Supporting Informations

A Copper Catalyzed Synthesis of 3-Aroylindoles via a sp^3 C–H Bond Activation Followed by C–C and C–O Bond Formation

Anupal Gogoi, Srimanta Guin, Saroj Kumar Rout and Bhisma K. Patel*

Department of Chemistry, Indian Institute of Technology Guwahati

Email: patel@iitg.ernet.in

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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 (300 MHz and 400 MHz) $CDCl_3$ solvent as the internal standard for ^{13}C NMR (75 MHz and 100 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.

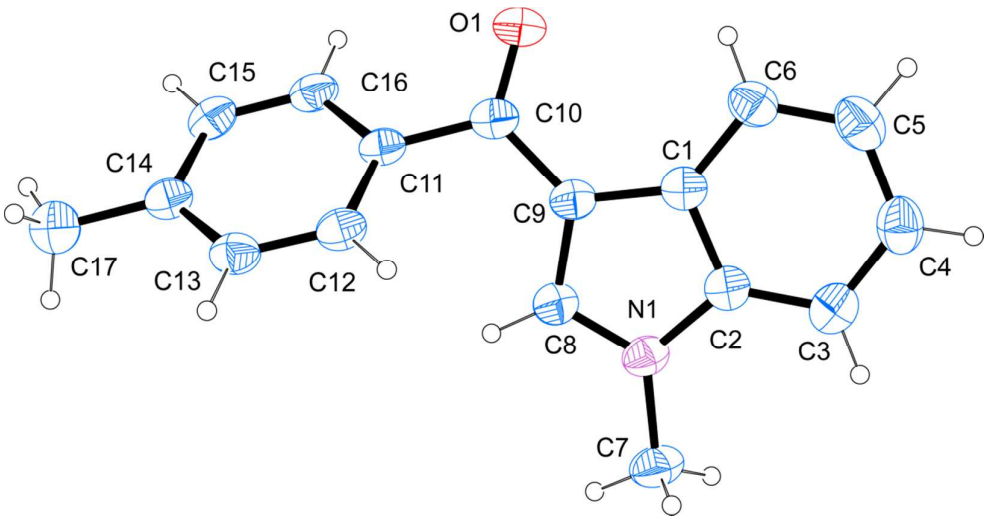
a. SMART V 4.043 Software for the CCD Detector System; Siemens Analytical Instruments Division: Madison, WI, 1995.

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 (1-Methyl-1*H*-indol-3-yl)(*p*-tolyl)methanone (1'b):

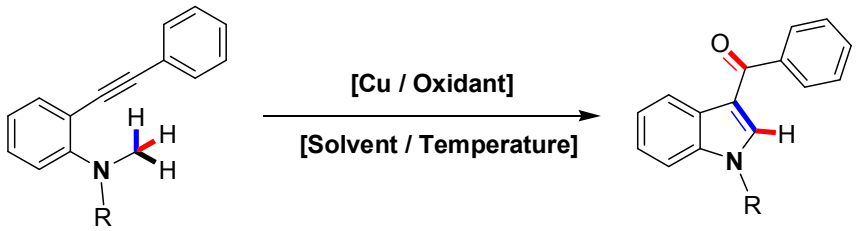
$C_{17}H_{15}NO$, crystal dimensions 0.41 x 0.35 x 0.26 mm, M_r = 249.30, Monoclinic, space group P21/n, a =11.1536(9), b = 7.2700(6), c = 16.7473(14) Å, α = 90 °, β = 101.080(3) °, γ = 90 °, V = 1332.67(19) Å^3, Z = 4, ρ_{calcd} = 1.242 mg/m^3, μ = 0.077 mm^{-1}, $F(000)$ = 528.0, reflection collected / unique = 3304 / 1785, refinement method = full-matrix least-squares on F^2, final R indices [$I > 2\sigma(I)$]: R_1 = 0.0493, wR_2 = 0.1117, R indices (all data): R_1 = 0.0872, wR_2 = 0.1201, goodness of fit = 0.997. CCDC-917715 for (1-Methyl-1*H*-indol-3-yl)(*p*-tolyl)methanone (**1'b**) 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.



(1-Methyl-1*H*-indol-3-yl)(*p*-tolyl)methanone (1'b)

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**) (110.65 mg, 0.5 mmol) in DMSO (2 mL) was added CuBr (7.17 mg, 0.05 mmol), followed by TBHP 70 % wt in water (215 µl, 1.5 mmol) and the resultant mixture was put into a preheated oil bath (80 ^{o}C) for 3.5 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**) (90.58 mg, 77 % yield).

Table S1. Screening of Reaction Condition

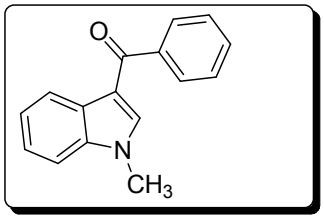


Entry	Catalyst (mol %)	Solvent	Oxidant (equiv)	Temp (^{o}C)	Yield (%)[a]
1	CuBr (10)	Toluene	5-6 M decane solution of TBHP (1)	80	45
2	CuBr (10)	Toluene	70% aq TBHP (1)	80	55
3	CuBr (10)	Toluene	70% aq TBHP (2)	80	62
4	CuBr (10)	Toluene	70% aq TBHP (3)	80	70
5	$CuBr_2$ (10)	Toluene	70% aq TBHP (3)	80	58
6	CuCl (10)	Toluene	70% aq TBHP (3)	80	55
7	CuI (10)	Toluene	70% aq TBHP (3)	80	68
8	$Cu(OAc)_2$ (10)	Toluene	70% aq TBHP (3)	80	40
9	$CuCl_2$ (10)	Toluene	70% aq TBHP (3)	80	25
10	CuBr (5)	Toluene	70% aq TBHP (3)	80	52
11	**CuBr (10)**	**DMSO**	70% aq **TBHP (3)**	**80**	**77**
12	CuBr (10)	*o*xylene	70% aq TBHP (3)	80	66
13	CuBr (10)	dioxane	70% aq TBHP (3)	80	62
14	CuBr (10)	DMF	70% aq TBHP (3)	80	25
15	CuBr (10)	THF	70% aq TBHP (3)	80	10
16	CuBr (10)	DMSO	70% aq TBHP (3)	100	60
17	CuBr (10)	DMSO	70% aq TBHP (3)	60	43
18	nil	DMSO	70% aq TBHP (3)	80	0
19	CuBr (10)	DMSO	Nil	80	0
20	$Pd(OAc)_2$ (10)	DMSO	70% aq TBHP (3)	80	35
21	$CoCl_2$ (10)	DMSO	70% aq TBHP (3)	80	50
22	$FeCl_3$ (10)	DMSO	70% aq TBHP (3)	80	45

[a]Isolalated yield.

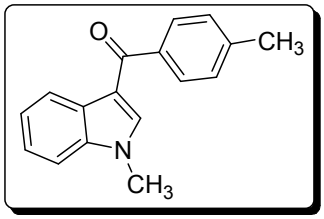
Spectral Data

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



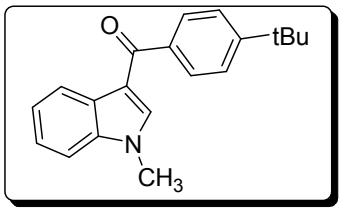
^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 3.82 (s, 3H), 7.31–7.38 (m, 3H), 7.44–7.53 (m, 3H), 7.78–7.81 (m, 2H), 8.40–8.42 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 33.7, 109.8, 115.8, 122.9, 123.8, 127.4, 128.5, 128.9, 131.3,132.4, 137.7, 138.1, 141.1, 191.1; IR (KBr): 2923, 2851, 1621, 1575, 1524, 1465, 1368, 1233, 1155, 1124, 1070, 872, 746, 716 cm^{-1}; HRMS (ESI): calcd. for $C_{16}H_{13}NO$ (MH^+) 236.1070; found 236.1065.

(1-Methyl-1*H*-indol-3-yl)(*p*-tolyl)methanone (1'b):



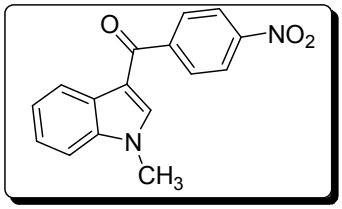
^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 2.42 (s, 3H), 3.83 (s, 3H), 7.27 (d, 2H, *J* = 7.6 Hz), 7.31–7.35 (m, 3H), 7.52 (s, 1H), 7.72 (d, 2H, *J* = 8.0 Hz), 8.38–8.40 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 21.7, 33.7, 109.8, 115.9, 122.8, 122.9, 123.7, 127.4, 129.0, 129.1, 137.7, 137.8, 138.3, 141.7, 190.9; IR (KBr): 2925, 2851, 1731, 1619, 1523, 1465, 1369, 1230, 1123, 1070, 875, 771, 776 cm^{-1}; HRMS (ESI): calcd. for $C_{17}H_{15}NO$ (MH^+) 250.1226; found 250.1224.

(4-Tert-butylphenyl)(1-methyl-1*H*-indol-3-yl)methanone (1'c):



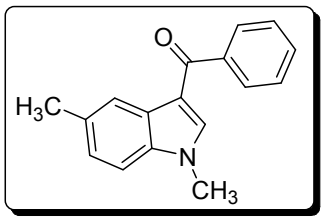
^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.36 (s, 9H), 3.84 (s, 3H), 7.32–7.36 (m, 3H), 7.48 (d, 2H, *J* = 8.4 Hz), 7.56 (s, 1H), 7.76 (d, 2H, *J* = 8.4 Hz), 8.41-8.43 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 29.9, 31.4, 35.1, 109.8, 115.9, 122.8, 123.0, 123.8, 125.4, 127.5, 128.9, 137.7, 138.0, 138.3, 154.8, 190.9; 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 292.1699.

(1-Methyl-1*H*-indol-3-yl) (4-nitrophenyl) methanone (1'd):



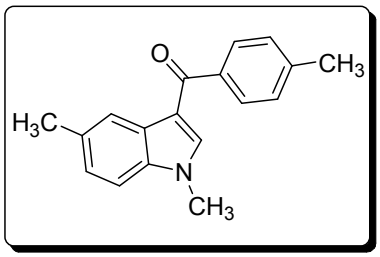
^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 3.87 (s, 3H), 7.35–7.40 (m, 3H), 7.49 (s, 1H), 7.91–7.93(m, 2H), 8.30–8.32(m, 2H), 8.38–8.40 (m, 1H) ; ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 33.7, 109.9, 115.3, 122.6, 123.3, 123.6, 124.2, 126.8, 126.9, 127.6, 128.5, 129.4, 137.7, 138.1, 146.3, 149.1, 188.4; IR (KBr): 2915, 2853, 1734, 1592, 1381, 1244, 1172, 1076, 982, 832, 742, 716 cm^{-1}; Anal. calcd for $C_{16}H_{12}N_2O_3$: C 68.56, H 4.32, N 9.99; found C 68.52, H 4.25, N 9.90.

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



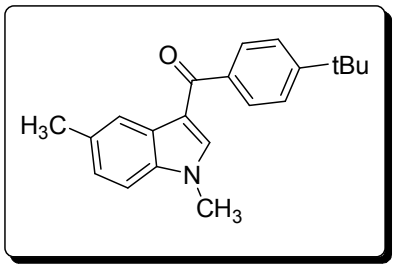
^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 2.51 (s, 3H) 3.81 (s, 3H), 7.18 (d, 1H, *J* = 8.4 Hz), 7.24–7.27 (m, 1H), 7.45–7.49 (m, 3H), 7.53 (d, 1H, *J* = 7.6 Hz), 7.80 (d, 2H, *J* = 8.0 Hz), 8.257–8.26 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 21.7, 33.6, 109.4, 115.2, 122.5, 125.3, 127.5, 128.3, 128.7, 131.0, 132.5, 136.1, 138.2, 141.2, 190.9; IR (KBr): 2924, 2852, 1627, 1522, 1361, 1268, 1237, 1117, 741 cm^{-1}; HRMS (ESI): calcd. for $C_{17}H_{15}NO$ (MH^+) 250.1226; found 250.1221.

(1,5-Dimethyl-1*H*-indol-3-yl)(*p*-tolyl)methanone (2'b):



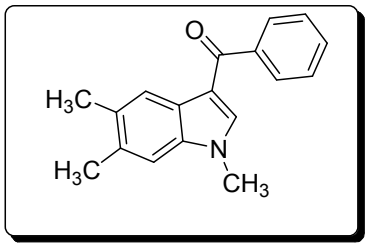
^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 2.44 (s, 3H), 2.51 (s, 3H), 3.81 (s, 3H), 7.17 (d, 1H, *J* = 8.4 Hz), 7.26–7.29 (m, 3H), 7.48 (s, 1H), 7.72 (d, 2H, *J* = 8.0 Hz), 8.24–8.25 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 21.5, 21.6, 33.5, 109.4, 115.2, 122.4, 125.1, 127.6, 128.9, 129.0, 132.3, 136.0, 137.9, 138.3, 141.5, 190.8; IR (KBr): 3027, 2921, 1618, 1523, 1484, 1458, 1237, 1141, 1119, 1064, 845, 787, 738 cm^{-1}; HRMS (ESI): calcd. for $C_{18}H_{17}NO$ (MH^+) 264.1383; found 264.1381.

(4-Tert-butylphenyl)(1,5-Dimethyl-1*H*-indol-3-yl)methanone (2'c):



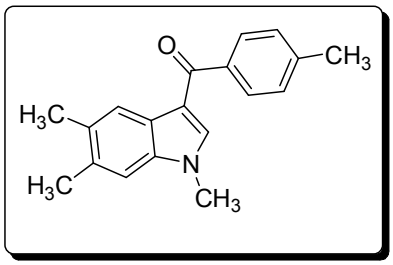
^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.37 (s, 9H), 2.51(s, 3H), 3.81 (s, 3H), 7.17 (d, 1H, *J* = 9.6 Hz), 7.25 (d, 1H, *J* = 8.4 Hz), 7.48–7.51 (m, 3H), 7.76 (d, 2H, *J* = 8.4 Hz), 8.28 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 21.7, 31.4, 33.6, 35.1, 109.4, 115.3, 122.6, 125.2, 125.3, 127.6, 128.7, 132.4, 136.1, 138.1, 138.4, 154.5, 190.8; IR (KBr): 2961, 2852, 1621, 1524, 1461, 1363, 1237, 1190, 1144, 1106, 1064, 848, 831, 709 cm^{-1}; HRMS (ESI): calcd. for $C_{21}H_{23}NO$ (MH^+) 306.1852; found 306.1862.

(1,5,6-Trimethy-l*H*-indol-3-yl)(phenyl)methanone (3'a):



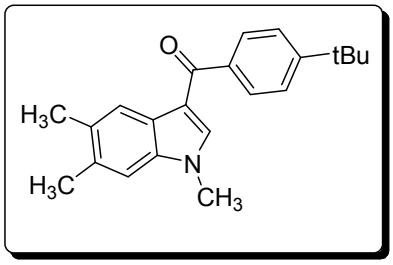
^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 2.39 (s, 3H), 2.40 (s, 3H), 3.78 (s, 3H), 7.12 (s, 1H), 7.40 (s, 1H), 7.43–7.51 (m, 3H), 7.77–7.79 (m, 2H), 8.19 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 20.3, 20.8, 33.6, 110.1, 115.3, 122.9, 125.6, 128.3, 128.8, 131.0, 131.9, 133.0, 136.7, 137.6, 141.3, 191.0; IR (KBr): 2928, 2851, 1624, 1523, 1465, 1363, 1262, 1240, 1119, 1064, 982, 842, 739, 716 cm^{-1}; HRMS (ESI): calcd. for $C_{18}H_{17}NO$ (MH^+) 264.1383; found 264.1376.

