

Supporting Informations

Benzylamine as arylcarboxy surrogate: A copper catalysed *o*-benzoylation of 2-phenylpyridines using benzyl amines

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General information:

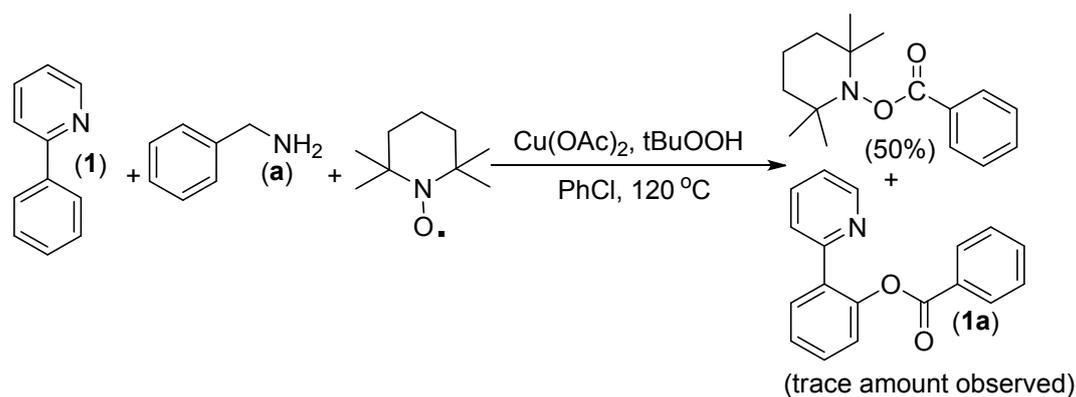
All the reagents were commercial grade and purified according to the established procedures. Organic extracts were dried over anhydrous sodium sulphate. Solvents were removed in a rotary evaporator under reduced pressure. Silica gel (60–120 mesh size) was used for the column chromatography. Reactions were monitored by TLC on silica gel 60 F₂₅₄ (0.25 mm). NMR spectra were recorded in CDCl₃ with tetramethylsilane as the internal standard for ¹H NMR (400 and 600 MHz) CDCl₃ solvent as the internal standard for ¹³C NMR (100 and 150 MHz). Mass spectra were recorded using WATERS MS system, Q-tof premier and data analyzed using Mass Lynx 4.1. IR spectra were recorded in KBr or neat on a Nicolet Impact 410 spectrophotometer.

General Procedure for the Synthesis of 2-(Pyridin-2-yl)phenyl benzoate (1a):

A mixture of 2-phenylpyridine (**1**) (77.5 mg, 0.5 mmol), Cu(OAc)₂ (18 mg, 20 mol %), benzylamine (**a**) (107 mg, 1 mmol) in chlorobenzene (2 mL) were taken in an oven dried round bottom flask fitted with a reflux condenser. To this mixture a decane solution of TBHP

(5–6 M) (1200 μ L, 6 equivalent with respect to benzylamine) was added and the reaction mixture was heated in an oil bath at 120 °C for 16 h. The reaction mixture was cooled to room temperature and admixed with ethyl acetate (15 mL) and the residual particles were filtered through a filter paper which was washed with ethyl acetate (2 x 2.5 mL). The ethyl acetate layer was washed with a 5% solution of sodium bicarbonate (2 x 5 mL) and water (2 x 5 mL) and the organic layer was dried over anhydrous Na_2SO_4 and the solvent was evaporated under reduced pressure. The crude product was purified over a column of silica gel and eluted with (92:8, hexane/ethyl acetate) to afford 2-(pyridine-2-yl)phenyl benzoate (**1a**) (89 mg, 65% yield).

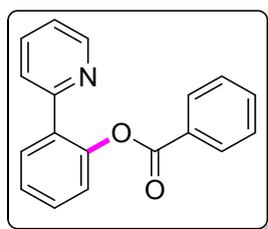
Mechanistic investigation in the presence of radical scavenger TEMPO: An oven-dried round bottom flask fitted with a reflux condenser was charged with 2-phenylpyridine (**1**) (77.5 mg, 0.5 mmol), benzylamine (**a**) (54 mg, 0.5 mmol), $\text{Cu}(\text{OAc})_2$ (18 mg, 0.1 mmol), TBHP in decane (5–6 M) (600 μ L, 6 equivalent with respect to benzylamine), TEMPO (78 mg, 0.5 mmol) in chlorobenzene (1 mL). The resultant reaction mixture was stirred in a preheated oil bath at 120 °C for 15 h. The reaction mixture was cooled to room temperature and admixed with ethyl acetate (15 mL) and the residual particles were filtered through a filter paper which was washed with ethyl acetate (2 x 2.5 mL). The ethyl acetate layer was washed with a 5% solution of sodium bicarbonate (2 x 5 mL) and water (2 x 5 mL) and the organic layer was dried over anhydrous Na_2SO_4 and the solvent was evaporated under reduced pressure. The crude product was purified over a column of silica gel which afforded the benzoyl-TEMPO adduct 2,2,6,6-tetramethylpiperidin-1-yl benzoate (**F**) (65 mg, 50% yield) and traces (<6%) of the desired product (**1a**) was observed. This experiment supports the formation of benzoyl radical (**B'**) in the medium from benzylamine.



Scheme S1: Trapping the intermediate with TEMPO

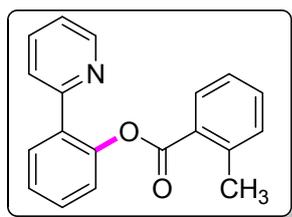
Spectral Data

2-(Pyridine-2-yl)phenyl benzoate (1a):



^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.14–7.17 (m, 1H), 7.29–7.32 (m, 1H), 7.38–7.43 (m, 2H), 7.45–7.48 (m, 2H), 7.55–7.64 (m, 3H), 7.77–7.79 (m, 1H), 8.07–8.09 (m, 2H), 8.59–8.60 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 122.3, 123.5, 123.9, 126.6, 128.7, 129.7, 129.9, 130.3, 131.1, 133.5, 133.6, 136.3, 148.5, 149.8, 155.8, 165.3; IR (KBr): 3442, 2918, 2853, 1736, 1634, 1585, 1446, 1262, 1194, 1061, 847, 754, 706, 614 cm^{-1} ; HRMS (ESI): calcd. for $\text{C}_{18}\text{H}_{13}\text{NO}_2$ (MH^+) 276.1019; found 276.1062.

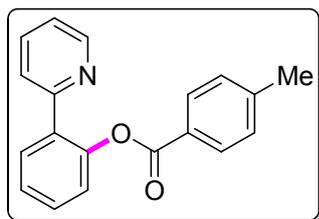
2-(Pyridin-2-yl)phenyl 2-methylbenzoate (1b):



^1H NMR (400 MHz, CDCl_3): δ (ppm) 2.53 (s, 3H), 7.17–7.20 (m, 1H), 7.25–7.30 (m, 3H), 7.38–7.51 (m, 3H), 7.54–7.57 (m, 1H), 7.60–7.67 (m, 1H), 7.74–7.77 (m, 1H), 7.98–8.02 (m,

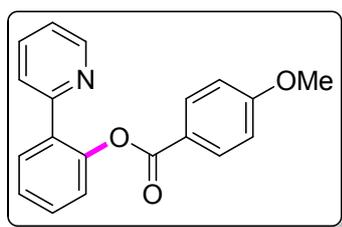
1H), 8.61–8.63 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 21.8, 122.3, 123.6, 123.9, 125.9, 126.5, 128.7, 129.9, 131.0, 131.2, 131.9, 132.7, 133.6, 136.4, 141.3, 148.5, 149.6, 155.9, 165.8; IR (KBr): 3062, 2962, 2856, 1743, 1585, 1492, 1467, 1426, 1289, 1250, 1197, 1115, 1040, 1021, 884, 794, 693, 616 cm^{-1} ; HRMS (ESI): calcd. for $\text{C}_{19}\text{H}_{15}\text{NO}_2$ (MH^+) 290.1176; found 290.1171.

2-(Pyridin-2-yl)phenyl 4-methylbenzoate (1c):

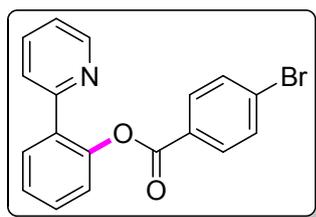


^1H NMR (400 MHz, CDCl_3): δ (ppm) 2.43 (s, 3H), 7.14–7.18 (m, 1H), 7.26 (d, 2H, $J = 8.0$ Hz), 7.29–7.31 (m, 1H), 7.38–7.42 (m, 1H), 7.46–7.50 (m, 1H), 7.54–7.57 (m, 1H), 7.60–7.64 (m, 1H), 7.77–7.80 (m, 1H), 7.96–7.98 (m, 2H), 8.60–8.62 (m, 1H); ^{13}C NMR (150 MHz, CDCl_3): δ (ppm) 21.9, 122.3, 123.6, 123.9, 126.5, 127.0, 129.4, 129.9, 130.4, 131.1, 133.6, 136.3, 144.5, 148.6, 149.8, 155.8, 165.4; IR (KBr): 3436, 2917, 1733, 1643, 1582, 1454, 1265, 1193, 1066, 985, 894, 748, 677 cm^{-1} ; HRMS (ESI): calcd. for $\text{C}_{19}\text{H}_{15}\text{NO}_2$ (MH^+) 290.1176; found 290.1167.

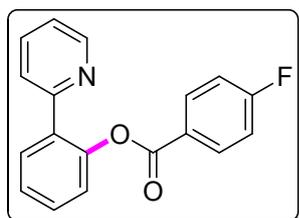
2-(Pyridin-2-yl)phenyl 4-methoxybenzoate (1d):



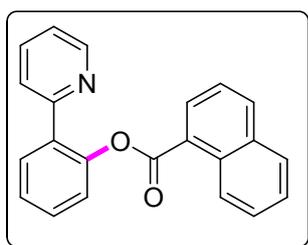
^1H NMR (400 MHz, CDCl_3): δ (ppm) 3.88 (s, 3H), 6.93 (d, 2H, $J = 9.2$ Hz), 7.15–7.18 (m, 1H), 7.28–7.31 (m, 1H), 7.37–7.41 (m, 1H), 7.46–7.50 (m, 1H), 7.56 (d, 1H, $J = 8.0$ Hz), 7.60–7.64 (m, 1H), 7.77–7.79 (m, 1H), 8.04 (d, 2H, $J = 8.8$ Hz), 8.62 (d, 1H, $J = 4.4$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 55.7, 113.9, 122.0, 122.3, 123.6, 124.0, 126.4, 129.9, 131.1, 132.5, 133.5, 136.3, 148.6, 149.8, 155.8, 164.0, 165.0; IR (KBr): 3413, 2925, 1731, 1605, 1511, 1463, 1254, 1166, 1067, 846, 752, 697, 572 cm^{-1} ; HRMS (ESI): calcd. for $\text{C}_{19}\text{H}_{15}\text{NO}_3$ (MH^+) 306.1125; found 306.1133.

2-(Pyridin-2-yl)phenyl 4-bromobenzoate (1e):

^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.15–7.18 (m, 1H), 7.29 (d, 1H, $J = 8.4$ Hz), 7.39–7.43 (m, 1H), 7.46–7.53 (m, 2H), 7.58–7.66 (m, 3H), 7.74–7.76 (m, 1H), 7.93 (d, 2H, $J = 8.8$ Hz), 8.56 (d, 1H, $J = 8.8$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 122.4, 123.4, 123.8, 126.7, 128.6, 128.7, 128.9, 130.3, 131.1, 131.8, 132.0, 136.4, 148.3, 149.7, 155.7, 164.7; IR (KBr): 3052, 2925, 2850, 1733, 1587, 1492, 1482, 1465, 1450, 1423, 1395, 1261, 1186, 1166, 1068, 1058, 1023, 1008, 849, 795, 761, 749 cm^{-1} ; HRMS (ESI): calcd. for $\text{C}_{18}\text{H}_{12}\text{BrNO}_2$ (MH^+) 354.0124; found 354.0117.

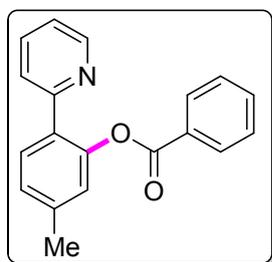
2-(Pyridin-2-yl)phenyl 4-fluorobenzoate (1f):

^1H NMR (600 MHz, CDCl_3): δ (ppm) 7.08–7.12 (m, 4H), 7.14–7.16 (m, 1H), 7.27–7.40 (m, 1H), 7.45–7.48 (m, 1H), 7.51 (d, 1H, $J = 7.8$ Hz), 7.60–7.75 (m, 1H), 8.06–8.09 (m, 2H), 8.56 (d, 1H, $J = 3.0$ Hz); ^{13}C NMR (150 MHz, CDCl_3): δ (ppm) 115.8, 116.0, 122.4, 123.5, 123.9, 126.0, 126.7, 130.0, 131.1, 132.9, 133.0, 133.5, 136.4, 148.4, 149.7, 155.8, 164.4, 165.4, 167.1; IR (KBr): 3419, 2929, 1739, 1633, 1501, 1462, 1263, 1193, 1068, 860, 753, 682, 573 cm^{-1} ; HRMS (ESI): calcd. for $\text{C}_{18}\text{H}_{12}\text{FNO}_2$ (MH^+) 294.0925; found 294.0965.

2-(Pyridin-2-yl)phenyl 1-naphthoate (1g):

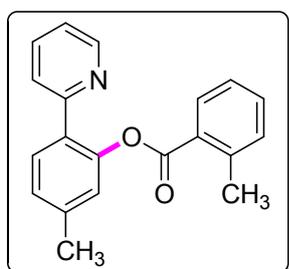
^1H NMR (600 MHz, CDCl_3): δ (ppm) 7.14–7.15 (m, 1H), 7.37 (d, 1H, $J = 7.8$ Hz), 7.42–7.44 (m, 1H), 7.49–7.55 (m, 3H), 7.56–7.63 (m, 2H), 7.78–7.79 (m, 2H), 7.89 (d, 1H, $J = 7.6$ Hz), 8.05 (d, 1H, $J = 7.8$ Hz), 8.30 (d, 1H, $J = 7.8$ Hz), 8.58–8.59 (m, 1H), 8.86 (d, 1H, $J = 8.4$ Hz); ^{13}C NMR (150 MHz, CDCl_3): δ (ppm) 122.4, 123.7, 123.9, 124.7, 125.9, 126.2, 126.5, 126.7, 128.2, 128.7, 130.0, 131.1, 131.2, 131.8, 133.8, 134.0, 134.2, 136.5, 148.6, 149.8, 156.1, 165.9; IR (KBr): 3058, 2919, 2846, 1732, 1602, 1586, 1509, 1493, 1471, 1463, 1452, 1425, 1276, 1240, 1186, 1120, 1059, 982, 885, 813, 780, 659, cm^{-1} ; HRMS (ESI): calcd. for $\text{C}_{22}\text{H}_{15}\text{NO}_2$ (MH^+) 326.1176; found 326.1179.

5-Methyl-2-(pyridin-2-yl)phenyl benzoate (2a):



^1H NMR (600 MHz, CDCl_3): δ (ppm) 2.43 (s, 3H), 7.12 (d, 2H, $J = 9.6$ Hz), 7.20 (d, 1H, $J = 7.2$ Hz), 7.45 (t, 2H, $J = 7.8$ Hz), 7.53 (d, 1H, $J = 7.8$ Hz), 7.57–7.60 (m, 2H), 7.68 (d, 1H, $J = 7.8$ Hz), 8.08–8.10 (m, 2H), 8.57 (d, 1H, $J = 4.8$ Hz); ^{13}C NMR (150 MHz, CDCl_3): δ (ppm) 21.4, 122.1, 123.7, 124.0, 127.5, 128.7, 129.8, 130.3, 130.6, 130.8, 133.6, 136.3, 140.4, 148.3, 149.7, 155.8, 165.5; IR (KBr): 3505, 2916, 1737, 1622, 1586, 1465, 1256, 1131, 1062, 892, 784, 707, 683, 545 cm^{-1} ; HRMS (ESI): calcd. for $\text{C}_{19}\text{H}_{15}\text{NO}_2$ (MH^+) 290.1176; found 290.1159.

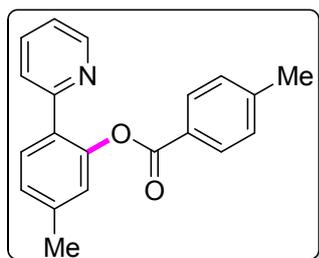
5-Methyl-2-(pyridin-2-yl)phenyl 2-methylbenzoate (2b):



^1H NMR (400 MHz, CDCl_3): δ (ppm) 2.43 (s, 3H), 2.53 (s, 3H), 7.09 (s, 1H), 7.11–7.15 (m, 1H), 7.18–7.25 (m, 3H), 7.40 (t, 1H, $J = 7.6$ Hz), 7.51–7.53 (m, 1H), 7.58–7.66 (m, 2H), 8.01

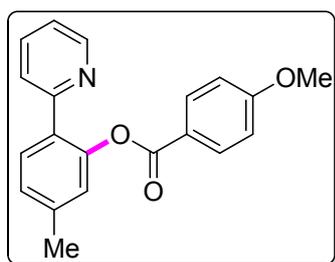
(d, 1H, $J = 7.6$ Hz), 8.57–8.59 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 21.4, 21.8, 122.1, 123.8, 124.0, 125.9, 127.4, 128.9, 130.8, 131.2, 131.9, 132.6, 136.3, 140.4, 141.3, 148.3, 149.7, 156.0, 166.0; IR (KBr) 3062, 2961, 2926, 1737, 1623, 1586, 1573, 1466, 1431, 1288, 1245, 1151, 1135, 1045, 893, 782, 736, 691 cm^{-1} ; HRMS (ESI): calcd. for $\text{C}_{20}\text{H}_{17}\text{NO}_2$ (MH^+) 304.1332; found 304.1335.

5-Methyl-2-(pyridin-2-yl)phenyl 4-methylbenzoate (2c):



^1H NMR (400 MHz, CDCl_3): δ (ppm) 2.428 (s, 3H), 2.434 (s, 3H), 7.11–7.15 (m, 1H), 7.20 (d, 1H, $J = 7.6$ Hz), 7.25 (d, 3H, $J = 6.8$ Hz), 7.53 (d, 1H, $J = 7.6$ Hz), 7.57–7.61 (m, 1H), 7.68 (d, 1H, $J = 8.0$ Hz), 7.97 (d, 2H, $J = 8.4$ Hz), 8.59 (d, 1H, $J = 4.4$ Hz); ^{13}C NMR (150 MHz, CDCl_3): δ (ppm) 21.4, 21.9, 122.1, 123.8, 124.0, 127.1, 127.4, 129.4, 130.4, 130.7, 130.9, 136.3, 140.4, 144.4, 148.4, 149.8, 155.9, 165.5; IR (KBr): 3442, 2923, 1735, 1612, 1586, 1464, 1257, 1130, 1069, 925, 831, 746, 668, 543 cm^{-1} ; HRMS (ESI): calcd. for $\text{C}_{20}\text{H}_{17}\text{NO}_2$ (MH^+) 304.1332; found 304.1348.

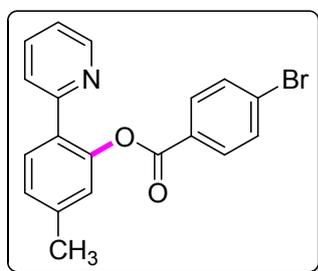
5-Methyl-2-(pyridin-2-yl)phenyl 4-methoxybenzoate (2d):



^1H NMR (600 MHz, CDCl_3): δ (ppm) 2.43 (s, 3H), 3.87 (s, 3H), 6.92–6.94 (m, 2H), 7.10–7.14 (m, 2H), 7.20 (d, 1H, $J = 7.8$ Hz), 7.53 (d, 1H, $J = 7.8$ Hz), 7.57–7.60 (m, 1H), 7.68 (d, 1H, $J = 7.8$ Hz), 8.03–8.05 (m, 2H), 8.59 (d, 1H, $J = 4.8$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 21.4, 55.7, 113.9, 122.0, 122.1, 123.8, 124.0, 127.3, 130.6, 130.8, 132.5, 136.2, 140.3, 148.4, 149.7, 155.9, 164.0, 165.2; IR (KBr): 3464, 2918, 1731, 1606, 1581,

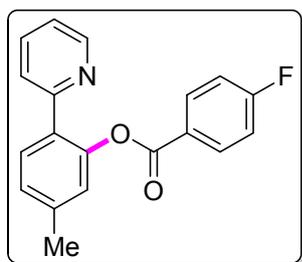
1464, 1254, 1167, 1069, 845, 774, 693, 569. cm^{-1} ; HRMS (ESI): calcd. for $\text{C}_{20}\text{H}_{17}\text{NO}_3$ (MH^+) 320.1281; found 320.1276.

5-Methyl-2-(pyridin-2-yl)phenyl 4-bromobenzoate (2e):

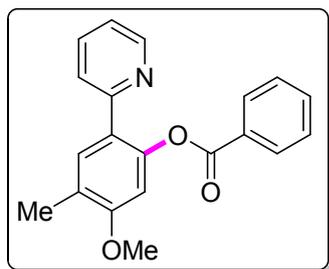


^1H NMR (400 MHz, CDCl_3): δ (ppm) 2.42 (s, 3H), 7.08–7.13 (m, 2H), 7.19 (d, 1H, $J = 8.0$ Hz), 7.47 (d, 1H, $J = 8.0$ Hz), 7.57 (d, 3H, $J = 8.8$ Hz), 7.63 (d, 1H, $J = 8.0$ Hz), 7.91 (d, 2H, $J = 8.8$ Hz), 8.51–8.52 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 21.4, 122.2, 123.6, 123.9, 127.6, 128.7, 128.8, 130.4, 130.8, 131.8, 132.0, 136.4, 140.5, 148.1, 149.7, 155.7, 164.8; IR (KBr): 2955, 2922, 2853, 1737, 1621, 1589, 1465, 1431, 1397, 1258, 1173, 1152, 1131, 1071, 1027, 1010, 783, 747, 678 cm^{-1} ; HRMS (ESI): calcd. for $\text{C}_{19}\text{H}_{14}\text{BrNO}_2$ (MH^+) 368.0281; found 368.0275.

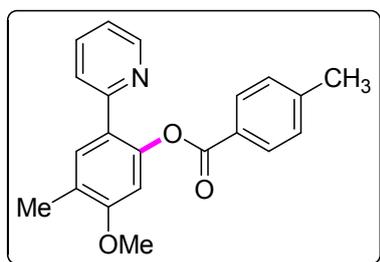
5-Methyl-2-(pyridin-2-yl)phenyl 4-fluorobenzoate (2f):



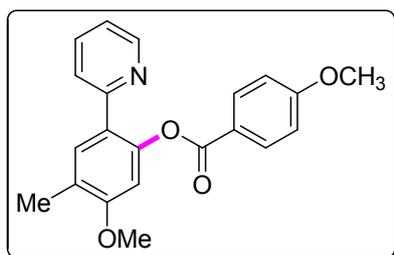
^1H NMR (600 MHz, CDCl_3): δ (ppm) 2.42 (s, 3H), 7.09–7.12 (m, 4H), 7.19 (d, 1H, $J = 8.4$ Hz), 7.49 (d, 1H, $J = 7.8$ Hz), 7.59 (t, 1H, $J = 7.2$ Hz), 7.64 (d, 1H, $J = 7.8$ Hz), 8.07–8.09 (m, 2H), 8.53 (d, 1H, $J = 4.8$ Hz); ^{13}C NMR (150 MHz, CDCl_3): δ (ppm) 21.4, 115.8, 115.9, 122.1, 123.9, 126.1, 127.6, 127.7, 130.6, 130.8, 132.9, 133.0, 136.4, 140.5, 148.2, 149.7, 155.9, 164.6, 165.4, 167.1; IR (KBr): 3722, 2920, 1739, 1604, 1507, 1226, 1151, 1071, 782, 684 cm^{-1} ; HRMS (ESI): calcd. for $\text{C}_{19}\text{H}_{17}\text{FNO}_2$ (MH^+) 308.1081; found 308.1073.

