Supporting Informations

A metal free domino synthesis of 3-aroylindoles via two sp^3 C-H activation

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General information:

All the reagents were commercial grade and used without purification. 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 F_{254} (0.25mm). NMR spectra were recorded in $CDCl_3$ with tetramethylsilane as the internal standard for ^1H NMR (600 MHz), $CDCl_3$ solvent as the internal standard for ^{13}C NMR (150 MHz). HRMS spectra were recorded using ESI mode. IR spectra were recorded in KBr or neat.

Crystallographic Description:

Crystal data were collected with Bruker Smart Apex-II CCD diffractometer using graphite monochromated MoKα radiation (λ = 0.71073 Å) at 298 K. Cell parameters were retrieved using SMART [a] software and refined with SAINT[a] on all observed reflections. Data reduction was performed with the SAINT software and corrected for Lorentz and polarization effects. Absorption corrections were applied with the program SADABS[b]. The structure was solved by direct methods implemented in SHELX-97[c] program and refined by full-matrix

least-squares methods on F2. All non-hydrogen atomic positions were located in difference Fourier maps and refined anisotropically. The hydrogen atoms were placed in their geometrically generated positions. Colourless crystals were isolated in rectangular shape from methanol at room temperature.

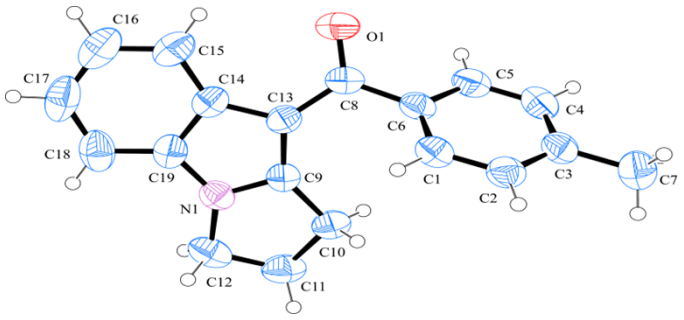
a. SMART V 4.043 Software for the CCD Detector System; Siemens Analytical Instruments Division: Madison, WI, 1995.

b. SAINT V 4.035 Software for the CCD Detector System; Siemens Analytical Instruments Division: Madison, WI, 1995.

c. Sheldrick, G. M. SHELXL-97, Program for the Refinement of Crystal Structures; University of Göttingen: Göttingen (Germany), 1997.

Crystallographic description of (2,3-Dihydro-1*H*-pyrrolo[1,2-a]indol-9-yl)(p-tolyl)methanone (5'g):

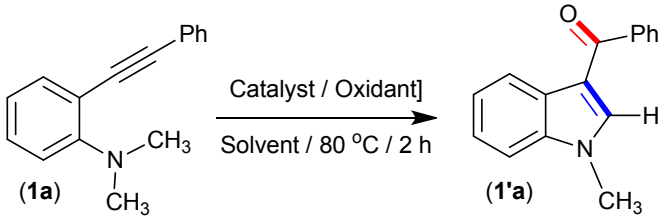
$C_{19}H_{17}NO$, crystal dimensions 0.41 x 0.35 x 0.28 mm, M_r = 275.34, Triclinic, space group P-1, a = 7.5607(4), b = 9.6755(6), c = 11.352(1) Å, α = 107.554(5) °, β = 102.789(5) °, γ = 103.850(4) °, V = 729.07(10) Å^3, Z = 2, ρ_{calcd} = 1.254 mg/m^3, μ = 0.077 mm^{-1}, $F(000)$ = 292.0, reflection collected / unique = 3682 / 2529, refinement method = full-matrix least-squares on F^2, final R indices [$I > 2\sigma(I)$]: R_1 = 0.0487, wR_2 = 0.1733, R indices (all data): R_1 = 0.0634, wR_2 = 0.1981, goodness of fit = 0.932. CCDC-1006843 for (2,3-Dihydro-1*H*-pyrrolo[1,2-a]indol-9-yl)(p-tolyl)methanone (**5'g**) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.



(2,3-Dihydro-1*H*-pyrrolo[1,2-a]indol-9-yl)(p-tolyl)methanone (5'g)

General procedure for the synthesis of (1-methyl-1*H*-indol-3-yl)(phenyl)methanone (1'a): To a solution of *N*, *N*-dimethyl-2-(phenylethynyl) aniline (**1a**) (55.28 mg, 0.25 mmol) in DMSO (1 mL) was added TBAI (18.47 mg, 0.05 mmol), followed by TBHP 70 % wt in water (180 µl, 1.25 mmol) and the resultant mixture was put into a preheated oil bath (80 ^{o}C) for 2 h. The resultant reaction mixture was admixed with water (5 mL) and the product was extracted with ethyl acetate (2 x 20 mL). The organic phase was dried over anhydrous sodium sulphate and concentrated in vacuo. The crude product was purified over a column of silica gel and eluted with (9:1 hexane / ethyl acetate to give (1-methyl-1*H*-indol-3-yl)(phenyl)methanone (**1'a**) (43.53 mg, 74 % yield).

Table S1. Screening of Reaction Conditions[a,b]

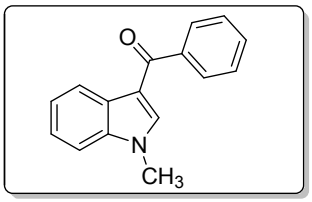


Entry	Catalyst (mol%)	Oxidant (equiv)	Solvent	Yield %
1	TBAI (20)	TBHP[c] (3)	DMSO	52
2	TBAI (20)	TBHP[c] (4)	DMSO	59
3	**TBAI (20)**	**TBHP[c] (5)**	**DMSO**	**74**
4	KI (20)	TBHP[c] (5)	DMSO	64
5	I_2 (20)	TBHP[c] (5)	DMSO	49
6	TBAB (20))	TBHP[c] (5)	DMSO	58
7	TBAI (20)	TBHP[d] (5)	DMSO	69
8	TBAI (20)	DTBP (5)	DMSO	<5
9	TBAI (20)	H_2O_2[e] (5)	DMSO	22
10	TBAI (20)	TBHP[c] (5)	DMF	62
11	TBAI (20)	TBHP[c] (5)	Toluene	46
12	TBAI (20)	TBHP[c] (5)	1,4-Dioxane	54
13	TBAI (20)	TBHP[c] (5)	DCE	37
14	TBAI (15)	TBHP[c] (5)	DMSO	56
15	TBAI (20)		DMSO	0
16		TBHP[c] (5)	TBHP[c] (5)	0

[a]Reaction conditions: *N*, *N*-dimethyl-2-(phenylethynyl) aniline (**1a**) (0.25 mmol), time 2 h, temperature 80 ^{o}C. [b]Isolated yield. [c]70% aqueous solution. [d]Decane solution (5-6 M). [e]50% aqueous solution.

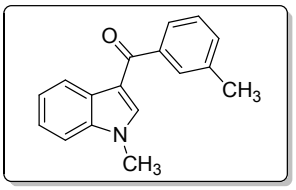
Spectral Data

(1-Methyl-1*H*-indol-3-yl)(phenyl)methanone (1′a):



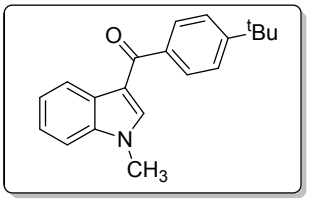
^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 3.79 (s, 3H), 7.32–7.33 (m, 3H), 7.46 (t, 2H, *J* = 7.2 Hz), 7.48 (s, 1H), 7.52 (t, 1H, *J* = 7.2 Hz), 7.79 (d, 2H, *J* = 7.2 Hz), 8.41–8.43 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 33.7, 109.8, 115.7, 122.8, 122.9, 123.8, 127.4, 128.4, 128.8, 131.2, 137.7, 138.1, 141.1, 191.0; IR (KBr): 2923, 2851, 1621, 1575, 1524, 1465, 1368, 1233, 1155, 1124, 1070, 872, 746, 716 cm^{-1}; HRMS (ESI): calcd. for $C_{16}H_{13}NO$ (MH^+) 236.1070; found 236.1077.

(1-Methyl-1*H*-indol-3-yl)(m-tolyl)methanone (1′b):



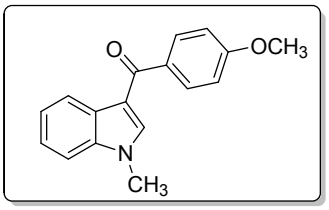
^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 2.42 (s, 3H), 3.83 (s, 3H), 7.32–7.36 (m, 5H), 7.51 (s, 1H), 7.57–7.59 (m, 1H), 7.61 (s, 1H), 8.40–8.41 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 21.6, 33.7, 109.8, 116.0, 122.9, 123.0, 123.8, 126.1, 127.4, 128.2, 129.4, 132.0, 137.8, 138.0, 138.3, 141.2, 191.3; IR (KBr): 2950, 2924, 2857, 1617, 1587, 1521, 1465, 1367, 1268, 1241, 1202, 1120, 1070, 751 cm^{-1}; HRMS (ESI): calcd. for $C_{17}H_{15}NO$ (MH^+) 250.1226; found 250.1232.

(4-(*tert*-Butyl)phenyl)(1-methyl-1*H*-indol-3-yl)methanone (1′c):



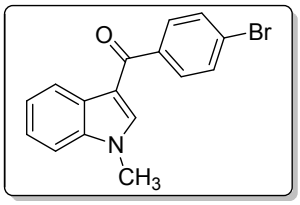
^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 1.36 (s, 9H), 3.82 (s, 3H), 7.32–7.35 (m, 3H), 7.48 (d, 2H, *J* = 8.4 Hz), 7.55 (s, 1H), 7.76 (d, 2H, *J* = 8.4 Hz), 8.42–8.44 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 31.5, 33.7, 35.2, 109.7, 115.9, 122.8, 123.0, 123.8, 125.4, 127.5, 128.9, 137.7, 137.9, 138.4, 154.8, 190.8; IR (KBr): 2963, 1689, 1612, 1524, 1464, 1367, 1268, 1235, 1185, 1125, 881, 745, 709 cm^{-1}; HRMS (ESI): calcd. for $C_{20}H_{21}NO$ (MH^+) 292.1696; found 292.1693.

(4-Methoxyphenyl)(1-methyl-1*H*-indol-3-yl)methanone (1′d):



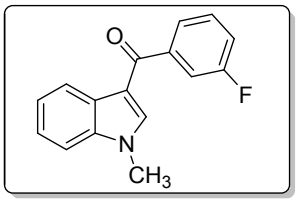
^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 3.80 (s, 3H), 3.85 (s, 3H), 6.95 (d, 2H, *J* = 8.4 Hz), 7.29–7.34 (m, 3H), 7.50 (s, 1H), 7.81 (d, 2H, *J* = 9.0 Hz), 8.35–8.37 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 33.6, 55.6, 109.7, 113.7, 115.8, 122.6, 122.8, 123.6, 127.5, 131.0, 133.6, 137.3, 137.6, 162.3, 189.9; IR (KBr): 3042, 2917, 1614, 1599, 1567, 1528, 1505, 1461, 1371, 1252, 1234, 1169, 1151, 1122, 1023, 878, 845, 748 cm^{-1}; HRMS (ESI): calcd. for $C_{17}H_{15}NO_2$ (MH^+) 266.1176; found 266.1172.

(4-Bromophenyl)(1-methyl-1*H*-indol-3-yl)methanone (1′e):



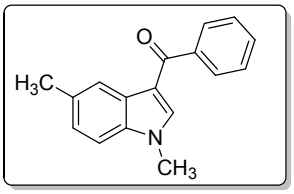
^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 3.79 (s, 3H), 7.31–7.33 (m, 3H), 7.45 (s, 1H), 7.57 (d, 2H, *J* = 7.8 Hz), 7.64 (d, 2H, *J* = 8.4 Hz), 8.36–8.38 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 33.7, 109.9, 115.4, 122.7, 123.0, 123.9, 125.8, 127.2, 130.4, 131.6, 137.7, 137.9, 139.7, 189.6; IR (KBr): 3081, 2925, 1624, 1582, 1520, 1459, 1395, 1370, 1266, 1233, 1155, 1125, 1070, 1034, 1003, 877, 840, 772, 751 cm^{-1}; HRMS (ESI): calcd. for $C_{16}H_{12}BrNO$ (MH^+) 314.0175; found 314.0184.

(3-Fluorophenyl)(1-methyl-1*H*-indol-3-yl)methanone (1′f):



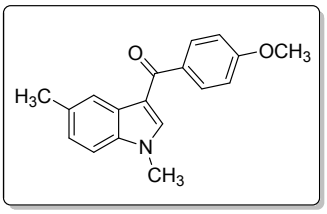
^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 3.85 (s, 3H), 7.23–7.26 (m, 1H), 7.34–7.38 (m, 3H), 7.43–7.47 (m, 1H), 7.50 (d, 1H, *J* = 9.0 Hz), 7.52 (s, 1H), 7.59 (d, 1H, *J* = 7.2 Hz), 8.40–8.42 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 33.8, 109.9, 115.5, 115.7, 115.8, 118.1, 118.2, 122.9, 123.1, 124.1, 124.5, 127.3, 130.1, 130.2, 137.8, 138.1, 143.17, 143.21, 161.9, 163.6, 189.3; IR (KBr): 3050, 2923, 1621, 1578, 1522, 1468, 1426, 1395, 1369, 1266, 1244, 1024, 1152, 1126, 1113, 1080, 833, 828, 769, 753 cm^{-1}; HRMS (ESI): calcd. for $C_{16}H_{12}FNO$ (MH^+) 254.0976; found 254.0980.

(1,5-Dimethyl-1*H*-indol-3-yl)(phenyl)methanone (2′a):



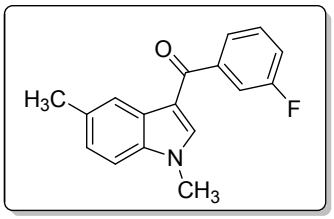
^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 2.50 (s, 3H), 3.77 (s, 3H), 7.16 (d, 1H, *J* = 8.4 Hz), 7.23 (t, 1H, *J* = 6.6 Hz), 7.43–7.47 (m, 3H), 7.51 (t, 1H, *J* = 7.8 Hz), 7.78 (d, 2H, *J* = 7.2 Hz), 8.26 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 21.7, 33.7, 109.4, 115.3, 122.6, 125.3, 127.6, 128.4, 128.8, 131.1, 132.6, 136.1, 138.2, 141.2, 191.0; IR (KBr): 3058, 2918, 1623, 1574, 1484, 1459, 1387, 1364, 1269, 1237, 1146, 1120, 1068, 1021, 907, 837, 795, 758, 718 cm^{-1}; HRMS (ESI): calcd. for $C_{17}H_{15}NO$ (MH^+) 250.1226; found 250.1222.

(1,5-Dimethyl-1*H*-indol-3-yl)(4-methoxyphenyl)methanone (2′d):



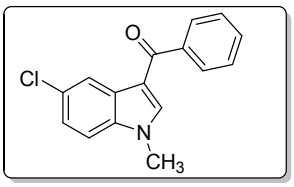
^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 2.50 (s, 3H), 3.83 (s, 3H), 3.89 (s, 3H), 6.98 (d, 2H, *J* = 8.4 Hz), 7.17 (d, 1H, *J* = 7.8 Hz), 7.25–7.26 (m, 1H), 7.49 (s, 1H), 7.83 (d, 2H, *J* = 8.4 Hz), 8.21 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 21.8, 33.7, 55.6, 109.4, 113.7, 115.5, 122.6, 125.3, 127.8, 131.0, 132.4, 133.9, 136.1, 137.4, 162.3, 190.0; IR (KBr): 2956, 2923, 1614, 1596, 1523, 1508, 1451, 1363, 1304, 1254, 1163, 1116, 1060, 1021, 910, 844, 775 cm^{-1}; HRMS (ESI): calcd. for $C_{18}H_{17}NO_2$ (MH^+) 280.1332; found 280.1335.

(1,5-Dimethyl-1*H*-indol-3-yl)(3-fluorophenyl)methanone (2′f):



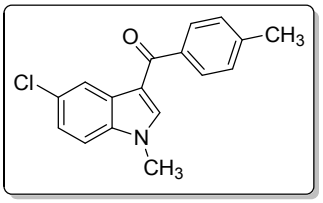
^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 2.52 (s, 3H), 3.82 (s, 3H),7.19 (d, 1H, *J* = 9.0 Hz), 7.22–7.25 (m, 1H), 7.26 (d, 1H, *J* = 8.4 Hz), 7.43–7.46 (m, 1H), 7.47 (s, 1H), 7.48–7.50 (m, 1H), 7.58 (d, 1H, *J* = 7.8 Hz), 8.25 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 21.7, 33.8, 109.6, 115.0, 115.6, 115.8, 118.0, 118.1, 122.6, 124.5, 125.6, 127.5, 130.09, 130.14, 132.9, 136.2, 138.2, 143.3, 143.4, 161.9, 163.6, 189.3; IR (KBr): 2922, 1624, 1581, 1523, 1482, 1452, 1428, 1364, 1269, 1244, 1206, 1149, 1116, 1065, 1032, 941, 893, 809, 792, 765, 739 cm^{-1}; HRMS (ESI): calcd. for $C_{17}H_{14}FNO$ (MH^+) 268.1132; found 268.1137.

(5-Chloro-1-methyl-1*H*-indol-3-yl)(phenyl)methanone (3′a):



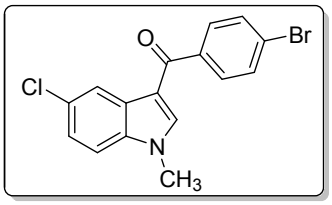
^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 3.82 (s, 3H), 7.24–7.28 (m, 2H), 7.48 (t, 2H, *J* = 7.8 Hz), 7.51 (s, 1H), 7.56 (t, 1H, *J* = 7.2 Hz), 7.78 (d, 2H, *J* = 7.2 Hz), 8.43 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 33.9, 110.9, 115.3, 122.4, 124.2, 128.4, 128.5, 128.8, 128.9, 131.5, 136.1, 138.8, 140.7, 190.7; IR (KBr): 3050, 2928, 1610, 1598, 1575, 1528, 1470, 1449, 1362, 1235, 1179, 1082, 1023, 891, 812, 717, 698 cm^{-1}; HRMS (ESI): calcd. for $C_{16}H_{12}ClNO$ (MH^+) 270.0680; found 270.0678.

(5-Chloro-1-methyl-1*H*-indol-3-yl)(p-tolyl)methanone (3′g):



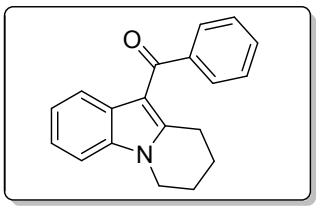
^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 2.44 (s, 3H), 3.82 (s, 3H), 7.25-7.28 (m, 4H), 7.52 (s, 1H), 7.70 (d, 2H, *J* = 6.6 Hz), 8.41 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 21.7, 33.9, 110.8, 115.4, 122.4, 124.1, 128.4, 128.8, 128.9, 129.2, 136.0, 137.9, 138.5, 142.0, 190.4; IR (KBr): 3056, 2917, 1614, 1601, 1566, 1525, 1471, 1448, 1368, 1236, 1182, 1144, 1131, 1082, 1034, 892, 873, 838, 787, 763, 740, 702 cm^{-1}; HRMS (ESI): calcd. for $C_{17}H_{14}ClNO$ (MH^+) 284.0837; found 284.0841.

(4-Bromophenyl)(5-chloro-1-methyl-1*H*-indol-3-yl)methanone (3′e):



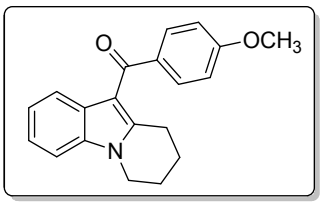
^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 3.84 (s, 3H), 7.26–7.30 (m, 2H), 7.49 (s, 1H), 7.61 (d, 2H, *J* = 9.0 Hz), 7.66 (d, 2H, *J* = 8.4 Hz), 8.39 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 34.0, 110.9, 115.1, 122.4, 124.4, 126.2, 128.3, 129.2, 130.4, 131.8, 136.2, 138.5, 139.4, 189.3; IR (KBr): 3056, 2924, 1605, 1586, 1525, 1470, 1364, 1234, 1085, 1033, 1010, 892, 842, 811, 765, 741 cm^{-1}; HRMS (ESI): calcd. for $C_{16}H_{11}BrClNO$ (MH^+) 347.9785; found 347.9782.

