Electronic Supplementary Material (ESI) for Green Chemistry.

Supporting Information for:

Visible-light-induced photocatalytic formyloxylation reactions of 3-bromooxindoles with water and DMF: scope and mechanism

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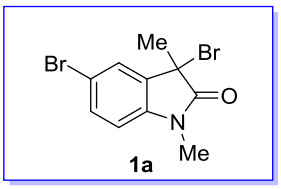
1. General Information

Unless otherwise noted, materials were purchased from commercial suppliers and used without further purification. All the solvents were treated according to general methods. Organic solutions were concentrated under reduced pressure on a Büchi rotary evaporator. Flash column chromatography (FC) was performed using 200-300 mesh silica gel. ^{1}H NMR spectra were recorded on Varian Mercury 600 (600 MHz) spectrophotometers. Chemical shifts (δ) are reported in ppm from the solvent resonance as the internal standard ($CDCl_3$: 7.26 ppm). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet), coupling constants (Hz) and integration. ^{13}C NMR spectra were recorded on Varian Mercury 400 (100 MHz) spectrophotometers ($CDCl_3$: 77.0 ppm) with complete proton decoupling. IR spectra were recorded on a BRUKER TENSOR 27 FT-IR spectrometer and are reported in terms of frequency of absorption (cm^{-1}). GC-MS was performed on a Thermo DSQ II 2000. High Resolution Mass spectra were obtained from the Shanghai Mass Spectrometry Center (Shanghai Institute of Organic Chemistry). Melt points were measured on Büchi Melting Point B-545. Fluorescence spectra were collected on Cary Eclipse Fluorescence spectrophotometer. For the ReactIR kinetic experiments, the reaction spectra were recorded using an IC 15 from Mettler-Toledo AutoChem.

2. General Procedure and Spectral Data

2.1 Spectral Data of Substrates 1a-1v



1a

3,5-Dibromo-1,3-dimethylindolin-2-one (yellow solid)

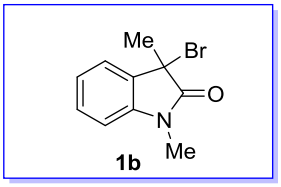
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.56 (d, *J* = 1.8 Hz, 1H), 7.46 (m, 1H), 6.73 (d, *J* = 8.3 Hz, 1H), 3.23 (s, 3H), 2.02 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 174.09, 140.70, 133.38, 132.82, 127.32, 115.80, 110.22, 51.22, 26.79, 26.17.

MS: m/z = 319.05 (M^+).

M.P.: 100.2-101.1 ^{o}C.

IR (in KBr): ῡ = 1718.75, 1606.92, 1486.33, 1232.55, 1107.57, 1046.68, 813.71, 646.04 cm^{-1}.



1b

3-Bromo-1,3-dimethylindolin-2-one (white solid)

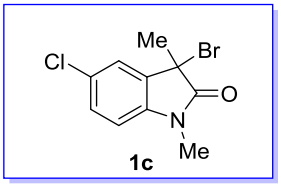
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.45 (d, *J* = 7.2 Hz, 1H), 7.34 (t, *J* = 7.3 Hz, 1H), 7.13 (t, *J* = 7.3 Hz, 1H), 6.85 (d, *J* = 7.7 Hz, 1H), 3.25 (s, 3H), 2.04 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 174.53, 141.58, 131.40, 129.99, 123.94, 123.23, 108.66, 52.36, 26.58, 26.22.

MS: m/z = 240.97 (M^+).

M.P.: 101.9-103.9 ^{o}C.

IR (in KBr): ṽ = 1716.37, 1610.74, 1467.80, 1233.71, 1103.40, 1036.29, 755.93, 669.73 cm^{-1}.



1c

3-Bromo-5-chloro-1,3-dimethylindolin-2-one (yellow solid)

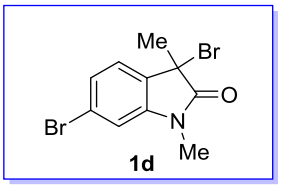
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.42 (s, 1H), 7.31 (d, *J* = 8.4 Hz, 1H), 6.77 (d, *J* = 8.3 Hz, 1H), 3.24 (s, 3H), 2.02 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 174.20, 140.20, 133.03, 129.93, 128.66, 124.57, 109.74, 51.32, 26.81, 26.16.

MS: m/z = 275.07 (M^+).

M.P.: 143.9-146.1 ^{o}C.

IR (in KBr): ṽ = 1725.12, 1610.21, 1488.37, 1232.82, 1110.50, 1044.75, 821.84, 680.85 cm^{-1}.



1d

3,6-Dibromo-1,3-dimethylindolin-2-one (white solid)

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.31 (d, *J* = 7.8 Hz, 1H), 7.26 (d, *J* = 8.3 Hz, 1H), 7.01 (s, 1H),

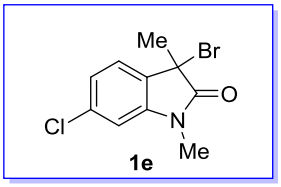
3.23 (s, 3H), 2.02 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 174.39, 142.89, 130.37, 126.10, 125.26, 123.68, 112.24, 51.37, 26.78, 26.08.

MS: m/z = 318.83 (M^+).

M.P.: 118.9-119.2 ^oC.

IR (in KBr): ṽ = 1728.14, 1605.24, 1489.69, 1366.71, 1105.62, 1056.70, 837.75, 674.48 cm^{-1}.



1e

3-Bromo-6-chloro-1,3-dimethylindolin-2-one (white solid)

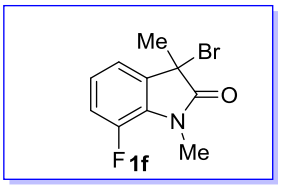
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.36 (d, *J* = 8.0 Hz, 1H), 7.10 (m, 1H), 6.85 (d, *J* = 1.0 Hz, 1H), 3.24 (s, 3H), 2.02 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 174.52, 142.83, 135.82, 129.84, 124.97, 123.15, 109.46, 51.39, 26.77, 26.15.

MS: m/z = 275.06 (M^+).

M.P.: 130.4-131.4 ^oC.

IR (in KBr): ṽ = 1718.46, 1608.36, 1492.90, 1370.12, 1108.05, 1060.68, 834.53, 689.78 cm^{-1}.



1f

3-Bromo-7-fluoro-1,3-dimethylindolin-2-one (yellow solid)

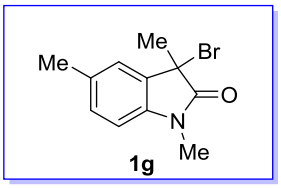
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.24 (m, 1H), 7.08 – 7.03 (m, 2H), 3.46 (d, *J* = 2.6 Hz, 3H), 2.03 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 174.30, 148.82, 146.39, 134.20, 128.54, 123.90, 123.84, 119.96, 117.94, 117.75, 51.65, 29.19, 26.38.

MS: m/z = 258.93 (M^+).

M.P.: 106.2-107.3 ^oC.

IR (in KBr): ṽ = 1727.07, 1630.10, 1478.13, 1374.96, 1280.69, 1055.27, 793.93, 729.91 cm^{-1}.



3-Bromo-1,3,5-trimethylindolin-2-one (yellow solid)

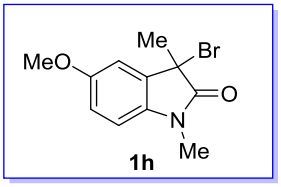
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.26 (s, 1H), 7.13 (d, *J* = 7.8 Hz, 1H), 6.73 (d, *J* = 7.9 Hz, 1H), 3.23 (s, 3H), 2.36 (s, 3H), 2.02 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 174.58, 139.26, 132.97, 131.44, 130.34, 124.70, 108.45, 52.73, 26.65, 26.32, 20.97.

MS: m/z = 254.99 (M^+).

M.P.: 104.8-105.0 ^{o}C.

IR (in KBr): ῡ = 1725.03, 1619.94, 1496.66, 1348.64, 1238.26, 1044.02, 812.83, 661.28 cm^{-1}.



