Supporting Informations

A Cu-catalysed synthesis of Substituted 3-Methyleneisoindolin-1-one

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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.

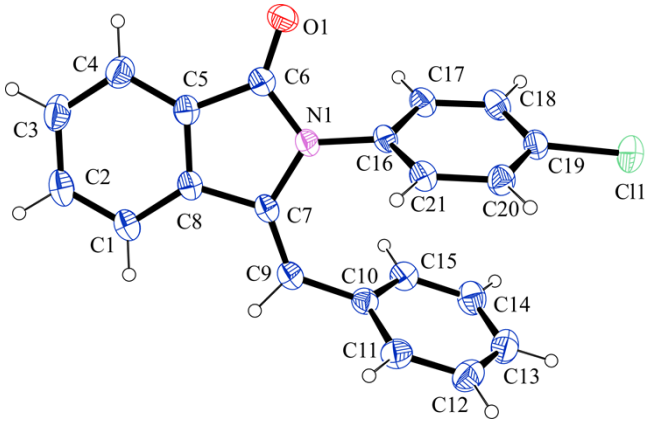
a. SMART V 4.043 Software for the CCD Detector System; Siemens Analytical Instruments Division: Madison, WI, 1995.

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 (*Z*)-3-Benzylidene-2-(4-chlorophenyl)isoindolin-1-one (5a):

$C_{21}H_{14}ClNO$, crystal dimensions 0.43 x 0.33 x 0.28 mm, M_r = 331.78, Triclinic, space group P-1, a = 7.6383(7), b = 9.0793(8), c = 12.1907(10) Å, α = 103.312(3) °, β = 93.496(3) °, γ = 96.408(3) °, V = 814.28(12) Å^3, Z = 2, ρ_{calcd} = 1.353 mg/m^3, μ = 0.241 mm^{-1}, F(000) = 344.0, reflection collected / unique = 4062/ 2881, refinement method = full-matrix least-squares on F^2, final R indices [$I > 2\sigma(I)$]: R_1 = 0.0412, wR_2 = 0.1122, R indices (all data): R_1 = 0542, wR_2 = 0.1201, goodness of fit = 1.001. CCDC-1024354 for (*Z*)-3-Benzylidene-2-(4-chlorophenyl)isoindolin-1-one (**5a**) 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.



(*Z*)-3-Benzylidene-2-(4-chlorophenyl)isoindolin-1-one (5a)

General procedure for the synthesis of (*Z*)-3-Benzylidene-2-phenylisoindolin-1-one (1a):

To a solution of 2-bromobenzamide (**1**) (138 mg, 0.5 mmol) in DMSO (2 mL) was added CuI (9.5 mg, 0.05 mmol), 1,10-phen (9 mg, 0.05 mmol), Cs_2CO_3 (245 mg, 0.75 mmol), phenyl propiolic acid (**a**) (87.6 mg, 0.6 mmol) and the resultant mixture was stirred in a preheated oil bath at 120 ^oC for 2 h. The reaction mixture was then cooled to room temperature, 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 (19:1 hexane / ethyl acetate to give (*Z*)-3-Benzylidene-2-phenylisoindolin-1-one (**1a**) (102.5 mg, 69% yield).

ESI-MS study for the detection of intermediates:

In order to detect the intermediates species in the reaction mixture an electrospray mass spectrometry was performed. In this study, after 15 minutes of reaction, aliquot (100 μL) was withdrawn and diluted with acetonitrile (1 mL). A 20 μL of the diluted solution was injected to run ESI-MS analysis. Various species were detected in the ESI-MS analysis as shown below in Figure S1-S5.

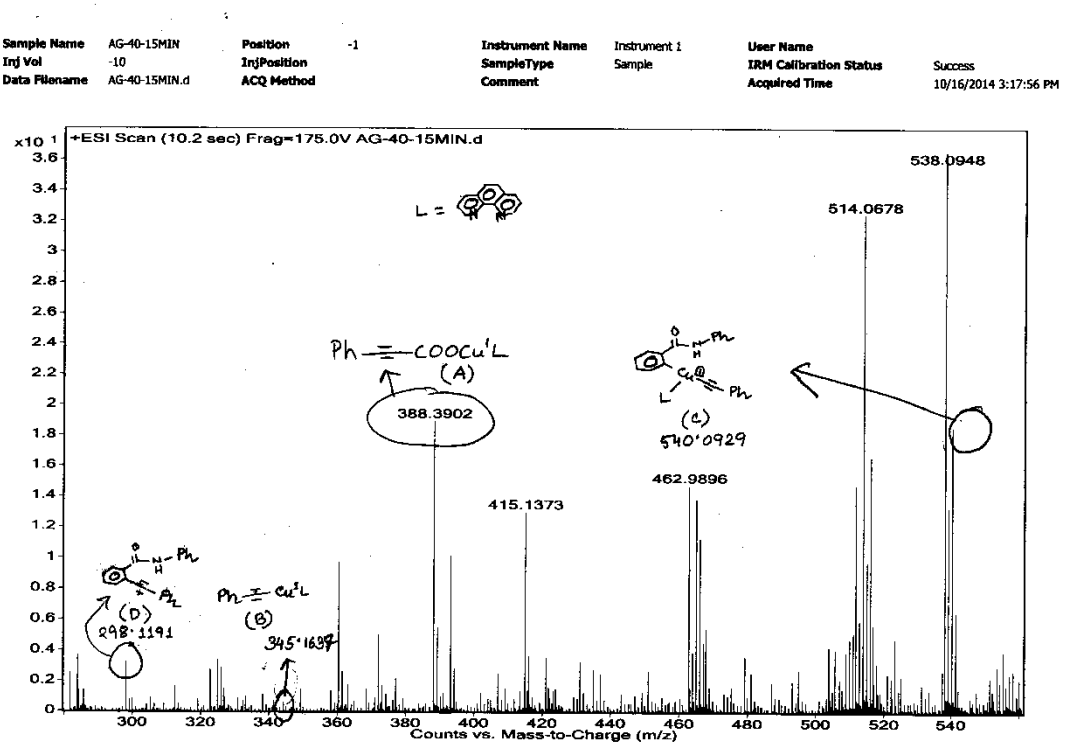


Figure S1: ESI-MS spectrum of the reaction mixture

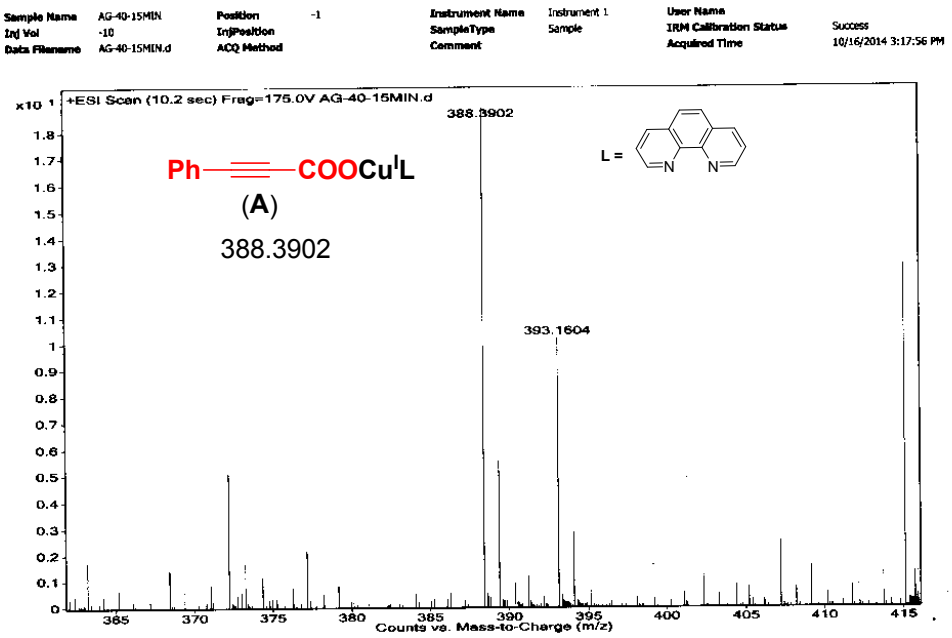


Figure S2: ESI-MS spectrum of the reaction mixture

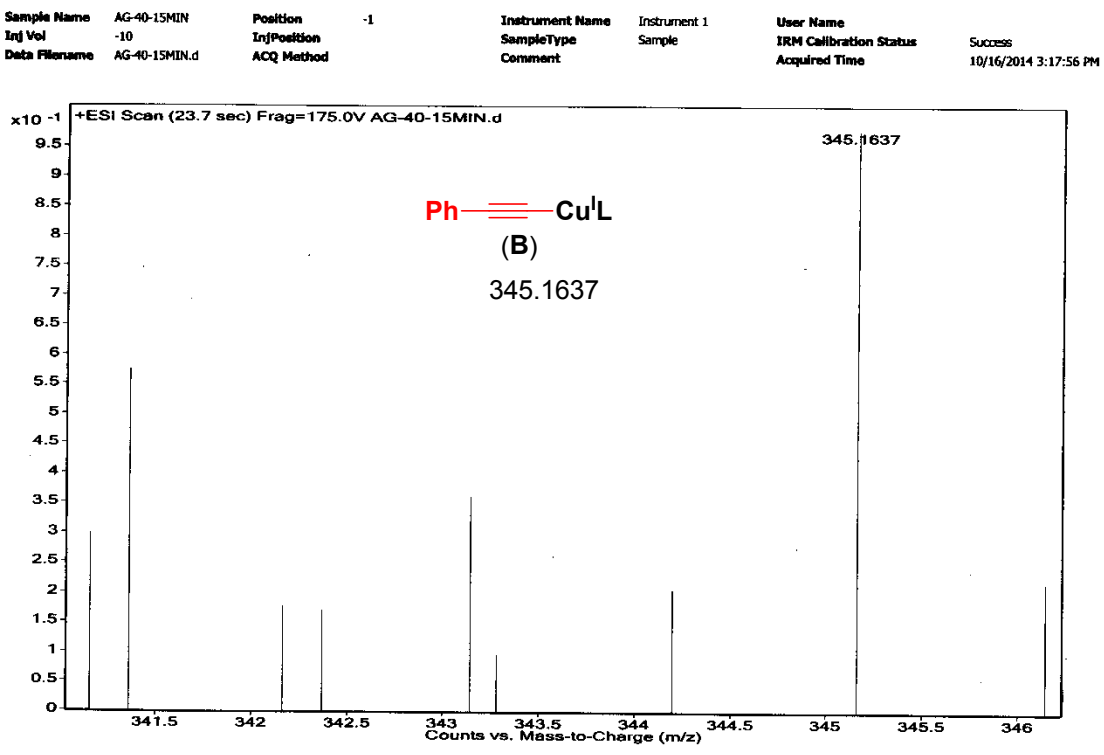


Figure S3: ESI-MS spectrum of the reaction mixture

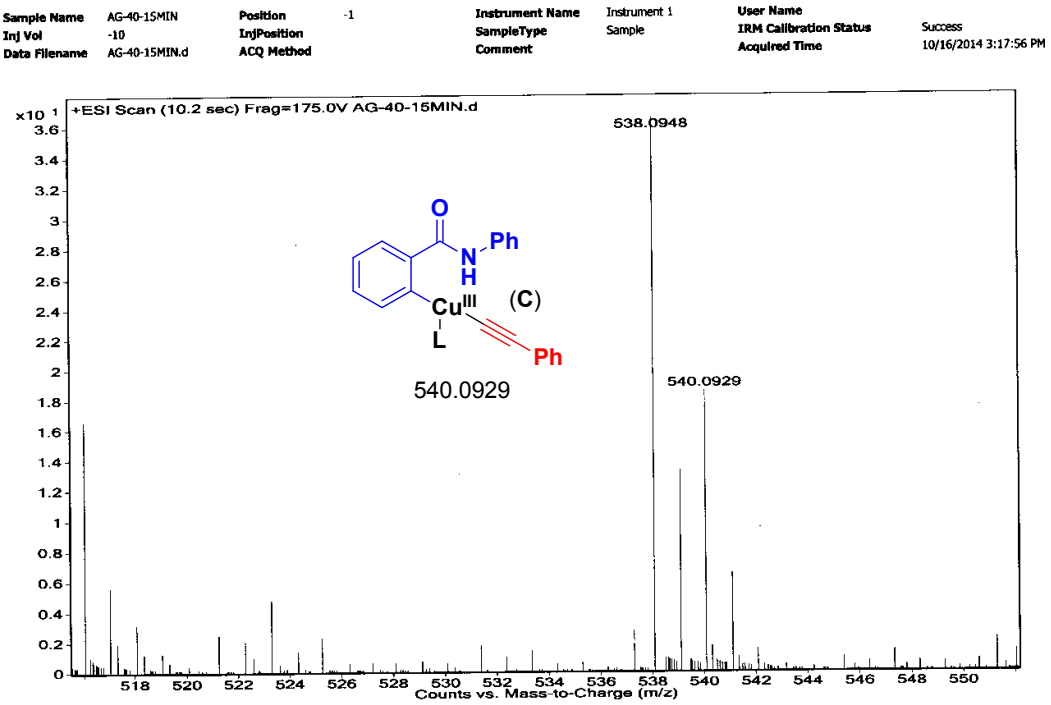


Figure S4: ESI-MS spectrum of the reaction mixture

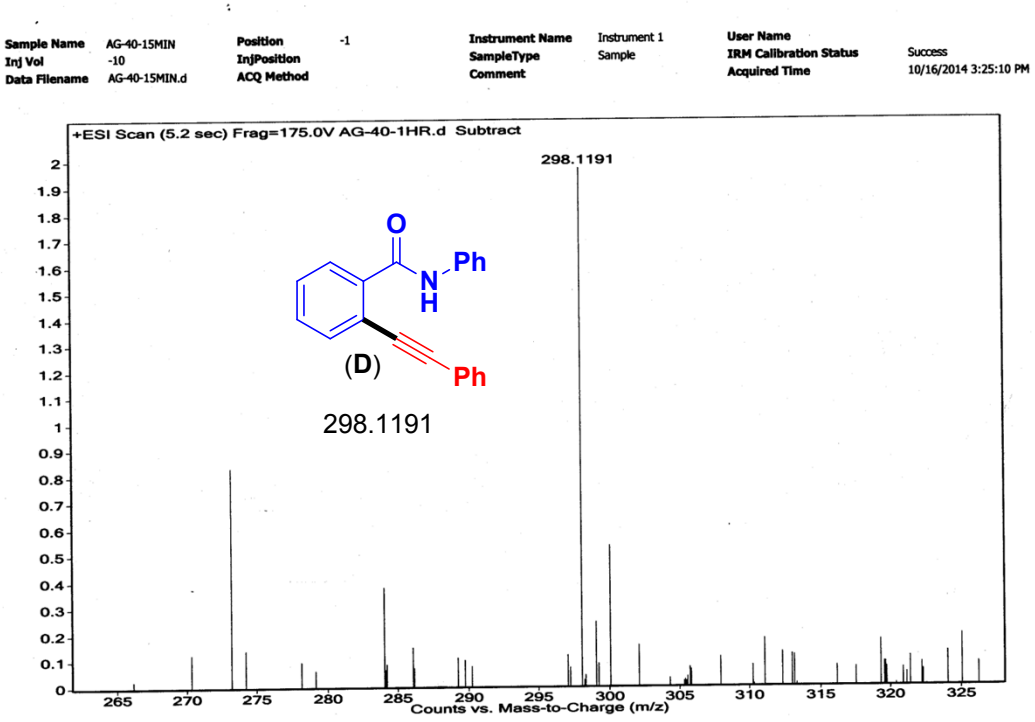
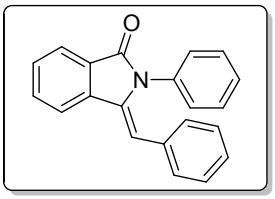


Figure S5: ESI-MS spectrum of the reaction mixture

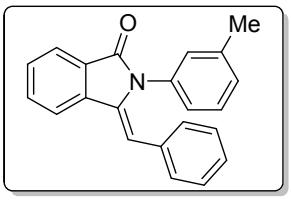
Spectral Data

(*Z*)-3-Benzylidene-2-phenylisoindolin-1-one (1a):



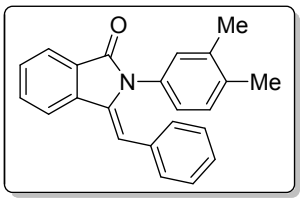
^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 6.82 (s, 1H), 6.84 (d, 2H, *J* = 7.8 Hz), 6.90 (t, 2H, *J* = 7.8 Hz), 6.95 (t, 1H, *J* = 7.8 Hz), 7.03 – 7.09 (m, 5H), 7.54 (t, 1H, *J* = 7.8 Hz), 7.66 (t, 1H, *J* = 7.2 Hz), 7.84 (d, 1H, *J* = 7.8 Hz), 7.93 (d, 1H, *J* = 7.8 Hz); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 107.8, 119.6, 124.1, 126.8, 126.9, 127.4, 128.0, 128.4, 129.3, 129.4, 132.6, 133.8, 134.6, 136.1, 138.9, 168.2; IR (KBr): 3029, 2922, 1705, 1647, 1494, 1469, 1388, 1297, 1123, 1069, 761, 693 cm^{-1}; HRMS (ESI): calcd. for $C_{21}H_{15}NO$ (MH^+) 298.1226; found 298.1232.

(*Z*)-3-Benzylidene-2-(*m*-tolyl)isoindolin-1-one (2a):



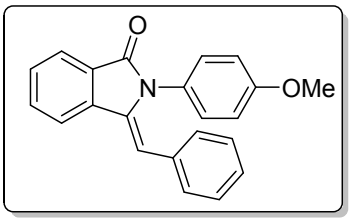
^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 2.06 (s, 3H), 6.77 (s, 1H), 6.81 (s, 1H), 6.84 (d, 3H, *J* = 7.2 Hz), 6.91 (t, 2H, *J* = 7.2 Hz), 6.93 – 6.96 (m, 2H), 6.99 (t, 1H, *J* = 7.8 Hz), 7.53 (t, 1H, *J* = 7.8 Hz), 7.65 (t, 1H, *J* = 7.2 Hz), 7.83, (d, 1H, *J* = 7.2 Hz), 7.93 (d, 1H, *J* = 8.4 Hz); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 21.1, 107.8, 119.5, 124.0, 124.6, 126.8, 127.3, 127.7, 128.1, 128.2, `28.3, 129.1, 129.4, 132.6, 134.0, 134.7, 135.8, 138.3, 138.8, 168.1; IR (KBr): 3048, 2921, 1707, 1631, 1489, 1449, 1402, 1351, 1300, 1184, 1120, 926, 798, 767, 701 cm^{-1}; HRMS (ESI): calcd. for $C_{22}H_{17}NO$ (MH^+) 312.1383; found 312.1391.

(*Z*)-3-Benzylidene-2-(3,4-dimethylphenyl)isoindolin-1-one (3a):



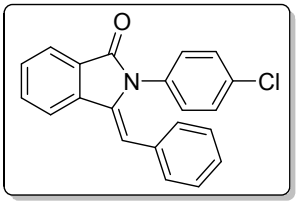
^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 1.95 (s, 3H), 2.10 (s, 3H), 6.71 (s, 1H), 6.79 (s, 1H), 6.83 – 6.86 (m, 4H), 6.88 (t, 2H, *J* = 7.2 Hz), 6.94 (t, 1H, *J* = 7.2 Hz), 7.52 (t, 1H, *J* = 7.8 Hz), 7.64 (t, 1H, *J* = 7.2 Hz), 7.82 (d, 1H, *J* = 7.8 Hz), 7.93 (d, 1H, *J* = 7.8 Hz); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 19.4, 19.5, 107.6, 119.5, 124.0, 124.9, 126.5, 127.1, 128.2, 128.8, 129.1, 129.3, 129.5, 132.4, 133.5, 134.0, 134.9, 135.4, 136.6, 138.8, 168.1; IR (KBr): 3018, 2966, 2918, 1710, 1634, 1606, 1500, 1468, 1446, 1394, 1341, 1302, 1184, 1112, 909, 811, 766, 693 cm^{-1}; HRMS (ESI): calcd. for $C_{23}H_{19}NO$ (MH^+) 326.1539; found 326.1536.

(*Z*)-3-Benzylidene-2-(4-methoxyphenyl)isoindolin-1-one (4a):



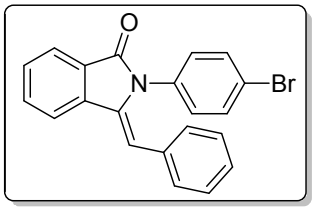
^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 3.71 (s, 3H), 6.62 (d, 2H, *J* = 7.2 Hz), 6.82 (s, 1H), 6.87 (d, 2H, *J* = 7.2 Hz), 6.94 – 7.01 (m, 5H), 7.55 (t, 1H, *J* = 7.8 Hz), 7.67 (t, 1H, *J* = 7.8 Hz), 7.85 (d, 1H, *J* = 7.8 Hz), 7.95 (d, 1H, *J* = 7.8 Hz); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 55.6, 107.6, 113.8, 119.5, 123.9, 126.6, 127.3, 128.0, 128.5, 128.9, 129.3, 132.5, 133.7, 134.8, 138.7, 158.5, 168.3; IR (KBr): 3014, 2929, 1714, 1640, 1607, 1511, 1467, 1445, 1391, 1298, 1248, 1123, 825, 766, 695 cm^{-1}; HRMS (ESI): calcd. for $C_{22}H_{17}NO_2$ (MH^+) 328.1332; found 328.1339.

(*Z*)-3-Benzylidene-2-(4-chlorophenyl)isoindolin-1-one (5a):



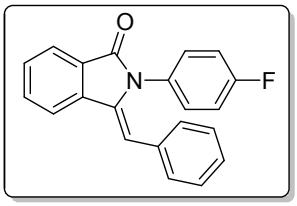
^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 6.83 – 6.85 (m, 3H), 6.95 – 6.99 (m, 4H), 7.01 – 7.04 (m, 3H), 7.54 (t, 1H, *J* = 7.2 Hz), 7.67 (t, 1H, *J* = 7.2 Hz), 7.84 (d, 1H, *J* = 7.8 Hz), 7.93 (d, 1H, *J* = 7.2 Hz); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 108.0, 119.7, 124.2, 127.1, 127.6, 127.8, 128.5, 128.6, 129.4, 129.6, 132.6, 132.9, 133.6, 134.4, 134.6, 138.7, 168.0; IR (KBr): 3050, 3021, 2927, 1701, 1643, 1471, 1442, 1384, 1342, 1314, 1189, 1129, 1085, 1012, 820, 760, 725, 694 cm^{-1}; HRMS (ESI): calcd. for $C_{21}H_{14}ClNO$ (MH^+) 332.0837; found 332.0832.

(*Z*)-3-Benzylidene-2-(4-bromophenyl)isoindolin-1-one (6a):



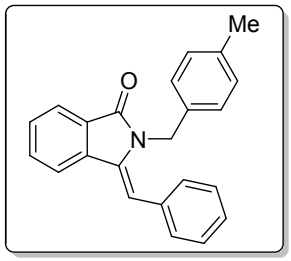
^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 6.83 – 685 (m, 3H), 6.91 – 6.93 (m, 2H), 6.96 (t, 2H, *J* = 7.2 Hz), 7.03 (t, 1H, *J* = 7.2 Hz), 7.16 – 7.18 (m, 2H), 7.54 (t, 1H, *J* = 7.8 Hz), 7.67 (t, 1H, *J* = 7.8 Hz), 7.84 (d, 1H, *J* = 7.2 Hz), 7.92 (d, 1H, *J* = 7.2 Hz); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 108.0, 119.7, 120.5, 124.2, 127.1, 127.6, 127.8, 128.9, 129.4, 129.6, 131.4, 132.9, 133.6, 134.4, 135.1, 138.7, 167.9; IR (KBr): 3051, 2923, 1710, 1638, 1487, 1394, 1342, 1302, 1183, 1122, 1066, 1007, 818, 762, 693 cm^{-1}; HRMS (ESI): calcd. for $C_{21}H_{14}BrNO$ (MH^+) 376.0332; found 376.0341.

(*Z*)-3-Benzylidene-2-(4-fluorophenyl)isoindolin-1-one (7a):



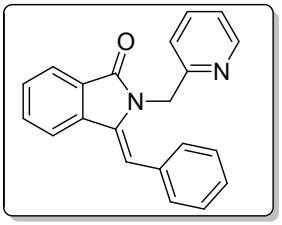
^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 6.74 – 6.77 (m, 2H), 6.83 – 685 (m, 3H), 6.95 (t, 2H, *J* = 7.8 Hz), 6.99 – 7.03 (m, 3H), 7.54 (t, 1H, *J* = 7.2 Hz), 7.67 (t, 1H, *J* = 7.2 Hz), 7.84 (d, 1H, *J* = 7.8 Hz), 7.93 (d, 1H, *J* = 7.8 Hz); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 107.8, 115.2, 115.3, 119.6, 124.1, 127.0, 127.5, 127.9, 129.0, 129.1, 129.4, 129.5, 132.1, 132.8, 133.6, 134.7, 138.7, 160.6, 162.2, 168.2; IR (KBr): 3054, 1706, 1640, 1604, 1505, 1471, 1446, 1379, 1301, 1217, 1121, 828, 765, 694 cm^{-1}; HRMS (ESI): calcd. for $C_{21}H_{14}FNO$ (MH^+) 316.1132; found 316.1135.

