-1.58 (m, 2H), 1.44-1.34 (m, 2H), 0.93 (t, J = 7.2 Hz, 3H) ppm;

^{13}C NMR (100 MHz, DMSO-d_6) δ = 133.35, 132.68, 131.14, 129.22, 128.55, 128.38, 127.06, 125.83, 125.45, 123.67, 122.34, 107.96, 32.86, 25.96, 22.17, 13.89 ppm.

HRMS (ESI) m/z calculated for $C_{20}H_{22}N$ $[M+H]^+$: 276.1752, found 276.1750.



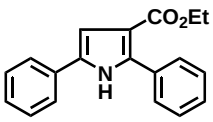
4j

ethyl 3,5-diphenyl-1*H*-pyrrole-2-carboxylate

This compound was prepared by the general procedure described above. Yield = 30%. ^{1}H NMR (400 MHz, DMSO-d_6) δ = 11.99 (s, 1H), 7.94 (d, J = 7.6 Hz, 2H), 7.57 (d, J = 7.2 Hz, 2H), 7.47-7.38 (m, 4H), 7.36-7.31 (m, 4H), 6.80 (d, J = 2.8 Hz, 1H), 4.22 (q, J = 7.1 Hz, 2H), 1.22 (t, J = 7.2 Hz, 3H) ppm;

^{13}C NMR (100 MHz, DMSO-d_6) δ = 160.57, 135.70, 135.34, 132.43, 131.07, 129.37, 128.65, 127.54, 127.46, 126.70, 125.43, 118.58, 109.83, 59.58, 14.12 ppm.

HRMS (ESI) m/z calculated for $C_{19}H_{18}O_2N$ $[M+H]^+$: 292.1338, found 292.1338.



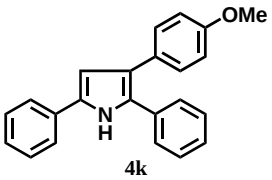
4j′

ethyl 2,5-diphenyl-1*H*-pyrrole-3-carboxylate

This compound was prepared by the general procedure described above. Yield = 43%. ^{1}H NMR (400 MHz, DMSO-d_6) δ = 11.89 (s, 1H), 7.83 (d, J = 7.2 Hz, 2H), 7.67 (d, J = 7.2 Hz, 2H), 7.50-7.40 (m, 5H), 7.27 (t, J = 7.6 Hz, 1H), 7.02 (d, J = 2.8 Hz, 1H), 4.16 (q, J = 7.1 Hz, 2H), 1.23 (t, J = 7.2 Hz, 3H) ppm;

^{13}C NMR (100 MHz, DMSO-d_6) δ = 164.04, 137.87, 131.79, 131.74, 131.55, 129.72, 128.73, 127.90, 127.61, 126.56, 124.28, 112.62, 108.61, 59.03, 14.22 ppm.

HRMS (ESI) m/z calculated for $C_{19}H_{18}O_2N$ $[M+H]^+$: 292.1338, found 292.1338.



4k

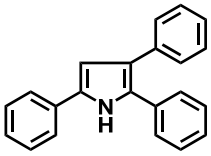
3-(4-methoxyphenyl)-2,5-diphenyl-1*H*-pyrrole

This compound was prepared by the general procedure described above. And the ratio of regioselectivity products was determined by crude NMR spectrum. Yield = 60%. ^{1}H NMR (400 MHz, DMSO-d_6) δ = 11.34 (d, J = 1.6 Hz, 1H), 7.83 (dd, J_1 = 8.4 Hz, J_2 = 0.8 Hz, 2H), 7.47-7.35 (m, 6H), 7.30-7.20 (m, 4H), 6.90 (dt, J_1 = 8.8 Hz, J_2 = 2.8 Hz, 2H), 6.73 (d, J = 2.4 Hz, 1H), 3.78 (s, 3H) ppm;

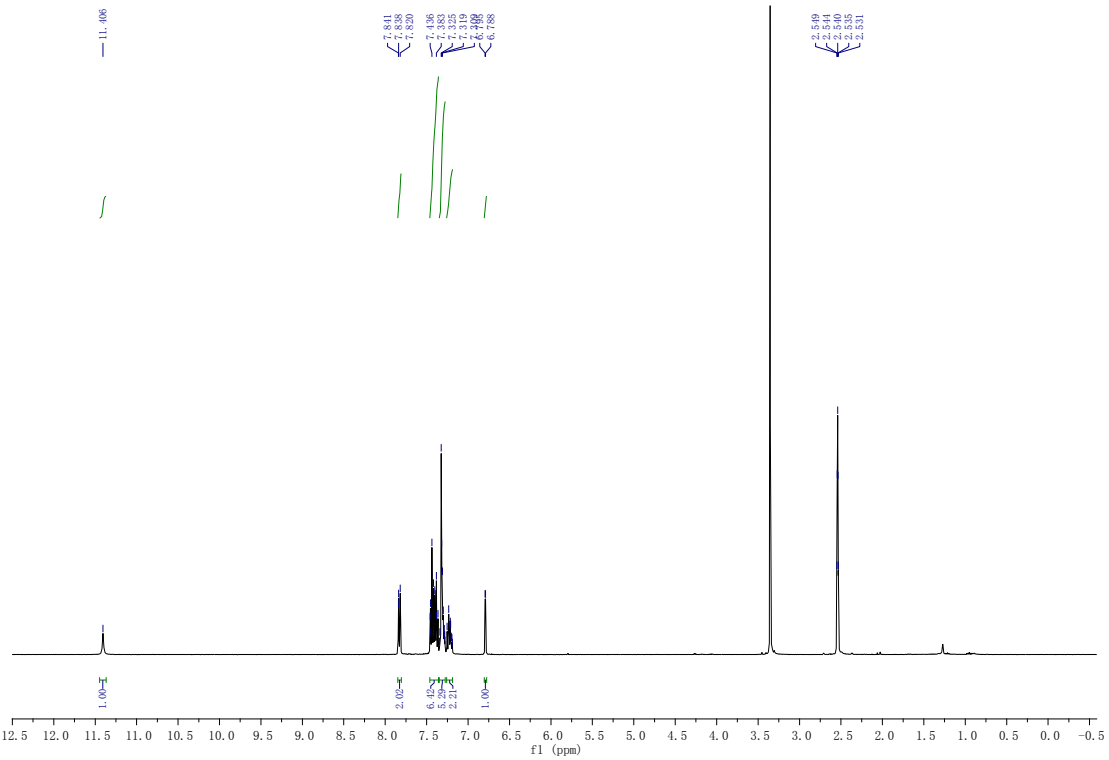
^{13}C NMR (100 MHz, DMSO-d_6) δ = 157.47, 133.09, 132.43, 131.83, 129.10, 129.01, 128.88, 128.64, 128.30, 127.98, 126.49, 125.84, 123.93, 122.53, 113.83, 108.12, 55.00 ppm.

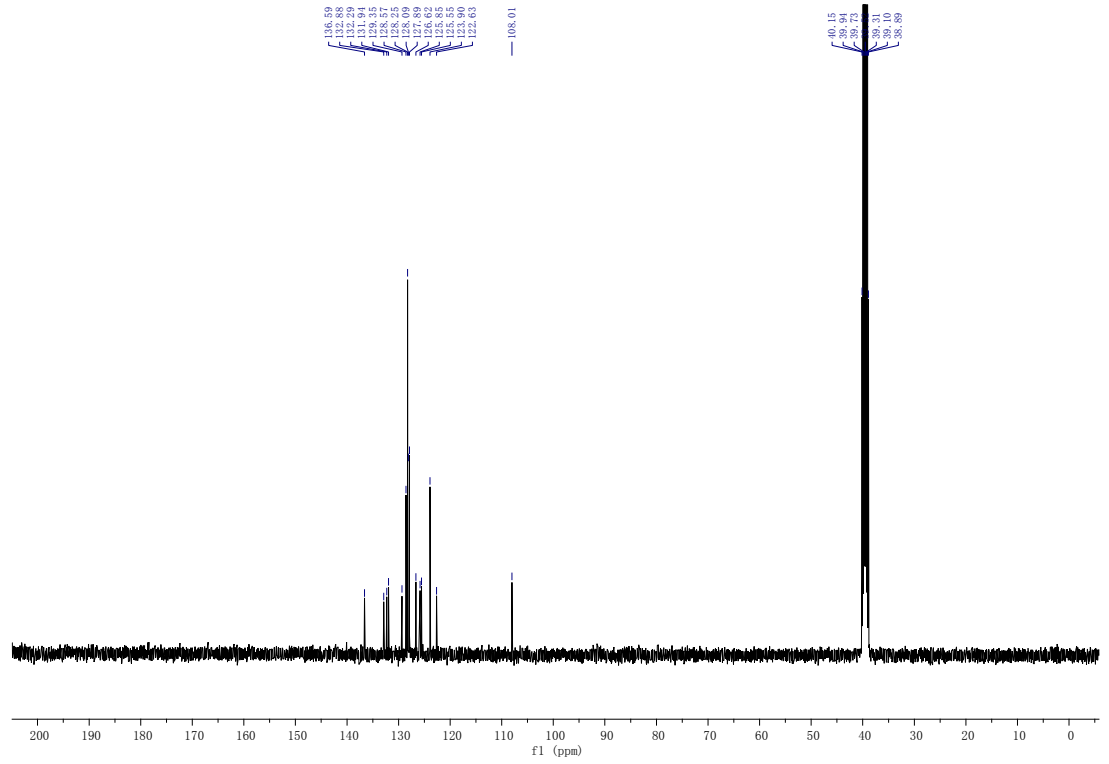
HRMS (ESI) m/z calculated for $C_{23}H_{20}NO$ $[M+Na]^+$: 348.1364, found 348.1366.

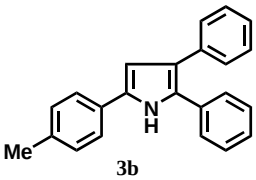
4. Copies of product NMR spectra



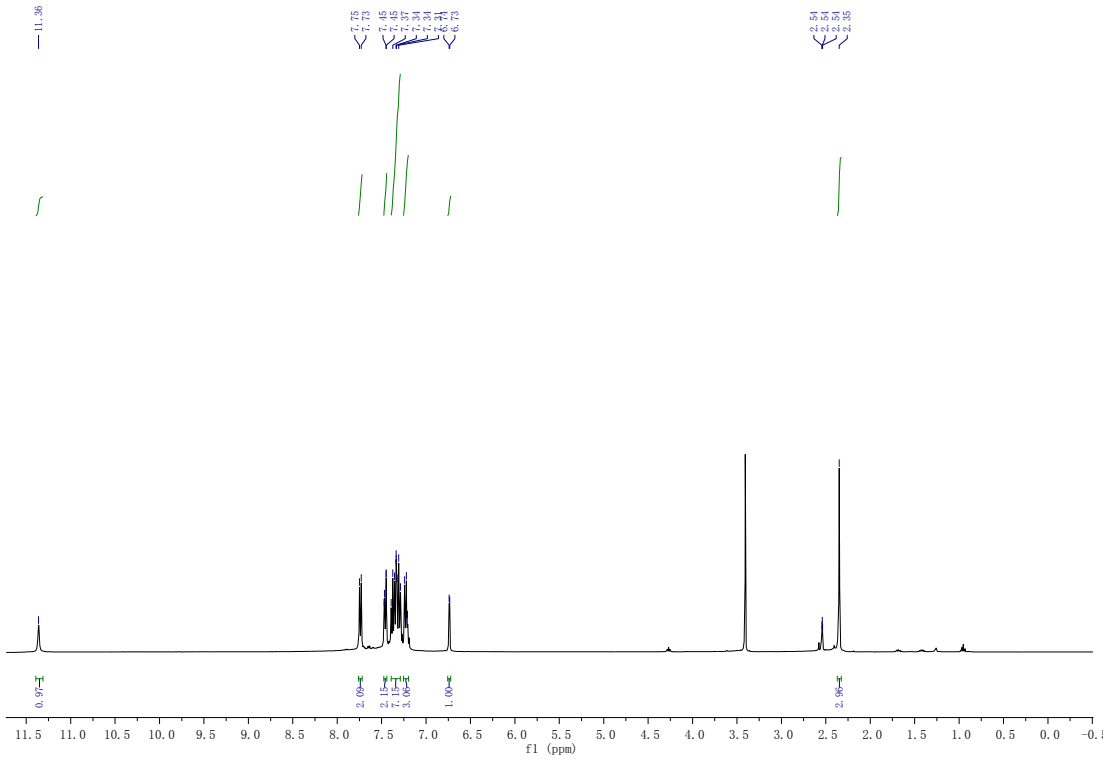
3a

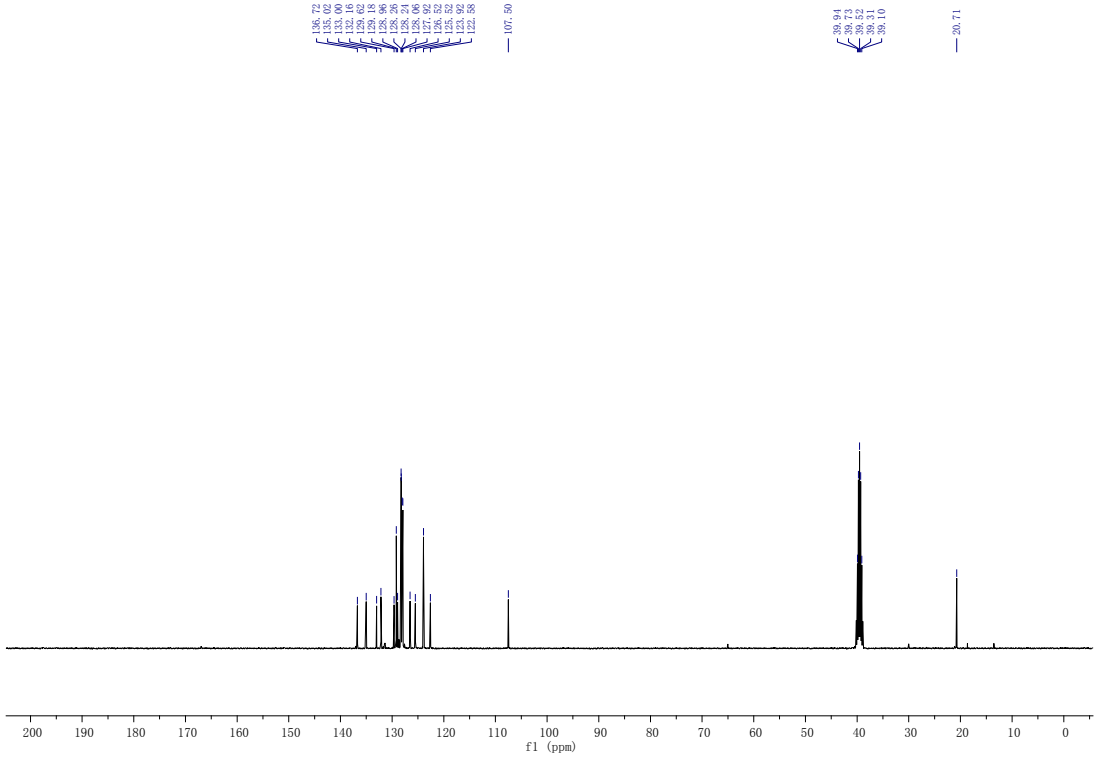


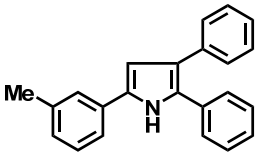



Me
N
H

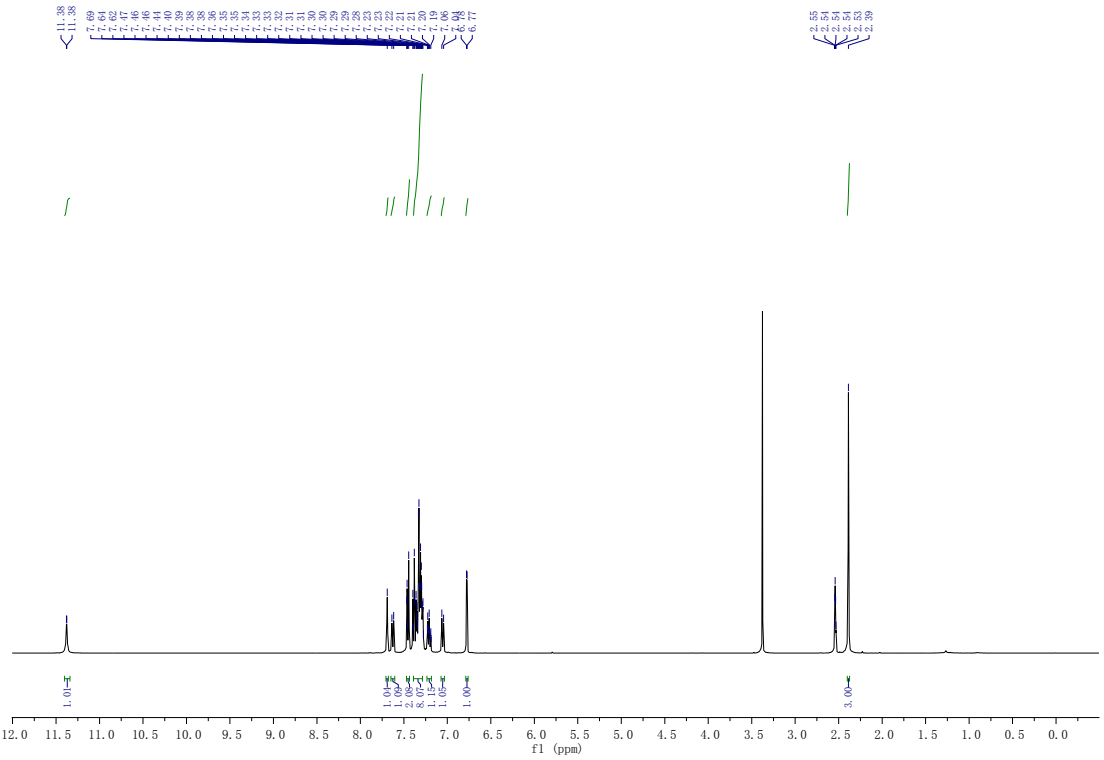
3b

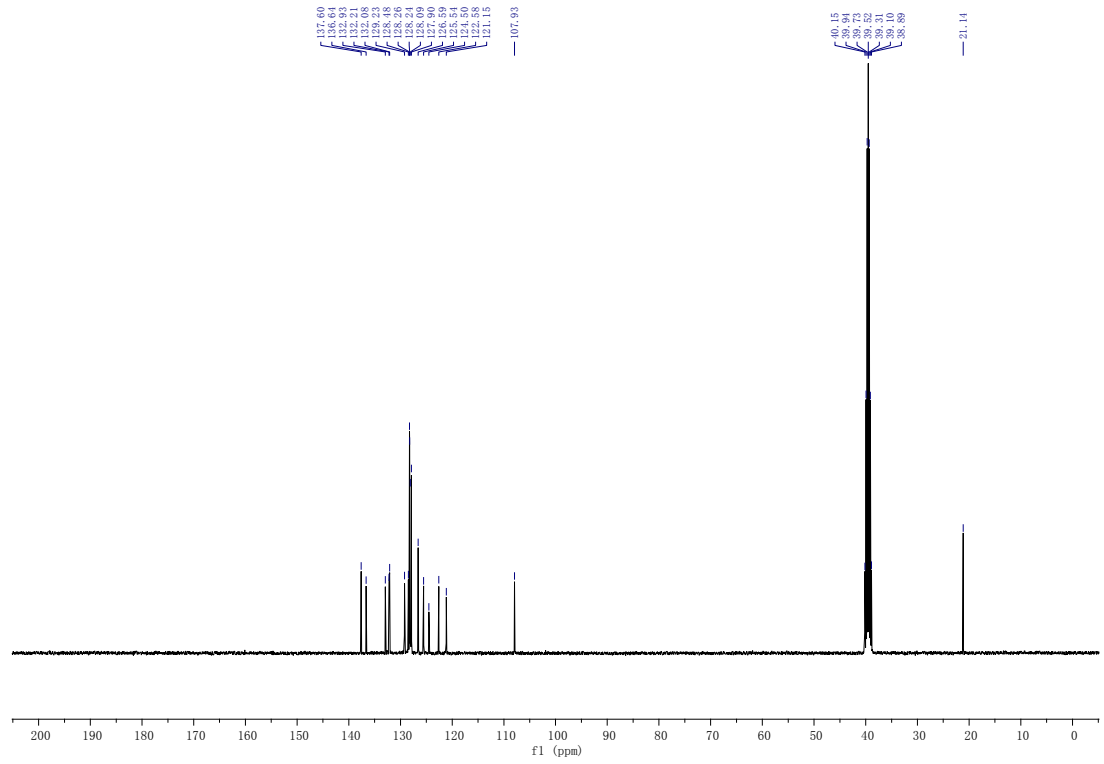

11.36
7.75
7.73
7.45
7.45
7.37
7.34
7.34
7.31
6.73
2.54
2.54
2.54
2.54
2.35
0.97
2.09
2.15
7.15
3.06
1.00
2.96
f1 (ppm)