3-Bromo-5-methoxy-1,3-dimethylindolin-2-one (yellow solid)

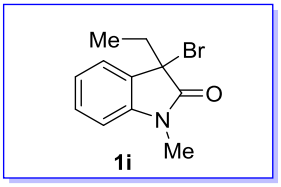
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.04 (d, *J* = 2.5 Hz, 1H), 6.86 (m, 1H), 6.75 (d, *J* = 8.5 Hz, 1H), 3.82 (s, 3H), 3.22 (s, 3H), 2.02 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 174.31, 156.39, 134.97, 132.53, 114.62, 110.94, 109.19, 55.78, 52.68, 26.67, 26.32.

MS: m/z = 269.15 (M^+).

M.P.: 107.8-108.0 ^{o}C.

IR (in KBr): ῡ = 1715.68, 1600.03, 1497.67, 1292.68, 1106.84, 1034.51, 860.92, 819.02 cm^{-1}.

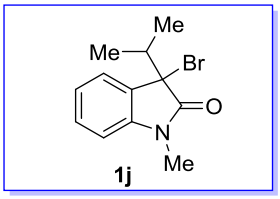


3-Bromo-3-ethyl-1-methylindolin-2-one (yellow solid)

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.40 (d, *J* = 7.5 Hz, 1H), 7.34 (t, *J* = 7.8 Hz, 1H), 7.12 (t, *J* = 7.5 Hz, 1H), 6.84 (d, *J* = 7.8 Hz, 1H), 3.25 (s, 3H), 2.44 – 2.37 (m, 2H), 0.79 (t, *J* = 7.4 Hz, 3H).

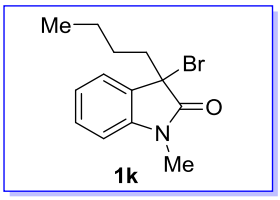
^{13}C NMR (100 MHz, $CDCl_3$) δ 174.03, 142.42, 129.92, 129.53, 124.38, 123.21, 108.61,

57.12, 32.71, 26.58, 9.80.
MS: m/z = 255.07 (M^+).
M.P.: 87.6-88.5 ^oC.
IR (in KBr): ṽ = 1724.00, 1615.05, 1492.71, 1346.63, 1111.78, 1080.02, 864.64, 749.02 cm^{-1}.



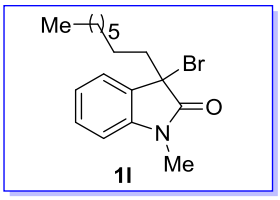
1j

3-Bromo-3-isopropyl-1-methylindolin-2-one (white solid)
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.42 (d, *J* = 7.5 Hz, 1H), 7.33 (t, *J* = 7.8 Hz, 1H), 7.09 (t, *J* = 7.6 Hz, 1H), 6.84 (d, *J* = 7.8 Hz, 1H), 3.24 (s, 3H), 2.61 (m, 1H), 1.29 (d, *J* = 6.9 Hz, 3H), 0.86 (d, *J* = 6.7 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 174.20, 142.52, 129.75, 128.76, 125.28, 122.95, 108.49, 62.00, 36.73, 26.48, 18.05, 17.37.
MS: m/z = 267.13 (M^+).
M.P.: 74.5-75.9 ^oC.
IR (in KBr): ṽ = 1724.62, 1611.93, 1472.89, 1367.94, 1082.93, 982.12, 763.99, 683.73 cm^{-1}.



1k

3-Bromo-3-butyl-1-methylindolin-2-one (yellow oil)
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.39 (d, *J* = 7.4 Hz, 1H), 7.33 (t, *J* = 7.7 Hz, 1H), 7.12 (t, *J* = 7.6 Hz, 1H), 6.84 (d, *J* = 7.8 Hz, 1H), 3.24 (s, 3H), 2.44 – 2.32 (m, 2H), 1.27 (m, 2H), 1.13 – 0.98 (m, 2H), 0.82 (t, *J* = 7.4 Hz, 3H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 173.84, 142.07, 129.73, 129.53, 124.08, 123.00, 108.48, 56.24, 38.95, 27.18, 26.35, 22.10, 13.46.
MS: m/z = 283.18 (M^+).
IR (in KBr): ṽ = 1734.99, 1612.47, 1472.74, 1374.20, 1082.27, 937.60, 750.27, 669.06 cm^{-1}.



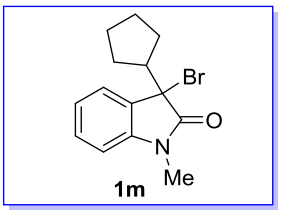
3-Bromo-1-methyl-3-octylindolin-2-one (yellow oil)

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.39 (d, *J* = 7.4 Hz, 1H), 7.33 (t, *J* = 7.7 Hz, 1H), 7.11 (t, *J* = 7.5 Hz, 1H), 6.83 (d, *J* = 7.7 Hz, 1H), 3.24 (s, 3H), 2.36 (m, 2H), 1.24 (s, 4H), 1.18 (s, 6H), 1.14 – 1.00 (m, 2H), 0.85 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 173.98, 142.19, 129.78, 129.70, 124.18, 123.08, 108.53, 56.30, 39.26, 31.50, 29.04, 28.90, 28.86, 26.44, 25.20, 22.36, 13.89.

MS: m/z = 339.30 (M^+).

IR (in KBr): ṽ = 1734.84, 1612.76, 1472.82, 1374.53, 1085.19, 1020.62, 879.90, 749.20 cm^{-1}.



3-Bromo-3-cyclopentyl-1-methylindolin-2-one (yellow solid)

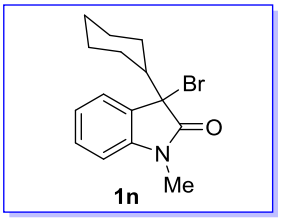
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.46 (d, *J* = 7.5 Hz, 1H), 7.32 (t, *J* = 7.7 Hz, 1H), 7.09 (t, *J* = 7.5 Hz, 1H), 6.83 (d, *J* = 7.8 Hz, 1H), 3.23 (s, 3H), 2.79 (m, 1H), 1.96 – 1.89 (m, 1H), 1.77 – 1.70 (m, 1H), 1.70 – 1.62 (m, 2H), 1.60 – 1.53 (m, 3H), 1.37 – 1.28 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 174.05, 142.29, 129.72, 125.08, 123.00, 108.44, 59.47, 48.12, 28.91, 28.14, 26.51, 25.62, 25.43.

MS: m/z = 295.23 (M^+).

M.P.: 49.8-50.6 ^{o}C.

IR (in KBr): ṽ = 1723.85, 1609.29, 1469.15, 1368.01, 1135.30, 1090.16, 752.62, 684.77 cm^{-1}.



3-Bromo-3-cyclohexyl-1-methylindolin-2-one (yellow solid)

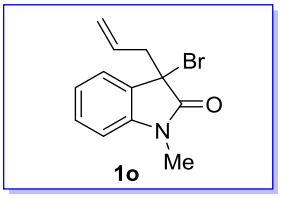
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.41 (d, *J* = 7.5 Hz, 1H), 7.32 (t, *J* = 7.7 Hz, 1H), 7.09 (t, *J* = 7.6 Hz, 1H), 6.82 (d, *J* = 7.8 Hz, 1H), 3.23 (s, 3H), 2.22 (t, *J* = 11.7 Hz, 2H), 1.83 (d, *J* = 11.6 Hz, 1H), 1.63 (d, *J* = 12.1 Hz, 3H), 1.34 – 1.23 (m, 3H), 1.05 (m, 1H), 0.88 – 0.80 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 174.28, 142.46, 129.64, 129.28, 125.37, 122.94, 108.46, 62.14, 46.11, 27.94, 27.76, 26.50, 26.23, 25.82, 25.78.

MS: m/z = 307.25 (M^+).

M.P.: 64.5-65.0 ^oC.

IR (in KBr): ῡ = 1723.08, 1609.72, 1470.23, 1347.88, 1104.91, 973.61, 755.22, 688.21 cm^{-1}.



1o

3-Allyl-3-bromo-1-methylindolin-2-one (yellow solid)

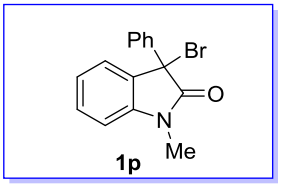
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.42 (d, *J* = 7.4 Hz, 1H), 7.33 (t, *J* = 7.7 Hz, 1H), 7.11 (t, *J* = 7.6 Hz, 1H), 6.83 (d, *J* = 7.8 Hz, 1H), 5.56 – 5.48 (m, 1H), 5.09 (m, 2H), 3.23 (s, 3H), 3.08 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 173.63, 142.22, 130.79, 129.99, 129.35, 124.68, 123.11, 120.59, 108.59, 54.92, 43.23, 26.57.

