Supporting Information
for

Copper-promoted hydration and annulation of 2-fluorophenylacetylene derivatives: from alkynes to benzo[*b*]furans and benzo[*b*]thiophenes

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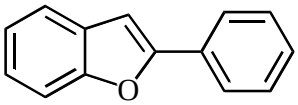
A. General methods

Unless otherwise noted, all commercial materials and solvents were used without further purification and all the reactions were carried out in a Schlenk tube equipped with a magnetic stir bar. ^{1}H NMR spectra were recorded in $CDCl_3$ at 400 MHz and ^{13}C NMR spectra were recorded in $CDCl_3$ at 100 MHz, respectively, ^{1}H and ^{13}C NMR were referenced to $CDCl_3$ at δ 7.26 and 77.0, respectively. GC–MS was obtained using electron ionization. HRMS was carried out on a MAT 95XP (Thermo). IR spectra were performed using potassium bromide pellets or liquid films between two potassium bromide pellets and a Brucker Vector 22 spectrometer. TLC was performed using commercially prepared 100–400 mesh silica gel plates (GF_{254}), and visualization was effected at 254 nm. All the other chemicals were purchased from Aldrich Chemicals. Commercial reagents were used without further purification.

B Typical procedure for the copper-promoted reaction of 2-fluorophenylacetylene derivatives synthesis of benzo[*b*]furans

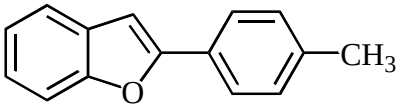
A mixture of 1-fluoro-2-(2-phenylethynyl)benzene (1 mmol), CuI (20 mg, 0.1 mmol), KOH (112 mg, 2 mmol), KI (33 mg, 0.2 mmol) and DMSO (3 mL), was added successively in a 20 mL Schlenk tube. After stirring for 4 h at 80 °C, the solution was filtered though a small amount of silica gel. Then the residue was concentrated in vacuo and the crude was purified by flash chromatography with *n*-hexane/ethyl acetate (20/1, v/v) to afford the 2-phenylbenzofuran as a pale-yellow solid. All spectral data correspond to those given in the literature.

*2-Phenylbenzofuran (**2a**)* [1]



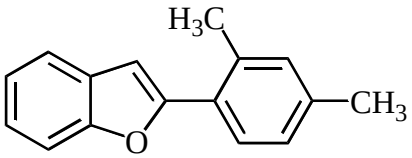
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.86 (d, J = 8.0 Hz, 2H), 7.57 (d, J = 7.6 Hz, 1H), 7.52 (d, J = 8.0 Hz, 1H), 7.43 (t, J = 7.8 Hz, 2H), 7.33 (t, J = 7.6 Hz, 1H), 7.29-7.20 (m, 2H), 7.00 (s, 1H); ^{13}C NMR ($CDCl_3$,100 MHz) δ 155.9, 154.9, 130.5, 129.2, 128.8 (2C), 128.5, 124.9 (2C), 124.2, 122.9, 120.9, 111.2, 101.3; MS (EI, 70 eV) m/z (%): 194, 165, 139, 97, 82.

*2-p-Tolylbenzofuran (**2b**)* [1]



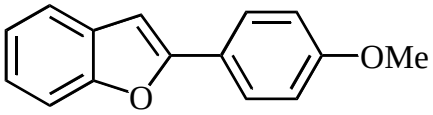
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.63 (d, J = 8.0 Hz, 2H), 7.56 (dd, J = 7.2 Hz, 16.8, 2H), 7.17−7.10 (m, 4H), 6.82 (s, 1H), 2.26 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 156.2, 154.8, 138.5, 129.4 (2C), 129.3, 127.7, 124.9 (2C), 124.0, 122.8, 120.7, 111.1, 100.5, 21.3; MS (EI, 70 eV) m/z (%): 208, 178, 165, 152, 104, 89.

*2-(2,4-Dimethylphenyl)benzofuran (**2c**)* [1]



^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.73 (d, J = 7.6 Hz, 1H), 7.55 (d, J = 7.2 Hz, 1H), 7.49 (d, J = 7.6 Hz, 1H), 7.17−7.18 (m, 2H), 7.12−7.06 (m, 2H), 6.80 (s, 1H), 2.51 (s, 3H), 2.32 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 155.6, 154.2, 138.4, 135.6, 132.0, 129.3, 128. 0, 127.1, 126.8, 124.0, 122.7, 120.7, 111.0, 104.4, 21.8, 21.1; MS (EI, 70 eV) m/z (%): 222, 207, 189, 178, 165, 152, 111; HRMS EI (m/z): calcd for $C_{16}H_{14}O$, 222.1045; found, 222.1041.

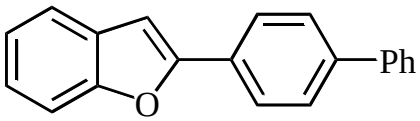
*2-(4-Methoxyphenyl)benzofuran (**2d**)* [1]



^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.80 (d, J = 8.0 Hz, 2H), 7.56 (d, J = 7.6 Hz, 1H), 7.50 (d, J = 7.6 Hz, 1H), 7.28−7.20 (m, 2H), 6.99 (d, J = 8.0 Hz, 2H), 6.89 (s, 1H) 3.87 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 160.0,

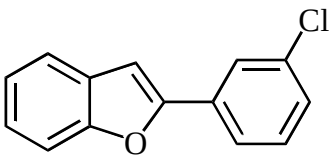
156.0, 154.7, 129.5, 126.4 (2C), 123.7, 123.3, 122.8, 120.5, 114.2 (2C), 111.0, 99.7, 55.4; MS (EI, 70 eV) m/z (%): 224, 209, 181, 152, 112.

*2-(Biphenyl-4-yl)benzofuran (**2e**)* [1]



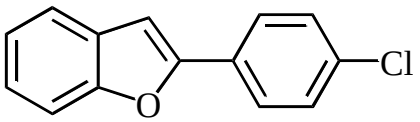
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.95 (d, *J* = 7.2 Hz, 2H), 7.68 (dd, *J* = 16.2, 7.2 Hz, 4H), 7.58 (dd, *J* = 21.8, 7.2 Hz, 2H), 7.48 (t, *J* =7.2 Hz, 2H), 7.39 (d, *J* = 6.2 Hz, 1H), 7.31-7.26 (m, 2H), 7.07 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 155.7, 155.0, 141.2, 140.4, 129.4, 129.3, 128.9 (2C), 127.6, 127.4 (2C), 127.0 (2C), 125.3 (2C), 124.3, 123.0, 120.9, 111.2, 101.4; MS (EI, 70 eV) m/z (%): 270, 239, 165, 135, 96, 73.

*2-(3-Chlorophenyl)benzofuran (**2f**)* [1]



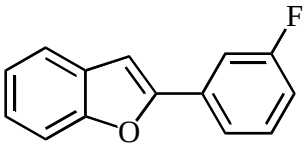
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.81 (s, 1H), 7.66 (d, *J* = 7.2 Hz, 1H), 7.54 (d, *J* = 7.6 Hz, 1H), 7.48 (d, *J* = 8.0 Hz, 1H), 7.32-7.19 (m, 4H), 6.96 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 154.9, 154.2, 134.8, 132.1, 130.0, 128.9, 128.3, 124.8, 124.7, 123.1, 122.9, 121.1, 111.2, 102.3; MS (EI, 70 eV) m/z (%): 228, 199, 165, 139, 114, 82.

*2-(4-Chlorophenyl)benzofuran (**2g**)* [1]



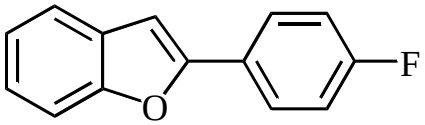
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.72 (d, *J* = 8.8 Hz, 2H), 7.53 (d, *J* = 7.2 Hz, 1H), 7.48 (d, *J* = 8.0 Hz, 1H), 7.36 (d, J = 8.8 Hz, 2H), 7.29−7.19 (m, 2H), 6.92 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 154.9, 154.7, 134.2, 129.0, 129.0 (2C), 128.9, 126.1 (2C), 124.5, 123.1, 121.0, 111.2, 101.7; MS (EI, 70 eV) m/z (%): 228, 199, 165, 139, 114.

*2-(3-Fluorophenyl)benzofuran (**2h**)* [2]



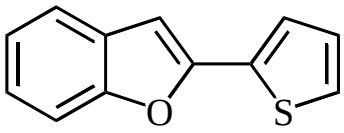
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60-7.49 (m, 4H), 7.34 (dd, J = 14.3, 7.5 Hz, 1H), 7.24 (dt, J = 25.0, 7.2 Hz, 2H), 7.00 (t, J = 8.4 Hz, 1H), 6.99 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 163.1 (d, J_{C-F} = 244.2 Hz), 154.9, 154.4 (d, J_{C-F} = 3.0 Hz), 132.5 (d, J_{C-F} = 8.4 Hz), 130.3 (d, J_{C-F} = 8.4 Hz), 128.9, 124.7, 123.1, 121.1, 120.5 (d, J_{C-F} = 2.9 Hz), 115.3 (d, J = 21.2 Hz), 111.9, 111.5 (d, J_{C-F} = 23.5 Hz), 111.2, 102.3; MS (EI, 70 eV) m/z (%): 212, 183, 157, 106, 91.

*2-(4-Fluorophenyl)benzofuran (**2i**)* [3]



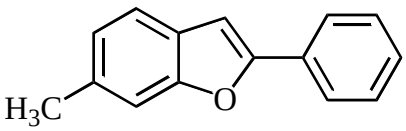
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.84−7.81 (m, 2H), 7.57 (d, J = 7.6 Hz, 1H), 7.50 (d, J = 8.1 Hz, 1H), 7.27 (t, J = 7.5 Hz, 1H), 7.22 (t, J = 7.8 Hz, 1H), 7.13 (t, J = 8.7 Hz, 2H), 6.94 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 162.9 (d, J_{C-F} = 247.3 Hz), 155.1, 154.9, 129.2, 126.8 (d, J_{C-F} = 3.8 Hz, 2C), 126.7, 124.3, 123.0, 120.9, 115.9 (d, J_{C-F} = 22.9 Hz, 2C), 111.2, 101.0 (d, J_{C-F} = 1.5 Hz); MS (EI, 70 eV) m/z (%): 212, 183, 157, 106, 91, 77.

*2-(Thiophen-2-yl)benzofuran (**2j**)* [4]



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51-7.44 (m, 3H), 7.23 (ddd, J = 19.6, 12.5, 6.1 Hz, 3H), 7.05 (t, J = 4.2 Hz, 1H), 6.81 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.5, 151.2, 133.2, 129.1, 127.8, 125.7, 124.6, 124.2, 123.1, 120.7, 111.0, 101.1; MS (EI, 70 eV) m/z (%): 200, 171, 155, 145, 127, 100.

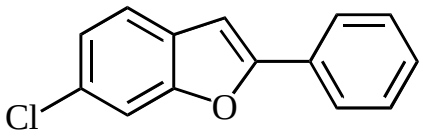
*6-Methyl-2-phenylbenzofuran (**2k**)* [5]



^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.77 (d, J = 8.0 Hz, 2H), 7.35 (t, J = 6.0 Hz, 3H), 7.26-7.23 (m, 2H), 6.97 (d, J = 7.6 Hz, 1H), 6.89 (s, 1H), 2.4

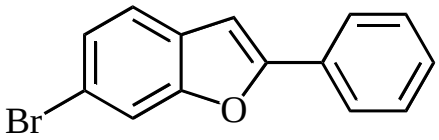
(s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 155.3, 155.3, 134.5, 130.7, 128.7 (2C), 128.3, 126.7, 124.7 (2C), 124.3, 120.3, 111.4, 101.2, 21.7; MS (EI, 70 eV) m/z (%): 208, 178, 165, 152, 104, 77.

*6-Chloro-2-phenylbenzofuran (**2l**)* [6]



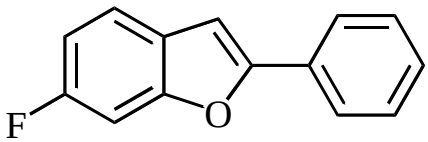
^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.83 (d, J = 7.6 Hz, 2H), 7.53 (s, 1H), 7.49-7.43 (m, 2H), 7.38 (t, J = 8.8 Hz, 1H), 7.27-7.20 (m, 2H), 6.98 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 156.7, 154.9, 129.9, 128.8 (3C), 128.7, 127.9, 124.9 (2C), 123.7, 121.3, 111.7, 101.0; MS (EI, 70 eV) m/z (%): 228, 199, 165, 139, 114, 77.

*6-Bromo-2-phenylbenzofuran (**2m**)*



IR (KBr): ν_{max} = 3091, 1448, 1019, 919, 868, 822, 762 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.82 (d, J = 7.2 Hz, 2H), 7.68 (s, 1H), 7.46-7.40 (m, 3H), 7.38-7.33 (m, 2H), 6.95 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 156.6, 155.1, 129.9, 128.8 (3C), 126.3, 124.9 (2C), 121.7, 117.3, 114.6, 101.0; MS (EI, 70 eV) m/z (%): 274, 272, 193, 165, 139, 115, 82; HRMS EI (m/z): calcd for $C_{14}H_9BrO$, 271.9837; found, 271.9833.

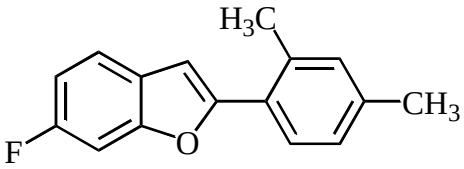
*6-Fluoro-2-phenylbenzofuran (**2n**)*



IR (KBr): ν_{max} = 3104, 3084, 2924, 1601, 1450, 1132, 853, 821, 761 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.81 (d, J = 7.6 Hz, 2H), 7.48-7.41 (m, 3H), 7.35-7.32 (m, 1H), 7.23 (d, J = 8.4 Hz, 1H), 6.99 (t, J = 9.2 Hz, 1H), 6.95 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 160.8 (d, J = 240.7 Hz), 156.7 (d, J = 4.3 Hz), 154.8 (d, J = 13.6 Hz), 130.2, 128.8 (2C), 128.6, 124.7 (2C), 123.7, 121.1 (d, J = 9.9 Hz), 111.2 (d, J = 23.8 Hz), 100.9, 99.0 (d, J = 26.6 Hz); MS

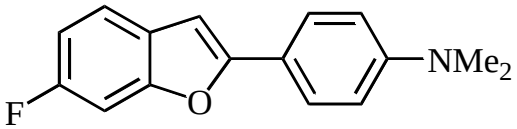
(EI, 70 eV) m/z (%): 212, 183, 157, 106, 91; HRMS EI (m/z): calcd for $C_{14}H_9FO$, 212.0637; found, 212.0631.

*6-Fluoro-2-(2,4-dimethylphenyl)benzofuran (**2o**)*



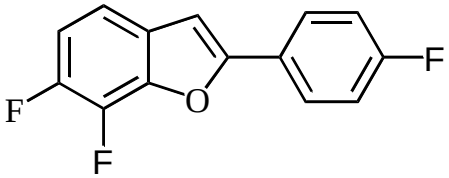
IR (KBr): v_{max} = 3037, 2959, 2924, 1599, 1486, 1267, 838, 810 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.69 (d, *J* = 8.8 Hz, 1H), 7.47 (dd, *J* = 8.8, 5.4 Hz, 1H), 7.25-7.17 (m, 1H), 7.10 (s, 1H), 7.09 (s, 1H), 7.03-6.93 (m, 1H), 6.78 (s, 1H), 2.51 (s, 3H), 2.35 (s, 3H)；^{13}C NMR ($CDCl_3$, 100 MHz) δ 160.7 (d, *J* = 240.3 Hz), 156.7 (d, *J* = 4.3 Hz), 154.2 (d, *J* = 13.5 Hz), 138.5, 135.4, 132.0, 127.9, 126.9 (2C), 125.5, 120.9 (d, *J* = 9.9 Hz), 111.2 (d, *J* = 23.9 Hz), 104.1, 98.7 (d, *J* = 36.4 Hz), 21.8, 21.1; MS (EI, 70 eV) m/z (%): 240, 225, 196, 120, 98; HRMS EI (m/z): calcd for $C_{16}H_{13}FO$, 240.0950; found, 240.0945.

*2-(4-Dimethylaminophenyl)-6-fluorobenzofuran (**2p**)*



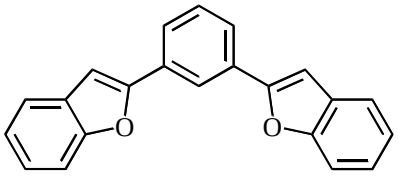
IR (KBr): v_{max} = 3105, 3036, 2921, 1614, 1495, 1453, 1256, 1170, 1019, 798, 749 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 7.61 (d, *J* = 8.0 Hz, 2H), 7.32 (t, *J* = 6.8 Hz, 1H), 7.12 (d, *J* = 8.8 Hz, 1H), 6.87 (t, *J* = 9.2 Hz, 1H), 6.69 (s, 1H), 6.67 (s, 2H), 2.93 (s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 160.2 (d, *J* = 238.9 Hz), 157.8 (d, *J* = 3.7 Hz), 154.4 (d, *J* = 3.5 Hz), 150.5, 126.0 (d, *J* = 1.2 Hz), 125.9 (4C), 120.1 (d, *J* = 9.8 Hz,), 112.2, 110.7 (d, *J* = 23.7 Hz), 98.7 (d, *J* = 25.5 Hz), 97.7, 40.3 (2C); MS (EI, 70 eV) m/z (%): 255, 212, 239, 183, 127; HRMS EI (m/z): calcd for $C_{16}H_{14}FNO$, 255.1059; found, 255.1053.