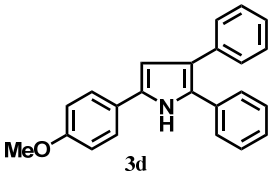

136.72
135.02
133.00
132.16
129.62
129.14
128.96
128.26
128.24
126.96
126.92
126.52
125.52
123.92
122.98
107.50
39.94
39.73
39.52
39.31
39.10
20.71
f1 (ppm)



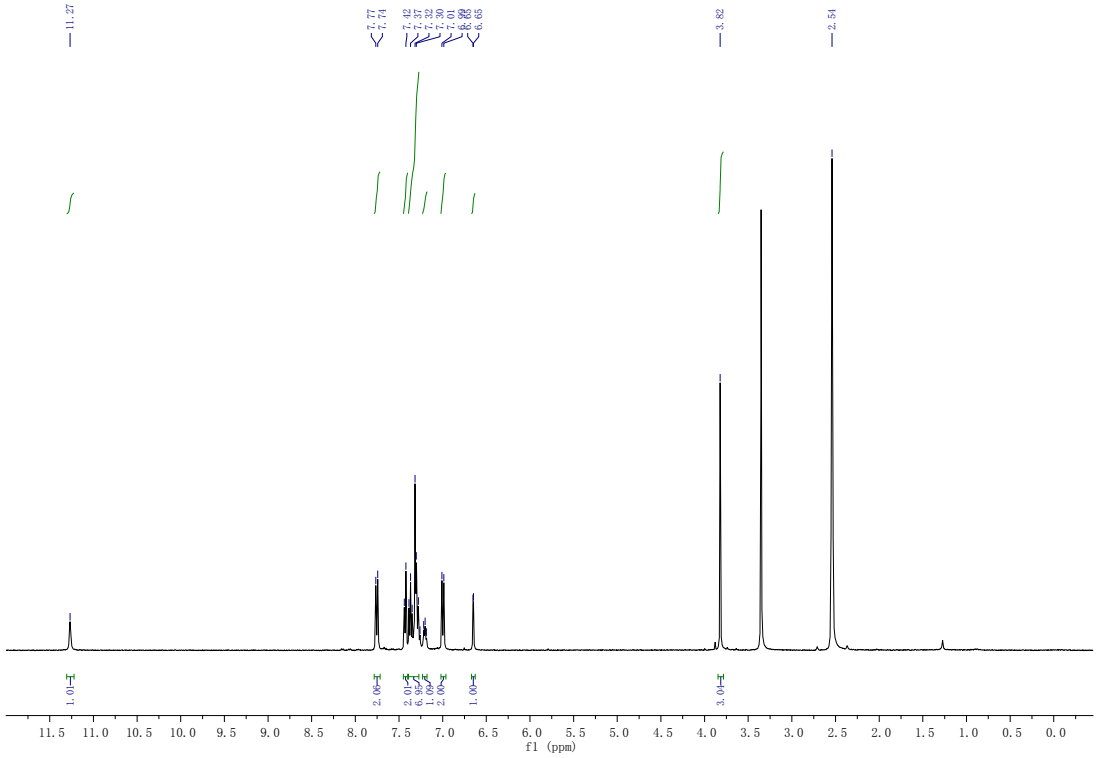
3c

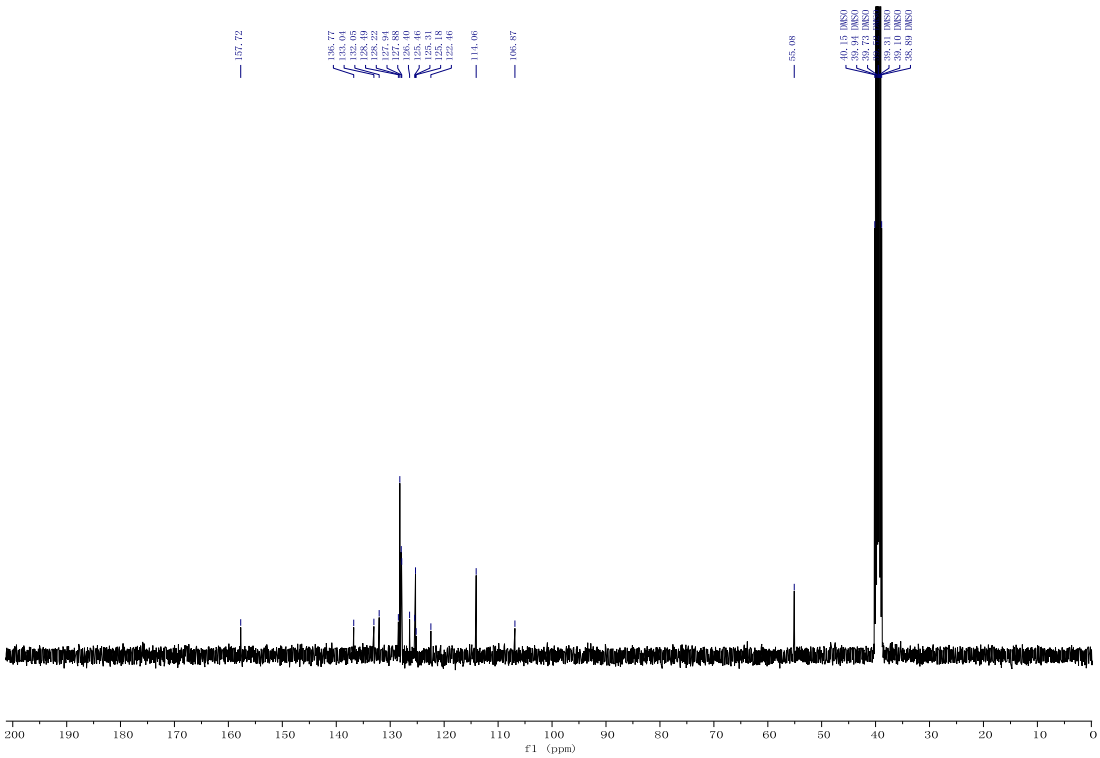


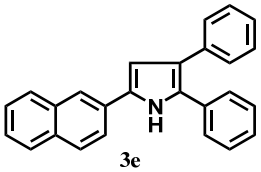




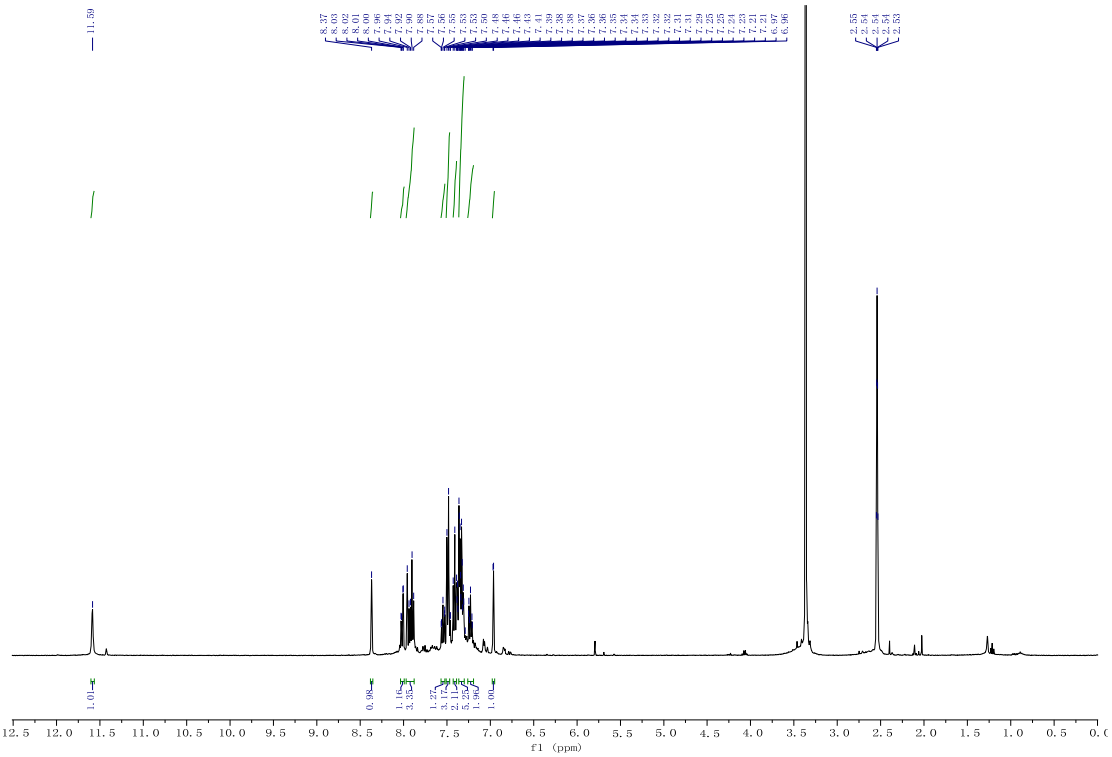
3d

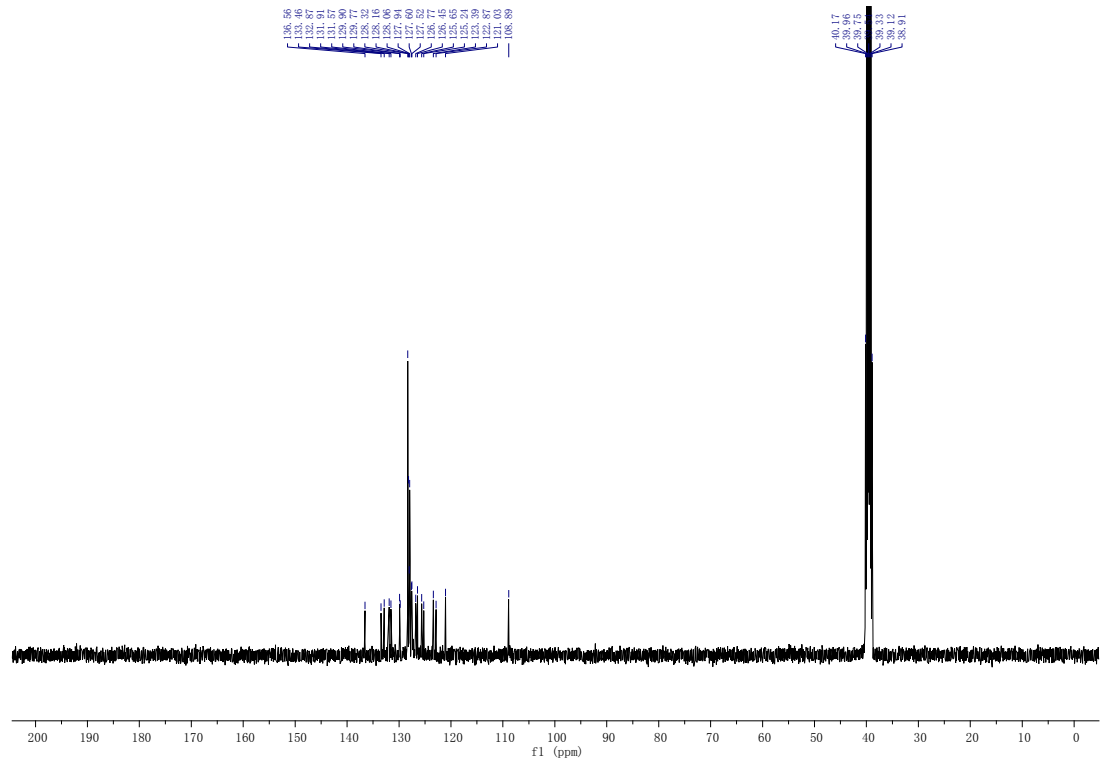


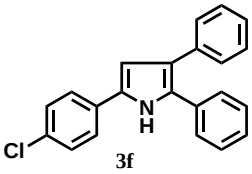




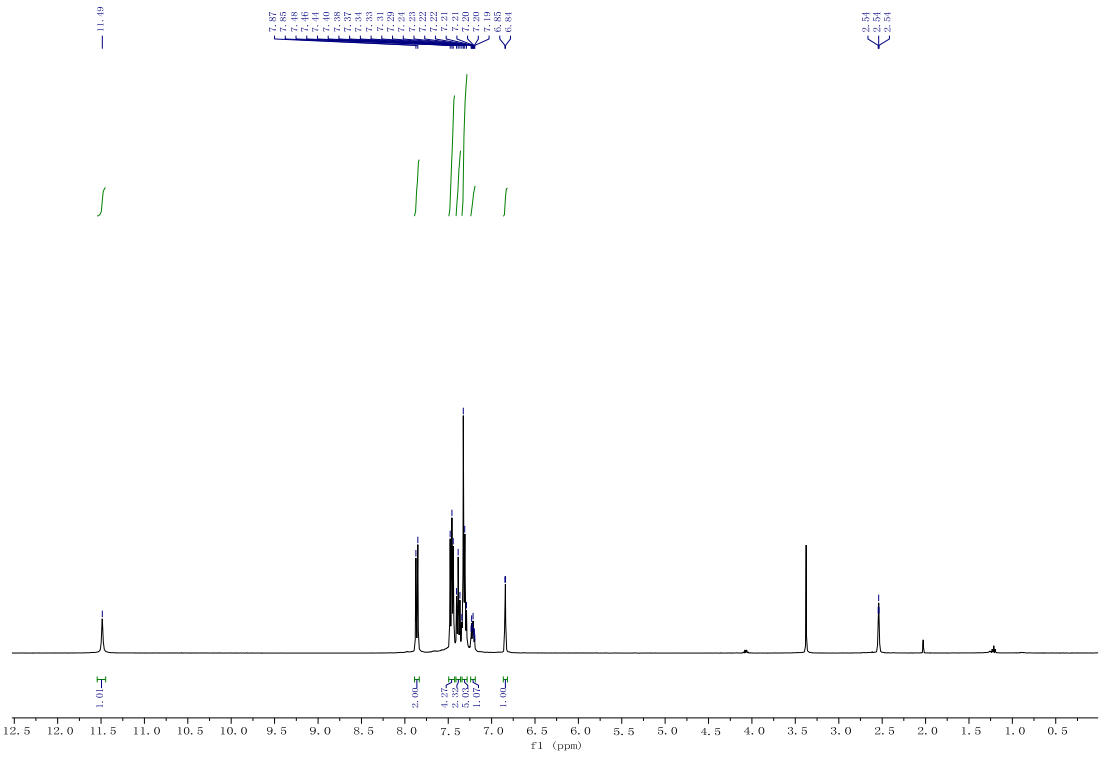
3e

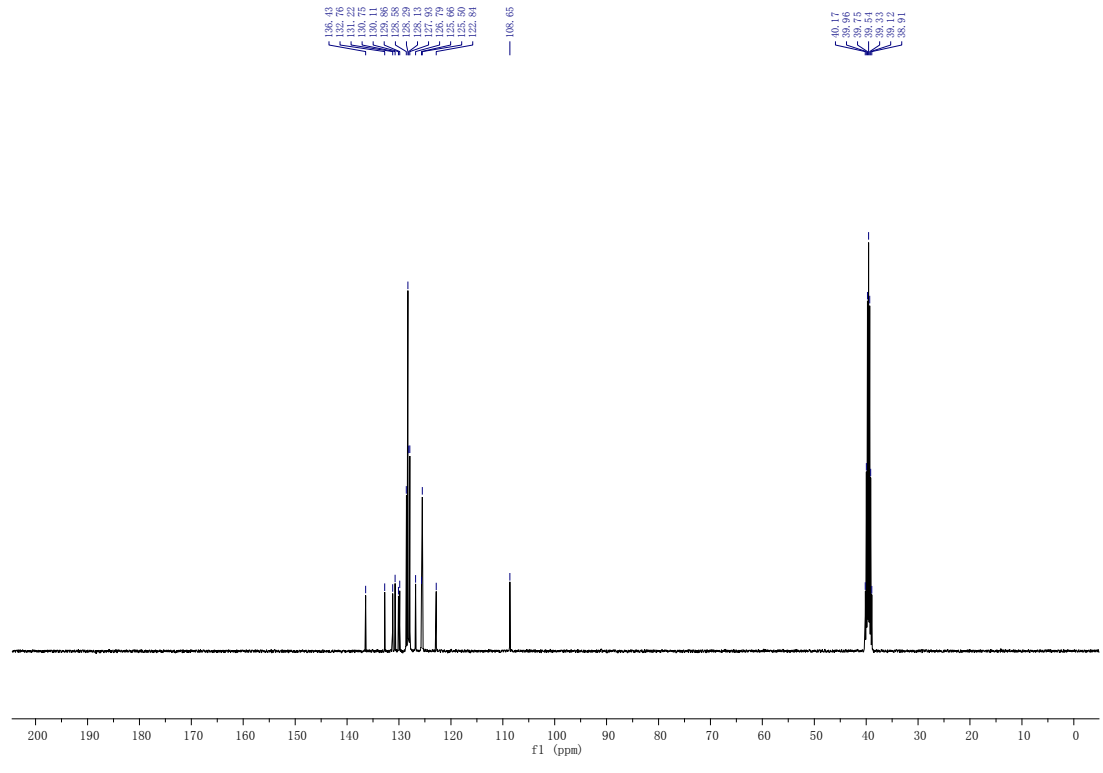


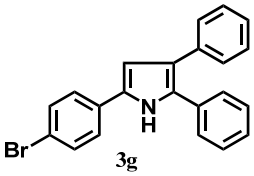




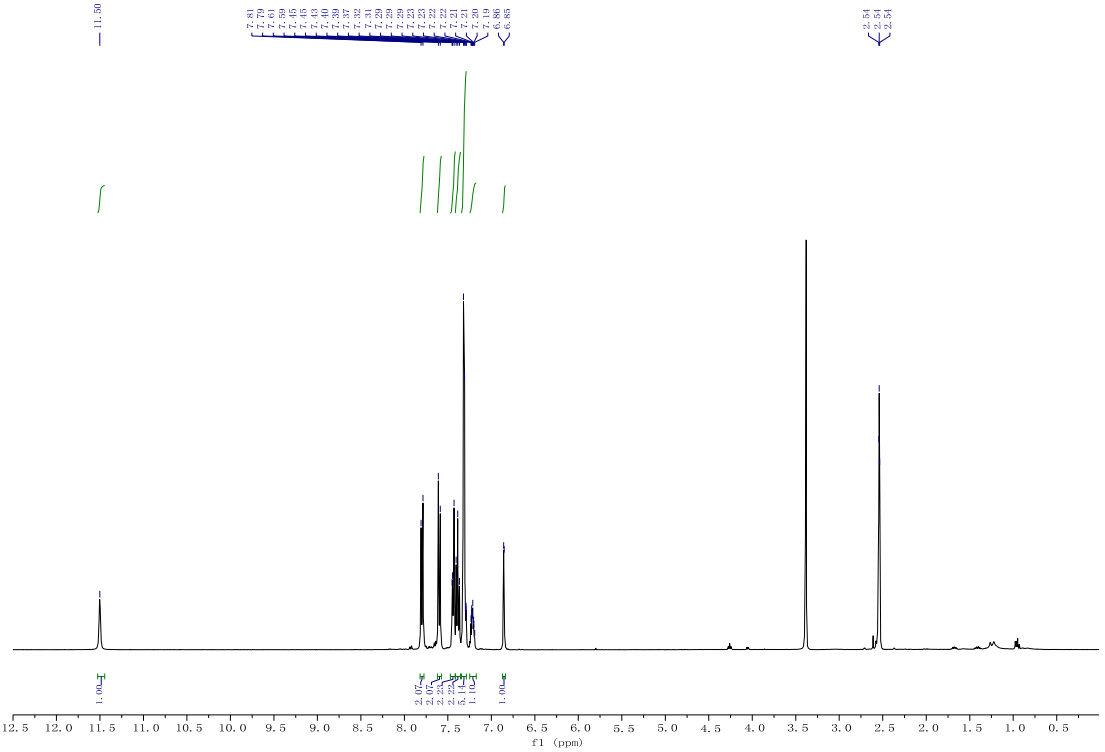
3f

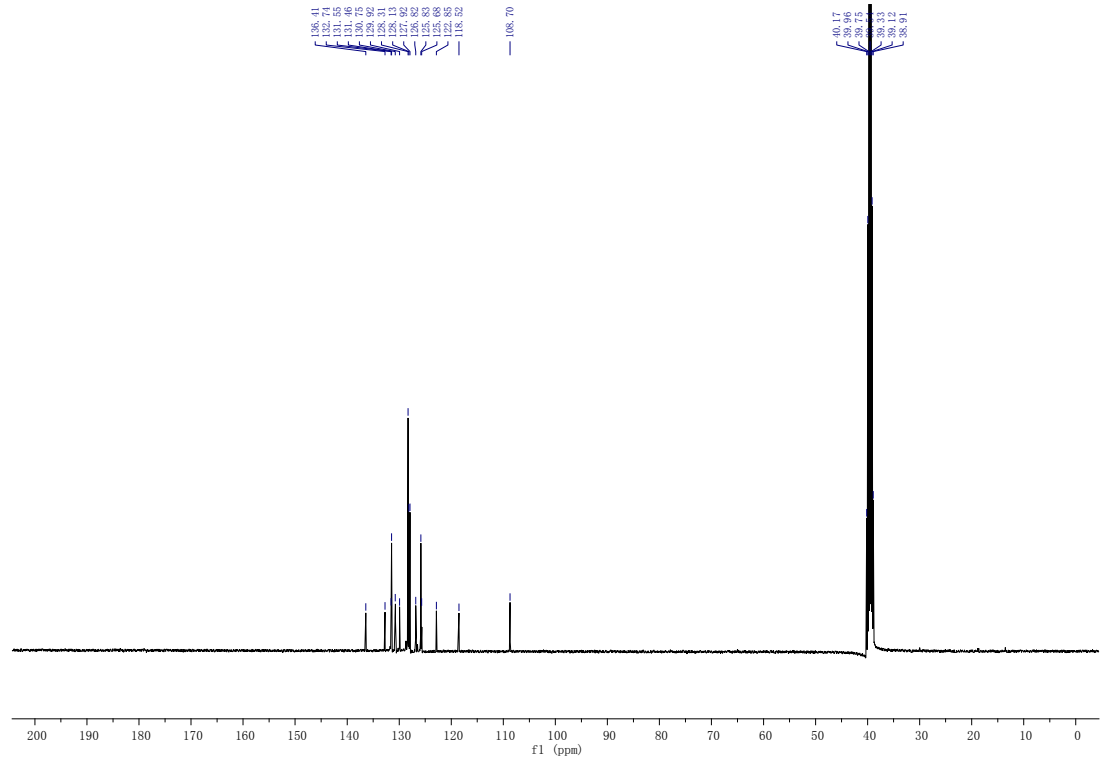


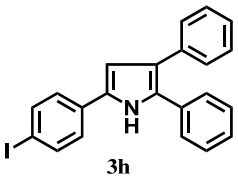