5-Methoxy-4-methyl-2-(pyridin-2-yl)phenyl benzoate (3a):

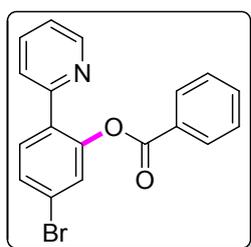
^1H NMR (400 MHz, CDCl_3): δ (ppm) 2.26 (s, 3H), 3.85 (s, 3H), 6.72 (s, 1H), 7.06–7.10 (m, 1H), 7.45 (t, 2H, $J = 7.6$ Hz), 7.49–7.53 (m, 1H), 7.55–7.61 (m, 3H), 8.08–8.10 (m, 2H), 8.55–8.56 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 16.0, 55.8, 105.4, 121.7, 123.6, 125.0, 125.2, 128.7, 129.8, 130.4, 132.3, 133.6, 136.2, 147.3, 149.7, 155.7, 158.8, 165.5; IR (KBr): 3443, 2925, 1736, 1618, 1589, 1464, 1260, 1143, 1060, 968, 890, 747, 612, 574 cm^{-1} ; HRMS (ESI): calcd. for $\text{C}_{20}\text{H}_{17}\text{NO}_3$ (MH^+) 320.1281; found 320.1293.

5-Methoxy-4-methyl-2-(pyridin-2-yl)phenyl 4-methylbenzoate (3c):

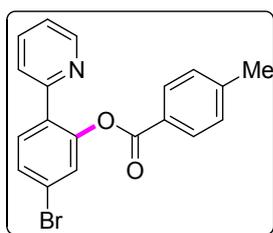
^1H NMR (400 MHz, CDCl_3): δ (ppm) 2.28 (s, 3H), 2.43 (s, 3H), 3.87 (s, 3H), 6.74 (s, 1H), 7.08–7.12 (m, 1H), 7.27 (d, 2H, $J = 8.0$ Hz), 7.51–7.58 (m, 2H), 7.61 (s, 1H), 8.00 (d, 2H, $J = 8.0$ Hz), 8.58 (d, 1H, $J = 4.4$ Hz); ^{13}C NMR (150 MHz, CDCl_3): δ (ppm) 16.0, 21.9, 55.8, 105.4, 121.7, 123.7, 125.0, 125.1, 127.0, 129.4, 130.5, 132.3, 136.2, 144.5, 147.3, 149.7, 155.7, 158.8, 165.6; IR (KBr): 3442, 2924, 1735, 1614, 1507, 1464, 1263, 1143, 1069, 968, 835, 747, 667, 571 cm^{-1} ; HRMS (ESI): calcd. for $\text{C}_{21}\text{H}_{19}\text{NO}_3$ (MH^+) 334.1438; found 334.1430.

5-Methoxy-4-methyl-2-(pyridin-2-yl)phenyl 4-methoxybenzoate (3d):

^1H NMR (400 MHz, CDCl_3): δ (ppm) 2.28 (s, 3H), 3.87 (s, 3H), 3.88 (s, 3H), 6.73 (s, 1H), 6.94 (d, 2H, $J = 9.2$ Hz), 7.10 (t, 1H, $J = 5.6$ Hz), 7.50–7.60 (m, 3H), 8.06 (d, 2H, $J = 9.2$ Hz), 8.59 (d, 1H, $J = 4.8$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 15.8, 55.5, 55.6, 105.2, 113.8, 121.5, 121.8, 123.5, 124.7, 124.8, 132.1, 132.3, 136.0, 147.1, 149.5, 155.5, 158.5, 163.8, 165.0; IR (KBr): 3402, 2922, 1730, 1606, 1511, 1464, 1256, 1167, 1069, 965, 895, 781, 610, 574 cm^{-1} ; HRMS (ESI): calcd. for $\text{C}_{21}\text{H}_{19}\text{NO}_4$ (MH^+) 350.1387; found 350.1356.

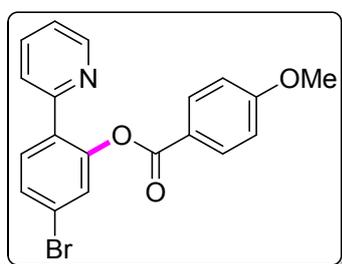
5-Bromo-2-(pyridin-2-yl)phenyl benzoate (4a):

^1H NMR (400 MHz, CDCl_3): δ (ppm) 7.14–7.17 (m, 1H), 7.43–7.48 (m, 3H), 7.51–7.53 (m, 2H), 7.57–7.63 (m, 2H), 7.66 (d, 1H, $J = 8.8$ Hz), 8.03–8.06 (m, 2H), 8.56–8.57 (m, 1H); ^{13}C NMR (150 MHz, CDCl_3): δ (ppm) 122.6, 122.9, 123.8, 126.9, 128.8, 129.2, 129.8, 130.4, 132.2, 132.6, 133.9, 136.5, 148.9, 149.9, 154.8, 164.9; IR (KBr): 3512, 2918, 1740, 1643, 1595, 1461, 1254, 1195, 1056, 868, 706, 551 cm^{-1} ; HRMS (ESI): calcd. for $\text{C}_{18}\text{H}_{12}\text{BrNO}_2$ (MH^+) 354.0124; found 354.0132.

5-Bromo-2-(pyridin-2-yl)phenyl 4-methylbenzoate (4c):

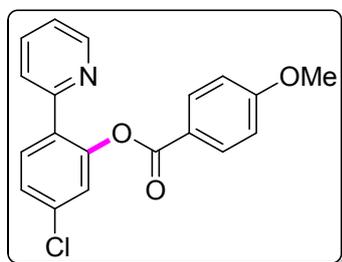
^1H NMR (600 MHz, CDCl_3): δ (ppm) 2.43 (s, 3H), 7.16–7.18 (m, 1H), 7.26 (d, 2H, $J = 7.8$ Hz), 7.490–7.493 (m, 1H), 7.52–7.54 (m, 2H), 7.59–7.63 (m, 1H), 7.69 (d, 1H, $J = 8.4$ Hz), 7.95 (d, 2H, $J = 7.8$ Hz), 8.60 (d, 1H, $J = 4.8$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 21.9, 122.6, 122.8, 123.8, 126.4, 126.9, 129.5, 129.7, 130.5, 132.2, 132.6, 136.5, 144.8, 148.9, 149.9, 154.8, 165.0; IR (KBr): 3438, 2917, 1738, 1612, 1595, 1462, 1259, 1176, 1061, 987, 830, 744, 668, 545 cm^{-1} ; HRMS (ESI): calcd. for $\text{C}_{19}\text{H}_{14}\text{BrNO}_2$ (MH^+) 368.0281; found 368.0274.

5-Bromo-2-(pyridin-2-yl)phenyl 4-methoxybenzoate (4d):



^1H NMR (600 MHz, CDCl_3): δ (ppm) 3.87 (s, 3H), 6.92–6.94 (m, 2H), 7.16–7.18 (m, 1H), 7.486–7.489 (m, 1H), 7.51–7.54 (m, 2H), 7.59–7.63 (m, 1H), 7.68 (d, 1H, $J = 8.4$ Hz), 8.01–8.03 (m, 2H), 8.60 (d, 1H, $J = 4.2$ Hz); ^{13}C NMR (100 MHz, CDCl_3): δ (ppm) 55.7, 114.1, 121.4, 122.6, 122.8, 123.8, 126.9, 129.7, 132.2, 132.5, 132.6, 136.4, 149.1, 149.9, 154.8, 164.2, 164.6; IR (KBr): 3422, 2926, 1734, 1605, 1511, 1462, 1254, 1166, 1058, 874, 781, 692, 583 cm^{-1} ; HRMS (ESI): calcd. for $\text{C}_{19}\text{H}_{14}\text{BrNO}_3$ (MH^+) 384.0230; found 384.0259.

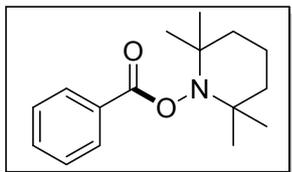
5-Chloro-2-(pyridin-2-yl)phenyl 4-methoxybenzoate (5d)



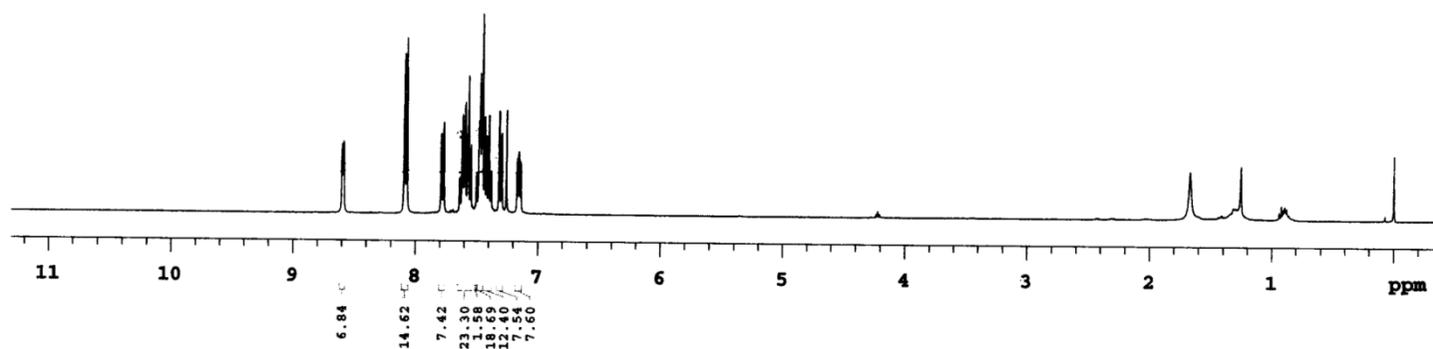
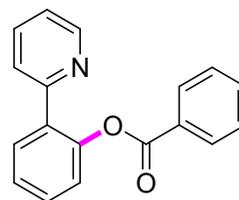
^1H NMR (400 MHz, CDCl_3): δ (ppm) 3.87 (s, 3H), 6.94 (d, 2H, $J = 8.8$ Hz), 7.16–7.19 (m, 1H), 7.34–7.38 (m, 2H), 7.53 (d, 1H, $J = 7.6$ Hz), 7.62 (t, 1H, $J = 7.2$ Hz), 7.75 (d, 1H, $J = 8.4$ Hz), 8.02 (d, 2H, $J = 8.8$ Hz), 8.61 (d, 1H, $J = 4.8$ Hz); ^{13}C NMR (150 MHz, CDCl_3): δ (ppm) 55.7, 114.1, 121.5, 122.6, 123.9, 124.1, 126.8, 131.9, 132.2, 132.6, 135.1, 136.4,

149.0, 149.9, 154.8, 164.2, 164.6; IR (KBr): 3442, 2924, 1733, 1604, 1461, 1253, 1166, 1059, 844, 762, 646, 587 cm^{-1} ; HRMS (ESI): calcd. for $\text{C}_{19}\text{H}_{14}\text{ClNO}_3$ (MH^+) 340.0735; found 340.0748.

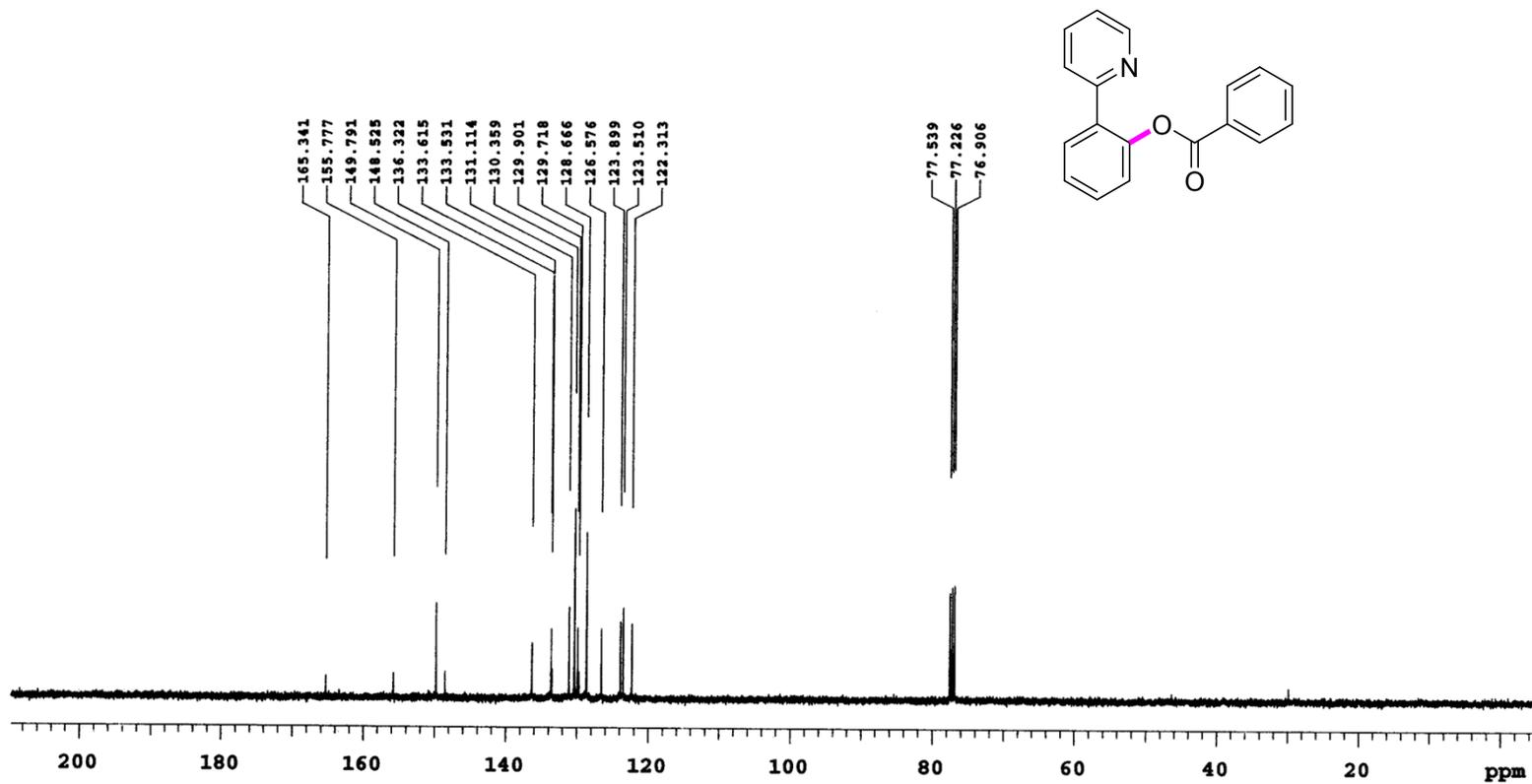
2,2,6,6-Tetramethylpiperidin-1-yl benzoate (F):



White solid; ^1H NMR (600 MHz, CDCl_3): δ (ppm) 1.12 (s, 6H), 1.26 (s, 6H), 1.42–1.45 (m, 1H), 1.55–1.58 (m, 2H), 1.66–1.78 (m, 3H), 7.43 (t, 2H, $J = 7.8$ Hz), 7.54 (t, 1H, $J = 7.8$ Hz), 8.03–8.06 (m, 2H); ^{13}C NMR (150 MHz, CDCl_3): δ (ppm) 17.2, 21.0, 32.1, 39.2, 60.6, 128.6, 129.7, 129.9, 133.0, 166.6; IR (KBr): 3007, 2973, 2940, 1741, 1641, 1452, 1365, 1253, 1238, 1083, 1062, 1026, 913, 718 cm^{-1} ; HRMS (ESI): calcd. for $\text{C}_{16}\text{H}_{23}\text{NO}_2$ (MH^+) 262.1802; found 262.1801.

2-(Pyridin-2-yl)phenyl benzoate (1a): ^1H NMR (400 MHz, CDCl_3)

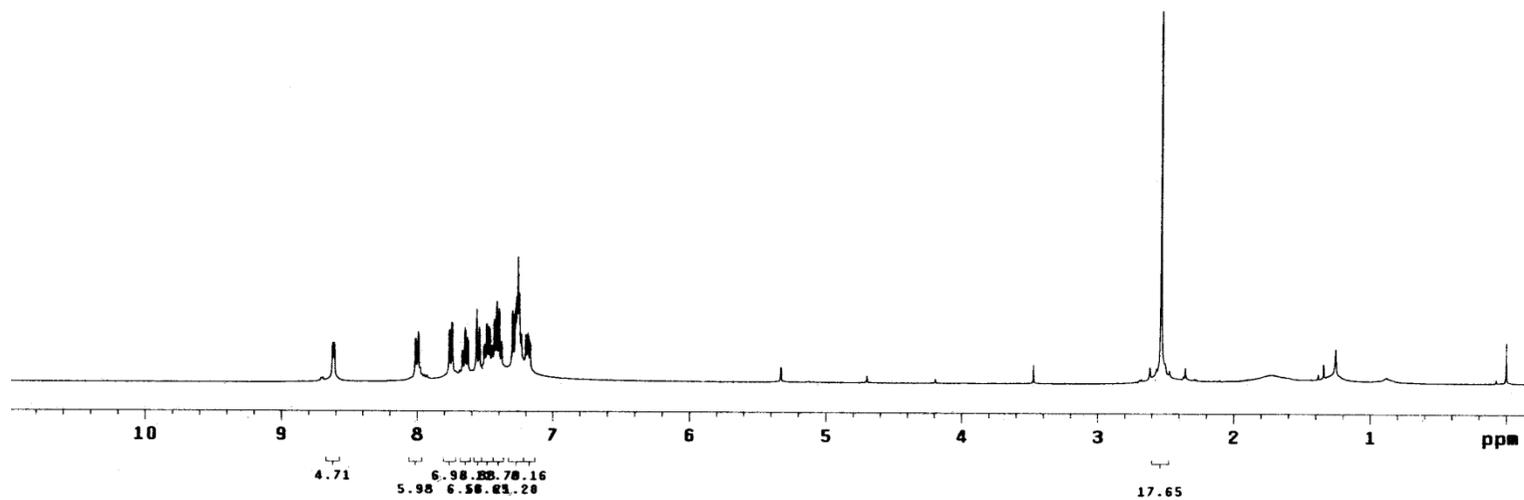
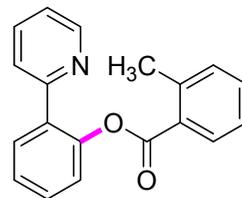
PULSE SEQUENCE: zgpg30 Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 2.561 sec Width 6398.0 Hz 32 repetitions	OBSERVE H1, 399.8509632 MHz FT size 32768 Total time 1 minutes	SR-01-S Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 "IITG-NMR"
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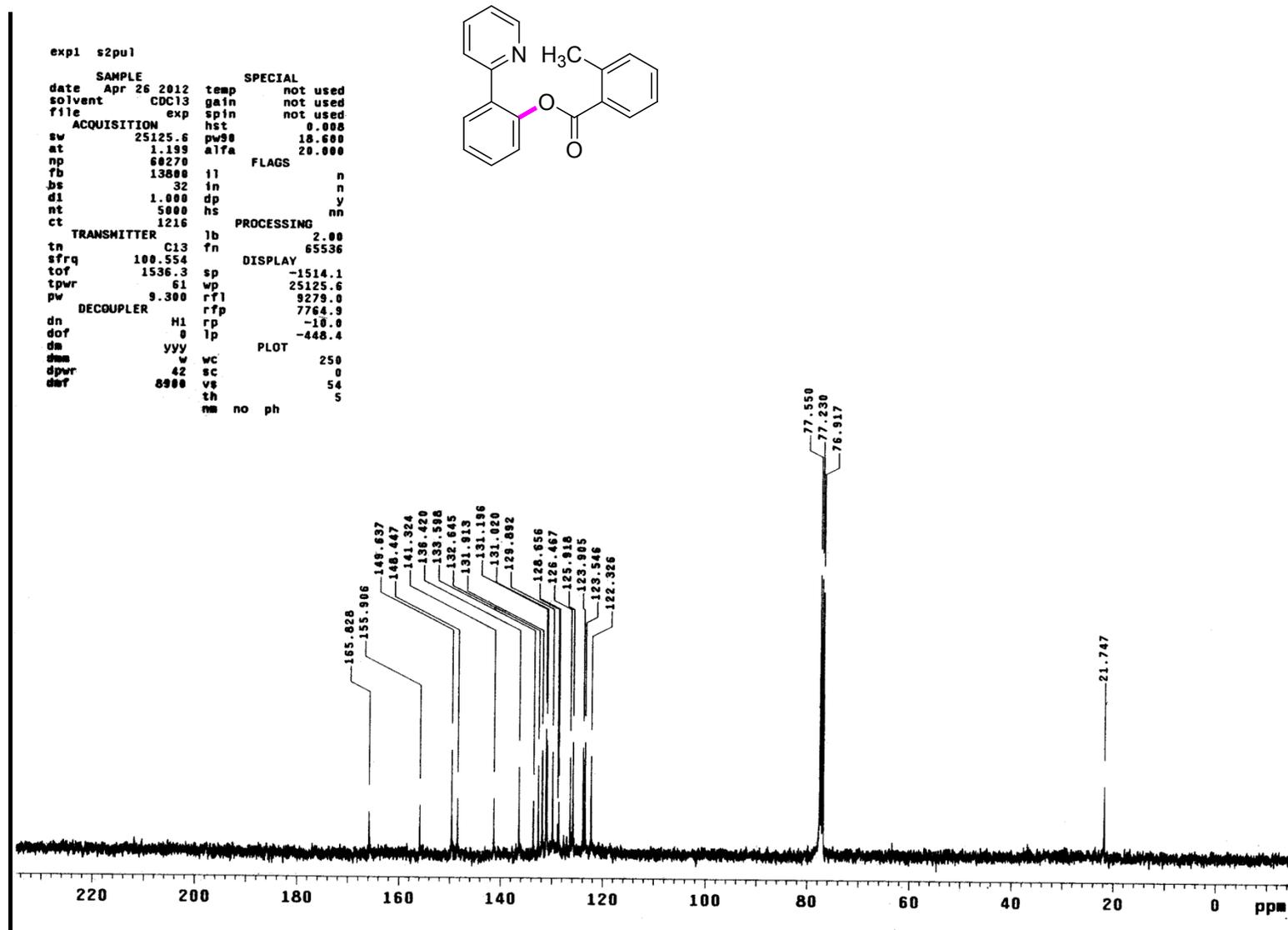
2-(Pyridin-2-yl)phenyl benzoate (1a): ^{13}C NMR (100 MHz, CDCl_3)