(1,5,6-Trimethy-l*H*-indol-3-yl)(*p*-tolyl)methanone (3'b):



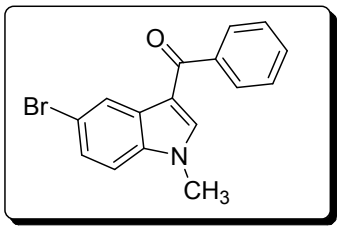
^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 2.41 (s, 3H), 2.42 (s, 3H), 2.44 (s, 3H), 3.80 (s, 3H), 7.14 (s, 1H), 7.27 (d, 2H, *J* = 10 Hz), 7.43 (s, 1H), 7.72 (d, 2H, *J* = 8.0 Hz), 8.20 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 20.2, 20.7, 21.6, 33.5, 110.0, 115.2, 122.7, 125.5, 128.8, 128.9, 131.6, 132.8, 136.5, 137.3, 138.4, 141.3, 190.7; IR (KBr): 2923, 2857, 1618, 1525, 1470, 1363, 1256, 1240, 1177, 1116, 982, 836, 768 cm^{-1}; HRMS (ESI): calcd. for $C_{19}H_{19}NO$ (MH^+) 278.1539; found 278.1530.

(4-Tert-butylphenyl)(1,5,6-trimethyl-1*H*-indol-3-yl)methanone (3'c):



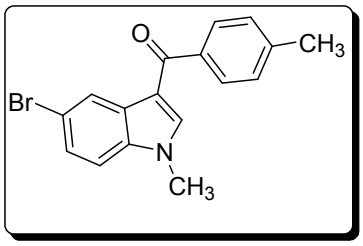
^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm)1.37 (s, 9H), 2.41 (s, 3H), 2.42 (s, 3H), 3.79 (s, 3H), 7.14 (s, 1H), 7.45 (s, 1H), 7.49 (d, 2H, *J* = 8.4 Hz), 7.76 (d, 2H, *J* = 8.4 Hz), 8.23 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ (ppm) 20.2, 20.8, 31.3, 33.5, 34.9, 110.0, 115.1, 122.8, 125.2, 125.5, 128.6, 131.6, 132.8, 136.5, 137.4, 138.4, 154.4, 190.7; IR (KBr): 2962, 2847, 1620, 1519, 1462, 1356, 1252, 1235, 1170, 1112, 978, 834, 765 cm^{-1}; Anal. calcd for $C_{22}H_{25}NO$: C 82.72, H 7.89, N 4.38; found C 82.65, H 7.95, N 4.30.

(5-Bromo-1-methyl-1*H*-indol-3-yl)(phenyl)methanone (4'a):



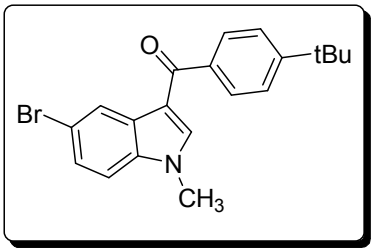
^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 3.82 (s, 3H), 7.22 (d, 1H, *J* = 8.8 Hz), 7.42 (d, 1H *J* = 8.8 Hz), 7.45–7.50 (m, 3H), 7.53 (d, 1H, *J* = 7.2Hz), 7.77 (d, 2H, *J* = 8.4 Hz), 8.58 (d, 1H, *J* = 1.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 33.9, 111.3, 115.2, 116.6, 125.4, 126.8, 128.5, 128.7, 128.9, 131.5, 136.4, 138.6, 140.7, 190.6; IR (KBr): 3055, 2928, 1612, 1575, 1527, 1470, 1446, 1365, 1235, 1190, 1079, 1023, 803, 717, 699, 670 cm^{-1}; HRMS (ESI): calcd. for $C_{16}H_{12}BrNO$ (MH^+) 314.0175; found 314.0179.

(5-Bromo-1-methyl-1*H*-indol-3-yl)(*p*-tolyl)methanone (4'b):



^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 2.42 (s, 3H), 3.81 (s, 3H), 7.21 (d, 1H, *J* = 8.4 Hz), 7.27 (d, 2H, *J* = 8.0 Hz), 7.40–7.43 (m, 1H), 7.50 (s, 1H), 7.69 (d, 2H, *J* = 8.4 Hz), 8.57 (d, 1H, *J* = 1.6Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 21.6, 33.8, 111.2, 115.1, 116.3, 125.3, 126.5, 128.8, 129.1, 129.4, 136.2, 137.8, 138.3, 141.9, 190.3; IR (KBr): 2924, 2857, 1616, 1602, 1523, 1470, 1446, 1365, 1235, 1179, 1079, 1034, 883, 806, 763, 740 cm^{-1}; HRMS (ESI): calcd. for $C_{17}H_{14}BrNO$ (MH^+) 328.0332; found 328.0338.

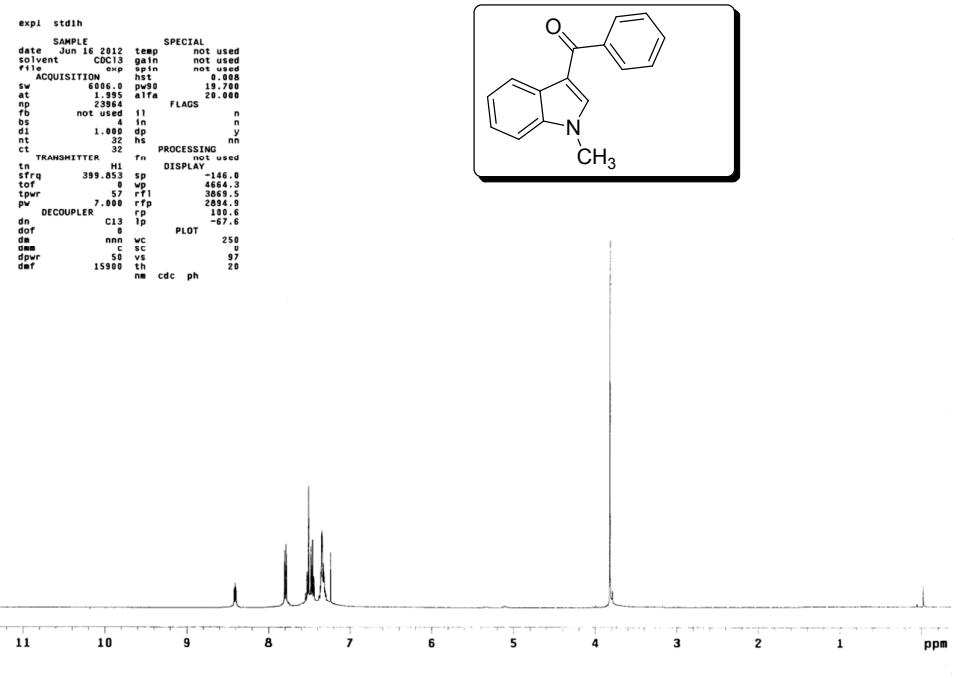
(4-Tert-butylphenyl)(5-bromo-1-methyl-1*H*-indol-3-yl)methanone (4'c):



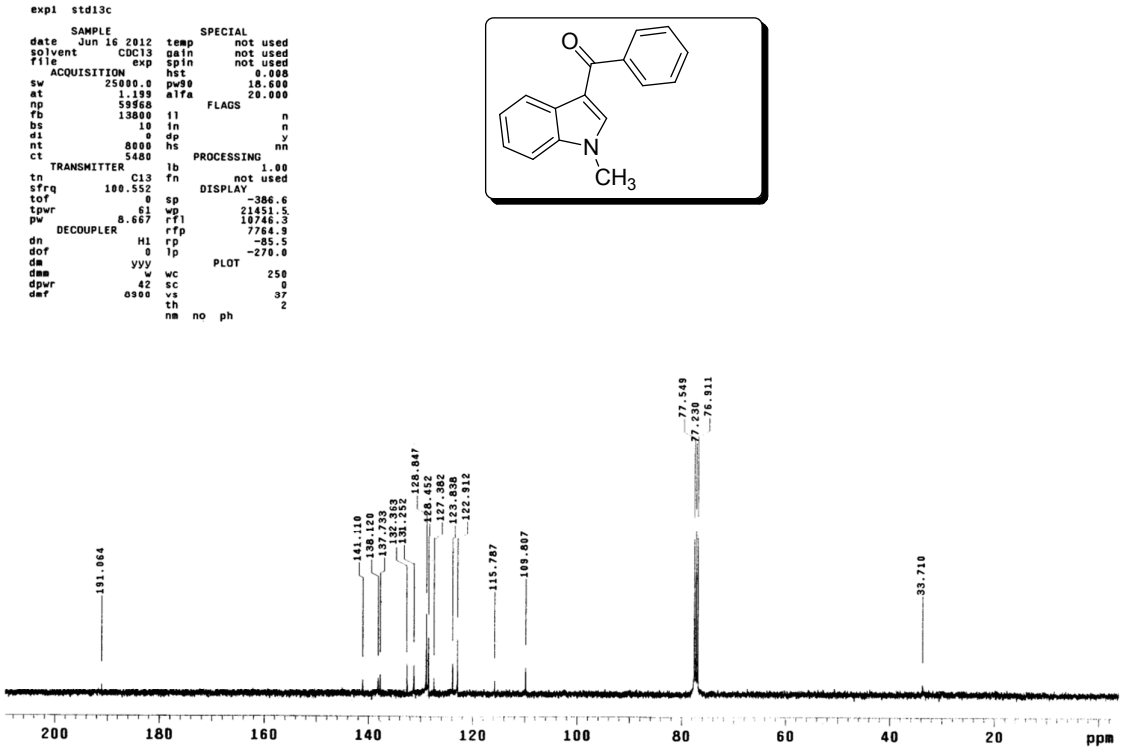
^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.36 (s, 9H), 3.81 (s, 3H), 7.21 (d, 1H J = 8.4 Hz), 7.40–7.43 (m, 1H), 7.48 (d, 2H, J = 8.4 Hz), 7.53 (s, 1H), 7.73 (d, 2H, J = 8.4 Hz), 8.59 (d, 1H, J = 2.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) 31.4, 33.9, 35.2, 111.2, 115.3, 116.6, 125.5, 126.7, 128.6, 128.8, 130.3, 133.8, 136.4, 137.9, 138.5, 155.1, 190.5; IR (KBr): 2961, 2853, 1626, 1524, 1463, 1364, 1267, 1235, 1105, 886, 798, 741, 709 cm^{-1}; HRMS (ESI): calcd. for $C_{20}H_{20}BrNO$ (MH^+) 370.0801; found 370.0809.

SPECTRA

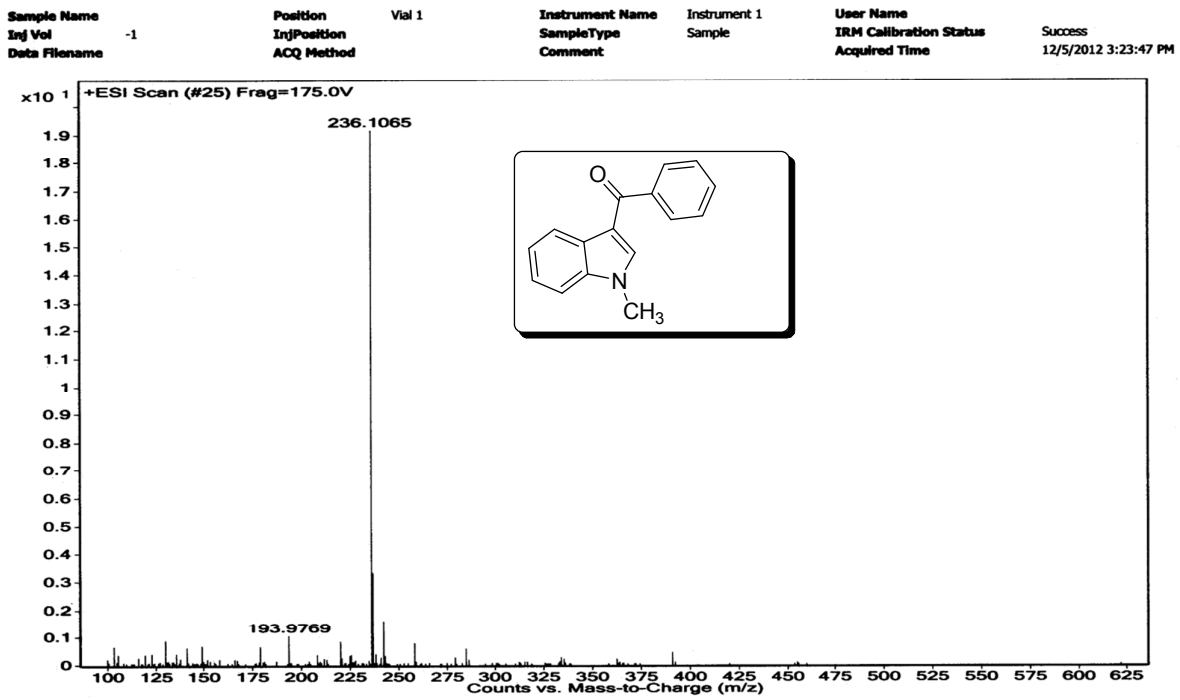
(1-Methyl-1*H*-indol-3-yl)(phenyl)methanone (1'a): ^{1}H NMR (400 MHz, $CDCl_3$)



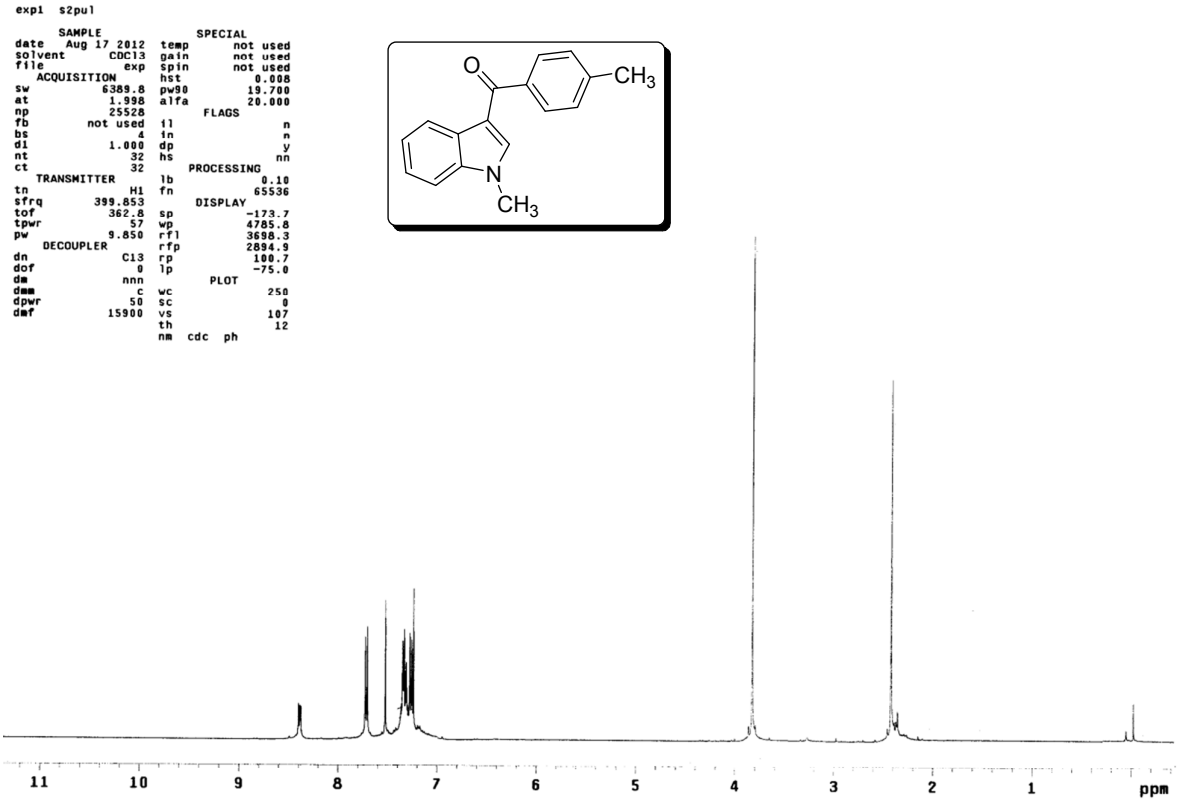
(1-Methyl-1*H*-indol-3-yl)(phenyl)methanone (1'a): ^{13}C NMR (100 MHz, $CDCl_3$)