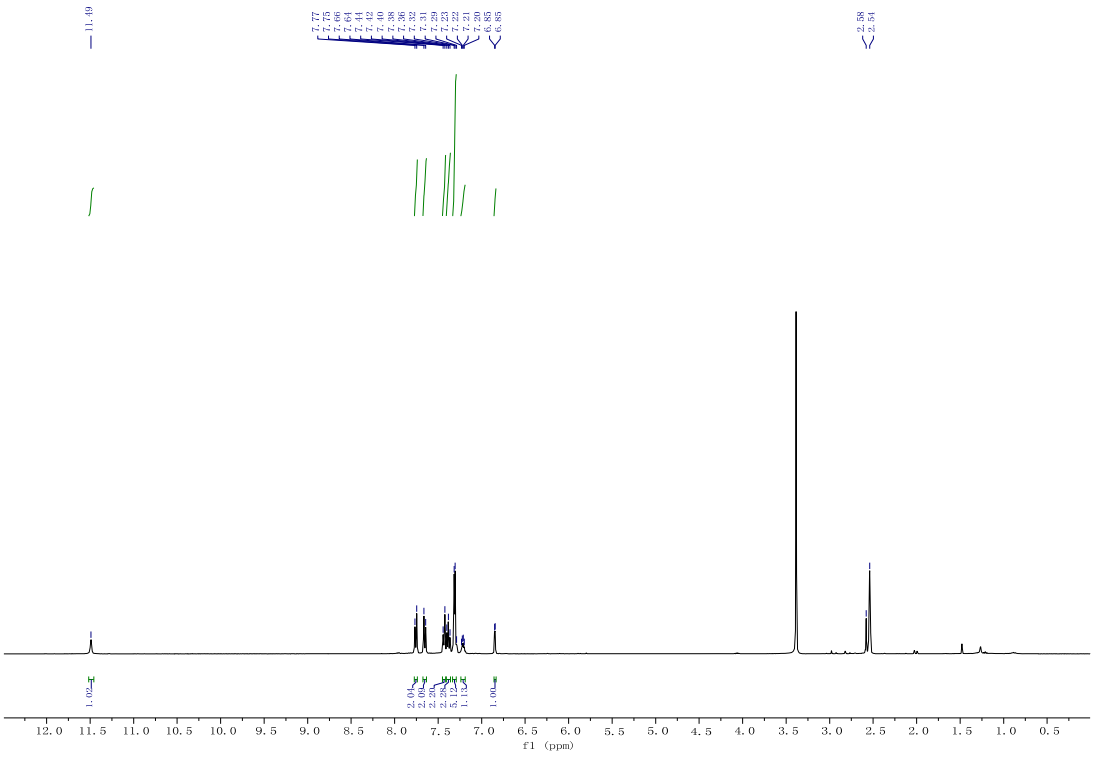
3g







3h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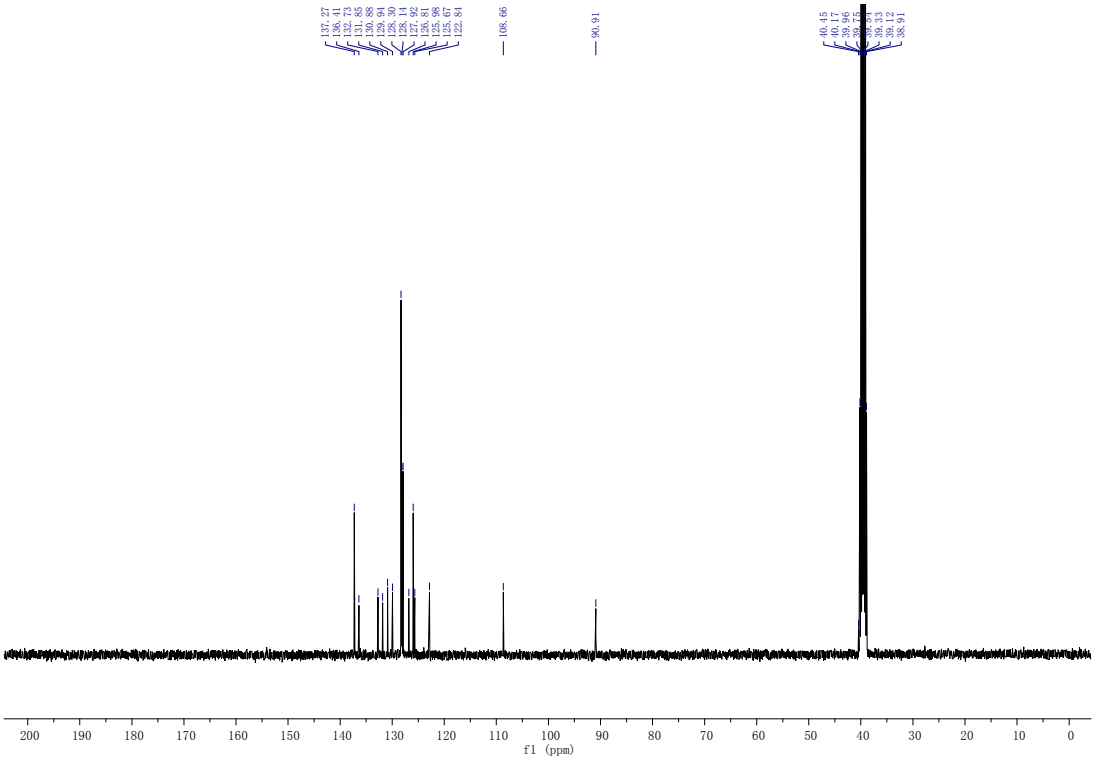
7.77
7.75
7.66
7.64
7.44
7.43
7.40
7.38
7.36
7.32
7.31
7.29
7.23
7.22
7.21
7.20
6.85
6.85
3.58
2.54
1.02
2.04
2.09
2.20
2.28
1.15
1.13
1.00
f1 (ppm)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131.85
130.88
129.94
128.30
128.14
127.92
126.51
125.98
125.67
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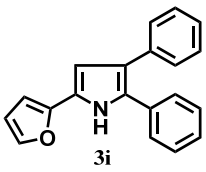
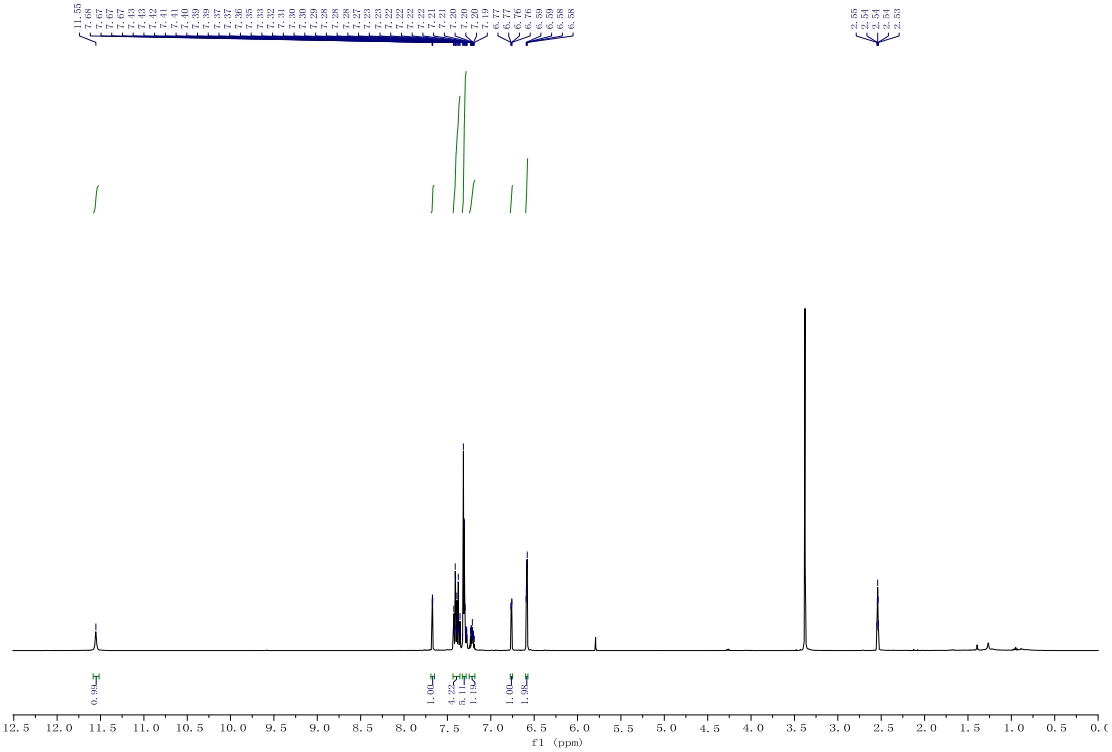
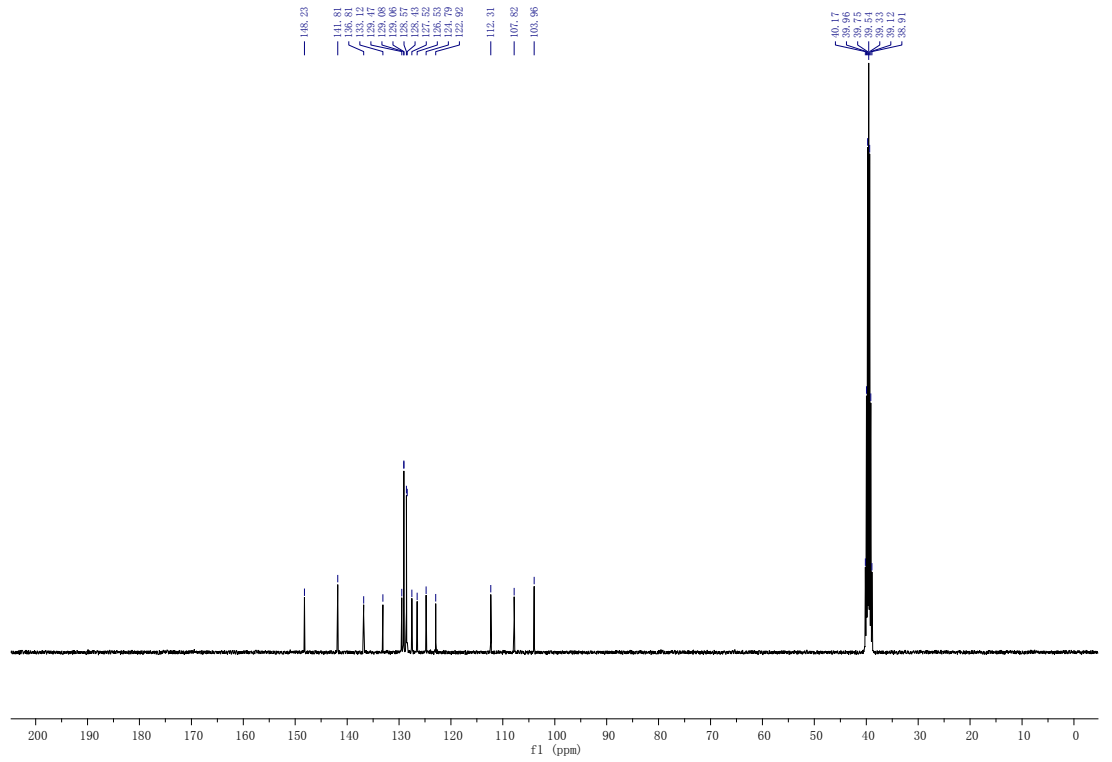
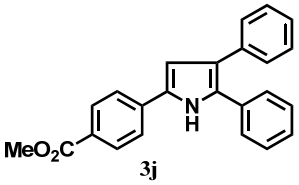
39.54
39.33
39.12
38.91
f1 (ppm)



3i







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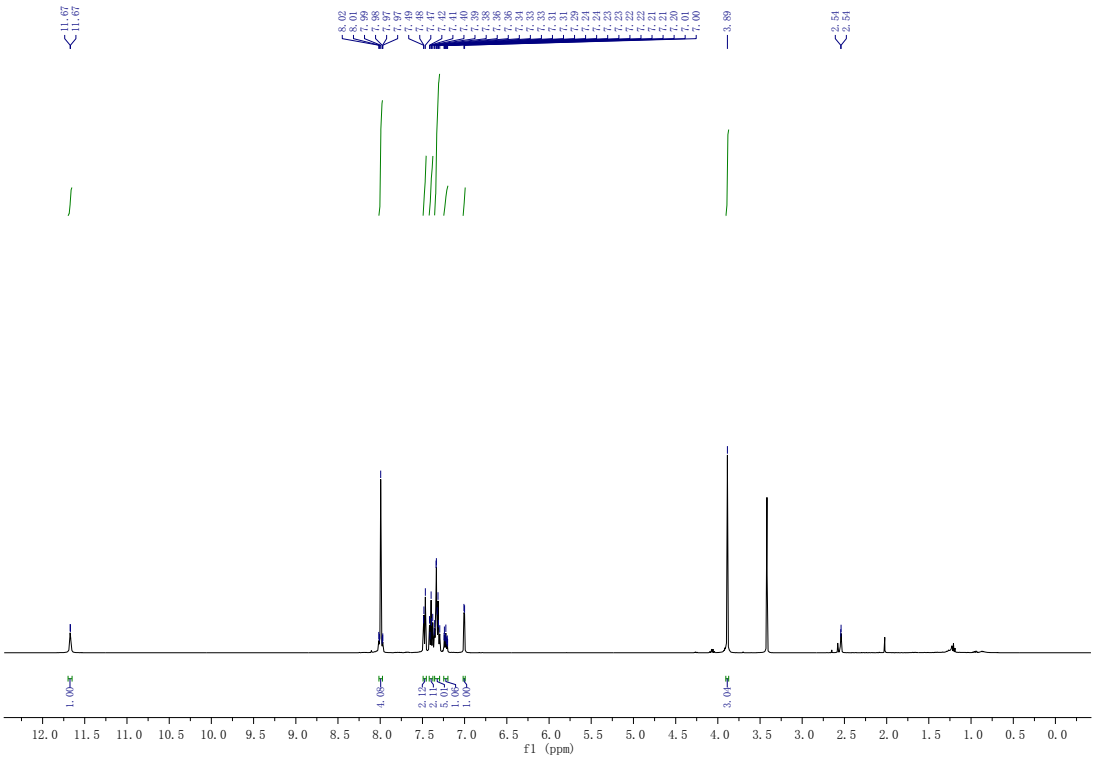