Phenyl(6,7,8,9-tetrahydropyrido[1,2-a]indol-10-yl)methanone (4′a):



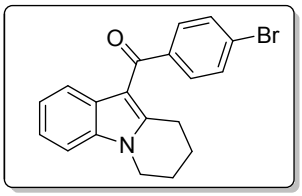
^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 1.87–1.92 (m, 2H), 2.09–2.13 (m, 2H), 3.15(t, 2H, *J* = 6.6 Hz), 4.11 (t, 2H, *J* = 6.6 Hz), 7.07 (t, 1H, *J* = 6.6 Hz), 7.18 (t, 1H, *J* = 7.2 Hz), 7.28–7.30 (m, 2H), 7.43 (t, 2H, *J* = 7.8 Hz), 7.51 (t, 1H, *J* = 7.8 Hz), 7.71 (d, 2H, *J* = 7.2 Hz); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 20.4, 22.7, 25.4, 42.8, 109.2, 112.3, 121.1, 121.9, 122.1, 127.2, 128.4, 128.8, 131.2, 136.3, 142.1, 146.5, 192.6; IR (KBr): 3055, 2928, 1617, 1511, 1487, 1472, 1456, 1437, 1419, 1374, 1315, 1225, 1160, 1057, 929, 880, 740, 731 cm^{-1}; HRMS (ESI): calcd. for $C_{19}H_{17}NO$ (MH^+) 276.1383; found 276.1385.

(4-Methoxyphenyl)(6,7,8,9-tetrahydropyrido[1,2-a]indol-10-yl)methanone (4′d):



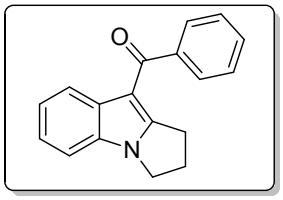
^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 1.87–1.91 (m, 2H), 2.09–2.13 (m, 2H), 3.16 (t, 2H, *J* = 6.6 Hz), 3.87 (s, 3H), 4.10 (t, 2H, *J* = 6.6 Hz), 6.92 (d, 2H, *J* = 9.0 Hz), 7.08 (t, 1H, *J* = 7.8 Hz), 7.17 (t, 1H, *J* = 7.8 Hz), 7.28 (d, 1H, *J* = 7.8 Hz), 7.36 (d, 1H, *J* = 8.4 Hz), 7.75 (d, 2H, *J* = 8.4 Hz); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 20.5, 22.8, 25.3, 42.7, 55.6, 109.2, 112.4, 113.5, 121.1, 121.7, 121.8, 127.3, 131.4, 134.4, 136.2, 145.7, 162.5, 191.5; IR (KBr): 2926, 1601, 1510, 1557, 1422, 1373, 1318, 1252, 1230, 1161, 1059, 933, 928, 884, 840, 779, 746 cm^{-1}; HRMS (ESI): calcd. for $C_{20}H_{19}NO_2$ (MH^+) 306.1489; found 306.1493.

(4-Bromophenyl)(6,7,8,9-tetrahydropyrido[1,2-a]indol-10-yl)methanone (4′e):



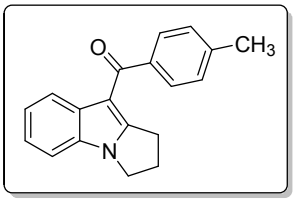
^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 1.91–1.95 (m, 2H), 2.12–2.16 (m, 2H), 3.18 (t, 2H, *J* = 6.6 Hz), 4.13 (t, 2H, *J* = 6.0 Hz), 7.10 (t, 1H, *J* = 7.8 Hz), 7.20 (t, 1H, *J* = 7.2 Hz), 7.26 (d, 1H, *J* = 4.2 Hz), 7.31 (d, 1H, *J* = 7.8 Hz), 7.60 (q, 4H, *J* = 8.4 Hz); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 20.3, 22.7, 25.5, 42.8, 109.3, 112.0, 121.0, 122.1, 122.3, 125.9, 127.0, 130.6, 131.7, 136.4, 140.8, 146.9, 191.2; IR (KBr): 2934, 1614, 1587, 1505, 1491, 1455, 1413, 1392, 1361, 1320, 1272, 1221, 1162, 1069, 1011, 929, 884, 836, 769, 746, 735 cm^{-1}; HRMS (ESI): calcd. for $C_{19}H_{16}BrNO$ (MH^+) 354.0488; found 354.0485.

(2,3-Dihydro-1*H*-pyrrolo[1,2-a]indol-9-yl)(phenyl)methanone (5′a):



^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 2.56 (quin, 2H, *J* = 7.2 Hz), 2.87 (t, 2H, *J* = 7.2 Hz), 4.12 (t, 2H, *J* = 7.2 Hz), 7.21–7.25 (m, 2H), 7.26–7.28 (m, 1H), 7.44–7.47 (m, 2H), 7.50–7.53 (m, 1H), 7.68–7.69 (m, 2H), 8.03–8.05 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 26.9, 27.1, 44.6, 109.5, 109.9, 122.4, 122.5, 128.1, 128.3, 130.8, 131.5, 133.3, 142.0, 153.6, 191.9; IR (KBr): 3049, 2928, 1608, 1570, 1508, 1451, 1437, 1420, 1384, 1304, 1215, 1043, 1009, 960, 927, 841, 746 cm^{-1}; HRMS (ESI): calcd. for $C_{18}H_{15}NO$ (MH^+) 262.1226; found 262.1221.

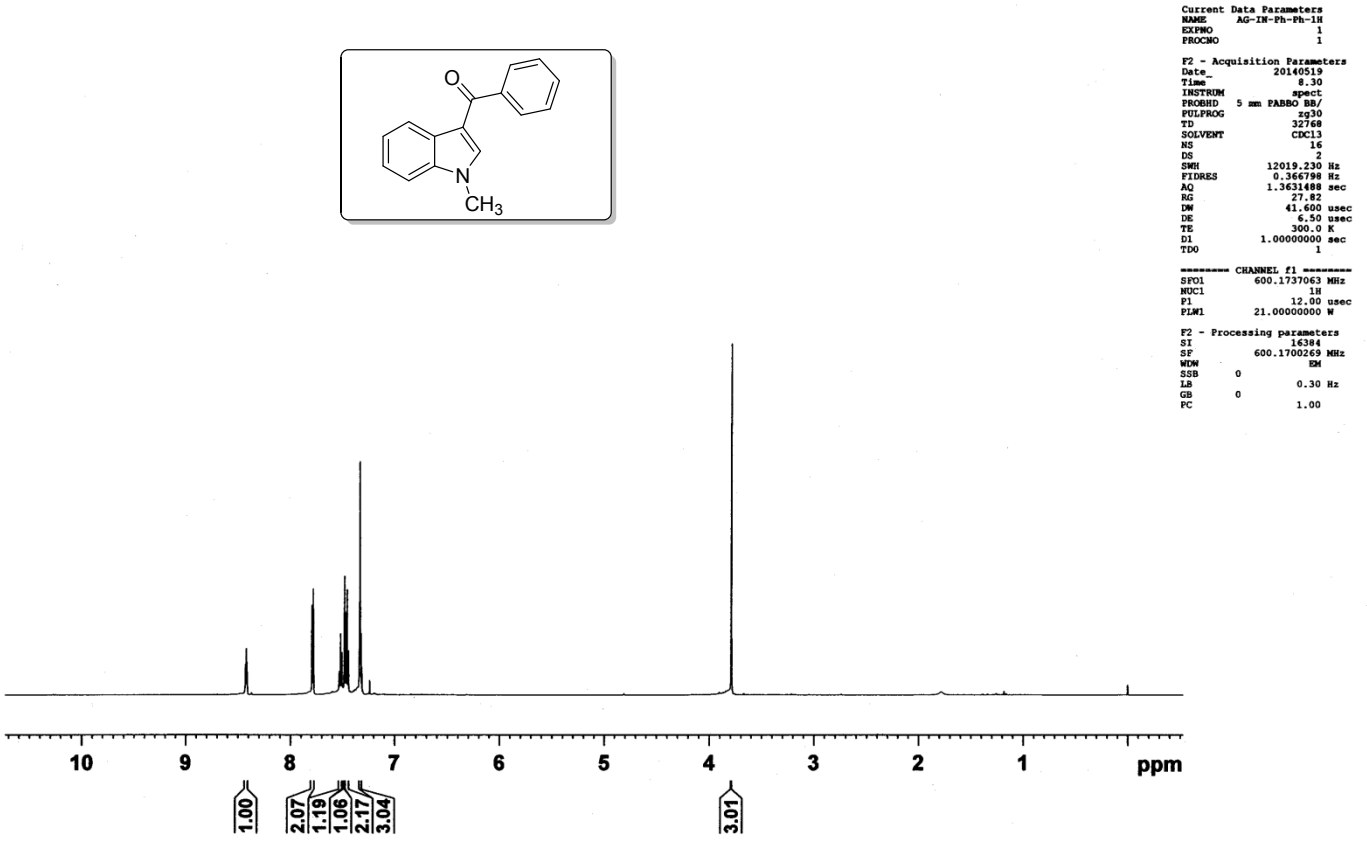
(2,3-Dihydro-1*H*-pyrrolo[1,2-a]indol-9-yl)(p-tolyl)methanone (5′g):



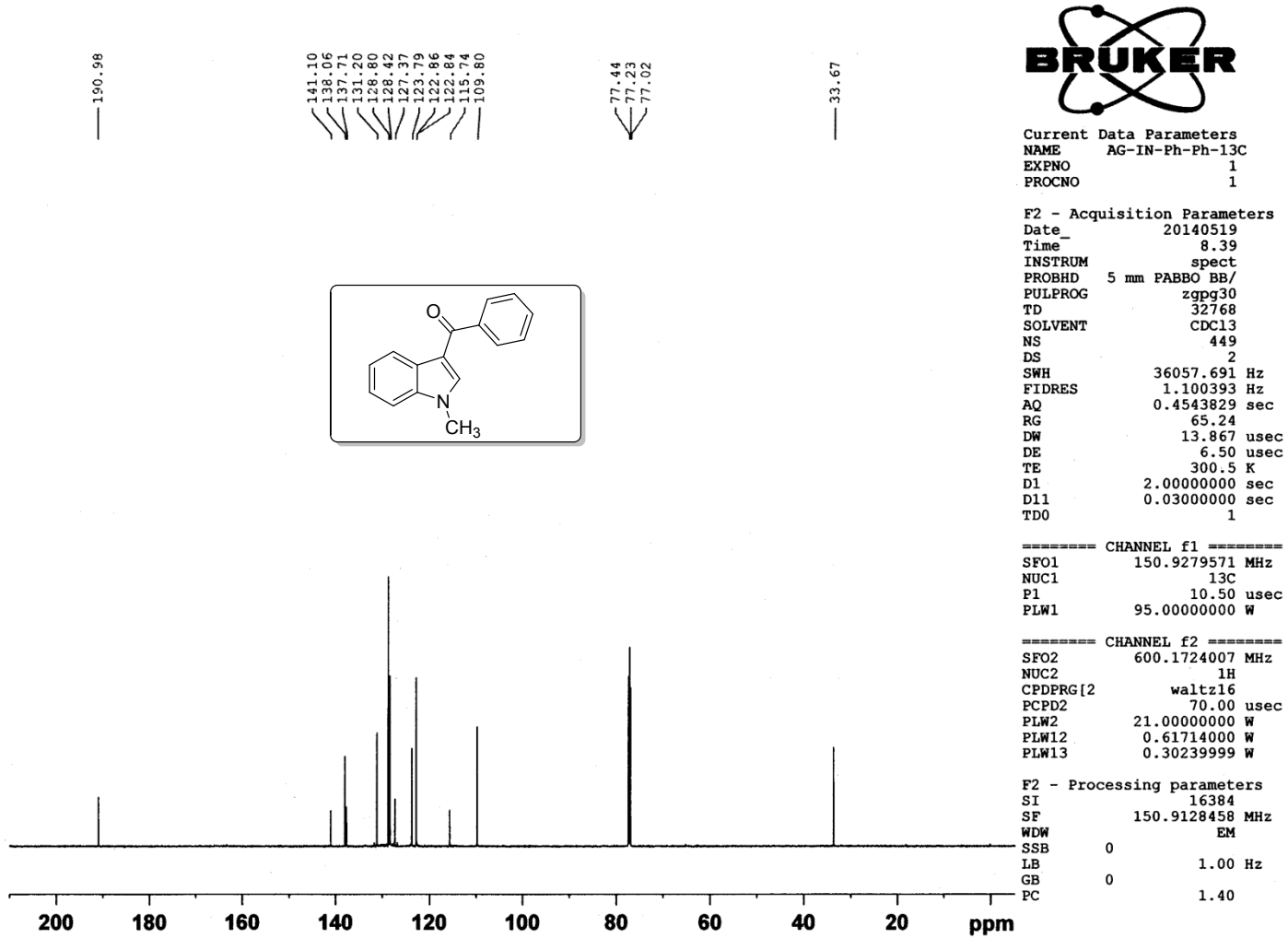
^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 2.44 (s, 3H), 2.54 (quin, 2H, *J* = 7.2 Hz), 2.90 (t, 2H, *J* = 7.2 Hz), 4.10 (t, 2H, *J* = 7.2 Hz), 7.20–7.23 (m, 2H), 7.24–7.26 (m, 3H), 7.61 (d, 2H, *J* = 7.8 Hz), 8.03–8.04 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 21.7, 27.0, 27.2, 44.6, 109.6, 109.9, 122.2, 122.35, 122.42, 128.5, 129.0, 131.5, 133.2, 139.1, 141.3, 153.3, 191.8; IR (KBr): 3049, 2983, 1614, 1602, 1570, 1520, 1464, 1448, 1437, 1419, 1382, 1305, 1220, 1205, 1137, 1043, 1010, 962, 828, 771, 745 cm^{-1}; HRMS (ESI): calcd. for $C_{19}H_{17}NO$ (MH^+) 276.1383; found 276.1389.

SPECTRA

(1-Methyl-1*H*-indol-3-yl)(phenyl)methanone (1′a): ^{1}H NMR (600 MHz, $CDCl_3$)



(1-Methyl-1*H*-indol-3-yl)(phenyl)methanone (1′a): ^{13}C NMR (150 MHz, $CDCl_3$)

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Current Data Parameters
NAME      AG-IN-Ph-Ph-13C
EXPNO                   1
PROCNO                  1

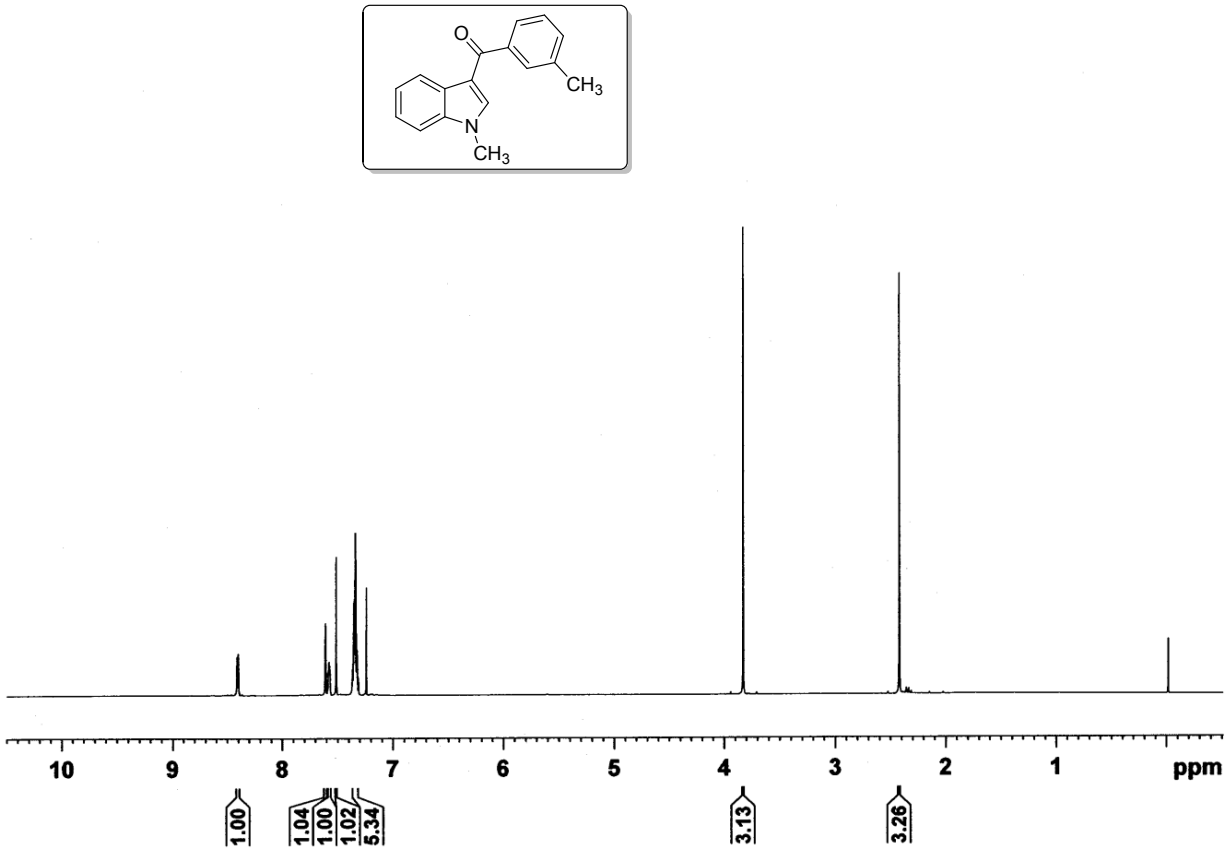
F2 - Acquisition Parameters
Date_           20140519
Time                8.39
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  449
DS                    2
SWH           36057.691 Hz
FIDRES         1.100393 Hz
AQ            0.4543829 sec
RG                65.24
DW               13.867 usec
DE                6.50 usec
TE               300.5 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          150.9128458 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

(1-Methyl-1*H*-indol-3-yl)(m-tolyl)methanone (1′b): ^{1}H NMR (600 MHz, $CDCl_3$)



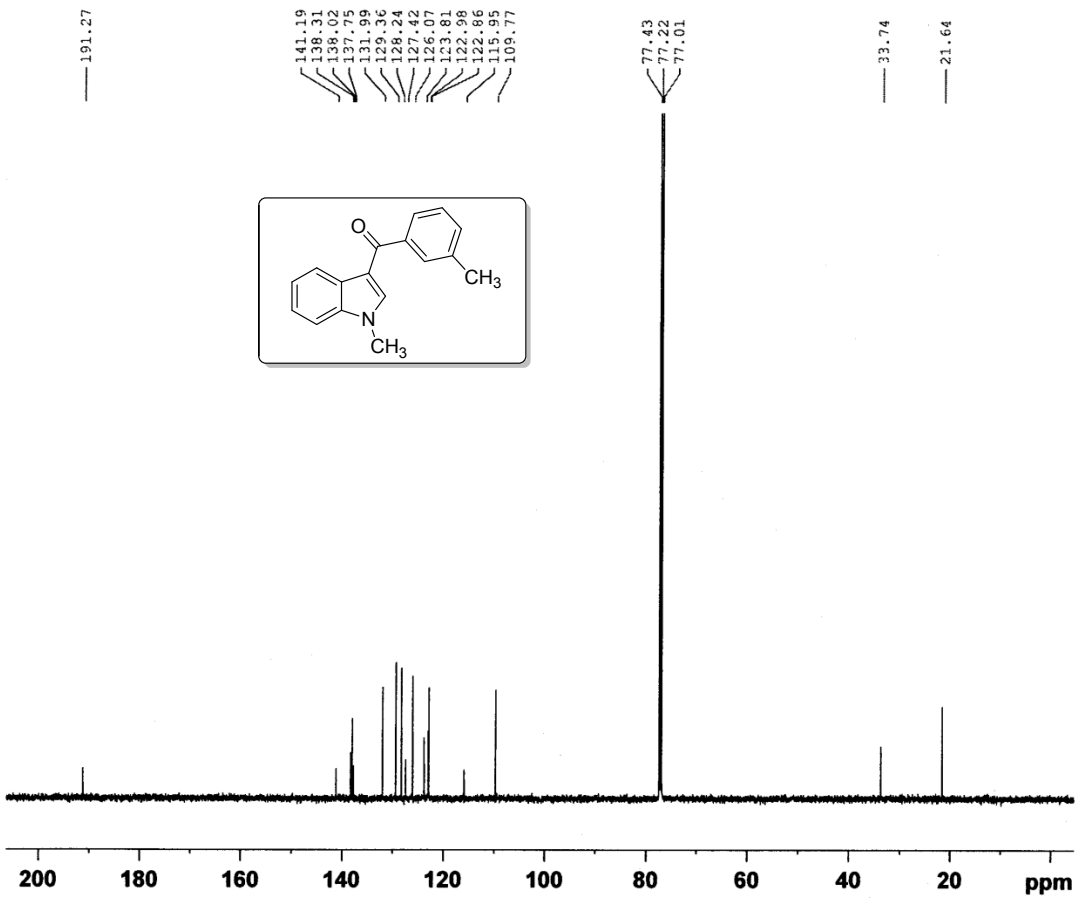

```
Current Data Parameters
NAME          AG-DPD-3-1H
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_          20140324
Time              8.52
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               299.5 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           600.1700268 MHz
WDW                EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

(1-Methyl-1*H*-indol-3-yl)(m-tolyl)methanone (1′b): ^{13}C NMR (150 MHz, $CDCl_3$)



BRUKER