MS: m/z = 267.13 (M^+).

M.P.: 76.7-77.0 ^oC.

IR (in KBr): ῡ = 1719.93, 1610.77, 1469.02, 1346.70, 1099.13, 946.60, 752.33, 663.75 cm^{-1}.



1p

3-Bromo-1-methyl-3-phenylindolin-2-one (yellow solid)

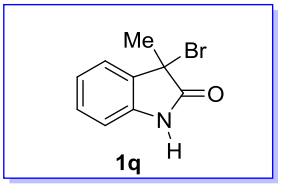
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.66 (m, 2H), 7.50 (d, *J* = 7.5 Hz, 1H), 7.38 (t, *J* = 7.8 Hz, 1H), 7.36 – 7.30 (m, 3H), 7.17 (t, *J* = 7.6 Hz, 1H), 6.89 (d, *J* = 7.9 Hz, 1H), 3.25 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 173.44, 142.12, 136.29, 130.24, 128.82, 128.42, 126.47, 123.44, 108.98, 56.85, 26.88.

MS: m/z = 301.20 (M^+).

M.P.: 124.2-126.1 ^oC.

IR (in KBr): ῡ = 1722.56, 1611.89, 1471.26, 1365.62, 1162.44, 927.58, 749.28, 698.14 cm^{-1}.



1q

3-Bromo-3-methylindolin-2-one (white solid)

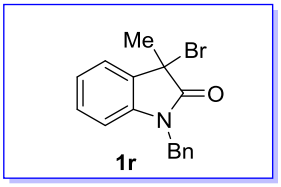
^{1}H NMR (600 MHz, $CDCl_3$) δ 9.17 (s, 1H), 7.43 (d, *J* = 7.5 Hz, 1H), 7.30 – 7.26 (m, 1H), 7.10 (t, *J* = 7.6 Hz, 1H), 6.97 (d, *J* = 7.8 Hz, 1H), 2.07 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 177.78, 139.09, 131.97, 130.11, 124.22, 123.35, 111.01, 53.03, 26.16.

MS: m/z = 225.09 (M^+).

M.P.: 127.3-129.2 ^{o}C.

IR (in KBr): ṽ = 3164.33, 1734.23, 1474.61, 1331.57, 1207.42, 1047.08, 750.64, 670.16 cm^{-1}.



1r

1-Benzyl-3-bromo-3-methylindolin-2-one (white solid)

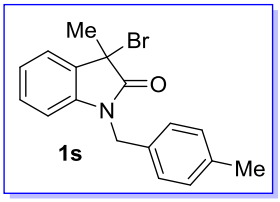
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.45 (d, *J* = 7.4 Hz, 1H), 7.31 (m, 5H), 7.20 (t, *J* = 7.7 Hz, 1H), 7.08 (t, *J* = 7.5 Hz, 1H), 6.70 (d, *J* = 7.8 Hz, 1H), 5.03 (d, *J* = 15.8 Hz, 1H), 4.85 (d, *J* = 15.8 Hz, 1H), 2.10 (s, 4H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 174.83, 140.73, 135.08, 131.49, 129.93, 128.81, 127.72, 127.02, 124.07, 123.32, 109.73, 52.45, 43.86, 26.22.

MS: m/z = 316.96 (M^+).

M.P.: 80.5-80.8 ^{o}C.

IR (in KBr): ṽ = 1725.76, 1613.68, 1469.06, 1356.95, 1185.15, 993.33, 749.21, 698.37 cm^{-1}.



1s

3-Bromo-3-methyl-1-(4-methylbenzyl)indolin-2-one (pink solid)

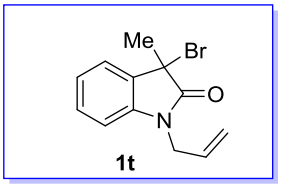
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.44 (d, *J* = 7.4 Hz, 1H), 7.19 (d, *J* = 6.5 Hz, 3H), 7.13 (d, *J* = 7.4 Hz, 2H), 7.07 (t, *J* = 7.5 Hz, 1H), 6.71 (d, *J* = 7.8 Hz, 1H), 4.98 (d, *J* = 15.6 Hz, 1H), 4.81 (d, *J* = 15.6 Hz, 1H), 2.31 (s, 3H), 2.09 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 174.86, 140.92, 137.49, 132.15, 131.65, 129.94, 129.53, 127.13, 124.08, 123.28, 109.80, 52.50, 43.77, 26.30, 21.06.

MS: m/z = 331.03 (M^+).

M.P.: 57.9-58.2 ^oC.

IR (in KBr): ῡ = 1728.36, 1612.23, 1487.81, 1355.61, 1180.25, 1050.03, 882.50, 754.55 cm^{-1}.



1t

1-Allyl-3-bromo-3-methylindolin-2-one (red solid)

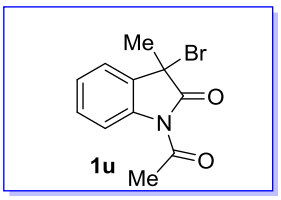
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.46 (d, *J* = 7.4 Hz, 1H), 7.30 (t, *J* = 7.7 Hz, 1H), 7.11 (t, *J* = 7.5 Hz, 1H), 6.83 (d, *J* = 7.8 Hz, 1H), 5.90 – 5.81 (m, 1H), 5.25 (d, *J* = 14.2 Hz, 2H), 4.42 – 4.30 (m, 2H), 2.06 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 174.39, 140.82, 131.46, 130.57, 129.91, 124.07, 123.24, 117.63, 109.56, 52.33, 42.40, 26.22.

MS: m/z = 266.94 (M^+).

M.P.: 35.0-35.8 ^oC.

IR (in KBr): ῡ = 1715.25, 1609.88, 1468.30, 1357.40, 1186.46, 1107.84, 925.82, 752.61 cm^{-1}.



1u

1-Acetyl-3-bromo-3-methylindolin-2-one (white solid)

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.22 (d, *J* = 8.2 Hz, 1H), 7.50 (d, *J* = 7.6 Hz, 1H), 7.39 (t, *J* = 7.9 Hz, 1H), 7.27 (m, 1H), 2.72 (s, 3H), 2.12 (s, 3H).

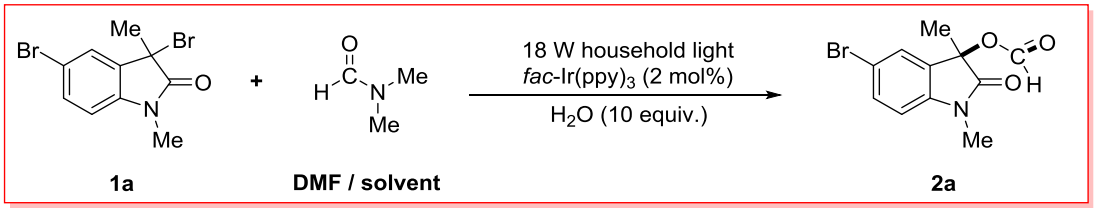
^{13}C NMR (100 MHz, $CDCl_3$) δ 174.86, 170.55, 137.99, 130.56, 130.47, 125.85, 123.77, 116.94, 52.40, 26.41, 26.34.

MS: m/z = 269.12 (M^+).

M.P.: 109.0-110.0 ^oC.

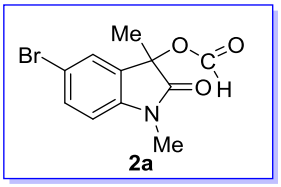
IR (in KBr): ῡ = 1755.18, 1720.59, 1464.48, 1373.76, 1183.84, 1013.72, 770.19, 757.10 cm^{-1}.