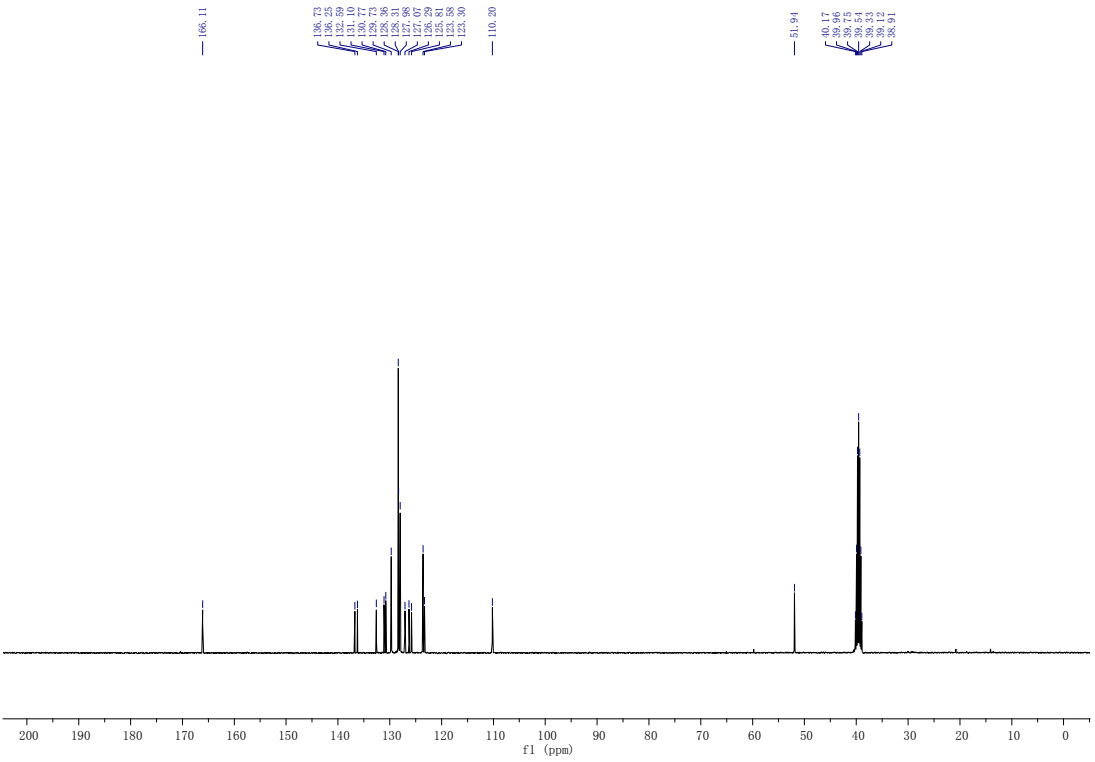

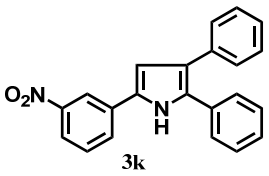

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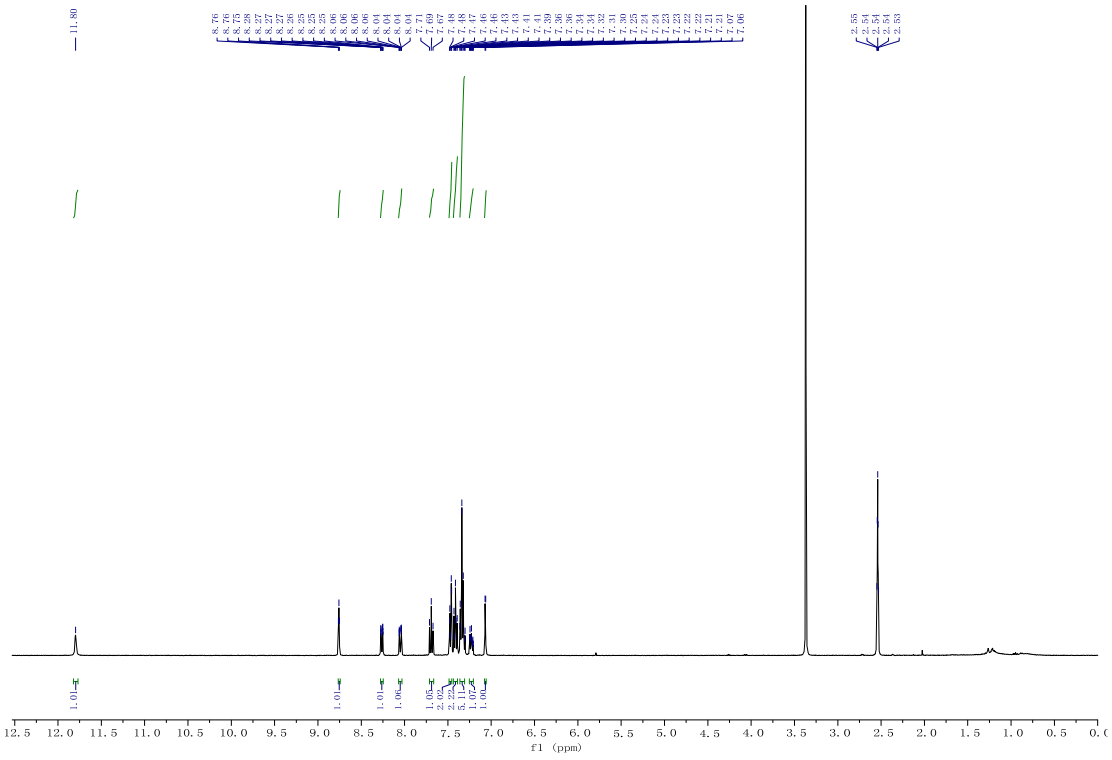

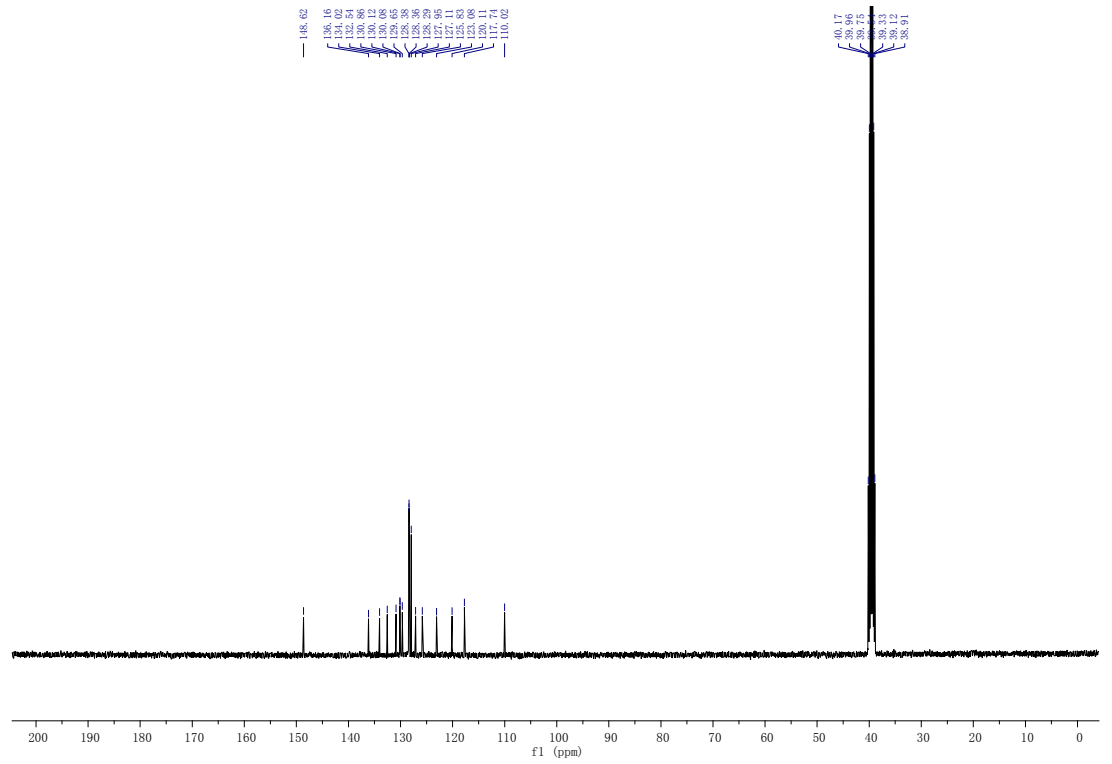

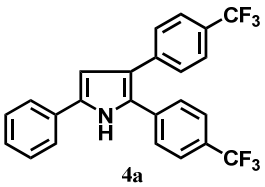

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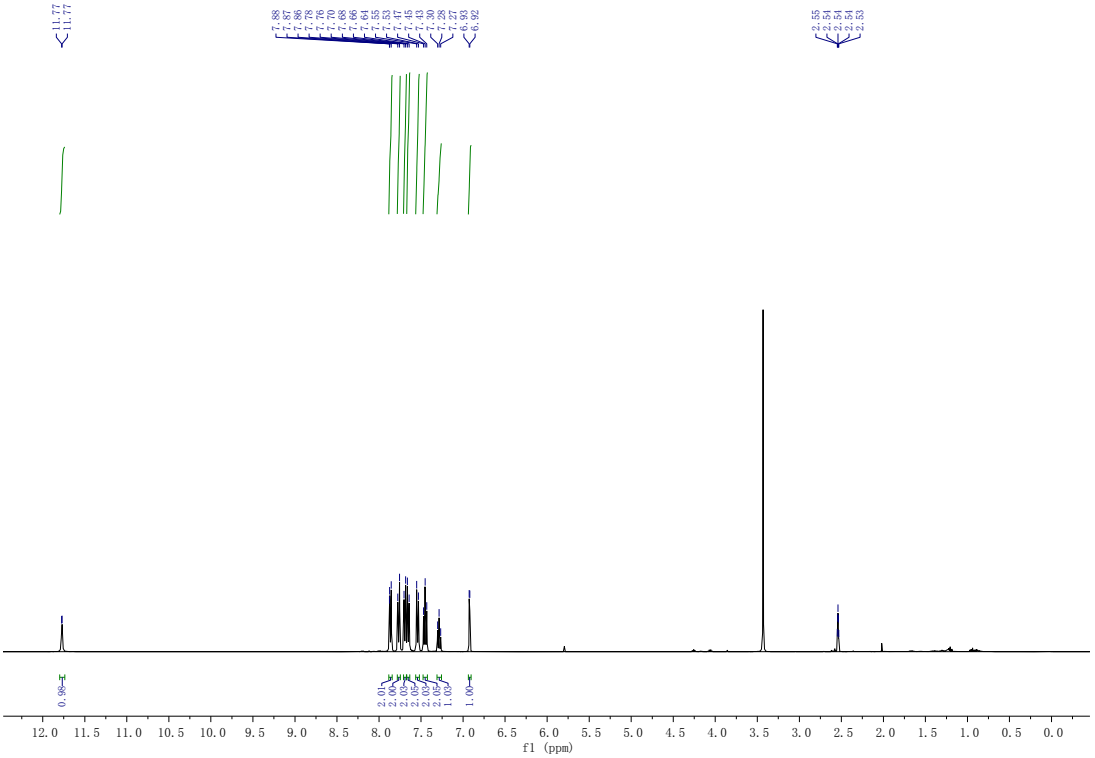

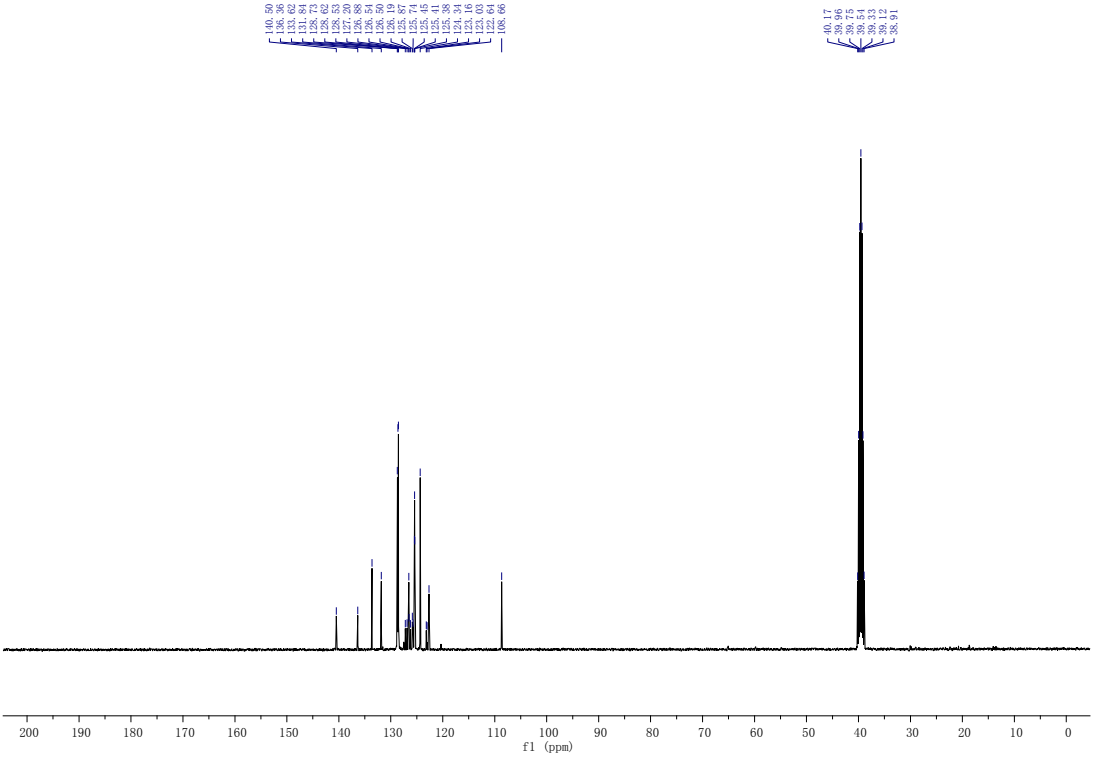

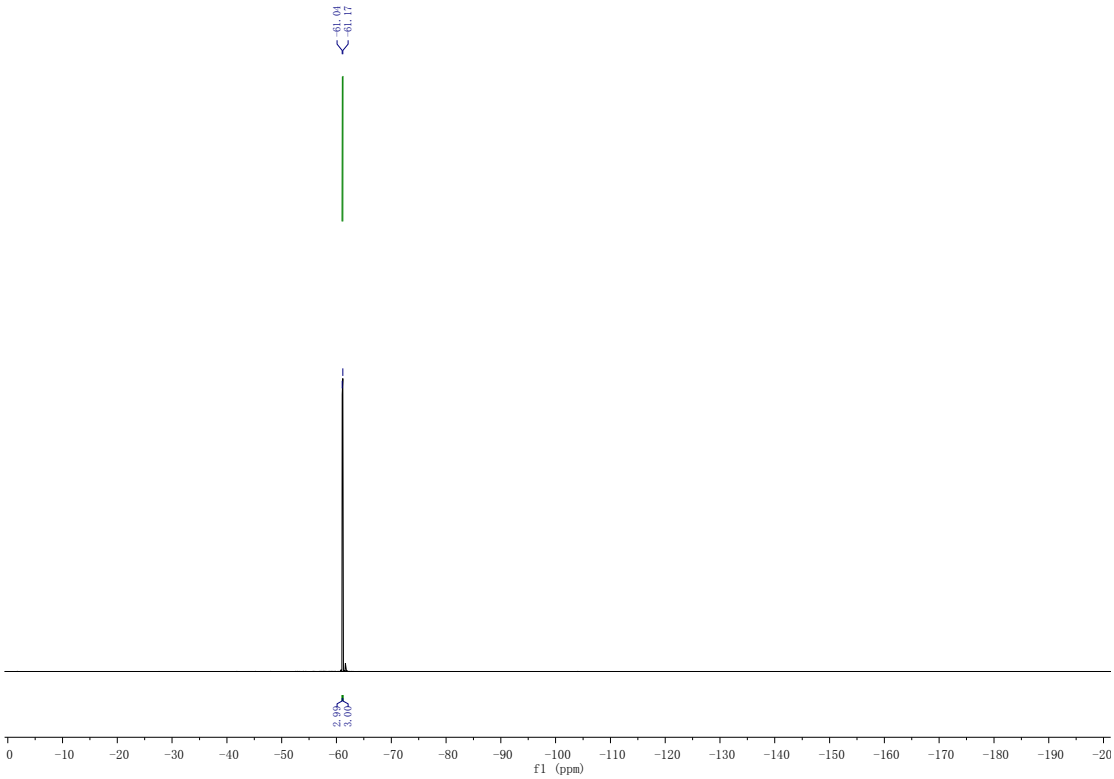

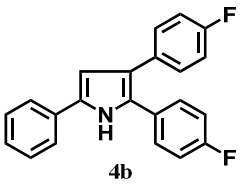

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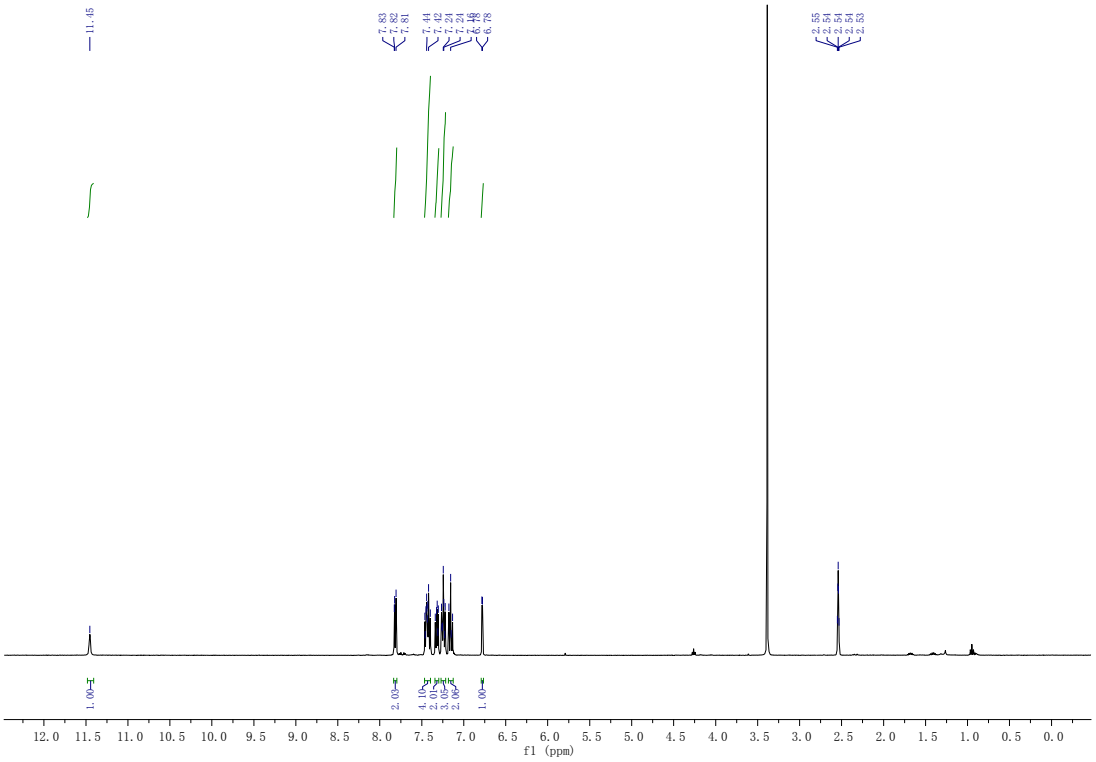

