

Supporting Information

A Convenient Synthesis of 2-Arylbenzo[*b*]furans from Aryl Halides and 2-Halophenols by Catalytic One-Pot Cascade Method

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Experimental

Materials

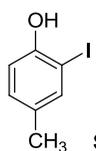
Experiments with air and moisture sensitive materials were carried under argon atmosphere. Glassware was oven dried for several hours, assembled hot, and cooled in a stream of argon. Silica gel 60, Merck 230–400 mesh, was used for preparative column flash chromatography. Analytical TLC was performed using Merck TLC Silica gel 60 F₂₅₄ 0.2 mm plates. Reagents were commercially available from Sigma-Aldrich, Merck or Fluorochem and were used without further purification. Palladium catalysts and copper(I) iodide was purchased from Sigma-Aldrich. Acetonitrile, triethylamine, morpholine, piperidine, dichloromethane, chloroform, ethyl acetate, methanol, *n*-heptane, petroleum ether, diethyl ether, 1,4-dioxane, toluene, DMF, DMSO, acetic acid, and THF were purchased from Avantor and Sigma-Aldrich. 1,4-Dioxane, toluene and THF were distilled from sodium benzophenone ketyl prior to use, DMF and DMSO were stirred over CaH₂ overnight, filtered, and distilled at 20 mmHg prior to use. Diisopropylamine, TMSA, iodine monochloride, TMEDA, ammonium hydroxide, sodium hypochlorite, iodobenzene, phenols and their derivatives were purchased from Sigma-Aldrich and used without further purification. Commercially unavailable or expensive halophenols (**S1-S21**) were synthesized as described below. ¹H and ¹³C NMR spectra were recorded on a Bruker Advance III 400 MHz or Bruker Advance III 700 MHz instrument at ambient temperature. Chemical shifts are reported in parts per million (δ scale), coupling constants (*J* values) are listed in Hertz. The following abbreviations were used to explain the multiplicities: s=singlet, d=doublet, t=triplet, q=quartet, p=pentet, sext=sextet, sep=septet, m=multiplet b=broad. IR spectra were recorded on Perkin Elmer FT-IR Spectrometer Spectrum Two. Melting points were determined with a Büchi SMP 32 and Barnstead-Thermolyne Mel-Temp II apparatus in open capillaries and are uncorrected. Elemental analyses were performed at Elementary Analyssysteme GmbH VarioMACRO CHNanalyzer.

Synthesis of 2-iodophenols

2-Iodophenols by reaction of phenols with sodium iodide and sodium hypochlorite¹

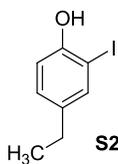
General procedure

In a round bottom flask equipped with magnetic stirring bar and dropping funnel, an appropriate phenol (10 mmol), sodium iodide (1.50 g; 10 mmol), and sodium hydroxide (0.48 g; 12 mmol), in methanol (30 mL) were cooled to 0 °C and stirred for 5 min. 5% aqueous solution of sodium hypochlorite (17.86 g, 12 mmol) was added dropwise during 15 min. The mixture was stirred under air until the substrate was consumed, as judged by TLC. The cooling bath was removed and 5% aqueous sodium thiosulfate solution (14 mL) was added. The mixture was neutralized with 2M HCl to pH<7 and extracted with diethyl ether (3×20 mL). The combined extracts were washed with water and brine and dried with anhydrous magnesium sulfate. Solvent was removed by rotary evaporation and the crude product was purified using flash chromatography.

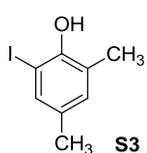


2-Iodo-4-methylphenol (S1): Flash, AcOEt:PE - 1:1. White crystals (69% yield), mp 30-31 °C (Lit.² 34.5-35.5 °C). ¹H NMR (CDCl₃, 400 MHz), δ ppm: 2.25 (s, 3H, CH₃), 5.11 (s, 1H, OH), 6.88 (d, *J*=8.2 Hz, 1H, CH_{Ar}), 7.04 (dd, *J*=8.2 Hz, *J*=2.2 Hz, 1H, CH_{Ar}), 7.47 (dd, *J*=2.2 Hz, *J*=0.4 Hz, 1H, CH_{Ar}). ¹³C NMR (CDCl₃, 100 MHz), δ ppm: 20.0 (CH₃), 85.4 (C_{Ar}), 114.7

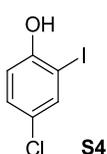
(CH_{Ar}), 130.8 (CH_{Ar}), 131.9 (C_{Ar}), 138.3 (CH_{Ar}), 152.7 (C_{Ar}). IR-ATR, cm⁻¹: 3235, 1578, 1399, 1276, 1234, 1218, 1202, 1140, 1037, 857, 808, 754, 665, 541, 464.



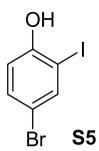
4-Ethyl-2-iodophenol (S2): Flash, DCM:*n*-heptane - 1:1. Light yellow oil (67% yield). ¹H NMR (CDCl₃, 400 MHz), δ ppm: 1.20 (t, *J*=7.6 Hz, 3H, CH₃), 2.54 (q, *J*=7.6 Hz, 2H, CH₂), 5.20 (bs, 1H, OH), 6.91 (d, *J*=8.2 Hz, 1H, CH_{Ar}), 7.07 (dd, *J*=8.2 Hz, *J*=2.1 Hz, 1H, CH_{Ar}), 7.49 (d, *J*=2.1 Hz, 1H, CH_{Ar}). ¹³C NMR (CDCl₃, 100 MHz), δ ppm: 15.7 (CH₃), 27.5 (CH₂), 85.6 (C_{Ar}), 114.8 (CH_{Ar}), 129.7 (CH_{Ar}), 137.2 (CH_{Ar}), 138.5 (C_{Ar}), 152.8 (C_{Ar}). IR-ATR cm⁻¹: 3454, 2963, 1499, 1486, 1285, 1202, 1174, 818, 740.



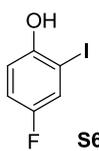
2-Iodo-4,6-dimethylphenol (S3): Flash, DCM:PE - 6:4. Yellow oil, bp=120-121 °C/15 mm Hg, (Lit.³ 123-124 °C/16 mm Hg) (67% yield). ¹H NMR (CDCl₃, 400 MHz), δ ppm: 2.22 (s, 3H, CH₃), 2.27 (s, 3H, CH₃), 5.12 (bs, 1H, OH), 6.89 (bs, 1H, CH_{Ar}), 7.30 (bs, 1H, CH_{Ar}). ¹³C NMR (CDCl₃, 100 MHz), δ ppm: 17.1 (CH₃), 19.9 (CH₃), 85.7 (C_{Ar}), 124.4 (C_{Ar}), 131.6 (C_{Ar}), 132.3 (CH_{Ar}), 135.6 (CH_{Ar}), 150.7 (C_{Ar}). IR-ATR, cm⁻¹: 3489, 2921, 1473, 1316, 1284, 1244, 1229, 1200, 1183, 1111, 850, 753, 713, 612.



4-Chloro-2-iodophenol (S4): Flash, DCM:PE - 6:4. White crystals (70% yield), mp 74.5-75.5 °C, (Lit.⁴ 75-76 °C). ¹H NMR (CDCl₃, 400 MHz), δ ppm: 5.28 (s, 1H, OH), 6.92 (d, *J*=8.8 Hz, 1H, CH_{Ar}), 7.22 (dd, *J*=8.8 Hz, *J*=2.4 Hz, 1H, CH_{Ar}), 7.63 (d, *J*=2.4 Hz, 1H, CH_{Ar}). ¹³C NMR (CDCl₃, 100 MHz), δ ppm: 85.4 (C_{Ar}), 115.7 (CH_{Ar}), 126.1 (C_{Ar}), 130.1 (CH_{Ar}), 137.1 (CH_{Ar}), 153.8 (C_{Ar}). IR-ATR, cm⁻¹: 3292, 1576, 1487, 1401, 1346, 1266, 1225, 1206, 1101, 1031, 871, 807, 683, 645, 540.



4-Bromo-2-iodophenol (S5): Flash, DCM:*n*-heptane - 4:6. White crystals (64% yield), mp 68-69 °C (lit.⁵ 69-70 °C). ¹H NMR (CDCl₃, 400 MHz) δ ppm: 5.30 (s, 1H, OH), 6.87 (d, *J*=8.7 Hz, 1H, CH_{Ar}), 7.35 (dd, *J*=8.7 Hz, *J*=2.3 Hz, 1H, CH_{Ar}), 7.77 (d, *J*=2.3 Hz, 1H, CH_{Ar}). ¹³C NMR (CDCl₃, 100 MHz), δ ppm: 86.2 (C_{Ar}), 113.1 (C_{Ar}), 116.3 (CH_{Ar}), 133.1 (CH_{Ar}), 139.8 (CH_{Ar}), 154.2 (C_{Ar}). IR-ATR, cm⁻¹: 3297, 1570, 1474, 1395, 1338, 1237, 1267, 1205, 1081, 1028, 871, 805, 666, 621, 533.



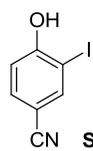
4-Fluoro-2-iodophenol (S6): Flash, DCM. White crystals (64% yield), mp 59.5-61 °C, (Lit.⁶ 62 °C). ¹H NMR (CDCl₃, 400 MHz), δ ppm: 5.11 (s, 1H, OH), 6.91-7.01 (m, 2H, 2CH_{Ar}), 7.38 (dd, *J*=7.6 Hz, *J*=2.8 Hz, 1H, CH_{Ar}). ¹³C NMR (CDCl₃, 100 MHz), δ ppm: 84.2 (C_{Ar}), 115.1 (d, *J*=7.9 Hz, CH_{Ar}), 116.9 (d, *J*=22.8 Hz, CH_{Ar}), 125.3 (d, *J*=25.3 Hz, CH_{Ar}), 151.5 (d, *J*=2.3 Hz, C_{Ar}), 155.2 (C_{Ar}), 156.4 (d, *J*=241.8 Hz, C_{Ar}). IR-ATR, cm⁻¹: 3350, 1496, 1408, 1264, 1179, 859, 814, 803, 762, 666, 462.

2-Iodophenols by reaction of phenols with iodine and ammonium hydroxide⁷

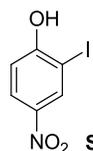
General procedure

In a round bottom flask equipped with magnetic stirring bar and dropping funnel, an appropriate phenol (10 mmol) was dissolved in methanol (25 mL), 20% ammonium hydroxide (25 mL) was added and solution of iodine (3.176 g; 12.5 mmol) in methanol (25 mL) was added dropwise. The mixture was stirred

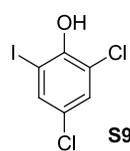
at rt until the substrate was consumed, as judged by TLC (~2h). Methanol was removed by rotary evaporation, water (100 mL) was added and the mixture was acidified with 2M HCl to pH=2. Product was extracted with ethyl acetate (3×25 mL). The combined extracts were washed with water, 5% aqueous sodium thiosulfate solution, brine and dried with anhydrous magnesium sulfate. Solvent was removed by rotary evaporation and the crude product was purified using flash chromatography.



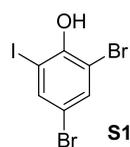
4-Hydroxy-3-iodobenzonitrile (S7): Flash, DCM:MeOH - 99:1. White crystals (64% yield), mp 145.5-146 °C (Lit.⁸ 144-146 °C). ¹H NMR (DMSO-d₆, 400 MHz), δ ppm: 6.97 (d, *J*=8.4 Hz, 1H, CH_{Ar}), 7.66 (dd, *J*=8.4 Hz, *J*=2.0 Hz, 1H, CH_{Ar}), 8.15 (d, *J*=2.0 Hz, 1H, CH_{Ar}), 11.53 (s, 1H, OH). ¹³C NMR (DMSO-d₆, 100 MHz), δ ppm: 85.6 (C_{Ar}), 103.4 (C_{Ar}), 115.7 (CH_{Ar}), 118.5 (C_{Ar}), 133.5 (CH_{Ar}), 143.0 (CH_{Ar}), 161.6 (C_{Ar}). IR-ATR, cm⁻¹: 3256, 2224, 1591, 1496, 1396, 1292, 1206, 1189, 1133, 1041, 894, 821, 730, 642, 580.



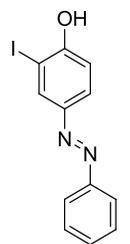
2-Iodo-4-nitrophenol (S8): Flash, DCM:PE - 8:2. Light yellow solid (50% yield), mp 86-88 °C, (Lit.⁹ 85-87 °C). ¹H NMR (DMSO-d₆, 400 MHz), δ ppm: 6.97 (d, *J*=8.8 Hz, 1H, CH_{Ar}), 8.12 (dd, *J*=8.8 Hz, *J*=3.0 Hz, 1H, CH_{Ar}), 8.49 (d, *J*=3.0 Hz, 1H, CH_{Ar}), 11.97 (bs, 1H, OH). ¹³C NMR (CDCl₃, 175 MHz), δ ppm: 85.3 (C_{Ar}), 114.9 (CH_{Ar}), 126.3 (CH_{Ar}), 135.0 (CH_{Ar}), 140.3 (C_{Ar}), 164.1 (C_{Ar}). IR-ATR, cm⁻¹: 3552, 1490, 1323, 1274, 1113, 900, 882, 821, 745, 681, 637.



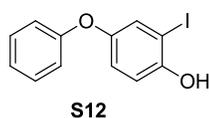
2,4-Dichloro-6-iodophenol (S9): Due to the high purity of the crude product the flash chromatography was not performed. White solid (95% yield), mp 56-57 °C; (Lit.¹⁰ 60 °C). ¹H NMR (CDCl₃, 400 MHz), δ ppm: 5.96 (bs, 1H, OH), 7.36 (s, 1H, CH_{Ar}), 7.63 (s, 1H, CH_{Ar}). ¹³C NMR (CDCl₃, 100 MHz), δ ppm: 83.2 (C_{Ar}), 119.2 (C_{Ar}), 126.3 (C_{Ar}), 129.3 (CH_{Ar}), 137.0 (CH_{Ar}), 150.0 (C_{Ar}). IR-ATR, cm⁻¹: 3321, 1452, 1380, 1318, 1260, 1218, 1147, 854, 754, 699, 561.



2,4-Dibromo-6-iodophenol (S10): Due to the high purity of the crude product the flash chromatography was not performed. Beige solid (94% yield), mp 101-102 °C; (Lit.¹¹ 105 °C). ¹H NMR (CDCl₃, 400 MHz) δ ppm: 5.35 (bs, 1H, OH), 7.60 (d, *J*=2.1 Hz, 1H, CH_{Ar}), 7.78 (d, *J*=2.1 Hz, 1H, CH_{Ar}). ¹³C NMR (CDCl₃, 100 MHz), δ ppm: 90.4 (C_{Ar}), 111.8 (2C_{Ar}), 135.2 (CH_{Ar}), 140.2 (CH_{Ar}), 154.5 (C_{Ar}). IR-ATR, cm⁻¹: 3435, 1443, 1375, 1310, 1225, 1144, 853, 719, 701, 660, 548.

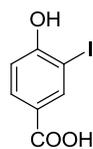


2-Iodo-4-(phenyldiazenyl)phenol (S11): Flash, DCM:*n*-heptane - 1:1 (77% yield), mp 140-141 °C; (Lit.¹² 138 °C). ¹H NMR (CDCl₃, 700 MHz), δ ppm: 5.64 (s, 1H, OH), 7.13 (d, *J*=7.0, 1H, CH_{Ar}), 7.45-7.47 (m, 1H, CH_{Ar}), 7.49-7.52 (m, 2H, 2CH_{Ar}), 7.87-7.88 (m, 2H, 2CH_{Ar}), 7.91 (dd, *J*=7.0, 1H, CH_{Ar}), 8.30 (d, *J*=7.0, 1H, CH_{Ar}). ¹³C NMR (CDCl₃, 100 MHz) δ ppm: 86.3 (C_{Ar}), 115.0 (CH_{Ar}), 122.7 (2CH_{Ar}), 126.3 (CH_{Ar}), 129.1 (2CH_{Ar}), 130.9 (CH_{Ar}), 132.1 (CH_{Ar}), 147.7 (C_{Ar}), 152.4 (C_{Ar}), 157.0 (C_{Ar}). IR-ATR, cm⁻¹: 3052, 1566, 1468, 1441, 1411, 1255, 1223, 1161, 828, 762, 682, 669.

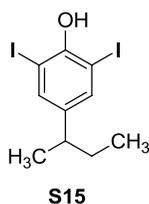
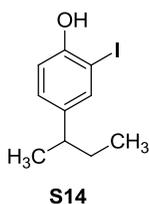


2-Iodo-4-phenoxyphenol (S12): Flash, DCM:*n*-heptane - 3:7. Light yellow oil (58% yield). ¹H NMR (CDCl₃, 700 MHz) δ ppm: 5.30 (bs, 1H, OH), 6.94-6.96 (m, 2H, 2CH_{Ar}), 6.96-6.97 (m, 2H, 2CH_{Ar}), 7.07-7.09 (m, 1H, CH_{Ar}), 7.31-7.34 (m, 2H, 2CH_{Ar}), 7.34-7.35 (m, 1H, CH_{Ar}). ¹³C NMR (CDCl₃, 100 MHz) δ ppm: 85.2 (C_{Ar}),

115.3 (CH_{Ar}), 118.0 (2CH_{Ar}), 121.7 (CH_{Ar}), 123.1 (CH_{Ar}), 129.0 (2CH_{Ar}), 129.9 (CH_{Ar}), 150.6 (C_{Ar}), 151.4 (C_{Ar}), 157.9 (C_{Ar}). IR-ATR, cm⁻¹: 3141, 1679, 1595, 1574, 1506, 1434, 1362, 1290, 1239, 1196, 1152, 1128, 1041, 901, 827, 768, 708, 666, 615.



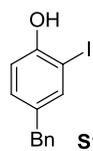
4-Hydroxy-3-iodobenzoic acid (S13): Due to the high purity of the crude product the flash chromatography was not performed. Gray solid (96% yield), mp 168-170 °C; (Lit.¹³ 172 -175 °C). ¹H NMR (DMSO-d₆, 700 MHz) δ ppm: 6.96 (d, *J*=8.4 Hz, 1H, CH_{Ar}), 7.81 (d, *J*=7.6 Hz, 1H, CH_{Ar}), 8.23-8.24 (m, 1H, CH_{Ar}), 11.21 (s, 1H, OH), 12.78 (s, 1H, OH). ¹³C NMR (CDCl₃, 100 MHz) δ ppm: 84.2 (C_{Ar}), 114.6 (CH_{Ar}), 123.4 (C_{Ar}), 131.3 (CH_{Ar}), 140.4 (CH_{Ar}), 160.8 (C_{Ar}), 166.0 (C). IR-ATR, cm⁻¹: 3142, 1679, 1595, 1574, 1506, 1434, 1362, 1290, 1041, 901, 827, 768, 708, 666, 615.



4-(sec-Butyl)-2-iodophenol (S14) and 4-(sec-butyl)-2,6-diiodophenol (S15):

Products were separated by flash chromatography, DCM:*n*-heptane - 1:1. **S14** - light yellow oil, 27% yield. ¹H NMR (CDCl₃, 400 MHz) δ ppm: 0.81 (t, *J*=7.0 Hz, 3H, CH₃), 1.19 (d, *J*=7.0 Hz, 3H, CH₃), 1.50-1.58 (m, 2H, CH₂), 2.49 (sext, *J*=7.0 Hz, 1H, CH), 5.36 (bs, 1H, OH), 6.91 (d, *J*=8.3 Hz, 1H, CH_{Ar}), 7.05 (dd, *J*=8.3 Hz, *J*=2.1 Hz, 1H, CH_{Ar}), 7.47 (d, *J*=2.1 Hz, 1H, CH_{Ar}). ¹³C NMR (CDCl₃, 100 MHz) δ ppm: 12.1 (CH₃), 21.9 (CH₃), 31.2 (CH₂), 40.5 (CH), 85.6 (C_{Ar}), 114.8 (CH_{Ar}), 128.8 (CH_{Ar}), 136.5 (CH_{Ar}), 142.0 (C_{Ar}), 152.8 (C_{Ar}). IR-ATR, cm⁻¹: 3453, 2960, 1488, 1455, 1400, 1309, 1179, 1151, 868, 703. Anal. Calcd. for C₁₀H₁₃IO: C, 43.50; H, 4.75. Found: C, 43.36; H, 4.71.

S15 - 50% yield. ¹H NMR (CDCl₃, 400 MHz) δ ppm: 0.83 (t, *J*=7.0 Hz, 3H, CH₃), 1.20 (d, *J*=7.0 Hz, 3H, CH₃), 1.50-1.58 (m, 2H, CH₂), 2.48 (sext, *J*=7.0 Hz, 1H, CH), 5.60 (s, 1H, OH), 7.49 (s, 2H, 2CH_{Ar}). ¹³C NMR (CDCl₃, 100 MHz) δ ppm: 12.1 (CH₃), 21.8 (CH₃), 31.1 (CH₂), 40.2 (CH), 82.2 (2C_{Ar}), 137.8 (2CH_{Ar}), 143.9 (C_{Ar}), 151.5 (C_{Ar}). IR-ATR, cm⁻¹: 3433, 2961, 2927, 1543, 1452, 1398, 1306, 1247, 1225, 1146, 866, 703. Anal. Calcd. for C₁₀H₁₂I₂O: C, 29.88; H, 3.01. Found: C, 30.11; H, 3.06.

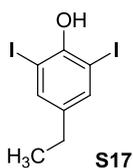


4-Benzyl-2-iodophenol (S16): Flash, DCM. White solid (66% yield), mp 48-48.5 °C. ¹H NMR (CDCl₃, 700 MHz), δ ppm: 3.87 (s, 2H, 2CH₂), 5.17 (s, 1H, OH), 6.90 (d, *J*=8.2 Hz, 1H, CH_{Ar}), 7.06 (dd, *J*=7.2 Hz, *J*=2.1 Hz, 1H, CH_{Ar}), 7.16 (d, *J*=7.2 Hz, 2H, 2CH_{Ar}), 7.21 (m, 1H, CH_{Ar}), 7.30 (m, 2H, 2CH_{Ar}), 7.48 (d, *J*=2.1 Hz, 1H, CH_{Ar}). ¹³C NMR (CDCl₃, 175 MHz), δ ppm: 41.5 (CH₂), 85.7 (C_{Ar}), 116.0 (CH_{Ar}), 127.3 (CH_{Ar}), 129.6 (2CH_{Ar}), 129.8 (2CH_{Ar}), 131.8 (CH_{Ar}), 136.4 (C_{Ar}), 139.2 (CH_{Ar}), 141.5 (C_{Ar}), 154.2 (C_{Ar}). IR-ATR, cm⁻¹: 3308, 1493, 1419, 1230, 1035, 831, 797, 728, 710, 692, 665, 616. Anal. Calcd. for C₁₃H₁₁IO: C, 50.35; H, 3.58. Found: C, 50.03; H, 3.49.

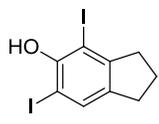
2,6-Diiodophenols by reaction of phenols with iodine and ammonium hydroxide

General procedure

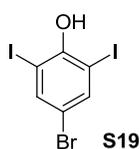
2,6-Diiodophenols were obtained using procedure 1.2.2 except that to the reaction was taken larger amount of iodine (5.336 g; 21 mmol).



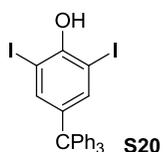
4-Ethyl-2,6-diiodophenol (S17): Flash, DCM:*n*-heptane - 1:1. Light green solid (89% yield), mp 31-32 °C; (lit.¹⁴ 29-30 °C). ¹H NMR (CDCl₃, 700 MHz) δ ppm: 1.18 (t, *J*=7.6 Hz, 3H, CH₃), 2.52 (q, *J*=7.6 Hz, 2H, CH₂), 5.58 (s, 1H, OH), 7.50 (s, 2H, 2 CH_{Ar}). ¹³C NMR (CDCl₃, 100 MHz) δ ppm: 15.5 (CH₃), 27.0 (CH₂), 82.1 (2C_{Ar}), 138.6 (2CH_{Ar}), 140.3 (C_{Ar}), 151.5 (C_{Ar}). IR-ATR, cm⁻¹: 3444, 2961, 1543, 1452, 1398, 1306, 1247, 1180, 703.



4,6-Diiodo-2,3-dihydro-1H-inden-5-ol (S18): Flash, DCM. Beige solid (73% yield), mp 76-76.5 °C. ¹H NMR (CDCl₃, 700 MHz), δ ppm: 2.09 (p, *J*=7.7 Hz 2H, CH₂), 2.86 (t, *J*=7.7 Hz, 2H, CH₂), 3.00 (t, *J*=7.7 Hz, 2H, CH₂), 5.62 (s, 1H, OH), 7.46 (s, 1H, CH_{Ar}). ¹³C NMR (CDCl₃, 100 MHz), δ ppm: 24.6 (CH₂), 33.6 (CH₂), 38.9 (CH₂), 78.8 (C_{Ar}), 82.0 (C_{Ar}), 133.7 (CH_{Ar}), 138.3 (C_{Ar}), 151.1 (C_{Ar}), 151.4 (C_{Ar}). IR-ATR, cm⁻¹: 3477, 2944, 2885, 2840, 1436, 1395, 1320, 1267, 1222, 1156, 1116, 858, 747, 579. Anal. Calcd. for C₉H₉I₂O: C, 28.01; H, 2.09. Found: C, 28.23; H, 2.03.

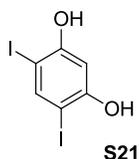


4-Bromo-2,6-diiodophenol (S19): Due to the high purity of the crude product the flash chromatography was not performed. White solid (93% yield), mp 125-126 °C, (Lit.¹⁵ 126-128 °C). ¹H NMR (CDCl₃, 400 MHz,) δ ppm: 5.73 (s, 1H, OH), 7.79 (s, 2H, 2CH_{Ar}). ¹³C NMR (CDCl₃, 175 MHz) δ ppm: 82.0 (2C_{Ar}), 113.2 (C_{Ar}), 140.5 (2CH_{Ar}), 152.7 (C_{Ar}). IR-ATR, cm⁻¹: 3458, 1435, 1376, 1305, 1230, 1174, 1145, 856, 699, 653, 540.



2,6-Diiodo-4-tritylphenol (S20): Flash, DCM/*n*-heptane - 1:1. Light pink solid (68% yield), mp 123-123.5 °C. ¹H NMR (DMSO-d₆, 700 MHz) δ ppm: 7.13 (d, *J*=7.7 Hz, 6H, 6CH_{Ar}), 7.25 (t, *J*=7.3 Hz, 3H, 3CH_{Ar}), 7.35 (t, *J*=7.7 Hz, 6H, 6CH_{Ar}), 7.42 (s, 2H, 2CH_{Ar}). ¹³C NMR (DMSO-d₆, 100 MHz) δ ppm: 66.4 (C), 87.7 (2C_{Ar}), 127.8 (3CH_{Ar}), 129.4 (6CH_{Ar}), 131.7 (6CH_{Ar}), 142.4 (2CH_{Ar}), 143.7 (C_{Ar}), 147.2 (3C_{Ar}), 155.2 (C_{Ar}). IR-ATR, cm⁻¹: 3469, 1490, 1459, 1442, 1318, 1260, 1239, 1489, 1153, 1083, 750, 698. Anal. Calcd. for C₂₅H₁₈I₂O: C, 51.05; H, 3.08. Found: C, 50.74; H, 3.12.

4,6-Diiodobenzene-1,3-diol by reaction of resorcinol with iodine monochloride¹⁶

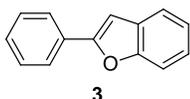


4,6-Diiodobenzene-1,3-diol (S21): To a solution of resorcinol (1.101 g; 10 mmol) in diethyl ether (10 mL) iodine monochloride (3.248 g; 20 mmol) was added at RT and stirred for 1 h. Reaction was quenched with water (30 mL), sodium sulfite (1.0 g; 7.9 mmol) was added and the mixture was transferred to separatory funnel. It was extracted with diethyl ether (3×20 mL), combined extracts were washed with water, brine and dried with anhydrous magnesium sulfate. Solvent was removed by rotary evaporation and the crude product was purified using flash chromatography, DCM:AcOH - 95:5 to give 2.160 g (60%) of white crystalline solid, mp 152-153 °C, (Lit.¹⁷ 156-160 °C). ¹H NMR (CDCl₃, 700 MHz), δ ppm: 5.26 (s, 2H, OH), 6.71 (s, 1H, CH_{Ar}), 7.84 (s, 1H, CH_{Ar}). ¹H NMR (DMSO-d₆, 700 MHz), δ ppm: 6.56 (s, 1H, CH_{Ar}), 7.75 (s, 1H, CH_{Ar}), 10.36 (s, 2H, OH). ¹³C NMR (DMSO-d₆, 100 MHz), δ ppm: 73.4 (2C_{Ar}), 102.6 (CH_{Ar}), 145.9 (CH_{Ar}), 158.2 (2C_{Ar}). IR-ATR, cm⁻¹: 3490, 1571, 1477, 1289, 1262, 1144, 1034, 988, 875, 824, 818, 627, 579.

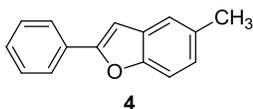
One-pot synthesis of 2-arylbenzofurans substituted in benzofuran moiety

General procedure

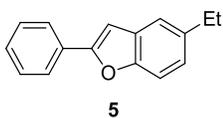
In a Schlenk tube equipped with magnetic stirring bar and reflux condenser, Pd(dppf)Cl₂ (0.0293 g; 0.04 mmol), CuI (0.0076 g; 0.04 mmol), and iodobenzene (0.408 g; 2 mmol) were added under argon atmosphere followed by dry degassed toluene (3 mL) and diisopropylamine (1.50 mL; 11 mmol). The mixture was stirred for 5 min. and TMSA (0.245 g; 2.5 mmol) in toluene (2 mL) was added at RT. It was stirred at this temperature until all iodobenzene was consumed (GC, ~10 min.). TBAF 1M in THF (4 mL; 4 mmol) was added followed by appropriate 2-iodophenole derivative (3 mmol). Temperature was increased to 80 °C, and the mixture was stirred at this temperature for 2-24 h (TLC). Reaction was quenched with 10% aqueous citric acid (20 mL) and extracted with DCM (3×20 mL). Combined extracts were washed with 10% aqueous NaOH (20 mL), water and dried with anhydrous magnesium sulfate. Solvent was removed by rotary evaporation and the crude product was purified using flash chromatography.



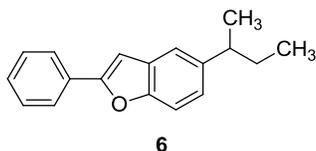
2-Phenylbenzofuran (3): Reaction time - 2 h. Flash, AcOEt/PE - 95:5. White solid (81% yield), mp 115.5-116.5 °C, (Lit.¹⁸ 116 °C). ¹H NMR (CDCl₃, 700 MHz), δ ppm: 7.03 (d, *J*=0.8 Hz, 1H, CH_{Ar}), 7.24 (td, *J*=7.3 Hz, *J*=0.8 Hz, 1H, CH_{Ar}), 7.27-7.30 (m, 1H, CH_{Ar}), 7.34-7.37 (m, 1H, CH_{Ar}), 7.44-7.47 (m, 2H, CH_{Ar}), 7.53 (dd, *J*=8.2 Hz, *J*=0.9 Hz, 1H, CH_{Ar}), 7.59 (d, *J*=7.7 Hz, 1H, CH_{Ar}), 7.88 (dd, *J*=8.6 Hz, *J*=0.9 Hz, 2H, CH_{Ar}). ¹³C NMR (CDCl₃, 100 MHz), δ ppm: 101.3 (CH_{Ar}), 111.2 (CH_{Ar}), 120.9 (CH_{Ar}), 122.9 (CH_{Ar}), 124.2 (CH_{Ar}), 124.9 (2CH_{Ar}), 128.5 (CH_{Ar}), 128.8 (2CH_{Ar}), 129.2 (C_{Ar}), 130.5 (C_{Ar}), 154.9 (C_{Ar}), 155.9 (C_{Ar}). IR-ATR, cm⁻¹: 2977, 1455, 1440, 1257, 1169, 1020, 918, 806, 765, 742, 688, 495.



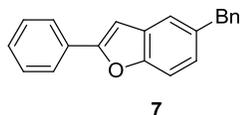
5-Methyl-2-phenylbenzofuran (4): Reaction time - 2 h. Flash, AcOEt/PE - 95:5. White solid (79% yield), mp 129-130 °C, (Lit.¹⁹ 129-130 °C). ¹H NMR (CDCl₃, 700 MHz), δ ppm: 2.45 (s, 3H, CH₃), 6.96 (d, *J*=0.7 Hz, 1H, CH_{Ar}), 7.10 (dd, *J*=7.7 Hz, *J*=1.4 Hz, 1H, CH_{Ar}), 7.33-7.36 (m, 1H, CH_{Ar}), 7.36-7.37 (m, 1H, CH_{Ar}), 7.40 (d, *J*=8.2 Hz, 1H, CH_{Ar}), 7.43-7.46 (m, 2H, 2CH_{Ar}), 7.86 (dd, *J*=8.6 Hz, *J*=1.4 Hz, 2H, 2CH_{Ar}). ¹³C NMR (CDCl₃, 175 MHz), δ ppm: 21.3 (CH₃), 101.1 (CH_{Ar}), 110.6 (CH_{Ar}), 120.7 (CH_{Ar}), 124.9 (2CH_{Ar}), 125.5 (CH_{Ar}), 128.4 (CH_{Ar}), 128.7 (2CH_{Ar}), 129.3 (C_{Ar}), 130.6 (C_{Ar}), 132.3 (C_{Ar}), 153.3 (C_{Ar}), 156.0 (C_{Ar}). IR-ATR, cm⁻¹: 2916, 1465, 1444, 1264, 1039, 1020, 914, 802, 758, 742, 688, 657, 495.



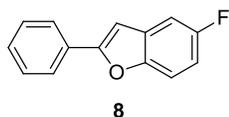
5-Ethyl-2-phenylbenzofuran (5): Reaction time - 4 h. Flash, DCM/PE - 3:7. White solid (73% yield), mp 98-99 °C. ¹H NMR (CDCl₃, 400 MHz) δ ppm: 1.30 (t, *J*=7.7 Hz, 3H, CH₃), 2.75 (q, *J*=7.7 Hz, 2H, CH₂), 6.97 (d, *J*=0.7 Hz, 1H, CH_{Ar}), 7.12 (dd, *J*=8.4 Hz, *J*=1.7 Hz, 1H, CH_{Ar}), 7.32-7.36 (m, 1H, CH_{Ar}), 7.40-7.46 (m, 4H, 4CH_{Ar}), 7.85-7.87 (m, 2H, 2CH_{Ar}). ¹³C NMR (CDCl₃, 173 MHz,) δ ppm: 15.9 (CH₃), 28.5 (CH₂), 100.8 (CH_{Ar}), 110.4 (CH_{Ar}), 119.2 (CH_{Ar}), 124.2 (CH_{Ar}), 124.5 (2CH_{Ar}), 128.0 (CH_{Ar}), 128.4 (2CH_{Ar}), 128.9 (C_{Ar}), 130.3 (C_{Ar}), 138.6 (C_{Ar}), 153.1 (C_{Ar}), 155.7 (C_{Ar}). IR-ATR, cm⁻¹: 2960, 1740, 1466, 1443, 1266, 1210, 1019, 911, 814, 807, 757, 749, 685. Anal. Calcd. for C₁₆H₁₄O: C, 86.45; H, 6.35. Found: C, 86.31; H, 6.37.



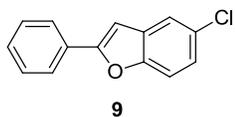
5-(sec-Butyl)-2-phenylbenzofuran (6): Reaction time - 4 h. Flash, DCM/PE - 2:8. White solid (69% yield), mp 63.5-64.5 °C. ¹H NMR (CDCl₃, 400 MHz) δ ppm: 0.86 (t, *J*=7.3 Hz, 3H, CH₃), 1.31 (d, *J*=7.0 Hz, 3H, CH₃), 1.63-1.70 (p, *J*=7.3 Hz, 2H, CH₂), 2.72 (sext, *J*=7.0 Hz, 1H, CH), 6.99 (d, *J*=0.8 Hz, 1H, CH_{Ar}), 7.13 (dd, *J*=8.5 Hz, *J*=1.8 Hz, 1H, CH_{Ar}), 7.34-7.40 (m, 2H, 2CH_{Ar}), 7.44-7.48 (m, 3H, 3CH_{Ar}), 7.86-7.89 (m, 2H, 2CH_{Ar}). ¹³C NMR (CDCl₃, 100 MHz) δ ppm: 12.4 (CH₃), 22.4 (CH₃), 31.6 (CH₂), 41.7 (CH), 101.3 (CH_{Ar}), 110.8 (CH_{Ar}), 118.8 (CH_{Ar}), 123.7 (CH_{Ar}), 124.9 (2CH_{Ar}), 128.4 (CH_{Ar}), 128.8 (2CH_{Ar}), 129.9 (C_{Ar}), 130.7 (C_{Ar}), 142.5 (C_{Ar}), 153.6 (C_{Ar}), 156.0 (C_{Ar}). IR-ATR, cm⁻¹: 2958, 1467, 1444, 1374, 1355, 1260, 1092, 1072, 1038, 1019, 912, 804, 761, 748, 657. Anal. Calcd. for C₁₈H₁₈O: C, 86.36; H, 7.25. Found: C, 86.51; H, 7.31.



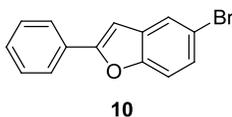
5-Benzyl-2-phenylbenzofuran (7): Reaction time - 3 h. Flash, DCM/PE - 2:8. Light yellow solid (88% yield), mp 79-80 °C. ¹H NMR (CDCl₃, 700 MHz), δ ppm: 4.08 (s, 2H, CH₂), 6.97 (d, *J*=0.9 Hz, 1H, CH_{Ar}), 7.12 (dd, *J*=8.5 Hz, *J*=2.2 Hz, 1H, CH_{Ar}), 7.19-7.23 (m, 3H, 3CH_{Ar}), 7.28-7.31 (m, 2H, 2CH_{Ar}), 7.33-7.36 (m, 1H, CH_{Ar}), 7.38-7.39 (m, 1H, CH_{Ar}), 7.42-7.45 (m, 3H, 3CH_{Ar}), 7.84-7.85 (m, 2H, 2CH_{Ar}). ¹³C NMR (CDCl₃, 100 MHz), δ ppm: 42.5 (CH₂), 102.2 (CH_{Ar}), 112.0 (CH_{Ar}), 121.9 (CH_{Ar}), 125.9 (2CH_{Ar}), 126.5 (CH_{Ar}), 127.0 (CH_{Ar}), 129.4 (2CH_{Ar}), 129.5 (CH_{Ar}), 129.8 (2CH_{Ar}), 129.9 (2CH_{Ar}), 130.4 (C_{Ar}), 131.6 (C_{Ar}), 136.8 (C_{Ar}), 142.6 (C_{Ar}), 154.7 (C_{Ar}), 157.2 (C_{Ar}). IR-ATR, cm⁻¹: 2977, 1450, 1439, 1260, 1159, 1050, 1020, 805, 762, 739, 687, 661. Anal. Calcd. for C₂₁H₁₆O: C, 88.70; H, 5.67. Found: C, 88.89; H, 5.70.



5-Fluoro-2-phenylbenzofuran (8): Reaction time - 2 h. Flash, DCM/PE - 2:8. White solid (94% yield), mp 171-172.5 °C, (Lit.²⁰ 175-177 °C, ²¹ 130-131 °C, ²² 133-135). ¹H NMR (CDCl₃, 400 MHz), δ ppm: 6.97-7.02 (m, 2H, 2CH_{Ar}), 7.23 (dd, *J*=8.4 Hz, *J*=2.6 Hz, 1H, CH_{Ar}), 7.35-7.40 (m, 1H, CH_{Ar}), 7.42-7.49 (m, 3H, 3CH_{Ar}), 7.85 (m, 2H, 2CH_{Ar}). ¹³C NMR (CDCl₃, 100 MHz), δ ppm: 101.4 (d, *J*=3.9 Hz, CH_{Ar}), 106.3 (d, *J*=25.1 Hz, CH_{Ar}), 111.7 (d, *J*=9.8 Hz, CH_{Ar}), 111.8 (d, *J*=26.4 Hz, CH_{Ar}), 125.0 (2CH_{Ar}), 128.8 (2CH_{Ar}), 128.9 (CH_{Ar}), 130.0 (d, *J*=10.9 Hz, C_{Ar}), 130.1 (C_{Ar}), 151.2 (C_{Ar}), 157.7 (C_{Ar}), 159.4 (d, *J*=159.4 Hz, C_{Ar}). IR-ATR, cm⁻¹: 2978, 1461, 1442, 1187, 1127, 915, 809, 801, 762, 737, 689, 493.

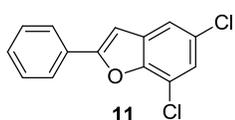


5-Chloro-2-phenylbenzofuran (9): Reaction time - 2 h. Flash, DCM/PE - 2:8. White solid (80% yield), mp 146-147 °C, (Lit.²³ 143.5-147 °C). ¹H NMR (CDCl₃, 400 MHz), δ ppm: 6.97 (d, *J*=1.0 Hz, 1H, CH_{Ar}); 7.24 (dd, *J*=8.6 Hz, *J*=2.2 Hz, 1H, CH_{Ar}); 7.35-7.40 (m, 1H, CH_{Ar}); 7.42-7.49 (m, 3H, 3CH_{Ar}); 7.55 (dd, *J*=2.2 Hz, *J*=0.4 Hz, 1H, CH_{Ar}); 7.84-7.87 (m, 2H, 2CH_{Ar}). ¹³C NMR (CDCl₃, 100 MHz), δ ppm: 100.8 (CH_{Ar}); 112.1 (CH_{Ar}); 120.4 (CH_{Ar}); 124.4 (CH_{Ar}); 125.0 (2CH_{Ar}); 128.5 (C_{Ar}); 128.8 (2CH_{Ar}); 129.0 (CH_{Ar}); 130.0 (C_{Ar}); 130.6 (C_{Ar}); 153.3 (C_{Ar}); 157.4 (C_{Ar}). IR-ATR, cm⁻¹: 2982, 1451, 1160, 1062, 1020, 904, 879, 806, 762, 739, 687, 661, 493.

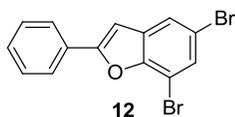


5-Bromo-2-phenylbenzofuran (10): Reaction time - 2.5 h. Flash, AcOEt/PE - 85:15. Light yellow solid (92% yield), mp 157-158 °C, (Lit.²⁴ 156-158 °C). ¹H NMR (CDCl₃, 700 MHz) δ ppm: 6.97 (s, 1H, CH_{Ar}); 7.36-7.40 (m, 3H, 3CH_{Ar}); 7.46 (m, 2H, 2CH_{Ar}); 7.71 (d, *J*=1.9 Hz, 1H, CH_{Ar}); 7.84-7.86 (m, 2H, 2CH_{Ar}). ¹³C NMR (CDCl₃, 100 MHz), δ ppm: 101.6 (CH_{Ar}), 113.6 (CH_{Ar}), 117.0 (C_{Ar}), 124.5 (CH_{Ar}), 126.1 (2CH_{Ar}), 128.1 (CH_{Ar}), 129.9 (2CH_{Ar}), 130.0 (CH_{Ar}), 130.9 (C_{Ar}), 132.2 (C_{Ar}), 154.6 (C_{Ar}), 158.3 (C_{Ar}). IR-ATR,

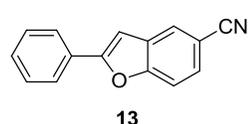
cm⁻¹: 3095, 1605, 1579, 1491, 1451, 1437, 1435, 1325, 1277, 1261, 1205, 1157, 1117, 1074, 1051, 1021, 921, 894, 879, 806, 761, 689, 579, 491.



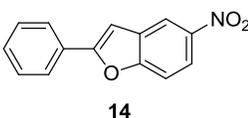
5,7-Dichloro-2-phenylbenzofuran (11): Reaction time - 2 h. Flash, AcOEt/PE - 90:10. Light yellow solid (87% yield), mp 124-126 °C, (Lit.²⁵ 127-128 °C). ¹H NMR (CDCl₃, 400 MHz) δ ppm: 6.99 (s, 1H, CH_{Ar}); 7.29 (d, *J*=2.0 Hz, 1H, CH_{Ar}); 7.40-7.43 (m, 1H, CH_{Ar}); 7.45-7.50 (m, 3H, 3CH_{Ar}); 7.87-7.90 (m, 2H, 2CH_{Ar}). ¹³C NMR (CDCl₃, 100 MHz,) δ ppm: 101.2 (CH_{Ar}), 117.2 (C_{Ar}), 119.0 (CH_{Ar}), 124.3 (CH_{Ar}), 125.3 (2CH_{Ar}), 128.7 (C_{Ar}), 128.3 (2CH_{Ar}), 129.4 (C_{Ar}), 129.4 (CH_{Ar}), 131.5 (C_{Ar}), 149.3 (C_{Ar}), 158.2 (C_{Ar}). IR-ATR, cm⁻¹: 3086, 1609, 1578, 1488, 1455, 1437, 1409, 1328, 1171, 1037, 909, 866, 837, 758, 679.



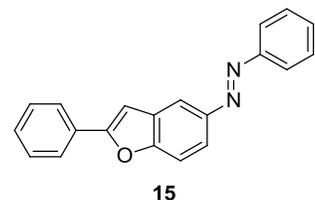
5,7-Dibromo-2-phenylbenzofuran (12): Reaction time - 2 h. Flash, AcOEt/PE - 90:10. Light yellow solid (72% yield), mp 134-136 °C. ¹H NMR (CDCl₃, 400 MHz) δ ppm: 7.00 (s, 1H, CH_{Ar}); 7.38-7.42 (m, 1H, CH_{Ar}); 7.45-7.50 (m, 2H, 2CH_{Ar}); 7.57 (d, *J*=2.0 Hz, 1H, CH_{Ar}); 7.64 (d, *J*=2.0 Hz, 1H, CH_{Ar}); 7.87-7.89 (m, 2H, 2CH_{Ar}). ¹³C NMR (CDCl₃, 100 MHz) δ ppm: 101.2 (CH_{Ar}), 104.6 (C_{Ar}), 116.1 (C_{Ar}), 122.6 (CH_{Ar}), 125.2 (2CH_{Ar}), 128.9 (2CH_{Ar}), 129.3 (C_{Ar}), 129.4 (CH_{Ar}), 129.5 (CH_{Ar}), 131.8 (C_{Ar}), 151.0 (C_{Ar}), 157.9 (C_{Ar}). IR-ATR, cm⁻¹: 3076, 1600, 1571, 1488, 1451, 1432, 1403, 1325, 1235, 1166, 1068, 1020, 905, 841, 758, 729, 683. Anal. Calcd. for C₁₄H₈Br₂O: C, 47.77; H, 2.29. Found: C, 47.51; H, 2.29.



2-Phenylbenzofuran-5-carbonitrile (13): Reaction time - 2 h. Flash, DCM/PE - 1:1. White solid (98% yield), mp 145-146 °C, (Lit.²⁶ 143-145 °C). ¹H NMR (CDCl₃, 400 MHz), δ ppm: 7.06 (d, *J*=0.8 Hz, 1H, CH_{Ar}); 7.40-7.44 (m, 1H, CH_{Ar}); 7.46-7.50 (m, 2H, CH_{Ar}); 7.55-7.61 (m, 2H, CH_{Ar}); 7.86-7.89 (m, 2H, CH_{Ar}); 7.92 (dd, *J*=1.6 Hz, *J*=0.8 Hz, 1H, CH_{Ar}). ¹³C NMR (CDCl₃, 100 MHz), δ ppm: 100.7 (CH_{Ar}); 106.9 (C_{Ar}); 112.3 (CH_{Ar}); 119.5 (C_{Ar}); 125.3 (2CH_{Ar}); 125.7 (CH_{Ar}); 127.9 (CH_{Ar}); 129.0 (2CH_{Ar}); 129.3 (C_{Ar}); 129.6 (CH_{Ar}); 129.9 (C_{Ar}); 156.5 (C_{Ar}); 158.4 (C_{Ar}). IR-ATR, cm⁻¹: 2982, 2225, 1464, 1268, 1020, 895, 824, 802, 766, 746, 738, 690, 618, 484.

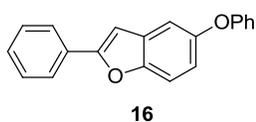


5-Nitro-2-phenylbenzofuran (14): Reaction time - 2 h. Flash, DCM/PE - 1:1. Yellow solid (91% yield), mp 150-151 °C, (Lit.²⁷ 151-152 °C). ¹H NMR (CDCl₃, 700 MHz), δ ppm: 7.14 (d, *J*=0.9 Hz, 1H, CH_{Ar}); 7.42-7.45 (m, 1H, CH_{Ar}); 7.48-7.51 (m, 2H, CH_{Ar}); 7.60 (d, *J*=9.1 Hz, 1H, CH_{Ar}); 7.89 (m, 2H, CH_{Ar}); 8.22 (dd, *J*=9.1 Hz, *J*=2.1 Hz, 1H, CH_{Ar}); 8.51 (d, *J*=2.1 Hz, 1H, CH_{Ar}). ¹³C NMR (CDCl₃, 175 MHz), δ ppm: 101.6 (CH_{Ar}); 111.4 (CH_{Ar}); 117.3 (CH_{Ar}); 120.1 (CH_{Ar}); 125.3 (2CH_{Ar}); 129.0 (2CH_{Ar}); 129.2 (C_{Ar}); 129.6 (C_{Ar}); 129.7 (CH_{Ar}); 144.4 (C_{Ar}); 157.6 (C_{Ar}); 159.3 (C_{Ar}). IR-ATR, cm⁻¹: 2982, 1514, 1347, 1335, 1265, 910, 904, 823, 803, 765, 748, 687, 488.



1-Phenyl-2-(2-phenylbenzofuran-5-yl)diazene (15): Reaction time - 4 h. Flash, DCM/PE - 2:8. Orange solid (77% yield), mp 149-150 °C. ¹H NMR (CDCl₃, 400 MHz) δ ppm: 7.15 (d, *J*=0.9 Hz, 1H, CH_{Ar}); 7.39-7.43 (m, 1H, CH_{Ar}); 7.48-7.57 (m, 5H, 5CH_{Ar}); 7.64-7.66 (m, 1H, CH_{Ar}); 7.91-7.99 (m, 5H, 5CH_{Ar}); 8.20 (dd, *J*=2.0 Hz, *J*=0.4 Hz, 1H, CH_{Ar}). ¹³C NMR (CDCl₃, 100 MHz) δ ppm: 102.0 (CH_{Ar}), 111.6 (CH_{Ar}), 116.3 (CH_{Ar}), 119.6 (CH_{Ar}), 122.7 (2CH_{Ar}), 125.1 (2CH_{Ar}), 128.9 (2CH_{Ar}), 128.9 (CH_{Ar}), 129.1 (2CH_{Ar}), 129.8 (C_{Ar}), 130.1 (C_{Ar}), 130.7 (CH_{Ar}), 149.3 (C_{Ar}), 152.7 (C_{Ar}), 156.5 (C_{Ar}), 157.5 (C_{Ar}). IR-ATR, cm⁻¹: 1470, 1443, 1274, 1262, 1206, 1096, 1019,

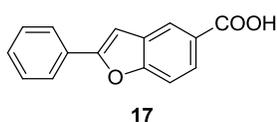
920, 897, 831, 808, 761, 745, 685. Anal. Calcd. for C₂₀H₁₄N₂O: C, 80.52; H, 4.73. Found: C, 80.21; H, 4.69.



5-Phenoxy-2-phenylbenzofuran (16): Reaction time - 3 h. Flash, DCM/PE - 2:8.

White solid (58% yield), mp 120-122 °C. ¹H NMR (CDCl₃, 700 MHz) δ ppm: 6.97 (d, *J*=0.7 Hz, 1H, CH_{Ar}); 6.99-7.01 (m, 3H, 3CH_{Ar}); 7.06-7.08 (m, 1H, CH_{Ar}); 7.22 (d, *J*=7.0 Hz, 1H, CH_{Ar}); 7.32-7.34 (m, 2H, 2CH_{Ar}); 7.36-7.38 (m, 1H, CH_{Ar});

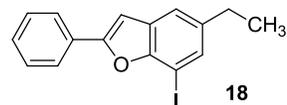
7.45-7.49 (m, 3H, 3CH_{Ar}), 7.85-7.87 (m, 2H, 2CH_{Ar}). ¹³C NMR (CDCl₃, 100 MHz) δ ppm: 101.0 (CH_{Ar}), 110.8 (CH_{Ar}), 111.5 (CH_{Ar}), 116.5 (CH_{Ar}), 117.5 (2CH_{Ar}), 122.2 (CH_{Ar}), 124.6 (2CH_{Ar}), 128.3 (CH_{Ar}), 128.4 (2CH_{Ar}), 129.3 (2CH_{Ar}), 129.8 (C_{Ar}), 129.9 (C_{Ar}), 151.1 (C_{Ar}), 152.2 (C_{Ar}), 156.8 (C_{Ar}), 158.2 (C_{Ar}). IR-ATR, cm⁻¹: 1586, 1488, 1459, 1441, 1219, 1205, 1188, 1128, 915, 848, 784, 743, 761, 692. Anal. Calcd. for C₂₀H₁₄O₂: C, 83.90; H, 4.93. Found: C, 83.56; H, 4.91.



2-Phenylbenzofuran-5-carboxylic acid (17): Reaction time - 24 h. Flash, DCM.

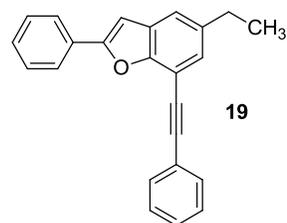
White solid (26% yield), mp 151-152 °C. ¹H NMR (CDCl₃, 400 MHz) δ ppm: 7.09 (s, 1H, CH_{Ar}); 7.38-7.41 (m, 1H, CH_{Ar}); 7.46-7.48 (m, 2H, 2CH_{Ar}); 7.57 (d, *J*=7.0 Hz, 1H, CH_{Ar}); 7.87-7.88 (m, 2H, 2CH_{Ar}); 8.07 (dd, *J*=8.5

Hz, *J*=1.7 Hz, 1H, CH_{Ar}); 8.38 (d, *J*=1.7 Hz 1H, CH_{Ar}). ¹³C NMR (DMSO-d₆, 100 MHz) δ ppm: 103.8 (CH_{Ar}), 112.6 (CH_{Ar}), 124.8 (CH_{Ar}), 126.2 (2CH_{Ar}), 127.7 (CH_{Ar}), 130.3 (C_{Ar}), 130.5 (C_{Ar}), 130.5 (2CH_{Ar}), 130.6 (CH_{Ar}), 130.7 (C_{Ar}), 158.0 (C_{Ar}), 158.1 (C_{Ar}), 169.0 (COOH). IR-ATR, cm⁻¹: 2962, 1683, 1594, 1491, 1444, 1402, 1259, 1171, 1091, 1018, 912, 866, 767, 751, 687, 667, 558, 526, 488. Anal. Calcd. for C₁₅H₁₀O₃: C, 75.62; H, 4.23. Found: C, 76.12; H, 4.16.



5-Ethyl-7-iodo-2-phenylbenzofuran (18) and 5-ethyl-2-phenyl-7-(phenylethynyl)benzofuran (19): When 4-ethyl-2,6-diiodophenol (**S17**) was taken to the reaction according to the general procedure two products were isolated. Reaction time 3 h. Flash, DCM/PE - 2:8. (**18**): white solid (46% yield),

mp 98-100 °C. ¹H NMR (CDCl₃, 400 MHz) δ ppm: 1.29 (t, *J*=8.0 Hz, 3H, CH₃); 2.72 (q, *J*=8.0 Hz, 2H, CH₂); 7.07 (s, 1H, CH_{Ar}); 7.35-7.36 (m, 1H, CH_{Ar}); 7.37-7.41 (m, 1H, CH_{Ar}); 7.46-7.48 (m, 2H, 2CH_{Ar}); 7.50-7.51 (m, 1H, CH_{Ar}); 7.88-7.91 (m, 2H, 2CH_{Ar}). ¹³C NMR (CDCl₃, 175 MHz,) δ ppm: 15.8 (CH₃), 28.1 (CH₂), 74.0 (C_{Ar}), 101.6 (CH_{Ar}), 119.4 (CH_{Ar}), 124.7 (2CH_{Ar}), 128.4 (2CH_{Ar}),

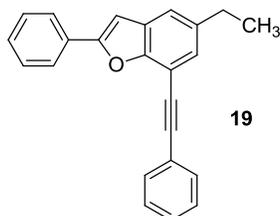


128.4 (CH_{Ar}), 128.9 (C_{Ar}), 129.8 (C_{Ar}), 132.9 (CH_{Ar}), 140.7 (C_{Ar}), 153.3 (C_{Ar}), 156.0 (C_{Ar}). IR-ATR, cm⁻¹: 2959, 1738, 1462, 1440, 1407, 1371, 1234, 1217, 1196, 1020, 910, 890, 857, 847, 761, 735, 684, 656. Anal. Calcd. for C₁₆H₁₃IO₂: C, 55.19; H, 3.76. Found: C, 55.12; H, 3.74. (**19**): Yellow solid (37%), mp 74-75 °C. ¹H NMR (CDCl₃, 400 MHz) δ ppm: 1.33 (t, *J*=8.0 Hz, 3H, CH₃); 2.77 (q, *J*=8.0 Hz, 2H, CH₂); 7.01 (s, 1H, CH_{Ar}); 7.33-7.34 (m, 1H, CH_{Ar}); 7.36-7.45 (m, 5H, 5CH_{Ar}); 7.46-7.50 (m, 2H, 2CH_{Ar}); 7.66-7.69 (m, 2H, 2CH_{Ar}); 7.92-7.94 (m, 2H, 2CH_{Ar}). ¹³C NMR (CDCl₃, 175 MHz,) δ ppm: 15.8 (CH₃), 28.3 (CH₂), 84.0 (C), 93.2 (C), 101.0 (CH_{Ar}), 106.5 (C_{Ar}), 119.9 (CH_{Ar}), 123.1 (C_{Ar}), 124.7 (2CH_{Ar}), 127.6 (CH_{Ar}), 128.0 (3CH_{Ar}), 128.3 (CH_{Ar}), 128.4 (2CH_{Ar}), 129.1 (C_{Ar}), 129.9 (C_{Ar}), 131.4 (2CH_{Ar}), 138.7 (C_{Ar}), 152.9 (C_{Ar}), 156.1 (C_{Ar}). IR-ATR, cm⁻¹: 2960, 1568, 1462, 1441, 1235, 1169, 1128, 1021, 911, 857, 761, 735, 684. Anal. Calcd. for C₂₄H₁₈O: C, 89.41; H, 5.63. Found: C, 89.67; H, 5.60.

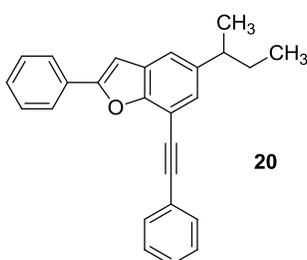
One-pot synthesis of 2-aryl-7-(phenylethynyl)benzofurans substituted in benzofuran moiety

General procedure

2-Aryl-7-(phenylethynyl)benzofurans were obtained using procedure 1.3 except that to the reaction were taken smaller amounts of 2,6-diiodophenol derivatives (1.3 mmol).

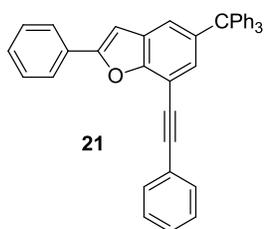


5-Ethyl-2-phenyl-7-(phenylethynyl)benzofuran (19): Reaction time 3 h. Flash, DCM/PE - 2:8. Light yellow solid (73% yield). Physical and spectral data identical as above.



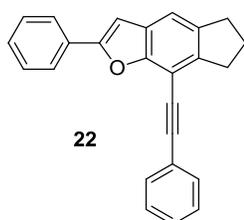
5-(sec-Butyl)-2-phenyl-7-(phenylethynyl)benzofuran (20): Reaction time 18 h. Flash, DCM/PE - 2:8. Yellow solid (67% yield), mp 79-82 °C. ¹H NMR (CDCl₃, 400 MHz) δ ppm: 0.88 (t, *J*=7.4 Hz, 3H, CH₃); 1.33 (d, *J*=7.0 Hz, 3H, CH₃); 1.69 (p, *J*=7.3 Hz, 2H, CH₂); 2.72 (sext, *J*=7.0 Hz, 1H, CH); 7.01 (s, 1H, CH_{Ar}); 7.33-7.34 (m, 1H, CH_{Ar}); 7.37-7.45 (m, 5H, 5CH_{Ar}); 7.46-7.51 (m, 2H, 2CH_{Ar}); 7.67-7.71 (m, 2H, 2CH_{Ar}); 7.93-7.95 (m, 2H, 2CH_{Ar}). ¹³C NMR (CDCl₃, 100 MHz,) δ ppm: 12.3 (CH₃), 22.3

(CH₃), 31.5 (CH₂), 41.6 (CH), 84.4 (C_{Ar}), 93.4 (C_{Ar}), 101.4 (CH_{Ar}), 106.8 (C_{Ar}), 119.6 (CH_{Ar}), 123.5 (C_{Ar}), 125.1 (2CH_{Ar}), 127.1 (CH_{Ar}), 128.4 (3CH_{Ar}), 128.6 (CH_{Ar}), 128.8 (2CH_{Ar}), 129.4 (C_{Ar}), 130.4 (C_{Ar}), 131.8 (2CH_{Ar}), 142.6 (C_{Ar}), 153.4 (C_{Ar}), 156.6 (C_{Ar}). IR-ATR, cm⁻¹: 2595, 1488, 1466, 1422, 1412, 1228, 1069, 1039, 1020, 911, 855, 804, 793, 761, 746, 687, 579, 520, 491. Anal. Calcd. for C₂₆H₂₂O: C, 89.11; H, 6.33. Found: C, 88.88; H, 6.37.



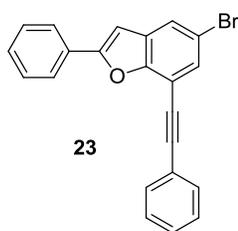
2-Phenyl-7-(phenylethynyl)-5-tritylbenzofuran (21): Reaction time 3 h. Flash, DCM/PE - 2:8. Yellow solid (36% yield), mp 91-93 °C. ¹H NMR (CDCl₃, 400 MHz) δ ppm: 6.94 (s, 1H, CH_{Ar}); 7.22-7.25 (m, 3H, 3CH_{Ar}); 7.26-7.28-7.30 (m, 12H, 12CH_{Ar}); 7.35-7.39 (m, 4H, 4CH_{Ar}); 7.42-7.43 (m, 1H, CH_{Ar}); 7.45-7.47 (m, 3H, 3CH_{Ar}); 7.60-7.62 (m, 2H, 2CH_{Ar}), 7.86-7.88 (m, 2H, 2CH_{Ar}). ¹³C NMR (CDCl₃, 176 MHz) δ ppm: 64.5 (C), 83.9 (C_{Ar}), 93.3 (C_{Ar}), 101.5 (CH_{Ar}),

105.8 (C_{Ar}), 122.8 (C_{Ar}), 123.3 (CH_{Ar}), 124.6 (2CH_{Ar}), 125.6 (3CH_{Ar}), 127.2 (6CH_{Ar}), 127.9 (2CH_{Ar}), 128.0 (CH_{Ar}), 128.2 (C_{Ar}), 128.3 (CH_{Ar}), 128.4 (2CH_{Ar}), 129.8 (C_{Ar}), 130.8 (6CH_{Ar}), 131.2 (CH_{Ar}), 131.4 (2CH_{Ar}), 141.6 (C_{Ar}), 146.6 (3C_{Ar}), 152.6 (C_{Ar}), 156.3 (C_{Ar}). IR-ATR, cm⁻¹: 1489, 1442, 1259, 1228, 1038, 1019, 912, 866, 796, 747, 716, 700, 687, 666, 642, 626, 572. Anal. Calcd. for C₄₁H₂₈O: C, 91.76; H, 5.26. Found: C, 91.55; H, 5.29.



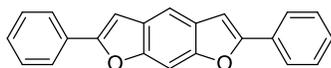
2-Phenyl-8-(phenylethynyl)-6,7-dihydro-5H-indeno[5,6-b]furan (22): Reaction time 4 h. Flash, DCM/PE - 2:8. Light yellow solid (76% yield), mp 66.5-68 °C. ¹H NMR (CDCl₃, 400 MHz), δ ppm: 2.16 (p, *J*=7.4 Hz, 2H, CH₂); 3.01 (t, *J*=7.4 Hz, 2H, CH₂); 3.13 (t, *J*=7.4 Hz, 2H, CH₂); 7.04 (s, 1H, CH_{Ar}); 7.27 (s, 1H, CH_{Ar}); 7.31-7.38 (m, 4H, CH_{Ar}); 7.42-7.47 (m, 2H, CH_{Ar}); 7.52-7.55 (m, 2H, CH_{Ar}); 7.86-7.89 (m, 2H, CH_{Ar}). ¹³C NMR (CDCl₃, 100 MHz), δ ppm: 25.1 (CH₂); 34.2 (CH₂);

37.6 (CH₂); 73.9 (C_{Ar}); 74.0 (C_{Ar}); 81.6 (C_{Ar}); 102.1 (CH_{Ar}); 115.6 (CH_{Ar}); 121.8 (C_{Ar}); 124.8 (2CH_{Ar}); 127.9 (C_{Ar}); 128.5 (2CH_{Ar}); 128.5 (CH_{Ar}); 128.8 (2CH_{Ar}); 129.2 (CH_{Ar}); 130.3 (C_{Ar}); 132.5 (2CH_{Ar}); 139.7 (C_{Ar}); 145.6 (C_{Ar}); 154.4 (C_{Ar}); 155.7 (C_{Ar}). IR-ATR, cm⁻¹: 2982, 1338, 1184, 1069, 1021, 886, 803, 756, 734, 684, 654, 625, 505. Anal. Calcd. for C₂₅H₁₈O: C, 89.79; H, 5.43. Found: C, 89.99; H, 5.48.



23

5-Bromo-2-phenyl-7-(phenylethynyl)benzofuran (23): Reaction time 2 h at 40 °C and 1 h at 80 °C. Flash, DCM/PE - 2:8. Yellow solid (75% yield), mp 139-141 °C. ¹H NMR (CDCl₃, 700 MHz) δ ppm: 6.98 (s, 1H, CH_{Ar}); 7.38-7.43 (m, 4H, 4CH_{Ar}); 7.46-7.49 (m, 2H, 2CH_{Ar}); 7.56-7.57 (m, 1H, CH_{Ar}); 7.64-7.68 (m, 3H, 3CH_{Ar}); 7.89-7.92 (m, 2H, 2CH_{Ar}). ¹³C NMR (CDCl₃, 176 MHz) δ ppm: 82.2 (C_{Ar}), 94.7 (C_{Ar}), 100.3 (CH_{Ar}), 108.7 (C_{Ar}), 115.1 (C_{Ar}), 122.4 (C_{Ar}), 123.3 (CH_{Ar}), 124.9 (2CH_{Ar}), 128.1 (2CH_{Ar}), 128.4 (CH_{Ar}), 128.5 (2CH_{Ar}), 128.9 (CH_{Ar}), 129.2 (C_{Ar}), 129.5 (CH_{Ar}), 130.7 (C_{Ar}), 131.5 (2CH_{Ar}), 153.0 (C_{Ar}), 157.2 (C_{Ar}). IR-ATR, cm⁻¹: 1738, 1575, 1488, 1441, 1365, 1226, 1071, 1020, 912, 854, 799, 763, 753, 744, 685, 569, 516, 487. Anal. Calcd. for C₂₂H₁₃BrO: C, 70.79; H, 3.51. Found: C, 71.12; H, 3.47.



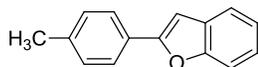
24

2,6-Diphenylbenzo[1,2-*b*:5,4-*b'*]difuran (24): Reaction time 24 h. Flash, AcOEt/PE - 8:92. Light orange solid (55% yield), mp 269-270 °C, (Lit.²⁸ 272-273 °C). ¹H NMR (CDCl₃, 700 MHz), δ ppm: 7.09 (d, *J*=0.9 Hz, 1H, CH_{Ar}); 7.33-7.38 (m, 3H, CH_{Ar}); 7.45-7.48 (m, 4H, CH_{Ar}); 7.52-7.55 (m, 1H, CH_{Ar}); 7.67 (m, 2H, CH_{Ar}); 7.89 (m, 3H, CH_{Ar}). ¹³C NMR (CDCl₃, 175 MHz), δ ppm: 94.3 (CH_{Ar}); 101.1 (2CH_{Ar}); 110.8 (CH_{Ar}); 124.7 (2CH_{Ar}); 126.2 (2C_{Ar}); 128.4 (2CH_{Ar}); 128.8 (4CH_{Ar}); 130.6 (2C_{Ar}); 131.6 (CH_{Ar}); 132.5 (CH_{Ar}); 153.5 (2C_{Ar}); 156.2 (2C_{Ar}). IR-ATR, cm⁻¹: 2922, 1260, 1091, 1072, 1016, 842, 798, 757, 747, 687, 652, 490.

One-pot synthesis of 2-arylbenzofurans substituted at 2-aryl position.