*6,7-Difluoro-2-(4-fluorophenyl)benzofuran (**2q**)*



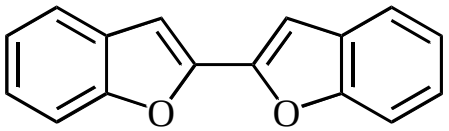
IR (KBr): v_{max} = 3116, 3056, 2921, 2849, 1609, 1499, 1306, 1229, 1036, 838, 815 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.82 (dd, *J* = 8.6, 5.4 Hz, 2H), 7.22 (dd, *J* = 8.6, 4.4 Hz, 1H), 7.15 (t, *J* = 8.6 Hz, 2H), 7.10-7.03 (m, 1H), 6.91 (d, *J* = 2.8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 163.1 (d, *J* = 248.1 Hz), 157.0 (d, *J* = 4.1 Hz), 148.2 (dd, *J* = 9.4 Hz, 241.2 Hz), 142.4 (dd, *J* = 4.8, 8.0 Hz), 140.0 (d, *J* = 16.7, 251.1 Hz), 127.9, 126.8 (d, *J* = 8.2 Hz, 2C), 125.9 (d, *J* = 3.4 Hz), 116.0 (d, *J* = 220.0 Hz, 2C), 115.1 (dd, *J* = 8.1, 4.6 Hz), 112.6 (d, *J* = 20.1 Hz), 100.8 (d, *J* = 1.8 Hz)；MS (EI, 70 eV) m/z (%): 248, 219, 201, 124; HRMS EI (m/z): calcd for $C_{14}H_7F_3O$, 248.0449; found, 248.0442.

*2-(3-(Benzofuran-2-yl)phenyl)benzofuran (**2r**)*



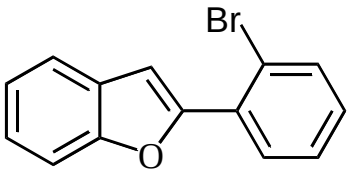
IR (KBr): v_{max} = 3031, 2922, 2851, 1704, 1450, 1367, 1257, 1212, 747 cm^{-1}; ^{1}H NMR (CDCl3, 400 MHz) δ 8.38 (s, 1H), 7.84 (d, *J* = 7.6 Hz, 2H), 7.63-7.52 (m, 6H), 7.34-7.28 (m, 3H), 7.2 (s, 2H); ^{13}C NMR (CDCl3, 100 MHz) δ 155.4, 155.0, 131.1, 129.3, 129.1, 124.9, 124.5, 123.0, 121.2, 121.0, 111.3, 102.0; MS (EI, 70 eV) m/z (%): 310, 252, 191, 155, 126, 96, 73; HRMS EI (m/z): calcd for $C_{22}H_{14}O_2$, 310.0994; found, 310.0988.

*2-(Benzofuran-2-yl)benzofuran (**2s**)* [7]



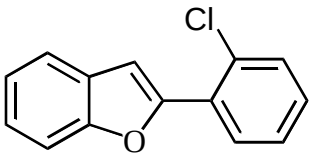
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.63 (d, *J* = 7.2 Hz, 2H), 7.54 (d, *J* = 8.0 Hz, 2H), 7.34 (t, *J* = 7.6 Hz, 2H), 7.29-7.26 (m, 2H), 7.17 (s, 2H); ^{13}C NMR (100 MHz, CDCl3) δ = 155.1, 147.7, 128.5, 125.1, 123.3, 121.4, 111.3, 103.7; MS (EI, 70 eV) m/z (%): 234, 205, 176, 152, 117.

*2-(2-Bromophenyl)benzofuran (**2t**)* [8]



^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.74-7.69 (m, 2H), 7.56 (d, *J* = 7.6 Hz, 1H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.41 (t, *J* = 8.0 Hz, 1H), 7.29 (t, *J* = 7.2 Hz, 1H), 7.22 (t, *J* = 7.2 Hz, 1H), 7.16 (d, *J* = 8.0 Hz, 1H), 7.01 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 154.9, 154.1, 149.7, 132.4, 130.2, 128.9, 124.9, 123.2, 123.1, 121.2, 120.6, 117.3, 111.3, 102.6; MS (EI, 70 eV) m/z (%): 274, 272, 165, 137, 83.

*2-(2-Chlorophenyl)benzofuran (**2v**)* [9]

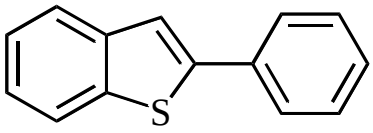


^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.03 (d, *J* = 8.0 Hz, 1H), 7.61 (d, *J* = 7.6 Hz, 1H), 7.52-7.45 (m, 3H), 7.36−7.28 (m, 2H), 7.25-7.20 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 154.1, 151.9, 131.3, 130.8, 129.0, 129.0, 128.9, 128.9, 126.9, 124.9, 122.9, 121.4, 111.0, 107.3; MS (EI, 70 eV) m/z (%): 228, 199, 165, 139, 114, 82.

C Typical procedure for the copper-promoted reaction of 2-fluorophenylacetylene derivatives synthesis of benzo[*b*]thiophenes

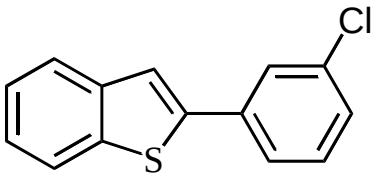
A mixture of 2-fluorophenylacetylenes (1 mmol), CuI (20 mg, 0.1 mmol), $Na_2S{\cdot}9H_2O$ (2 mmol) and DMSO (3 mL), was added successively in a 20 mL Schlenk tube. After stirring for 8 h at 60 °C, the solution was filtered though a small amount of silica gel. Then the residue was concentrated in vacuo and the crude was purified by flash chromatography with *n*-hexane/ethyl acetate (20/1, v/v) to afford the benzothiophenes **3a**–**c** as a pale-yellow solid. All spectral data correspond to those given in the literature.

*2-phenylbenzo[b]thiophene (**3a**)*[10]



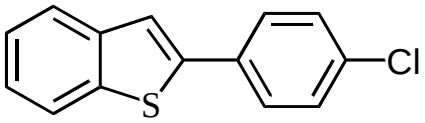
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.78 (dd, *J* = 23.0, 7.8 Hz, 2H), 7.70 (d, *J* = 7.8 Hz, 2H), 7.52 (s, 1H), 7.40 (t, *J* = 7.6 Hz, 2H), 7.31-7.35 (m, 3H); ^{13}C NMR (100 MHz, CDCl3) δ = 144.2, 140.7, 139.5, 134.3, 128.9 (2C), 128.2, 126.5 (2C), 124.5, 124.3, 123.5, 122.2, 119.4; MS (EI, 70 eV) m/z (%): 210, 202, 178, 165.

*2-(3-chlorophenyl)benzo[b]thiophene (**3b**)*[10]



^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.76 (dd, *J* = 22.4, 7.6 Hz, 2H), 7.67 (s, 1H), 7.53 (d, *J* = 6.8 Hz, 1H), 7.49 (s, 1H), 7.36-7.24 (m, 4H); ^{13}C NMR (100 MHz, CDCl3) δ = 142.4, 140.4, 139.5, 136.0, 134.8, 130.1, 128.1, 126.4, 124.7, 124.6, 124.6, 123.7, 122.3, 120.3; MS (EI, 70 eV) m/z (%): 246, 244.

*2-(4-chlorophenyl)benzo[b]thiophene (**3c**)*[10]



^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.78 (dd, *J* = 22.5, 7.6 Hz, 2H), 7.61 (d, *J* = 8.2 Hz, 2H), 7.50 (s, 1H), 7.41-7.28 (m, 4H); ^{13}C NMR (100 MHz, CDCl3) δ = 142.8, 140.6, 139.5, 134.1, 132.8, 129.1 (2C), 127.6 (2C), 124.7, 124.6, 123.6, 122.3, 119.9; MS (EI, 70 eV) m/z (%):246, 244.

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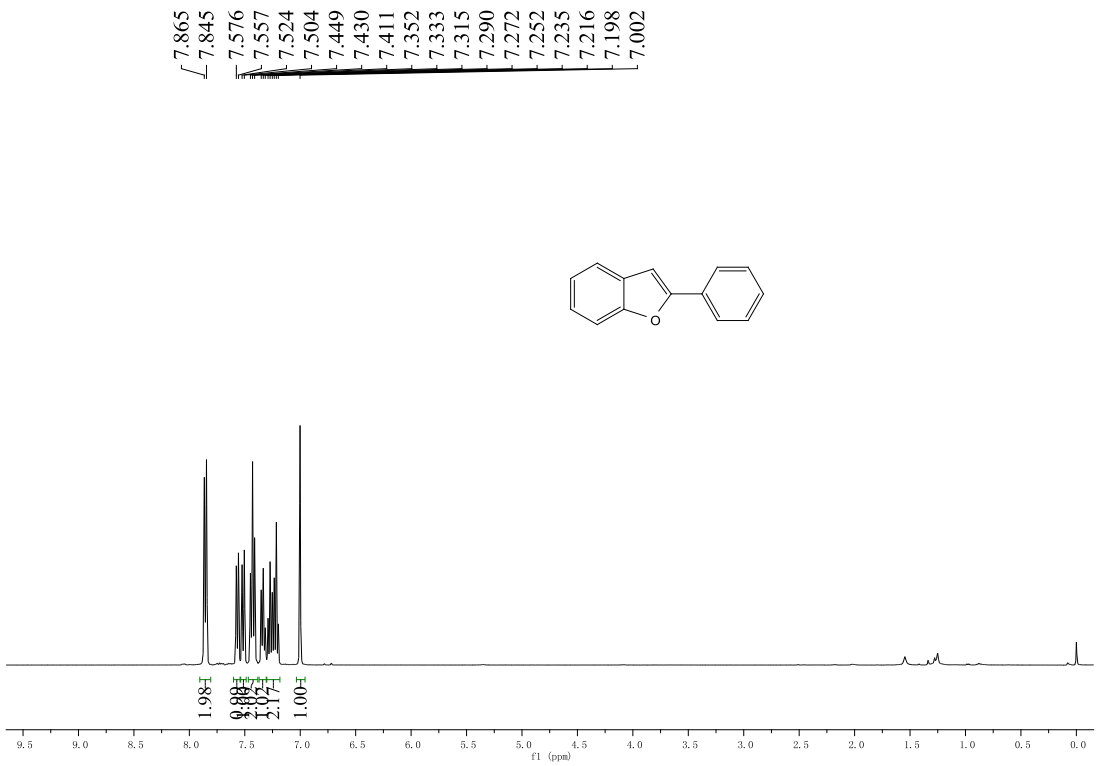
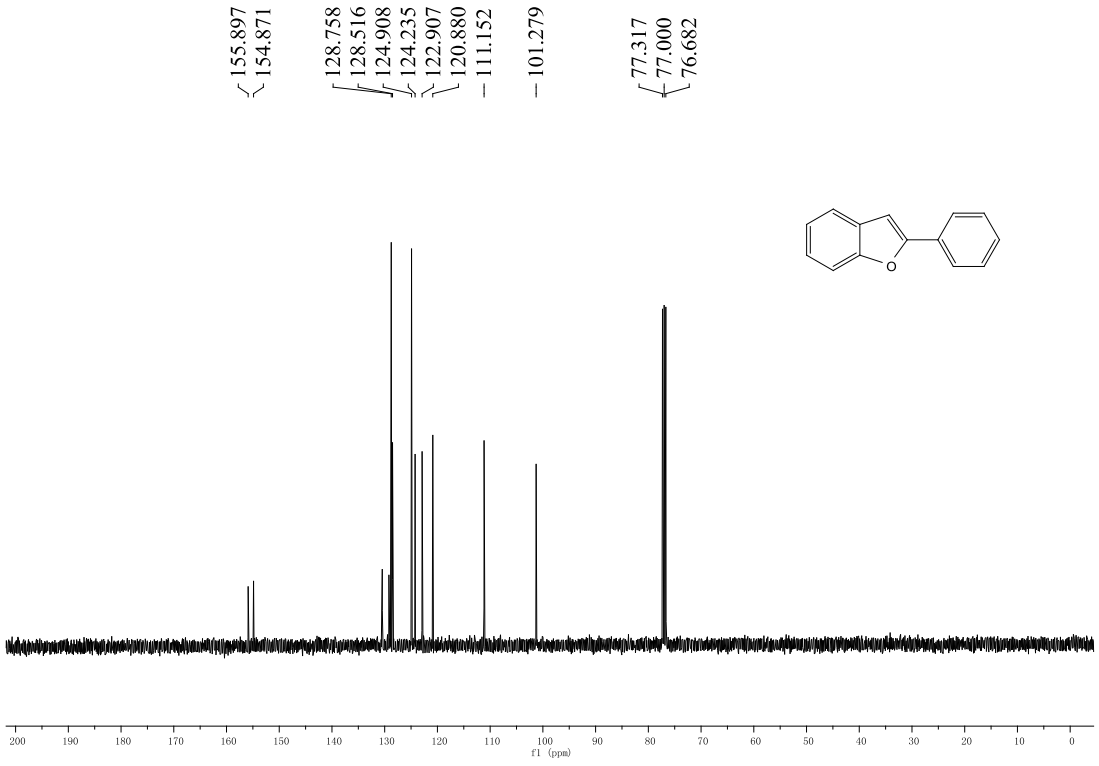
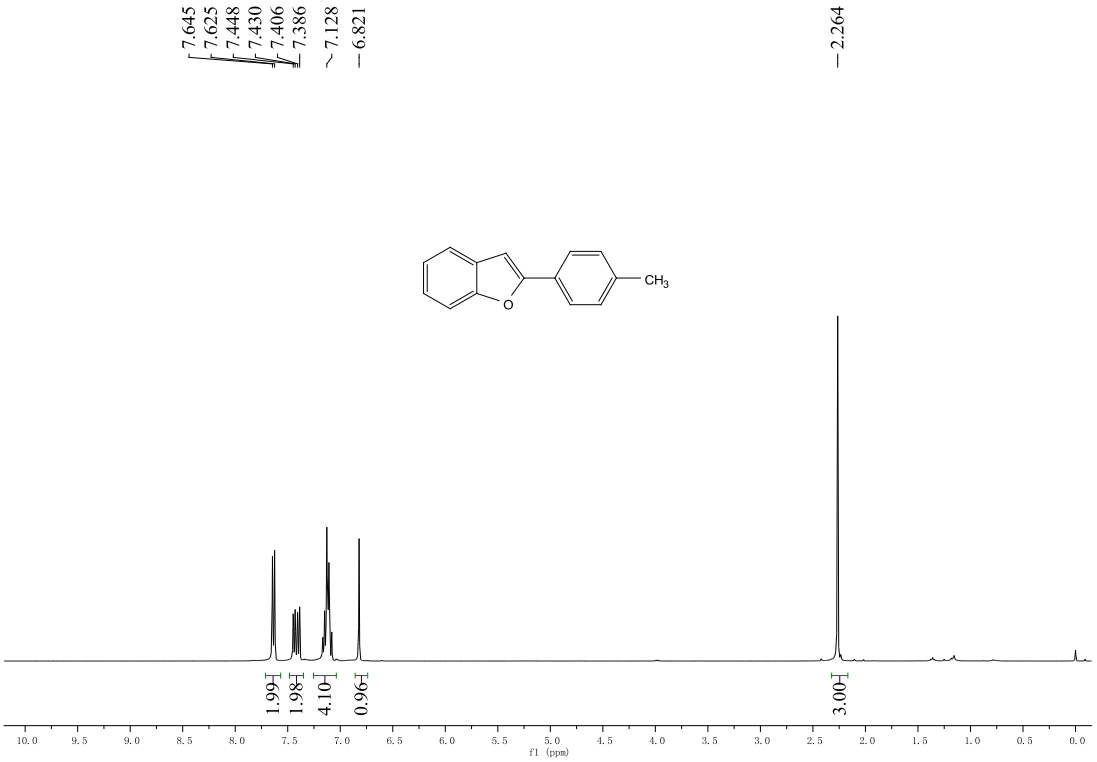
D ^{1}H NMR and ^{13}C NMR spectra for products



