DMTSF-mediated electrophilic cyclization for the synthesis of 3-thiomethyl substituted benzo[b]furan derivatives

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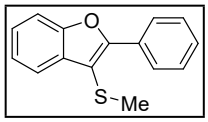
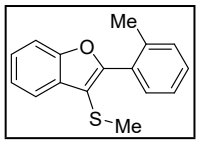
General. The ^{1}H and ^{13}C NMR spectra were recorded at 400 and 100 MHz, respectively. Thin layer chromatography was performed using commercially prepared 60-mesh silica gel plates, utilizing short wavelength UV light (254 nm) for effective visualization. All obtained melting points are uncorrected**.**

Reagents. All reagents were used directly as obtained commercially unless otherwise noted.

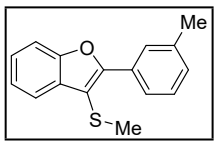
General Procedure for synthesis of benzofurans: To a 6-dram vial, a substituted (o-methoxy) phenylacetylene (100mg, 0.48mol), dimethyl(methylthio)sulfonium tetrafluoroborate (54.2mg, 0.58mol), and 5mL of dichloromethane was added. The reaction was monitored by TLC and stirred at room temperature for 12 hours. The reaction mixture was filtered and absorbed in silica gel before purification via column chromatography using hexanes and ethyl acetate as the eluent.



3-(methylsulfanyl)-2-phenyl-1-benzofuran (3): Column chromatography was performed using hexanes and ethyl acetate (40:1) as the eluent. Light yellow viscous liquid; 0.0928g, 83%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (dd, J = 8.4, 1.4 Hz, 2H), 7.74 – 7.69 (m, 1H), 7.53 – 7.44 (m, 3H), 7.41 – 7.36 (m, 1H), 7.35 – 7.26 (m, 2H), 2.37 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.31, 153.73, 131.19, 130.36, 129.02, 128.57, 127.32, 125.07, 123.21, 120.07, 111.38, 109.24, 18.46; FTIR (Salt Plate) cm^{-1} 3066, 2992, 2921, 2859, 1888, 1779, 1594, 1552, 1489, 1474, 1454, 1442, 1342, 1336, 1276, 1254, 1201, 1182, 1108, 1084, 1067, 1032, 1014, 1006, 970, 927, 888, 822;

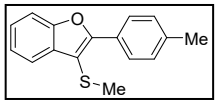


2-(2-methylphenyl)-3-(methylsulfanyl)-1-benzofuran (6): Column chromatography was performed using hexanes and ethyl acetate (40:1) as the eluent. White solid; 0.1099g, 95%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 – 7.63 (m, 1H), 7.46 (d, J = 7.6 Hz, 1H), 7.45 – 7.41 (m, 1H), 7.30 – 7.21 (m, 5H), 2.31 (s, 3H), 2.21 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.47, 154.30, 138.19, 131.07, 130.61, 130.00, 129.68, 129.50, 125.48, 124.74, 123.07, 119.99, 111.51, 110.84, 20.48, 18.33; FTIR (ATR) cm^{-1} 3065, 2921, 2858, 1729, 1590, 1447, 1382, 1246, 1196, 1071, 1041, 1007, 970, 890, 830, 762, 746, 721.

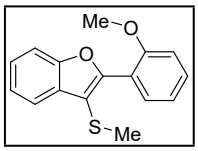


2-(3-methylphenyl)-3-(methylsulfanyl)-1-benzofuran (7): Column chromatography was performed using hexanes and ethyl acetate (40:1) as the eluent. Colorless visous liquid; 0.1115g, 95%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, J = 8.2 Hz, 1H), 8.06 (t, J = 1.8 Hz, 1H), 7.78 – 7.68 (m, 1H), 7.55 – 7.45 (m, 1H), 7.37 (t, J = 7.7 Hz, 1H), 7.31 (ddd, J = 6.4, 4.1, 1.6 Hz, 2H), 7.24 – 7.14 (m, 1H), 2.44 (s, 3H), 2.37 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.50, 153.69,

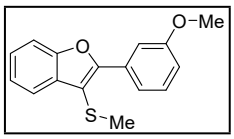
138.20, 131.21, 130.25, 129.86, 128.47, 127.84, 124.98, 124.58, 123.15, 120.03, 111.34, 109.07, 21.66, 18.44; FTIR (Salt Plate) cm^{-1} 3070, 2908, 2875, 2430, 1710, 1576, 1430, 1382, 1260, 1213, 1052, 1023, 1014, 963, 922, 897, 837, 750, 731, 707.



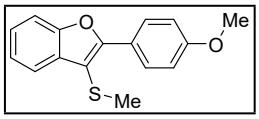
2-(4-methylphenyl)-3-(methylsulfanyl)-1-benzofuran (8): Column chromatography was performed using hexanes and ethyl acetate (40:1) as the eluent. White solid; 0.0933g, 81%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, J = 8.3 Hz, 2H), 7.74 – 7.67 (m, 1H), 7.53 – 7.48 (m, 1H), 7.33 – 7.27 (m, 4H), 2.42 (s, 3H), 2.38 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.64, 153.61, 139.15, 131.23, 129.25, 127.54, 127.22, 124.79, 123.09, 119.87, 111.26, 108.37, 21.48, 18.40; FTIR (ATR) cm^{-1} 3068, 2926, 2886, 1695, 1574, 1416, 1389, 1265, 1214, 1057, 1017, 1008, 951, 913, 829, 736;



2-(2-methoxyphenyl)-3-(methylsulfanyl)-1-benzofuran (9): Column chromatography was performed using hexanes and ethyl acetate (40:1) as the eluent. Coloress viscous liquid; 0.1012g, 96%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 – 7.70 (m, 1H), 7.55 (ddd, J = 9.0, 7.2, 1.5 Hz, 2H), 7.46 (ddd, J = 8.3, 7.4, 1.8 Hz, 1H), 7.37 – 7.29 (m, 2H), 7.09 (td, J = 7.6, 1.0 Hz, 1H), 7.05 (d, J = 8.4 Hz, 1H), 3.87 (s, 3H), 2.34 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.83, 154.69, 154.53, 131.89, 131.17, 130.10, 124.56, 122.88, 120.39, 119.92, 119.19, 111.57, 111.53, 111.42, 55.74, 18.14; FTIR (Salt Plate) cm^{-1} 3057, 2996, 2956, 2925, 2834, 2044, 1934, 1786, 1697, 1585, 1491, 1451, 1436, 1343, 1281, 1250, 1199, 1122, 1062, 1028, 971, 891;

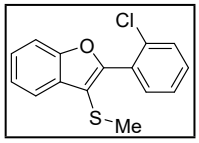


2-(3-methoxyphenyl)-3-(methylsulfanyl)-1-benzofuran (10): Column chromatography was performed using hexanes and ethyl acetate (40:1) as the eluent. Yellow viscous liquid; 0.1088g, 91%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 – 7.92 (m, 2H), 7.81 – 7.72 (m, 1H), 7.61 – 7.52 (m, 1H), 7.44 (t, J = 8.3 Hz, 1H), 7.41 – 7.32 (m, 2H), 7.00 (ddd, J = 8.3, 2.5, 1.1 Hz, 1H), 3.94 (s, 3H), 2.44 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.68, 155.03, 153.64, 131.53, 131.17, 129.60, 125.11, 123.19, 120.07, 119.78, 115.09, 112.38, 111.36, 109.50, 55.41, 18.41; FTIR (Salt Plate) cm^{-1} 3016, 2943, 2923, 2852, 1466, 1380, 1289, 1263, 1216, 1179, 1050, 975; HRMS (EI-ion trap) *m/z* $[M]^+$ calcd for $(C_{16}H_{14}O_2S)^+$ 270.0715, found 270.0718.

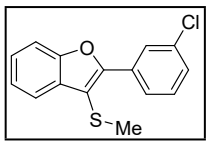


2-(4-methoxyphenyl)-3-(methylsulfanyl)-1-benzofuran (11): Column chromatography was performed using hexanes and ethyl acetate (40:1) as the eluent. White solid; 0.0944g, 89%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, J = 8.4 Hz, 2H), 7.61 – 7.55 (m, 1H), 7.41 – 7.34 (m, 1H), 7.18 (p, J = 5.5 Hz, 2H), 6.89 (d, J = 8.4 Hz, 2H), 3.73 (s, 3H), 2.25 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.24, 155.59, 153.55, 131.38, 128.85, 124.61, 123.12,

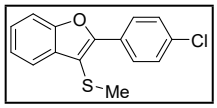
123.08, 119.76, 114.03, 111.19, 107.35, 55.37, 18.41; FTIR (ATR) cm^{-1} 3056, 2961, 2914, 2831, 1886, 1745, 1610, 1497, 1450, 1348, 1293, 1291, 1244, 1176, 1075, 1039, 981, 890, 829;



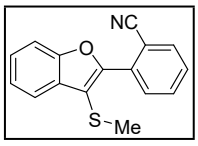
2-(2-chlorophenyl)-3-(methylsulfanyl)-1-benzofuran (12): Column chromatography was performed using hexanes and ethyl acetate (40:1) as the eluent. Light yellow viscous liquid; 0.0996g, 88%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 – 7.71 (m, 1H), 7.58 (dd, J = 7.0, 2.3 Hz, 1H), 7.53 (ddd, J = 6.9, 4.3, 1.5 Hz, 2H), 7.43 – 7.30 (m, 4H), 2.32 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.55, 154.43, 134.53, 132.68, 130.91, 130.15, 129.67, 129.36, 126.51, 125.22, 123.23, 120.21, 112.46, 111.76, 18.19; FTIR (Salt Plate) cm^{-1} 3066, 2980, 2843, 1583, 1572, 1431, 1309, 1261, 1213, 1207, 1105, 1013, 945, 912, 834, 812;



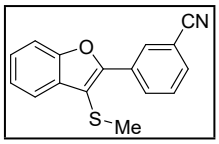
2-(3-chlorophenyl)-3-(methylsulfanyl)-1-benzofuran (13): Column chromatography was performed using hexanes and ethyl acetate (40:1) as the eluent. Light yellow solid; 0.1085g, 92%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (t, J = 1.9 Hz, 1H), 8.21 (dt, J = 7.6, 1.5 Hz, 1H), 7.74 – 7.69 (m, 1H), 7.53 – 7.47 (m, 1H), 7.40 (t, J = 7.8 Hz, 1H), 7.37 – 7.28 (m, 3H), 2.39 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.72, 153.52, 134.59, 132.01, 130.94, 129.81, 128.88, 127.04, 125.52, 125.24, 123.37, 120.24, 111.45, 110.54, 18.42; FTIR (ATR) cm^{-1} 3063, 2971, 2855, 1596, 1588, 1448, 1422, 1252, 1202, 1095, 1020, 972, 884, 839, 782, 741;



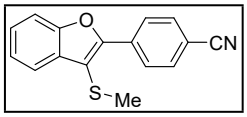
2-(4-chlorophenyl)-3-(methylsulfanyl)-1-benzofuran (14): Column chromatography was performed using hexanes and ethyl acetate (40:1) as the eluent. Light yellow solid; 0.1132g, 99%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 – 7.45 (m, 3H), 7.34 – 7.28 (m, 3H), 6.98 – 6.88 (m, 2H), 3.91 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.97, 134.07, 133.58, 132.88, 130.02, 128.60, 122.13, 120.54, 112.13, 110.73, 92.27, 86.74, 55.85; FTIR (ATR) cm^{-1} 3063, 2925, 2865, 1484, 1449, 1403, 1342, 1312, 1250, 1202, 1095, 1075, 1012, 968, 932, 830, 755, 743, 725.



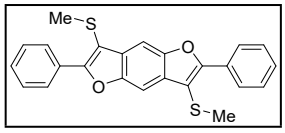
2-[3-(methylsulfanyl)-1-benzofuran-2-yl]benzonitrile (15): Column chromatography was performed using hexanes and ethyl acetate (40:1) as the eluent. Off-white solid; 0.0570g, 50%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (dd, J = 7.9, 1.2 Hz, 1H), 7.86 (dd, J = 7.9, 1.4 Hz, 1H), 7.83 – 7.77 (m, 1H), 7.74 (td, J = 7.8, 1.3 Hz, 1H), 7.65 – 7.60 (m, 1H), 7.56 (td, J = 7.7, 1.2 Hz, 1H), 7.41 (dtd, J = 20.1, 7.3, 1.3 Hz, 2H), 2.46 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.53, 152.31, 134.10, 132.95, 132.35, 130.84, 129.86, 129.29, 126.00, 123.56, 120.55, 118.10, 113.29, 112.12, 111.99, 18.09; FTIR (ATR) cm^{-1} 3070, 2926, 2855, 2225, 1728, 1598, 1448, 1343, 1266, 1246, 1202, 1082, 1037, 964, 892, 828; HRMS (EI-ion trap) *m/z* $[M]^+$ calcd for $(C_{16}H_{11}NOS)^+$ 265.0561, found 265.0559.



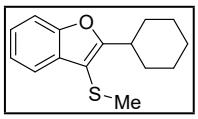
3-[3-(methylsulfanyl)-1-benzofuran-2-yl]benzonitrile (16): Column chromatography was performed using hexanes and ethyl acetate (40:1) as the eluent. White solid; 0.0924g, 80%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (td, J = 1.7, 0.6 Hz, 1H), 8.49 (dt, J = 8.0, 1.5 Hz, 1H), 7.70 – 7.64 (m, 1H), 7.59 (dt, J = 7.7, 1.4 Hz, 1H), 7.52 (td, J = 7.8, 0.6 Hz, 1H), 7.50 – 7.44 (m, 1H), 7.32 (td, J = 8.2, 7.7, 1.6 Hz, 1H), 7.27 (td, J = 7.4, 1.2 Hz, 1H), 2.35 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.82, 152.37, 131.88, 131.61, 130.97, 130.71, 130.50, 129.42, 125.96, 123.59, 120.41, 118.61, 112.96, 111.57, 18.44; FTIR (ATR) cm^{-1} 3064, 2974, 2942, 2874, 2229, 1753, 1600, 1583, 1494, 1311, 1293, 1243, 1124, 1086, 1053, 1023, 950, 880, 845; HRMS (EI-ion trap) *m/z* $[M]^+$ calcd for $(C_{16}H_{11}NOS)^+$ 265.0561, found 265.0548.



4-[3-(methylsulfanyl)-1-benzofuran-2-yl]benzonitrile (17): Column chromatography was performed using hexanes and ethyl acetate (40:1) as the eluent. White solid; 0.0548g, 49% ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42 (d, J = 8.5 Hz, 2H), 7.73 (ddd, J = 8.6, 4.2, 1.5 Hz, 3H), 7.55 – 7.49 (m, 1H), 7.36 (dtd, J = 21.5, 7.3, 1.2 Hz, 2H), 2.41 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.90, 152.50, 134.35, 132.24, 130.74, 127.22, 126.18, 123.60, 120.49, 118.72, 112.71, 111.81, 111.57, 18.41; FTIR (ATR) cm^{-1} 3033, 2949, 2928, 2856, 2226, 1741, 1608, 1538, 1490, 1451, 1410, 1342, 1253, 1202, 1074, 1013, 973, 888, 838, 833; HRMS (EI-ion trap) *m/z* $[M]^+$ calcd for $(C_{16}H_{11}NOS)^+$ 265.0561, found 265.0558.

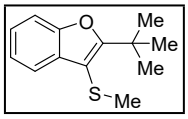


3,7-bis(methylsulfanyl)-2,6-diphenylbenzo[1,2-b:4,5-b']difuran (18): Column chromatography was performed using hexanes and ethyl acetate (40:1) as the eluent. Pale yellow solid; 0.0620g, 99%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (d, J = 7.2 Hz, 3H), 7.72 (s, 2H), 7.44 (t, J = 7.6 Hz, 4H), 7.35 (t, J = 7.4 Hz, 2H), 7.18 (s, 1H), 2.35 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.31, 150.98, 130.36, 130.18, 129.08, 128.58, 127.23, 109.32, 101.24, 18.38; FTIR (ATR) cm^{-1} 3022, 2909, 2868, 1711, 1642, 1565, 1518, 1459, 1417, 1380, 1216, 1109, 1033, 934, 856; HRMS (EI-ion trap) *m/z* $[M]^+$ calcd for $(C_{24}H_{18}O_2S_2)^+$ 402.0748, found 402.0744.

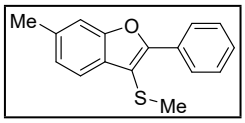


2-cyclohexyl-3-(methylsulfanyl)-1-benzofuran (22): Column chromatography was performed using hexanes and ethyl acetate (80:1) as the eluent. Colorless viscous liquid; 0.0500g, 41%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 – 7.61 (m, 1H), 7.51 – 7.42 (m, 1H), 7.33 – 7.27 (m, 3H), 3.25 (tt, J = 11.8, 3.6 Hz, 1H), 2.35 (s, 3H), 1.97 – 1.84 (m, 4H), 1.78 (qd, J = 12.3, 3.5 Hz, 3H), 1.54 – 1.33 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.61, 153.91, 130.01, 123.77, 122.78, 119.29, 111.15, 106.71, 36.32, 31.35, 26.28, 25.88, 19.24; FTIR (Salt Plate) cm^{-1} 3022, 2961, 2925, 2853,

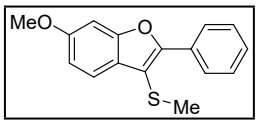
2405, 1581, 1539, 1480, 1430, 1216, 1105, 1000, 932, 801; HRMS (EI-ion trap) *m/z* $[M]^+$ calcd for $(C_{15}H_{18}OS)^+$ 246.1077, found 246.1078.



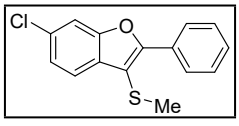
2-*tert*-butyl-3-(methylsulfanyl)-1-benzofuran (23): Column chromatography was performed using hexanes and ethyl acetate (80:1) as the eluent. Yellow viscous liquid. 0.0306g, 47%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 – 7.50 (m, 1H), 7.39 – 7.30 (m, 1H), 7.22 – 7.13 (m, 2H), 2.24 (s, 3H), 1.47 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.20, 152.97, 131.14, 123.85, 122.70, 119.18, 111.03, 106.49, 34.84, 29.50, 19.31. FTIR (Salt Plate) cm^{-1} 2959, 2923, 2852, 2362, 1734, 1501, 1465, 1375, 1221, 1087, 1037, 972, 827; HRMS (EI-ion trap) *m/z* $[M]^+$ calcd for $(C_{13}H_{16}OS)^+$ 220.0922, found 220.0923.



6-Methyl-3-(methylthio)-2-phenyl-1-benzofuran (25): Column chromatography was performed using hexanes and ethyl acetate (80:1) as the eluent. White solid. 0.097.9g, 87%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 – 8.34 (m, 2H), 7.68 (d, J = 7.9 Hz, 1H), 7.56 (t, J = 7.7 Hz, 2H), 7.51 – 7.42 (m, 1H), 7.40 (s, 1H), 7.21 (d, J = 7.9 Hz, 1H), 2.57 (s, 3H), 2.46 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.68, 154.16, 135.49, 130.58, 128.80, 128.74, 128.56, 127.18, 124.65, 119.58, 111.65, 109.19, 77.47, 77.36, 77.16, 76.84, 21.83, 18.47. FTIR (Salt Plate) cm^{-1} 3055, 2921, 2856, 1621, 1549, 1485, 1445, 1332, 1288, 1210, 1129, 1065, 1030, 967, 936, 851, 807; HRMS (EI-ion trap) *m/z* $[M]^+$ calcd for $(C_{16}H_{14}OS)^+$ 254.0765, found 254.0765.

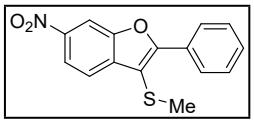


6-Methoxy-3-(methylthio)-2-phenyl-1-benzofuran (26): Column chromatography was performed using hexanes and ethyl acetate (40:1) as the eluent. Brown liquid. 0.1003g, 88%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 – 8.23 (m, 2H), 7.60 (dd, J = 8.5, 0.5 Hz, 1H), 7.56 – 7.46 (m, 2H), 7.43 – 7.37 (m, 1H), 7.09 (d, J = 2.1 Hz, 1H), 6.97 (dd, J = 8.6, 2.2 Hz, 1H), 3.91 (s, 3H), 2.41 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.68, 154.65, 130.53, 128.51, 126.81, 124.48, 120.20, 112.15, 95.98, 77.35, 77.03, 76.71, 29.72, 18.44. FTIR (Salt Plate) cm^{-1} 3746, 2921, 1621, 1488, 1343, 1276, 1199, 1150, 1112, 1062, 1029, 967, 821; HRMS (EI-ion trap) *m/z* $[M]^+$ calcd for $(C_{16}H_{14}O_2S)^+$ 270.0715, found 270.0715.

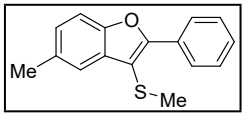


6-Chloro-3-(methylthio)-2-phenyl-1-benzofuran (27): Column chromatography was performed using hexanes and ethyl acetate (80:1) as the eluent. Off-white solid. 0.1096g, 97%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 – 8.27 (m, 2H), 7.65 (d, J = 8.4 Hz, 1H), 7.58 – 7.49 (m, 3H), 7.49 – 7.41 (m, 1H), 7.32 (dd, J = 8.3, 1.8 Hz, 1H), 2.40 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.38, 153.65, 131.23, 129.92, 129.26, 128.62, 127.21, 123.96, 120.58, 111.90,

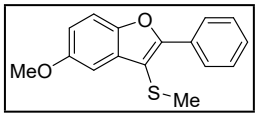
109.17, 77.41, 77.09, 76.78, 18.42. FTIR (Salt Plate) cm^{-1} 3063, 2921, 1606, 1465, 1417, 1327, 1285, 1200, 1122, 1060, 1030, 968, 913, 843, 810; HRMS (EI-ion trap) *m/z* $[M]^+$ calcd for $(C_{15}H_{11}ClOS)^+$ 274.0219, found 274.0219.