```
Current Data Parameters
NAME        AG-DPD-3-13C
EXPNO                  1
PROCNO                 1

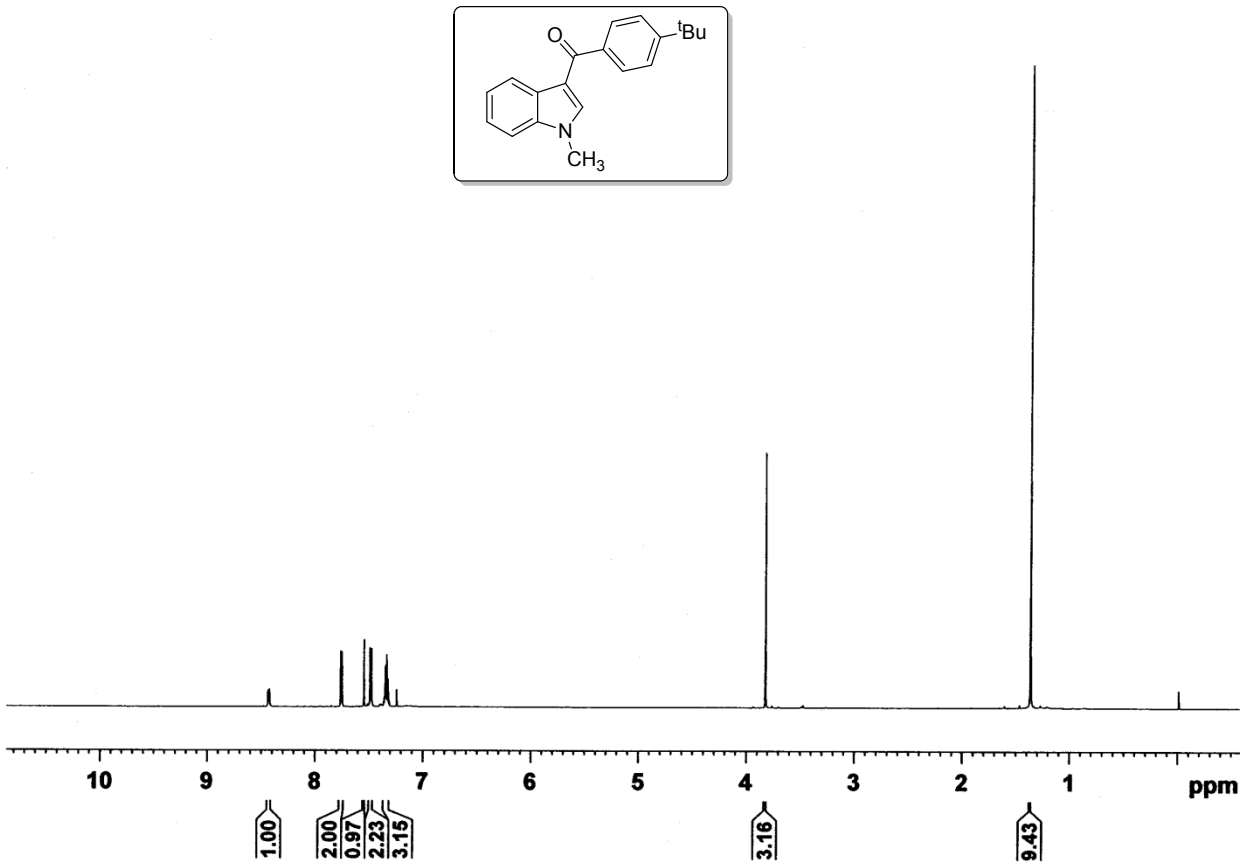
F2 - Acquisition Parameters
Date_           20140324
Time                9.01
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  305
DS                    2
SWH           36057.691 Hz
FIDRES         1.100393 Hz
AQ            0.4543829 sec
RG                65.24
DW               13.867 usec
DE                6.50 usec
TE               300.6 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          150.9128370 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

(4-(tert-Butyl)phenyl)(1-methyl-1*H*-indol-3-yl)methanone (1′c): ^{1}H NMR (600 MHz, $CDCl_3$)



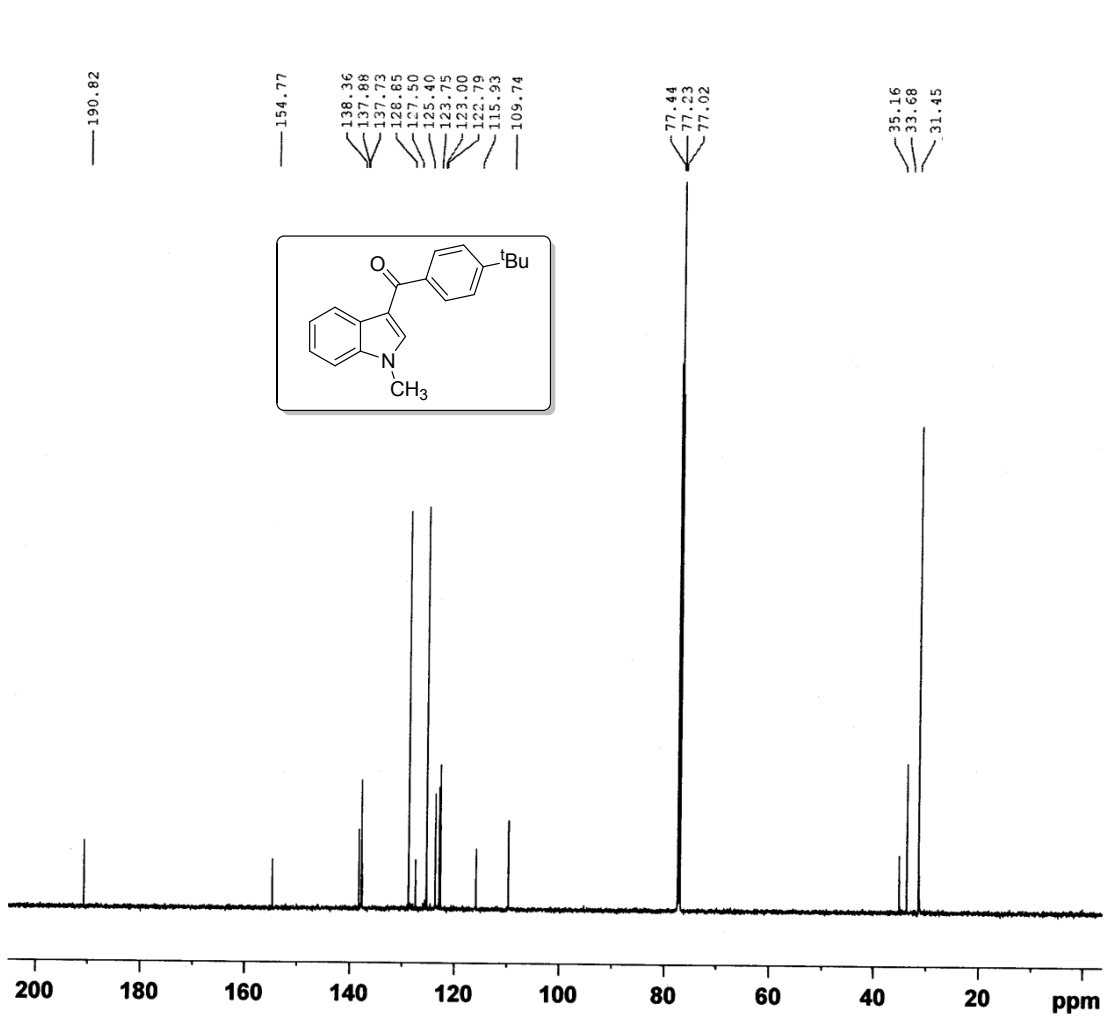

```
Current Data Parameters
NAME          AG-260-R-1H
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_          20140324
Time               9.16
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                65.24
DW               41.600 usec
DE                6.50 usec
TE                299.8 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                0.30 Hz
GB        0
PC                1.00
```

(4-(tert-Butyl)phenyl)(1-methyl-1*H*-indol-3-yl)methanone (1′c): ^{13}C NMR (150 MHz, $CDCl_3$)



BRUKER

```
Current Data Parameters
NAME          AG-260-R-13C
EXPNO                    1
PROCNO                   1

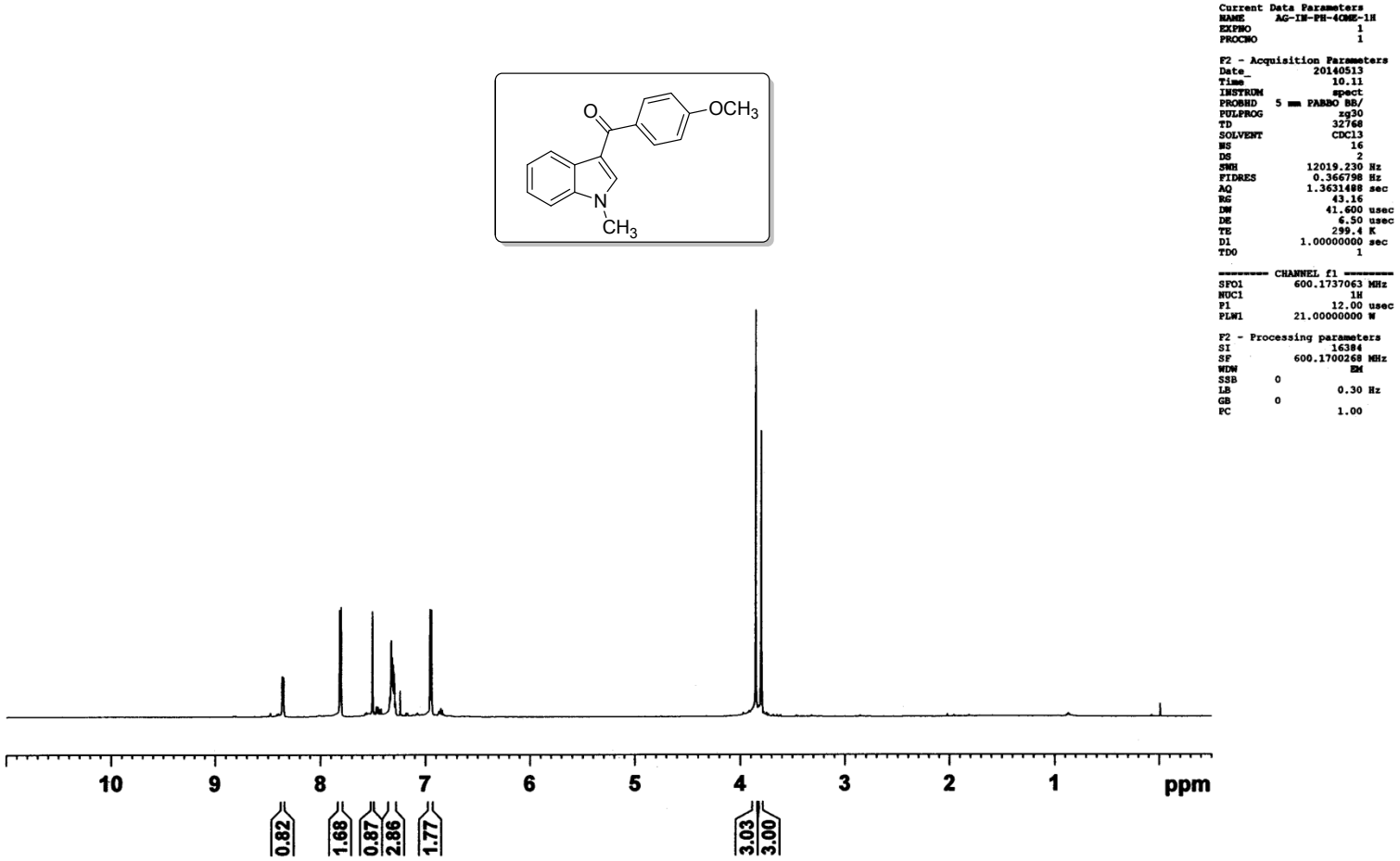
F2 - Acquisition Parameters
Date_             20140321
Time                 9.16
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 32768
SOLVENT             CDCl3
NS                    576
DS                      2
SWH           36057.691 Hz
FIDRES         1.100393 Hz
AQ             0.4543829 sec
RG                 65.24
DW                13.867 usec
DE                 6.50 usec
TE                302.1 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            150.9128370 MHz
WDW                     EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

(4-Methoxyphenyl)(1-methyl-1*H*-indol-3-yl)methanone (1′d): ^{1}H NMR (600 MHz, $CDCl_3$)



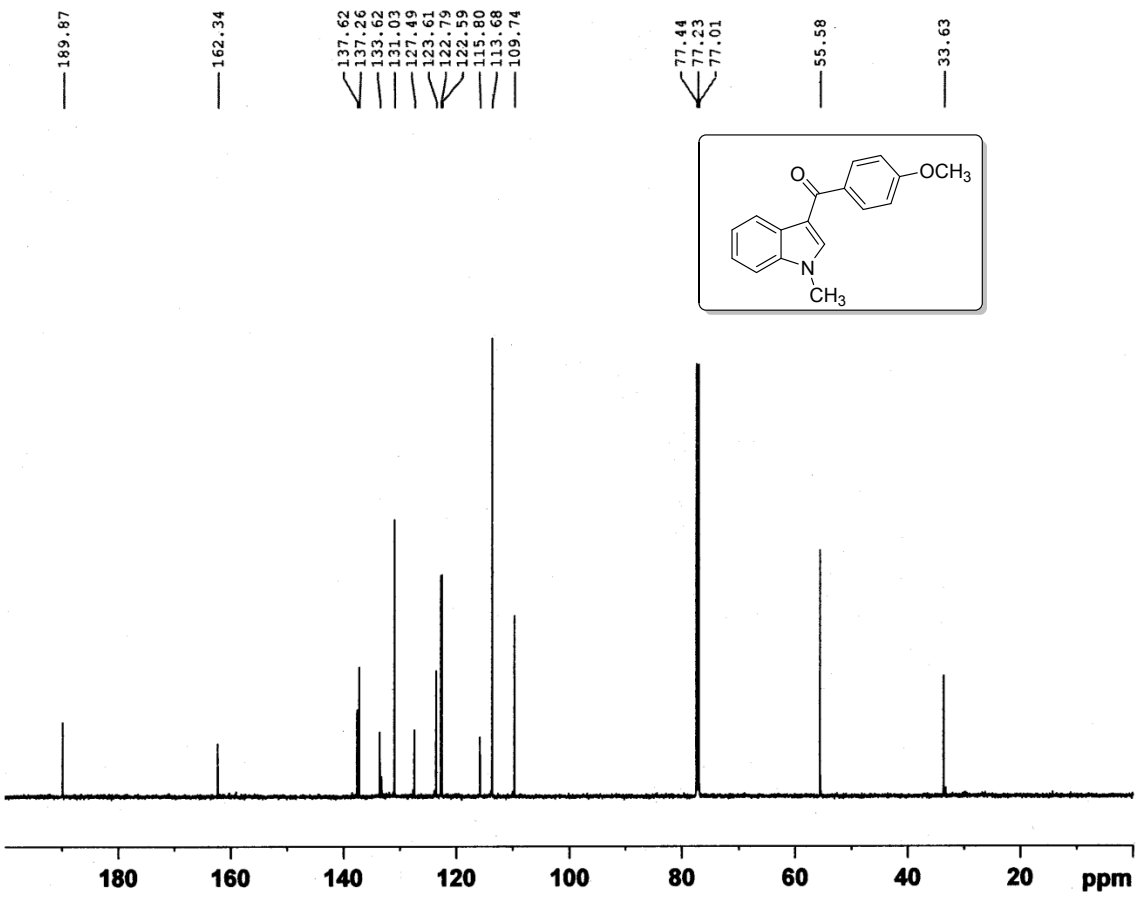

```
Current Data Parameters
NAME        AG-IN-PH-4OME-1H
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_               20140513
Time                   10.11
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                      43.16
DW                     41.600 usec
DE                      6.50 usec
TE                     299.4 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              600.1700268 MHz
WDW                       EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