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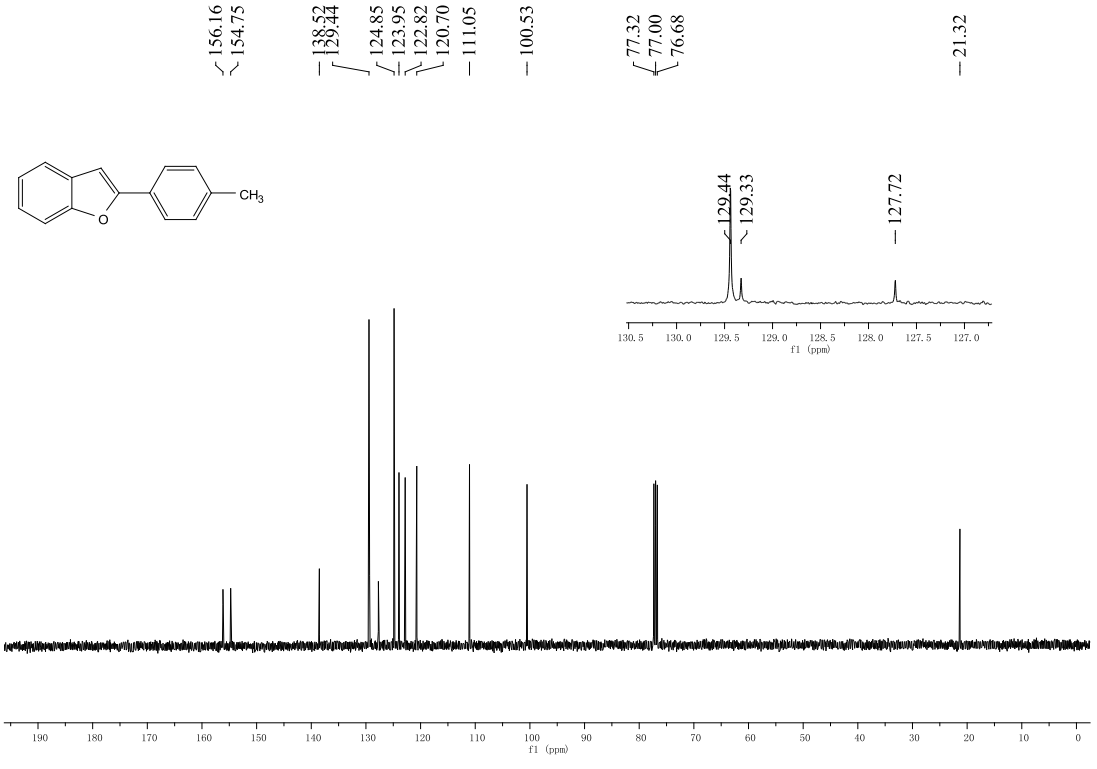
7.625
7.448
7.430
7.406
7.386
7.128
6.821
2.264
CH3
O
1.99
1.98
4.10
0.96
3.00
f1 (ppm)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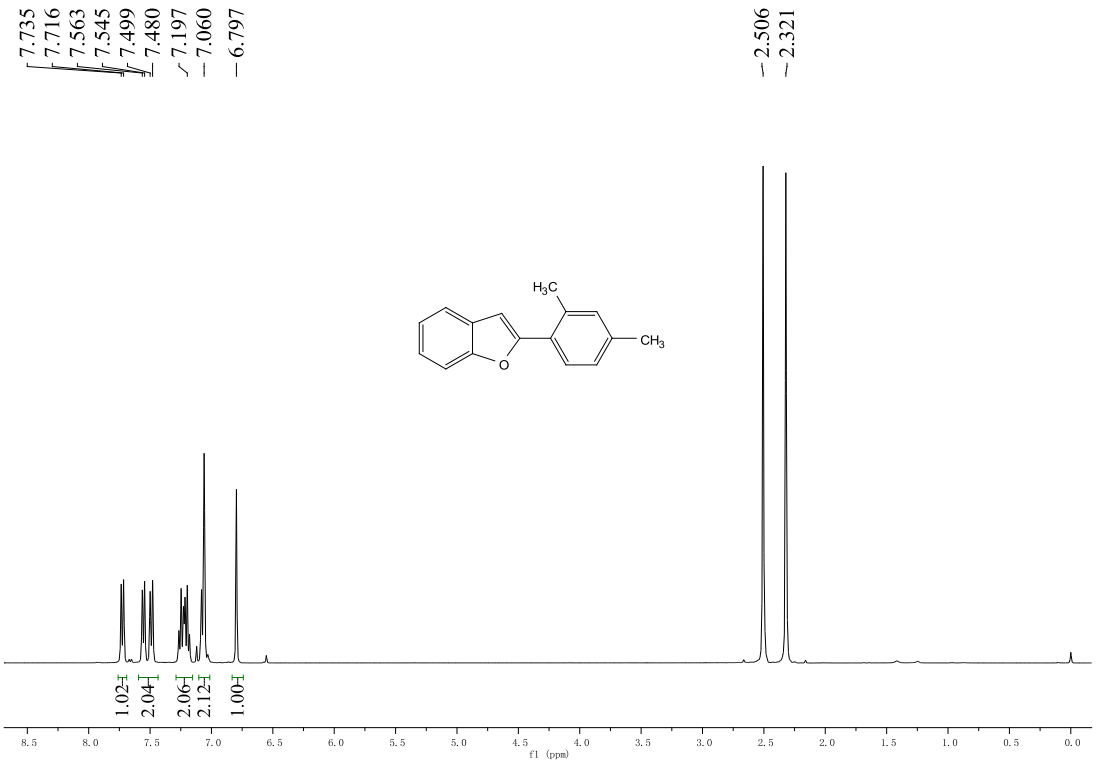
154.75
138.52
129.44
124.85
123.95
122.82
120.70
111.05
100.53
77.32
77.00
76.68
21.32
CH3
O
129.44
129.33
127.72
f1 (ppm)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7.716
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7.499
7.480
7.197
7.060
6.797
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2.321
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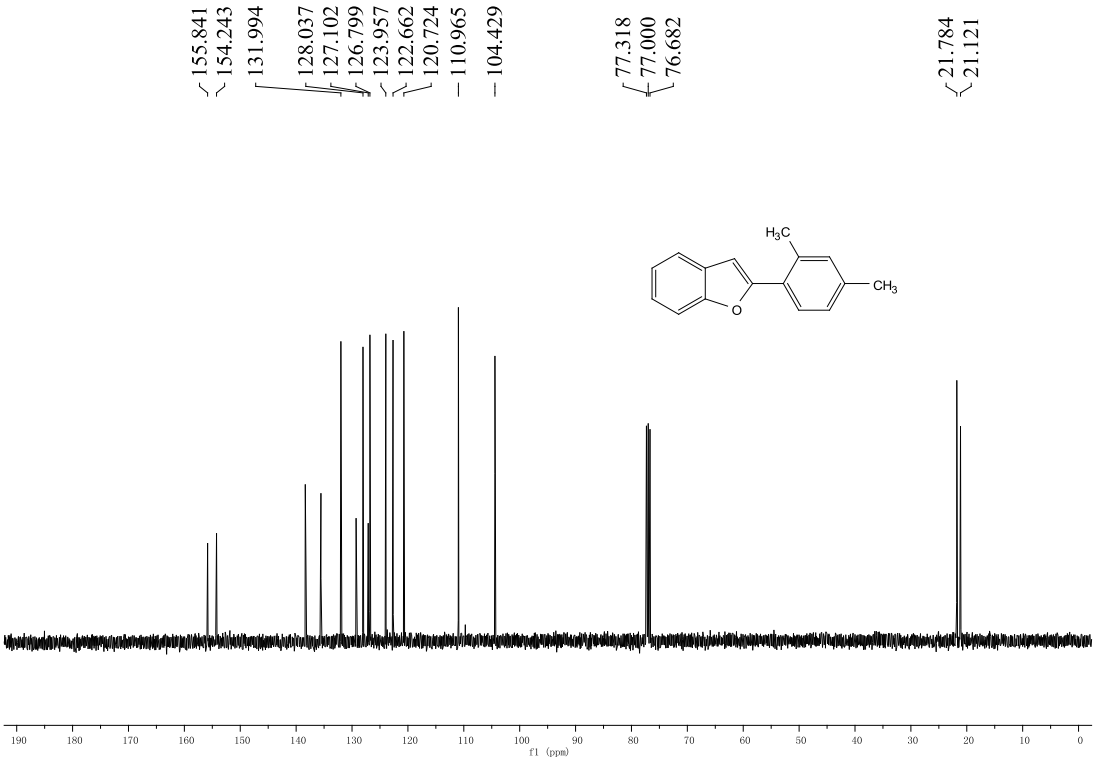
CH3
O
1.02
2.04
2.06
2.12
1.00
f1 (ppm)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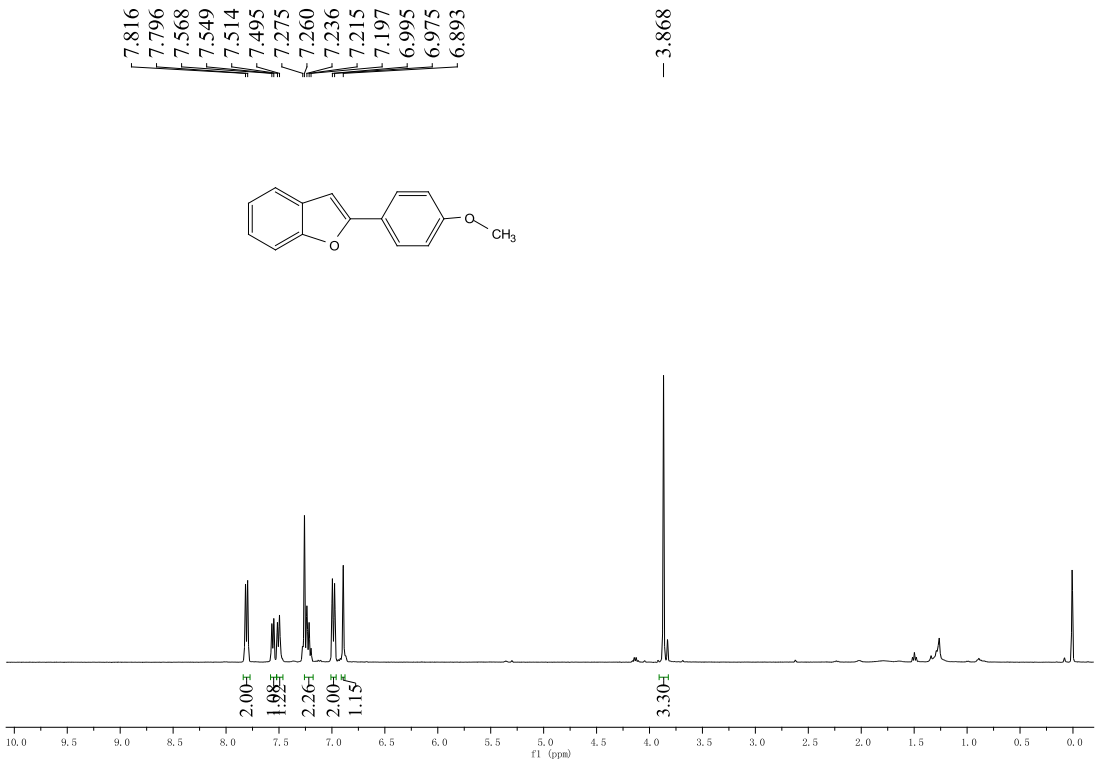
127.102
126.799
123.957
122.662
120.724
110.965
104.429
77.318
77.000
76.682
21.784
21.121
H3C
CH3
O
f1 (ppm)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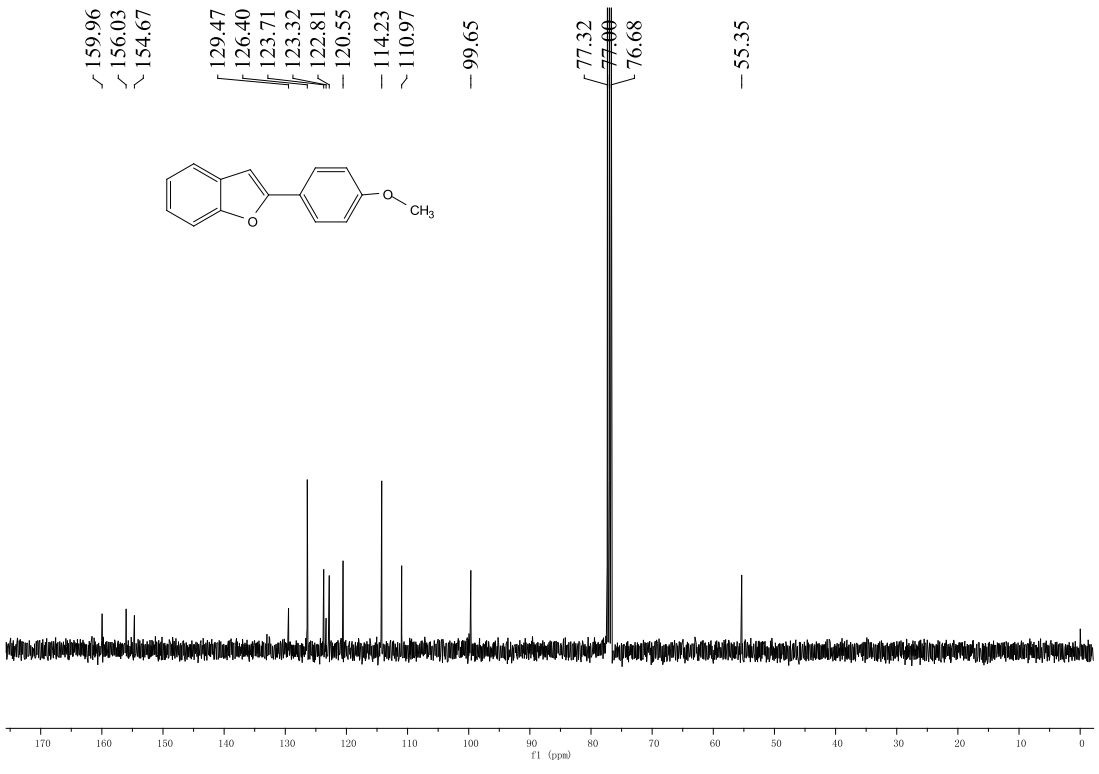
7.796
7.568
7.549
7.514
7.495
7.275
7.260
7.236
7.215
7.197
6.995
6.975
6.893
3.868
O
CH3
2.00
1.08
1.02
2.26
2.00
1.15
3.30
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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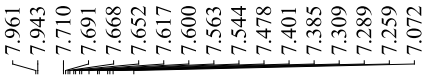
156.03
154.67
129.47
126.40
123.71
123.32
122.81
120.55
114.23
110.97
99.65
77.32
77.00
76.68
55.35
O
CH3
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.710
7.691
7.668
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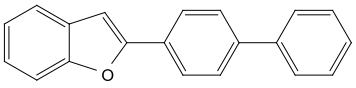
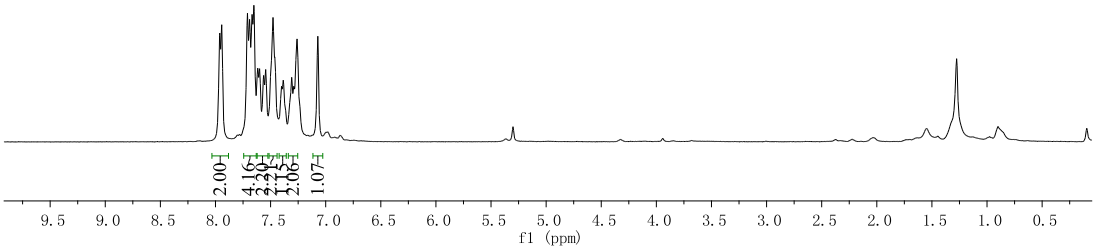
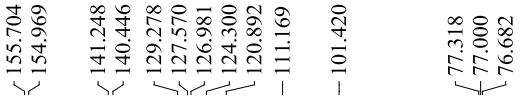
7.544
7.478
7.401
7.385
7.309
7.289
7.259
7.072