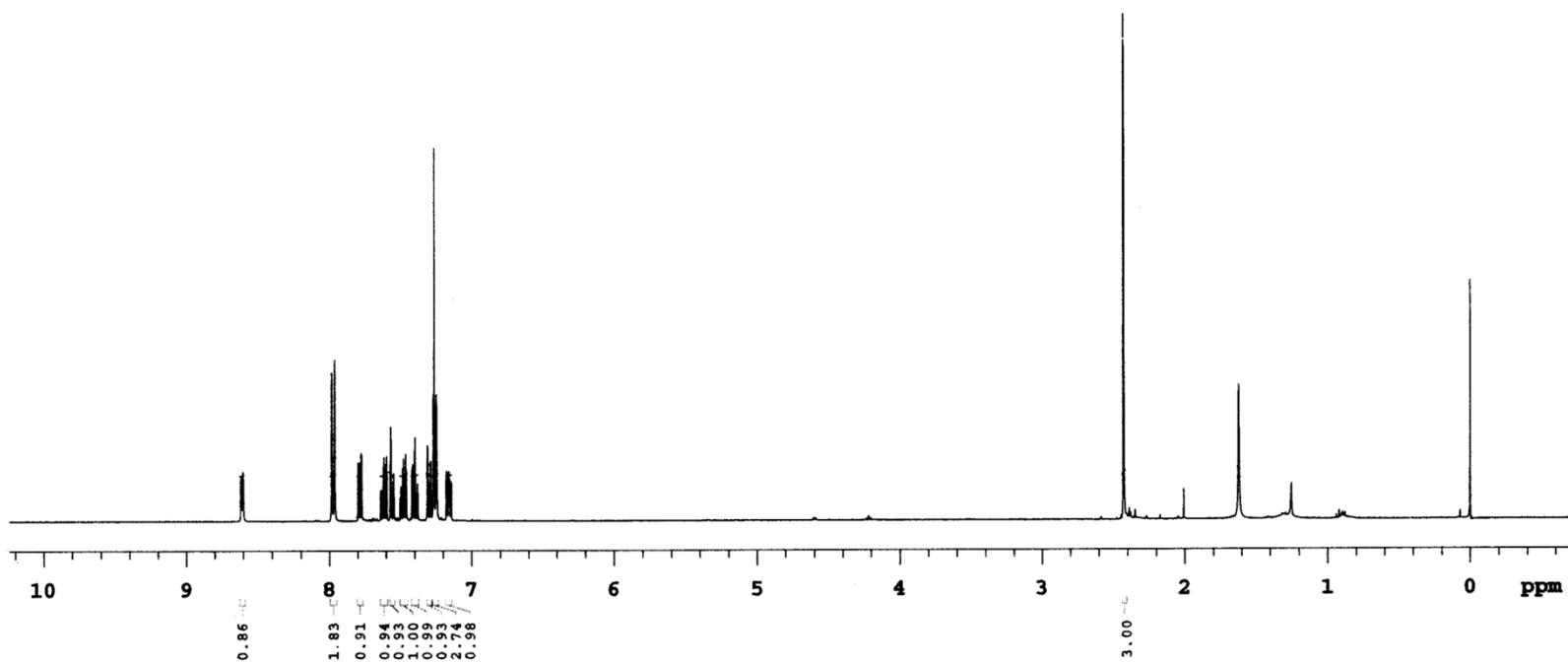
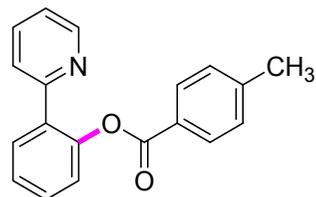
PULSE SEQUENCE DATA PROCESSING OBSERVE C13, 100.5425844 Relax. delay 1.000 sec Pulse 45.0 degree Acq. time 1.304 sec Width 25125.6 Hz 464 repetitions	DECOUPLE H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	DATA PROCESSING SR-01 Line broadening 0.5 Hz FT size 65536 Total time 17 minutes	SR-01-S Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 "IITG-NMR"
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2-(Pyridin-2-yl)phenyl 2-methylbenzoate (1b): ^1H NMR (400 MHz, CDCl_3)

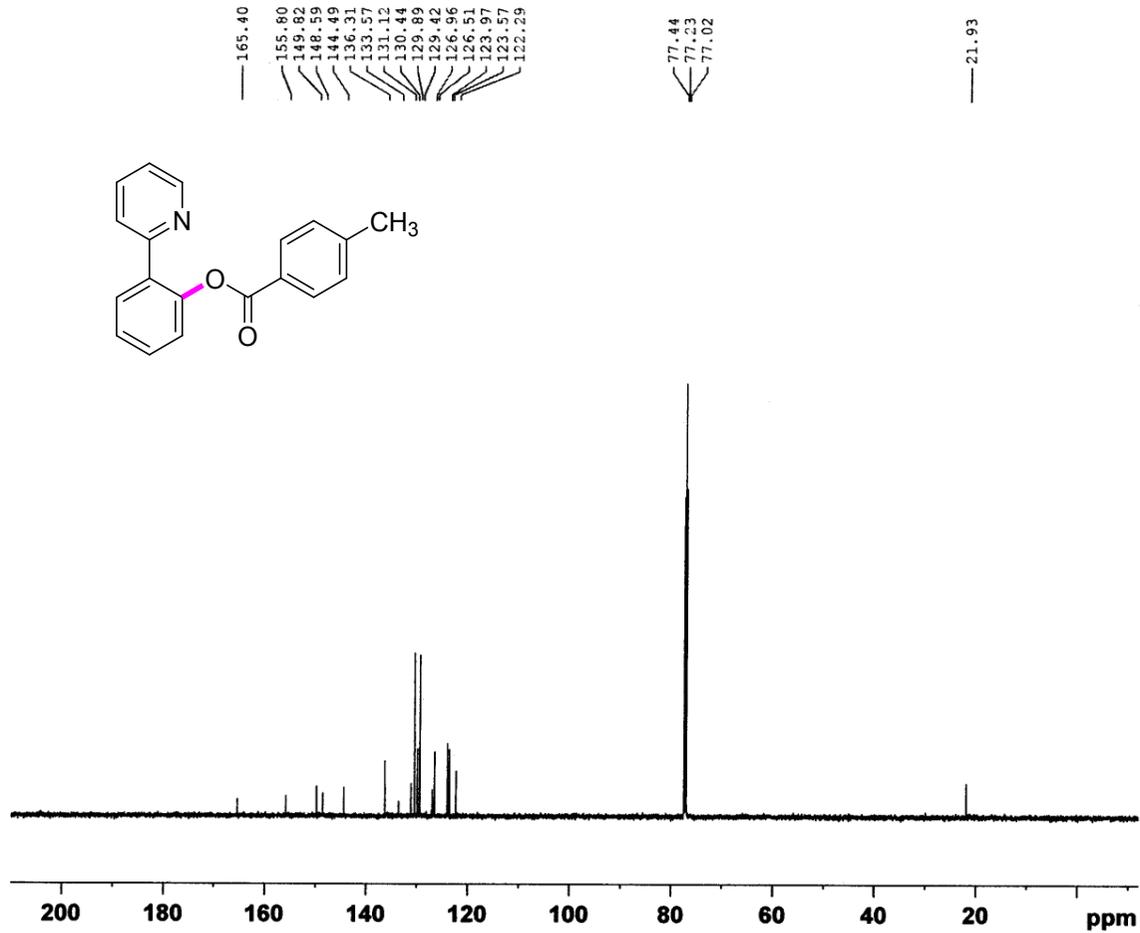
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file exp spin not used
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at 1.998 pwr0 19.700
np 25528 alfa 20.000
fb not used
bs 4
di 1.000 dp
nt 32 hs
ct 32
TRANSMITTER lb 0.10
tn H1 fn 65536
sfrq 399.853
tof 362.8 sp
tpwr 57 wp 4458.4
pw 9.850 rfp 795.8
DECOUPLER C13 rfp 0
dn 0 rp 102.0
dof 0 ip -87.3
da nnn
dmm c
dpwr 50 wc 250
daf 15900 vs 0
nm cdc ph th 65
          nm cdc ph 5
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2-(Pyridin-2-yl)phenyl-2-methylbenzoate(1b):¹³CNMR (100 MHz, CDCl₃)

2-(Pyridin-2-yl)phenyl 4-methylbenzoate (1c): ^1H NMR (400 MHz, CDCl_3)

PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 2.561 sec Width 6398.0 Hz 32 repetitions	DATA PROCESSING Observed F1, 399.8509627	DATA PROCESSING FT size 32768 Total time 1 minutes	Solvent: cdcl3 Temp: 25.0 C / 298.1 K Operator: chem Mercury-400 "IITG-NMR"
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2-(Pyridin-2-yl)phenyl-4-methylbenzoate (1c): ^{13}C NMR (150MHz, CDCl_3)

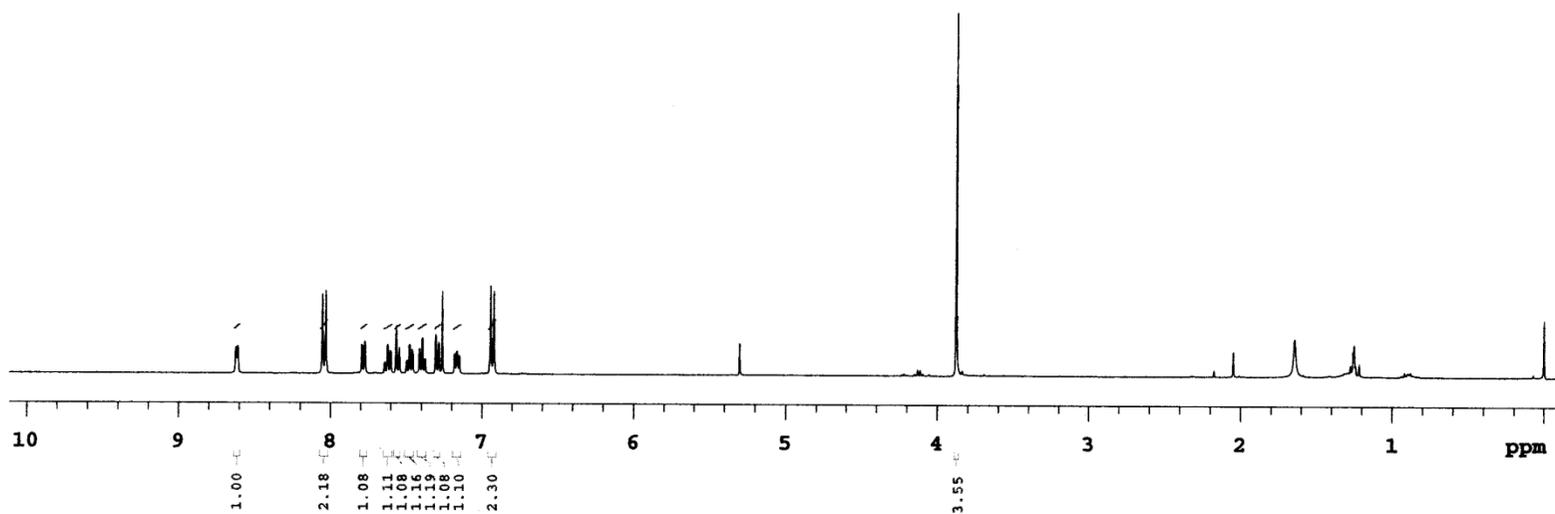
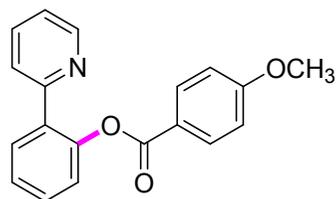
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 TD0 1

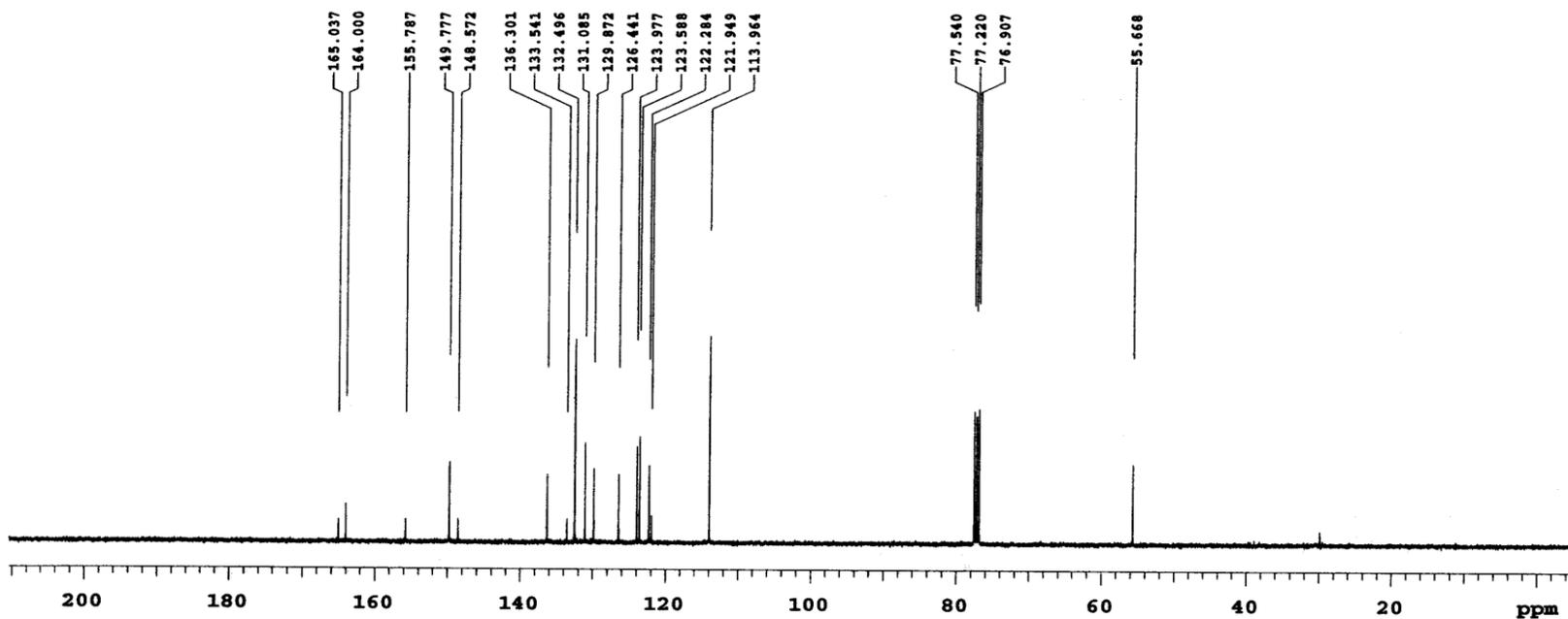
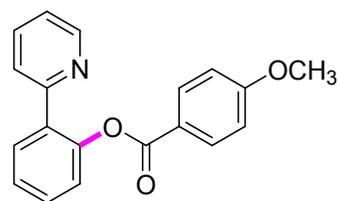
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 CPDPRG[2] waltz16
 PCPD2 70.00 usec
 PLW2 21.00000000 W
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 PLW13 0.30239999 W

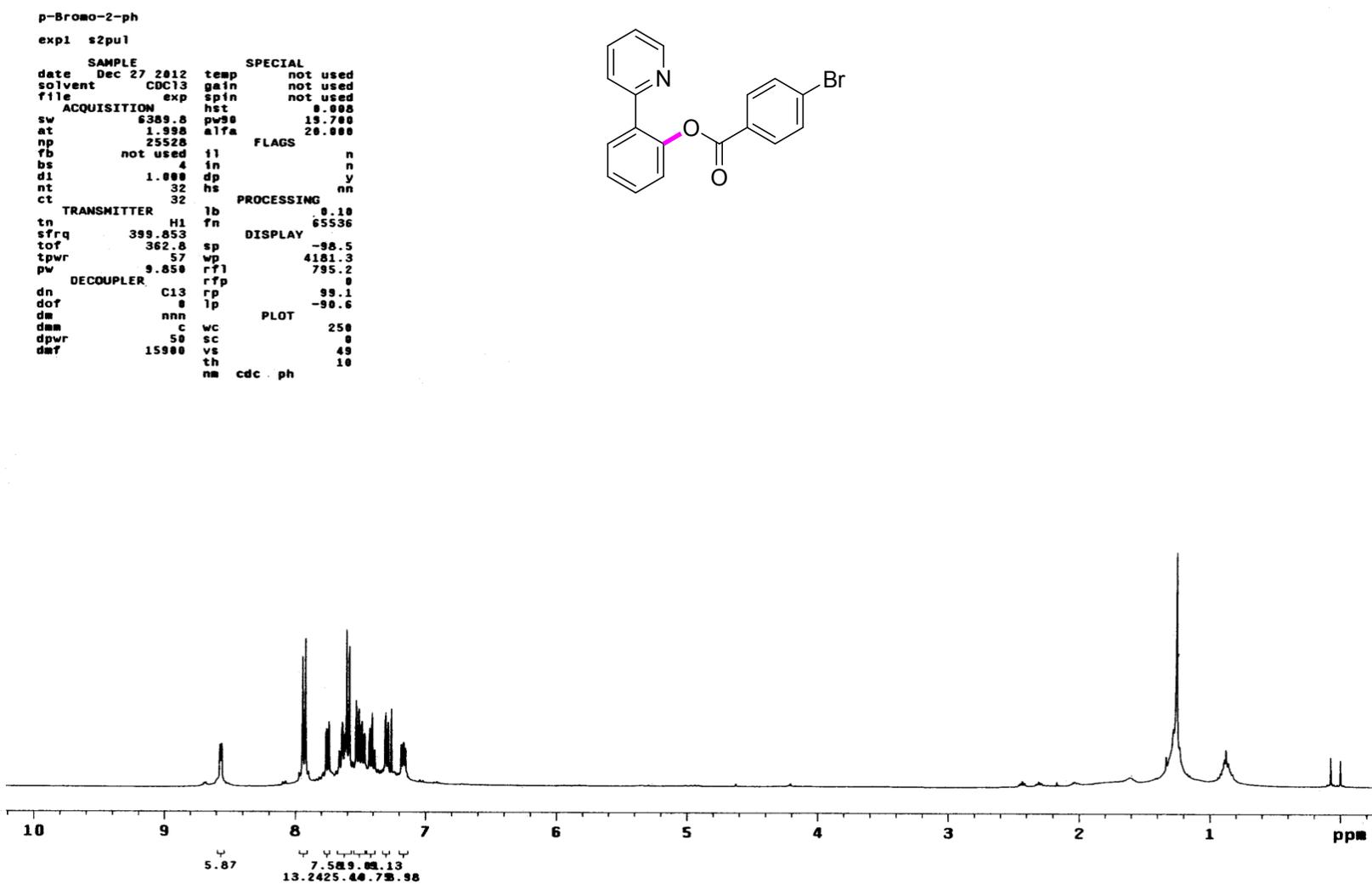
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 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

2-(Pyridin-2-yl)phenyl 4-methoxybenzoate (1d): ^1H NMR (400 MHz, CDCl_3)

PULSE SEQUENCE DATA PROCESSING Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 2.561 sec Width 6398.0 Hz 32 repetitions	OBSERVE H1, 399.8509621	DATA PROCESSING F1 size 32768 Total time 1 minutes	sr-01-ome Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 "IITG-NMR"
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2-(Pyridin-2-yl)phenyl 4-methoxybenzoate (1d): ^{13}C NMR (100 MHz, CDCl_3)

PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 1000 repetitions	DECOUPLE H1 , 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 0.5 Hz FT size 65536 Total time 38 minutes	Solvent : 'cdcl3' Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 "IITG-NMR"
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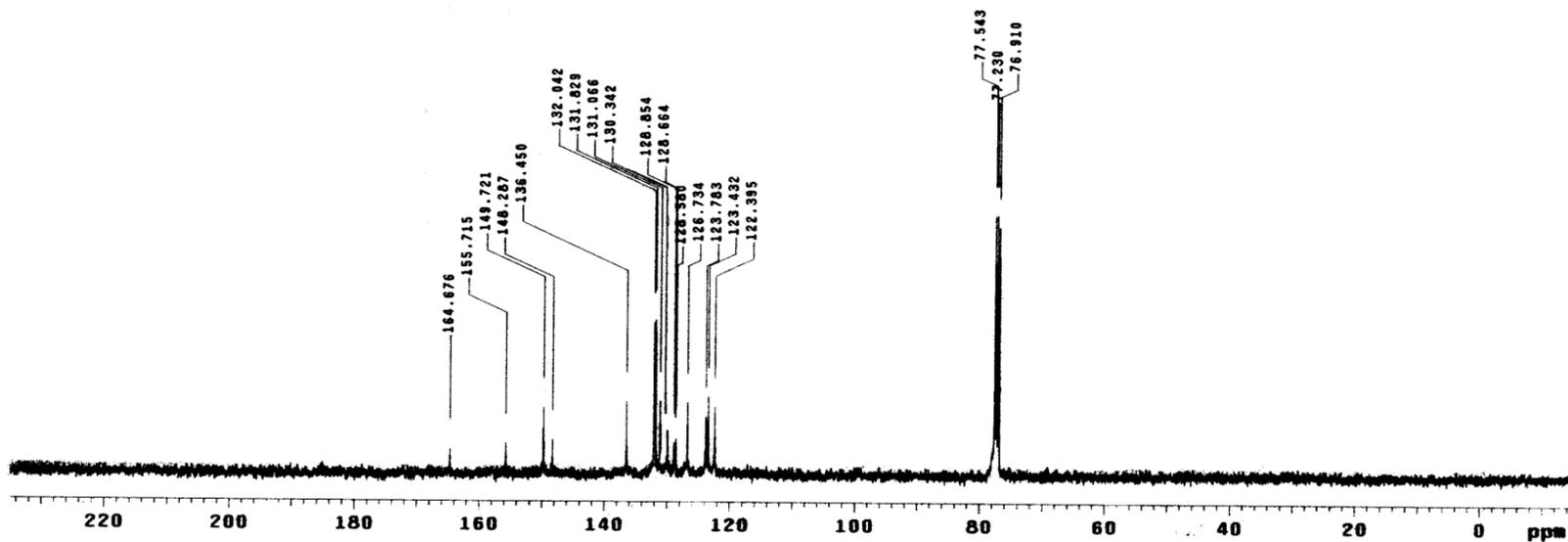
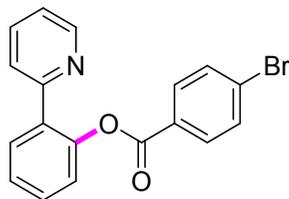
2-(Pyridin-2-yl)phenyl -4-bromobenzoate (1e): ^1H NMR (400 MHz, CDCl_3)