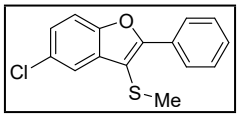
6-Nitro-3-(methylthio)-2-phenyl-1-benzofuran (28): Column chromatography was performed using hexanes and ethyl acetate (40:1) as the eluent. Yellow solid. 0.1095g, 96%. ^1H NMR (400 MHz, $CDCl_3$) δ 8.44 (d, J = 1.9 Hz, 1H), 8.40 – 8.32 (m, 2H), 8.27 (dd, J = 8.6, 2.0 Hz, 1H), 7.82 (d, J = 8.6 Hz, 1H), 7.60 – 7.51 (m, 3H), 2.42 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.43, 152.22, 145.42, 137.25, 130.33, 129.16, 128.82, 128.45, 127.63, 119.90, 119.09, 109.76, 107.81, 77.35, 77.24, 77.03, 76.72, 18.46. FTIR (Salt Plate) cm^{-1} 3094, 2958, 2917, 2846, 2342, 1605, 1513, 1481, 1424, 1338, 1198, 1121, 1061, 1029, 969, 938, 878, 819; HRMS (EI-ion trap) *m/z* $[M]^+$ calcd for $(C_{15}H_{11}NO_3S)^+$ 285.0460, found 285.0460.



5-Methyl-3-(methylthio)-2-phenyl-1-benzofuran (29): Column chromatography was performed using hexanes and ethyl acetate (80:1) as the eluent. White solid. 0.0980g, 86%. ^1H NMR (400 MHz, $CDCl_3$) δ 8.41 – 8.34 (m, 2H), 7.56 (t, J = 7.7 Hz, 2H), 7.46 (dd, J = 8.0, 6.6 Hz, 2H), 7.21 (dd, J = 8.4, 1.8 Hz, 1H), 2.57 (s, 3H), 2.46 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.44, 152.18, 132.79, 131.26, 130.53, 128.92, 128.56, 127.26, 126.36, 119.84, 110.93, 108.94, 77.46, 77.14, 76.82, 21.52, 18.50. FTIR (Salt Plate) cm^{-1} 2919, 2227, 2083, 1895, 1813, 1734, 1643, 1599, 1468, 1443, 1336, 1261, 1202, 1159, 1067, 1025, 966, 831; HRMS (EI-ion trap) *m/z* $[M]^+$ calcd for $(C_{16}H_{14}OS)^+$ 254.0765, found 254.0765.

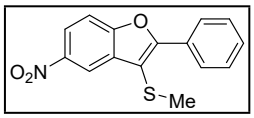


5-Methoxy-3-(methylthio)-2-phenyl-1-benzofuran (30): Column chromatography was performed using hexanes and ethyl acetate (40:1) as the eluent. Brown liquid. 0.1081g, 95%. ^1H NMR (400 MHz, $CDCl_3$) δ 8.35 – 8.30 (m, 2H), 7.57 – 7.48 (m, 2H), 7.48 – 7.38 (m, 2H), 7.20 (d, J = 2.6 Hz, 1H), 6.97 (dd, J = 8.9, 2.6 Hz, 1H), 3.94 (s, 3H), 2.41 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.55, 156.17, 148.86, 131.94, 130.43, 128.96, 128.54, 127.16, 113.95, 111.93, 109.20, 102.12, 77.39, 77.28, 76.76, 56.01, 18.42. FTIR (Salt Plate) cm^{-1} 3062, 2994, 2923, 2832, 1608, 1547, 1468, 1290, 1201, 1168, 1087, 1034, 968, 938, 836; HRMS (EI-ion trap) *m/z* $[M]^+$ calcd for $(C_{16}H_{14}O_2S)^+$ 270.0715, found 270.0715.

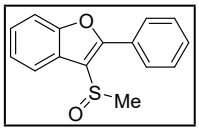


5-Chloro-3-(methylthio)-2-phenyl-1-benzofuran (31): Column chromatography was performed using hexanes and ethyl acetate (80:1) as the eluent. Off-white solid. 0.1261g, 95%. ^1H NMR (400 MHz, $CDCl_3$) δ 8.36 – 8.28 (m, 2H), 7.72 (d, J = 2.2

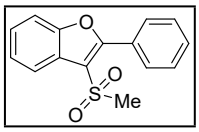
Hz, 1H), 7.58 – 7.49 (m, 2H), 7.50 – 7.42 (m, 2H), 7.31 (dd, J = 8.6, 2.2 Hz, 1H), 2.41 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.77, 152.02, 132.73, 129.88, 129.40, 129.02, 128.63, 127.32, 125.24, 119.68, 112.37, 108.87, 77.44, 77.13, 76.81, 18.45. FTIR (Salt Plate) cm^{-1} 3063, 2989, 2922, 1728, 1607, 1580, 1549, 1442, 1319, 1255, 1198, 1066, 1027, 968, 913, 866; HRMS (EI-ion trap) *m/z* $[M]^+$ calcd for $(C_{15}H_{11}ClOS)^+$ 274.0219, found 274.0219.



5-Nitro-3-(methylthio)-2-phenyl-1-benzofuran (32): Column chromatography was performed using hexanes and ethyl acetate (40:1) as the eluent. Yellow solid. 0.1049g, 93%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.61 (d, J = 2.4 Hz, 1H), 8.34 – 8.28 (m, 2H), 8.25 (dd, J = 9.0, 2.4 Hz, 1H), 7.61 – 7.43 (m, 4H), 2.42 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.43, 156.37, 144.55, 131.95, 130.01, 129.12, 128.76, 127.37, 120.86, 116.51, 111.71, 110.08, 77.43, 77.11, 76.79, 18.49. FTIR (Salt Plate) cm^{-1} 3148, 3096, 2916, 2843, 1765, 1643, 1578, 1522, 1482, 1441, 1344, 1263, 1200, 1117, 1060, 1027, 968, 934, 891, 825; HRMS (EI-ion trap) *m/z* $[M]^+$ calcd for $(C_{15}H_{11}NO_3S)^+$ 285.0460, found 285.0460.

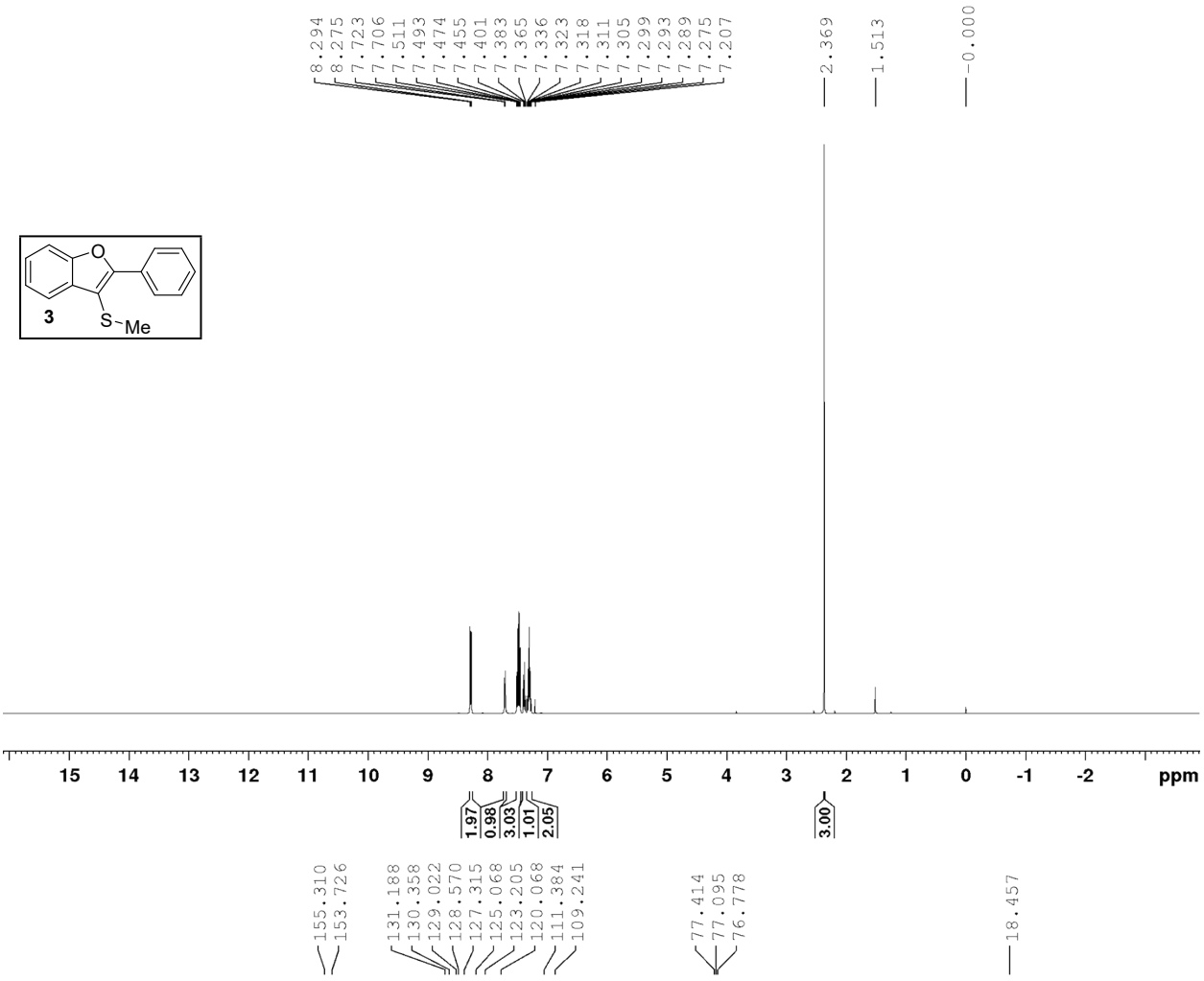


Synthesis of 3-(methanesulfinyl)-2-phenyl-1-benzofuran (48): To a 6 dram vial, 3-(methylsulfanyl)-2-phenyl-1-benzofuran (100mg, 0.42mol) and *m*-chloroperbenzoic acid (70mg, 0.41mol) was added. 4mL of dichloromethane was added. The reaction was stirred at room temperature for 24 hours. The reaction mixture was filtered and absorbed in silica gel before purification via column chromatography using hexanes and ethyl acetate (40:1) as the eluent. White solid; 0.0915g, 83%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 – 8.20 (m, 1H), 7.86 – 7.80 (m, 2H), 7.57 (d, J = 8.0 Hz, 1H), 7.53 – 7.43 (m, 3H), 7.42 – 7.32 (m, 2H), 3.10 (s, J = 1.1 Hz, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.72, 154.16, 130.34, 128.95, 128.54, 128.19, 125.85, 125.17, 124.02, 121.37, 118.51, 111.87, 40.25; FTIR (ATR) cm^{-1} 3088, 3086, 3084, 1605, 1460, 1433, 1429, 1411, 1358, 1270, 1255, 1196, 1131, 1016, 970, 873, 864, 855, 849; HRMS (EI-ion trap) *m/z* $[M]^+$ calcd for $(C_{15}H_{12}O_2S)^+$ 256.0558, found 256.0551.



Synthesis of 3-(methanesulfonyl)-2-phenyl-1-benzofuran (49): To a 6 dram vial, 3-(methylsulfanyl)-2-phenyl-1-benzofuran (100mg, 0.42mol) and *m*-chloroperbenzoic acid (180mg, 1.0mol) was added. 4mL of dichloromethane was added. The reaction was stirred at room temperature for 24 hours. The reaction mixture was filtered and absorbed in silica gel before purification via column chromatography using hexanes and ethyl acetate (40:1) as the eluent. White solid; 0.0710g, 86%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (t, J = 1.9 Hz, 1H), 8.00 – 7.96 (m, 1H), 7.93 (dt, J = 7.8, 1.3 Hz, 1H), 7.51 (dd, J = 2.2, 1.1 Hz, 2H), 7.47 (dd, J = 5.1, 1.9 Hz, 2H), 7.40 – 7.31 (m, 2H), 3.02 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 134.74, 133.90, 131.15, 130.96, 130.28, 129.86, 128.59, 128.33,