2.2 General Procedure for Visible Light Induced Formyloxylation Reaction



To a 10 mL Schlenk tube equipped with a magnetic stir bar and rubber septum was charged with 3,5-dibromo-1,3-dimethylindolin-2-one **1a** (0.20 mmol, 1.0 equiv.), tris-(2-phenylpyridinato-C2,*N*)iridium(III) (*fac*-Ir(ppy)$_3$) (0.004 mmol, 0.02 equiv.), water (2.0 mmol, 10.0 equiv.), and DMF (2.0 mL). The mixture was degassed via the freeze-pump-thaw method and placed at a distance of ~5 cm from two 18 W household light bulbs. After the reaction was complete (2.5 h, monitored by TLC analysis), H_2O (5.0 mL) was added into the reaction mixture. Then, the mixture was extracted with Et_2O and the combined organic layers were dried over Na_2SO_4 and concentrated in vacuo. The residue was purified by FC (silica gel, PE:EtOAc = 10:1-5:1) to give the desired product 5-bromo-1,3-dimethyl-2-oxoindolin-3-yl formate **2a** (44.8 mg, 79 % yield) as a white solid.

2.3 Spectral Data of Products 2a-2t



5-Bromo-1,3-dimethyl-2-oxoindolin-3-yl formate (white solid)

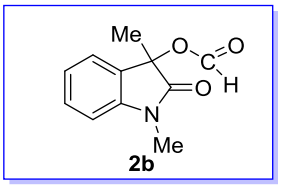
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.88 (s, 1H), 7.47 (d, *J* = 8.2 Hz, 1H), 7.38 (s, 1H), 6.76 (d, *J* = 7.9 Hz, 1H), 3.24 (s, 3H), 1.65 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 173.59, 158.37, 158.32, 142.09, 132.55, 130.10, 125.53, 115.26, 110.00, 76.68, 26.44, 22.72 (The carbon of formate unit resonates as a doublet).

HRMS (ESI) m/z calculated for $C_{11}H_{10}BrNNaO_3$ $[M+Na]^+$ 305.9736, found 305.9734.

M.P.: 174.0-175.2 ^oC.

IR (in KBr): $\tilde{\nu}$ = 1726.27, 1609.20, 1491.85, 1346.03, 1157.17, 1030.77, 828.07, 683.84 cm^{-1}.



2b

3-Methyl-2-oxoindolin-3-yl formate (white solid)

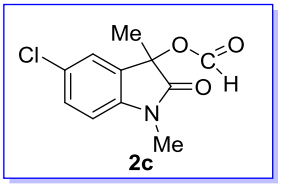
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.88 (s, 1H), 7.35 (t, *J* = 7.7 Hz, 1H), 7.27 (d, *J* = 7.8 Hz, 1H), 7.08 (t, *J* = 7.5 Hz, 1H), 6.88 (d, *J* = 7.8 Hz, 1H), 3.26 (s, 3H), 1.66 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 174.32, 158.46, 143.24, 129.93, 128.38, 122.89, 122.39, 108.54, 77.52, 26.46, 22.97.

HRMS (ESI) m/z calculated for $C_{11}H_{11}NNaO_3$ $[M+Na]^+$ 228.0631, found 228.0627.

M.P.: 98.8-100.9 ^{o}C.

IR (in KBr): ῡ = 1735.28, 1617.14, 1473.04, 1353.23, 1164.73, 1030.75, 840.61, 769.73 cm^{-1}.



2c

5-Chloro-1,3-dimethyl-2-oxoindolin-3-yl formate (white solid)

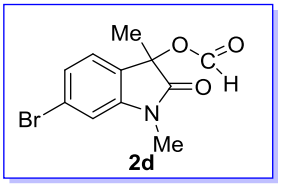
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.87 (s, 1H), 7.31 (d, *J* = 8.3 Hz, 1H), 7.24 (s, 1H), 6.80 (d, *J* = 8.3 Hz, 1H), 3.24 (s, 3H), 1.65 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 173.86, 158.46, 158.40, 141.71, 129.87, 129.78, 128.26, 122.96, 109.58, 77.32, 26.59, 22.84 (The carbon of formate unit resonates as a doublet).

HRMS (ESI) m/z calculated for $C_{11}H_{10}ClNNaO_3$ $[M+Na]^+$ 262.0241, found 262.0236.

M.P.: 156.7-158.4 ^{o}C.

IR (in KBr): ῡ = 1726.31, 1612.44, 1493.64, 1344.95, 1160.88, 1028.92, 825.82, 693.48 cm^{-1}.



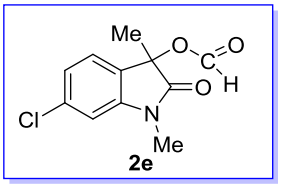
2d

6-Bromo-1,3-dimethyl-2-oxoindolin-3-yl formate (white solid)

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.86 (s, 1H), 7.21 (d, *J* = 7.8 Hz, 1H), 7.13 (d, *J* = 7.8 Hz, 1H), 7.03 (s, 1H), 3.24 (s, 3H), 1.64 (s, 3H).

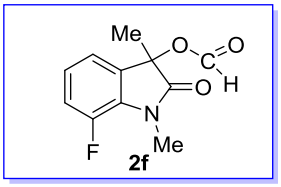
^{13}C NMR (100 MHz, $CDCl_3$) δ 174.03, 158.45, 158.40, 144.44, 127.16, 125.64, 123.62,

112.12, 76.68, 26.54, 22.71 (The carbon of formate unit resonates as a doublet).
HRMS (ESI) m/z calculated for $C_{11}H_{10}BrNNaO_3$ $[M+Na]^+$ 305.9736, found 305.9731.
M.P.: 142.4-144.2 ^oC.
IR (in KBr): ṽ = 1720.44, 1608.71, 1494.25, 1370.09, 1166.70, 1030.72, 817.83, 704.52 cm^{-1}.



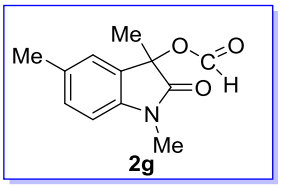
2e

6-Chloro-1,3-dimethyl-2-oxoindolin-3-yl formate (white solid)
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.86 (s, 1H), 7.19 (d, *J* = 7.8 Hz, 1H), 7.05 (d, *J* = 7.9 Hz, 1H), 6.88 (s, 1H), 3.25 (s, 3H), 1.64 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 174.14, 158.45, 144.37, 135.71, 126.61, 123.31, 122.66, 109.34, 76.68, 26.53, 22.76.
HRMS (ESI) m/z calculated for $C_{11}H_{10}ClNNaO_3$ $[M+Na]^+$ 262.0241, found 262.0236.
M.P.: 138.2-139.8 ^oC.
IR (in KBr): ṽ = 1722.90, 1612.22, 1467.65, 1371.18, 1169.66, 1055.61, 926.86, 819.63 cm^{-1}.



2f

7-Fluoro-1,3-dimethyl-2-oxoindolin-3-yl formate (white solid)
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.88 (s, 1H), 7.06 (m, 2H), 7.00 (m, 1H), 3.47 (s, 3H), 1.65 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 174.01, 158.45, 158.40, 148.96, 146.53, 131.16, 129.77, 123.58, 123.52, 118.10, 118.03, 117.84, 77.32, 28.99, 23.05 (The carbon of formate unit resonates as a doublet).
HRMS (ESI) m/z calculated for $C_{11}H_{10}FNNaO_3$ $[M+Na]^+$ 246.0537, found 246.0530.
M.P.: 155.9-156.9 ^oC.
IR (in KBr): ṽ = 1739.38, 1716.54, 1481.32, 1246.92, 1169.64, 1055.59, 852.98, 732.05 cm^{-1}.



2g

1,3,5-Trimethyl-2-oxoindolin-3-yl formate (white solid)

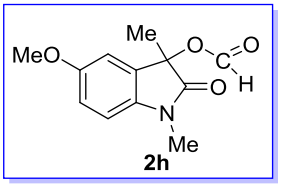
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.88 (s, 1H), 7.14 (d, *J* = 7.9 Hz, 1H), 7.08 (s, 1H), 6.76 (d, *J* = 7.8 Hz, 1H), 3.24 (s, 3H), 2.33 (s, 3H), 1.64 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 174.23, 158.45, 140.73, 132.45, 130.09, 128.26, 123.14, 108.25, 77.60, 26.42, 22.97, 20.95.

HRMS (ESI) m/z calculated for $C_{12}H_{13}NNaO_3$ $[M+Na]^+$ 242.0788, found 242.0779.