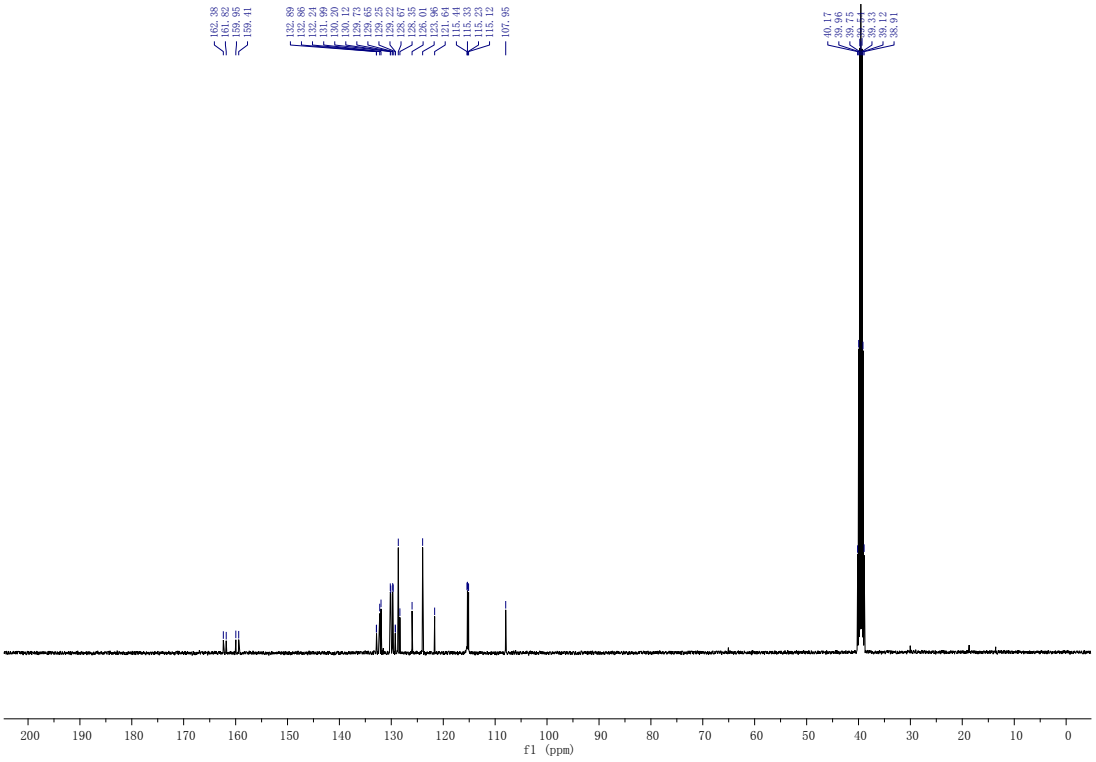

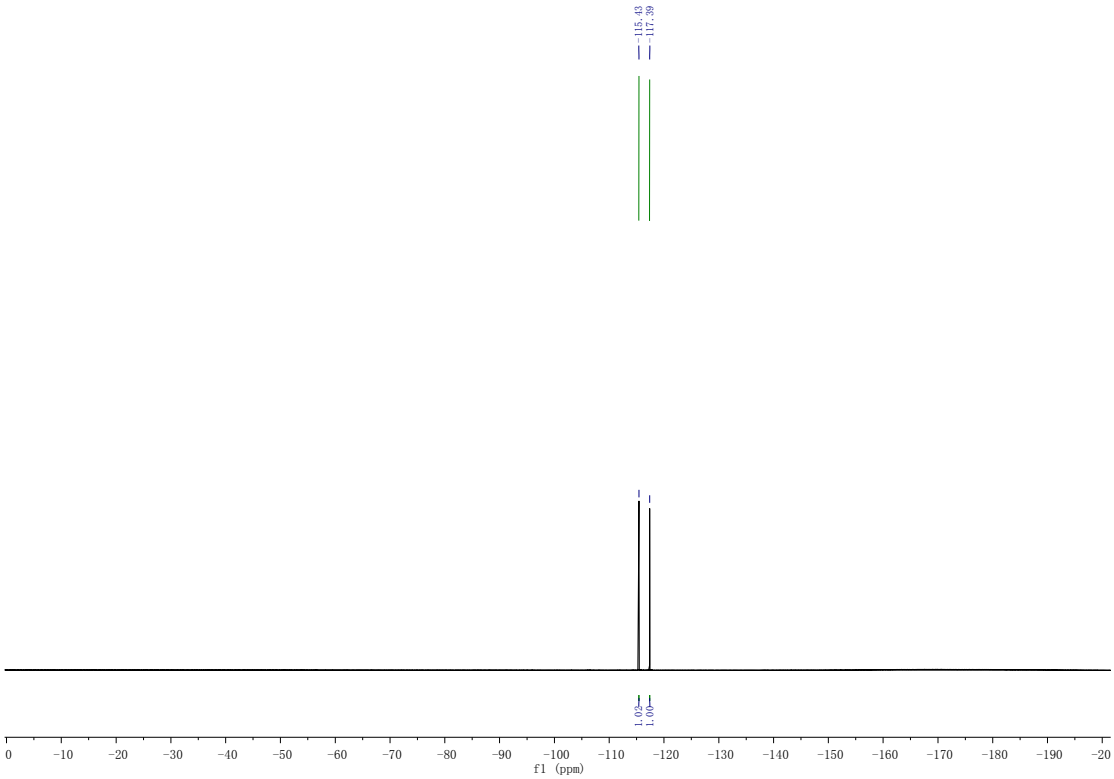

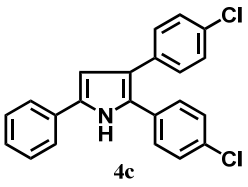

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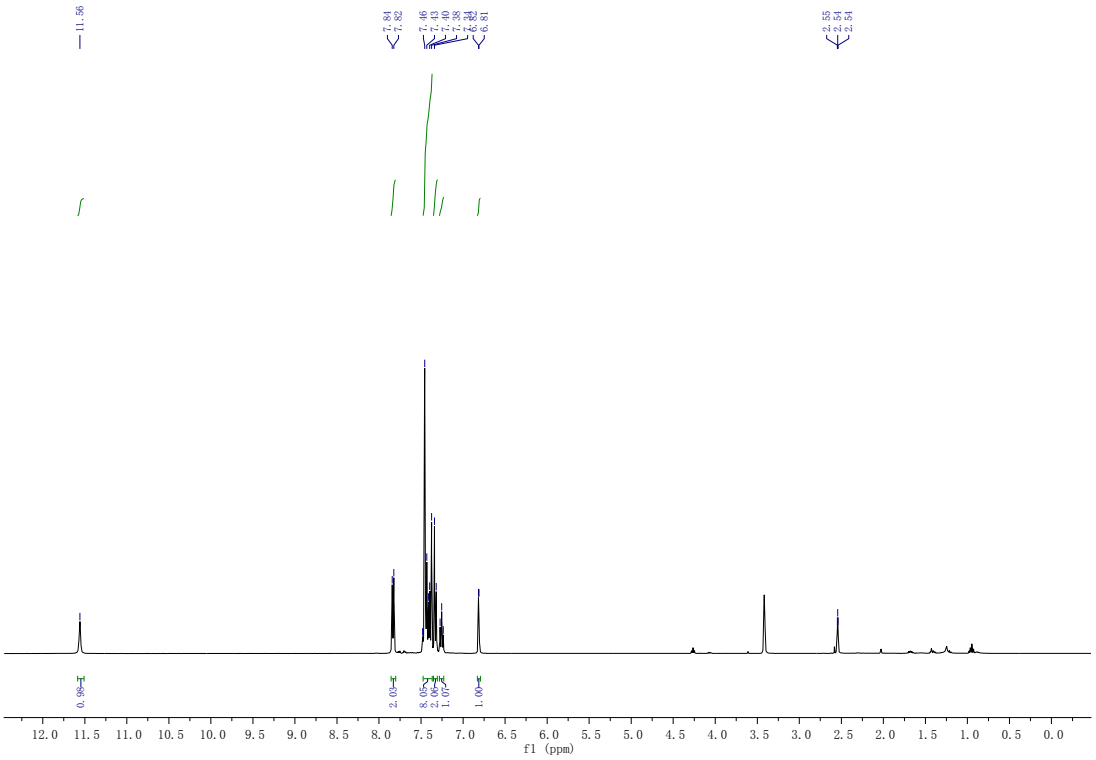

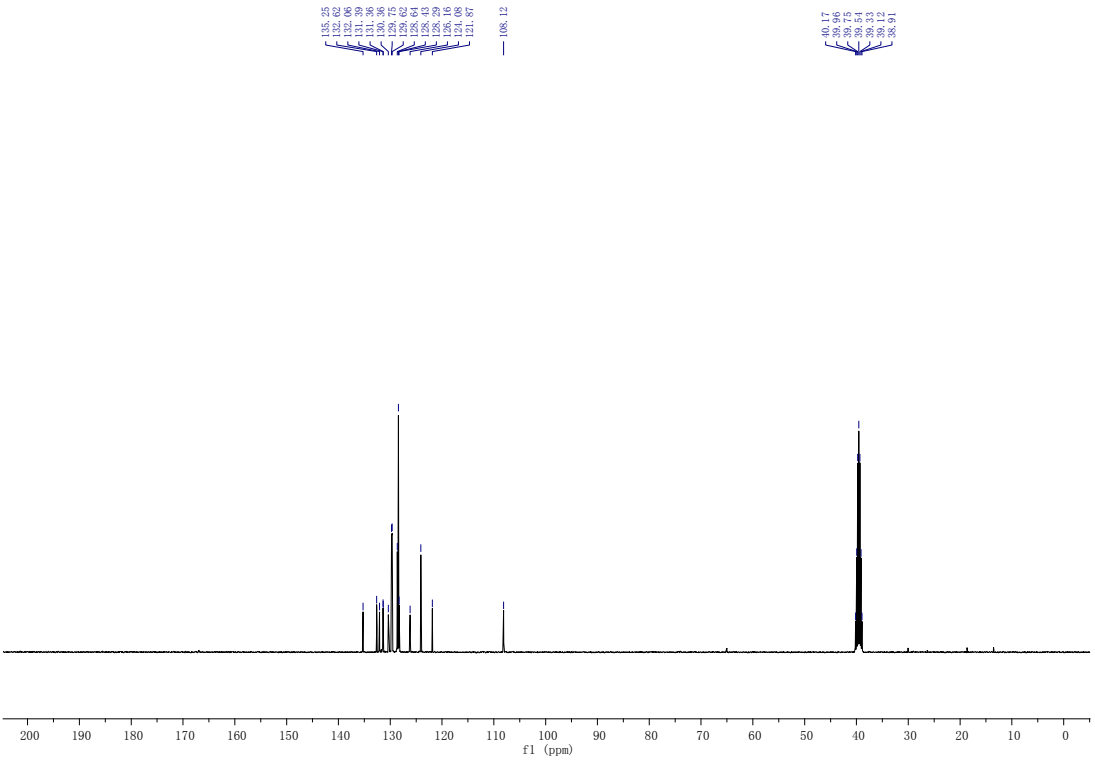

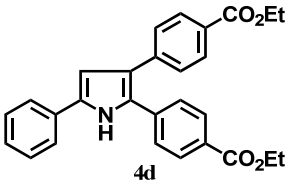

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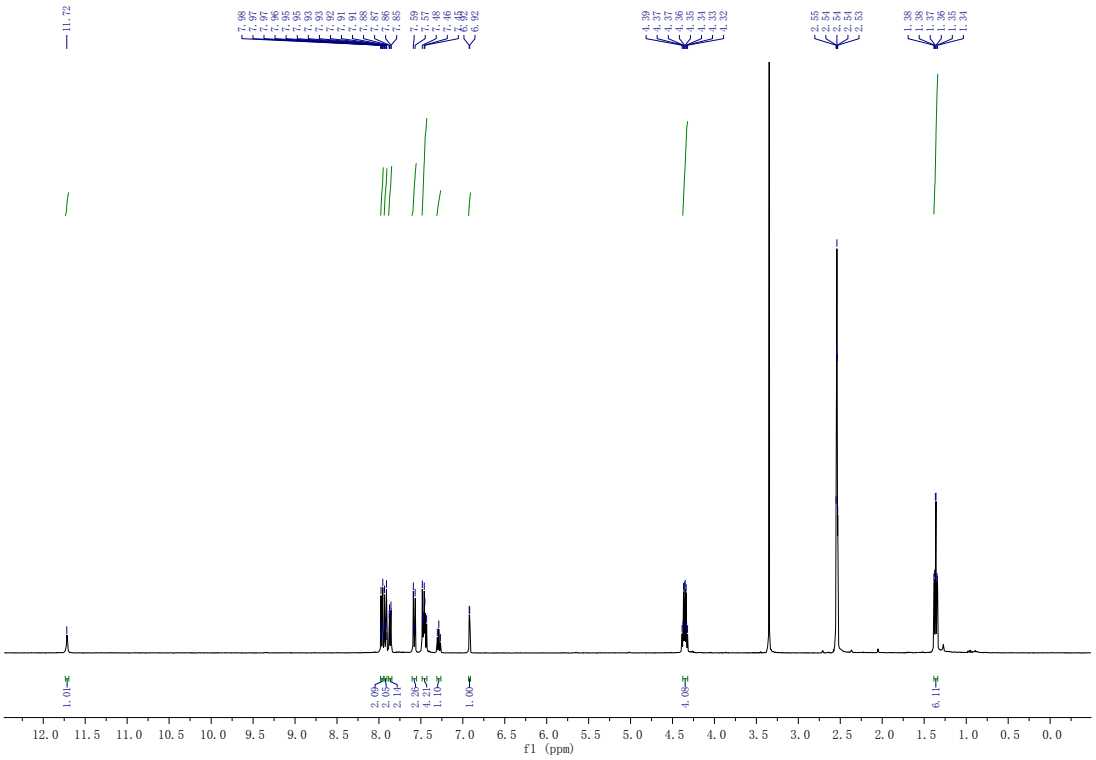