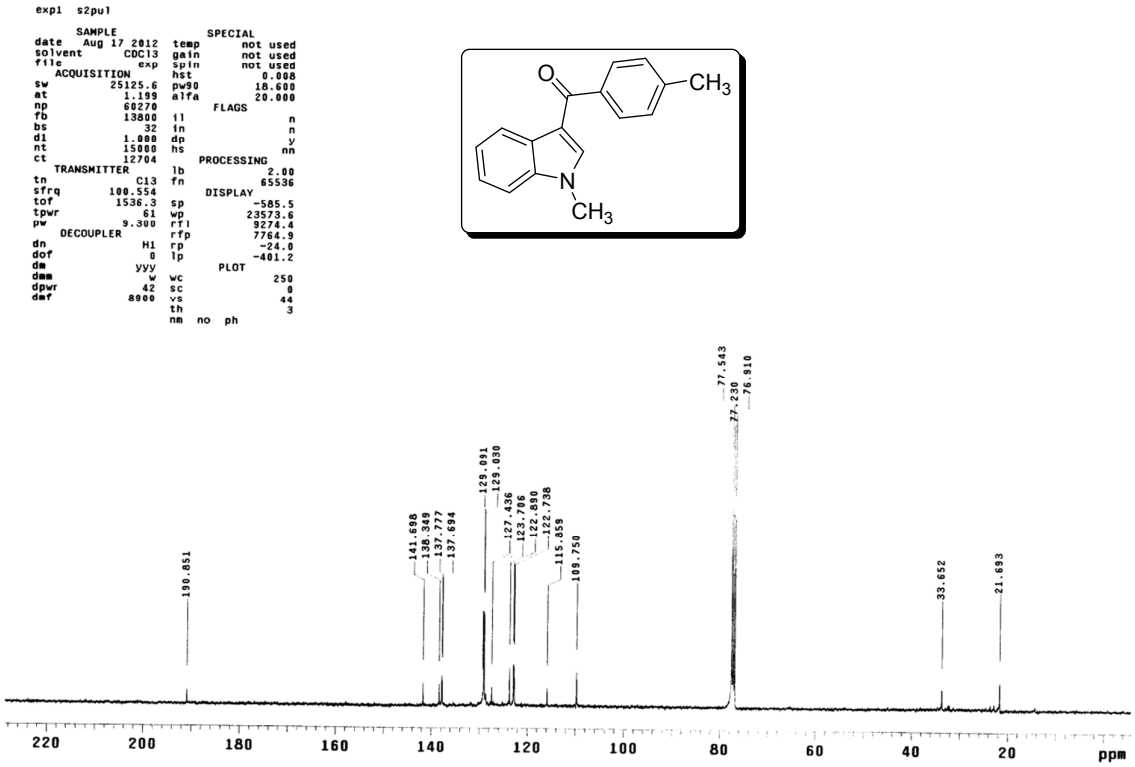
(1-Methyl-1*H*-indol-3-yl)(phenyl)methanone (1'a): HRMS



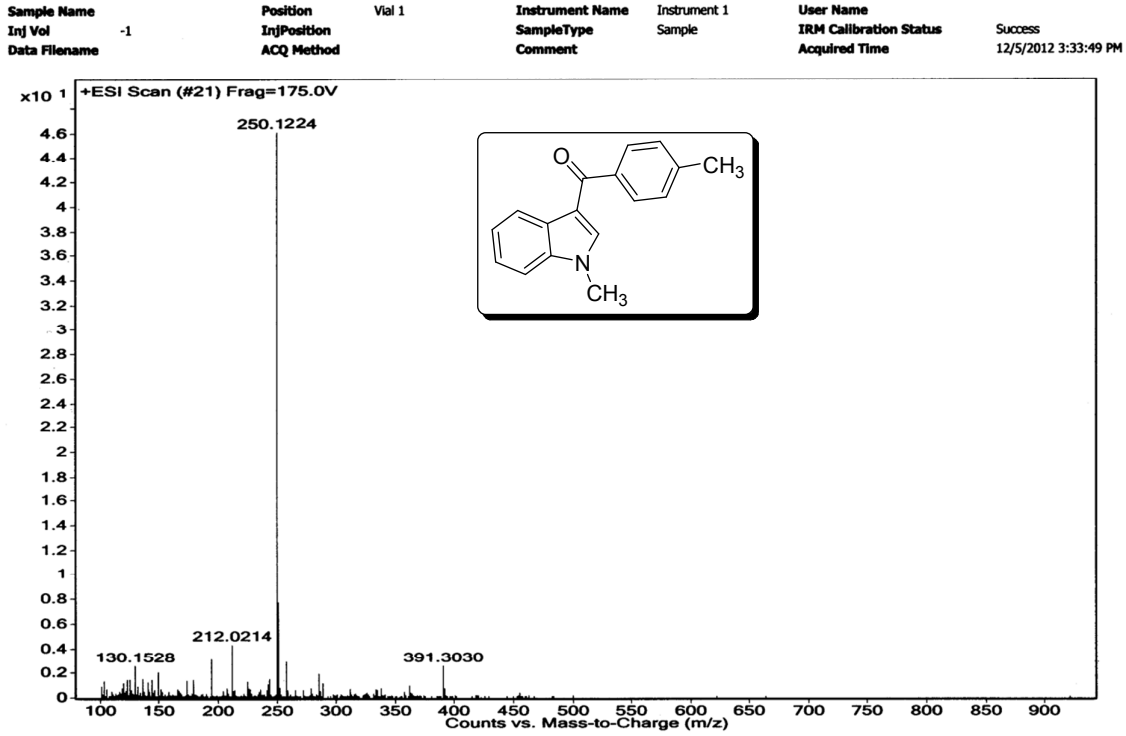
(1-Methyl-1*H*-indol-3-yl)(*p*-tolyl)methanone (1'b): ^{1}H NMR (400 MHz, $CDCl_3$)



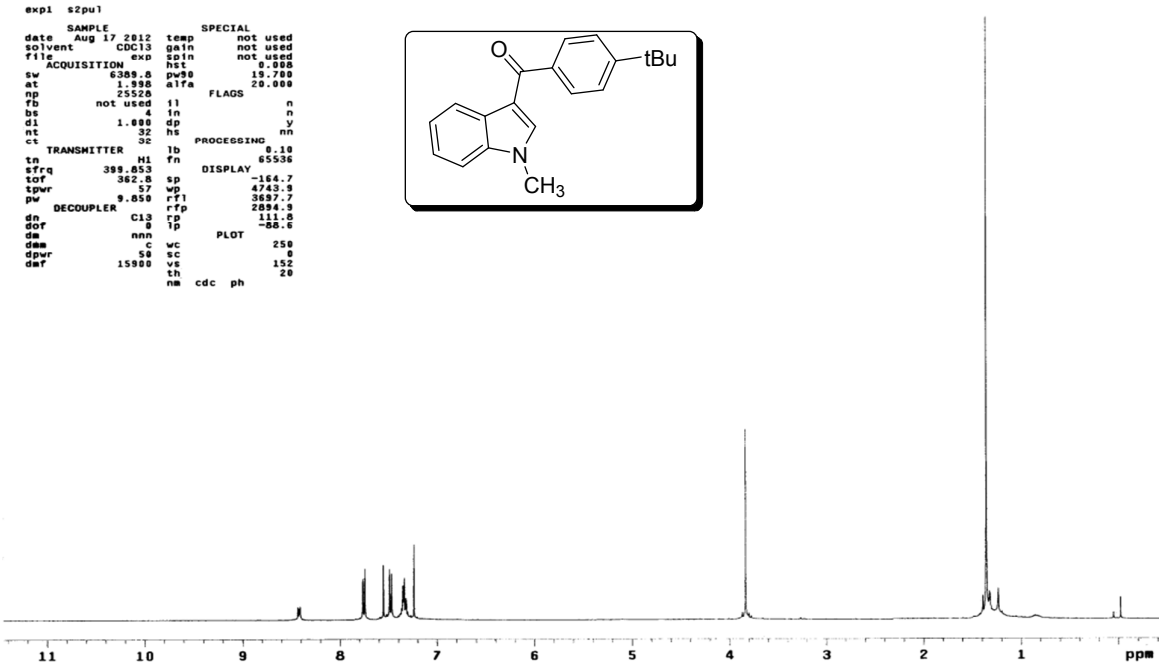
(1-Methyl-1*H*-indol-3-yl)(*p*-tolyl)methanone (1'b): ^{13}C NMR (100 MHz, $CDCl_3$)



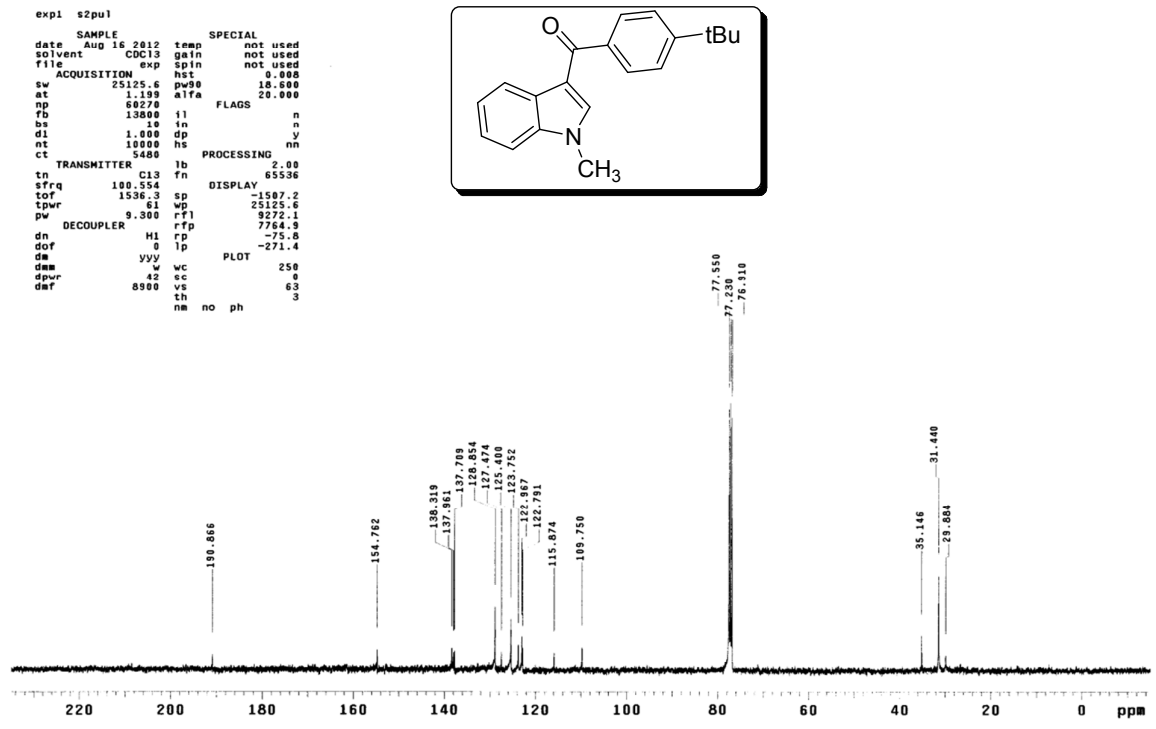
(1-Methyl-1*H*-indol-3-yl)(*p*-tolyl)methanone (1'b): HRMS



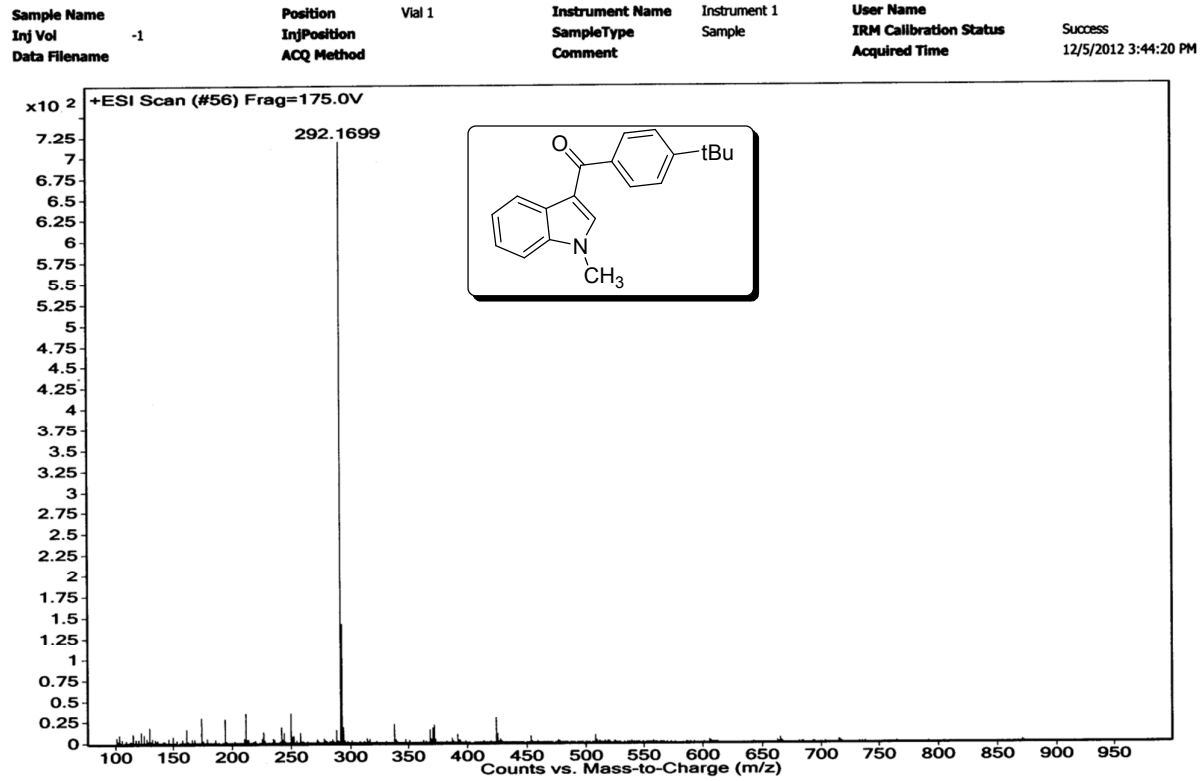
(4-Tert-butylphenyl)(1-methyl-1*H*-indol-3-yl)methanone (1'c): ^{1}H NMR (400 MHz, $CDCl_3$)