M.P.: 141.9-142.8 °C.

IR (in KBr): ṽ = 1732.30, 1625.28, 1500.45, 1246.35, 1164.75, 1051.37, 822.62, 704.18 cm^{-1}.



2h

5-Methoxy-1,3-dimethyl-2-oxoindolin-3-yl formate (white solid)

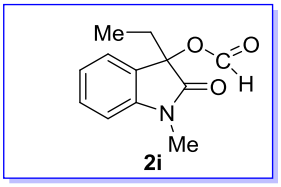
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.88 (s, 1H), 6.88 (d, *J* = 2.0 Hz, 1H), 6.87 – 6.84 (m, 1H), 6.77 (d, *J* = 8.4 Hz, 1H), 3.79 (s, 3H), 3.23 (s, 3H), 1.65 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 173.99, 158.43, 158.38, 156.14, 136.47, 129.49, 113.84, 109.87, 108.95, 77.70, 55.70, 26.49, 23.02 (The carbon of formate unit resonates as a doublet).

HRMS (ESI) m/z calculated for $C_{12}H_{13}NNaO_4$ $[M+Na]^+$ 258.0737, found 258.0732.

M.P.: 156.9-159.9 °C.

IR (in KBr): ṽ = 1724.06, 1604.03, 1470.29, 1286.73, 1158.74, 1039.56, 880.55, 815.31 cm^{-1}.



2i

3-Ethyl-1-methyl-2-oxoindolin-3-yl formate (white solid)

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.89 (s, 1H), 7.34 (t, *J* = 7.4 Hz, 1H), 7.23 (d, *J* = 7.3 Hz, 1H), 7.07 (t, *J* = 7.5 Hz, 1H), 6.86 (d, *J* = 7.8 Hz, 1H), 3.25 (s, 3H), 2.11 (m, 1H), 2.02 (m, 1H),

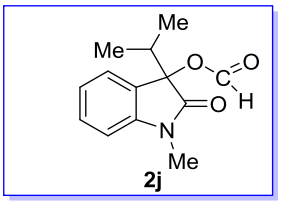
0.83 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 173.88, 158.47, 158.42, 143.74, 129.79, 126.67, 122.70, 122.63, 108.30, 80.51, 29.56, 26.27, 6.48 (The carbon of formate unit resonates as a doublet).

HRMS (ESI) m/z calculated for $C_{12}H_{13}NNaO_3$ $[M+Na]^+$ 242.0788, found 242.0784.

M.P.: 82.7-83.8 °C.

IR (in KBr): ṽ = 1724.65, 1612.47, 1471.96, 1350.38, 1156.41, 1069.62, 854.54, 751.42 cm^{-1}.



2j

3-Isopropyl-1-methyl-2-oxoindolin-3-yl formate (white solid)

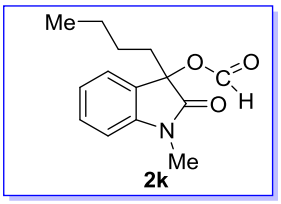
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.90 (s, 1H), 7.34 (m, 1H), 7.22 (d, *J* = 7.3 Hz, 1H), 7.05 (t, *J* = 7.5 Hz, 1H), 6.85 (d, *J* = 7.8 Hz, 1H), 3.24 (s, 3H), 2.41 (m, 1H), 1.09 (d, *J* = 6.8 Hz, 3H), 0.76 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 173.96, 158.55, 158.50, 144.26, 129.76, 125.30, 123.41, 122.35, 108.14, 82.72, 34.48, 26.17, 15.77, 15.28 (The carbon of formate unit resonates as a doublet).

HRMS (ESI) m/z calculated for $C_{13}H_{15}NNaO_3$ $[M+Na]^+$ 256.0944, found 256.0940.

M.P.: 76.1-76.9 °C.

IR (in KBr): ṽ = 1715.74, 1613.25, 1470.47, 1375.43, 1170.65, 1123.70, 983.01, 767.56 cm^{-1}.



2k

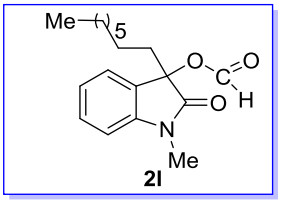
3-Butyl-1-methyl-2-oxoindolin-3-yl formate (colorless oil)

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.88 (s, 1H), 7.34 (t, *J* = 7.7 Hz, 1H), 7.24 (d, *J* = 7.3 Hz, 1H), 7.07 (t, *J* = 7.5 Hz, 1H), 6.87 (d, *J* = 7.8 Hz, 1H), 3.25 (s, 3H), 2.05 (m, 1H), 1.97 (m, 1H), 1.29 – 1.21 (m, 3H), 1.16 – 1.10 (m, 1H), 0.84 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 174.06, 158.47, 158.42, 143.68, 129.77, 127.01, 122.72, 122.64, 108.32, 80.15, 36.12, 26.30, 23.95, 22.47, 13.66 (The carbon of formate unit resonates as a doublet).

HRMS (ESI) m/z calculated for $C_{14}H_{17}NNaO_3$ $[M+Na]^+$ 270.1101, found 270.1093.

IR (in KBr): ṽ = 1729.94, 1615.54, 1471.55, 1374.71, 1167.83, 1121.93, 976.33, 753.81 cm^{-1}.



2l

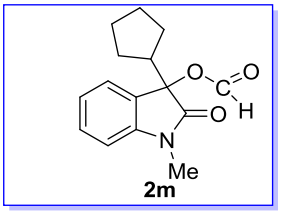
1-Methyl-3-octyl-2-oxoindolin-3-yl formate (colorless oil)

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.88 (s, 1H), 7.34 (t, *J* = 7.7 Hz, 1H), 7.23 (d, *J* = 7.3 Hz, 1H), 7.07 (t, *J* = 7.4 Hz, 1H), 6.86 (d, *J* = 7.8 Hz, 1H), 3.25 (s, 3H), 2.04 (t, *J* = 12.2 Hz, 1H), 1.95 (m, 1H), 1.25 – 1.12 (m, 12H), 0.85 (t, *J* = 7.0 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 174.02, 158.44, 158.39, 143.66, 129.74, 127.01, 122.69, 122.60, 108.29, 80.13, 36.33, 31.60, 29.32, 29.07, 28.98, 26.27, 22.44, 21.84, 13.94 (The carbon of formate unit resonates as a doublet).

HRMS (ESI) m/z calculated for $C_{18}H_{25}NNaO_3$ $[M+Na]^+$ 326.1727, found 326.1721.

IR (in KBr): ṽ = 1746.61, 1616.16, 1470.99, 1374.93, 1157.49, 1122.59, 973.38, 752.59 cm^{-1}.



2m

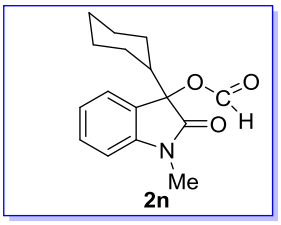
3-Cyclopentyl-1-methyl-2-oxoindolin-3-yl formate (colorless oil)

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.89 (s, 1H), 7.33 (t, *J* = 7.8 Hz, 1H), 7.25 (d, *J* = 7.4 Hz, 1H), 7.03 (t, *J* = 7.5 Hz, 1H), 6.85 (d, *J* = 7.8 Hz, 1H), 3.23 (s, 3H), 2.56 – 2.50 (m, 1H), 1.79 (m, 1H), 1.66 – 1.62 (m, 2H), 1.56 – 1.52 (m, 2H), 1.49 – 1.46 (m, 2H), 1.24 – 1.18 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 174.09, 158.58, 144.02, 129.69, 126.48, 123.23, 122.41, 108.15, 81.65, 45.71, 26.26, 26.20, 25.62, 25.13, 24.91.

HRMS (ESI) m/z calculated for $C_{15}H_{17}NNaO_3$ $[M+Na]^+$ 282.1101, found 282.1099.

IR (in KBr): ṽ = 1722.41, 1611.37, 1465.42, 1371.50, 1147.11, 1077.51, 856.65, 757.95 cm^{-1}.