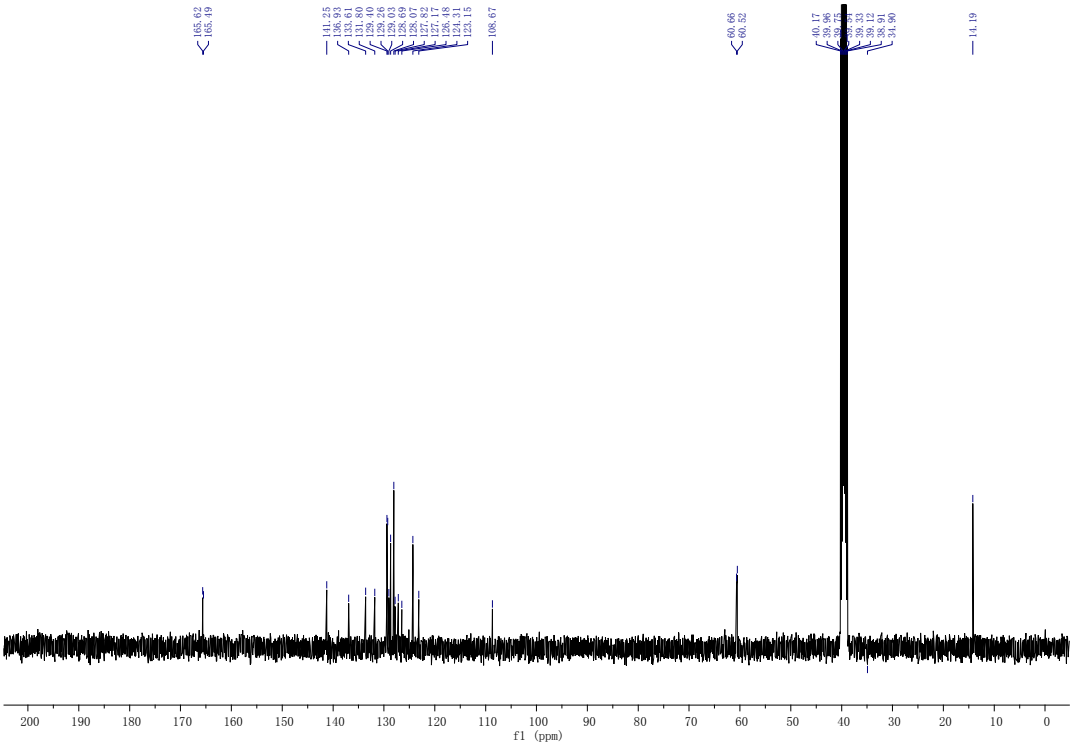

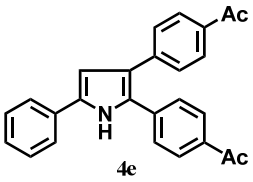

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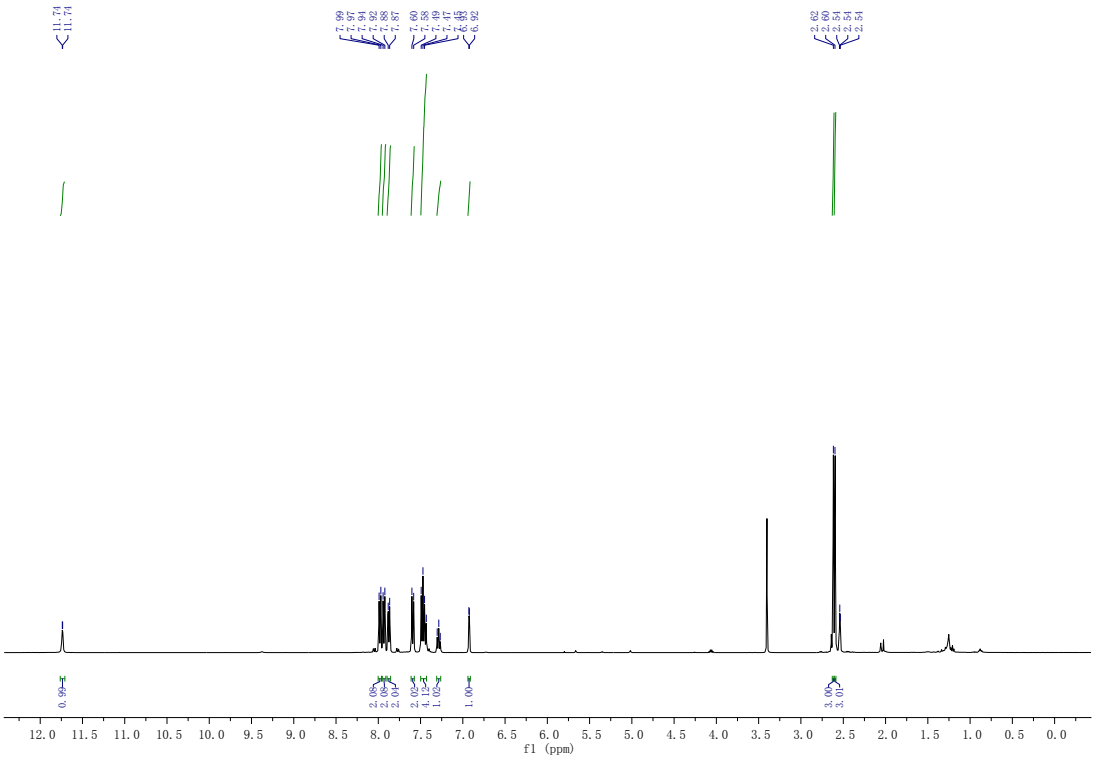
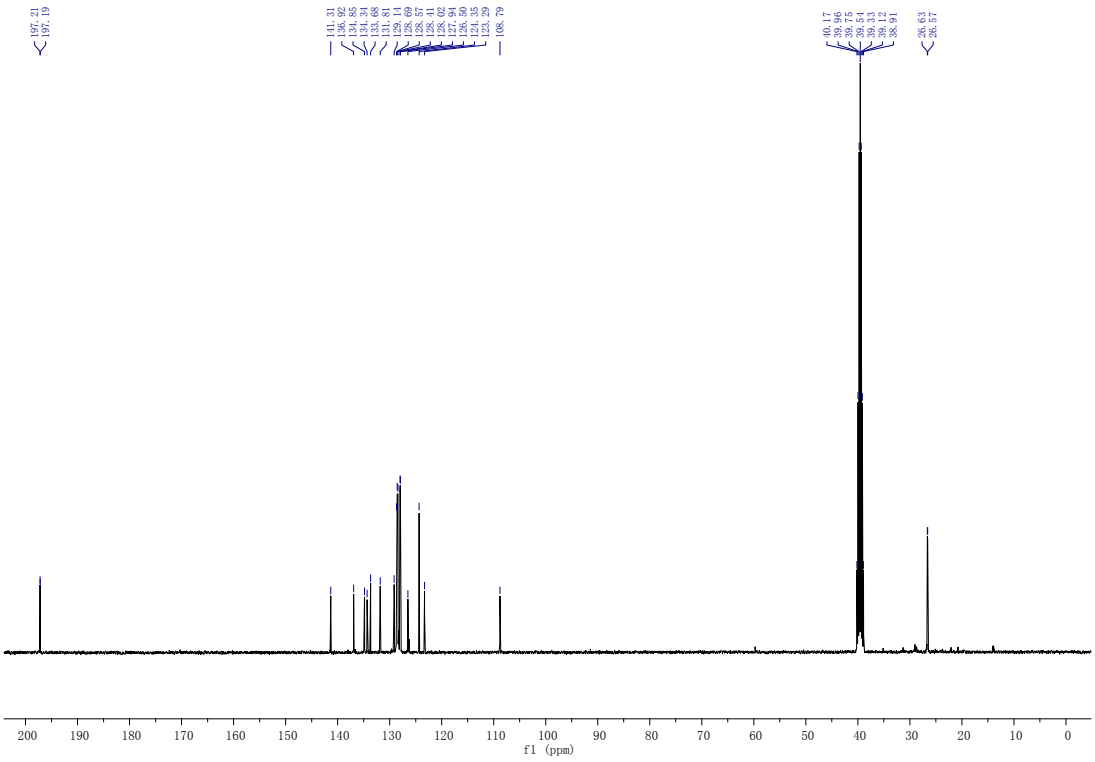
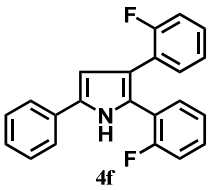
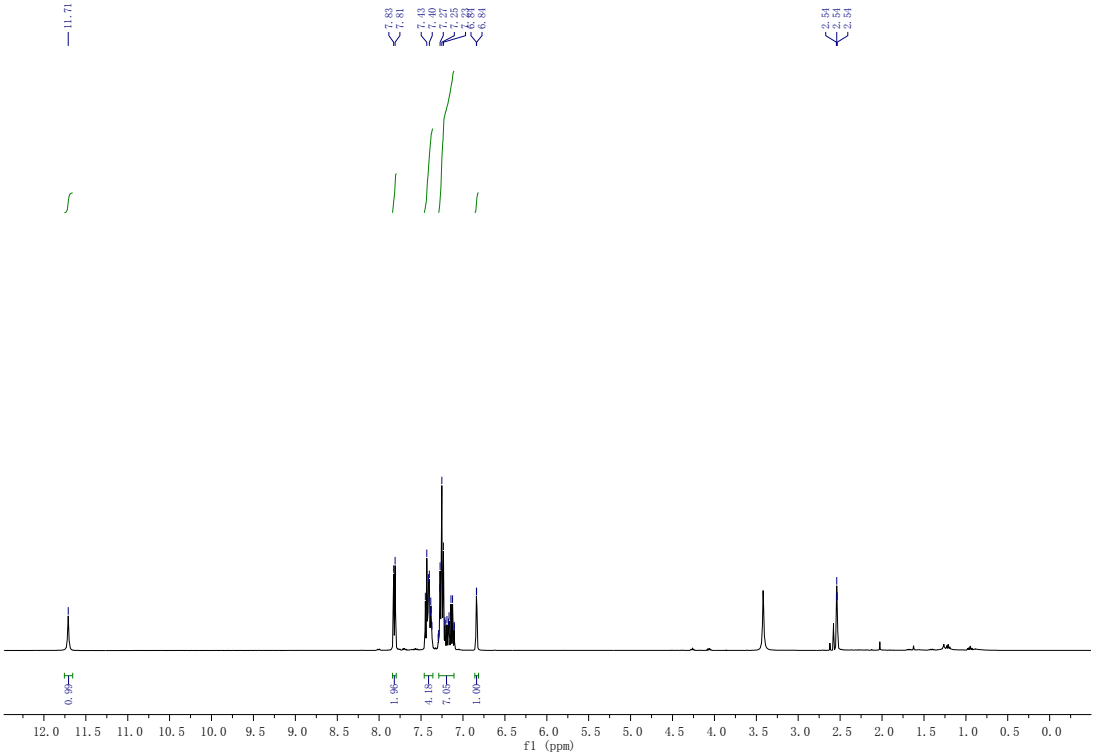
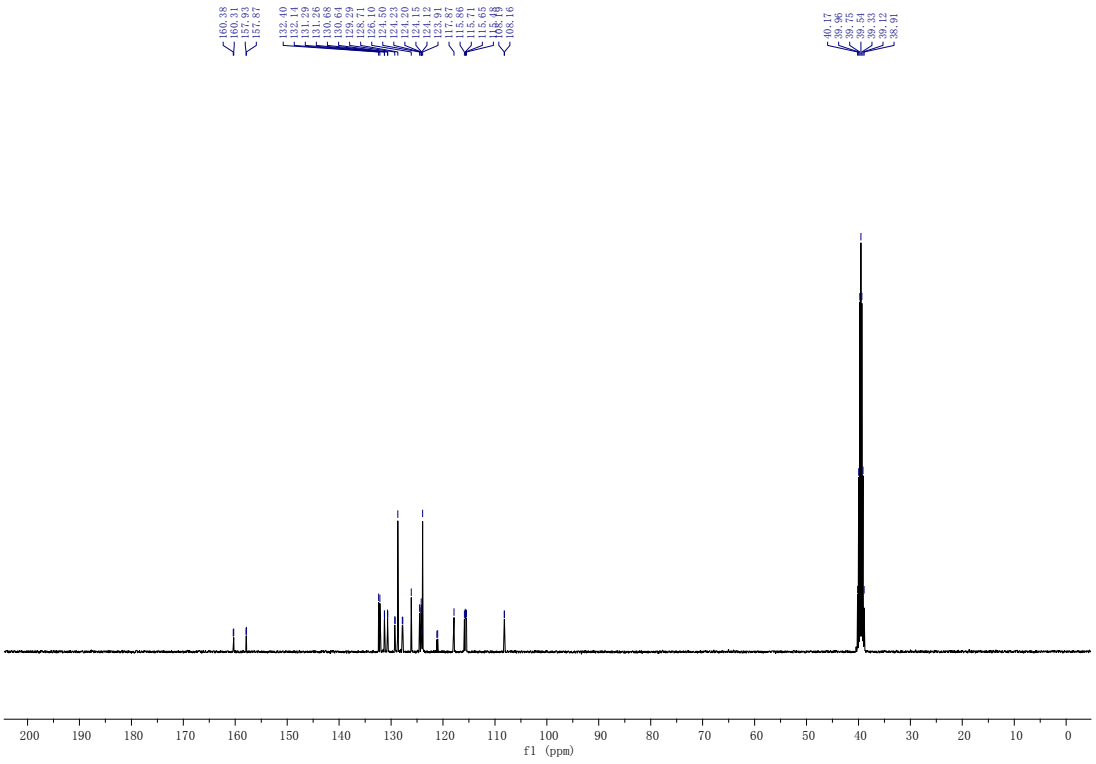


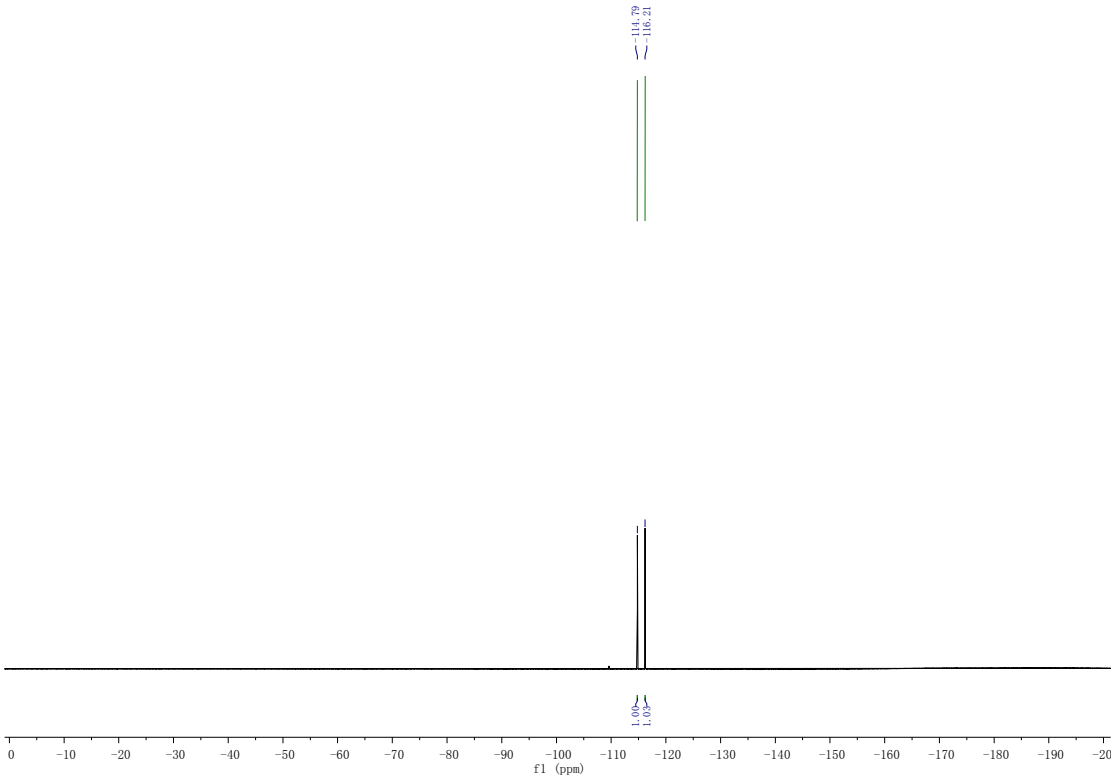


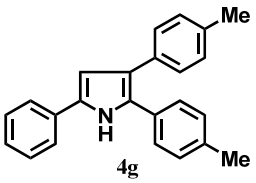

F
N
H
F

4f

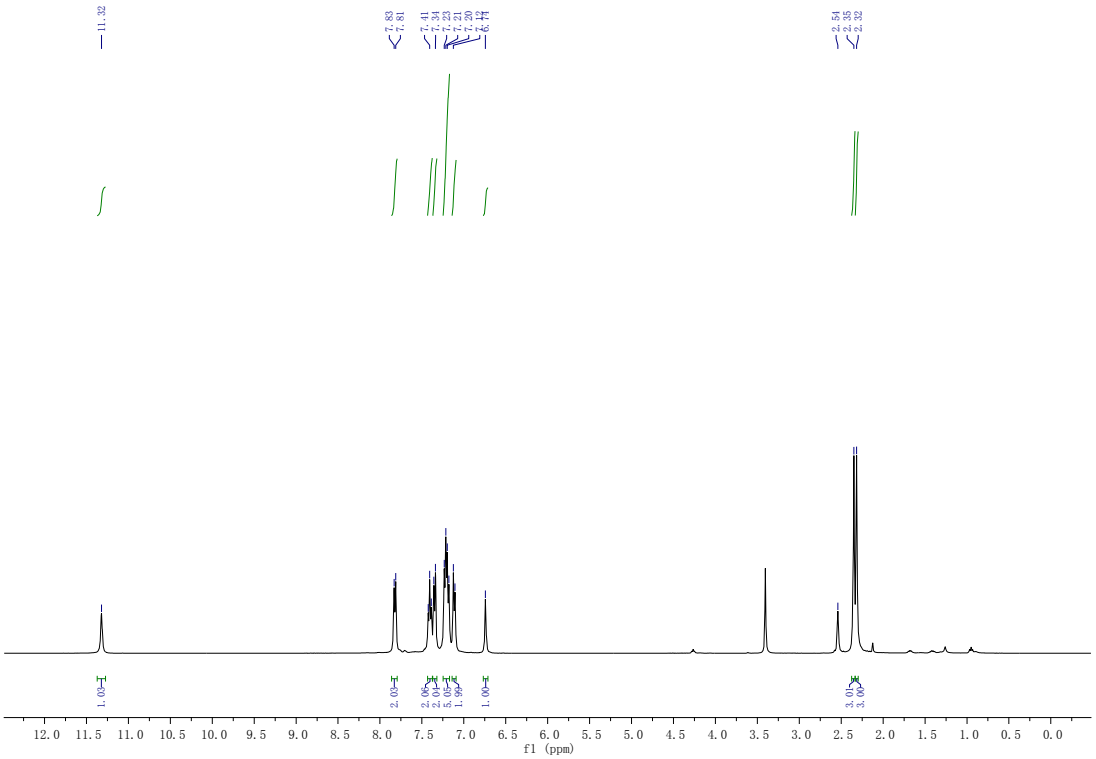

11.71
7.83
7.81
7.43
7.40
7.27
7.25
6.87
6.84
2.54
2.54
2.54
0.99
1.96
4.18
7.05
1.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

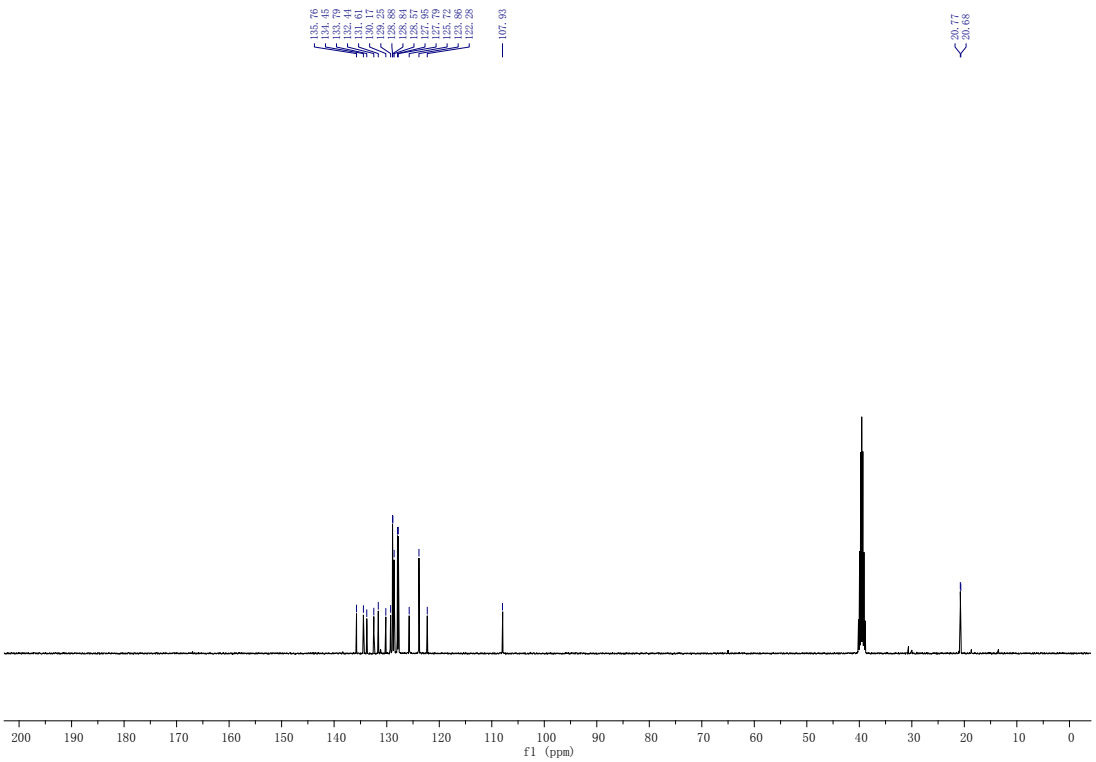

160.38
160.31
157.93
151.87
132.40
132.14
131.29
131.26
130.68
130.64
129.29
128.71
126.10
125.50
124.23
124.20
124.15
123.12
123.11
117.87
115.86
115.71
115.45
108.19
108.16
40.17
39.96
39.75
39.54
39.33
39.12
38.91
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

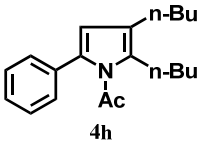



Me
N
H
Me

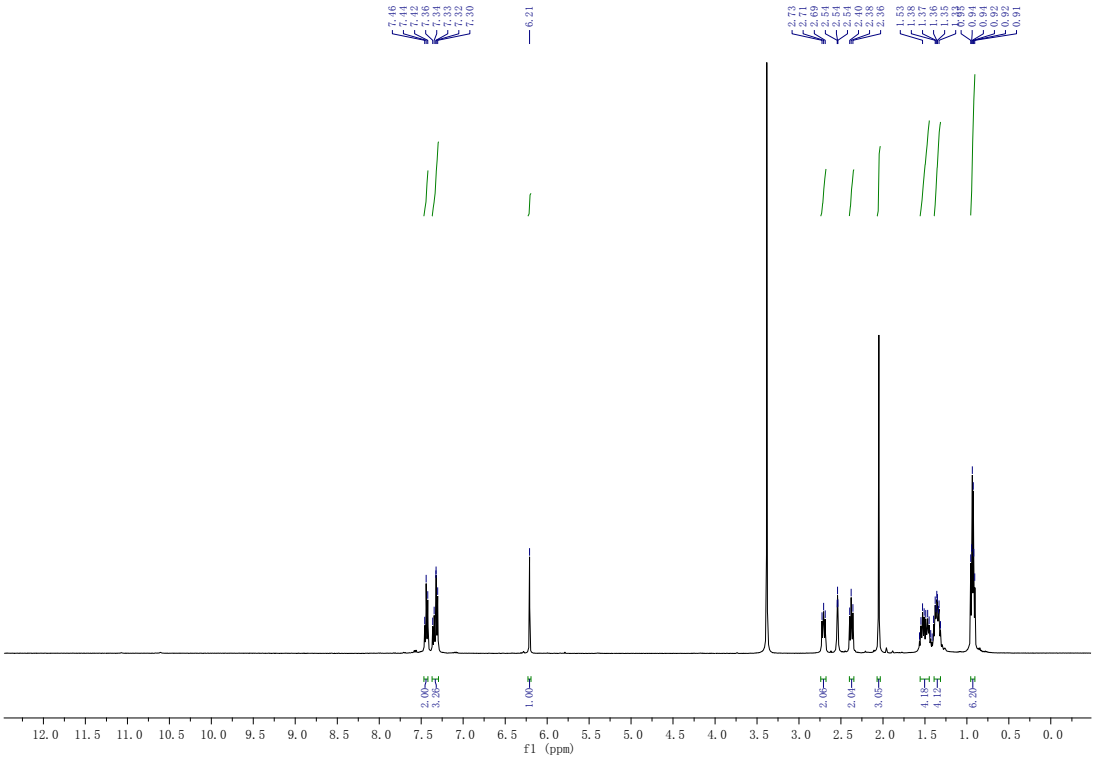
4g


11.32
7.83
7.81
7.41
7.34
7.23
7.21
7.20
7.19
6.74
2.54
2.35
2.32
1.03
2.03
2.06
2.04
5.05
1.99
1.00
3.01
3.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