(*Z*)-3-Benzylidene-2-(4-methylbenzyl)isoindolin-1-one (8a):



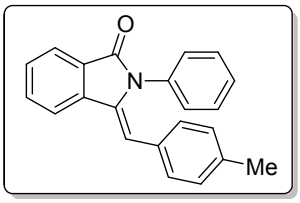
^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 2.26 (s, 3H), 4.94 (s, 2H), 6.48 (d, 2H, *J* = 7.8 Hz), 6.74 (s, 1H), 6.90 (d, 2H, *J* = 7.2 Hz), 7.14 (d, 2H, *J* = 8.4 Hz), 7.29 – 7.32 (m, 3H), 7.54 (t, 1H, *J* = 7.8 Hz), 7.62 (t, 1H, *J* = 7.2 Hz), 7.75 (d, 1H, *J* = 7.8 Hz), 7.96 (d, 1H, *J* = 7.2 Hz); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 21.2, 44.8, 107.6, 119.6, 123.6, 126.6, 127.5, 128.1, 128.3, 128.8, 129.1, 129.9, 132.2, 134.0, 134.5, 134.8, 136.4, 138.7, 169.2; IR (KBr): 3049, 2920, 1706, 1655, 1620, 1471, 1429, 1395, 1343, 1288, 1108, 958, 786, 757, 695 cm^{-1}; HRMS (ESI): calcd. for $C_{23}H_{19}NO$ (MH^+) 326.1539; found 326.1535.

(*Z*)-3-Benzylidene-2-(pyridin-2-ylmethyl)isoindolin-1-one (9a):



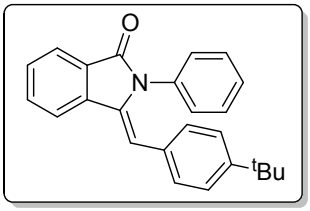
^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 4.98 (s, 2H), 6.57 (d, 1H, *J* = 7.8 Hz), 6.73 (s, 1H), 6.95 (d, 2H, *J* = 7.8 Hz), 6.98 – 7.00 (m, 1H), 7.12 (t, 2H, *J* = 7.8 Hz), 7.19 (t, 1H, *J* = 7.8 Hz), 7.40 (t, 1H, *J* = 7.2 Hz), 7.52 (t, 1H, *J* = 7.8 Hz), 7.62 (t, 1H, *J* = 7.8 Hz), 7.75 (d, 1H, *J* = 7.8 Hz), 7.92 (d, 1H, *J* = 7.8 Hz), 8.26 (d, 1H, *J* = 4.8 Hz); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 47.0, 107.5, 119.7, 120.3, 121.7, 123.8, 127.6, 128.0, 128.4, 129.3, 129.4, 132.4, 134.3, 134.9, 136.3, 138.6, 149.3, 156.5, 169.1; IR (KBr): 3059, 3008, 2932, 1702, 1654, 1591, 1473, 1431, 1399, 1366, 1344, 1119, 984, 949, 753, 697 cm^{-1}; HRMS (ESI): calcd. for $C_{21}H_{16}N_2O$ (MH^+) 313.1335; found 313.1343.

(*Z*)-3-(4-Methylbenzylidene)-2-phenylisoindolin-1-one (1b):



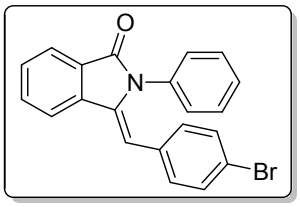
^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 2.17 (s, 3H), 6.71 (q, 4H, *J* = 4.2 Hz), 6.79 (s, 1H), 7.05 – 7.09 (m, 5H), 7.52 (t, 1H, *J* = 7.8 Hz), 7.64 (t, 1H, *J* = 7.2 Hz), 7.83 (d, 1H, *J* = 7.8 Hz), 7.93 (d, 1H, *J* = 7.8 Hz); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 21.3, 108.1, 119.5, 124.1, 126.8, 127.4, 127.9, 128.1, 128.4, 129.2, 129.3, 130.8, 132.6, 134.0, 136.2, 136.7, 139.0, 168.2; IR (KBr): 3034, 3023, 2920, 1706, 1647, 1495, 1468, 1386, 1339, 1299, 1183, 1122, 922, 827, 758, 693 cm^{-1}; HRMS (ESI): calcd. for $C_{22}H_{17}NO$ (MH^+) 312.1383; found 312.1389.

(*Z*)-3-(4-(*tert*-butyl)benzylidene)-2-phenylisoindolin-1-one (1c):



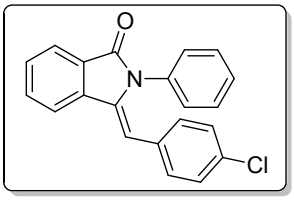
^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 1.19 (s, 9H), 6.73 (d, 2H, *J* = 7.8 Hz), 6.83 (s, 1H), 6.89 (d, 2H, *J* = 7.8 Hz), 7.00 – 7.04 (m, 5H), 7.52 (t, 1H, *J* = 7.8 Hz), 7.65 (t, 1H, *J* = 6.6 Hz), 7.83 (d, 1H, *J* = 7.8 Hz), 7.92 (d, 1H, *J* = 7.2 Hz); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 31.4, 34.6, 108.0, 119.5, 124.1, 124.3, 126.7, 127.5, 128.0, 128.2, 128.9, 129.25, 129.33, 130.8, 132.6, 134.4, 136.1, 138.9, 150.0, 168.1; IR (KBr): 3054, 2960, 1712, 1599, 1495, 1469, 1380, 1338, 1300, 1182, 1111, 1063, 1017, 844, 758, 693 cm^{-1}; HRMS (ESI): calcd. for $C_{25}H_{23}NO$ (MH^+) 354.1852; found 354.1849.

(*Z*)-3-(4-bromobenzylidene)-2-phenylisoindolin-1-one (1d):



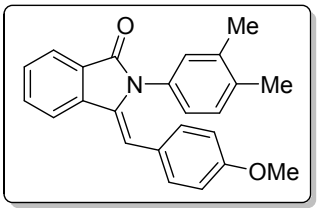
^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 6.69 (t, 3H, *J* = 4.2 Hz), 7.02 (d, 2H, *J* = 7.8 Hz), 7.04 – 7.06 (m, 2H), 7.10 – 7.12 (m, 3H), 7.54 (t, 1H, *J* = 7.8 Hz), 7.66 (t, 1H, *J* = 7.2 Hz), 7.82 (d, 1H, *J* = 7.8 Hz), 7.93 (d, 1H, *J* = 7.8 Hz); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 106.2, 119.6, 120.9, 124.1, 127.2, 127.4, 127.9, 128.6, 129.6, 130.5, 130.7, 132.7, 135.1, 135.9, 138.6, 168.1; IR (KBr): 3055, 2923, 1708, 1638, 1593, 1486, 1391, 1300, 1181, 1123, 1070, 1007, 845, 810, 763, 694 cm^{-1}; HRMS (ESI): calcd. for $C_{21}H_{14}BrNO$ (MH^+) 376.0322; found 376.0327.

(*Z*)-3-(4-chlorobenzylidene)-2-phenylisoindolin-1-one (1e):



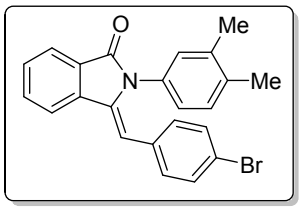
^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 6.72 (s, 1H), 6.76 (d, 2H, *J* = 8.4 Hz), 6.86 (d, 2H, *J* = 7.8 Hz), 7.05 – 7.06 (m, 2H), 7.10 – 7.13 (m, 3H), 7.54 (t, 1H, *J* = 7.8 Hz), 7.66 (t, 1H, *J* = 7.2 Hz), 7.82 (d, 1H, *J* = 7.2 Hz), 7.93 (d, 1H, *J* = 7.2 Hz); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 106.2, 119.6, 124.2, 127.2, 127.5, 127.6, 128.0, 128.6, 129.6, 130.5, 132.3, 132.70, 132.74, 135.2, 136.0, 138.7, 168.1; IR (KBr): 3057, 2922, 1708, 1647, 1596, 1488, 1388, 1297, 1120, 1088, 905, 760, 697 cm^{-1}; HRMS (ESI): calcd. for $C_{21}H_{14}ClNO$ (MH^+) 332.0837; found 332.0833.

(*Z*)-2-(3,4-dimethylphenyl)-3-(4-methoxybenzylidene)isoindolin-1-one (3f):



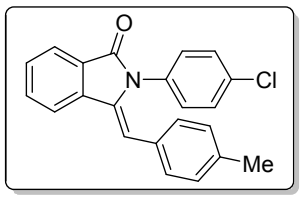
^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 1.99 (s, 3H), 2.13 (s, 3H), 3.68 (s, 3H), 6.43 (d, 2H, *J* = 9.0 Hz), 6.73 – 6.76 (m, 4H), 6.86 (d, 1H, *J* = 7.2 Hz), 6.90 (t, 1H, *J* = 8.4 Hz), 7.51 (t, 1H, *J* = 7.2 Hz), 7.62 (t, 1H, *J* = 7.2 Hz), 7.80 (d, 1H, *J* = 7.8 Hz), 7.91 (d, 1H, *J* = 7.8 Hz); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 19.5, 19.6, 55.4, 107.6, 114.2, 119.4, 124.0, 124.9, 126.5, 128.1, 128.8, 129.0, 129.5, 130.5, 130.9, 132.4, 133.7, 133.8, 135.3, 136.6, 139.0, 158.6, 168.2; IR (KBr): 2918, 1713, 1632, 1601, 1507, 1468, 1386, 1342, 1302, 1247, 1175, 1107, 1024, 910, 837, 759, 692 cm^{-1}; HRMS (ESI): calcd. for $C_{24}H_{21}NO_2$ (MH^+) 356.1645; found 356.1656.

(*Z*)-3-(4-bromobenzylidene)-2-(3,4-dimethylphenyl)isoindolin-1-one (3g):



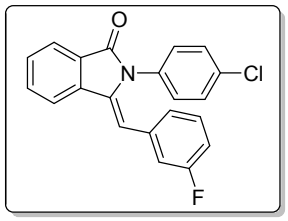
^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 1.98 (s, 3H), 2.17 (s, 3H), 6.61 (s, 1H), 6.66 – 6.68 (m, 3H), 6.85 (d, 1H, *J* = 7.8 Hz), 6.93 (d, 1H, *J* = 7.8 Hz), 7.00 (d, 2H, *J* = 8.4 Hz), 7.53 (t, 1H, *J* = 7.2 Hz), 7.64 (t, 1H, *J* = 7.2 Hz), 7.80 (d, 1H, *J* = 7.8 Hz), 7.93 (d, 1H, *J* = 7.8 Hz); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 19.4, 19.5, 105.9, 119.5, 120.6, 124.0, 125.0, 128.1, 128.7, 129.5, 129.6, 130.1, 130.4, 132.5, 133.0, 133.2, 135.6, 136.0, 136.7, 138.4, 167.9; IR (KBr): 3027, 2919, 1705, 1647, 1500, 1484, 1385, 1309, 1184, 1114, 1070, 1010, 915, 818, 757, 693 cm^{-1}; HRMS (ESI): calcd. for $C_{23}H_{18}BrNO$ (MH^+) 404.0645; found 404.0652.

(*Z*)-2-(4-Chlorophenyl)-3-(4-methylbenzylidene)isoindolin-1-one (5b):



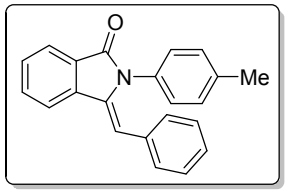
^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 2.22 (s, 3H), 6.72 (d, 2H, *J* = 7.8 Hz), 6.77 (d, 2H, *J* = 8.4 Hz), 6.81 (s, 1H), 6.98 (d, 2H, *J* = 7.2 Hz), 7.03 (d, 2H, *J* = 7.2 Hz), 7.52 (t, 1H, *J* = 7.8 Hz), 7.65 (t, 1H, *J* = 7.2 Hz), 7.82 (d, 1H, *J* = 7.2 Hz), 7.91 (d, 1H, *J* = 7.2 Hz); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 21.3, 108.3, 119.6, 124.1, 127.7, 128.3, 128.4, 128.6, 129.3, 129.4, 130.6, 132.5, 132.8, 133.9, 134.7, 137.2, 138.8, 168.0; IR (KBr): 3043, 2918, 1713, 1637, 1492, 1471, 1396, 1343, 1304, 1182, 1122, 1084, 912, 832, 759, 691 cm^{-1}; HRMS (ESI): calcd. for $C_{22}H_{16}ClNO$ (MH^+) 346.0993; found 346.0985.

(*Z*)-2-(4-Chlorophenyl)-3-(3-fluorobenzylidene)isoindolin-1-one (5h):



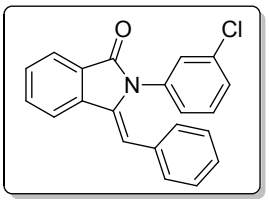
^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 6.56 (d, 1H, *J* = 9.6 Hz), 6.62 (d, 1H, *J* = 7.8 Hz), 6.71 – 6.74 (m, 2H), 6.92 (q, 1H, *J* = 7.8 Hz), 6.99 (d, 2H, *J* = 9.0 Hz), 7.07 (d, 2H, *J* = 7.2 Hz), 7.55 (t, 1H, *J* = 7.8 Hz), 7.67 (t, 1H. *J* = 7.8 Hz), 7.82 (d, 1H, *J* = 7.8 Hz), 7.92 (d, 1H, *J* = 7.8 Hz); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 106.2, 113.9, 114.0, 116.1, 116.3, 119.7, 124.2, 125.2, 127.8, 128.5, 128.6, 129.0, 129.1, 129.8, 132.9, 133.0, 134.5, 135.4, 135.8, 135.9, 138.4, 161.3, 162.9, 167.9; IR (KBr): 3056, 3023, 1703, 1645, 1580, 1488, 1388, 1313, 1127, 1088, 871, 819, 762, 697 cm^{-1}; HRMS (ESI): calcd. for $C_{21}H_{13}ClFNO$ (MH^+) 350.0742; found 350.0735.

(*Z*)-3-Benzylidene-2-(*p*-tolyl)isoindolin-1-one (2´a):



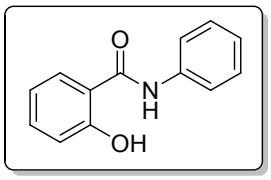
^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 2.21 (s, 3H), 6.79 (s, 1H), 6.83 – 6.94 (m, 8H), 6.96 (t, 1H, *J* = 7.8 Hz), 7.52 (t, 1H, *J* = 7.2 Hz), 7.65 (t, 1H. *J* = 6.6 Hz), 7.83 (d, 1H, *J* = 7.8 Hz), 7.92 (d, 1H, *J* = 7.2 Hz); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 21.2, 107.7, 119.6, 124.0, 126.6, 127.25, 127.34, 128.1, 129.0, 129.3, 129.4, 132.5, 133.5, 133.8, 134.8, 136.8, 138.9, 168.2; IR (KBr): 3044, 3021, 2920, 1707, 1641, 1512, 1469, 1389, 1341, 1301, 1186, 1126, 1073, 925, 809, 760, 692 cm^{-1}; HRMS (ESI): calcd. for $C_{22}H_{17}NO$ (MH^+) 312.1383; found 312.1389.

(*Z*)-3-Benzylidene-2-(3-chlorophenyl)isoindolin-1-one (3´a):



^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 6.85 (s, 1H), 6.87 (d, 2H, *J* = 7.8 Hz), 6.96 – 7.02 (m, 7H), 7.54 (t, 1H, *J* = 7.8 Hz), 7.67 (t, 1H. *J* = 7.8 Hz), 7.84 (d, 1H, *J* = 7.8 Hz), 7.93 (d, 1H, *J* = 7.2 Hz); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 108.1, 119.7, 124.2, 125.6, 127.0, 127.2, 127.6, 127.8, 127.9, 129.1, 129.2, 129.6, 132.9, 133.6, 134.0, 134.3, 137.1, 138.7, 167.9; IR (KBr): 3070, 1706, 1632, 1588, 1473, 1401, 1350, 1298, 1183, 1126, 1072, 925, 905, 798, 767, 702, 690 cm^{-1}; HRMS (ESI): calcd. for $C_{21}H_{14}ClNO$ (MH^+) 332.0837; found 332.0841.

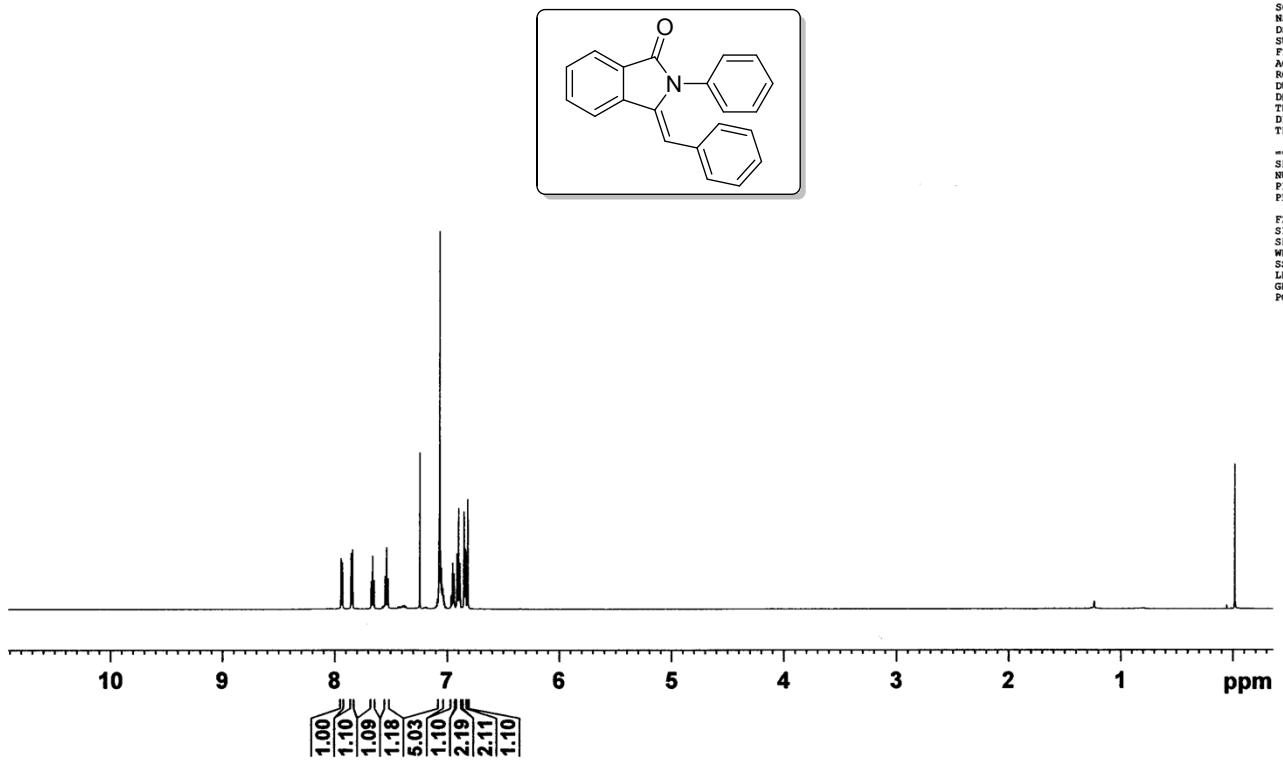
2-Hydroxy-*N*-phenylbenzamide (1a′):



^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) 6.92 (t, 1H, *J* = 7.2 Hz), 7.04 (d, 1H, *J* = 7.8 Hz), 7.22 (t, 1H, *J* = 7.2 Hz), 7.40 (t, 2H, *J* = 7.8 Hz), 7.45 (t, 1H, *J* = 7.2 Hz), 7.55 – 7.59 (m, 3H), 8.08 (s, 1H), 12.01 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 114.8, 119.1, 119.2, 121.5, 125.6, 125.7, 129.4, 134.9, 136.8, 162.0, 168.6; IR (KBr): 3299, 2923, 1621, 1556, 1500, 1455, 1375, 1332, 1201, 1158, 894, 753 cm^{-1}. HRMS (ESI): calcd. for $C_{13}H_{11}NO_2$ (MH^+) 214.0823; found 214.0863.

SPECTRA

(*Z*)-3-Benzylidene-2-phenylisoindolin-1-one (1a): ^{1}H NMR (600 MHz, $CDCl_3$)

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Current Data Parameters
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EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
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Time                8.46
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                   113
DW                41.600 usec
DE                 6.50 usec
TE                299.3 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           600.1700267 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
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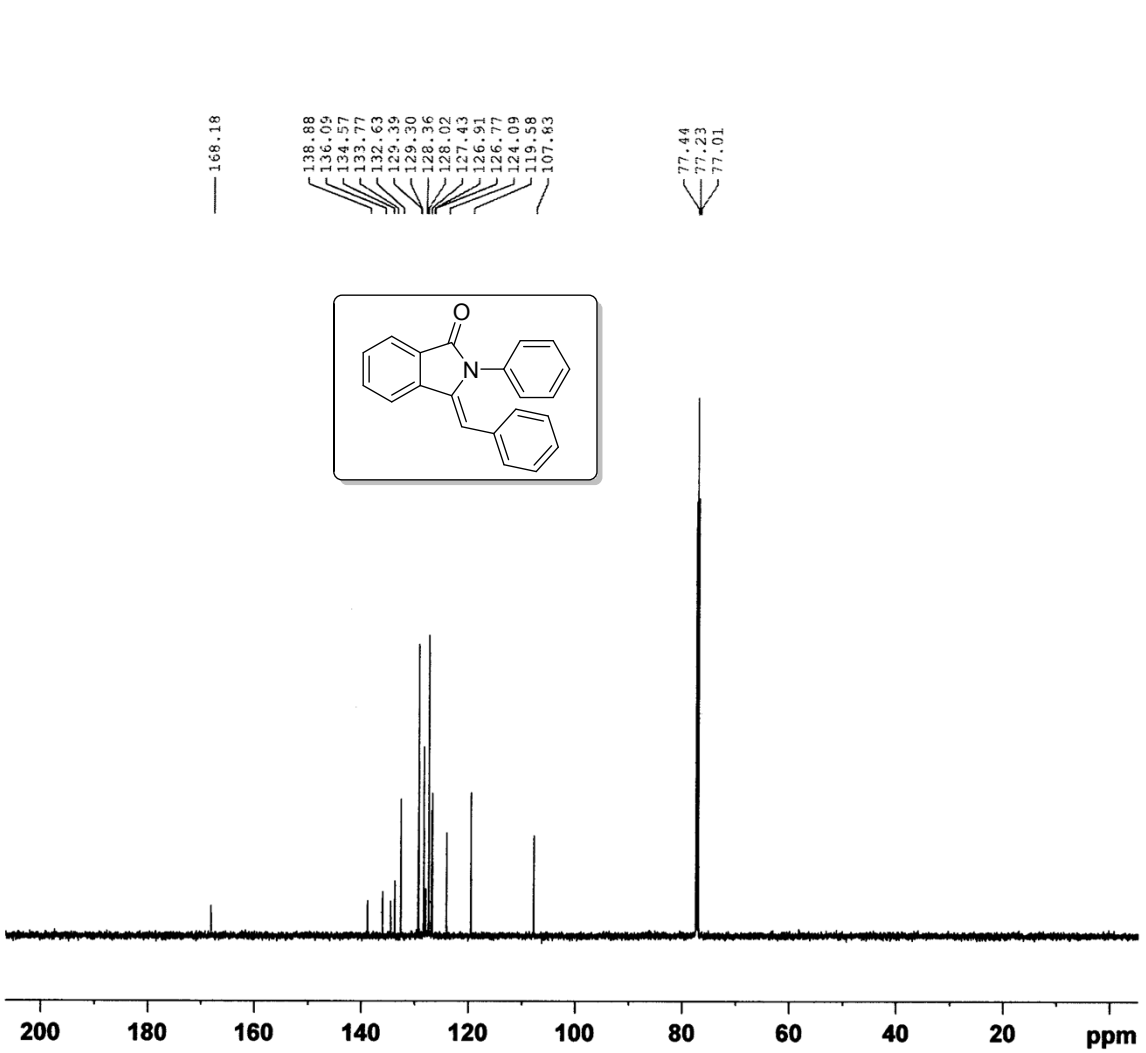
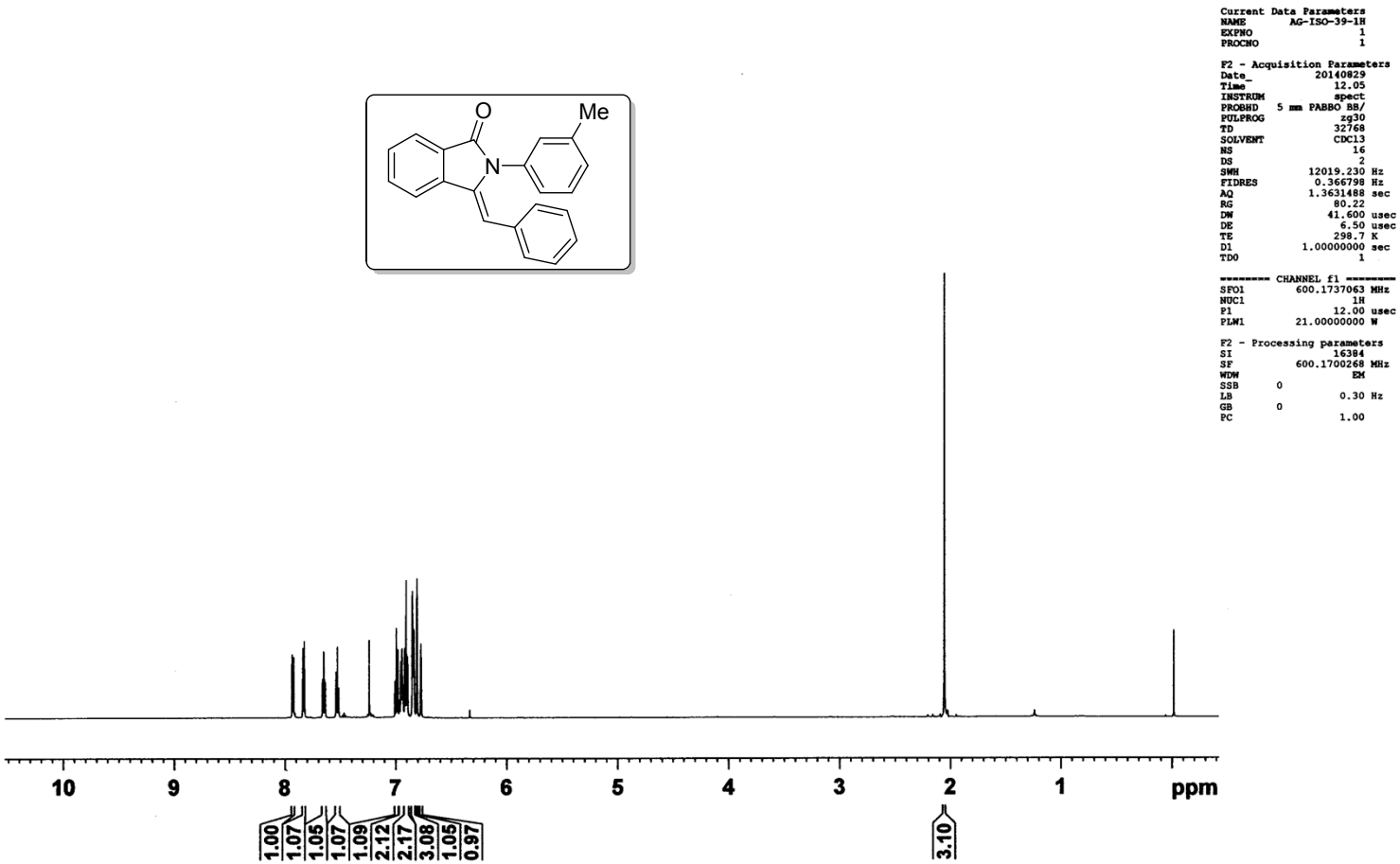
(*Z*)-3-Benzylidene-2-phenylisoindolin-1-one (1a): ^{13}C NMR (150 MHz, $CDCl_3$)