General procedure

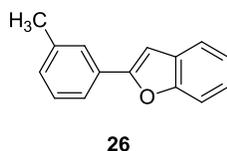
In a Schlenk tube equipped with magnetic stirring bar and reflux condenser, Pd(dppf)Cl₂ (0.0293 g; 0.04 mmol), CuI (0.0076 g; 0.04 mmol), and appropriate iodobenzene derivative (2 mmol) were added under argon atmosphere followed by dry degassed toluene (3 mL) and diisopropylamine (1.50 mL; 11 mmol). The mixture was stirred for 5 min. and TMSA (0.245 g; 2.5 mmol) in toluene (2 mL) was added at RT. It was stirred at this temperature until all iodobenzene derivative was consumed (GC, 5-15 min.). TBAF 1M in THF (4 mL; 4 mmol) was added followed by 2-iodophenole (3 mmol). Temperature was increased to 80 °C, and the mixture was stirred at this temperature for 2-24 h (TLC). Reaction was quenched with 10% aqueous citric acid (20 mL) and extracted with DCM (3×20 mL). Combined extracts were washed with 10% aqueous NaOH (20 mL), water and dried with anhydrous magnesium sulfate. Solvent was removed by rotary evaporation and the crude product was purified using flash chromatography.



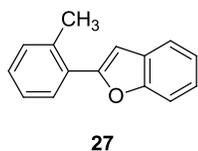
25

2-(*p*-Tolyl)benzofuran (25): Reaction time 2 h. Flash, DCM/PE - 2:8. White solid (84% yield), mp 123-124 °C, (Lit.²⁹ 122-124 °C). ¹H NMR (CDCl₃, 700 MHz),

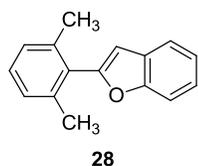
δ ppm: 2.40 (s, 3H, CH₃); 6.97 (d, $J=0.7$ Hz, 1H, CH_{Ar}); 7.21-7.23 (m, 1H, CH_{Ar}); 7.25-7.27 (m, 3H, CH_{Ar}); 7.50-7.52 (m, 1H, CH_{Ar}); 7.56-7.58 (m, 1H, CH_{Ar}); 7.75-7.78 (m, 2H, CH_{Ar}). ¹³C NMR (CDCl₃, 175 MHz), δ ppm: 22.5 (CH₃); 100.2 (CH_{Ar}); 110.7 (CH_{Ar}); 120.3 (CH_{Ar}); 122.5 (CH_{Ar}); 123.6 (CH_{Ar}); 124.5 (2CH_{Ar}); 127.4 (C_{Ar}); 129.0 (C_{Ar}); 129.1 (2CH_{Ar}); 138.2 (C_{Ar}); 154.4 (C_{Ar}); 155.8 (C_{Ar}). IR-ATR, cm⁻¹: 2979, 1504, 1449, 1254, 1168, 1105, 1033, 919, 823, 800, 748, 736, 501.



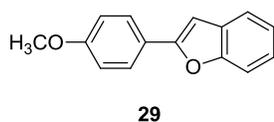
2-(m-Tolyl)benzofuran (26): Reaction time 2 h. Flash, DCM/PE - 2:8. White solid (75% yield), mp 76-77 °C, (Lit.²⁹ 76-78 °C). ¹H NMR (CDCl₃, 700 MHz), δ ppm: 2.44 (s, 3H, CH₃); 7.02 (d, $J=0.9$ Hz, 1H, CH_{Ar}); 7.18 (d, $J=7.3$ Hz, 1H, CH_{Ar}); 7.22-7.25 (m, 1H, CH_{Ar}); 7.27-7.30 (m, 1H, CH_{Ar}); 7.33-7.36 (m, 1H, CH_{Ar}); 7.53 (d, $J=8.2$ Hz, 1H, CH_{Ar}); 7.58-7.59 (m, 1H, CH_{Ar}); 7.68 (d, $J=7.7$ Hz, 1H, CH_{Ar}); 7.71 (s, 1H, CH_{Ar}). ¹³C NMR (CDCl₃, 175 MHz), δ ppm: 21.4 (CH₃); 101.2 (CH_{Ar}); 111.1 (CH_{Ar}); 120.8 (CH_{Ar}); 122.1 (CH_{Ar}); 122.9 (CH_{Ar}); 124.1 (CH_{Ar}); 125.2 (CH_{Ar}); 128.7 (CH_{Ar}); 129.3 (C_{Ar}); 129.3 (CH_{Ar}); 130.4 (C_{Ar}); 138.4 (C_{Ar}); 154.9 (C_{Ar}); 156.1 (C_{Ar}). IR-ATR, cm⁻¹: 2982, 1448, 1256, 1169, 1090, 1047, 932, 881, 807, 782, 745, 691, 664.



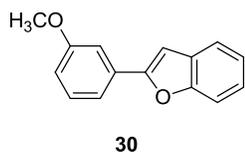
2-(o-Tolyl)benzofuran (27): Reaction time 2 h. Flash, DCM/PE - 2:8. White solid (75% yield), mp 97-98 °C (Lit.³⁰ 96-98 °C). ¹H NMR (CDCl₃, 700 MHz), δ ppm: 2.55 (s, 3H, CH₃); 6.86 (d, $J=0.9$ Hz, 1H, CH_{Ar}); 7.19-7.22 (m, 1H, CH_{Ar}); 7.25-7.29 (m, 4H, CH_{Ar}); 7.50 (d, $J=8.2$ Hz, 1H, CH_{Ar}); 7.58 (d, $J=7.7$ Hz, 1H, CH_{Ar}); 7.81 (d, $J=7.7$ Hz, 1H, CH_{Ar}). ¹³C NMR (CDCl₃, 175 MHz), δ ppm: 21.9 (CH₃); 105.1 (CH_{Ar}); 111.1 (CH_{Ar}); 120.9 (CH_{Ar}); 122.8 (CH_{Ar}); 124.2 (CH_{Ar}); 126.1 (CH_{Ar}); 128.1 (CH_{Ar}); 128.5 (CH_{Ar}); 129.1 (C_{Ar}); 129.9 (C_{Ar}); 131.2 (CH_{Ar}); 135.9 (C_{Ar}); 154.3 (C_{Ar}); 155.6 (C_{Ar}). IR-ATR, cm⁻¹: 2979, 1452, 1256, 1169, 1120, 1018, 921, 886, 804, 760, 746, 719, 452.



2-(2,6-Dimethylphenyl)benzofuran (28): Reaction time 8 h. Flash, AcOEt/PE - 1:9. Light yellow oil (90% yield). ¹H NMR (CDCl₃, 400 MHz) δ ppm: 2.26 (s, 6H, 2CH₃); 6.67 (d, $J=0.9$ Hz, 1H, CH_{Ar}); 7.14-7.16 (m, 2H, 2CH_{Ar}); 7.24-7.25 (m, 1H, CH_{Ar}); 7.27-7.33 (m, 2H, 2CH_{Ar}); 7.51-7.53 (m, 1H, CH_{Ar}); 7.62-7.64 (m, 1H, CH_{Ar}). ¹³C NMR (CDCl₃, 100 MHz) δ ppm: 20.6 (2CH₃); 106.1 (CH_{Ar}); 111.2 (CH_{Ar}); 120.8 (CH_{Ar}); 122.7 (CH_{Ar}); 123.8 (CH_{Ar}); 127.6 (2CH_{Ar}); 128.8 (C_{Ar}); 129.2 (CH_{Ar}); 130.6 (C_{Ar}); 138.6 (2C_{Ar}); 154.8 (C_{Ar}); 154.8 (C_{Ar}). IR-ATR, cm⁻¹: 2959, 1467, 1446, 1256, 1202, 1160, 1109, 1005, 917, 826, 771, 748.

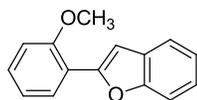


2-(4-Methoxyphenyl)benzofuran (29): Reaction time 2 h. Flash, DCM/PE - 3:7. White solid (86% yield), mp 143-144 °C, (Lit.³¹ 143-145 °C). ¹H NMR (CDCl₃, 700 MHz), δ ppm: 3.87 (s, 3H, CH₃); 6.89 (d, $J=0.9$ Hz, 1H, CH_{Ar}); 6.97-7.00 (m, 2H, CH_{Ar}); 7.20-7.23 (m, 1H, CH_{Ar}); 7.24-7.27 (m, 1H, CH_{Ar}); 7.50 (m, 1H, CH_{Ar}); 7.56 (m, 1H, CH_{Ar}); 7.79-7.82 (m, 2H, CH_{Ar}). ¹³C NMR (CDCl₃, 175 MHz), δ ppm: 55.4 (CH₃); 99.7 (CH_{Ar}); 111.0 (CH_{Ar}); 114.2 (2CH_{Ar}); 120.5 (CH_{Ar}); 122.8 (CH_{Ar}); 123.3 (C_{Ar}); 123.7 (CH_{Ar}); 126.4 (2CH_{Ar}); 129.5 (C_{Ar}); 154.7 (C_{Ar}); 156.0 (C_{Ar}); 159.9 (C_{Ar}). IR-ATR, cm⁻¹: 2982, 1610, 1505, 1451, 1243, 1178, 1169, 1022, 1006, 836, 818, 800, 749, 742, 520.



2-(3-Methoxyphenyl)benzofuran (30): Reaction time 2 h. Flash, DCM/PE - 3:7. White solid (88% yield), mp 50.5-51 °C, (Lit.¹⁸ 50-51 °C). ¹H NMR (CDCl₃, 700 MHz), δ ppm: 3.90 (s, 3H, CH₃); 6.91 (ddd, $J=8.2$ Hz, $J=2.6$ Hz, $J=0.7$ Hz, 1H,

CH_{Ar}); 7.03 (d, *J*=0.8 Hz, 1H, CH_{Ar}); 7.22-7.25 (m, 1H, CH_{Ar}); 7.28-7.31 (m, 1H, CH_{Ar}); 7.36 (t, *J*=8.2 Hz, 1H, CH_{Ar}); 7.41-7.42 (m, 1H, CH_{Ar}); 7.46-7.47 (m, 1H, CH_{Ar}); 7.53 (d, *J*=8.4 Hz, 1H, CH_{Ar}); 7.58-7.59 (m, 1H, CH_{Ar}). ¹³C NMR (CDCl₃, 175 MHz), δ ppm: 55.3 (CH₃); 101.6 (CH_{Ar}); 110.1 (CH_{Ar}); 111.1 (CH_{Ar}); 114.4 (CH_{Ar}); 117.5 (CH_{Ar}); 120.9 (CH_{Ar}); 122.9 (CH_{Ar}); 124.3 (CH_{Ar}); 129.1 (C_{Ar}); 129.8 (CH_{Ar}); 131.7 (C_{Ar}); 154.8 (C_{Ar}); 155.7 (C_{Ar}); 159.8 (C_{Ar}). IR-ATR, cm⁻¹: 2971, 1258, 1233, 1165, 1083, 1047, 1010, 806, 794, 748, 736, 688, 455.



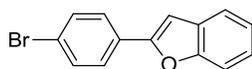
31

2-(2-Methoxyphenyl)benzofuran (31): Reaction time 2 h. Flash, DCM/PE - 3:7.

White solid (59% yield), mp 77-78 °C, (Lit.¹⁸ 77-78 °C). ¹H NMR (CDCl₃, 700 MHz), δ ppm: 4.02 (s, 3H, CH₃); 7.02 (d, *J*=8.2 Hz, 1H, CH_{Ar}); 7.08-7.10 (m, 1H, CH_{Ar});

7.21-7.23 (m, 1H, CH_{Ar}); 7.26-7.29 (m, 1H, CH_{Ar}); 7.32-7.34 (m, 1H, CH_{Ar}); 7.36 (s,

1H, CH_{Ar}); 7.52 (d, *J*=8.2 Hz, 1H, CH_{Ar}); 7.60 (d, *J*=7.5 Hz, 1H, CH_{Ar}); 8.08 (dd, *J*=7.7 Hz, *J*=1.7 Hz, 1H, CH_{Ar}). ¹³C NMR (CDCl₃, 175 MHz), δ ppm: 55.4 (CH₃); 106.3 (CH_{Ar}); 110.8 (CH_{Ar}); 111.0 (CH_{Ar}); 119.3 (C_{Ar}); 120.7 (CH_{Ar}); 121.0 (CH_{Ar}); 122.6 (CH_{Ar}); 124.1 (CH_{Ar}); 127.0 (CH_{Ar}); 129.2 (CH_{Ar}); 129.8 (C_{Ar}); 152.1 (C_{Ar}); 153.9 (C_{Ar}); 156.5 (C_{Ar}). IR-ATR, cm⁻¹: 2961, 1259, 1249, 1165, 1119, 1087, 1055, 1024, 1014, 800, 759, 740, 662.

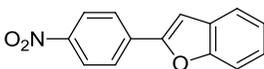


32

2-(4-Bromophenyl)benzofuran (32): Reaction time 4 h. Flash, DCM/PE - 2:8.

Light yellow solid (82% yield), mp 150-151 °C; (Lit.²⁰ 149-150 °C). ¹H NMR (CDCl₃, 700 MHz) δ ppm: 7.03 (d, *J*=0.8 Hz, 1H, CH_{Ar}); 7.23-7.25 (m, 1H, CH_{Ar});

7.29-7.31 (m, 1H, CH_{Ar}); 7.51-7.52 (m, 1H, CH_{Ar}); 7.57-7.60 (m, 3H, 3CH_{Ar}); 7.72-7.74 (m, 2H, 2CH_{Ar}). ¹³C NMR (CDCl₃, 176 MHz) δ ppm: 101.5 (CH_{Ar}), 110.8 (CH_{Ar}), 120.6 (CH_{Ar}), 122.1 (C_{Ar}), 122.7 (CH_{Ar}), 124.2 (CH_{Ar}), 126.0 (2CH_{Ar}), 128.6 (C_{Ar}), 129.2 (C_{Ar}), 131.6 (2CH_{Ar}), 154.4 (C_{Ar}), 154.5 (C_{Ar}). IR-ATR, cm⁻¹: 1735, 1486, 1448, 1340, 1258, 1169, 1105, 1071, 1006, 919, 801, 749, 743, 502.

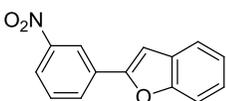


33

2-(4-Nitrophenyl)benzofuran (33): Reaction time 6 h. Flash, DCM/PE - 2:8.

Yellow solid (83% yield), mp 181-182 °C (lit.³² 181-183 °C). ¹H NMR (CDCl₃, 400 MHz) δ ppm: 7.24 (d, *J*=0.9 Hz, 1H, CH_{Ar}); 7.26-7.31 (m, 1H, CH_{Ar}); 7.35-

7.40 (m, 1H, CH_{Ar}); 7.55-7.57 (m, 1H, CH_{Ar}); 7.64-7.66 (m, 1H, CH_{Ar}); 8.00-8.03 (m, 2H, 2CH_{Ar}); 8.30-8.33 (m, 2H, 2CH_{Ar}). ¹³C NMR (CDCl₃, 100 MHz) δ ppm: 105.1 (CH_{Ar}), 111.5 (CH_{Ar}), 121.6 (CH_{Ar}), 123.5 (CH_{Ar}), 124.3 (2CH_{Ar}), 125.2 (2CH_{Ar}), 125.8 (CH_{Ar}), 128.7 (C_{Ar}), 136.3 (C_{Ar}), 147.3 (C_{Ar}), 153.3 (C_{Ar}), 155.5 (C_{Ar}). IR-ATR, cm⁻¹: 1598, 1514, 1447, 1301, 1335, 1279, 1180, 1168, 1106, 1030, 851, 808, 759, 750, 690.

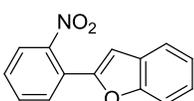


34

2-(3-Nitrophenyl)benzofuran (34): Reaction time 6 h. Flash, DCM/PE - 2:8. Light

yellow solid (68% yield), mp 136-138 °C, (lit.³³ 136-138 °C). ¹H NMR (CDCl₃, 400 MHz) δ ppm: 7.19 (d, *J*=0.9 Hz, 1H, CH_{Ar}); 7.26-7.30 (m, 1H, CH_{Ar}); 7.33-7.38

(m, 1H, CH_{Ar}); 7.55-7.58 (m, 1H, CH_{Ar}); 7.61-7.65 (m, 2H, 2CH_{Ar}); 8.15-8.20 (m, 2H, 2CH_{Ar}); 8.70-8.71 (m, 1H, CH_{Ar}). ¹³C NMR (CDCl₃, 100 MHz) δ ppm: 103.2 (CH_{Ar}), 111.0 (CH_{Ar}), 119.3 (CH_{Ar}), 121.0 (CH_{Ar}), 122.4 (CH_{Ar}), 123.0 (CH_{Ar}), 125.0 (CH_{Ar}), 128.3 (C_{Ar}), 129.5 (CH_{Ar}), 129.9 (CH_{Ar}), 131.7 (C_{Ar}), 148.4 (C_{Ar}), 152.7 (C_{Ar}), 154.7 (C_{Ar}). IR-ATR, cm⁻¹: 1524, 1478, 1449, 1345, 1304, 798, 761, 734, 678.

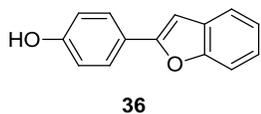


35

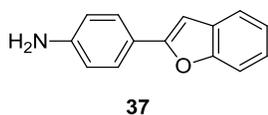
2-(2-Nitrophenyl)benzofuran (35): Reaction time 6 h. Flash, DCM/PE - 2:8. Light

yellow oil (48% yield). ¹H NMR (CDCl₃, 400 MHz) δ ppm: 7.02 (d, *J*=0.9 Hz, 1H, CH_{Ar}); 7.24-7.29 (m, 1H, CH_{Ar}); 7.31-7.36 (m, 1H, CH_{Ar}); 7.49-7.53

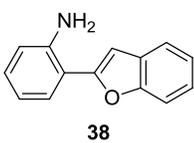
(m, 2H, 2CH_{Ar}); 7.61-7.67 (m, 2H, 2CH_{Ar}); 7.78 (dd, *J*=8.0 Hz, *J*=1.2 Hz, 1H, CH_{Ar}); 7.87 (dd, *J*=8.0 Hz, *J*=1.2 Hz, 1H, CH_{Ar}). ¹³C NMR (CDCl₃, 100 MHz) δ ppm: 107.1 (CH_{Ar}), 121.4 (CH_{Ar}), 122.5 (CH_{Ar}), 124.3 (CH_{Ar}), 125.0 (CH_{Ar}), 125.2 (C_{Ar}), 126.4 (CH_{Ar}), 129.5 (C_{Ar}), 130.3 (CH_{Ar}), 130.9 (CH_{Ar}), 133.0 (CH_{Ar}), 149.3 (C_{Ar}), 151.4 (C_{Ar}), 156.2 (C_{Ar}). IR-ATR, cm⁻¹: 1527, 1449, 1442, 1361, 1254, 1201, 1163, 1018, 921, 813, 783, 743, 699.



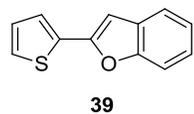
4-(Benzofuran-2-yl)phenol (36): Reaction time 2 h. Flash, DCM/PE - 2:8. Light yellow solid (54% yield), mp 192.5-194 °C, (Lit.³⁴ 194-195 °C). ¹H NMR (CDCl₃, 700 MHz), δ ppm: 4.89 (s, 1H, OH); 6.88 (d, *J*=0.9 Hz, 1H, CH_{Ar}); 6.90-6.93 (m, 2H, CH_{Ar}); 7.20-7.23 (m, 1H, CH_{Ar}); 7.24-7.27 (m, 1H, CH_{Ar}); 7.49-7.50 (m, 1H, CH_{Ar}); 7.55-7.56 (m, 1H, CH_{Ar}); 7.75-7.78 (m, 2H, CH_{Ar}). ¹³C NMR (CDCl₃, 175 MHz), δ ppm: 99.3 (CH_{Ar}); 110.6 (CH_{Ar}); 115.3 (2CH_{Ar}); 120.2 (CH_{Ar}); 122.4 (CH_{Ar}); 123.3 (C_{Ar}); 123.4 (CH_{Ar}); 126.3 (2CH_{Ar}); 129.0 (C_{Ar}); 154.3 (C_{Ar}); 155.9 (2C_{Ar}). IR-ATR, cm⁻¹: 3407, 2982, 1610, 1502, 1430, 1247, 1211, 1169, 1106, 1032, 832, 804, 750, 740, 516.



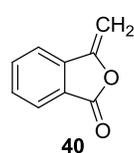
4-(Benzofuran-2-yl)aniline (37): Reaction time 2 h. Flash, DCM/PE - 2:8. Light beige solid (45% yield), mp 149-150 °C, (Lit.³³ 149-151 °C). ¹H NMR (CDCl₃, 700 MHz), δ ppm: 3.84 (bs, 2H, NH₂); 6.73-6.76 (m, 2H, CH_{Ar}); 6.81 (d, *J*=0.7 Hz, 1H, CH_{Ar}); 7.18-7.24 (m, 2H, CH_{Ar}); 7.47-7.48 (m, 1H, CH_{Ar}); 7.52-7.53 (m, 1H, CH_{Ar}); 7.66-7.69 (m, 2H, CH_{Ar}). ¹³C NMR (CDCl₃, 175 MHz), δ ppm: 98.2 (CH_{Ar}); 110.5 (CH_{Ar}); 114.7 (2CH_{Ar}); 119.9 (CH_{Ar}); 120.7 (C_{Ar}); 122.3 (CH_{Ar}); 123.0 (CH_{Ar}); 126.0 (2CH_{Ar}); 129.3 (C_{Ar}); 146.6 (C_{Ar}); 154.1 (C_{Ar}); 156.3 (C_{Ar}). IR-ATR, cm⁻¹: 3386, 2977, 1614, 1505, 1452, 1295, 1254, 1163, 833, 797, 747, 515, 468.



2-(Benzofuran-2-yl)aniline (38): Reaction time 2 h. Flash, DCM/PE - 2:8. Gray solid (88% yield), mp 65-66 °C, (Lit.³⁵ 64-66 °C). ¹H NMR (CDCl₃, 700 MHz), δ ppm: 4.50 (bs, 2H, NH₂); 6.80 (dd, *J*=8.4 Hz, *J*=0.9 Hz, 1H, CH_{Ar}); 6.84-6.87 (m, 1H, CH_{Ar}); 6.95 (d, *J*=0.9 Hz, 1H, CH_{Ar}); 7.18-7.21 (m, 1H, CH_{Ar}); 7.25-7.28 (m, 1H, CH_{Ar}); 7.28-7.31 (m, 1H, CH_{Ar}); 7.53-7.54 (m, 1H, CH_{Ar}); 7.60-7.61 (m, 1H, CH_{Ar}); 7.64 (dd, *J*=7.7 Hz, *J*=1.4 Hz, 1H, CH_{Ar}). ¹³C NMR (CDCl₃, 175 MHz), δ ppm: 103.0 (CH_{Ar}); 111.0 (CH_{Ar}); 115.5 (C_{Ar}); 116.8 (CH_{Ar}); 118.5 (CH_{Ar}); 120.7 (CH_{Ar}); 123.0 (CH_{Ar}); 124.0 (CH_{Ar}); 128.6 (CH_{Ar}); 128.9 (C_{Ar}); 129.8 (CH_{Ar}); 144.2 (C_{Ar}); 154.3 (C_{Ar}); 155.6 (C_{Ar}). IR-ATR, cm⁻¹: 3407, 2982, 1613, 1578, 1487, 1459, 1444, 1256, 1246, 1138, 1012, 796, 738, 469



2-(Thiophen-2-yl)benzofuran (39): Reaction time 4 h. Flash, DCM/PE - 2:8. Light gray solid (88% yield), mp 90-92 °C, (Lit.³⁶ 89-92 °C). ¹H NMR (CDCl₃, 700 MHz) δ ppm: 6.87 (d, *J*=0.8 Hz, 1H, CH_{Ar}), 7.10-7.12 (m, 1H, CH), 7.21-7.24 (m, 1H, CH_{Ar}), 7.26-7.29 (m, 1H, CH_{Ar}), 7.34-7.35 (m, 1H, CH_{Ar}), 7.49-7.50 (m, 2H, 2CH_{Ar}), 7.54-7.56 (m, 1H, CH_{Ar}). ¹³C NMR (CDCl₃, 176 MHz) δ ppm: 100.7 (CH_{Ar}), 110.7 (CH_{Ar}), 120.4 (CH_{Ar}), 122.7 (CH_{Ar}), 123.9 (CH_{Ar}), 124.2 (CH_{Ar}), 125.4 (CH_{Ar}), 127.5 (CH_{Ar}), 128.7 (C_{Ar}), 132.9 (C_{Ar}), 150.9 (C_{Ar}), 154.2 (C_{Ar}). IR-ATR, cm⁻¹: 1738, 1450, 1420, 1368, 1252, 1202, 996, 848, 801, 746, 700.

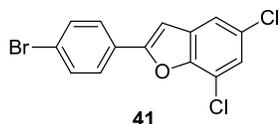


3-Methyleneisobenzofuran-1(3H)-one (40): Reaction time 18 h. Flash, DCM/PE - 2:8. Light gray solid (31% yield), mp 52-54 °C; (lit.³⁷ 54-56 °C). ¹H NMR (CDCl₃, 700 MHz) δ ppm: 5.22-5.23 (m, 2H, CH₂); 7.57-7.60 (m, 1H, CH_{Ar}); 7.73 (d, *J*=3.9 Hz, 2H, 2CH_{Ar}); 7.90-7.92 (m, 1H, CH_{Ar}). ¹³C NMR (CDCl₃, 176 MHz) δ ppm: 92.2 (CH₂), 121.6 (CH_{Ar}), 126.1 (C_{Ar}), 126.2 (CH_{Ar}), 131.5 (CH_{Ar}), 135.5 (CH_{Ar}), 140.0 (C_{Ar}), 152.8 (C), 167.8 (C=O).

One-pot synthesis of 2-arylbenzofurans substituted both at 2-aryl position and at benzofuran ring

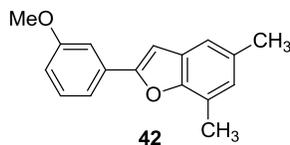
General procedure

2-Arylbenzofurans substituted both at 2-aryl position and at benzofuran ring were obtained according to procedure 1.3 except that appropriate iodobenzene derivative was taken to the reaction instead of iodobenzene.



2-(4-Bromophenyl)-5,7-dichlorobenzofuran (41): Reaction time 3 h. Flash, AcOEt/PE - 1:9. Orange solid (80% yield), mp 144.5-145 °C. ¹H NMR (CDCl₃, 700 MHz) δ ppm: 6.99 (s, 1H, CH_{Ar}); 7.29-7.30 (m, 1H, CH_{Ar}); 7.45 (m, 1H, CH_{Ar}); 7.59-7.61 (m, 2H, 2CH_{Ar}); 7.73-7.80 (m, 2H, 2CH_{Ar}). ¹³C NMR

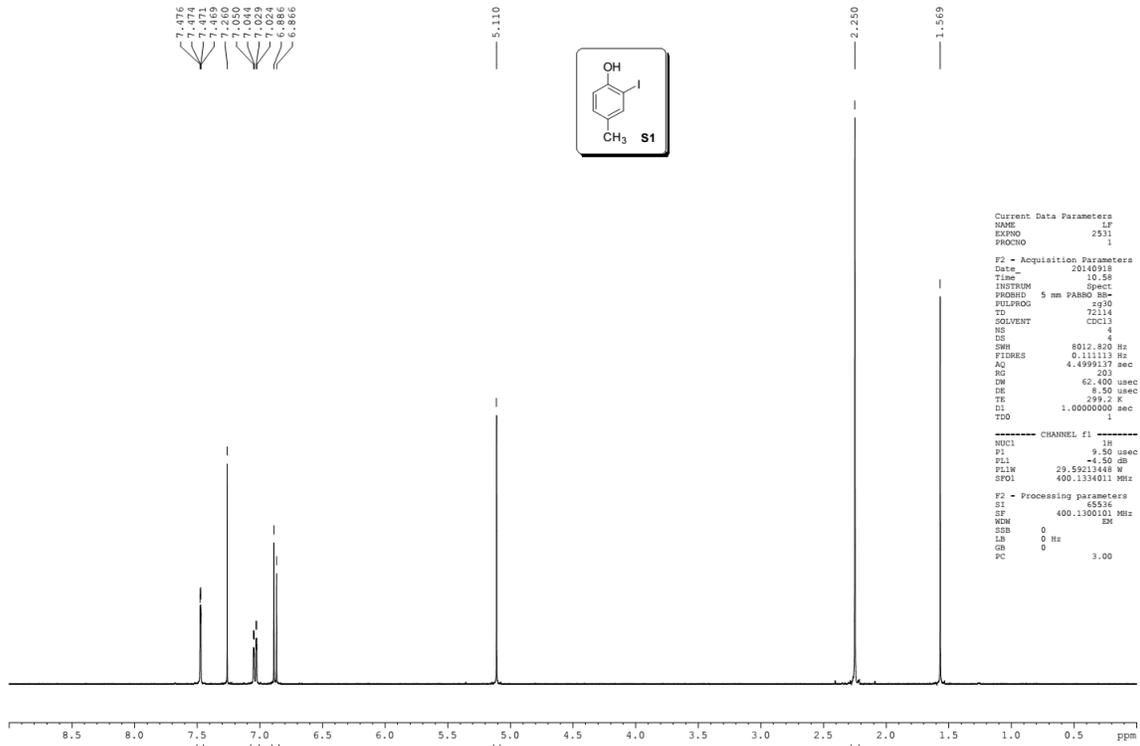
(CDCl₃, 100 MHz) δ ppm: 101.3 (CH_{Ar}), 116.8 (C_{Ar}), 118.7 (CH_{Ar}), 123.2 (C_{Ar}), 124.2 (CH_{Ar}), 126.3 (2CH_{Ar}), 127.8 (C_{Ar}), 128.5 (C_{Ar}), 130.9 (C_{Ar}), 131.7 (2CH_{Ar}), 148.9 (C_{Ar}), 156.6 (C_{Ar}). IR-ATR, cm⁻¹: 1603, 1573, 1482, 1442, 1411, 1399, 1169, 1109, 1035, 910, 859, 821, 785, 734, 485. Anal. Calcd. for C₁₄H₇BrCl₂O: C, 49.16; H, 2.06. Found: C, 48.88; H, 2.02.



2-(3-Methoxyphenyl)-5,7-dimethylbenzofuran (42): Reaction time 3 h. Flash, AcOEt/PE - 1:9. Yellow solid (82% yield), mp 58.5-59.5 °C. ¹H NMR (CDCl₃, 700 MHz), δ ppm: 2.42 (s, 3H, CH₃); 2.55 (s, 3H, CH₃); 3.90 (s, 3H, CH₃); 6.90 (dd, *J*=10.7 Hz, *J*=2.0 Hz, 1H, CH_{Ar}); 6.92 (s, 1H, CH_{Ar}); 6.95 (s,

1H, CH_{Ar}); 7.20 (s, 1H, CH_{Ar}); 7.35-7.38 (m, 1H, CH_{Ar}); 7.41-7.42 (m, 1H, CH_{Ar}); 7.41-7.47 (m, 1H, CH_{Ar}). ¹³C NMR (CDCl₃, 175 MHz), δ ppm: 14.3 (CH₃); 20.6 (CH₃); 54.6 (CH₃); 101.0 (CH_{Ar}); 109.6 (CH_{Ar}); 113.2 (CH_{Ar}); 116.7 (CH_{Ar}); 117.4 (CH_{Ar}); 120.1 (C_{Ar}); 126.0 (CH_{Ar}); 128.0 (C_{Ar}); 129.1 (CH_{Ar}); 131.4 (C_{Ar}); 131.6 (C_{Ar}); 151.6 (C_{Ar}); 154.7 (C_{Ar}); 159.2 (C_{Ar}). IR-ATR, cm⁻¹: 2982, 1480, 1229, 1207, 1173, 1162, 1051, 939, 846, 802, 790, 747, 687.

NMR Spectra



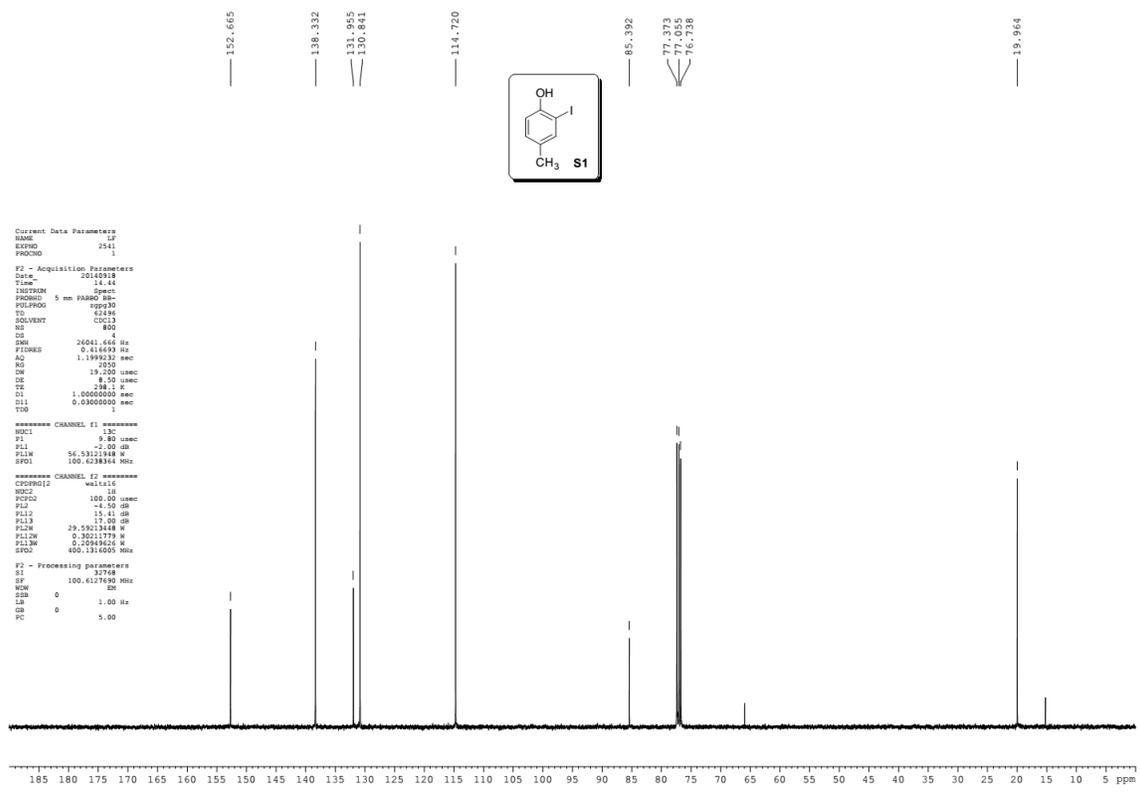
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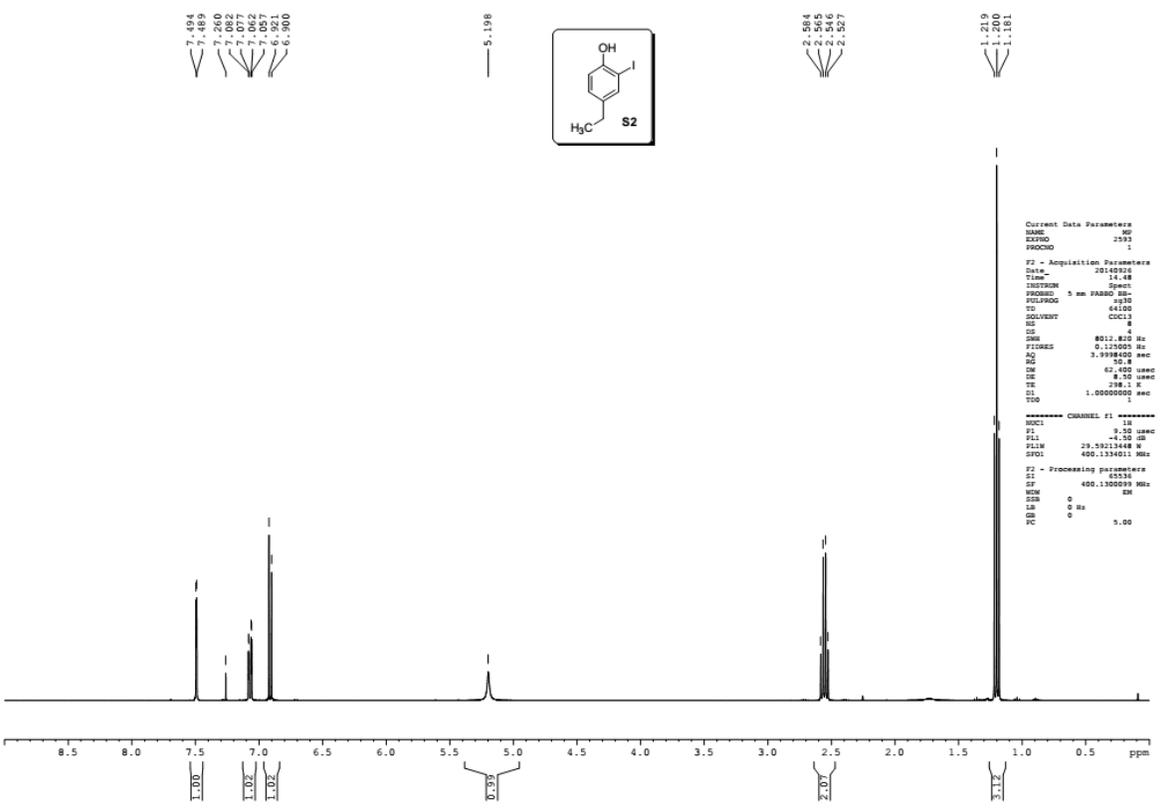
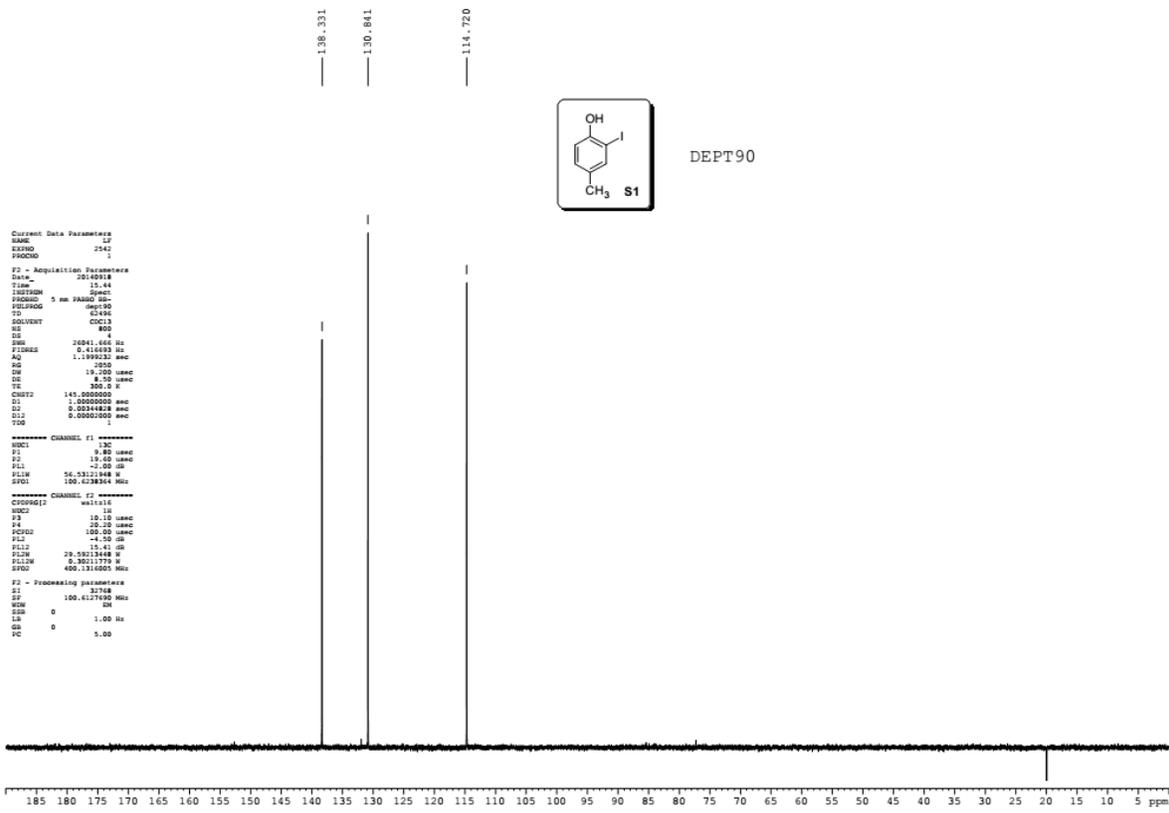
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PROCNO   1

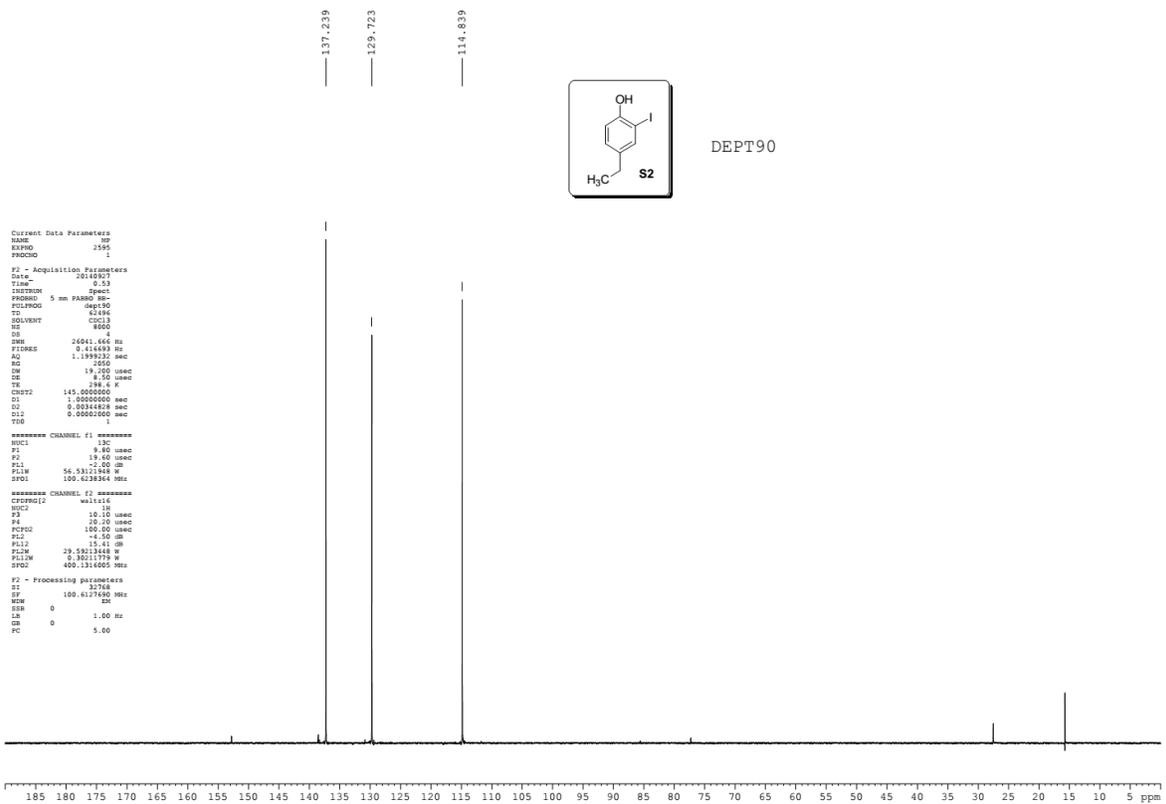
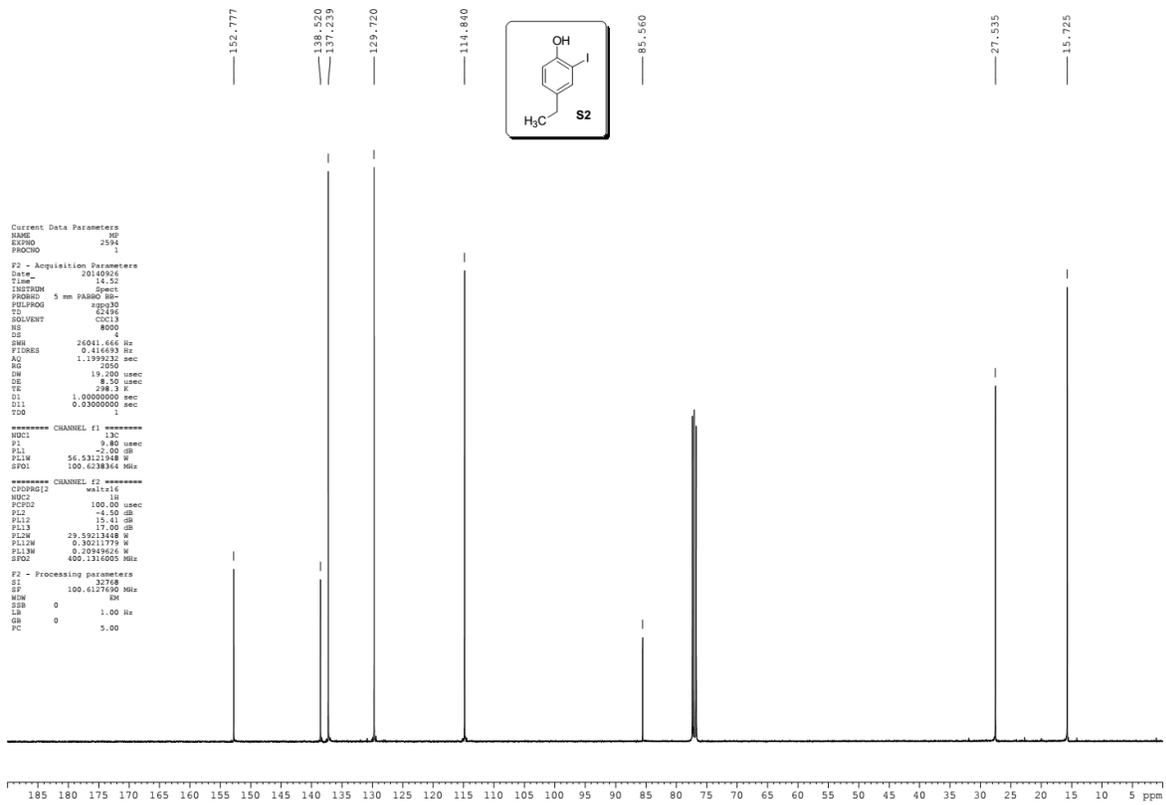
F2 - Acquisition Parameters
Date_    20100918
Time     14.41
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       4
DS       4
SWH      24041.644 Hz
FIDRES   0.614693 Hz
AQ       1.1998232 sec
RG       3250
DW       19.250 usec
DE       8.50 usec
TE       298.1 K
D1       1.00000000 sec
D11      0.03000000 sec
TD       1

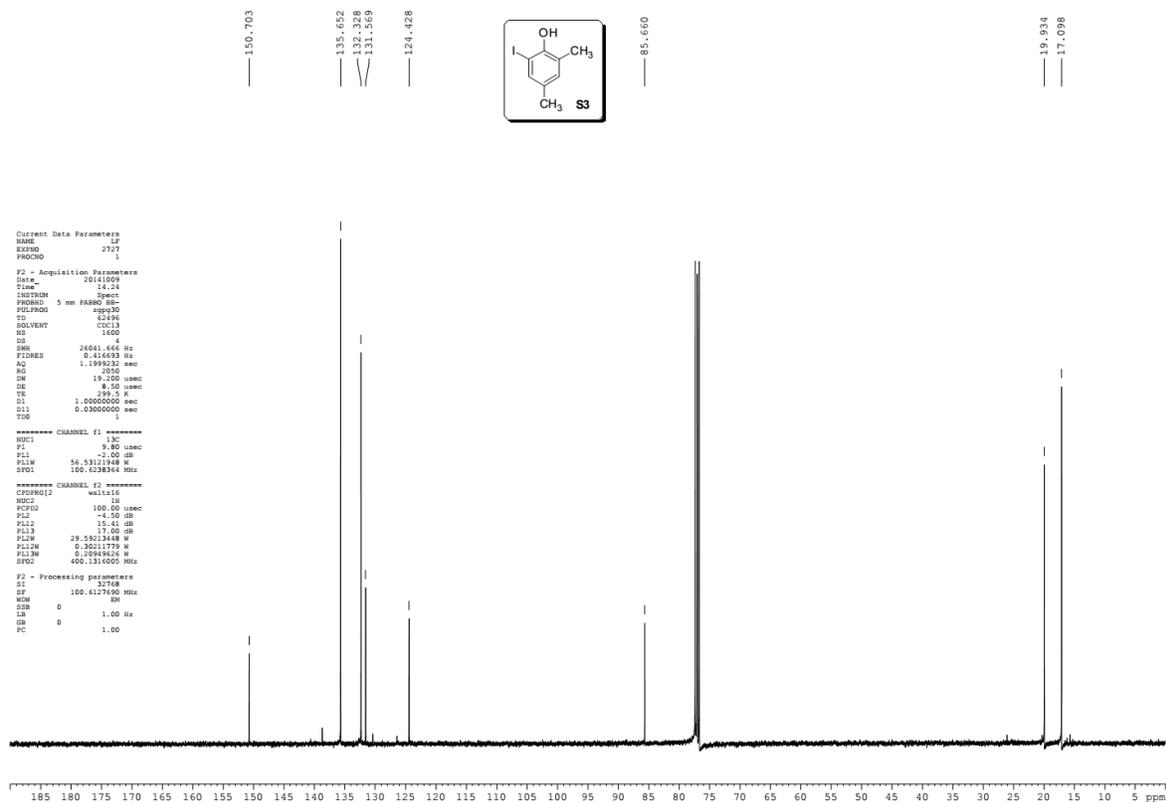
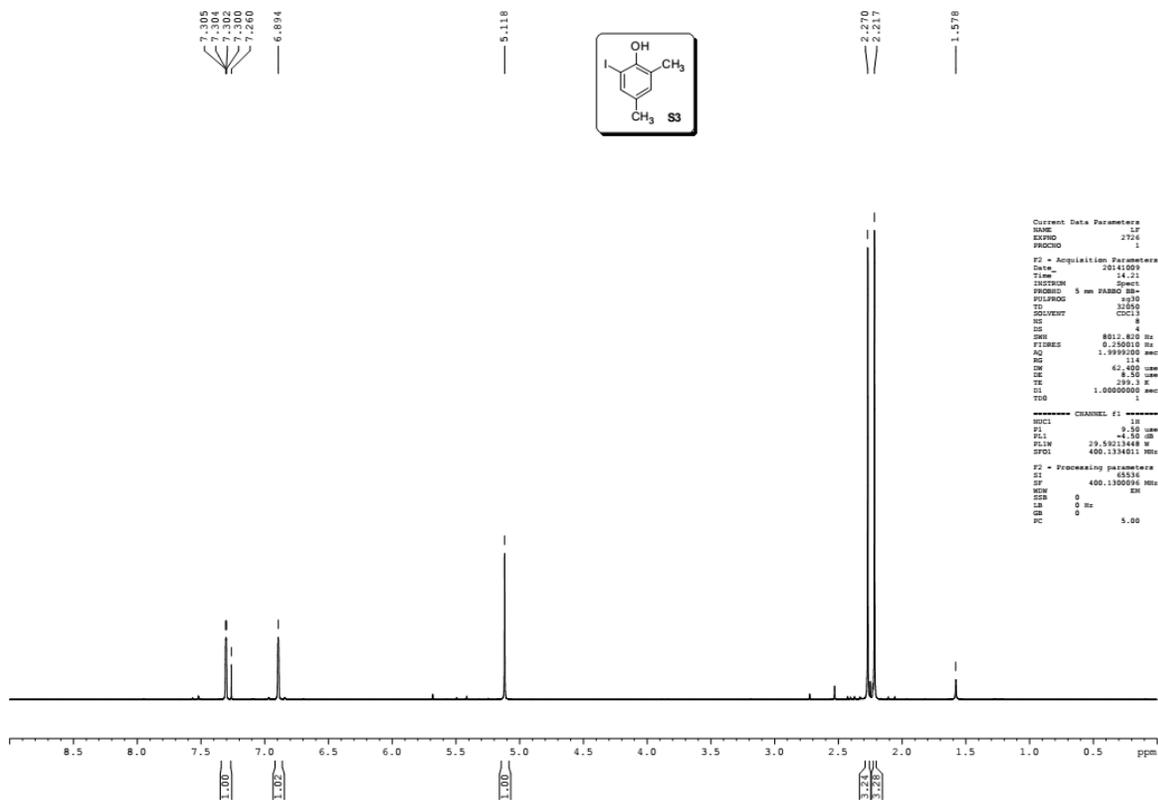
===== CHANNEL f1 =====
NUC1     13C
P1       9.80 usec
PL1     +1.00 dB
PL1W    56.53121948 W
SFO1    100.6218344 MHz

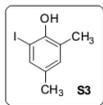
===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2     1H
PCPD2   100.00 usec
PL2     +1.50 dB
PL12    15.41 dB
PL1W    29.59213448 W
SFO2    400.1334011 MHz

F2 - Processing parameters
SI       65536
SF      100.6127950 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       5.00
    
```

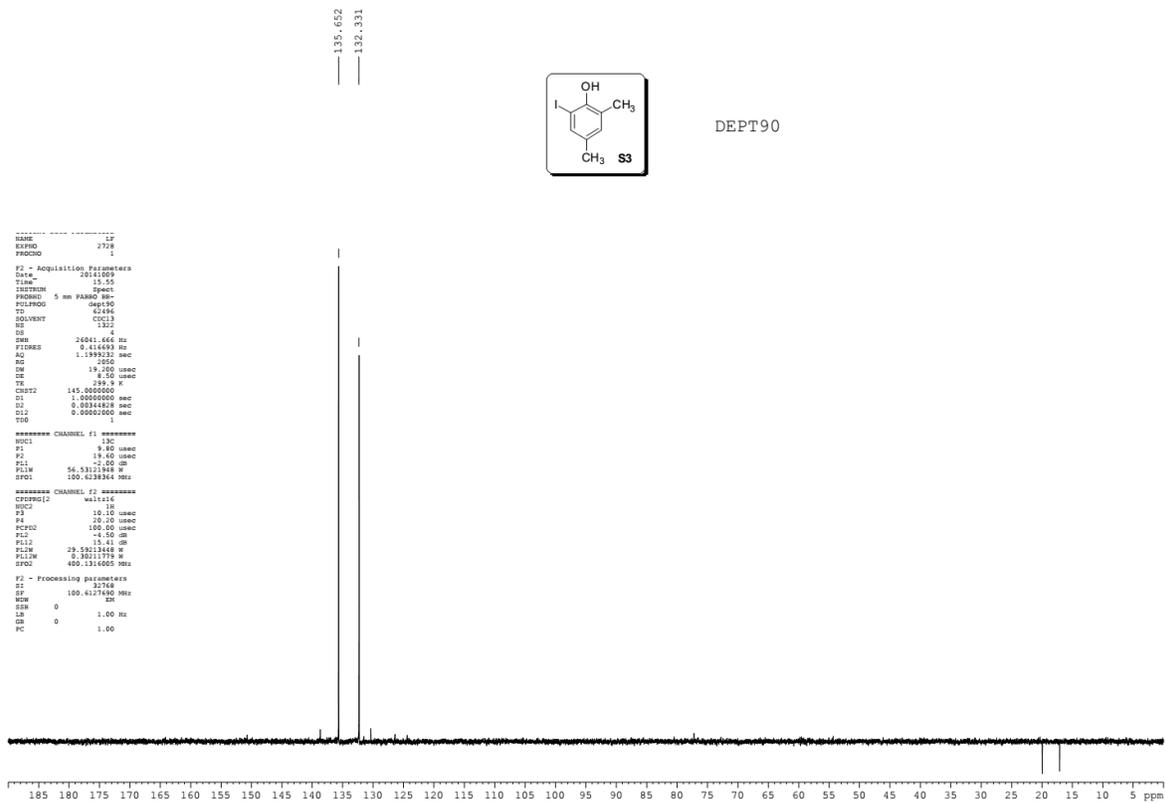








DEPT90



```

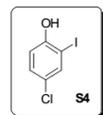
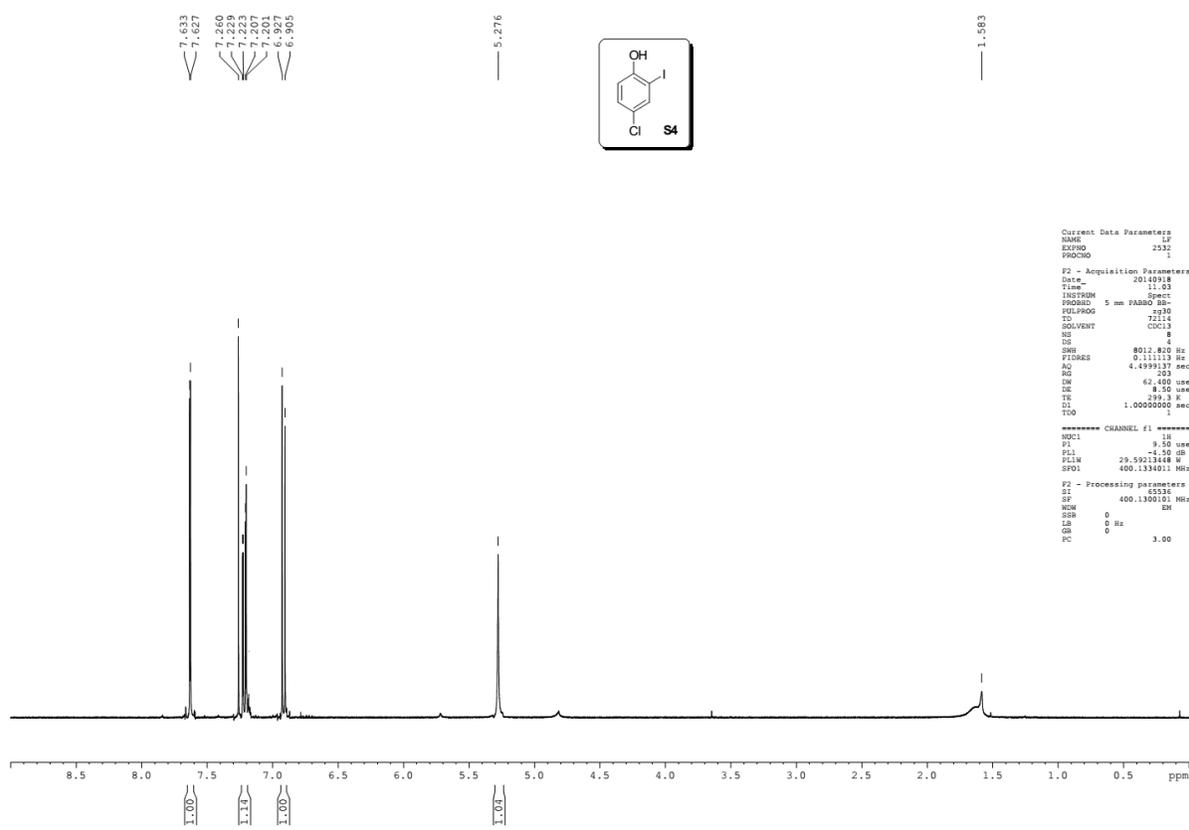
NAME      LF
EXPNO    2718
PROCNO   1

F2 - Acquisition Parameters
Date_    20141209
Time     15.55
INSTRUM  spect
PROBHD   5 mm PABBO BH-
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        4
DS        4
SFORES   26041.666 Hz
AQ        0.116493 Hz
RG        1.1899232 sec
WDW       2550
SS        19.200 usec
LB        8.50 usec
TE        299.9 K
CH2TZ    145.000000 sec
D1        1.00000000 sec
D12       0.00346428 sec
D13       0.00002000 sec
TDO       1

***** CHANNEL f1 *****
NUC1      13C
P1        9.80 usec
PC1       19.00 dB
PL1       -2.00 dB
PL12      56.5311788 W
SFO1      100.6238364 MHz

***** CHANNEL f2 *****
CPDPRG2  mult16
NUC2      13C
P2        10.10 usec
PC2       18.00 dB
PL2       -4.50 dB
PL12      29.5511348 W
SFO2      400.1334001 MHz

F2 - Processing parameters
SI        32768
SF        100.6127480 MHz
WDW       DM
SSB       0
LB        1.00 Hz
GB        0
PC        1.00
  
```



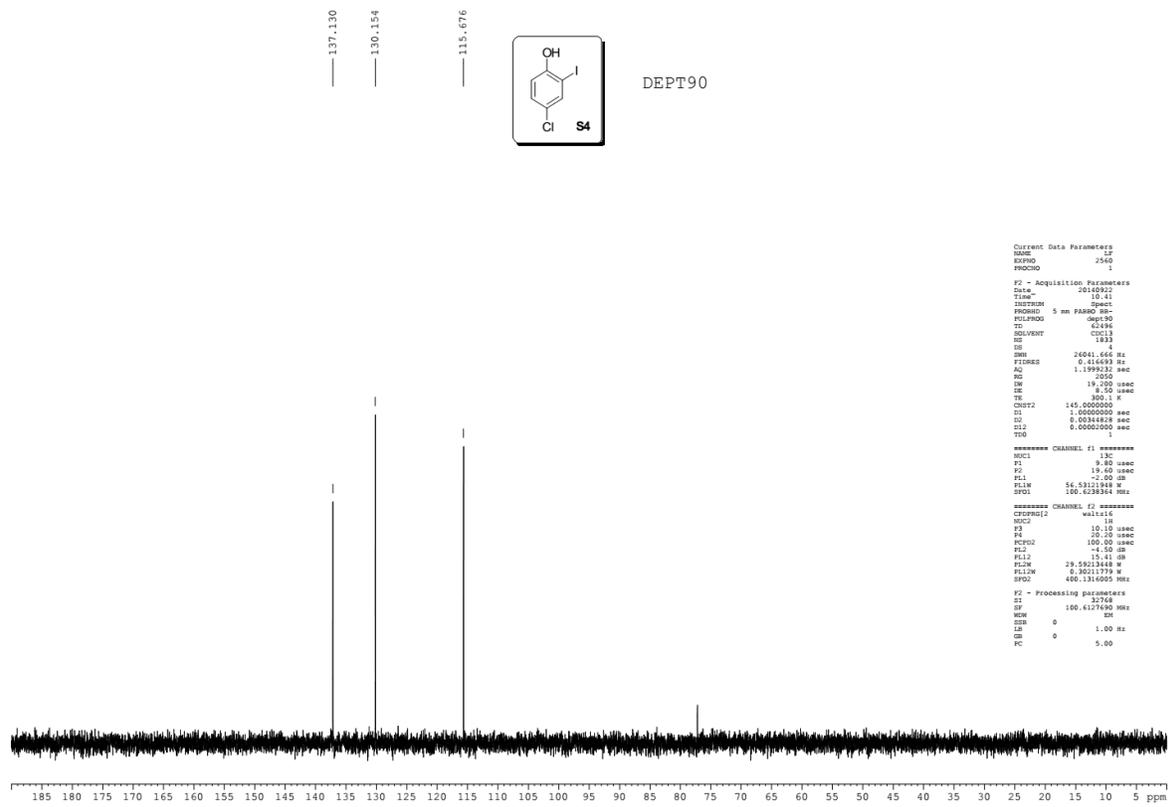
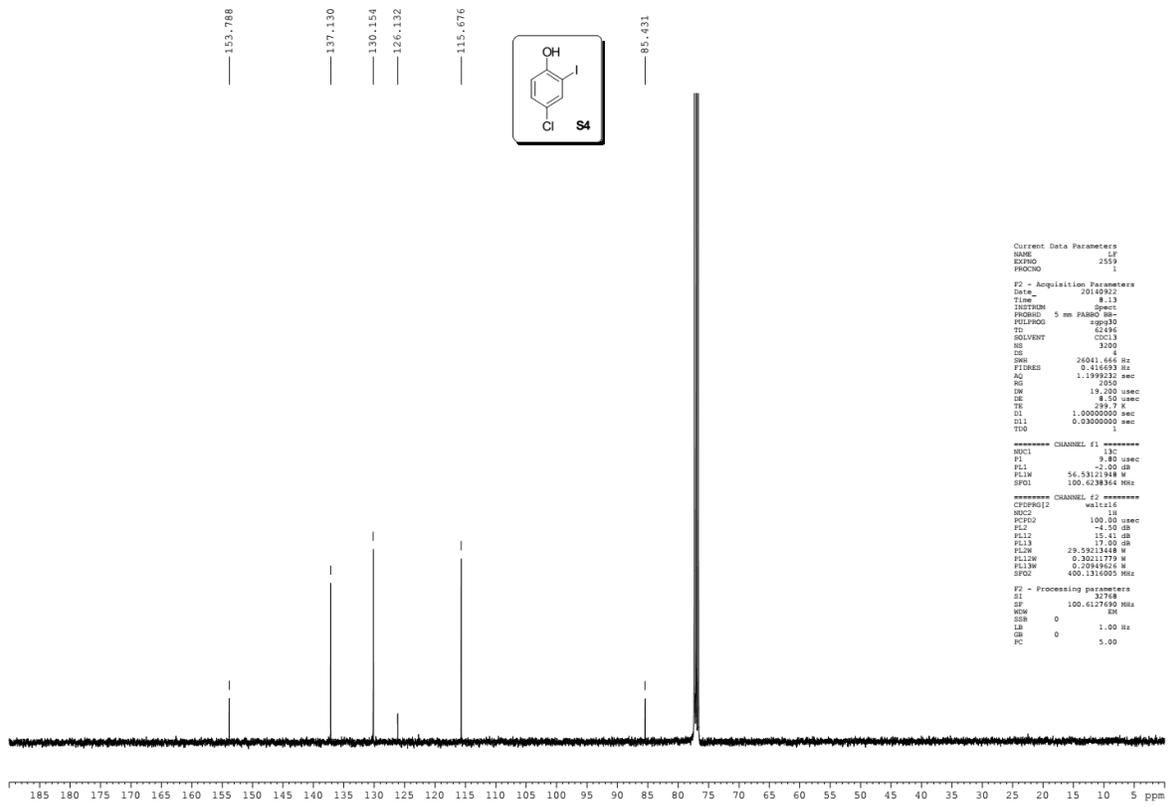
```

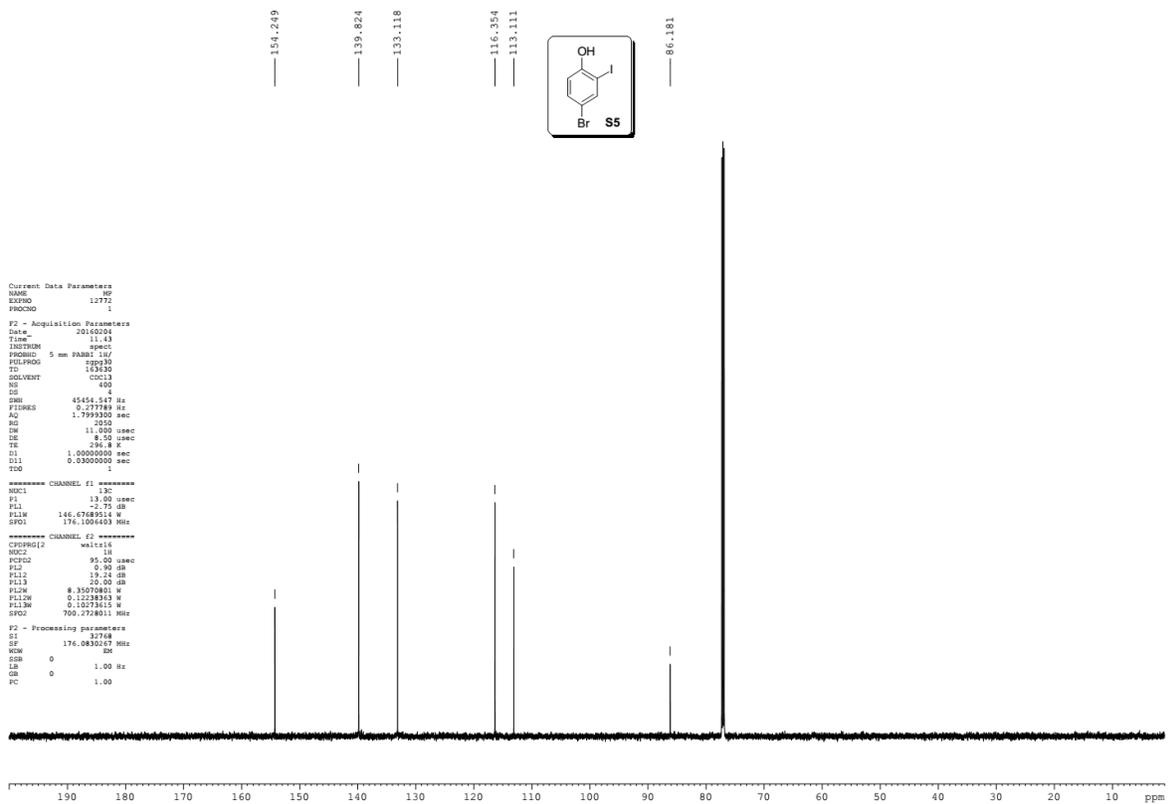
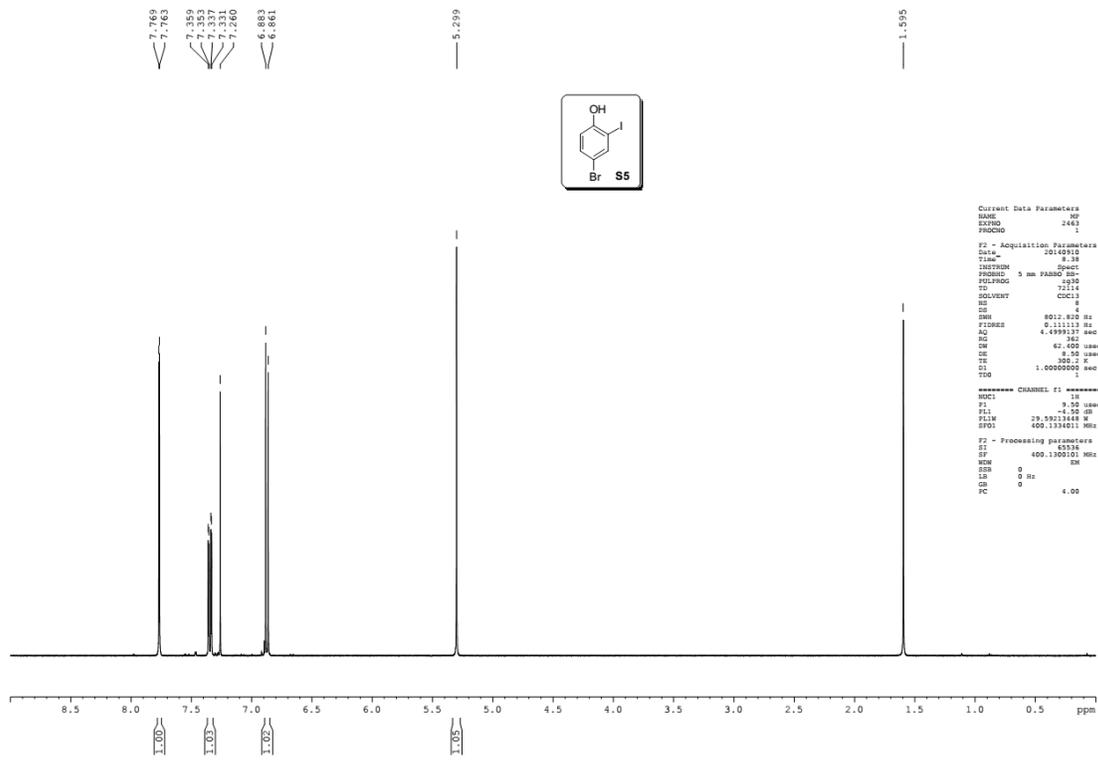
Current Data Parameters
NAME      LF
EXPNO    2532
PROCNO   1