135.76
134.45
133.79
132.44
131.61
130.17
129.25
128.88
128.84
128.57
127.95
127.79
125.72
123.86
122.28
107.93
20.77
20.68
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


n-Bu
n-Bu
N
Ac

4h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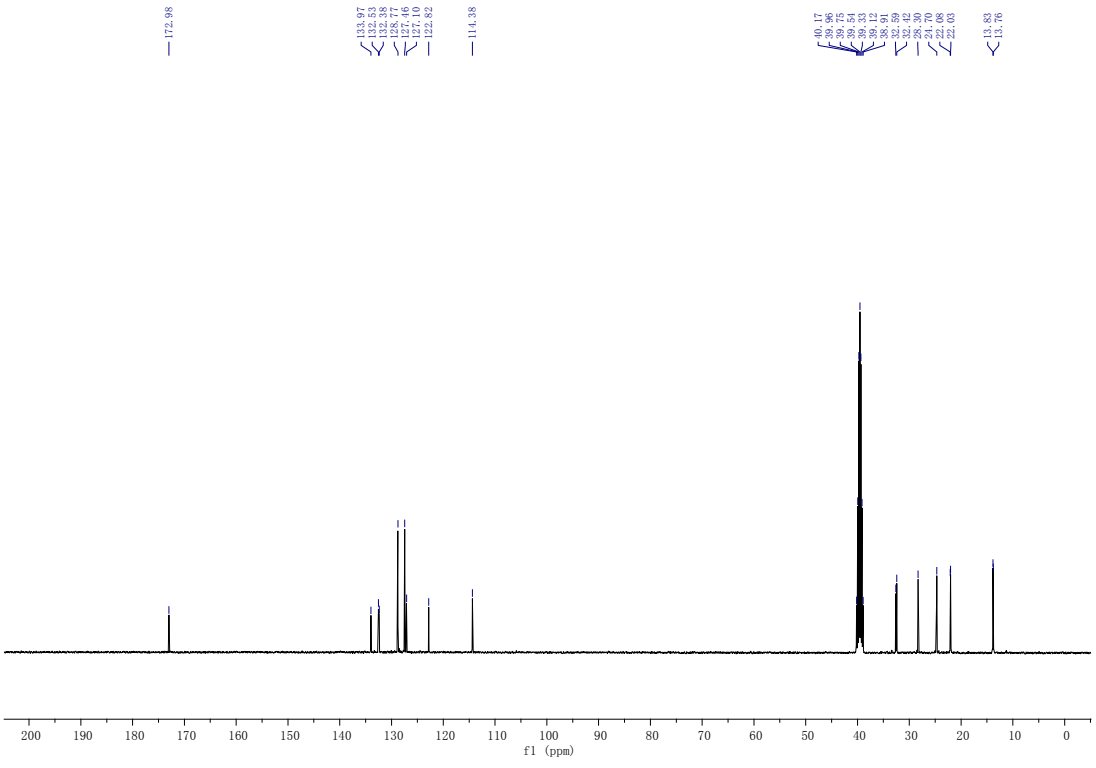
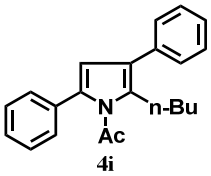
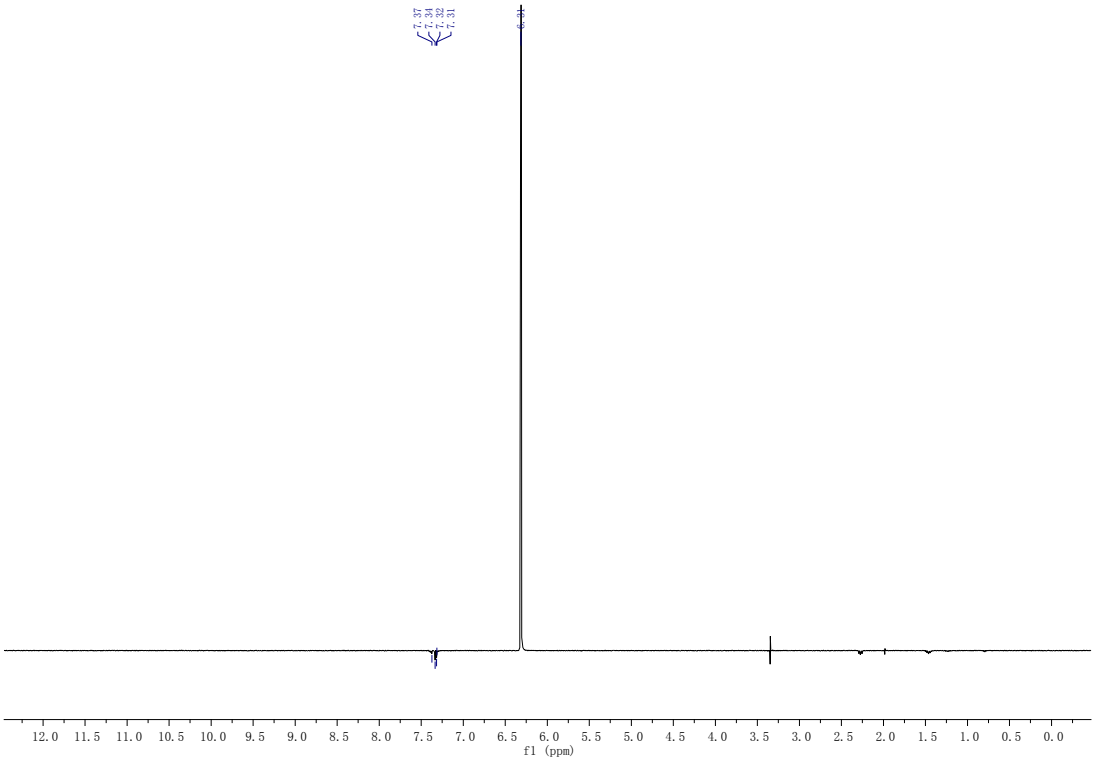
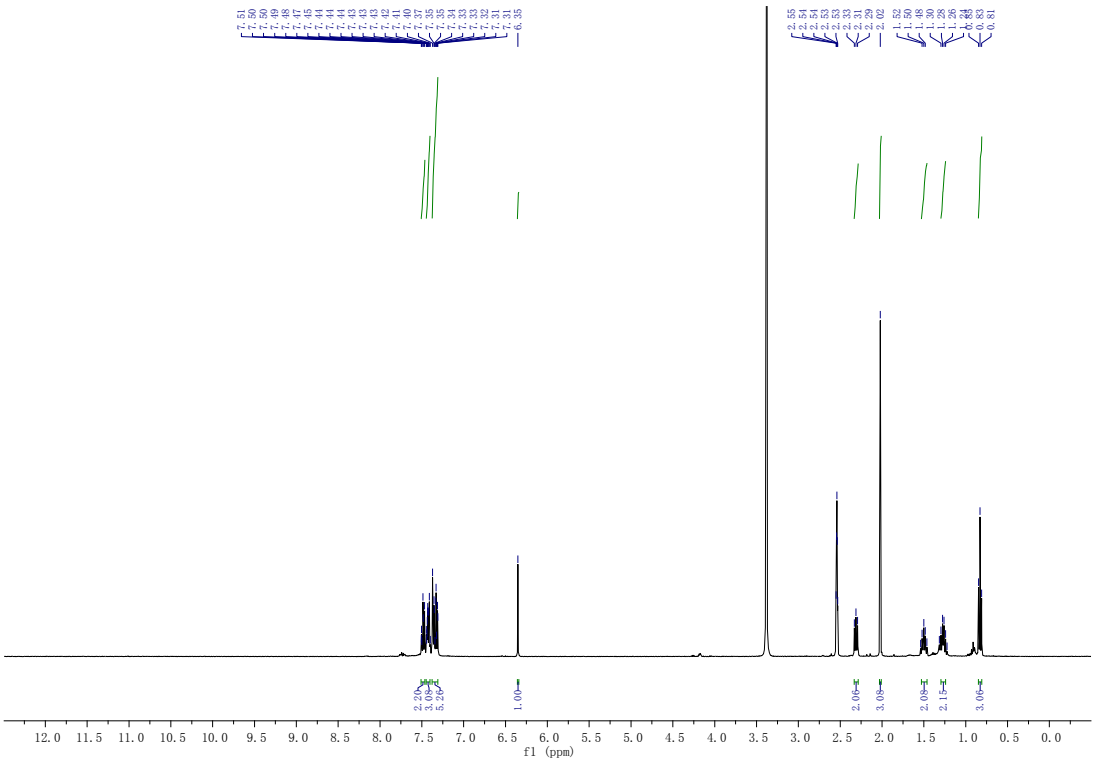
7.44
7.42
7.36
7.34
7.33
7.32
7.30
6.21
2.73
2.71
2.69
2.54
2.54
2.54
2.40
2.38
2.36
1.53
1.38
1.37
1.36
1.35
0.94
0.94
0.92
0.92
0.91
2.00
3.29
1.00
2.06
2.04
3.05
4.18
4.12
6.20
f1 (ppm)


172.98
133.97
132.53
132.38
128.77
127.46
127.10
122.82
114.38
40.17
39.96
39.75
39.54
39.33
39.12
38.91
32.59
32.42
28.30
24.70
22.08
22.03
13.83
13.76
f1 (ppm)


n-Bu
N
Ac

4i


7.37
7.34
7.32
7.31
6.35
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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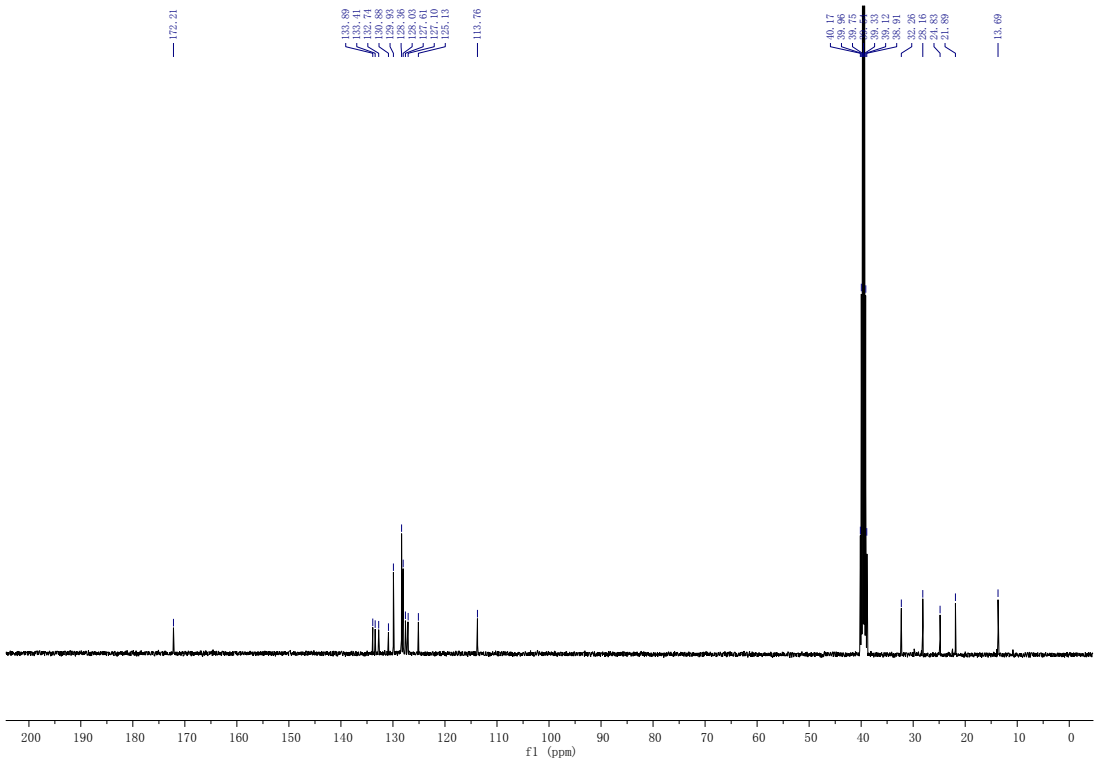
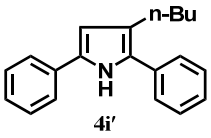
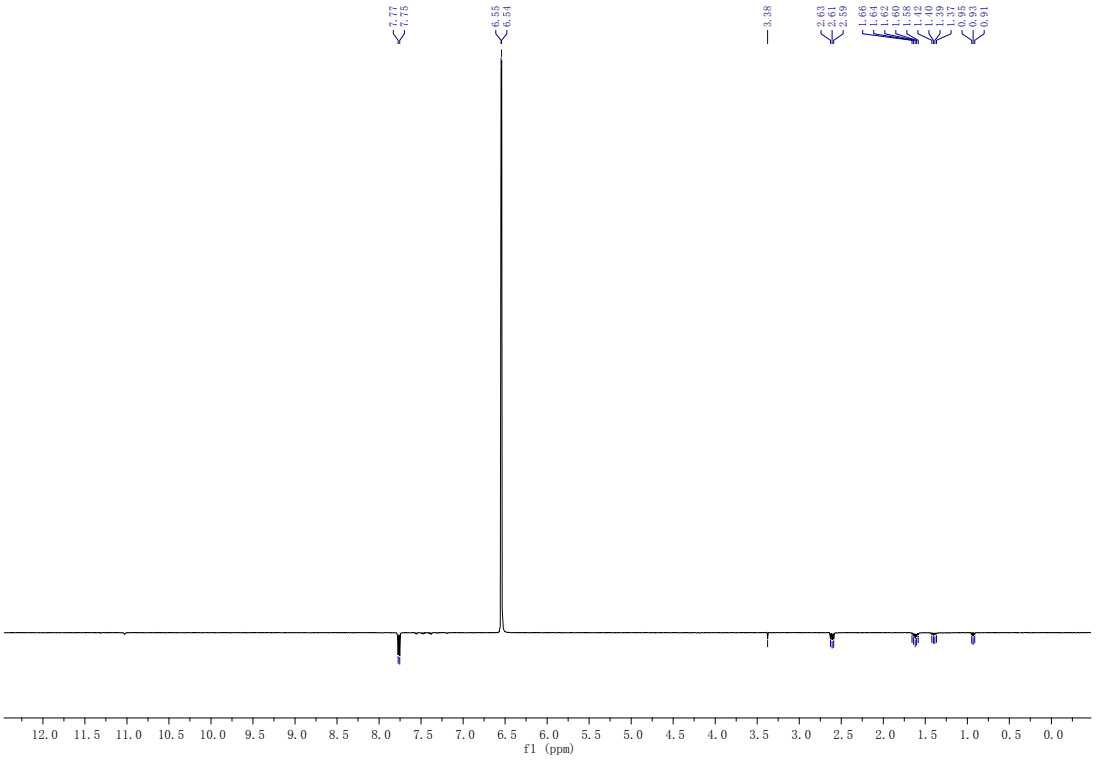
7.47
7.45
7.44
7.44
7.43
7.43
7.13
7.12
7.12
7.11
7.40
7.37
7.35
7.35
7.34
7.33
7.32
7.31
7.31
6.35
2.55
2.54
2.54
2.53
2.53
2.33
2.31
2.31
2.29
2.02
1.52
1.50
1.48
1.30
1.28
1.26
0.85
0.83
0.81
2.20
3.03
5.26
1.00
2.03
3.03
2.03
2.15
3.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)