126.19, 124.76, 121.59, 111.52, 44.61; FTIR (ATR) cm^{-1} 3099, 3098, 3097, 3088, 2134, 1551, 1459, 1410, 1307, 1281, 1269, 1269, 1256, 1133, 1118, 1104, 1014, 971, 898, 874, 863, 854, 848, 841; HRMS (EI-ion trap) *m/z* $[M]^+$ calcd for $(C_{15}H_{12}O_3S)^+$ 272.0507, found 272.0500.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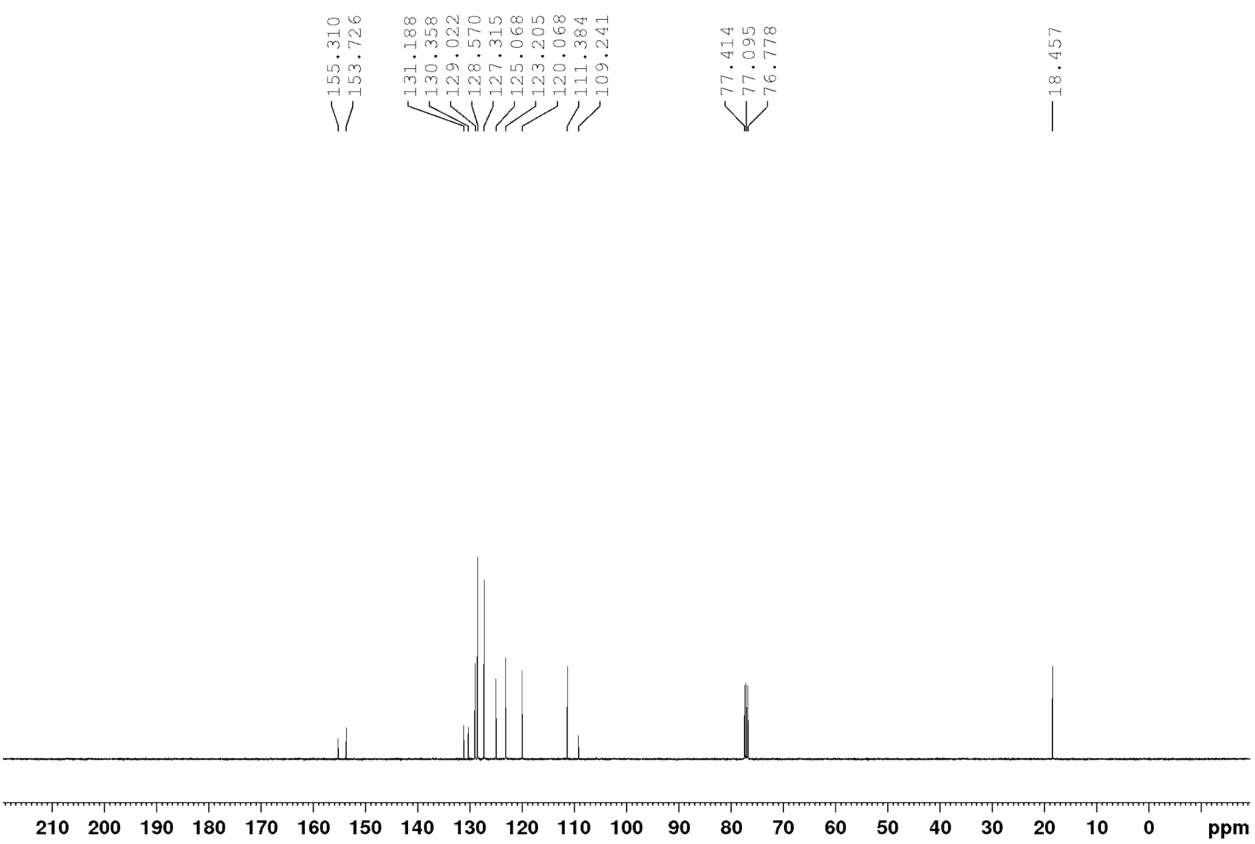
8.275
7.723
7.706
7.511
7.493
7.474
7.455
7.401
7.383
7.365
7.336
7.323
7.318
7.311
7.305
7.299
7.293
7.289
7.275
7.207
2.369
1.513
0.000
3
S
Me
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
1.97
0.98
3.03
1.01
2.05
3.00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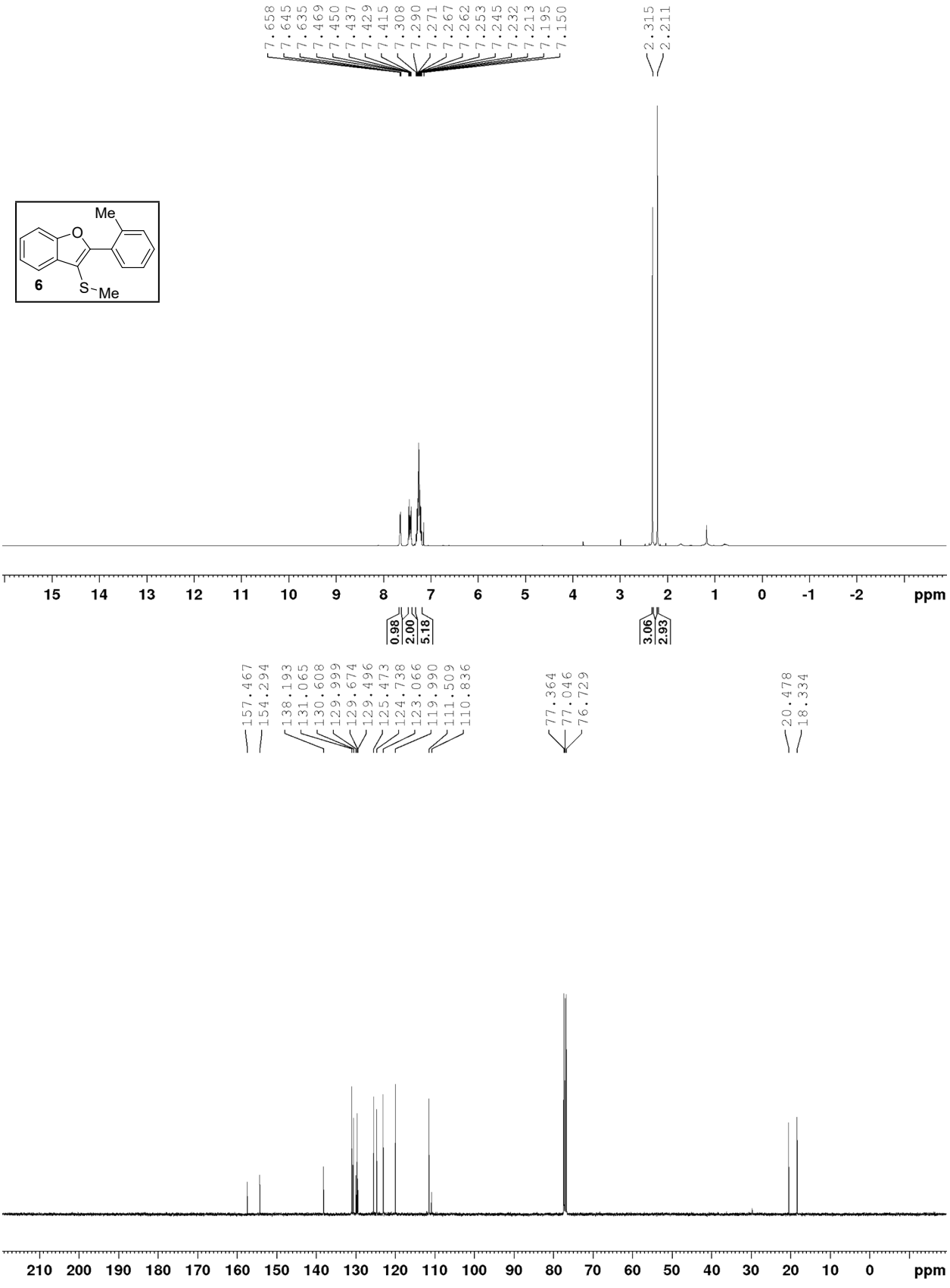
130.358
129.022
128.570
127.315
125.068
123.205
120.068
111.384
109.241
77.414
77.095
76.778
18.457
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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7.635
7.469
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7.437
7.429
7.415
7.308
7.290
7.271
7.267
7.262
7.253
7.245
7.232
7.213
7.195
7.150
2.315
2.211
Me
O
6
S
Me
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
0.98
2.00
5.18
3.06
2.93
157.467
154.294
138.193
131.065
130.608
129.999
129.674
129.496
125.473
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123.066
119.990
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77.046
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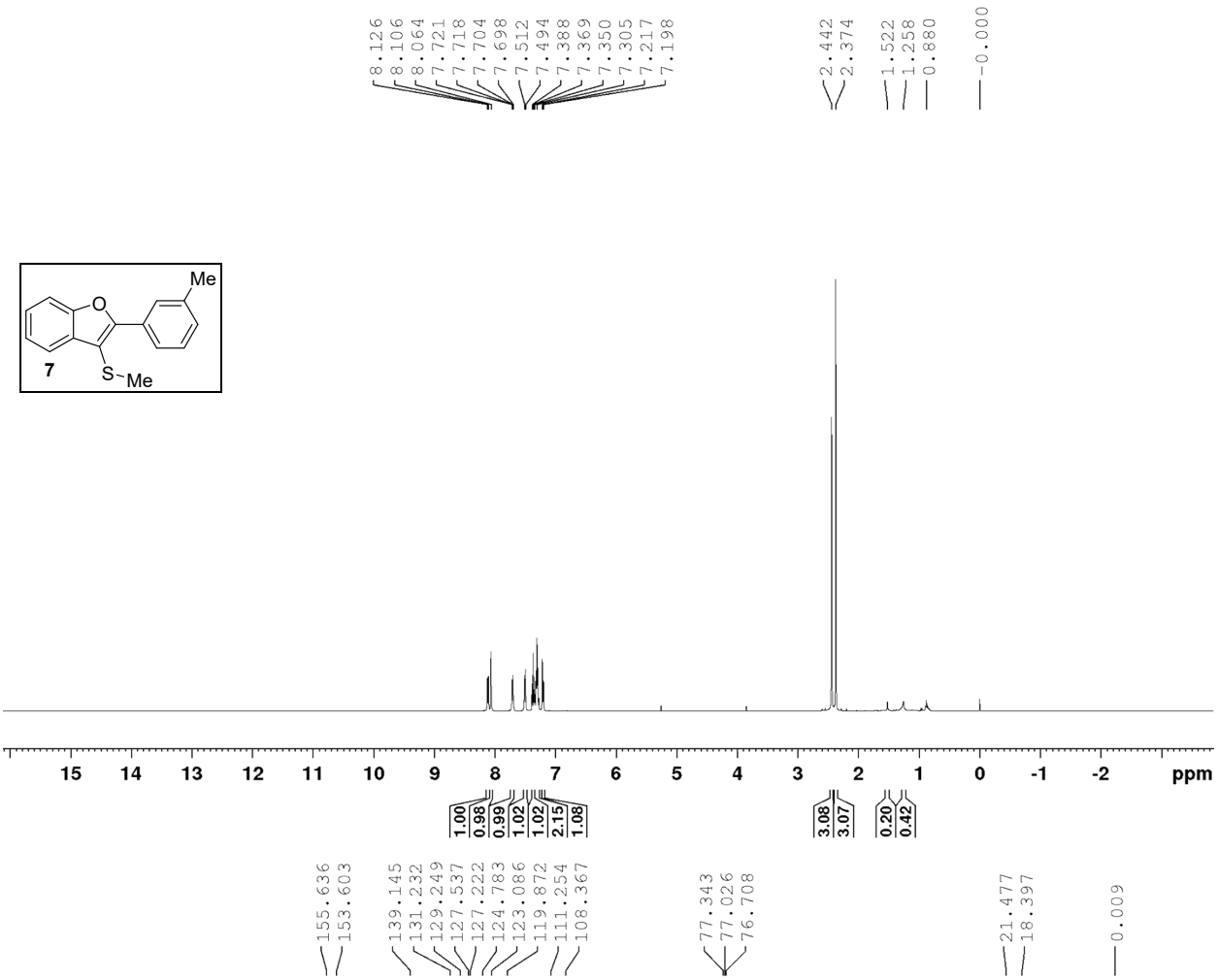
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8.106
8.064
7.721
7.718
7.704
7.698
7.512
7.494
7.388
7.369
7.350
7.305
7.217
7.198
2.442
2.374
1.522
1.258
0.880
-0.000
Me
O
7
S
Me
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
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0.98
0.99
1.02
1.02
2.15
1.08
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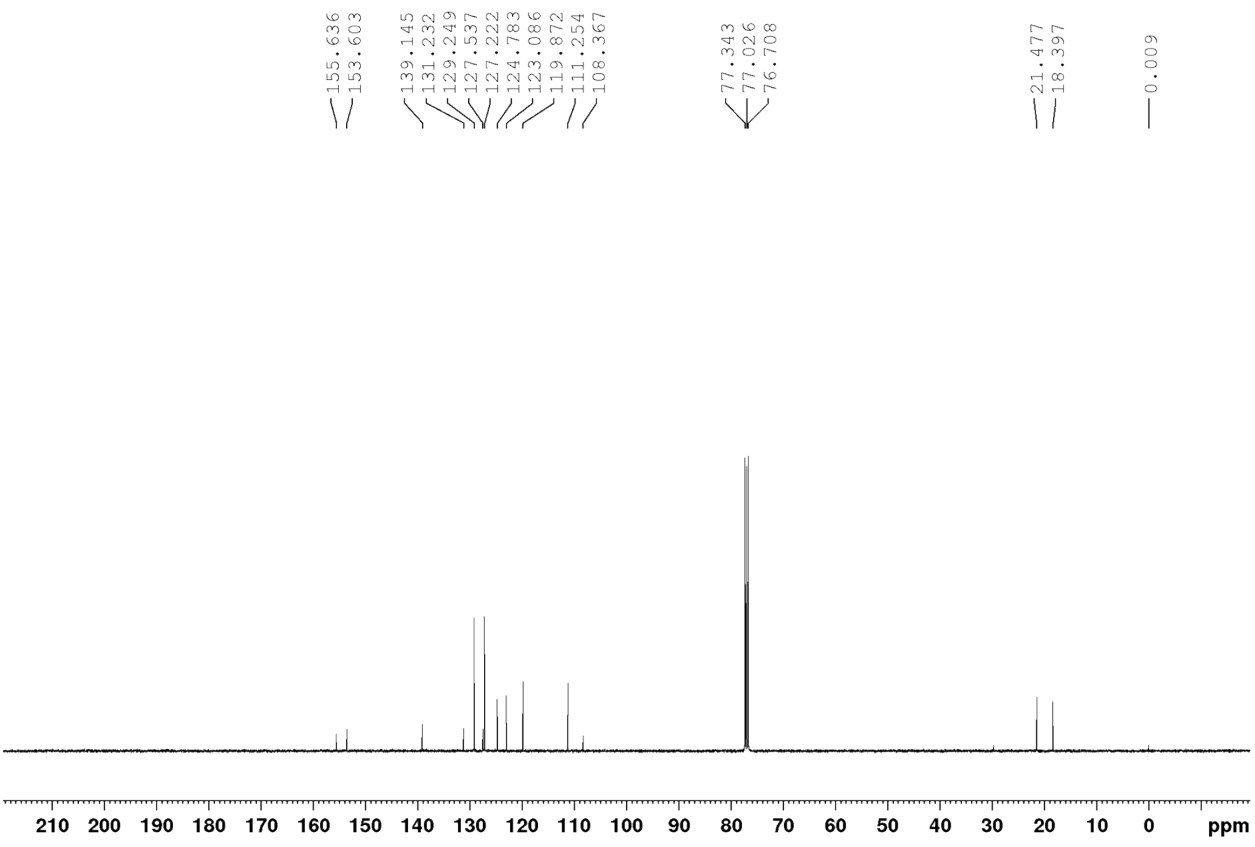
0.42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153.603
139.145
131.232
129.249
127.537
127.222
124.783
123.086
119.872
111.254
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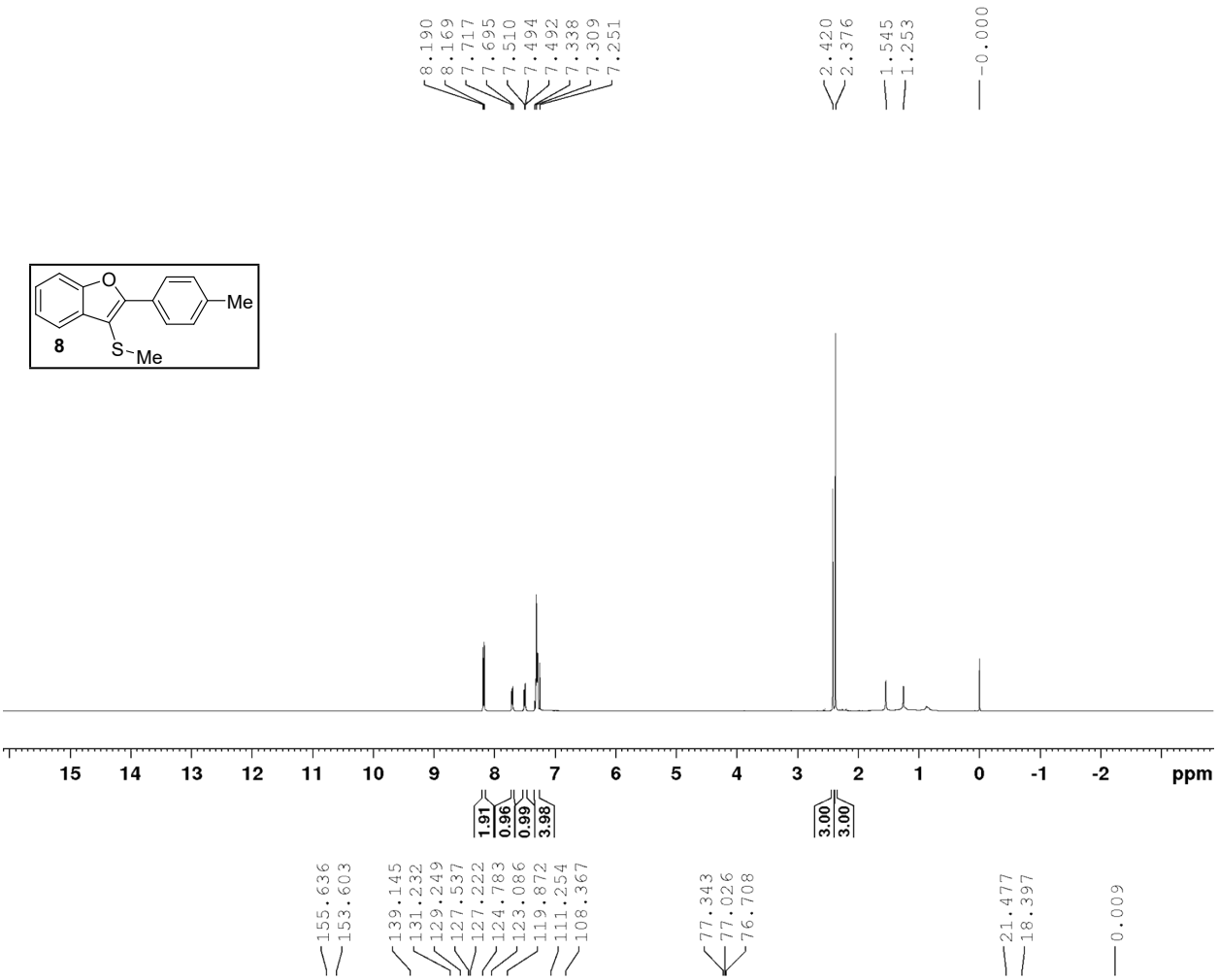
77.026
76.708
21.477
18.397
0.009
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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8.169
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7.695
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7.494
7.492
7.338
7.309
7.251
2.420
2.376
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1.253
-0.000
O
Me
8
S
Me
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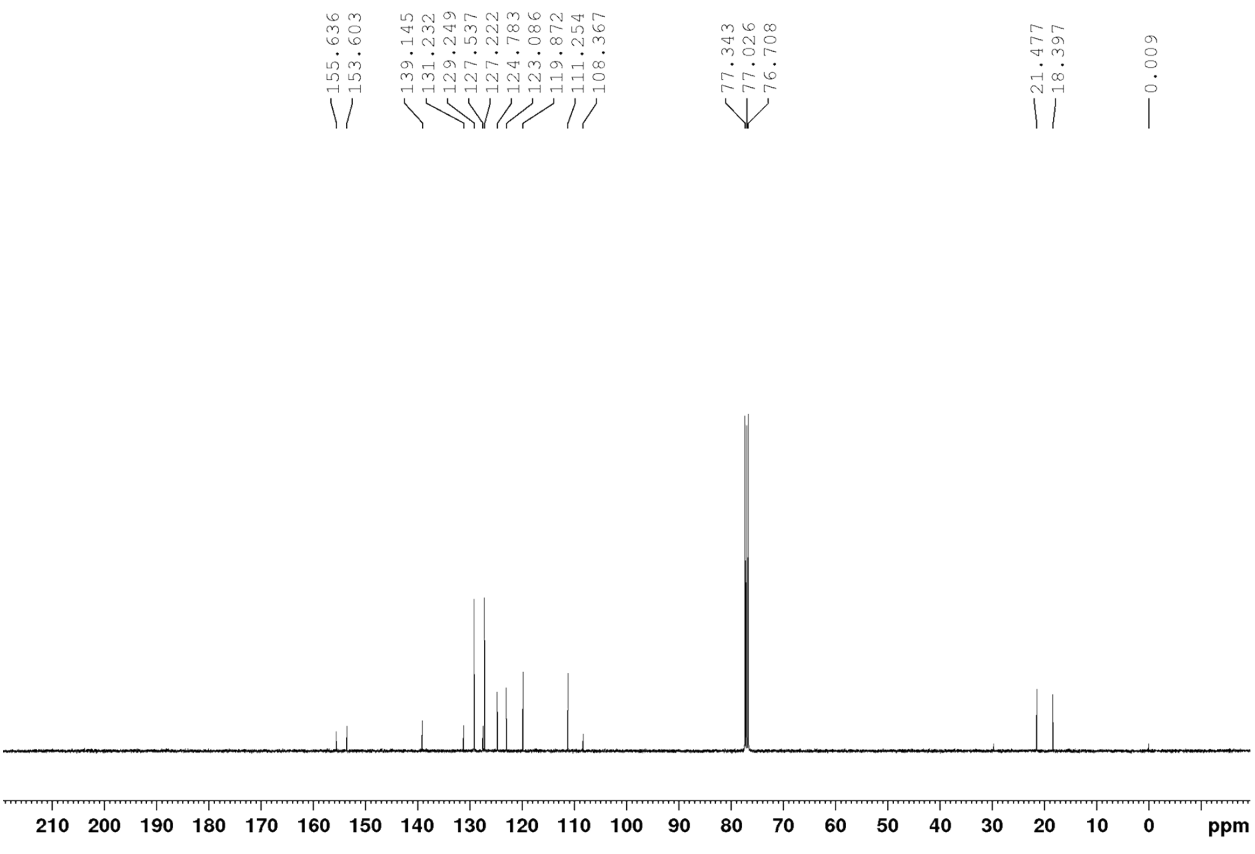
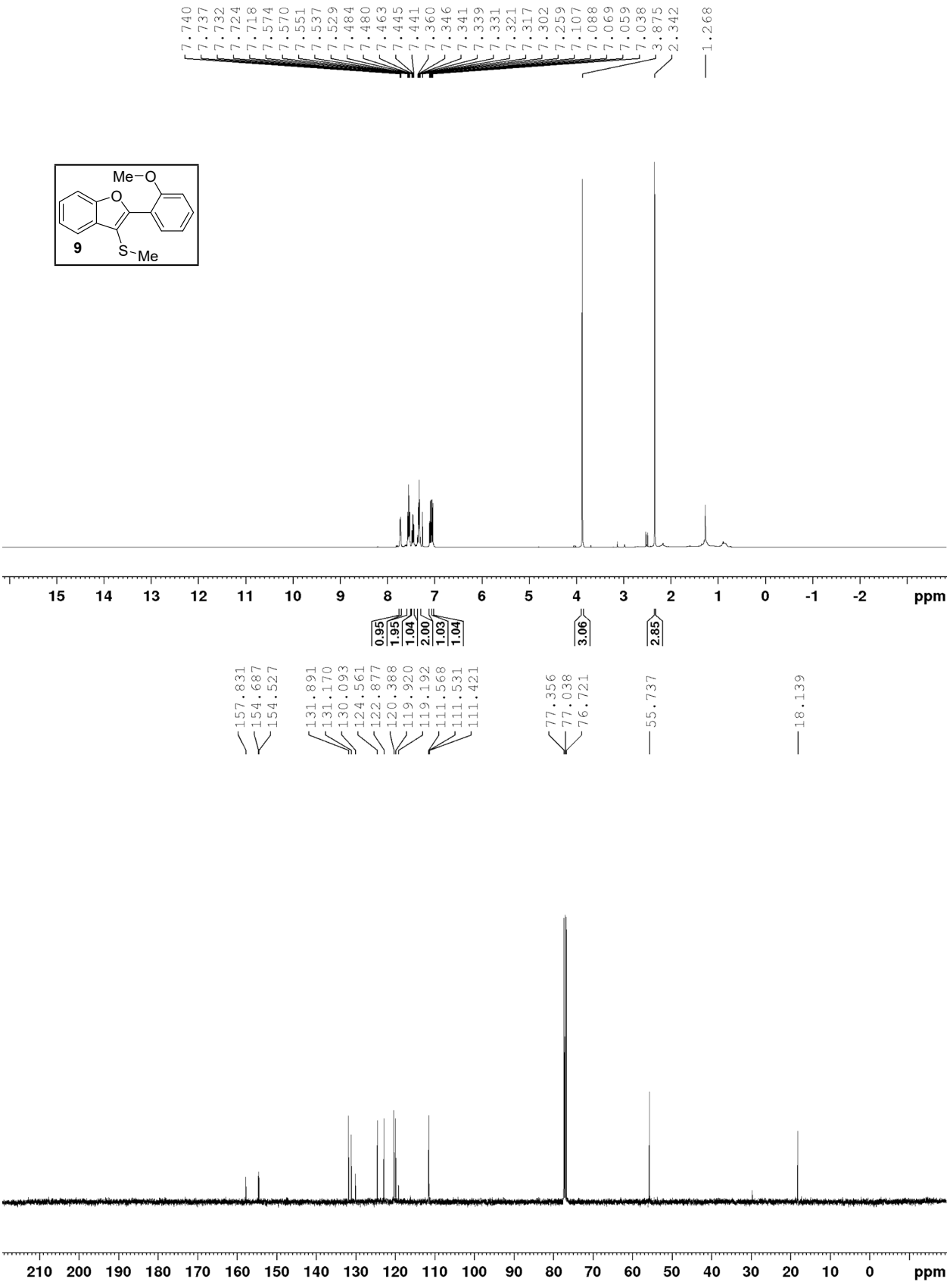
1.91
0.96
0.99
3.98
3.00
3.00