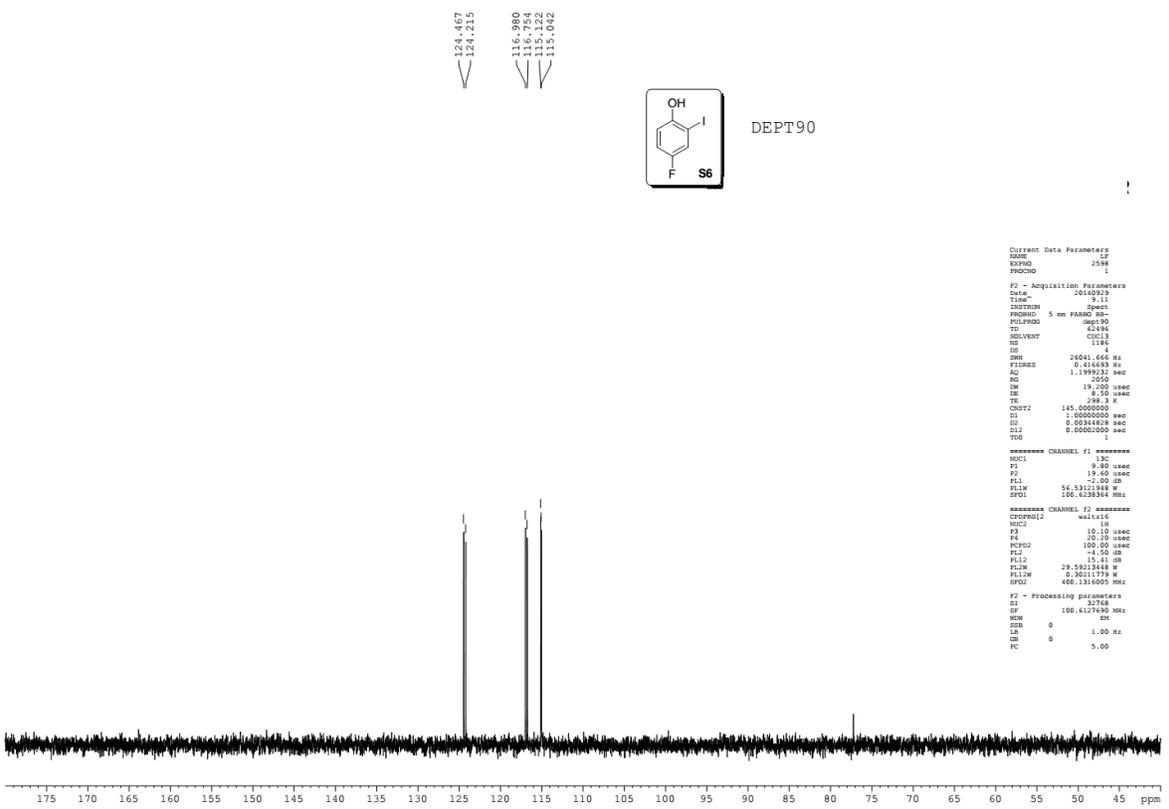
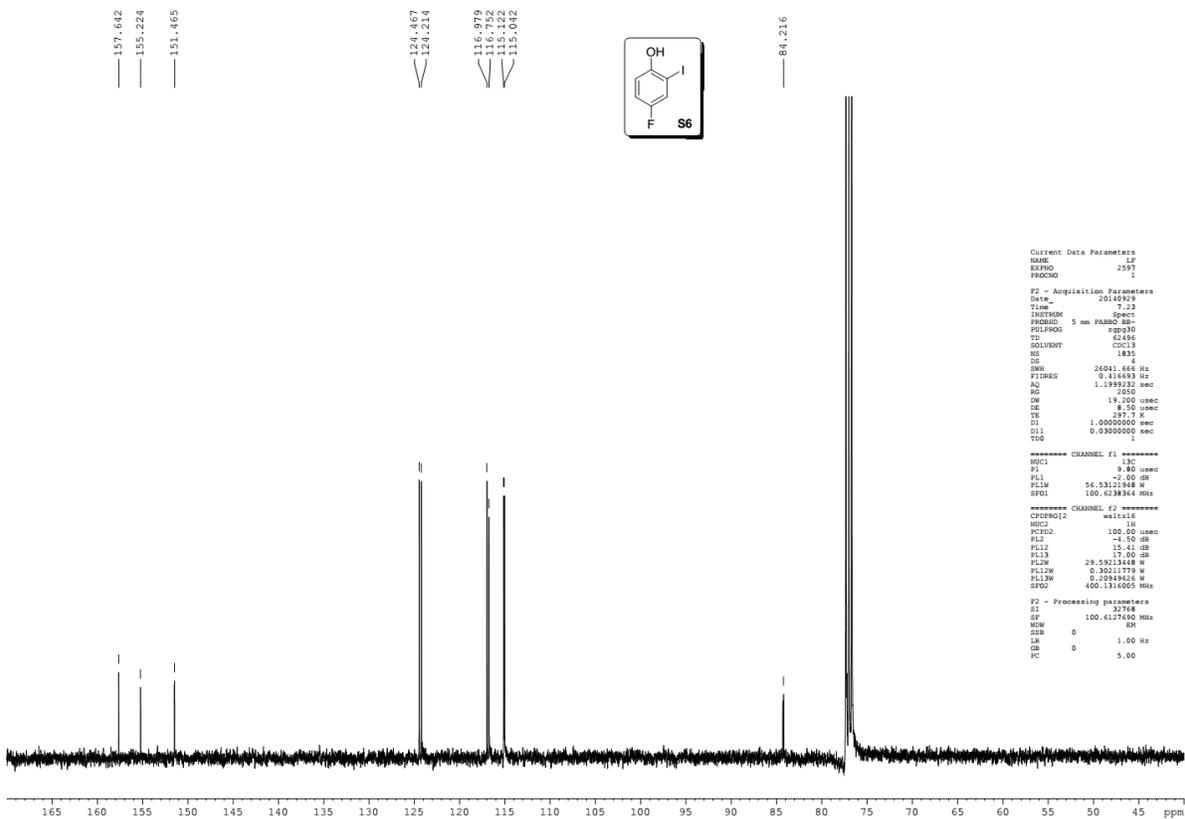
F2 - Acquisition Parameters
Date_    20140918
Time     11.03
INSTRUM  spect
PROBHD   5 mm PABBO BH-
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        4
DS        4
SFORES   801.820 Hz
AQ        0.111113 Hz
RG        4.4999372 sec
WDW       203
SS        62.400 usec
LB        8.50 usec
TE        299.9 K
D1        1.00000000 sec
TDO       1

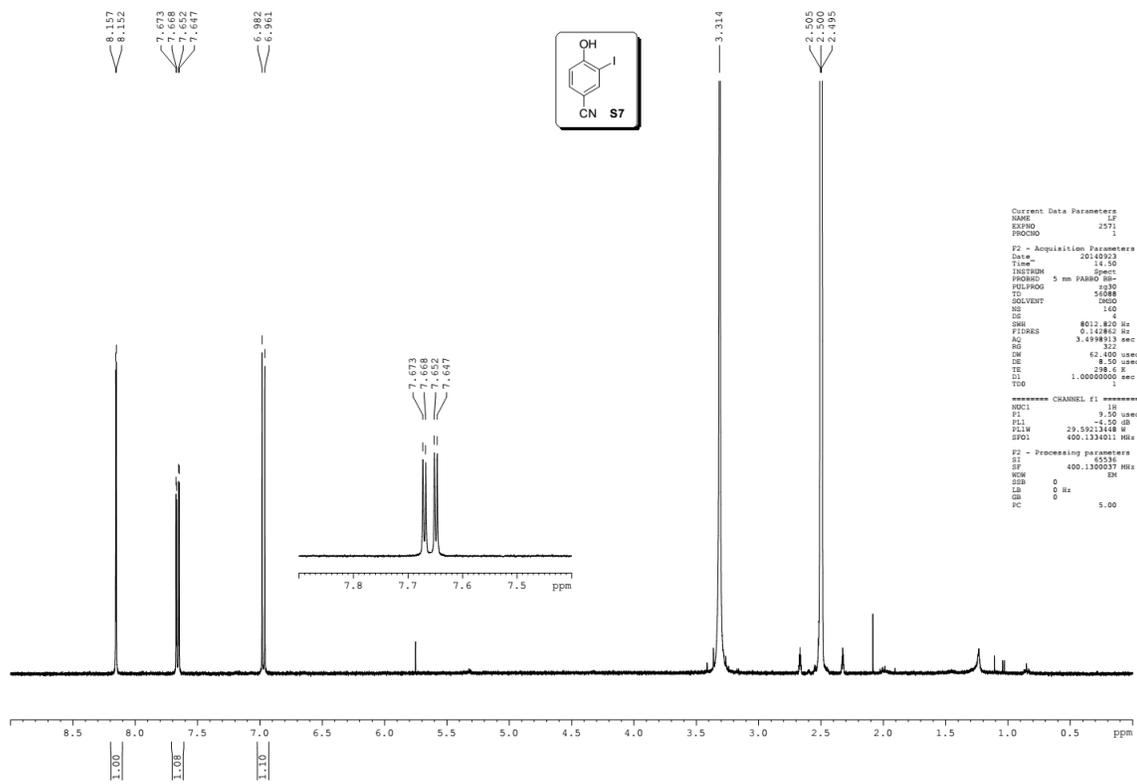
***** CHANNEL f1 *****
NUC1      1H
P1        9.50 usec
PC1       19.00 dB
PL1       -2.00 dB
PL12      29.5511348 W
SFO1      400.1334011 MHz

F2 - Processing parameters
SI        65536
SF        400.1300101 MHz
WDW       DM
SSB       0
LB        0 Hz
GB        0
PC        3.00
  
```









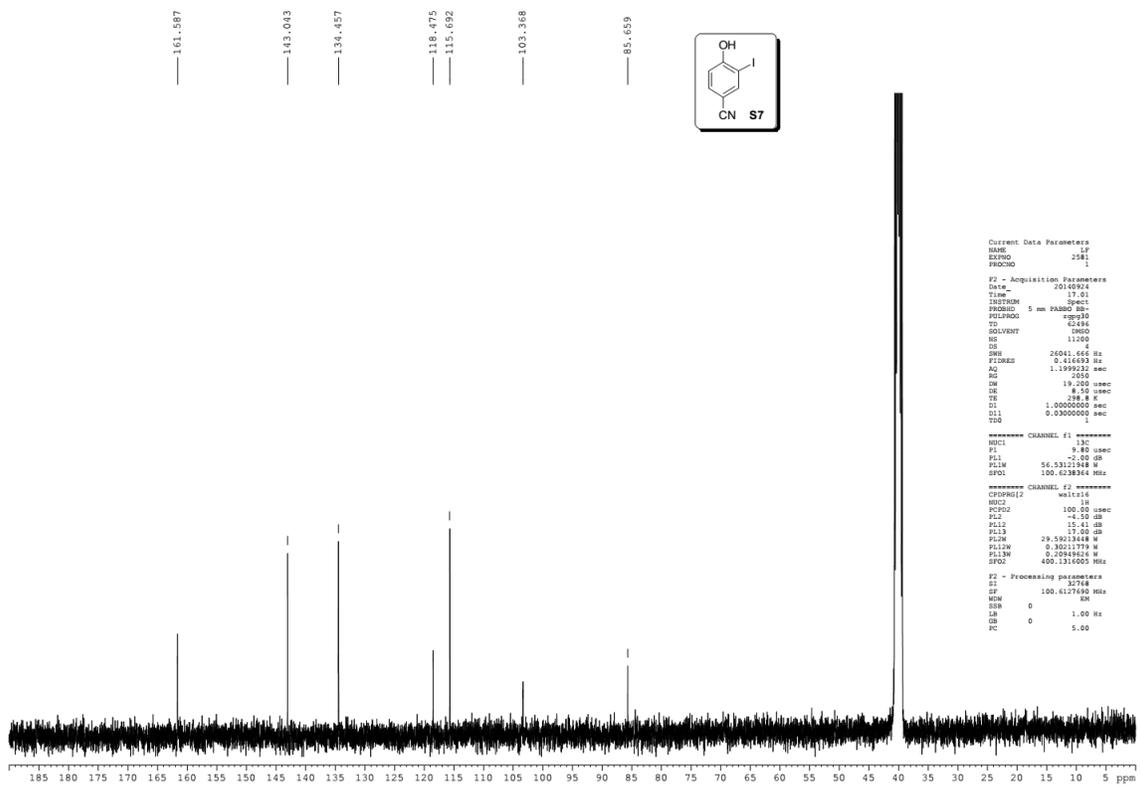
```

Current Data Parameters
NAME      LF
EXPNO    251
PROCNO   1

F2 - Acquisition Parameters
Date_    20140923
Time     14:50
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD        65536
SOLVENT  DMSO
NS        4
DS        4
SFORES   8012.820 Hz
AQ        0.142862 sec
RG        3.4598913 sec
DE        32
DM        62.400 usec
TE        8.50 usec
TE        288.6 K
D1        1.00000000 sec
D11       1
TDO       1

===== CHANNEL f1 =====
NUC1      13C
P1        9.50 usec
PL1       -4.50 dB
PL1W     29.5921348 W
SFO1      400.1304011 MHz

F2 - Processing parameters
SI        0
SF        400.1304011 MHz
WDW       EM
SSB       0
LB        0 Hz
GB        0
PC        5.00
  
```



```

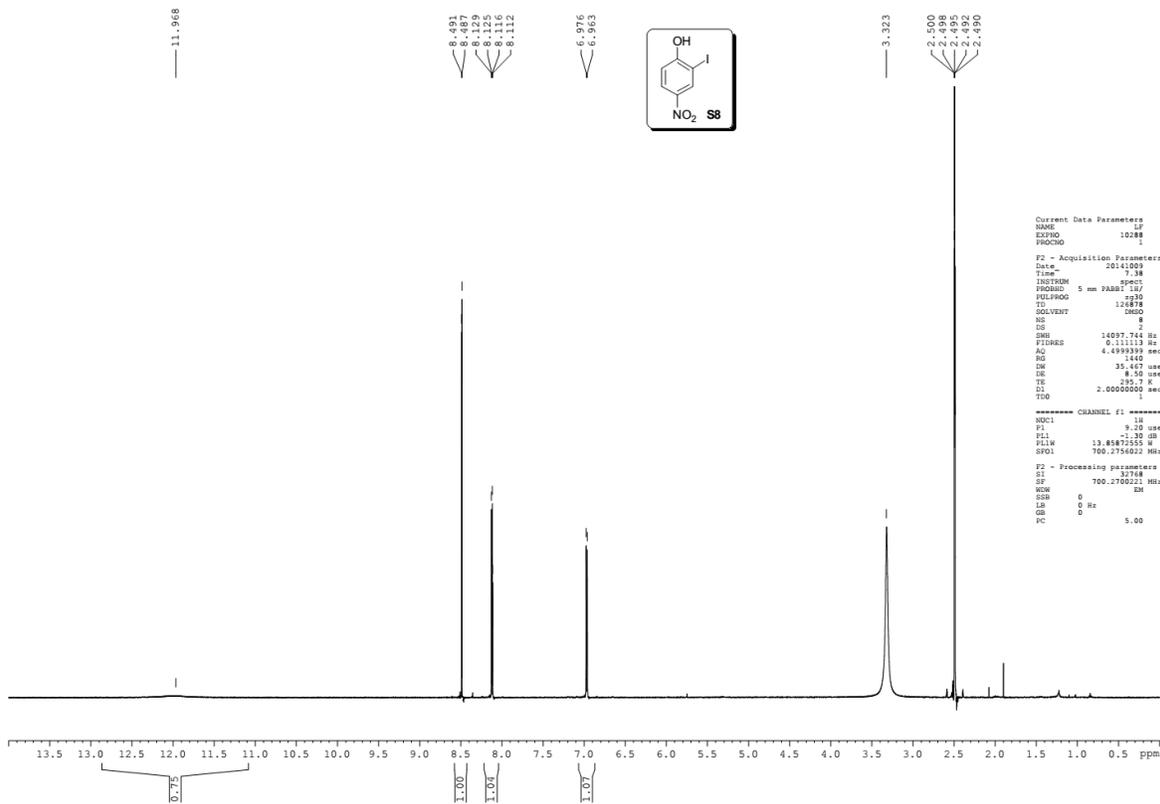
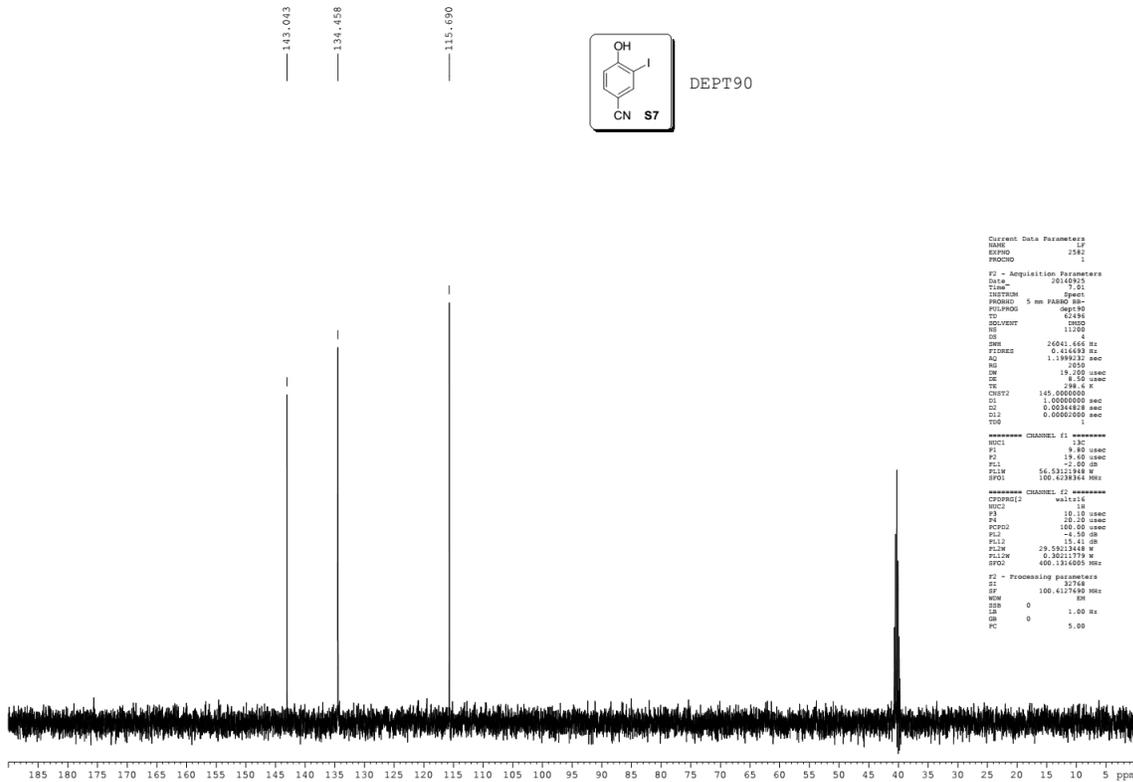
Current Data Parameters
NAME      LF
EXPNO    251
PROCNO   1

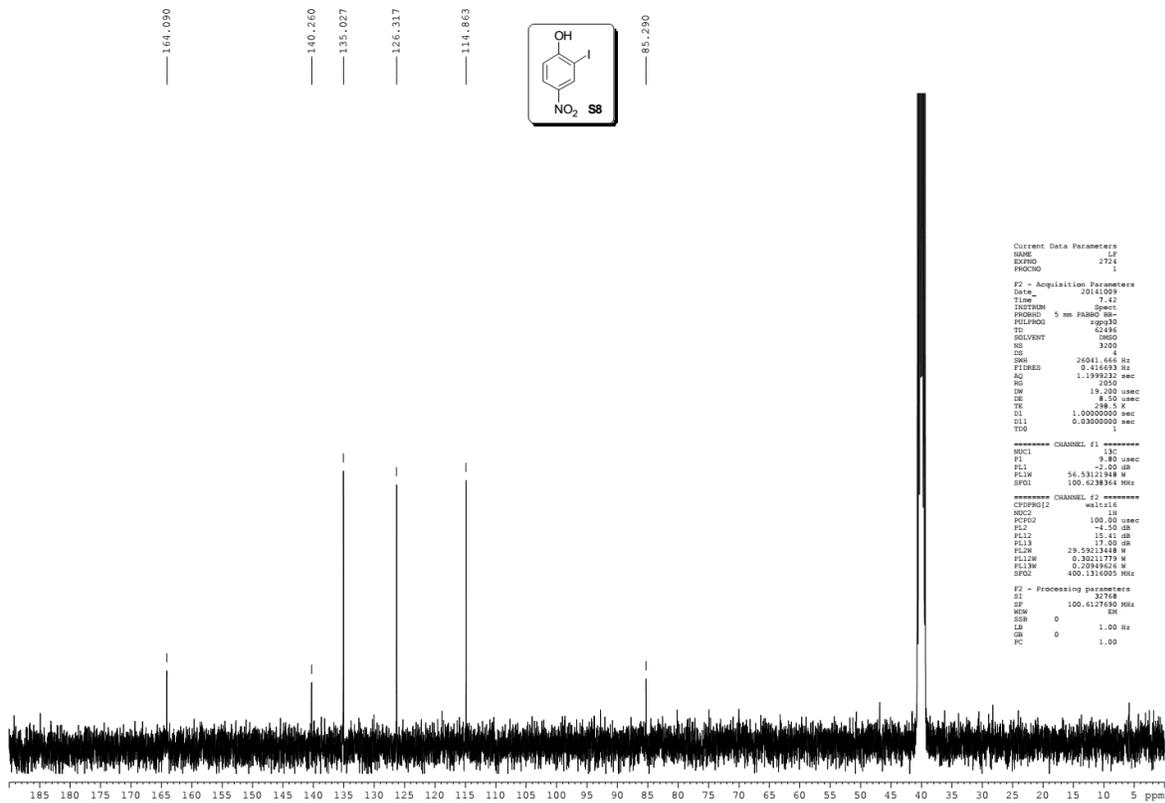
F2 - Acquisition Parameters
Date_    20140924
Time     17:01
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD        65536
SOLVENT  DMSO
NS        4
DS        4
SFORES   2641.666 Hz
AQ        0.416693 sec
RG        1.1999232 sec
DE        32
DM        18.200 usec
TE        8.50 usec
TE        288.6 K
D1        1.00000000 sec
D11       0.03000000 sec
TDO       1

===== CHANNEL f1 =====
NUC1      13C
P1        9.50 usec
PL1       -2.00 dB
PL1W     56.5312188 W
SFO1      100.6238344 MHz

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2      1H
PCPD2    100.00 usec
PL2       -6.50 dB
PL2W     15.41 dB
PL3       17.00 dB
PL3W     29.5921348 W
PL4W     0.3021179 W
PL1W     0.2944921 W
SFO2      400.1316095 MHz

F2 - Processing parameters
SI        0
SF        100.6107860 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        5.00
  
```





```

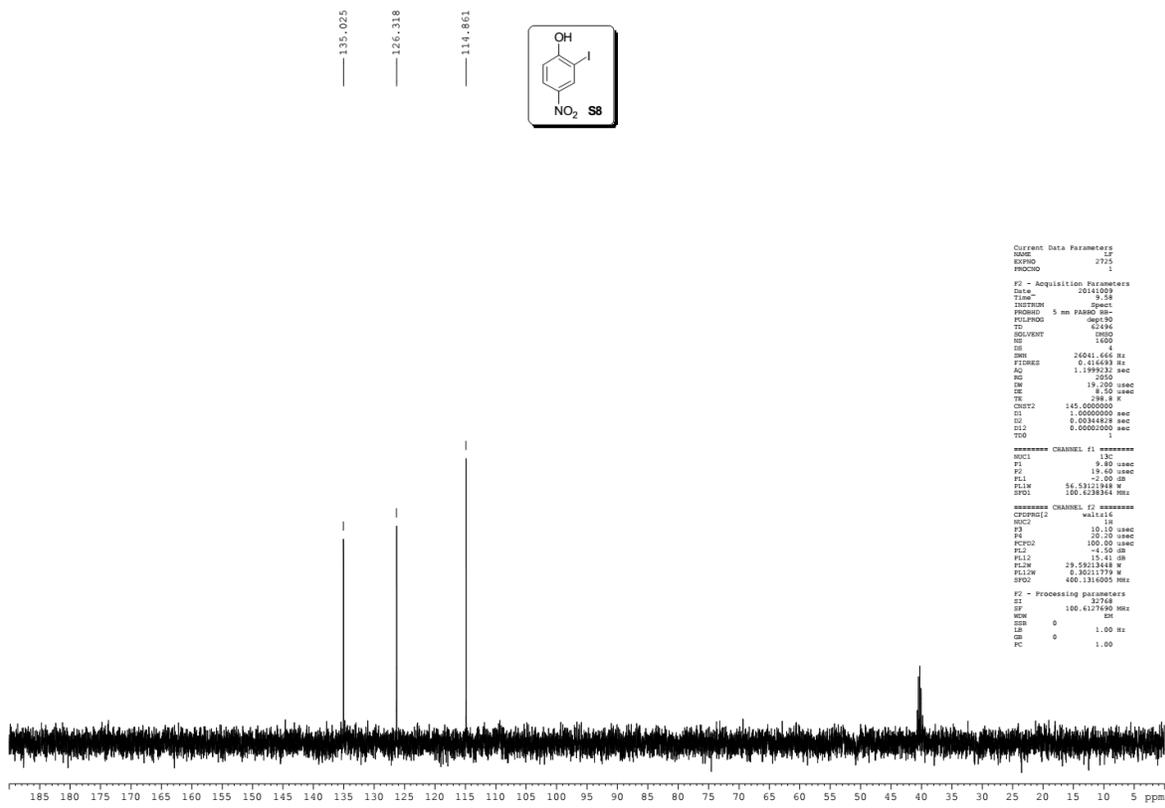
Current Data Parameters
NAME      LF
EXPNO    274
PROCNO   1

F2 - Acquisition Parameters
Date_    2014099
Time     7.42
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD        65496
SOLVENT  DMSO
NS        3200
DS        4
SWH       26041.666 Hz
FIDRES   0.416693 Hz
AQ        1.1999232 sec
RG        2050
WE        13.200 usec
DE        8.50 usec
TE        298.2 K
D1        1.00000000 sec
d11       0.03000000 sec
TOD       1

===== CHANNEL f1 =====
NUC1      13C
P1        9.30 usec
P2        -2.00 usec
PL1W     56.5312348 W
SFO1     100.6238364 MHz

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2      1H
P3        10.00 usec
P4        -4.50 usec
PL2W     15.41 usec
PL3W     17.00 usec
PL4W     29.5921348 W
PL12W    0.30211779 W
PL13W    0.2084968 W
SFO2     400.1316095 MHz

F2 - Processing parameters
SI        32768
SF        100.6127490 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.00
  
```



```

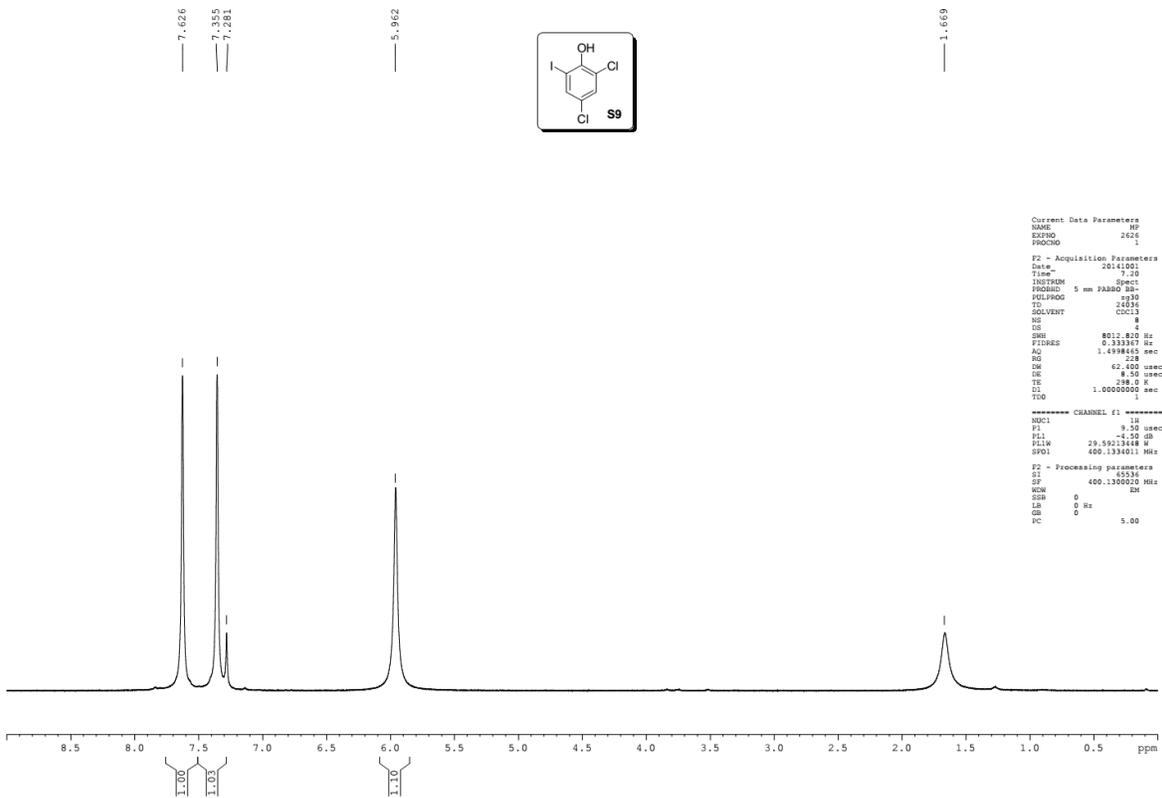
Current Data Parameters
NAME      LF
EXPNO    2725
PROCNO   1

F2 - Acquisition Parameters
Date_    2014099
Time     9.58
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD        65496
SOLVENT  DMSO
NS        1600
DS        4
SWH       26041.666 Hz
FIDRES   0.416693 Hz
AQ        1.1999232 sec
RG        2050
WE        13.200 usec
DE        8.50 usec
TE        298.2 K
D1        1.00000000 sec
D11       0.03000000 sec
D12       0.00000000 sec
TOD       1

===== CHANNEL f1 =====
NUC1      13C
P1        9.30 usec
P2        -2.00 usec
PL1W     56.5312348 W
SFO1     100.6238364 MHz

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2      1H
P3        10.10 usec
P4        -4.50 usec
PL2W     15.41 usec
PL3W     17.00 usec
PL4W     29.5921348 W
PL12W    0.30211779 W
PL13W    0.2084968 W
SFO2     400.1316095 MHz

F2 - Processing parameters
SI        32768
SF        100.6127490 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.00
  
```



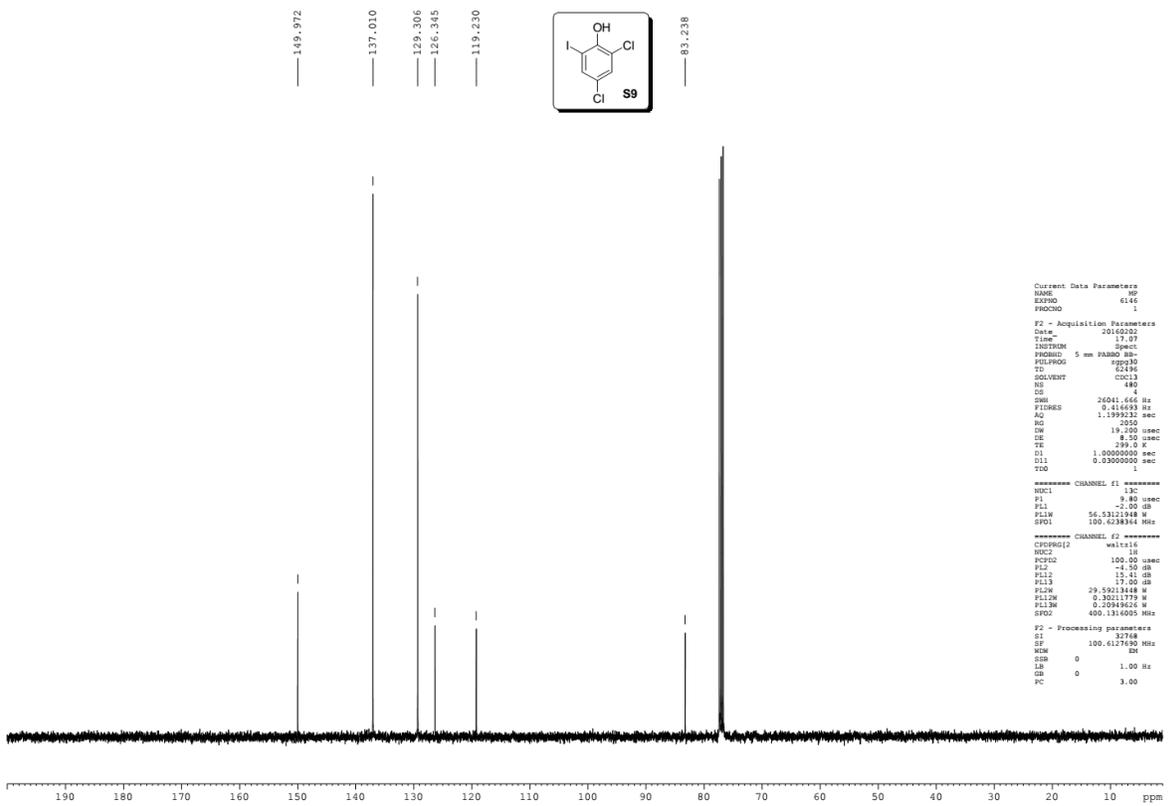
```

Current Data Parameters
NAME      RP
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20141001
Time     7.20
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        4
DS        4
SFB      801.820 Hz
FIDRES   0.33387 Hz
AQ        1.459865 sec
RG         228
OR        62.400 usec
DE        8.50 usec
TE        298.0
D1        1.0000000 sec
TD0       1

===== CHANNEL f1 =====
NUC1      1H
P1         9.50 usec
PL1       -4.50 dB
PL1W      29.5013148 W
SFO1      400.1334011 MHz

F2 - Processing parameters
SI         65536
SF         400.1300020 MHz
WDW        EM
SSB        0
LB         0 Hz
GB         0
PC         5.00
  
```



```

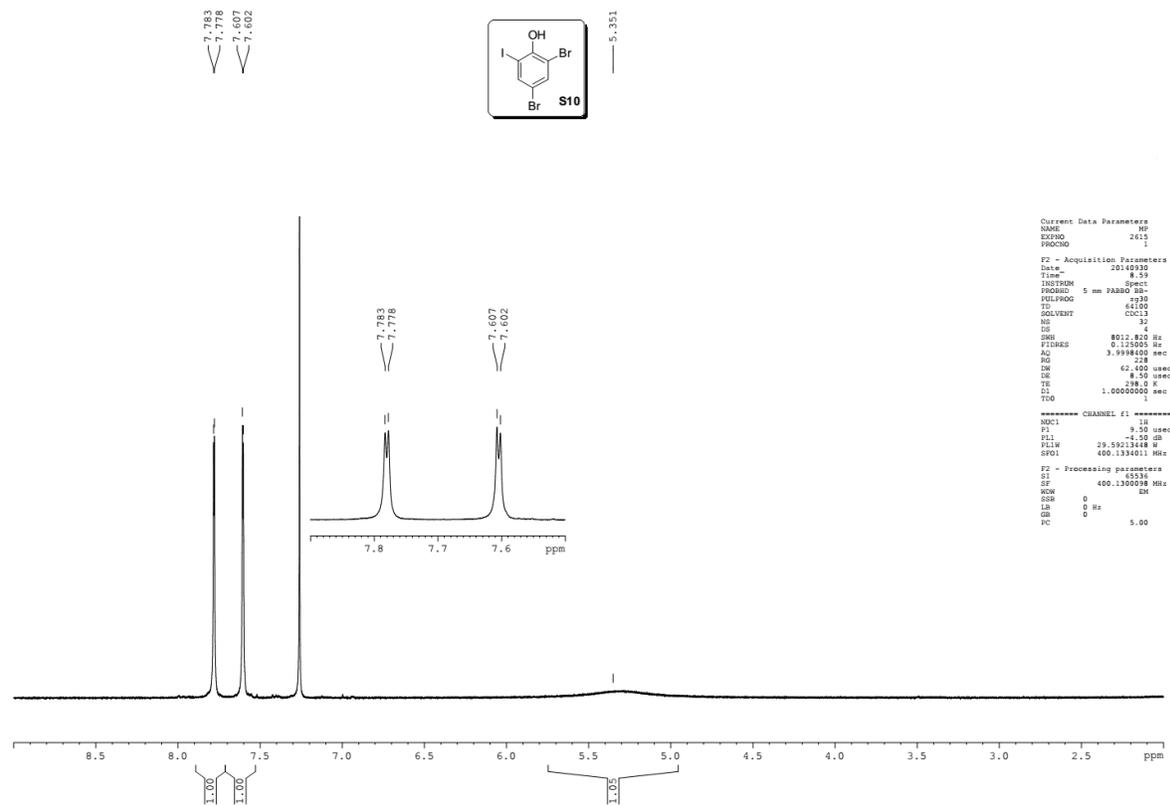
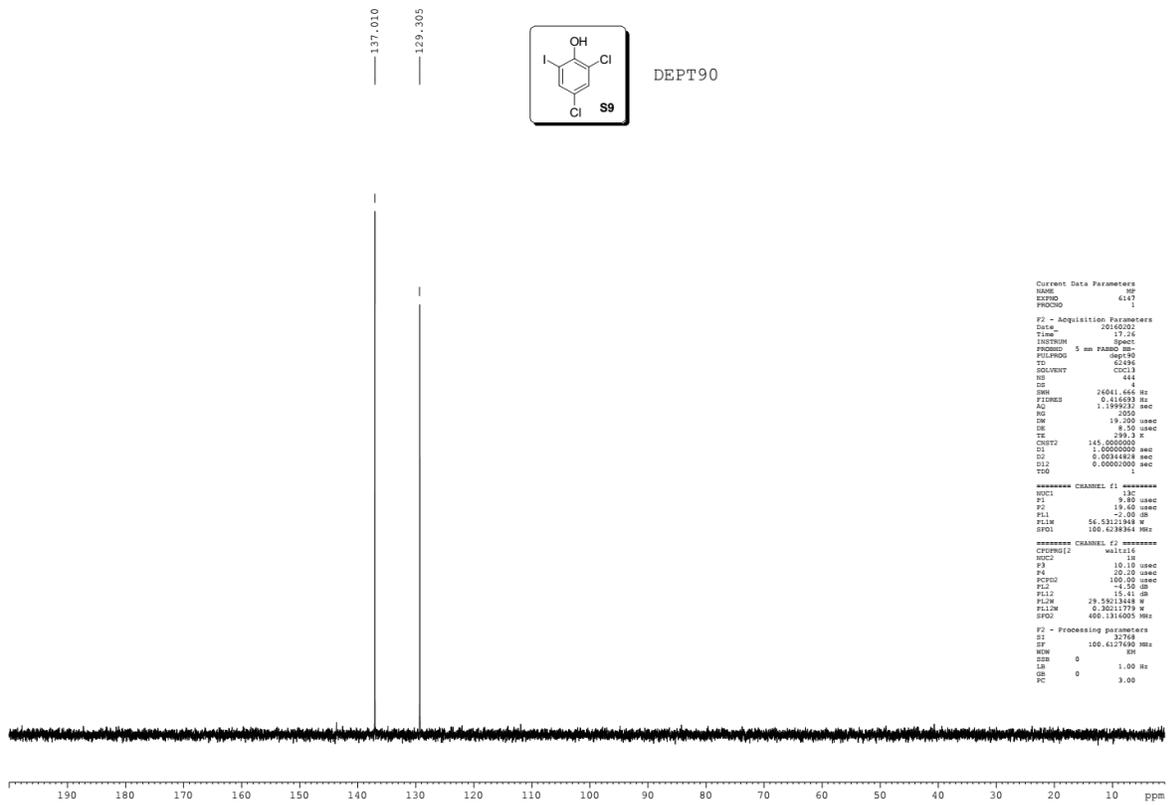
Current Data Parameters
NAME      RP
EXPNO    1
PROCNO   1

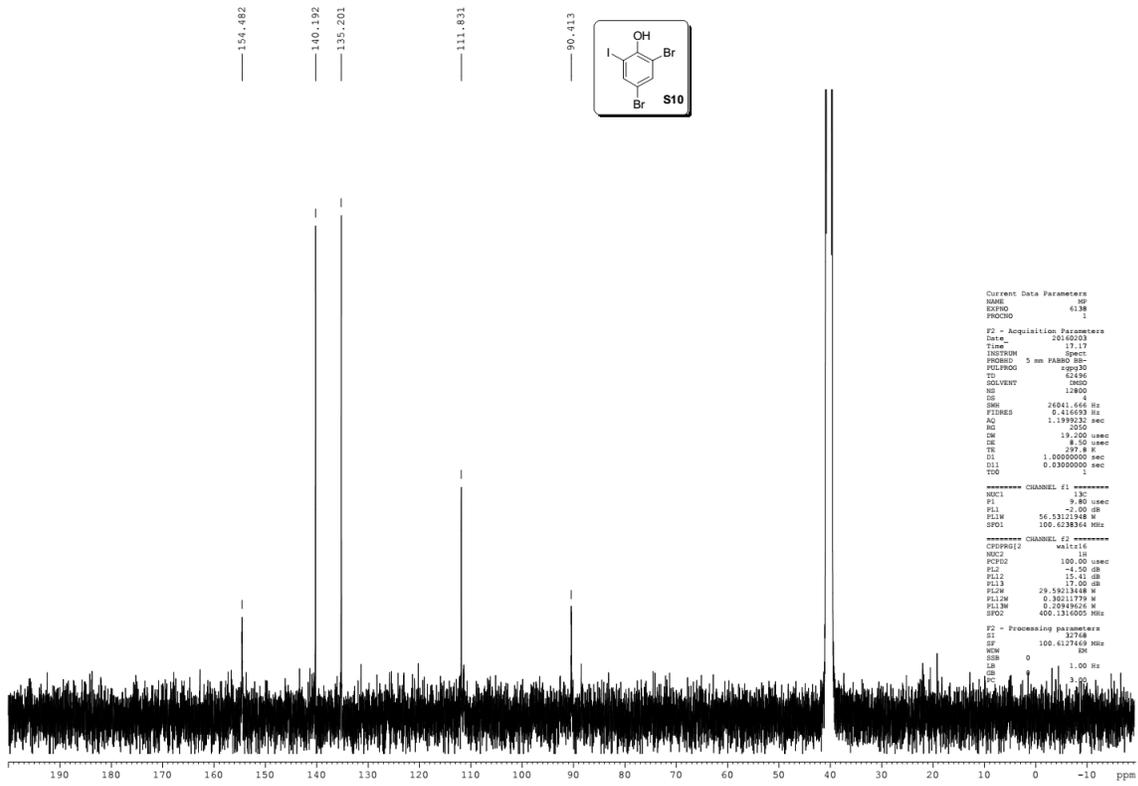
F2 - Acquisition Parameters
Date_    20160202
Time     17.07
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD        62496
SOLVENT  CDCl3
NS        4
DS        4
SFB      26041.600 Hz
FIDRES   0.416693 Hz
AQ        1.1999232 sec
RG         2050
OR        19.100 usec
DE        8.50 usec
TE        299.0
D1        1.0000000 sec
D11       0.2300000 sec
TD0       1

===== CHANNEL f1 =====
NUC1      13C
P1        13.5
PL1        0.00 usec
PL1W      56.53121948 W
SFO1      100.6283644 MHz

===== CHANNEL f2 =====
CPROG12  waltz16
NUC2      1H
P2        100.00 usec
PL2       -1.00 dB
PL12      17.00 dB
PL13      17.00 dB
PL1W      29.5013148 W
PL12W     0.30211779 W
PL13W     0.29494576 W
SFO2      400.1316005 MHz

F2 - Processing parameters
SI         32768
SF         100.6178930 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         3.00
  
```





```

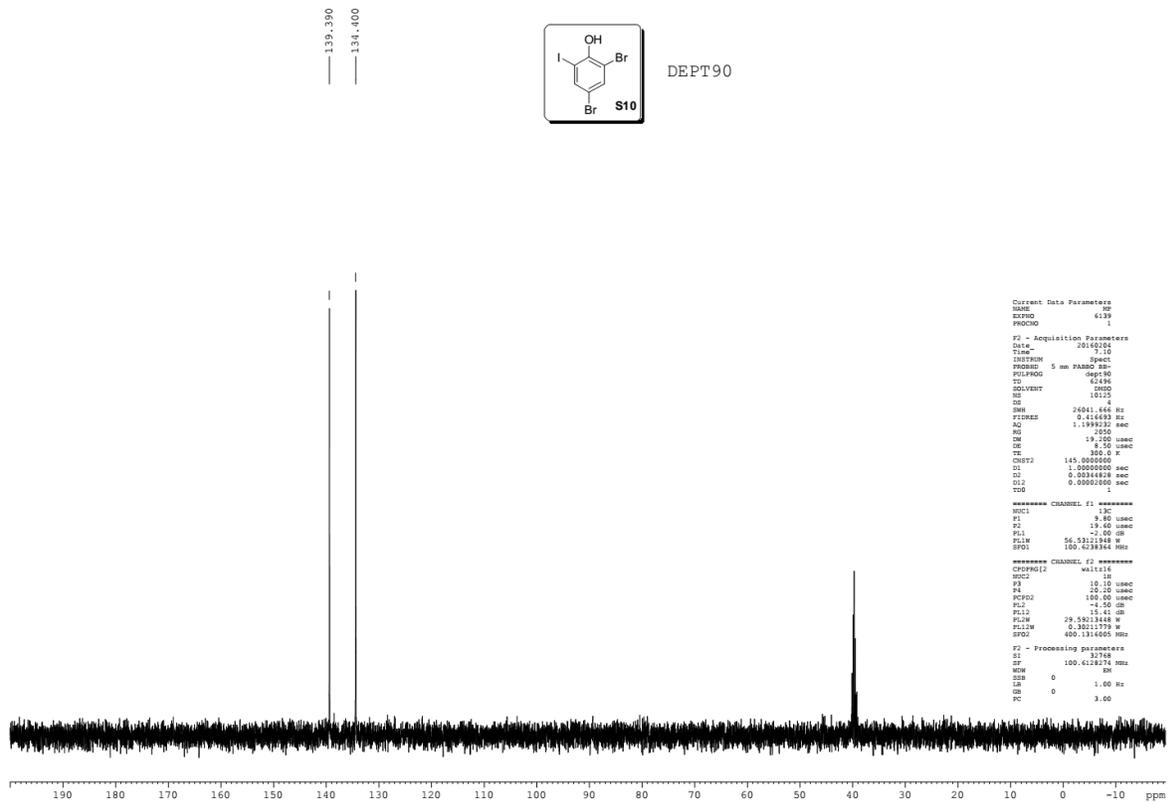
Current Data Parameters
NAME      S10
EXPNO    4139
PROCNO   1

F2 - Acquisition Parameters
Date_    20160203
Time     17.17
INSTRUM  spect
PROBHD   5 mm PABBO BBO
PULPROG  zgpg30
TD        65536
SOLVENT  DMSO
NS        4
DS        2
SFO      26041.664 Hz
FIDRES   0.416093 Hz
AQ        1.1999232 sec
RG        2050
DM        19.200 usec
DE        8.50 usec
TE        297.8 K
D1        1.0000000 sec
D11       0.0300000 sec
TD0       1

===== CHANNEL f1 =====
NUC1      13C
P1        9.80 usec
PL1       -2.00 dB
PL1W      56.53121948 W
SFO1      100.6238264 MHz

===== CHANNEL f2 =====
CPROG2   waltz16
NUC2      1H
PCPD2    100.00 usec
P2        -4.50 dB
PL2       15.41 dB
PL2W      17.00 dB
PL2W      29.59213448 W
PL2W      0.38211779 W
PL2W      0.20949626 W
SFO2      400.1314005 MHz

F2 - Processing parameters
SI        32768
SF        100.6182674 MHz
WDW       EM
SSB       0
GB        1.00 Hz
PC        3.00
  
```



```

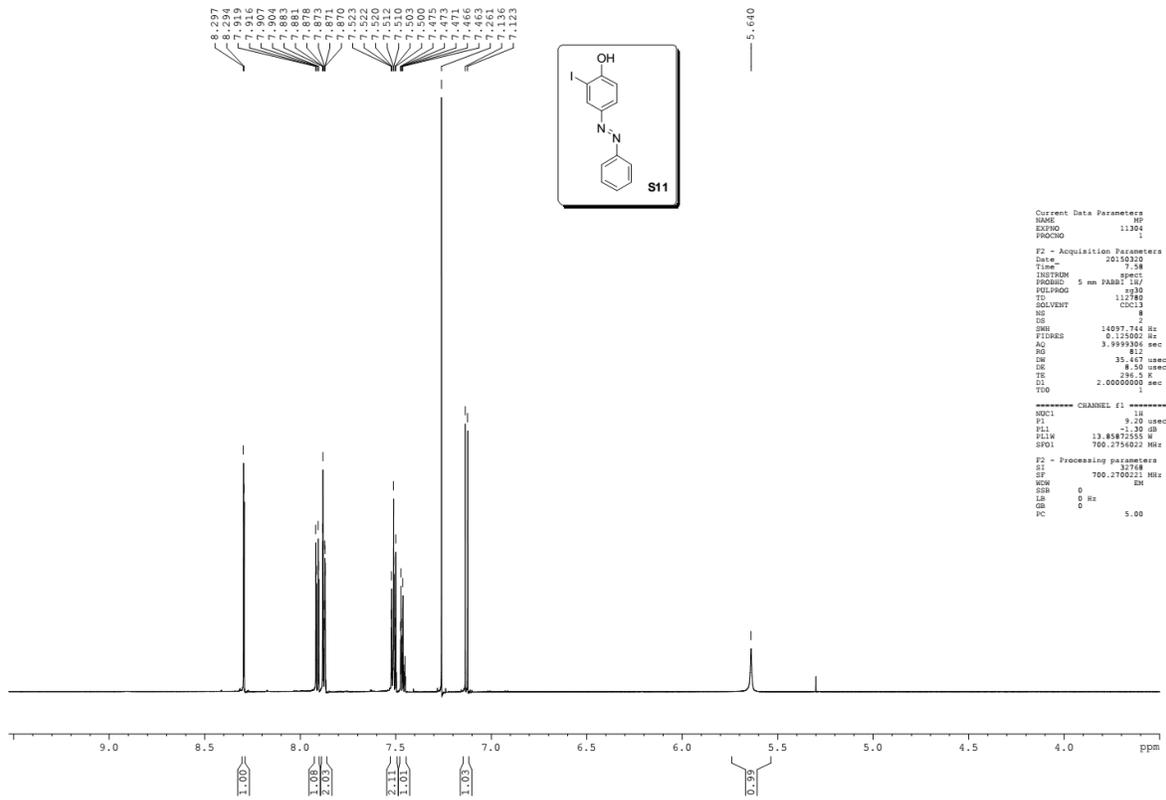
Current Data Parameters
NAME      S10
EXPNO    4139
PROCNO   1

F2 - Acquisition Parameters
Date_    20160204
Time     7.10
INSTRUM  spect
PROBHD   5 mm PABBO BBO
PULPROG  zgpg30
TD        65536
SOLVENT  DMSO
NS        4
DS        2
SFO      26041.664 Hz
FIDRES   0.416093 Hz
AQ        1.1999232 sec
RG        2050
DM        19.200 usec
DE        8.50 usec
TE        297.8 K
D1        1.0000000 sec
D11       0.0300000 sec
TD0       1

===== CHANNEL f1 =====
NUC1      13C
P1        9.80 usec
PL1       -2.00 dB
PL1W      56.53121948 W
SFO1      100.6238264 MHz

===== CHANNEL f2 =====
CPROG2   waltz16
NUC2      1H
PCPD2    100.00 usec
P2        -4.50 dB
PL2       15.41 dB
PL2W      17.00 dB
PL2W      29.59213448 W
PL2W      0.38211779 W
PL2W      0.20949626 W
SFO2      400.1314005 MHz

F2 - Processing parameters
SI        32768
SF        100.6182674 MHz
WDW       EM
SSB       0
GB        1.00 Hz
PC        3.00
  
```



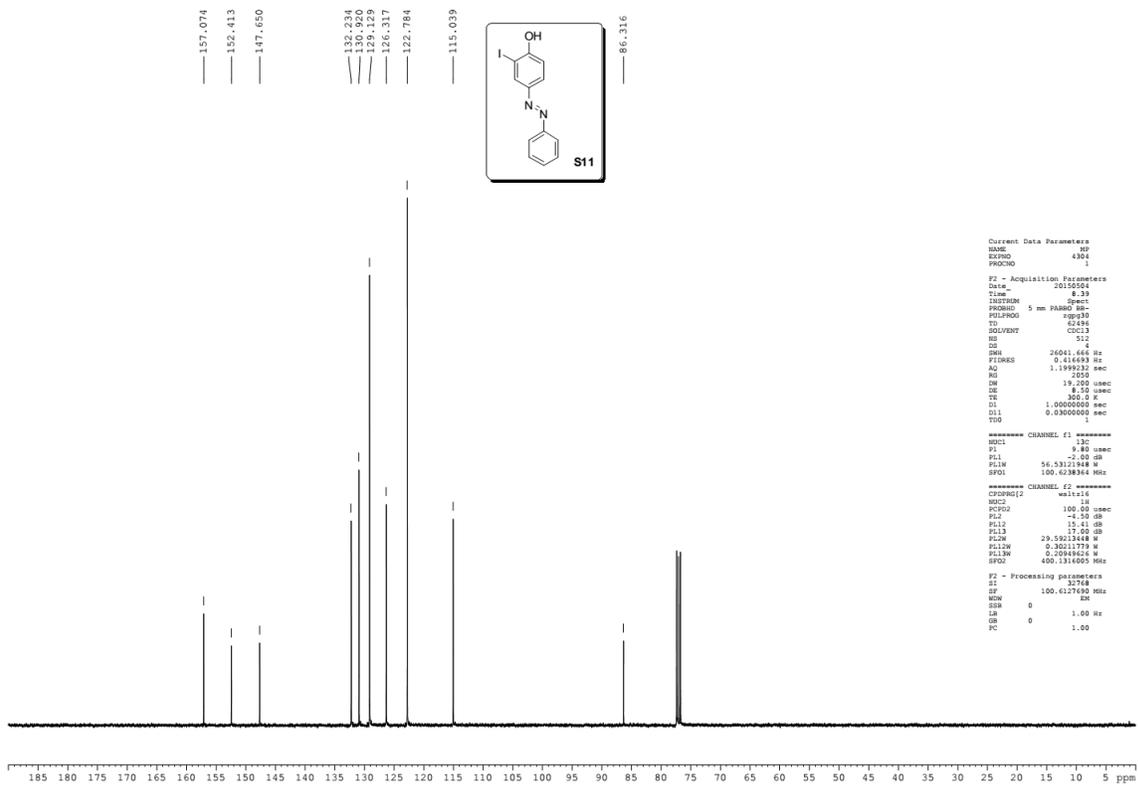
```

Current Data Parameters
NAME      RP
EXPNO    11304
PROCNO   1

F2 - Acquisition Parameters
Date_    20150310
Time     7:58
INSTRUM  spect
PROBHD   5 mm PABBI 1H/
PULPROG  zg30
TD       65536
SOLVENT  CDCl3
NS       8
DS       2
SWH      14097.744 Hz
FREQS    0.126822 Hz
AQ       3.9999206 sec
RG       612
DM       35.467 usec
DE       8.30 usec
TE       296.5 K
DQ1     2.00000000 sec
TOD     1

===== CHANNEL f1 =====
NUC1     1H
P1       9.20 usec
PL1     -1.30 dB
PL1W    13.88872355 W
SFO1    700.2754622 MHz

F2 - Processing parameters
SI       32768
SF       700.2700221 MHz
WDW      EM
SSB      0
LB       0 Hz
GB       0
PC       5.00
  
```



```

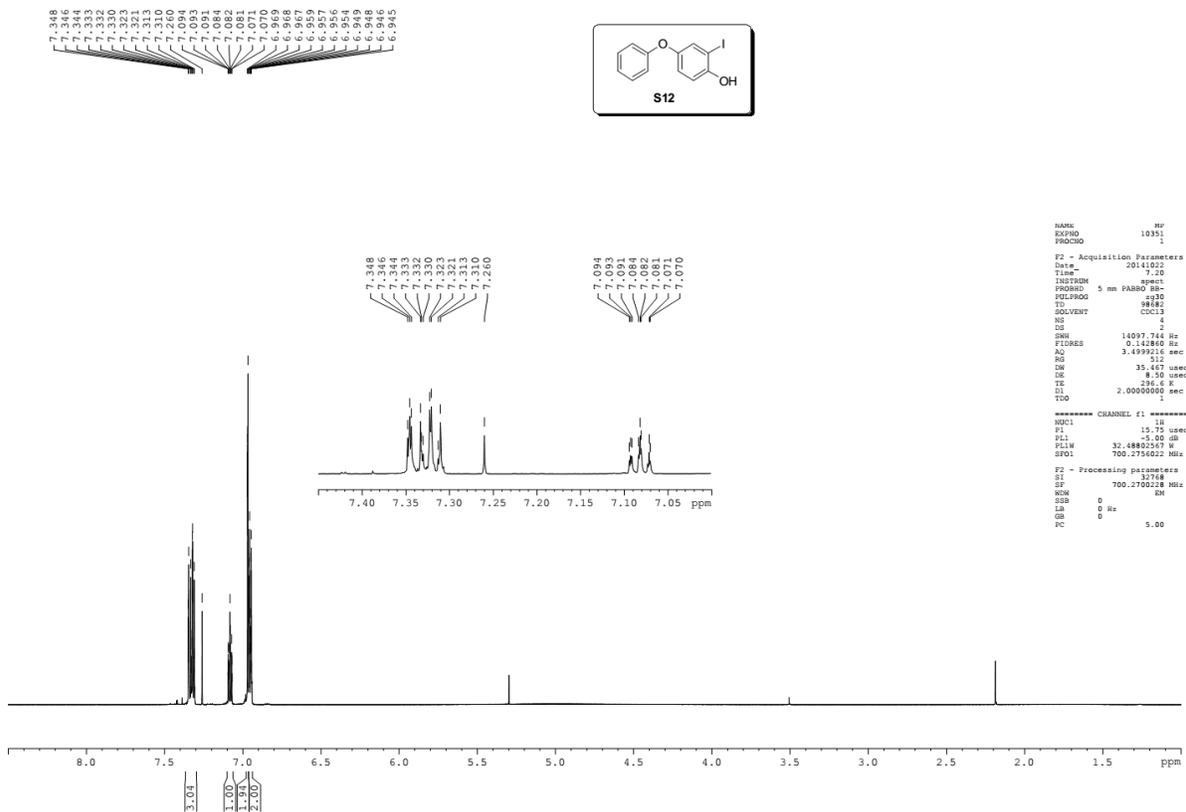
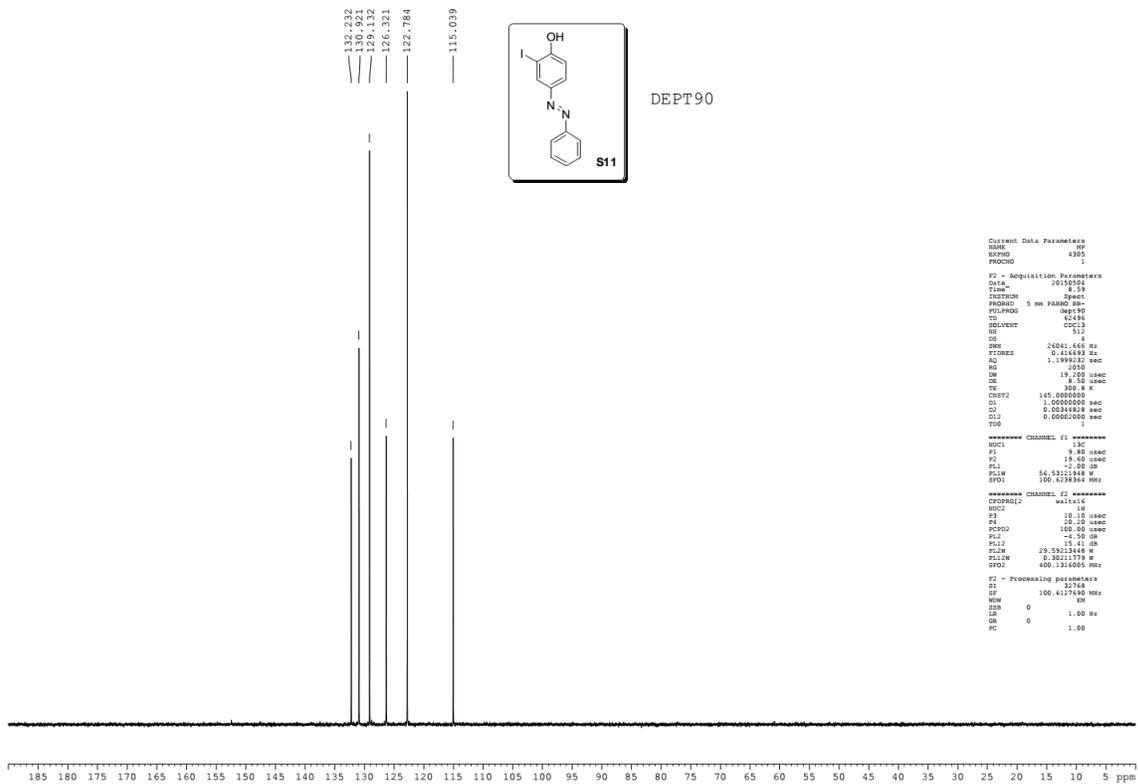
Current Data Parameters
NAME      RP
EXPNO    4304
PROCNO   1

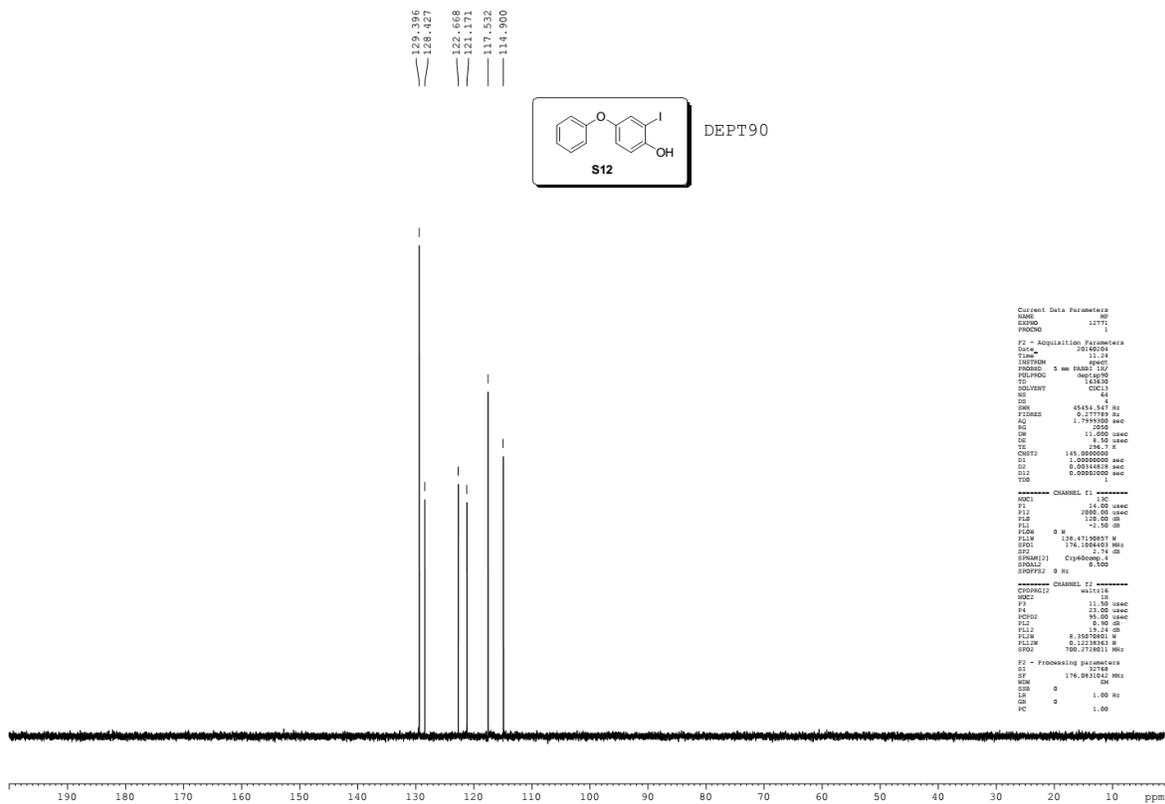
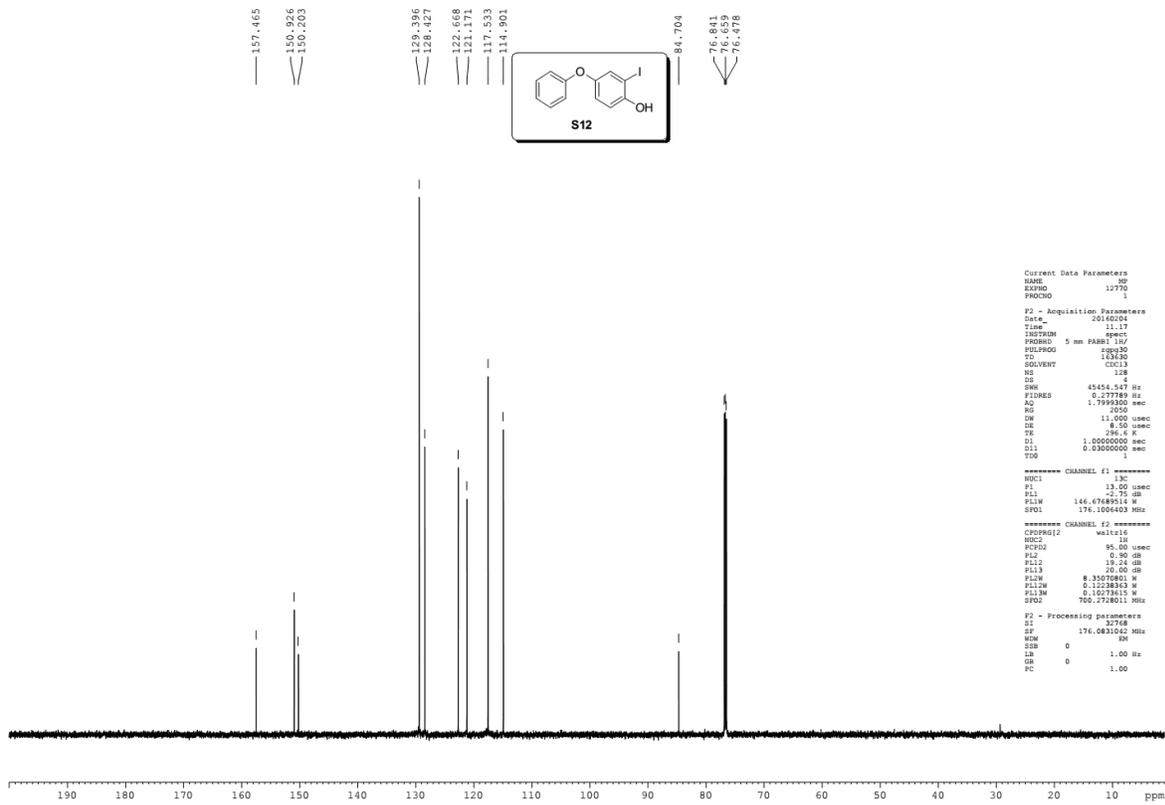
F2 - Acquisition Parameters
Date_    20150504
Time     6:39
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD       65496
SOLVENT  CDCl3
NS       4
DS       2
SWH      26041.644 Hz
FREQS    0.414493 Hz
AQ       1.1998232 sec
RG       2508
DM       19.700 usec
DE       8.10 usec
TE       300.0 K
DQ1     1.00000000 sec
DQ2     0.03000000 sec
TOD     1