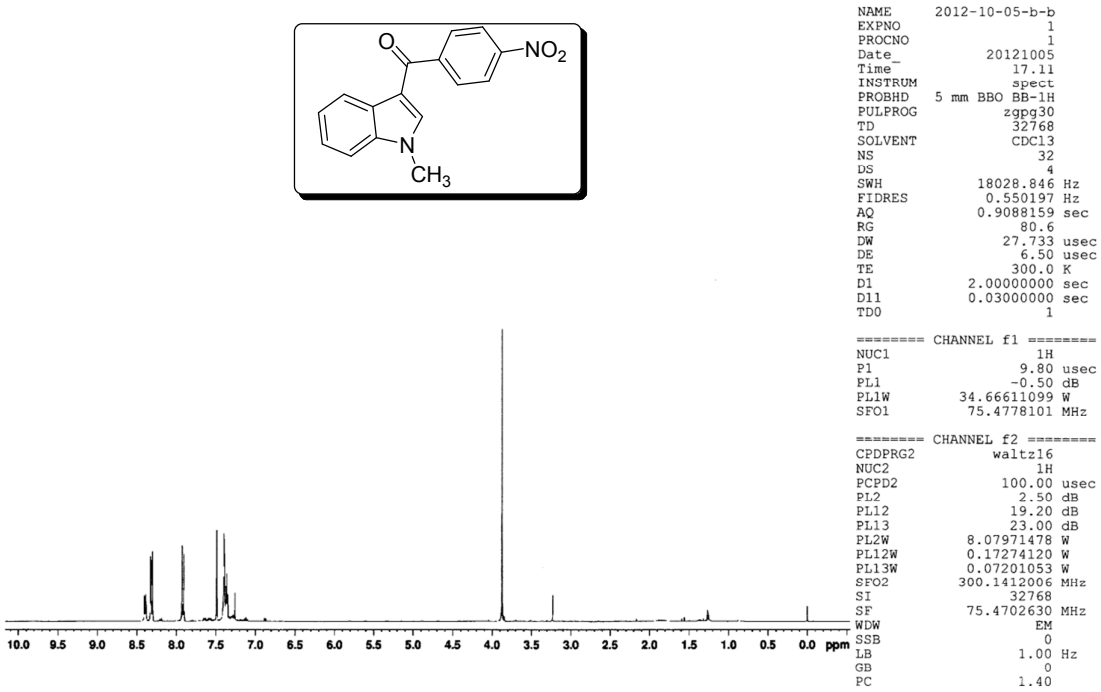
(4-Tert-butylphenyl)(1-methyl-1*H*-indol-3-yl)methanone (1'c): ^{13}C NMR (100 MHz, $CDCl_3$)



(4-Tert-butylphenyl)(1-methyl-1*H*-indol-3-yl)methanone (1'c): HRMS



(1-Methyl-1*H*-indol-3-yl)(4-nitrophenyl) methanone (1'd): ^{1}H NMR (300 MHz, $CDCl_3$)



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PROCNO	1
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TD	32768
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DS	4
SWH	18028.846 Hz
FIDRES	0.550197 Hz
AQ	0.9088159 sec
RG	80.6
DW	27.733 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
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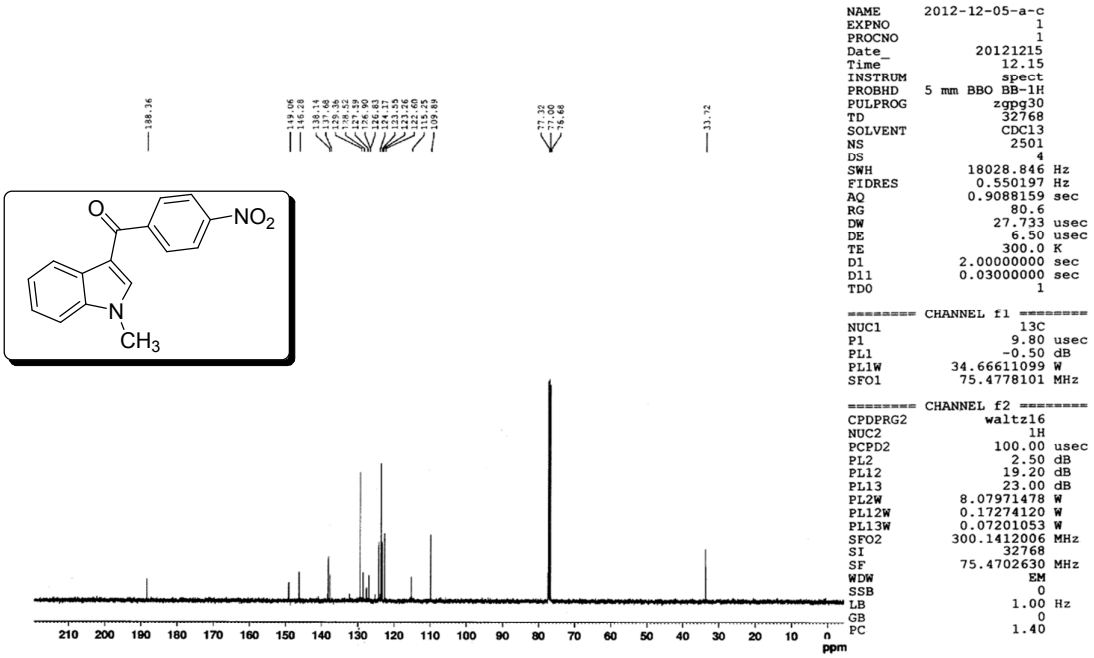
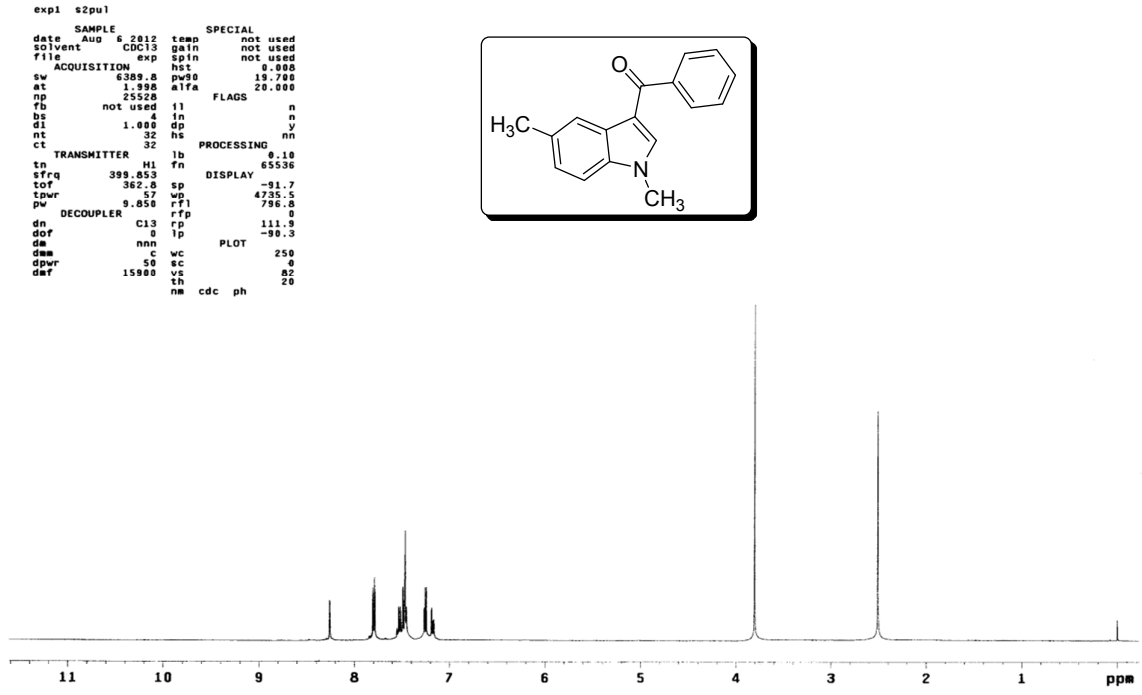
NUC1	1H
P1	9.80 usec
PL1	-0.50 dB
PL1W	34.66611099 W
SFO1	75.4778101 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	100.00 usec
PL2	2.50 dB
PL12	19.20 dB
PL13	23.00 dB
PL2W	8.07971478 W
PL12W	0.17274120 W
PL13W	0.07201053 W
SFO2	300.1412006 MHz
SI	32768
SF	75.4702630 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

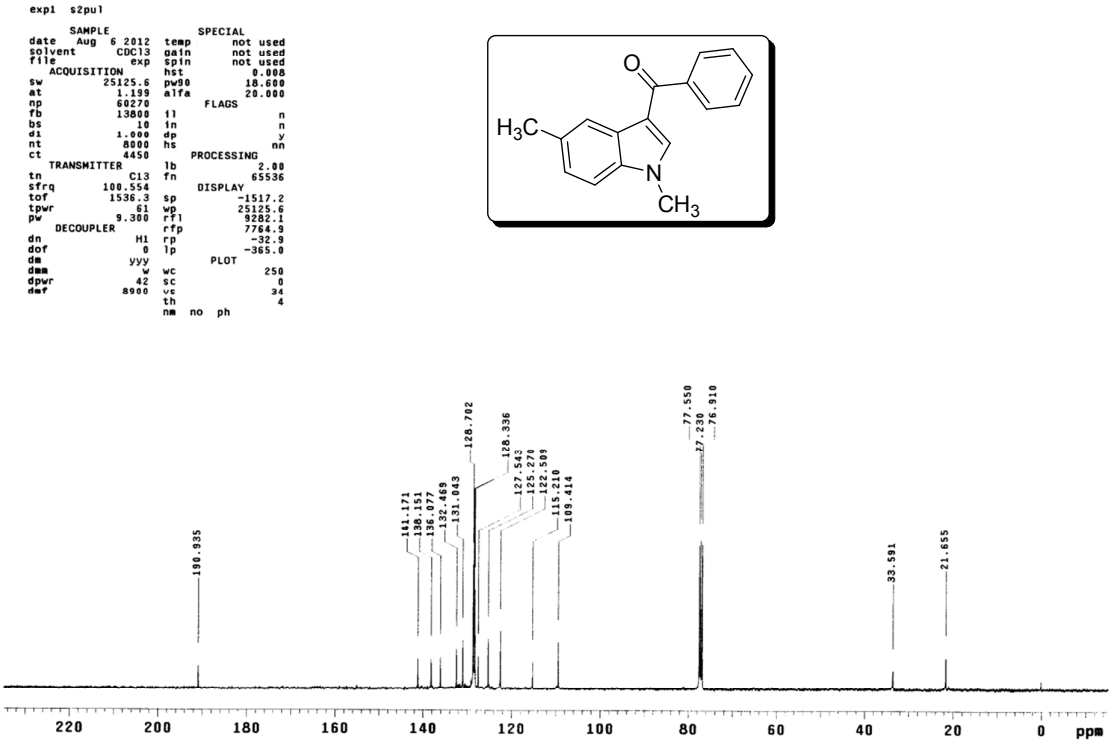
(1-Methyl-1*H*-indol-3-yl)(4-nitrophenyl) methanone (1'd): ^{13}C NMR (75 MHz, $CDCl_3$)



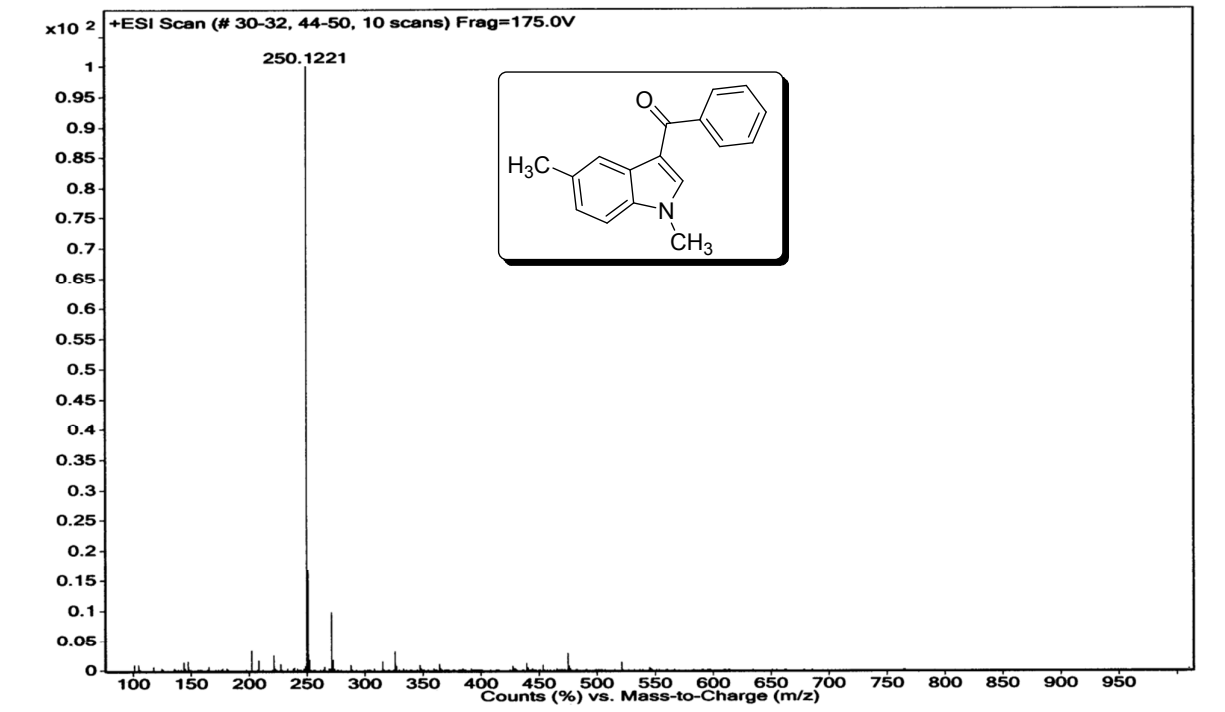
(1,5-Dimethyl-1*H*-indol-3-yl)(phenyl)methanone (2'a): ^{1}H NMR (400 MHz, $CDCl_3$)