BRUKER

```
Current Data Parameters
NAME       AG-ISO-40-13C
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20140901
Time              11.56
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                32768
SOLVENT           CDCl3
NS                  197
DS                    2
SWH           36057.691 Hz
FIDRES         1.100393 Hz
AQ            0.4543829 sec
RG                65.24
DW               13.867 usec
DE                6.50 usec
TE                301.6 K
D1           2.00000000 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          150.9128372 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

(*Z*)-3-Benzylidene-2-(*m*-tolyl)isoindolin-1-one (2a): ^{1}H NMR (600 MHz, $CDCl_3$)

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Current Data Parameters
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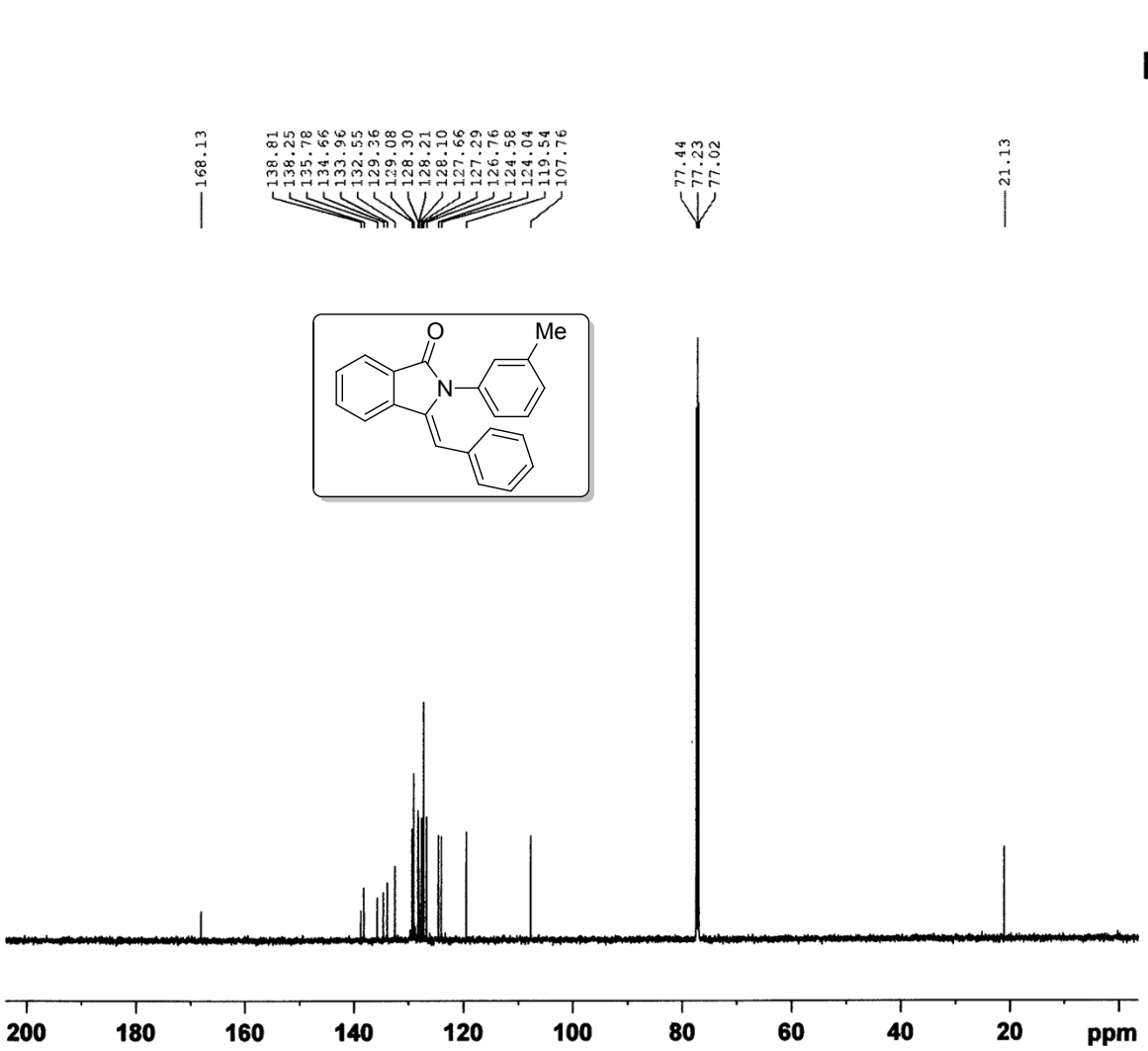
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_          20140829
Time              12.05
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               32768
SOLVENT          CDCl3
NS                  16
DS                   2
SWH           12019.230 Hz
FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG                80.22
DW               41.600 usec
DE                6.50 usec
TE               298.7 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          600.1700268 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

(*Z*)-3-Benzylidene-2-(*m*-tolyl)isoindolin-1-one (2a): ^{13}C NMR (150 MHz, $CDCl_3$)



BRUKER

```
Current Data Parameters
NAME       AG-ISO-39-13C
EXPNO                  1
PROCNO                 1

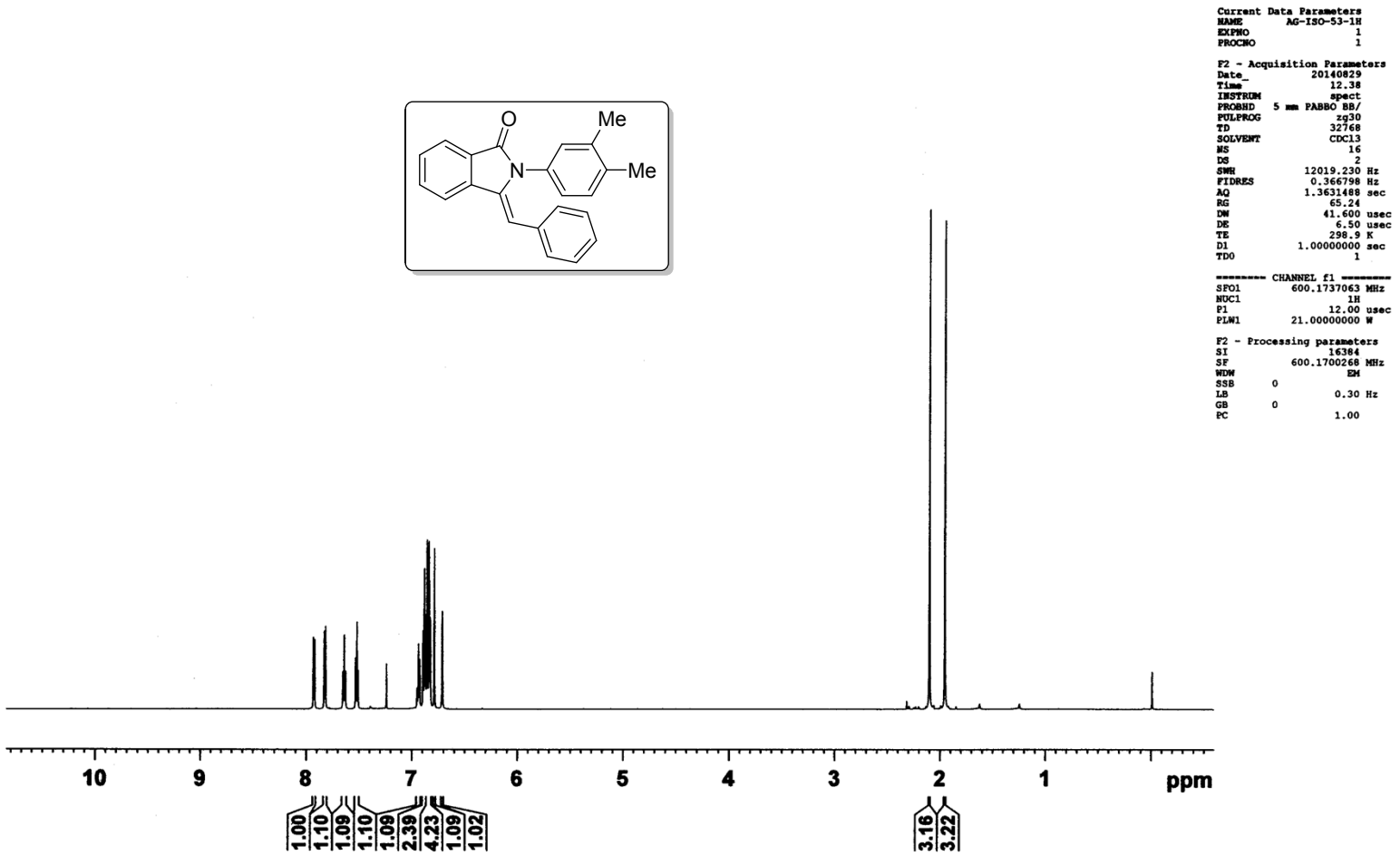
F2 - Acquisition Parameters
Date_           20140829
Time               12.12
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  265
DS                    2
SWH           36057.691 Hz
FIDRES         1.100393 Hz
AQ            0.4543829 sec
RG                65.24
DW               13.867 usec
DE                6.50 usec
TE               299.9 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
```

(*Z*)-3-Benzylidene-2-(3,4-dimethylphenyl)isoindolin-1-one (3a): ^{1}H NMR (600 MHz, $CDCl_3$)

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Current Data Parameters
NAME          AG-ISO-53-1H
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20140829
Time                  12.38
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                  298.9 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              600.1700268 MHz
WDW                     EM
SSB       0
LB                     0.30 Hz
GB        0
PC                     1.00
```
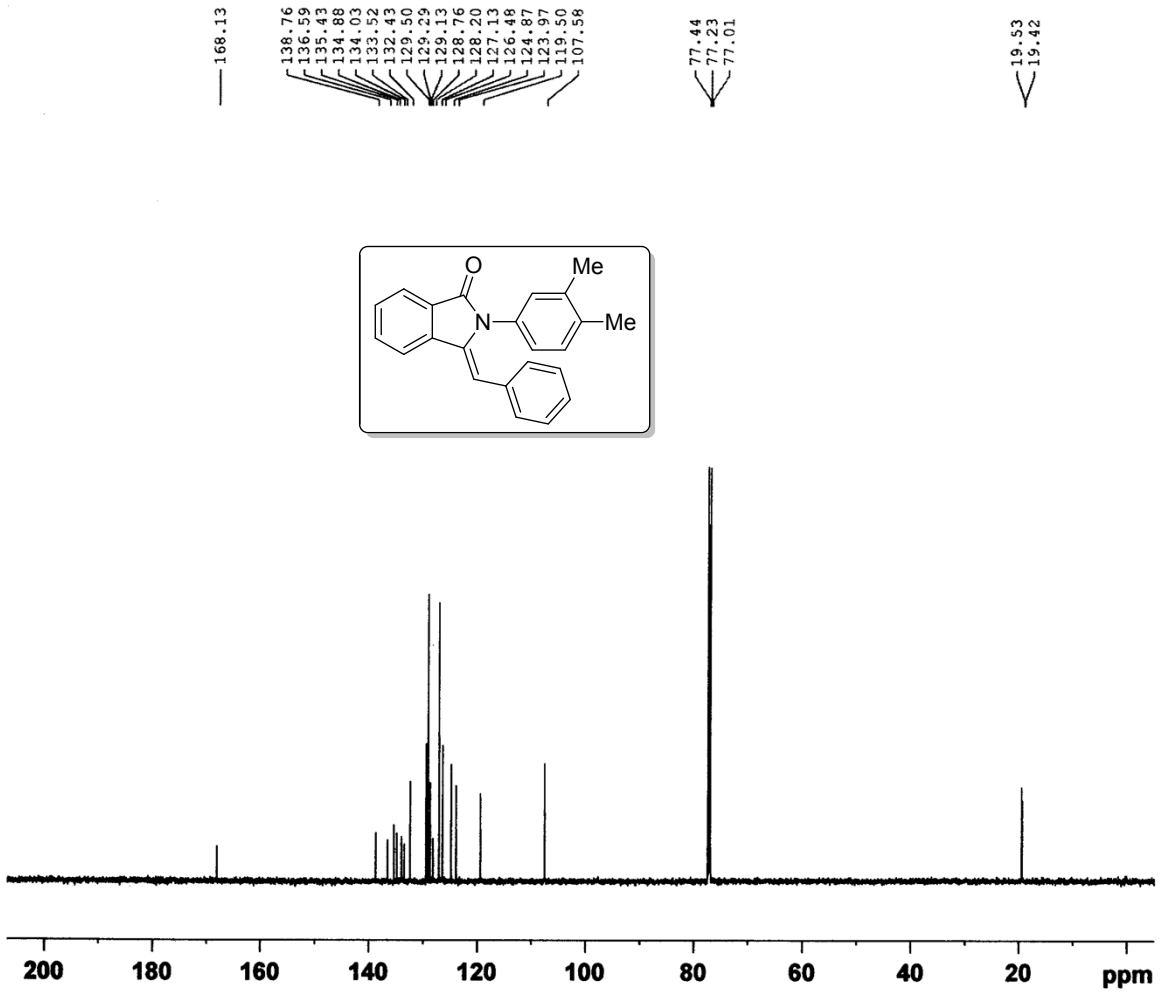

(*Z*)-3-Benzylidene-2-(3,4-dimethylphenyl)isoindolin-1-one (3a): ^{13}C NMR (150 MHz, $CDCl_3$)

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Current Data Parameters
NAME       AG-ISO-53-13C
EXPNO                 1
PROCNO                1

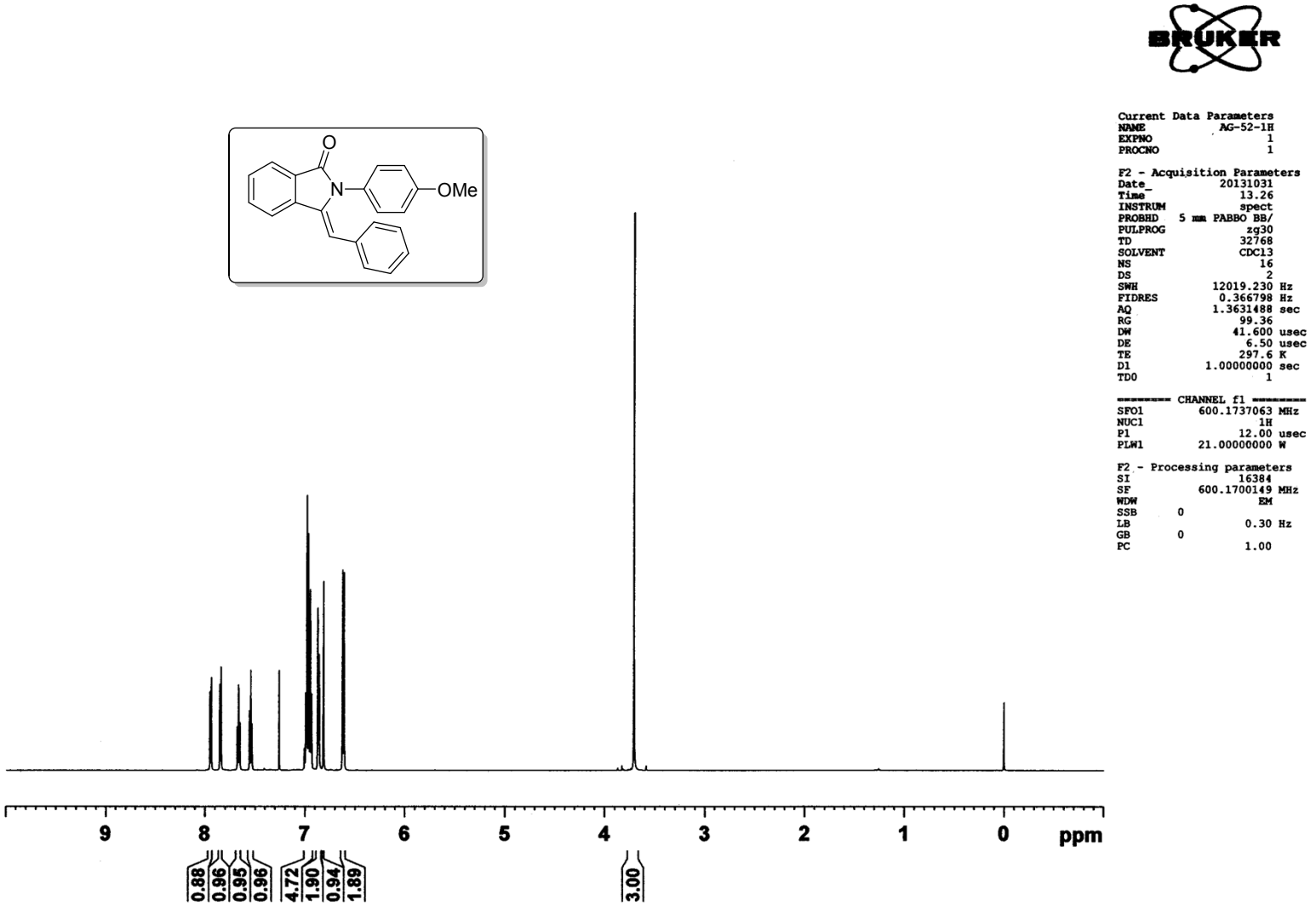
F2 - Acquisition Parameters
Date_          20140829
Time              12.46
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD              32768
SOLVENT          CDCl3
NS                 201
DS                   2
SWH          36057.691 Hz
FIDRES        1.100393 Hz
AQ           0.4543829 sec
RG               65.24
DW              13.867 usec
DE               6.50 usec
TE              300.1 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         150.9128391 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```

(*Z*)-3-Benzylidene-2-(4-methoxyphenyl)isoindolin-1-one (4a): ^{1}H NMR (600 MHz, $CDCl_3$)

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Current Data Parameters
NAME                  AG-52-1H
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20131031
Time                   13.26
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                    297.6 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              600.1700149 MHz
WDW                        EM
SSB          0
LB                      0.30 Hz
GB           0
PC                      1.00
```
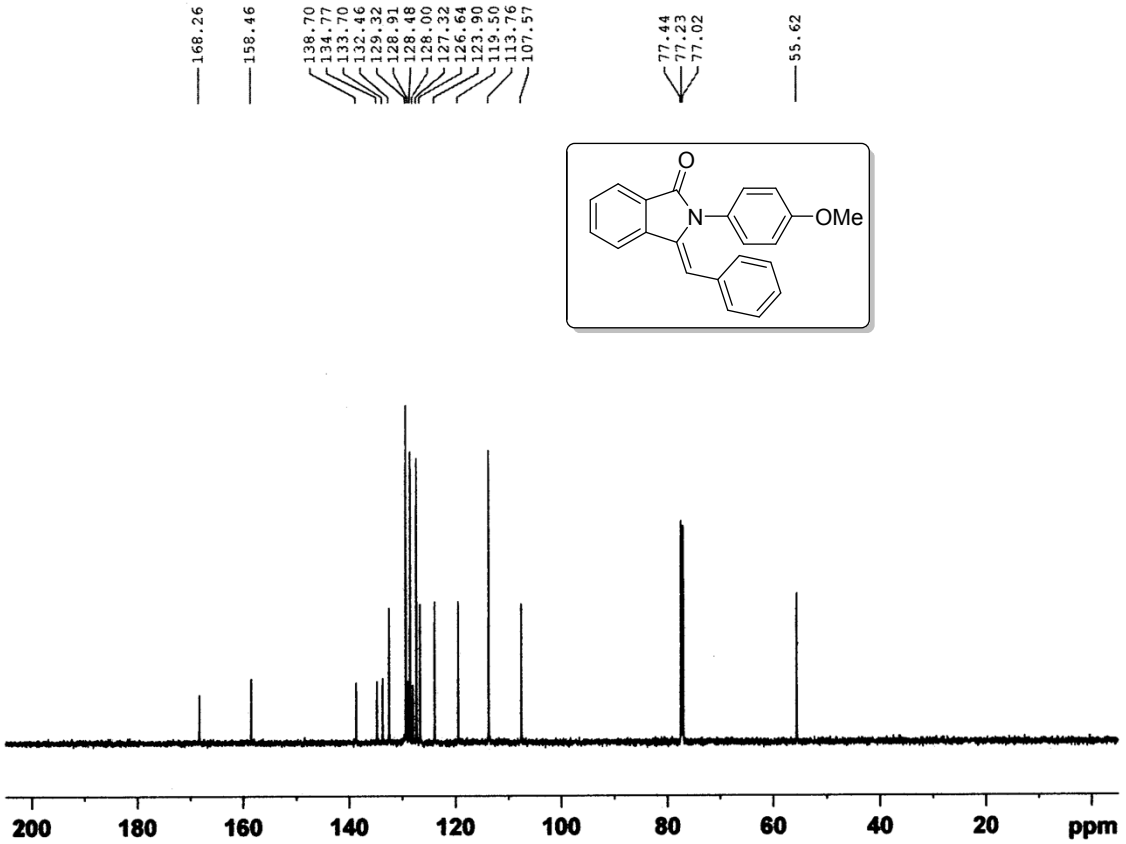
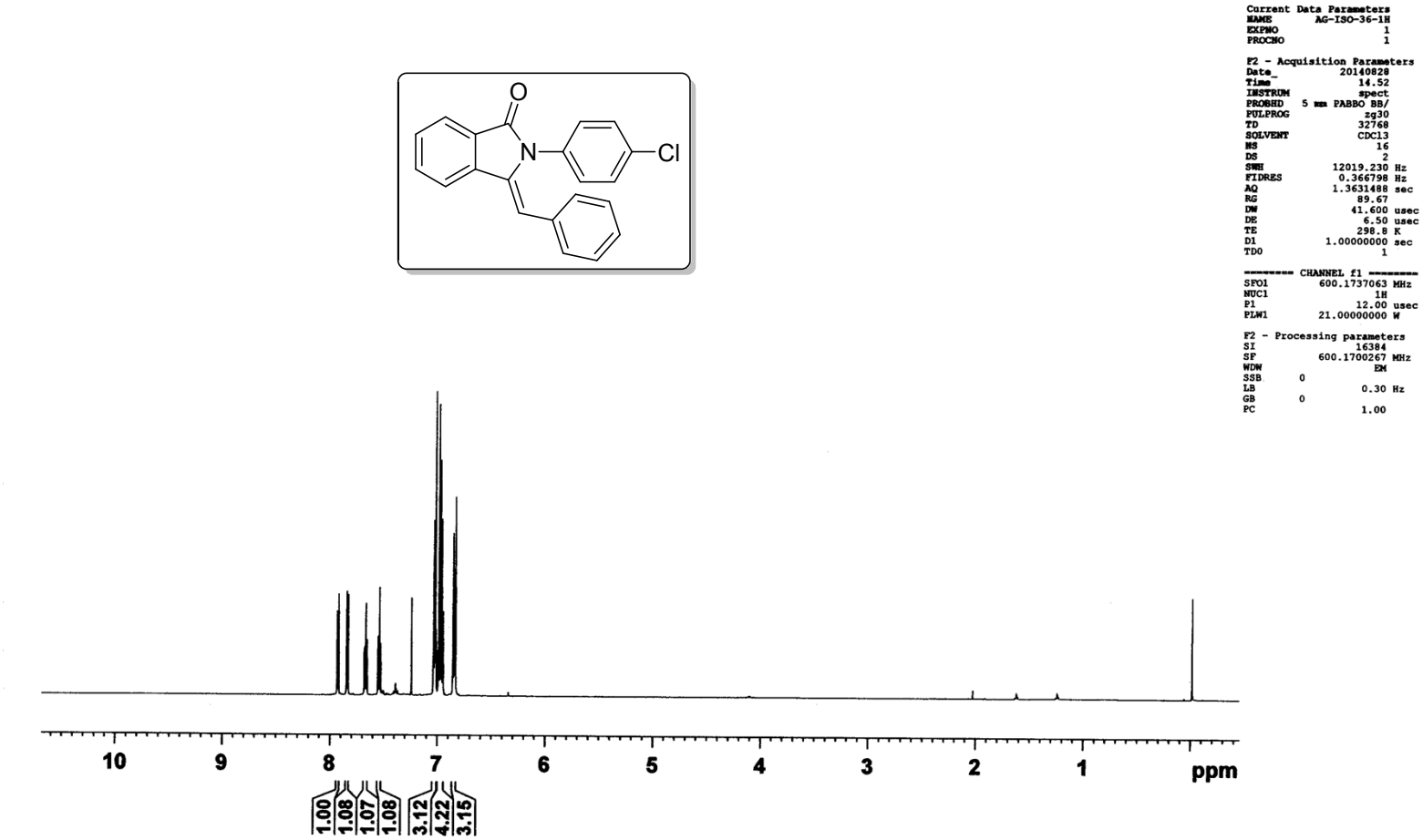

(*Z*)-3-Benzylidene-2-(4-methoxyphenyl)isoindolin-1-one (4a): ^{13}C NMR (150 MHz, $CDCl_3$)



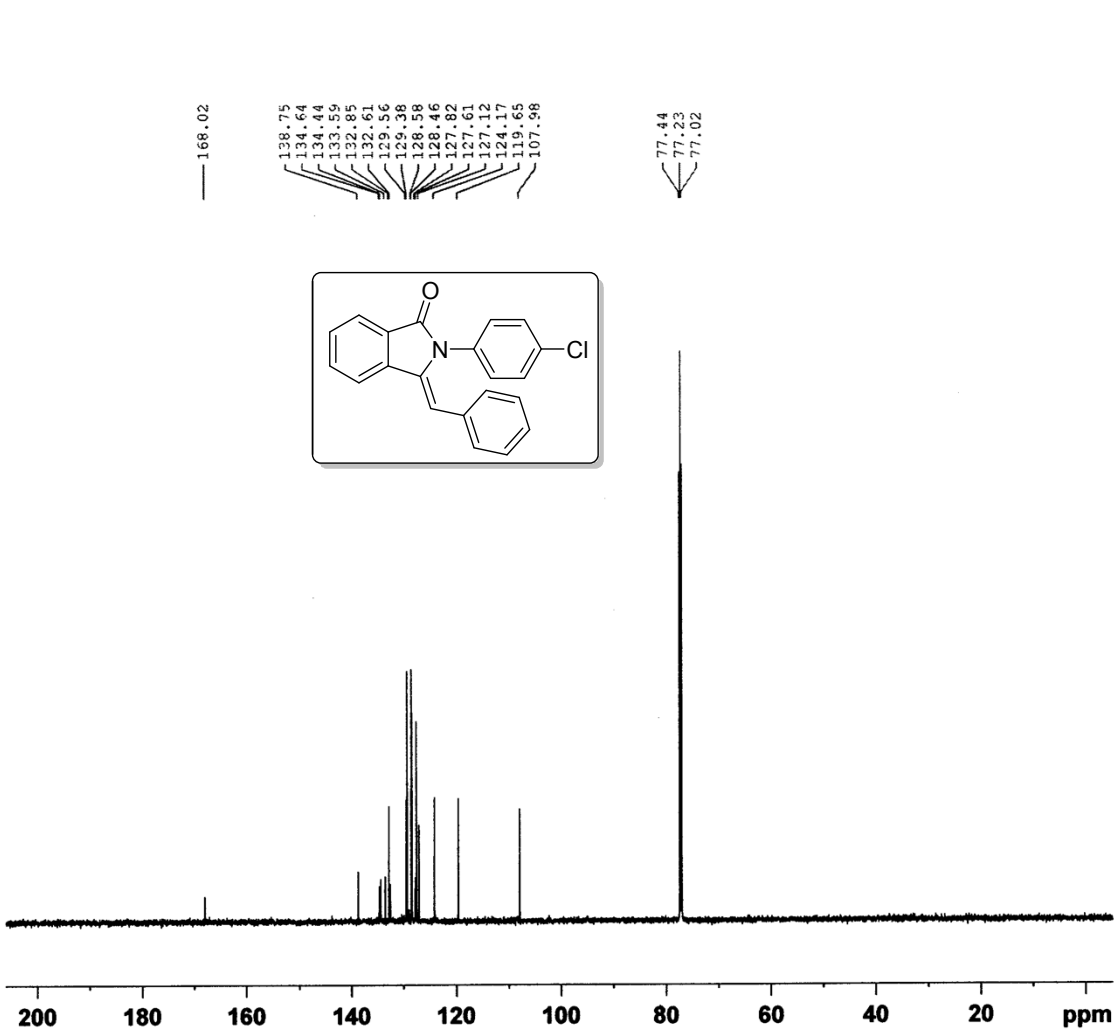