(4-Methoxyphenyl)(1-methyl-1*H*-indol-3-yl)methanone (1′d): ^{13}C NMR (150 MHz, $CDCl_3$)




```
Current Data Parameters
NAME      AG-IN-PH-4OME-13C
EXPNO                    1
PROCNO                   1

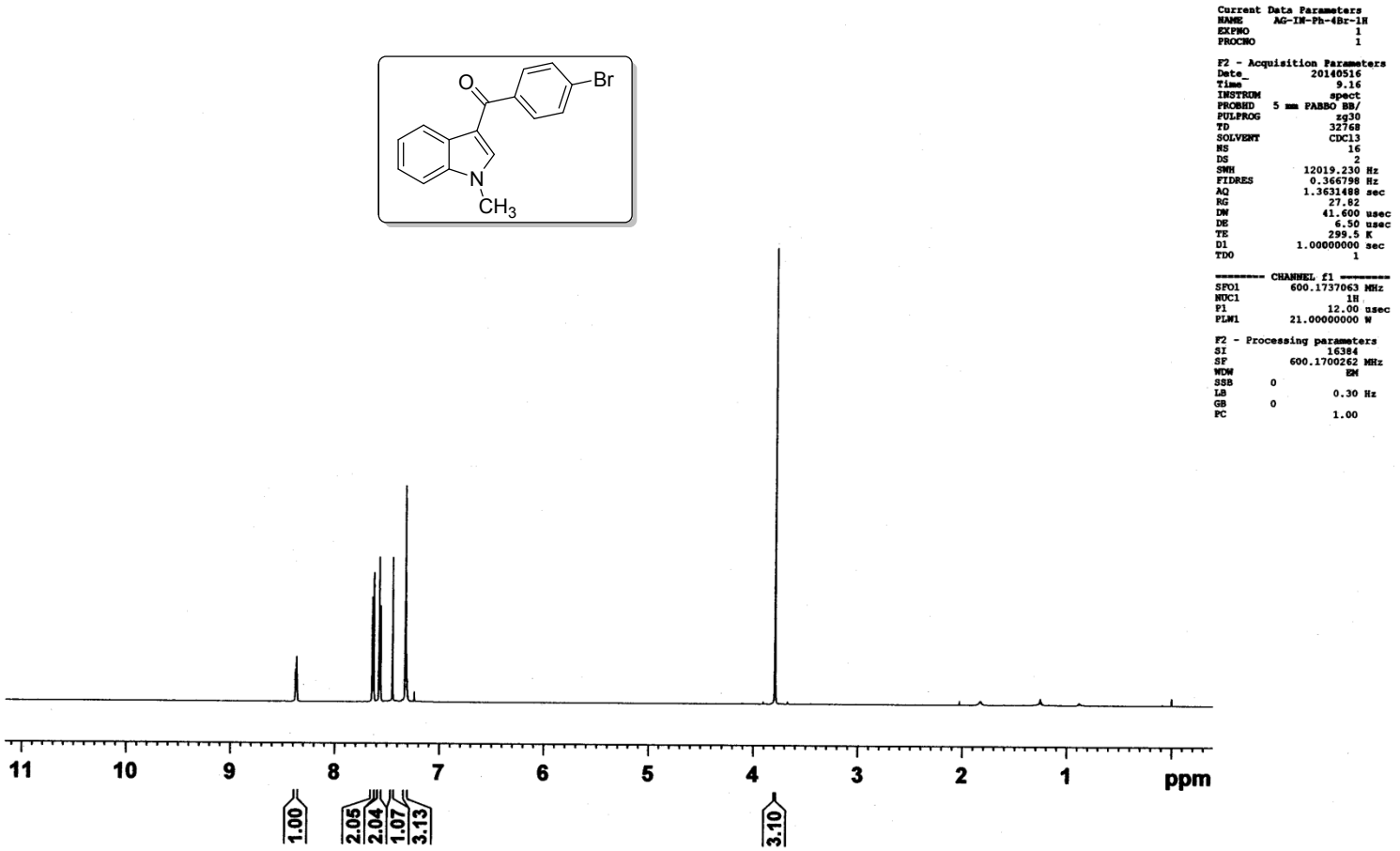
F2 - Acquisition Parameters
Date_              20140513
Time                 10.18
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG            zgpg30
TD                  32768
SOLVENT             CDCl3
NS                    313
DS                      2
SWH             36057.691 Hz
FIDRES           1.100393 Hz
AQ               0.4543829 sec
RG                   65.24
DW                 13.867 usec
DE                  6.50 usec
TE                 300.0 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            150.9128452 MHz
WDW                       EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```

(4-Bromophenyl)(1-methyl-1*H*-indol-3-yl)methanone (1′e): ^{1}H NMR (600 MHz, $CDCl_3$)



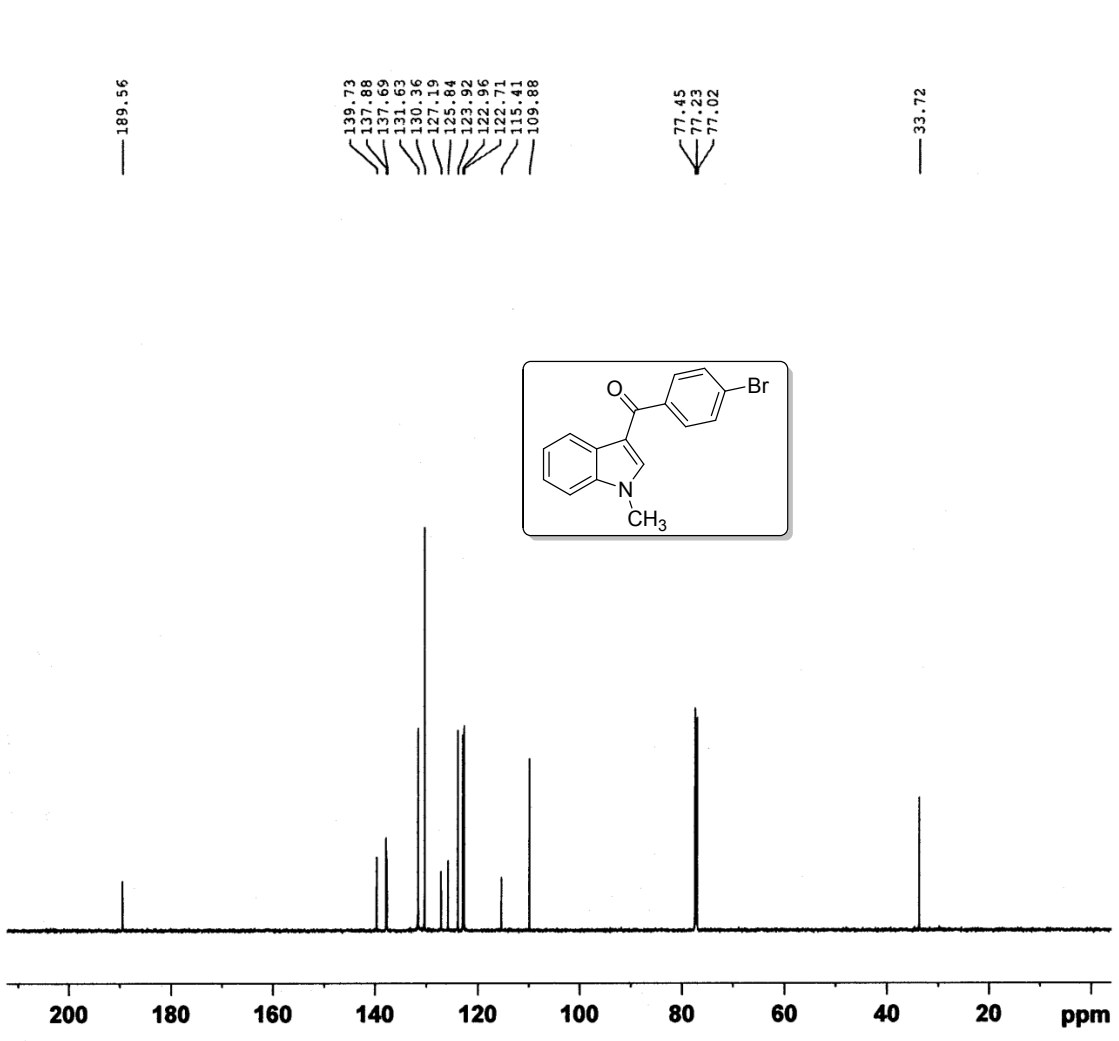

```
Current Data Parameters
NAME          AG-IN-Ph-4Br-1H
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_               20140516
Time                    9.16
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                     27.82
DW                    41.600 usec
DE                     6.50 usec
TE                    299.5 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             600.1700262 MHz
WDW                       EM
SSB                    0
LB                    0.30 Hz
GB                     0
PC                    1.00
```

(4-Bromophenyl)(1-methyl-1*H*-indol-3-yl)methanone (1′e): ^{13}C NMR (150 MHz, $CDCl_3$)




```
Current Data Parameters
NAME      AG-IN-Ph-4Br-13C
EXPNO                    1
PROCNO                   1

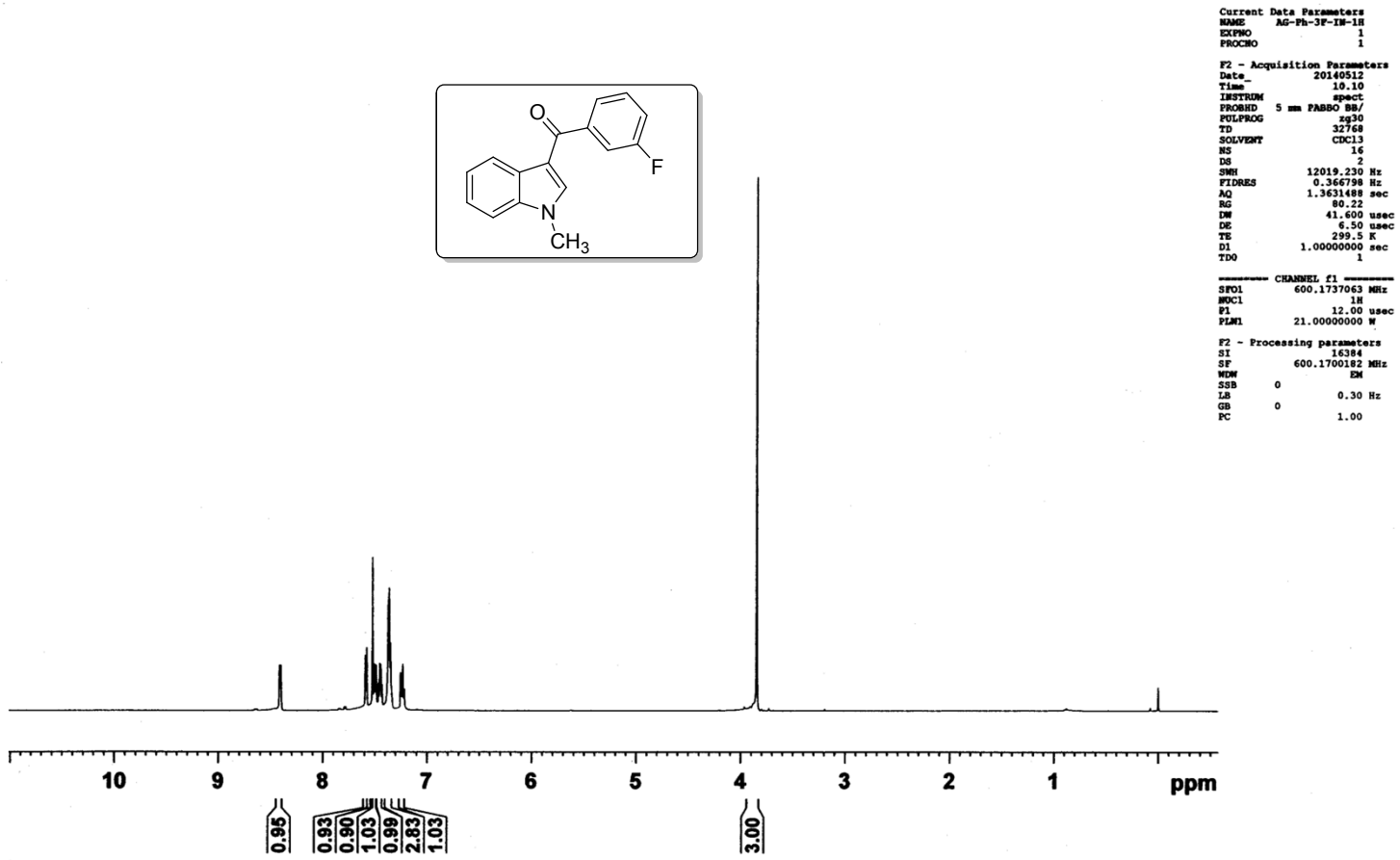
F2 - Acquisition Parameters
Date_             20140516
Time                 9.24
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                   125
DS                     2
SWH            36057.691 Hz
FIDRES          1.100393 Hz
AQ              0.4543829 sec
RG                  65.24
DW                13.867 usec
DE                 6.50 usec
TE                300.5 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           150.9128503 MHz
WDW                    EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

(3-Fluorophenyl)(1-methyl-1*H*-indol-3-yl)methanone (1′f): ^{1}H NMR (600 MHz, $CDCl_3$)

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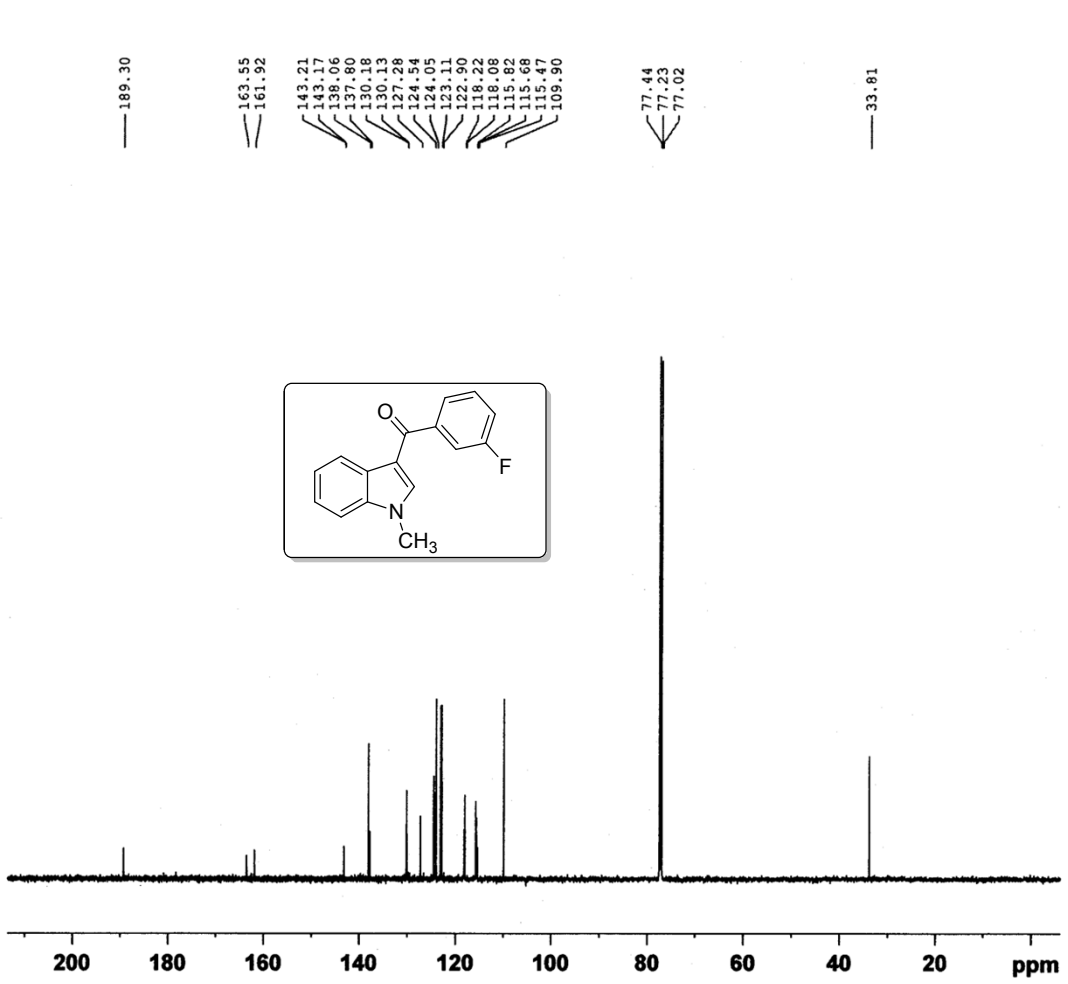
Current Data Parameters
NAME      AG-Ph-3F-IM-1H
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140512
Time_              10.10
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                299.5 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            600.1700182 MHz
WDW                    EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                 1.00
```

(3-Fluorophenyl)(1-methyl-1*H*-indol-3-yl)methanone (1′f): ^{13}C NMR (150 MHz, $CDCl_3$)

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Current Data Parameters
NAME      AG-Ph-3F-IN-R-13C
EXPNO                    1
PROCNO                   1

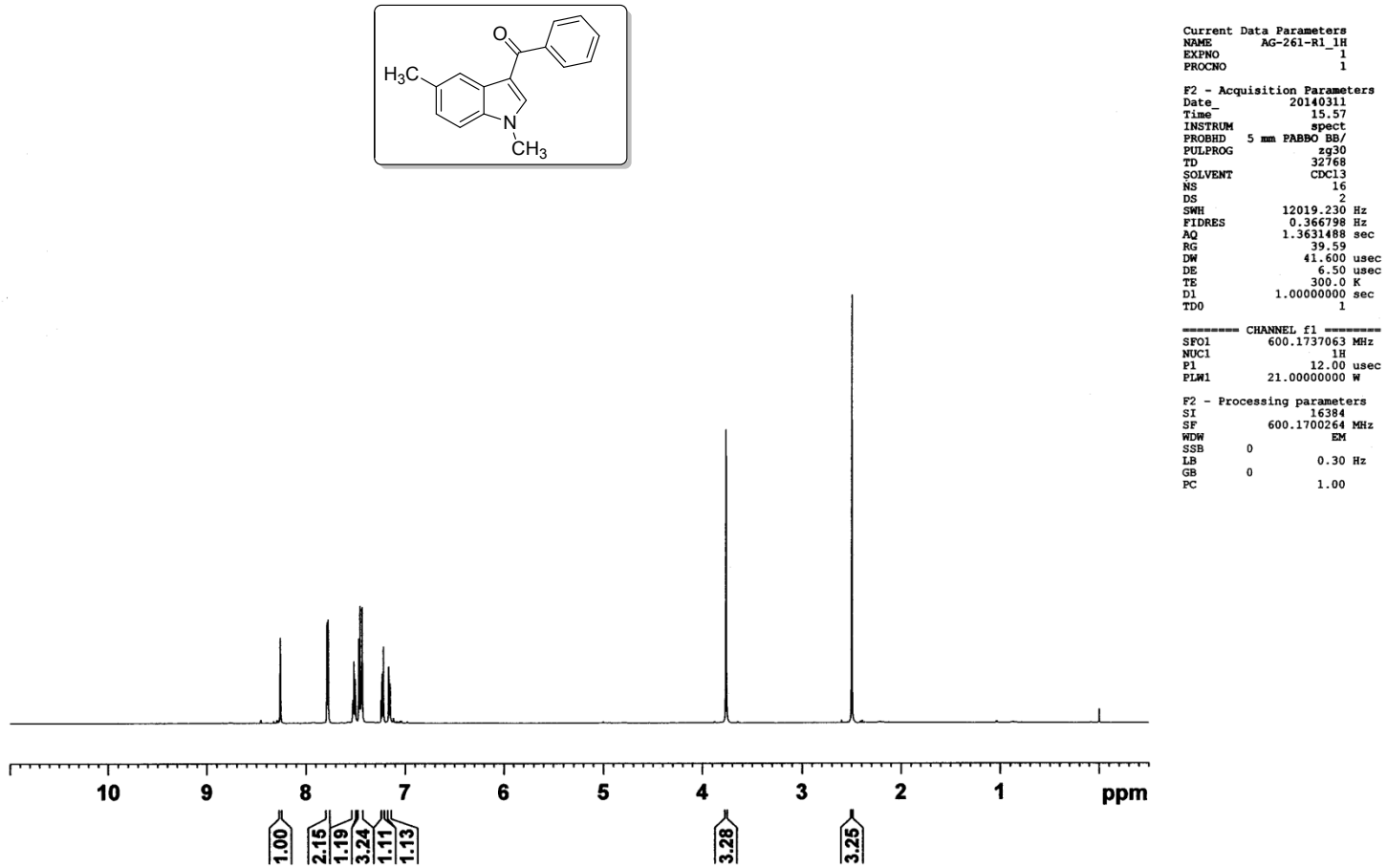
F2 - Acquisition Parameters
Date_             20140512
Time                 10.18
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG            zgpg30
TD                  32768
SOLVENT             CDCl3
NS                    504
DS                      2
SWH           36057.691 Hz
FIDRES         1.100393 Hz
AQ            0.4543829 sec
RG                 65.24
DW               13.867 usec
DE                6.50 usec
TE                300.0 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          150.9128384 MHz
WDW                    EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

(1,5-Dimethyl-1*H*-indol-3-yl)(phenyl)methanone (2′a): ^{1}H NMR (600 MHz, $CDCl_3$)



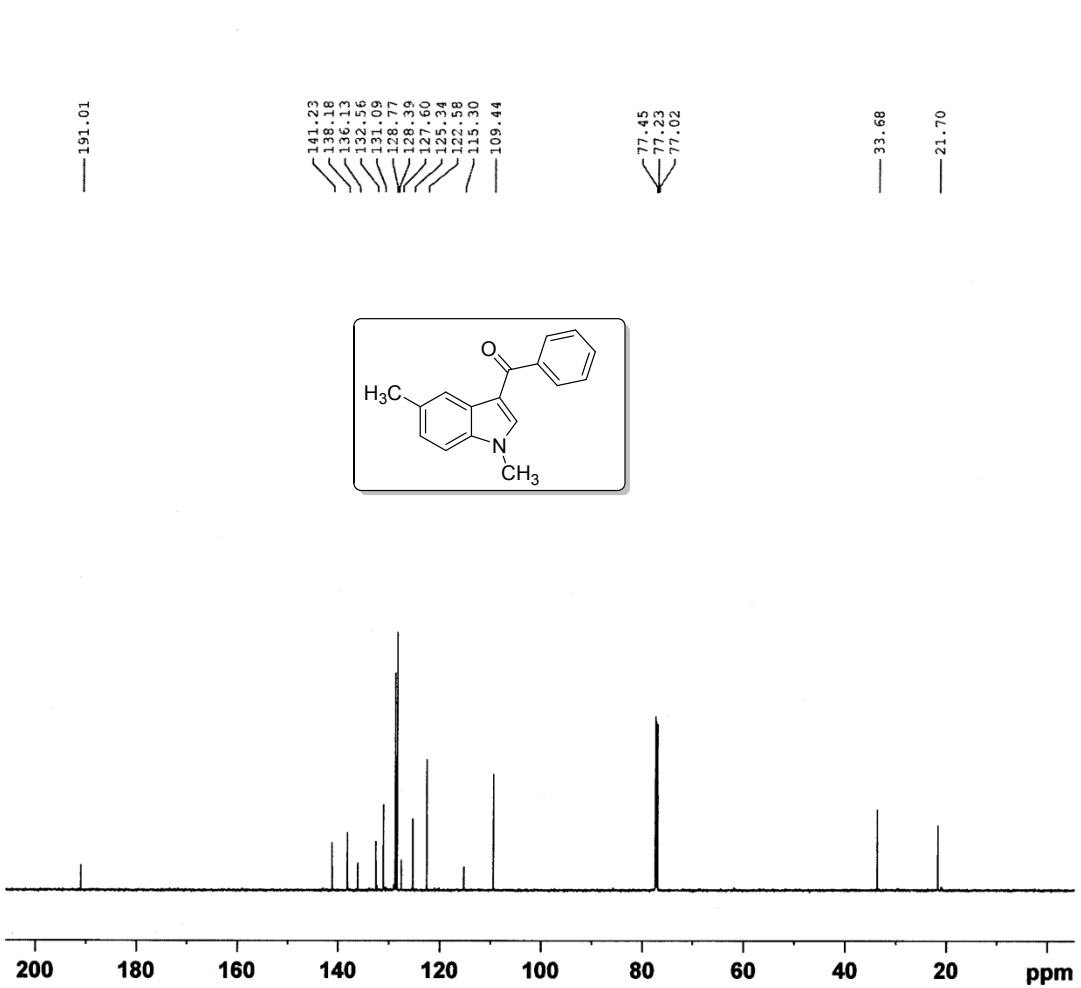