155.636
153.603
139.145
131.232
129.249
127.537
127.222
124.783
123.086
119.872
111.254
108.367
77.343
77.026
76.708
21.477
18.397
0.009
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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7.737
7.732
7.724
7.718
7.574
7.570
7.551
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7.529
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7.480
7.463
7.445
7.441
7.360
7.346
7.341
7.339
7.331
7.321
7.317
7.302
7.259
7.107
7.088
7.069
7.059
7.038
3.875
2.342
1.268
Me–O
O
9
S
Me
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
0.95
1.95
1.04
2.00
1.03
1.04
3.06
2.85
157.831
154.687
154.527
131.891
131.170
130.093
124.561
122.877
120.388
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119.192
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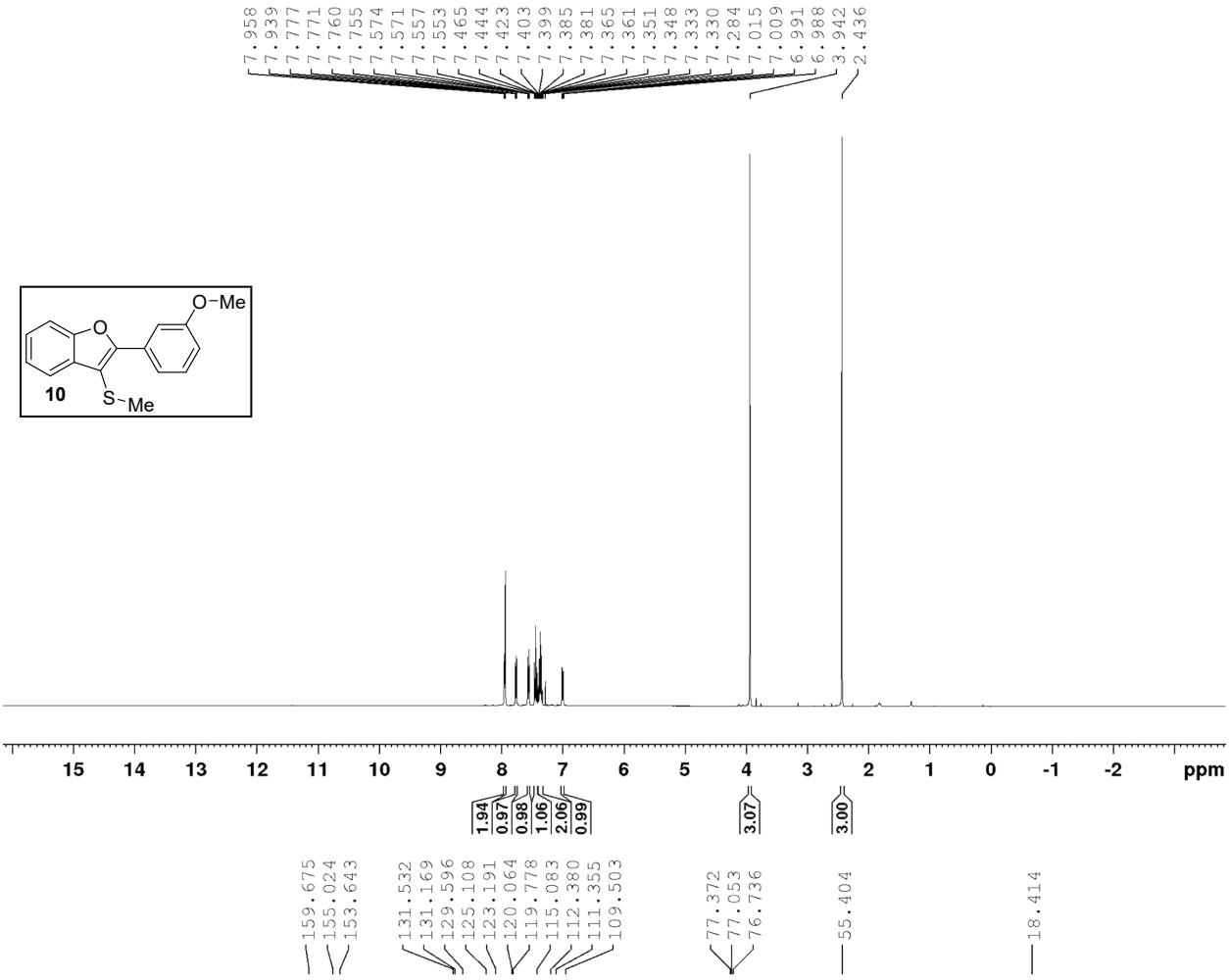
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7.361
7.351
7.348
7.333
7.330
7.284
7.015
7.009
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6.988
3.942
2.436
O–Me
O
10
S–Me
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
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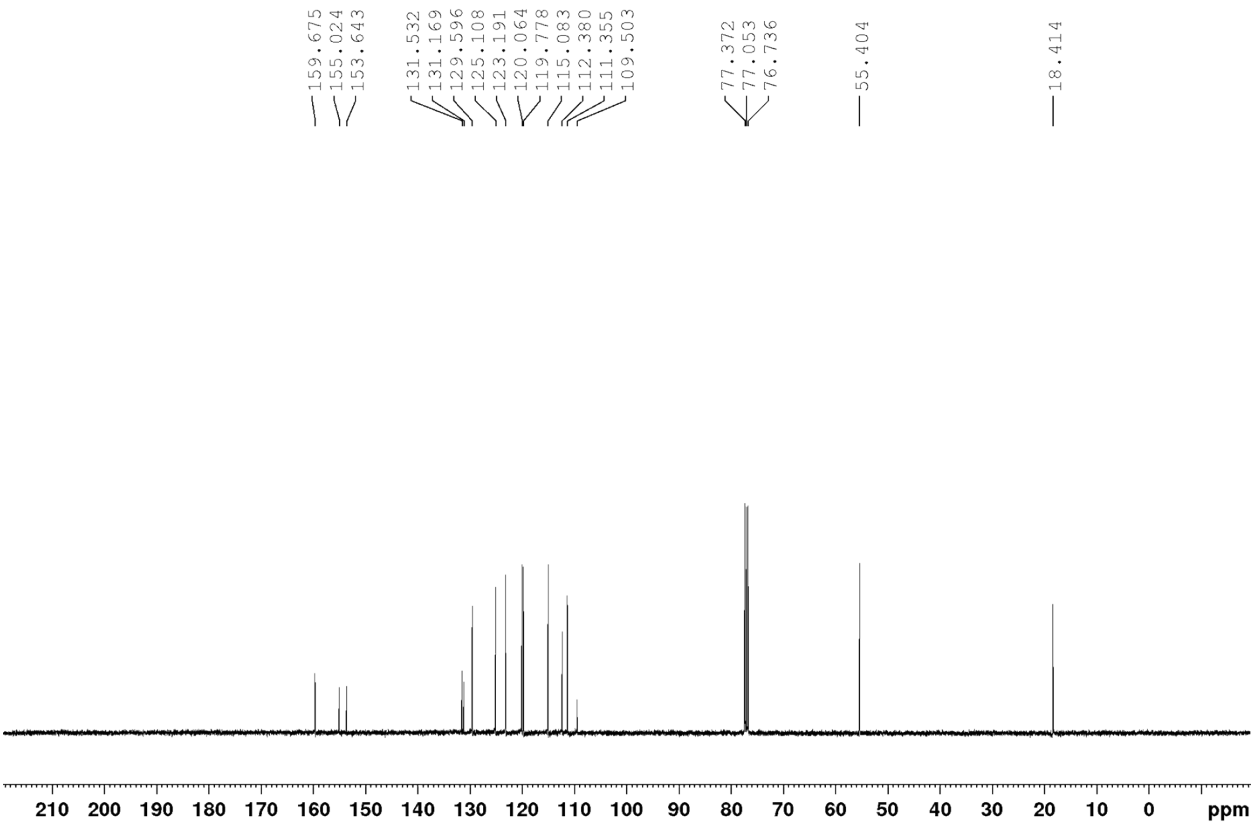
0.97
0.98
1.06
2.06
0.99
3.07
3.00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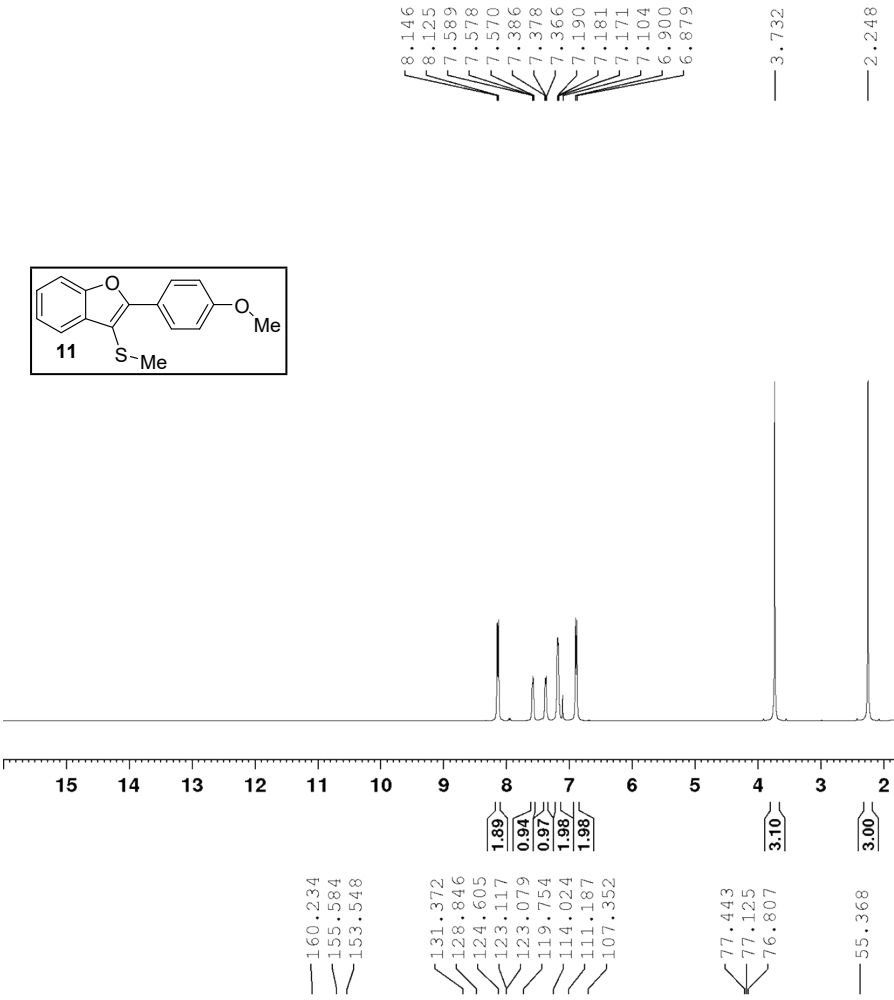
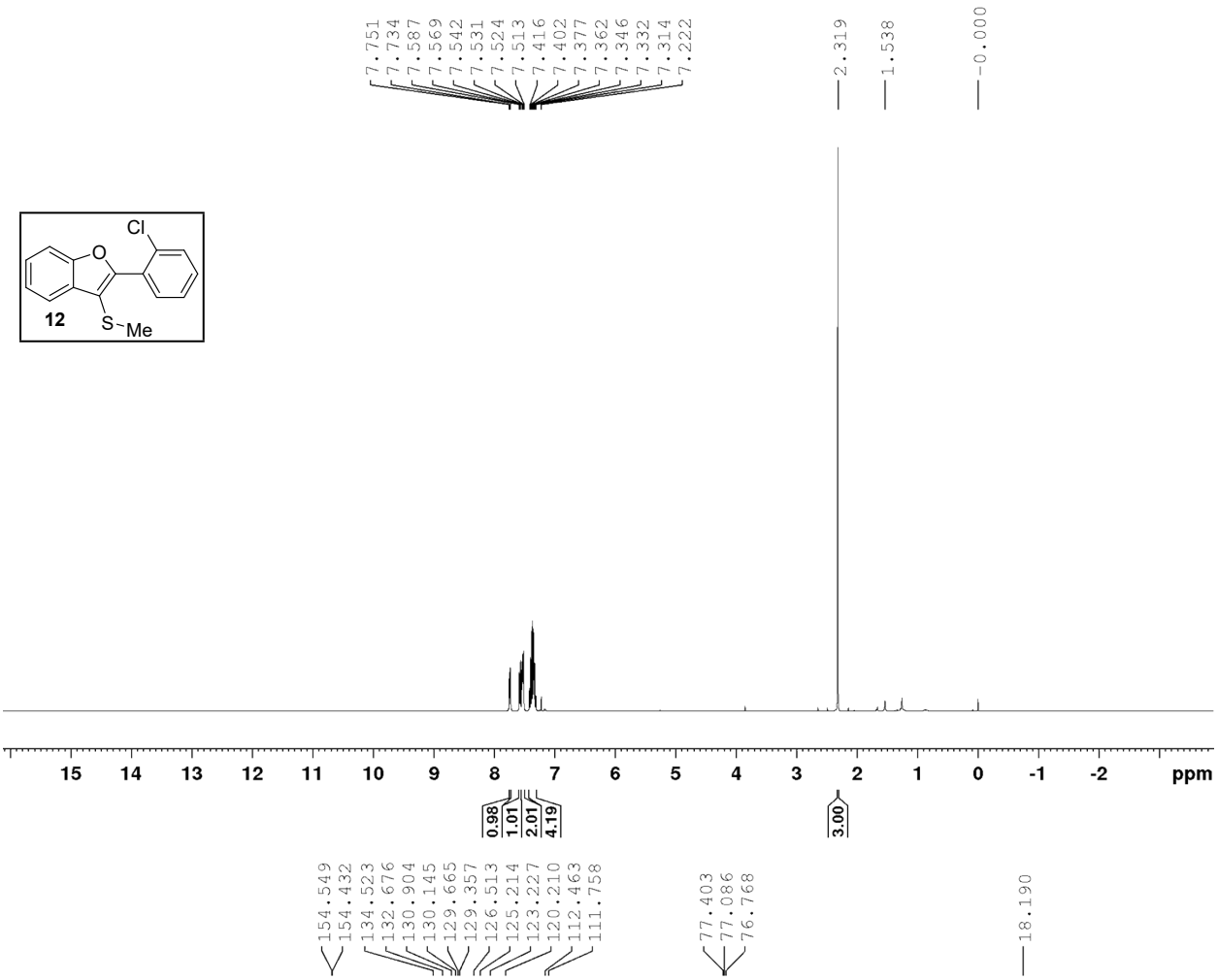
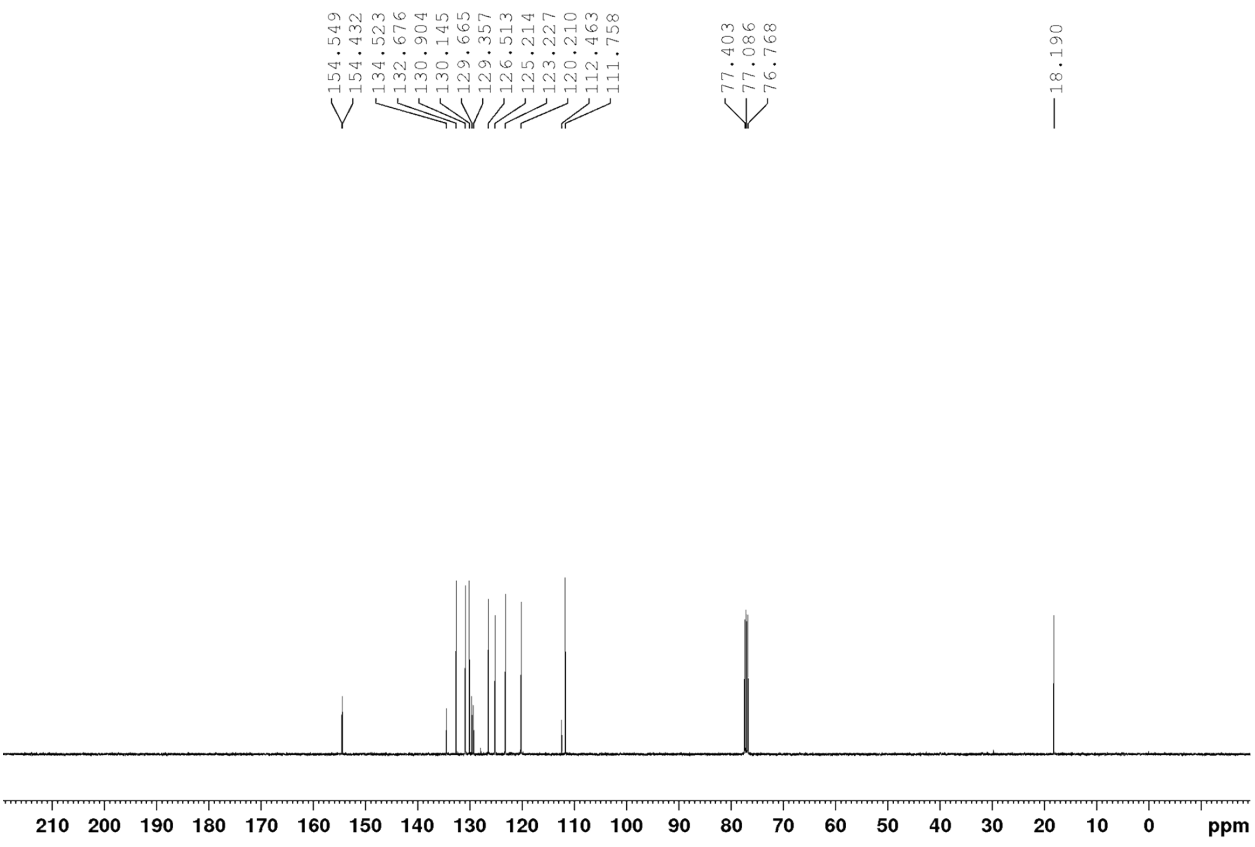
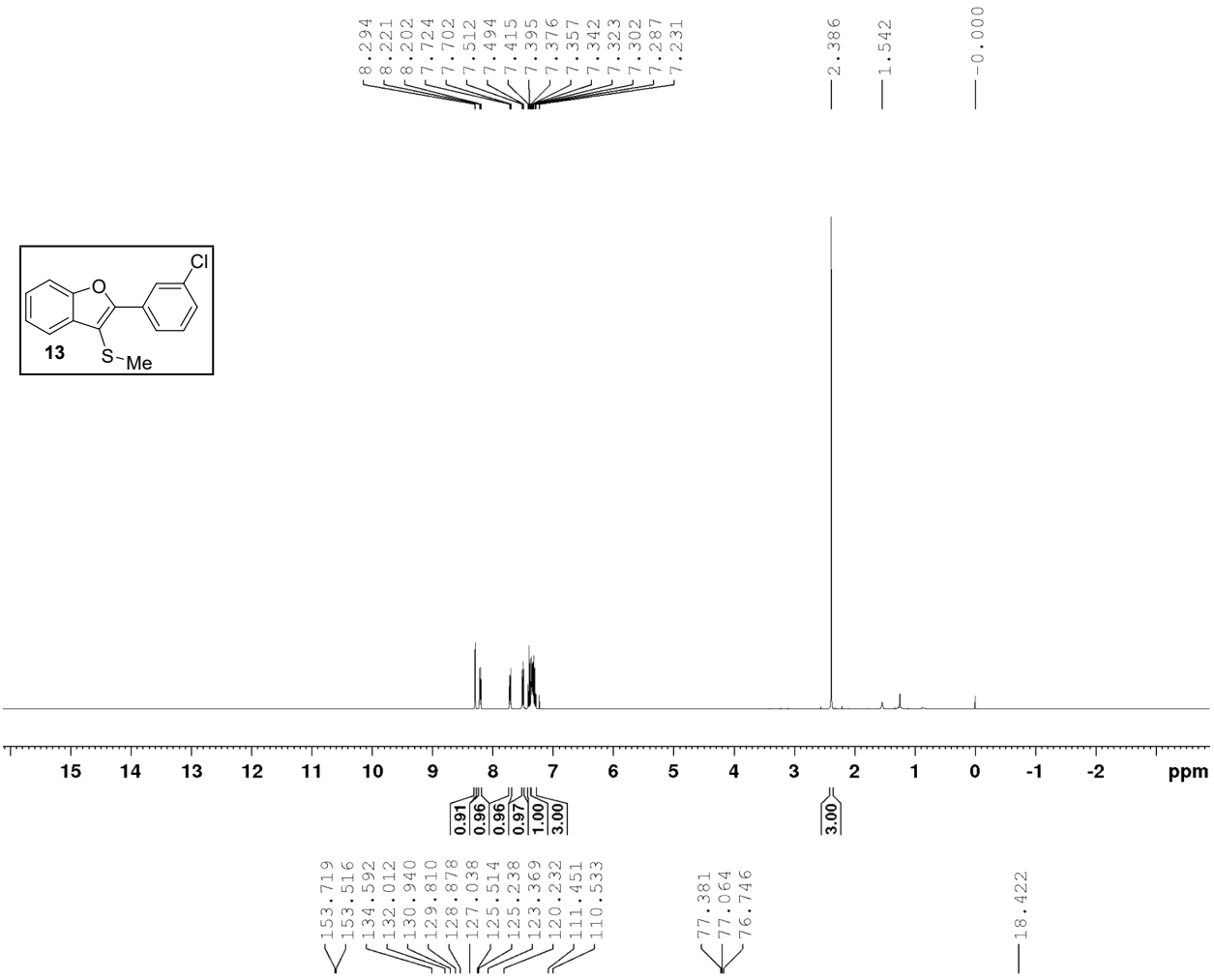
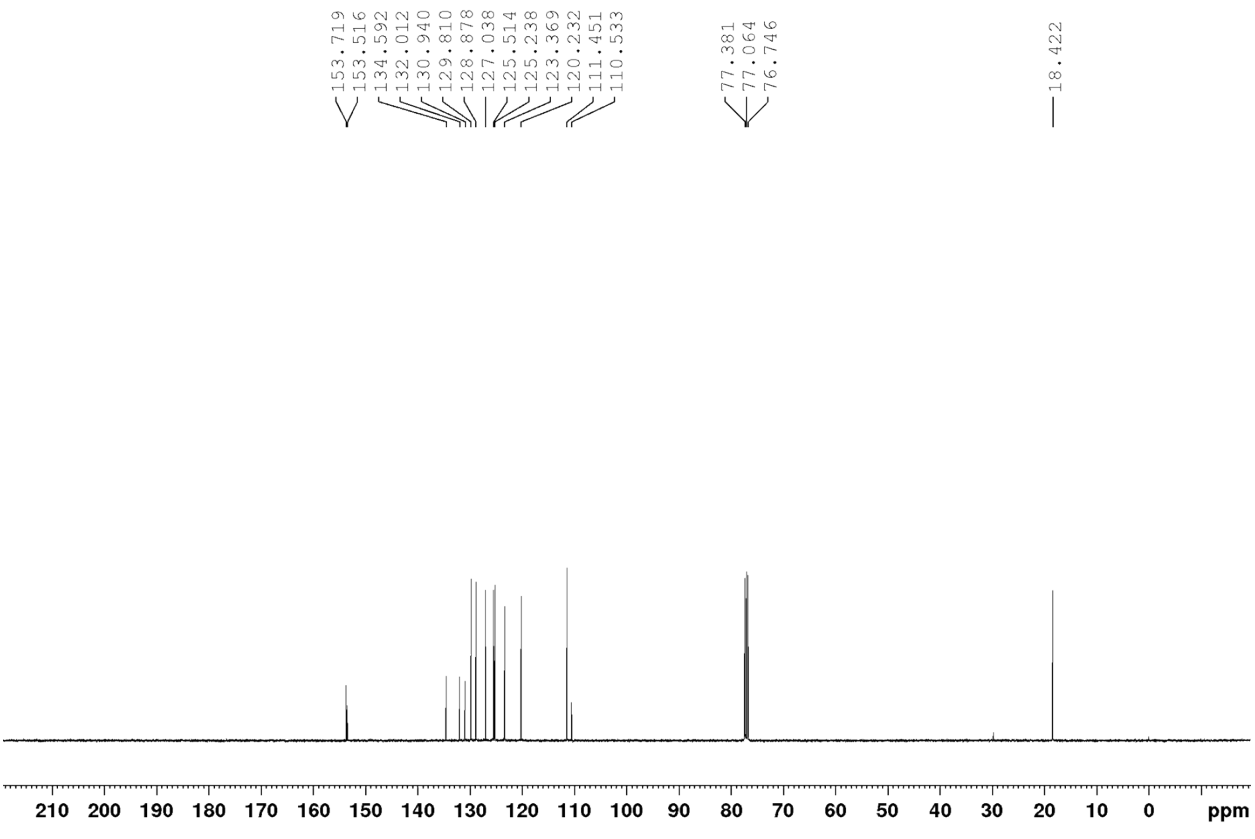
109.503
77.372
77.053
76.736
55.404
18.414
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

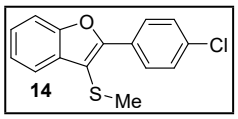

8.146
8.125
7.589
7.578
7.570
7.386
7.378
7.366
7.190
7.181
7.171
7.104
6.900
6.879
3.732
2.248
O
O
Me
11
S
Me
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
1.89
0.94
0.97
1.98
1.98
3.10
3.00
160.234
155.584
153.548
131.372
128.846
124.605
123.117
123.079
119.754
114.024
111.187
107.352
77.443
77.125
76.807
55.368
18.413
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