n-Bu
N
H

4i′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2.63
2.61
2.59
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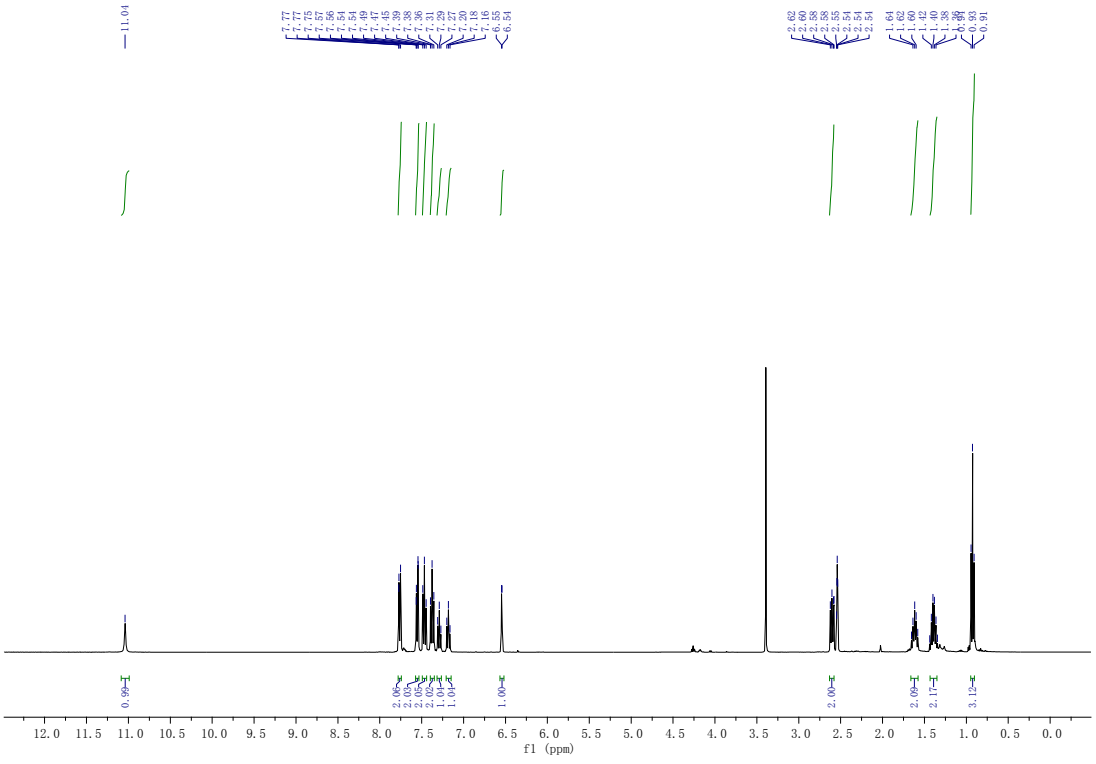
1.62
1.60
1.58
1.42
1.40
1.39
1.37
0.95
0.93
0.91
f1 (ppm)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7.56
7.54
7.54
7.49
7.47
7.45
7.38
7.36
7.31
7.29
7.27
7.20
7.18
6.55
6.54
2.62
2.60
2.58
2.55
2.54
2.54
2.54
1.64
1.62
1.60
1.42
1.40
1.38
0.95
0.93
0.91
0.99
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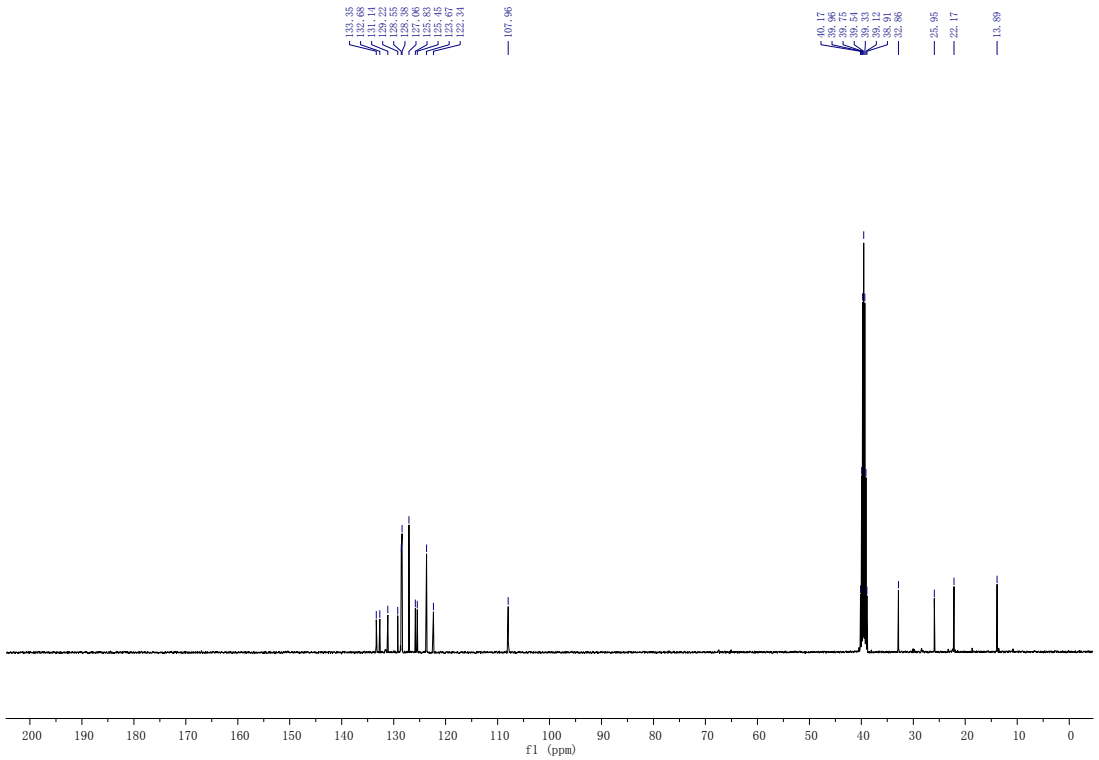
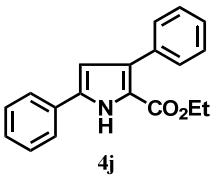
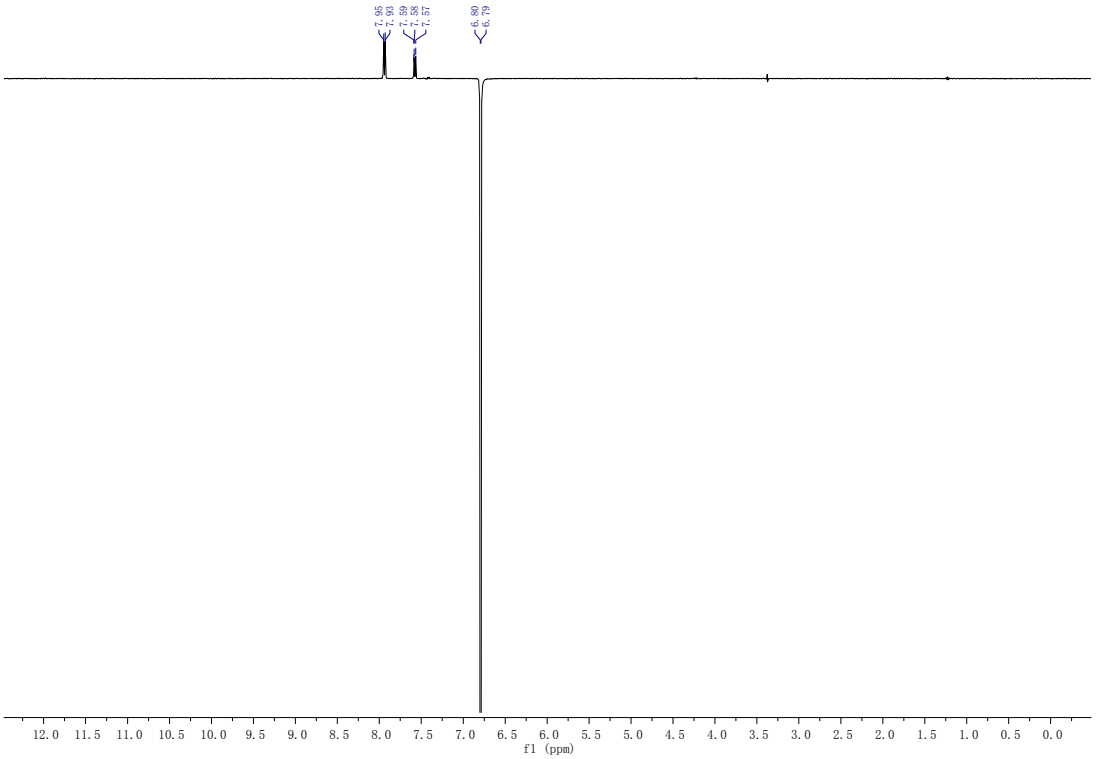
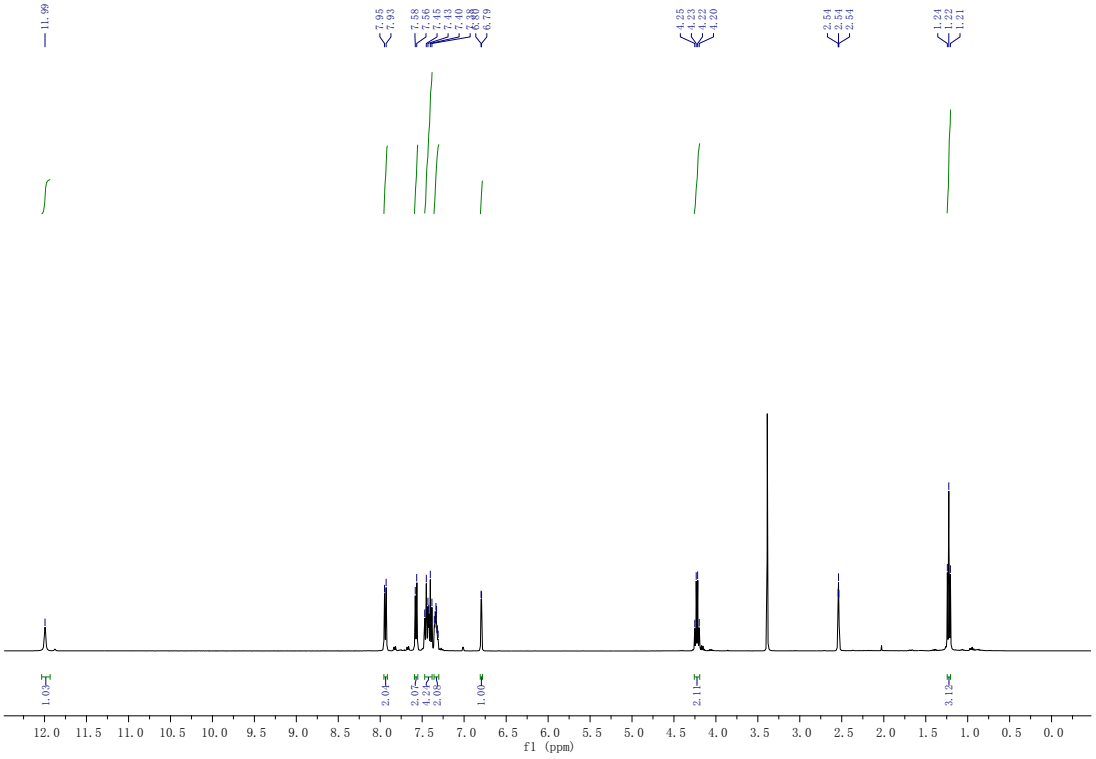
2.02
2.04
1.04
1.00
2.00
2.09
2.17
3.12
f1 (ppm)

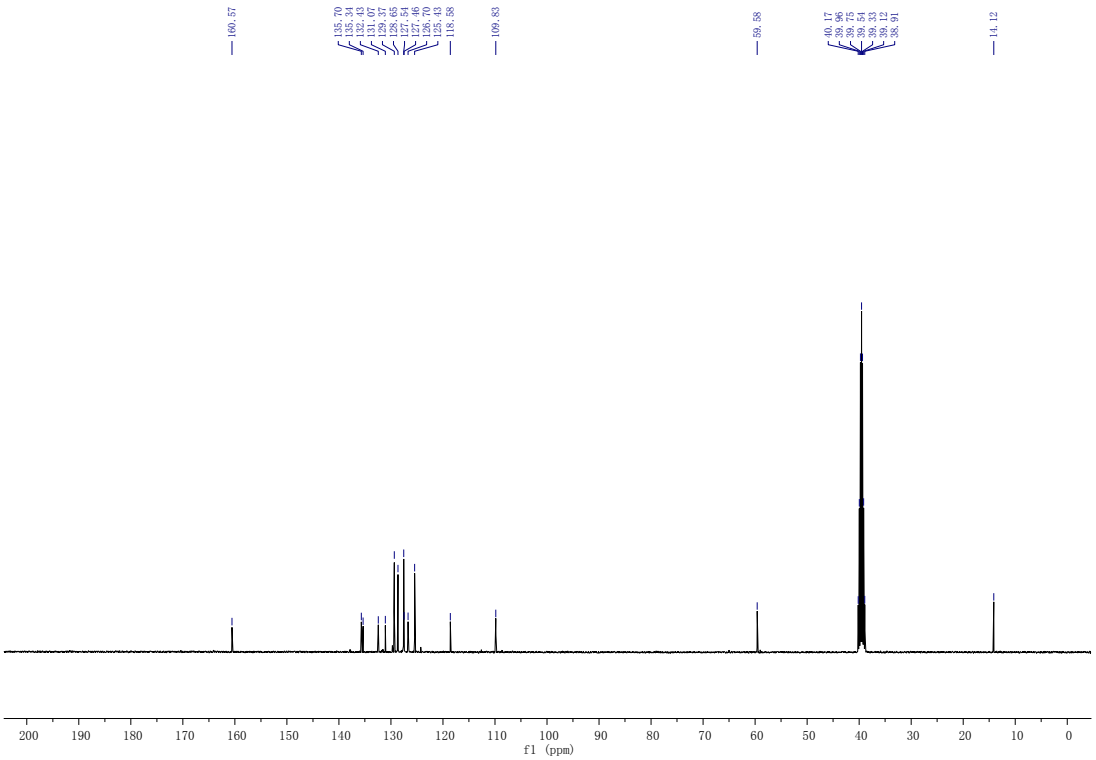


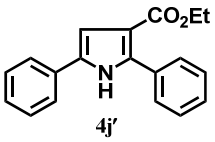


4j









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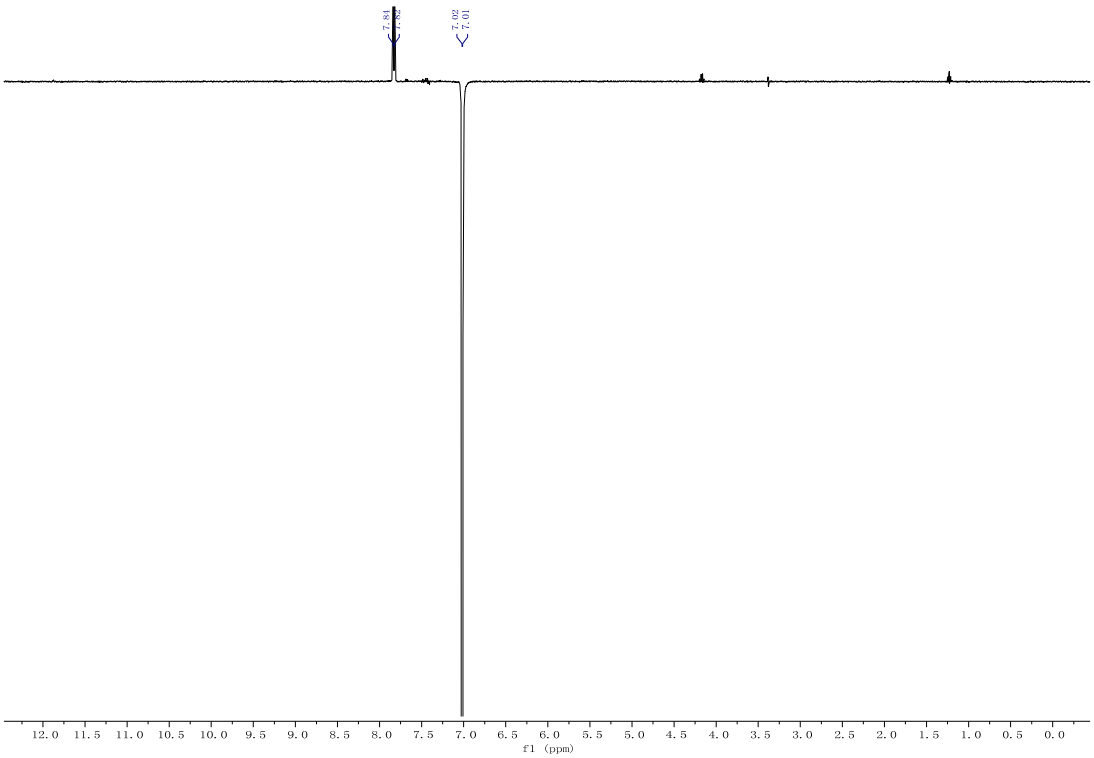

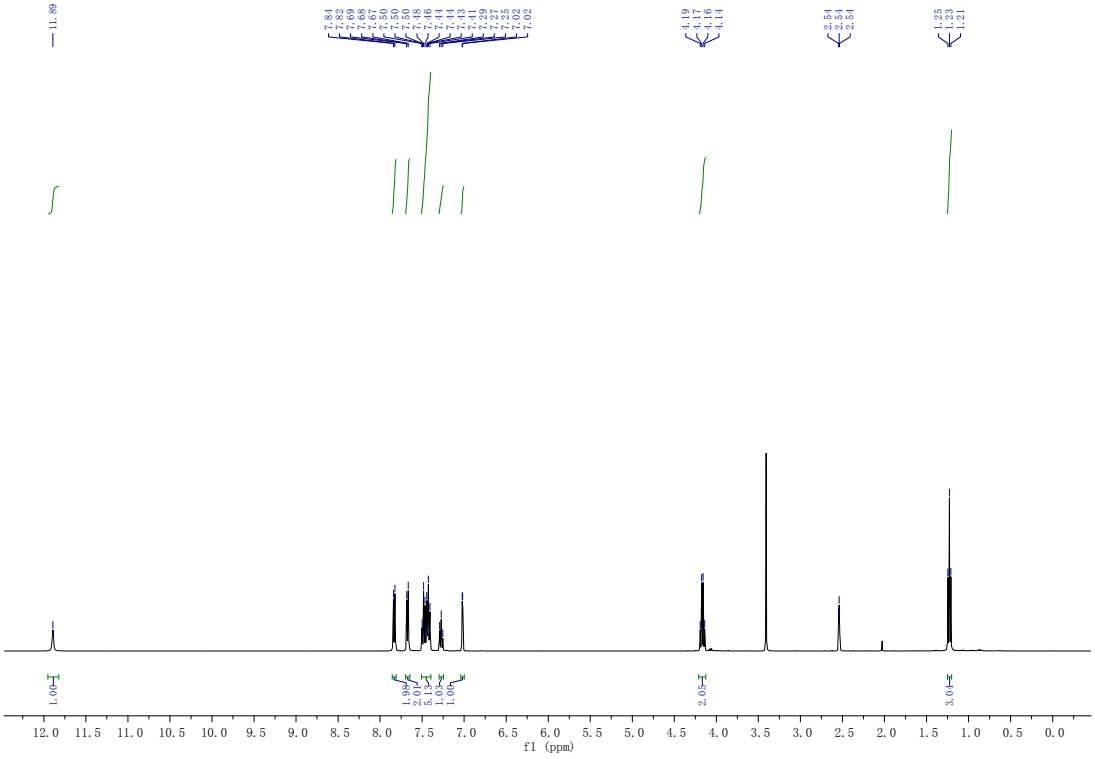

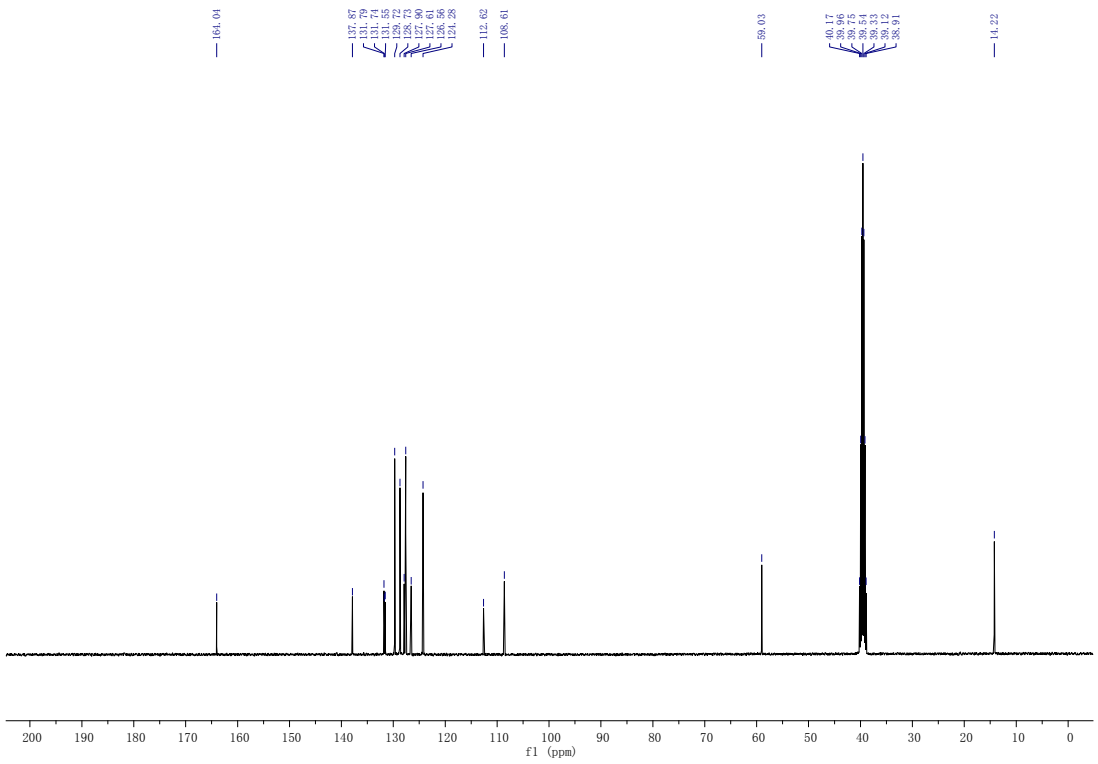

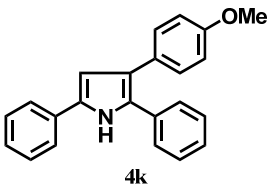

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