```
Current Data Parameters
NAME        AG-261-R1_1H
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140311
Time               15.57
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                 39.59
DW                41.600 usec
DE                 6.50 usec
TE                300.0 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            600.1700264 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

(1,5-Dimethyl-1*H*-indol-3-yl)(phenyl)methanone (2′a): ^{13}C NMR (150 MHz, $CDCl_3$)




```
Current Data Parameters
NAME       AG-261-R1_13C
EXPNO                  1
PROCNO                 1

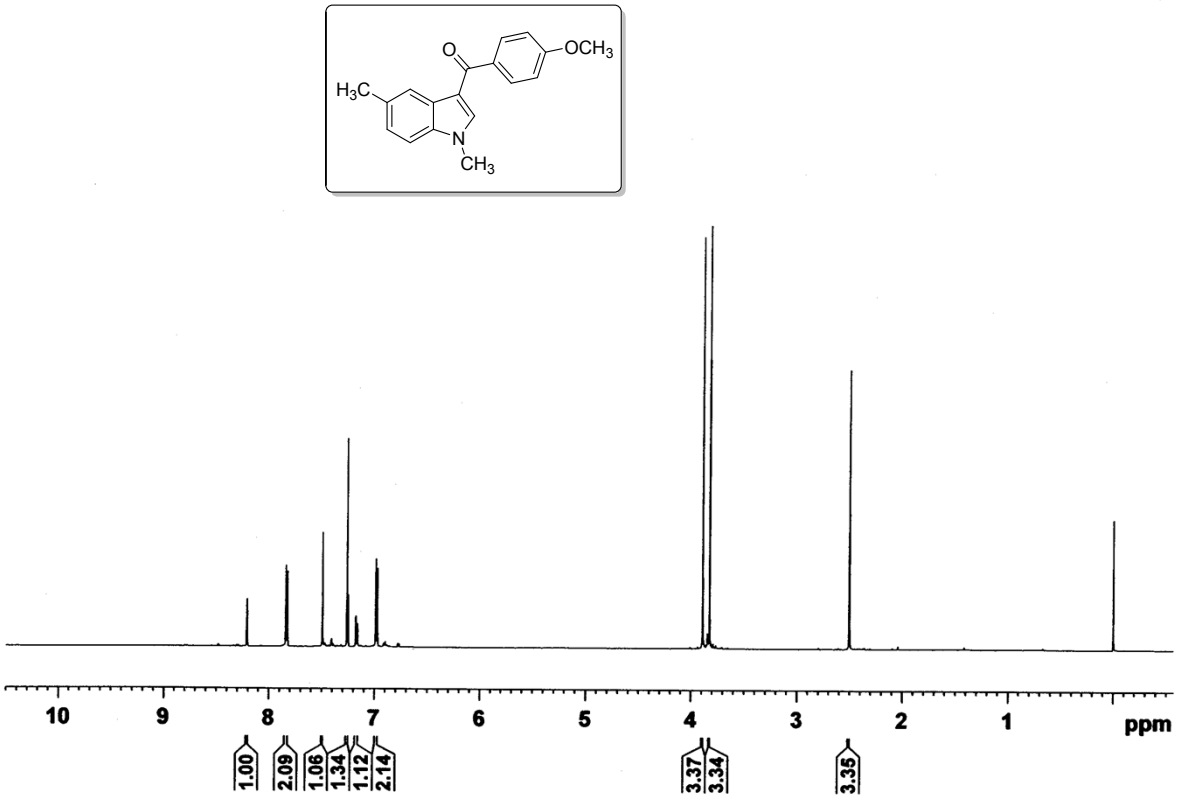
F2 - Acquisition Parameters
Date_           20140311
Time               16.04
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                32768
SOLVENT           CDCl3
NS                  146
DS                    2
SWH           36057.691 Hz
FIDRES         1.100393 Hz
AQ            0.4543829 sec
RG                65.24
DW               13.867 usec
DE                6.50 usec
TE                300.7 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          150.9128459 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

(1,5-Dimethyl-1*H*-indol-3-yl)(4-methoxyphenyl)methanone (2′d): ^{1}H NMR (600 MHz, $CDCl_3$)



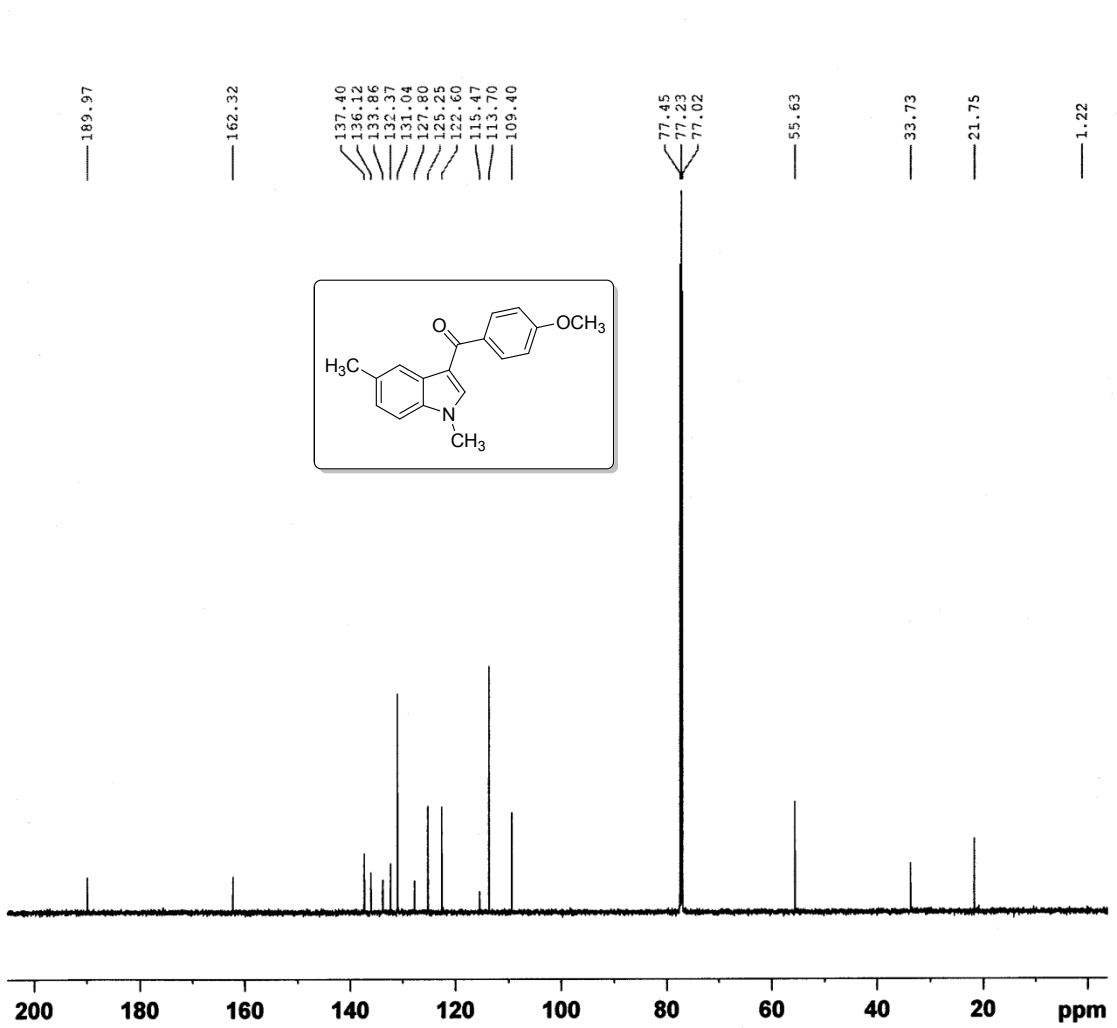

```
Current Data Parameters
NAME                  AG-DPD-2-1H
EXPNO                           1
PROCNO                          1

F2 - Acquisition Parameters
Date_                    20140321
Time                         8.41
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                        300.9 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                   600.1700152 MHz
WDW                           EM
SSB          0
LB                         0.30 Hz
GB           0
PC                         1.00
```

(1,5-Dimethyl-1*H*-indol-3-yl)(4-methoxyphenyl)methanone (2′d): ^{13}C NMR (150 MHz, $CDCl_3$)




```
Current Data Parameters
NAME        AG-DPD-2-13C
EXPNO                  1
PROCNO                 1

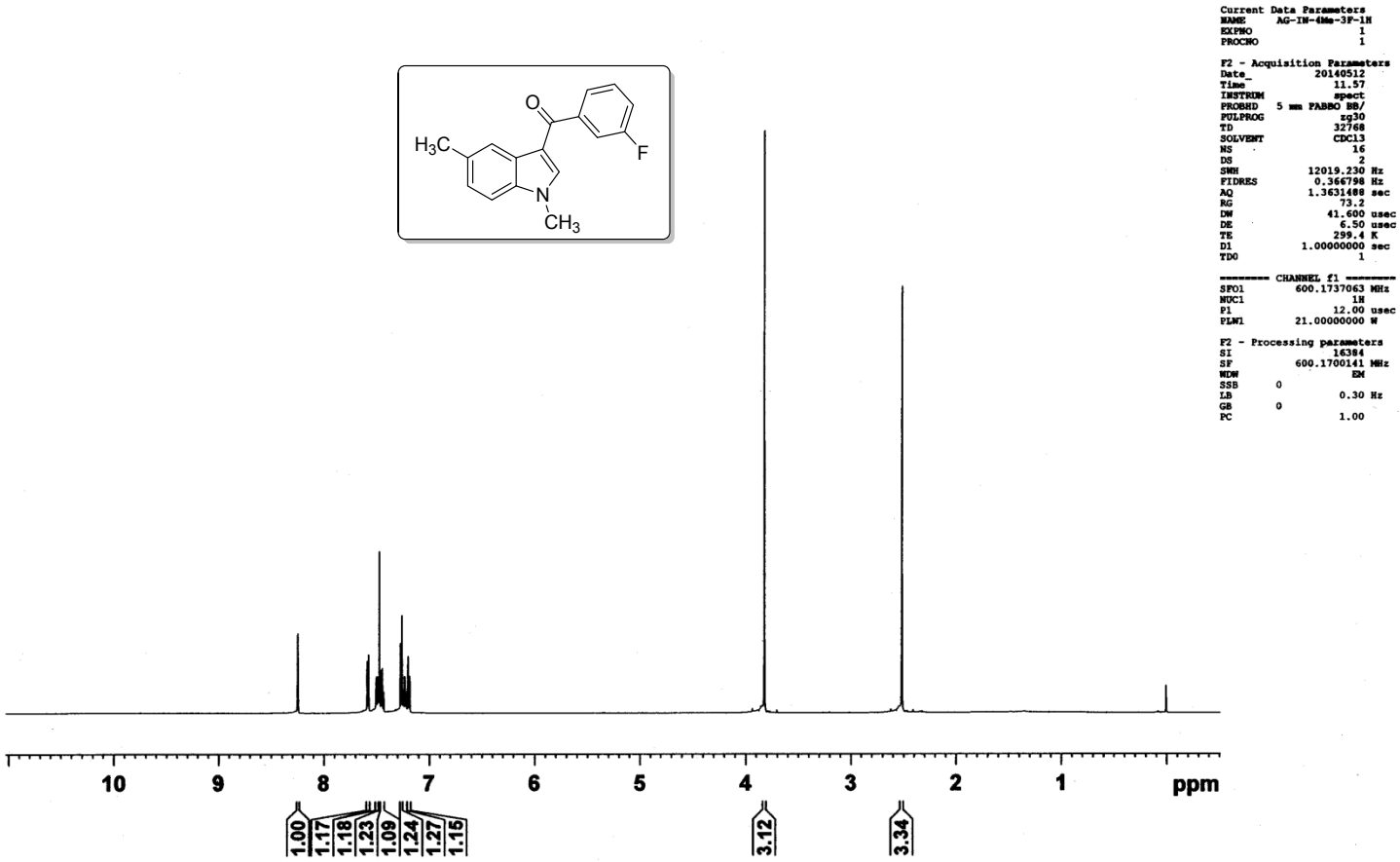
F2 - Acquisition Parameters
Date_           20140321
Time                8.55
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  405
DS                    2
SWH           36057.691 Hz
FIDRES         1.100393 Hz
AQ            0.4543829 sec
RG                65.24
DW               13.867 usec
DE                6.50 usec
TE               301.9 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          150.9128348 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

(1,5-Dimethyl-1*H*-indol-3-yl)(3-fluorophenyl)methanone (2′f): ^{1}H NMR (600 MHz, $CDCl_3$)



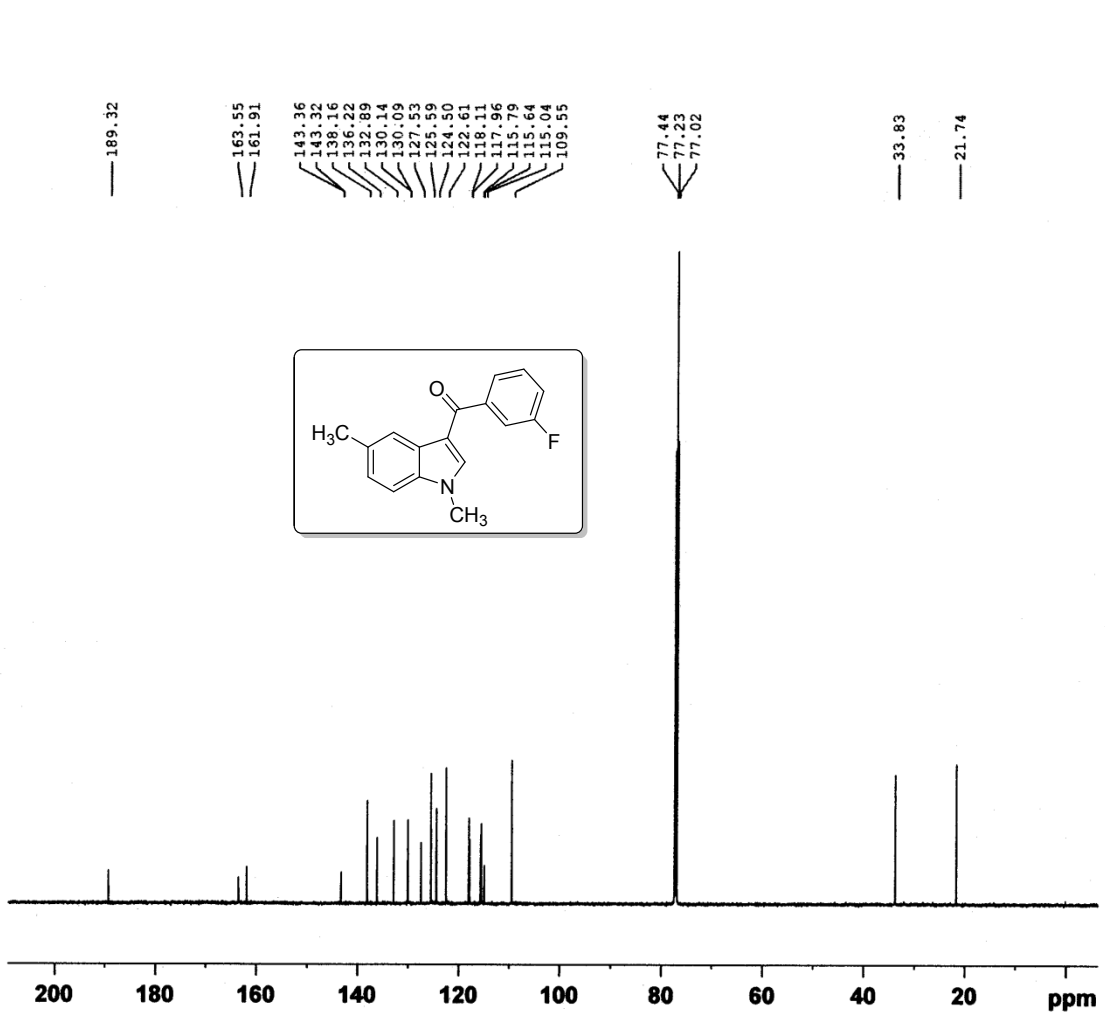

```
Current Data Parameters
NAME      AG-IN-4Me-3F-1H
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_              20140512
Time                 11.57
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                  299.4 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            600.1700141 MHz
WDW                     EM
SSB                  0
LB                   0.30 Hz
GB                   0
PC                   1.00
```