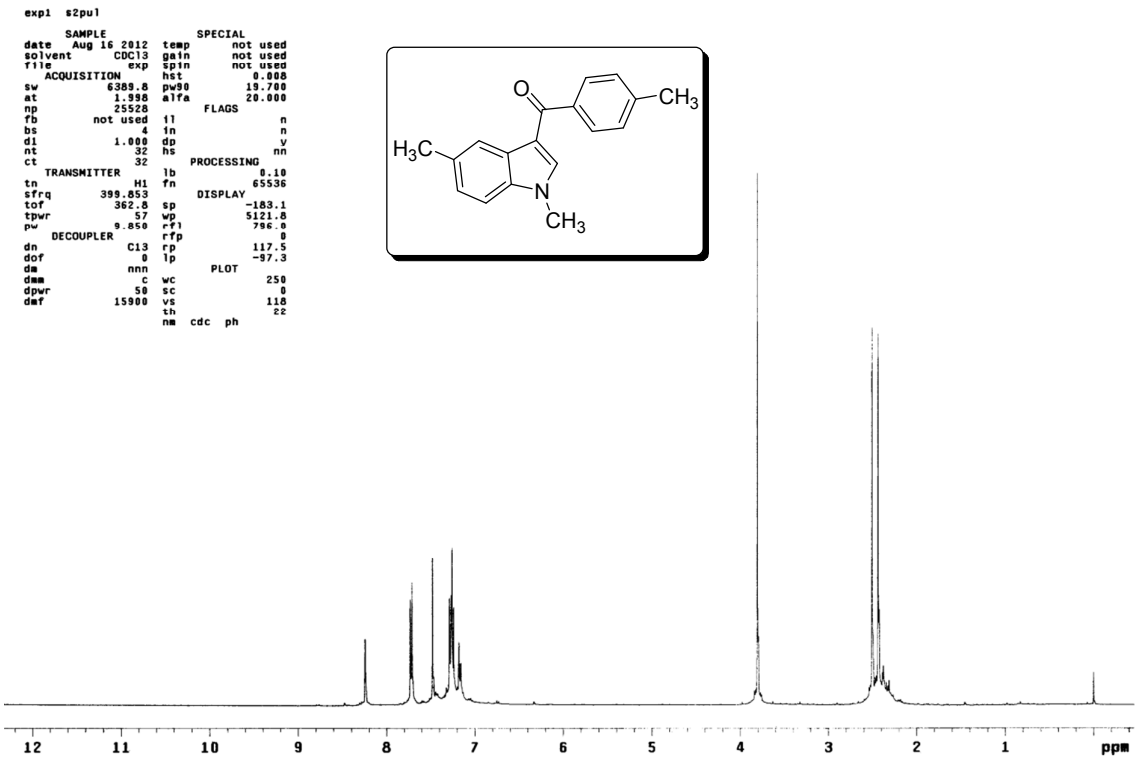
(1,5-Dimethyl-1*H*-indol-3-yl)(phenyl)methanone (2'a): ^{13}C NMR (100 MHz, $CDCl_3$)



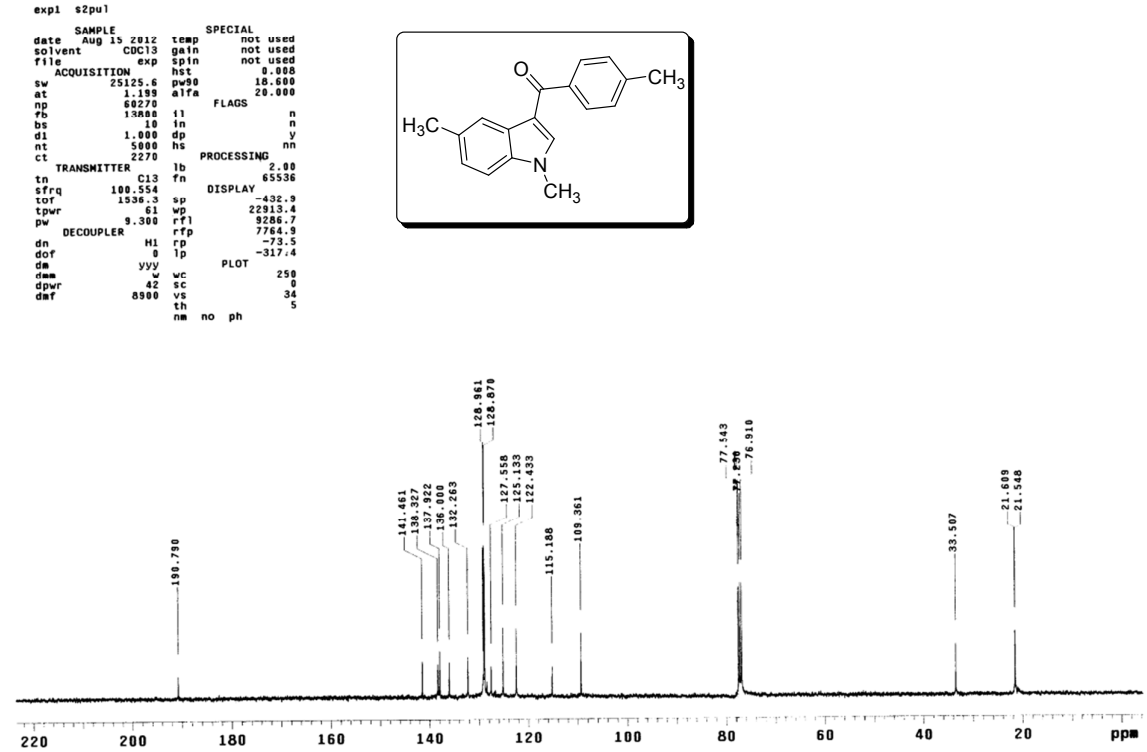
(1,5-Dimethyl-1*H*-indol-3-yl)(phenyl)methanone (2'a): HRMS



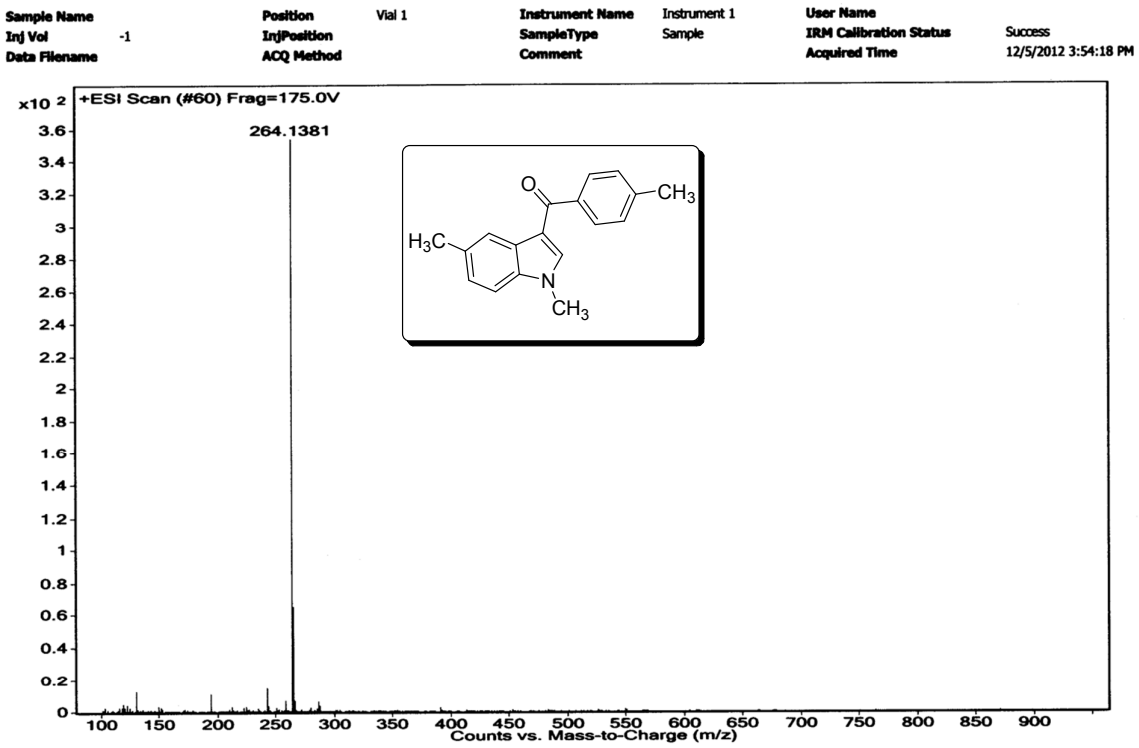
(1,5-Dimethyl-1*H*-indol-3-yl)(*p*-tolyl)methanone (2'b): ^{1}H NMR (400 MHz, $CDCl_3$)



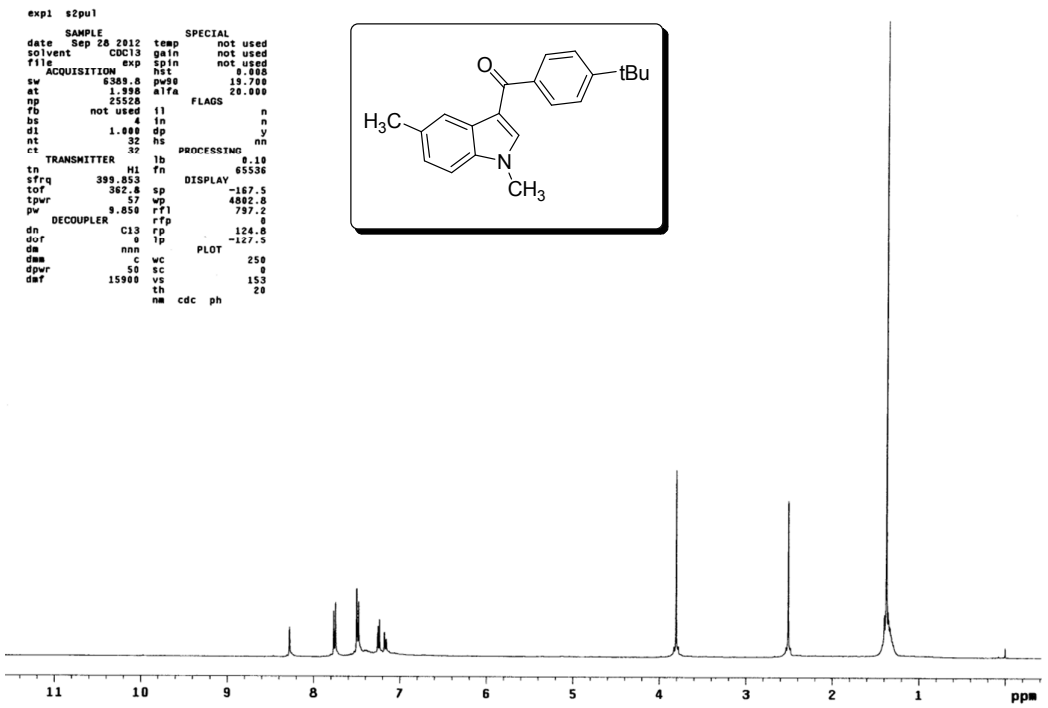
(1,5-Dimethyl-1*H*-indol-3-yl)(*p*-tolyl)methanone (2'b): ^{13}C NMR (100 MHz, $CDCl_3$)



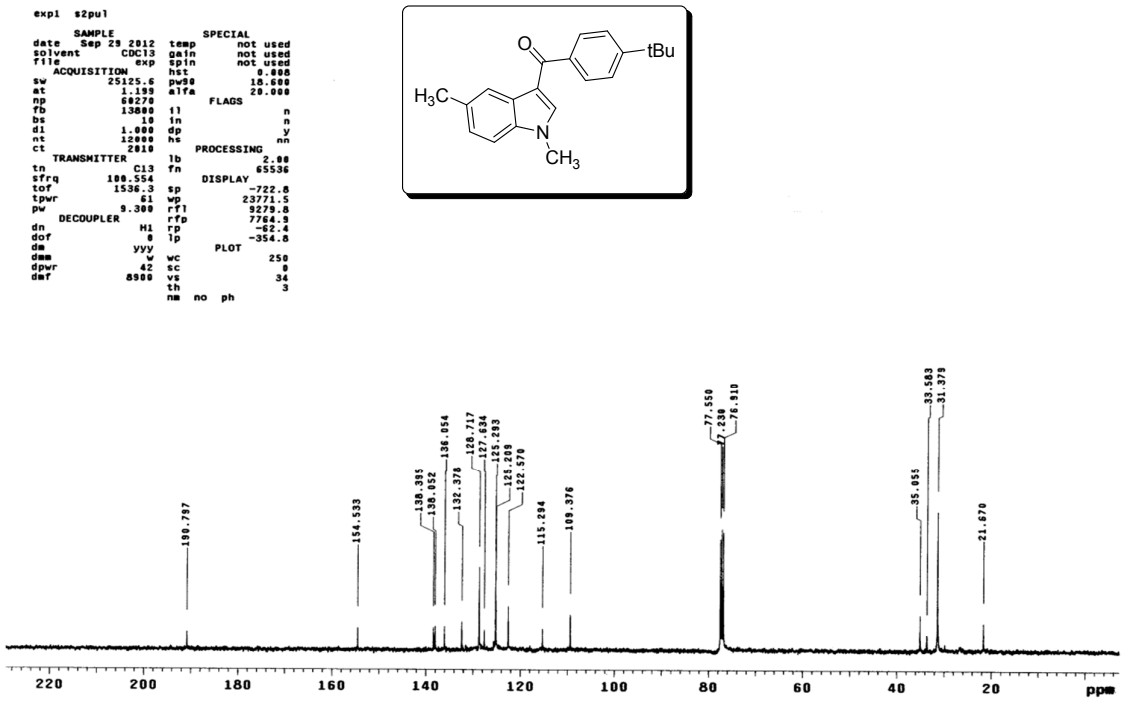
(1,5-Dimethyl-1*H*-indol-3-yl)(*p*-tolyl)methanone (2'b): HRMS



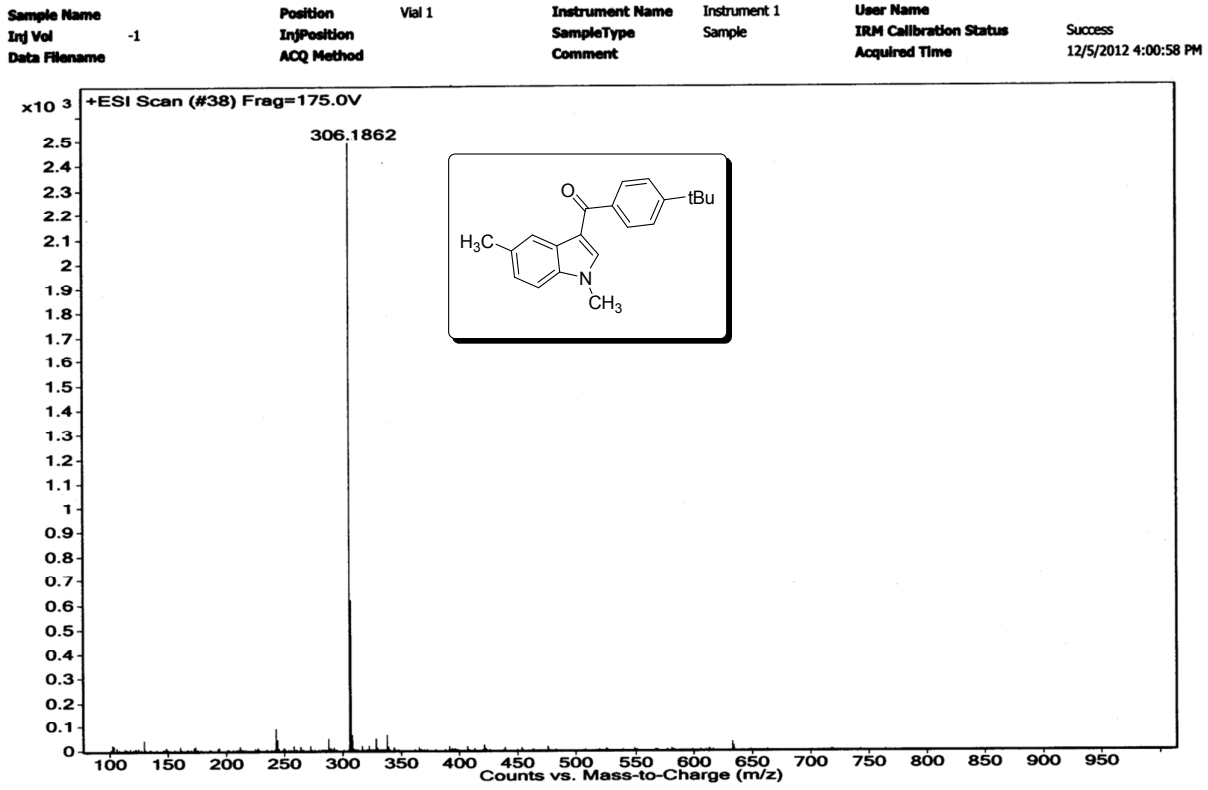
(4-Tert-butylphenyl)(1,5-Dimethyl-1*H*-indol-3-yl)methanone (2'c): ^{1}H NMR (400 MHz, $CDCl_3$)