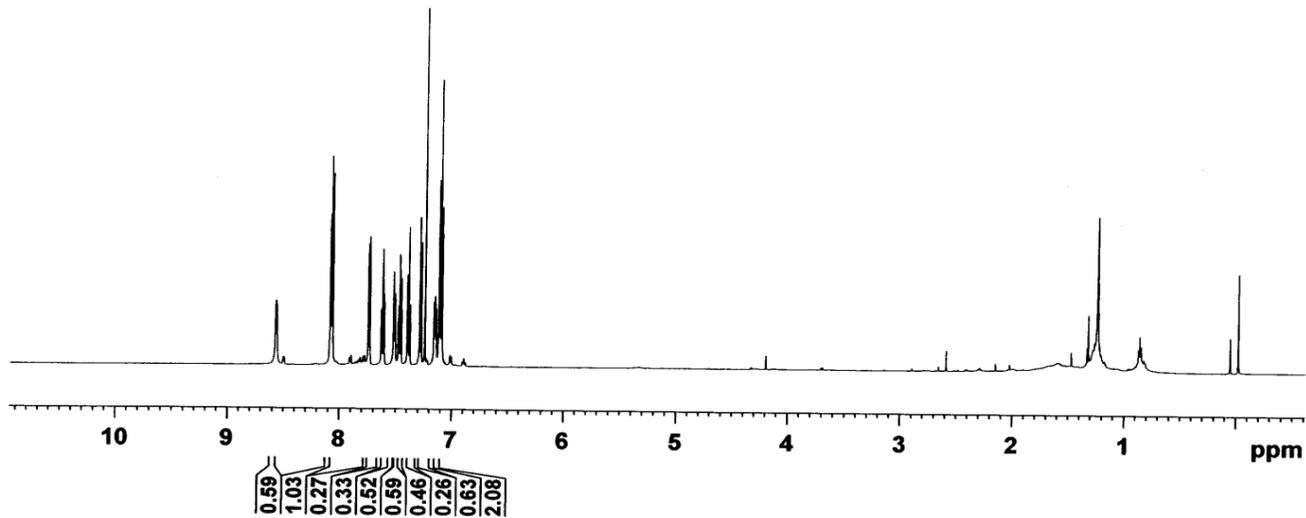
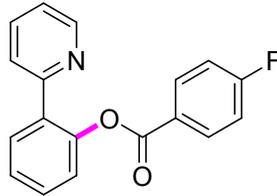
2-(Pyridin-2-yl)phenyl -4-bromobenzoate (1e): ^{13}C NMR (100 MHz, CDCl_3)

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solvent CDCl3 gain not used
file exp spin not used
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fb 13000 f1 FLAGS n
bs 32 f2 n
d1 1.000 dp y
nt 5000 hs PROCESSING nn
ct 2144
TRANSMITTER
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sfrq 100.554 fn 65536
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tpwr 61 wp 25125.6
pw 4.700 rfl 9274.4
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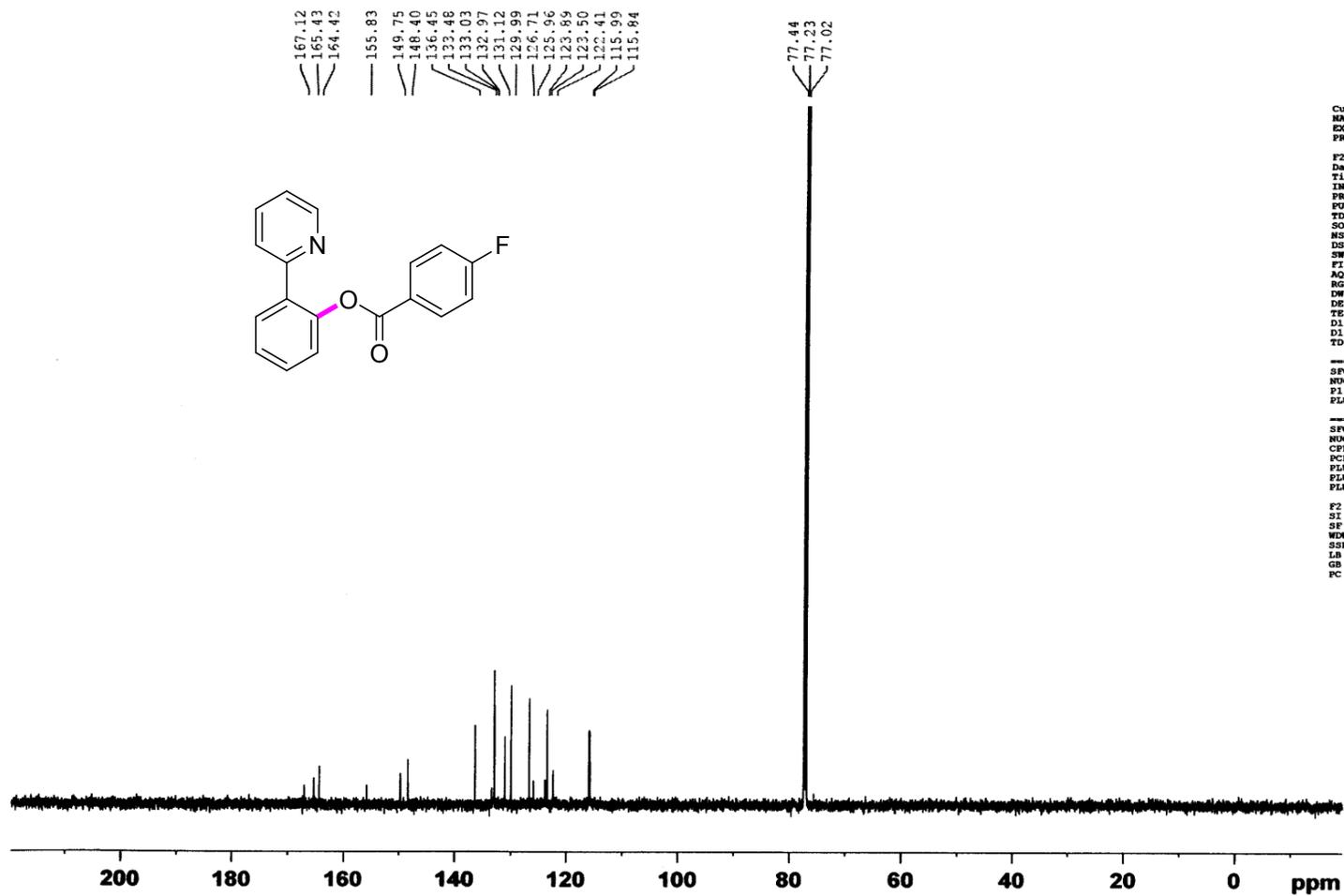
2-(Pyridin-2-yl)phenyl 4-fluorobenzoate (1f): ^1H NMR (600 MHz, CDCl_3)

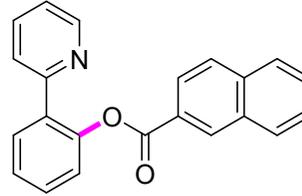
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F2 - Processing parameters
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2-(Pyridin-2-yl)phenyl 4-fluorobenzoate (1f): ^{13}C NMR (150 MHz, CDCl_3)

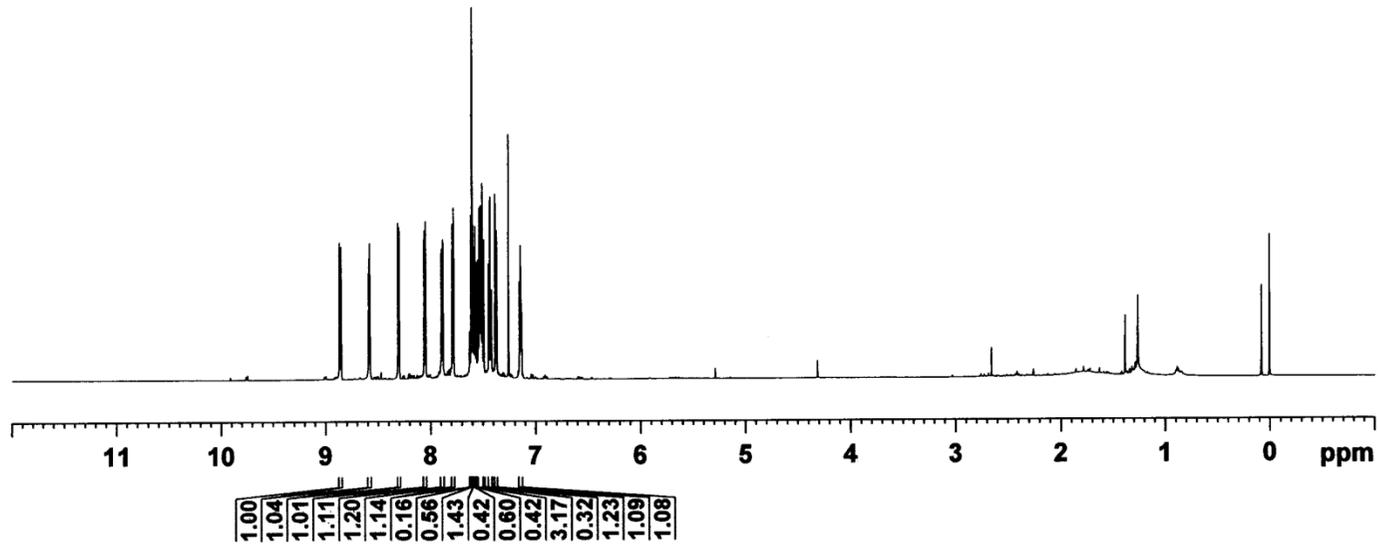
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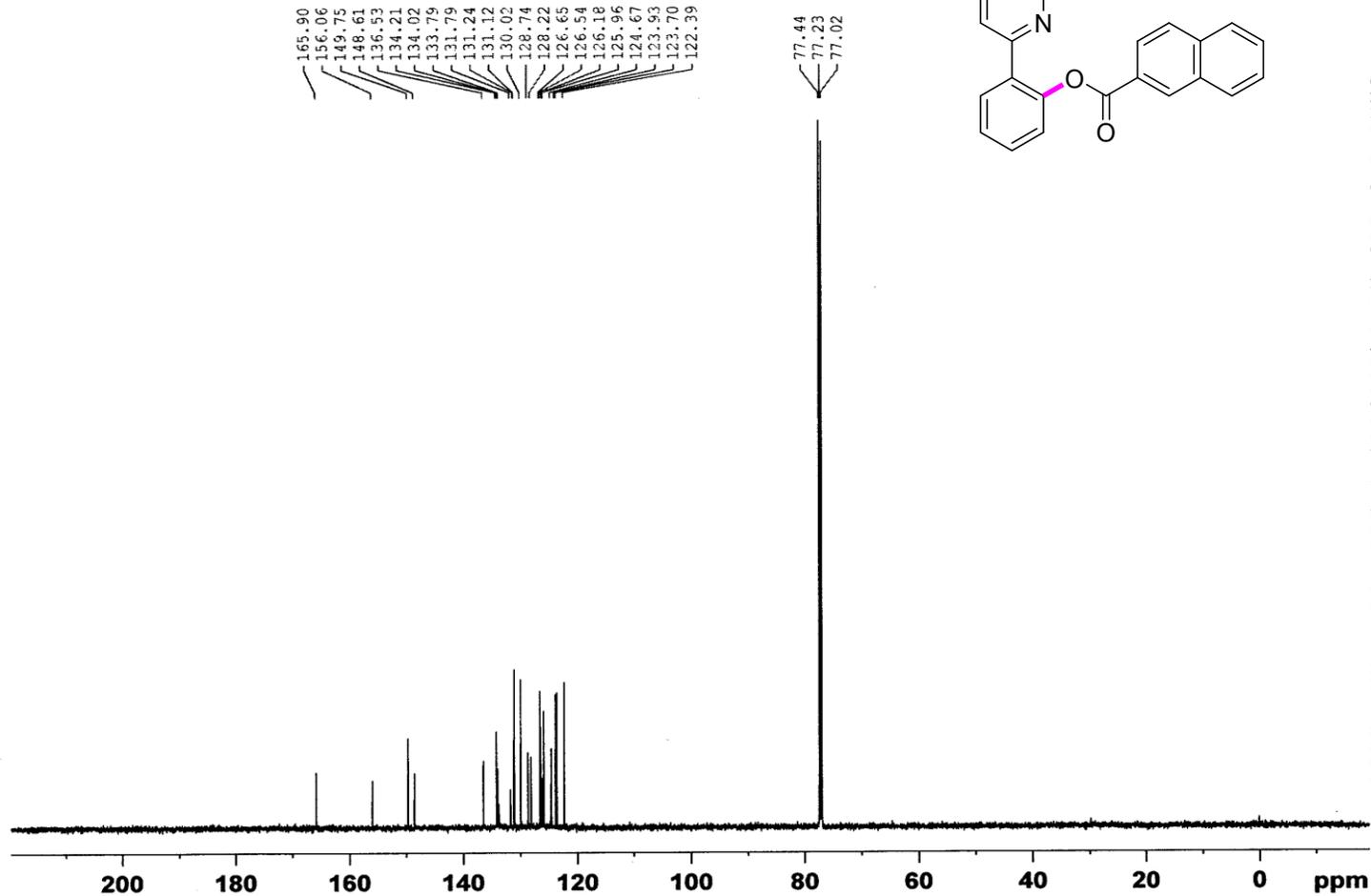
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 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
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 DS 2
 SWH 12019.230 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 65.24
 DW 41.600 usec
 DE 6.50 usec
 TE 299.3 K
 D1 1.00000000 sec
 TDO 1

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F2 - Processing parameters
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2-(Pyridin-2-yl)phenyl 2-naphthoate (1g): ^{13}C NMR (150 MHz, CDCl_3)

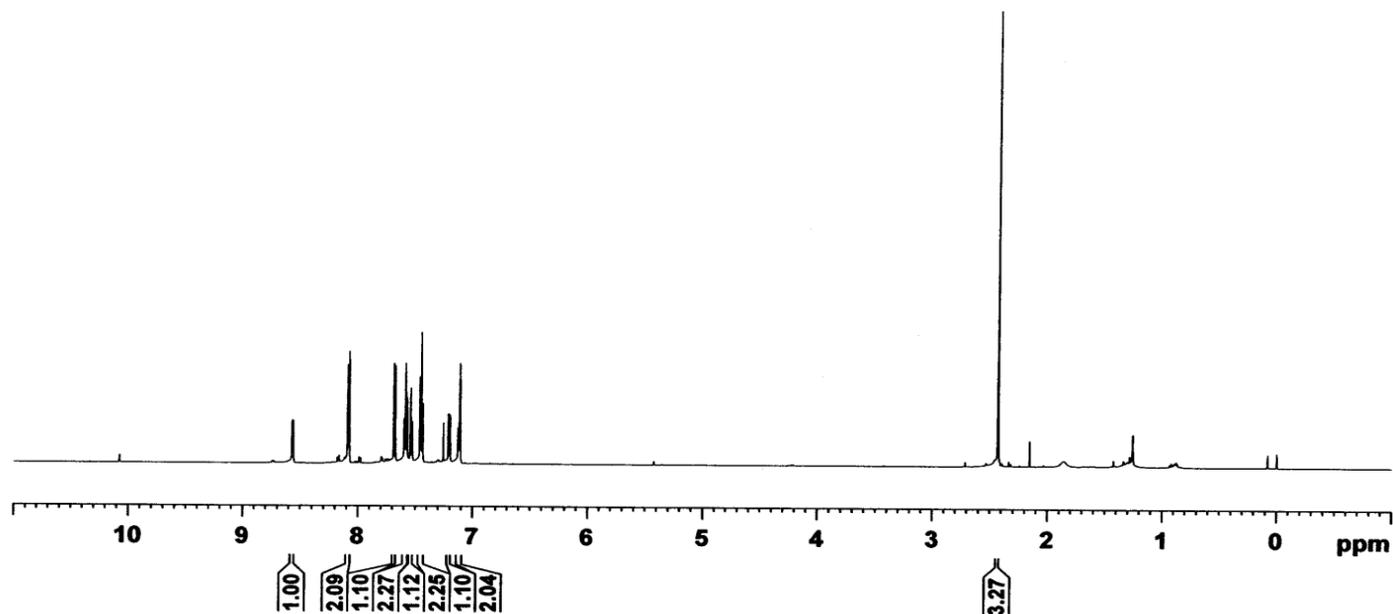
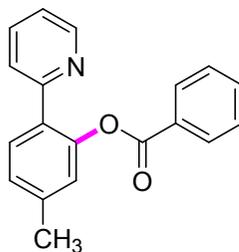
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 DE 6.50 usec
 TE 300.4 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

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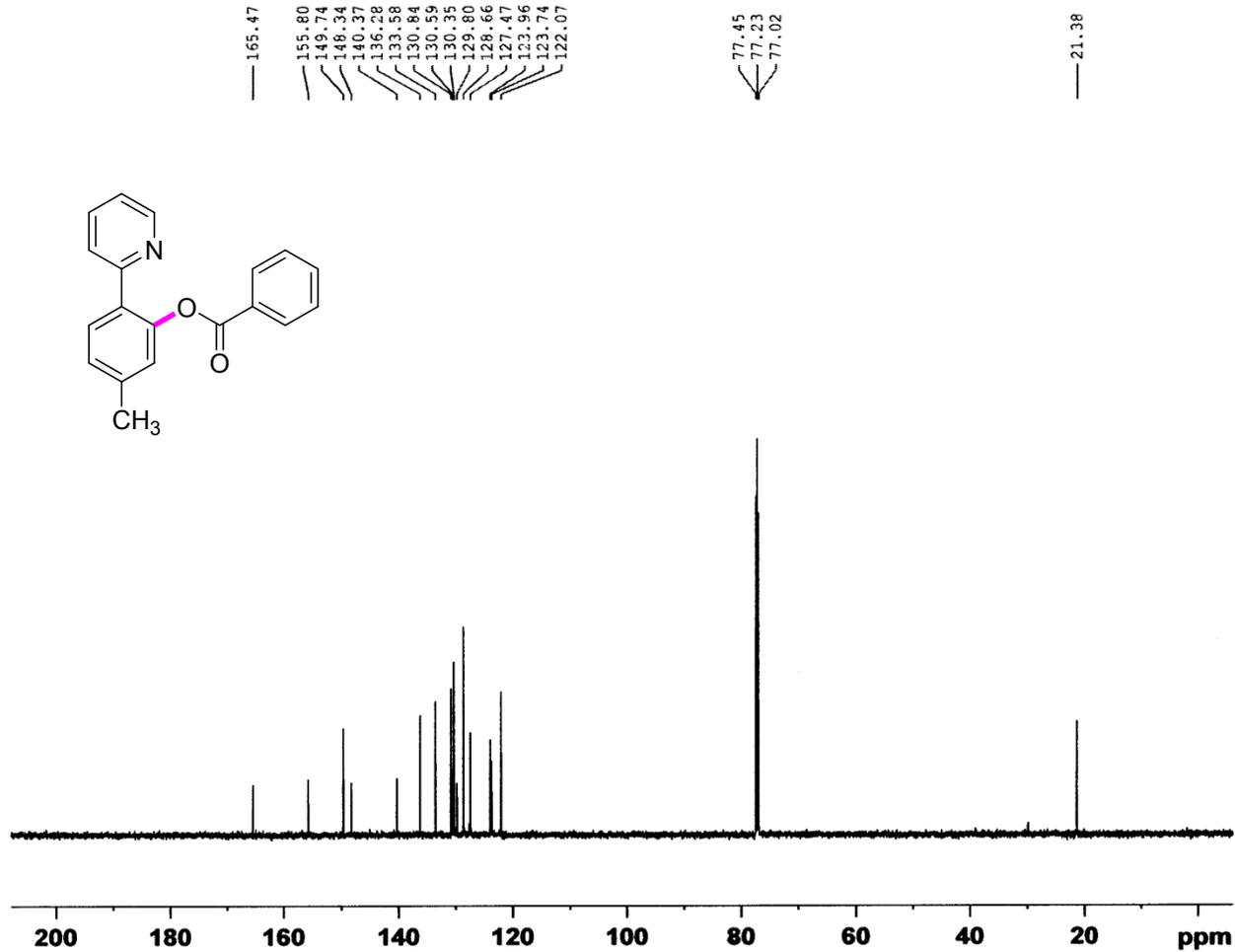
5-Methyl-2-(pyridine-2-yl)phenyl benzoate (2a): ^1H NMR (600 MHz, CDCl_3)

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PC        1.00
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5-Methyl-2-(pyridine-2-yl)phenyl benzoate (2a): ^{13}C NMR (150 MHz, CDCl_3)

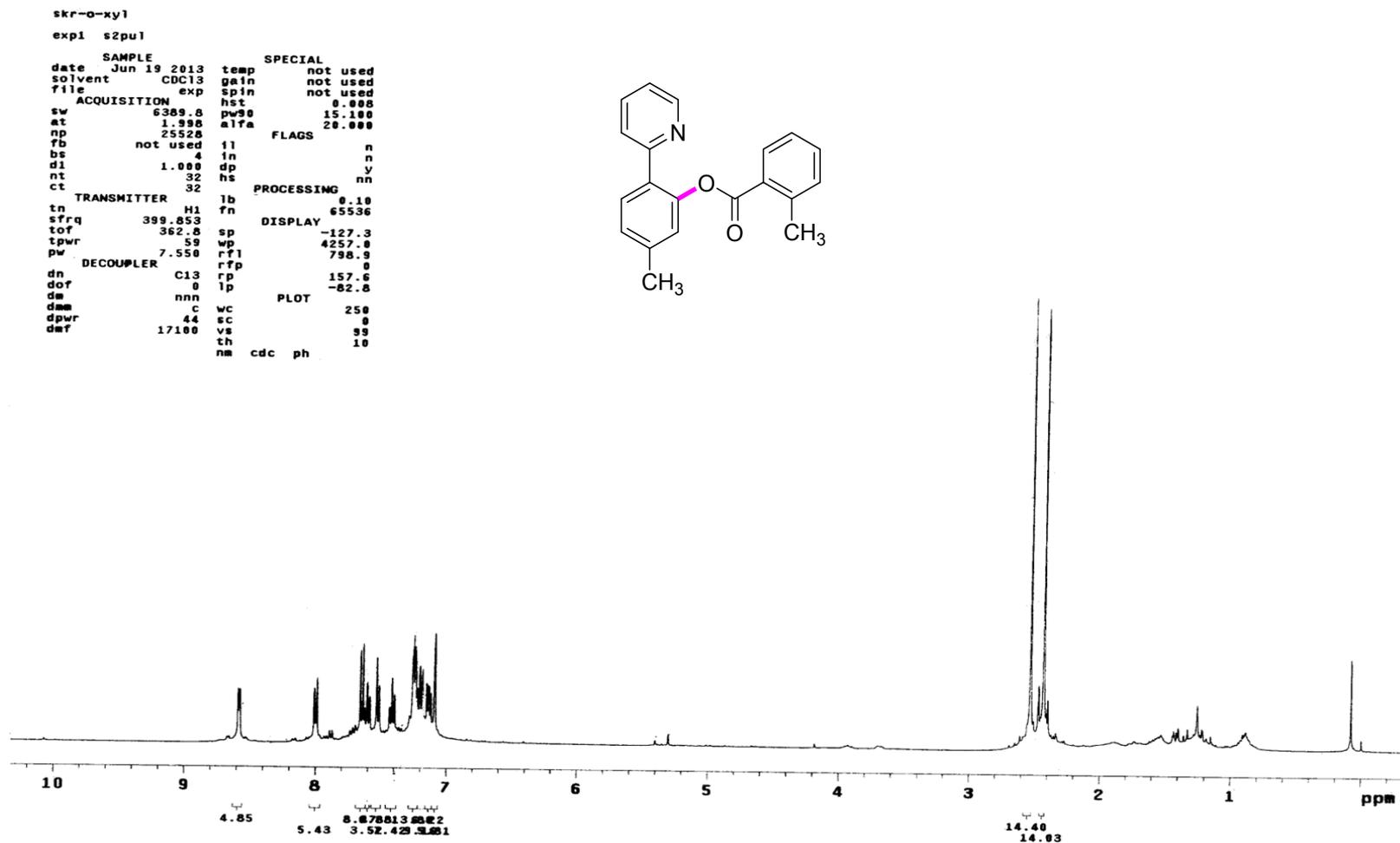
Current Data Parameters
 NAME SR-01-TS-13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140321
 Time_ 9.51
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl_3
 NS 90
 DS 2
 SWH 36057.691 Hz
 FIDRES 1.100393 Hz
 AQ 0.4543829 sec
 RG 65.24
 DW 13.867 usec
 DE 6.50 usec
 TE 301.8 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 150.9279571 MHz
 NUC1 13C
 P1 10.50 usec
 PLW1 95.00000000 W