(1,5-Dimethyl-1*H*-indol-3-yl)(3-fluorophenyl)methanone (2′f): ^{13}C NMR (150 MHz, $CDCl_3$)




```
Current Data Parameters
NAME      AG-IN-4Me-3F-13C
EXPNO                    1
PROCNO                   1

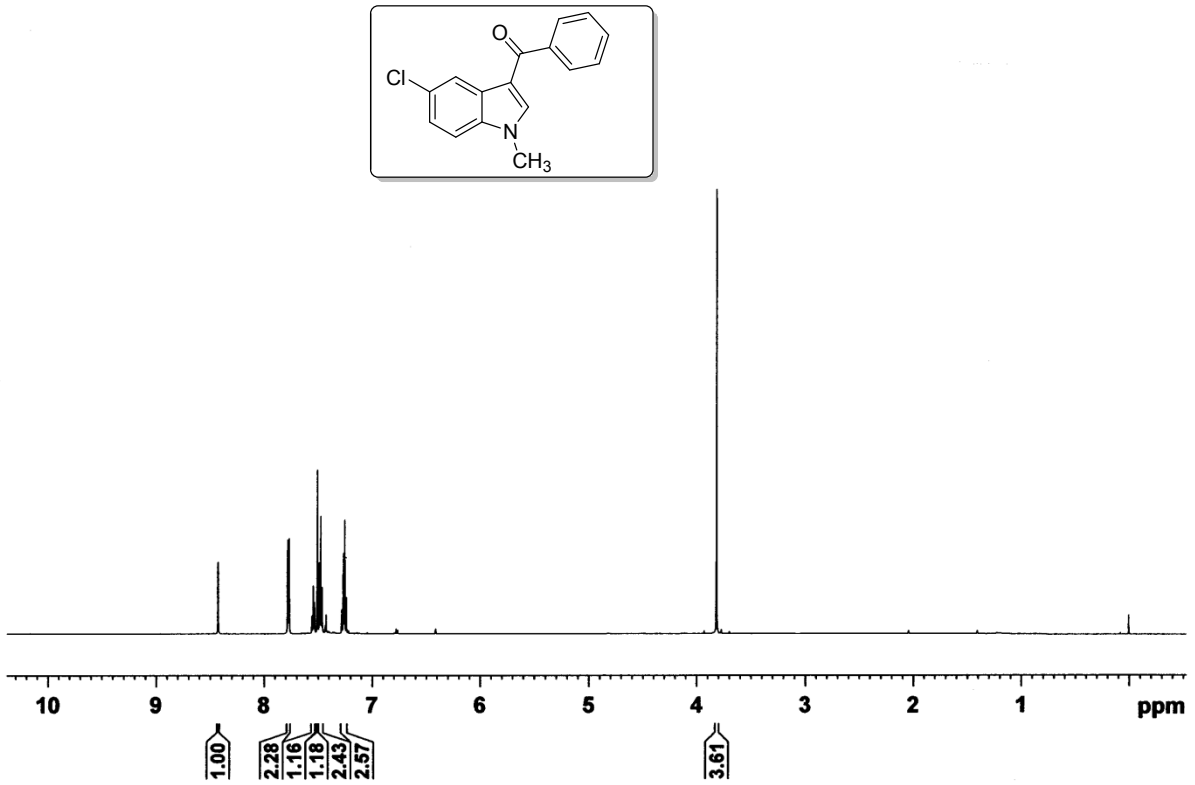
F2 - Acquisition Parameters
Date_              20140512
Time                 11.13
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   32768
SOLVENT              CDCl3
NS                     940
DS                       2
SWH              36057.691 Hz
FIDRES           1.100393 Hz
AQ               0.4543829 sec
RG                   65.24
DW                13.867 usec
DE                 6.50 usec
TE                299.7 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            150.9128371 MHz
WDW                       EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

(5-Chloro-1-methyl-1*H*-indol-3-yl)(phenyl)methanone (3′a): ^{1}H NMR (600 MHz, $CDCl_3$)



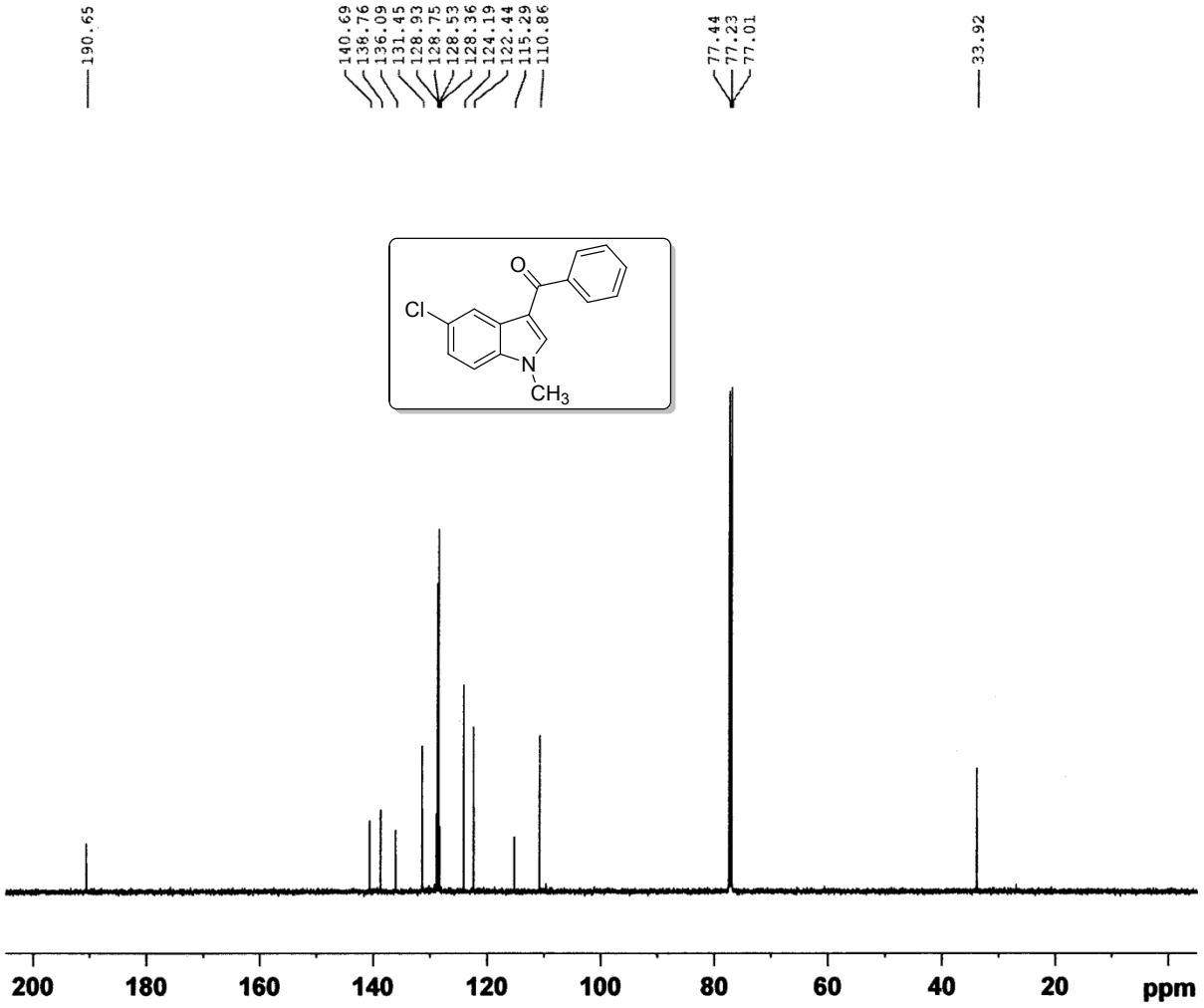

```
Current Data Parameters
NAME        AG-46,47-4-Cl+sim-TBAI-1H
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_         20131212
Time             12.59
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               54.94
DW              41.600 usec
DE               6.50 usec
TE              297.7 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          600.1700137 MHz
WDW                 EM
SSB          0
LB                0.30 Hz
GB           0
PC                1.00
```

(5-Chloro-1-methyl-1*H*-indol-3-yl)(phenyl)methanone (3′a): ^{13}C NMR (150 MHz, $CDCl_3$)




```
Current Data Parameters
NAME      AG-46,47-4-Cl+sim-TBAI-13C
EXPNO                 1
PROCNO                1

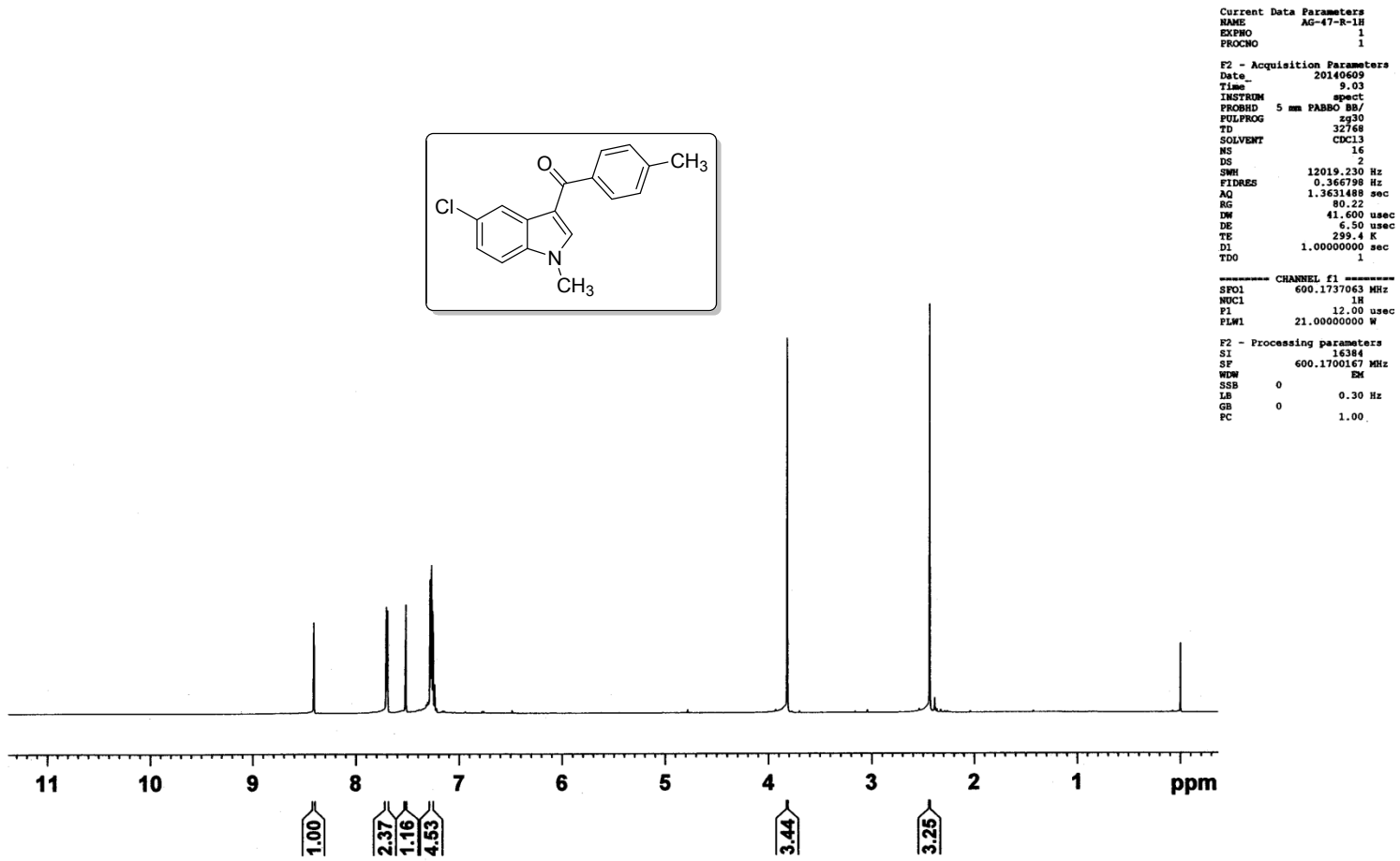
F2 - Acquisition Parameters
Date_          20131212
Time              13.05
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD              32768
SOLVENT           CDCl3
NS                  155
DS                    2
SWH           36057.691 Hz
FIDRES         1.100393 Hz
AQ             0.4543829 sec
RG                65.24
DW               13.867 usec
DE                6.50 usec
TE               298.2 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

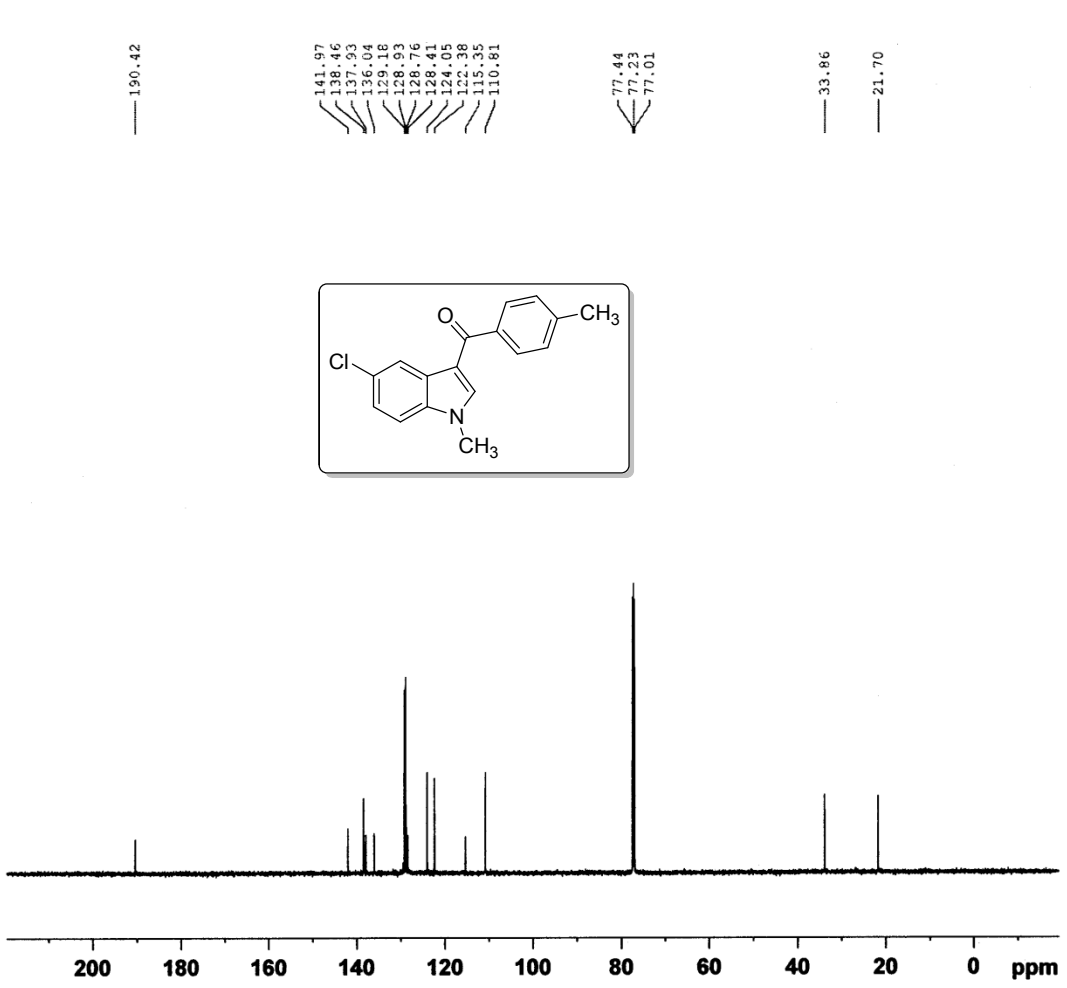
======== CHANNEL f2 ========
SFO2        600.1724007 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             70.00 usec
PLW2        21.00000000 W
PLW12        0.61714000 W
PLW13        0.30239999 W

F2 - Processing parameters
SI                 16384
SF          150.9128413 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

(5-Chloro-1-methyl-1*H*-indol-3-yl)(p-tolyl)methanone (3′g): ^{1}H NMR (600 MHz, $CDCl_3$)



(5-Chloro-1-methyl-1*H*-indol-3-yl)(p-tolyl)methanone (3′g): ^{13}C NMR (150 MHz, $CDCl_3$)




```
Current Data Parameters
NAME                  AG_47_13C
EXPNO                         1
PROCNO                        1

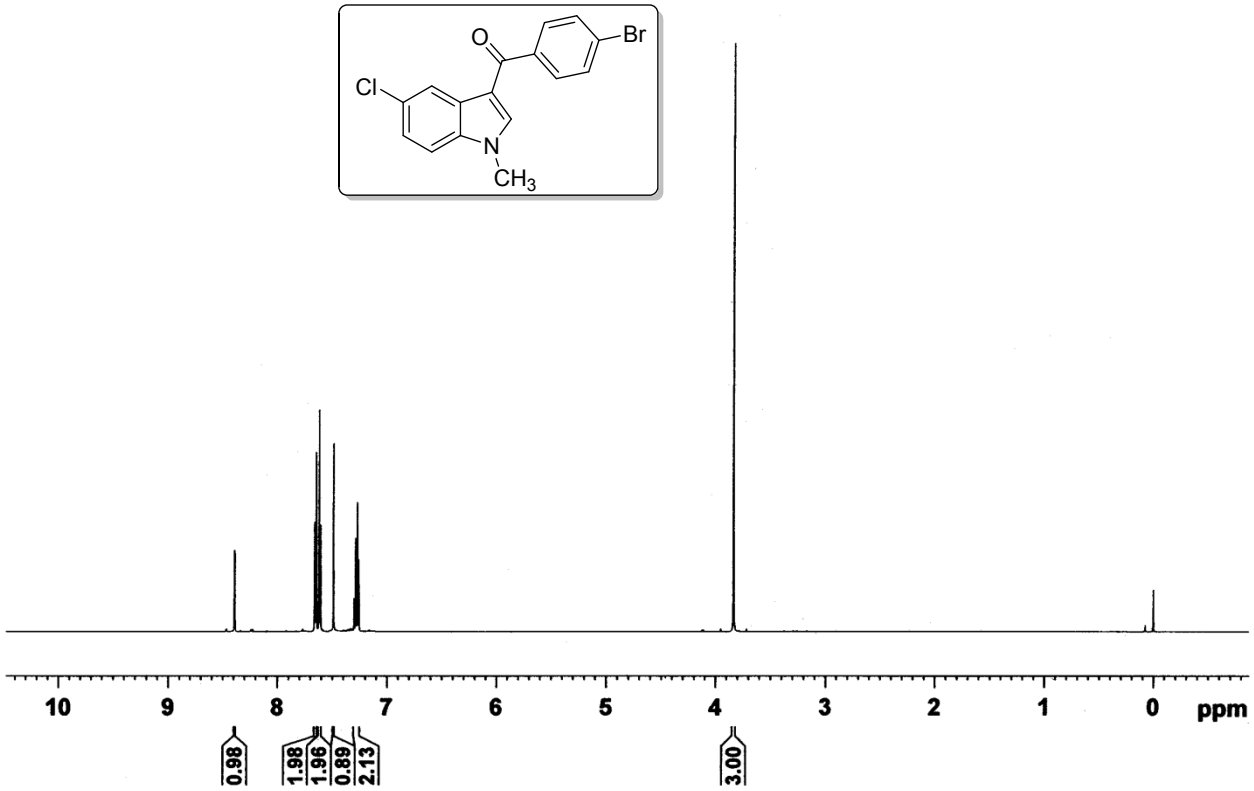
F2 - Acquisition Parameters
Date_                  20130926
Time                      15.58
INSTRUM                   spect
PROBHD    5 mm PABBO BB/
PULPROG                 zgpg30
TD                        32768
SOLVENT                   CDCl3
NS                          253
DS                            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                   2.00000000 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                  150.9128420 MHz
WDW                          EM
SSB       0
LB                         1.00 Hz
GB        0
PC                         1.40
```

(4-Bromophenyl)(5-Chloro-1-methyl-1*H*-indol-3-yl)methanone (3′e): ^{1}H NMR (600 MHz, $CDCl_3$)



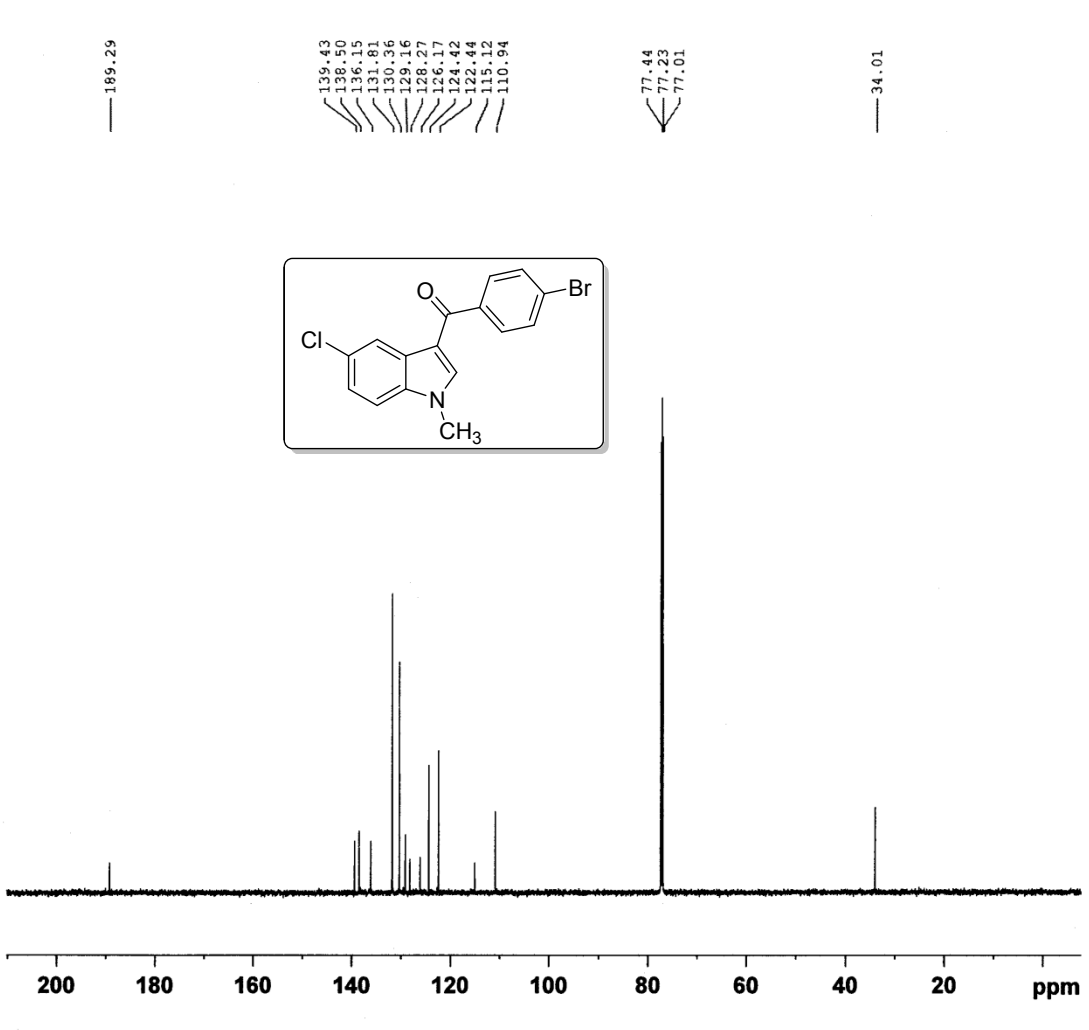

```
Current Data Parameters
NAME        AG_DPD_P1_1H
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140304
Time               16.16
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                89.67
DW               41.600 usec
DE                6.50 usec
TE               300.2 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           600.1700141 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

(4-Bromophenyl)(5-Chloro-1-methyl-1*H*-indol-3-yl)methanone (3′e): ^{13}C NMR (150 MHz, $CDCl_3$)



BRUKER