2n

3-Cyclohexyl-1-methyl-2-oxoindolin-3-yl formate (white solid)

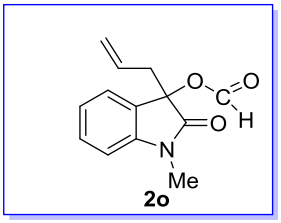
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.90 (s, 1H), 7.33 (t, *J* = 7.8 Hz, 1H), 7.21 (d, *J* = 7.4 Hz, 1H), 7.05 (t, *J* = 7.5 Hz, 1H), 6.84 (d, *J* = 7.8 Hz, 1H), 3.23 (s, 3H), 2.10 (t, *J* = 11.8 Hz, 1H), 1.95 (d, *J* = 10.7 Hz, 1H), 1.77 (s, 1H), 1.67 – 1.57 (m, 3H), 1.27 – 1.19 (m, 3H), 1.05 (t, *J* = 11.0 Hz, 1H), 0.77 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 174.10, 158.62, 158.57, 144.20, 129.66, 125.94, 123.45, 122.33, 108.10, 82.62, 44.31, 26.17, 25.98, 25.81, 25.63, 25.57, 25.11 (The carbon of formate unit resonates as a doublet).

M.P.: 111.5-112.6 ^{o}C.

HRMS (ESI) m/z calculated for $C_{16}H_{19}NNaO_3$ $[M+Na]^+$ 296.1257, found 296.1251.

IR (in KBr): ṽ = 1733.11, 1610.31, 1492.12, 1372.61, 1139.53, 1075.73, 858.79, 758.25 cm^{-1}.



2o

3-Allyl-1-methyl-2-oxoindolin-3-yl formate (white solid)

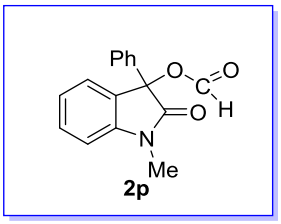
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.90 (s, 1H), 7.34 (m, 1H), 7.25 (d, *J* = 7.3 Hz, 1H), 7.06 (t, *J* = 7.5 Hz, 1H), 6.86 (d, *J* = 7.8 Hz, 1H), 5.60 (m, 1H), 5.09 (m, 2H), 3.24 (s, 3H), 2.87 (m, 1H), 2.62 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 173.40, 158.35, 158.30, 143.54, 129.92, 128.97, 126.33, 123.10, 122.57, 120.75, 108.34, 79.33, 40.56, 26.30 (The carbon of formate unit resonates as a doublet).

M.P.: 69.3-70.0 ^{o}C.

HRMS (ESI) m/z calculated for $C_{13}H_{13}NNaO_3$ $[M+Na]^+$ 254.0788, found 254.0787.

IR (in KBr): ṽ = 1730.24, 1613.03, 1470.40, 1373.16, 1165.80, 1082.20, 836.71, 762.83 cm^{-1}.



2p

1-Methyl-2-oxo-3-phenylindolin-3-yl formate (white solid)

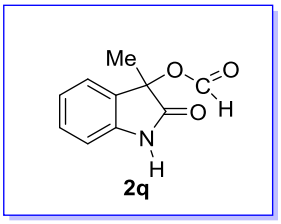
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.08 (s, 1H), 7.42 (m, 1H), 7.38 – 7.36 (m, 2H), 7.36 – 7.32 (m, 3H), 7.26 (s, 1H), 7.12 (t, *J* = 7.2 Hz, 1H), 6.94 (d, *J* = 7.9 Hz, 1H), 3.25 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 173.22, 158.63, 158.58, 144.55, 135.89, 130.45, 129.04, 128.60, 127.53, 126.31, 124.51, 123.15, 108.68, 81.29, 26.74 (The carbon of formate unit resonates as a doublet).

M.P.: 165.7-167.2 ^{o}C.

HRMS (ESI) m/z calculated for $C_{16}H_{13}NNaO_3$ $[M+Na]^+$ 290.0788, found 290.0783.

IR (in KBr): ṽ = 1719.12, 1615.15, 1471.46, 1367.95, 1155.69, 1014.93, 860.80, 762.92 cm^{-1}.



2q

3-Methyl-2-oxoindolin-3-yl formate (white solid)

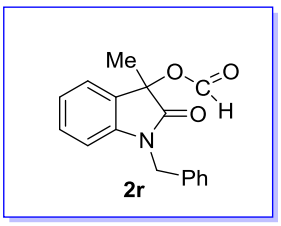
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.18 (s, 1H), 7.92 (s, 1H), 7.26 (t, *J* = 8.0 Hz, 2H), 7.06 (t, *J* = 7.2 Hz, 1H), 6.91 (d, *J* = 7.6 Hz, 1H), 1.69 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 176.66, 158.66, 140.34, 129.89, 128.67, 122.87, 122.58, 110.68, 77.90, 23.06.

M.P.: 146.1-148.1 ^{o}C.

HRMS (ESI) m/z calculated for $C_{10}H_9NNaO_3$ $[M+Na]^+$ 214.0475, found 214.0467.

IR (in KBr): ṽ = 1721.40, 1620.20, 1473.11, 1335.21, 1171.32, 1015.31, 824.21, 749.07 cm^{-1}.



2r

1-Benzyl-3-methyl-2-oxoindolin-3-yl formate (white solid)

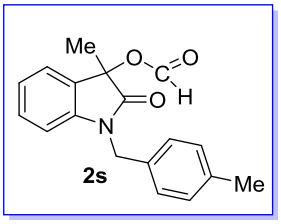
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.93 (s, 1H), 7.37 (d, *J* = 7.6 Hz, 2H), 7.33 (t, *J* = 7.4 Hz, 2H), 7.27 (d, *J* = 7.5 Hz, 2H), 7.19 (t, *J* = 7.8 Hz, 1H), 7.03 (t, *J* = 7.5 Hz, 1H), 6.69 (d, *J* = 7.9 Hz, 1H), 5.01 (d, *J* = 15.9 Hz, 1H), 4.92 (d, *J* = 15.9 Hz, 1H), 1.72 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 174.32, 158.42, 142.10, 135.36, 129.72, 128.70, 128.32, 127.56, 127.15, 122.91, 122.29, 109.66, 77.51, 43.97, 23.44.

M.P.: 150.1-152.0 °C.

HRMS (ESI) m/z calculated for $C_{17}H_{15}NNaO_3$ $[M+Na]^+$ 304.0944, found 304.0939.

IR (in KBr): ṽ = 1728.51, 1612.94, 1471.27, 1372.45, 1144.48, 1095.33, 896.77, 753.41 cm^{-1}.



2s

3-Methyl-1-(4-methylbenzyl)-2-oxoindolin-3-yl formate (pink solid)

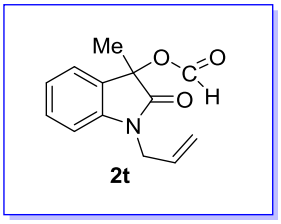
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.93 (s, 1H), 7.26 (s, 3H), 7.19 (t, *J* = 7.8 Hz, 1H), 7.14 (d, *J* = 7.7 Hz, 2H), 7.02 (t, *J* = 7.5 Hz, 1H), 6.71 (d, *J* = 7.9 Hz, 1H), 4.96 (d, *J* = 15.7 Hz, 1H), 4.88 (d, *J* = 15.7 Hz, 1H), 2.32 (s, 3H), 1.71 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 174.25, 158.38, 142.13, 137.19, 132.29, 129.67, 129.34, 128.30, 127.17, 122.81, 122.23, 109.66, 77.50, 43.72, 23.40, 21.03.

M.P.: 137.2-138.4 °C.

HRMS (ESI) m/z calculated for $C_{18}H_{17}NNaO_3$ $[M+Na]^+$ 318.1101, found 318.1096.

IR (in KBr): ṽ = 1717.41, 1612.77, 1490.13, 1368.67, 1146.53, 1093.15, 902.00, 752.26 cm^{-1}.