2.00
4.16
2.30
1.75
2.06
1.07
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
f1 (ppm)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140.446
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127.570
126.981
124.300
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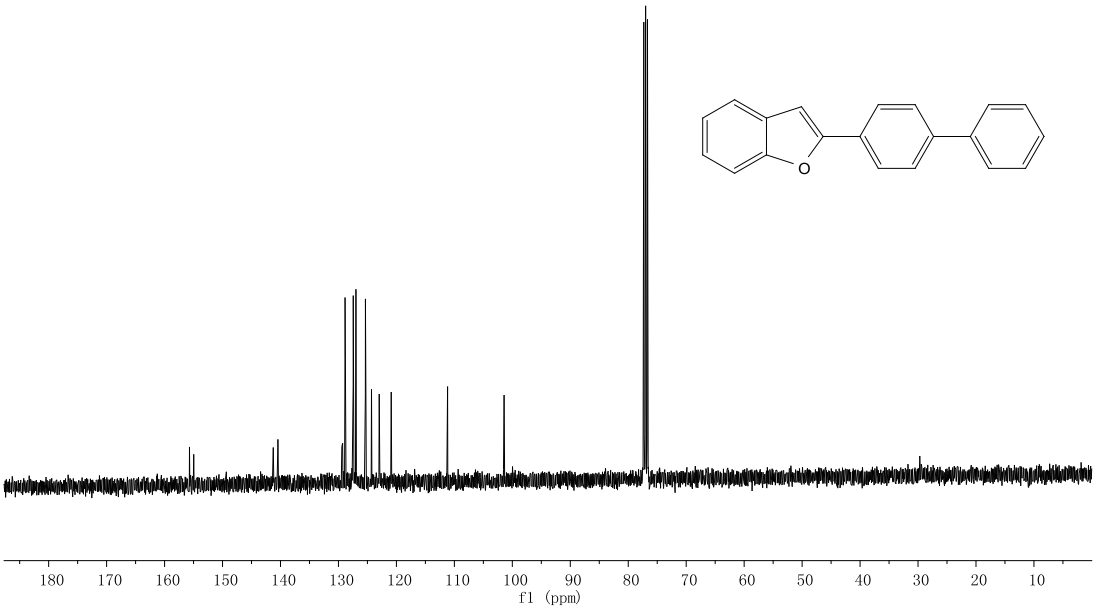
111.169
101.420
77.318
77.000
76.682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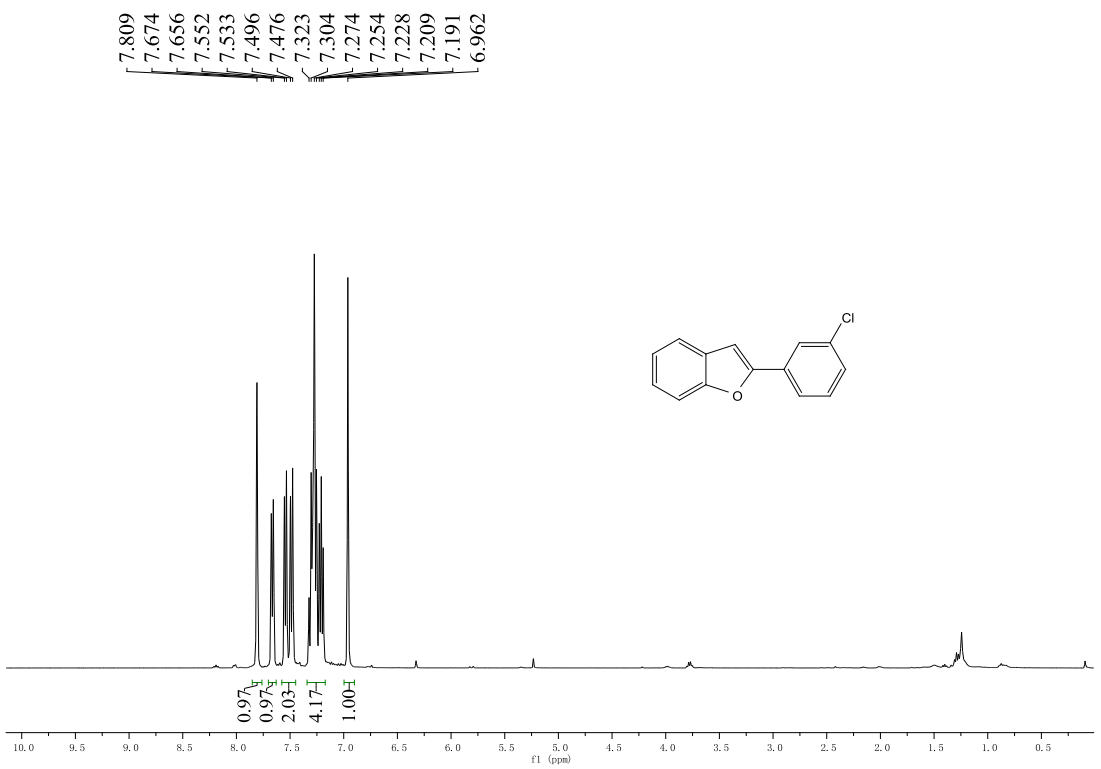
f1 (ppm)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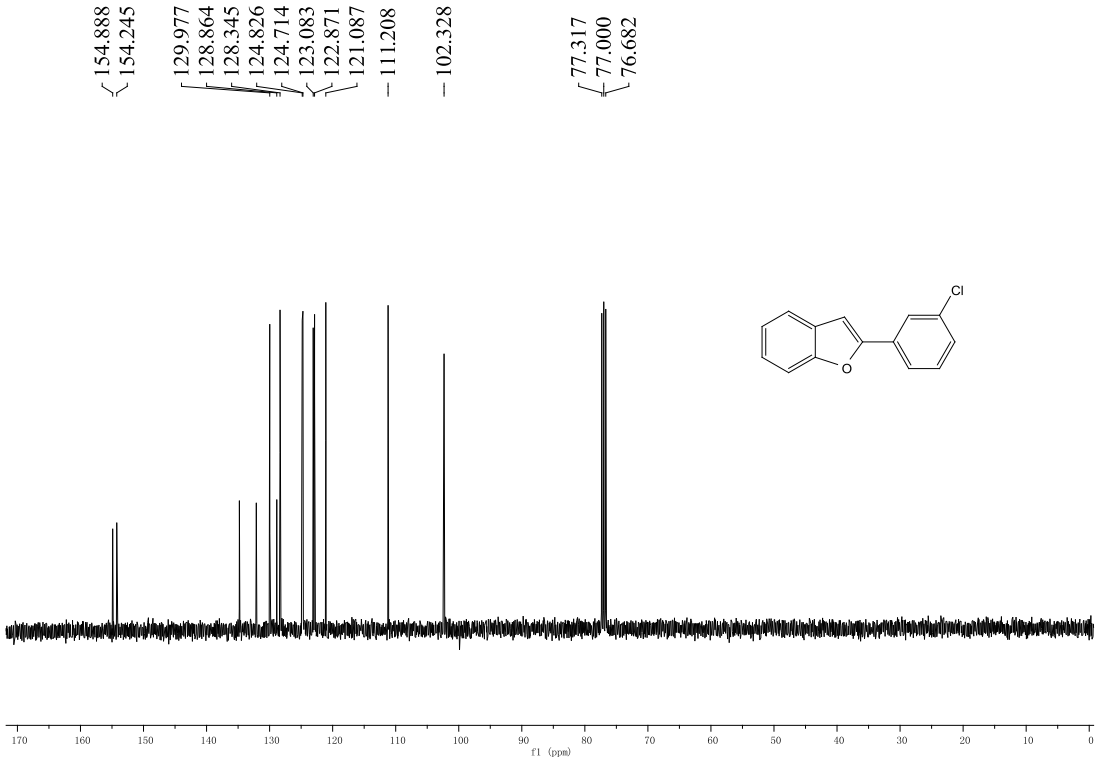
7.674
7.656
7.552
7.533
7.496
7.476
7.323
7.304
7.274
7.254
7.228
7.209
7.191
6.962
Cl
O
0.97
0.97
2.03
4.17
1.00
f1 (ppm)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77.000
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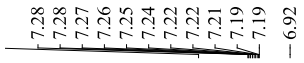
Cl
O
f1 (ppm)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7.27
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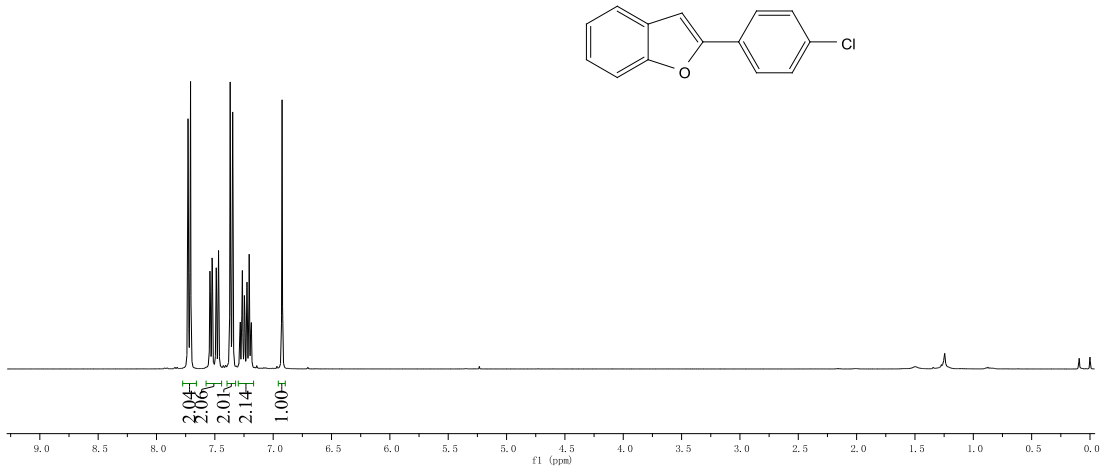
7.24
7.22
7.22
7.21
7.19
7.19
6.92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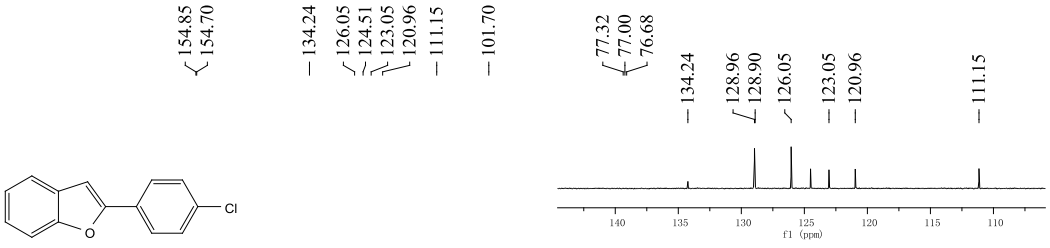
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124.51
123.05
120.96
111.15
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123.05
120.96
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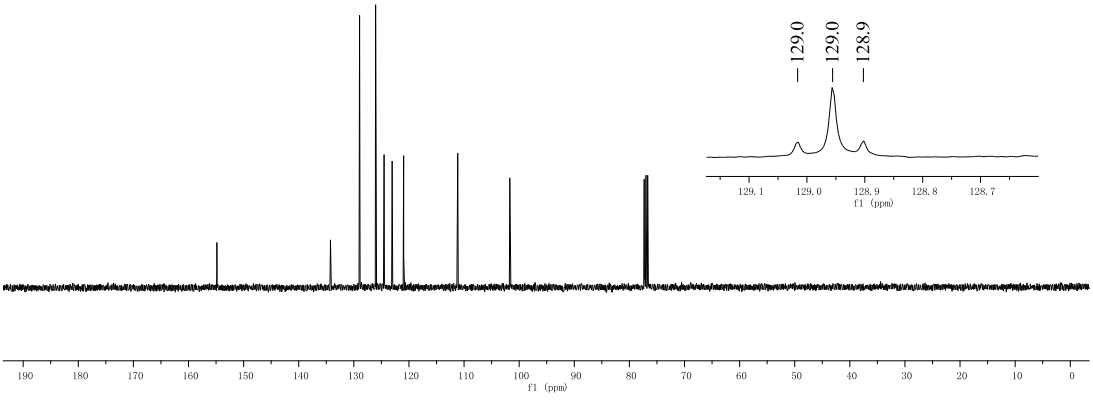
Cl
O
f1 (ppm)


129.0
129.0
128.9
f1 (ppm)
f1 (ppm)


7.602
7.583
7.566
7.546
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7.488
7.384
7.365
7.347
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7.301
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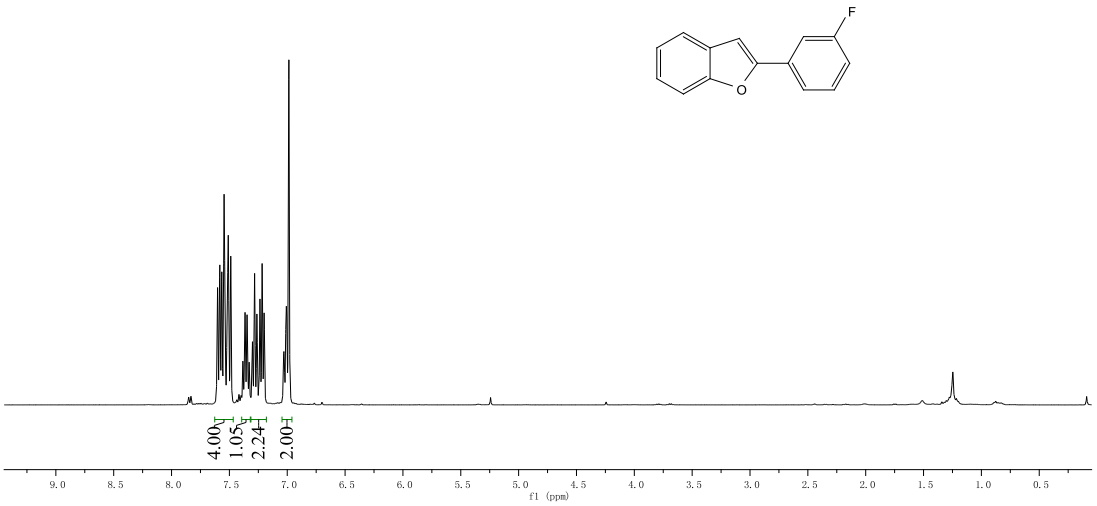
7.236
7.217
7.200
7.029
7.008
6.986


F
O
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1.05
2.24
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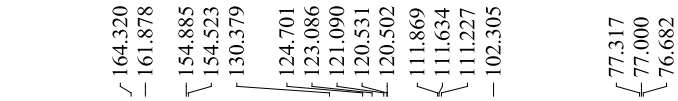
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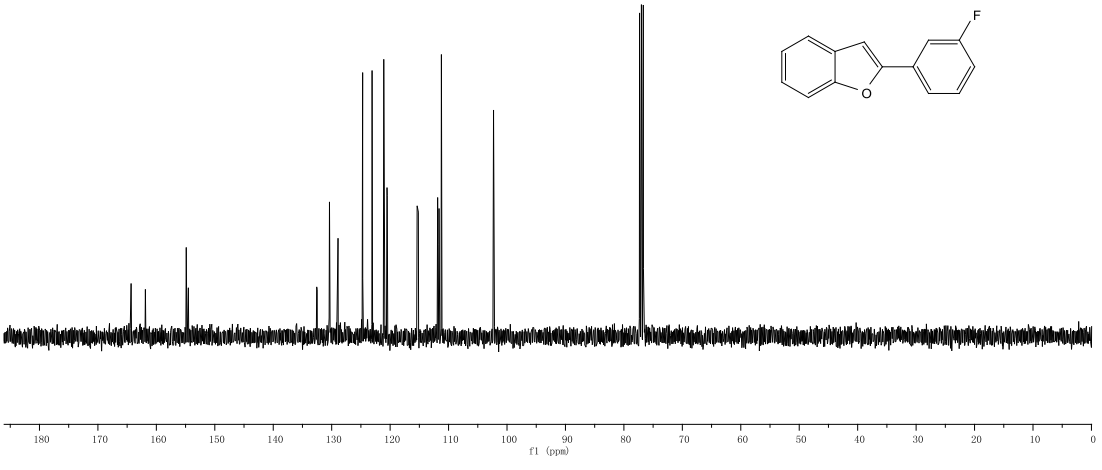
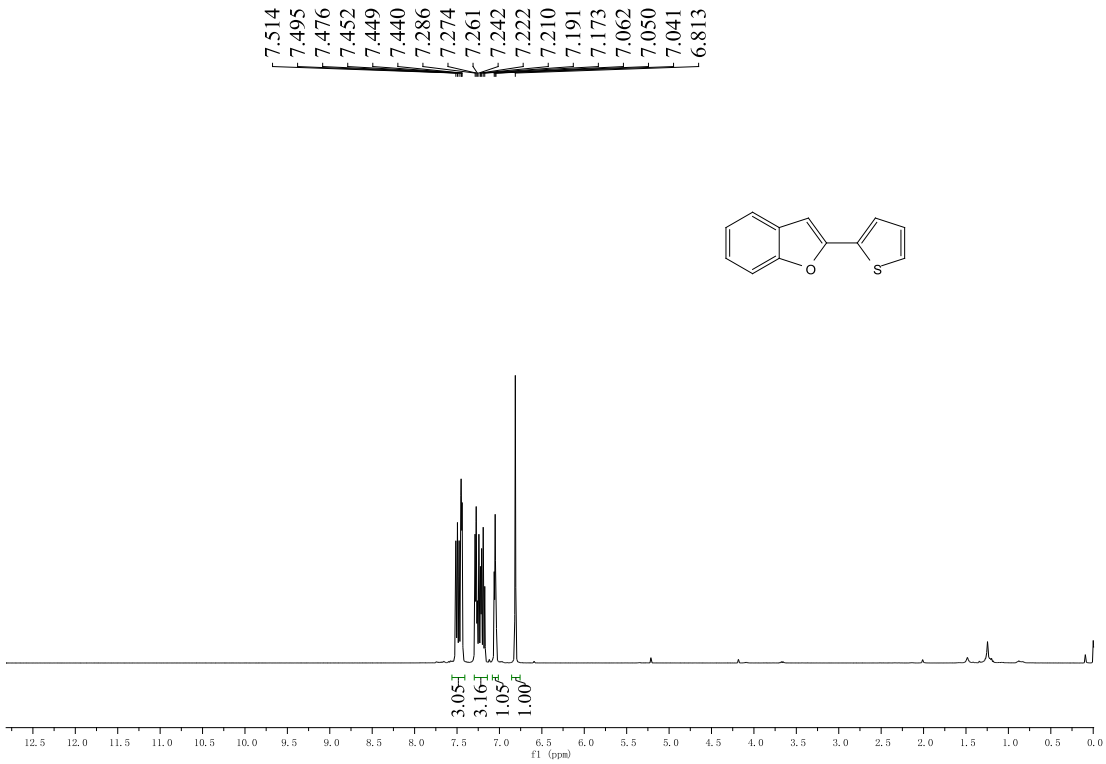
76.682