7.751
7.734
7.587
7.569
7.542
7.531
7.524
7.513
7.416
7.402
7.377
7.362
7.346
7.332
7.314
7.222
2.319
1.538
0.000
Cl
O
12
S
Me
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
0.98
1.01
2.01
4.19
3.00

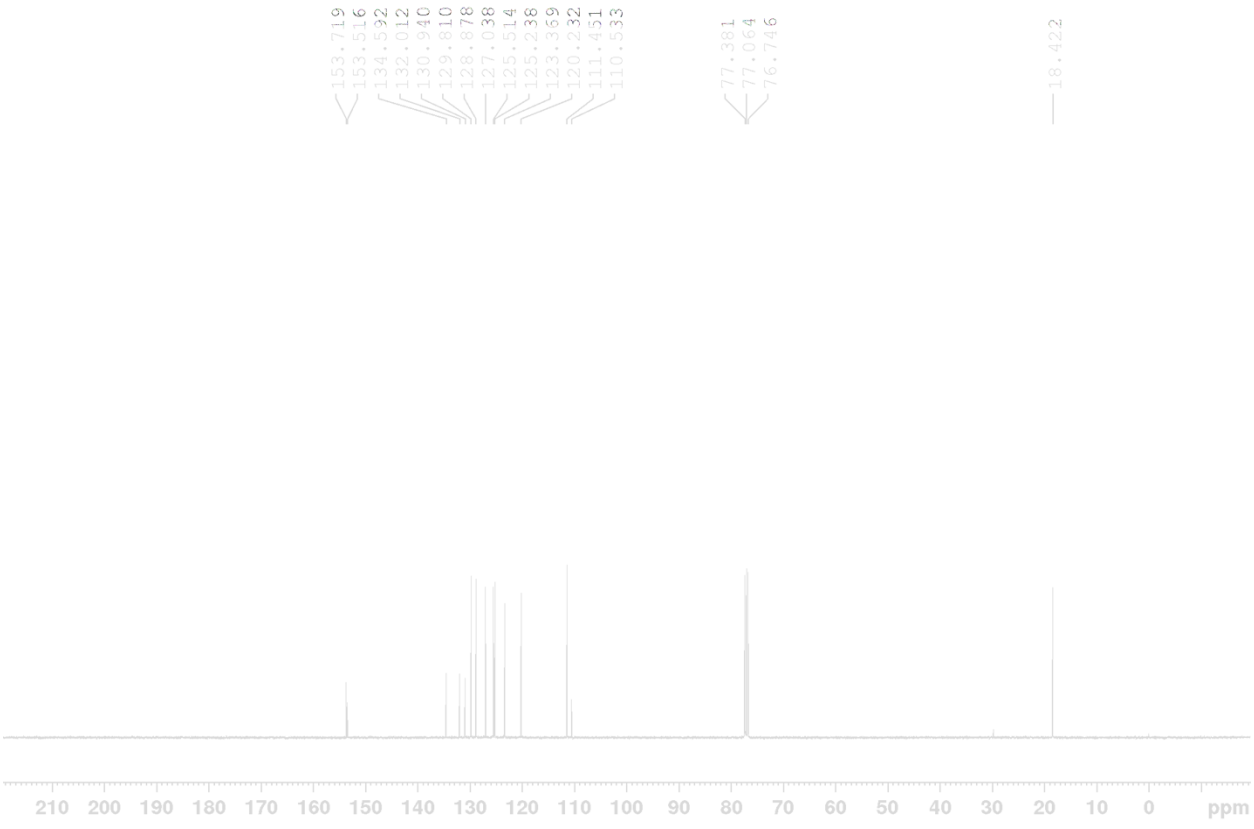

154.549
154.432
134.523
132.676
130.904
130.145
129.665
129.357
126.513
125.214
123.227
120.210
112.463
111.758
77.403
77.086
76.768
18.190
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

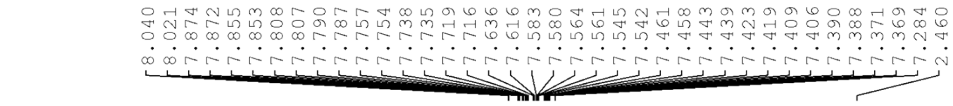

8.294
8.221
8.202
7.724
7.702
7.512
7.494
7.415
7.395
7.376
7.357
7.342
7.323
7.302
7.287
7.231
2.386
1.542
0.000
Cl
O
S
Me
13
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
0.91
0.96
0.96
0.97
1.00
3.00
3.00


153.719
153.516
134.592
132.012
130.940
129.810
128.878
127.038
125.514
125.238
123.369
120.232
111.451
110.533
77.381
77.064
76.746
18.422
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

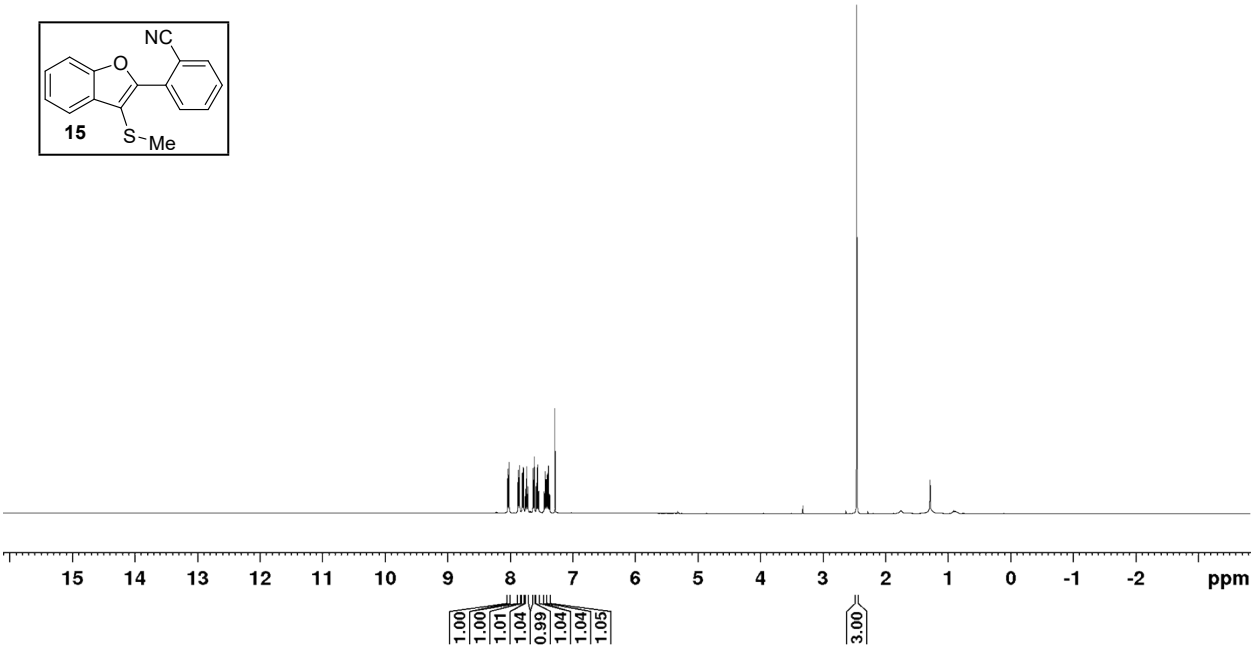

O
Cl
14
S
Me

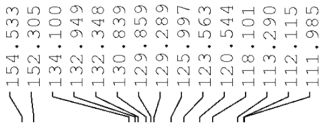
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

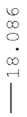

8.040
8.021
7.874
7.872
7.855
7.853
7.808
7.807
7.790
7.787
7.757
7.754
7.738
7.735
7.719
7.716
7.636
7.616
7.583
7.580
7.564
7.561
7.545
7.542
7.461
7.458
7.443
7.439
7.423
7.419
7.409
7.406
7.390
7.388
7.371
7.369
7.284
2.460

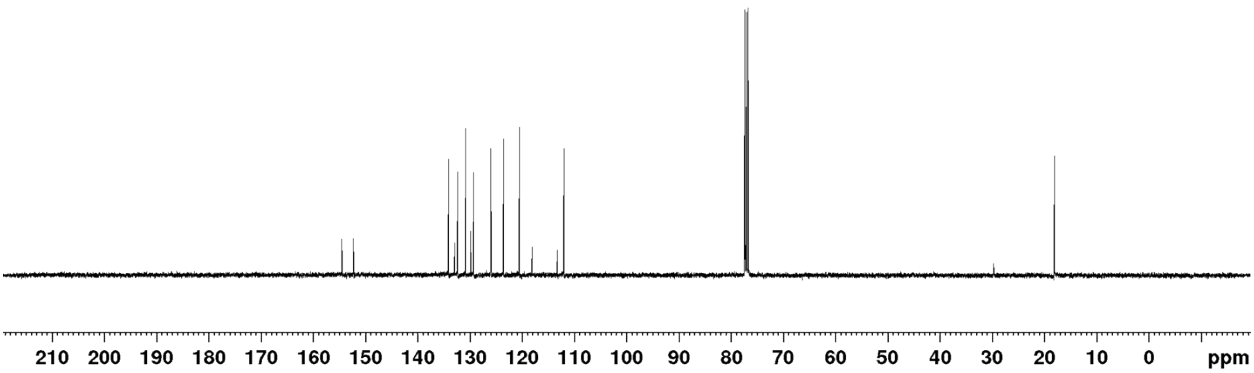
NC
O
15
S
Me

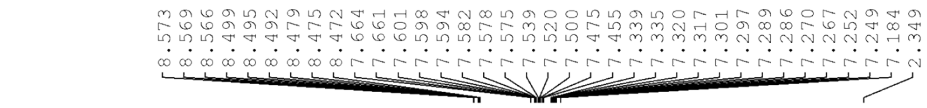

15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
1.00
1.00
1.01
1.04
0.99
1.04
1.04
1.05
3.00

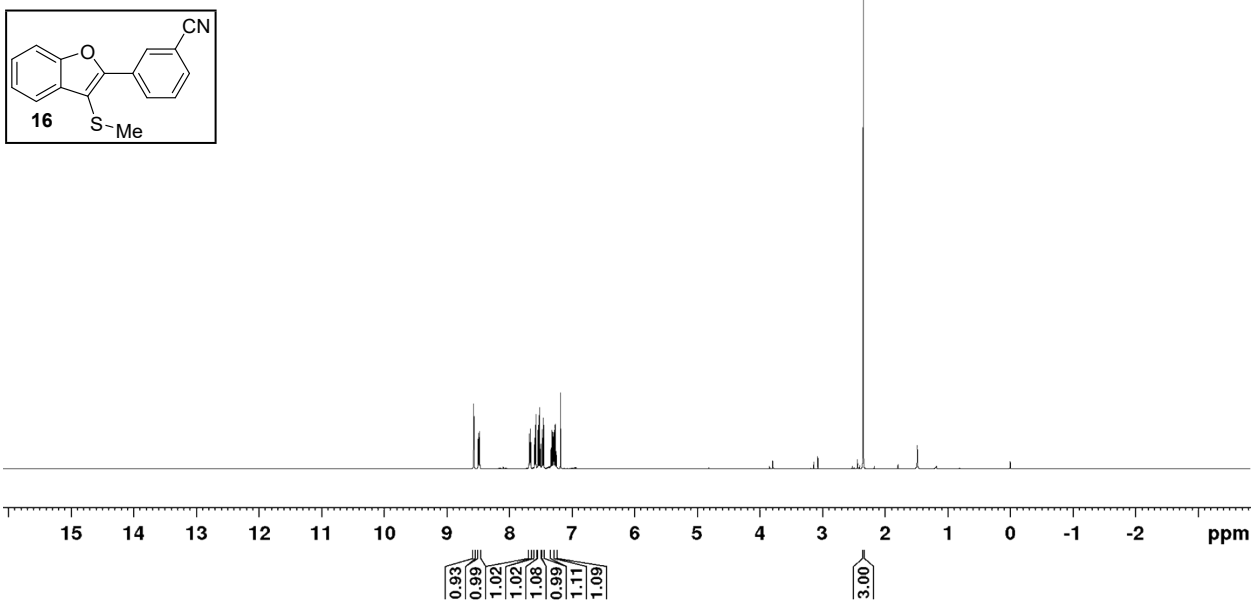

154.533
152.305
134.100
132.949
132.348
130.839
129.859
129.289
125.997
123.563
120.544
118.101
113.290
112.115
111.985