2t

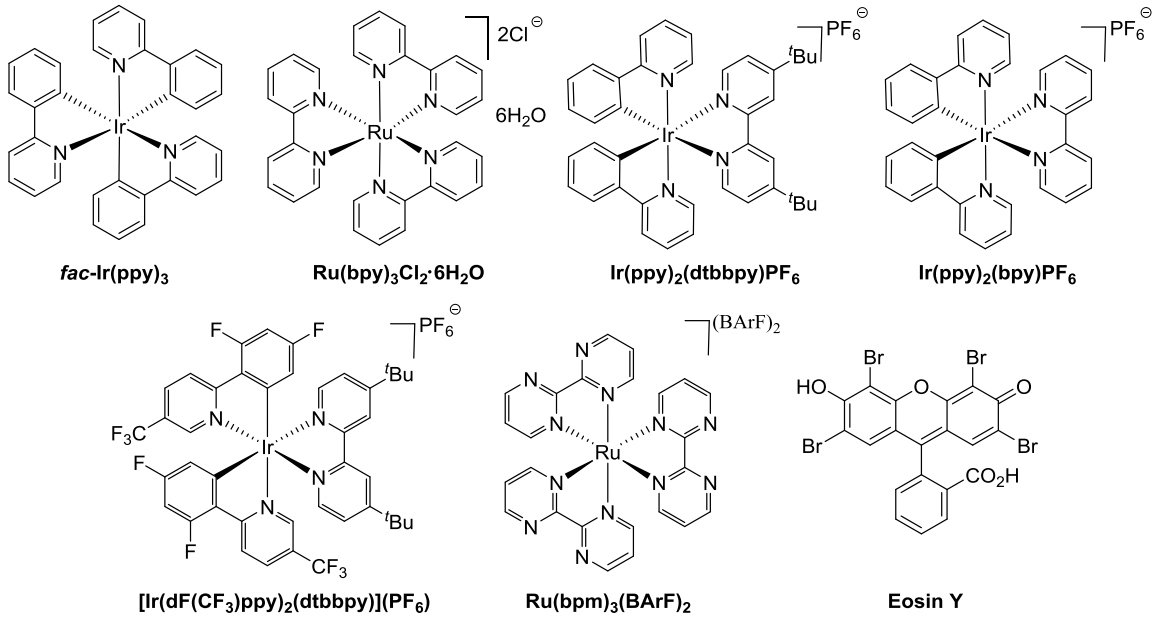
1-Allyl-3-methyl-2-oxoindolin-3-yl formate (pink oil)

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.89 (s, 1H), 7.32 – 7.26 (m, 2H), 7.06 (t, *J* = 7.4 Hz, 1H), 6.86 (d, *J* = 7.8 Hz, 1H), 5.90 – 5.82 (m, 1H), 5.34 (d, *J* = 17.3 Hz, 1H), 5.25 (d, *J* = 10.3 Hz, 1H), 4.43 (d, *J* = 16.2 Hz, 1H), 4.33 (m, 1H), 1.68 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 174.00, 158.41, 158.36, 142.20, 130.89, 129.71, 128.28, 122.82, 122.30, 117.62, 109.48, 77.41, 42.41, 23.20 (The carbon of formate unit

resonates as a doublet).
HRMS (ESI) m/z calculated for $C_{13}H_{13}NNaO_3$ $[M+Na]^+$ 254.0788, found 254.0781.
IR (in KBr): ṽ = 1715.11, 1613.44, 1471.28, 1370.20, 1148.49, 1017.48, 937.31, 753.07 cm^{-1}.

2.4 Structure of the Photocatalysts



3. Mechanism Studies

3.1 Fluorescence Quenching Experiment

Fluorescence spectra were collected on Cary Eclipse Fluorescence Spectrophotometer (Varian, USA). All *fac*-Ir(ppy)$_3$ solutions were excited at 385 nm and the emission intensity at 520 nm was observed. In a typical experiment, a 50 µM solution of *fac*-Ir(ppy)$_3$ in DMF was added to the appropriate amount of quencher in a quartz cuvette. After degassing with a stream of argon for 15 minutes, the emission spectrum of the sample was collected.

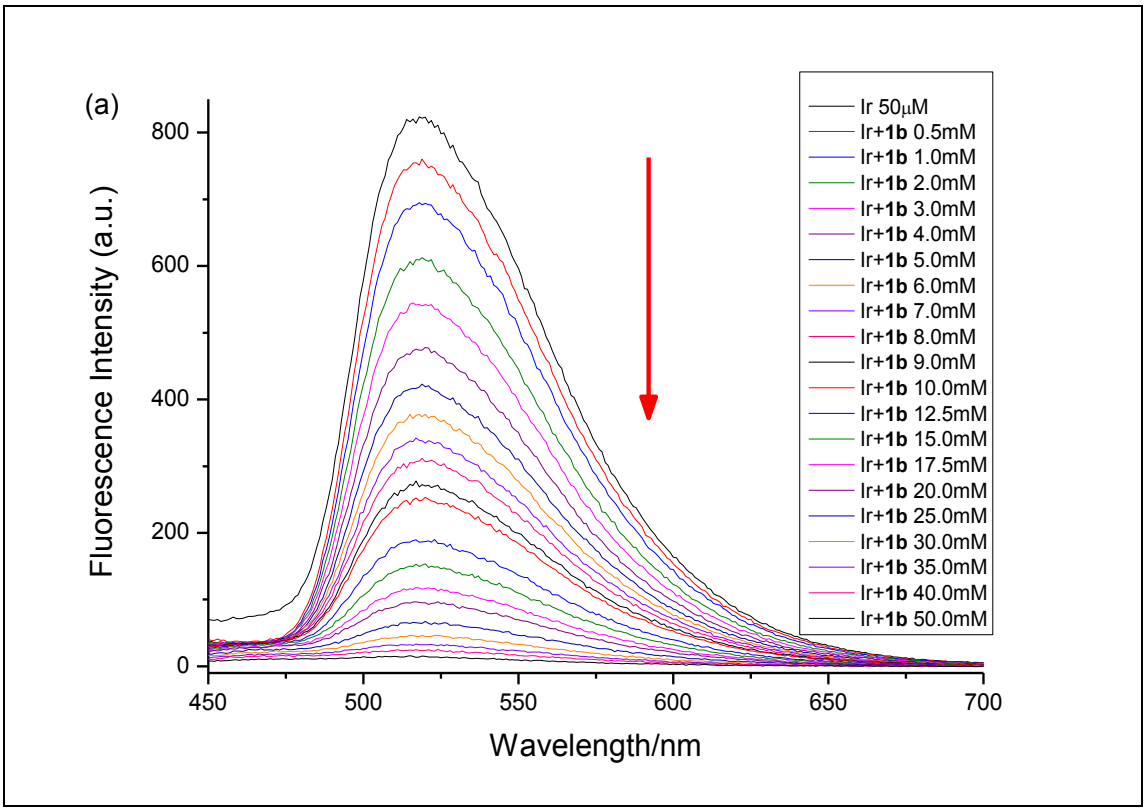


Figure (a). Emission spectra of 50 μM $Ir(ppy)_3$ at λ_{ex} = 385 nm showing the quenching effect of increasing concentrations of 3-bromo-1,3-dimethylindolin-2-one (**1b**).