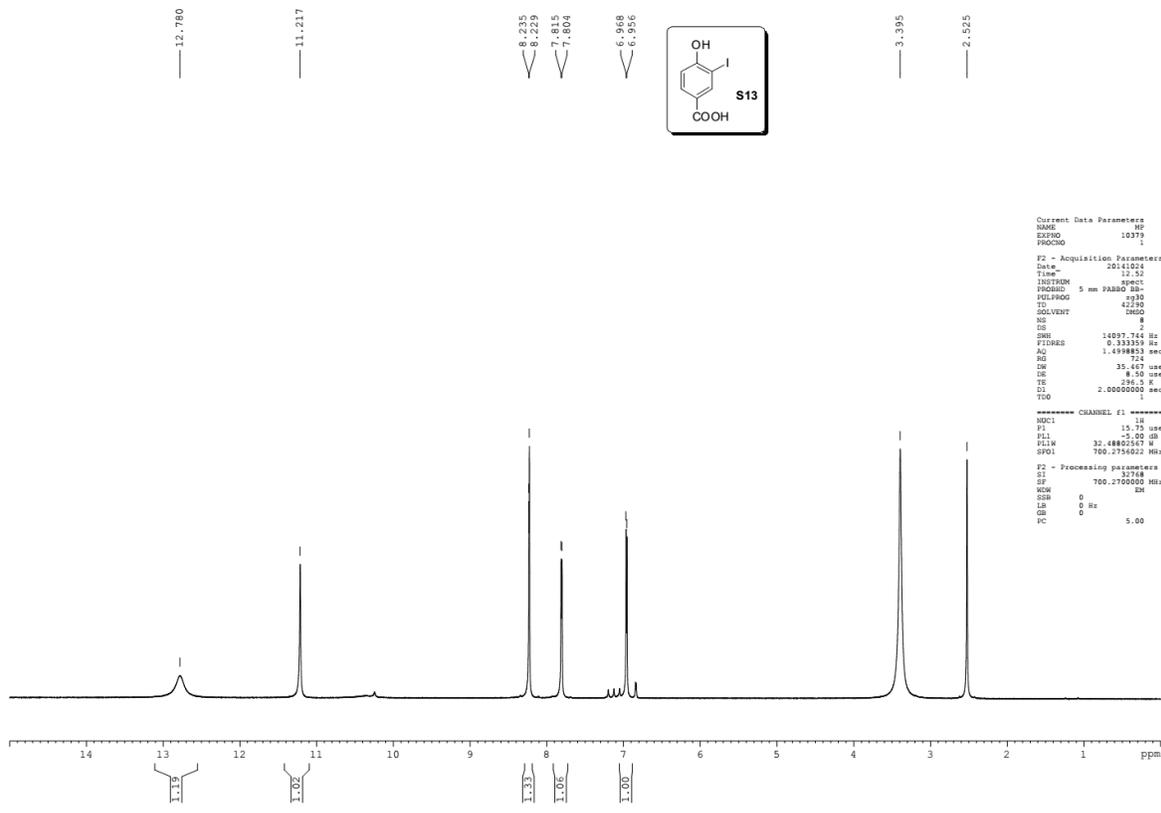
===== CHANNEL f1 =====
NUC1     13C
P1       9.80 usec
PL1     -1.00 dB
PL1W    56.53121248 W
SFO1    100.628364 MHz

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2     1H
PCPD2    100.00 usec
PL2     -1.00 dB
PL2W    17.00 dB
PL3     29.5621848 W
PL3W    0.30117779 W
SFO2    400.1316005 MHz

F2 - Processing parameters
SI       32768
SF       100.6127490 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.00
  
```







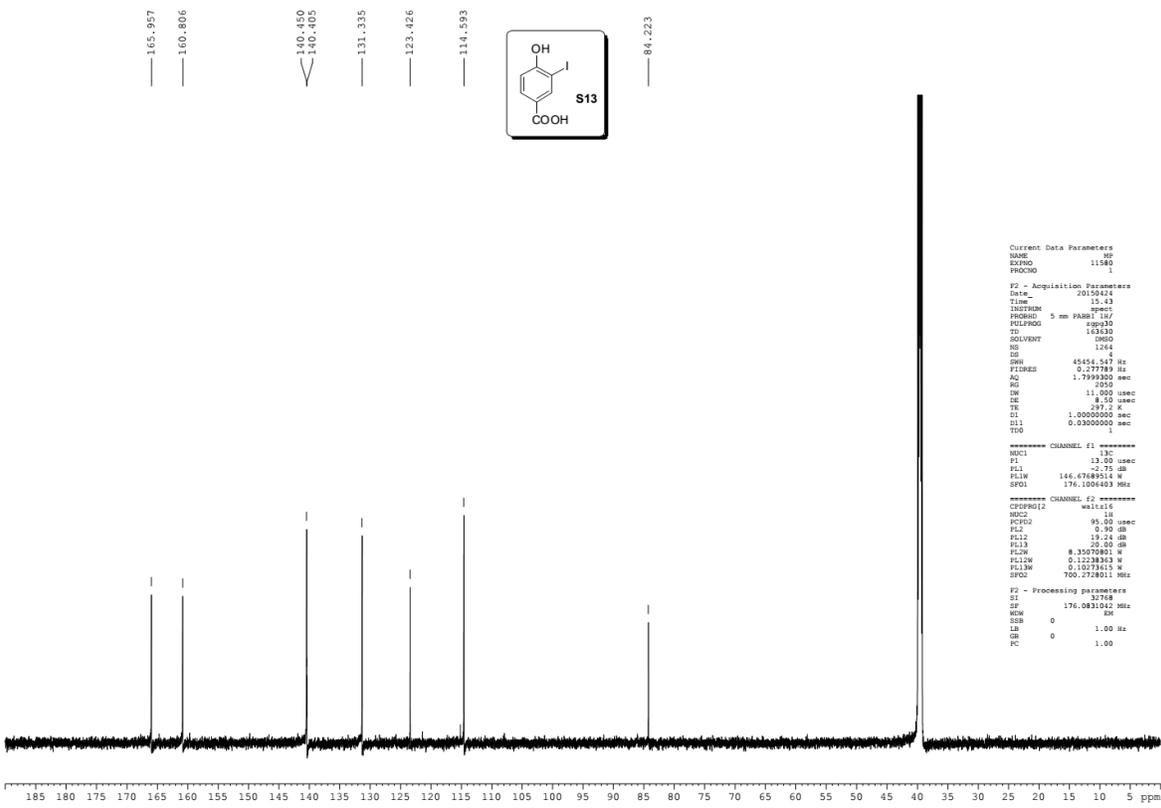
```

Current Data Parameters
NAME          RP
EXPNO        10379
PROCNO       1

F2 - Acquisition Parameters
Date_        20121024
Time         12.52
INSTRUM      spect
PROBHD       5 mm PABBO BB-
PULPROG      zg30
TD           42290
SOLVENT      DMSO
NS           8
DS           4
SWH          14097.744 Hz
FIDRES       0.333339 Hz
AQ           1.4598853 sec
RG           724
SQ           35.467 usec
DE           8.30 usec
TE           296.5
D1           2.0000000 sec
TOD         1

===== CHANNEL f1 =====
NUC1         1H
P1           15.70 usec
PL1         -3.00 dB
PL12        32.48802317 dB
SFO1        700.2754622 MHz

F2 - Processing parameters
SI           32768
SF           700.2700000 MHz
WDW          EM
SSB          0
LB           0 Hz
GB           0
PC           5.00
  
```



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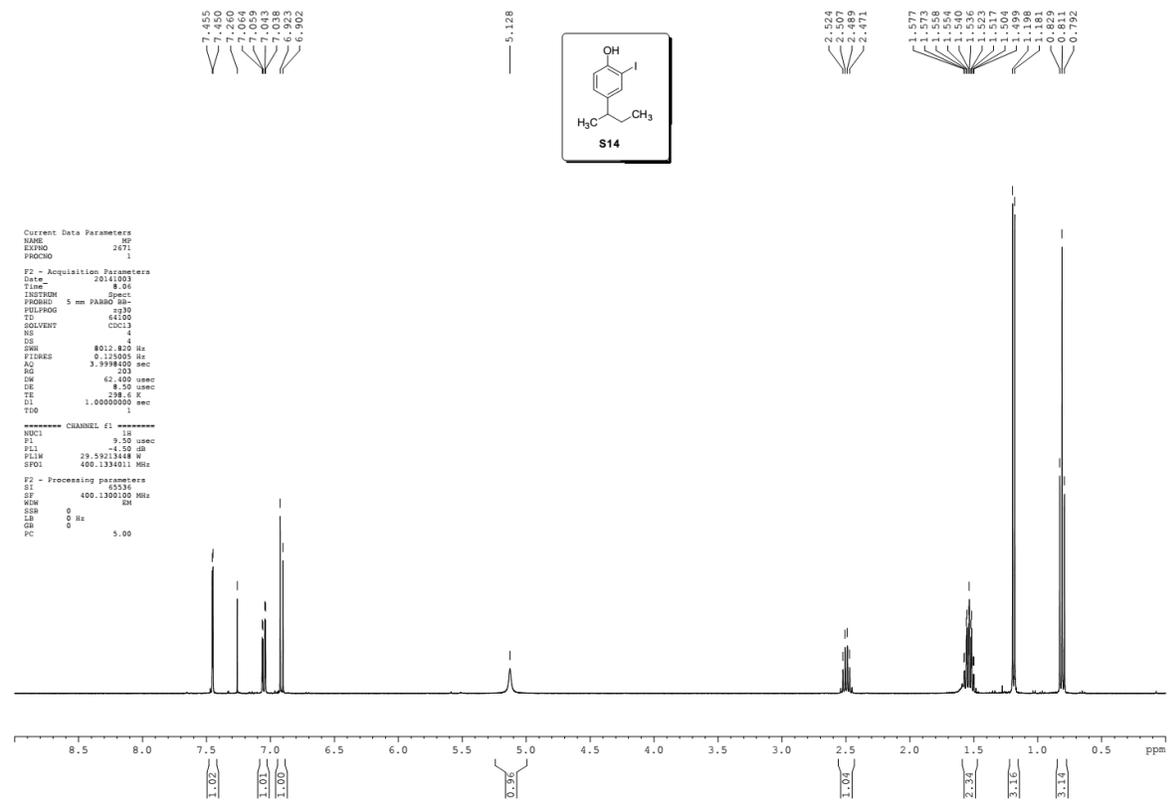
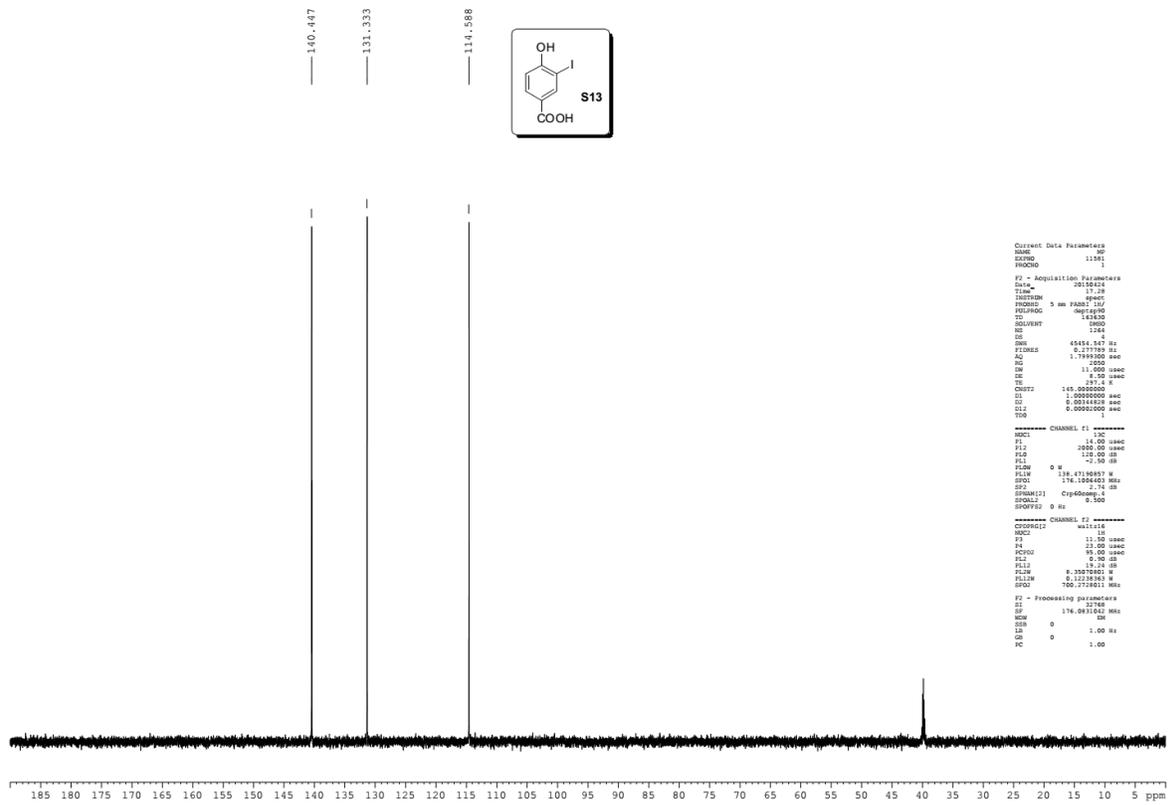
Current Data Parameters
NAME          RP
EXPNO        11580
PROCNO       1

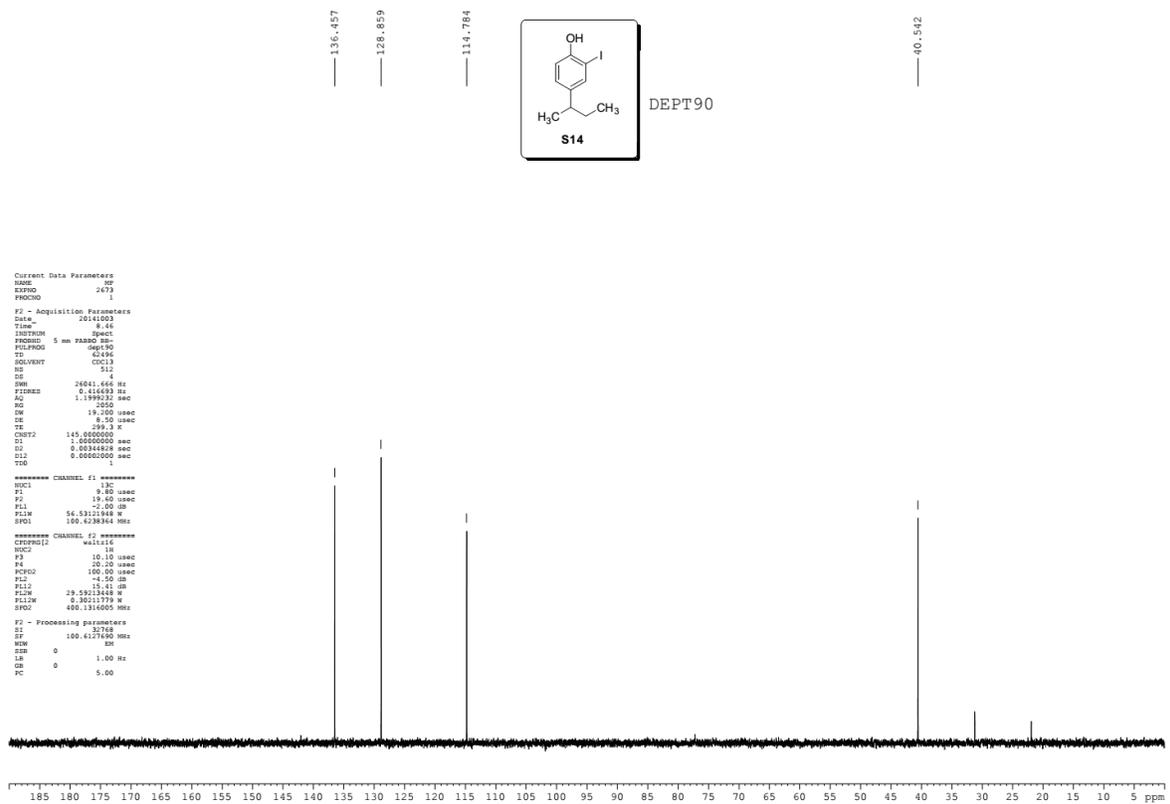
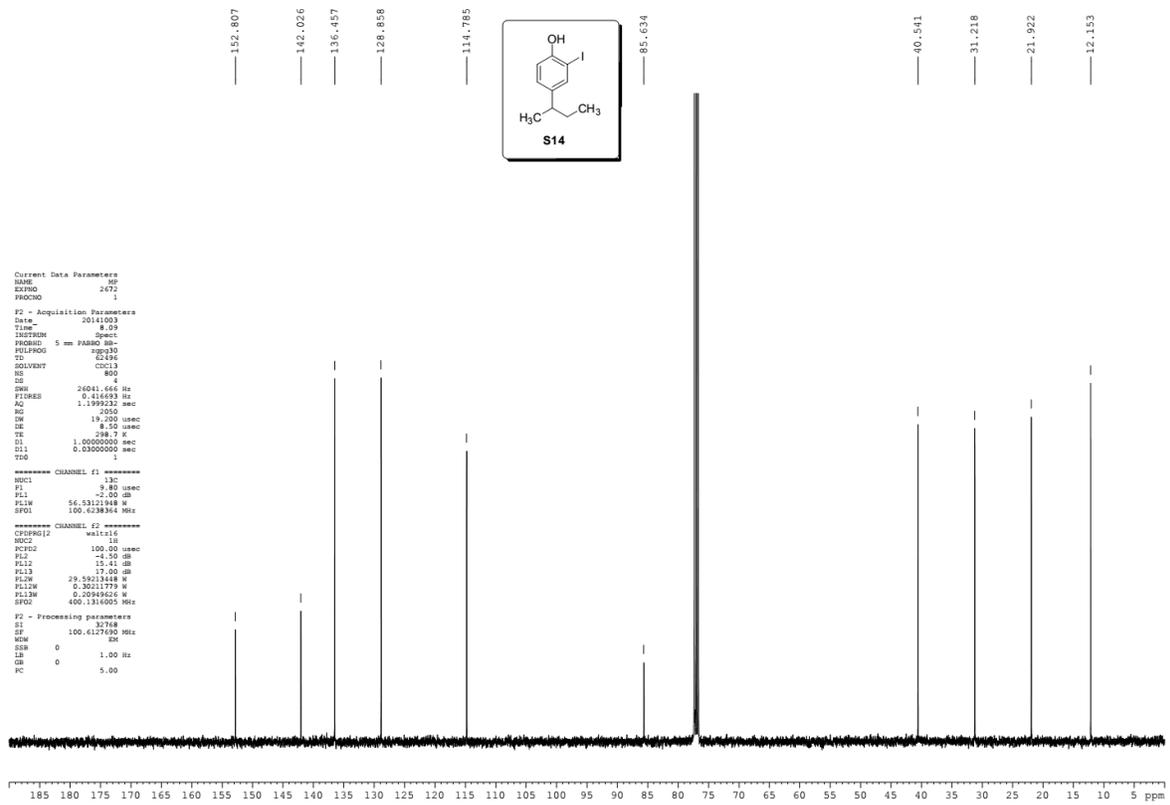
F2 - Acquisition Parameters
Date_        20150824
Time         15.43
INSTRUM      spect
PROBHD       5 mm PABBO BB-
PULPROG      zgpg30
TD           143830
SOLVENT      DMSO
NS           1244
DS           4
SWH          45454.547 Hz
FIDRES       0.277789 Hz
AQ           1.7599202 sec
RG           2000
SQ           11.000 usec
DE           8.10 usec
TE           297.2
D1           1.0000000 sec
D11         0.0300000 sec
TOD         1

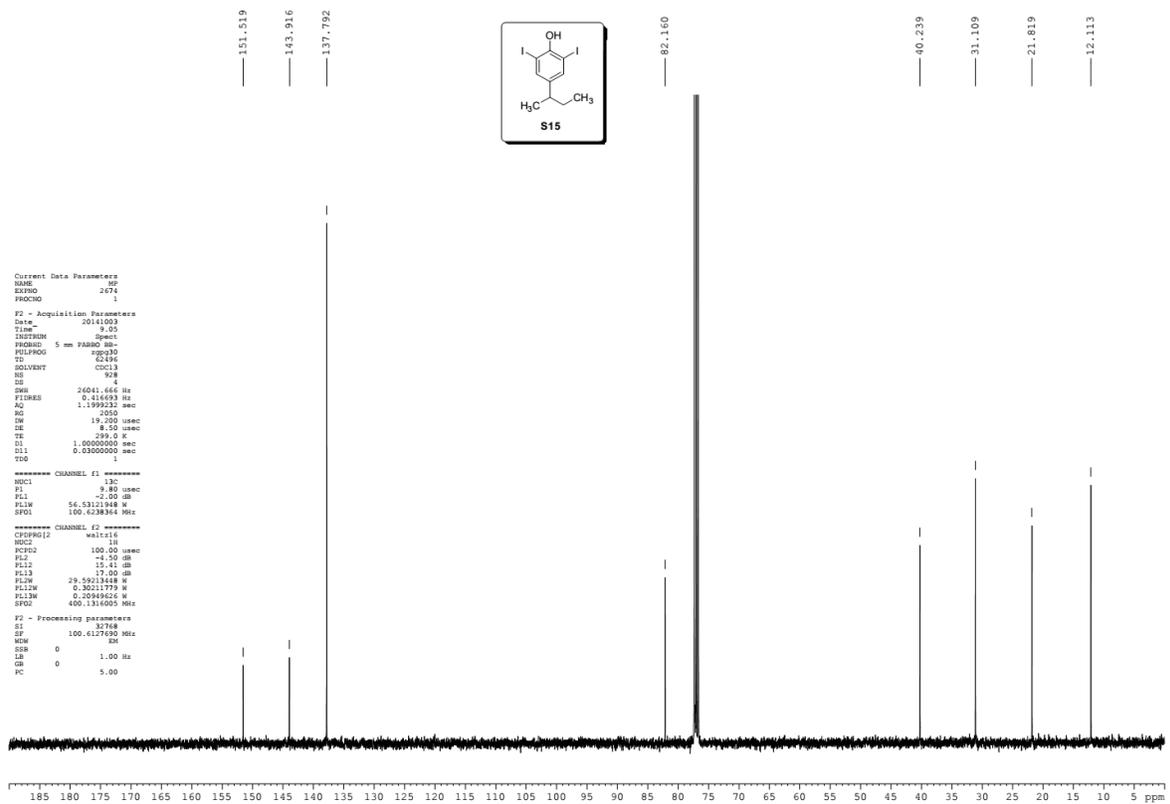
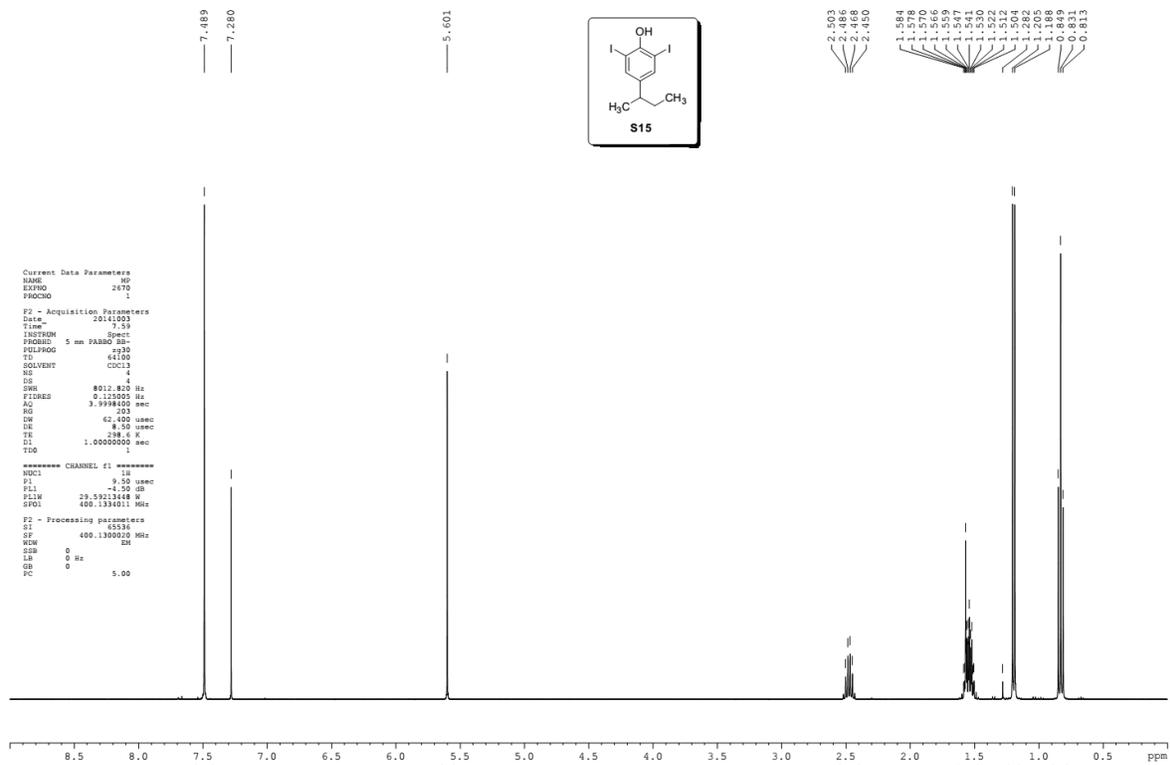
===== CHANNEL f1 =====
NUC1         13C
P1           13.00 usec
PL1         -2.75 dB
PL12        144.67488514 dB
SFO1        176.1006403 MHz

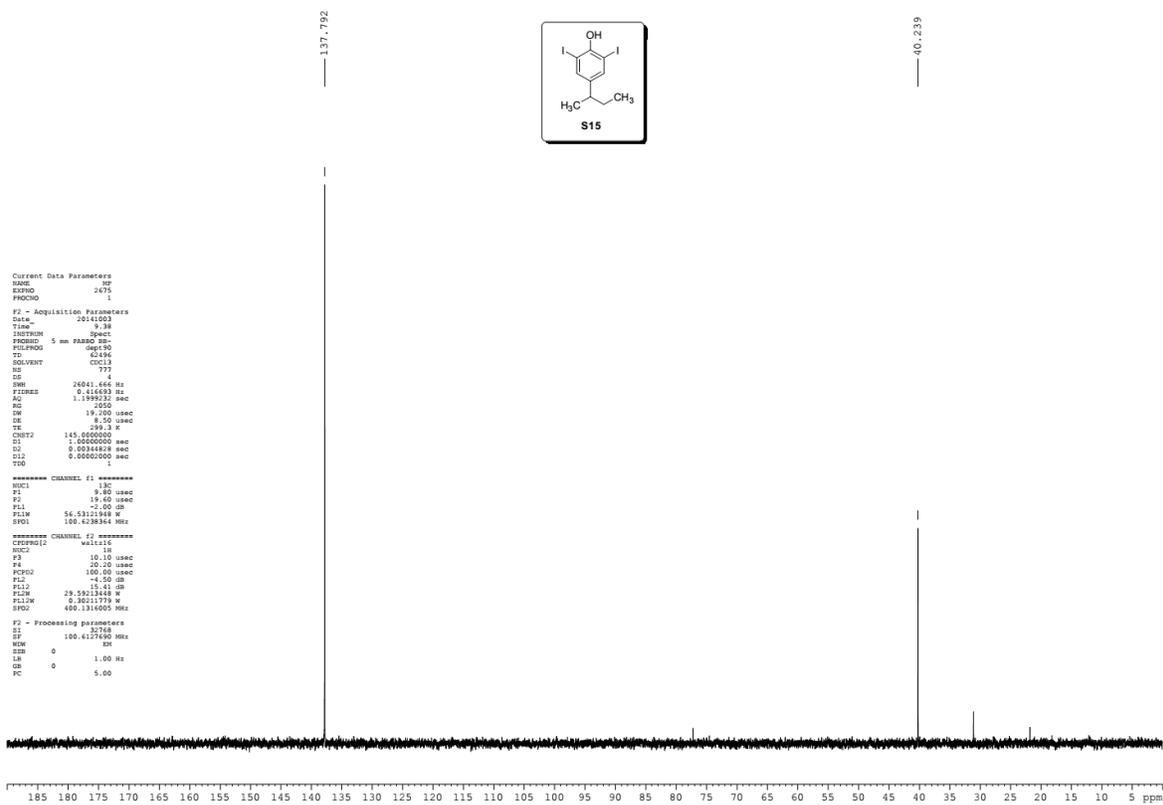
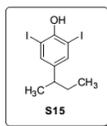
===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2         1H
PCPD2        95.00 usec
PL2          0.90 dB
PL12         19.24 dB
PL13         30.00 dB
PL14         8.35070891 dB
PL15W        0.12238343 W
PL16W        0.10778115 W
SFO2        700.2748011 MHz

F2 - Processing parameters
SI           32768
SF           176.0831042 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.00
  
```









```

Current Data Parameters
NAME          SF
EXPNO        2475
PROCNO       1

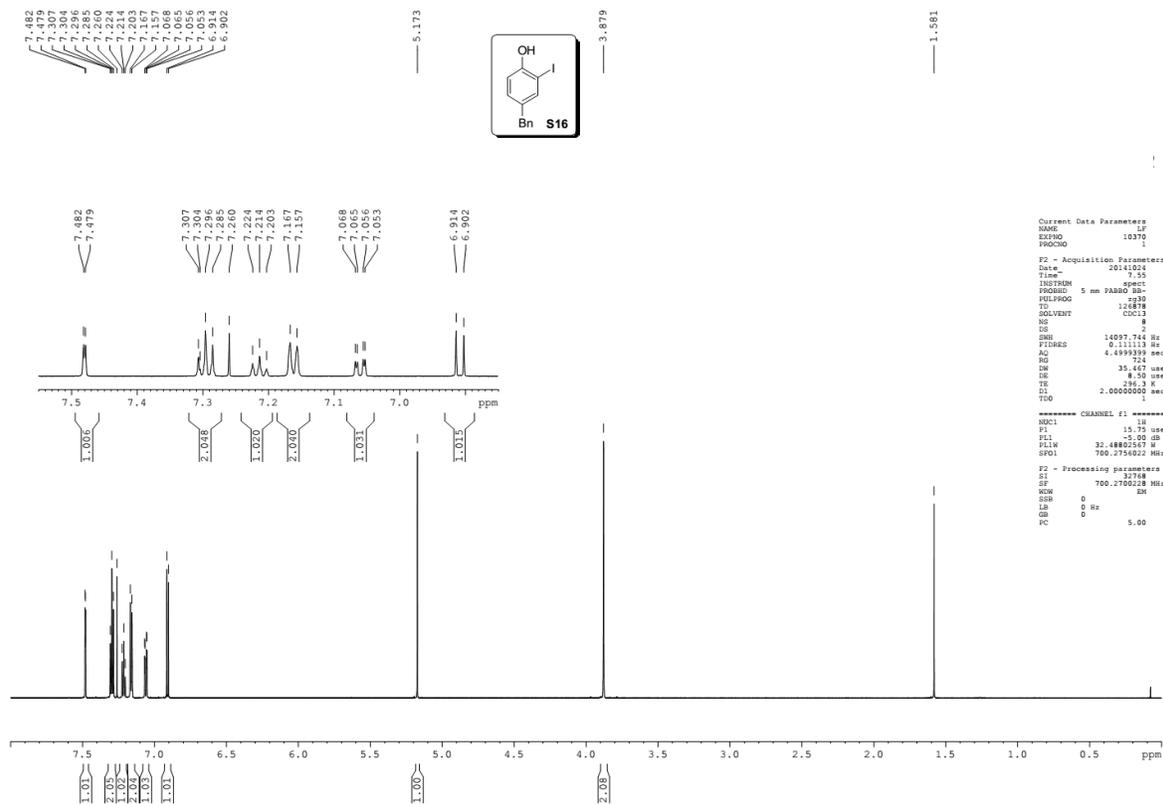
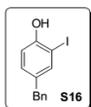
F2 - Acquisition Parameters
Date_        20141003
Time        9.38
INSTRUM      spect
PROBHD      5 mm PABBO BB-
PULPROG     zgpg30
TD           65536
SOLVENT     CDCl3
NS           4
DS           2
SWH          26041.666 Hz
F2FRES      6.41683 Hz
AQ           1.1999232 sec
RG           9.250
WDW          EM
SSB          0
GB           0
DC           0
CMB2        145.0000000
D1           1.0000000 sec
D2           0.00344828 sec
D12          0.0000000 sec
TD0          1

===== CHANNEL f1 =====
NUC1         13C
P1           2.32
PC1          19.60 usec
PL1          -1.50 dB
PL1W        56.53121948 W
SFO1        100.628354 Mhz

===== CHANNEL f2 =====
CFPROG2      waltz16
NUC2         1H
P2           10.10 usec
PC2          100.00 usec
PL2          -1.50 dB
PL2W        29.5821348 W
PL1W        5.30211779 W
SFO2        400.1316005 Mhz

F2 - Processing parameters
SI           32768
SF           100.6171900 Mhz
WDW          EM
SSB          0
GB           0
DC           0
CMB          0
PC           5.00
  
```

7.482
7.307
7.304
7.296
7.286
7.280
7.224
7.214
7.167
7.157
7.085
7.056
7.053
6.902



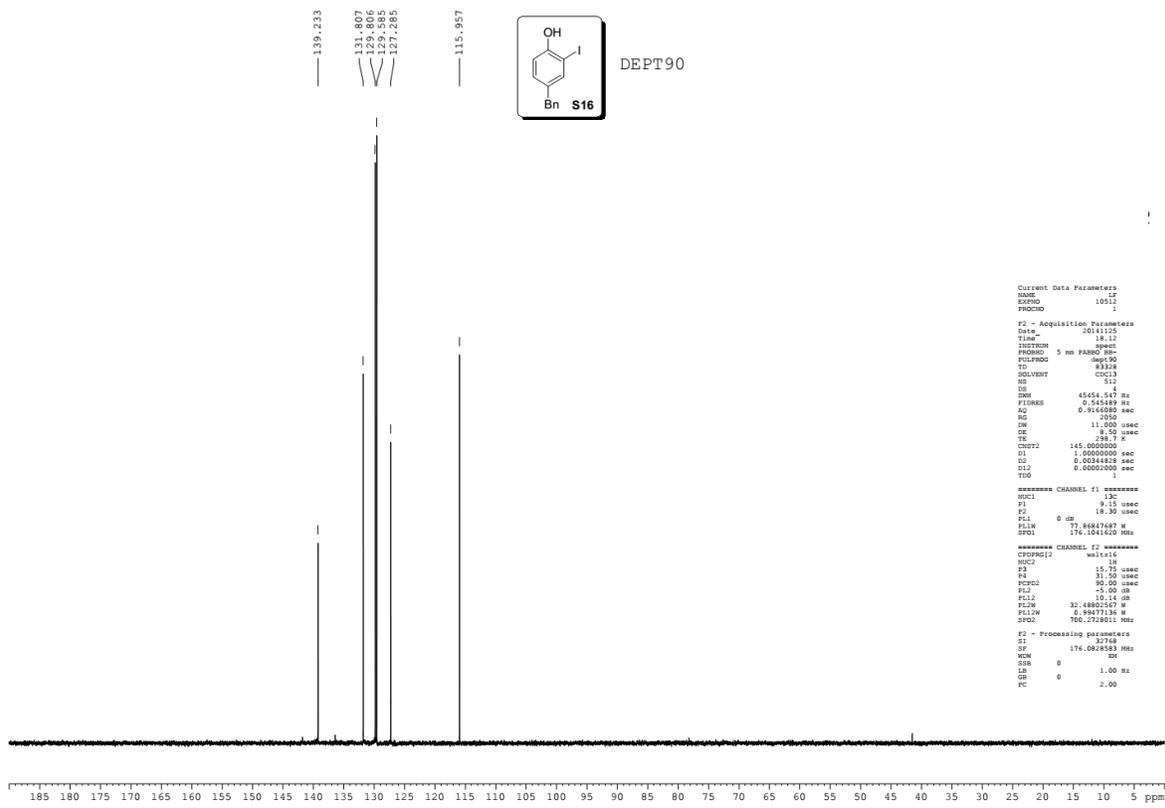
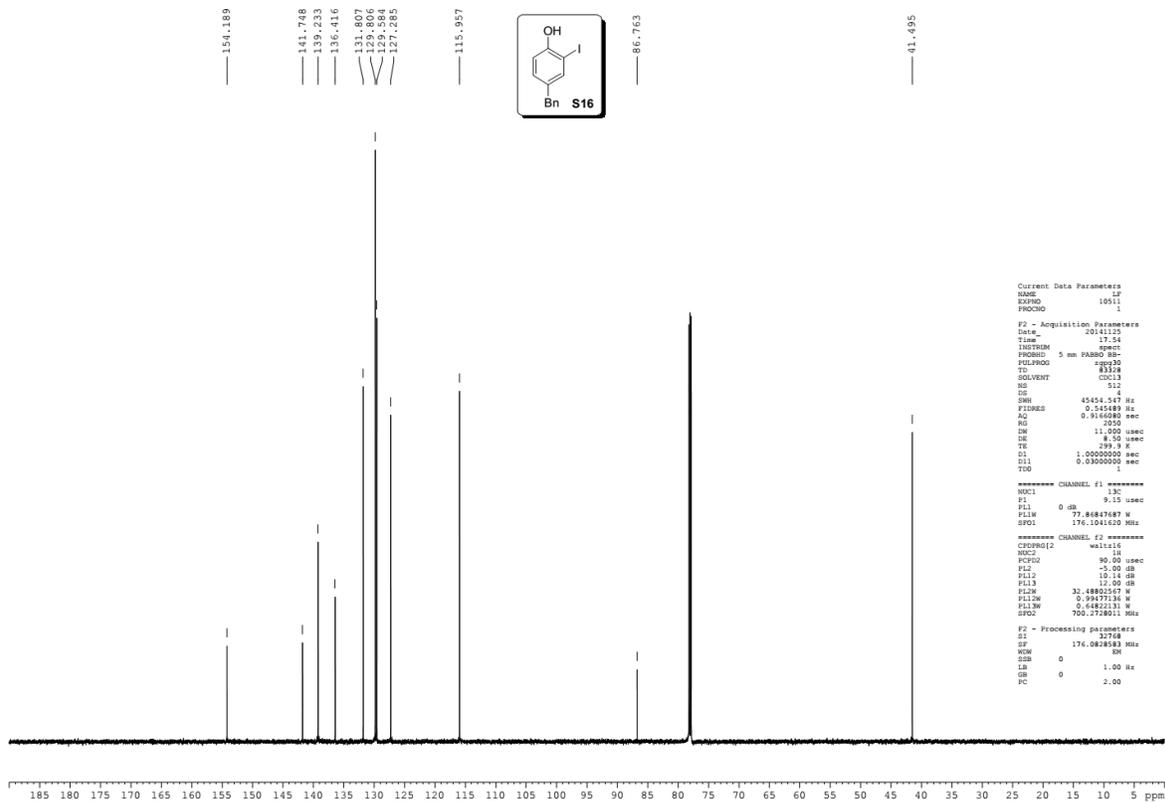
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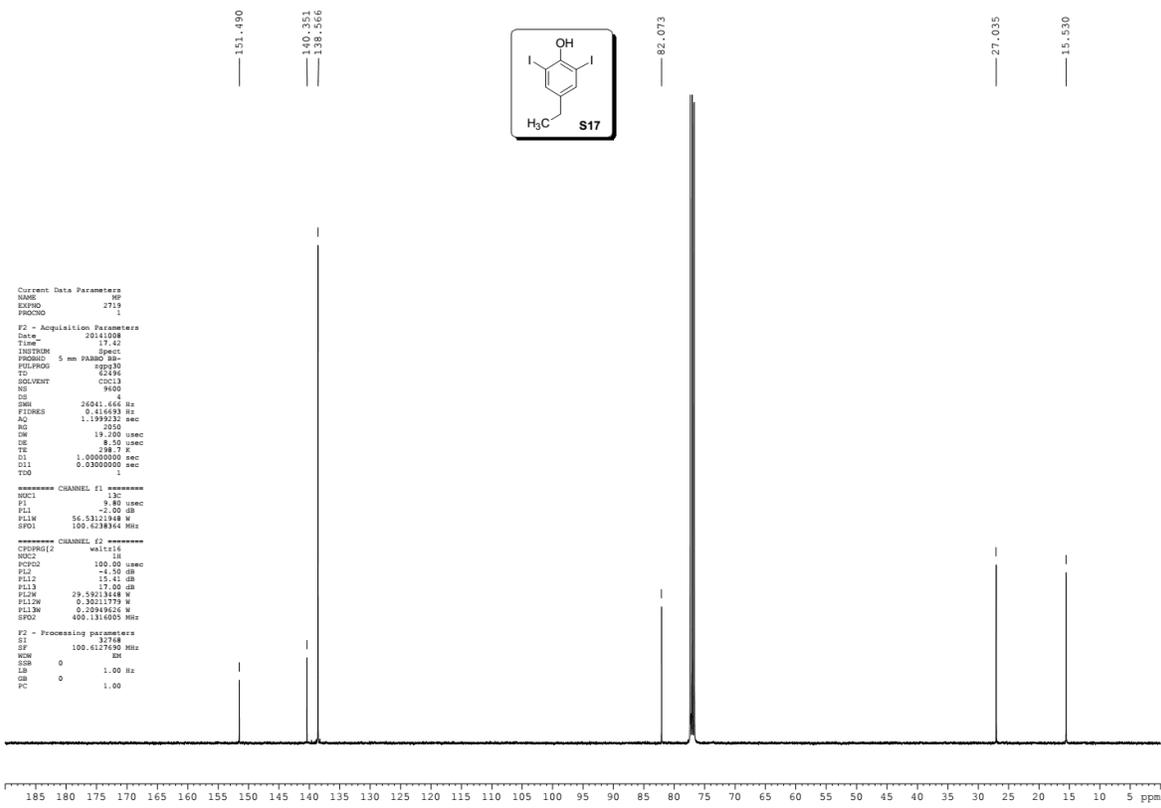
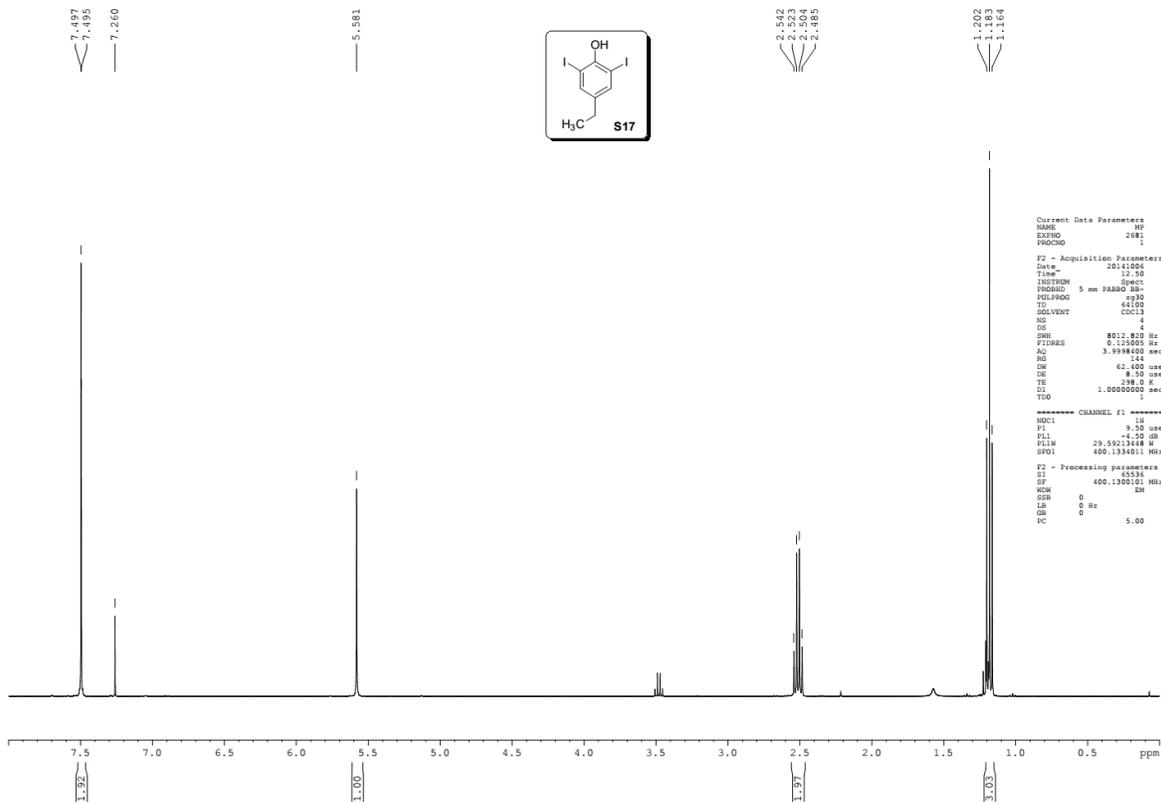
Current Data Parameters
NAME          SF
EXPNO        10370
PROCNO       1

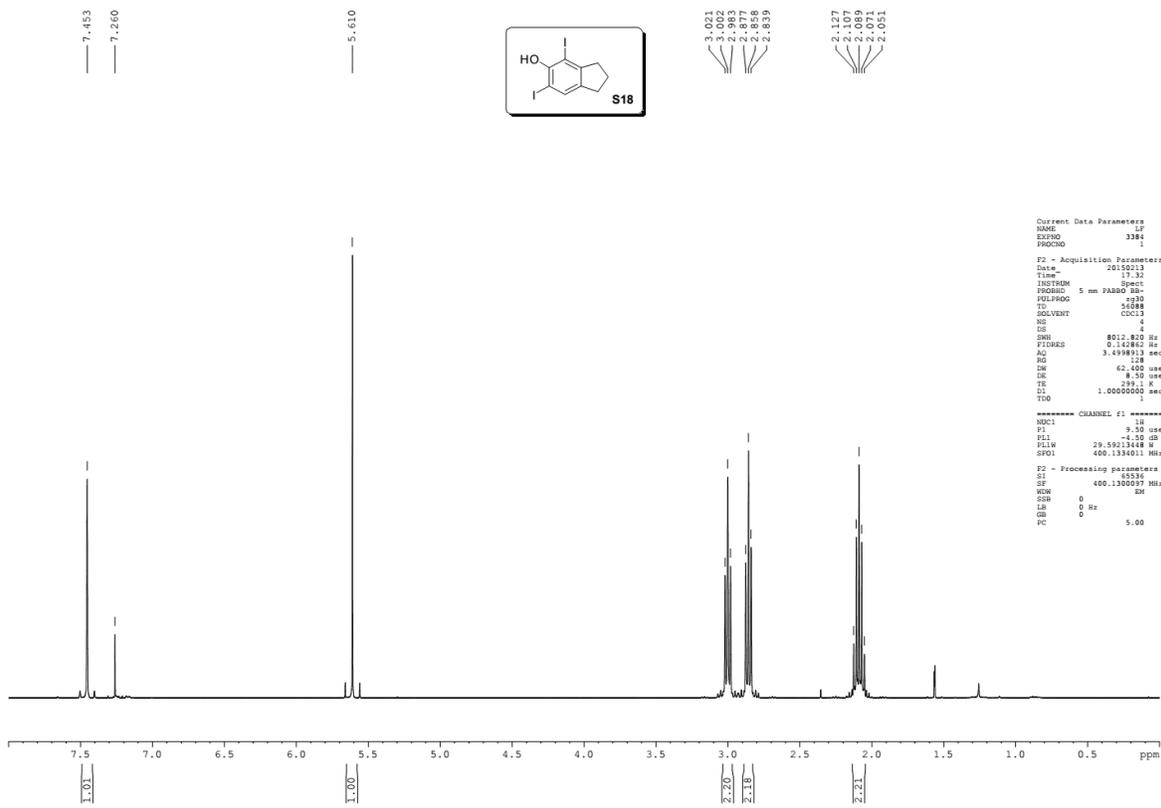
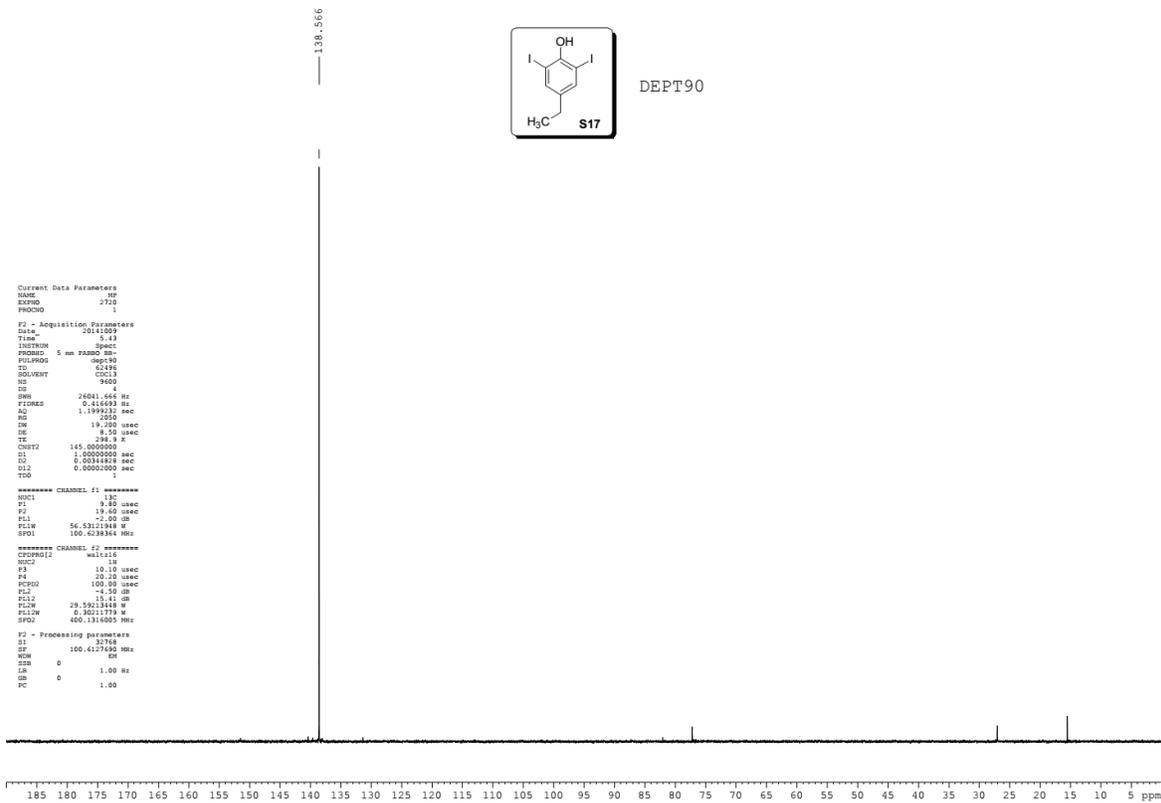
F2 - Acquisition Parameters
Date_        20141024
Time        7.55
INSTRUM      spect
PROBHD      5 mm PABBO BB-
PULPROG     zgpg30
TD           126878
SOLVENT     CDCl3
NS           8
DS           2
SWH          14097.764 Hz
F2FRES      0.11113 Hz
AQ           4.4993399 sec
RG           33.427
WDW          EM
SSB          0
GB           0
DC           0
CMB          0
PC           5.00

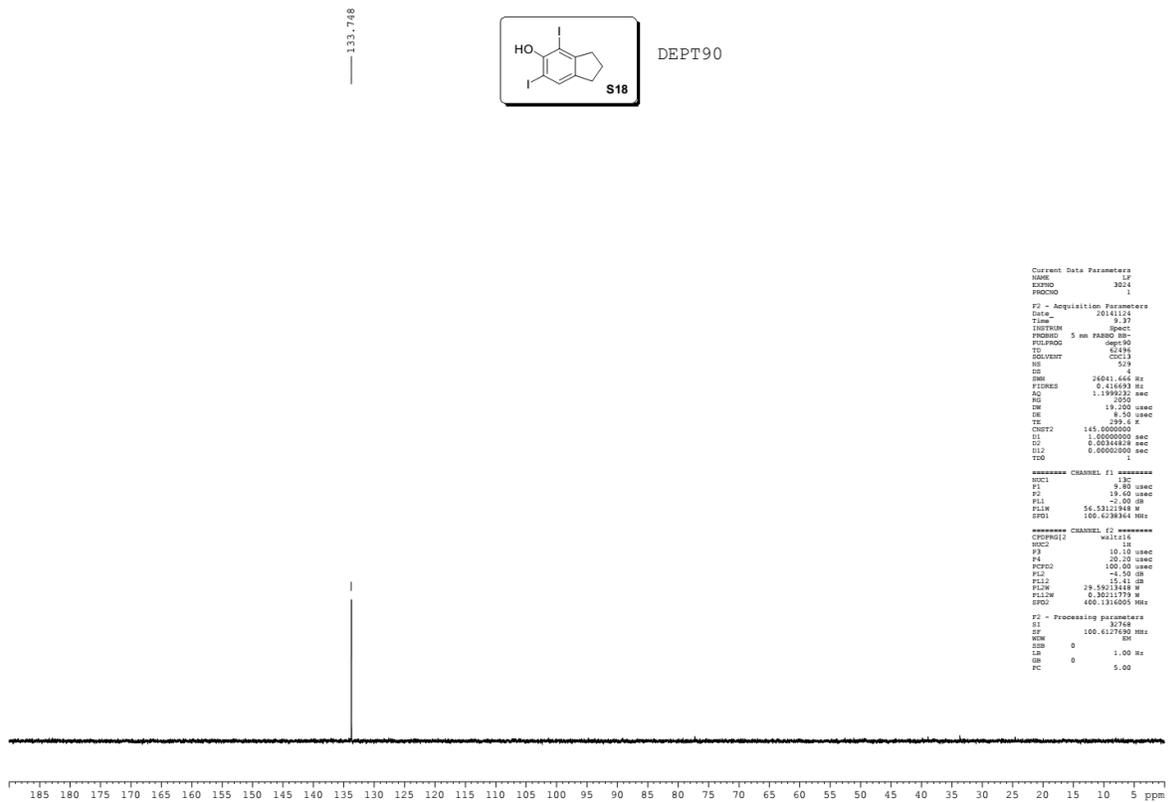
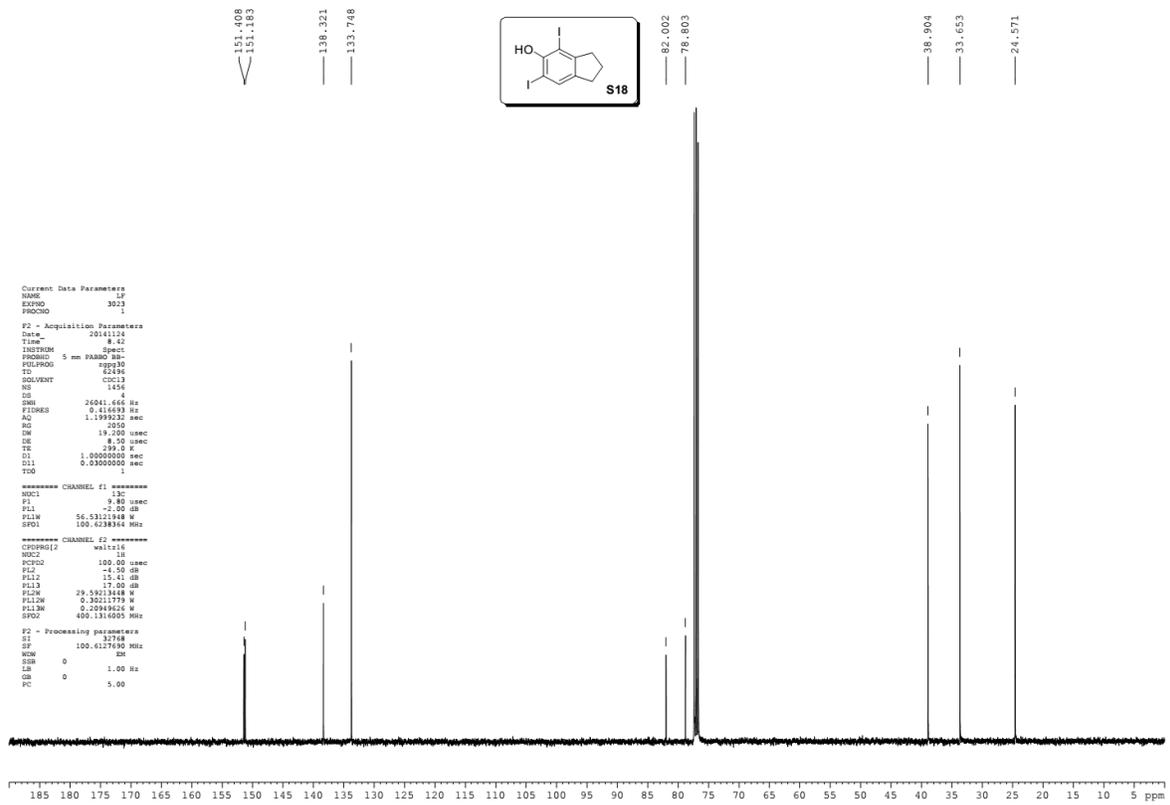
===== CHANNEL f1 =====
NUC1         1H
P1           18
PC1          19.60 usec
PL1          -5.00 dB
PL1W        31.4880557 W
SFO1        100.2756022 Mhz

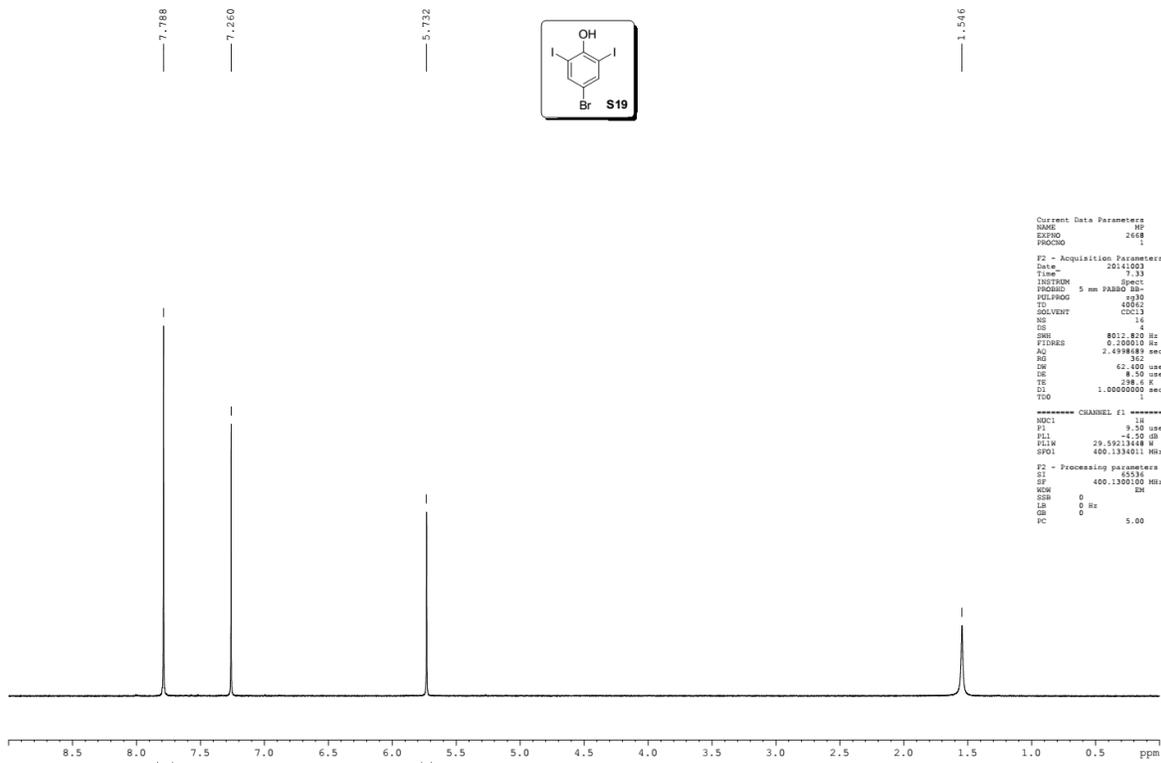
F2 - Processing parameters
SI           32768
SF           100.2700228 Mhz
WDW          EM
SSB          0
GB           0
DC           0
CMB          0
PC           5.00
  
```









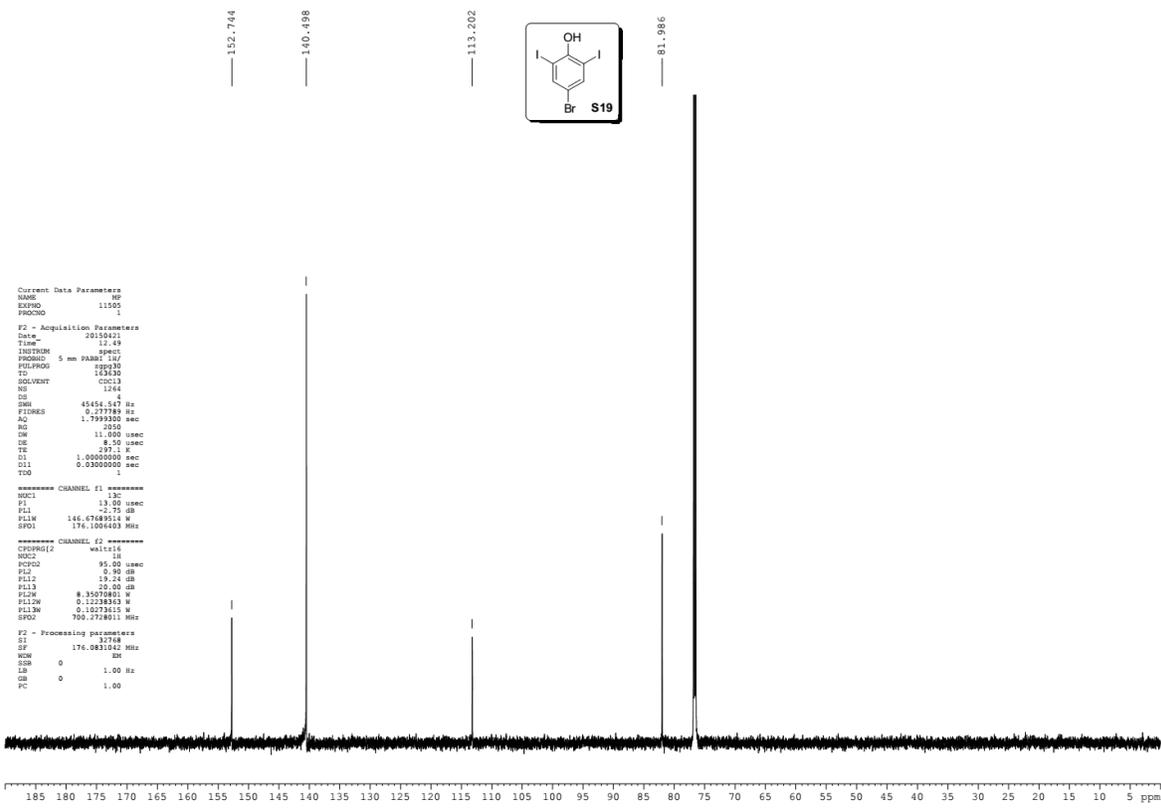


```

Current Data Parameters
NAME      KF
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    201203
Time     7.33
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        16
DS        4
SWH       8012.820 Hz
FIDRES    0.200010 Hz
AQ         2.4598889 sec
RG         322
SQ         62.400 usec
SE         8.30 usec
TE         298.6 K
SI         1.00000000 sec
D1         1
===== CHANNEL f1 =====
NUC1      1H
P1         9.50 usec
PL1       -1.50 dB
PL12      29.5013848 dB
SFO1      400.1334011 MHz

F2 - Processing parameters
SI         65536
SF         400.1300100 MHz
WDW        EM
SSB        0
LB         0 Hz
GB         0
PC         5.00
  
```



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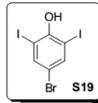
Current Data Parameters
NAME      KF
EXPNO    15501
PROCNO   1

F2 - Acquisition Parameters
Date_    2015021
Time     12.49
INSTRUM  spect
PROBHD   5 mm PABBO 1H/
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        1264
DS        4
SWH       45454.547 Hz
FIDRES    0.277788 Hz
AQ         1.7993000 sec
RG         2050
SQ         11.000 usec
SE         8.30 usec
TE         297.1 K
SI         1.00000000 sec
D1         0.03000000 sec
D11        1
===== CHANNEL f1 =====
NUC1      13C
P1        13.00 usec
PL1        0.00 dB
PL12      146.47689514 dB
SFO1      176.1004493 MHz

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2      1H
P2P2     95.00 usec
P12       0.00 dB
PL12      19.24 dB
PL13      10.00 dB
PL2W      8.35070861 W
PL2W      0.12238363 W
PL3W      0.10273615 W
SFO2      705.7738011 MHz

F2 - Processing parameters
SI         176.0810428 MHz
SF         176.0810428 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.00
  
```

140.196



DEPT90

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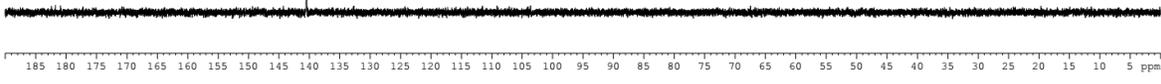
Current Data Parameters
NAME          RP
EXPNO        11504
PROCNO       1

F2 - Acquisition Parameters
Date_        20150212
Time         13.55
INSTRUM      spect
PROBHD       5 mm PABBO 1H/
PULPROG      zgpg30
TD           65536
SOLVENT      CDCl3
NS           512
DS           4
SWH           40454.147 Hz
FIDRES       0.277789 Hz
AQ           1.799789 sec
RG           2552
SW           11.900 usec
DE           8.50 usec
TE           297.2 K
CNU2         145.000000
SI           1.00000000 sec
SFO1         0.0034803 sec
SFO2         0.0000200 sec
TOD          1

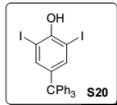
===== CHANNEL f1 =====
NUC1          13C
P1            14.00 usec
PL1           28.00 usec
SFO1         125.760350 MHz
SFO2         176.1004403 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2          1H
P2            11.50 usec
PL2           23.00 usec
SFO2         400.146401 MHz
PL12         0.90 usec
PL13         0.1238363 usec
PL14         8.3507080 usec
SFO1         0.1238363 MHz
SFO2         700.728011 MHz