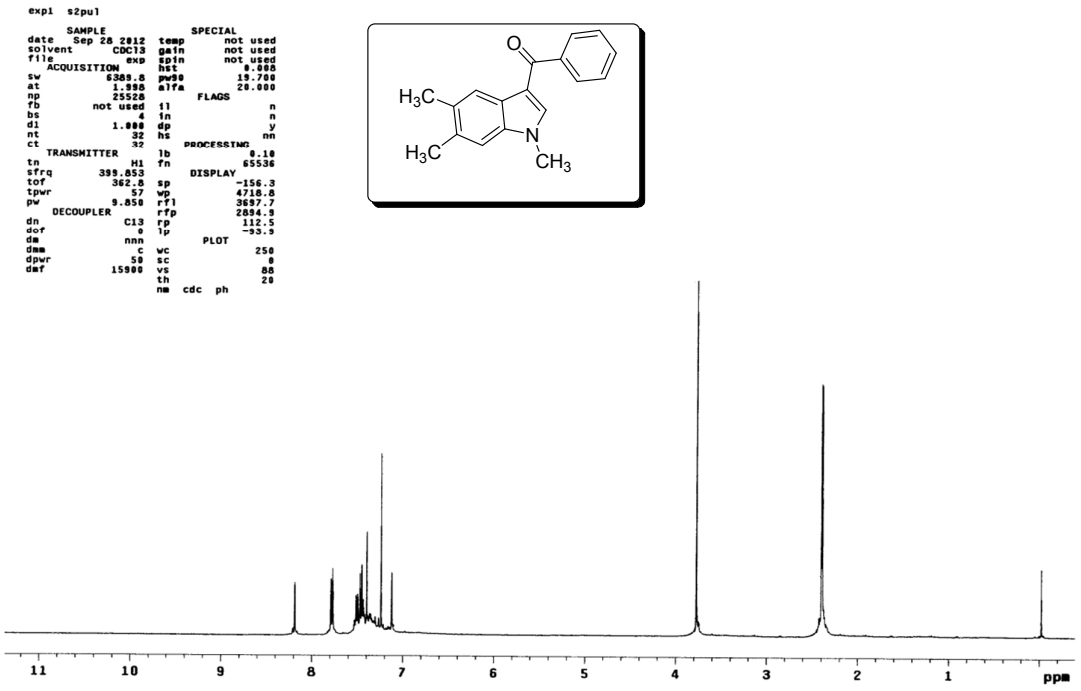
(4-Tert-butylphenyl)(1,5-Dimethyl-1*H*-indol-3-yl)methanone (2'c): ^{13}C NMR (100 MHz, $CDCl_3$)



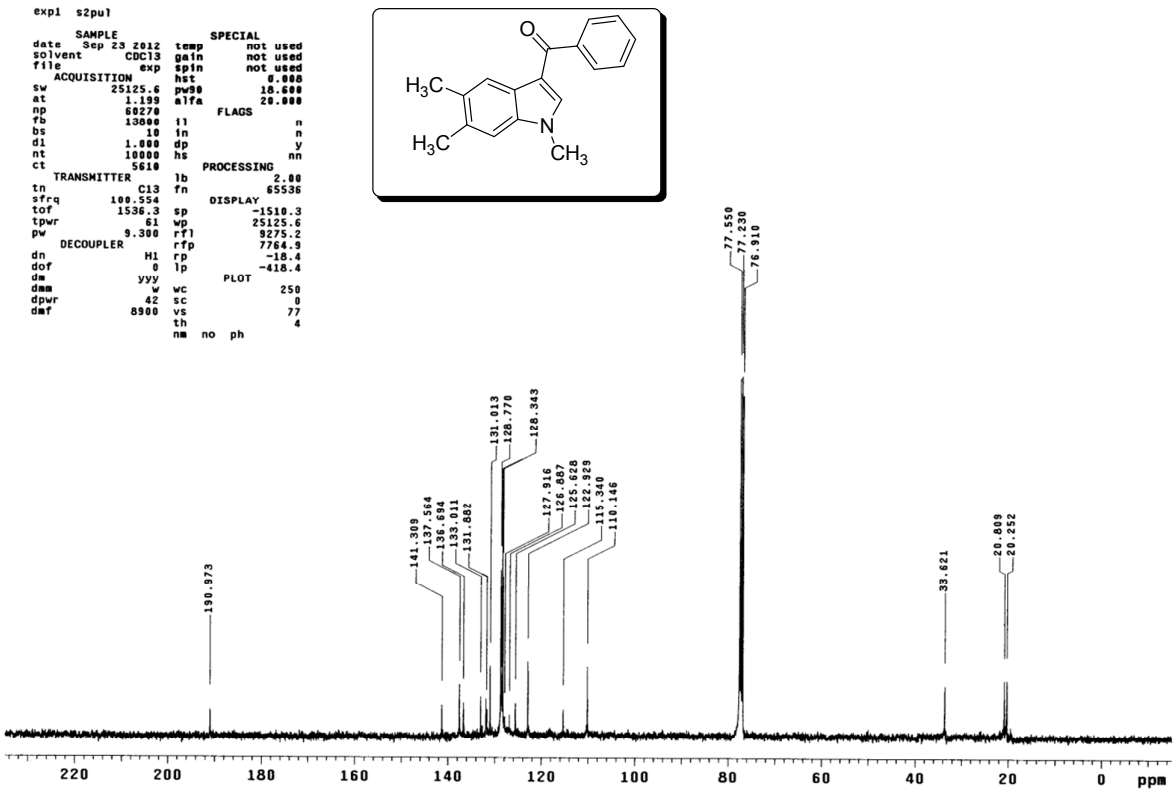
(4-Tert-butylphenyl)(1,5-Dimethyl-1*H*-indol-3-yl)methanone (2'c): HRMS



(1,5,6-Trimethy-l*H*-indol-3-yl)(phenyl)methanone (3'a): ^{1}H NMR (400 MHz, $CDCl_3$)

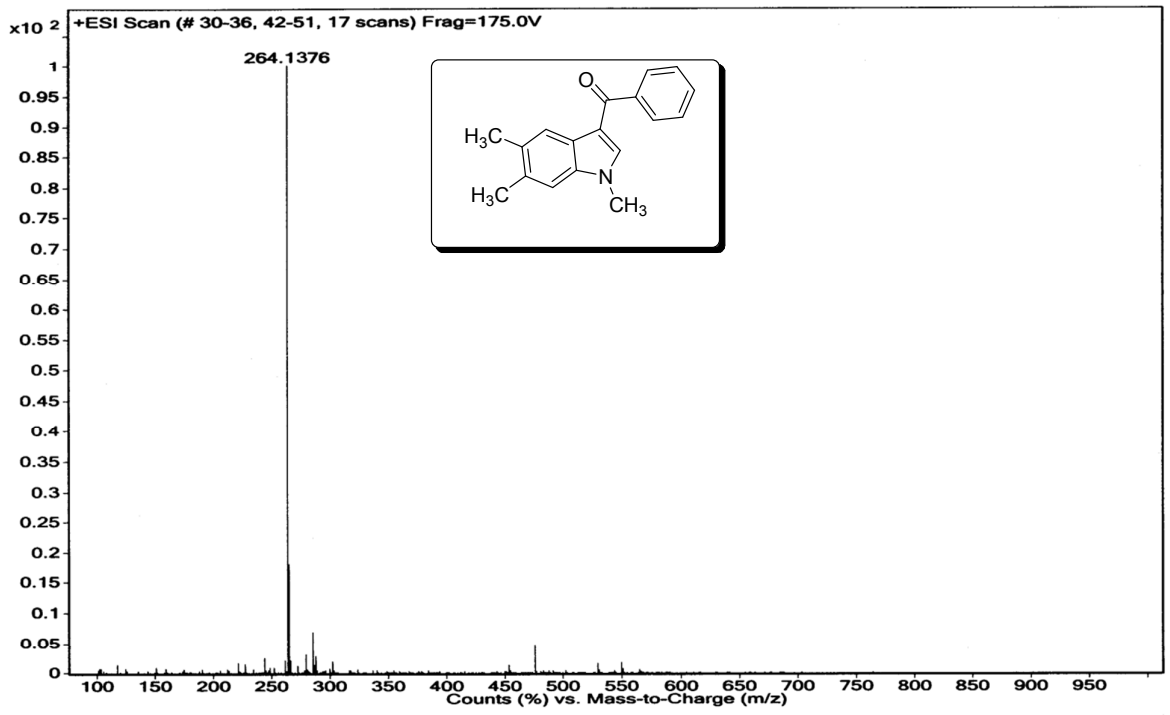


(1,5,6-Trimethy-l*H*-indol-3-yl)(phenyl)methanone (3'a): ^{13}C NMR (100 MHz, $CDCl_3$)



(1,5,6-Trimethy-l*H*-indol-3-yl)(phenyl)methanone (3'a): HRMS

Sample Name		**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename		**ACQ Method**		**Comment**		**Acquired Time**	12/5/2012 4:38:37 PM



(1,5,6-Trimethy-l*H*-indol-3-yl)(*p*-tolyl)methanone (3'b): ^{1}H NMR (400 MHz, $CDCl_3$)

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solvent       CDCl3     gain          not used
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              fid       pw90           19.700
    ACQUISITION         alfa           29.600
sw             6389.8           FLAGS
at              1.598   il                  n
np             25528    in                  n
fb         not used     dp                  y
bs                 4    ns                 nn
di             1.000        PROCESSING
nt                64    lb              0.10
ct                64    fn             65536
   TRANSMITTER               DISPLAY
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tof            362.8     rfl            795.2
tpwr              57     rfp                0
pw             9.850     rp             105.9
    DECOUPLER           lp             -98.6
dn                C13           PLOT
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dm               nnn    sc                0
dmm                c    vs               45
dpwr              50    th               20
dmf            15980    nm   cdc  ph
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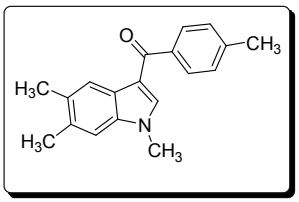
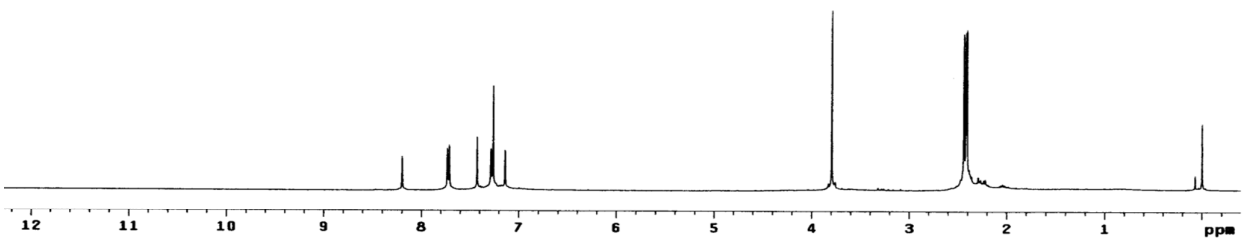
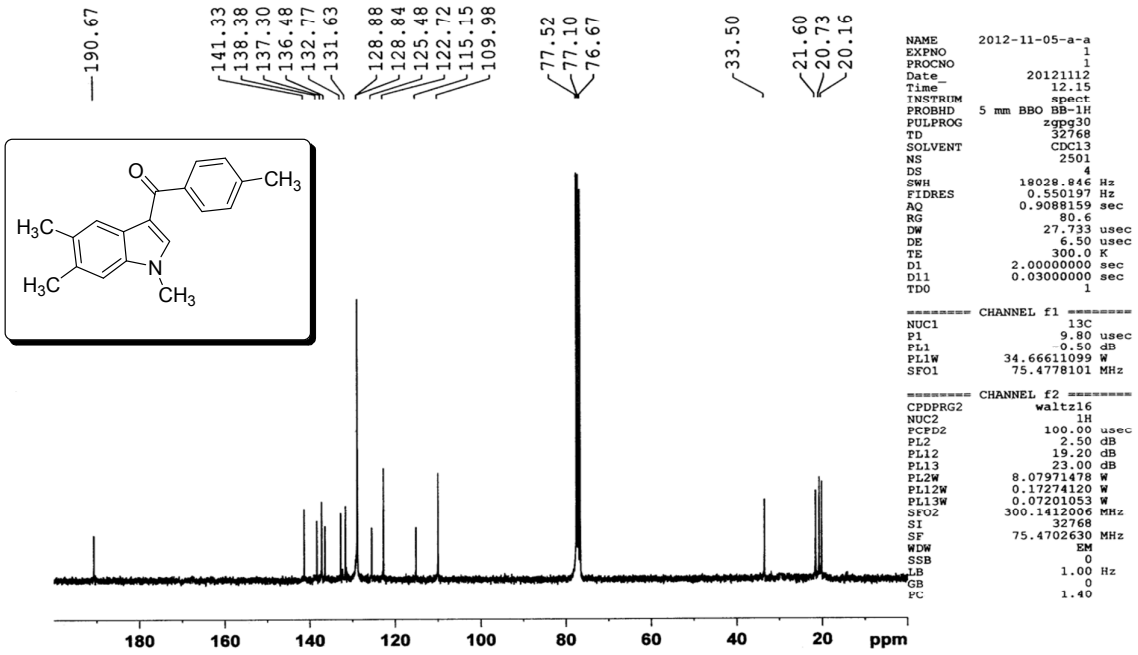
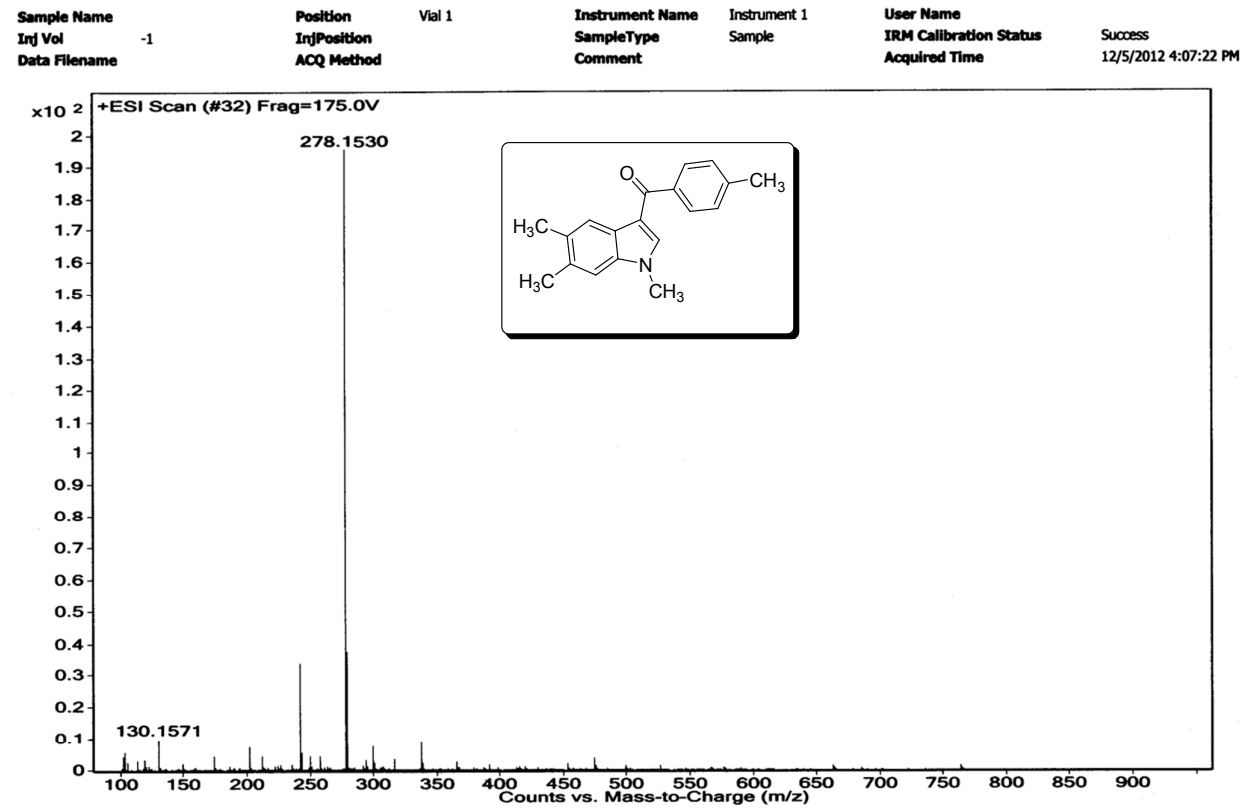