```
Current Data Parameters
NAME                 AG_52_13C
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20131003
Time                      9.35
INSTRUM                  spect
PROBHD     5 mm PABBO BB/
PULPROG                 zgpg30
TD                       32768
SOLVENT                  CDCl3
NS                         218
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                 150.9128486 MHz
WDW                         EM
SSB          0
LB                        1.00 Hz
GB           0
PC                        1.40
```

(*Z*)-3-Benzylidene-2-(4-chlorophenyl)isoindolin-1-one (5a): ^{1}H NMR (600 MHz, $CDCl_3$)



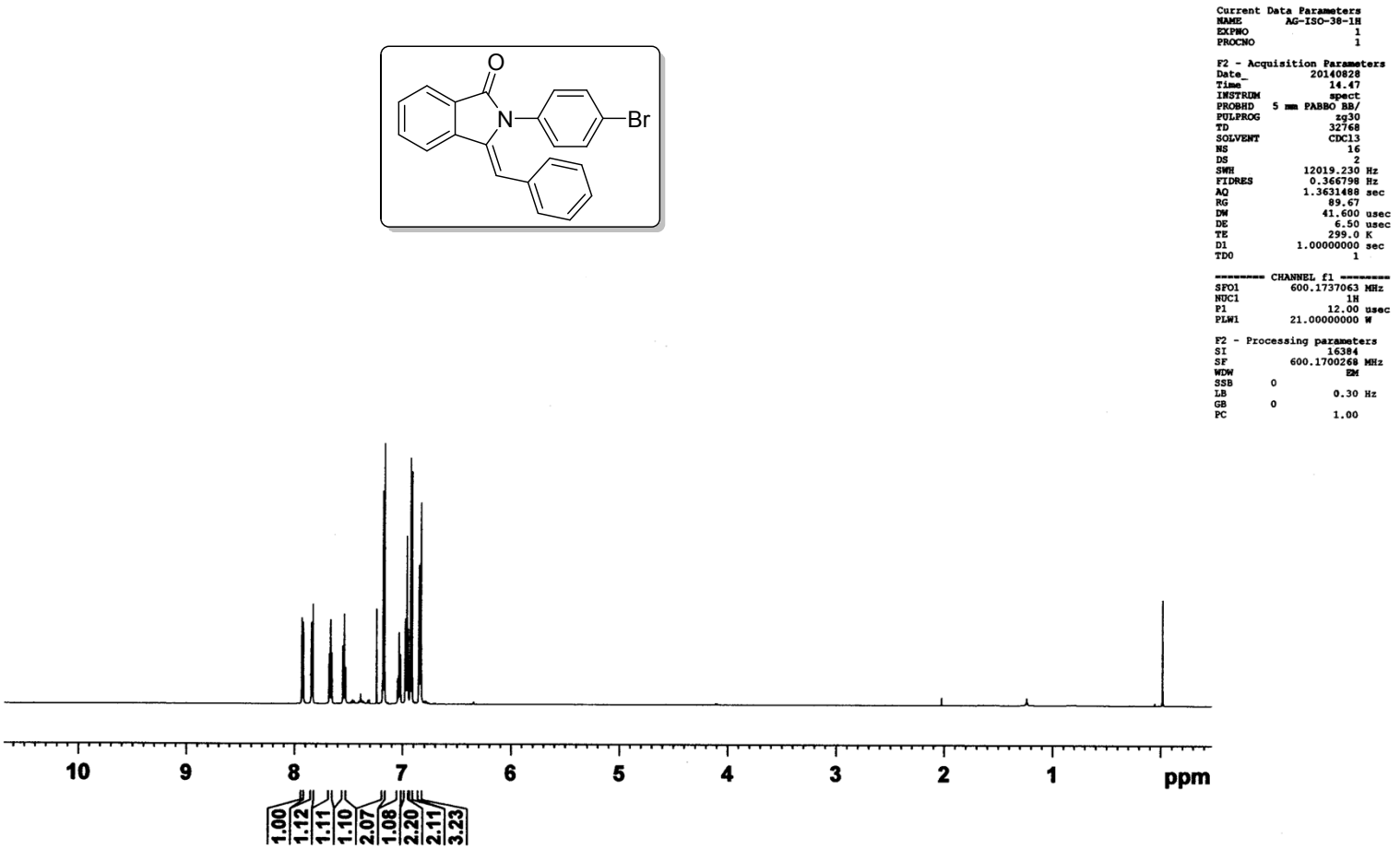

```
Current Data Parameters
NAME          AG-ISO-36-1H
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20140828
Time                 14.52
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                  89.67
DW                 41.600 usec
DE                  6.50 usec
TE                 298.8 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            600.1700267 MHz
WDW                    EM
SSB          0
LB                  0.30 Hz
GB           0
PC                  1.00
```

(*Z*)-3-Benzylidene-2-(4-chlorophenyl)isoindolin-1-one (5a): ^{13}C NMR (150 MHz, $CDCl_3$)



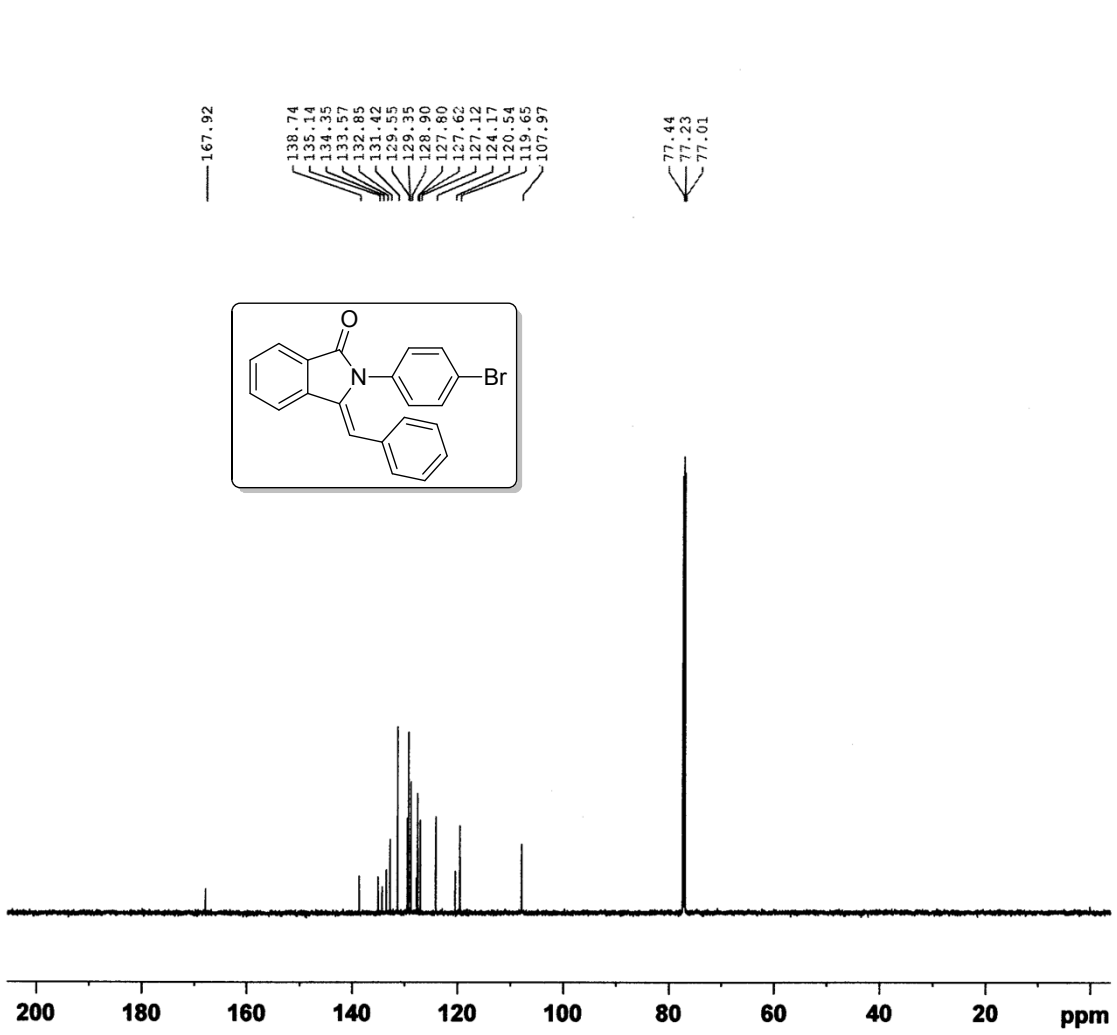

```
Current Data Parameters
NAME      AG-ISO-36-R-13C
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140901
Time              11.35
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                32768
SOLVENT           CDCl3
NS                  323
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                301.5 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          150.9128347 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

(*Z*)-3-Benzylidene-2-(4-bromophenyl)isoindolin-1-one (6a): ^{1}H NMR (600 MHz, $CDCl_3$)



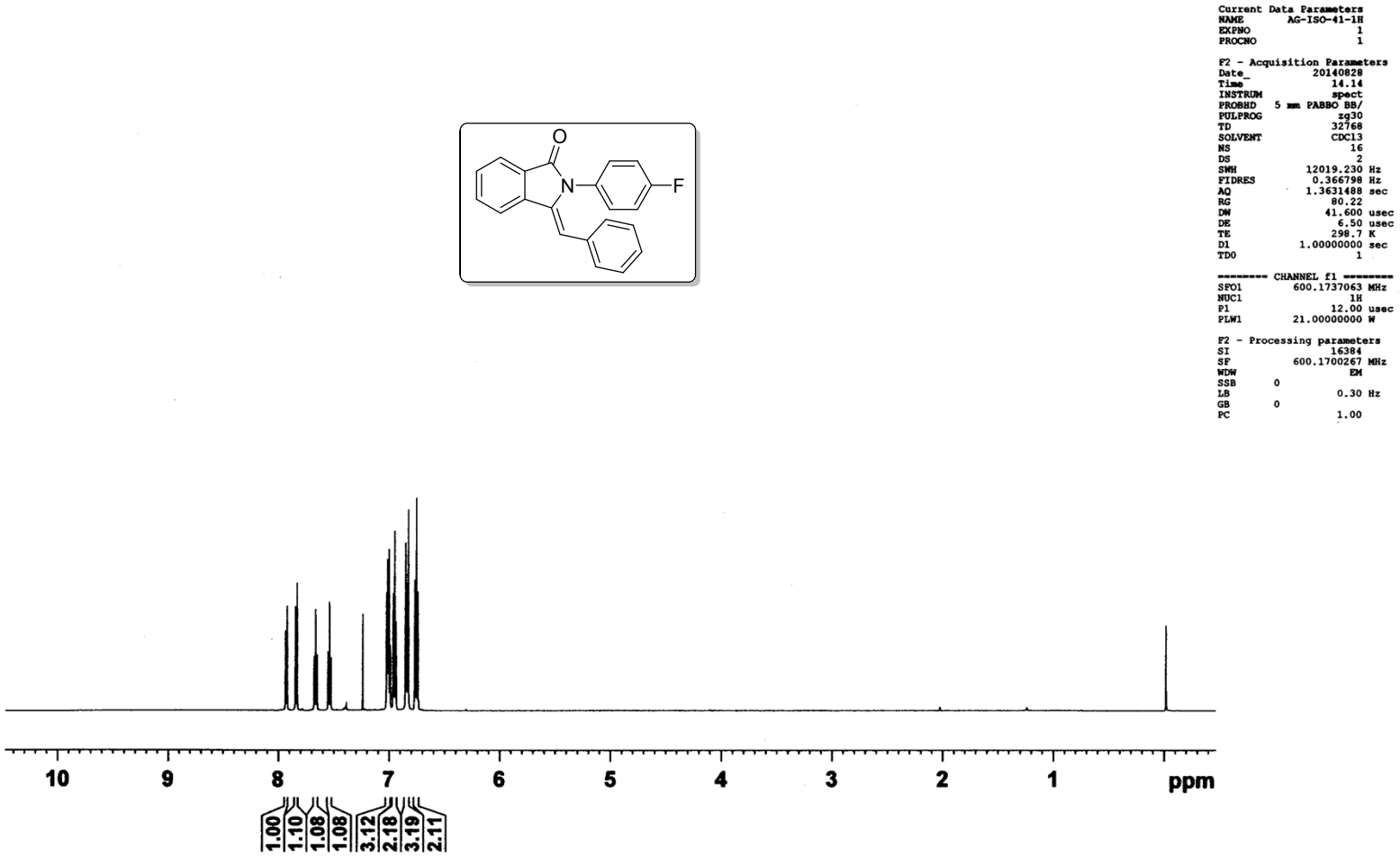

```
Current Data Parameters
NAME            AG-ISO-30-1H
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_           20140828
Time_              14.47
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                299.0 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            600.1700268 MHz
WDW                  EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
```

(*Z*)-3-Benzylidene-2-(4-bromophenyl)isoindolin-1-one (6a): ^{13}C NMR (150 MHz, $CDCl_3$)



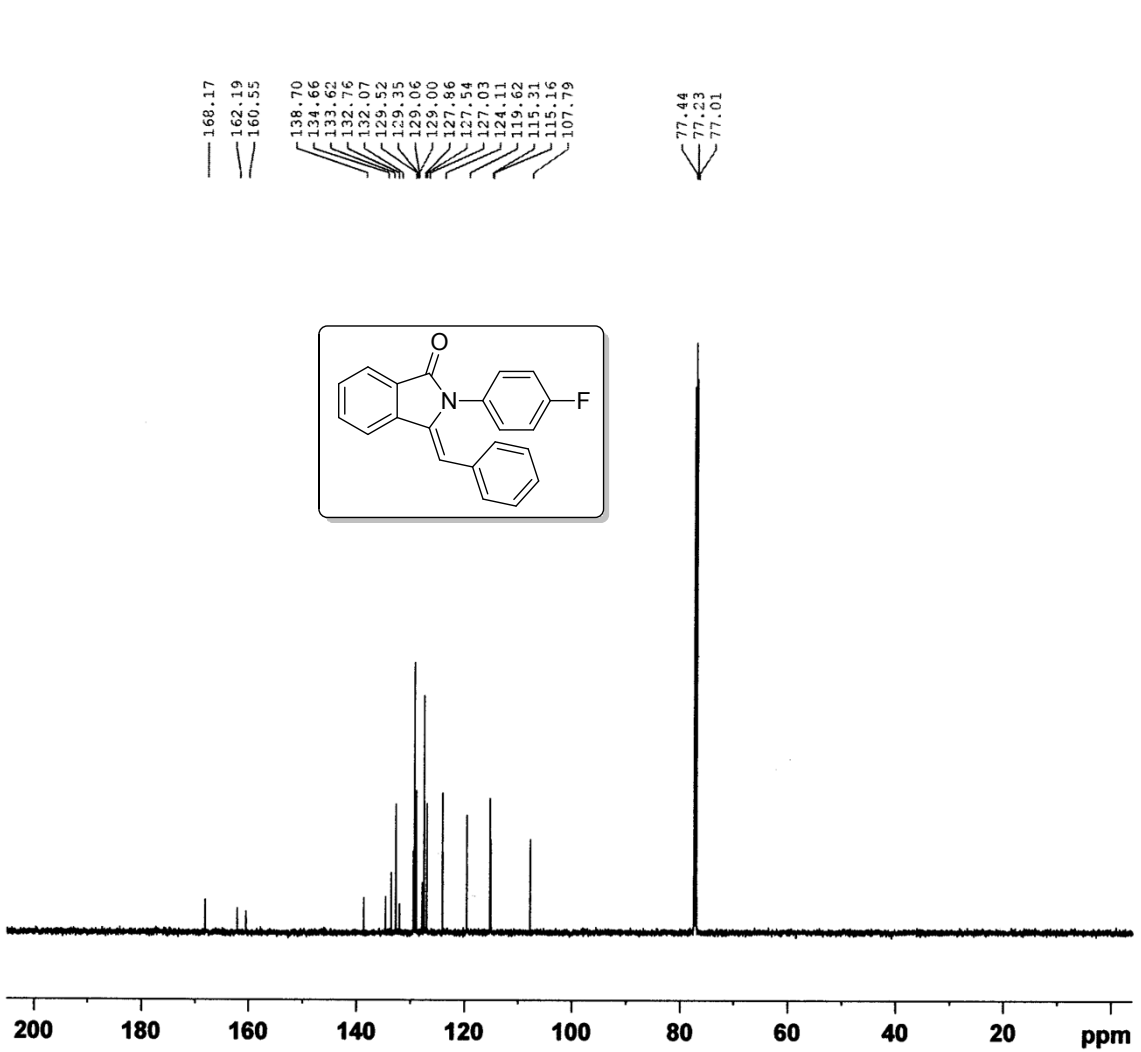

```
Current Data Parameters
NAME       AG-ISO-38-13C
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140828
Time               14.34
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  265
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                299.8 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          150.9128370 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

(*Z*)-3-Benzylidene-2-(4-fluorophenyl)isoindolin-1-one (7a): ^{1}H NMR (600 MHz, $CDCl_3$)