F2 - Processing parameters
SI            32768
SF           176.0931042 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.00
  
```



7.424
7.353
7.342
7.266
7.256
7.126
7.115



3.351

2.525

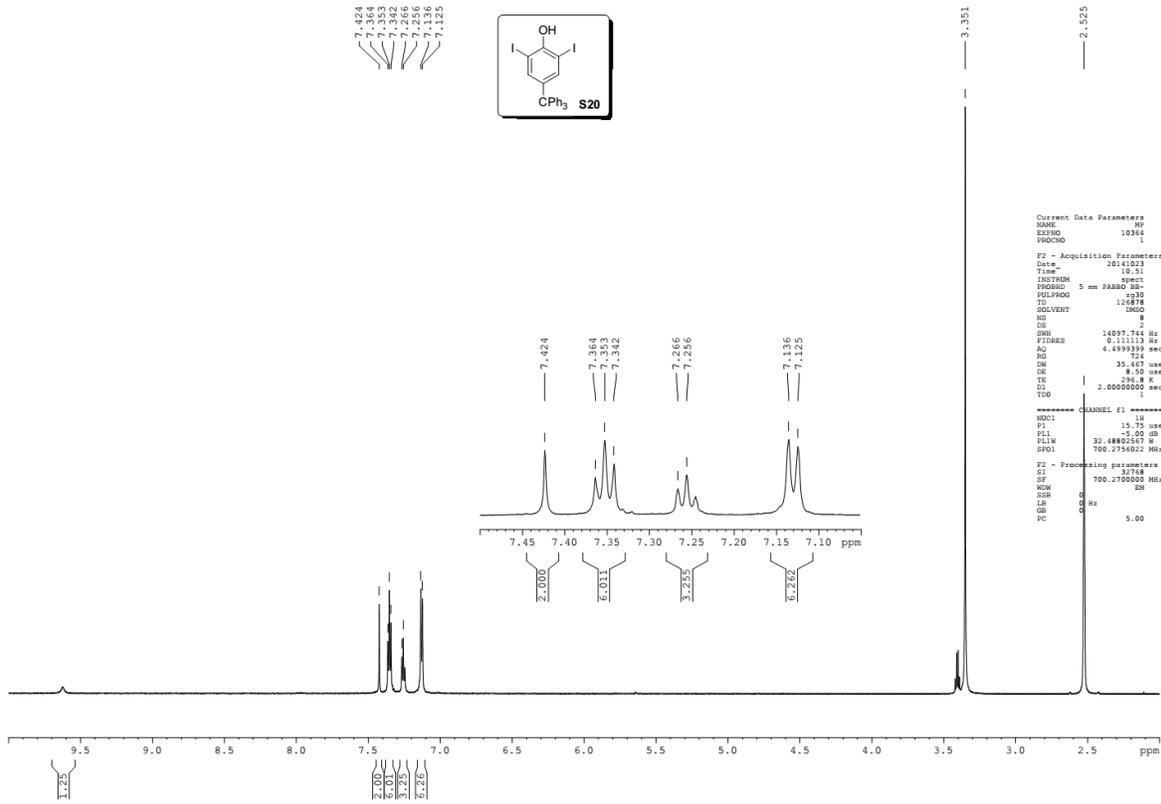
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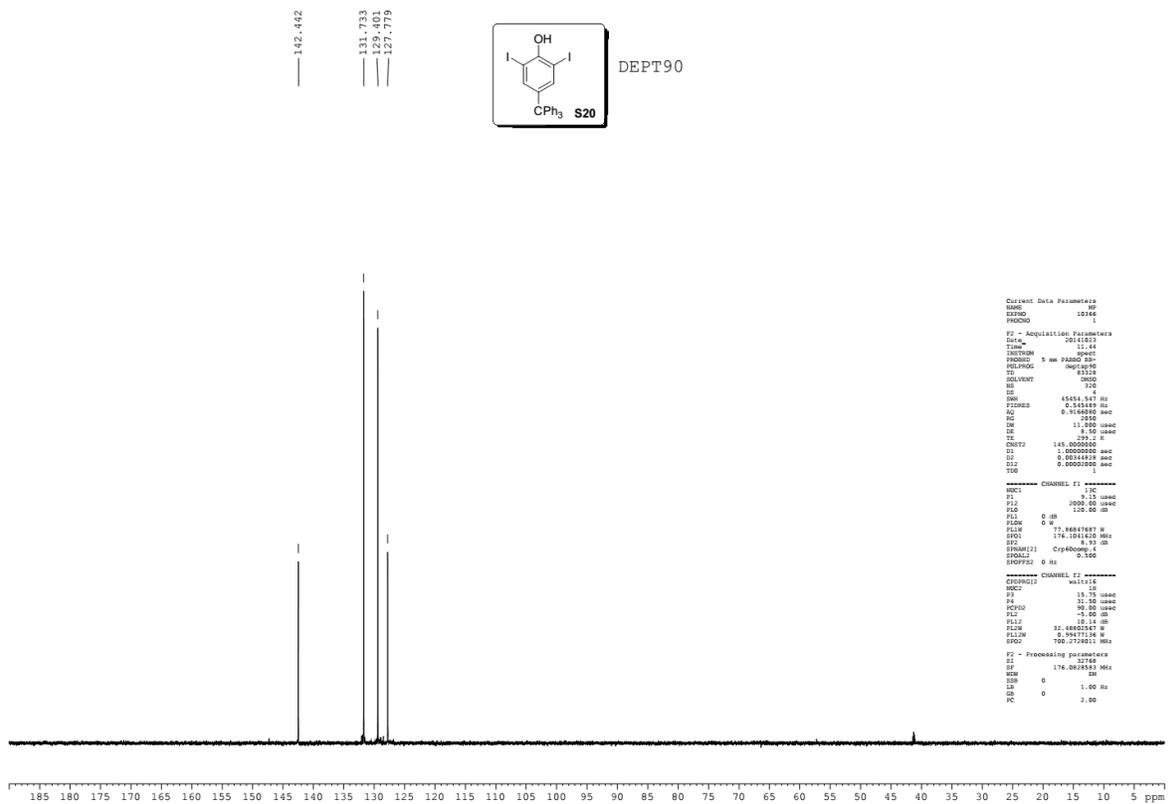
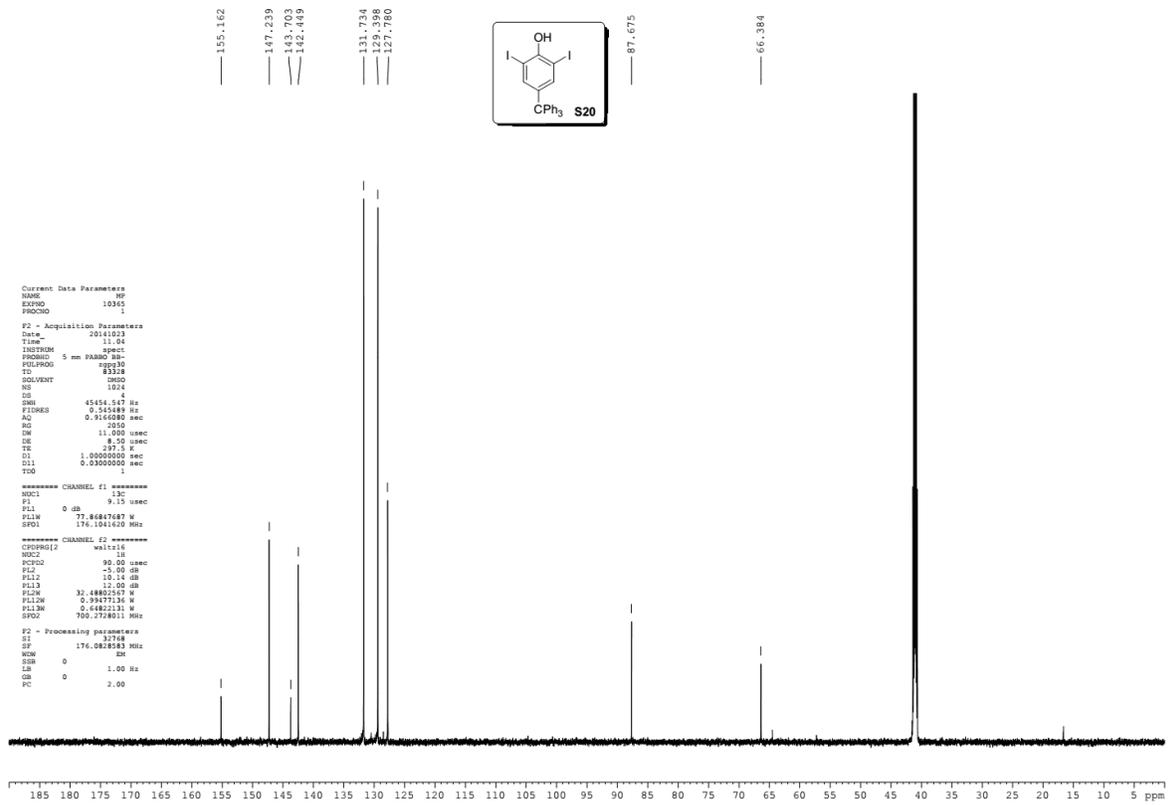
Current Data Parameters
NAME          RP
EXPNO        10344
PROCNO       1

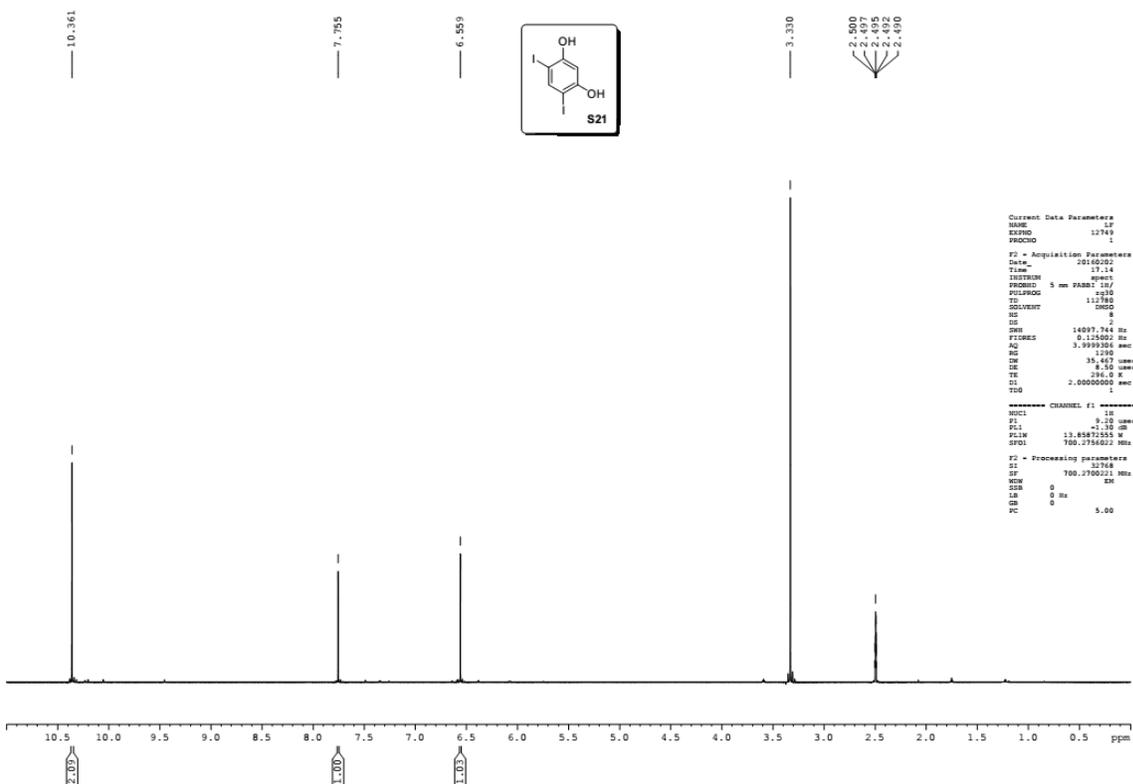
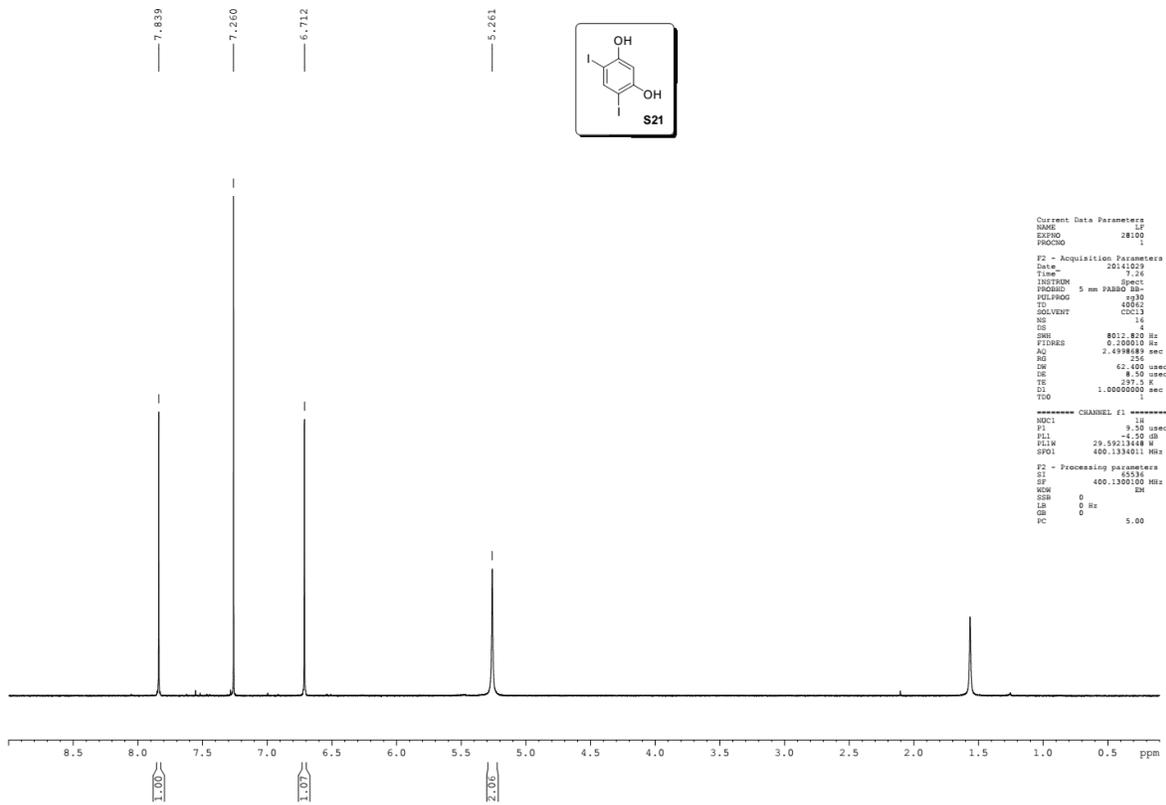
F2 - Acquisition Parameters
Date_        20141023
Time         10.51
INSTRUM      spect
PROBHD       5 mm PABBO 1H/
PULPROG      zgpg30
TD           132678
SOLVENT      DMSO
NS           8
DS           2
SWH           14097.764 Hz
FIDRES       0.111113 Hz
AQ           4.4999399 sec
RG           274
SW           33.462 usec
DE           8.50 usec
TE           296.8 K
SFO1         2.00000000 sec
SFO2         2.00000000 sec
TOD          1

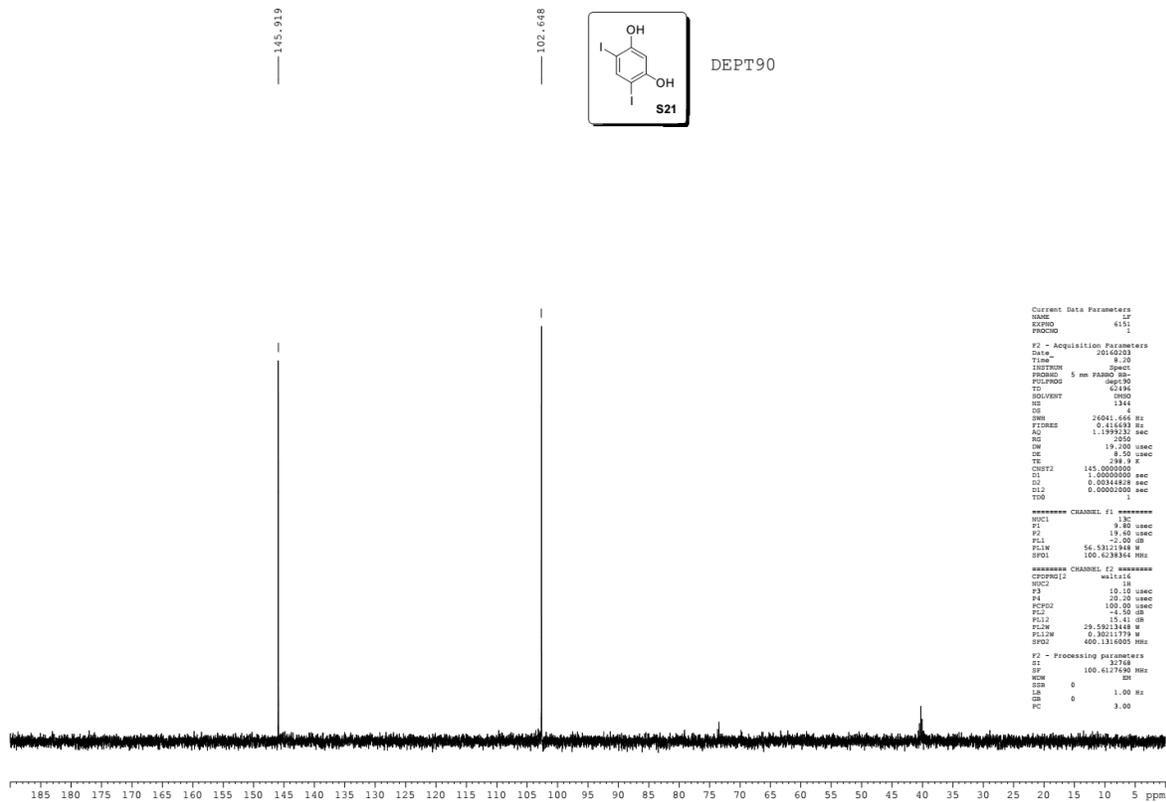
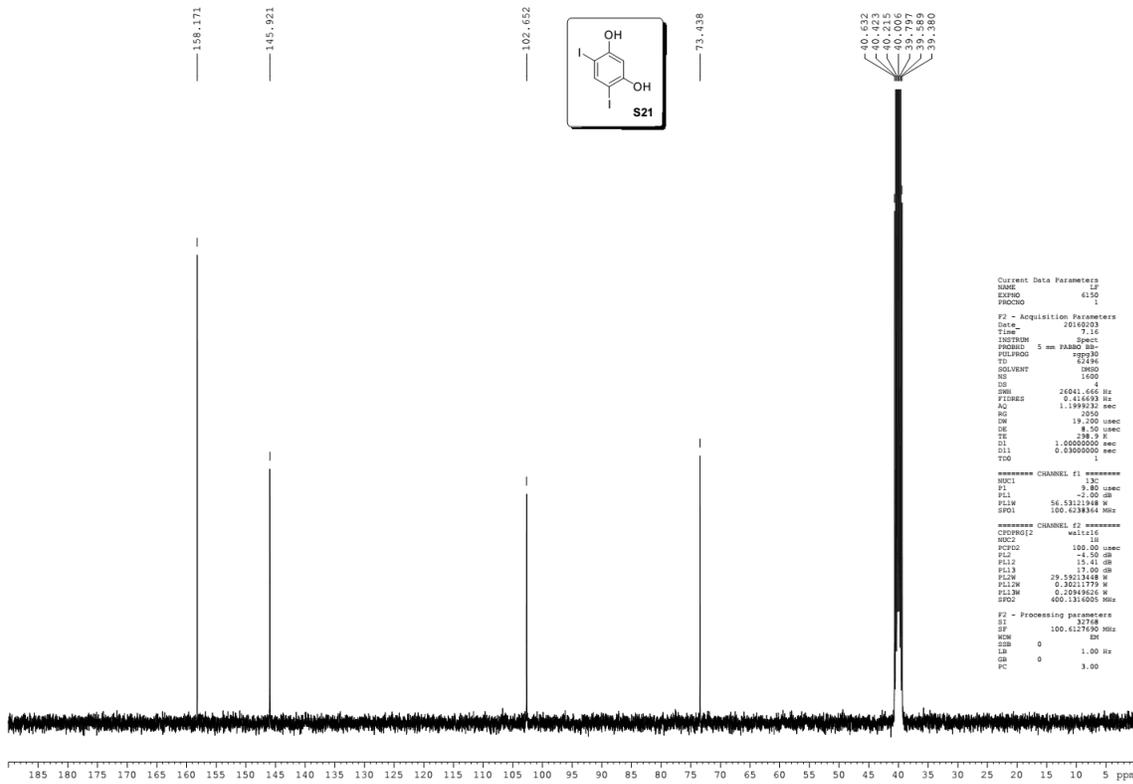
===== CHANNEL f1 =====
NUC1          1H
P1            15.10 usec
PL1           -5.00 usec
SFO1         30.4880507 MHz
SFO2         700.2756022 MHz

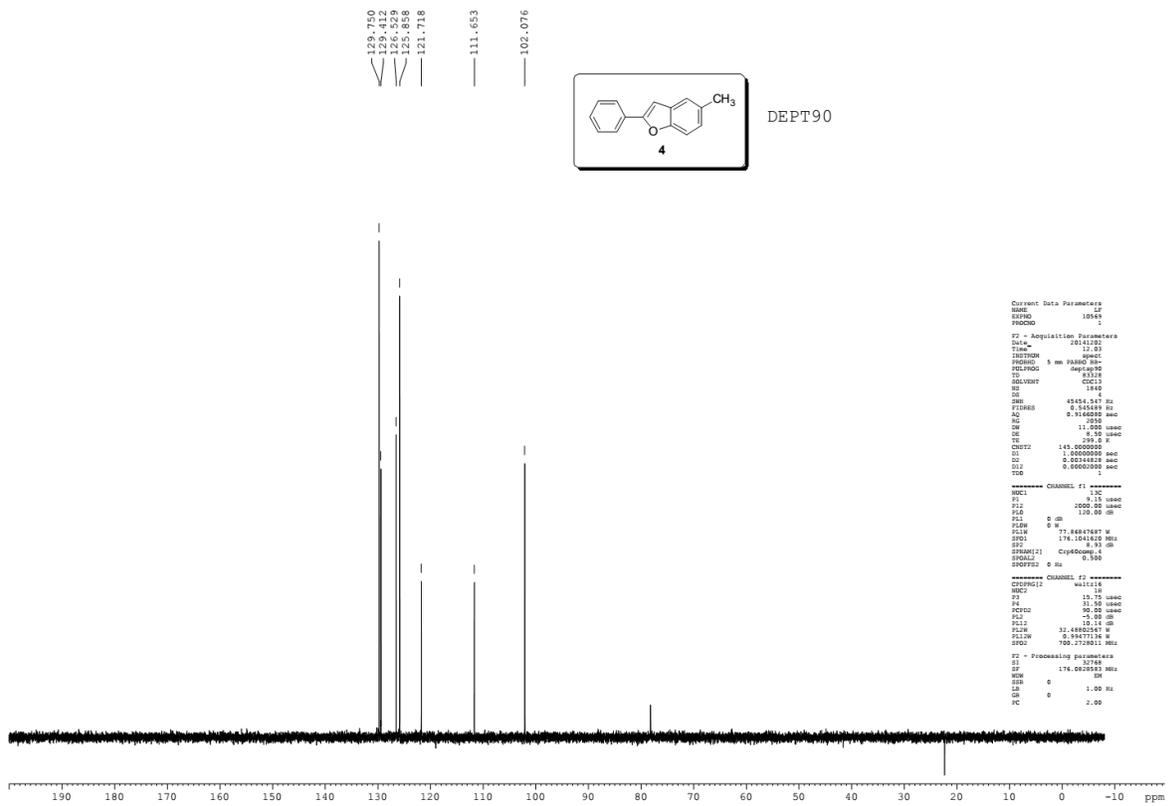
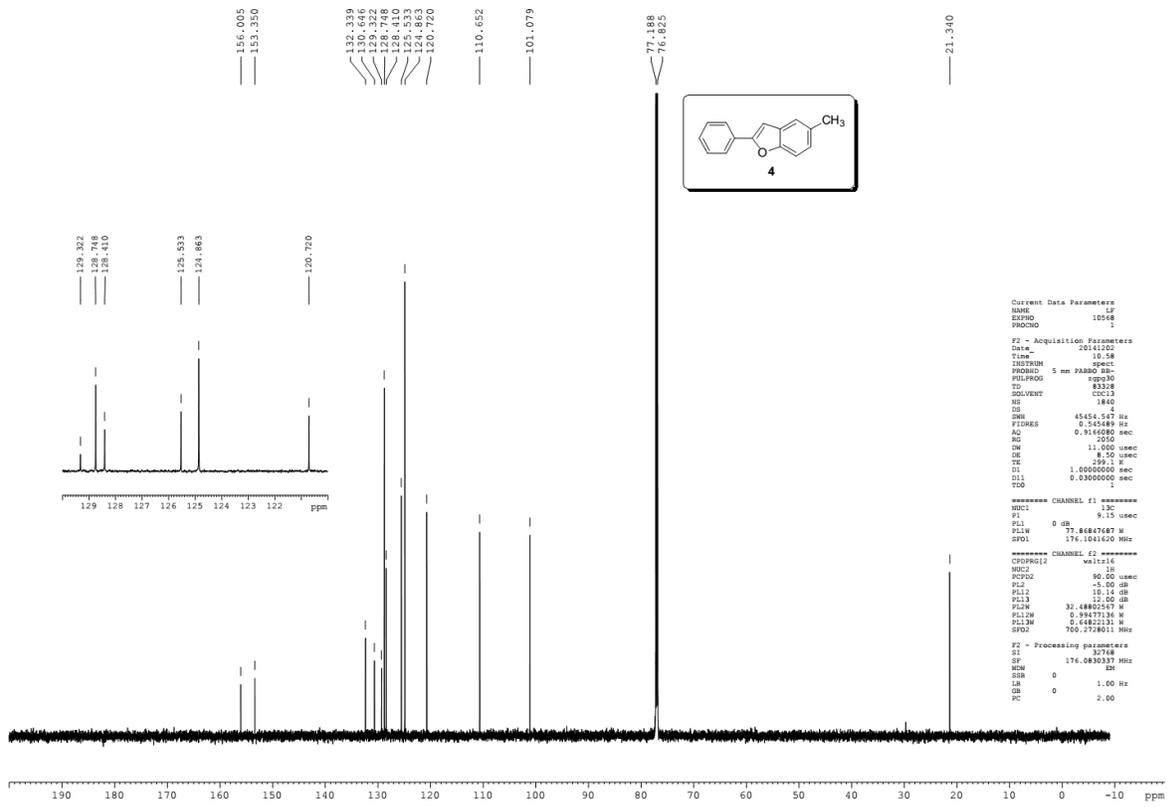
F2 - Processing parameters
SI            32768
SF           700.2700000 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            5.00
  
```

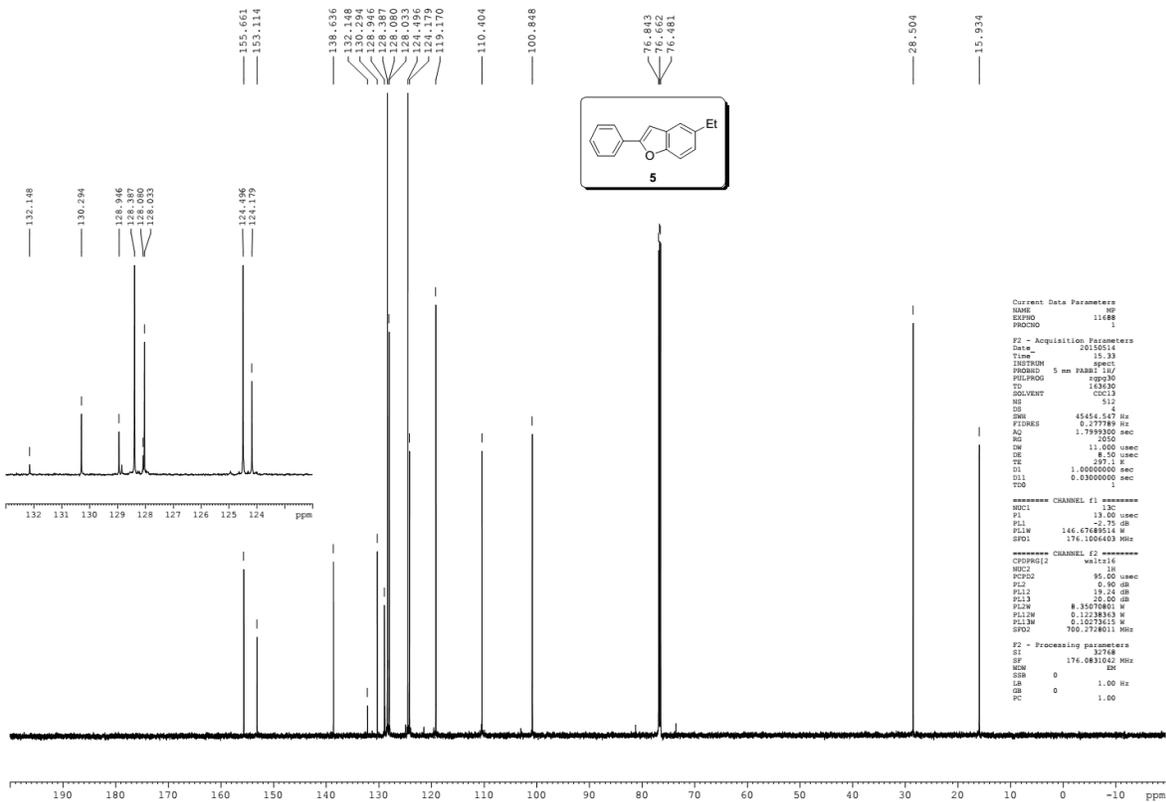
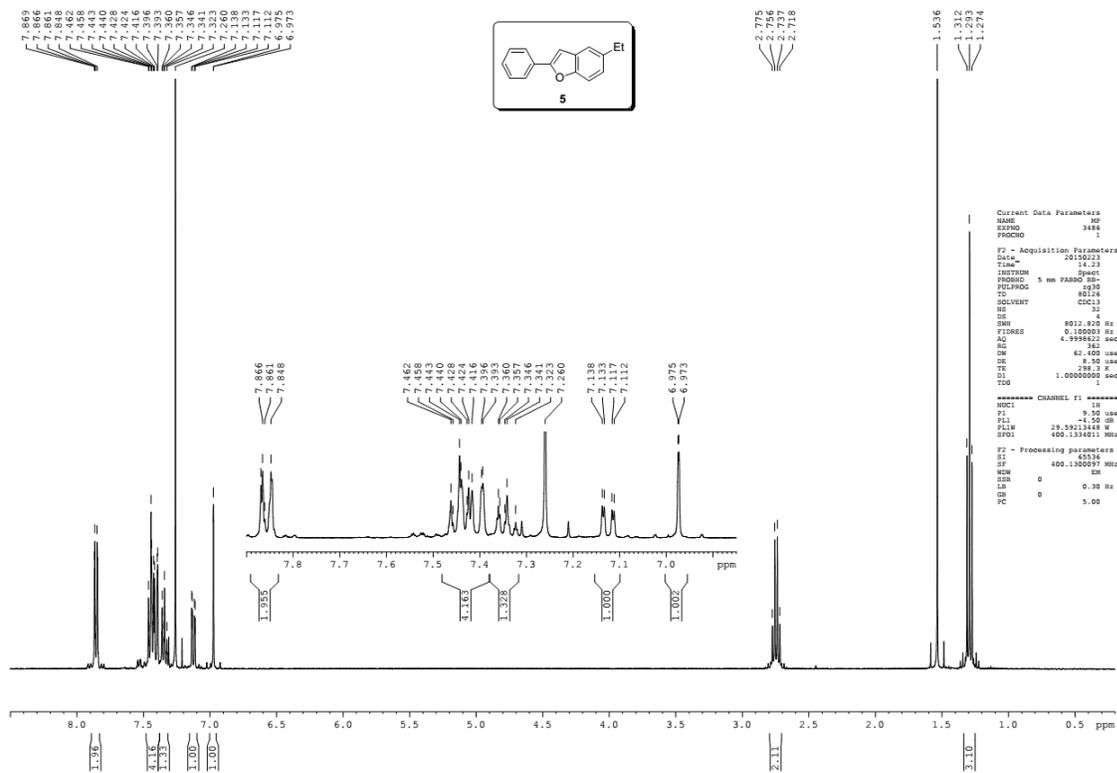


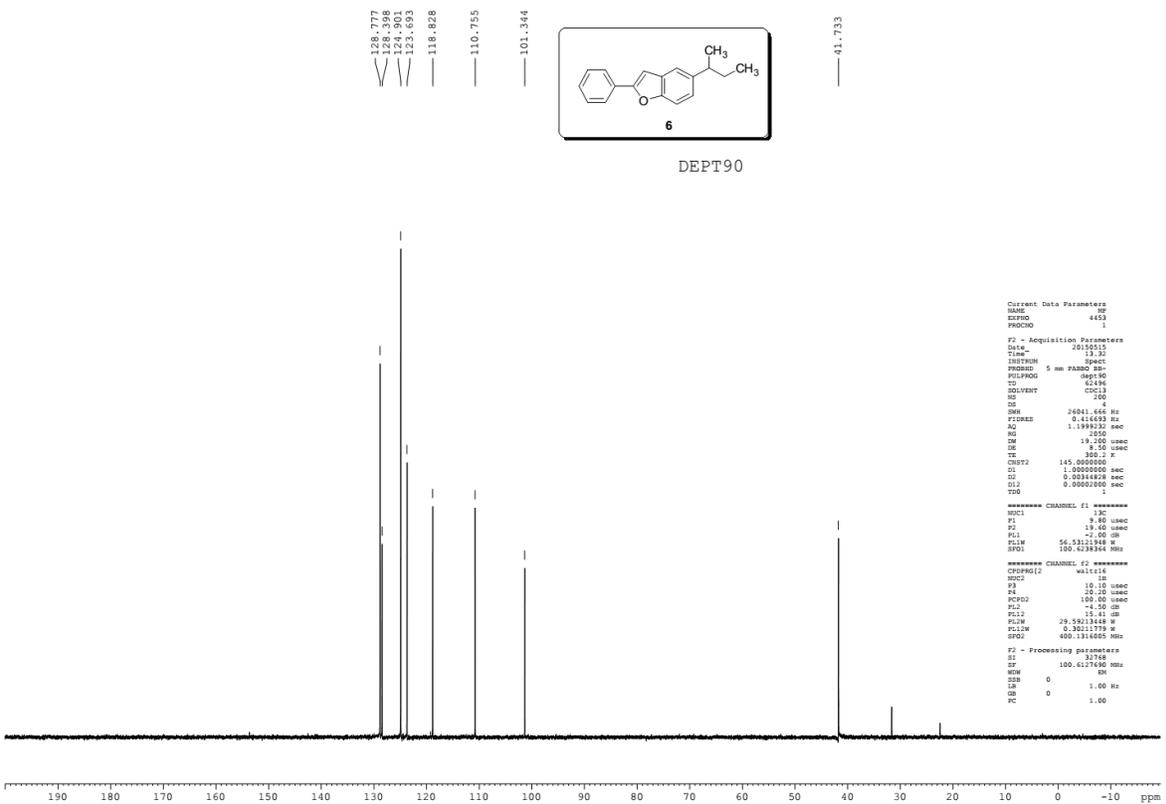
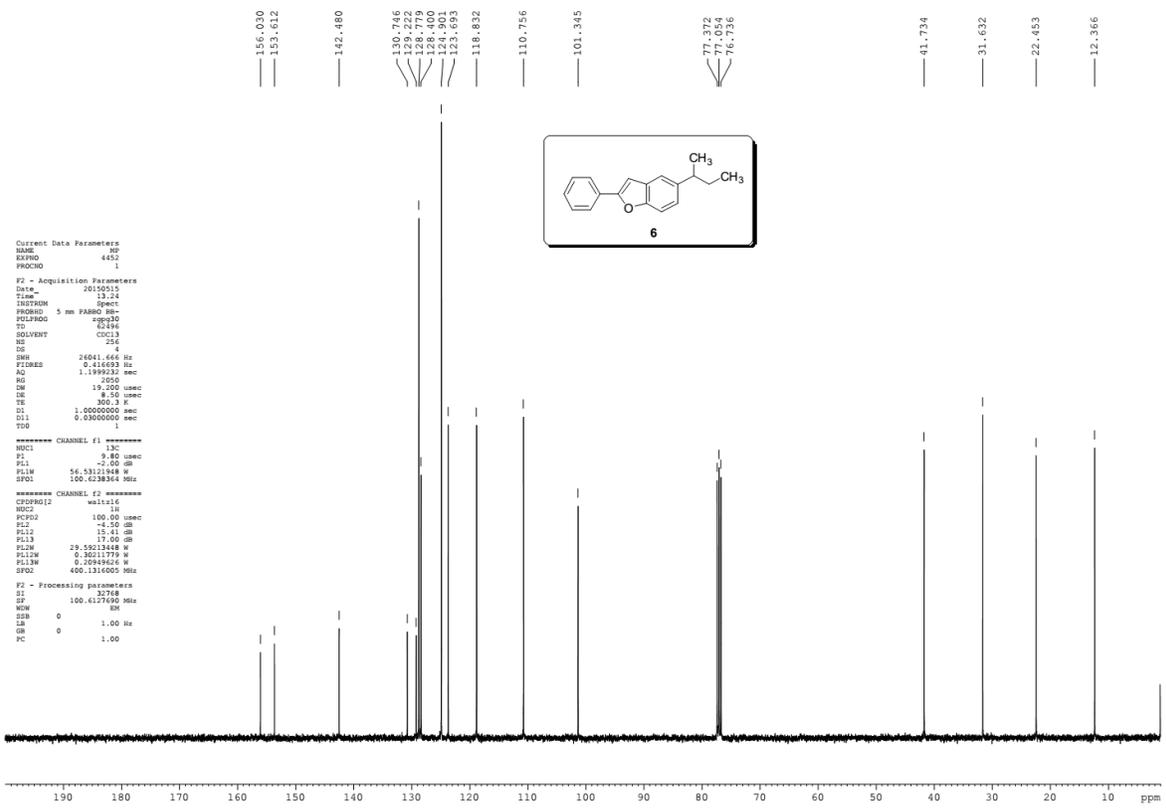


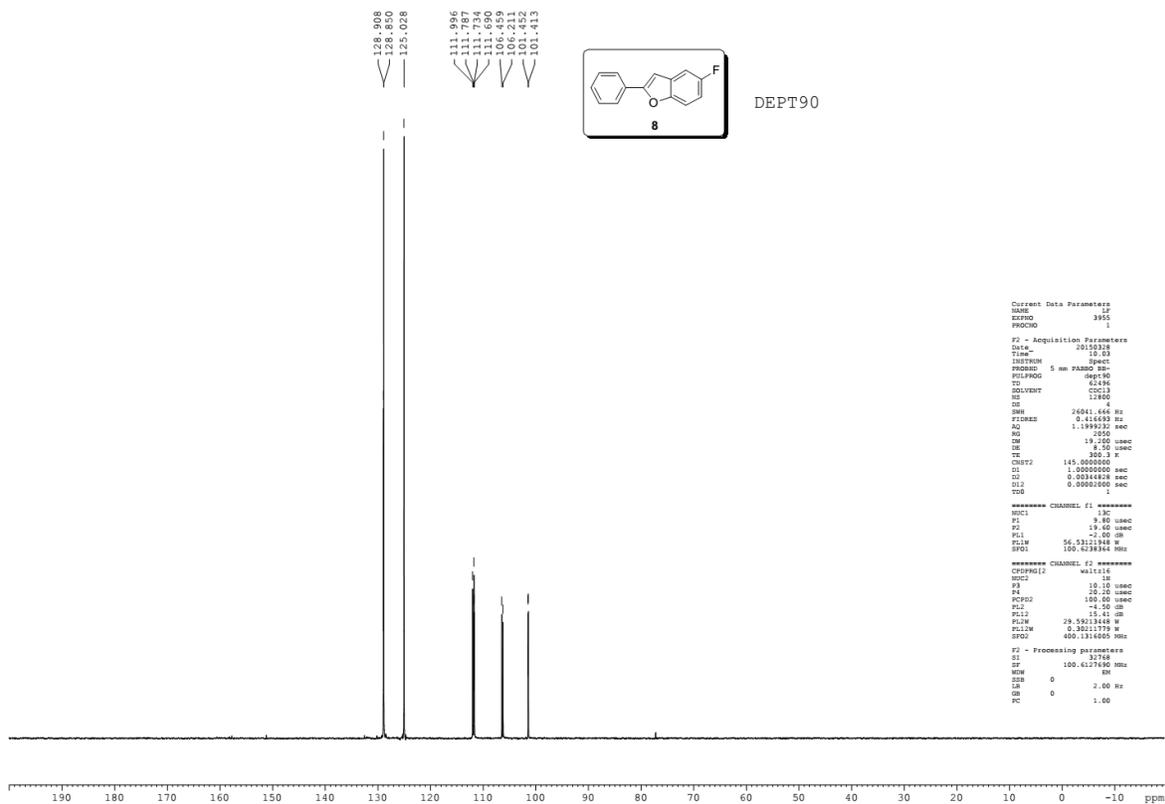
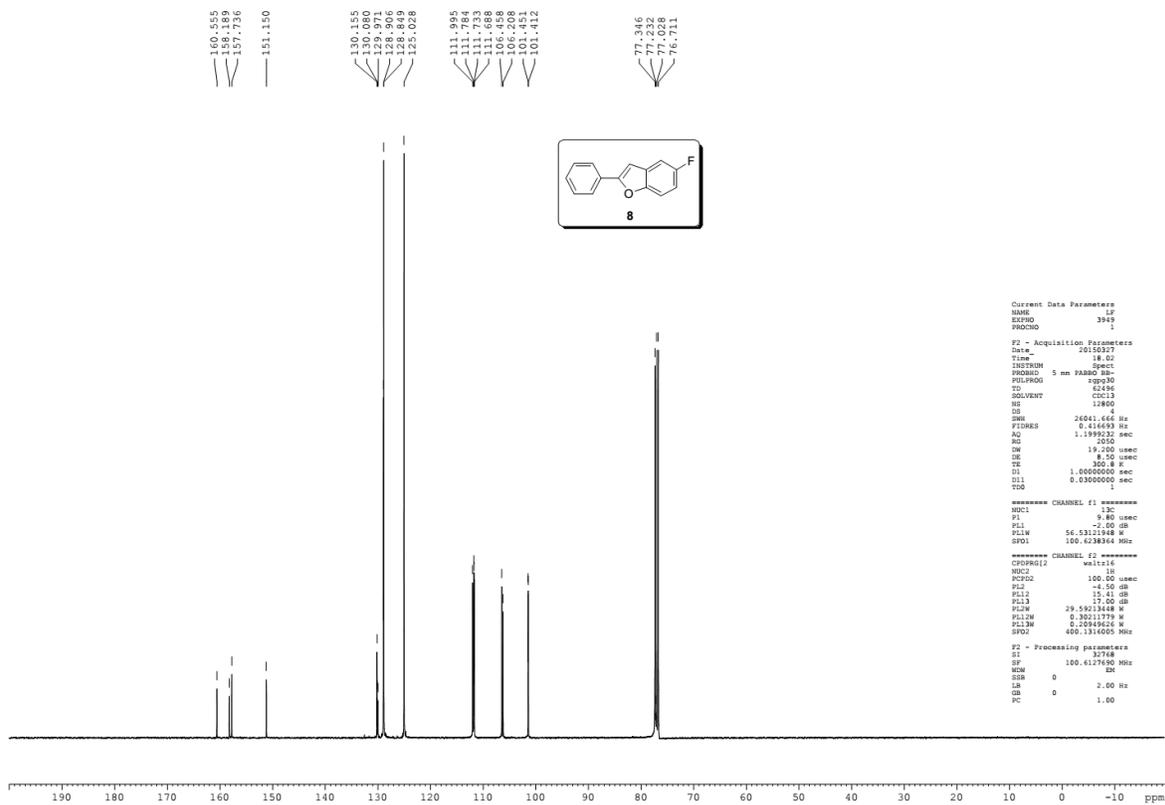




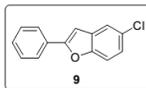




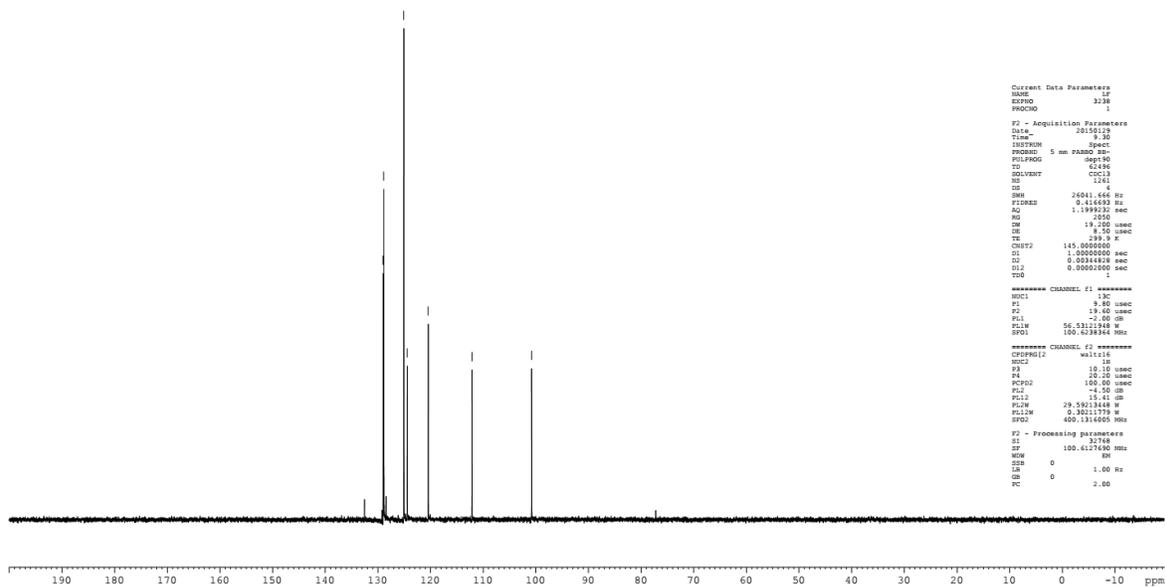




129.000
128.940
125.067
124.399
120.423
112.115
100.798



DEPT90



```

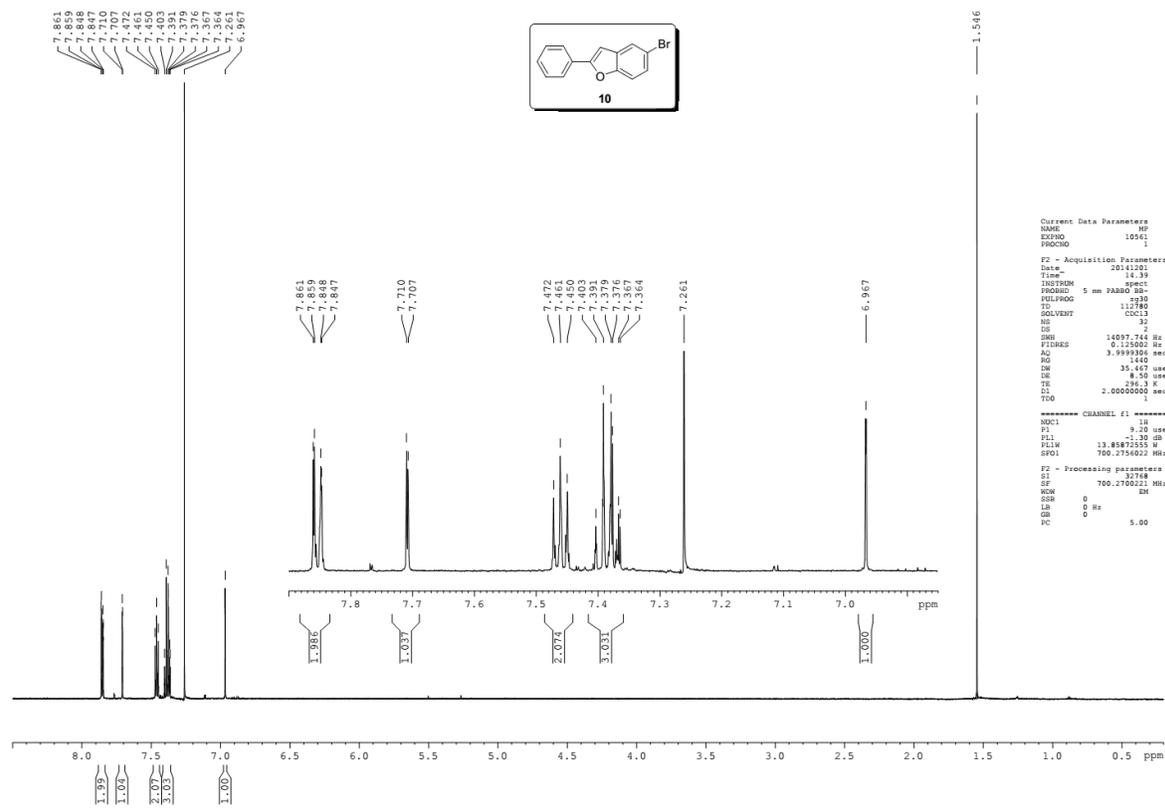
Current Data Parameters
NAME          15
EXPNO        3238
PROCNO       1

F2 - Acquisition Parameters
Date_        20150129
Time         8.30
INSTRUM      spect
PROBHD       5 mm PABBO BB-
PULPROG      zgpg30
TD           65496
SOLVENT      CDCl3
NS           128
DS           4
SWH          26041.666 Hz
FIDRES      0.414493 Hz
AQ          11.99932 sec
RG           2500
DE          19.200 usec
TE           8.50 usec
TD0          339.1
CHST2       145.0000000
SI           1.0000000 sec
SF           0.0038482 MHz
DQ           0.00001000 sec
TOD         1

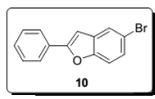
===== CHANNEL f1 =====
NUC1         13C
P1           18.00 usec
P2           19.60 usec
PL1         -2.00 dB
PL2         56.5311948 W
SFO1        100.6283616 MHz

===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2         1H
P3           18.18 usec
P4           10.20 usec
PCPD2       100.00 usec
PL3         -4.50 dB
PL4         8.3011779 W
PL5         29.5821348 W
PL6         8.3021379 W
PL7         400.1316005 MHz
SFO2        400.1316005 MHz

F2 - Processing parameters
SI           1
SF           100.6283616 MHz
WDW          EM
SSB          0
LB           0 Hz
GB           0 Hz
PC           2.00
  
```



7.861
7.859
7.848
7.847
7.817
7.707
7.472
7.450
7.403
7.391
7.376
7.367
7.284
6.967



1.546

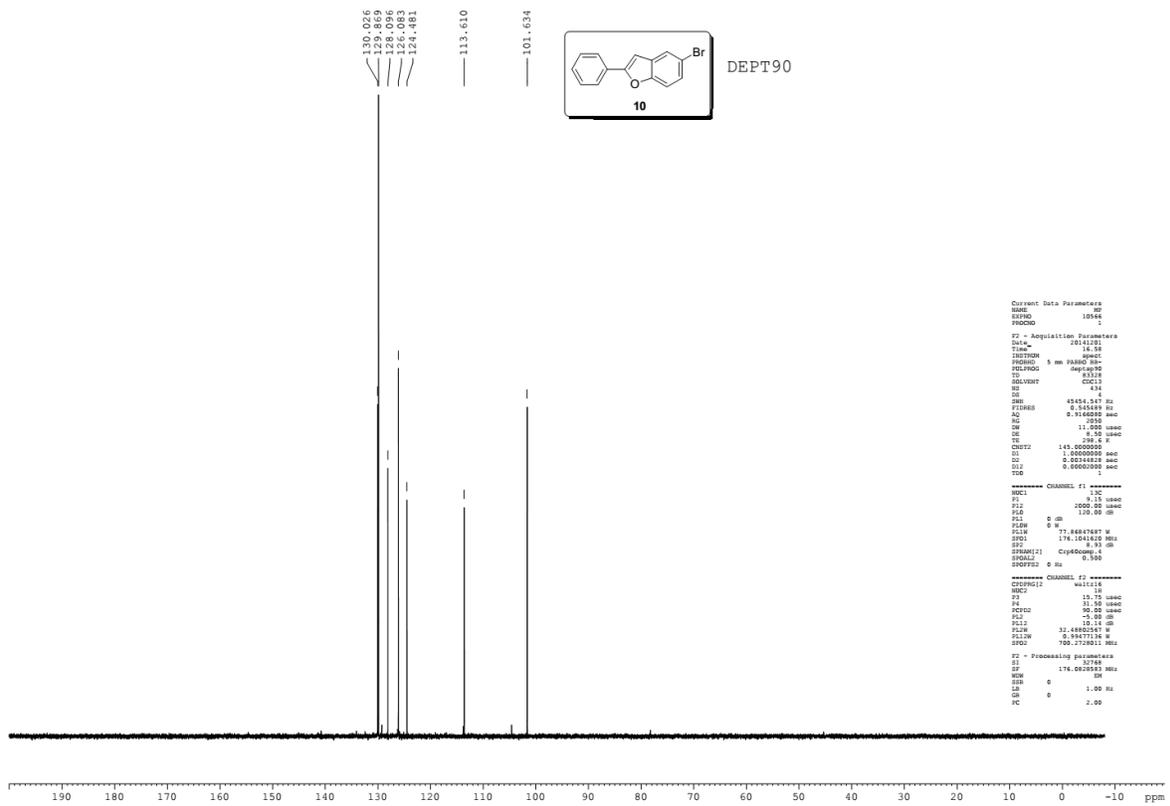
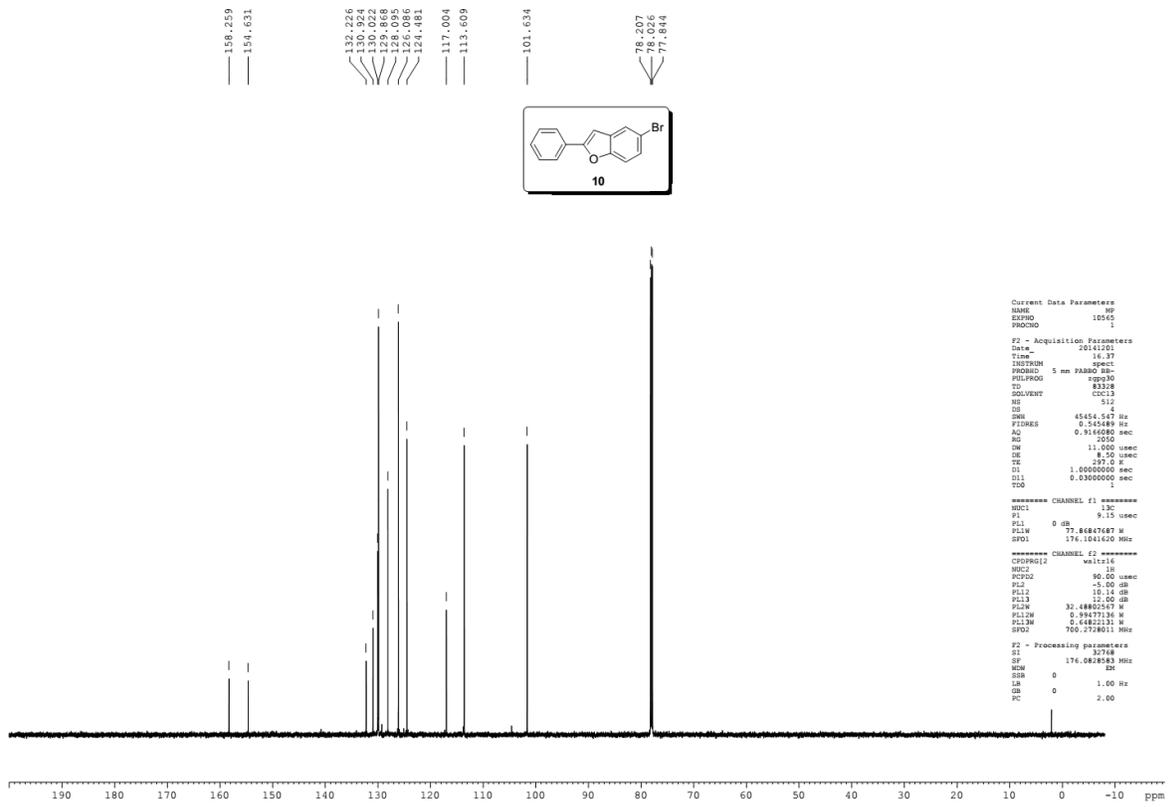
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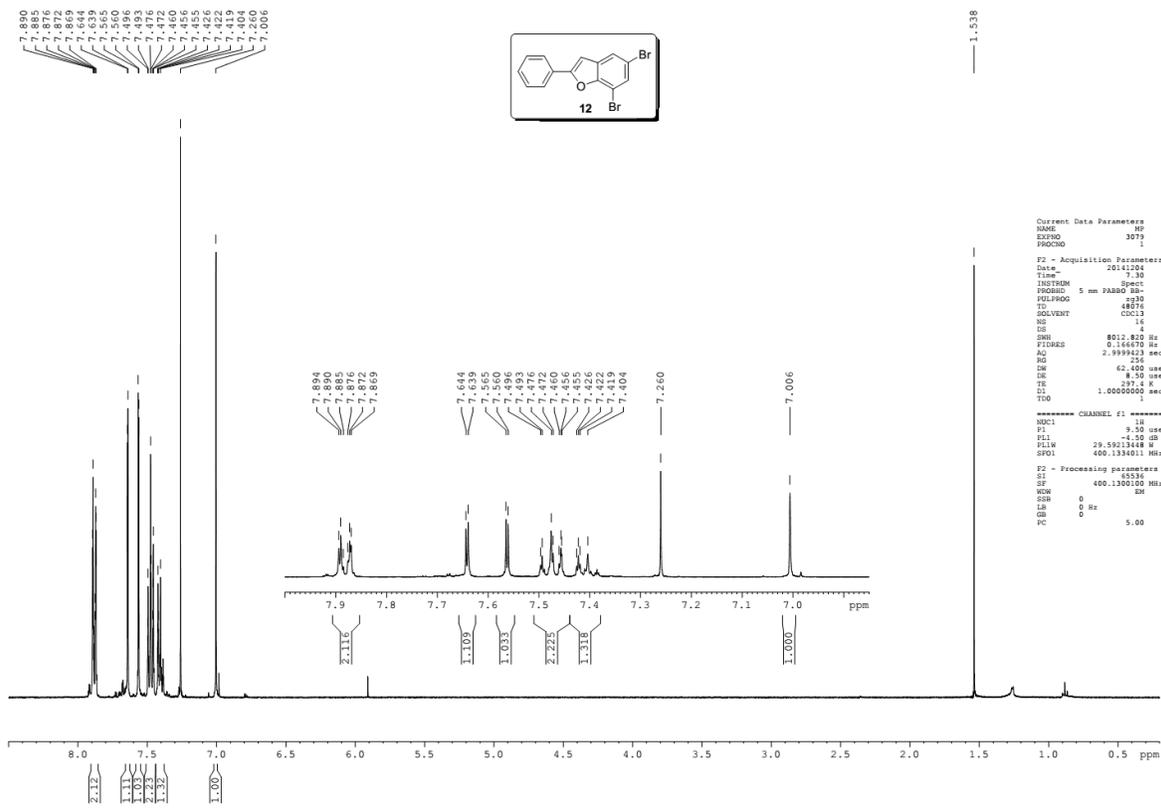
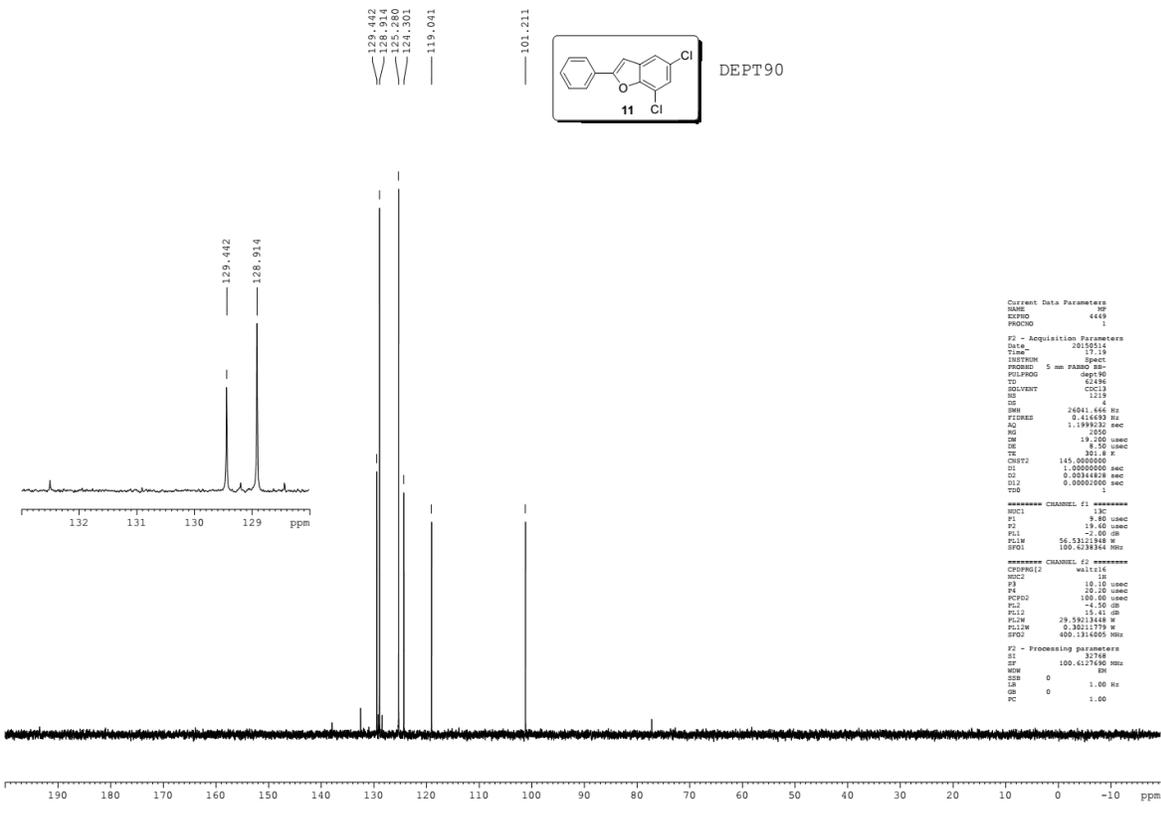
Current Data Parameters
NAME          10
EXPNO        10541
PROCNO       1

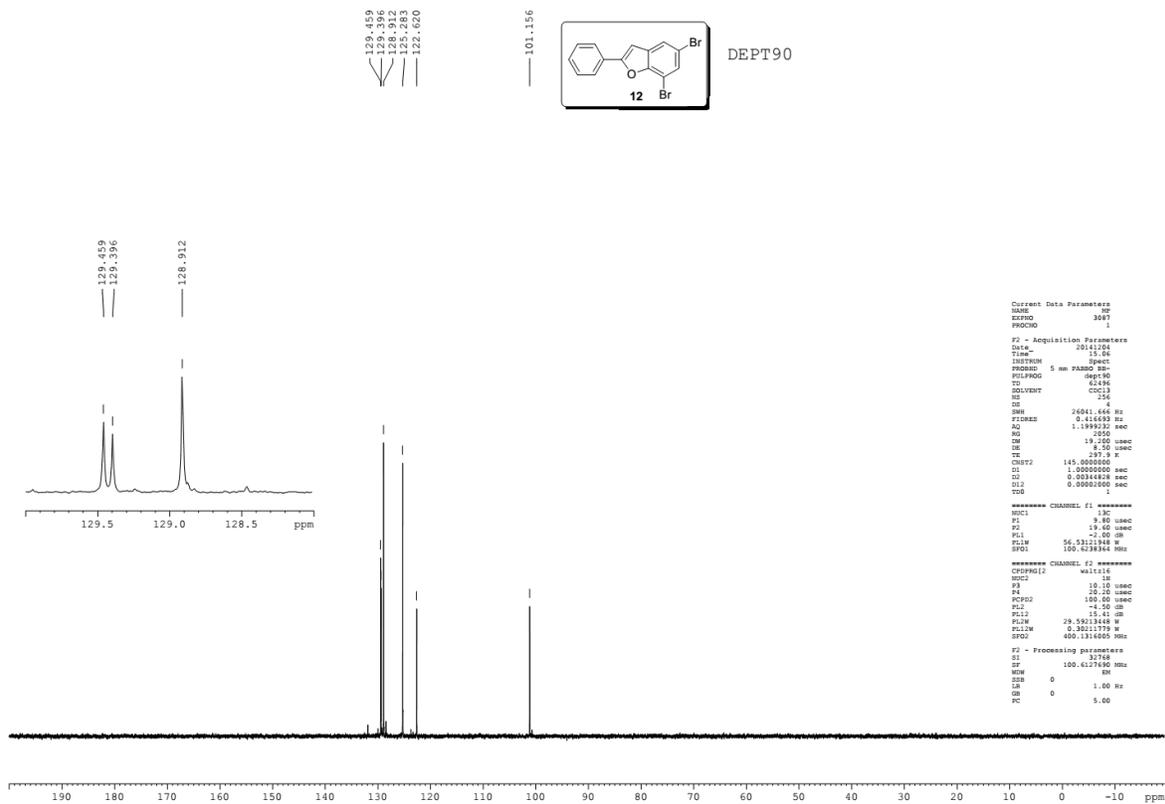
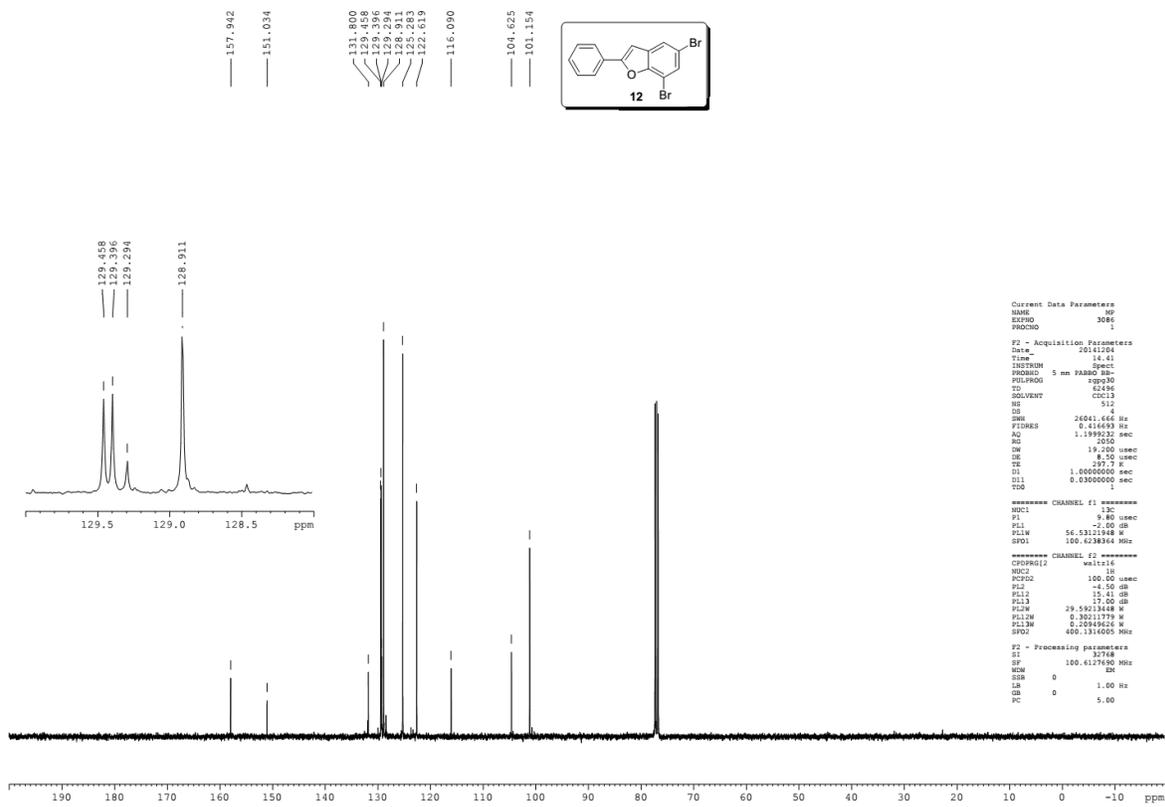
F2 - Acquisition Parameters
Date_        20141201
Time         14.39
INSTRUM      spect
PROBHD       5 mm PABBO BB-
PULPROG      zgpg30
TD           112780
SOLVENT      CDCl3
NS           32
DS           2
SWH          14097.764 Hz
FIDRES      0.125002 Hz
AQ          3.9999306 sec
RG           7440
DE          39.447 usec
TE           8.50 usec
TD0          28.18
CH1         2.00000000 sec
TOD         1

===== CHANNEL f1 =====
NUC1         1H
P1           9.10 usec
P2           -1.30 dB
PL1         13.85872555 W
SFO1        700.2756222 MHz

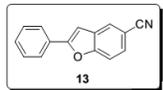
F2 - Processing parameters
SI           1
SF           700.2700221 MHz
WDW          EM
SSB          0
LB           0 Hz
GB           0 Hz
PC           5.00
  
```



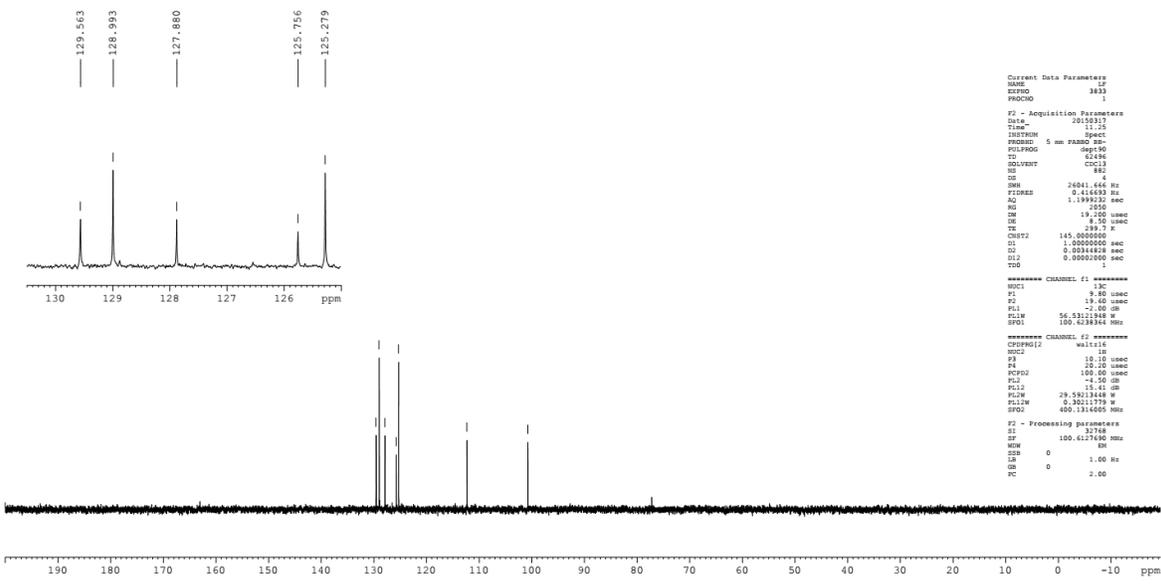




129.563
128.993
128.756
125.279
112.293
100.753



DEPT90