F
O
f1 (ppm)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7.286
7.274
7.261
7.242
7.222
7.210
7.191
7.173
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7.050
7.041
6.813
O
S
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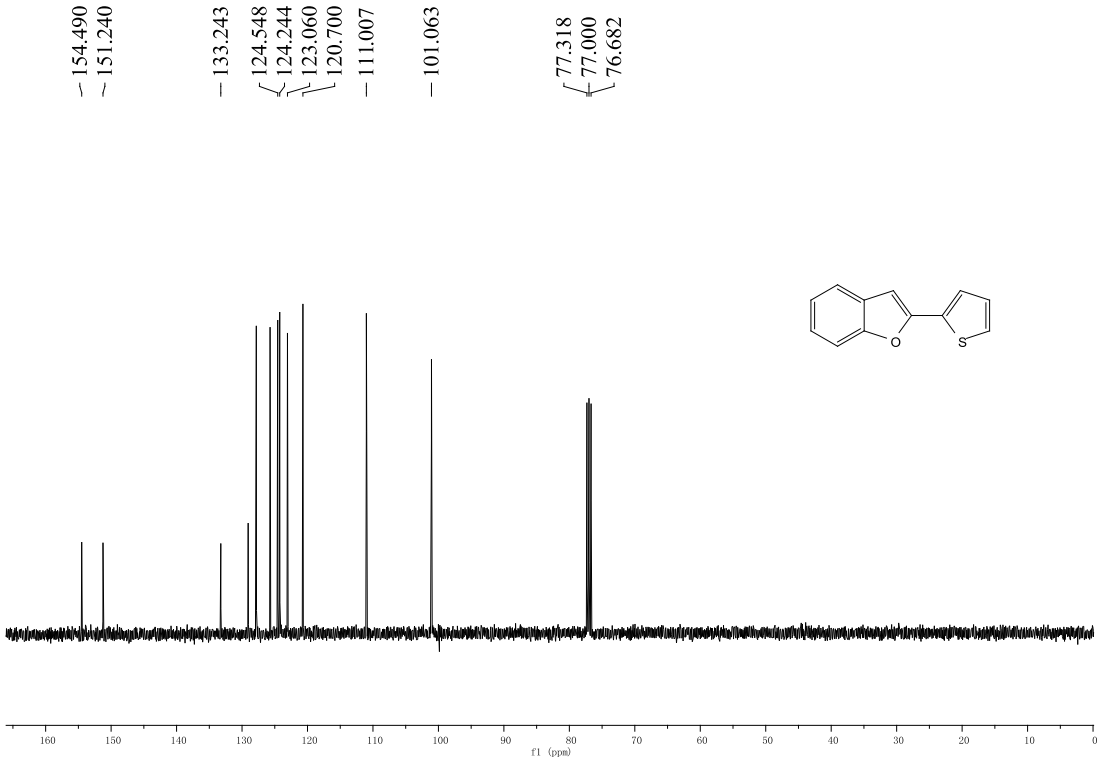
3.16
1.05
1.00
f1 (ppm)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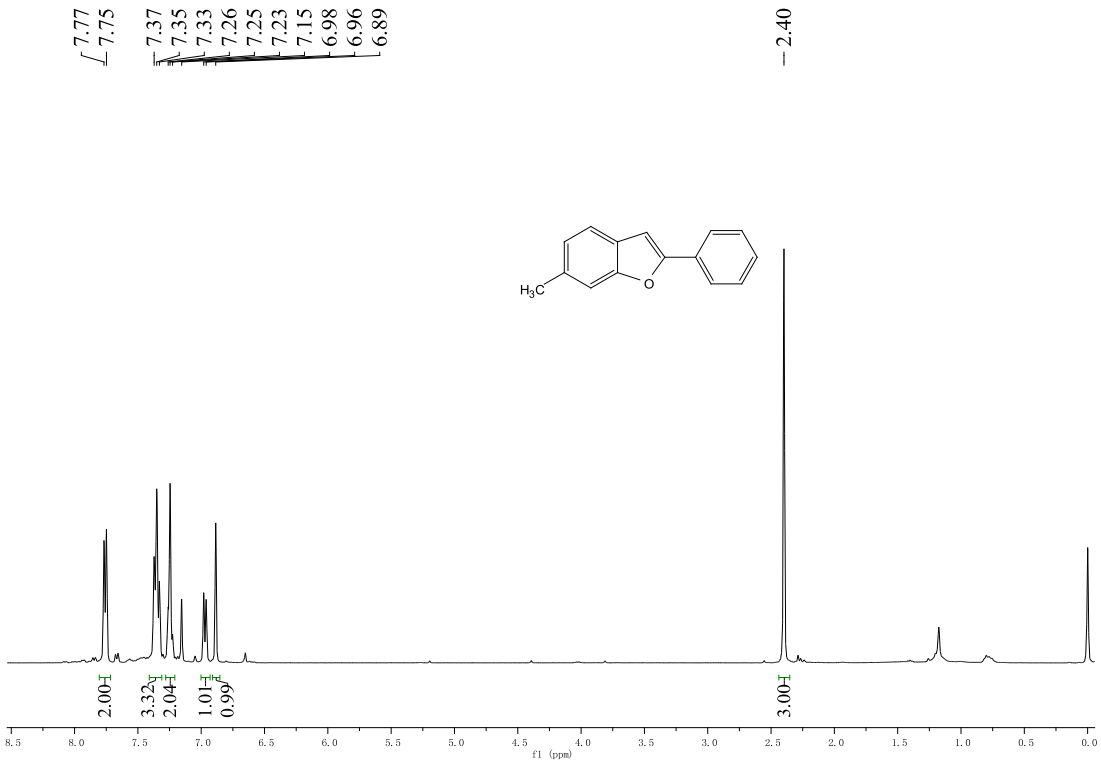
77.318
77.000
76.682
O
S
f1 (ppm)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7.33
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7.15
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6.96
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H3C
O
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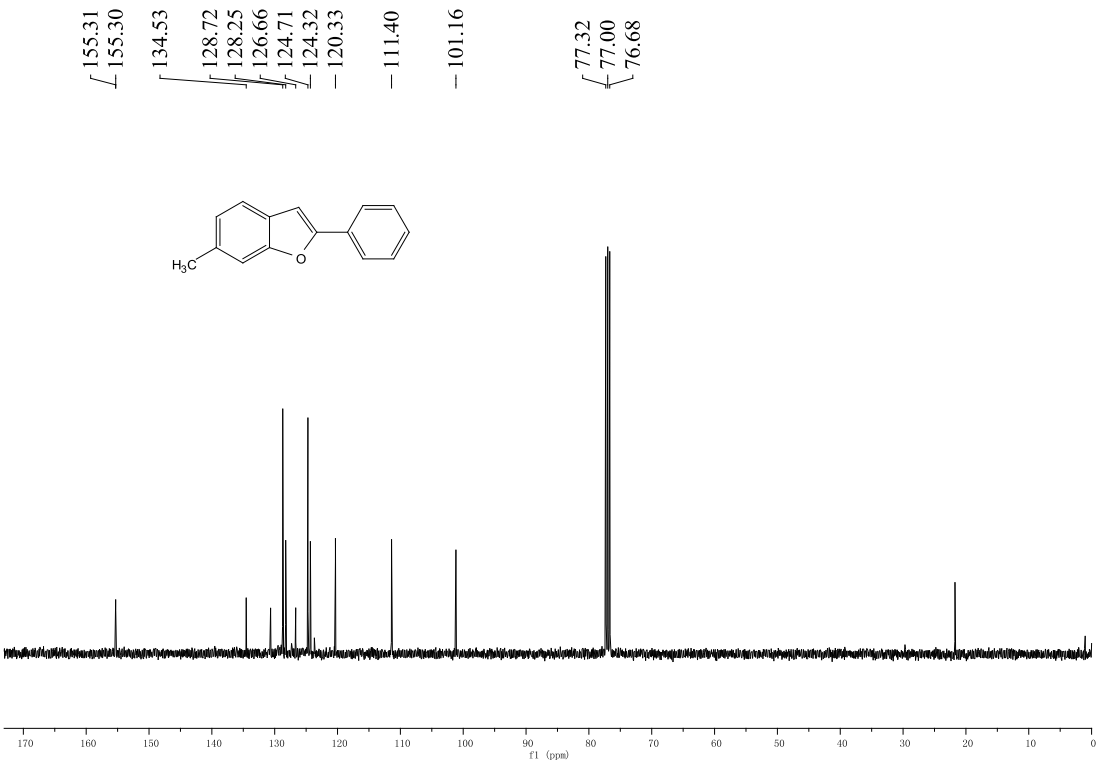
2.04
1.01
0.99
3.00
f1 (ppm)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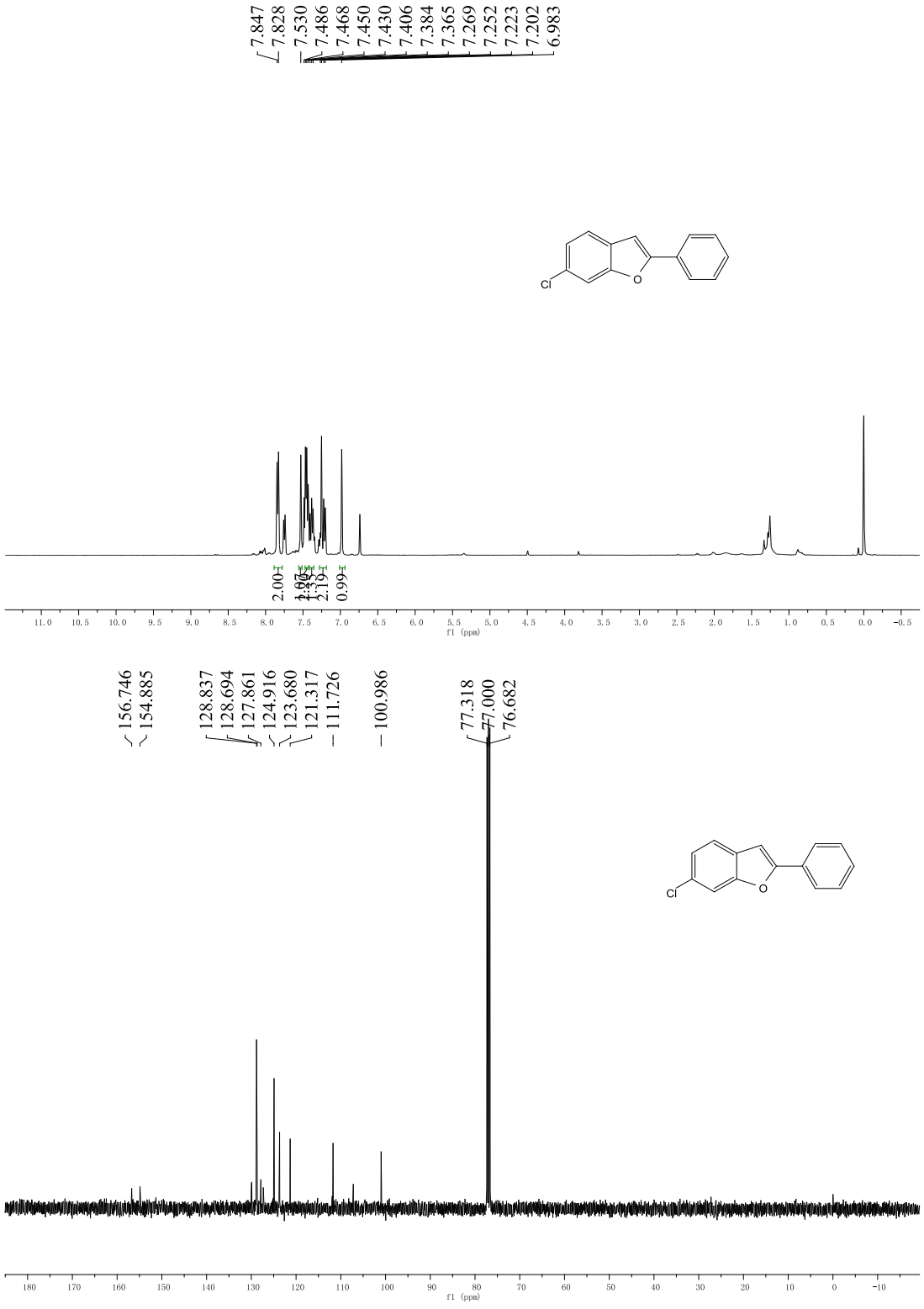
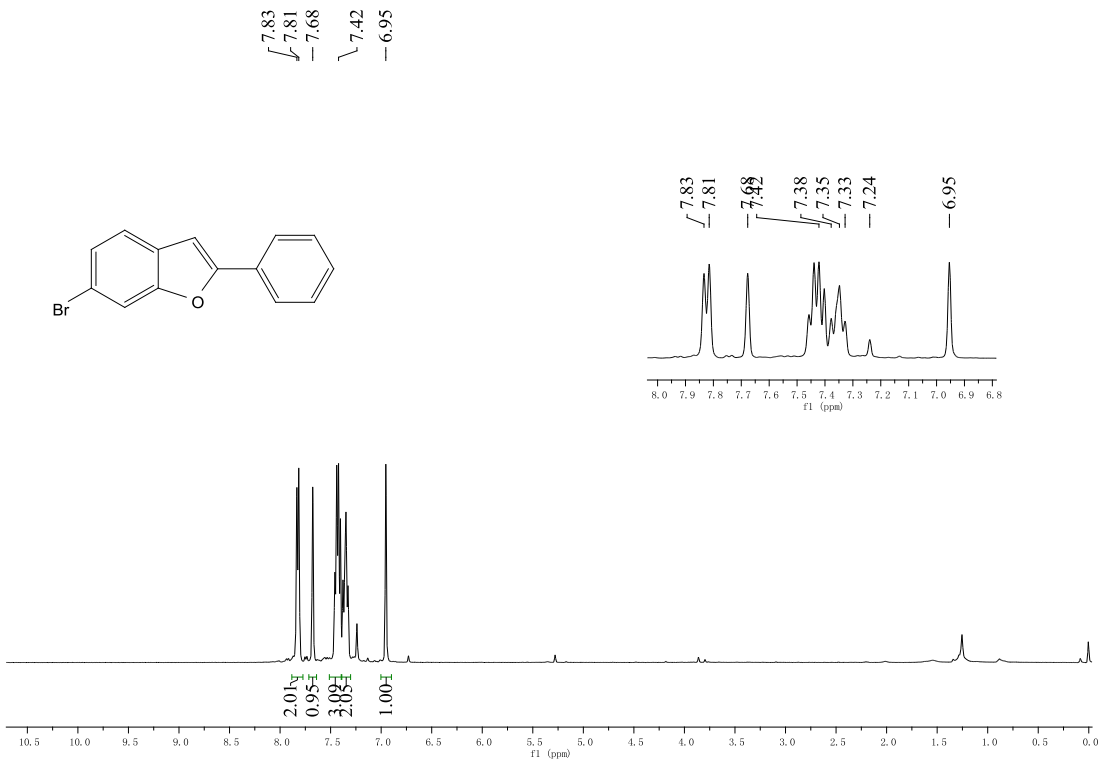
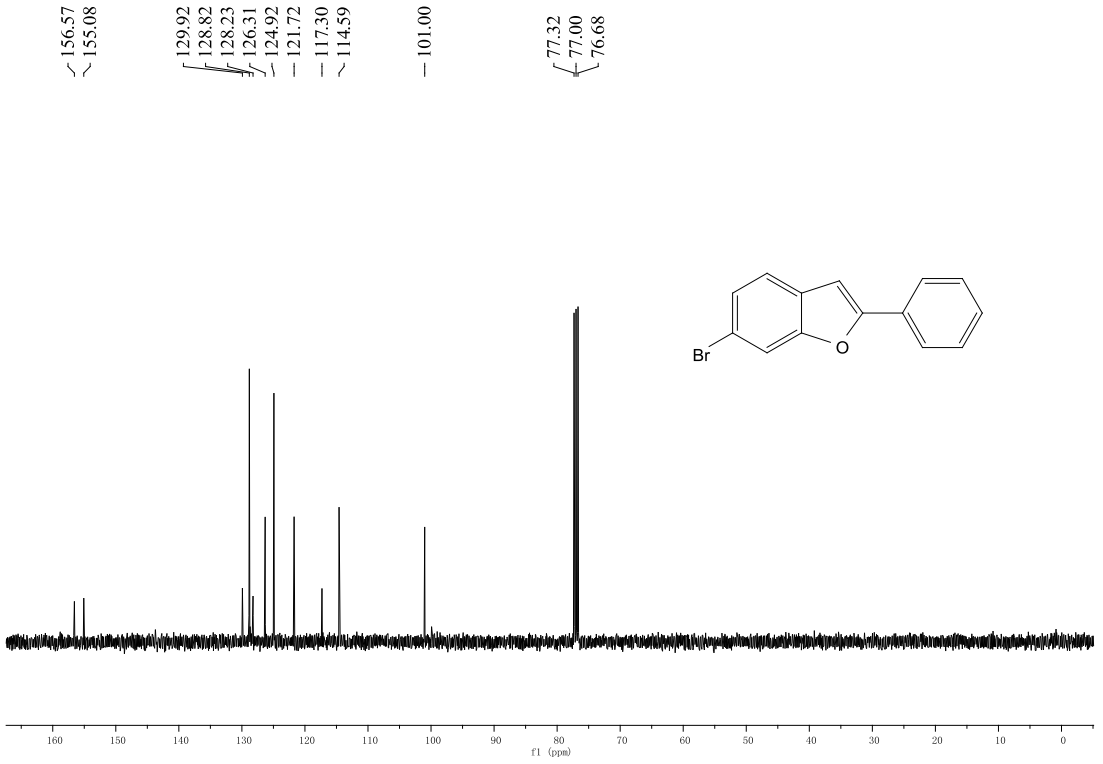
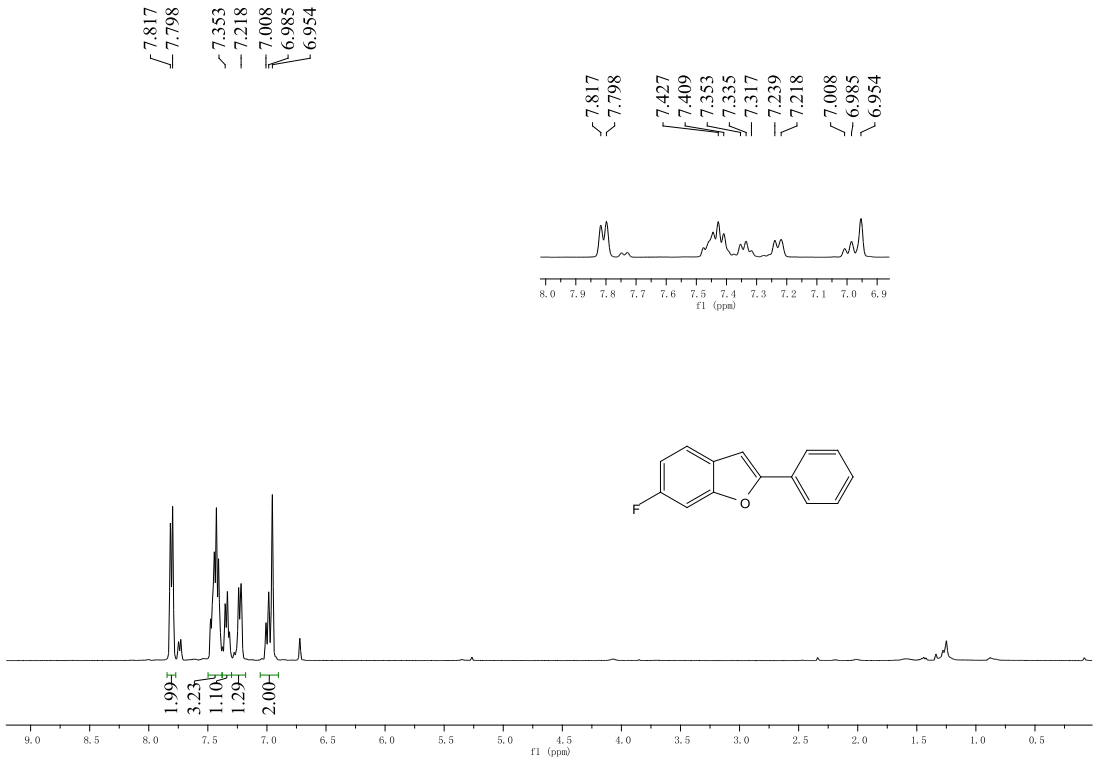
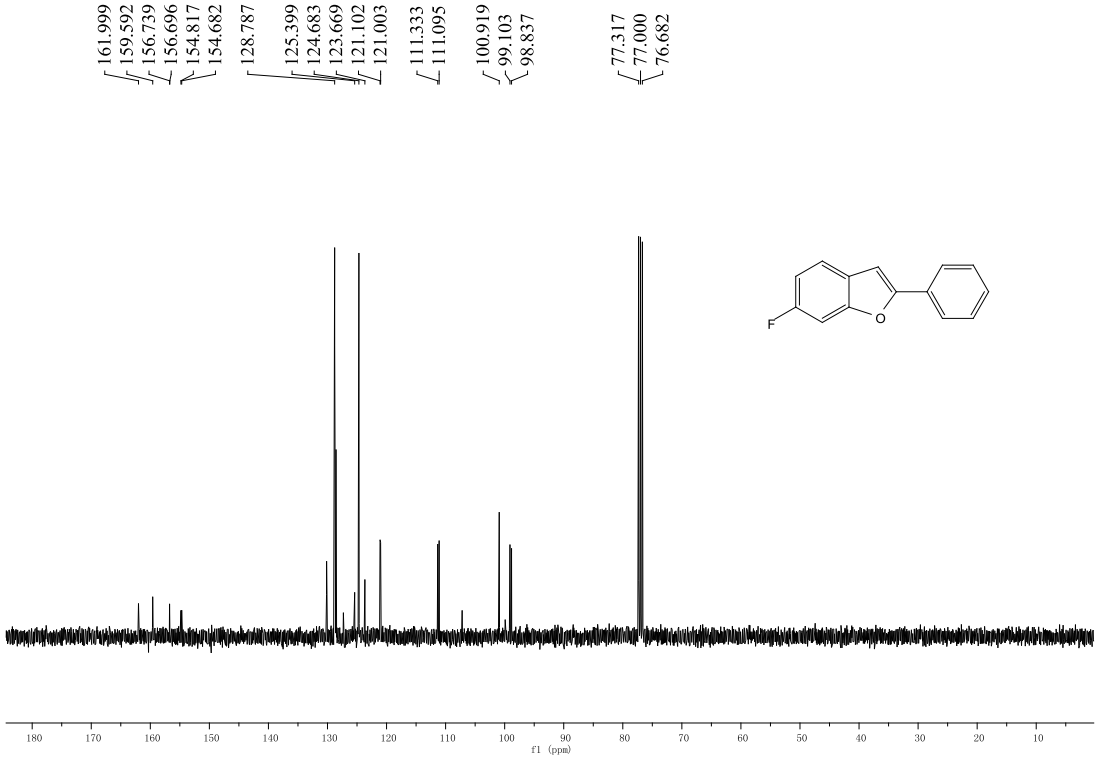
77.00
76.68
H3C
O
f1 (ppm)