```
Current Data Parameters
NAME          AG-ISO-41-1H
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20140828
Time                  14.14
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                  298.7 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               600.1700267 MHz
WDW                      EM
SSB          0
LB                        0.30 Hz
GB           0
PC                       1.00
```

(*Z*)-3-Benzylidene-2-(4-fluorophenyl)isoindolin-1-one (7a): ^{13}C NMR (150 MHz, $CDCl_3$)



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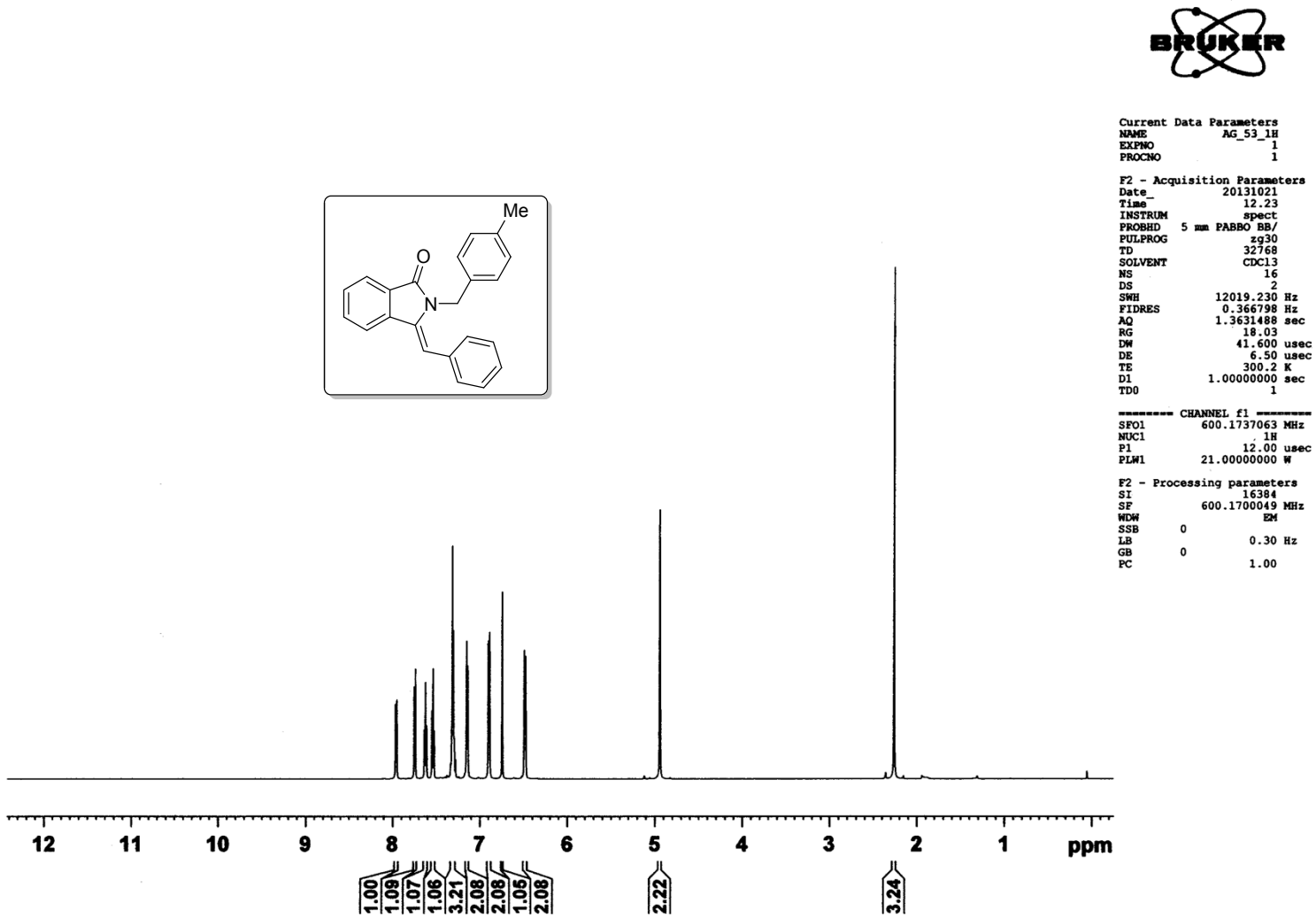
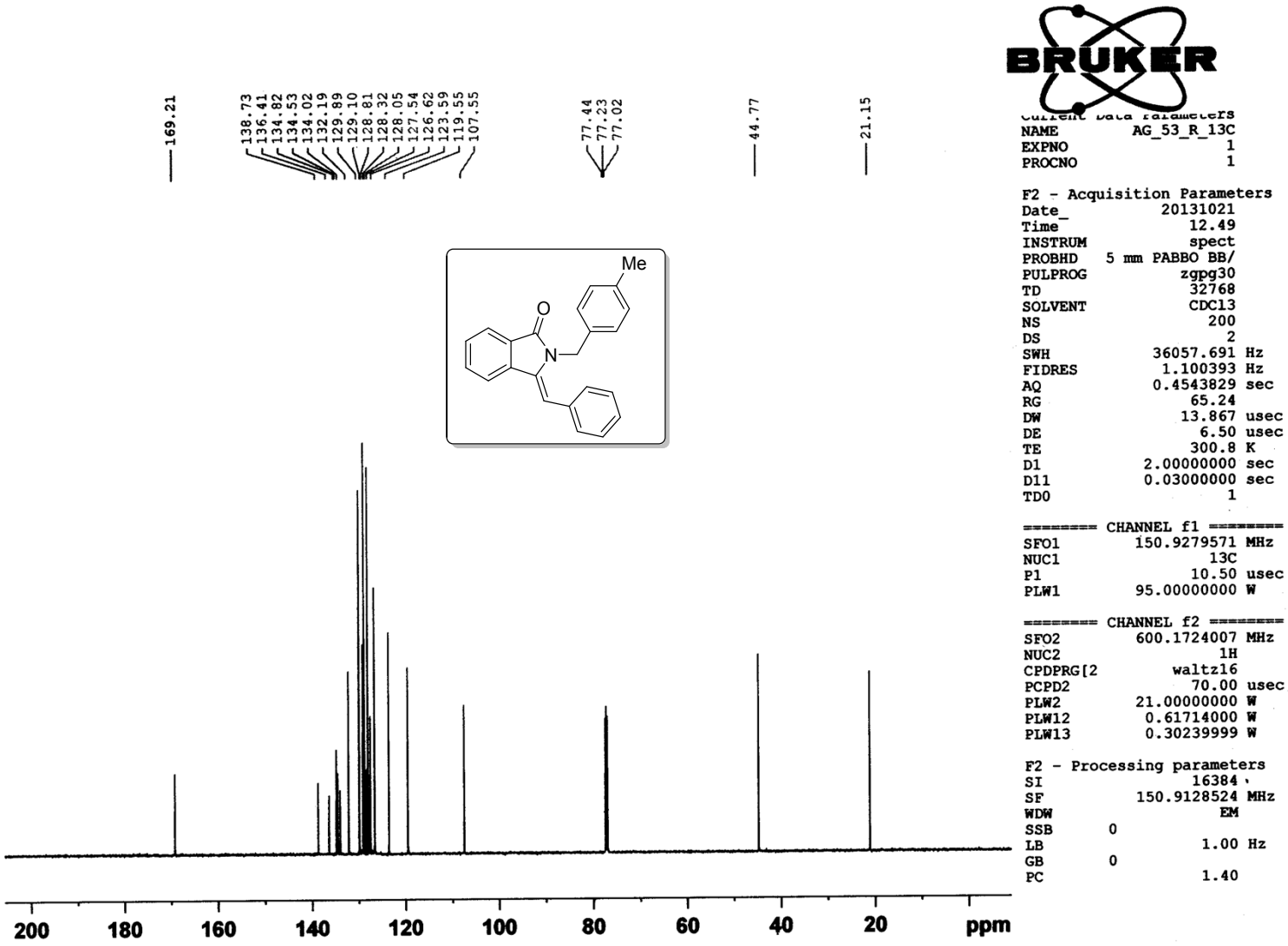
```
Current Data Parameters
NAME       AG-ISO-41-13C
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140828
Time               14.21
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                32768
SOLVENT            CDCl3
NS                   251
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           150.9128372 MHz
WDW                   EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

(*Z*)-3-Benzylidene-2-(4-methylbenzyl)isoindolin-1-one (8a): ^{1}H NMR (600 MHz, $CDCl_3$)




```
Current Data Parameters
NAME                  AG_53_1H
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20131021
Time                     12.23
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                        18.03
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                  600.1700049 MHz
WDW                         EM
SSB                  0
LB                        0.30 Hz
GB                   0
PC                        1.00
```

(*Z*)-3-Benzylidene-2-(4-methylbenzyl)isoindolin-1-one (8a): ^{13}C NMR (150 MHz, $CDCl_3$)



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Current Data Parameters

NAME	AG_53_R_13C
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20131021
Time	12.49
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zgpg30
TD	32768
SOLVENT	CDCl3
NS	200
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

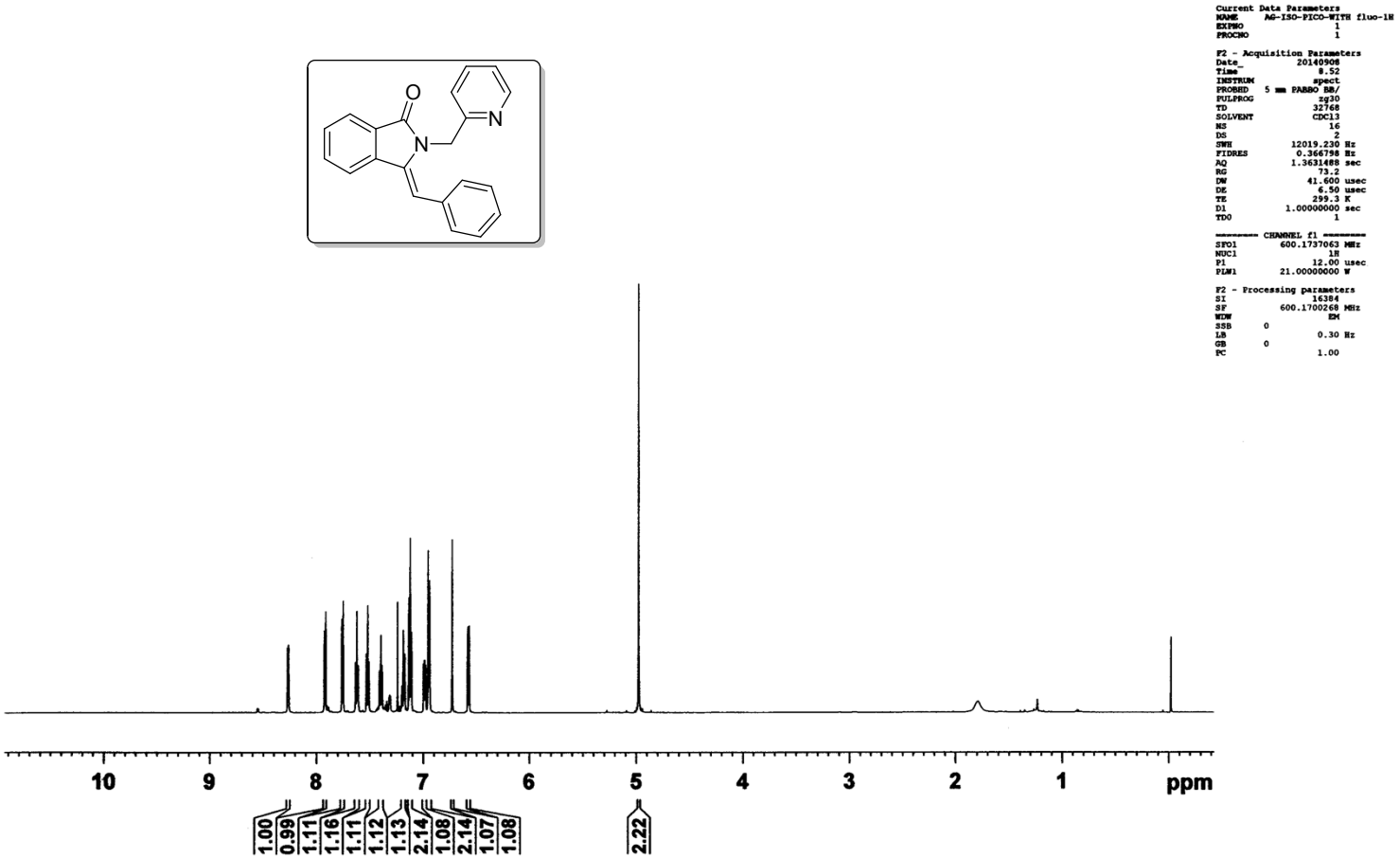
======== CHANNEL f2 ========

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

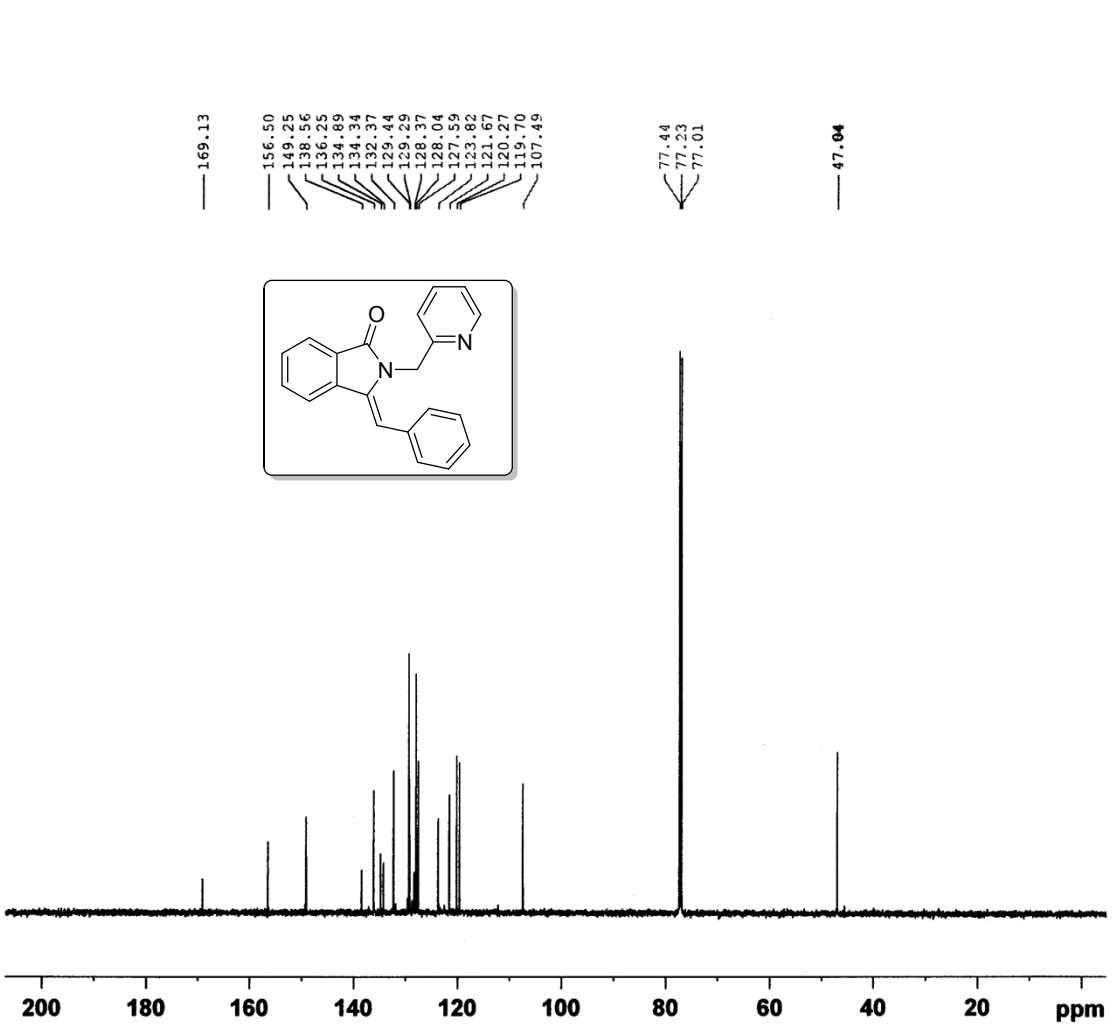
F2 - Processing parameters

SI	16384
SF	150.9128524 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

(*Z*)-3-Benzylidene-2-(pyridin-2-ylmethyl)isoindolin-1-one (9a): ^{1}H NMR (600 MHz, $CDCl_3$)

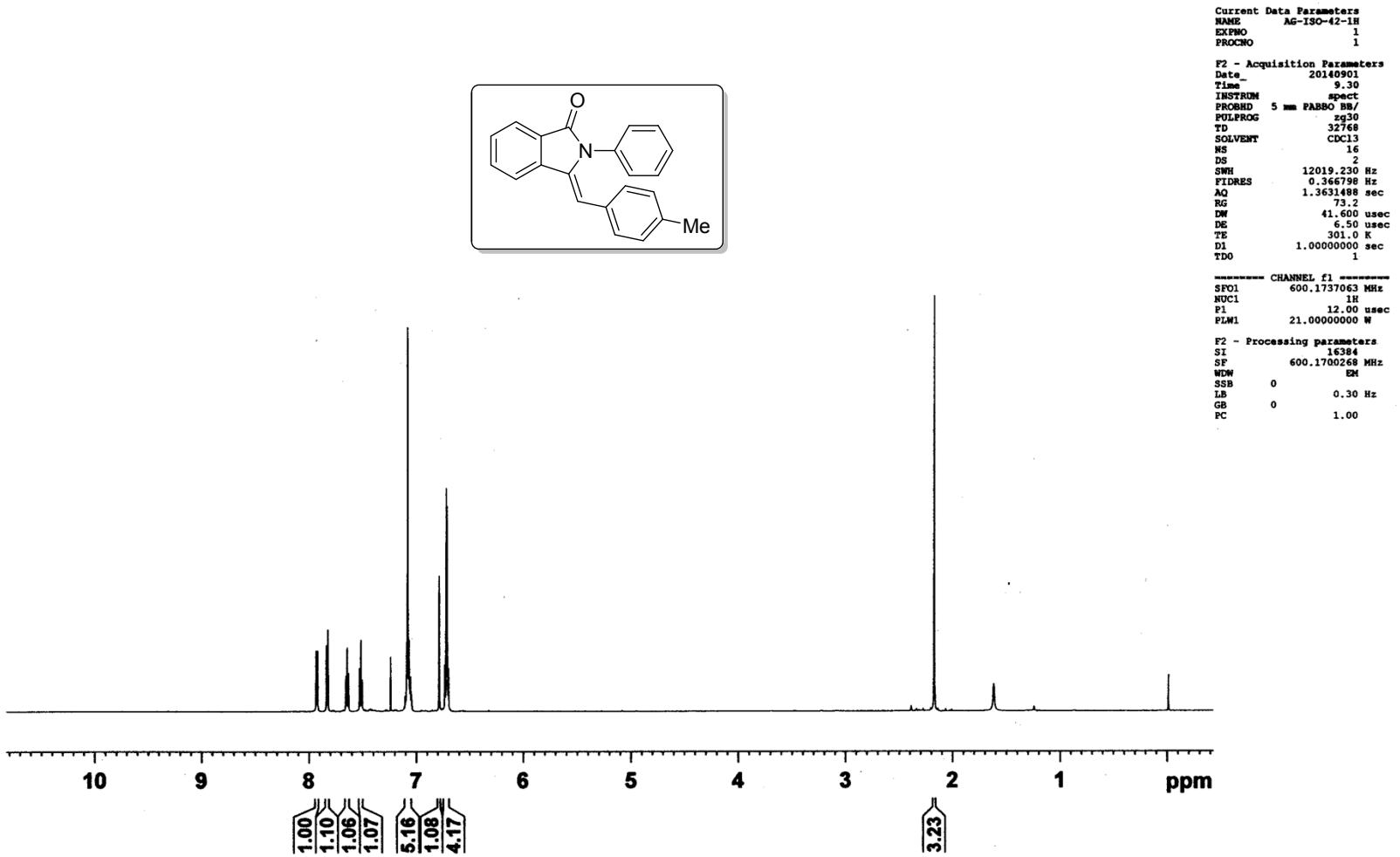


(*Z*)-3-Benzylidene-2-(pyridin-2-ylmethyl)isoindolin-1-one (9a): ^{13}C NMR (150 MHz, $CDCl_3$)



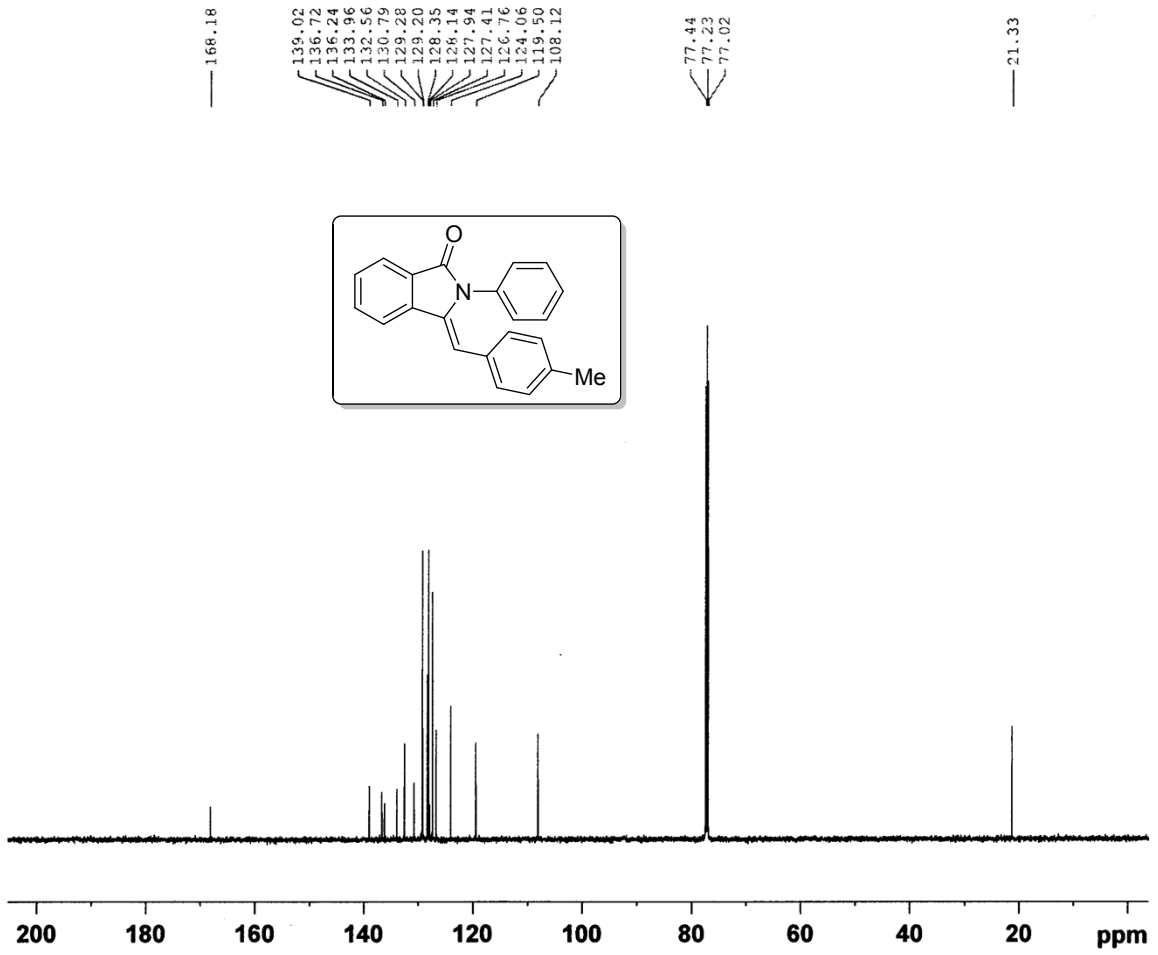

```
Current Data Parameters
NAME      AG-ISO-PICO-WITH fluo-13C
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20140908
Time                9.00
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  303
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          150.9128390 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

(*Z*)-3-(4-Methylbenzylidene)-2-phenylisoindolin-1-one (1b): ^{1}H NMR (600 MHz, $CDCl_3$)



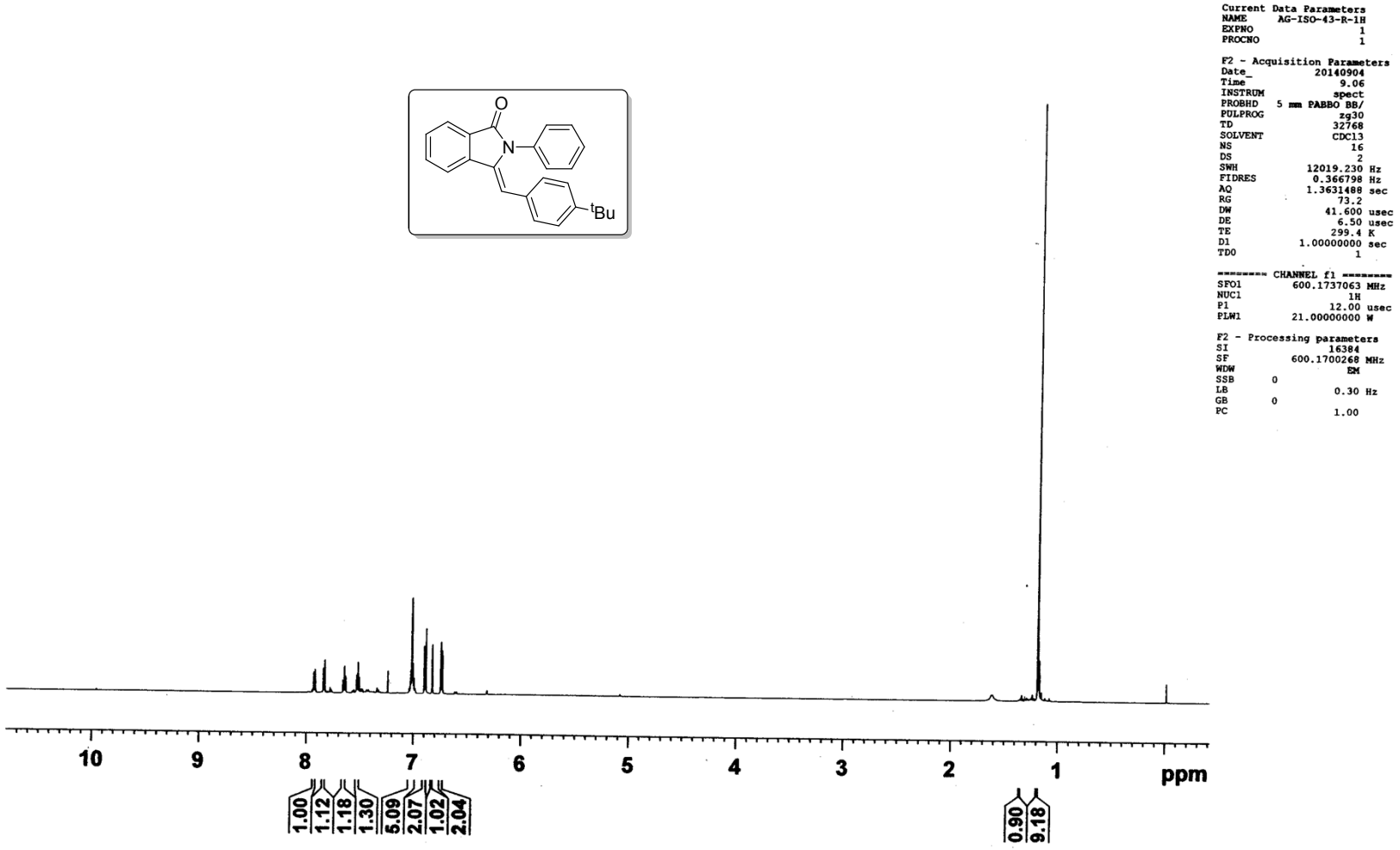

```
Current Data Parameters
NAME          AG-ISO-42-1H
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20140901
Time                 9.30
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                301.0 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            600.1700268 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

(*Z*)-3-(4-Methylbenzylidene)-2-phenylisoindolin-1-one (1b): ^{13}C NMR (150 MHz, $CDCl_3$)