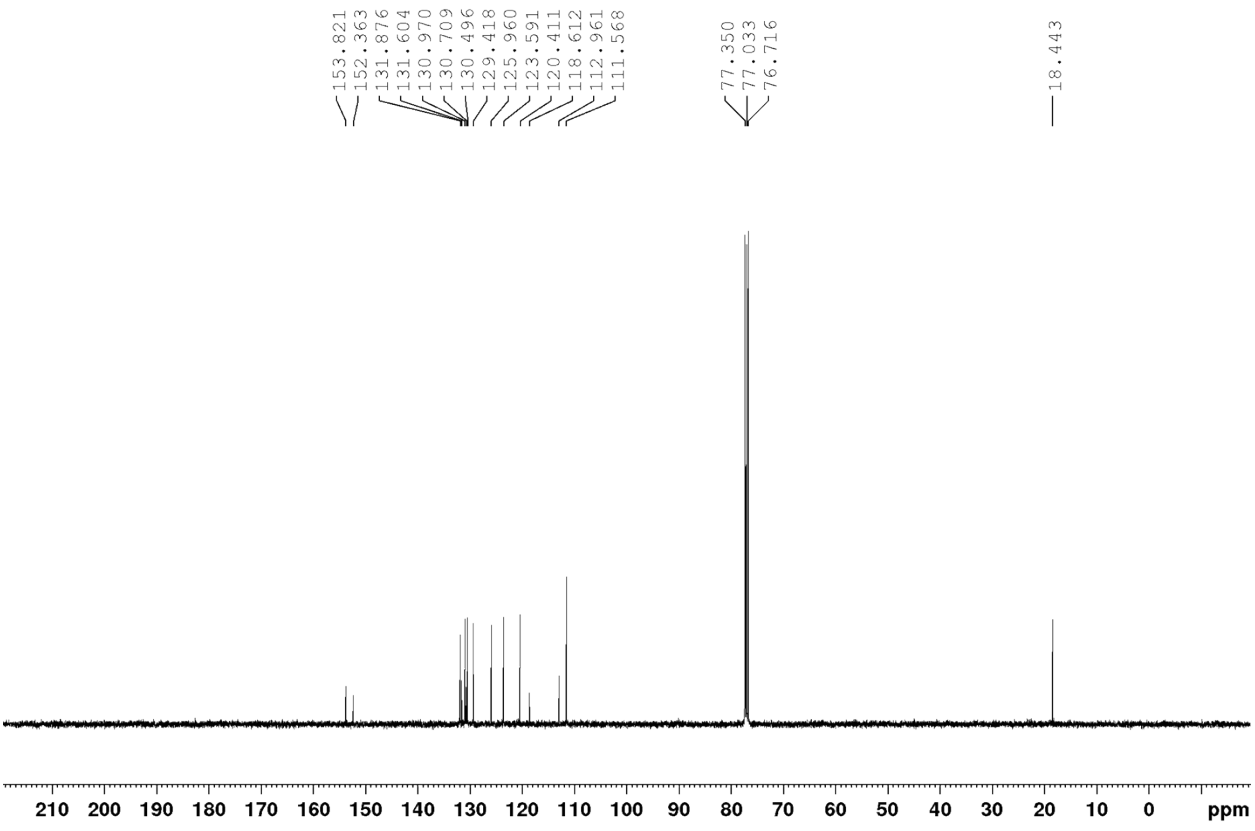

77.366
77.048
76.730

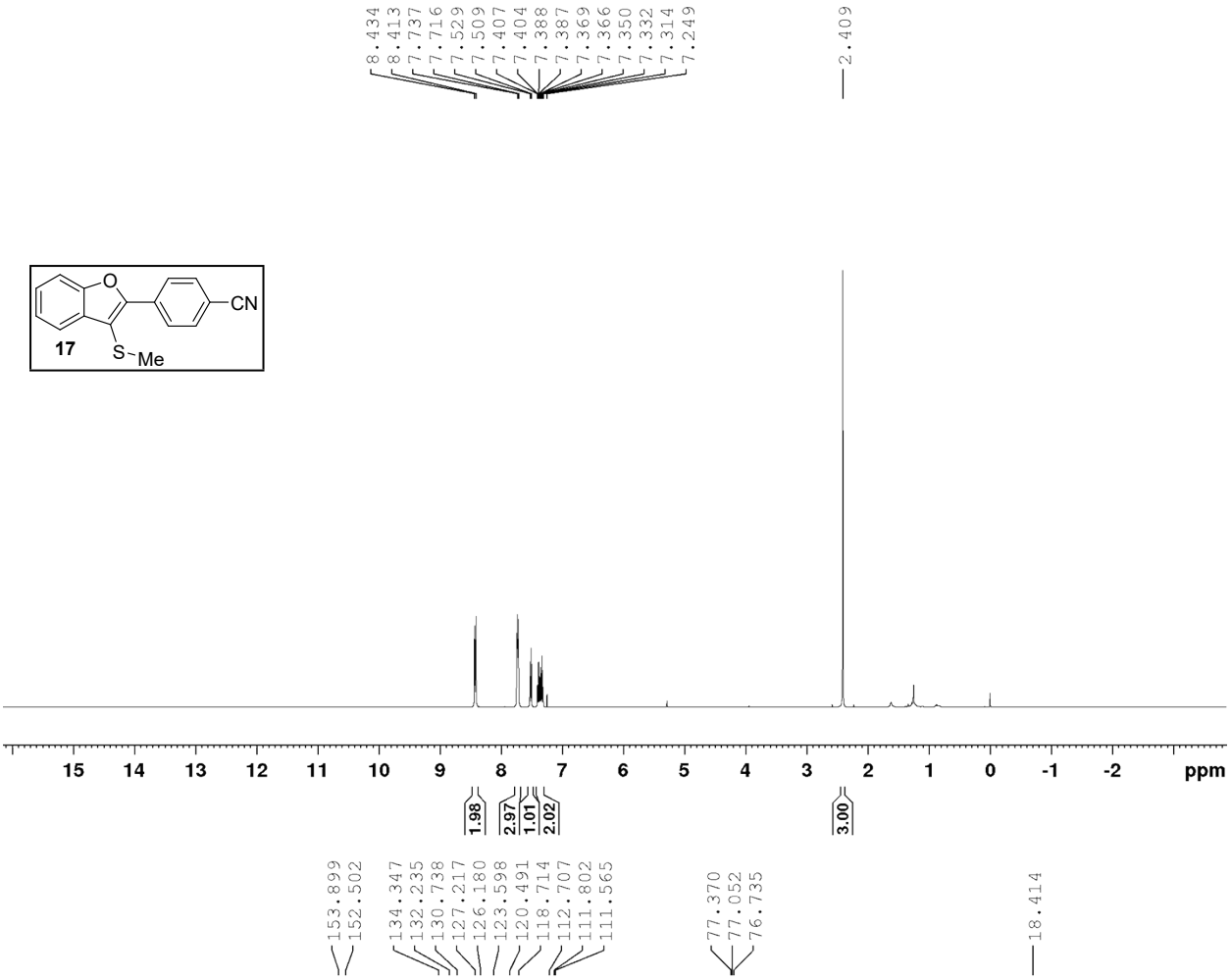

18.086

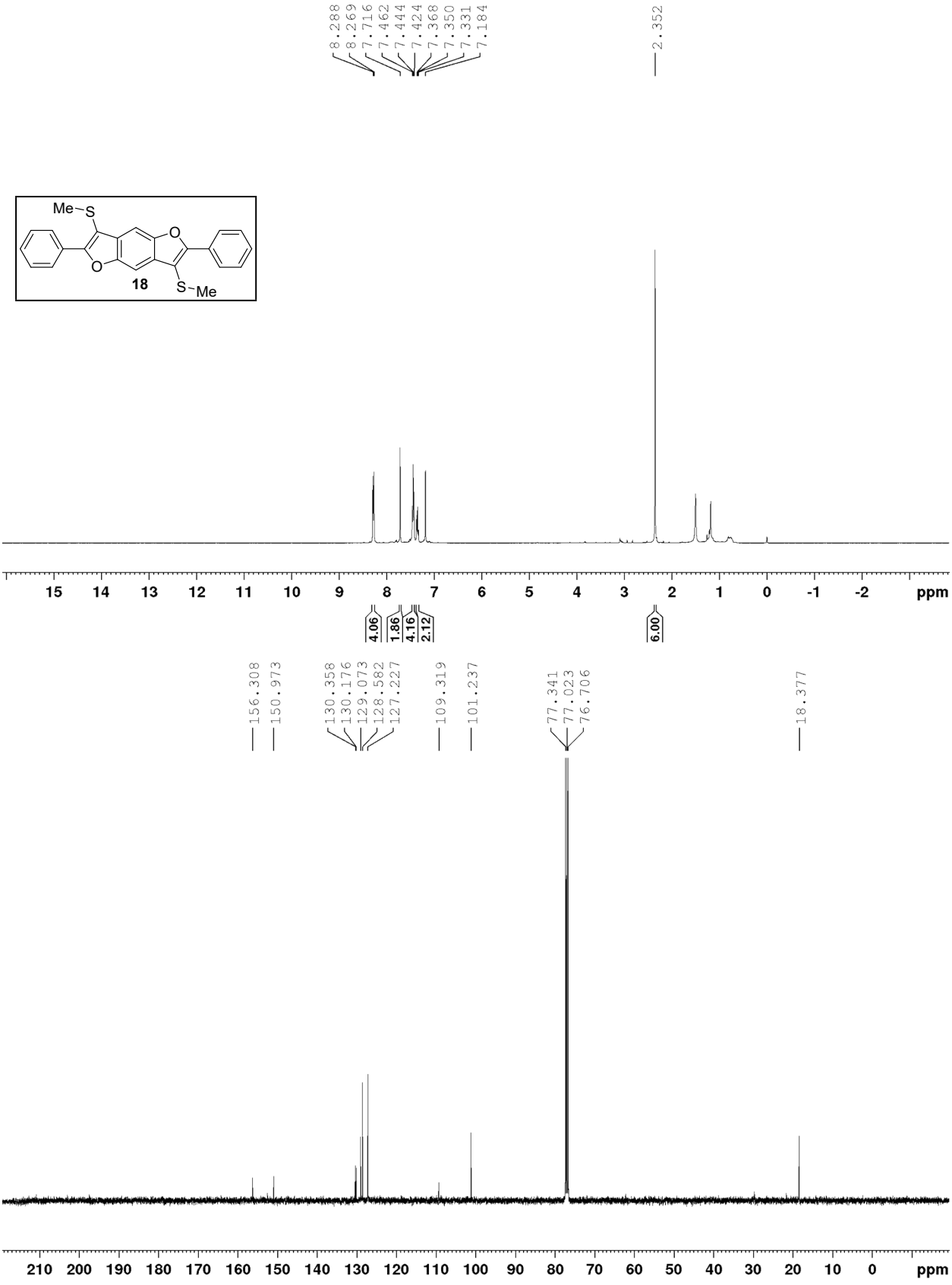

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

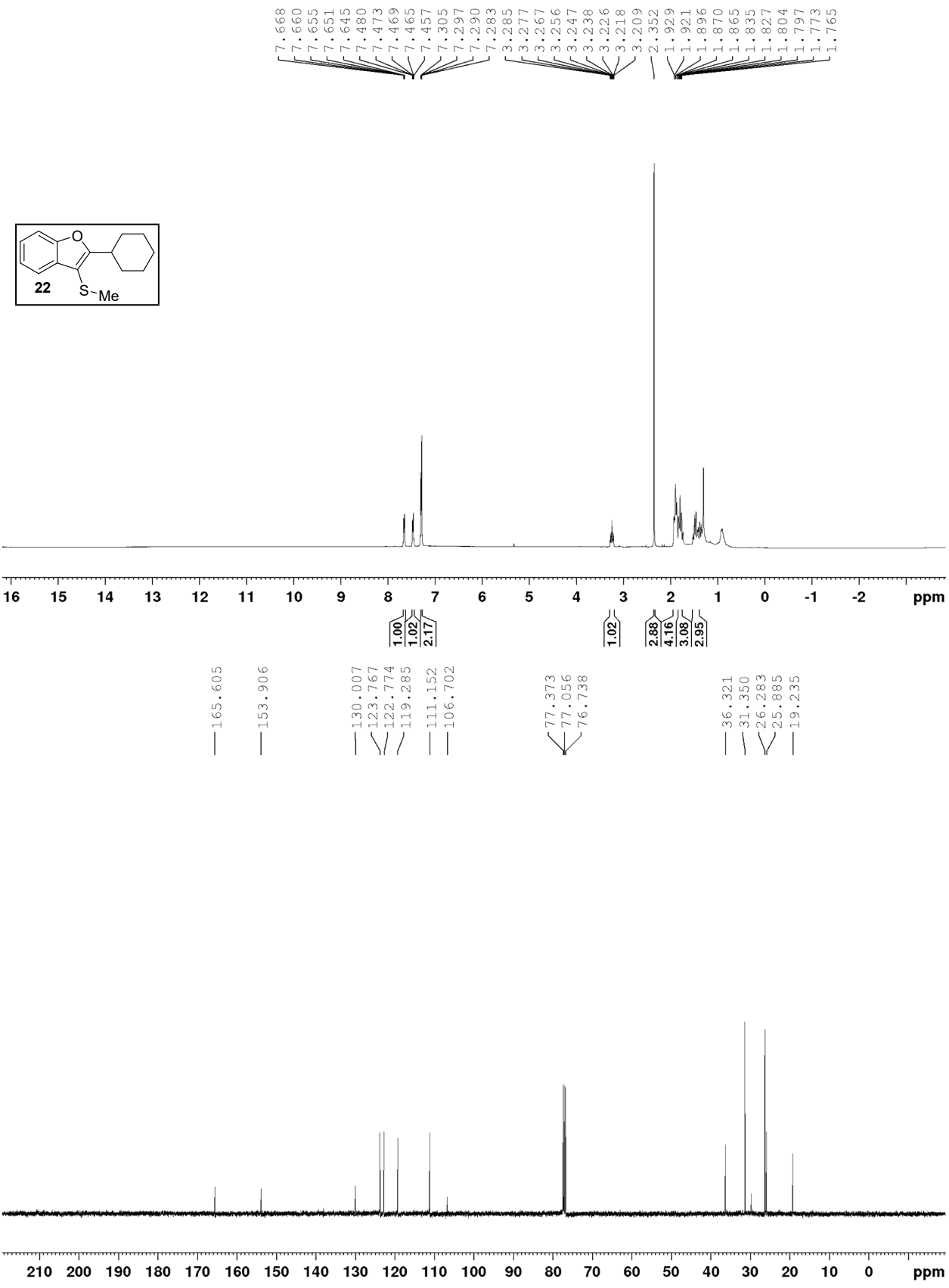

8.573
8.569
8.566
8.499
8.495
8.492
8.479
8.475
8.472
7.664
7.661
7.601
7.598
7.594
7.582
7.578
7.575
7.539
7.520
7.500
7.475
7.455
7.339
7.335
7.320
7.317
7.301
7.297
7.289
7.286
7.270
7.267
7.252
7.249
7.184
2.349

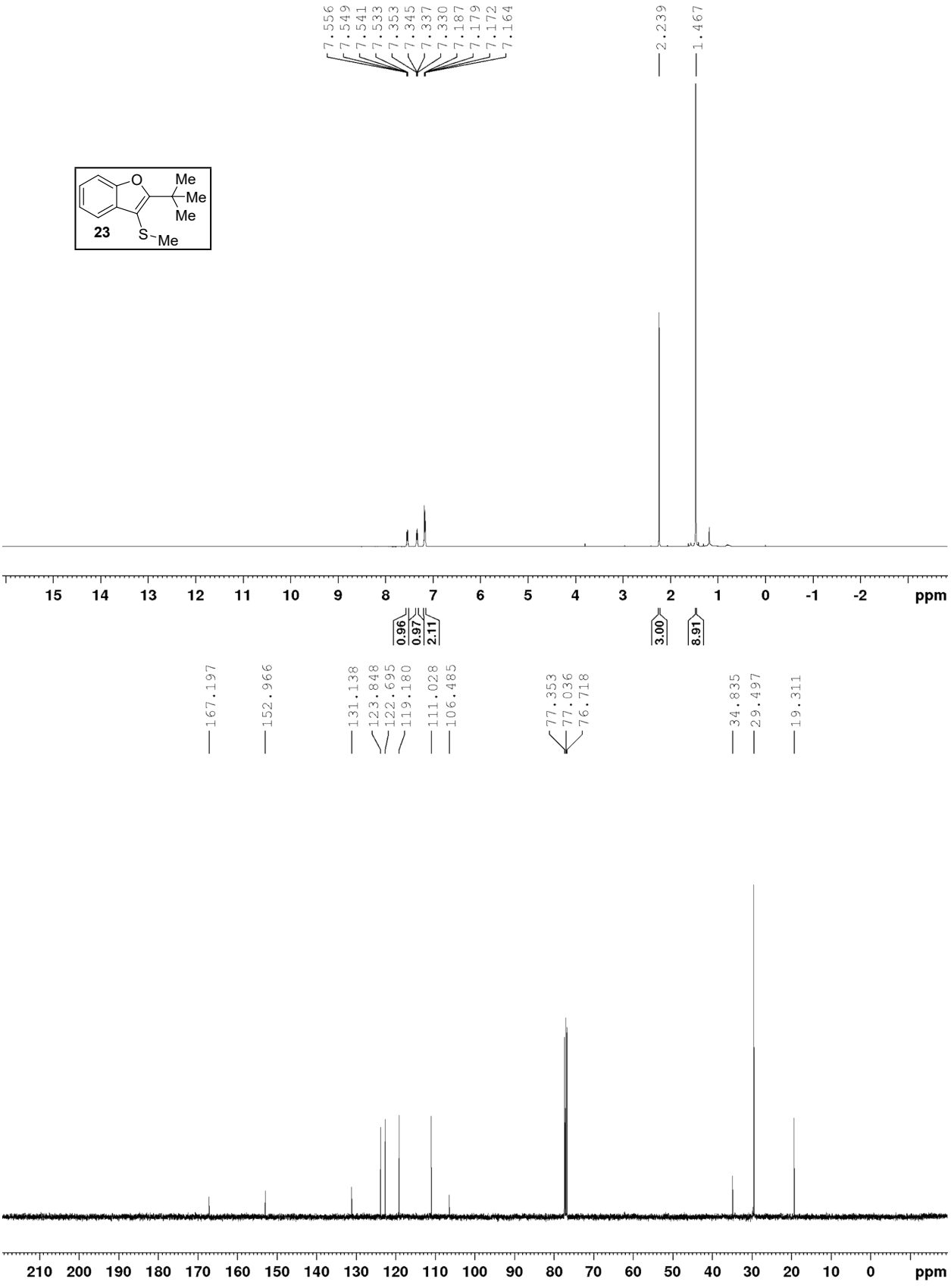

CN
O
16
S
Me
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
0.93
0.99
1.02
1.02
1.08
0.99
1.11
1.09
3.00


153.821
152.363
131.876
131.604
130.970
130.709
130.496
129.418
125.960
123.591
120.411
118.612
112.961
111.568
77.350
77.033
76.716
18.443
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

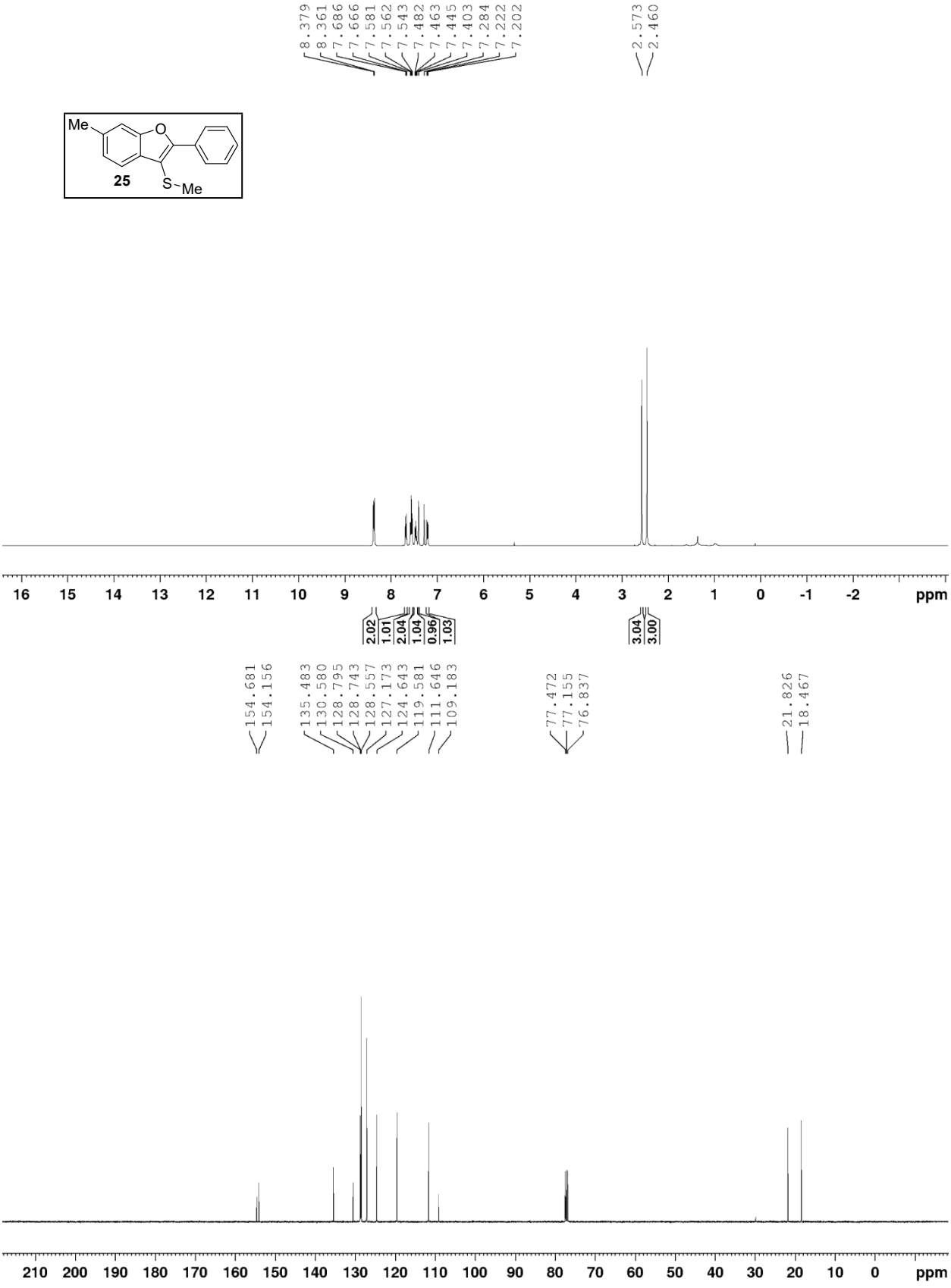

8.434
8.413
7.737
7.716
7.529
7.509
7.407
7.404
7.388
7.387
7.369
7.366
7.350
7.332
7.314
7.249
2.409
O
CN
17
S
Me
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
1.98
2.97
1.01
2.02
3.00
153.899
152.502
134.347
132.235
130.738
127.217
126.180
123.598
120.491
118.714
112.707
111.802
111.565
77.370
77.052
76.735
18.414
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

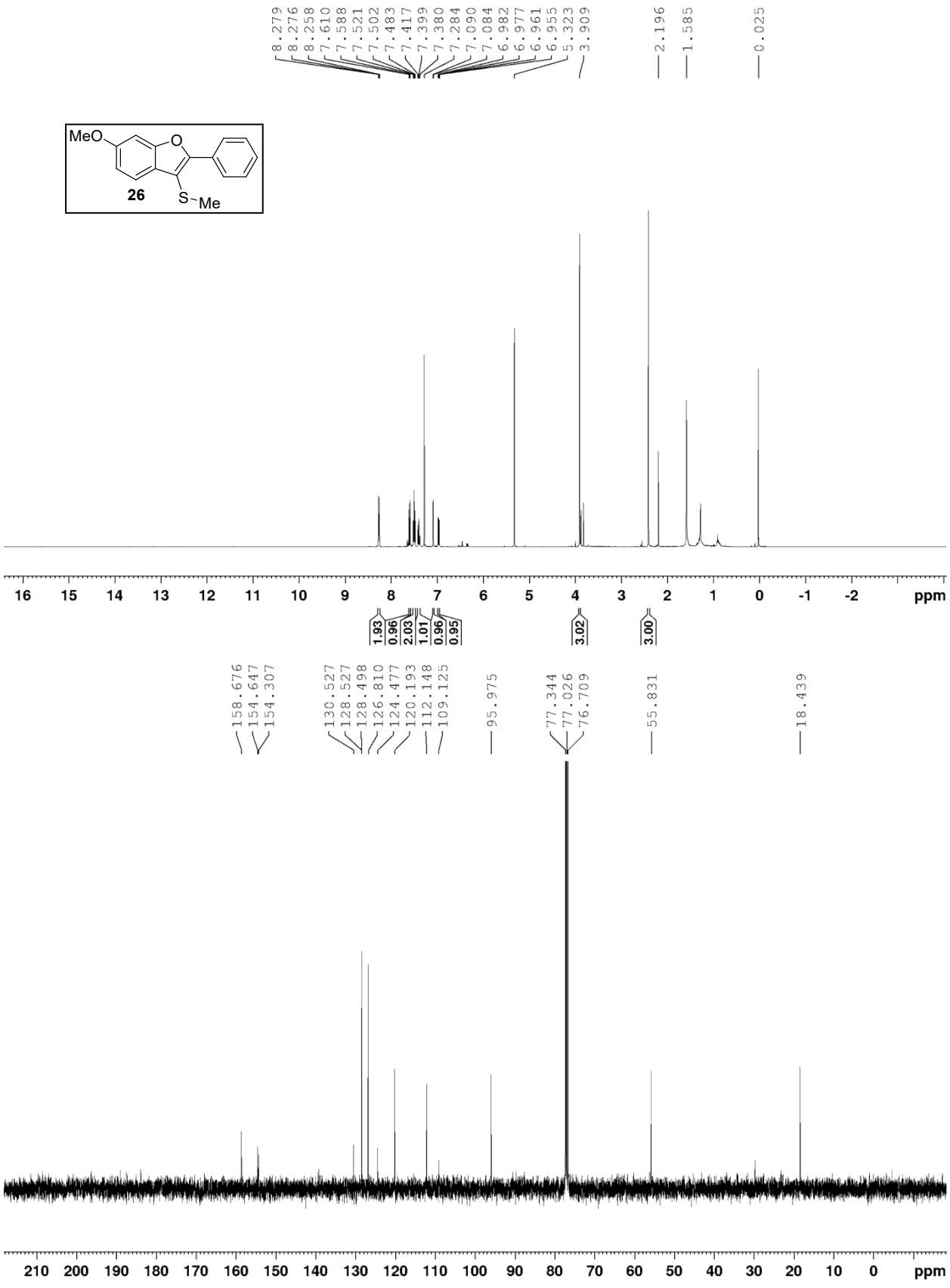

8.288
8.269
7.716
7.462
7.444
7.424
7.368
7.350
7.331
7.184
2.352
Me
S
O
O
S
Me
18
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
4.06
1.86
4.16
2.12
6.00
156.308
150.973
130.358
130.176
129.073
128.582
127.227
109.319
101.237
77.341
77.023
76.706
18.377
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

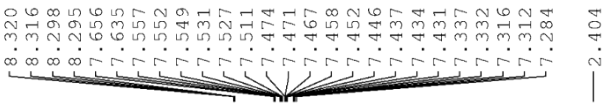

7.668
7.660
7.655
7.651
7.645
7.480
7.473
7.469
7.465
7.457
7.305
7.297
7.290
7.283
3.285
3.277
3.267
3.256
3.247
3.238
3.226
3.218
3.209
2.352
1.929
1.921
1.896
1.870
1.865
1.835
1.827
1.804
1.797
1.773
1.765
O
22
S
Me
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
1.00
1.02
2.17
1.02
2.88
4.16
3.08
2.95
165.605
153.906
130.007
123.767
122.774
119.285
111.152
106.702
77.373
77.056
76.738
36.321
31.350
26.283
25.885
19.235
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

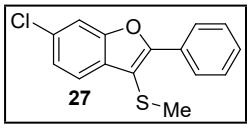

7.556
7.549
7.541
7.533
7.353
7.345
7.337
7.330
7.187
7.179
7.172
7.164
2.239
1.467
O
Me
Me
Me
23
S
Me
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
0.96
0.97
2.11
3.00
8.91
167.197
152.966
131.138
123.848
122.695
119.180
111.028
106.485
77.353
77.036
76.718
34.835
29.497
19.311
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

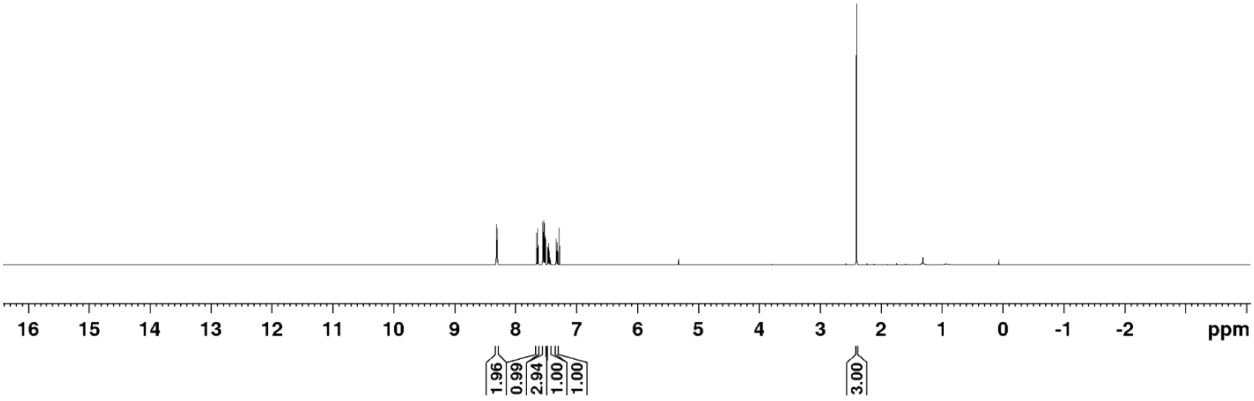
Me
O
25
S
Me


8.379
8.361
7.686
7.666
7.581
7.562
7.543
7.482
7.463
7.445
7.403
7.284
7.222
7.202
2.573
2.460
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
2.02
1.01
2.04
1.04
0.96
1.03
3.04
3.00
154.681
154.156
135.483
130.580
128.795
128.743
128.557
127.173
124.643
119.581
111.646
109.183
77.472
77.155
76.837
21.826
18.467
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