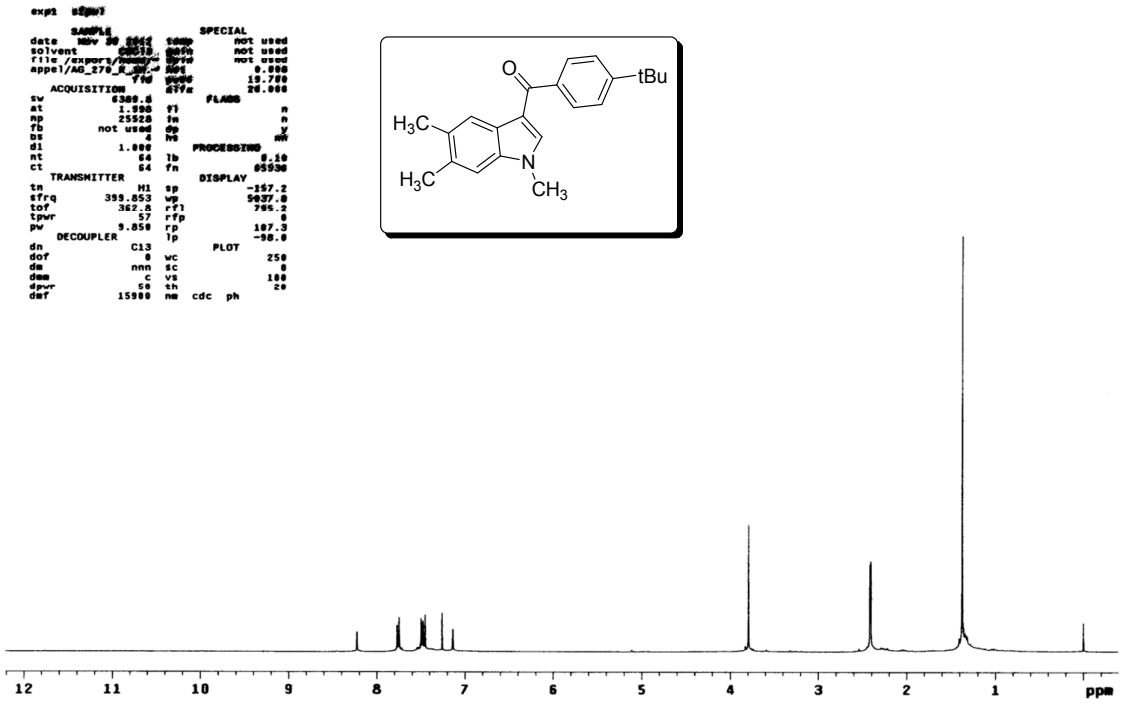
(1,5,6-Trimethy-l*H*-indol-3-yl)(*p*-tolyl)methanone (3'b): ^{13}C NMR (75 MHz, $CDCl_3$)



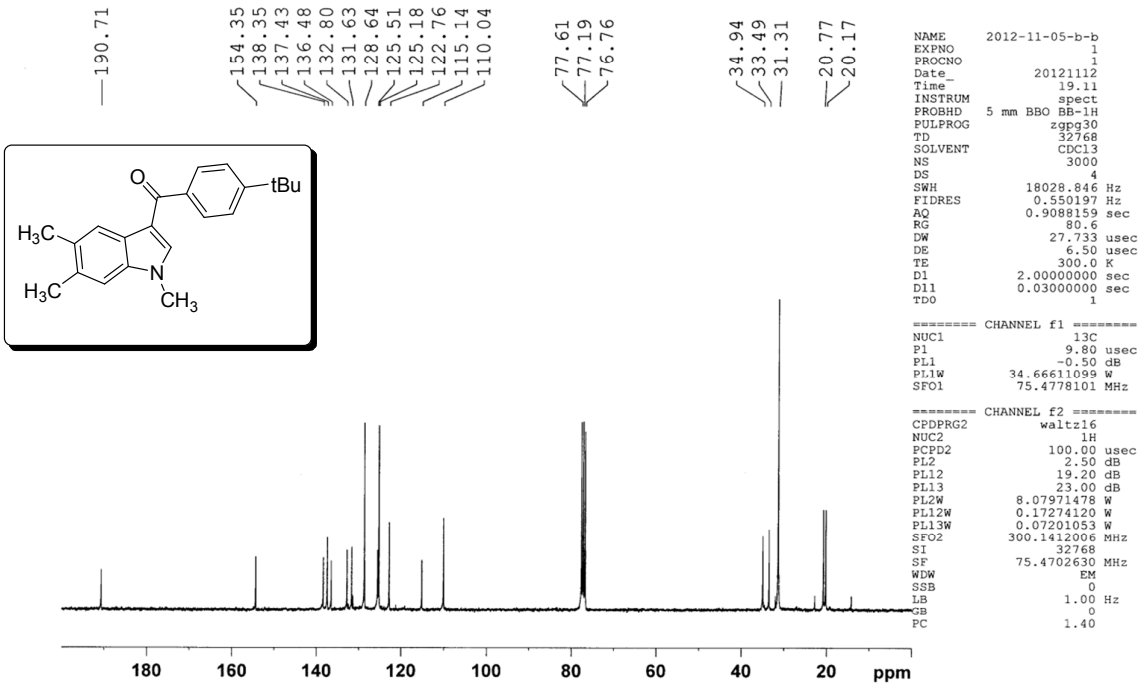
(1,5,6-Trimethy-l*H*-indol-3-yl)(*p*-tolyl)methanone (3'b): HRMS



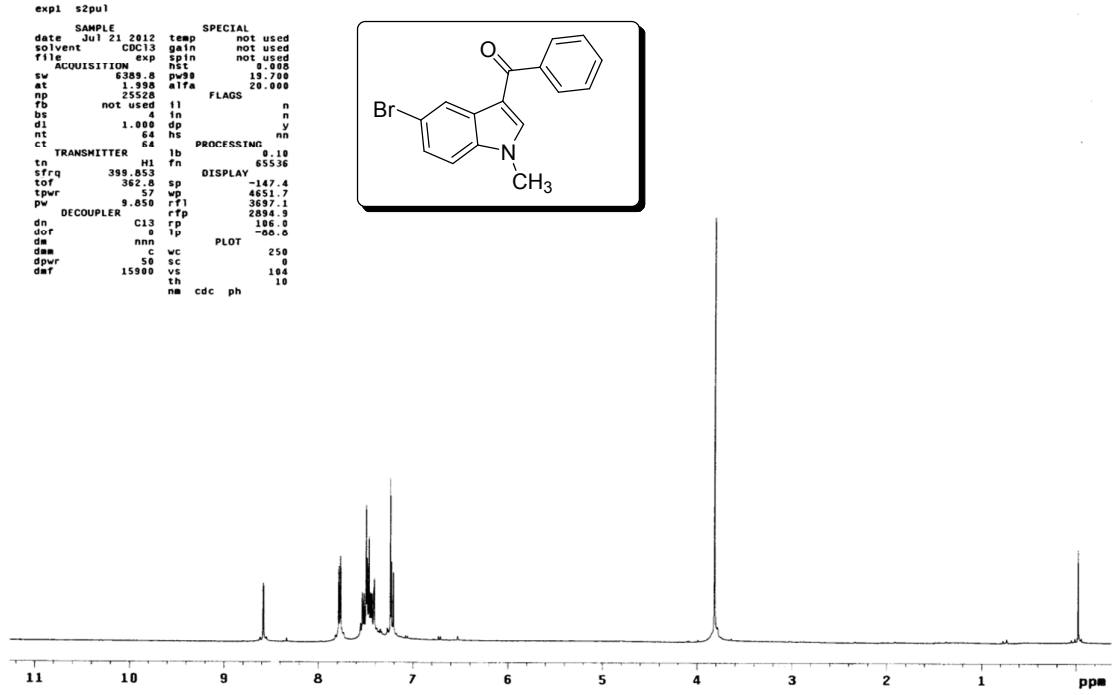
(4-Tert-butylphenyl)(1,5,6-trimethyl-1*H*-indol-3-yl)methanone (3'c): ^{1}H NMR (400 MHz, $CDCl_3$)



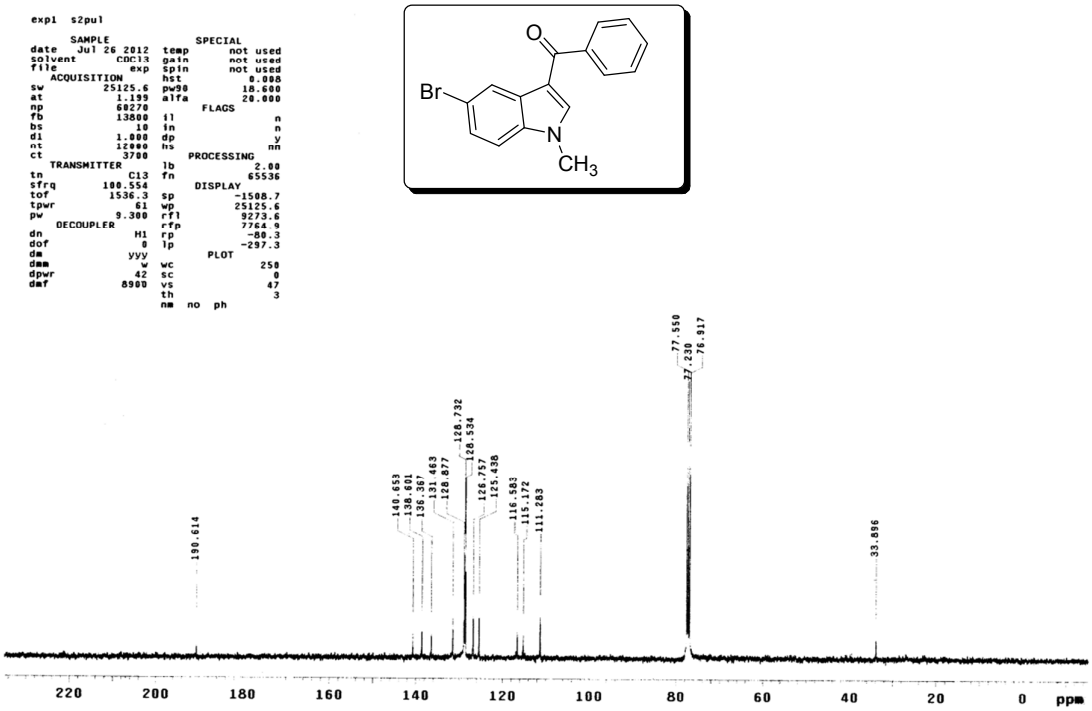
(4-Tert-butylphenyl)(1,5,6-trimethyl-1*H*-indol-3-yl)methanone (3'c): ^{13}C NMR (75 MHz, $CDCl_3$)



(5-Bromo-1-methyl-1*H*-indol-3-yl)(phenyl)methanone (4'a): ^{1}H NMR (400 MHz, $CDCl_3$)

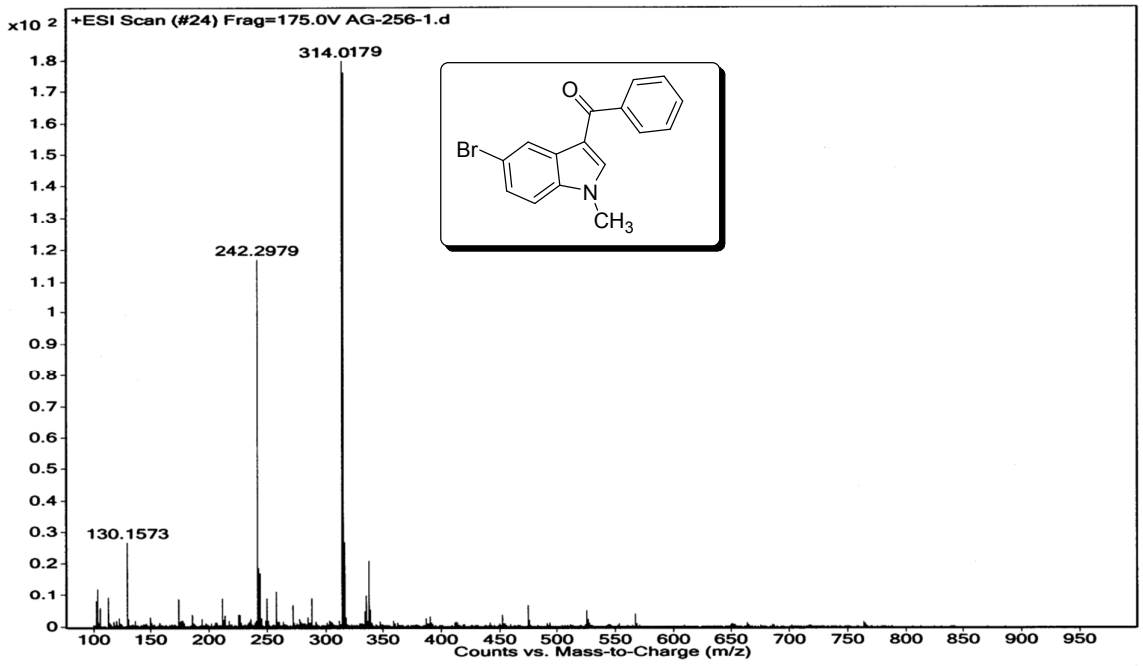


(5-Bromo-1-methyl-1*H*-indol-3-yl)(phenyl)methanone (4'a): ^{13}C NMR (100 MHz, $CDCl_3$)