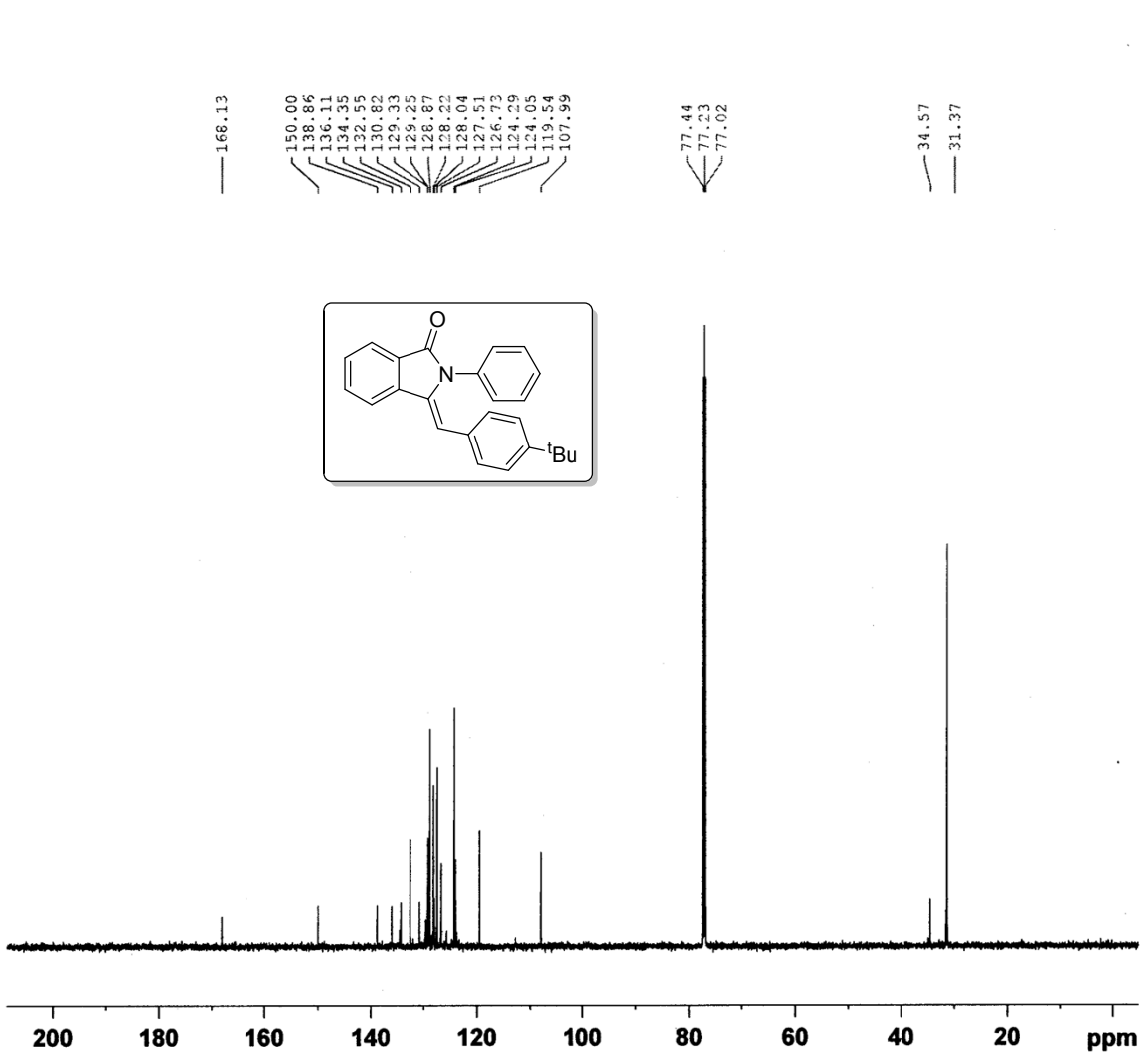

```
Current Data Parameters
NAME       AG-ISO-42-13C
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140901
Time                9.39
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  303
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               302.0 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          150.9128369 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

(*Z*)-3-(4-(*tert*-butyl)benzylidene)-2-phenylisoindolin-1-one (1c): ^{1}H NMR (600 MHz, $CDCl_3$)




```
Current Data Parameters
NAME      AG-ISO-43-R-1H
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140904
Time_               9.06
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            600.1700260 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

(*Z*)-3-(4-(*tert*-butyl)benzylidene)-2-phenylisoindolin-1-one (1c): ^{13}C NMR (150 MHz, $CDCl_3$)



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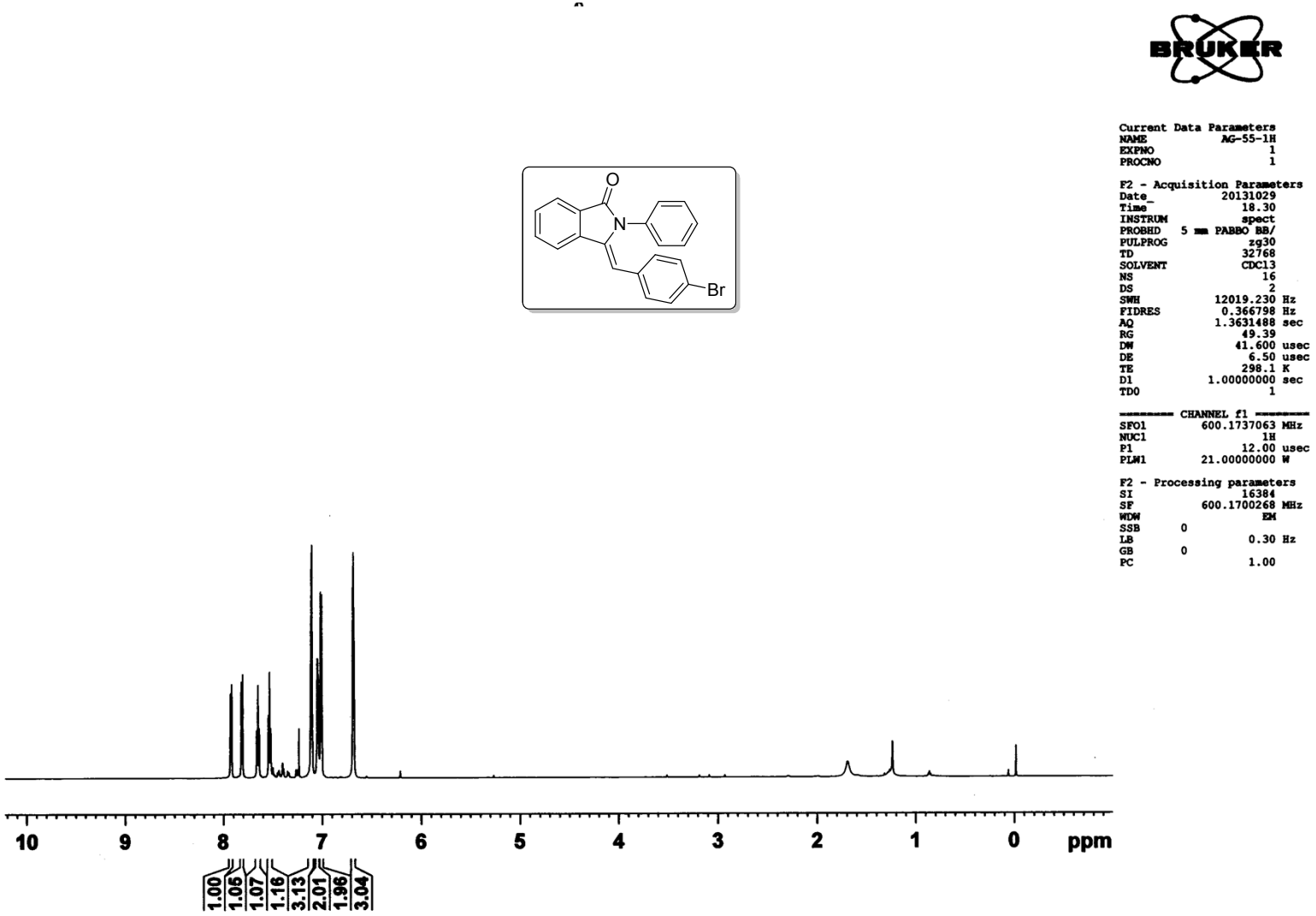
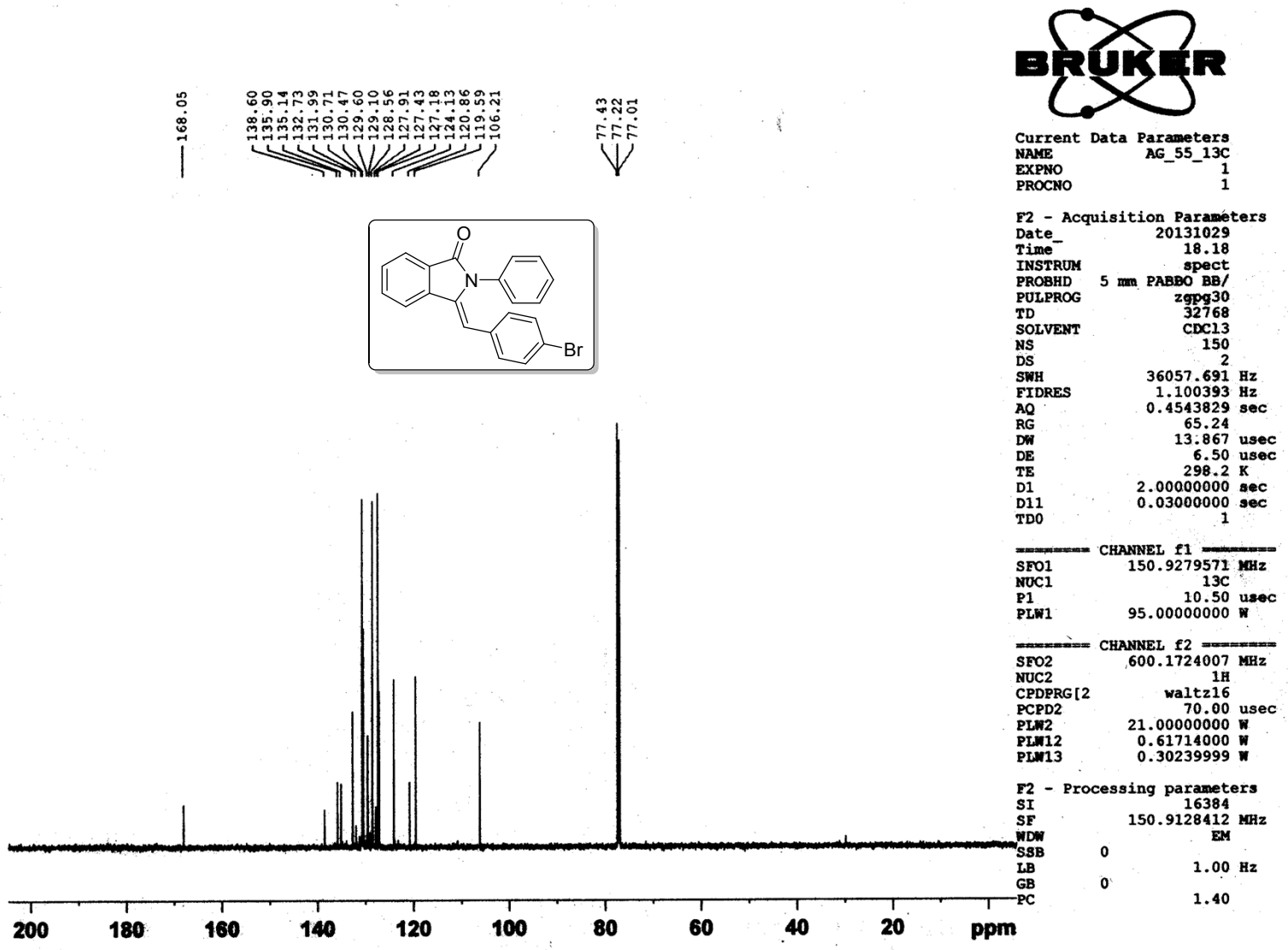
```
Current Data Parameters
NAME      AG-ISO-43-R-13C
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20140904
Time                9.17
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                32768
SOLVENT            CDCl3
NS                   452
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           150.9128348 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

(*Z*)-3-(4-bromobenzylidene)-2-phenylisoindolin-1-one (1d): ^{1}H NMR (600 MHz, $CDCl_3$)

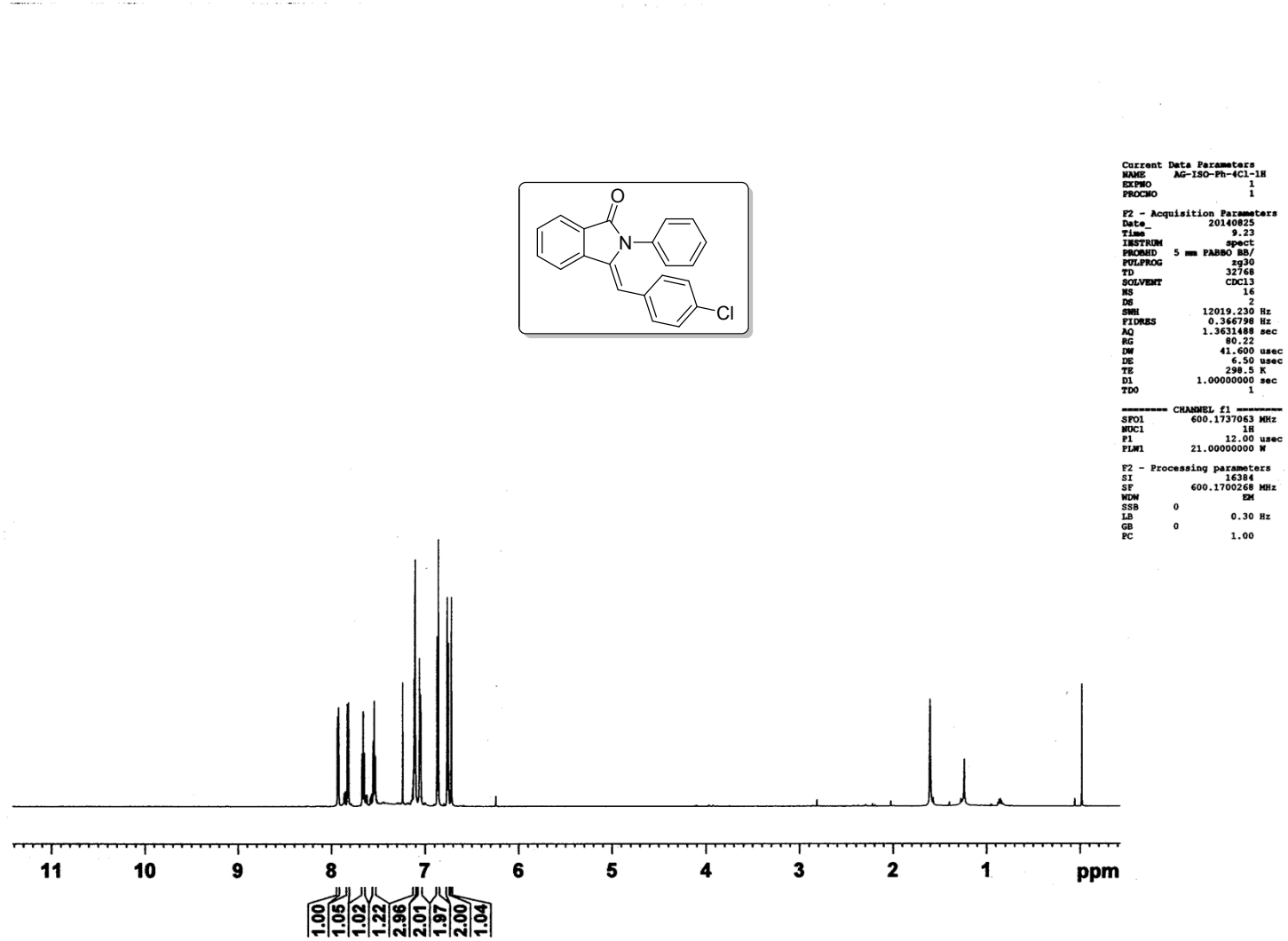


(*Z*)-3-(4-bromobenzylidene)-2-phenylisoindolin-1-one (1d): ^{13}C NMR (150 MHz, $CDCl_3$)

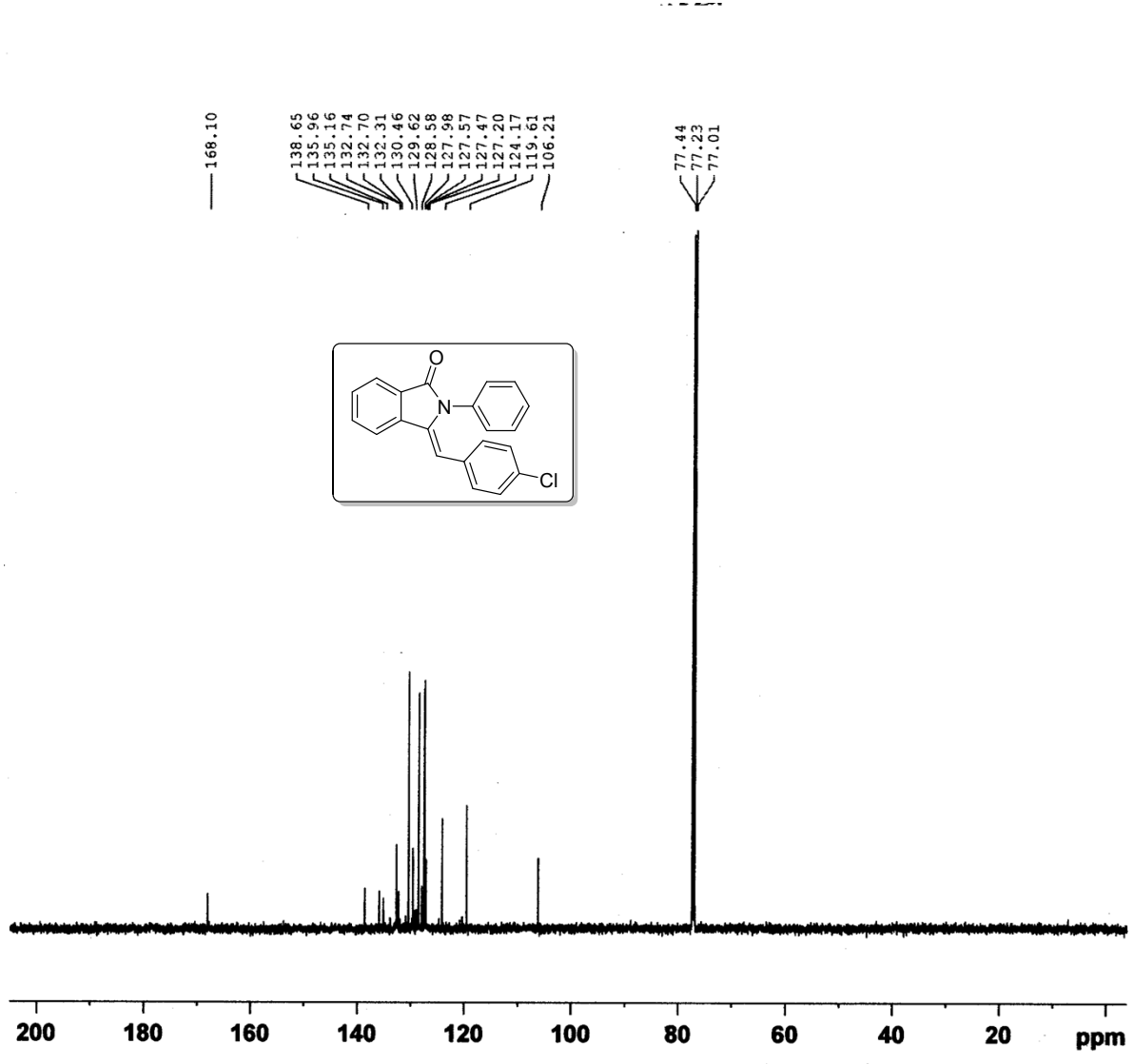



```
Current Data Parameters
NAME                  AG_55_13C
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20131029
Time                      18.18
INSTRUM                   spect
PROBHD    5 mm PABBO BB/
PULPROG                 zgpg30
TD                       32768
SOLVENT                  CDCl3
NS                         150
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                 150.9128412 MHz
WDW                           EM
SSB          0
LB                        1.00 Hz
GB           0
PC                        1.40
```

(*Z*)-3-(4-chlorobenzylidene)-2-phenylisoindolin-1-one (1e): ^{1}H NMR (600 MHz, $CDCl_3$)

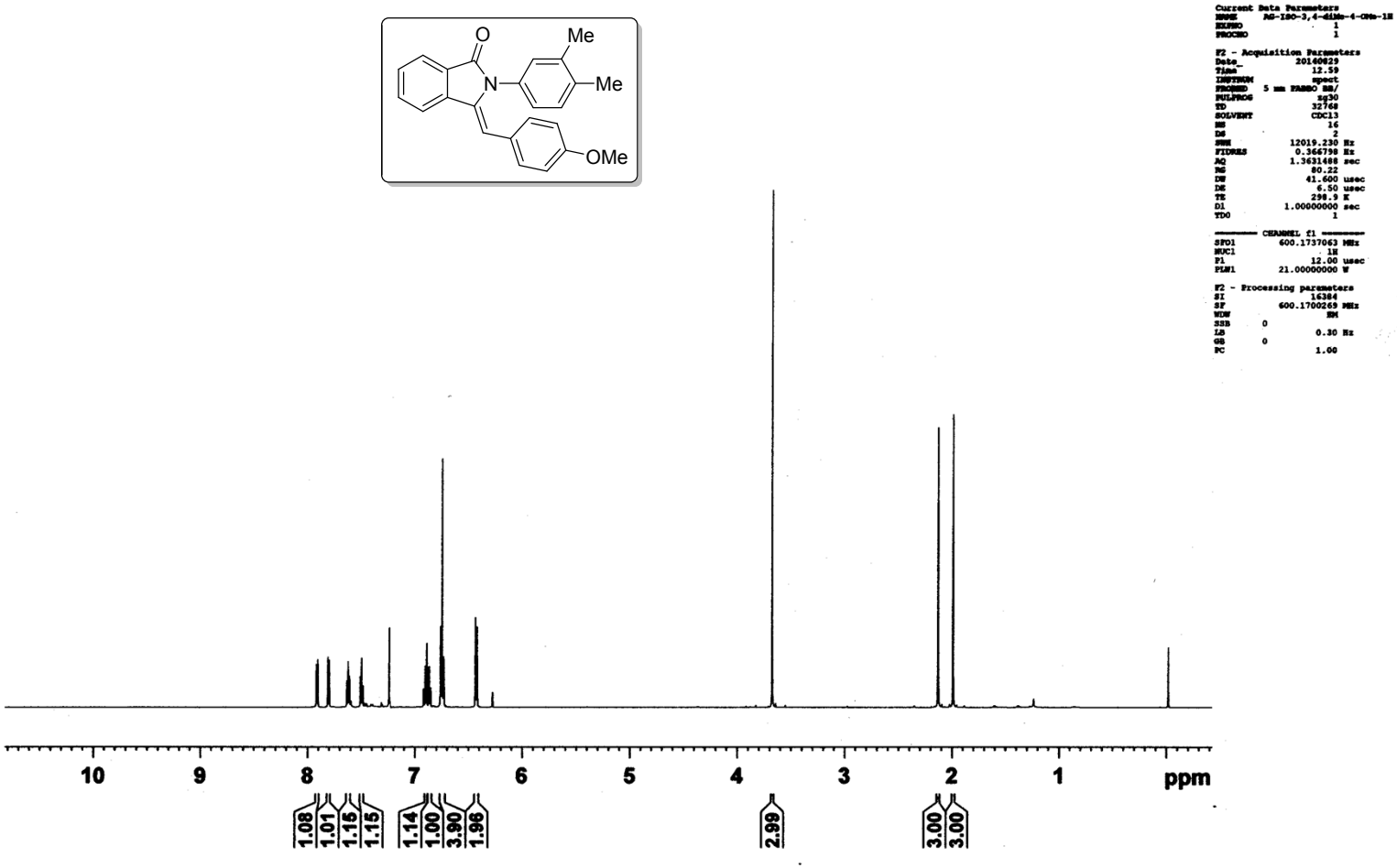


(*Z*)-3-(4-chlorobenzylidene)-2-phenylisoindolin-1-one (1e): ^{13}C NMR (150 MHz, $CDCl_3$)

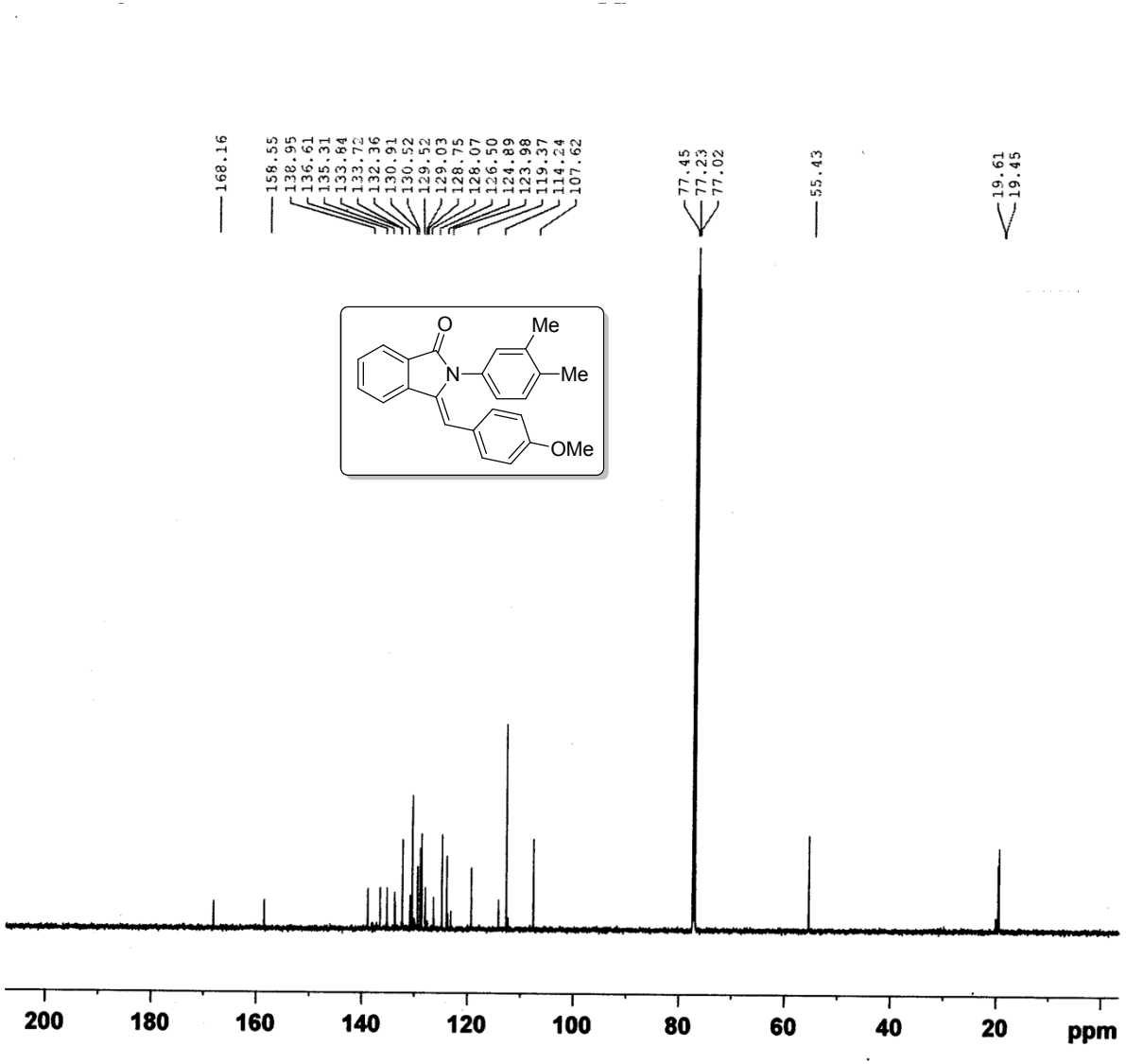