```

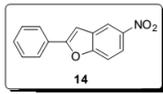
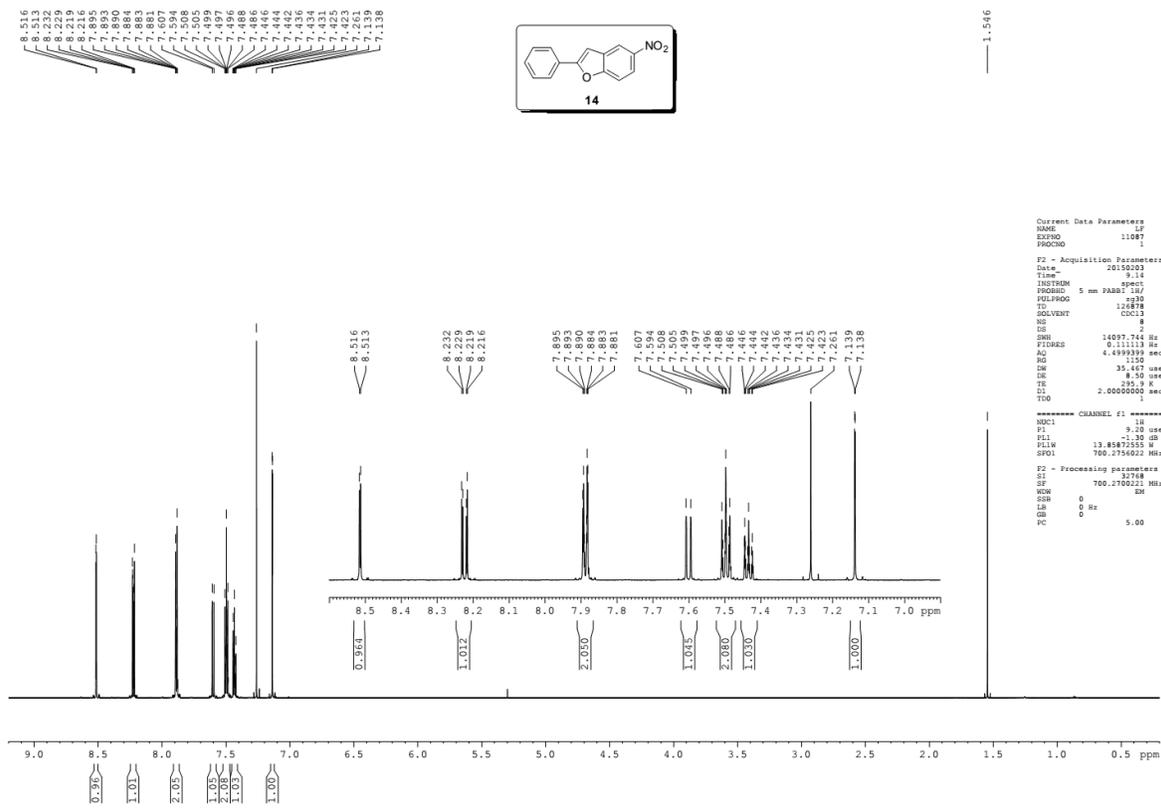
Current Data Parameters
NAME      13
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20130113
Time     11:25
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        8
DS        4
SWH       26041.666 Hz
FIDRES    0.414493 Hz
AQ        1.1999702 sec
RG        2500
PROBHD    5 mm
DE        19.200 usec
TE        300.2 K
DETC      8.50 usec
CHRG2     145.0000000
SI         1.000000000 sec
SF         0.003484280 MHz
DI2        0.000010000 sec
TOD        1

===== CHANNEL f1 =====
NUC1       13C
P1         19.00 usec
P2         19.40 usec
PL1        -2.00 dB
PL2        19.00 dB
PL12       56.5311948 MHz
SFO1       100.6283630 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
P3         18.18 usec
P4         18.20 usec
PCPD2     180.00 usec
PL3        -4.50 dB
PL4        -4.50 dB
PL123     29.5821344 MHz
PL124     8.28213778 MHz
SFO2       400.1314000 MHz
SFO3       400.1314000 MHz

F2 - Processing parameters
SI         100.6170000 MHz
SF         100.6170000 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         2.00
  
```



1.546

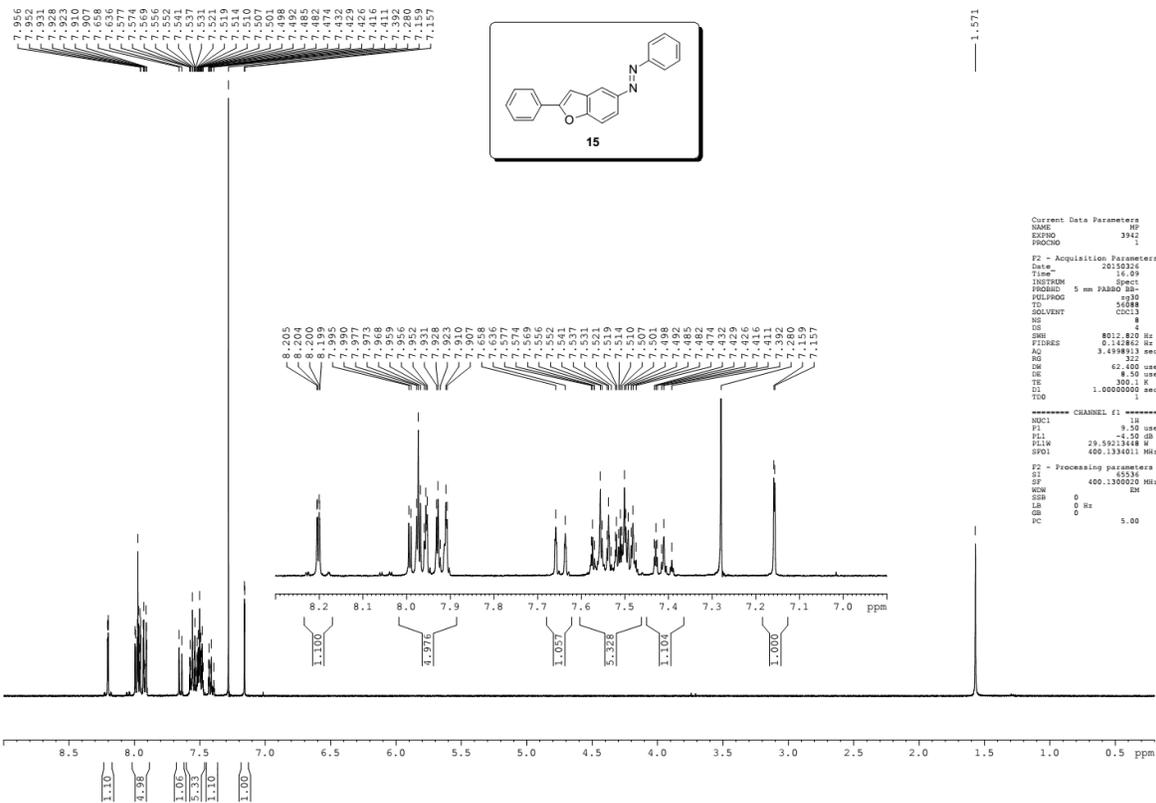
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Current Data Parameters
NAME      14
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20130203
Time     9:14
INSTRUM  spect
PROBHD   5 mm PABBO 1H/
PULPROG  zgpg30
TD        126878
SOLVENT  CDCl3
NS        8
DS        4
SWH       14097.944 Hz
FIDRES    0.111113 Hz
AQ        4.4999399 sec
RG        2500
PROBHD    5 mm
DE        19.200 usec
TE        300.2 K
DETC      8.50 usec
CHRG2     145.0000000
SI         1.000000000 sec
SF         0.003484280 MHz
DI2        0.000010000 sec
TOD        1

===== CHANNEL f1 =====
NUC1       1H
P1         9.10 usec
P2         -1.30 dB
PL1        13.8587555 MHz
SFO1       700.2756022 MHz

F2 - Processing parameters
SI         700.2700221 MHz
SF         700.2700221 MHz
WDW        EM
SSB        0
LB         0 Hz
GB         0
PC         5.00
  
```

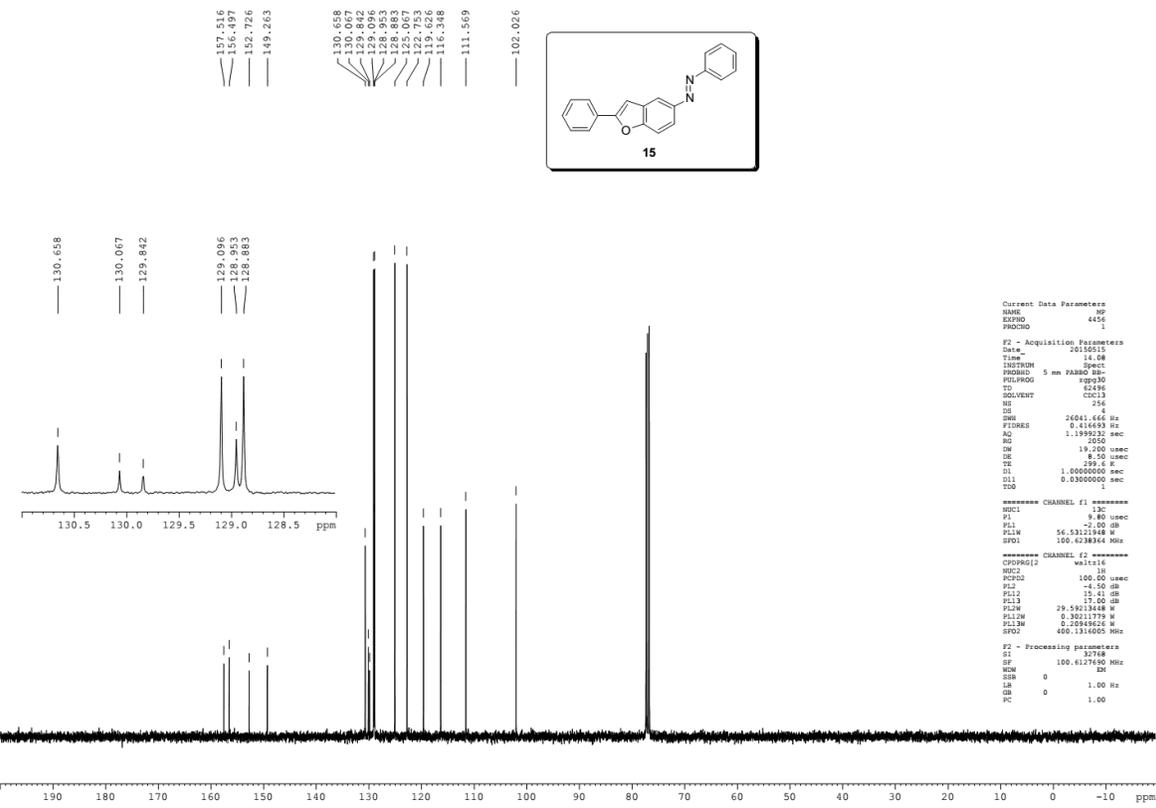
```

Current Data Parameters
NAME      39F
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20150316
Time     14.09
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS         4
DS         4
SWH       801.420 Hz
FIDRES    0.142842 Hz
AQ         3.499813 sec
RG         322
SQ         62.400 usec
SR         8.30 usec
TE         300.1
D1         1.0000000 sec
TOD        1

===== CHANNEL f1 =====
NUC1      1H
P1         9.50 usec
PL1       -1.50 dB
PL12      29.5013448 dB
SFO1      400.1334011 MHz

F2 - Processing parameters
SI         65536
SF         400.1300020 MHz
WDW        EM
SSB        0
LB         0 Hz
GB         0
PC         5.00
  
```



```

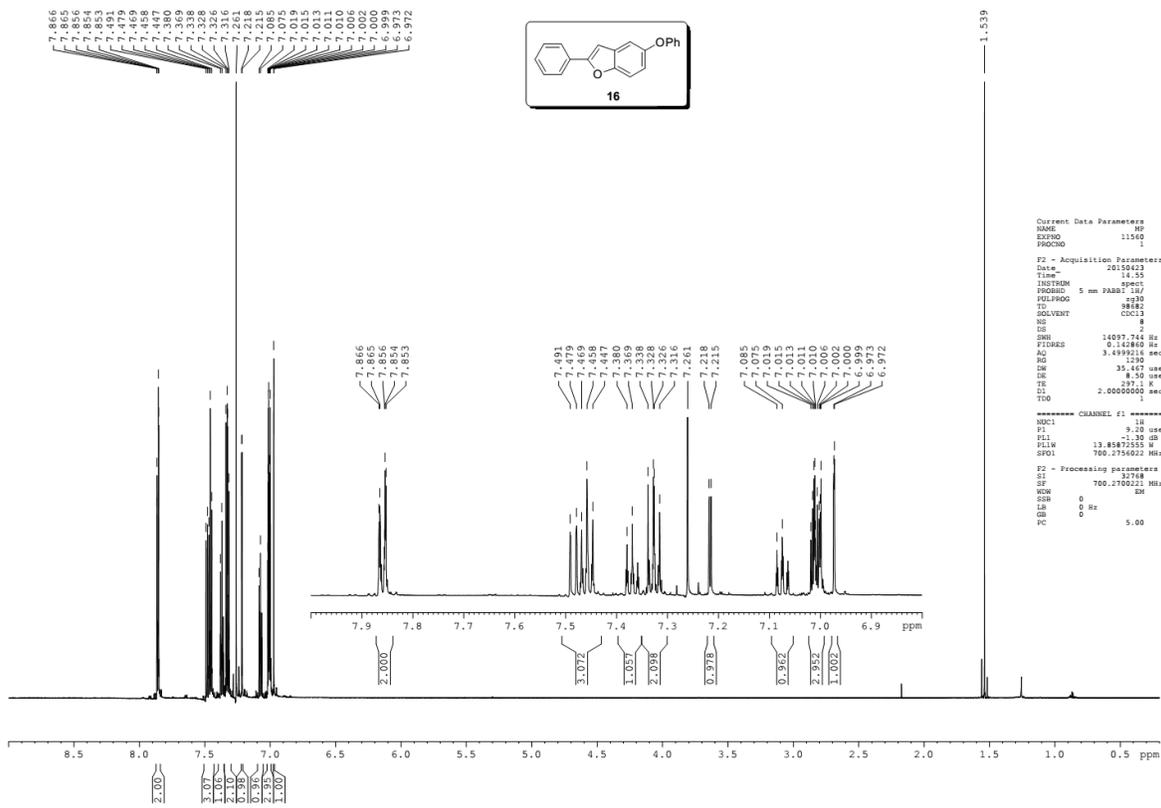
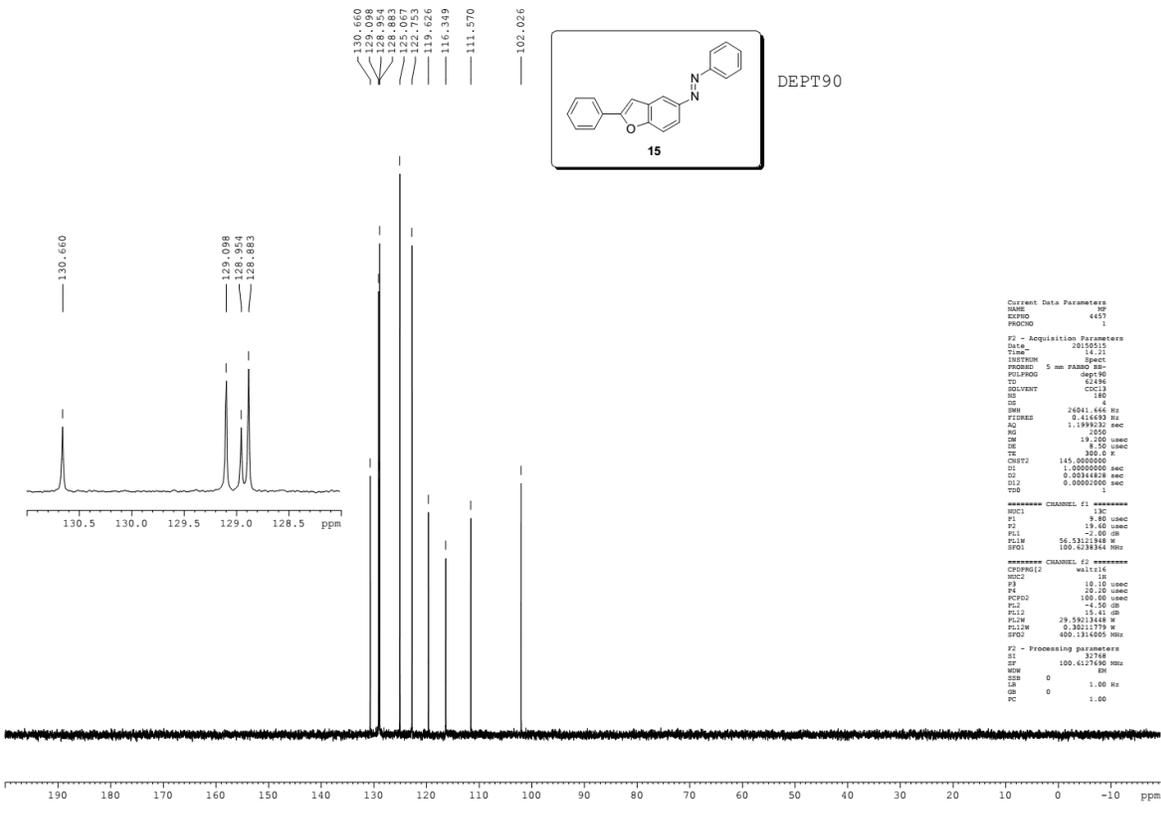
Current Data Parameters
NAME      445F
EXPNO    1
PROCNO   1

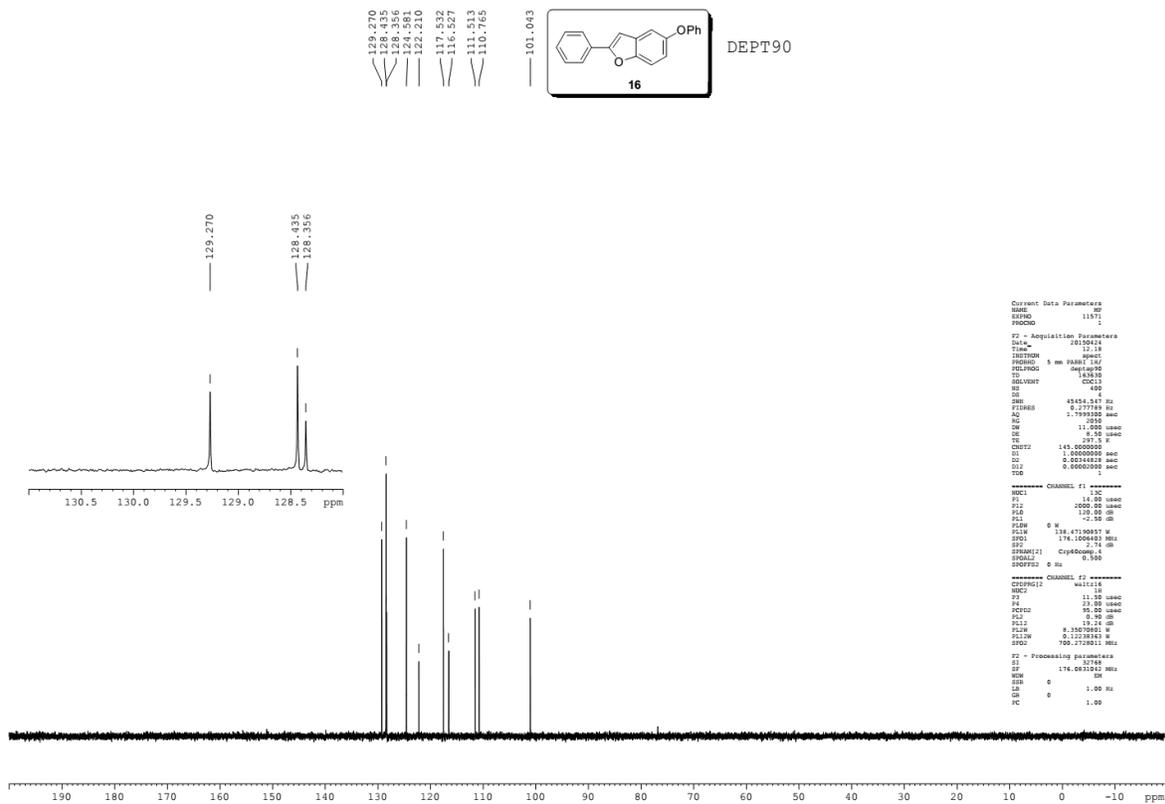
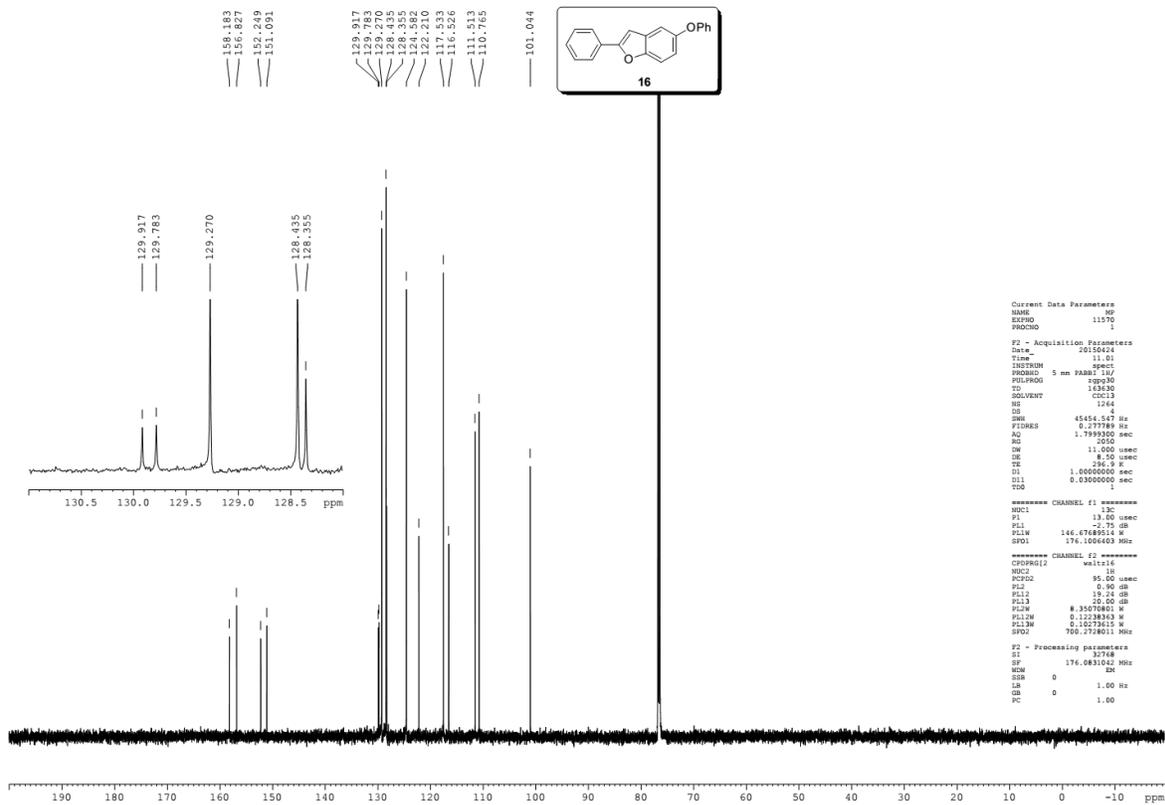
F2 - Acquisition Parameters
Date_    20150316
Time     14.08
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS         4
DS         4
SWH       26041.666 Hz
FIDRES    0.416693 Hz
AQ         1.1599230 sec
RG         2050
SQ         18.200 usec
SR         8.30 usec
TE         299.8
D1         1.0000000 sec
D11        0.03000000 sec
TOD        1

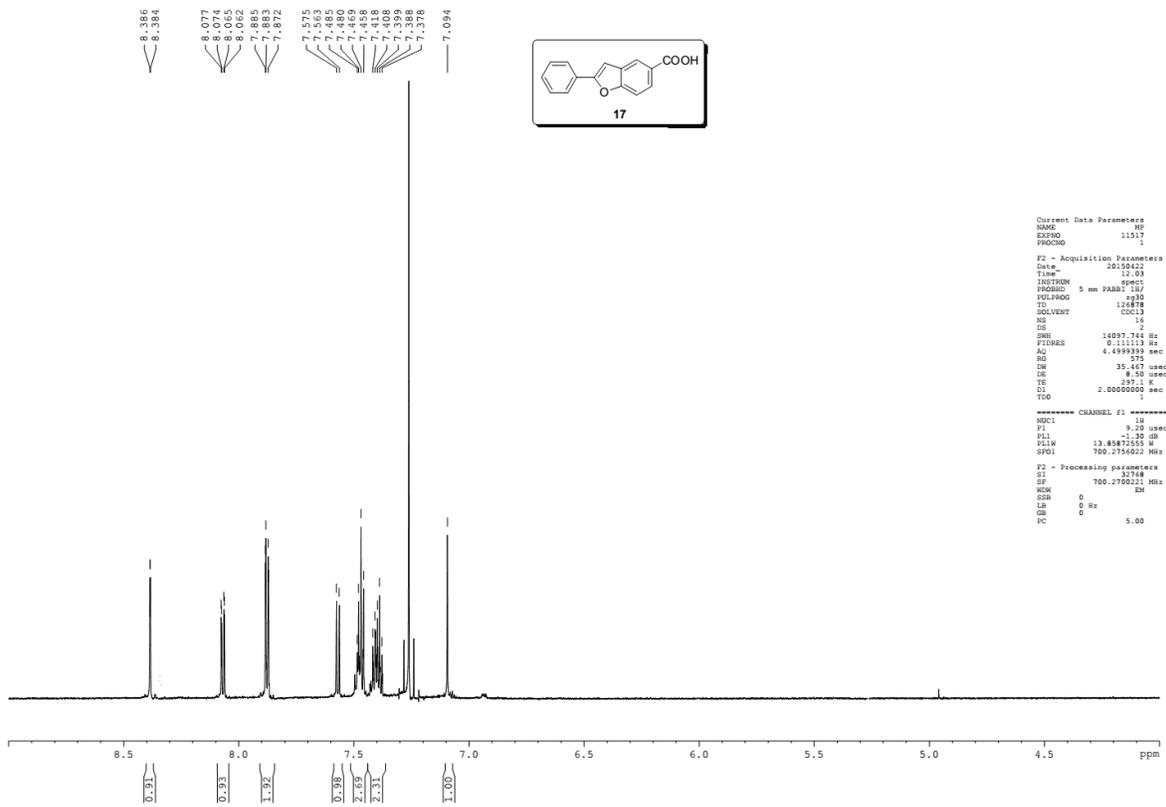
===== CHANNEL f1 =====
NUC1      13C
P1         9.80 usec
PL1       -2.00 dB
PL12      56.53121948 dB
SFO1      100.6219854 MHz

===== CHANNEL f2 =====
CPDPRG2  wait16
NUC2      13C
PCPD2    100.00 usec
PL2       -1.50 dB
PL12     15.41 dB
PL13     17.00 dB
PL14     17.00 dB
PL15     17.00 dB
PL16     17.00 dB
PL17     17.00 dB
PL18     17.00 dB
PL19     17.00 dB
PL20     17.00 dB
SFO2      100.6219854 MHz

F2 - Processing parameters
SI         65536
SF         100.6177430 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.00
  
```







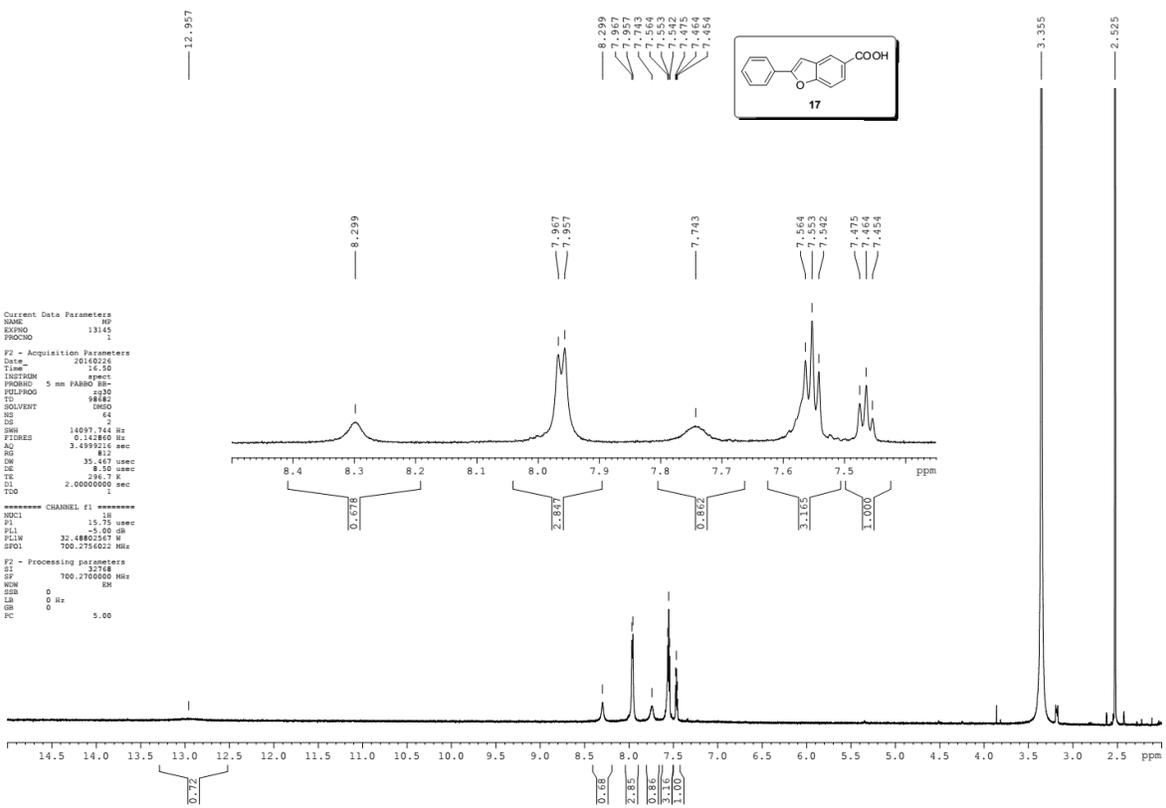
```

Current Data Parameters
NAME      HP
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20160226
Time     12.03
INSTRUM spect
PROBHD   5 mm PABBI 12/
PULPROG zgpg30
SOLVENT  CDCl3
TD        65536
SOLVENT  CDCl3
NS        2
DS        2
SWH      14097.744 Hz
FIDRES   0.111113 Hz
AQ        0.975
RG        4.4999999 sec
DE        35.467 usec
SE        8.30 usec
TE        297.1
D1        2.00000000 sec
T00       1

===== CHANNEL f1 =====
NUC1      13
P1         9.20 usec
PL1       -1.20 dB
PL12      13.86872555 dB
SFO1      700.2754622 MHz

F2 - Processing parameters
SI         32768
SF         700.2700221 MHz
WDW        EM
SSB        0
LB         0 Hz
GB         0
PC         5.00
  
```



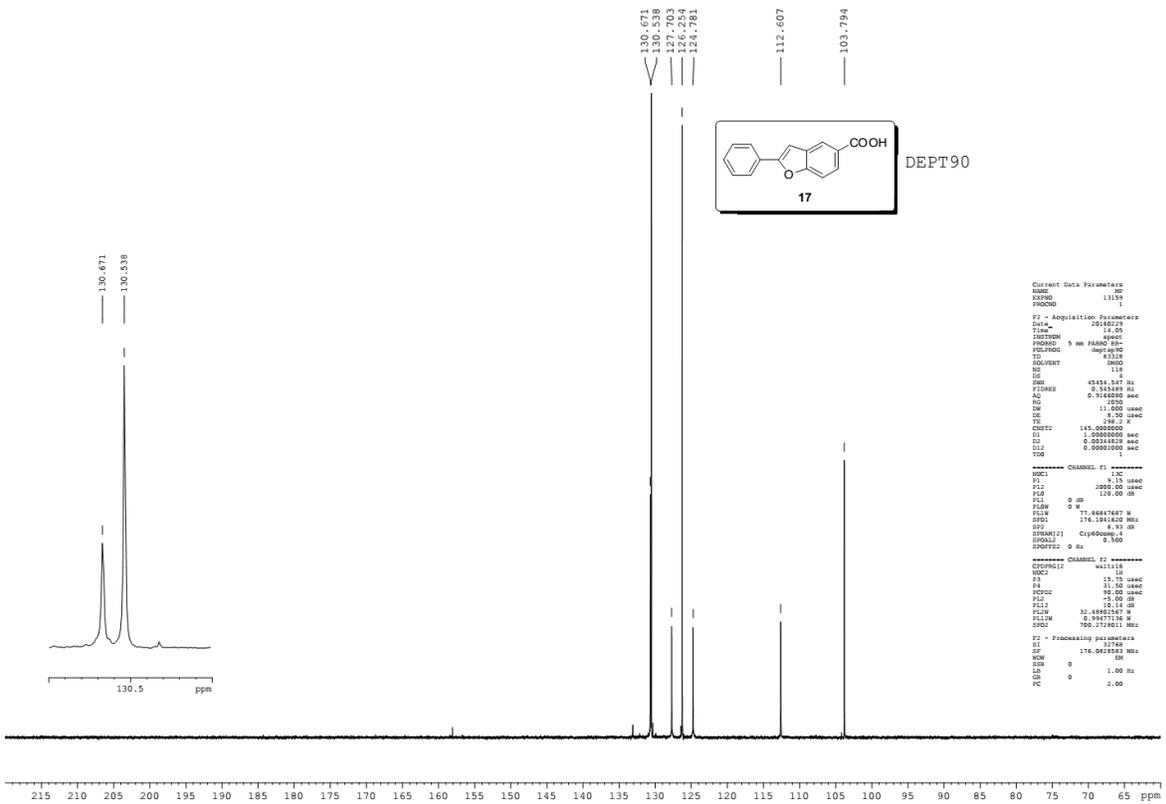
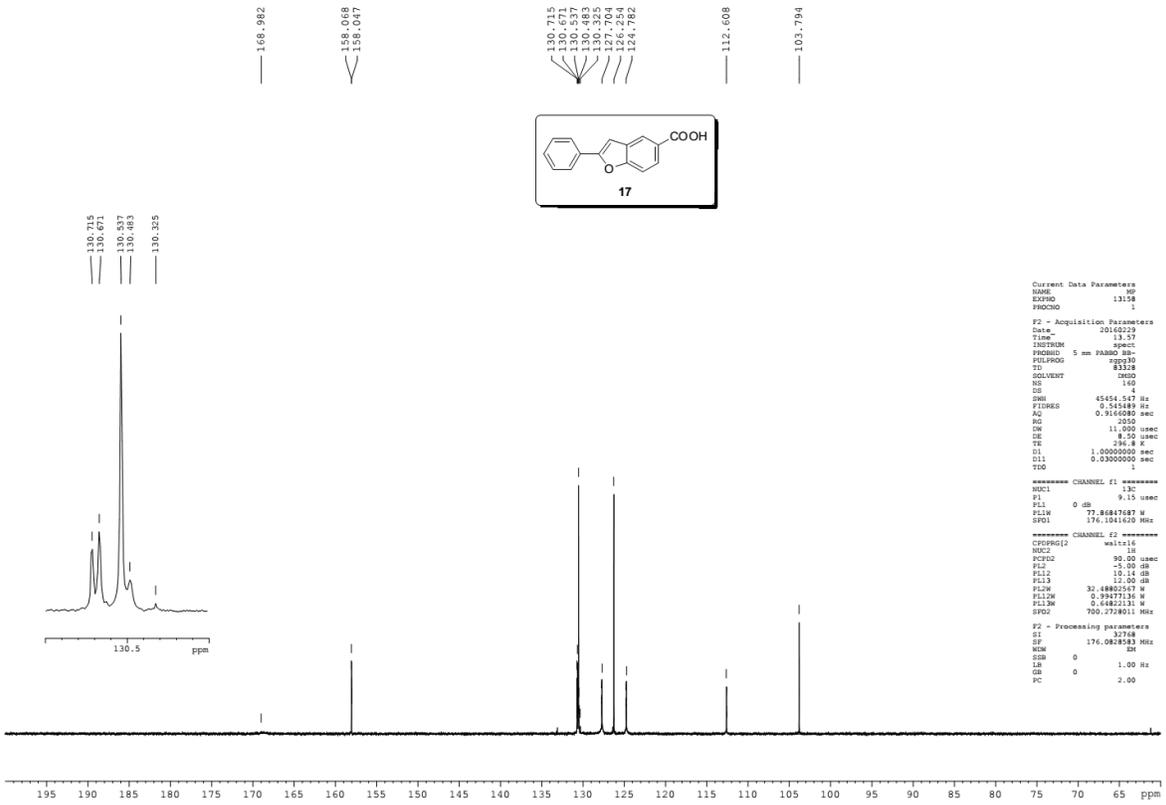
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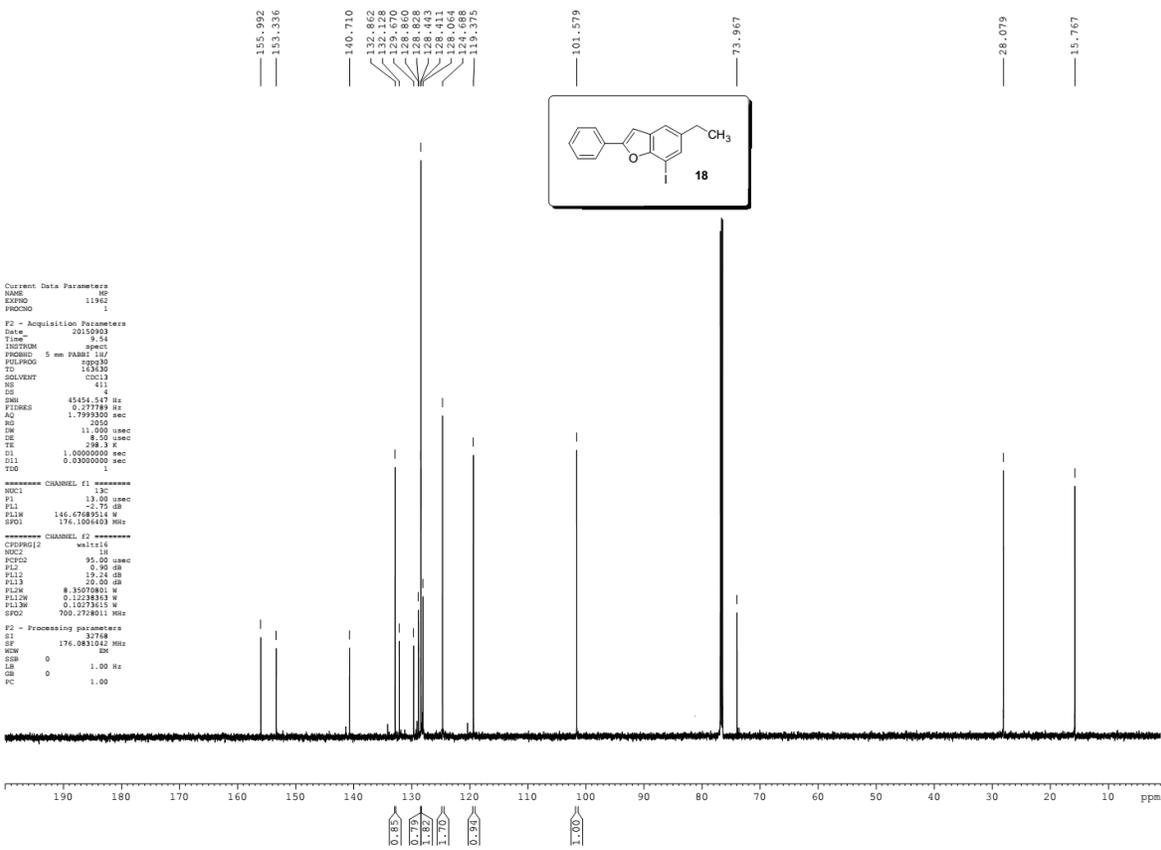
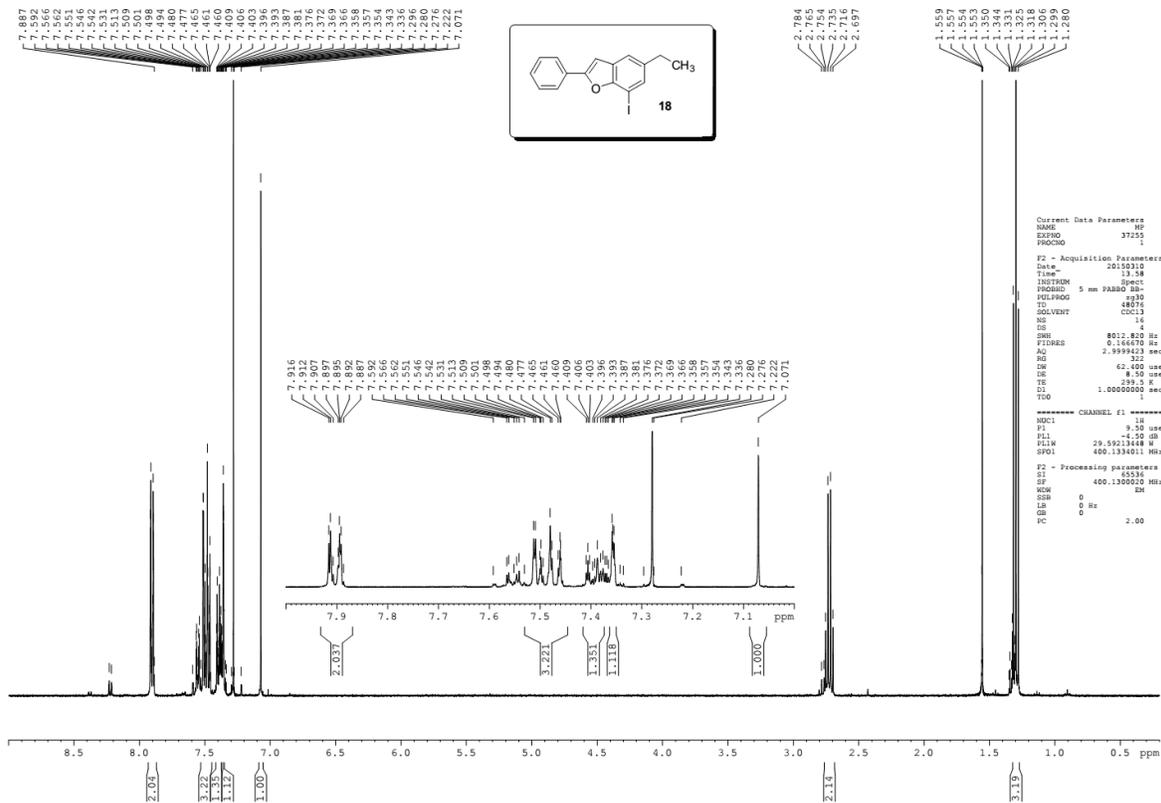
Current Data Parameters
NAME      HP
EXPNO    13145
PROCNO   1

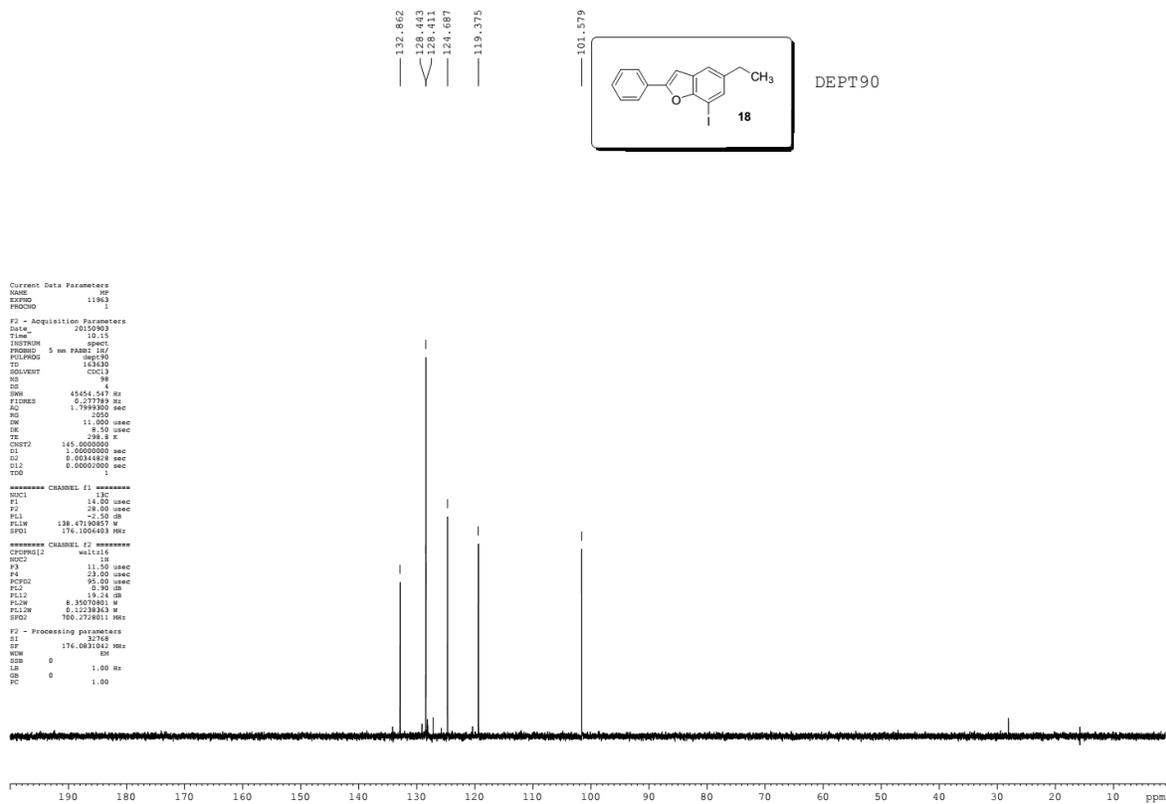
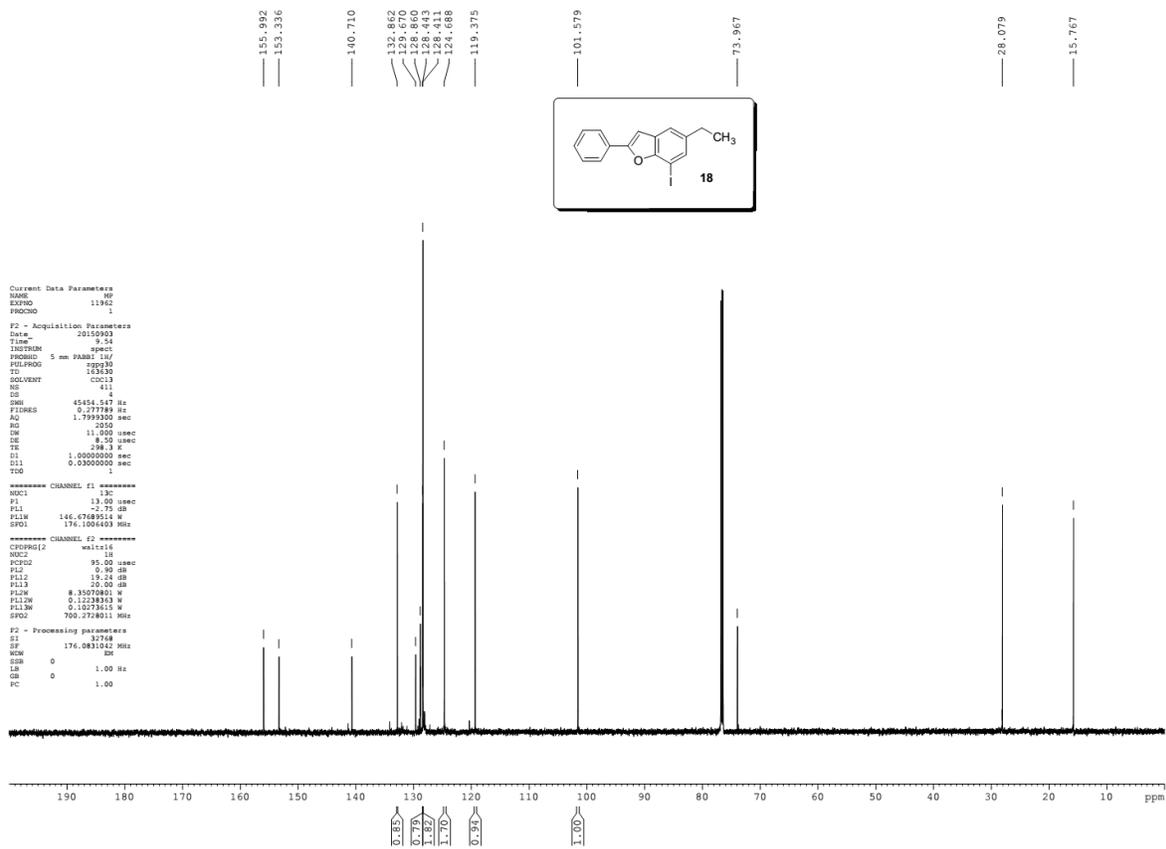
F2 - Acquisition Parameters
Date_    20160226
Time     16.10
INSTRUM spect
PROBHD   5 mm PABBI 12/
PULPROG zgpg30
SOLVENT  CDCl3
TD        65536
SOLVENT  CDCl3
NS        2
DS        2
SWH      14097.744 Hz
FIDRES   0.112810 Hz
AQ        0.975
RG        4.4999999 sec
DE        35.467 usec
SE        8.30 usec
TE        296.7
D1        2.00000000 sec
T00       1

===== CHANNEL f1 =====
NUC1      13
P1        15.75 usec
PL1       -5.00 dB
PL12      32.48802107 dB
SFO1      700.2754622 MHz

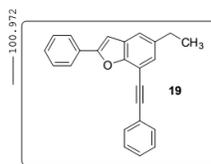
F2 - Processing parameters
SI         32768
SF         700.2700221 MHz
WDW        EM
SSB        0
LB         0 Hz
GB         0
PC         5.00
  
```







131.444
128.793
128.041
127.567
124.693
119.950



DEPT90

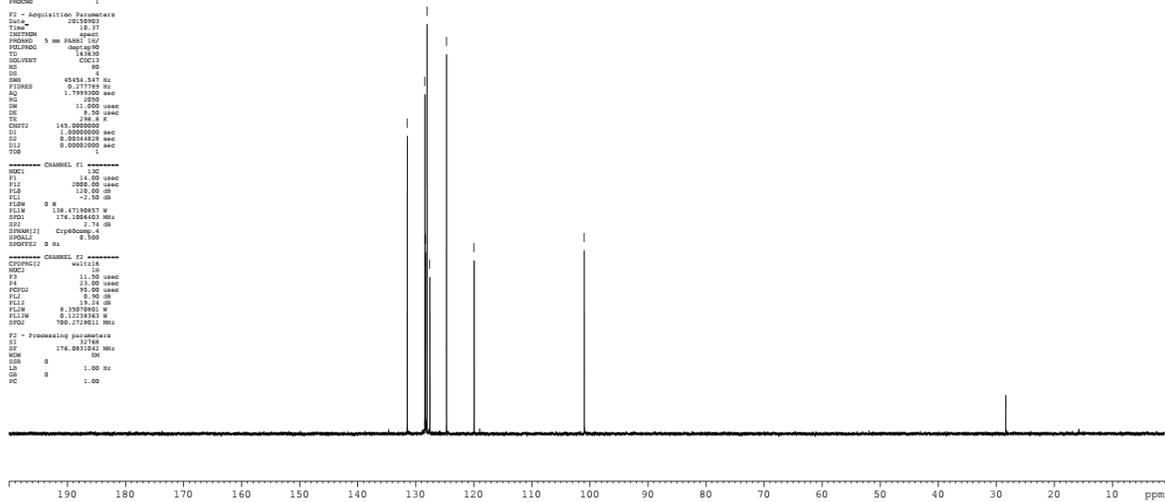
```

Current Data Parameters
NAME      MF
EXPNO    1144
PROCNO   1

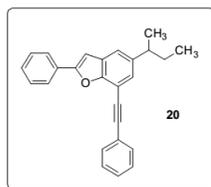
F2 - Acquisition Parameters
Date_    20100201
Time     10.37
INSTRUM  spect
PROBHD   5 mm PABBO-5B
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        4
DS        4
SWH       8012.820 Hz
FIDRES   0.111113 Hz
AQ        4.499937 sec
RG        101
DE        8.50 usec
TE        300.4 K
D1        1.0000000 sec
D2        0.0000000 sec
D3        0.0000000 sec
TD0       1

===== CHANNEL f1 =====
NUC1      1H
P1        14.00 usec
PL1       0.00 dB
PL2       10.00 usec
PL3       0.00 dB
PL4       0.00 dB
PL5       0.00 dB
PL6       0.00 dB
PL7       0.00 dB
PL8       138.4719687 MHz
SFO1      176.126402 MHz
SFO2      2.74 MHz
===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2      13C
P2        11.50 usec
PL2       0.00 dB
PL3       0.00 usec
PL4       0.00 dB
PL5       0.00 dB
PL6       8.3307801 MHz
PL7       0.1217861 MHz
SFO1      100.6278011 MHz

F2 - Processing parameters
SI         32768
SF         400.1334011 MHz
WDW        EM
SSB        0
LB         0.00 Hz
GB         0
PC         1.00
  
```

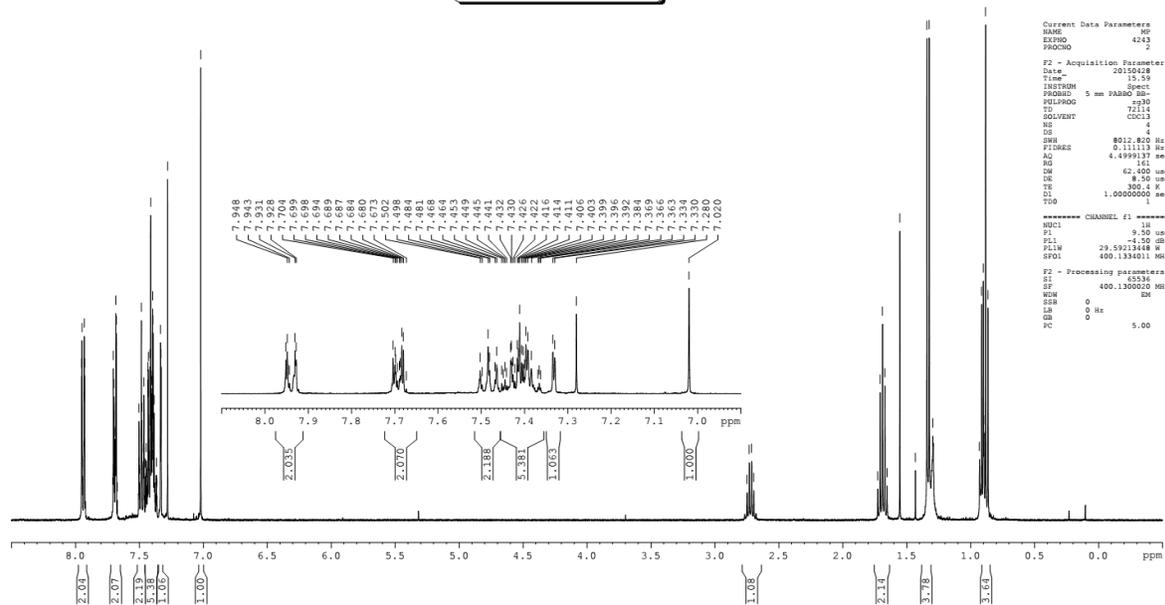


7.502
7.489
7.481
7.468
7.453
7.449
7.441
7.432
7.422
7.416
7.411
7.406
7.400
7.393
7.382
7.372
7.369
7.366
7.363
7.350
7.280
7.020



2.748
2.731
2.696

1.726
1.708
1.671
1.653
1.554
1.342
1.324
0.951
0.914
0.561
0.583
0.865



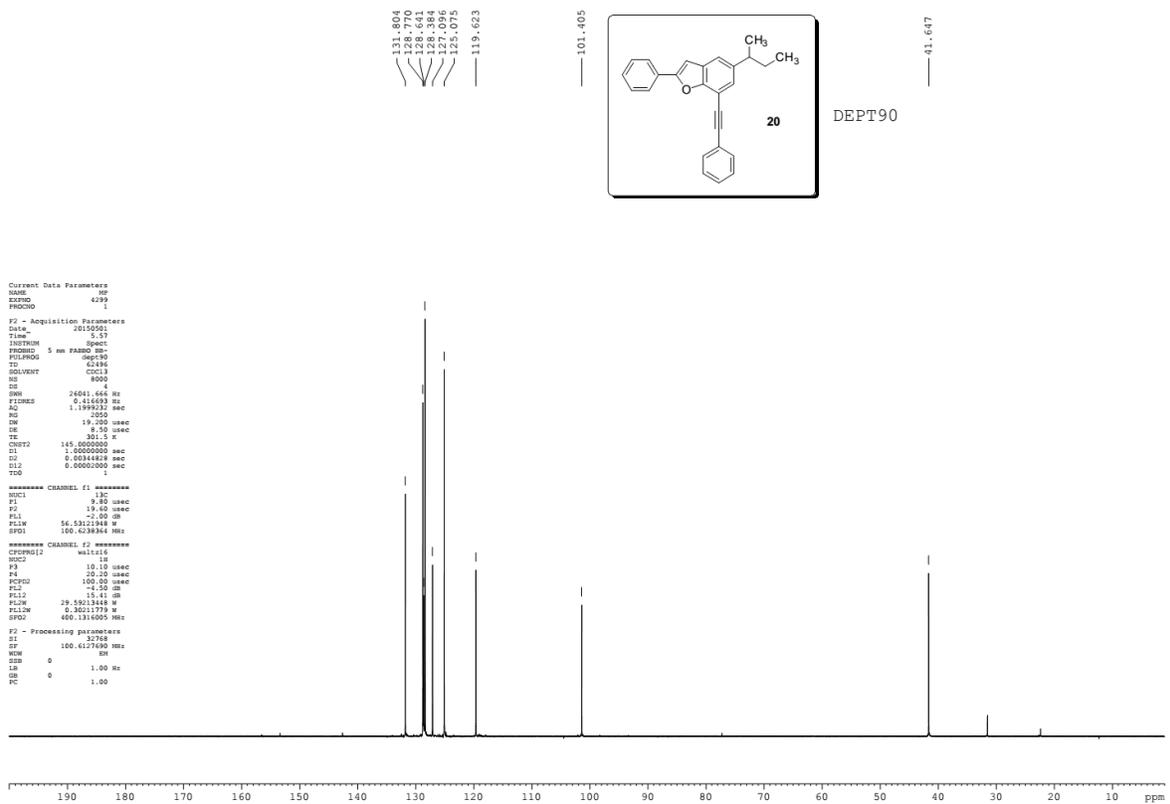
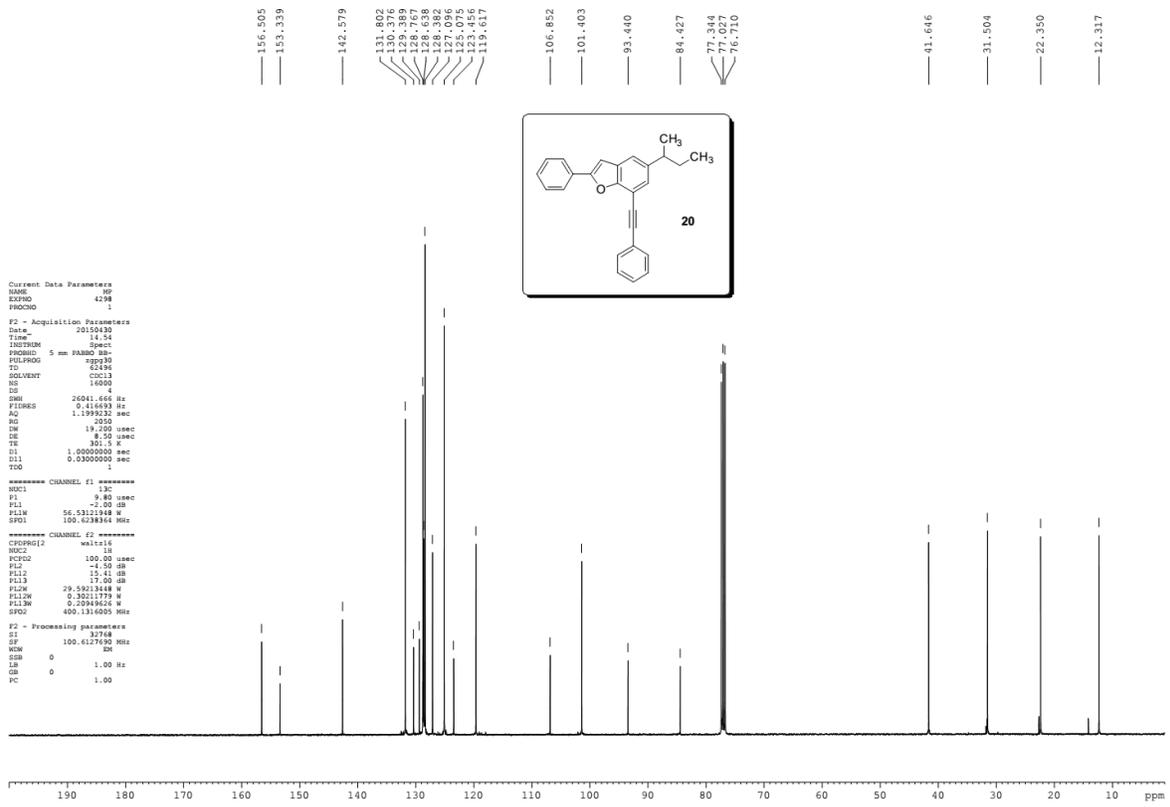
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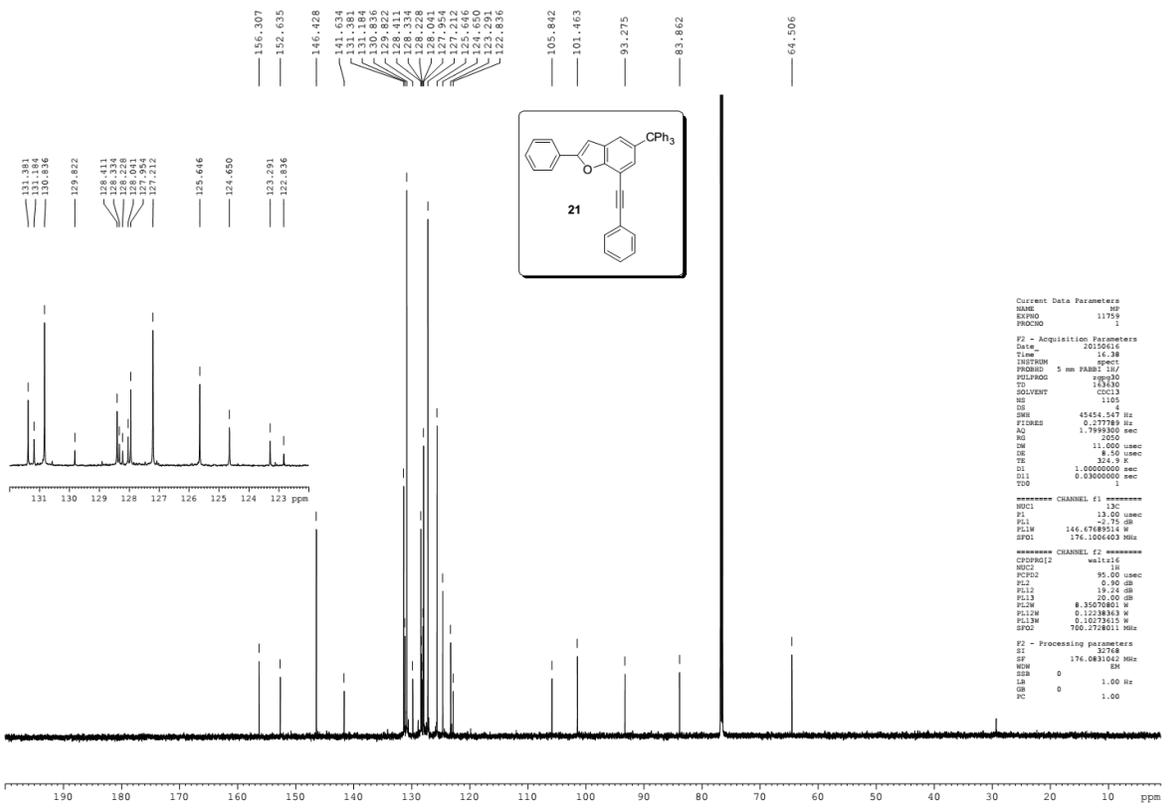
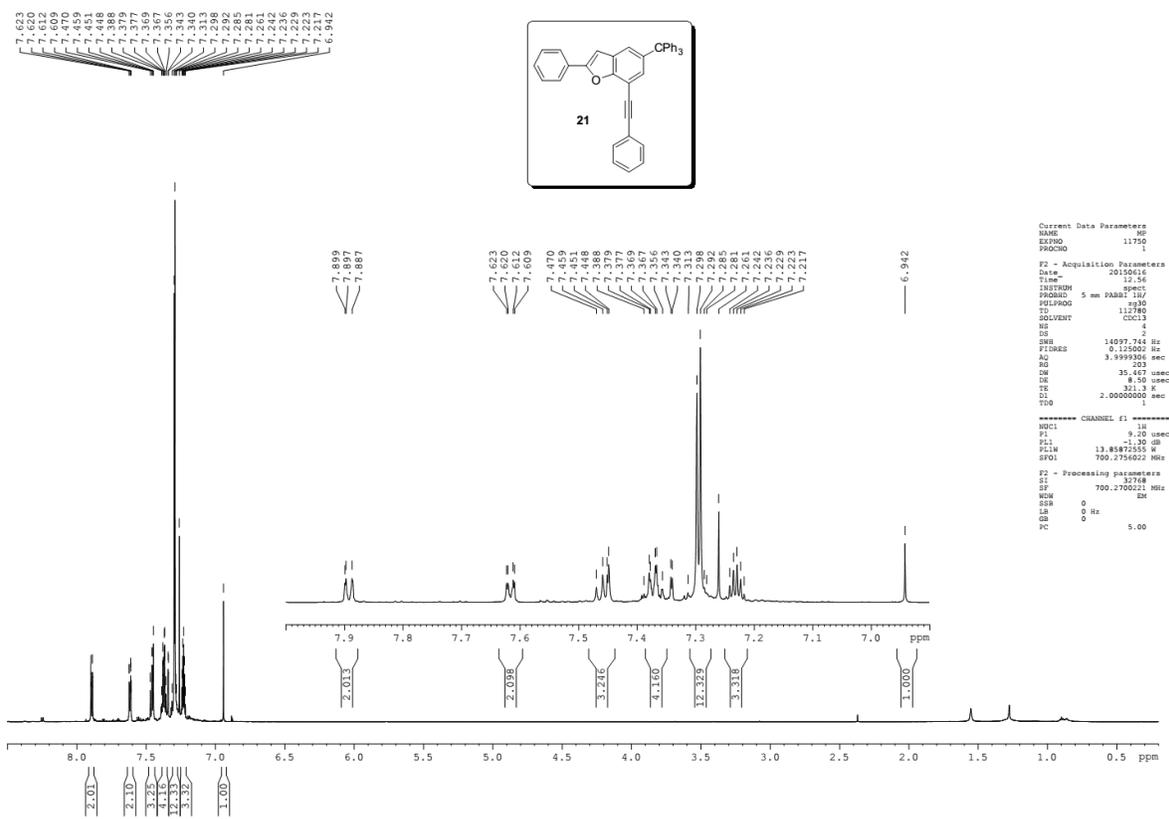
Current Data Parameters
NAME      MF
EXPNO    413
PROCNO   2

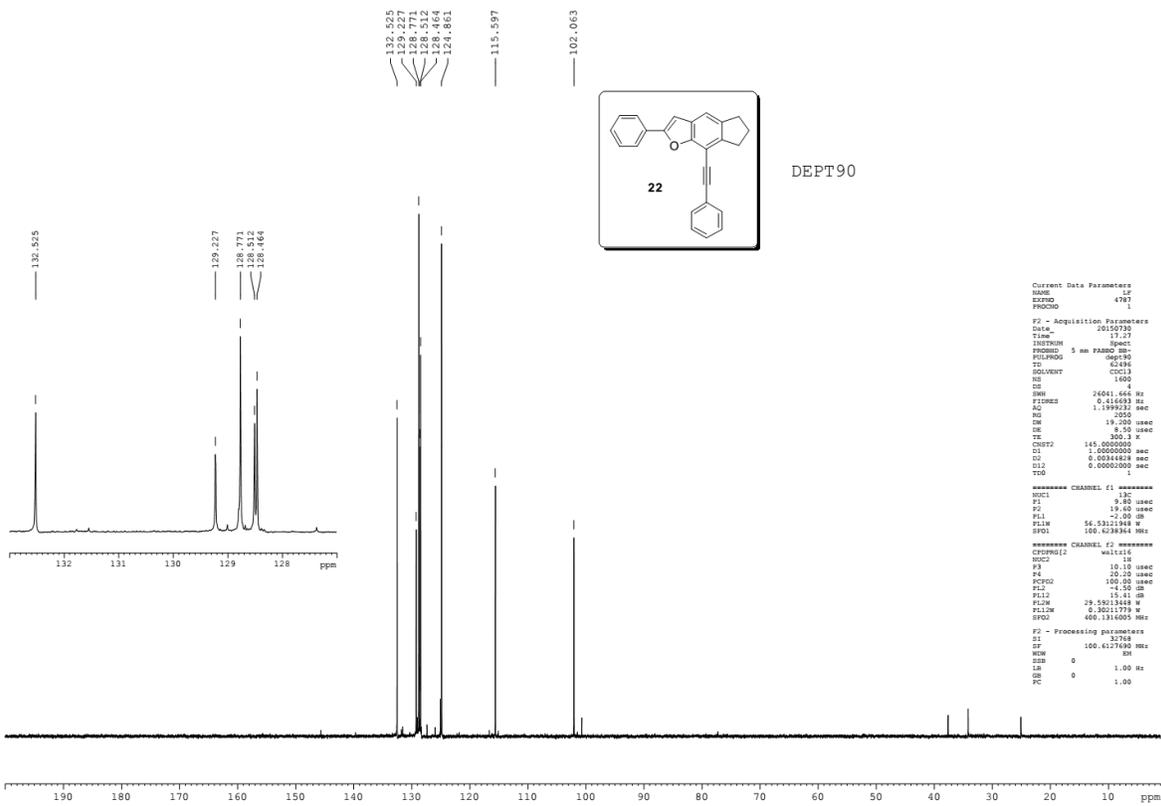
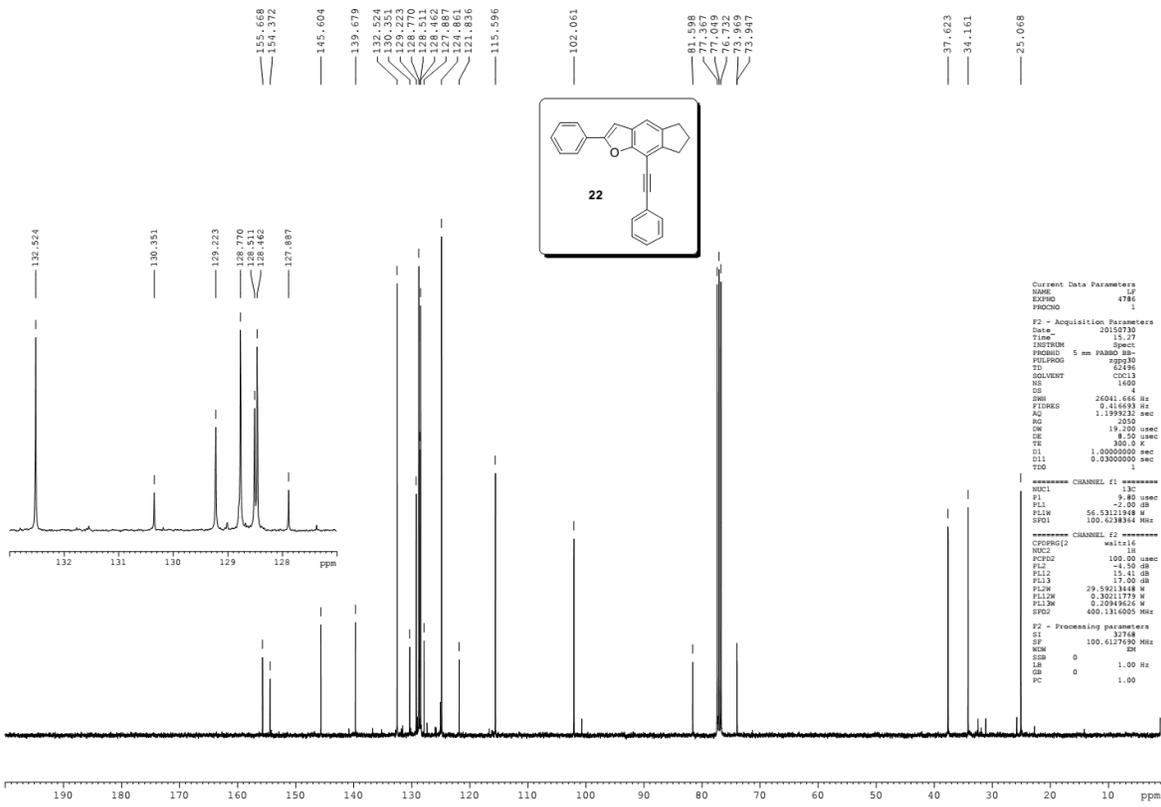
F2 - Acquisition Parameters
Date_    20100208
Time     15.59
INSTRUM  spect
PROBHD   5 mm PABBO-5B
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        4
DS        4
SWH       8012.820 Hz
FIDRES   0.111113 Hz
AQ        4.499937 sec
RG        101
DE        8.50 usec
TE        300.4 K
D1        1.0000000 sec
D2        0.0000000 sec
D3        0.0000000 sec
TD0       1

===== CHANNEL f1 =====
NUC1      1H
P1        9.50 usec
PL1       -4.50 dB
PL2       0.00 dB
PL3       29.5913448 MHz
PL4       400.1334011 MHz
SFO1      400.1330020 MHz

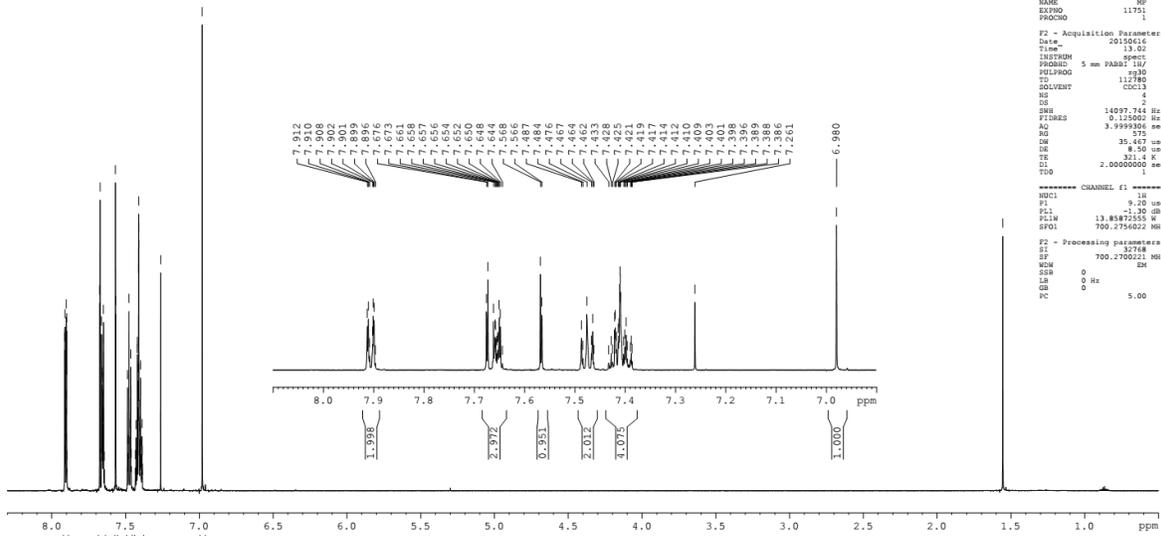
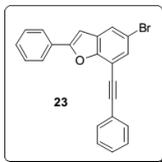
F2 - Processing parameters
SI         32768
SF         400.1330020 MHz
WDW        EM
SSB        0
LB         0.00 Hz
GB         0
PC         5.00
  