===== CHANNEL f2 =====
 SFO2 600.1724007 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 70.00 usec
 PLW2 21.00000000 W
 PLW12 0.61714000 W
 PLW13 0.30239999 W

F2 - Processing parameters
 SI 16384
 SF 150.9128392 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

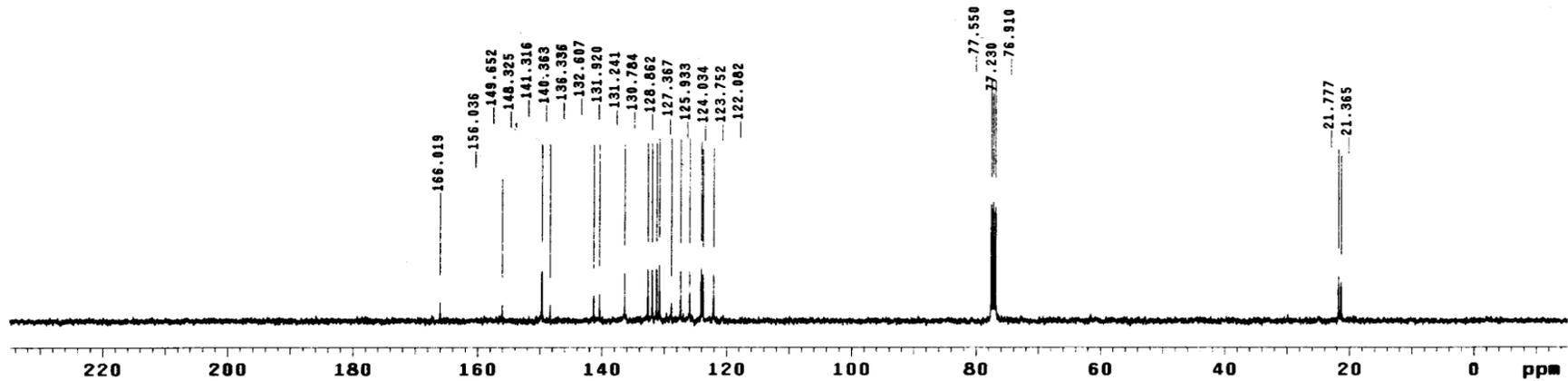
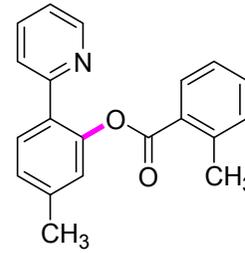
5-Methyl-2-(pyridine-2-yl)phenyl 2-methylbenzoate (2b): ^1H NMR (400 MHz, CDCl_3)

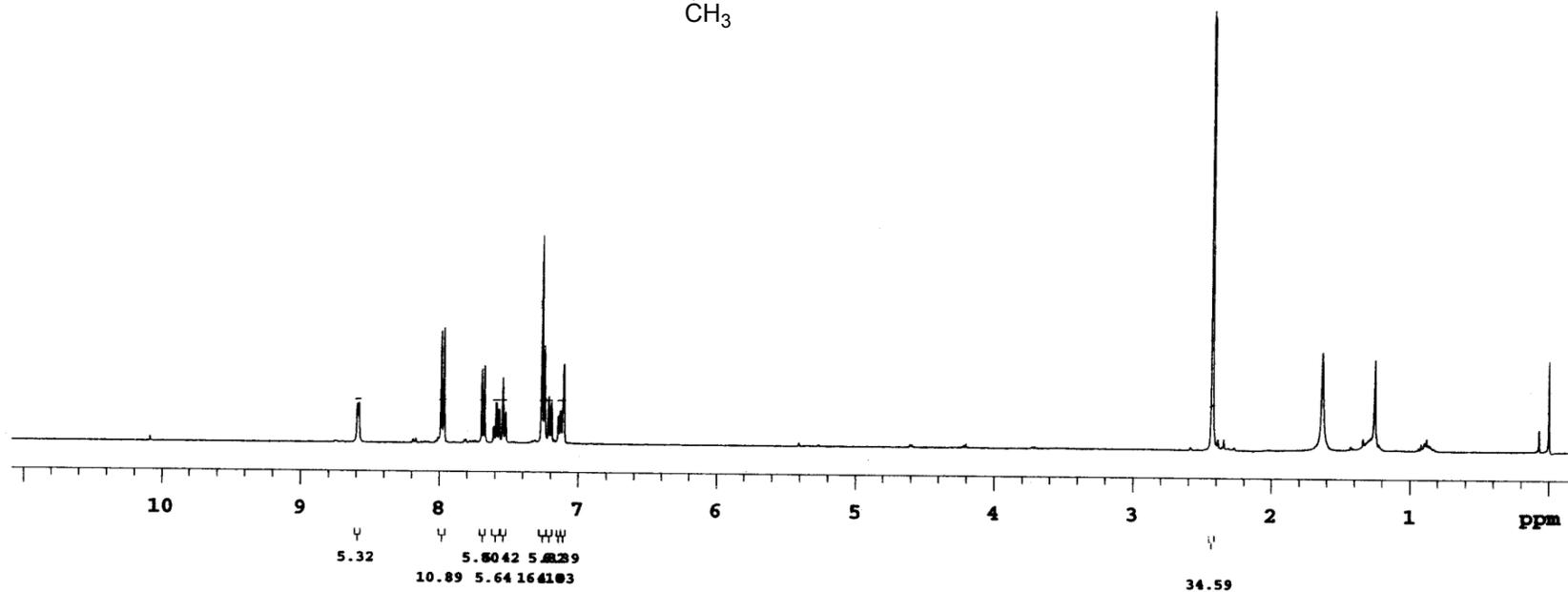
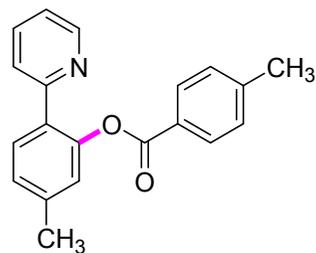
5-Methyl-2-(pyridine-2-yl)phenyl 2-methylbenzoate (2b): ^{13}C NMR (100 MHz, CDCl_3)

```

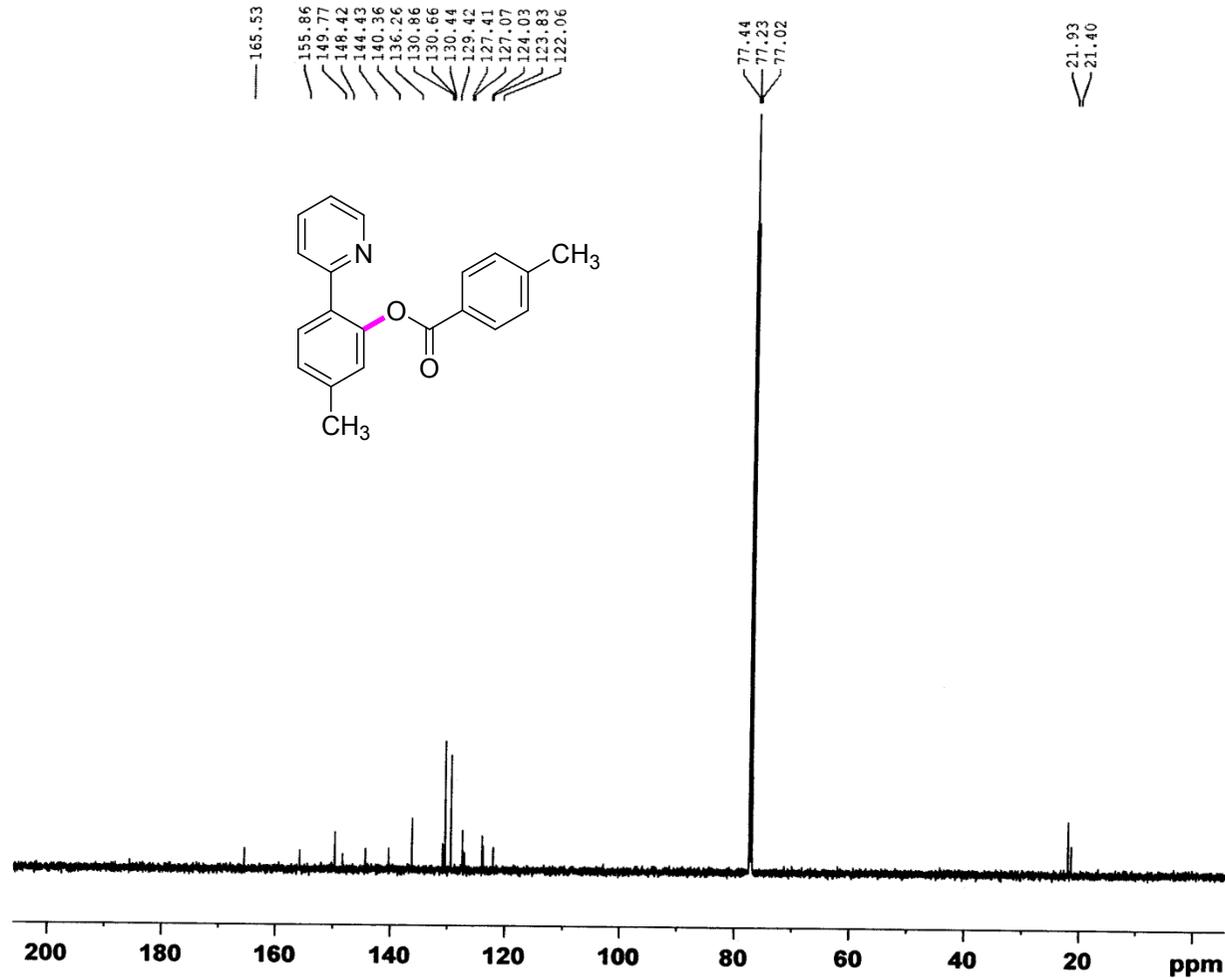
skr-o-xy1-13c
exp1 s2pu1
SAMPLE
#date Jun 19 2013 temp not used
#solvent CDCl3 gain not used
#file exp spin not used
ACQUISITION
sw 25125.6 hst 0.000
at 1.199 pws 0.400
np 60270 a1fa 20.000
fb 13800 il n
bs 32 in n
dl 1.000 dp y
nt 5000 hs nn
ct 1024
TRANSMITTER
tn C13 lb 2.00
sfrq 100.554 fn 65536
tof 1536.3 sp -1508.7
tpwr 61 wp 25125.6
pw 4.700 rfl 9273.6
DECOUPLER
dn H1 rfp 7764.9
dof 0 rp -74.2
dm yyy lp -271.4
dmm w wc 250
dpr 42 sc 0
dnt 8500 vs 22
th 2
nm no ph

```



5-Methyl-2-(pyridine-2-yl)phenyl 4-methylbenzoate (2c): ^1H NMR (400 MHz, CDCl_3)

PULSE SEQUENCE	DATA PROCESSING	SR01: TMR 1H
Relax. delay 1.000 sec	FT size 32768	Solvent: cdcl3
Pulse 45.0 degrees	Total time 1 minutes	Temp. 25.0 C / 298.1 K
Acq. time 2.561 sec		Operator: chem
Width 6398.0 Hz		Mercury-400 "IITG-NMR"
32 repetitions		

5-Methyl-2-(pyridine-2-yl)phenyl 4-methylbenzoate (2c): ^{13}C NMR (150 MHz, CDCl_3)

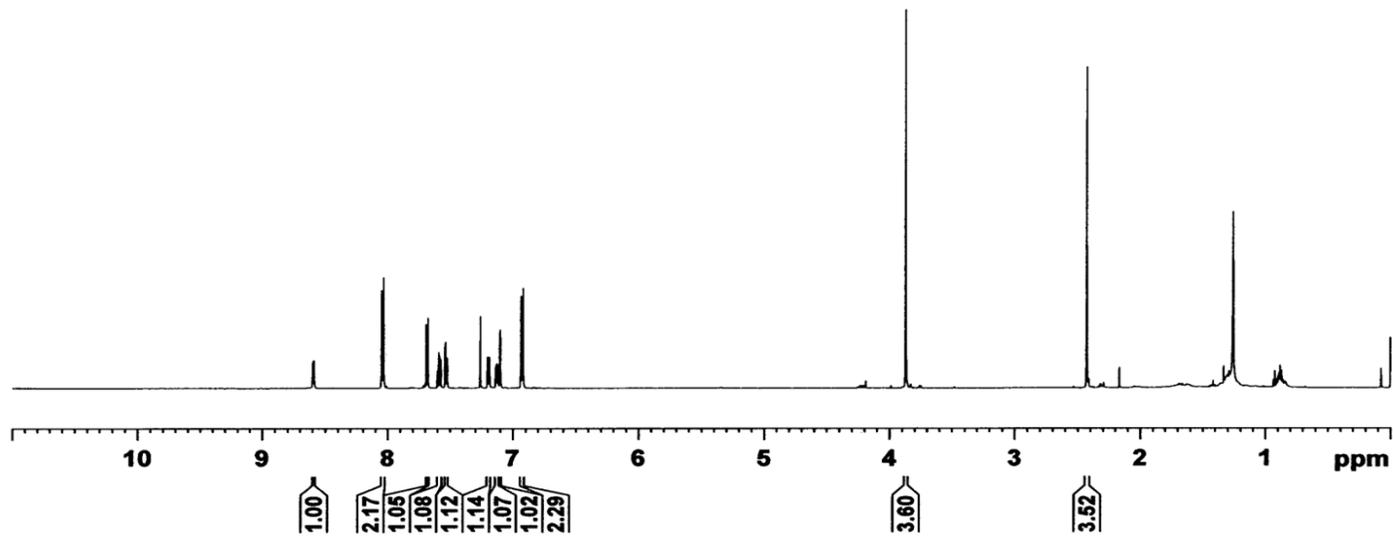
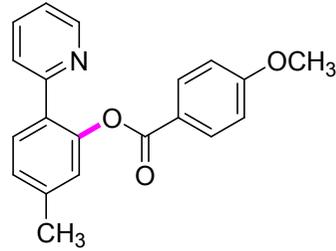
Current Data Parameters
 NAME SR-01-TME-13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140318
 Time 13.24
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl_3
 NS 260
 DS 2
 SWH 36057.691 Hz
 FIDRES 1.100393 Hz
 AQ 0.4543829 sec
 RG 65.24
 DW 13.867 usec
 DE 6.50 usec
 TE 303.3 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 150.9279571 MHz
 NUC1 13C
 P1 10.50 usec
 PLW1 95.00000000 W

===== CHANNEL f2 =====
 SFO2 600.1724007 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 70.00 usec
 PLW2 21.00000000 W
 PLW12 0.61714000 W
 PLW13 0.30239999 W

F2 - Processing parameters
 SI 16384
 SF 150.9128326 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

5-Methyl-2-(pyridine-2-yl)phenyl 4-methoxybenzoate (2d): ^1H NMR (600 MHz, CDCl_3)

```

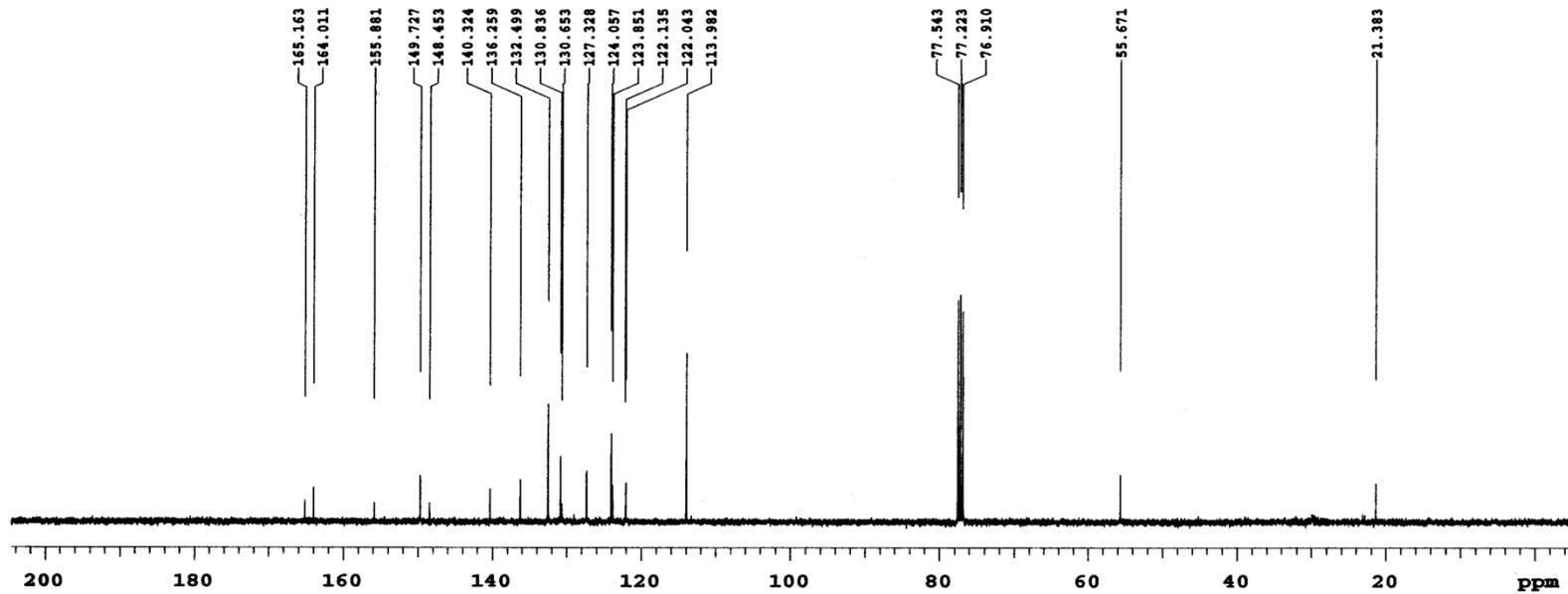
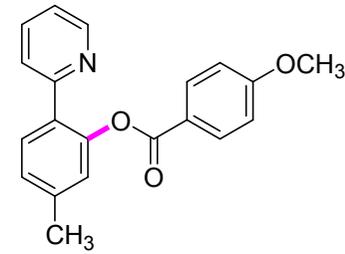
Current Data Parameters
NAME      SR-01-TOM-1H
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20140312
Time     14.04
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zg30
TD       32768
SOLVENT  CDCl3
NS       16
DS       2
SWH      12019.230 Hz
FIDRES   0.366798 Hz
AQ       1.3631488 sec
RG       73.2
DW       41.600 usec
DE       6.50 usec
TE       300.5 K
D1       1.00000000 sec
TDO      1

----- CHANNEL f1 -----
SF01    600.1737063 MHz
NUC1     1H
P1       12.00 usec
PLW1    21.00000000 W

F2 - Processing parameters
SI       16384
SF       600.1700148 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00

```

5-Methyl-2-(pyridine-2-yl)phenyl 4-methoxybenzoate (2d): ^{13}C NMR (100 MHz, CDCl_3)

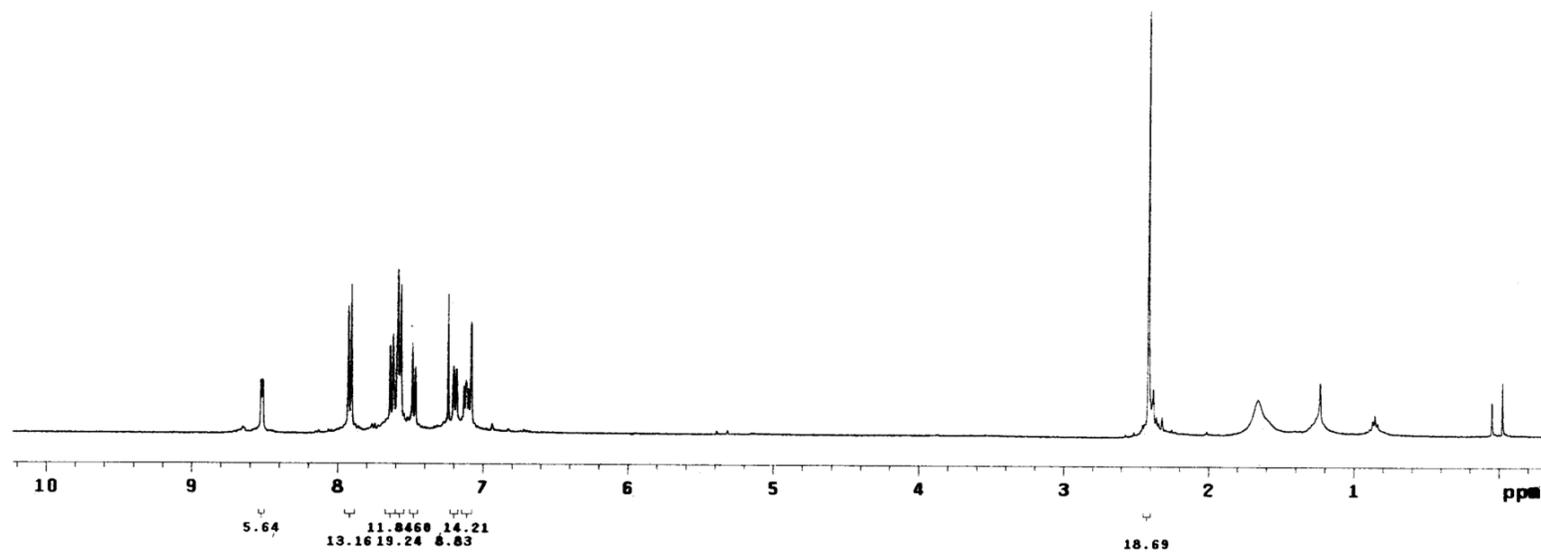
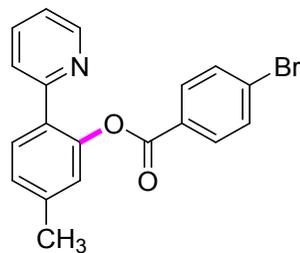
PULSE SEQUENCE DATA PROC Relax. delay 1.000 sec Pulse 45.0 degree Acq. time 1.304 sec Width 25125.6 Hz 992 repetitions	OBSERVE C13, 100.5425808 DECOUPLE H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 0.5 Hz FT size 65536 Total time 38 minutes	SR-01-TOM Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 "IITG-NMR"
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5-Methyl-2-(pyridin-2-yl)phenyl 4-bromobenzoate (2e): ^1H NMR (400 MHz, CDCl_3)

```

skr-p-br
exp1 s2pu1
SAMPLE
date Jun 19 2013 temp not used
solvent CDCl3 gain not used
file exp spin not used
ACQUISITION hst 8.988
sw 6389.8 pw90 15.100
at 1.498 alfa 20.000
np 25528
fb not used il FLAGS n
bs 4 in n
d1 1.000 dp y
nt 32 hs PROCESSING nn
ct 32
TRANSMITTER lb 6.10
tn H1 fn 65536
sfrq 399.853 DISPLAY -132.9
tof 362.8 wp 4223.4
tpwr 59 rfl 3689.5
pw 7.550 rfp 2894.9
DECOUPLER C13 rfp 152.7
dn C13 rp -69.9
dof 0 lp
dm nnn PLOT
dmc c wc 250
dpwr 44 sc 0
dmf 17100 vs 75
th 20
nm cdc ph