```
Current Data Parameters
NAME      AG-ISO-Ph-4Cl-13C
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20140825
Time                   9.29
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG              zgpg30
TD                    32768
SOLVENT               CDCl3
NS                      200
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                    299.6 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            150.9128371 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

(*Z*)-2-(3,4-dimethylphenyl)-3-(4-methoxybenzylidene)isoindolin-1-one (3f): ^{1}H NMR (600 MHz, $CDCl_3$)

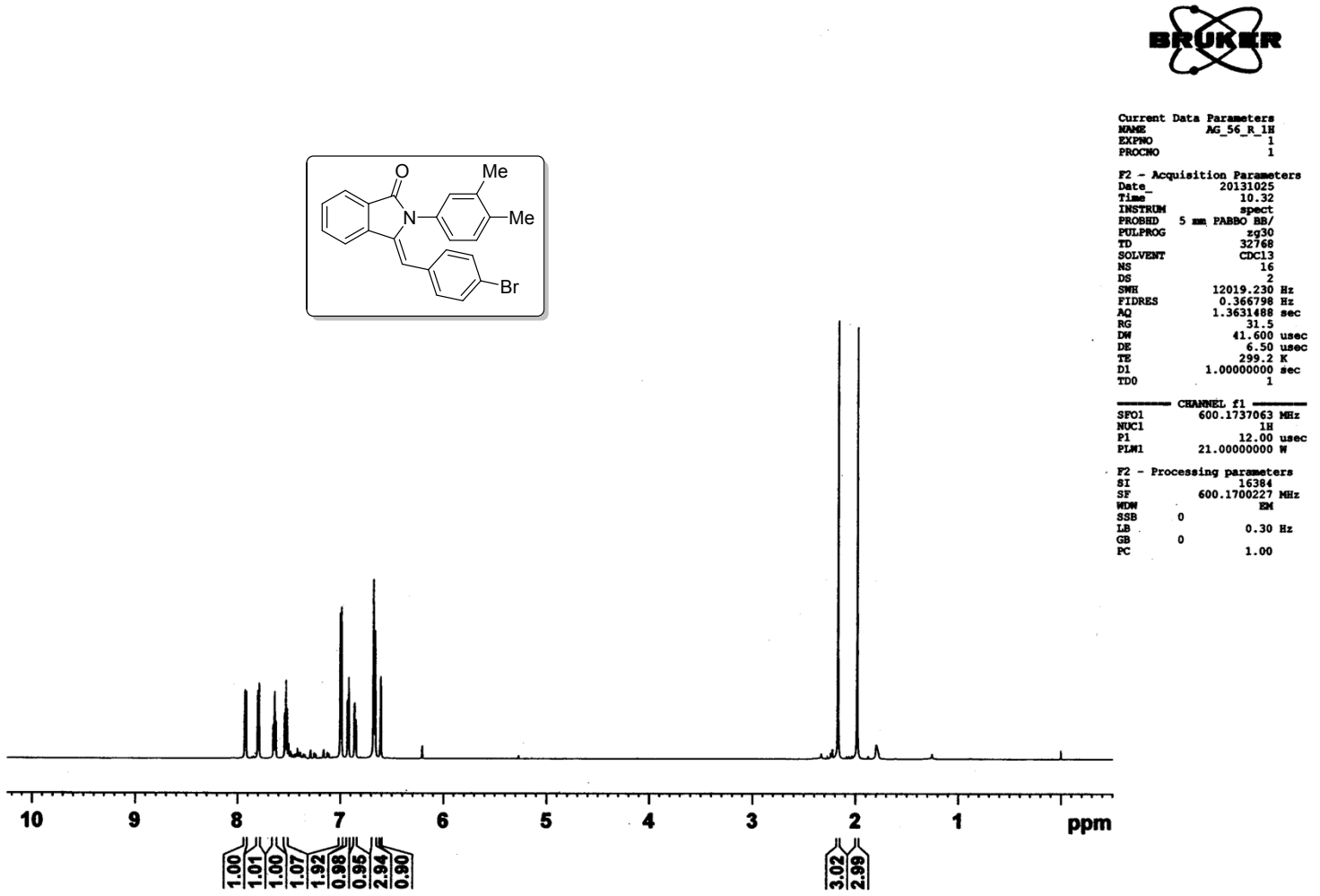


(*Z*)-2-(3,4-dimethylphenyl)-3-(4-methoxybenzylidene)isoindolin-1-one (3f): ^{13}C NMR (150 MHz, $CDCl_3$)



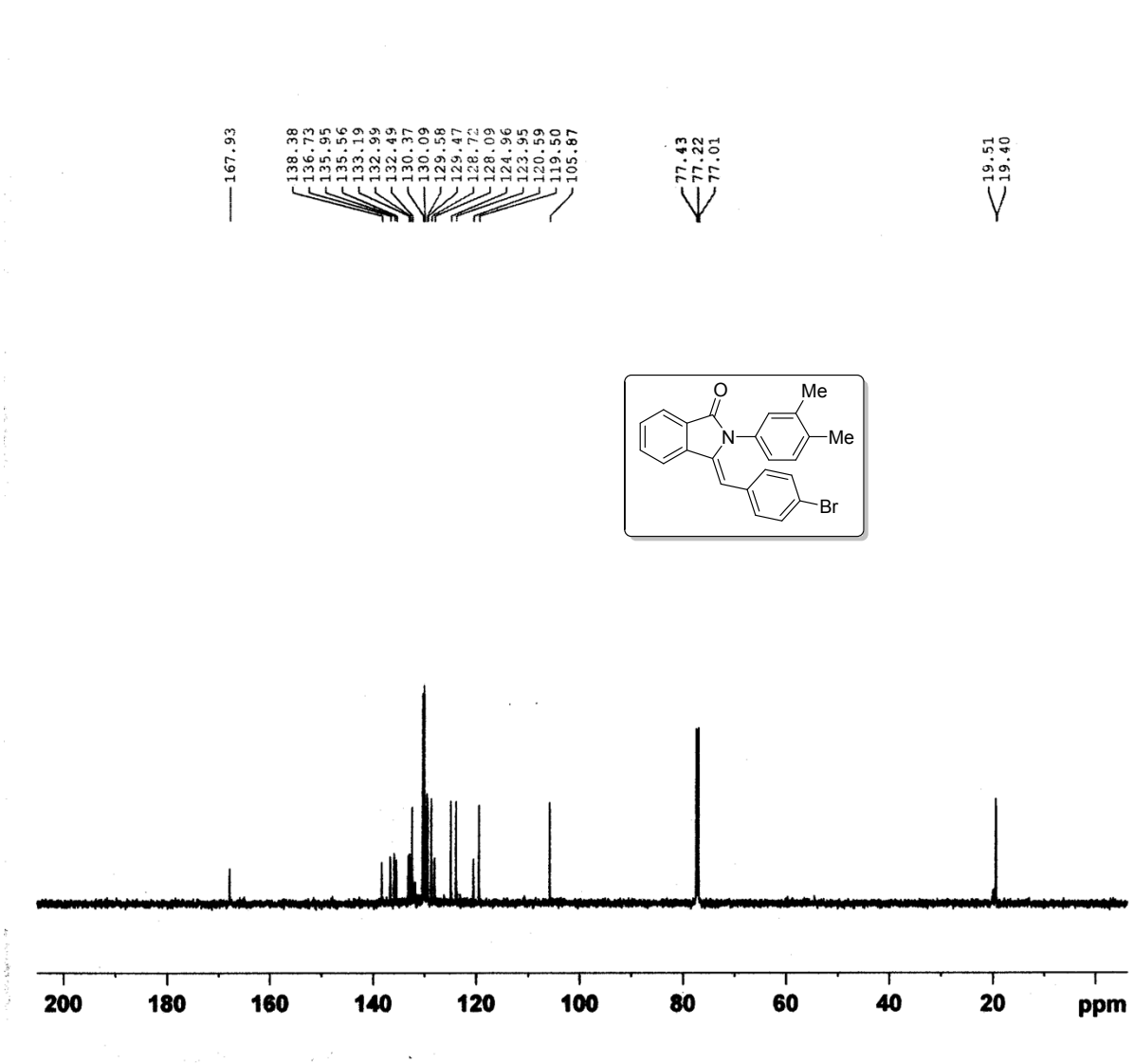

```
Current Data Parameters
NAME      AG-ISO-3,4-diMe-4-OMe-13C
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20140901
Time              11.09
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD              32768
SOLVENT           CDCl3
NS                  563
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               301.7 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          150.9128349 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

(*Z*)-3-(4-bromobenzylidene)-2-(3,4-dimethylphenyl)isoindolin-1-one (3g): ^{1}H NMR (600 MHz, $CDCl_3$)



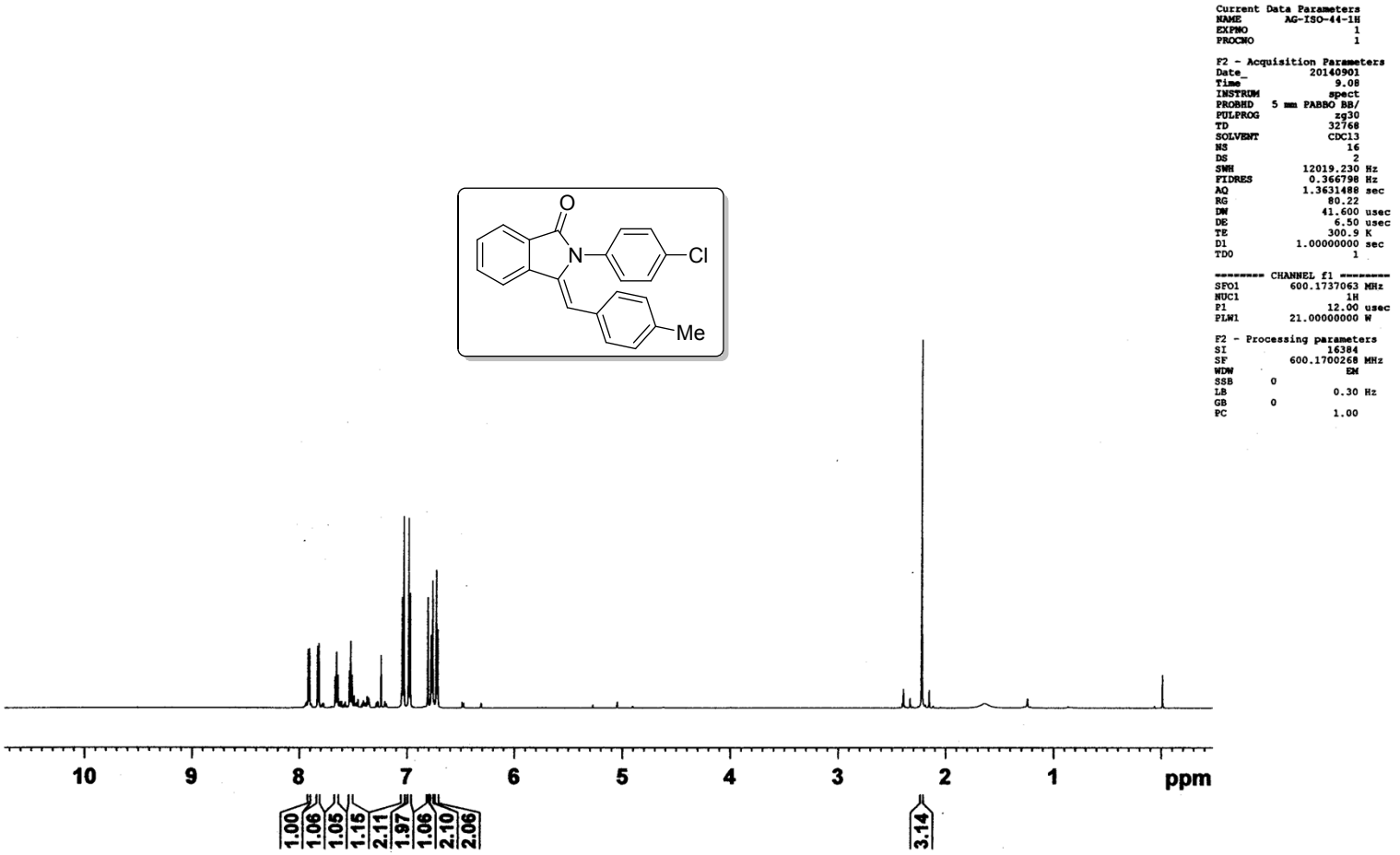

```
Current Data Parameters
NAME          AG_56_R_1H
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20131025
Time               10.32
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                 31.5
DW               41.600 usec
DE                6.50 usec
TE               299.2 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           600.1700227 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

(*Z*)-3-(4-bromobenzylidene)-2-(3,4-dimethylphenyl)isoindolin-1-one (3g): ^{13}C NMR (150 MHz, $CDCl_3$)



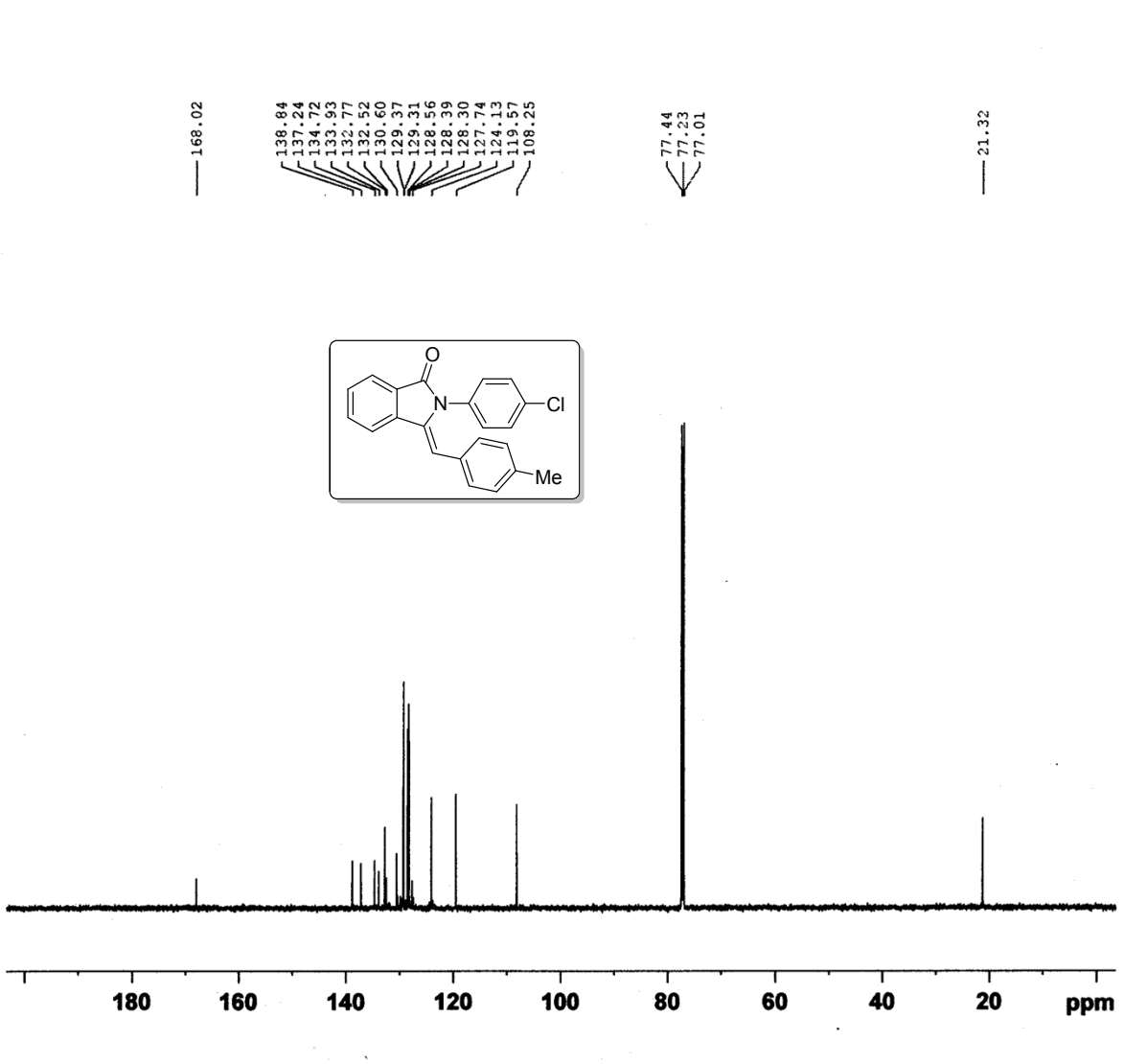

```
Current Data Parameters
NAME            AG_56_13C
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20131017
Time                17.15
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                  32768
SOLVENT             CDC13
NS                    100
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                 300.2 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            150.9128498 MHz
WDW                     EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

(*Z*)-2-(4-Chlorophenyl)-3-(4-methylbenzylidene)isoindolin-1-one (5b): ^{1}H NMR (600 MHz, $CDCl_3$)



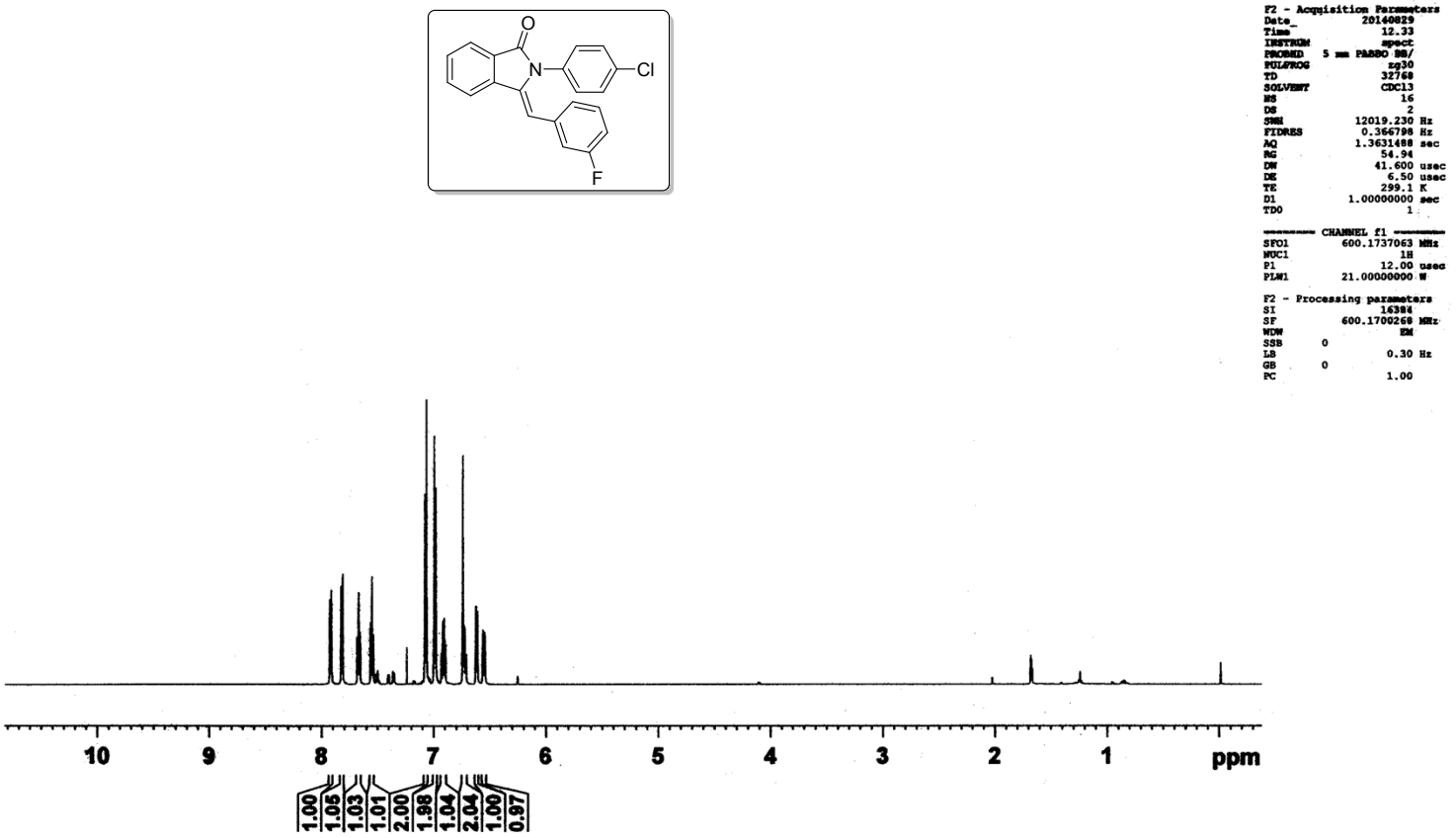

```
Current Data Parameters
NAME          AG-ISO-44-1H
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20140901
Time                  9.08
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                300.9 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           600.1700268 MHz
WDW                    EM
SSB          0
LB                 0.30 Hz
GB           0
PC                 1.00
```

(*Z*)-2-(4-Chlorophenyl)-3-(4-methylbenzylidene)isoindolin-1-one (5b): ^{13}C NMR (150 MHz, $CDCl_3$)



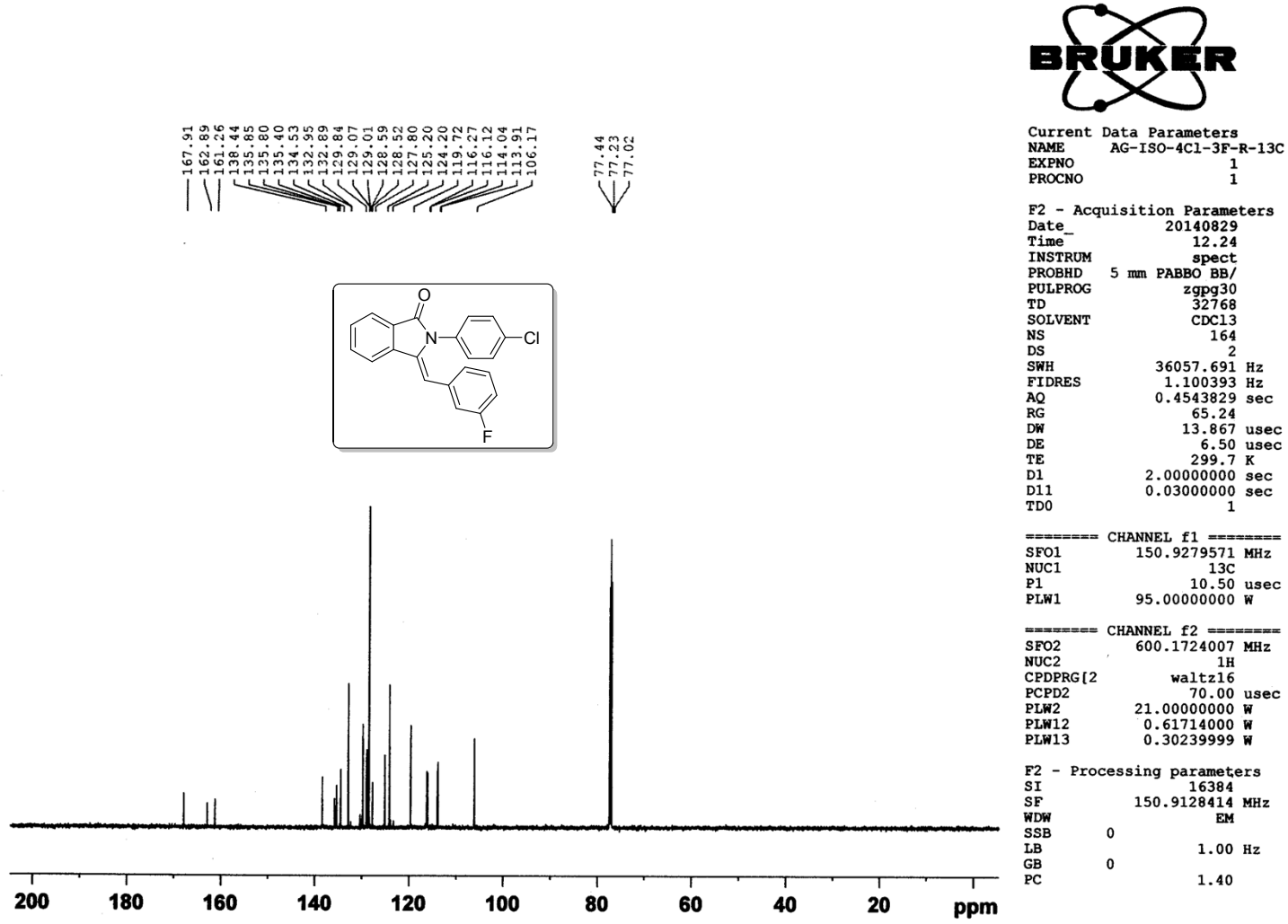