```







7.648
7.644
7.568
7.564
7.587
7.484
7.476
7.462
7.464
7.428
7.425
7.421
7.417
7.414
7.410
7.409
7.403
7.398
7.396
7.388
7.386
7.261
6.980

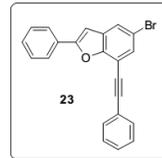
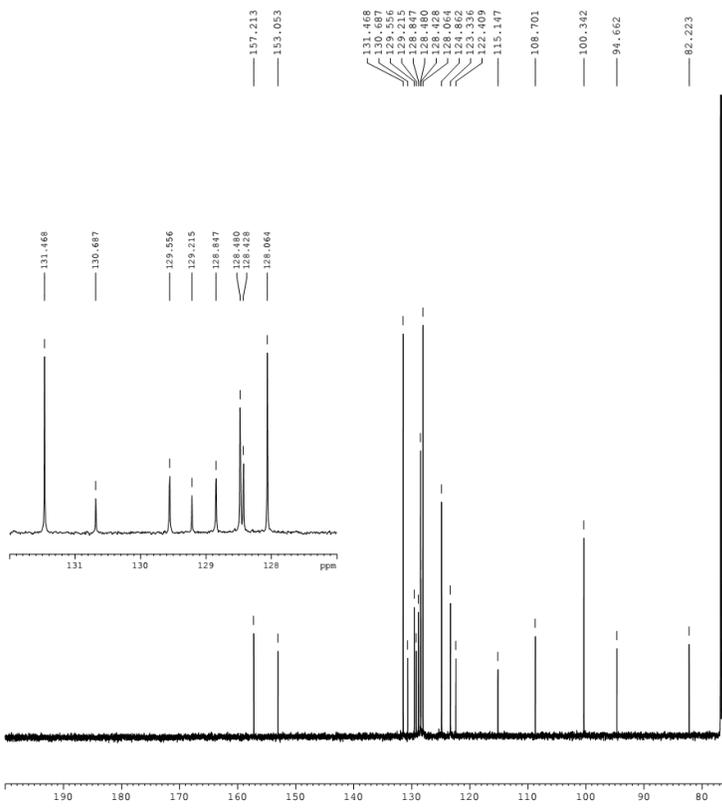


```
Current Data Parameters
NAME      MF
EXPNO    11751
PROCNO    1

F2 - Acquisition Parameters
Date_     2015016
Time      13.02
INSTRUM   spect
PROBHD    5 mm PABBI 1H/
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         4
DS         2
SFR        14097.744 Hz
AQ         0.125000 Hz
RG         3.999986 sec
AW         375
DE         35.467 usec
TE         8.50 usec
D1         301.4 Hz
D11        2.0000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         9.20 usec
PL1        -1.20 dB
PL12       13.8847355 dB
SFO1       700.2754022 MHz

F2 - Processing parameters
SI         32768
SF         700.2700221 MHz
WDW        EM
SSB        0 Hz
LB         0 Hz
GB         0 Hz
PC         5.00
```



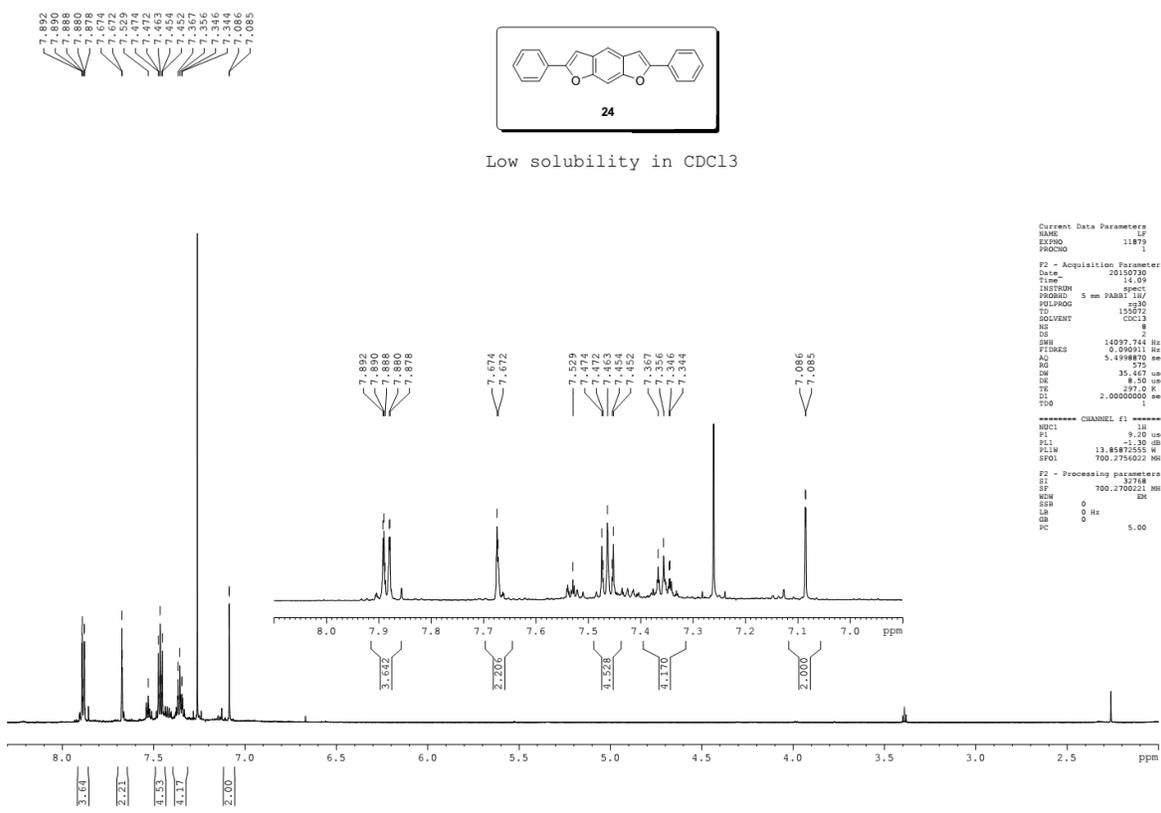
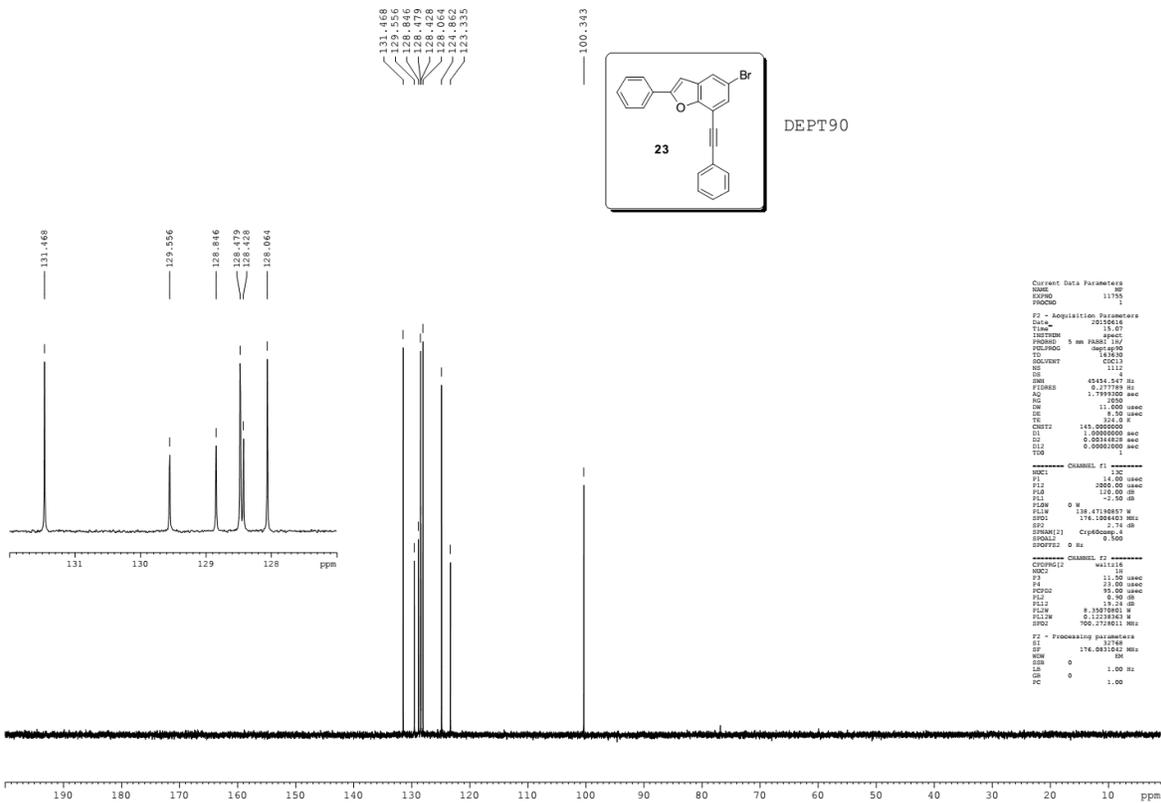
```
Current Data Parameters
NAME      11956
EXPNO    11956
PROCNO    1

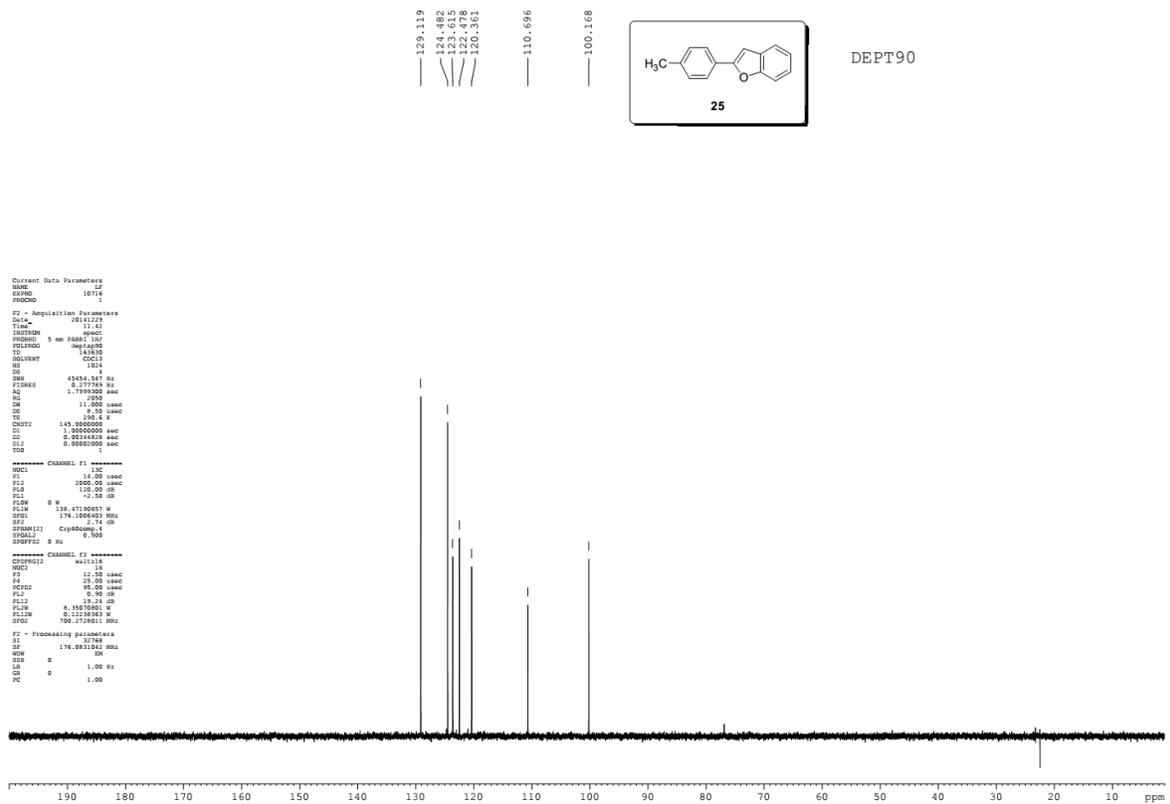
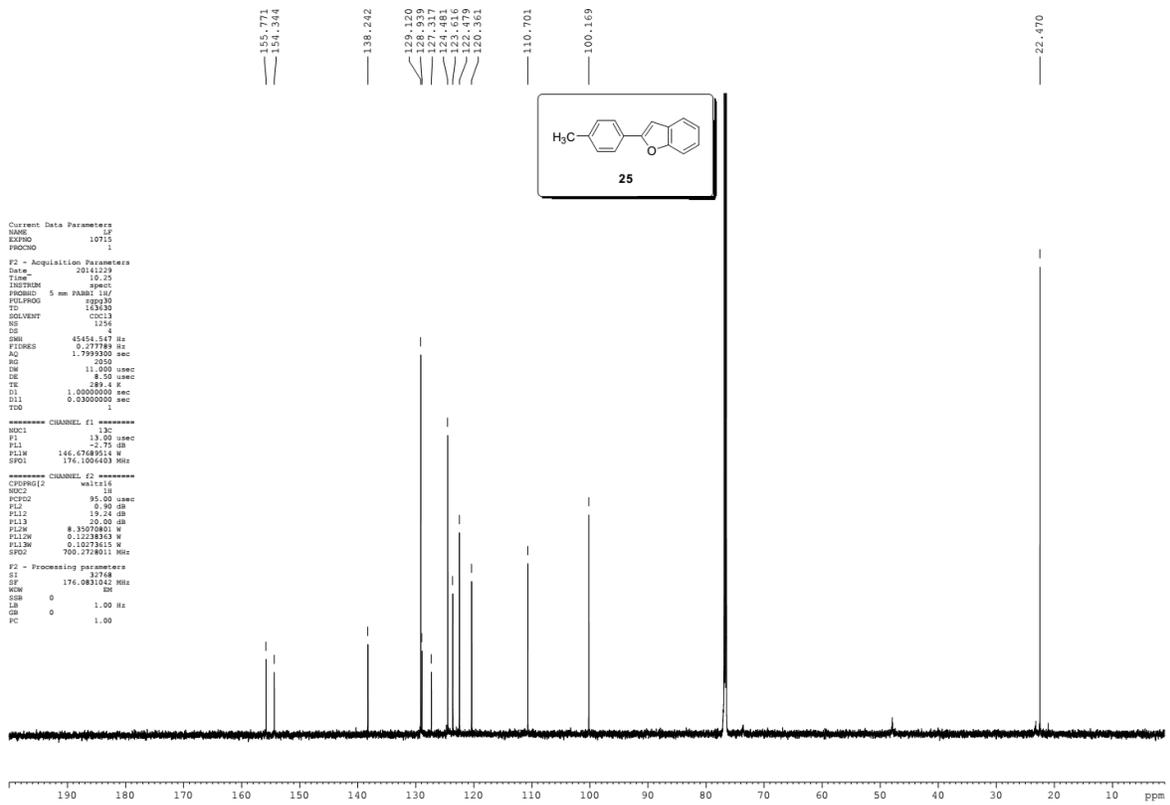
F2 - Acquisition Parameters
Date_     2015016
Time      14.04
INSTRUM   spect
PROBHD    5 mm PABBI 1H/
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         4
DS         2
SFR        45454.147 Hz
AQ         0.277988 Hz
RG         1.799990 sec
AW         2050
DE         11.900 usec
TE         8.50 usec
D1         1.0000000 sec
D11        0.2300000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1         13.00 usec
PL1        -2.75 dB
PL12       146.47689514 dB
SFO1       176.1004403 MHz

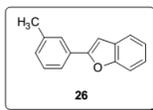
===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2     90.00 usec
PL2       0.00 dB
PL12      20.00 dB
PL13      20.00 dB
PL14      20.00 dB
PL15      20.00 dB
PL16      20.00 dB
PL17      20.00 dB
PL18      20.00 dB
PL19      20.00 dB
PL20      20.00 dB
PL21      20.00 dB
PL22      20.00 dB
PL23      20.00 dB
PL24      20.00 dB
PL25      20.00 dB
PL26      20.00 dB
PL27      20.00 dB
PL28      20.00 dB
PL29      20.00 dB
PL30      20.00 dB
SFO2       700.278011 MHz

F2 - Processing parameters
SI         32768
SF         176.0831042 MHz
WDW        EM
SSB        0 Hz
LB         1.00 Hz
GB         0 Hz
PC         1.00
```





129.433
127.592
125.599
124.223
122.905
122.905
120.911
111.188
101.251



DEPT90

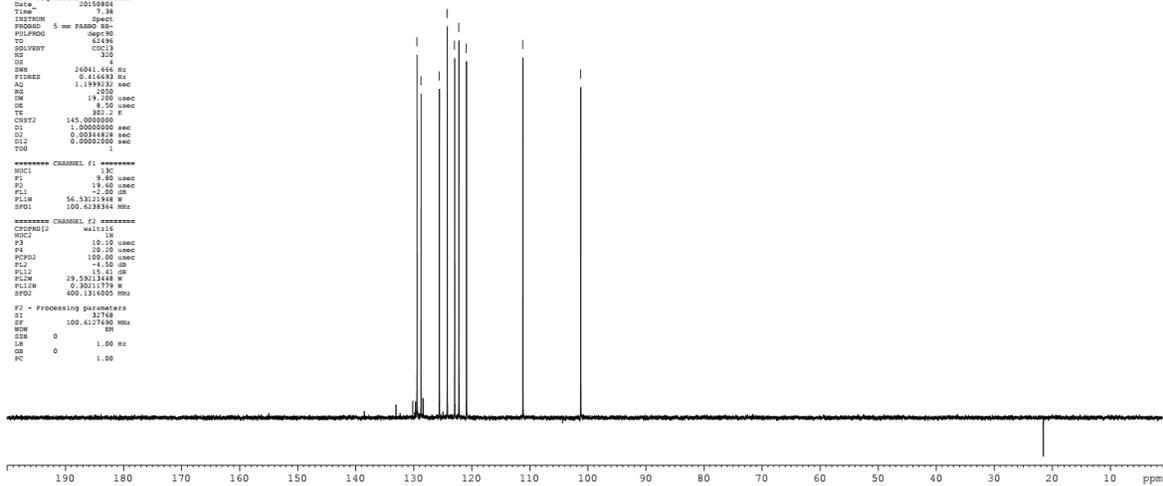
```
Current Data Parameters
NAME      IF
EXPNO    4790
PROCNO   1

F2 - Acquisition Parameters
Date_    20150804
Time_    7.38
INSTRUM  spect
PROBHD   5 mm PABBI 1H/
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       4
DS       4
SWH      26041.666 Hz
FIDRES   0.416893 Hz
AQ       1.1999232 sec
RG       2560
DM       19.700 usec
DC       8.50 usec
TE       302.2 K
CSTZ     145.0000000
D1       1.000000000 sec
D2       0.000000000 sec
D3       0.000000000 sec
TD0      1

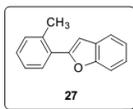
***** CHANNEL f1 *****
NUC1      13C
P1        9.80 usec
PL1       -1.00 dB
PC1       56.5311188 W
SFO1     100.628364 MHz

***** CHANNEL f2 *****
CPDPRG2  waltz16
NUC2      13C
P2        10.10 usec
PL2       -1.00 dB
PC2       56.5311188 W
SFO2     100.628364 MHz

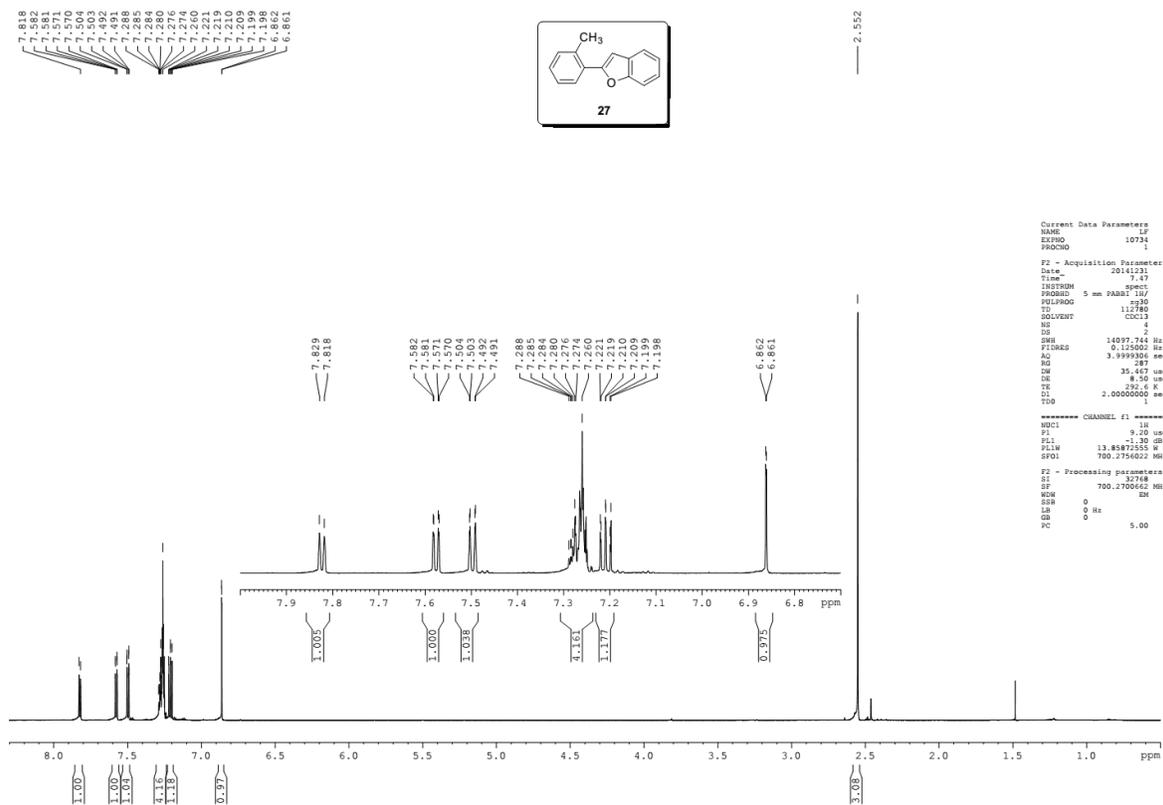
F2 - Processing parameters
SI        32768
SF        100.627430 MHz
WDW       EM
SSB       0
LA        1.00 Hz
GB        0
PC        1.00
```



7.582
7.581
7.577
7.570
7.504
7.503
7.503
7.491
7.488
7.285
7.280
7.276
7.266
7.260
7.221
7.219
7.209
7.199
7.182
6.862
6.861



2.552

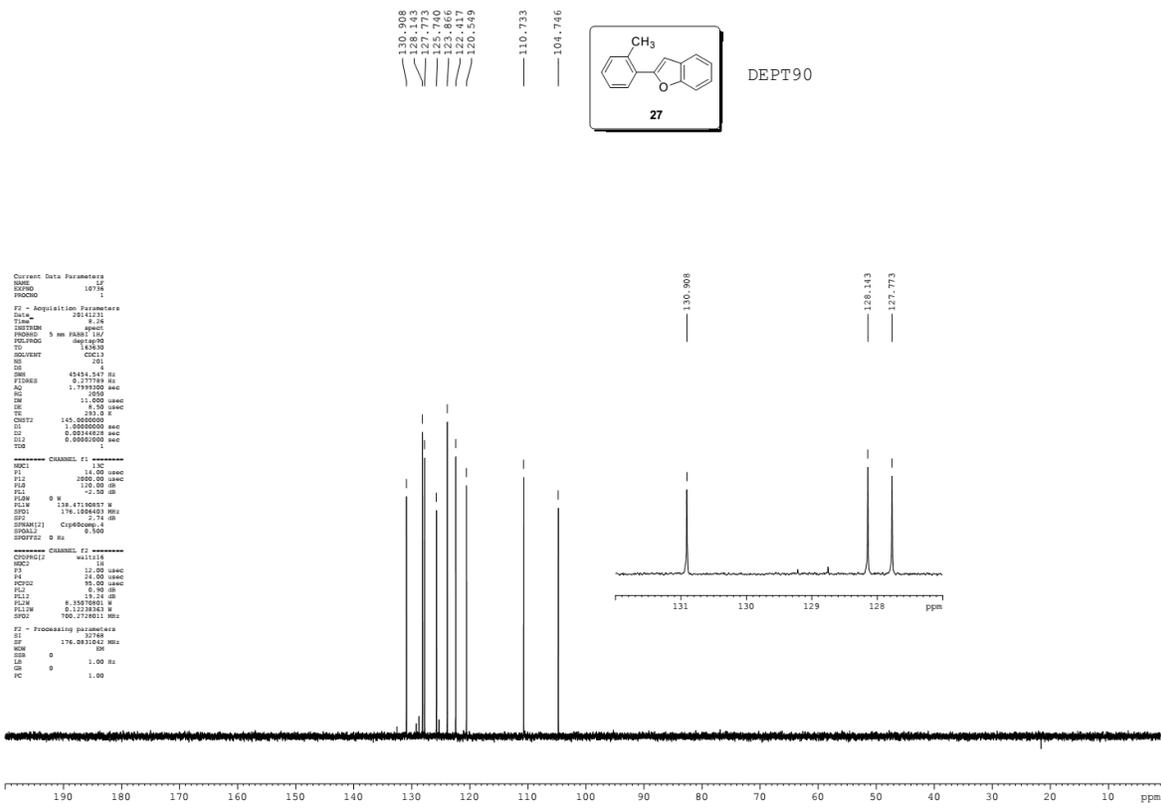
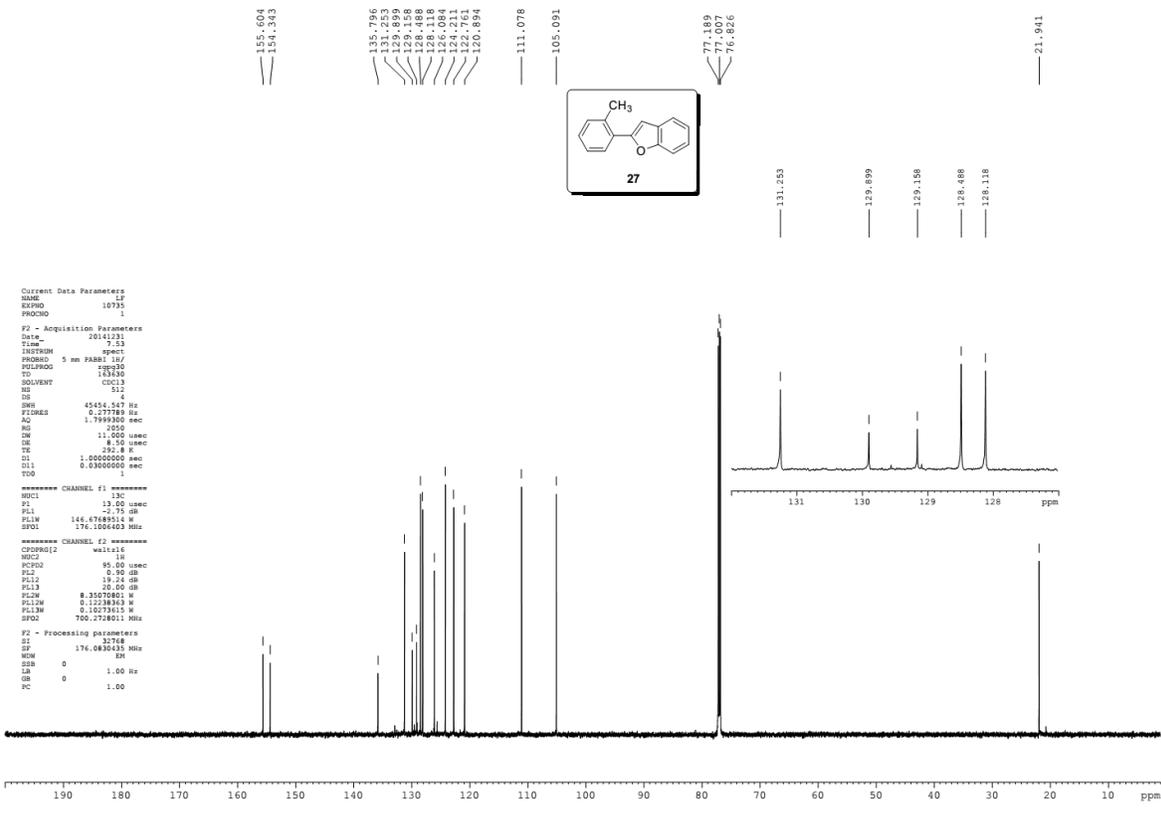


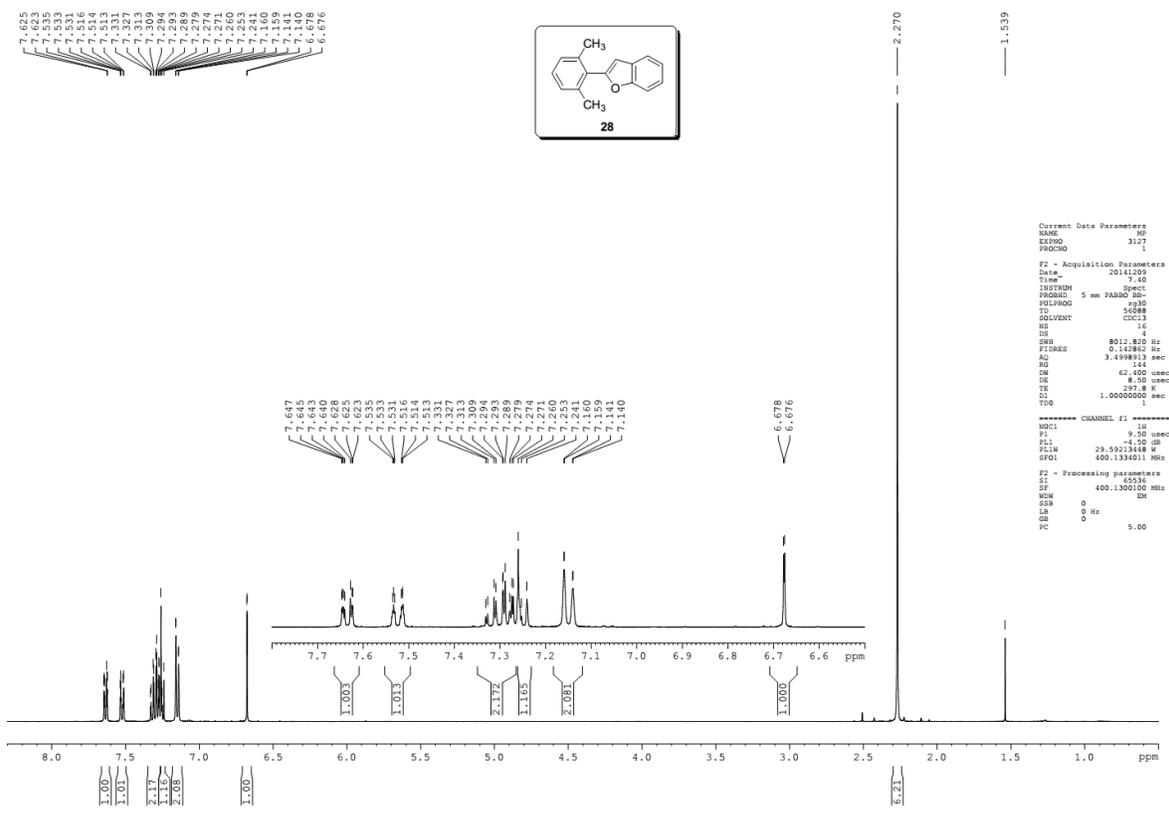
```
Current Data Parameters
NAME      IF
EXPNO    10734
PROCNO   1

F2 - Acquisition Parameters
Date_    20141231
Time_    7.47
INSTRUM  spect
PROBHD   5 mm PABBI 1H/
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       4
DS       4
SWH      14097.744 Hz
FIDRES   0.125002 Hz
RG       3.9999900 sec
DM       19.700 usec
DC       8.50 usec
TE       301.477 usec
CSTZ     145.0000000
D1       1.000000000 sec
D2       0.000000000 sec
TD0      1

***** CHANNEL f1 *****
NUC1      1H
P1        9.30 usec
PL1       -1.30 dB
PC1       13.85873555 W
SFO1     700.2756022 MHz

F2 - Processing parameters
SI        32768
SF        700.270062 MHz
WDW       EM
SSB       0
LA        0 Hz
GB        0
PC        5.00
```





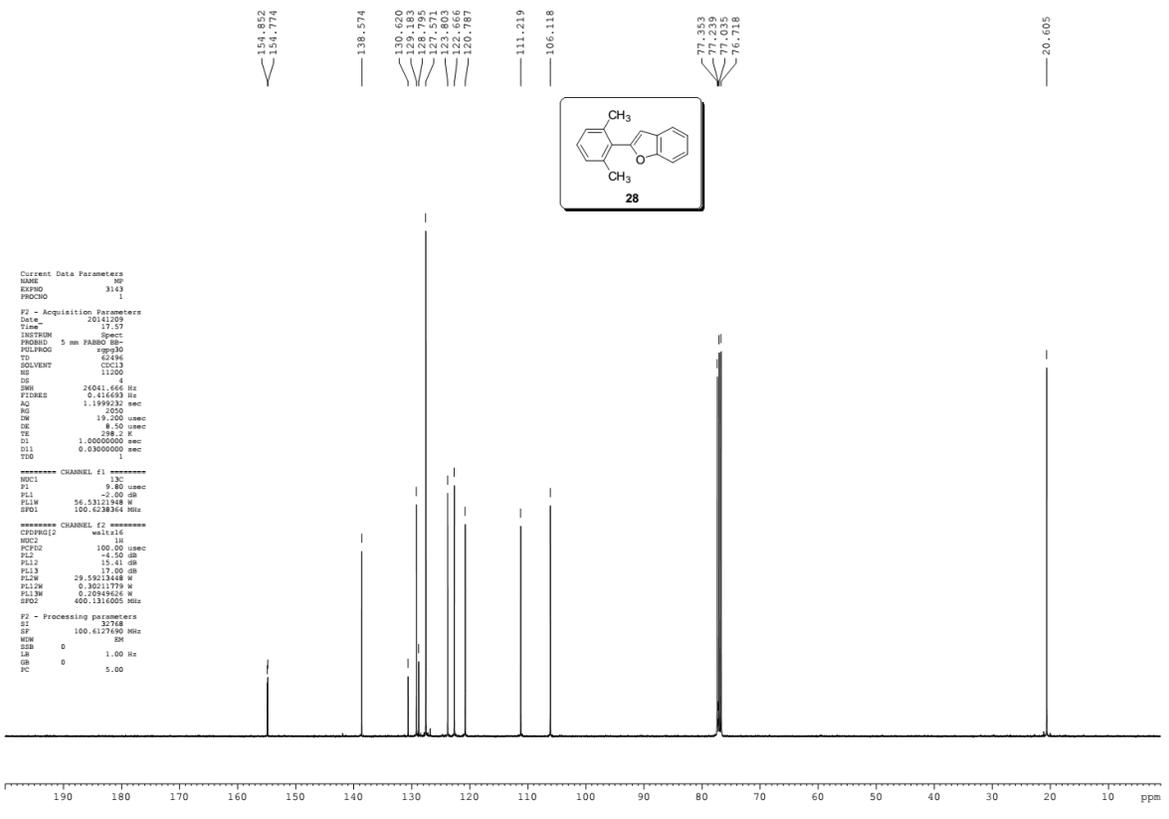
```

Current Data Parameters
NAME      MF
EXPNO    3127
PROCNO    1

F2 - Acquisition Parameters
Data      20141209
Time      7.40
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         4
SWH        8012.820 Hz
FIDRES     0.142862 Hz
AQ         3.4998913 sec
RG         654
DM         62.400 usec
DE         8.50 usec
TE         297.8 K
SI         1.00000000 sec
TOD        1

===== CHANNEL f1 =====
NUC1       1H
P1         16
PC1        4.50 usec
PL1        29.5813448 dB
PL1W       400.1334011 MHz
SFO1       400.1334011 MHz

F2 - Processing parameters
SI         65536
SF         400.1300100 MHz
SFR        0
SSB        0
LB         0 Hz
GB         0
PC         5.00
  
```



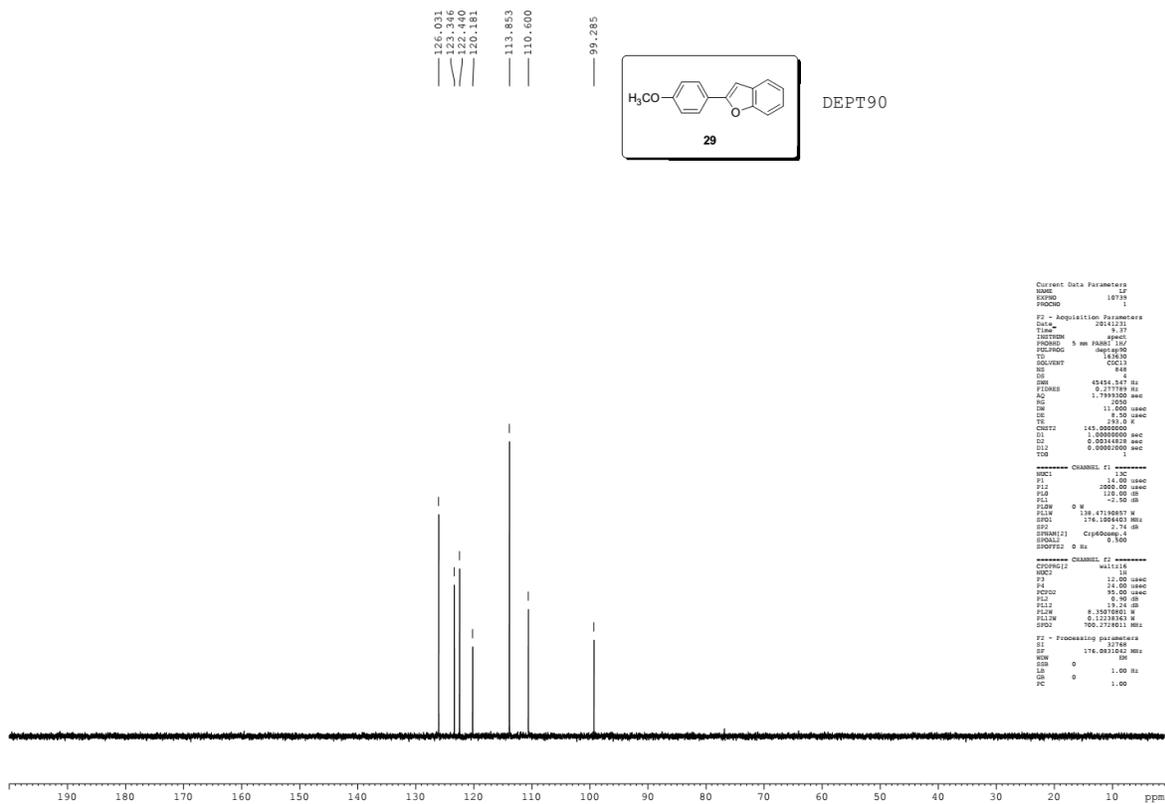
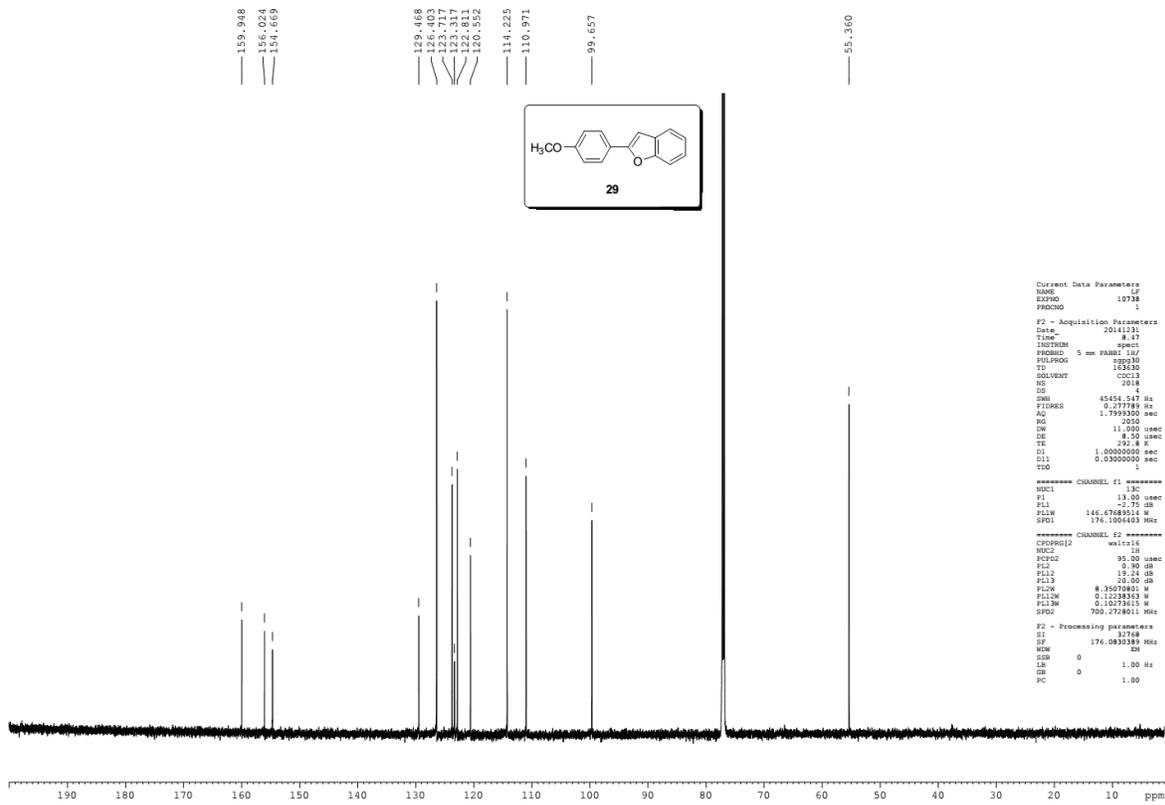
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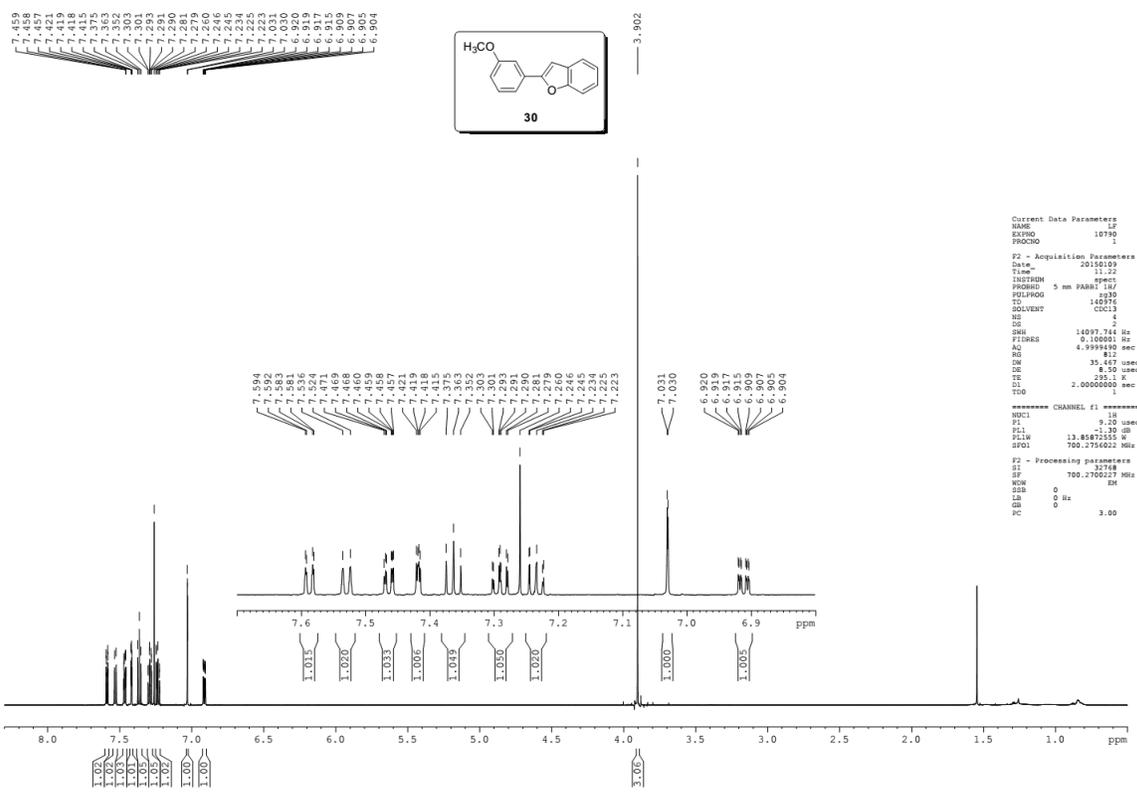
Current Data Parameters
NAME      MF
EXPNO    3143
PROCNO    1

F2 - Acquisition Parameters
Data      20141209
Time      17.57
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         11200
DS         4
SWH        26041.666 Hz
FIDRES     0.416403 Hz
AQ         1.1999232 sec
RG         2920
DM         19.200 usec
DE         8.50 usec
TE         298.2
SI         1.00000000 sec
SFO1       100.628364 MHz
SFO2       100.628364 MHz

===== CHANNEL f1 =====
NUC1       13C
P1         8.80 usec
PC1        4.50 usec
PL1        19.5813448 dB
PL1W       100.628364 MHz

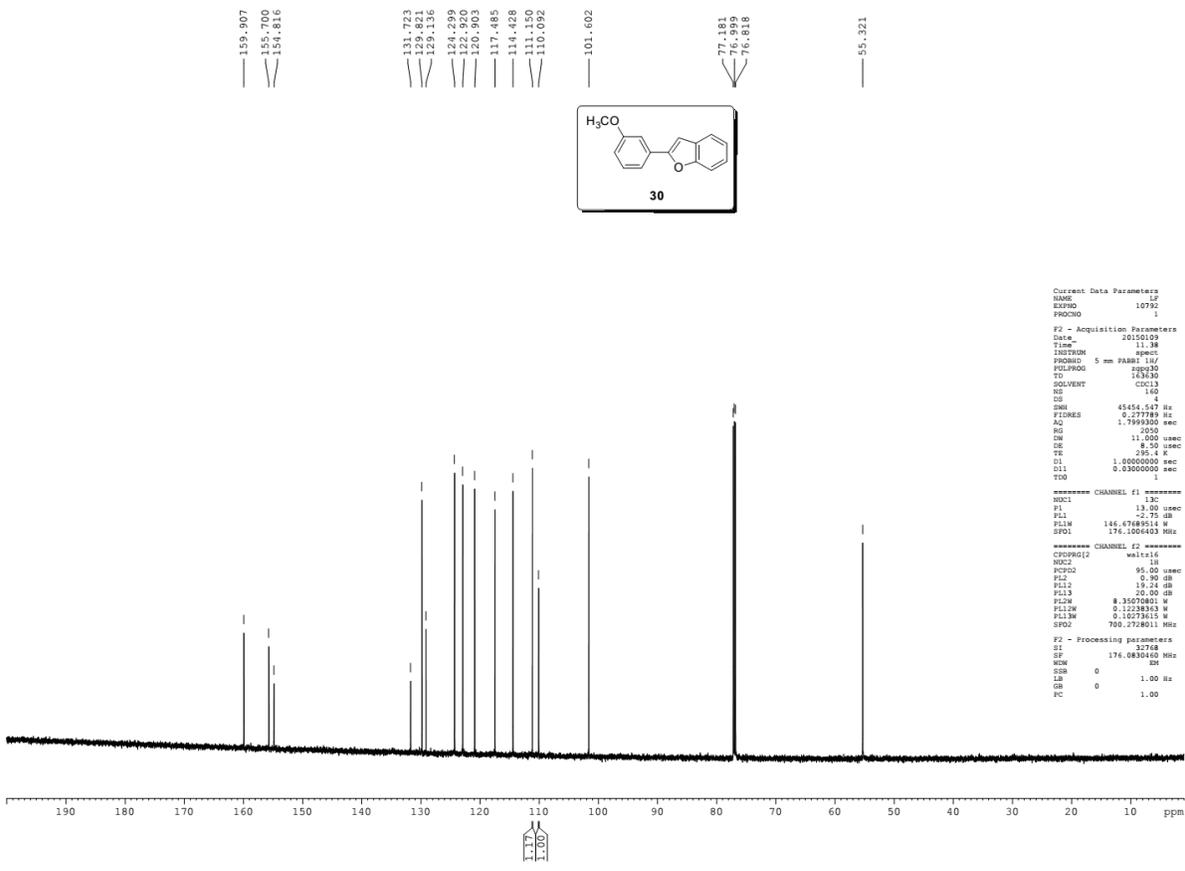
===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       13C
PCPD2     100.00 usec
PC2       4.50 usec
PL12      15.41 dB
PL13      17.00 dB
PL2W      29.5913448 dB
PL3W      0.3021779 dB
PL3W      0.2049626 dB
SFO2       100.627490 MHz
SFR        0
SSB        0
LB         1.00 Hz
GB         0
PC         5.00
  
```



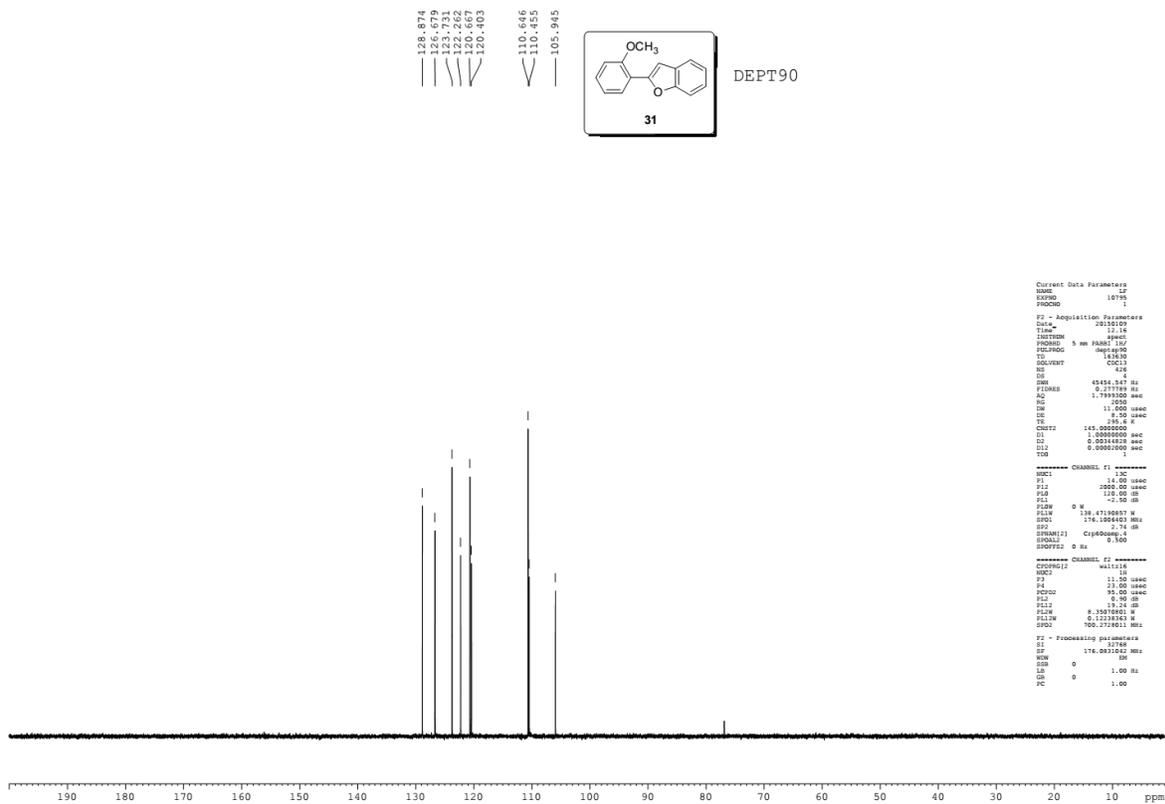
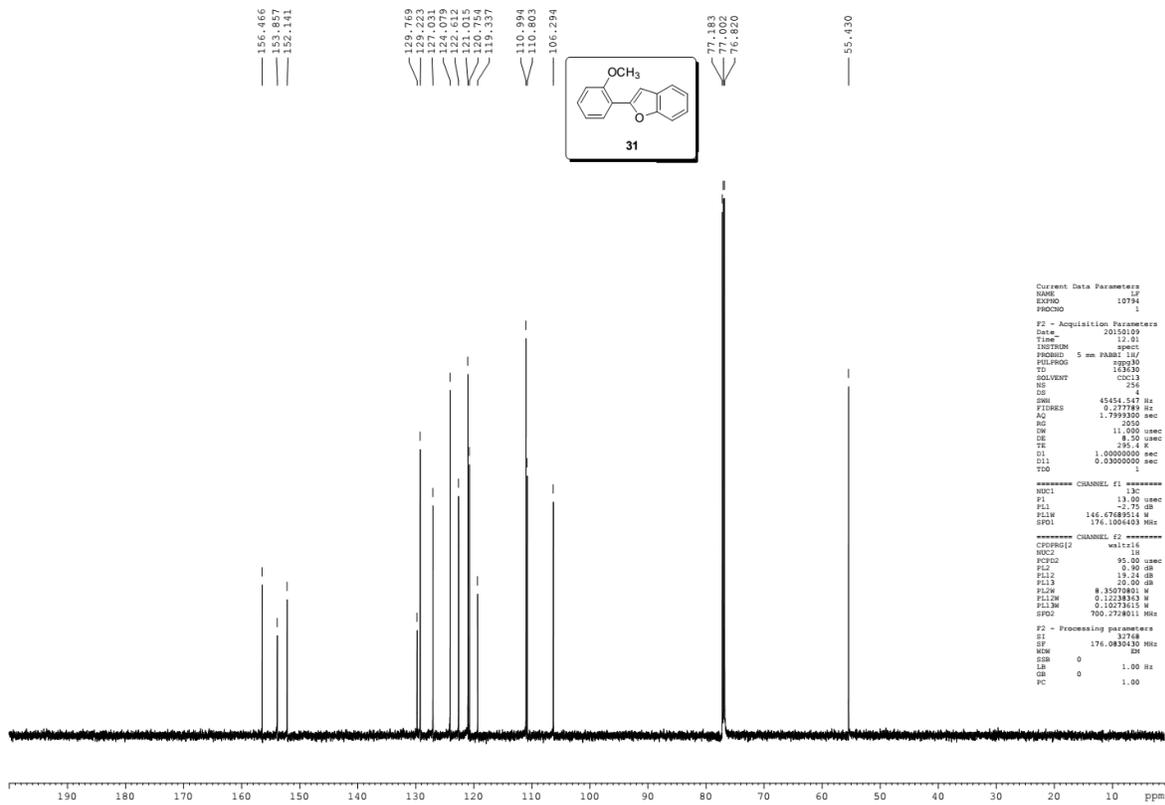
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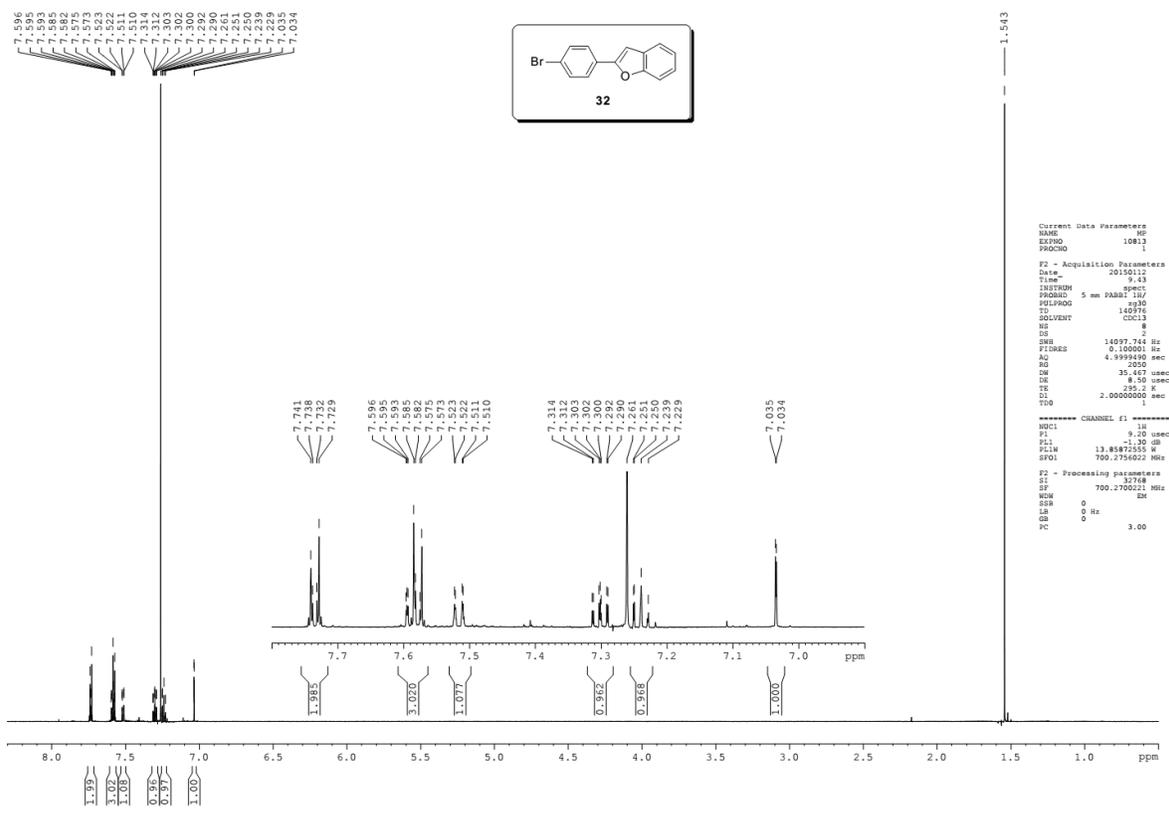
Current Data Parameters
NAME      1F
EXPNO    10790
PROCNO   1
F2 - Acquisition Parameters
Date_    20150109
Time     11.22
INSTRUM  spect
PROBHD   5 mm PABBI 1H/
PULPROG  zgpg30
TD        163830
SOLVENT  CDCl3
NS        140
DS        4
SFO      46454.547 Hz
FIDRES   0.177789 Hz
AQ        1.7999300 sec
RG        2050
SWH       11.0000 usec
SB        8.00 usec
TE        295.4 K
DE        1.00000000 sec
SI        0.03000000 sec
TD0       1
===== CHANNEL f1 =====
NUC1      1H
P1        9.20 usec
PC1       -1.20 dB
PL1W     13.81872555 W
SFO1     700.2746022 MHz
F2 - Processing parameters
SI        32768
SF        700.2746022 MHz
WDW       EM
SSB       0 Hz
GB        0
PC        3.00
  
```



```

Current Data Parameters
NAME      1F
EXPNO    10792
PROCNO   1
F2 - Acquisition Parameters
Date_    20150109
Time     11.38
INSTRUM  spect
PROBHD   5 mm PABBI 1H/
PULPROG  zgpg30
TD        163830
SOLVENT  CDCl3
NS        140
DS        4
SFO      46454.547 Hz
FIDRES   0.177789 Hz
AQ        1.7999300 sec
RG        2050
SWH       11.0000 usec
SB        8.00 usec
TE        295.4 K
DE        1.00000000 sec
SI        0.03000000 sec
TD0       1
===== CHANNEL f1 =====
NUC1      13C
P1        13.00 usec
PC1       -2.70 dB
PL1W     146.67889514 W
SFO1     176.1006403 MHz
===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2      13C
PCPD2    95.00 usec
PL2      0.80 dB
PL12     19.24 dB
PL13     20.00 dB
PL2W     8.35070801 W
PL1W     0.12238463 W
PL3W     0.10273615 W
SFO2     700.2746011 MHz
F2 - Processing parameters
SI        32768
SF        176.0830400 MHz
WDW       EM
SSB       0
GB        1.00 Hz
PC        1.00
  
```



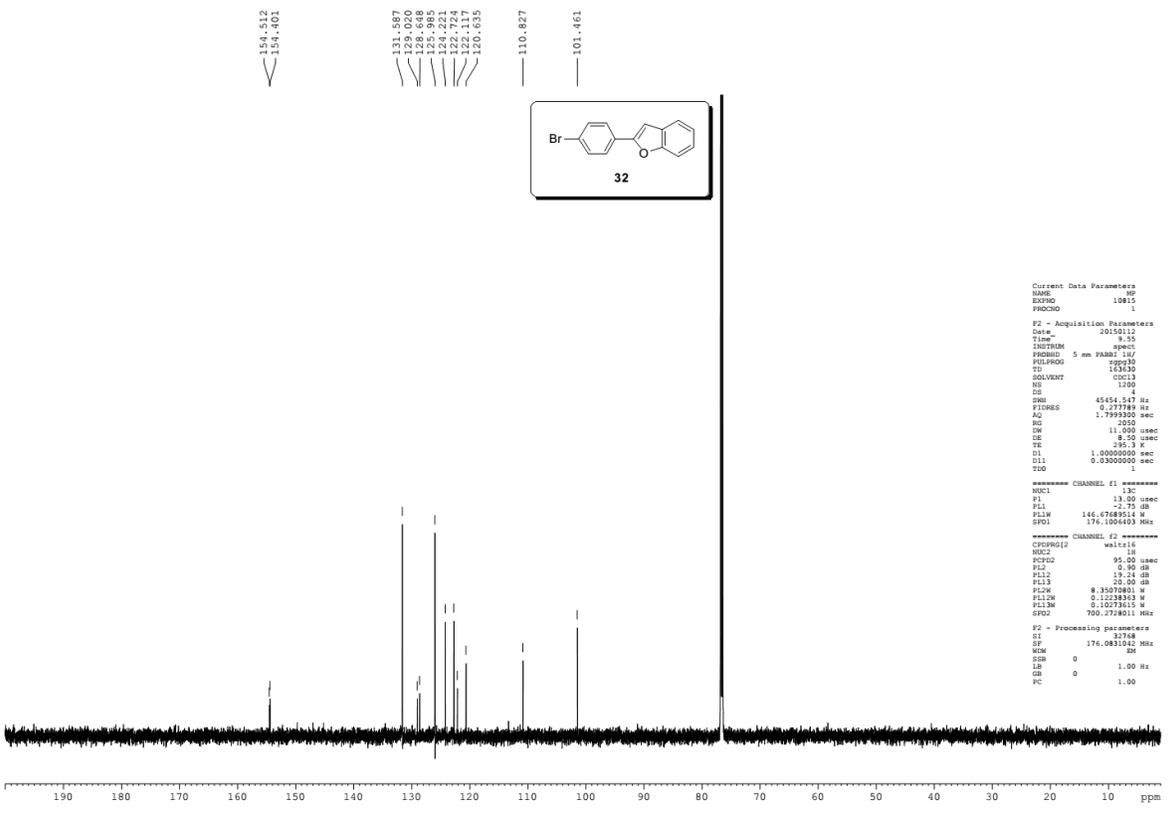
```

Current Data Parameters
NAME      MR1
EXPNO    10813
PROCNO   1

F2 - Acquisition Parameters
Date_    20150112
Time     9.43
INSTRUM  spect
PROBHD   5 mm PABBI 1H/
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        8
DS        2
SWS      14097.744 Hz
FIDRES   0.100001 Hz
AQ        4.9999490 sec
RG        2000
DM        35.467 usec
DE        8.50 usec
TE        295.2 K
D1        2.0000000 sec
TD0       1

===== CHANNEL f1 =====
NUC1      1H
P1         9.20 usec
PL1       -1.20 dB
PL12      13.88472355 W
SFO1      700.2754022 MHz

F2 - Processing parameters
SI
SF        700.2700221 MHz
WDW       EM
SSB       0
LB        0 Hz
GB        0
PC        3.00
  