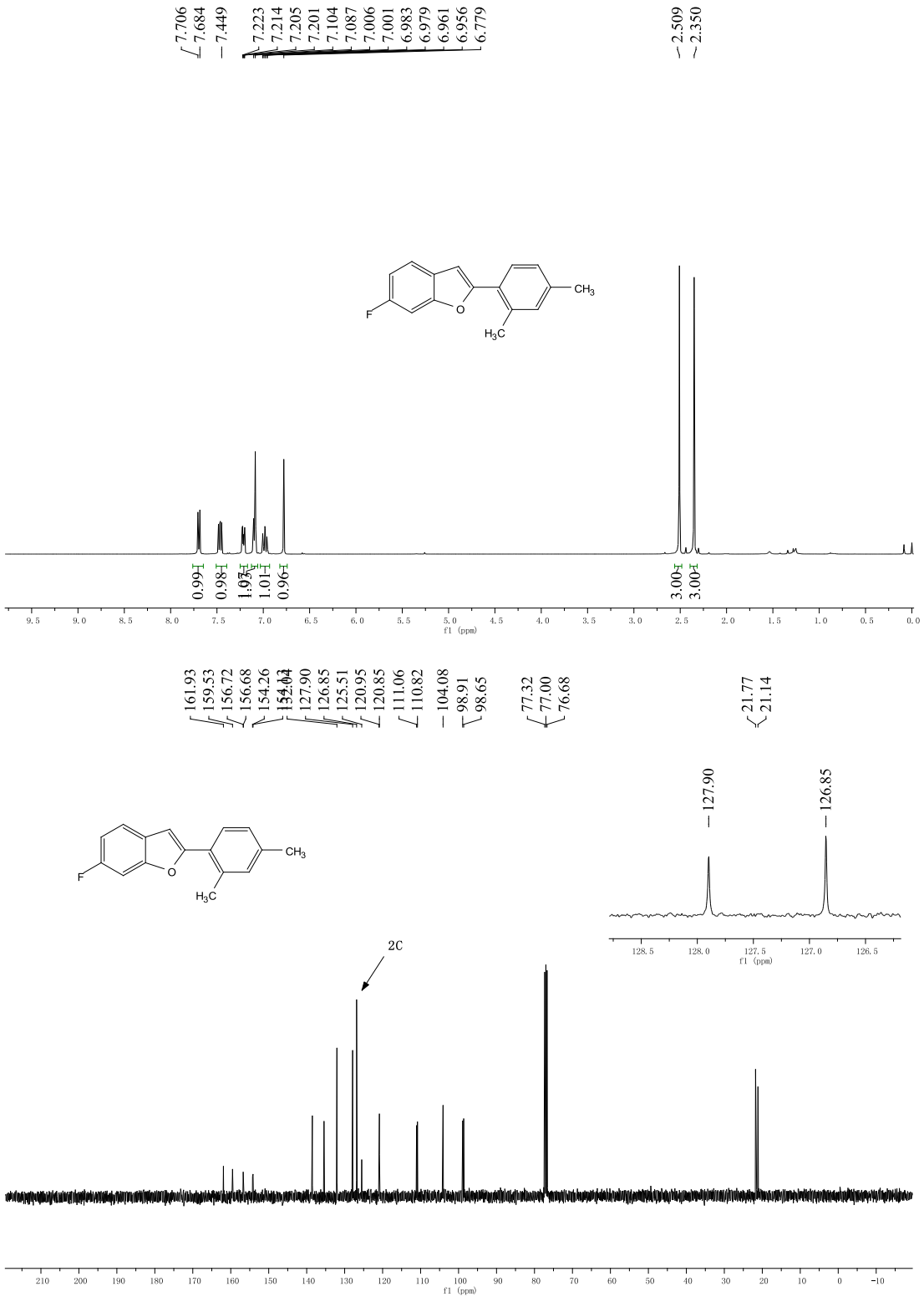

7.847
7.828
7.530
7.486
7.468
7.450
7.430
7.406
7.384
7.365
7.269
7.252
7.223
7.202
6.983
Cl
O
2.00
1.07
1.45
2.19
0.99
f1 (ppm)
156.746
154.885
128.837
128.694
127.861
124.916
123.680
121.317
111.726
100.986
77.318
77.000
76.682
Cl
O
f1 (ppm)

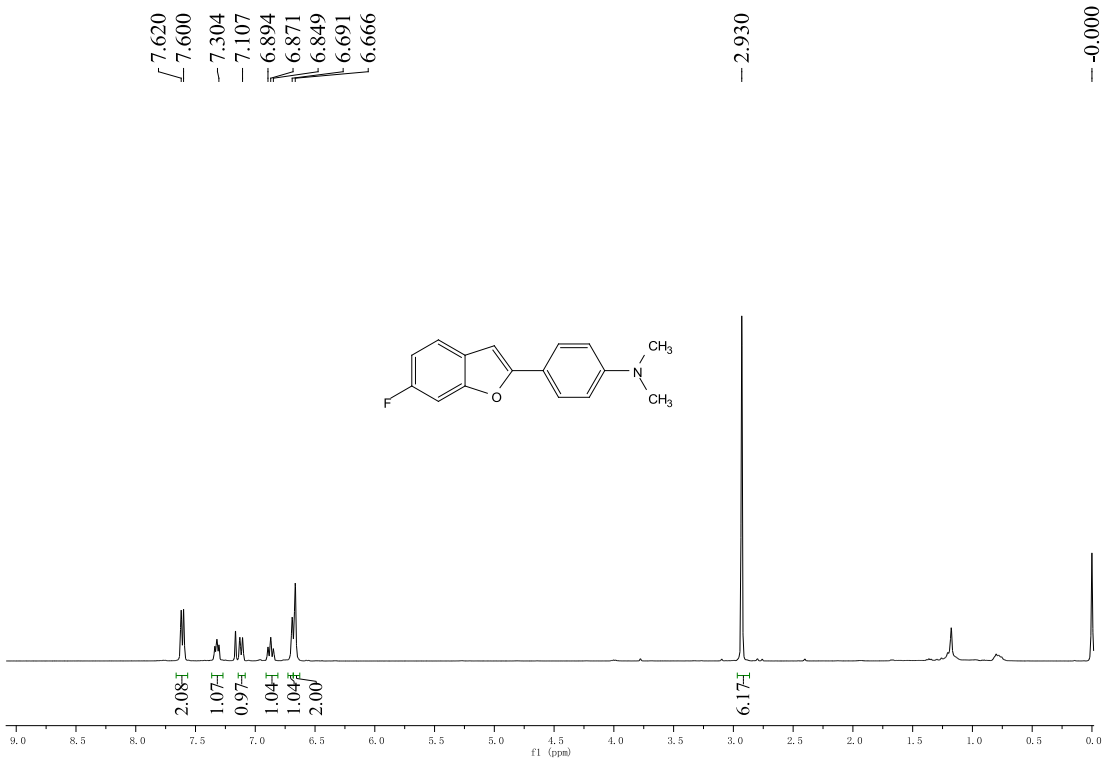

7.83
7.81
7.68
7.42
6.95
Br
O
7.38
7.35
7.33
7.24
f1 (ppm)
2.01
0.95
3.09
2.05
1.00
f1 (ppm)

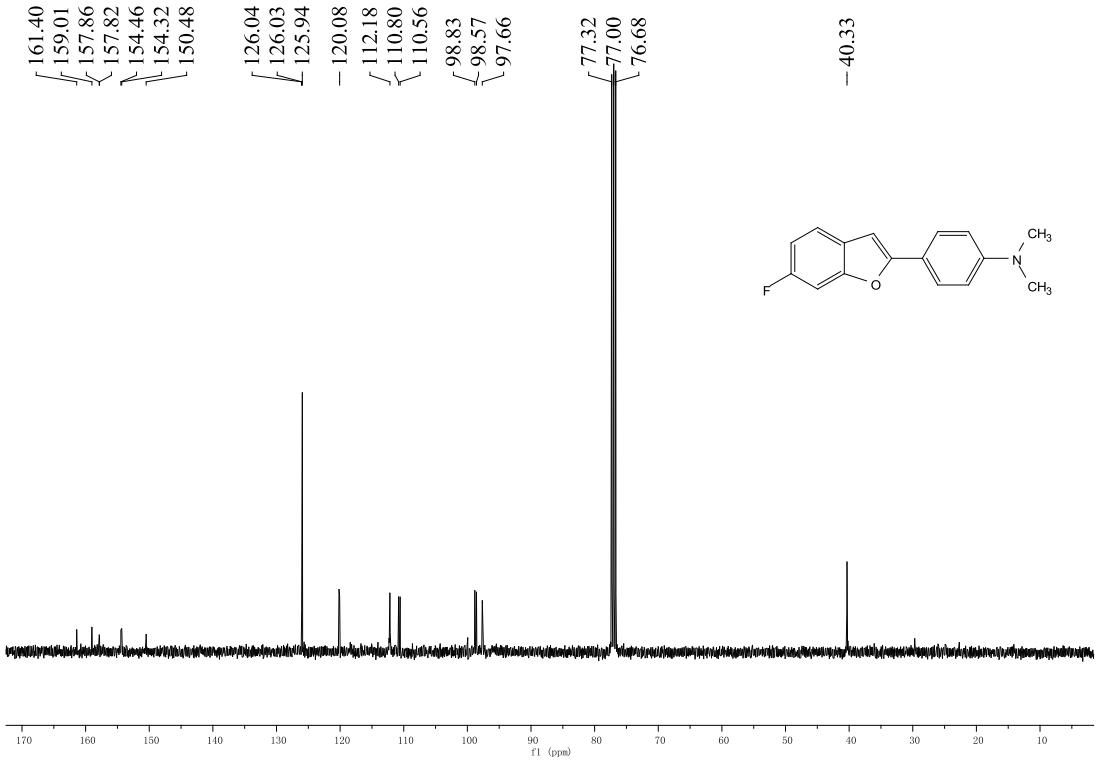

156.57
155.08
129.92
128.82
128.23
126.31
124.92
121.72
117.30
114.59
101.00
77.32
77.00
76.68
Br
O
f1 (ppm)