```
Current Data Parameters
NAME       AG-ISO-44-13C
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140901
Time               9.16
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                32768
SOLVENT           CDCl3
NS                  300
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          150.9128370 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

(*Z*)-2-(4-Chlorophenyl)-3-(3-fluorobenzylidene)isoindolin-1-one (5h): ^{1}H NMR (600 MHz, $CDCl_3$)



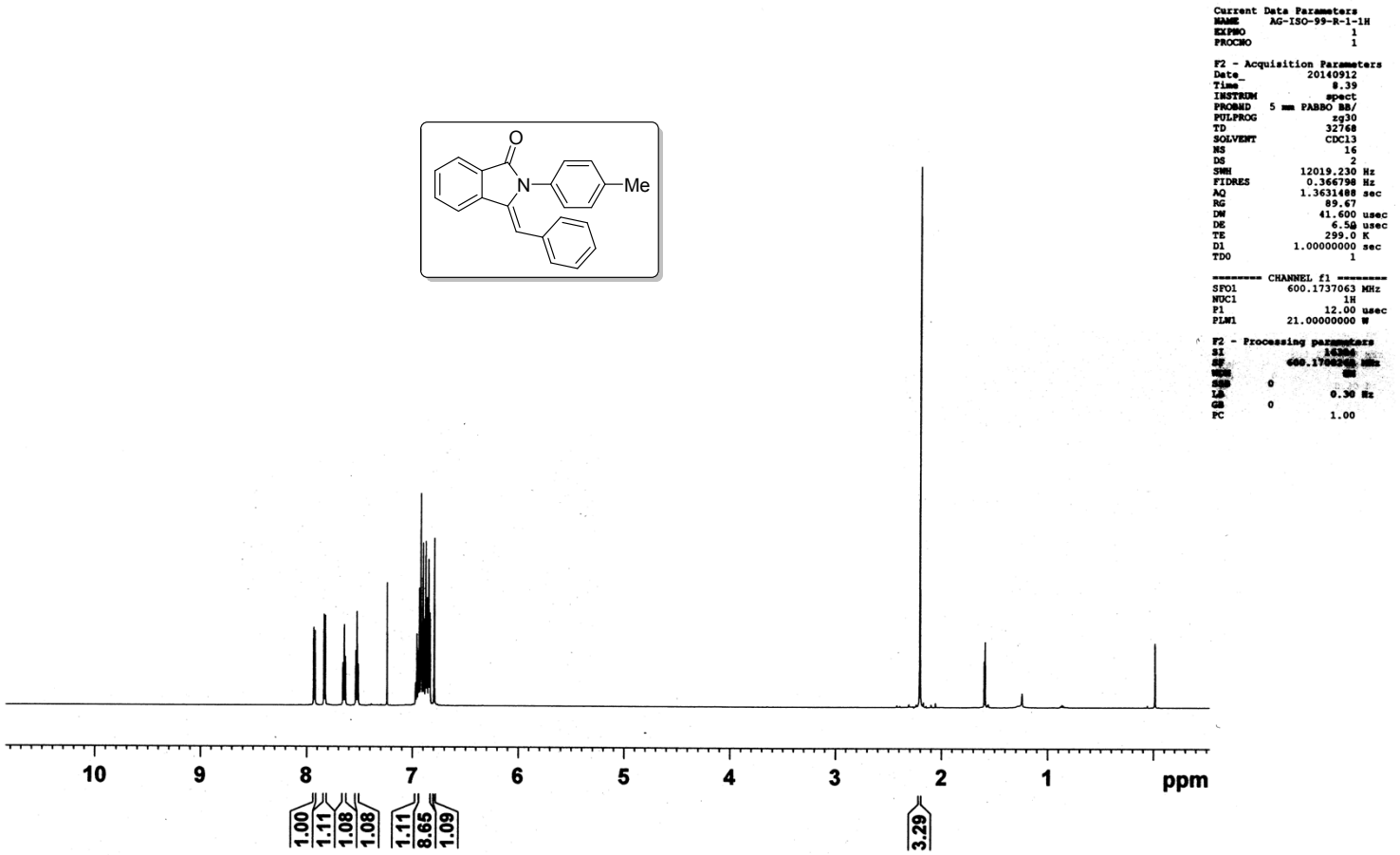

```
Current Data Parameters
NAME                  AG-ISO-4Cl-3F-R-1H
EXPNO                                  1
PROCNO                                 1

F2 - Acquisition Parameters
Date_                           20140829
Time                               12.33
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                                299.1 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                       600.1700260 MHz
WDW                                   EM
SSB                    0
LB                                 0.30 Hz
GB                     0
PC                                 1.00
```

(*Z*)-2-(4-Chlorophenyl)-3-(3-fluorobenzylidene)isoindolin-1-one (5h): ^{13}C NMR (150 MHz, $CDCl_3$)



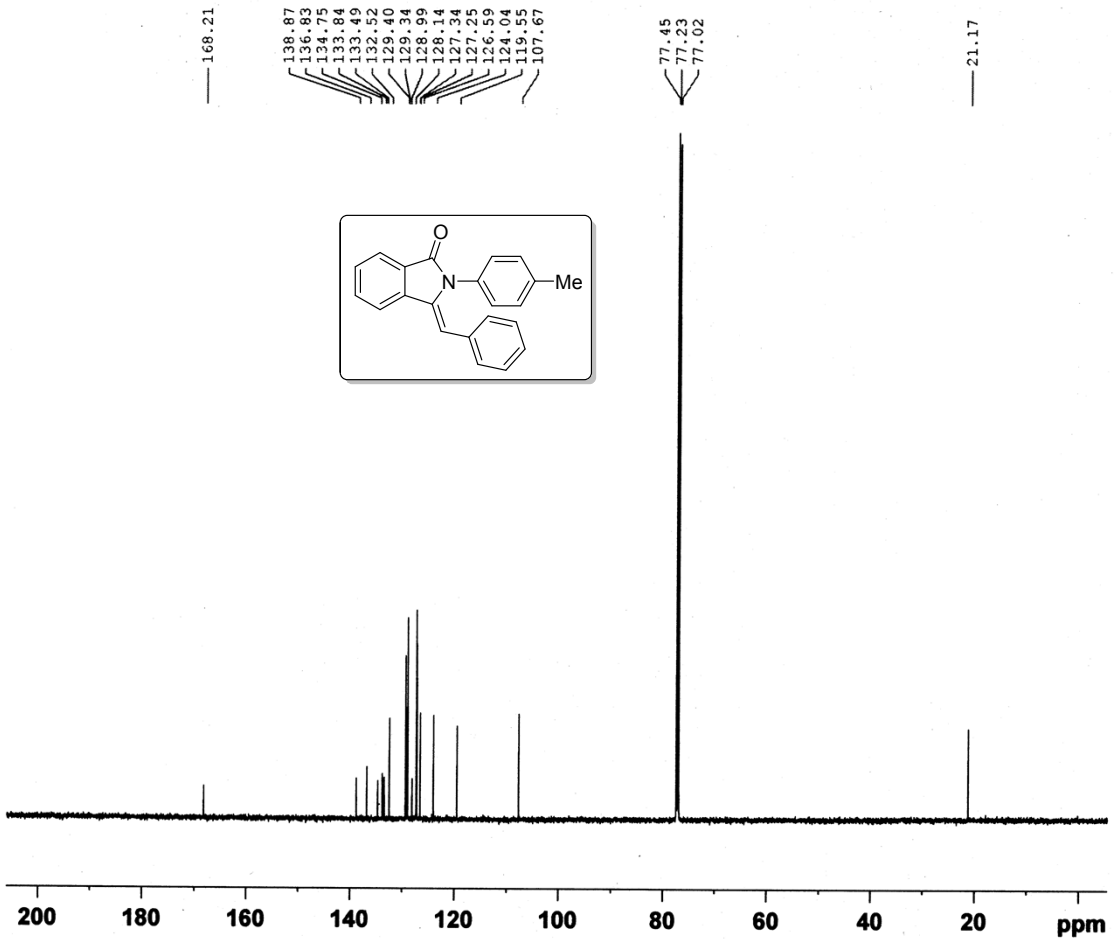

```
Current Data Parameters
NAME      AG-ISO-4Cl-3F-R-13C
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20140829
Time              12.24
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  164
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          150.9128414 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

(*Z*)-3-Benzylidene-2-(*p*-tolyl)isoindolin-1-one (2´a): ^{1}H NMR (600 MHz, $CDCl_3$)



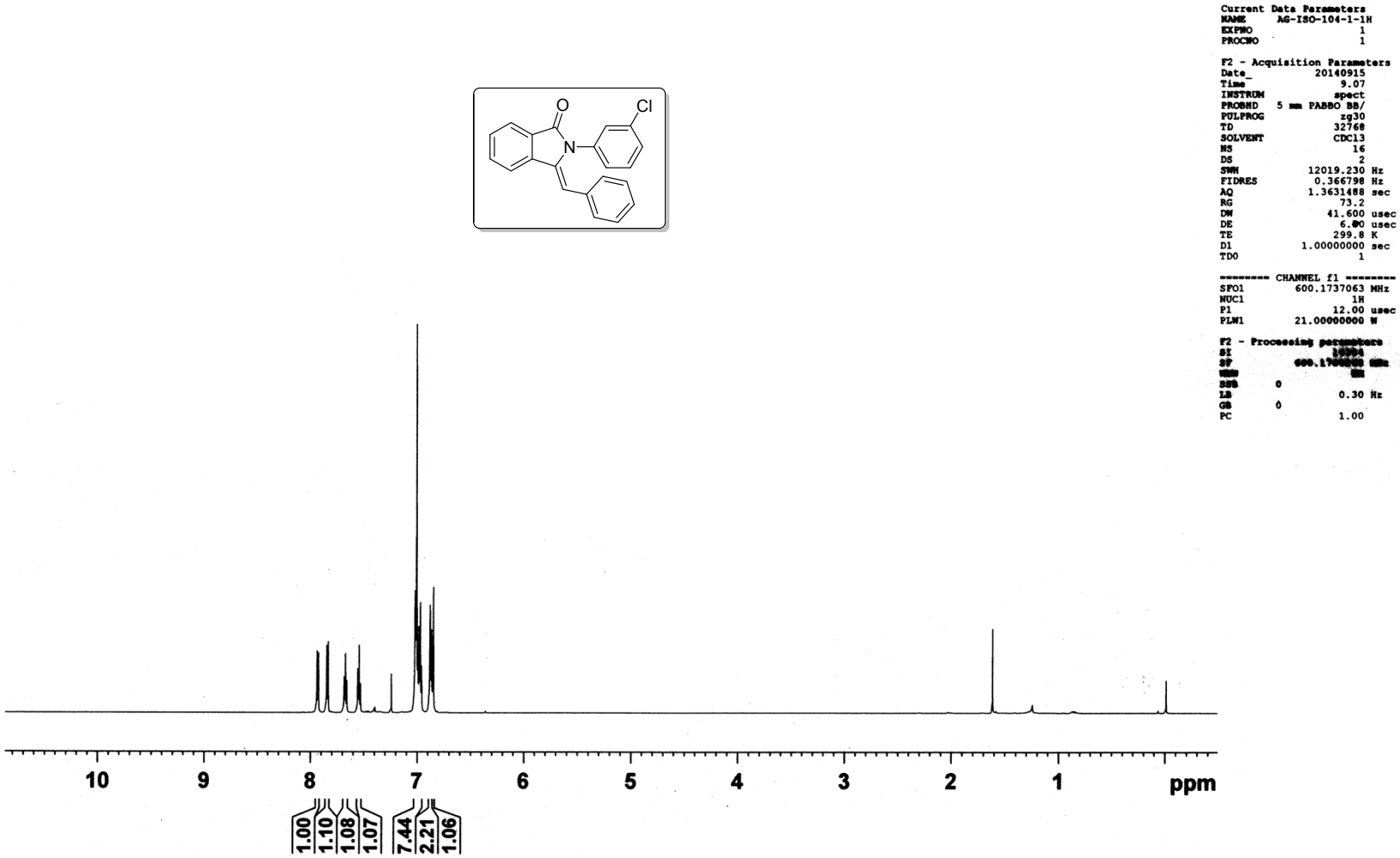

```
Current Data Parameters
NAME      AG-ISO-99-R-1-1H
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20140912
Time                   8.39
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                   299.0 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          600.1700000 MHz
WDW                     EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

(*Z*)-3-Benzylidene-2-(*p*-tolyl)isoindolin-1-one (2´a): ^{13}C NMR (150 MHz, $CDCl_3$)



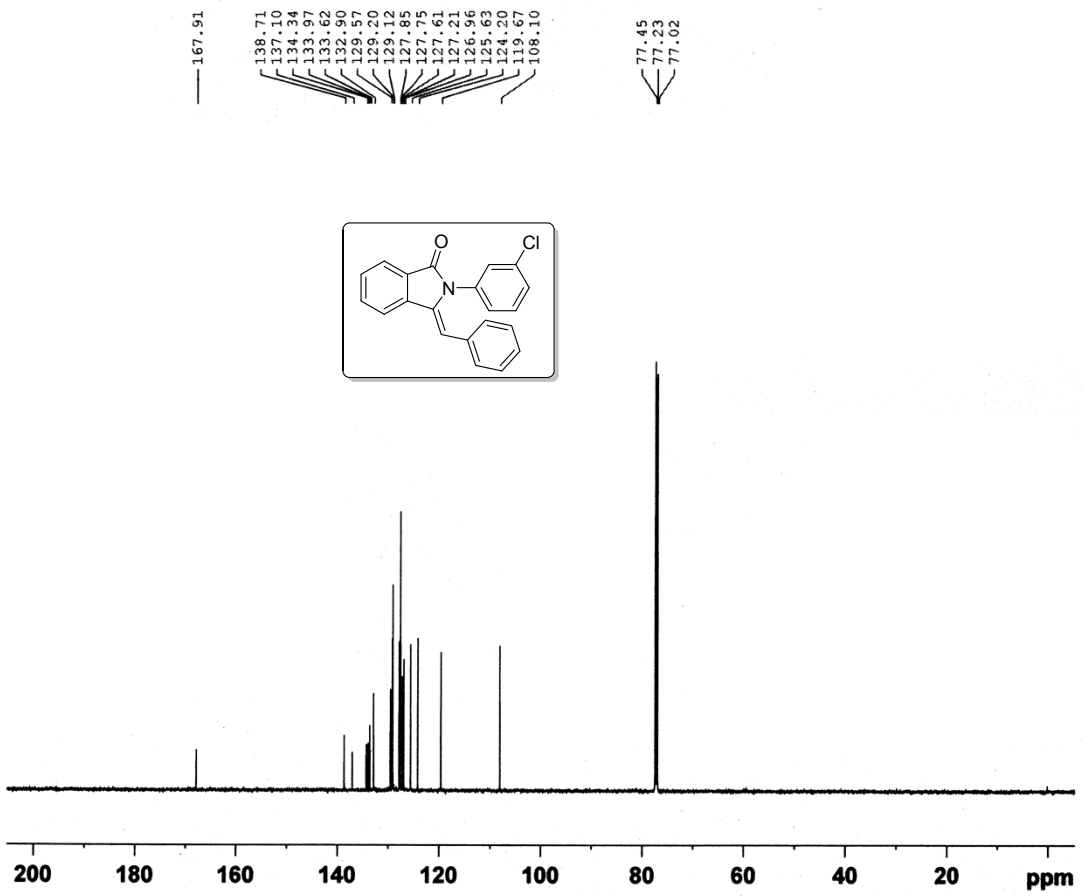

```
Current Data Parameters
NAME      AG-ISO-99-R-1-13C
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20140912
Time                  8.50
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   32768
SOLVENT              CDCl3
NS                     416
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            150.9128349 MHz
WDW                     EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

(*Z*)-3-Benzylidene-2-(3-chlorophenyl)isoindolin-1-one (3´a): ^{1}H NMR (600 MHz, $CDCl_3$)




```
Current Data Parameters
NAME       AG-ISO-104-1-1H
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20140915
Time               9.07
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               6.00 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               [illegible]
SF          [illegible] MHz
WDW                 [illegible]
SSB          0
LB                0.30 Hz
GB           0
PC                1.00
```

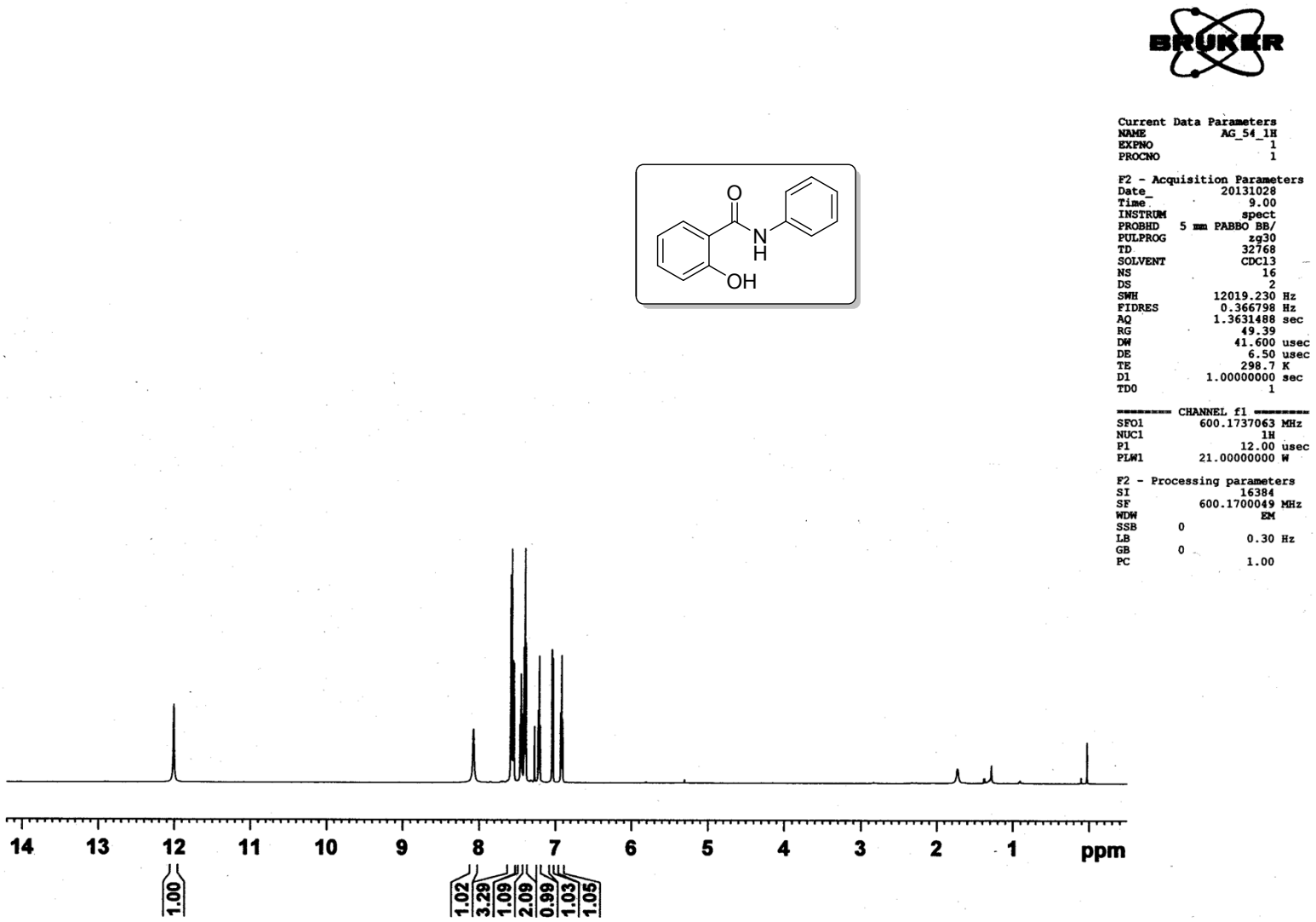
(*Z*)-3-Benzylidene-2-(3-chlorophenyl)isoindolin-1-one (3´a): ^{13}C NMR (150 MHz, $CDCl_3$)



BRUKER

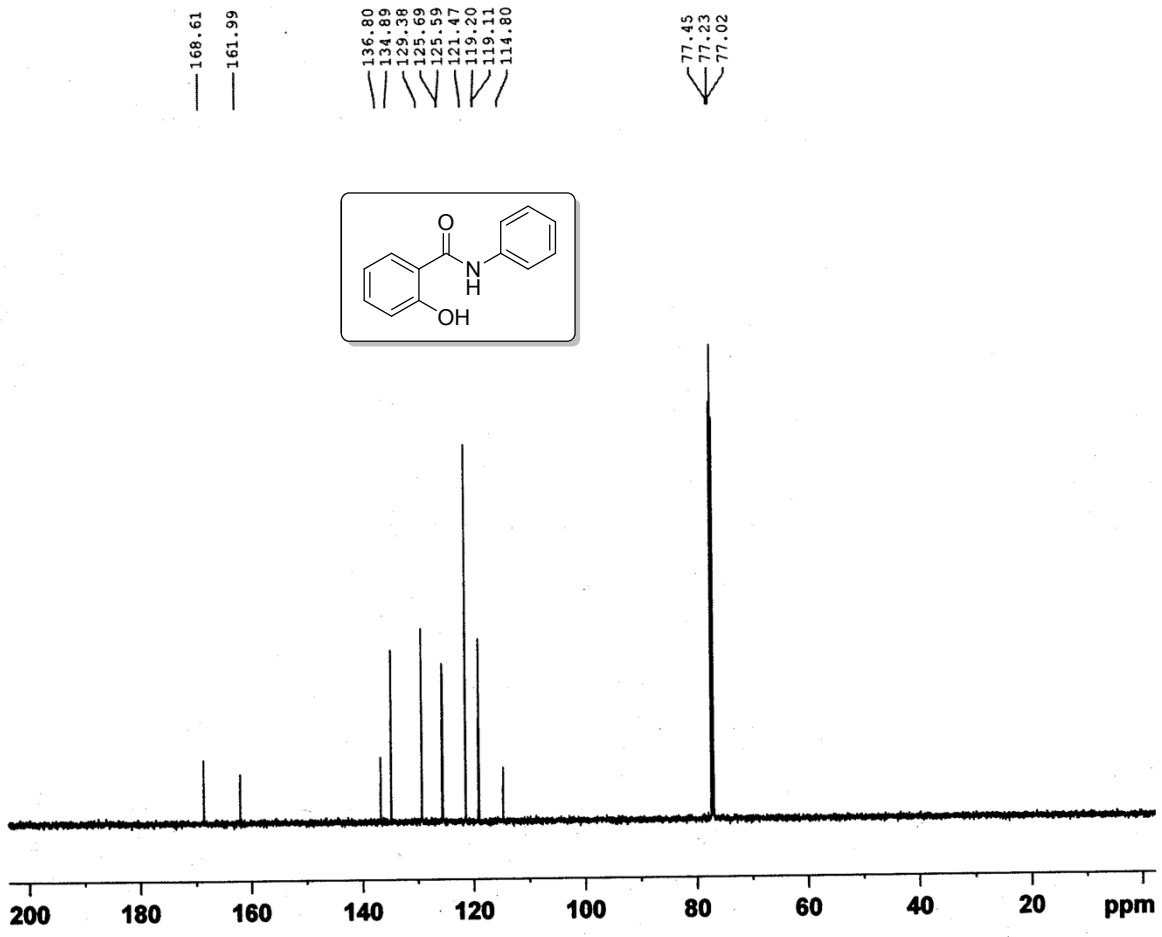
```
Current Data Parameters
NAME      AG-ISO-104-1-13C
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20140915
Time                   9.12
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   32768
SOLVENT              CDCl3
NS                     416
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            150.9128370 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

2-Hydroxy-*N*-phenylbenzamide (1a′): ^{1}H NMR (600 MHz, $CDCl_3$)




```
Current Data Parameters
NAME                  AG_54_1H
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_               20131028
Time                    9.00
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                    298.7 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               600.1700049 MHz
WDW                       EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

2-Hydroxy-*N*-phenylbenzamide (1a′): ^{13}C NMR (150 MHz, $CDCl_3$)




```
Current Data Parameters
NAME                  AG-54-13C
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20131029
Time                      18.38
INSTRUM                   spect
PROBHD     5 mm PABBO BB/
PULPROG                 zgpg30
TD                       32768
SOLVENT                  CDCl3
NS                         102
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              150.9128392 MHz
WDW                          EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
```