```

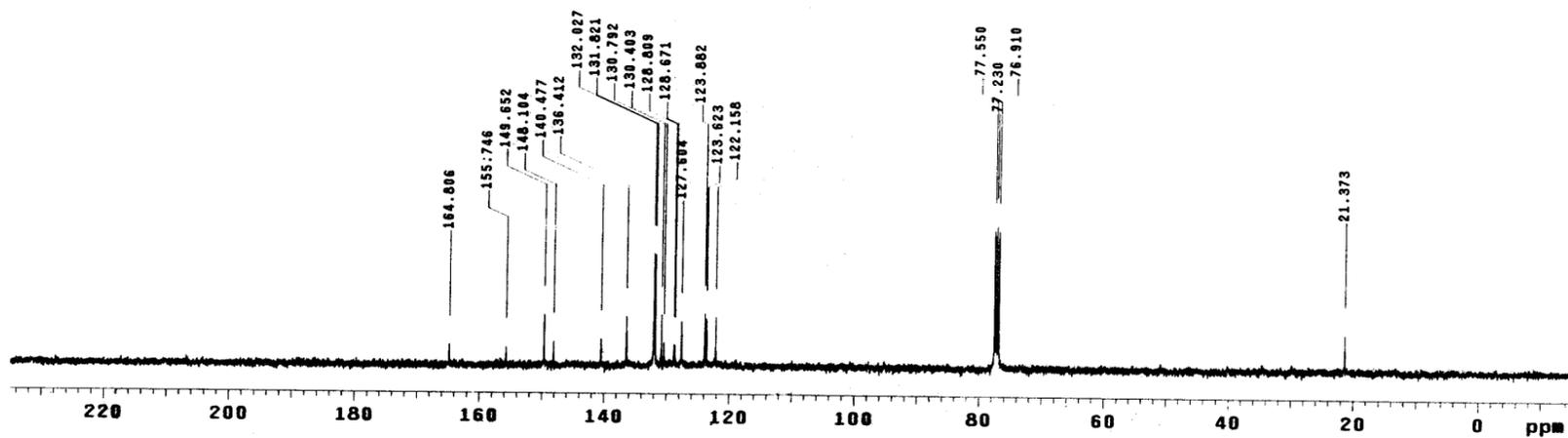
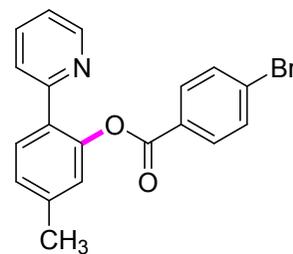


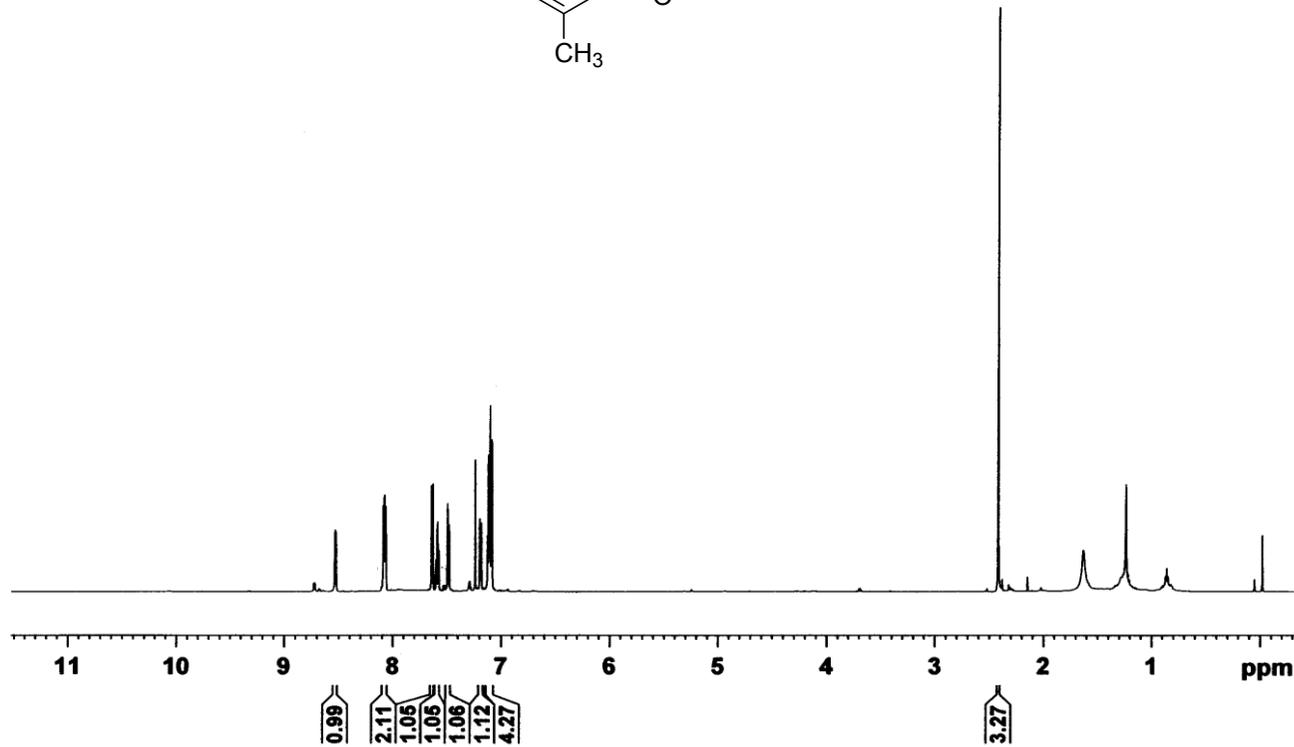
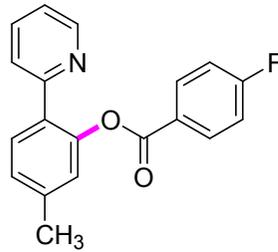
5-Methyl-2-(pyridine-2-yl)phenyl 4-bromobenzoate (2e): ^{13}C NMR (100 MHz, CDCl_3)

```

exp1 s2pu1
SAMPLE
date Jun 24 2013 temp not used
solvent CDCl3 gain not used
file exp spin not used
ACQUISITION
sw 25125.6 pw90 9.498
at 1.199 alfa 20.000
np 60270
fb 13800
bs 32
dl 1.000
nt 5000
ct 1024
TRANSMITTER
tn C13
sfrq 100.554
tof 1536.3
tpwr 61
pw 4.700
DECOUPLER
dn H1
dof 8
dms yyy
dpwr 42
dnt 8500
SPECIAL
flags n
in n
dp y
hs nn
PROCESSING
lb 2.00
fn 65536
DISPLAY
sp -1508.7
wp 25125.6
rf1 9273.6
rfp 7764.9
rp -58.3
tp -327.3
PLOT
wc 250
sc 0
vs 25
th 3
nm no ph

```



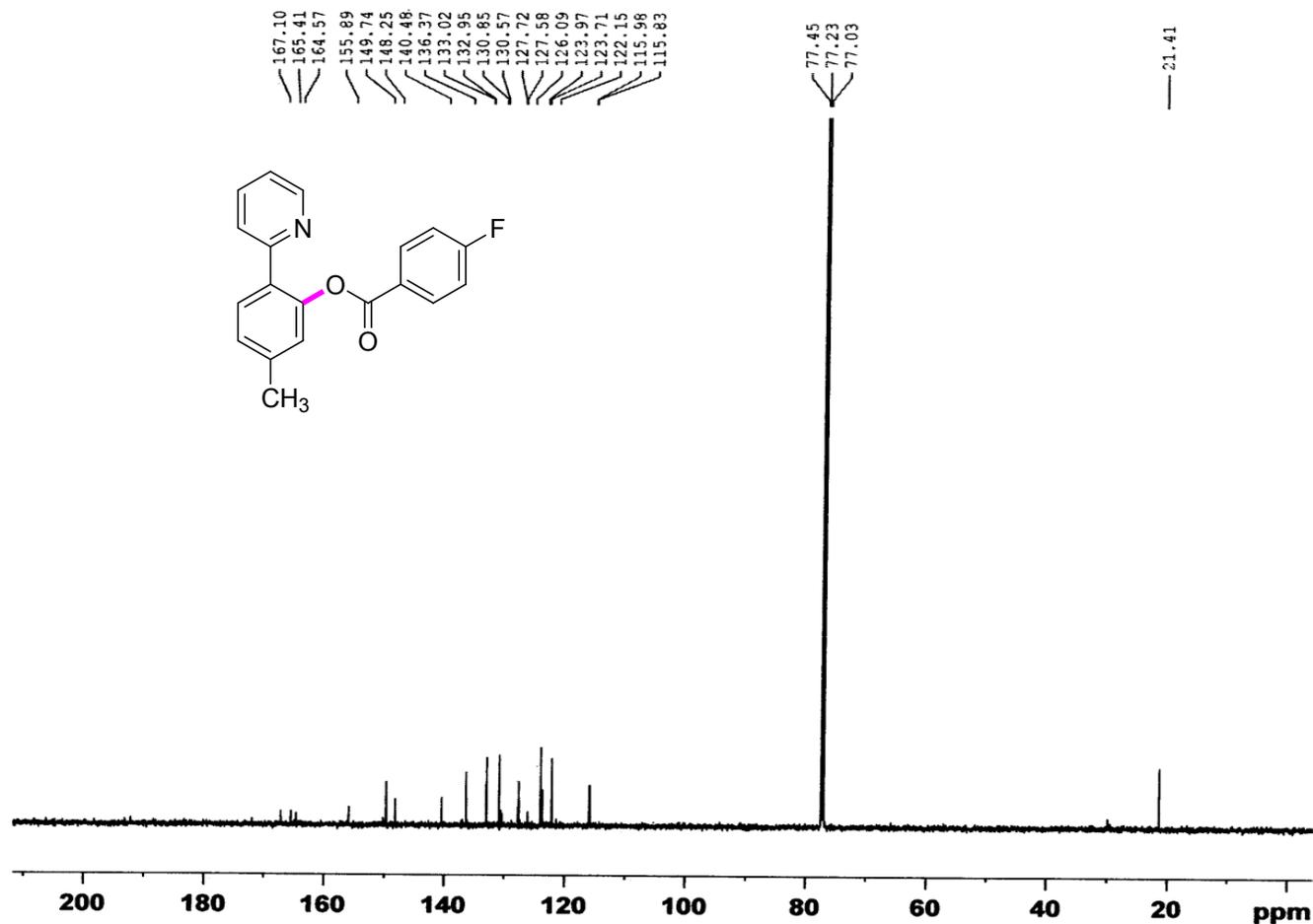
5-Methyl-2-(pyridin-2-yl)phenyl 4-fluorobenzoate (2f): ^1H NMR (600 MHz, CDCl_3)

Current Data Parameters
NAME SR-01-TE-1H
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140324
Time 12.48
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 80.22
DW 41.600 usec
DE 6.50 usec
TE 299.9 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
SFO1 600.1737063 MHz
NUC1 1H
P1 12.00 usec
PLW1 21.00000000 W

F2 - Processing parameters
SI 16384
SF 600.1700275 MHz
WDW EM
SSB 0
LB 0 0.30 Hz
GB 0
PC 1.00

5-Methyl-2-(pyridine-2-yl)phenyl 4-fluorobenzoate (2f): ^{13}C NMR (150 MHz, CDCl_3)

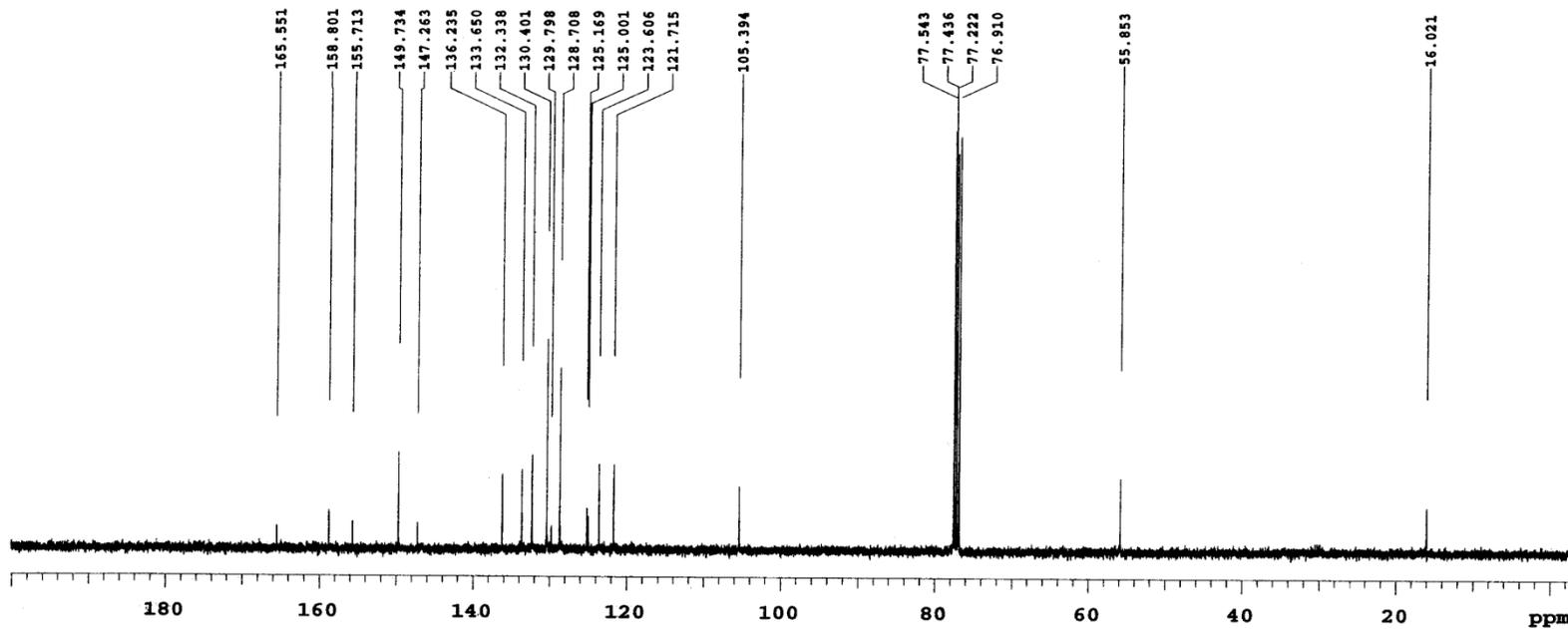
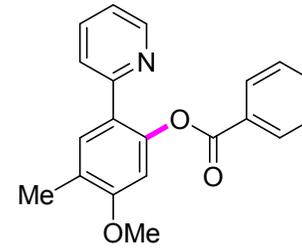
Current Data Parameters
 NAME SR-01-TF-13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140321
 Time 10.01
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl_3
 NS 392
 DS 2
 SWH 36057.691 Hz
 FIDRES 1.100393 Hz
 AQ 0.4543829 sec
 RG 65.24
 DW 13.867 usec
 DE 6.50 usec
 TE 301.6 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 150.9279571 MHz
 NUC1 ^{13}C
 P1 10.50 usec
 PLW1 95.0000000 W

===== CHANNEL f2 =====
 SFO2 600.1724007 MHz
 NUC2 ^1H
 CPDPRG[2] waltz16
 PCPD2 70.00 usec
 PLW2 21.0000000 W
 PLW12 0.61714000 W
 PLW13 0.30239999 W

F2 - Processing parameters
 SI 16384
 SF 150.9128326 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

5-Methoxy-4-methyl-2-(pyridin-2-yl)phenyl benzoate (3a):¹³C NMR (100 MHz, CDCl₃)

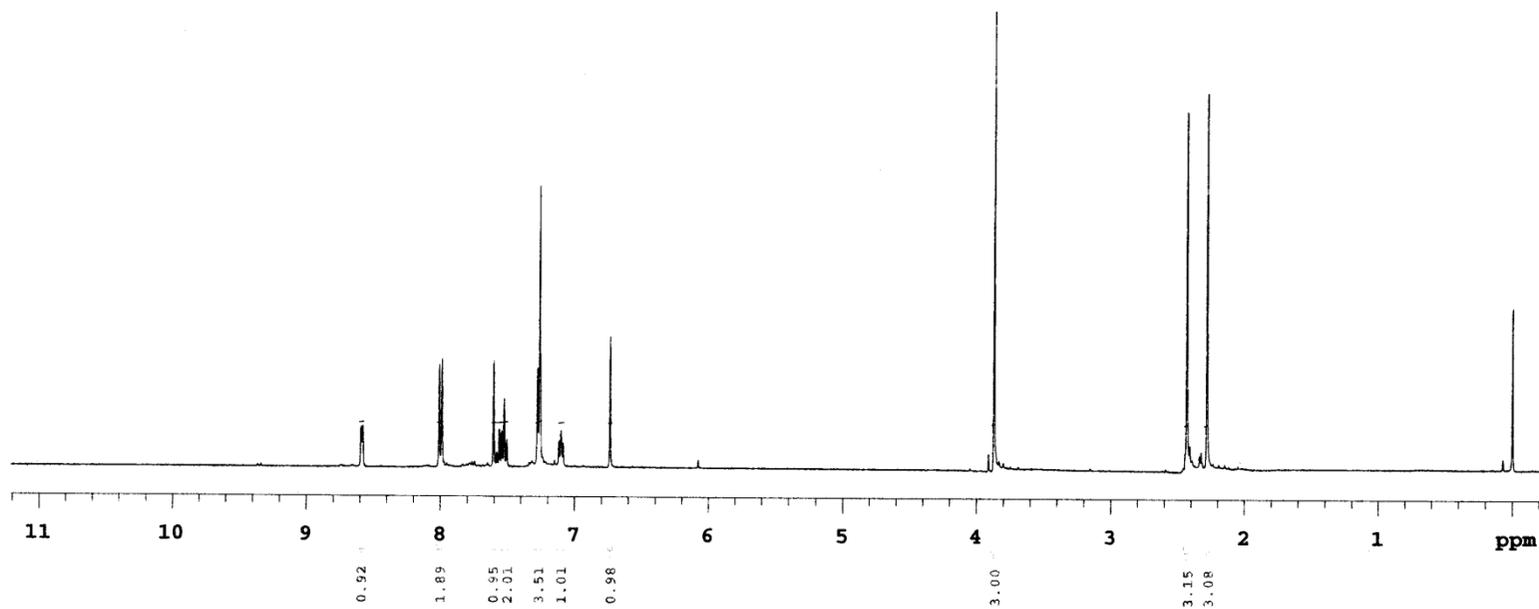
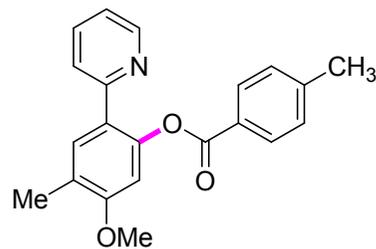
PULSE SEQUENCE: zgpg30
 Relaxation delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.304 sec
 Width 25125.6 Hz
 11200 repetitions

OBSERVED F1: 100.625817
 DECOUPLE H1, 399.8529994
 Power 42 dB
 continuously on
 WALTZ-16 modulated

DATA PROCESSING: FT-CON-13C
 Line broadening 0.5 Hz
 FT size 65536
 Total time 46 minutes

SR-01-SOM-13C

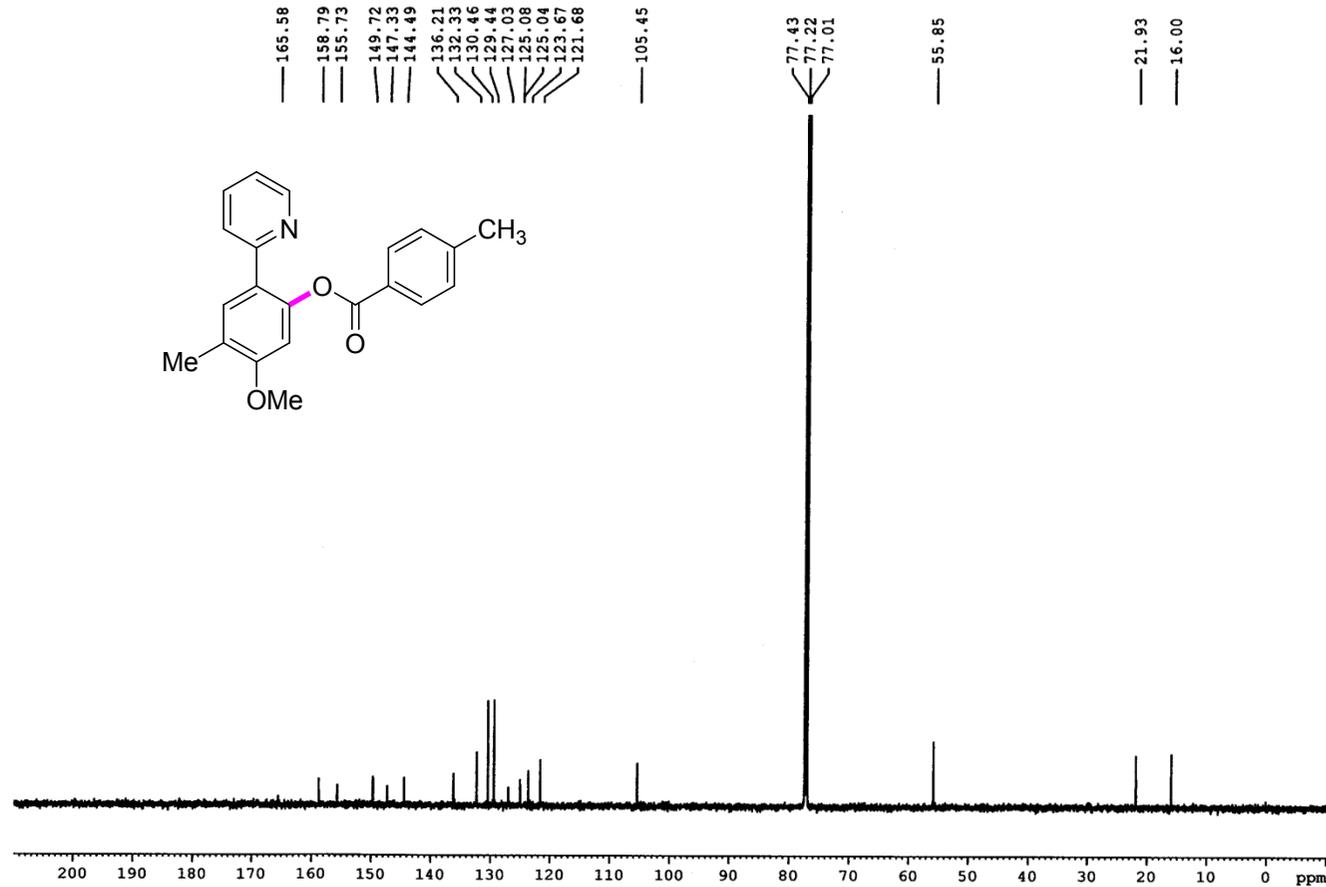
Solvent: cdcl3
 Temp. 25.0 C / 298.1 K
 Operator: chem
 Mercury-400 "IITG-NMR"

5-Methoxy-4-methyl-2-(pyridin-2-yl)phenyl 4-methylbenzoate (3c): ^1H NMR (400 MHz, CDCl_3)

PULSE SEQUENCE DATA PROCESSING OBSERVE MeH1, 399.8509625
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.561 sec
Width 6398.0 Hz
32 repetitions

DATA PROCESSING SR_01 Me2
FT size 32768
Total time 1 minutes

SR_01 Me2_1H
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: chem
Mercury-400 "IITG-NMR"