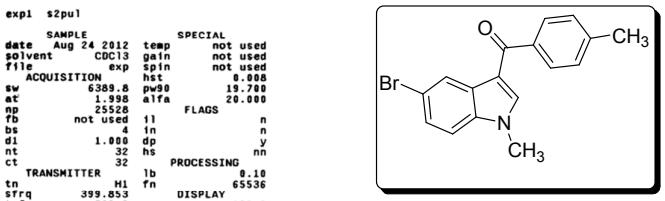


(5-Bromo-1-methyl-1*H*-indol-3-yl)(phenyl)methanone (4'a): HRMS

Sample Name		**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename		**ACQ Method**		**Comment**		**Acquired Time**	12/5/2012 4:15:32 PM



(5-Bromo-1-methyl-1*H*-indol-3-yl)(*p*-tolyl)methanone (4'b): ^{1}H NMR (400 MHz, $CDCl_3$)



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file             exp  spin          not used
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at                1.998  alfa          20.000
np                25528          FLAGS
fb            not used  il                 n
bs                   4  in                 n
d1               1.000  dp                 y
nt                  32  hs                nn
ct                  32      PROCESSING
   TRANSMITTER          lb              0.10
tn                  H1  fn             65536
sfrq          399.853       DISPLAY
tof               382.8  sp             -189.9
tpwr                57  wp             5197.3
pw                9.850  rfl            3697.7
    DECOUPLER          rfp            2894.9
dn                  C13  rp              97.8
dof                   0  lp             -71.8
dm                  nnn          PLOT
dmm                   c  wc              250
dpwr                 50  sc                0
dmf               15900  vs               71
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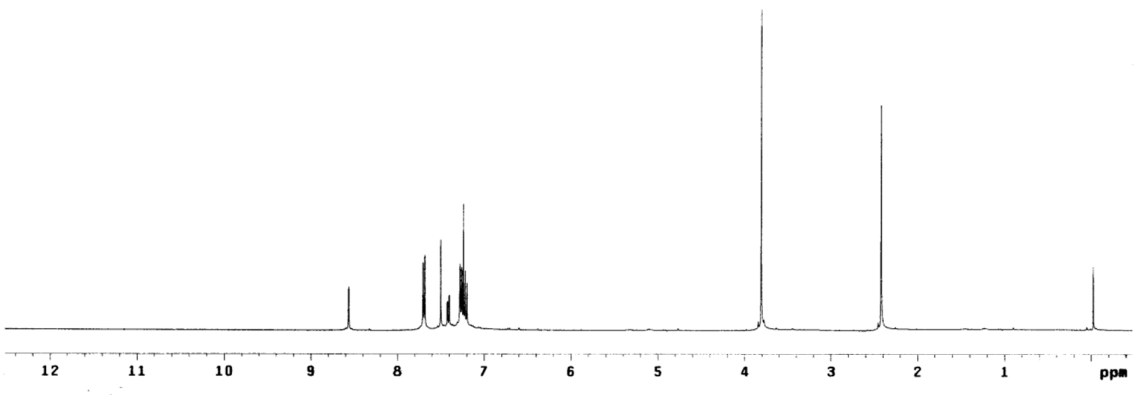
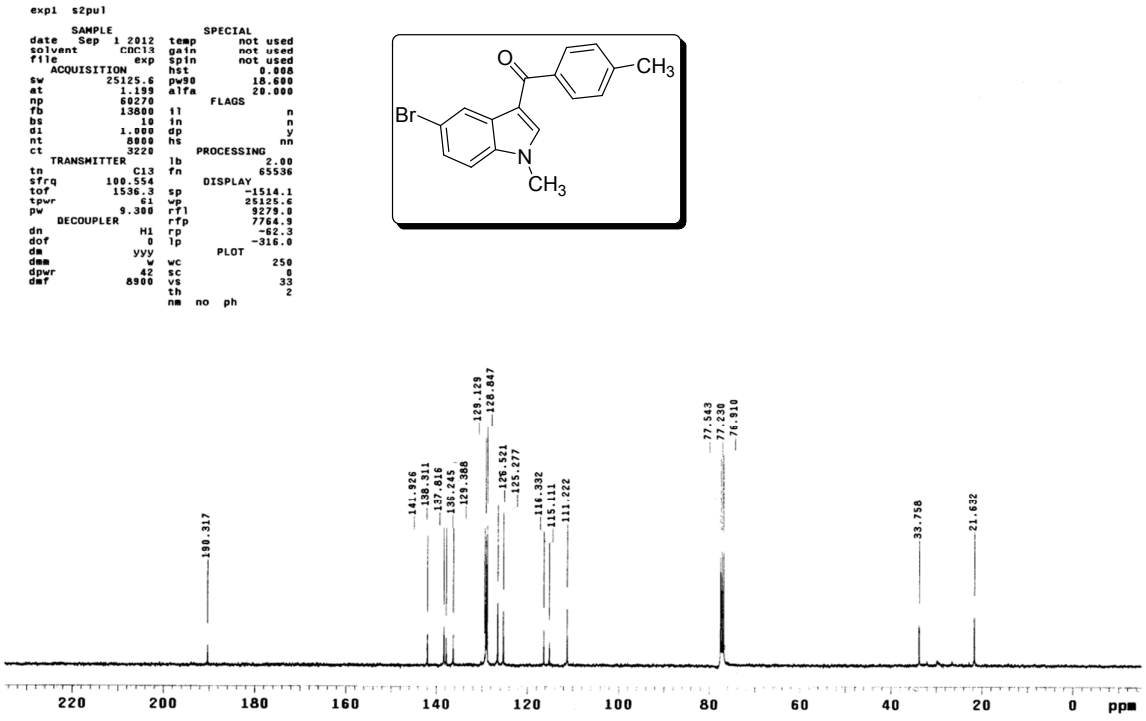
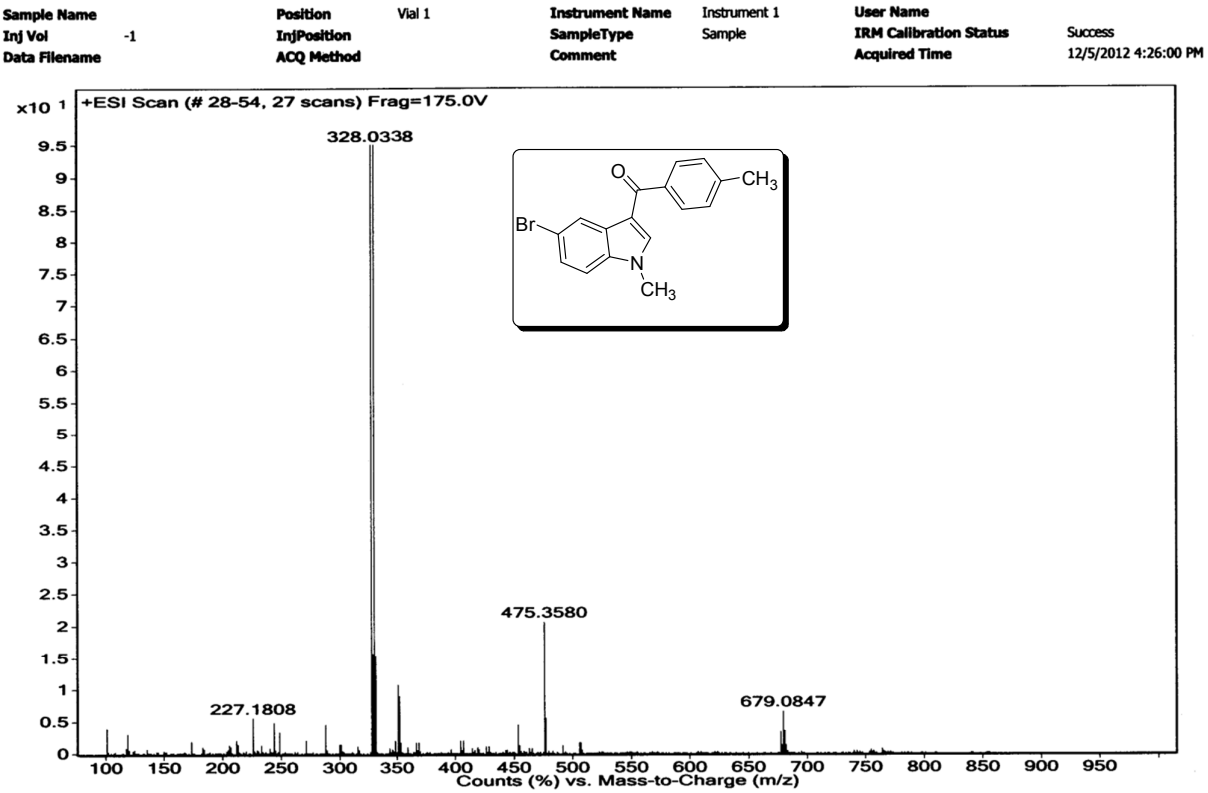


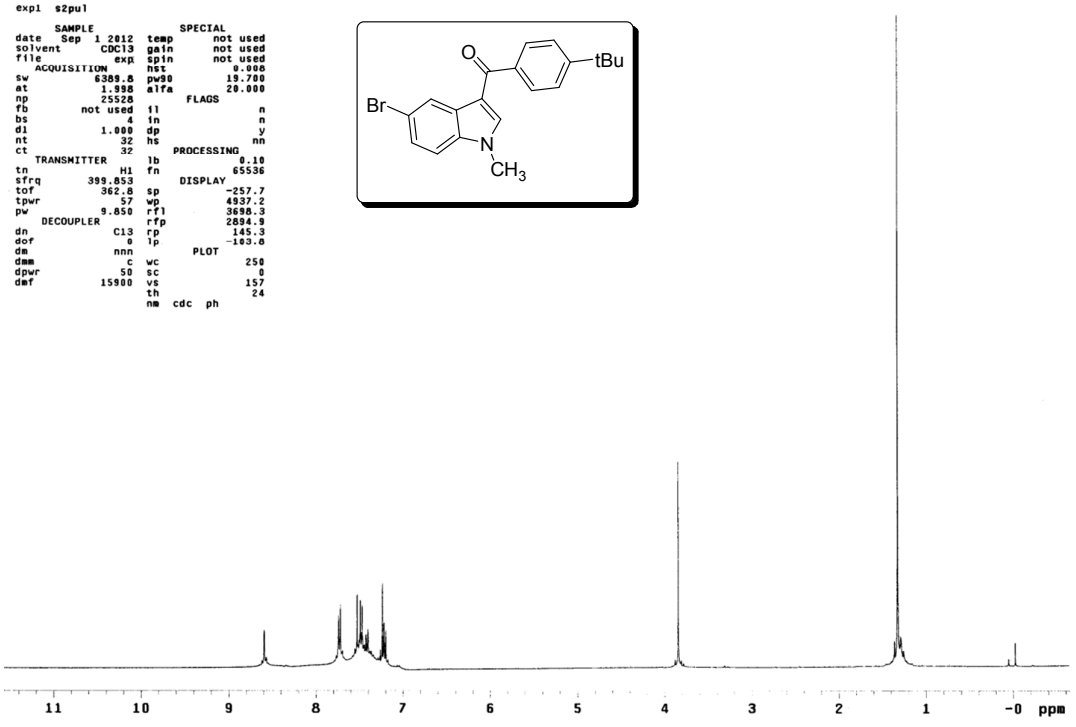
(5-Bromo-1-methyl-1*H*-indol-3-yl)(*p*-tolyl)methanone (4'b): ^{13}C NMR (100 MHz, $CDCl_3$)



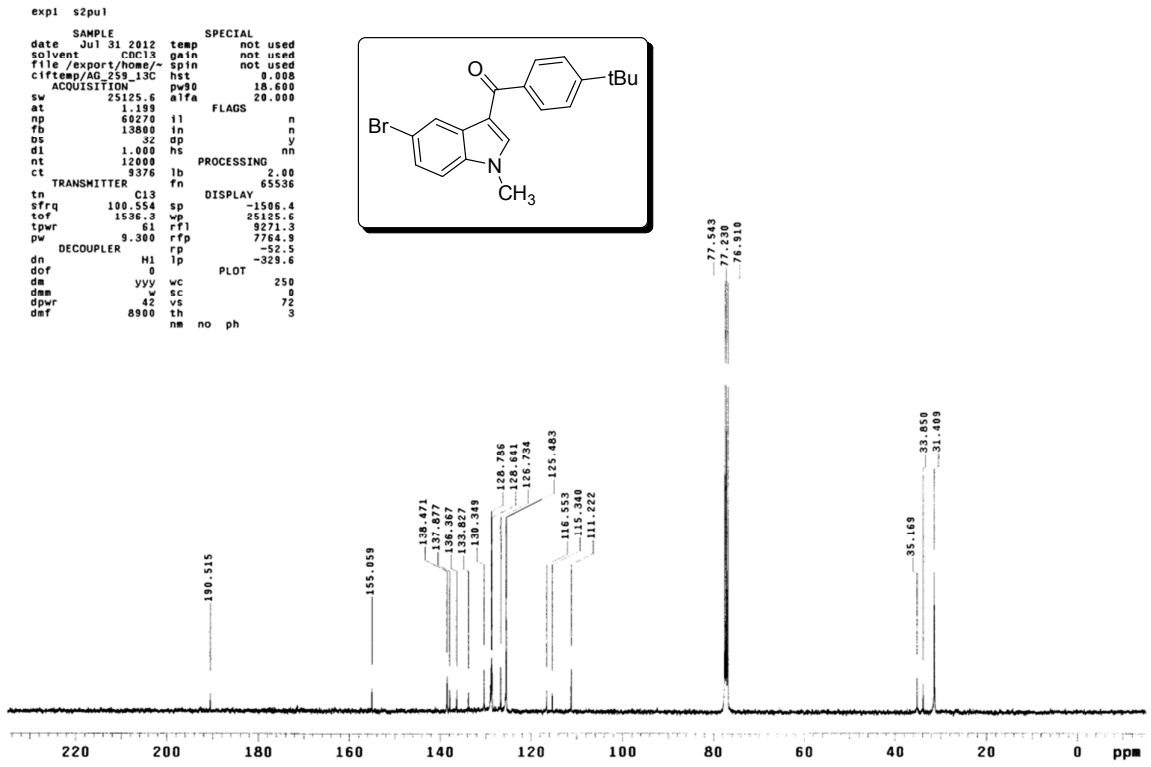
(5-Bromo-1-methyl-1*H*-indol-3-yl)(*p*-tolyl)methanone (4'b): HRMS



(4-Tert-butylphenyl)(5-bromo-1-methyl-1*H*-indol-3-yl)methanone (4'c): ^{1}H NMR (400 MHz, $CDCl_3$)



(4-Tert-butylphenyl)(5-bromo-1-methyl-1*H*-indol-3-yl)methanone (4'c): ^{13}C NMR (100 MHz, $CDCl_3$)



(4-Tert-butylphenyl)(5-bromo-1-methyl-1*H*-indol-3-yl)methanone (4'c): HRMS

Sample Name		**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename		**ACQ Method**		**Comment**		**Acquired Time**	12/5/2012 4:31:48 PM