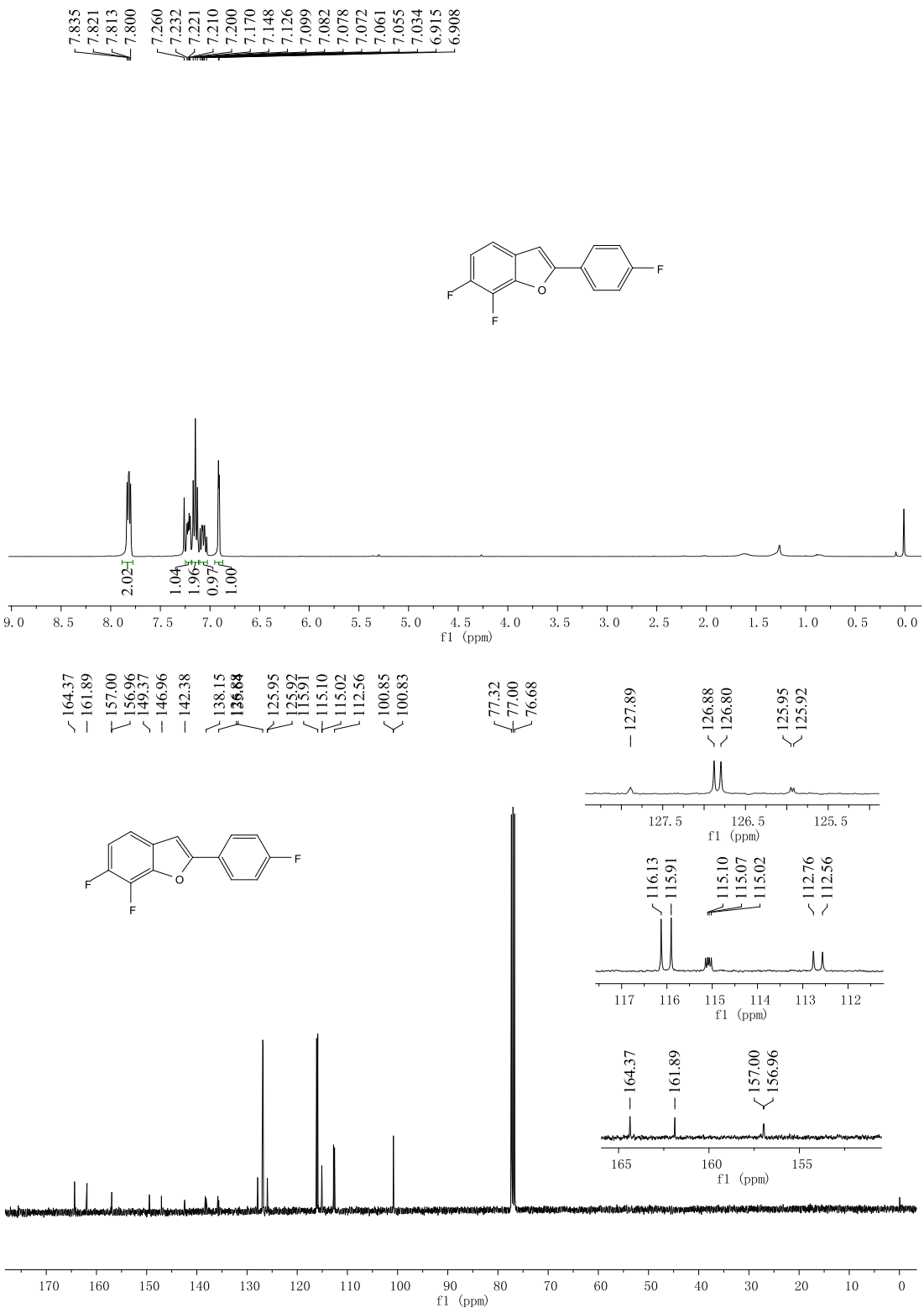

7.817
7.798
7.353
7.218
7.008
6.985
6.954
7.817
7.798
7.427
7.409
7.353
7.335
7.317
7.239
7.218
7.008
6.985
6.954
8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9
f1 (ppm)
F
O
1.99
3.23
1.10
1.29
2.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

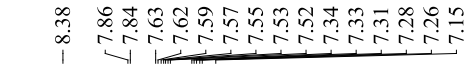

161.999
159.592
156.739
156.696
154.817
154.682
128.787
125.399
124.683
123.669
121.102
121.003
111.333
111.095
100.919
99.103
98.837
77.317
77.000
76.682
F
O
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

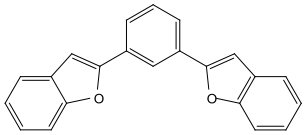

7.706
7.684
7.449
7.223
7.214
7.205
7.201
7.104
7.087
7.006
7.001
6.983
6.979
6.961
6.956
6.779
2.509
2.350
F
O
CH3
H3C
0.99
0.98
1.93
1.01
0.96
3.00
3.00
f1 (ppm)
161.93
159.53
156.72
156.68
154.26
127.90
126.85
125.51
120.95
120.85
111.06
110.82
104.08
98.91
98.65
77.32
77.00
76.68
21.77
21.14
127.90
126.85
2C
f1 (ppm)

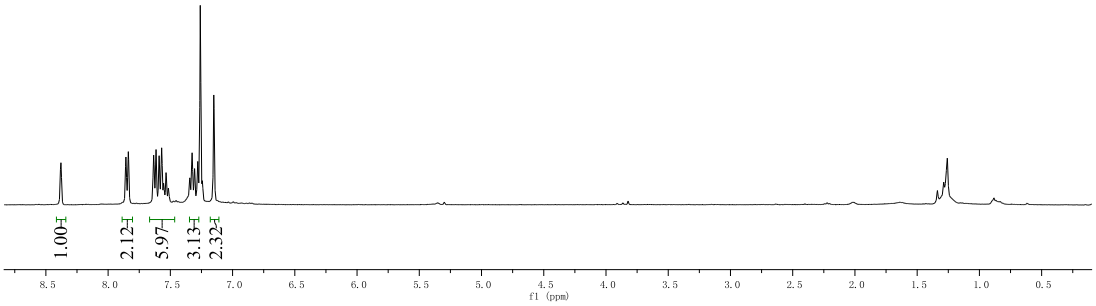

7.620
7.600
7.304
7.107
6.894
6.871
6.849
6.691
6.666
2.930
-0.000
2.08
1.07
0.97
1.04
1.04
2.00
6.17
f1 (ppm)

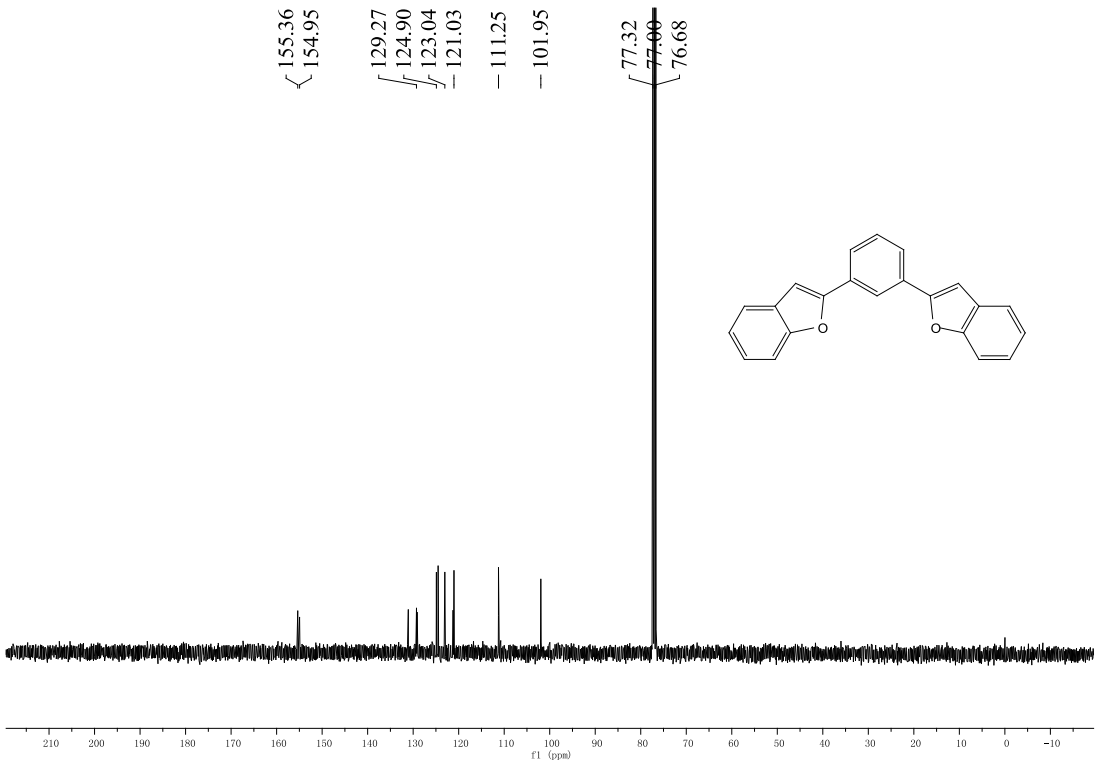

161.40
159.01
157.86
157.82
154.46
154.32
150.48
126.04
126.03
125.94
120.08
112.18
110.80
110.56
98.83
98.57
97.66
77.32
77.00
76.68
40.33
f1 (ppm)

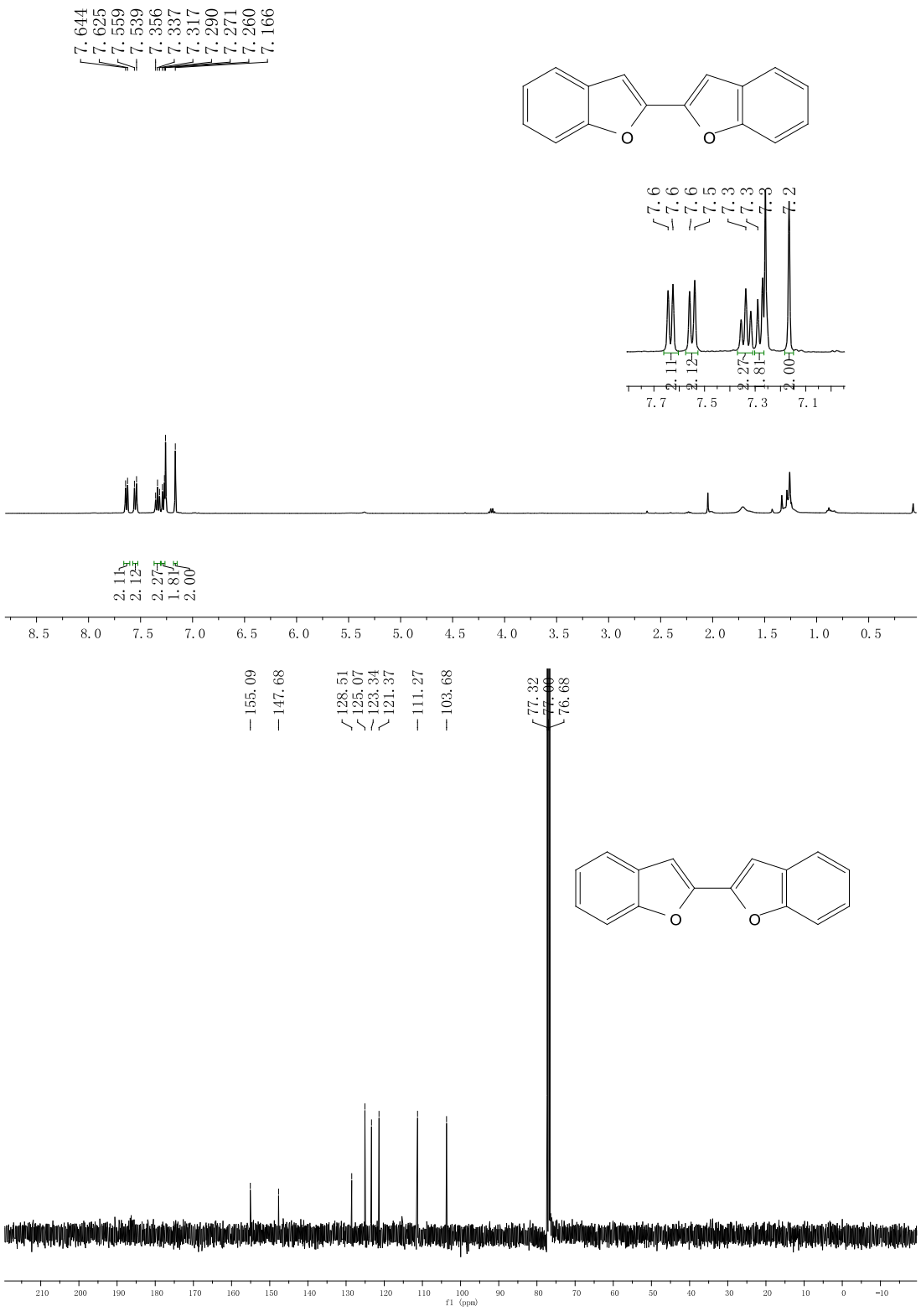

7.835
7.821
7.813
7.800
7.260
7.232
7.221
7.210
7.200
7.170
7.148
7.126
7.099
7.082
7.078
7.072
7.061
7.055
7.034
6.915
6.908
F
F
O
F
2.02
1.04
1.96
0.97
1.00
f1 (ppm)
164.37
161.89
157.00
156.96
149.37
146.96
142.38
138.15
125.95
125.92
115.91
115.10
115.02
112.56
100.85
100.83
77.32
77.00
76.68
127.89
126.88
126.80
125.95
125.92
116.13
115.91
115.10
115.07
115.02
112.76
112.56
164.37
161.89
157.00
156.96


8.38
7.86
7.84
7.63
7.62
7.59
7.57
7.55
7.53
7.52
7.34
7.33
7.31
7.28
7.26
7.15

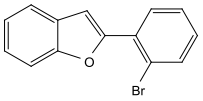


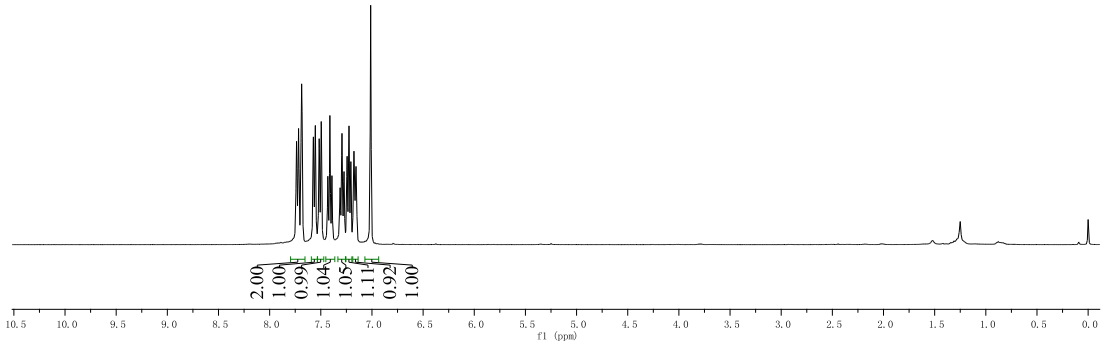

1.00
2.12
5.97
3.13
2.32
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


155.36
154.95
129.27
124.90
123.04
121.03
111.25
101.95
77.32
77.00
76.68
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

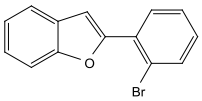

7.644
7.625
7.559
7.539
7.356
7.337
7.317
7.290
7.271
7.260
7.166
O
O
2.11
2.12
2.27
1.81
2.00
155.09
147.68
128.51
125.07
123.34
121.37
111.27
103.68
77.32
77.00
76.68
f1 (ppm)

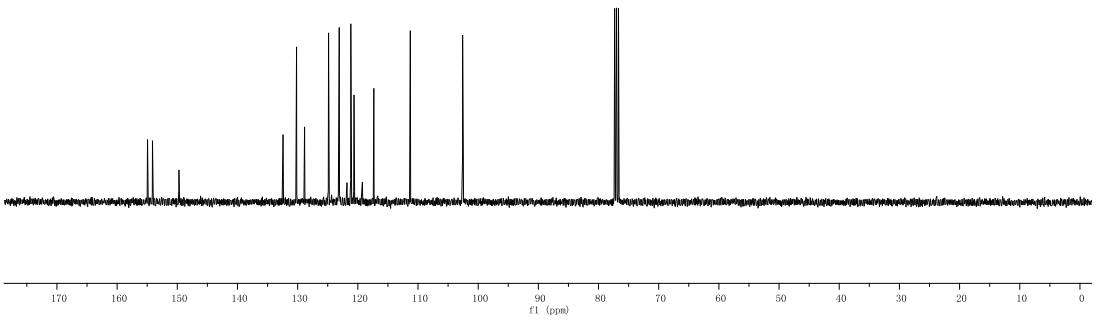

7.737
7.717
7.687
7.572
7.553
7.516
7.496
7.431
7.411
7.391
7.311
7.293
7.273
7.243
7.224
7.207
7.176
7.156
7.013