5-Methoxy-4-methyl-2-(pyridin-2-yl)phenyl 4-methylbenzoate (3c): ^{13}C NMR (150 MHz, CDCl_3)

```

Current Data Parameters
NAME      SR-01-ME2_13C
EXPNO     1
PROCNO    1

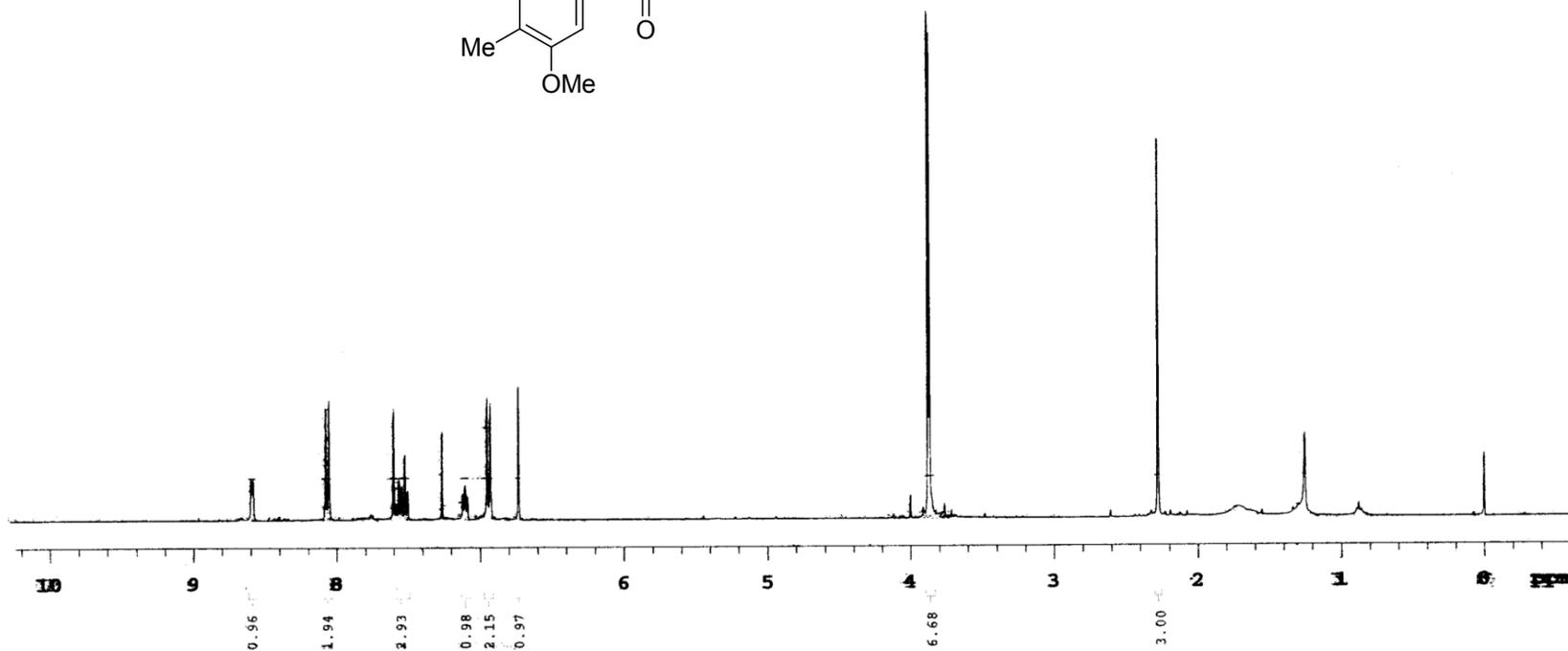
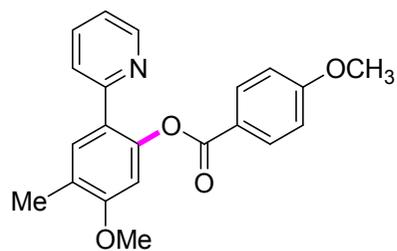
F2 - Acquisition Parameters
Date_     20140416
Time      11.13
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zgpg30
TD         32768
SOLVENT   CDCl3
NS         404
DS         2
SWH        36057.691 Hz
FIDRES     1.100393 Hz
AQ         0.4543829 sec
RG         65.24
DM         13.867 usec
DE         6.50 usec
TE         301.6 K
D1         2.00000000 sec
D11        0.03000000 sec
TDO        1

===== CHANNEL f1 =====
SFO1      150.9279571 MHz
NUC1       13C
P1         10.50 usec
PLW1       95.00000000 W

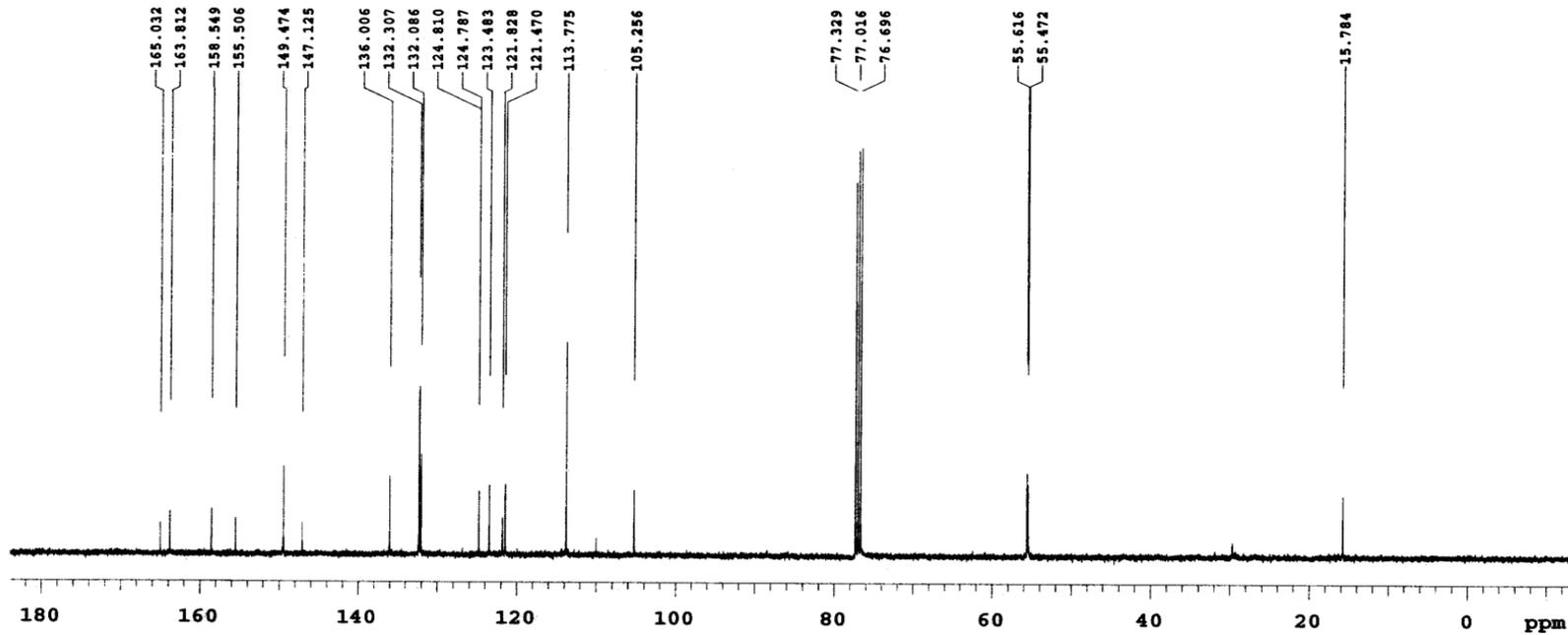
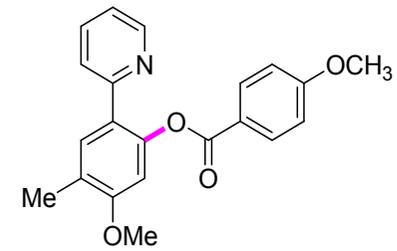
===== CHANNEL f2 =====
SFO2      600.1724007 MHz
NUC2        1H
CPDPRG2    waltz16
PCPD2      70.00 usec
PLW2       21.00000000 W
PLW12      0.61714000 W
PLW13      0.30239999 W

F2 - Processing parameters
SI         16384
SF         150.9128348 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

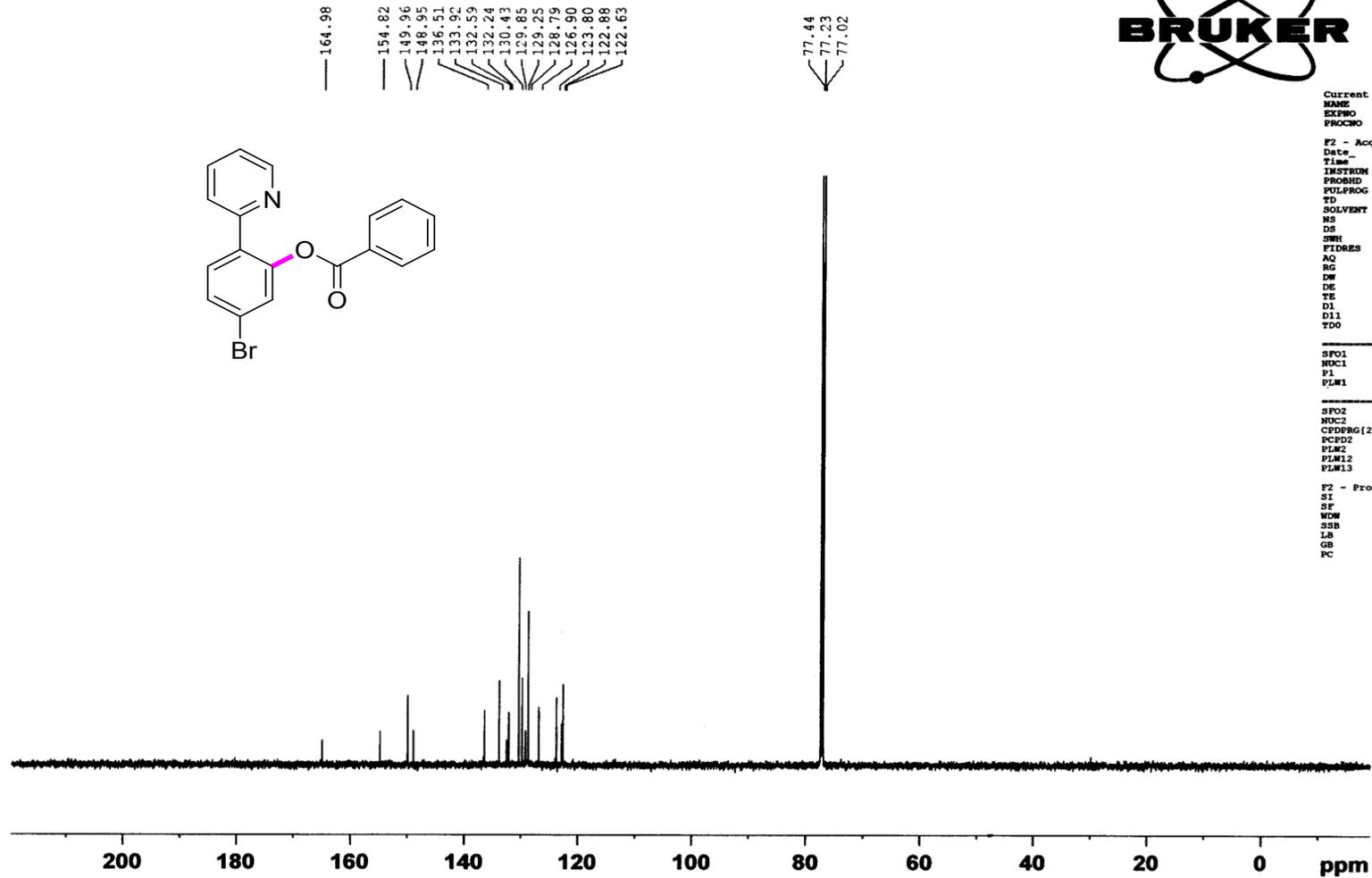
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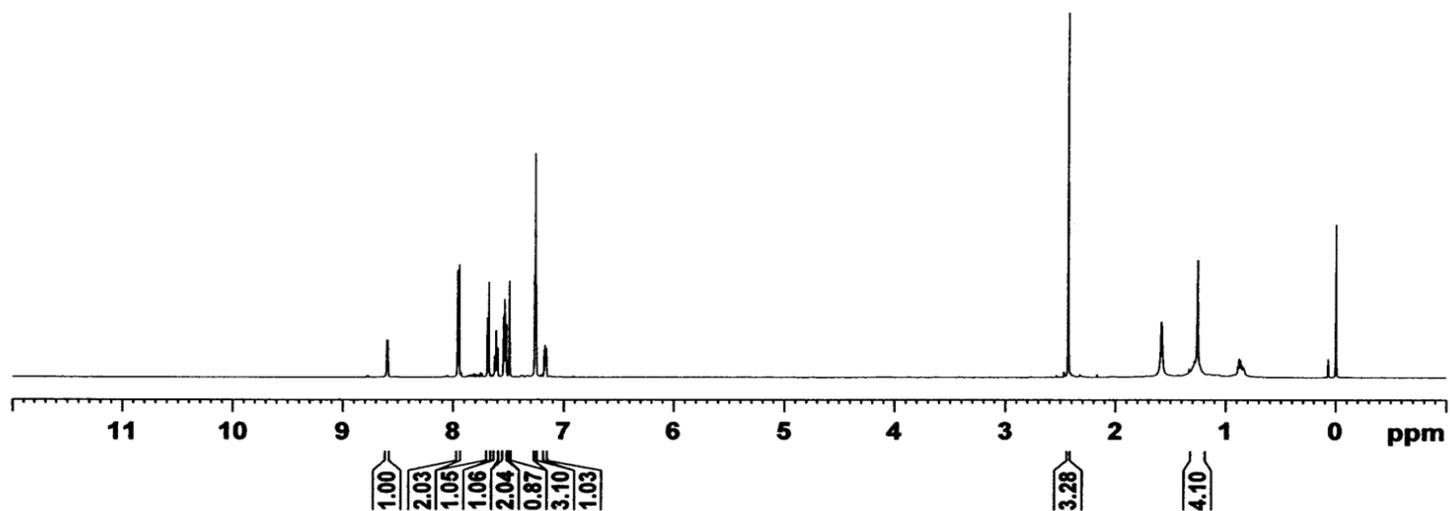
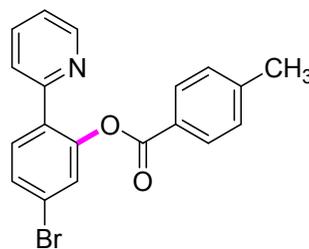
5-Methoxy-4-methyl-2-(pyridin-2-yl)phenyl 4-methoxybenzoate (3d): ^1H NMR (400 MHz, CDCl_3)

1H NMR (400 MHz, CDCl3) δ 8.5 (d, 1H, J = 2.0 Hz, H-6), 7.8 (d, 2H, J = 2.0 Hz, H-7, H-8), 7.5 (d, 2H, J = 2.0 Hz, H-9, H-10), 7.2 (d, 1H, J = 2.0 Hz, H-11), 7.1 (d, 2H, J = 2.0 Hz, H-12, H-13), 7.0 (d, 1H, J = 2.0 Hz, H-14), 3.8 (s, 3H, OCH3), 3.8 (s, 3H, OCH3).

5-Methoxy-4-methyl-2-(pyridin-2-yl)phenyl-4-methoxybenzoate (3d): ^{13}C NMR (100 MHz, CDCl_3)

<p> PULSE SEQUENCE Relax delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 2000 repetitions </p>	<p> OBSERVE C13, 100.5426047 DECOUPLE H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated </p>	<p> DATA PROCESSING Line broadening 0.5 Hz FT size 65536 Total time 76 minutes </p>	<p> SR-01-M02-13C Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 "IITG-NMR" </p>
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5-Bromo-2-(pyridin-2-yl)phenyl benzoate (4a):¹³C NMR (150 MHz, CDCl₃)

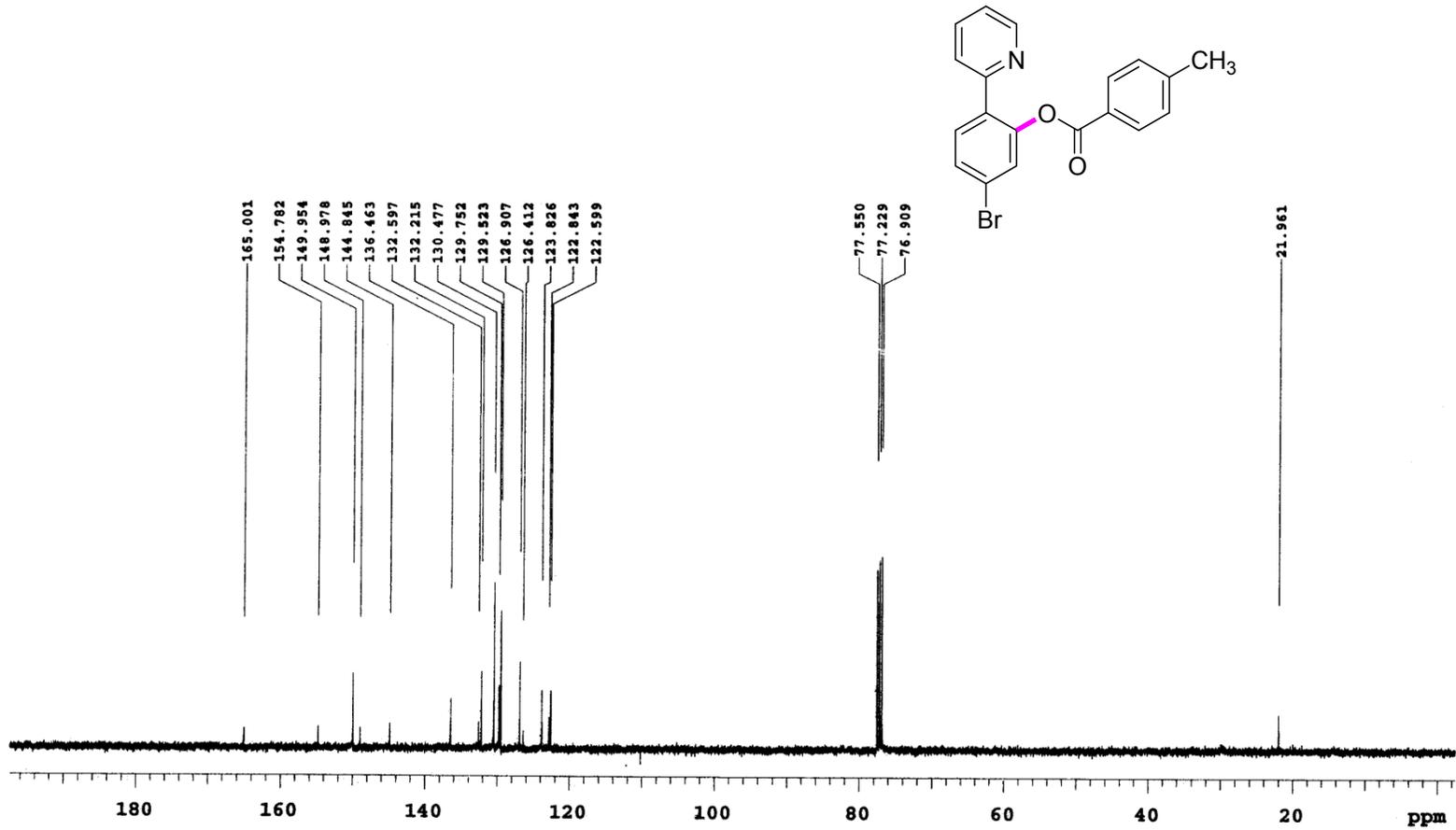
5-Bromo-2-(pyridin-2-yl)phenyl 4-methylbenzoate (4c): ^1H NMR (600 MHz, CDCl_3)

```
Current Data Parameters
NAME      SR-01-BRM-1H
EXPNO    1
PROCNO   1

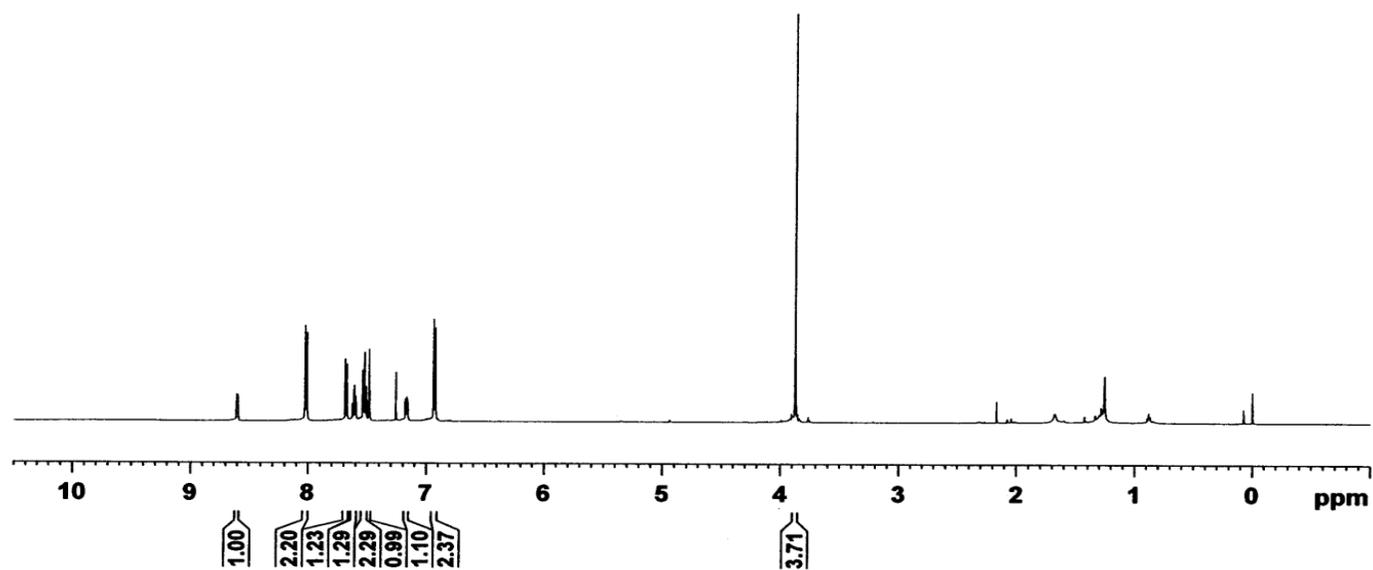
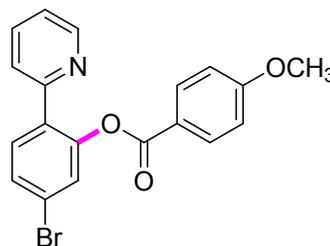
F2 - Acquisition Parameters
Date_    20140402
Time     17.05
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zg30
TD       32768
SOLVENT  CDCl3
NS       16
DS       2
SWH      12019.230 Hz
FIDRES   0.366798 Hz
AQ       1.3631488 sec
RG       127.57
DW       41.600 usec
DE       6.50 usec
TE       299.9 K
D1       1.00000000 sec
TDO      1

----- CHANNEL f1 -----
SF01    600.1737053 MHz
NUC1     1H
P1      12.00 usec
PLW1    21.00000000 W