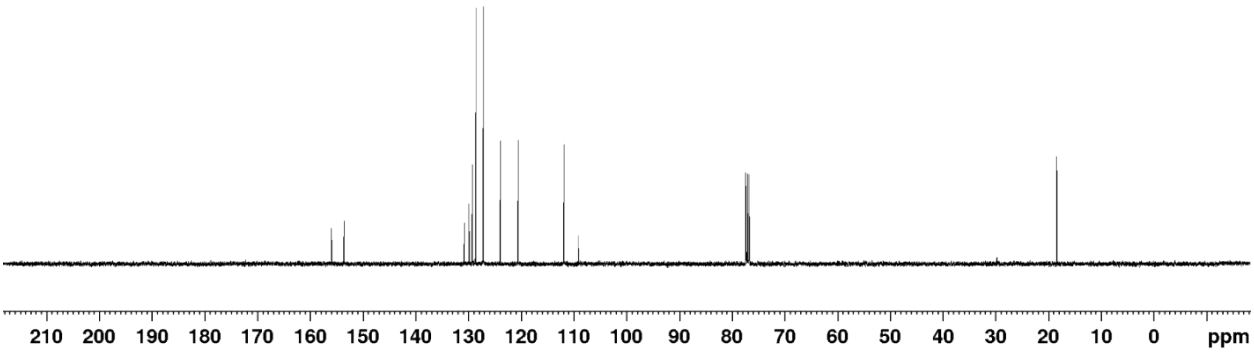

8.279
8.276
8.258
7.610
7.588
7.521
7.502
7.483
7.417
7.399
7.380
7.284
7.090
7.084
6.982
6.977
6.961
6.955
5.323
3.909
2.196
1.585
0.025
MeO
O
S
Me
26
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
1.93
0.96
2.03
1.01
0.96
0.95
3.02
3.00
158.676
154.647
154.307
130.527
128.527
128.498
126.810
124.477
120.193
112.148
109.125
95.975
77.344
77.026
76.709
55.831
18.439
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

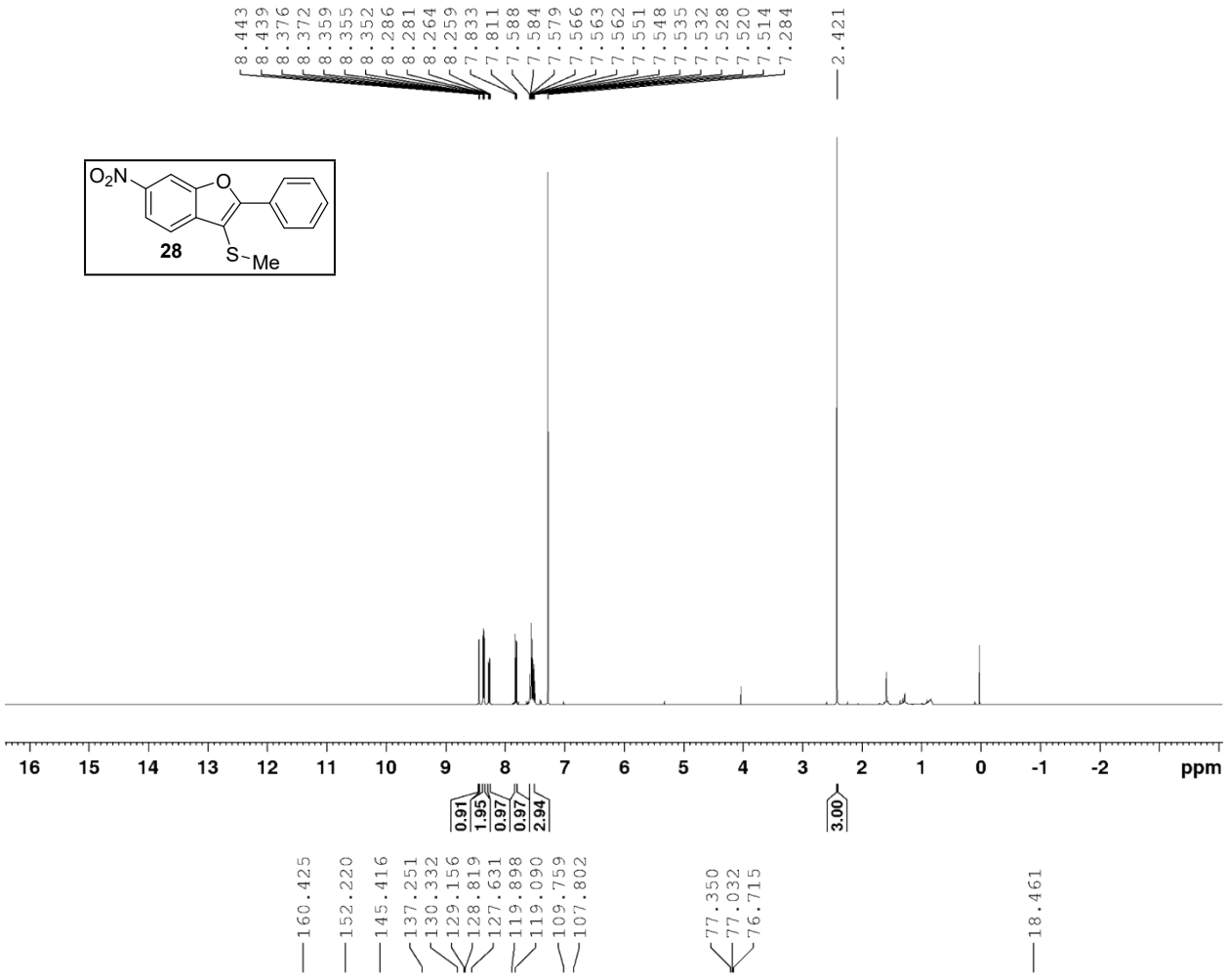

8.320
8.316
8.298
8.295
7.656
7.635
7.557
7.552
7.549
7.531
7.527
7.511
7.474
7.471
7.467
7.458
7.452
7.446
7.437
7.434
7.431
7.337
7.332
7.316
7.312
7.284
2.404

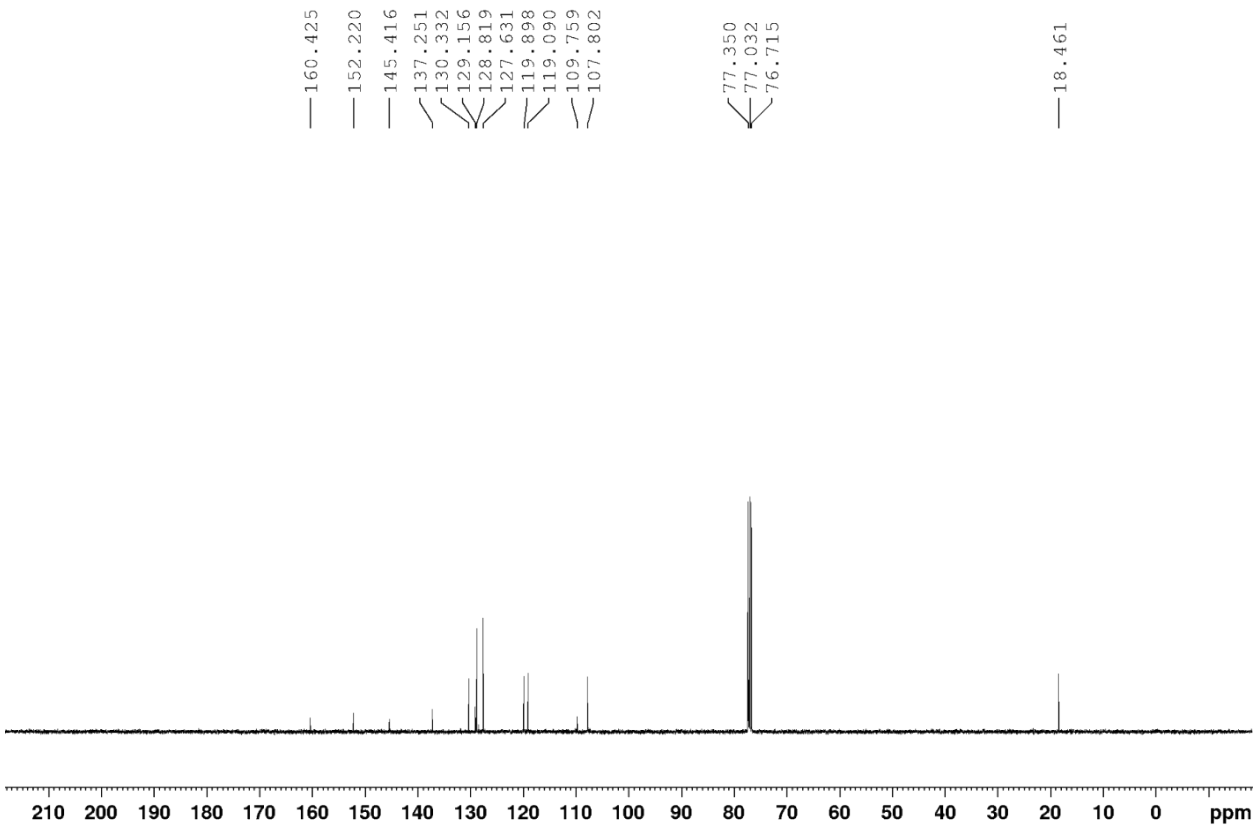

Cl
O
S
Me
27

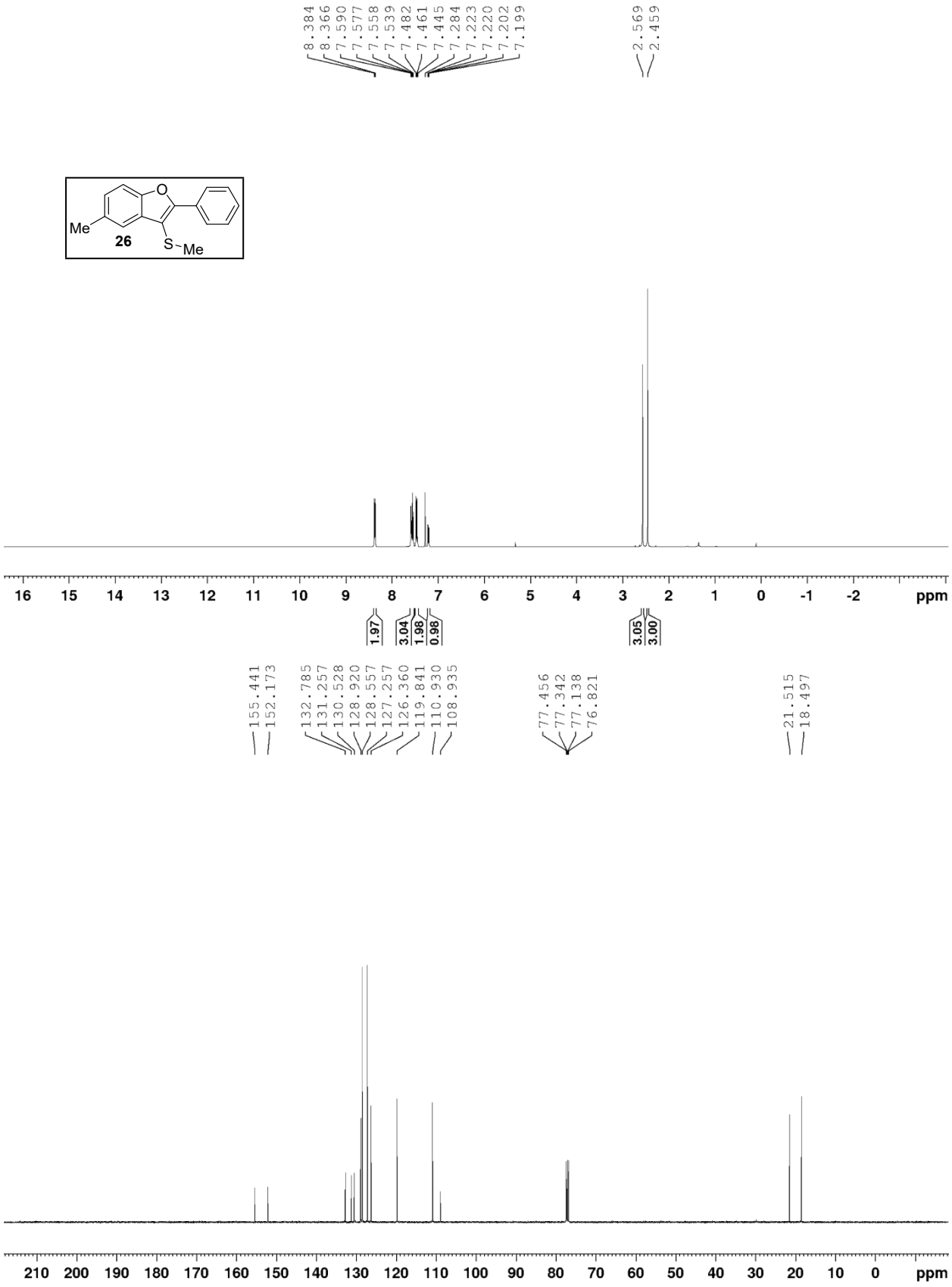

16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
1.96
0.99
2.94
1.00
1.00
3.00


155.977
153.650
130.791
129.921
129.261
128.615
127.207
123.956
120.578
111.903
109.168
77.409
77.091
76.774
18.423

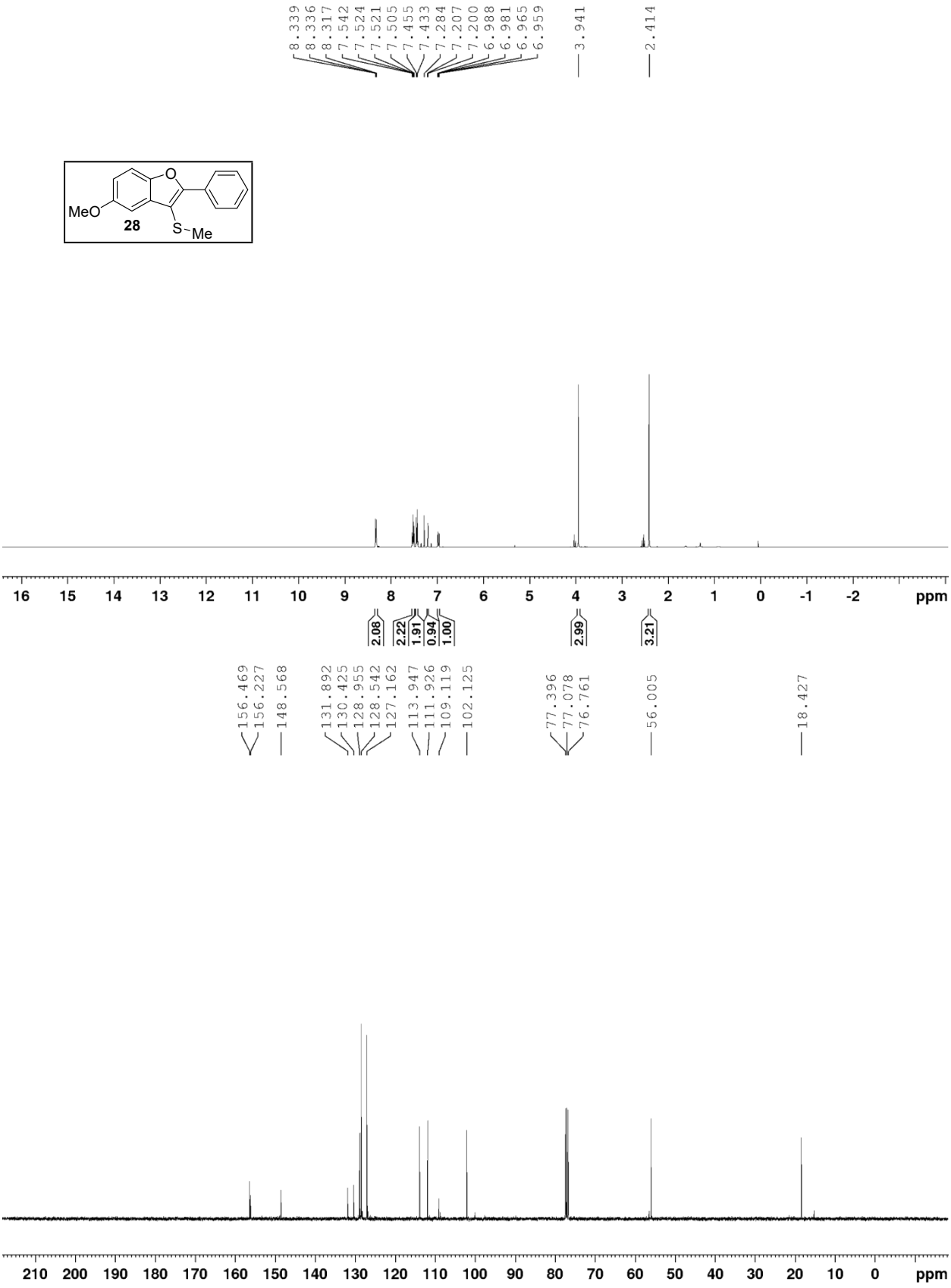

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

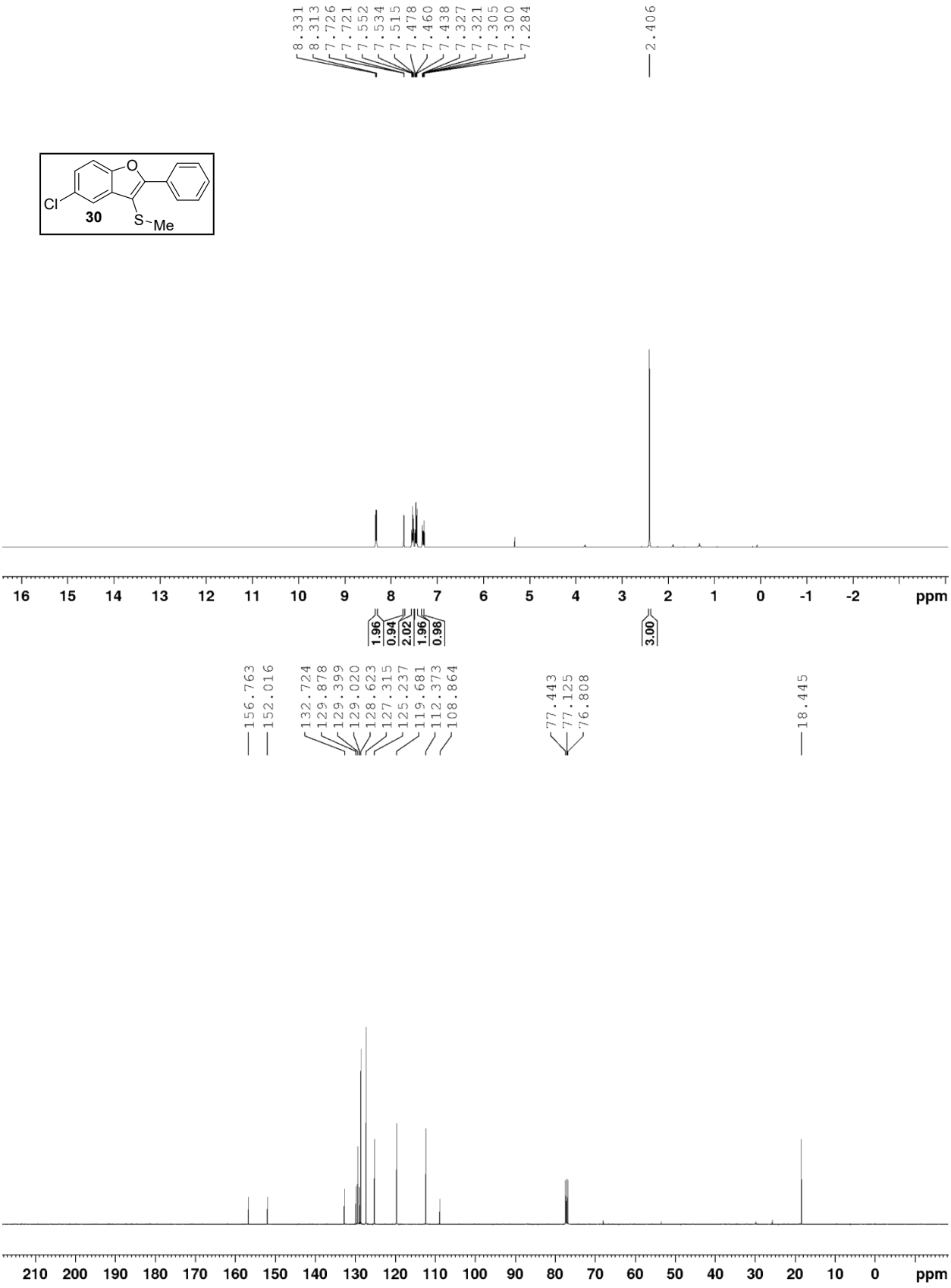

8.443
8.439
8.376
8.372
8.359
8.355
8.352
8.286
8.281
8.264
8.259
7.833
7.811
7.588
7.584
7.579
7.566
7.563
7.562
7.551
7.548
7.535
7.532
7.528
7.520
7.514
7.284
2.421
O2N
O
S
Me
28
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
0.91
1.95
0.97
0.97
2.94
3.00


160.425
152.220
145.416
137.251
130.332
129.156
128.819
127.631
119.898
119.090
109.759
107.802
77.350
77.032
76.715
18.461
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


8.384
8.366
7.590
7.577
7.558
7.539
7.482
7.461
7.445
7.284
7.223
7.220
7.202
7.199
2.569
2.459
Me
26
S
Me
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
1.97
3.04
1.98
0.98
3.05
3.00
155.441
152.173
132.785
131.257
130.528
128.920
128.557
127.257
126.360
119.841
110.930
108.935
77.456
77.342
77.138
76.821
21.515
18.497
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