```



```

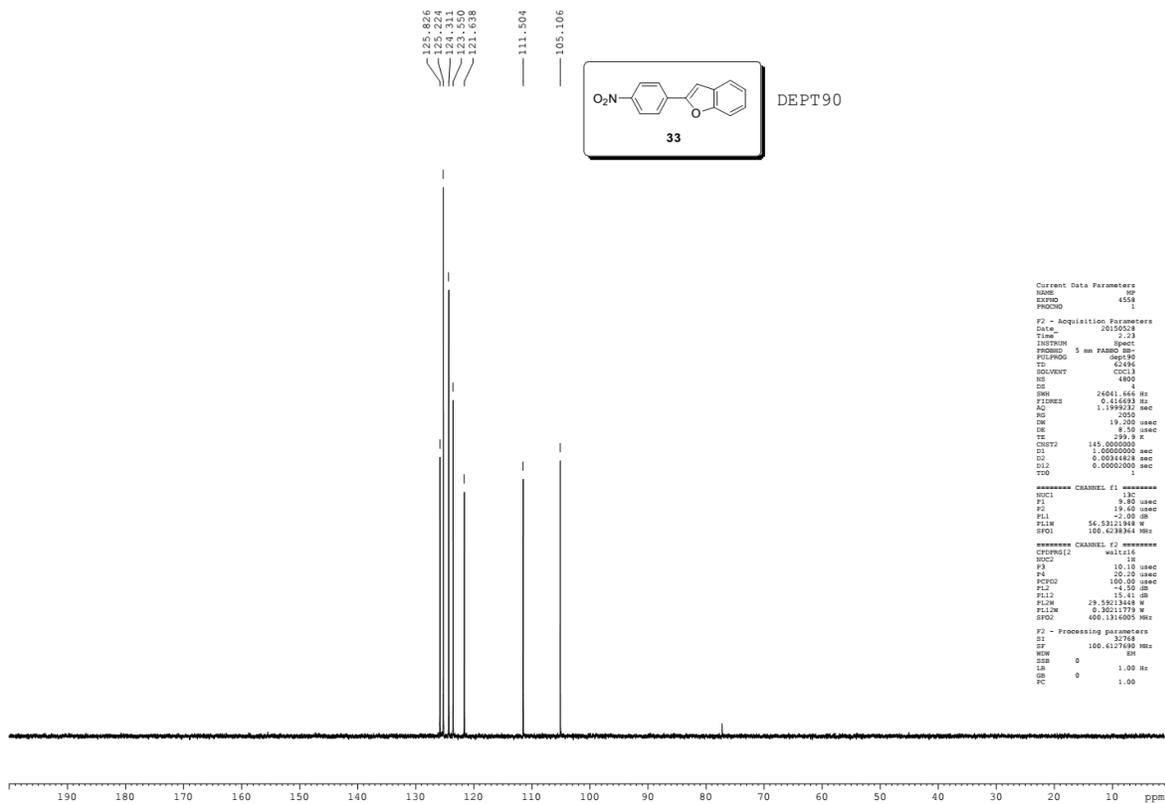
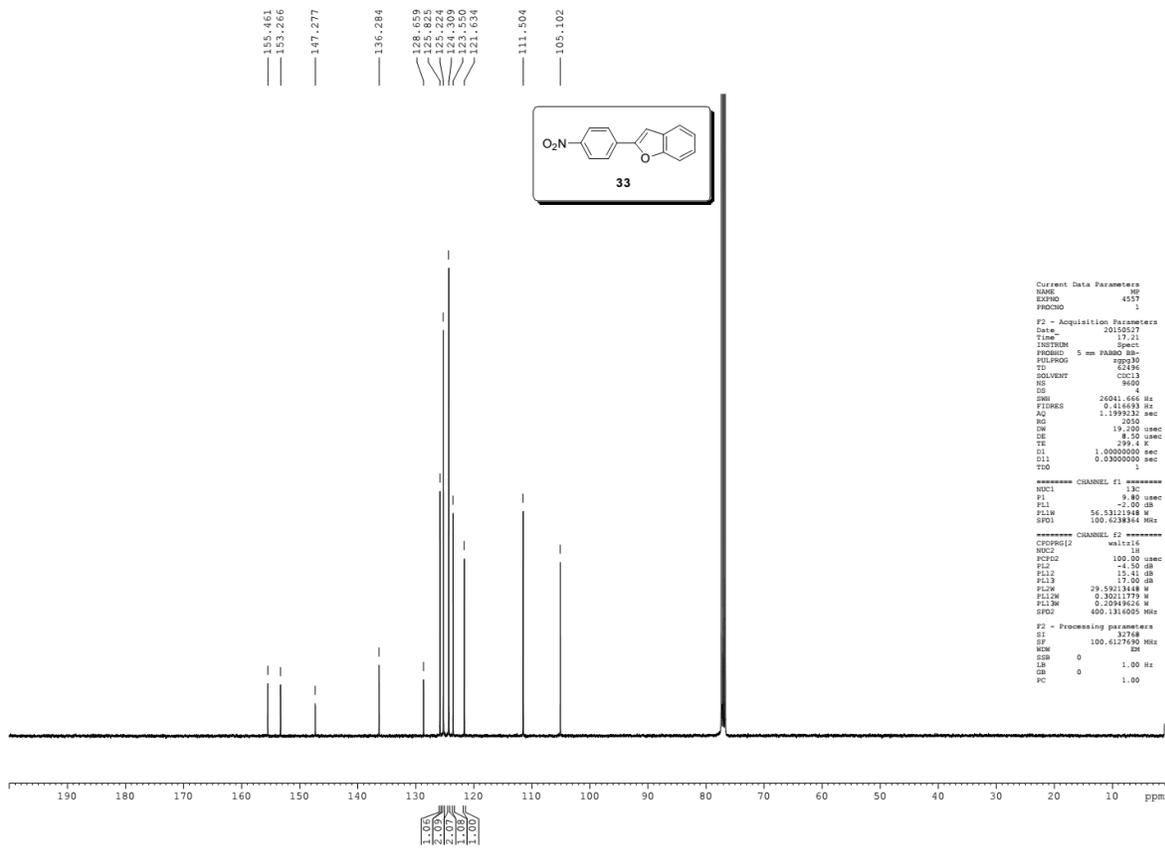
Current Data Parameters
NAME      MR15
EXPNO    10815
PROCNO   1

F2 - Acquisition Parameters
Date_    20150112
Time     9.55
INSTRUM  spect
PROBHD   5 mm PABBI 1H/
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        8
DS        2
SWS      45454.047 Hz
FIDRES   0.277783 Hz
AQ        1.7999300 sec
RG        2000
DM        11.900 usec
DE        8.50 usec
TE        295.2 K
D1        1.0000000 sec
D11       0.2300000 sec
TD0       1

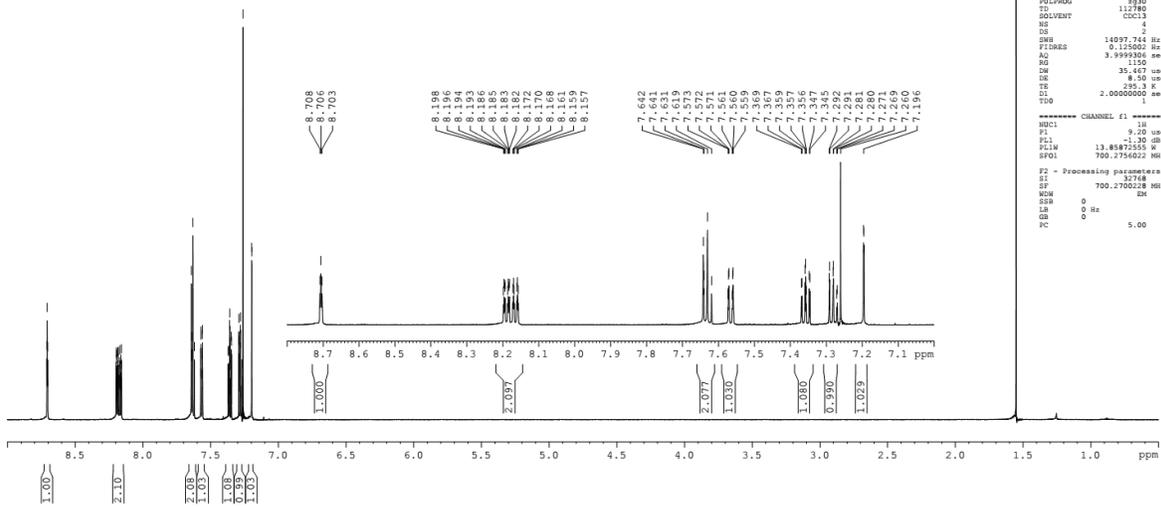
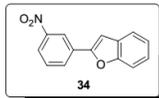
===== CHANNEL f1 =====
NUC1      13C
P1        13.00 usec
PL1       -2.75 dB
PL12      146.47689514 W
SFO1      176.1808463 MHz

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2      1H
PCPD2    90.00 usec
PL2       0.00 dB
PL13      20.00 dB
PL14      20.00 dB
PL15      20.00 dB
PL16      20.00 dB
PL17     0.2238363 W
PL18     0.2238363 W
SFO2      700.2728011 MHz

F2 - Processing parameters
SI
SF        176.0831042 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.00
  
```

8.185
8.182
8.177
8.170
8.168
8.161
8.157
8.157
7.642
7.641
7.631
7.619
7.573
7.571
7.561
7.560
7.369
7.367
7.347
7.337
7.356
7.347
7.291
7.291
7.280
7.271
7.269
7.269
7.196
7.195



Current Data Parameters
NAME MF
EXPNO 10660
PROCNO 1

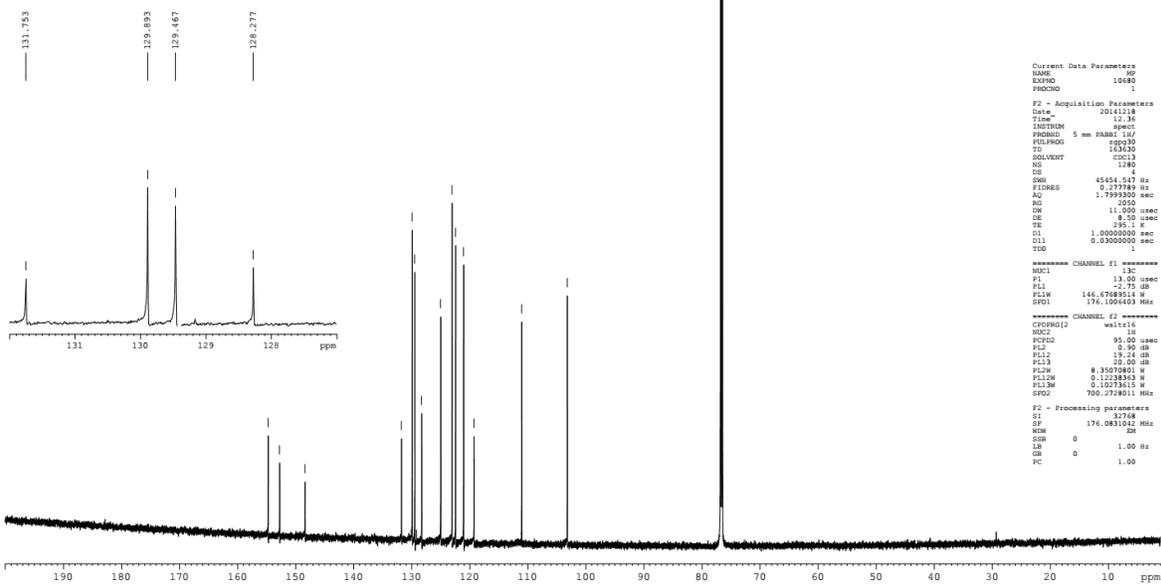
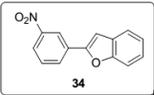
F2 - Acquisition Parameters
Date_ 20141217
Time 8.20
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zgpg30
TD 132800
SOLVENT CDCl3
NS 4
DS 2
SWH 14097.744 Hz
FIDRES 0.120002 Hz
AQ 3.9999306 sec
RG 1150
DM 35.467 usec
DE 8.50 usec
TE 299.3 K
D1 2.0000000 sec
TD0 1

***** CHANNEL f1 *****
NUC1 1H
P1 8.20 usec
PL1 -1.20 dB
PL1W 13.8847355 W
SFO1 700.2754022 MHz

F2 - Processing parameters
SI 32768
SF 700.2700228 MHz
WDW EM
SSB 0 Hz
LB 0 Hz
GB 5.00
PC 5.00

1.552

154.717
152.744
148.378
131.753
129.467
128.277
128.277
128.277
124.995
124.440
121.053
119.280
111.035
103.193



Current Data Parameters
NAME MF
EXPNO 10480
PROCNO 1

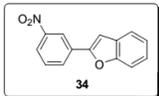
F2 - Acquisition Parameters
Date_ 20141218
Time 12.34
INSTRUM spect
PROBHD 5 mm PABBI 1H/
PULPROG zgpg30
TD 143520
SOLVENT CDCl3
NS 1940
DS 2
SWH 45454.647 Hz
FIDRES 0.277988 Hz
AQ 1.7999300 sec
RG 1050
DM 11.900 usec
DE 8.50 usec
TE 299.3 K
D1 1.0000000 sec
D11 0.2300000 sec
TD0 1

***** CHANNEL f1 *****
NUC1 13C
P1 13.00 usec
PL1 -2.15 dB
PL1W 146.47689514 W
SFO1 176.1004403 MHz

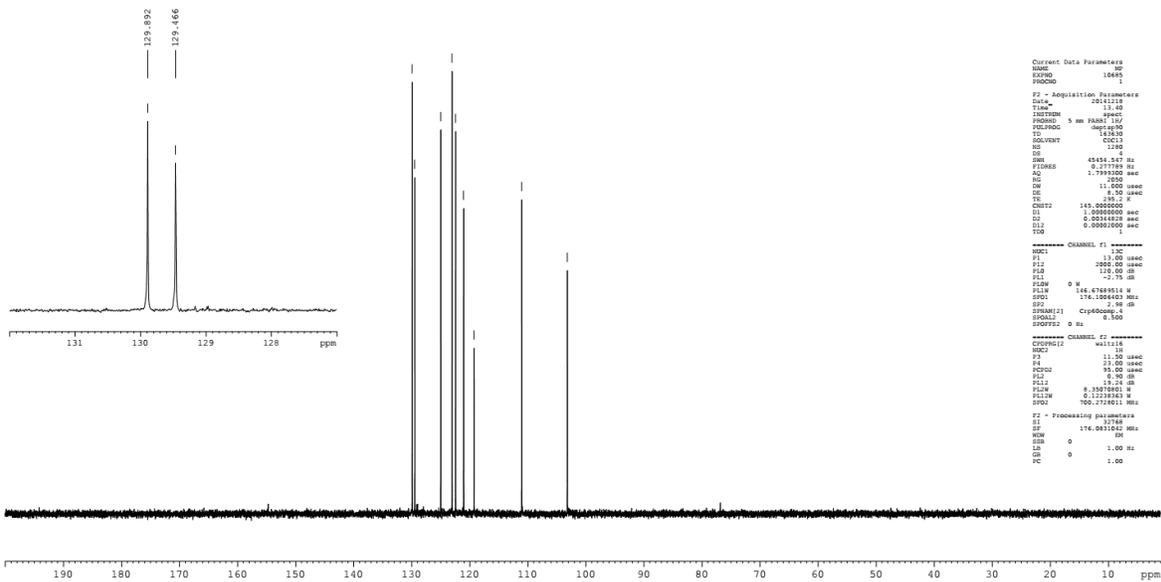
***** CHANNEL f2 *****
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL2W 0.00000000 W
PL3 20.00 dB
PL3W 8.36788000 W
PL1W 0.1278893 W
PL2W 0.1278893 W
SFO2 700.278011 MHz

F2 - Processing parameters
SI 32768
SF 176.081042 MHz
WDW EM
SSB 0 Hz
LB 1.00 Hz
GB 0 Hz
PC 1.00

129.892
129.896
129.896
123.046
122.439
119.052
119.289
111.033
103.189



DEPT90

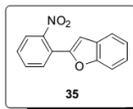
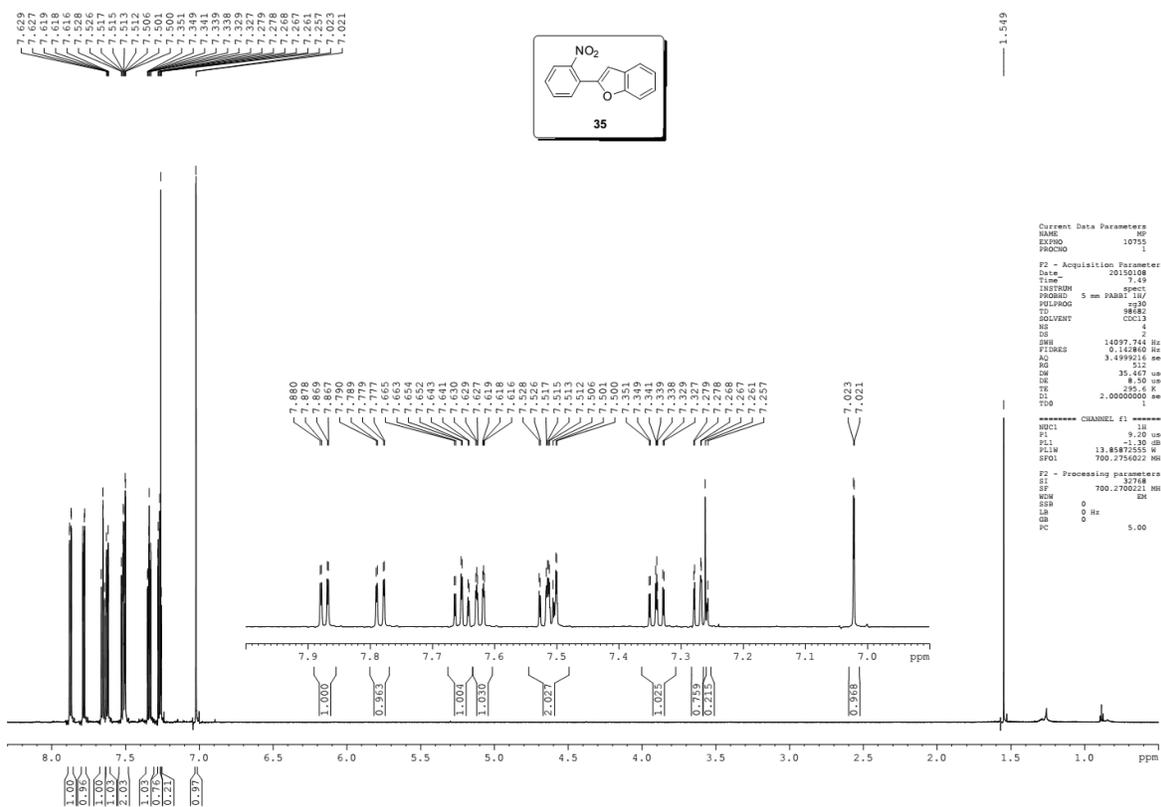


```

Current Data Parameters
NAME      1075
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20111218
Time     13:40
INSTRUM  spect
PROBHD   5 mm PABBI 1H/
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        4
DS        4
SWH       14097.744 Hz
FIDRES   0.142860 Hz
AQ        3.4999216 sec
RG        512
DE        8.50 usec
TE        30.403 usec
DQ        29.6 usec
DI        2.00000000 sec
TDI       1
===== CHANNEL f1 =====
NUC1      13C
P1        13.00 usec
PL1       0.00 dB
PL12      120.00 dB
PL13      -7.00 dB
PULSE    o w
PC        146.6788914 W
SFO1     176.1824000 MHz
SSB       0
SF02     700.2756022 MHz
===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2      1H
P2        11.00 usec
PL2       0.00 dB
PL22      95.00 dB
PL23      0.00 dB
PL24      0.00 dB
PL25      8.33570900 W
PULSE    zgpg30
PC        0.1219788 usec
SF02     700.2756022 MHz

F2 - Processing parameters
SI        32768
SF        176.1824000 MHz
WDW       EM
SSB       0
LB        0.00 Hz
GB        0
PC        1.00
  
```

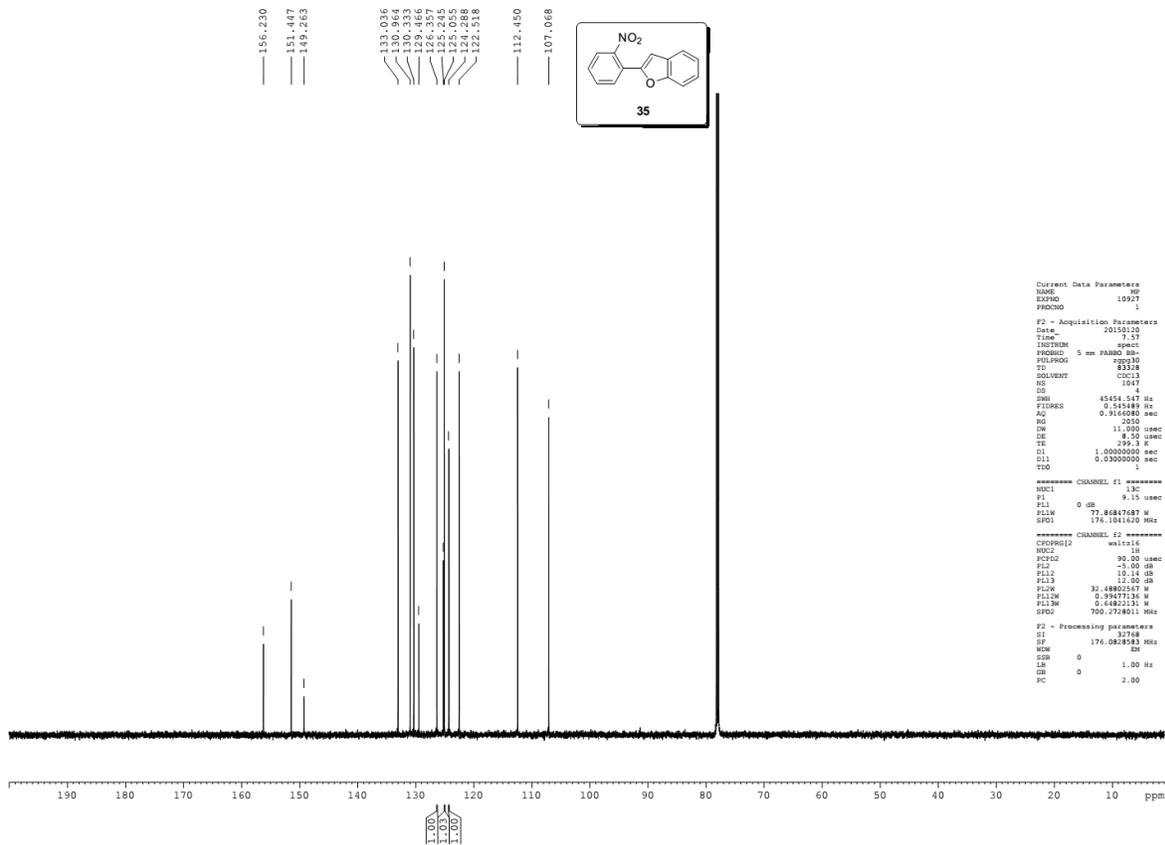


```

Current Data Parameters
NAME      1075
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20150108
Time     7:49
INSTRUM  spect
PROBHD   5 mm PABBI 1H/
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        4
DS        4
SWH       14097.744 Hz
FIDRES   0.142860 Hz
AQ        3.4999216 sec
RG        512
DE        8.50 usec
TE        30.403 usec
DQ        29.6 usec
DI        2.00000000 sec
TDI       1
===== CHANNEL f1 =====
NUC1      1H
P1        9.30 usec
PL1       -1.30 dB
PL12      13.85873555 W
PL13      700.2756022 MHz
===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2      13C
P2        11.00 usec
PL2       0.00 dB
PL22      95.00 dB
PL23      0.00 dB
PL24      0.00 dB
PL25      8.33570900 W
PULSE    zgpg30
PC        0.1219788 usec
SF02     700.2756022 MHz

F2 - Processing parameters
SI        32768
SF        176.1824000 MHz
WDW       EM
SSB       0
LB        0.00 Hz
GB        0
PC        5.00
  
```



```

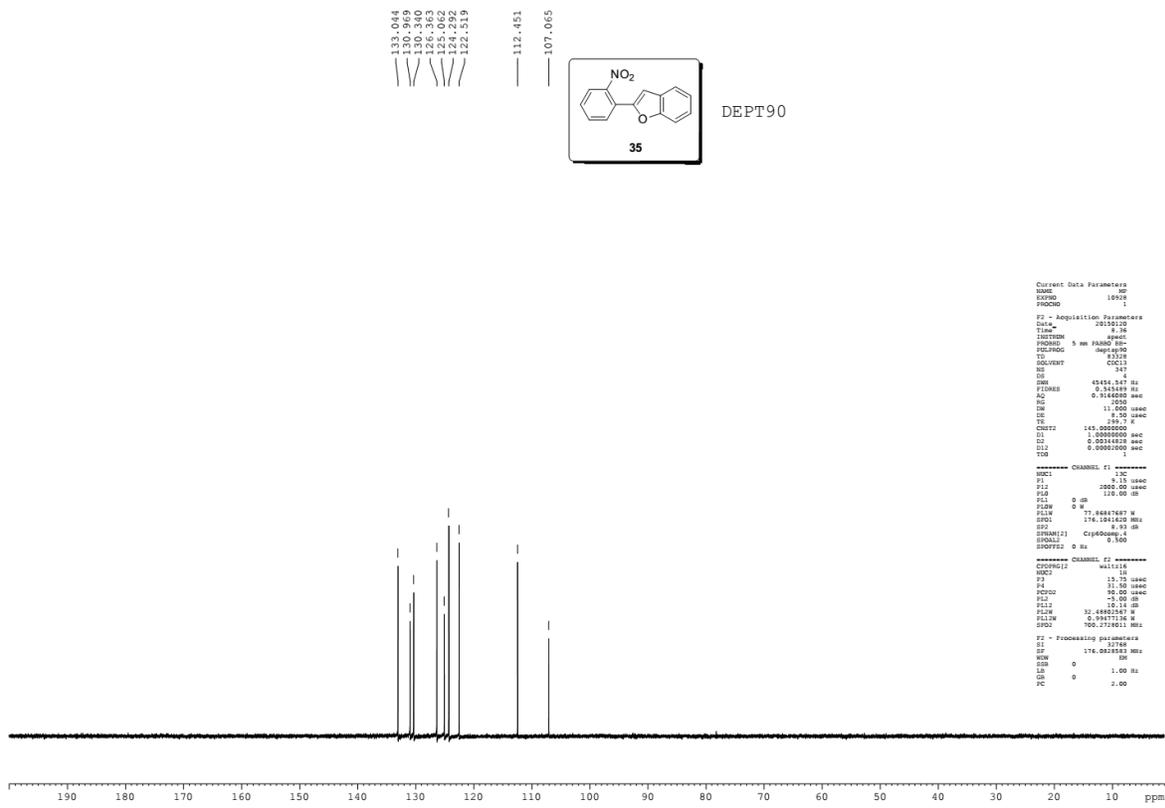
Current Data Parameters
NAME      35
EXPNO    10977
PROCNO    1

F2 - Acquisition Parameters
Date_     20150120
Time      7.57
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         83378
SOLVENT   CDCl3
NS         1047
DS         4
SMBR      45454.547 Hz
FIDRES    0.363488 Hz
AQ         0.916080 sec
RG         3000
DM         11.000 usec
DE         8.25 usec
TE         297.2 K
D1         1.00000000 sec
D11        0.03000000 sec
TD0

===== CHANNEL f1 =====
NUC1       13C
P1         9.15 usec
PL1        0 dB
PL1W       77.86847687 W
SFO1       176.1041620 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2        1H
PCPD2      90.00 usec
PL2         0.00 dB
PL12        10.14 dB
PL13         0.00 dB
PL1W        32.48802567 W
PL1W2       0.39877136 W
PL1W3       0.44821311 W
SFO2       700.770811 MHz

F2 - Processing parameters
SI         32768
SF         176.0828183 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         2.00
  
```



```

Current Data Parameters
NAME      35
EXPNO    19958
PROCNO    1

F2 - Acquisition Parameters
Date_     20150120
Time      8.16
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         83378
SOLVENT   CDCl3
NS         341
DS         4
SMBR      45454.547 Hz
FIDRES    0.363488 Hz
AQ         0.916080 sec
RG         3000
DM         11.000 usec
DE         8.25 usec
TE         297.2 K
D1         1.00000000 sec
D11        0.03000000 sec
TD0

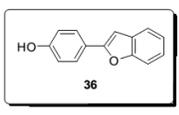
===== CHANNEL f1 =====
NUC1       13C
P1         9.15 usec
PL1        0 dB
PL1W       77.86847687 W
SFO1       176.1041620 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2        1H
PCPD2      90.00 usec
PL2         0.00 dB
PL12        10.14 dB
PL13         0.00 dB
PL1W        32.48802567 W
PL1W2       0.39877136 W
PL1W3       0.44821311 W
SFO2       700.770811 MHz

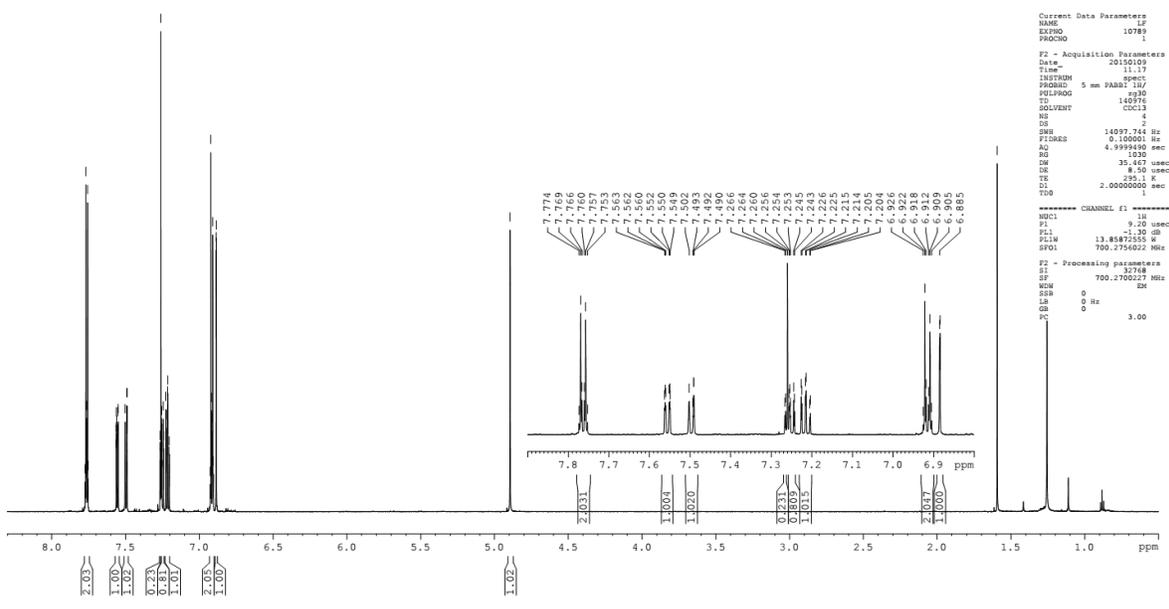
F2 - Processing parameters
SI         32768
SF         176.0828183 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         2.00
  
```

7.550
7.550
7.549
7.493
7.492
7.490
7.264
7.260
7.254
7.253
7.245
7.226
7.225
7.214
7.205
7.204
6.918
6.907
6.905
6.885

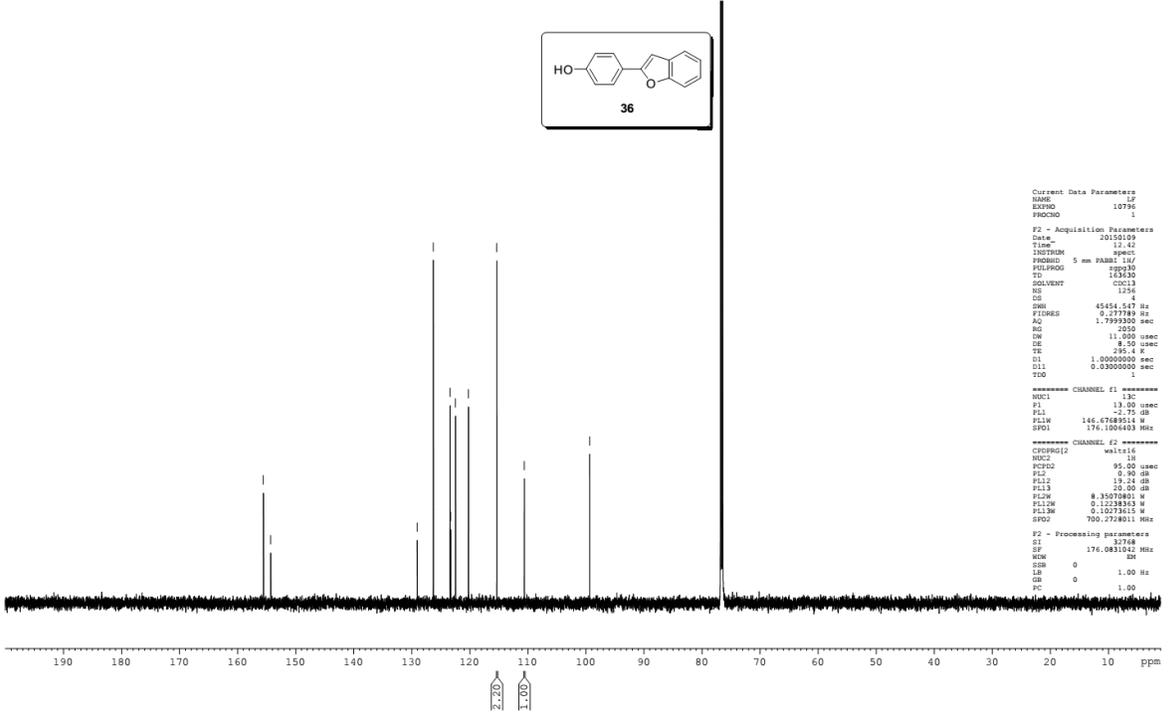
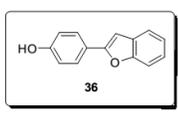
4.894

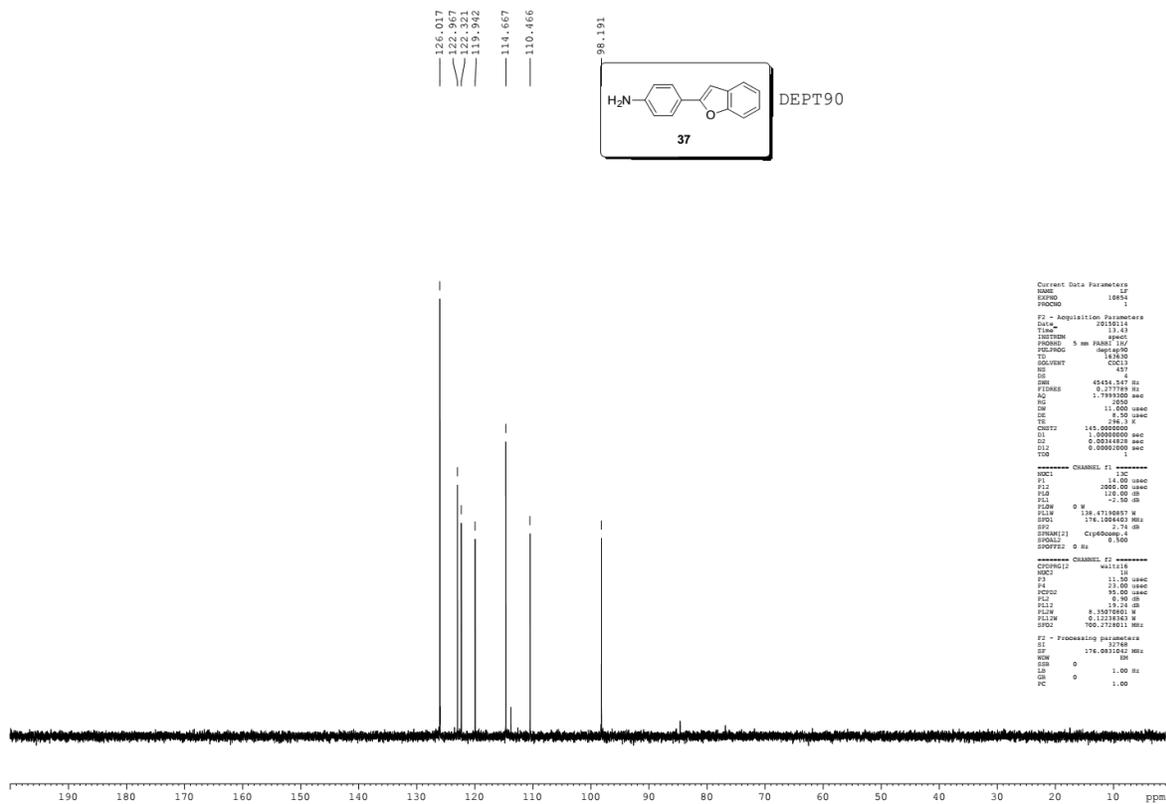
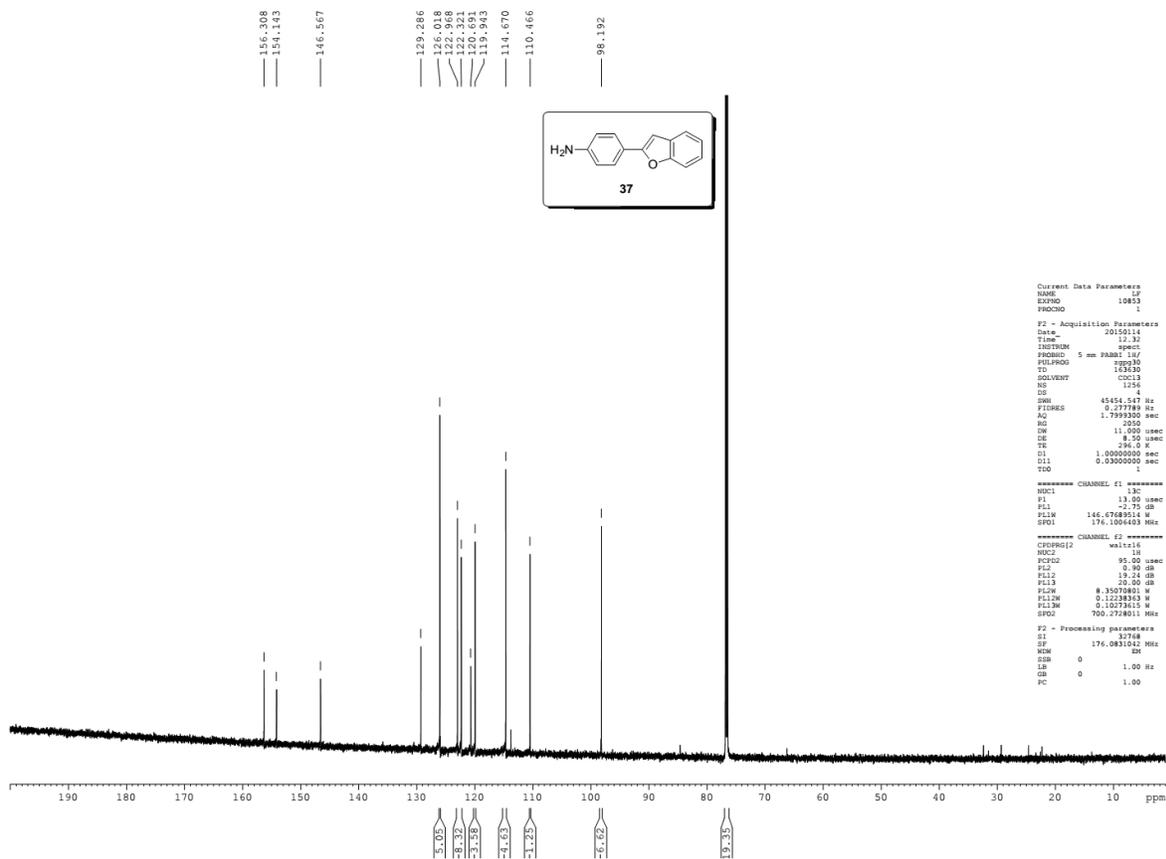


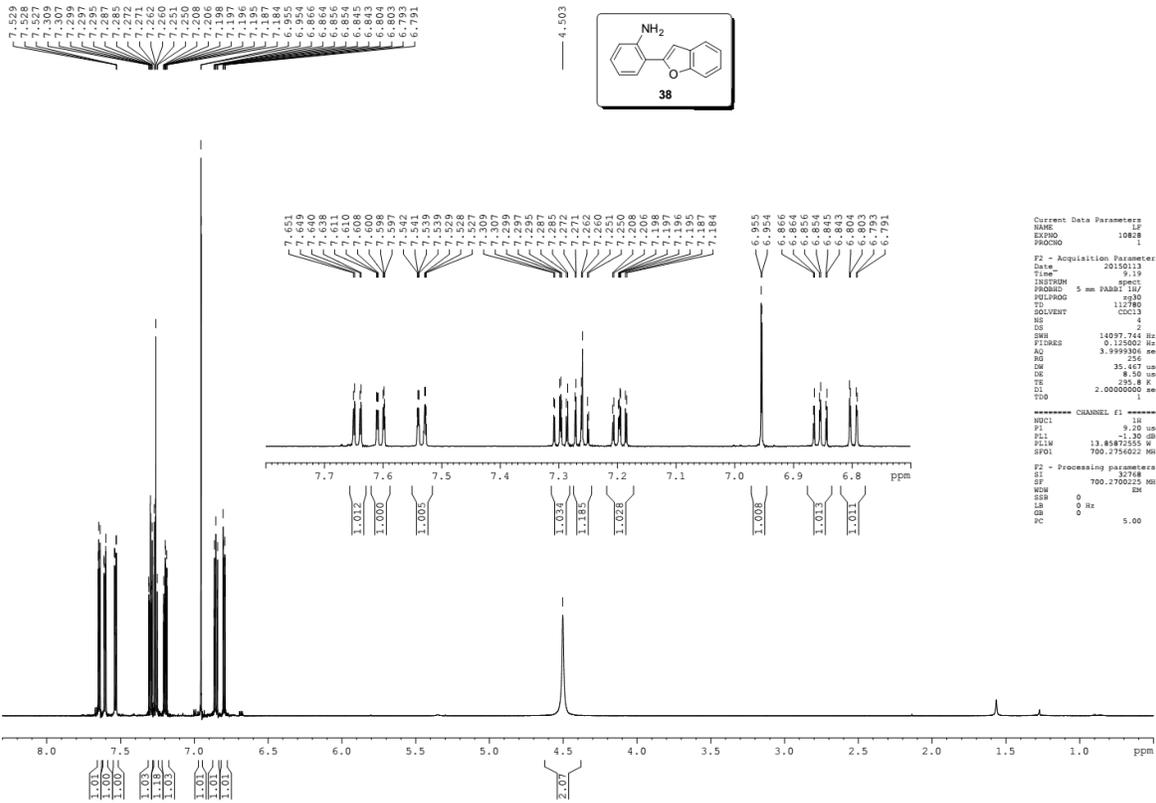
1.593



155.540
154.283
129.042
126.276
123.401
122.455
120.210
115.350
110.605
99.333







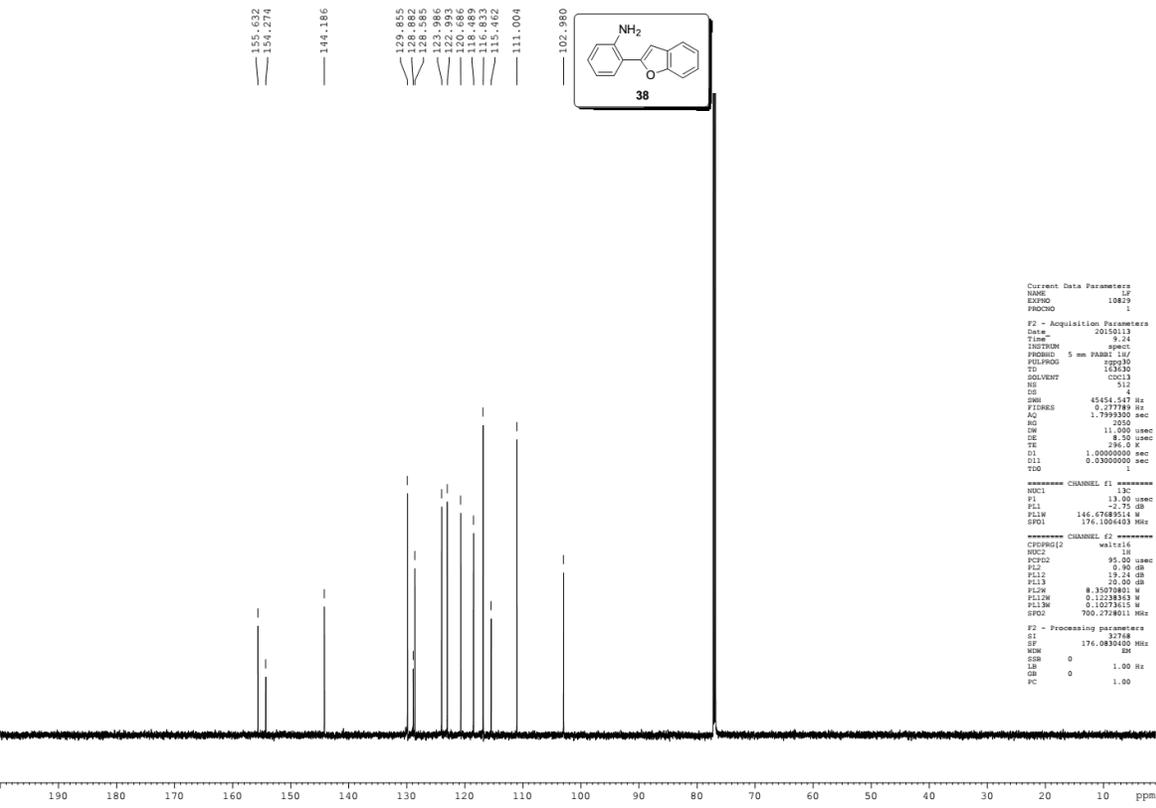
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Current Data Parameters
NAME          LF
EXPNO        1082
PROCNO       1

F2 - Acquisition Parameters
Date_         20150113
Time_        9.19
INSTRUM      spect
PROBHD      5 mm PABBI 1H/
PULPROG     zgpg30
TD           65536
SOLVENT     CDCl3
NS           4
DS           2
SWS         14097.744 Hz
FIDRES      0.125000 Hz
AQ          3.9999306 sec
RG          256
DM          35.467 usec
DE          8.50 usec
TE          295.8 K
D1          2.0000000 sec
TD0         1

===== CHANNEL f1 =====
NUC1         1H
P1           9.00 usec
PL1         -1.20 dB
PL1W        13.8847355 W
SFO1        700.2754022 MHz

F2 - Processing parameters
SI           32768
SF          700.2700225 MHz
WDW          EM
SSB          0
GB           0 Hz
PC          5.00
  
```



```

Current Data Parameters
NAME          LF
EXPNO        1082
PROCNO       1

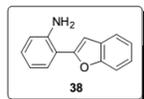
F2 - Acquisition Parameters
Date_         20150113
Time_        9.24
INSTRUM      spect
PROBHD      5 mm PABBI 1H/
PULPROG     zgpg30
TD           65536
SOLVENT     CDCl3
NS           4
DS           2
SWS         45454.547 Hz
FIDRES      0.277788 Hz
AQ          1.7999306 sec
RG          256
DM          11.900 usec
DE          8.50 usec
TE          295.8 K
D1          1.0000000 sec
D11         0.3300000 sec
TD0         1

===== CHANNEL f1 =====
NUC1         13C
P1          13.00 usec
PL1         -2.75 dB
PL1W        146.47689514 W
SFO1        176.1004403 MHz

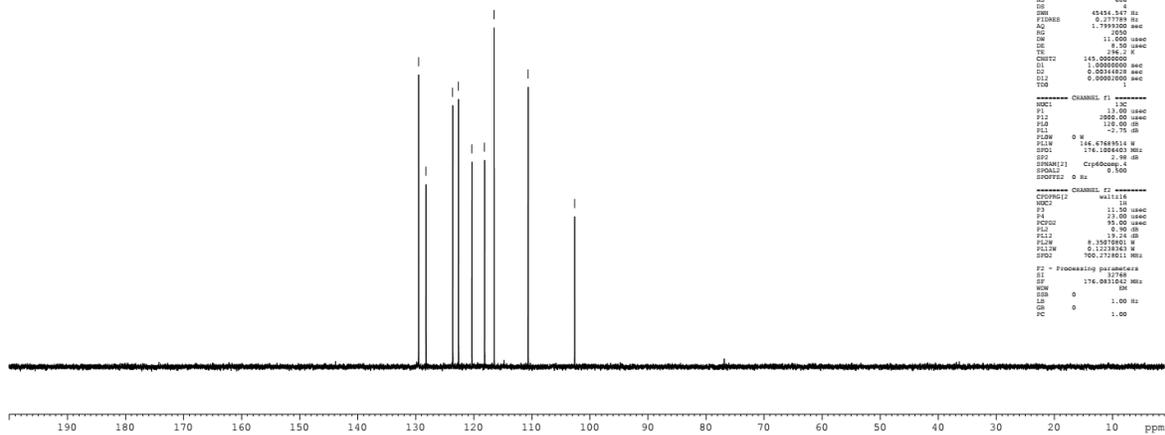
===== CHANNEL f2 =====
CPDPRG2     waltz16
NUC2         1H
PCPD2       90.00 usec
PL2         19.00 dB
PL2W        8.3838000 W
SFO2        400.1417701 MHz
PL1W        8.3838000 W
PL2W        0.12238363 W
PL1W2       0.1073811 W
SFO2        700.2728011 MHz

F2 - Processing parameters
SI           32768
SF          176.0830400 MHz
WDW          EM
SSB          0
GB           0 Hz
PC          1.00
  
```

129.490
128.217
123.621
122.628
118.321
116.468
110.639
102.616



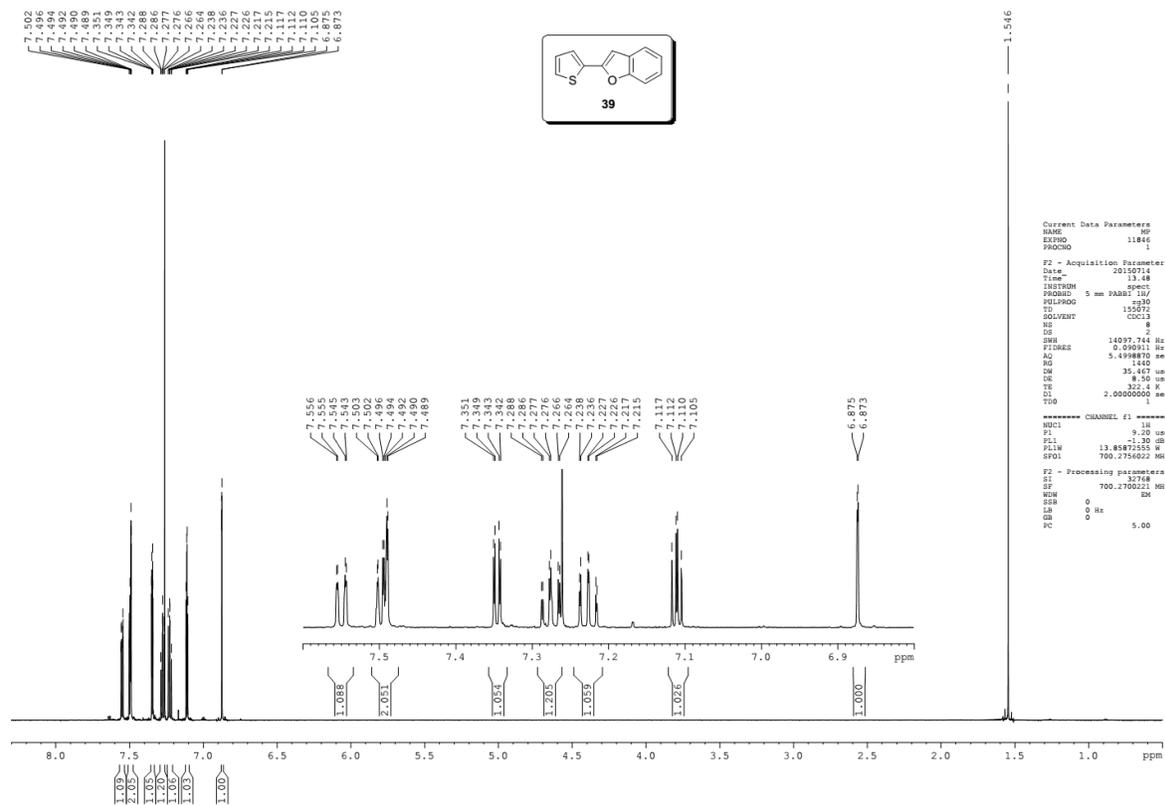
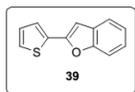
DEPT90



```

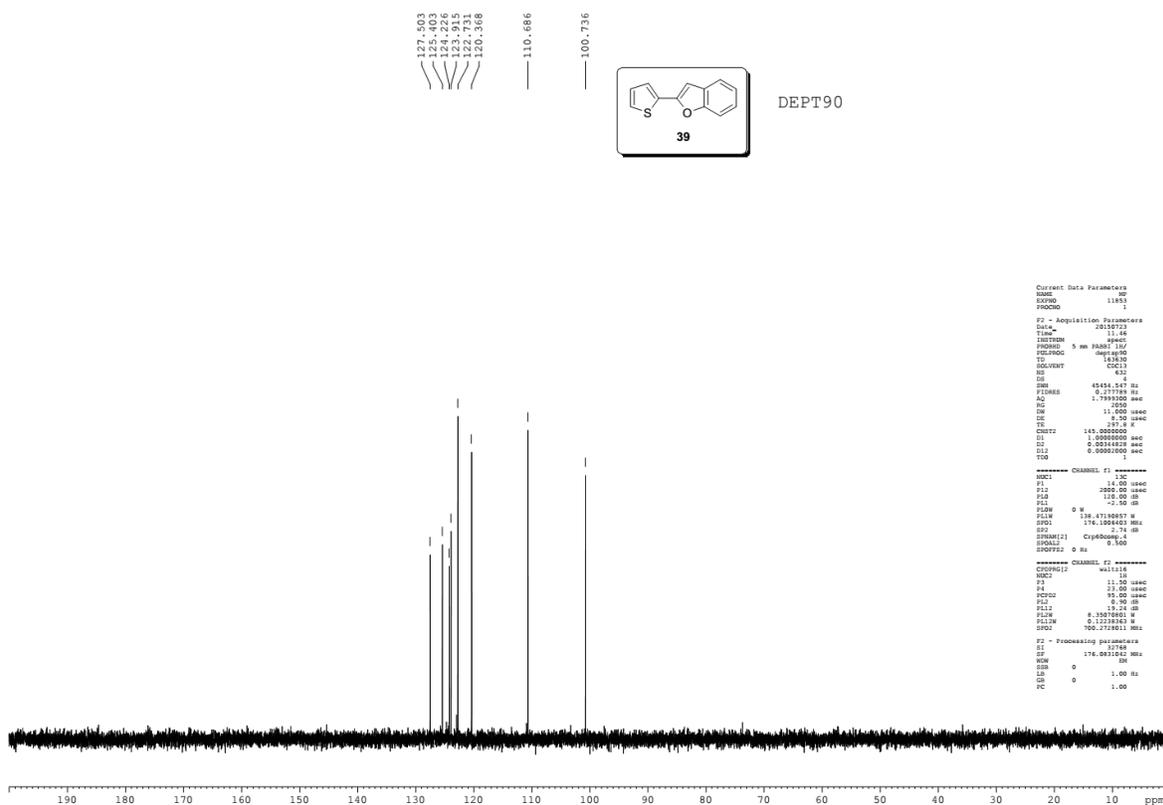
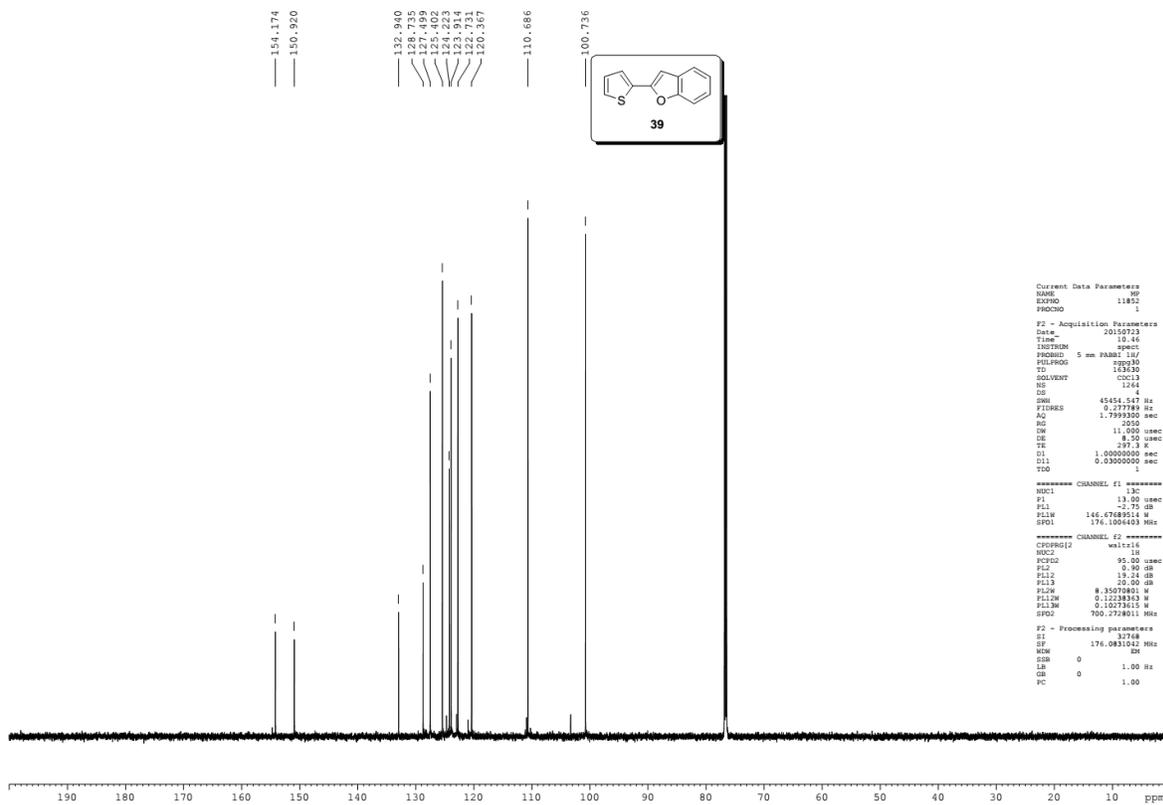
Current Data Parameters
NAME      RP
EXPNO    1
PROCNO   1
F2 - Acquisition Parameters
Date_    20150113
Time     9:28
INSTRUM  spect
PROBHD   5 mm PABBI 1H/
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        8
DS        4
SWH       14097.744 Hz
FIDRES    0.090311 Hz
AQ        5.4998810 sec
RG        321.410
DE        8.50 usec
TE        300.2 K
D1        2.00000000 sec
D11       0.00000000 sec
TD0       0.00001000 sec
===== CHANNEL f1 =====
NUC1      13C
P1        13.00 usec
PL1       0.00 dB
PC1       1.00 usec
PULSE    zgpg30
SFO1     101.25318 MHz
===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2      1H
P2        11.00 usec
PL2       0.00 dB
PC2       1.00 usec
PULSE    zgpg30
SFO2     500.13643 MHz
F2 - Processing parameters
SI        32768
SF        700.146400 MHz
WDW       EM
SSB       0
LB        0.00 Hz
GB        0
PC        1.00
  
```

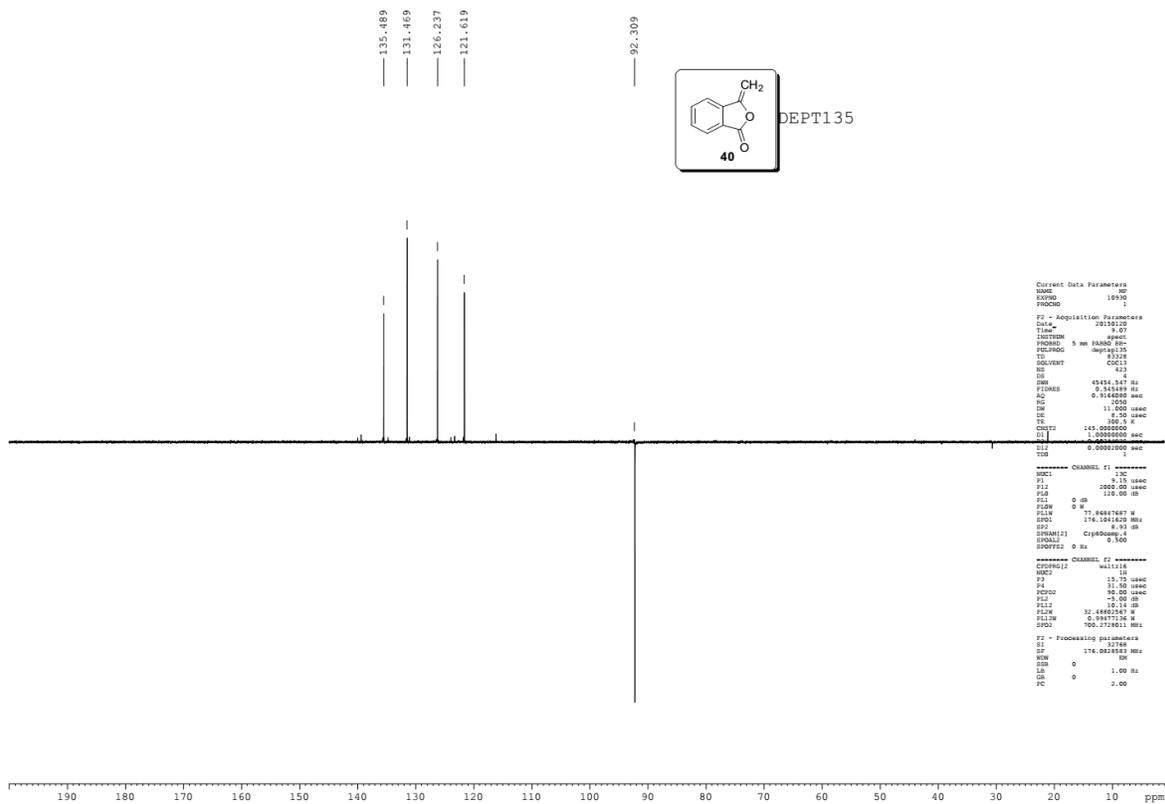
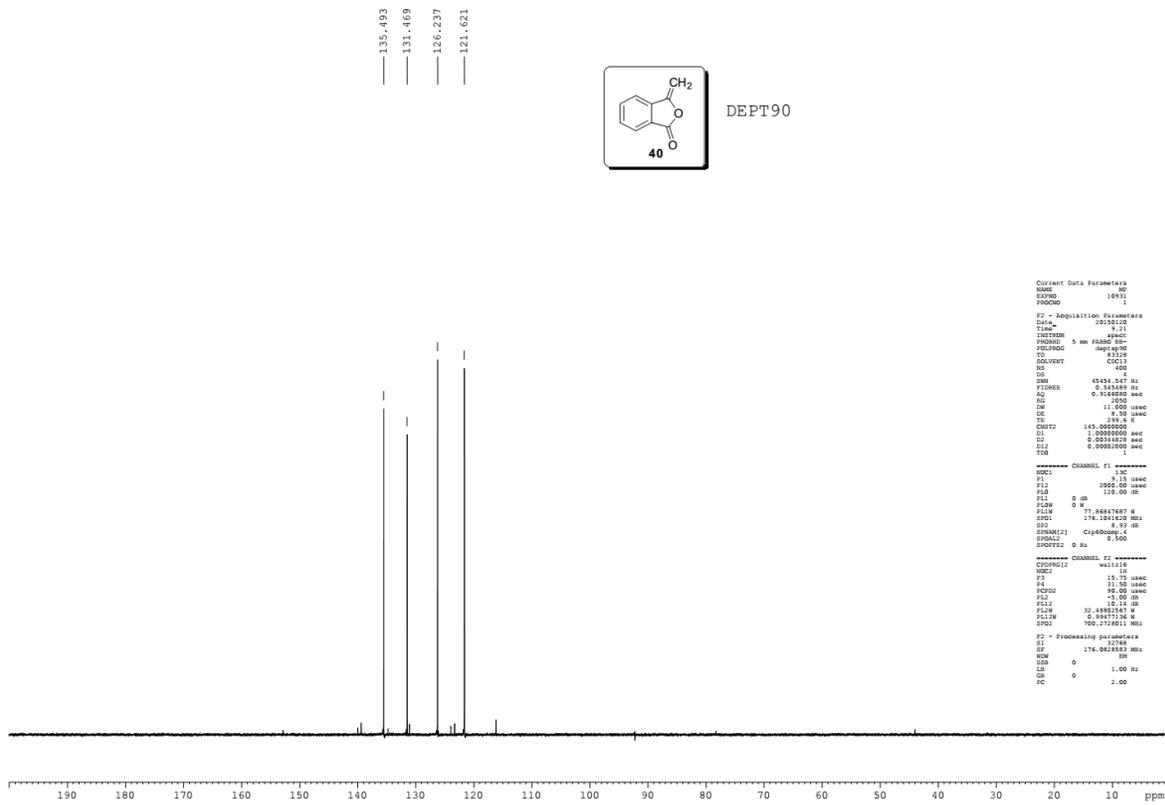
7.502
7.494
7.452
7.448
7.439
7.351
7.349
7.288
7.286
7.277
7.276
7.266
7.258
7.236
7.227
7.227
7.217
7.215
7.112
7.110
7.105
6.873



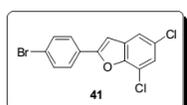
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Current Data Parameters
NAME      RP
EXPNO    1
PROCNO   1
F2 - Acquisition Parameters
Date_    20150714
Time     13:48
INSTRUM  spect
PROBHD   5 mm PABBI 1H/
PULPROG  zgpg30
TD        155072
SOLVENT  CDCl3
NS        8
DS        4
SWH       14097.744 Hz
FIDRES    0.090311 Hz
AQ        5.4998810 sec
RG        321.410
DE        8.50 usec
TE        300.2 K
D1        2.00000000 sec
D11       0.00000000 sec
TD0       0.00001000 sec
===== CHANNEL f1 =====
NUC1      1H
P1        9.30 usec
PL1       -1.30 dB
PC1       1.00 usec
PULSE    zgpg30
SFO1     500.13643 MHz
===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2      13C
P2        11.00 usec
PL2       0.00 dB
PC2       1.00 usec
PULSE    zgpg30
SFO2     101.25318 MHz
F2 - Processing parameters
SI        32768
SF        700.146400 MHz
WDW       EM
SSB       0
LB        0.00 Hz
GB        0
PC        1.00
  
```

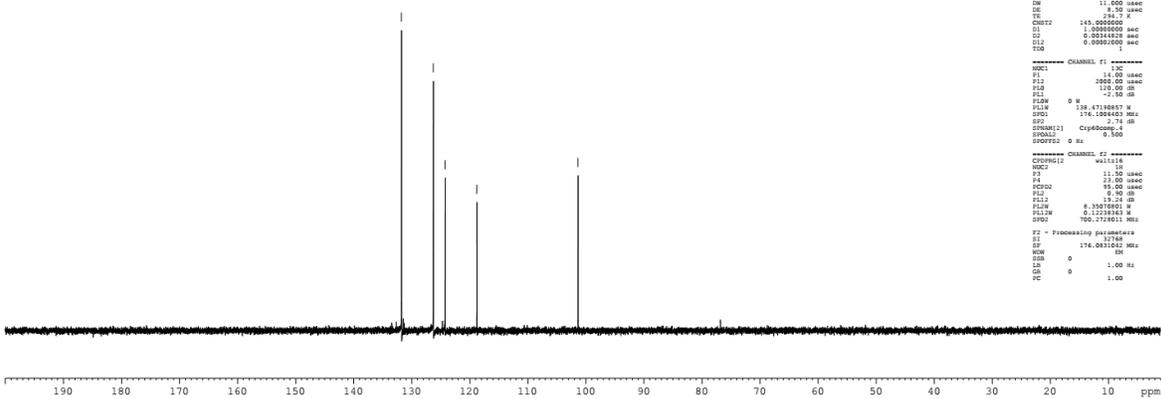




131.752
 126.268
 124.244
 118.761
 101.343



DEPT90



```

Current Data Parameters
NAME
EXPNO 1640
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111216
Time 14:13
INSTRUM spect
PROBHD 5 mm PABBO
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 371
DS 4
SWH 6431.742 Hz
AQ 0.779700 sec
RG 1050
RM 11.000 usec
DE 8.50 usec
TE 300.2
CHPZ 140.000000
DI 1.0000000 sec
DQ 0.0001000 sec
D12 0.00001000 sec
TD0
===== CHANNEL f1 =====
NUC1 13C
P1 14.00 usec
PL1 2000.00 usec
P2 110.00 usec
PL2 0.00 usec
PULSE O W
PL1W 138.4718097 W
SFO 176.1824000 MHz
SD 2.74 usec
SFO2 Ccp600MHz
SH100
SFOFF2 0 Hz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 13C
P3 11.00 usec
PL3 0.00 usec
PCPD 95.00 usec
P4 0.00 usec
PL4 0.00 usec
PL12 8.3367000 W
PULSE O W
PL1W 700.7118011 MHz
SFO 176.1824000 MHz
SD 1.00 usec
SFO2 700.7118011 MHz
F2 - Processing parameters
SI 32768
SF 176.182400 MHz
WDW EM
SSB 0
GB 0
AR 1.00 Hz
DR 0
FC 1.00
  
```

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