F2 - Processing parameters
SI      16384
SF      600.1700151 MHz
WDW     EM
SSB     0
LB      0.30 Hz
GB      0
PC      1.00
```

5-Bromo-2-(pyridin-2-yl)phenyl 4-methylbenzoate (4c): ^{13}C NMR (100 MHz, CDCl_3)

PULSE SEQUENCE	OBSERVE C13, 100.5425033	DATA PROCESSING	SR-01-Brm-13c
Relax. delay 1.000 sec	DECOUPLE H1, 399.8529994	Line broadening 0.5 Hz	
Pulse 45.0 degrees	Power 42 dB	FT size 65536	Solvent: cdcl3
Acq. time 1.304 sec	continuously on	Total time 19 minutes	Temp. 25.0 C / 298.1 K
Width 25125.6 Hz	WALTZ-16 modulated		Operator: chem
516 repetitions			Mercury-400 "ITG-NMR"

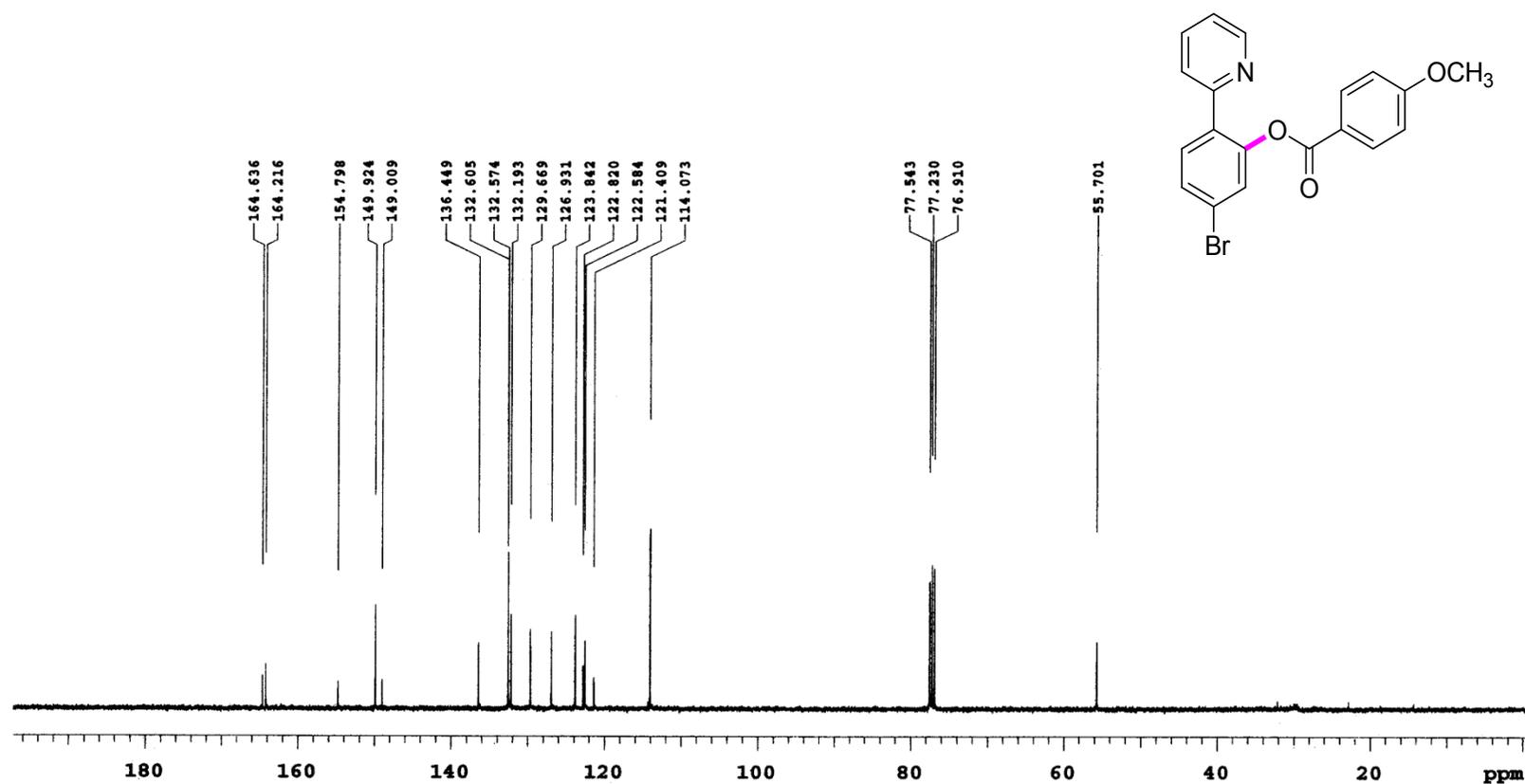
5-Bromo-2-(pyridin-2-yl)phenyl 4-methoxybenzoate (4d): ^1H NMR (600 MHz, CDCl_3)

```
Current Data Parameters
NAME      SR-01-BrO-1H
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20140327
Time      12.50
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zg30
TD         32768
SOLVENT   CDCl3
NS         16
DS         2
SWH        12019.230 Hz
FIDRES     0.366798 Hz
AQ         1.3631488 sec
RG         80.22
DW         41.600 usec
DE         6.50 usec
TE         299.3 K
D1         1.0000000 sec
TDO        1

===== CHANNEL f1 =====
SFO1      600.1737063 MHz
NUC1      1H
P1         12.00 usec
PLW1      21.0000000 W

F2 - Processing parameters
SI         16384
SF         600.1700145 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```

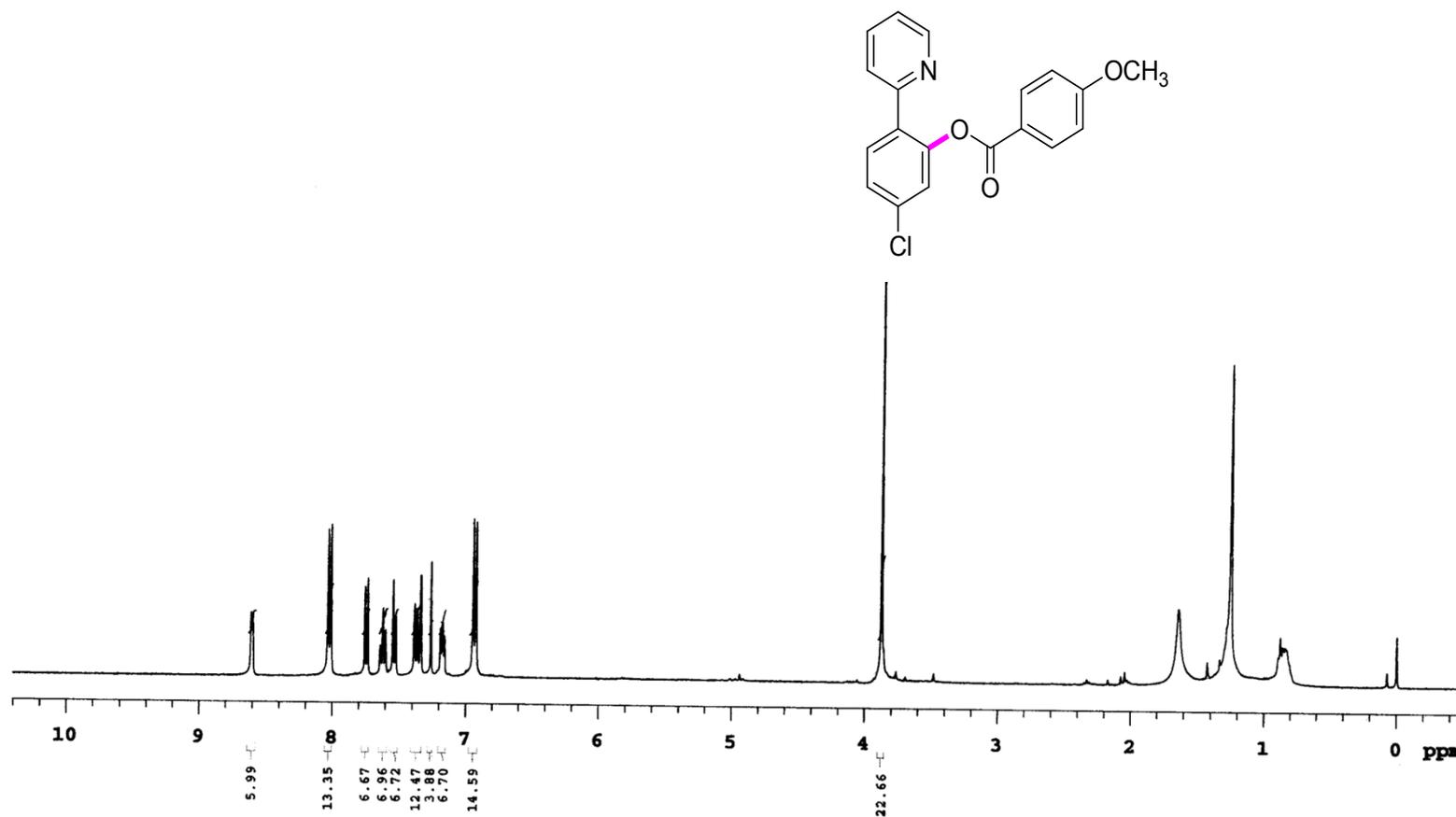
5-Bromo-2-(pyridin-2-yl)phenyl 4-methoxybenzoate (4d): ^{13}C NMR (100 MHz, CDCl_3)

DECOUPLE SEQUENCE
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.304 sec
 Width 25125.6 Hz
 1030 repetitions

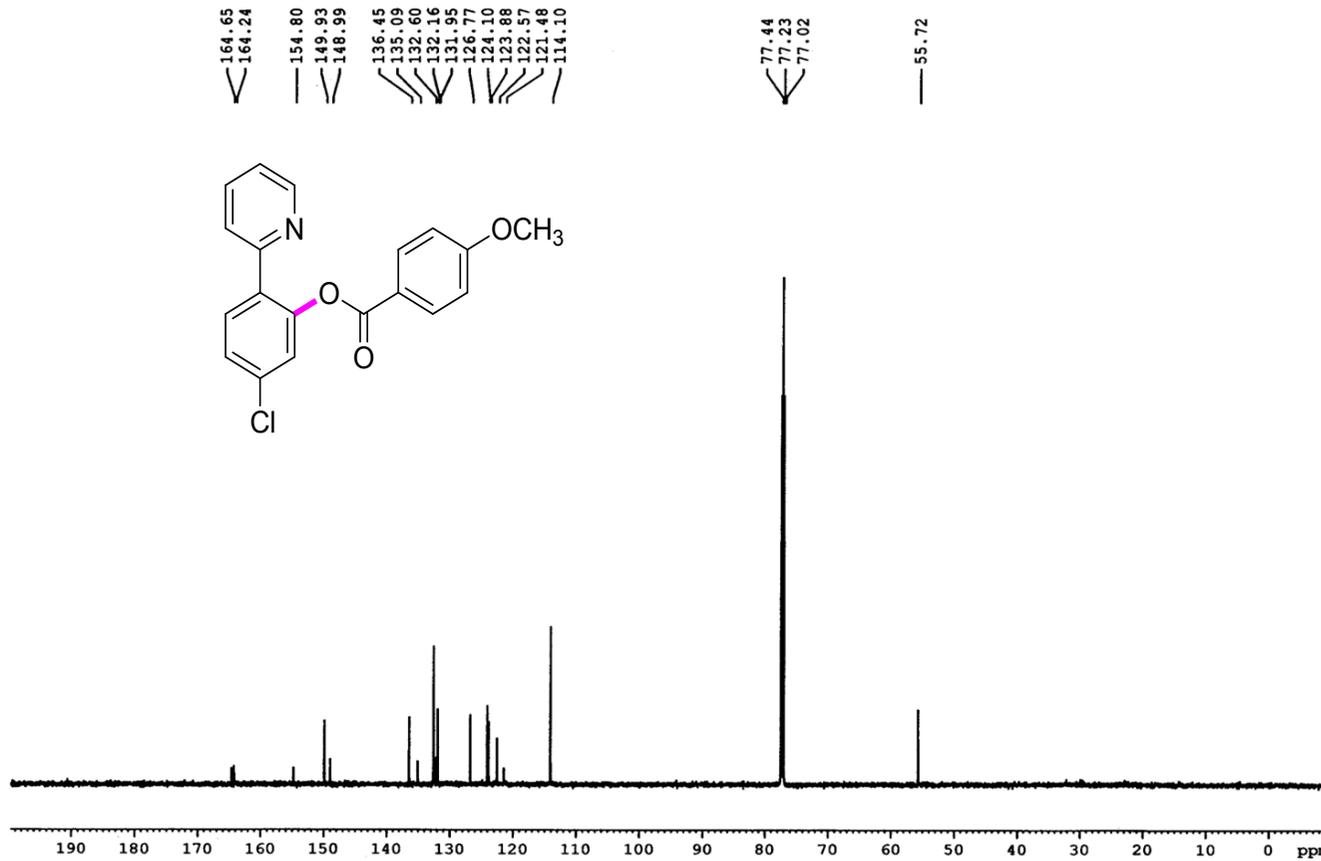
OBSERVE ^{13}C , 100.5425640
 DECOUPLE H1, 399.8529994
 Power 42 dB
 continuously on
 WALTZ-16 modulated

DATA PROCESSING SR-01-Bro-13C
 Line broadening 0.5 Hz
 FT size 65536
 Total time 39 minutes

SR-01-Bro-13C
 Solvent: cdcl3
 Temp. 25.0 C / 298.1 K
 Operator: chem
 Mercury-400 "IITG-NMR"

5-Chloro-2-(pyridin-2-yl)phenyl 4-methoxybenzoate (5d): ^1H NMR (400 MHz, CDCl_3)

NAME: 5d	DATA PROCESSING: 399:8909631	NAME: SR#01-001	DATA PROCESSING: SR#01-001
Relax. delay 1.000 sec	42768	FT size 32768	42768
Pulse 45.0 deg	1 minute	Total time 1 minute	1 minute
Acq. time 2.561 sec		solvent: cdcl3	
Width 6398.0 Hz		Temp. 25.0 C / 298.1 K	
32 repetitions		Operator: chem	
	Mercury-400	Mercury-400	Mercury-400 "IITG-NMR"

5-Chloro-2-(pyridin-2-yl)phenyl 4-methoxybenzoate (5d): ^{13}C NMR (150 MHz, CDCl_3)

```

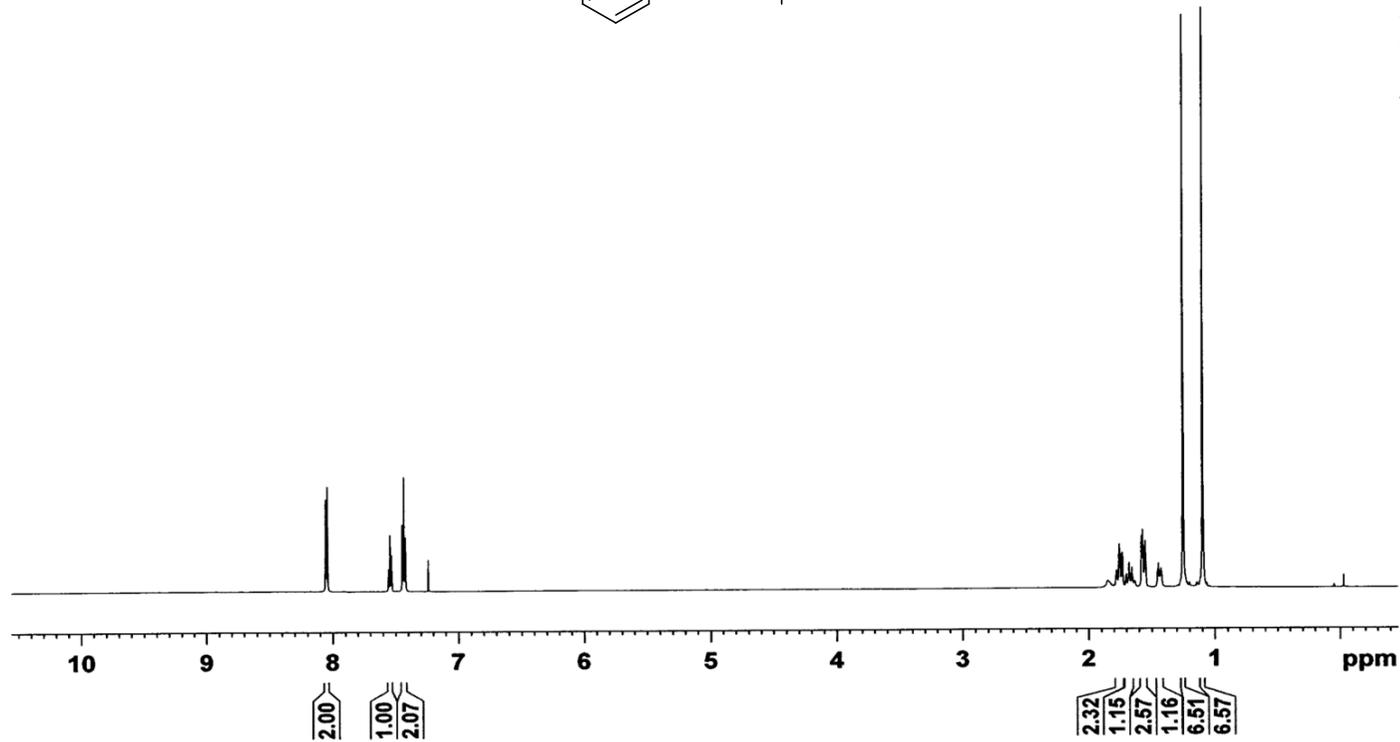
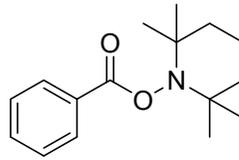
Current Data Parameters
NAME      SR-01-COM_13C
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20140606
Time      11.45
INSTRUM   spect
PROBHD    5 mm PABBO BB/
PULPROG   zgpg30
TD         32768
SOLVENT   CDCl3
NS         342
DS         2
SWH        36057.691 Hz
FIDRES     1.100393 Hz
AQ         0.4543829 sec
RG         65.24
DW         13.867 usec
DE         6.50 usec
TE         300.8 K
D1         2.0000000 sec
D11        0.0300000 sec
TD0        1

===== CHANNEL f1 =====
SFO1      150.9279571 MHz
NUC1       13C
P1         10.50 usec
PLW1       95.0000000 W

===== CHANNEL f2 =====
SFO2      600.1724007 MHz
NUC2       1H
CPDPRG[2] waltz16
PCPD2      70.00 usec
PLW2       21.0000000 W
PLW12      0.61714000 W
PLW13      0.30239999 W

F2 - Processing parameters
SI         16384
SF         150.9128348 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
  
```

2,2,6,6-Tetramethylpiperidin-1-yl benzoate (F): ^1H NMR (600 MHz, CDCl_3)

```

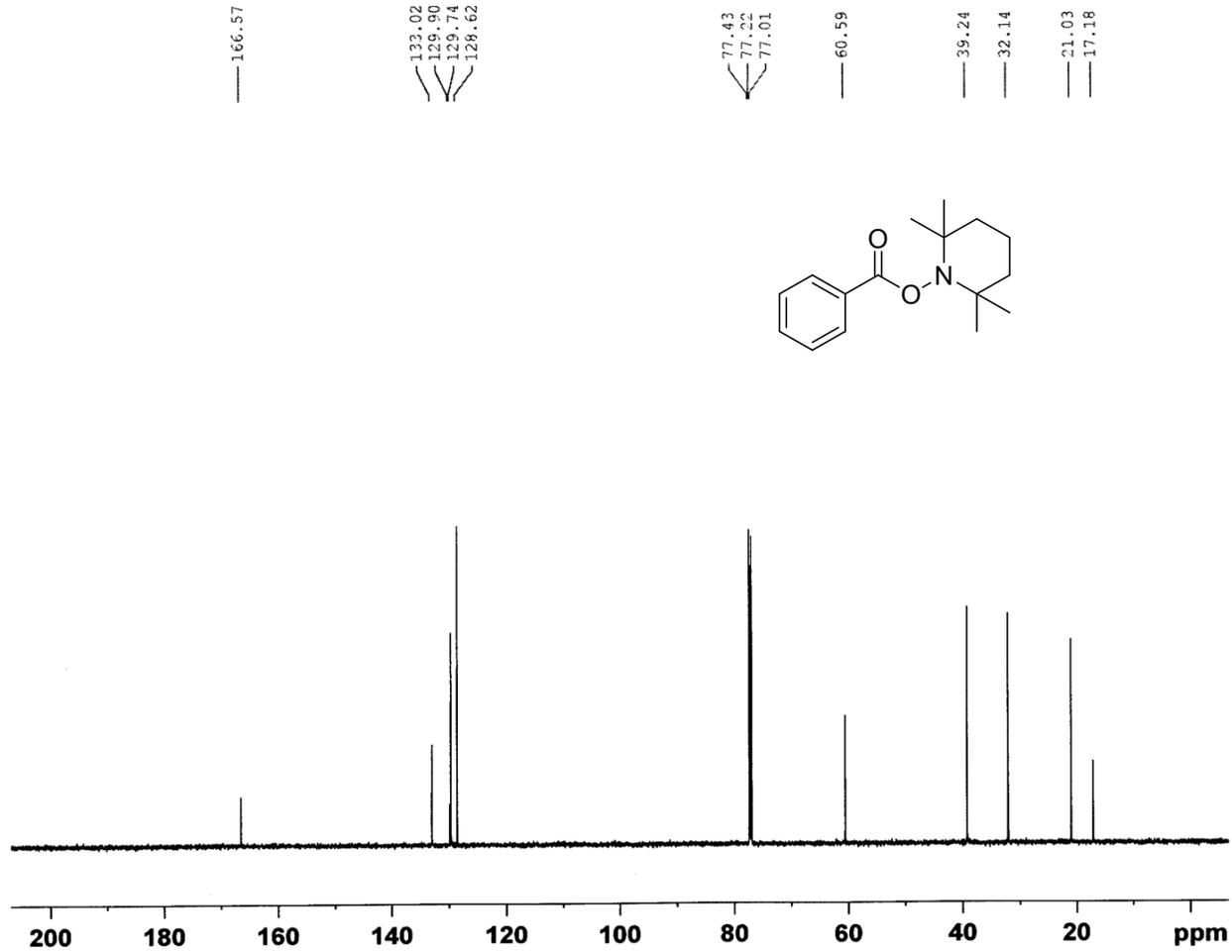
Current Data Parameters
NAME      SG-TEM-US-1H
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20131109
Time     10.51
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zg30
TD       32768
SOLVENT  CDCl3
NS       16
DS       2
SWH      12019.230 Hz
FIDRES   0.366798 Hz
AQ       1.3631488 sec
RG       34.76
DW       41.600 usec
DE       6.50 usec
TE       298.9 K
D1       1.00000000 sec
TDO      1

----- CHANNEL f1 -----
SF01    600.1737063 MHz
NUC1     1H
P1       12.00 usec
PLW1     21.00000000 W

F2 - Processing parameters
SI       16384
SF       600.1700268 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00

```

2,2,6,6-Tetramethylpiperidin-1-yl benzoate (F): ^{13}C NMR (150 MHz, CDCl_3)

Current Data Parameters
 NAME SG-TEM-US-13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20131109
 Time 10.59
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl_3
 NS 65
 DS 2
 SWH 36057.691 Hz
 FIDRES 1.100393 Hz
 AQ 0.4543829 sec
 RG 65.24
 DW 13.867 usec
 DE 6.50 usec
 TE 299.3 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 150.9279571 MHz
 NUC1 13C
 P1 10.50 usec
 PLW1 95.00000000 W

===== CHANNEL f2 =====
 SFO2 600.1724007 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 70.00 usec
 PLW2 21.00000000 W
 PLW12 0.61714000 W
 PLW13 0.30239999 W

F2 - Processing parameters
 SI 16384
 SF 150.9128415 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40