MeO
28
S
Me


8.339
8.336
8.317
7.542
7.524
7.521
7.505
7.455
7.433
7.284
7.207
7.200
6.988
6.981
6.965
6.959
3.941
2.414
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
2.08
2.22
1.91
0.94
1.00
2.99
3.21
156.469
156.227
148.568
131.892
130.425
128.955
128.542
127.162
113.947
111.926
109.119
102.125
77.396
77.078
76.761
56.005
18.427
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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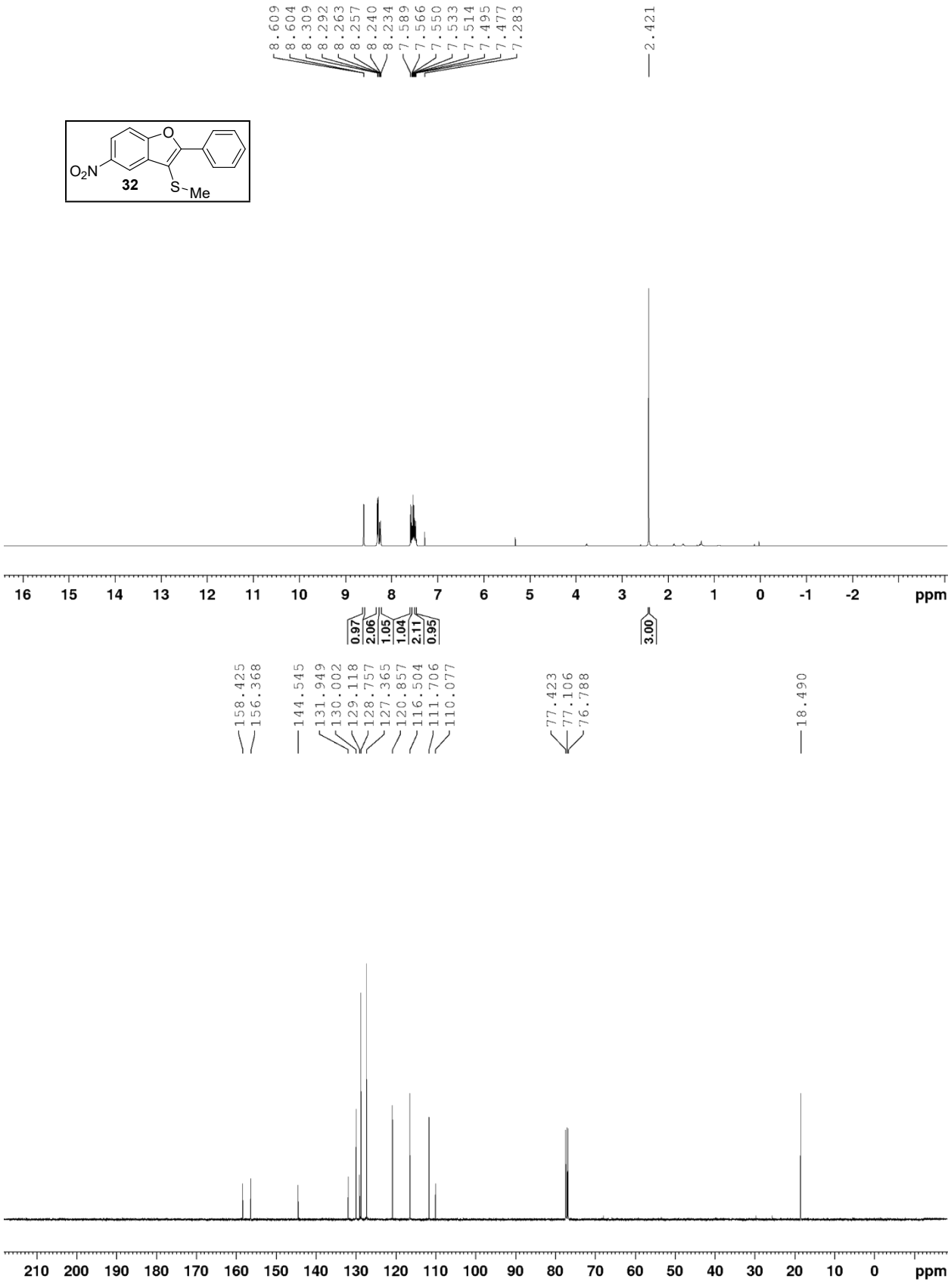
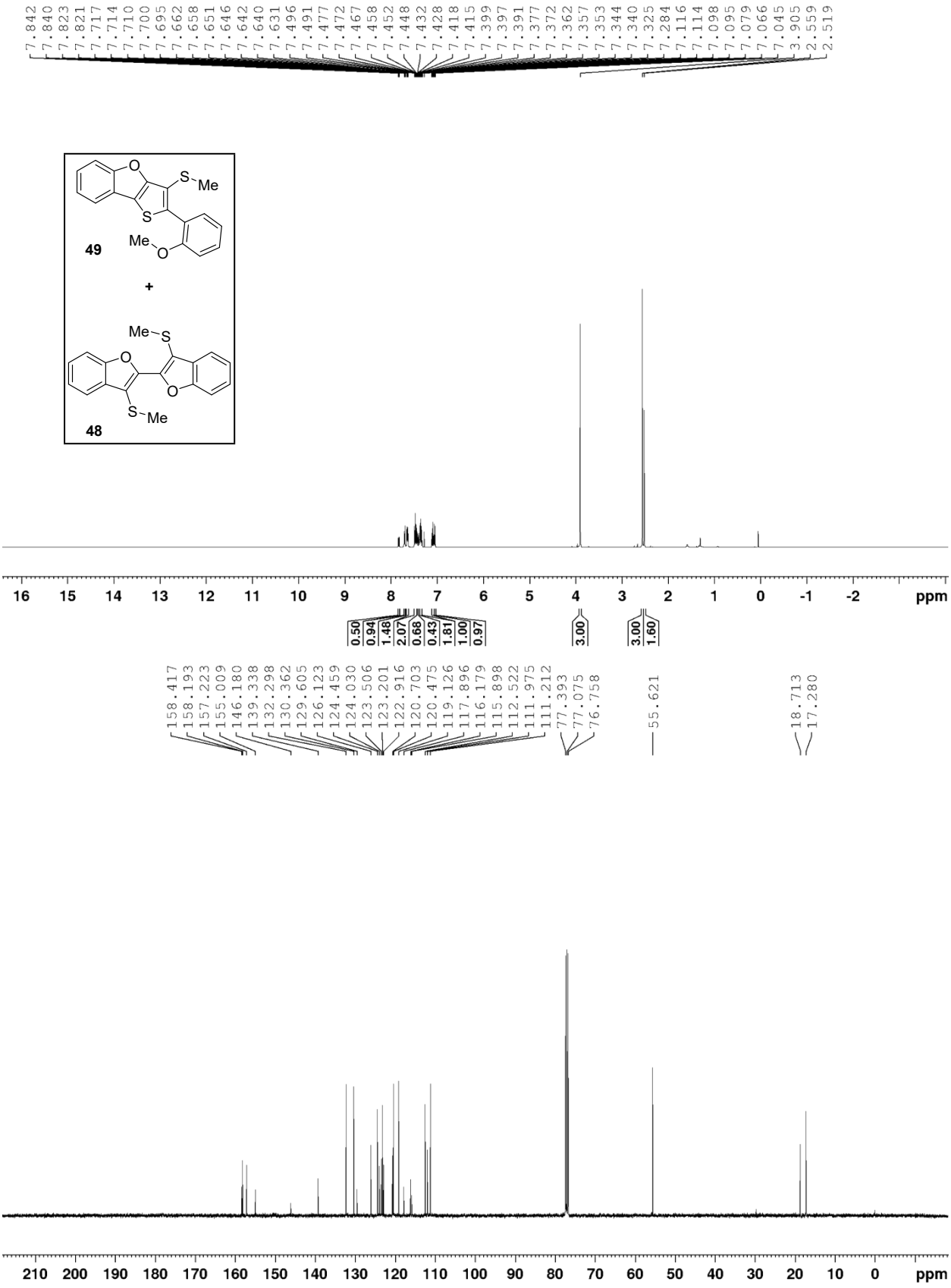
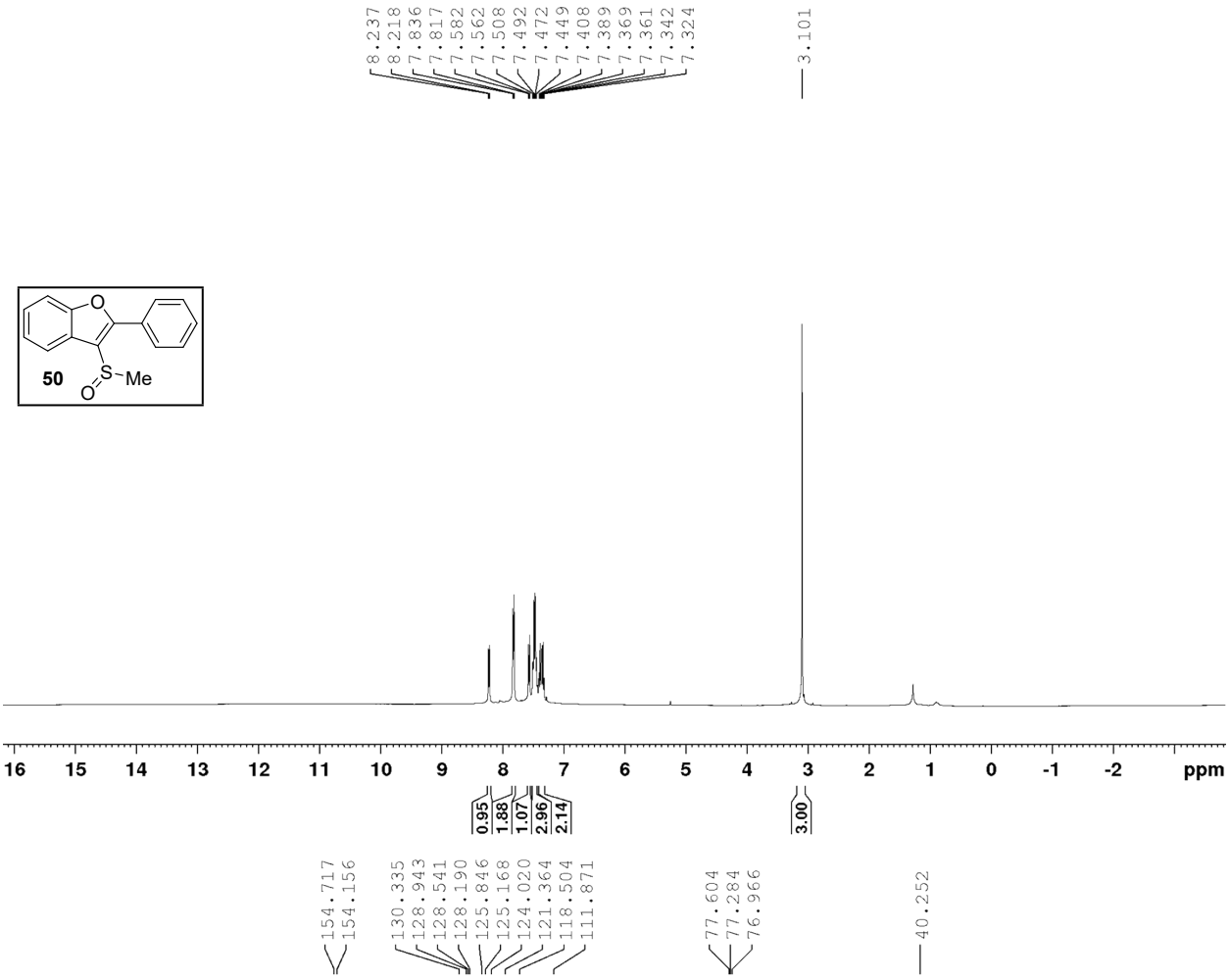
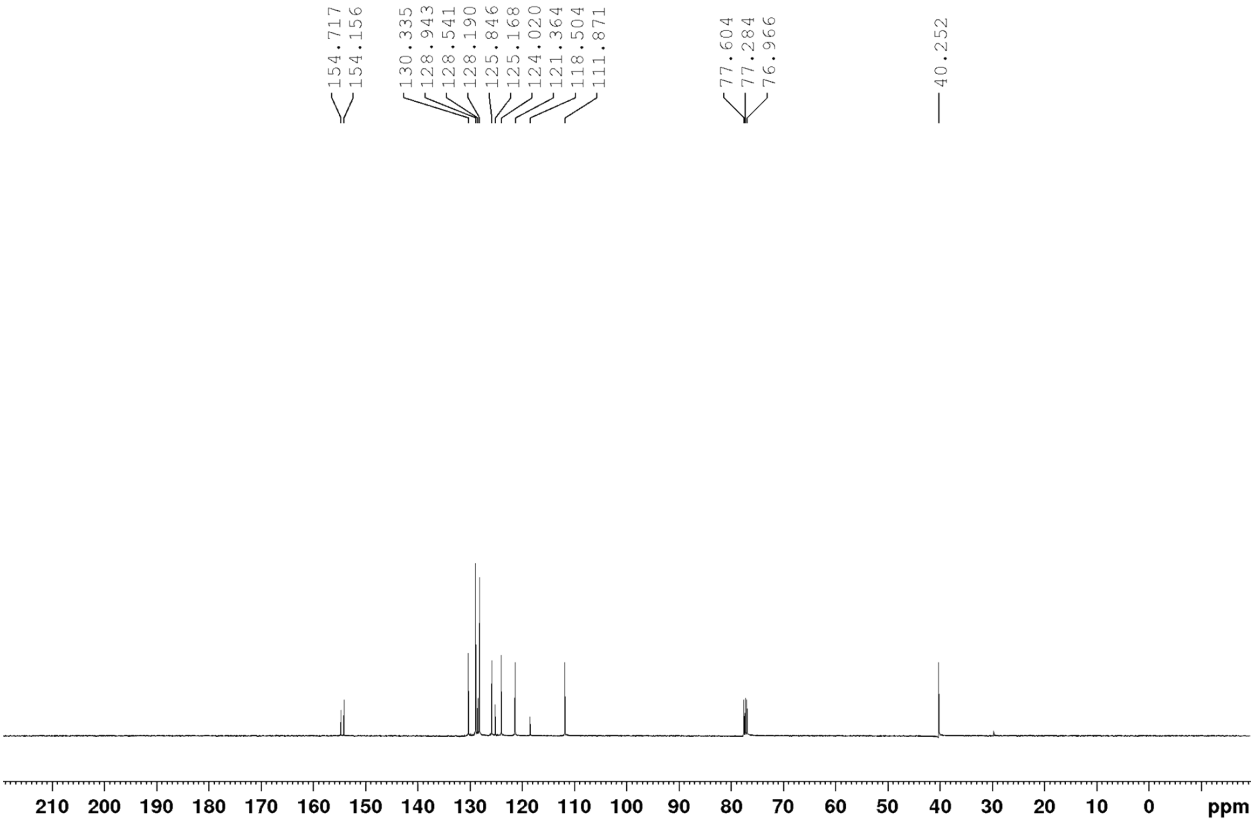
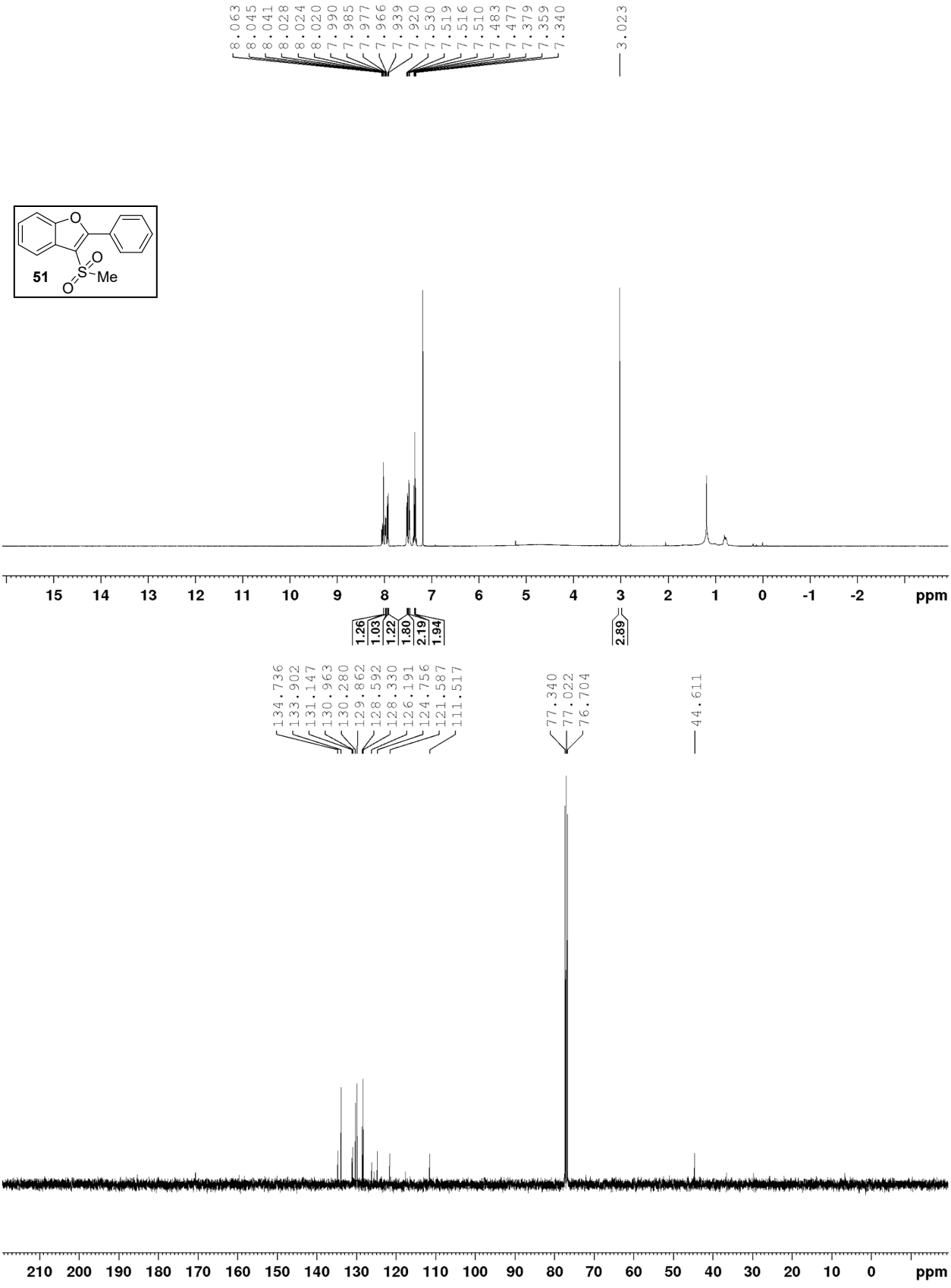
8.313
7.726
7.721
7.552
7.534
7.515
7.478
7.460
7.438
7.327
7.321
7.305
7.300
7.284
2.406
Cl
O
S
Me
30
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
1.96
0.94
2.02
1.96
0.98
3.00
156.763
152.016
132.724
129.878
129.399
129.020
128.623
127.315
125.237
119.681
112.373
108.864
77.443
77.125
76.808
18.445
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


8.609
8.604
8.309
8.292
8.263
8.257
8.240
8.234
7.589
7.566
7.550
7.533
7.514
7.495
7.477
7.283
2.421
O2N
32
S
Me
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
0.97
2.06
1.05
1.04
2.11
0.95
3.00
158.425
156.368
144.545
131.949
130.002
129.118
128.757
127.365
120.857
116.504
111.706
110.077
77.423
77.106
76.788
18.490
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


7.842
7.840
7.823
7.821
7.717
7.714
7.710
7.700
7.695
7.662
7.658
7.651
7.646
7.642
7.640
7.631
7.496
7.491
7.477
7.472
7.467
7.458
7.452
7.448
7.432
7.428
7.418
7.415
7.399
7.397
7.391
7.377
7.372
7.362
7.357
7.353
7.344
7.340
7.325
7.284
7.116
7.114
7.098
7.095
7.079
7.066
7.045
3.905
2.559
2.519
O
S
Me
S
Me
O
49
+
Me
S
O
O
S
Me
48
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
0.50 0.94 1.46 2.07 0.68 0.43 1.81 1.00 0.97
3.00
3.00 1.60
158.417
158.193
157.223
155.009
146.180
139.338
132.298
130.362
129.605
126.123
124.459
124.030
123.506
123.201
122.916
120.703
120.475
119.126
117.896
116.179
115.898
112.522
111.975
111.212
77.393
77.075
76.758
55.621
18.713
17.280
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


8.237
8.218
7.836
7.817
7.582
7.562
7.508
7.492
7.472
7.449
7.408
7.389
7.369
7.361
7.342
7.324
3.101
50
S
Me
O
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
0.95
1.88
1.07
2.96
2.14
3.00


154.717
154.156
130.335
128.943
128.541
128.190
125.846
125.168
124.020
121.364
118.504
111.871
77.604
77.284
76.966
40.252
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


8.063
8.045
8.041
8.028
8.024
8.020
7.990
7.985
7.977
7.966
7.939
7.920
7.530
7.519
7.516
7.510
7.483
7.477
7.379
7.359
7.340
3.023
51
Me
1.26
1.03
1.22
1.80
2.19
1.94
2.89
134.736
133.902
131.147
130.963
130.280
129.862
128.592
128.330
126.191
124.756
121.587
111.517
77.340
77.022
76.704
44.611
ppm
ppm