```
Current Data Parameters
NAME       AG_DPD_P1_13C
EXPNO                  1
PROCNO                 1

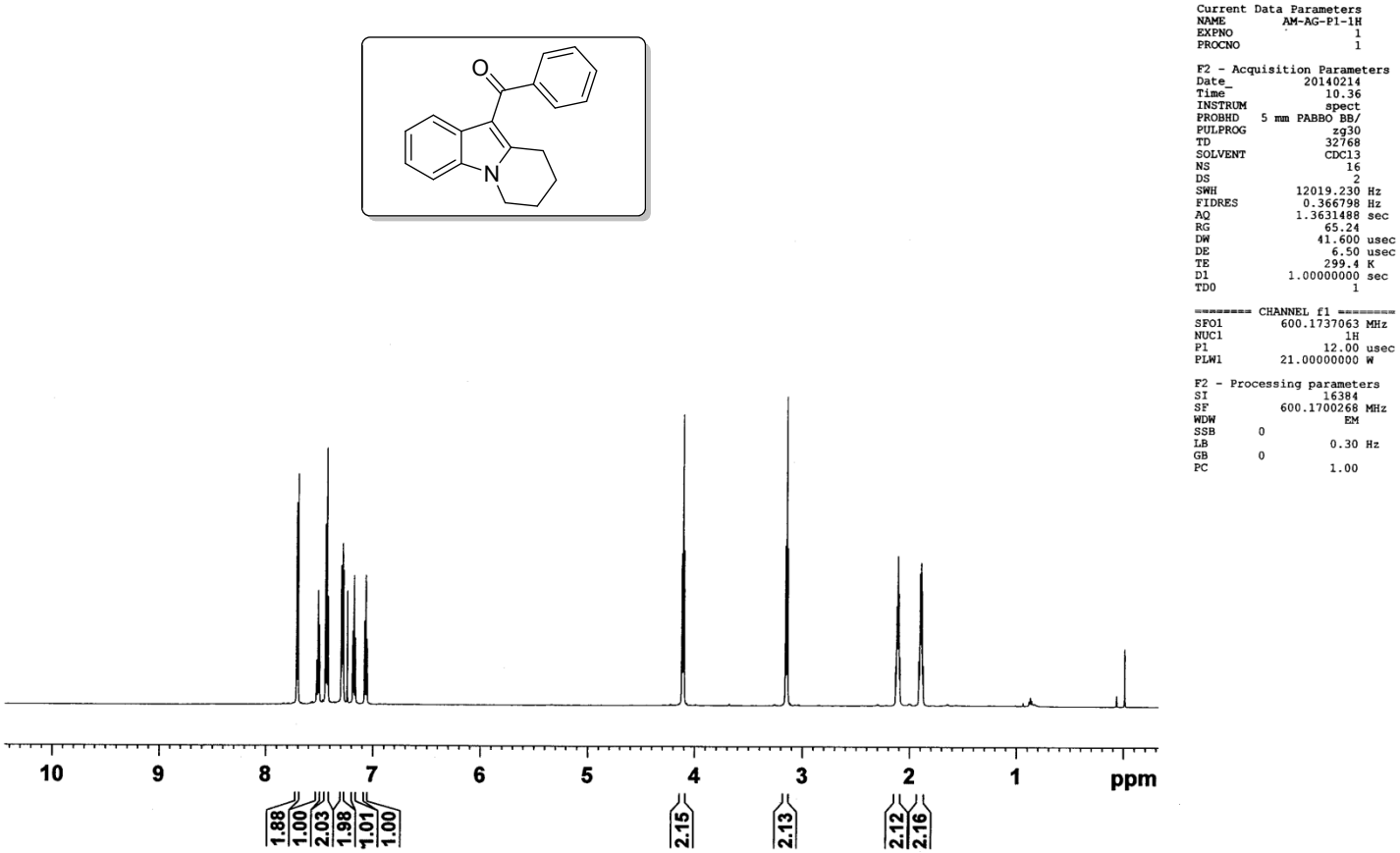
F2 - Acquisition Parameters
Date_           20140304
Time               12.52
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  204
DS                    2
SWH           36057.691 Hz
FIDRES         1.100393 Hz
AQ            0.4543829 sec
RG                65.24
DW               13.867 usec
DE                6.50 usec
TE               300.9 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          150.9128369 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

Phenyl(6,7,8,9-tetrahydropyrido[1,2-a]indol-10-yl)methanone (4′a): ^{1}H NMR (600 MHz, $CDCl_3$)



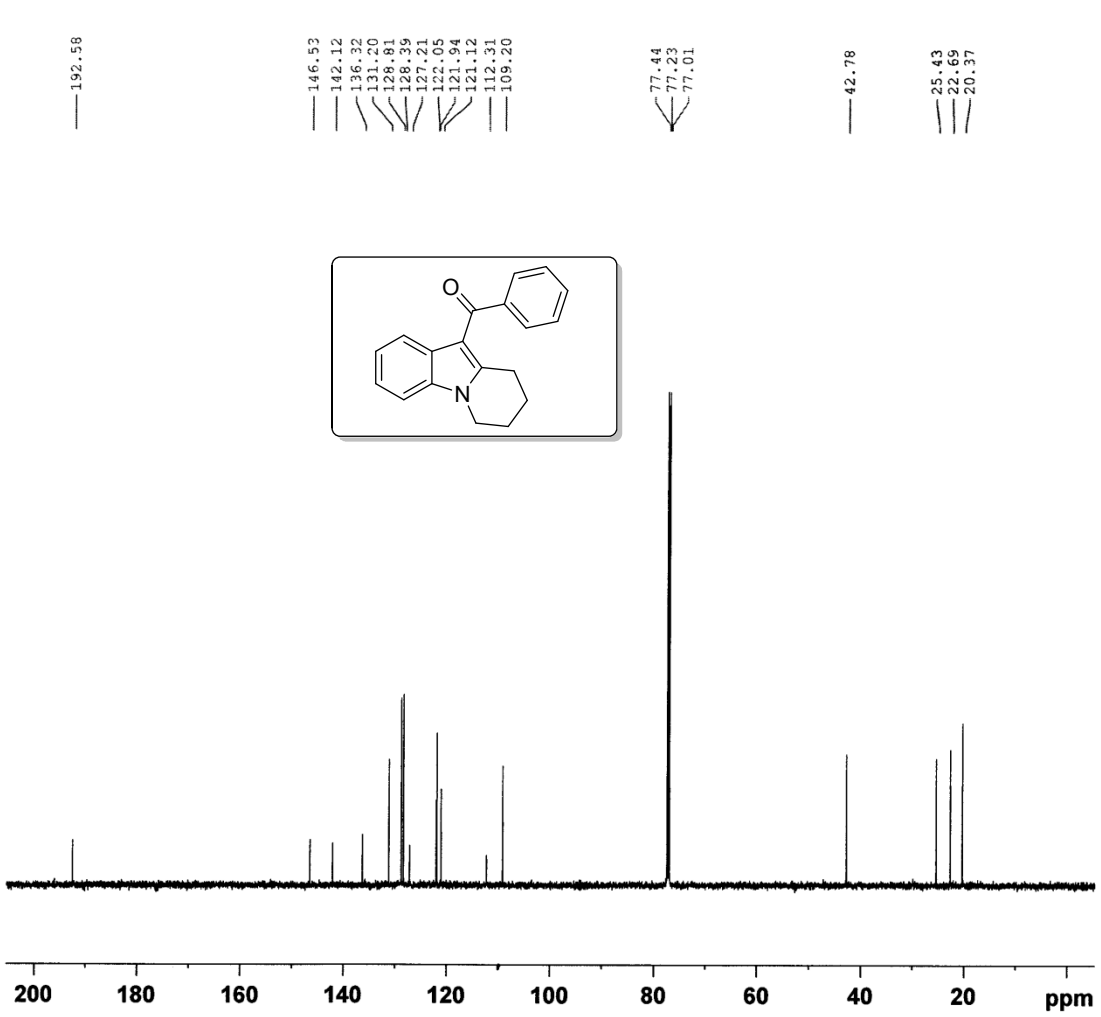

```
Current Data Parameters
NAME         AM-AG-P1-1H
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140214
Time                10.36
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                 65.24
DW                41.600 usec
DE                 6.50 usec
TE                299.4 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            600.1700268 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

(Phenyl(6,7,8,9-tetrahydropyrido[1,2-a]indol-10-yl)methanone (4′a): ^{13}C NMR (150 MHz, $CDCl_3$)




```
Current Data Parameters
NAME        AM-AG-P1-13C
EXPNO                  1
PROCNO                 1

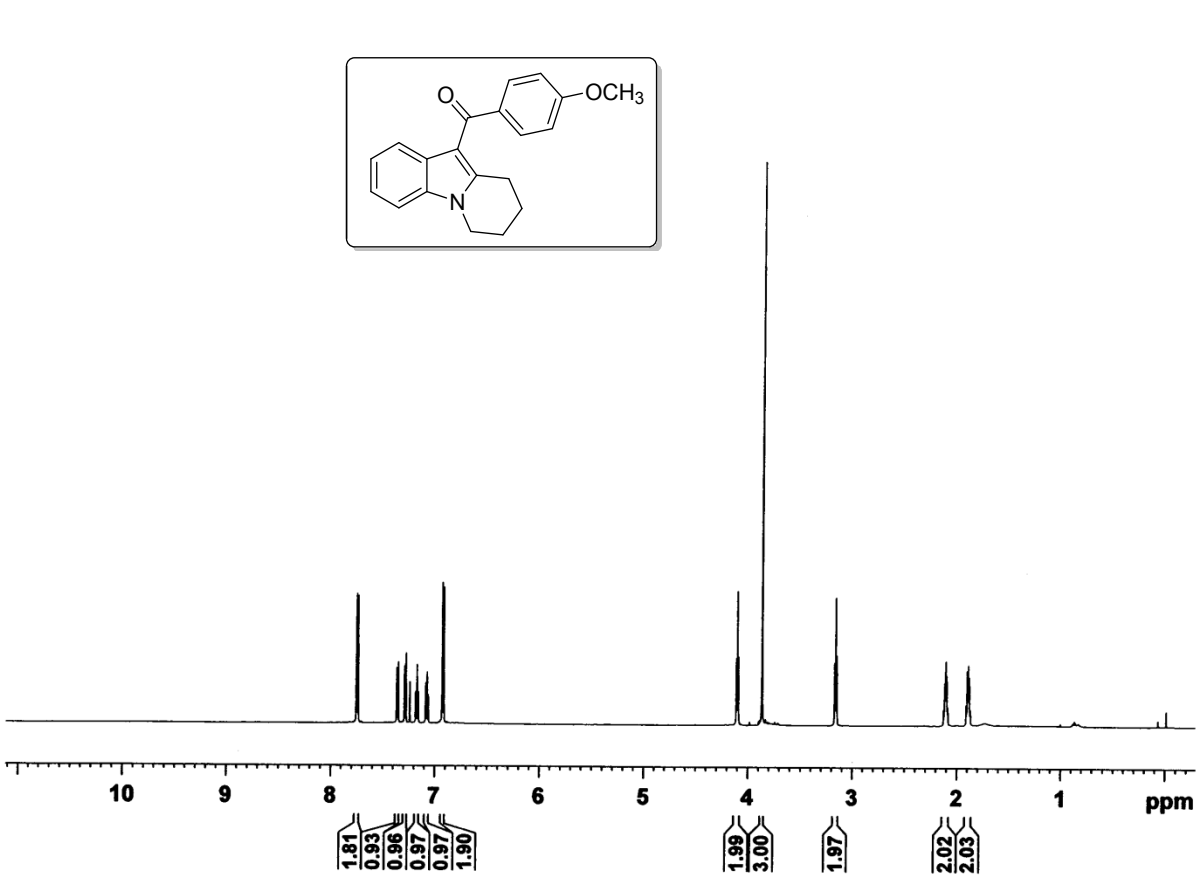
F2 - Acquisition Parameters
Date_           20140214
Time               10.43
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  158
DS                    2
SWH           36057.691 Hz
FIDRES         1.100393 Hz
AQ            0.4543829 sec
RG                65.24
DW               13.867 usec
DE                6.50 usec
TE                300.3 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          150.9128390 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

(4-Methoxyphenyl)(6,7,8,9-tetrahydropyrido[1,2-a]indol-10-yl)methanone (4′d): ^{1}H NMR (600 MHz, $CDCl_3$)



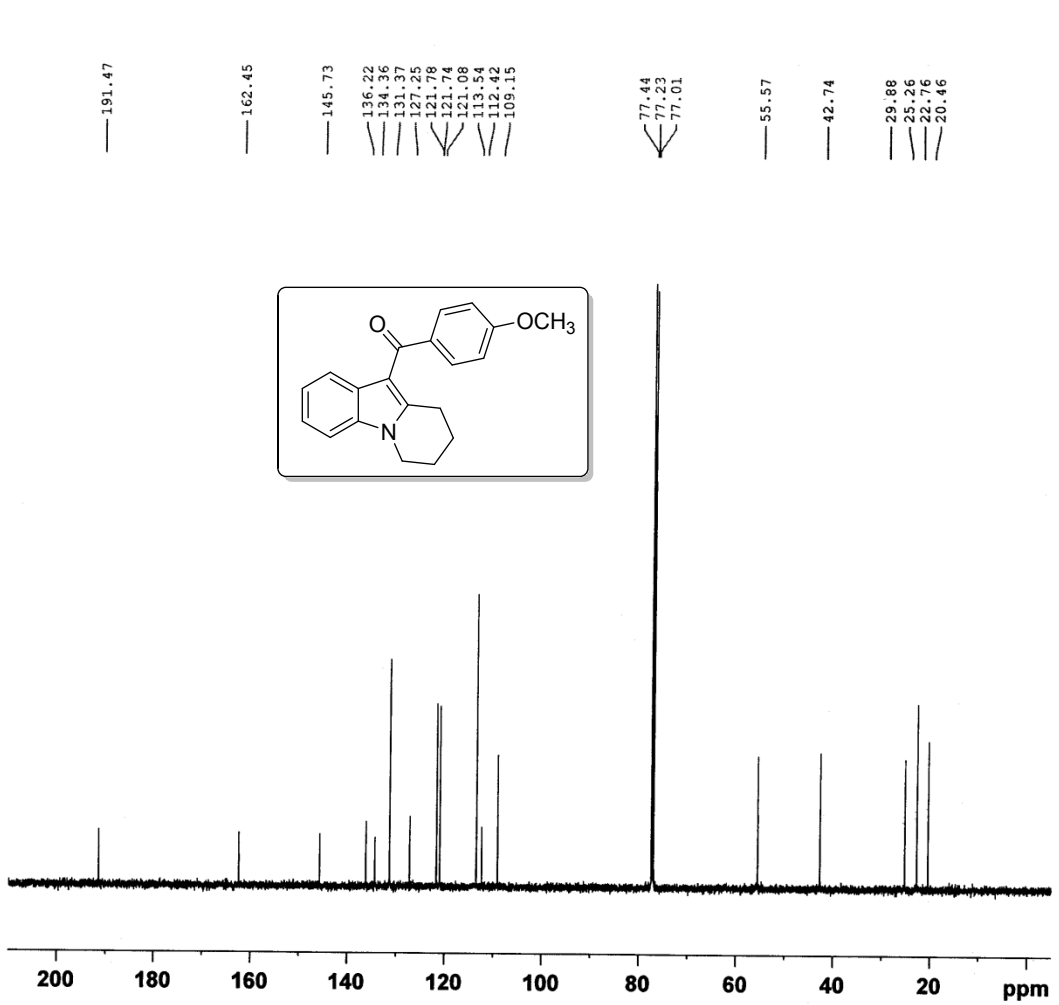

```
Current Data Parameters
NAME                  AM-OME-1H
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_              20140218
Time                   9.58
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                     43.16
DW                    41.600 usec
DE                     6.50 usec
TE                    300.2 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             600.1700268 MHz
WDW                      EM
SSB       0
LB                     0.30 Hz
GB        0
PC                     1.00
```

(4-Methoxyphenyl)(6,7,8,9-tetrahydropyrido[1,2-a]indol-10-yl)methanone (4′d): ^{13}C NMR (150 MHz, $CDCl_3$)




```
Current Data Parameters
NAME          AM-OME-13C
EXPNO                  1
PROCNO                 1

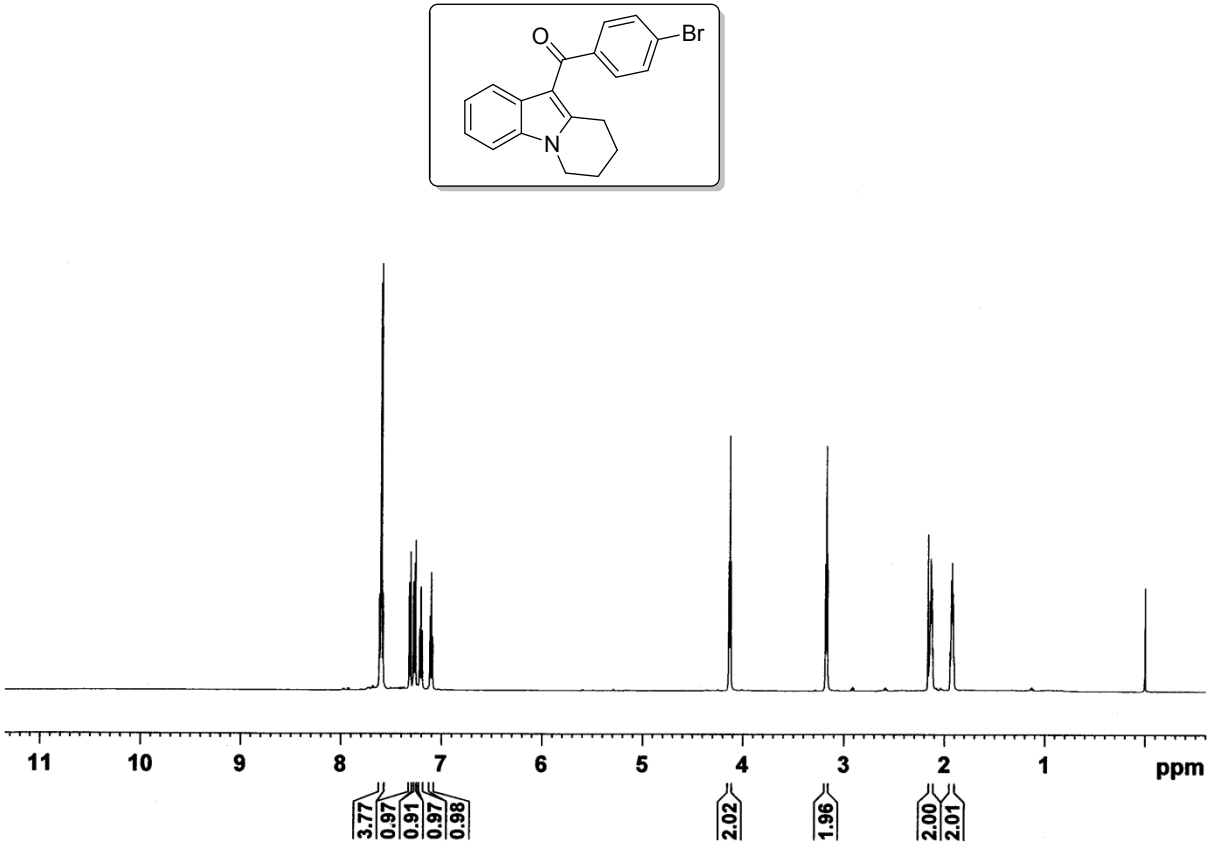
F2 - Acquisition Parameters
Date_           20140218
Time               9.47
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD              32768
SOLVENT          CDCl3
NS                 138
DS                   2
SWH          36057.691 Hz
FIDRES        1.100393 Hz
AQ           0.4543829 sec
RG               65.24
DW              13.867 usec
DE               6.50 usec
TE              300.7 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         150.9128412 MHz
WDW                EM
SSB      0
LB               1.00 Hz
GB       0
PC               1.40
```

(4-Bromophenyl)(6,7,8,9-tetrahydropyrido[1,2-a]indol-10-yl)methanone (4′e): ^{1}H NMR (600 MHz, $CDCl_3$)