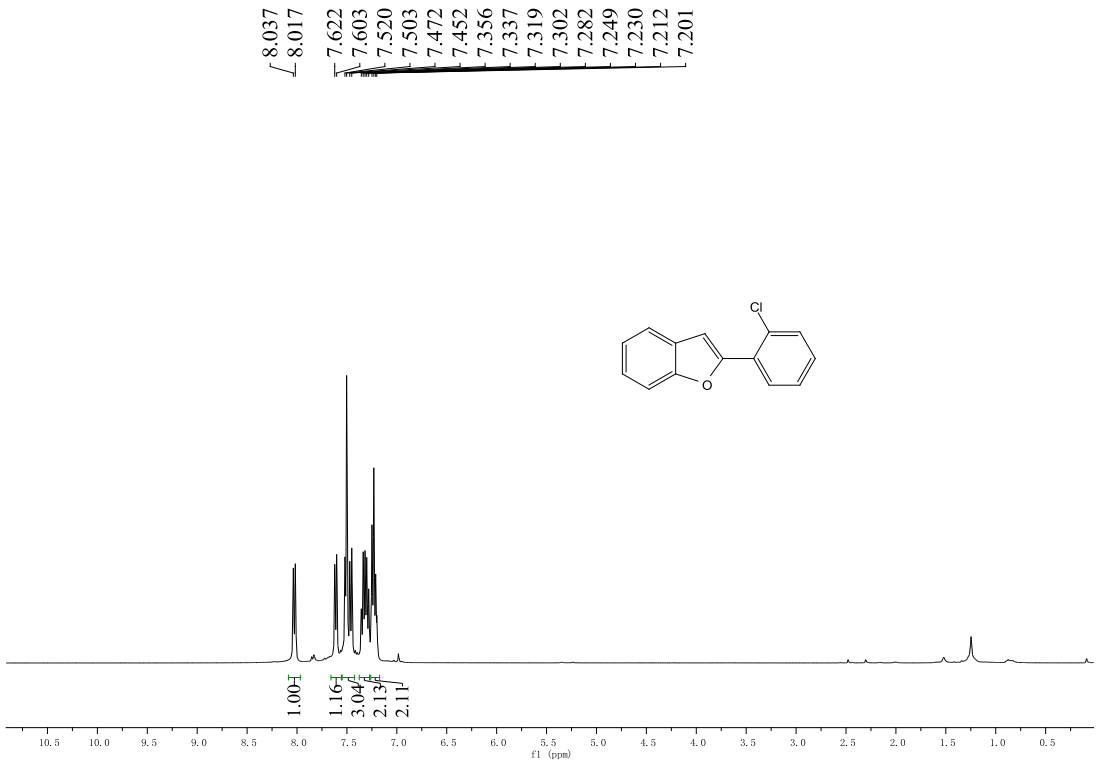

O
Br

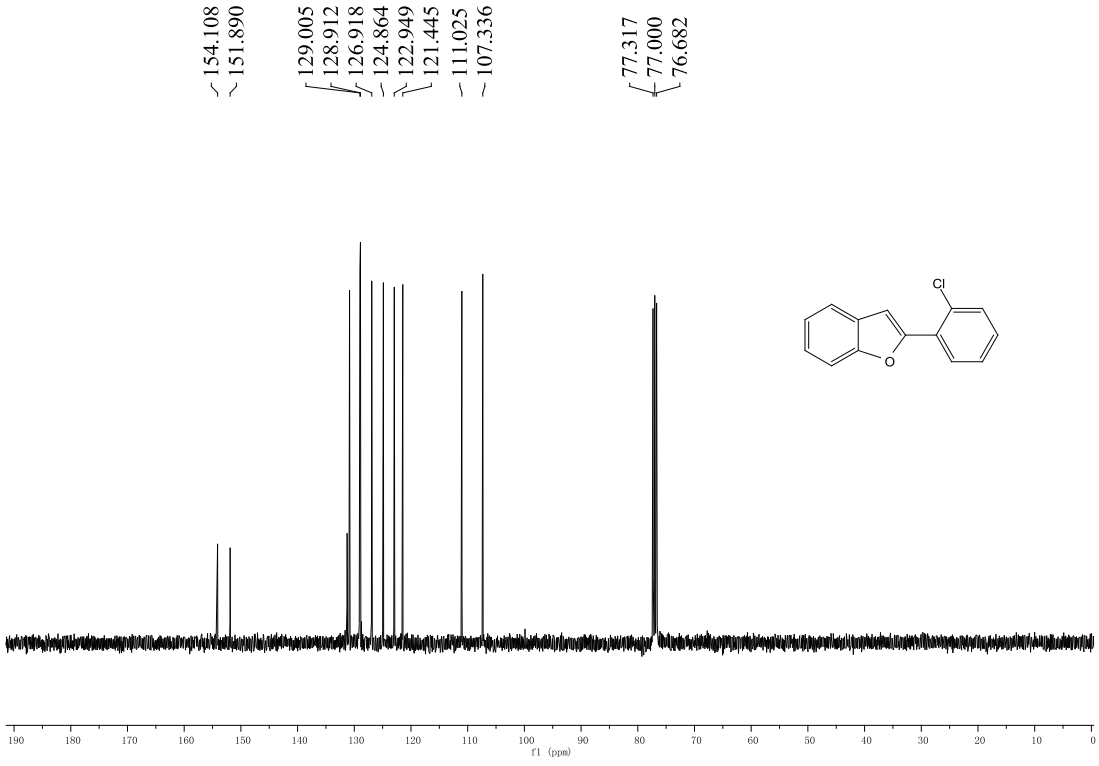

2.00
1.00
0.99
1.04
1.05
1.11
0.92
1.00
f1 (ppm)

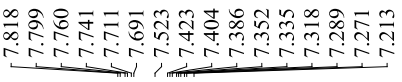

154.946
154.121
149.727
124.861
123.165
123.088
121.163
120.630
117.337
111.277
102.583
77.318
77.000
76.683

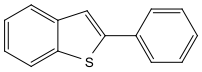

O
Br

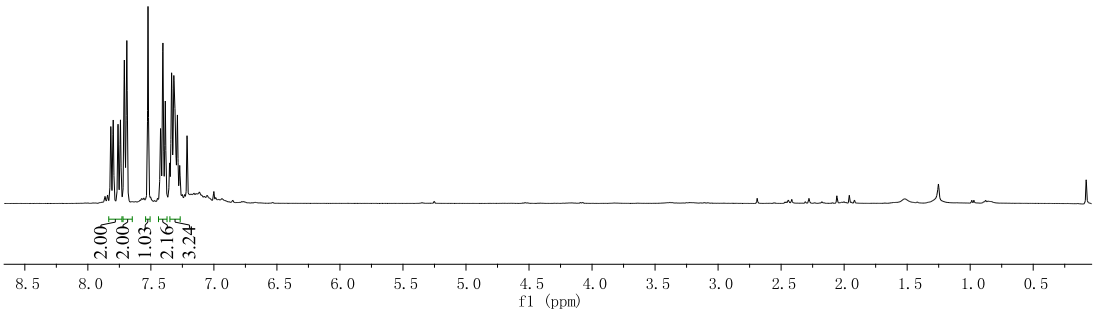

f1 (ppm)


8.037
8.017
7.622
7.603
7.520
7.503
7.472
7.452
7.356
7.337
7.319
7.302
7.282
7.249
7.230
7.212
7.201
Cl
O
1.00
1.16
3.04
2.13
2.11
f1 (ppm)


154.108
151.890
129.005
128.912
126.918
124.864
122.949
121.445
111.025
107.336
77.317
77.000
76.682
Cl
O
f1 (ppm)


7.818
7.799
7.760
7.741
7.711
7.691
7.523
7.423
7.404
7.386
7.352
7.335
7.318
7.289
7.271
7.213

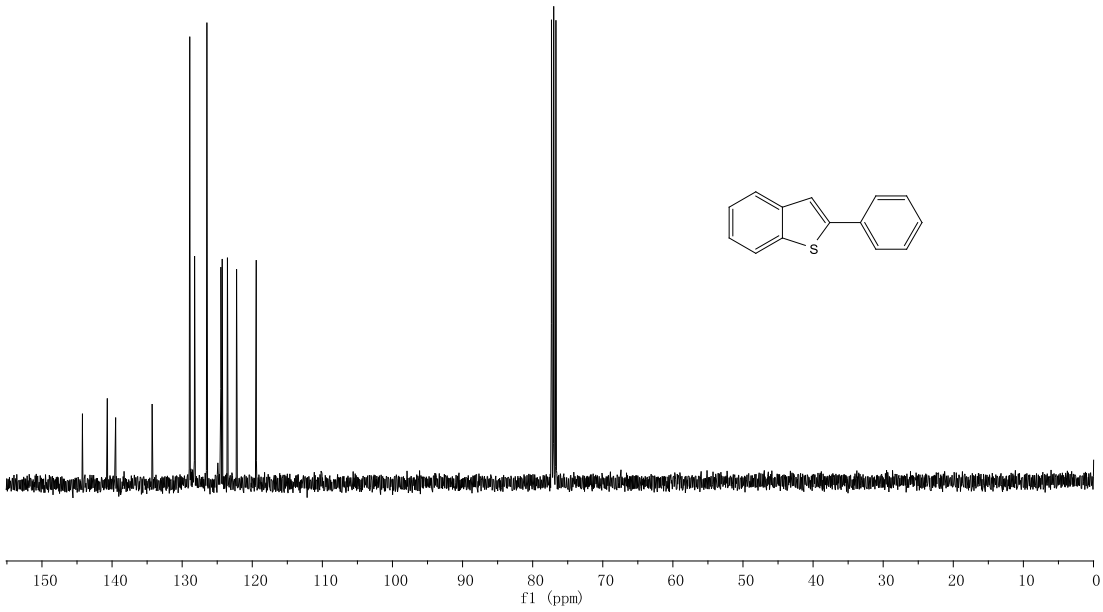

S


2.00
2.00
1.03
2.16
3.24
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
f1 (ppm)

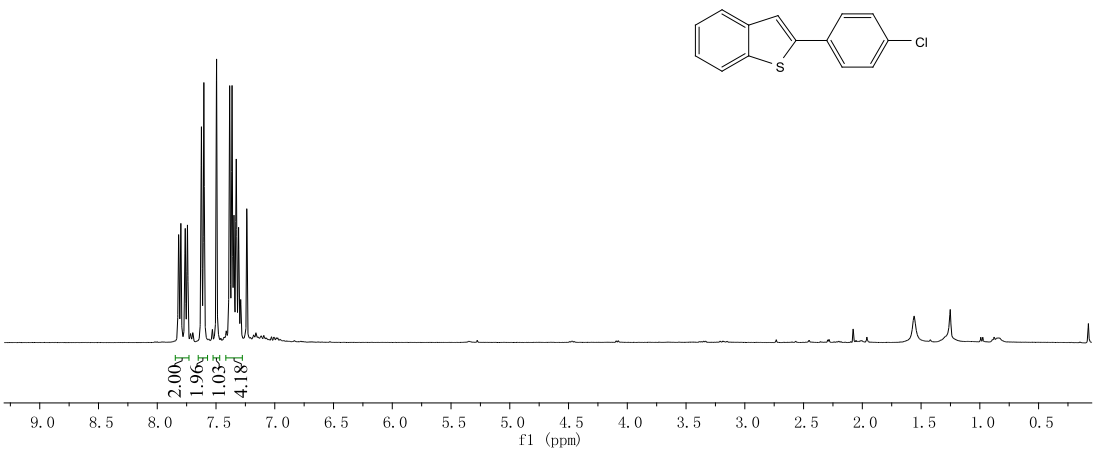

144.2
140.7
139.5
134.3
128.9
128.2
126.5
124.5
124.3
123.5
122.2
119.4

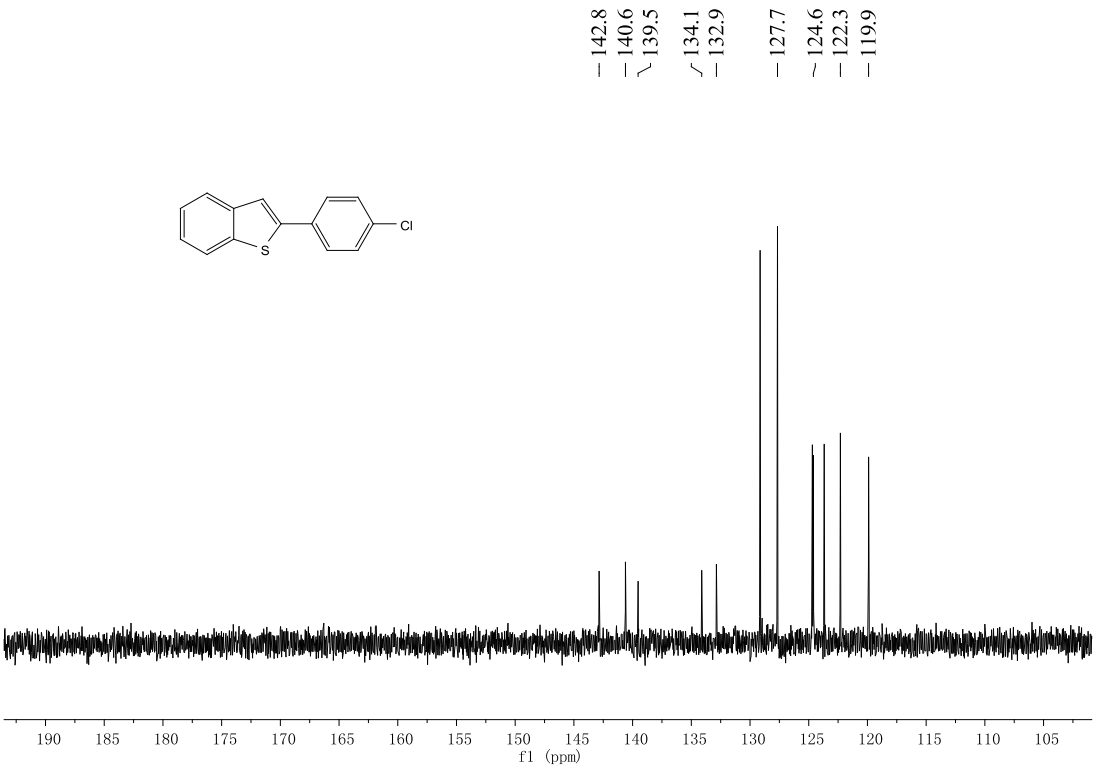

77.3
77.0
76.7

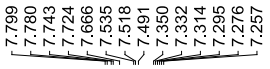
S

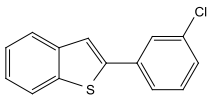

150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

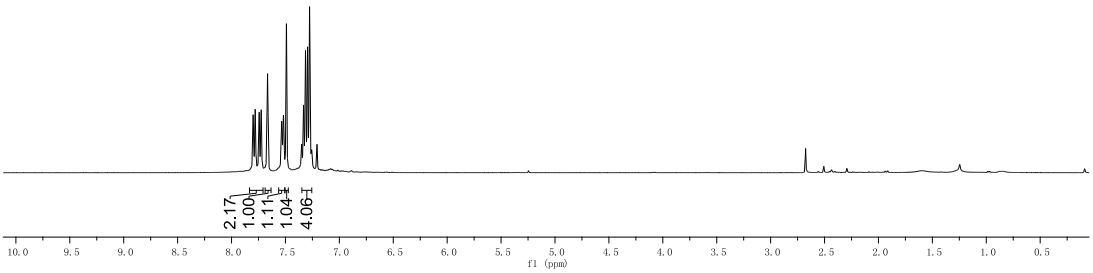

7.82
7.80
7.76
7.74
7.62
7.60
7.50
7.38
7.36
7.35
7.33
7.31
7.24

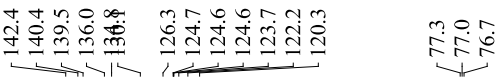

Cl
S
2.00
1.96
1.03
4.18
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

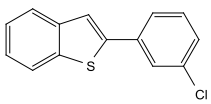

142.8
140.6
139.5
134.1
132.9
127.7
124.6
122.3
119.9
Cl
S
190 185 180 175 170 165 160 155 150 145 140 135 130 125 120 115 110 105
f1 (ppm)

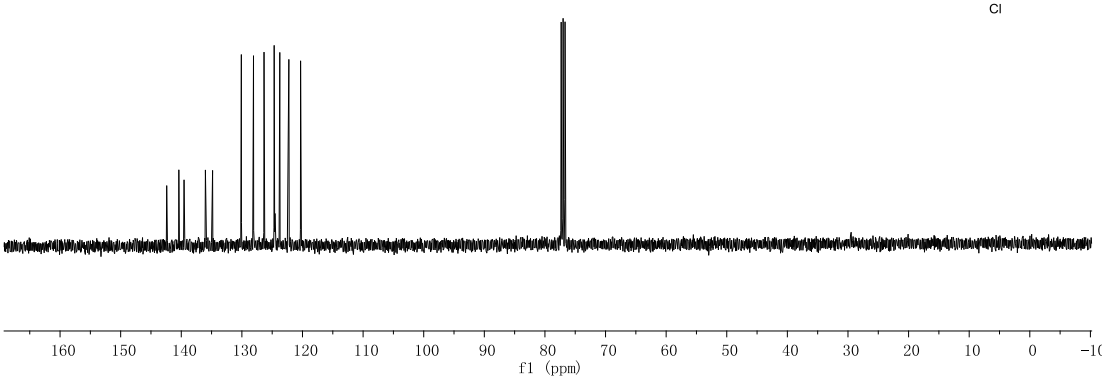

7.799
7.780
7.743
7.724
7.666
7.535
7.518
7.491
7.350
7.332
7.314
7.295
7.276
7.257


Cl
S


2.17
1.00
1.11
1.04
4.06
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
f1 (ppm)


142.4
140.4
139.5
136.0
126.3
124.7
124.6
123.7
122.2
120.3
77.3
77.0
76.7


S
Cl


160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)