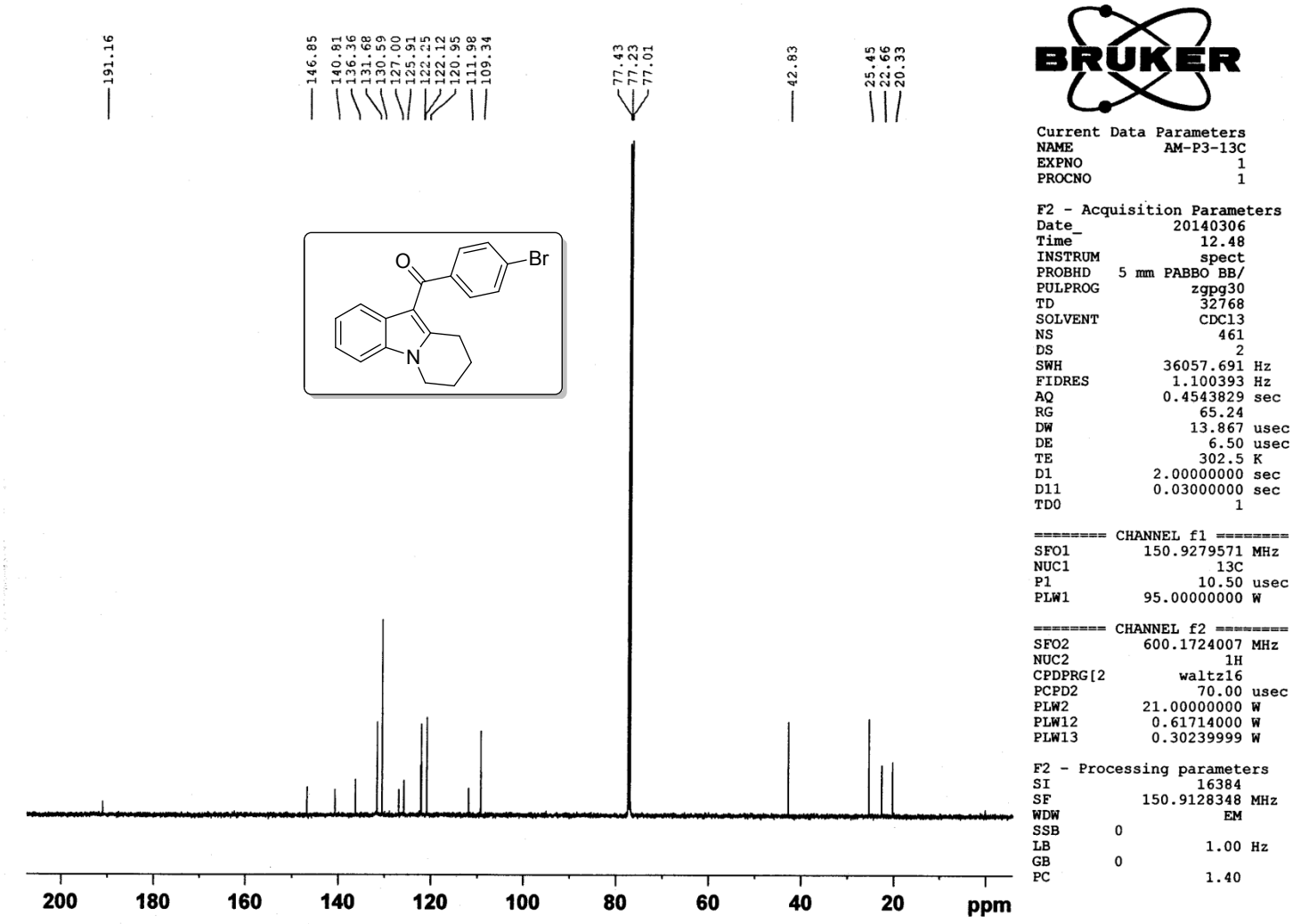

```
Current Data Parameters
NAME                  AM-P3-1H
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20140306
Time                     13.11
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                        99.36
DW                       41.600 usec
DE                        6.50 usec
TE                       301.9 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                  600.1700167 MHz
WDW                         EM
SSB                  0
LB                       0.30 Hz
GB                   0
PC                       1.00
```

(4-Bromophenyl)(6,7,8,9-tetrahydropyrido[1,2-a]indol-10-yl)methanone (4′e): ^{13}C NMR (150 MHz, $CDCl_3$)




```
Current Data Parameters
NAME                  AM-P3-13C
EXPNO                         1
PROCNO                        1

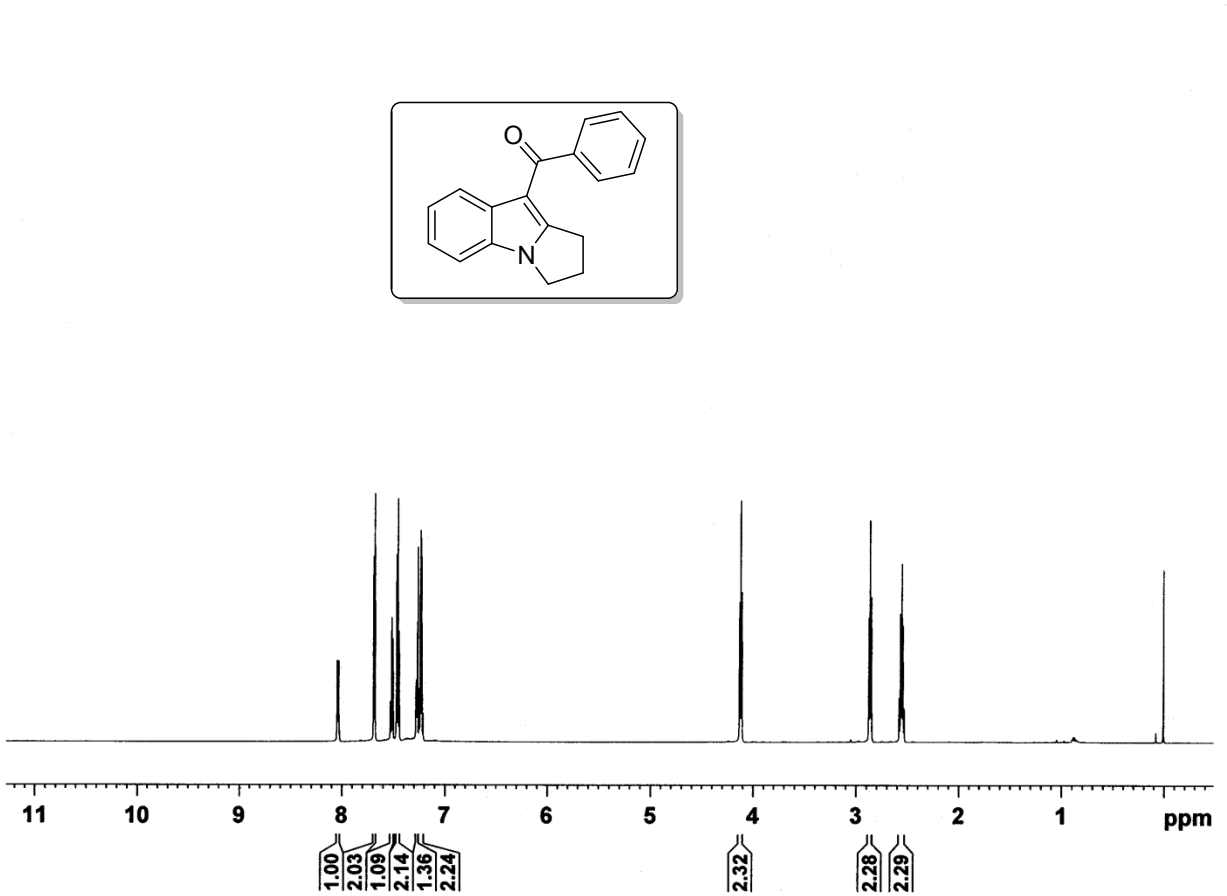
F2 - Acquisition Parameters
Date_                  20140306
Time                      12.48
INSTRUM                   spect
PROBHD    5 mm PABBO BB/
PULPROG                 zgpg30
TD                        32768
SOLVENT                   CDCl3
NS                          461
DS                            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                       302.5 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                 150.9128348 MHz
WDW                          EM
SSB          0
LB                        1.00 Hz
GB           0
PC                        1.40
```

(2,3-Dihydro-1*H*-pyrrolo[1,2-a]indol-9-yl)(phenyl)methanone (5′a): ^{1}H NMR (600 MHz, $CDCl_3$)



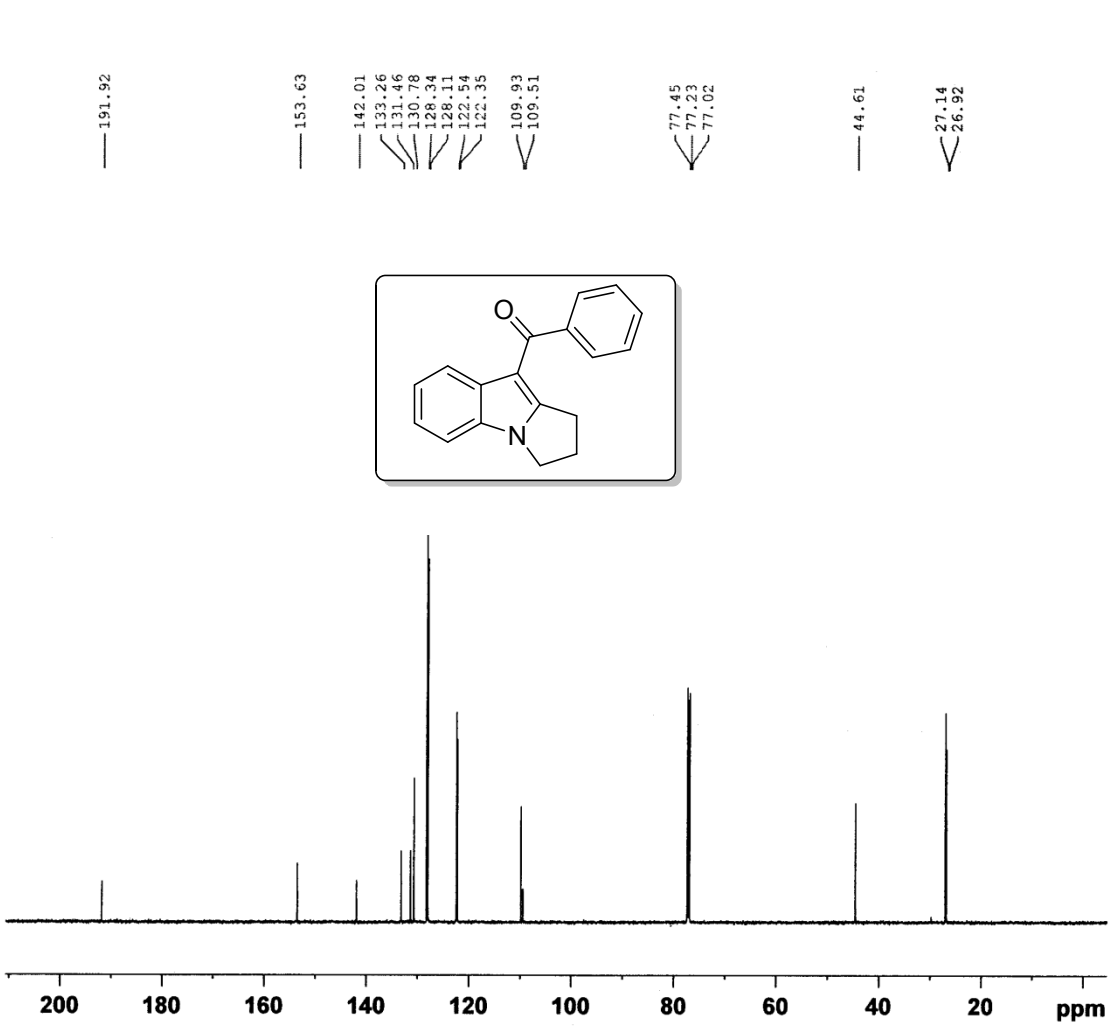

```
Current Data Parameters
NAME                  AM-P4-R_1H
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20140311
Time                       16.18
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                        300.1 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                  600.1700141 MHz
WDW                           EM
SSB                0
LB                         0.30 Hz
GB                 0
PC                         1.00
```

(2,3-Dihydro-1*H*-pyrrolo[1,2-a]indol-9-yl)(phenyl)methanone (5′a): ^{13}C NMR (150 MHz, $CDCl_3$)




```
Current Data Parameters
NAME                 AM-P4-13C
EXPNO                        1
PROCNO                       1

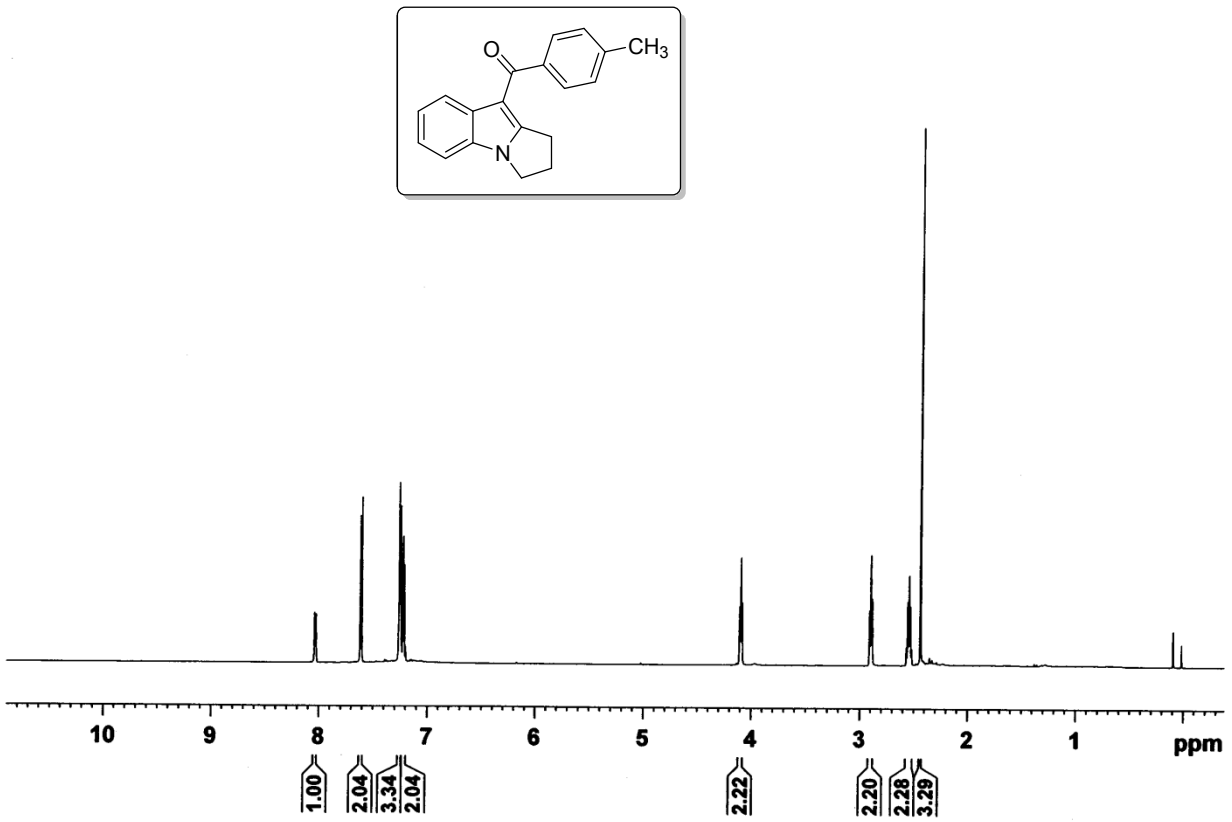
F2 - Acquisition Parameters
Date_                 20140310
Time                      8.53
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                 zgpg30
TD                       32768
SOLVENT                  CDC13
NS                         203
DS                           2
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                  2.00000000 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                 150.9128460 MHz
WDW                         EM
SSB          0
LB                        1.00 Hz
GB           0
PC                        1.40
```

(2,3-Dihydro-1*H*-pyrrolo[1,2-a]indol-9-yl)(p-tolyl)methanone (5′g): ^{1}H NMR (600 MHz, $CDCl_3$)



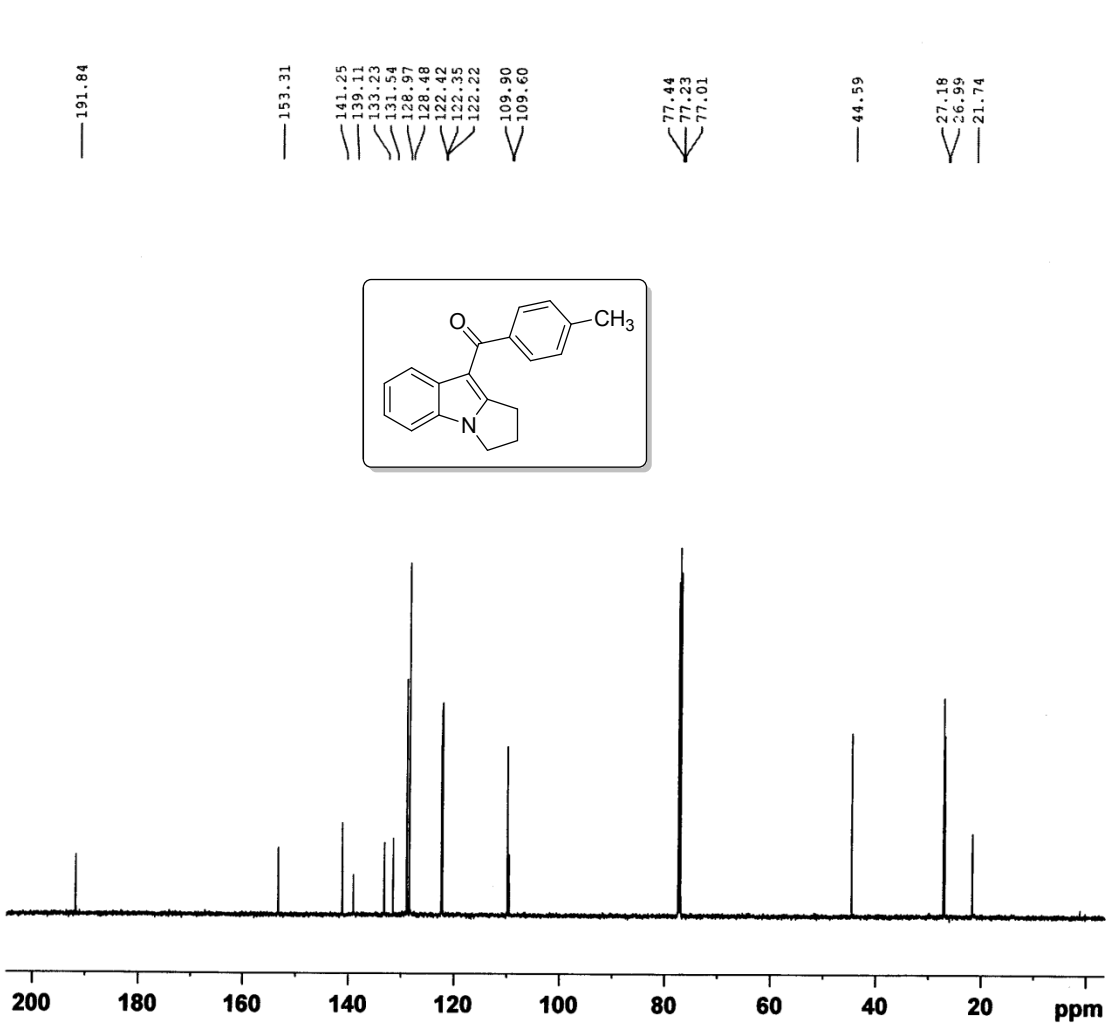

```
Current Data Parameters
NAME                  AG-AM-p6-1H
EXPNO                           1
PROCNO                          1

F2 - Acquisition Parameters
Date_                    20140324
Time                        10.02
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                          49.39
DW                         41.600 usec
DE                          6.50 usec
TE                         299.6 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                    600.1700141 MHz
WDW                           EM
SSB          0
LB                          0.30 Hz
GB           0
PC                          1.00
```

(2,3-Dihydro-1*H*-pyrrolo[1,2-a]indol-9-yl)(p-tolyl)methanone (5′g): ^{13}C NMR (150 MHz, $CDCl_3$)



BRUKER

```
Current Data Parameters
NAME          AG-AM-P6-13C
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20140324
Time                 12.37
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG            zgpg30
TD                  32768
SOLVENT             CDCl3
NS                    202
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                 300.9 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            150.9128436 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```