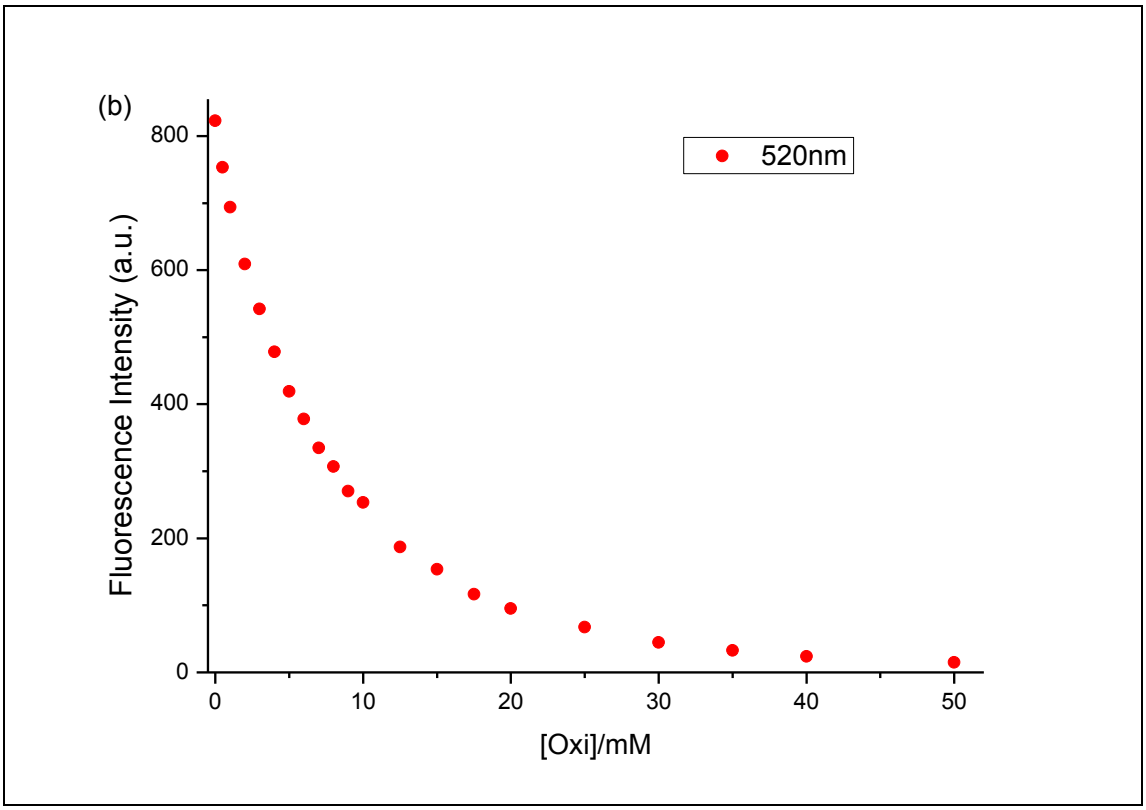


Figure (b). Relationship between the fluorescence intensity and the concentration of 3-bromo-1,3-dimethylindolin-2-one (**1b**).

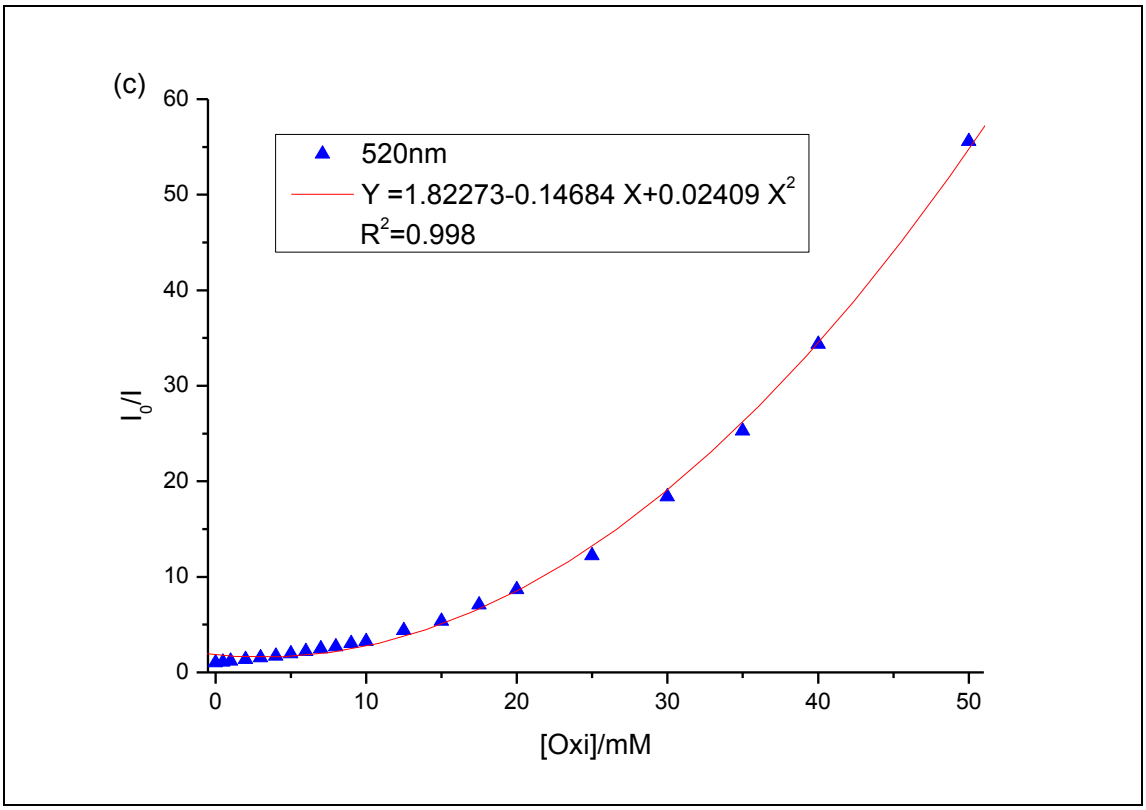


Figure (c). The cubic relationship of increasing concentrations of 3-bromo-1,3-dimethylindolin-2-one (**1b**).

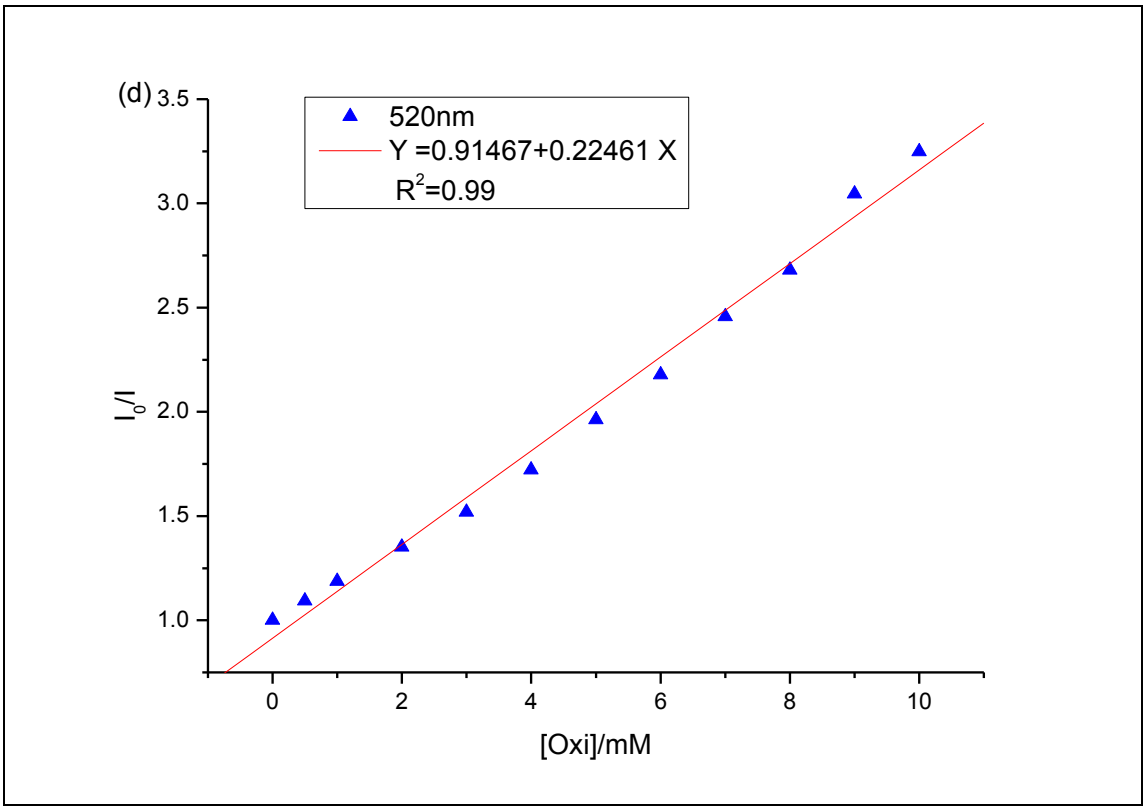
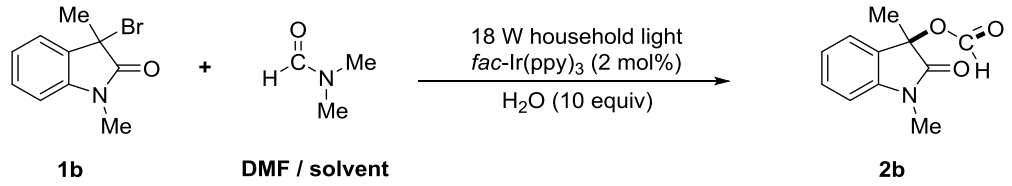
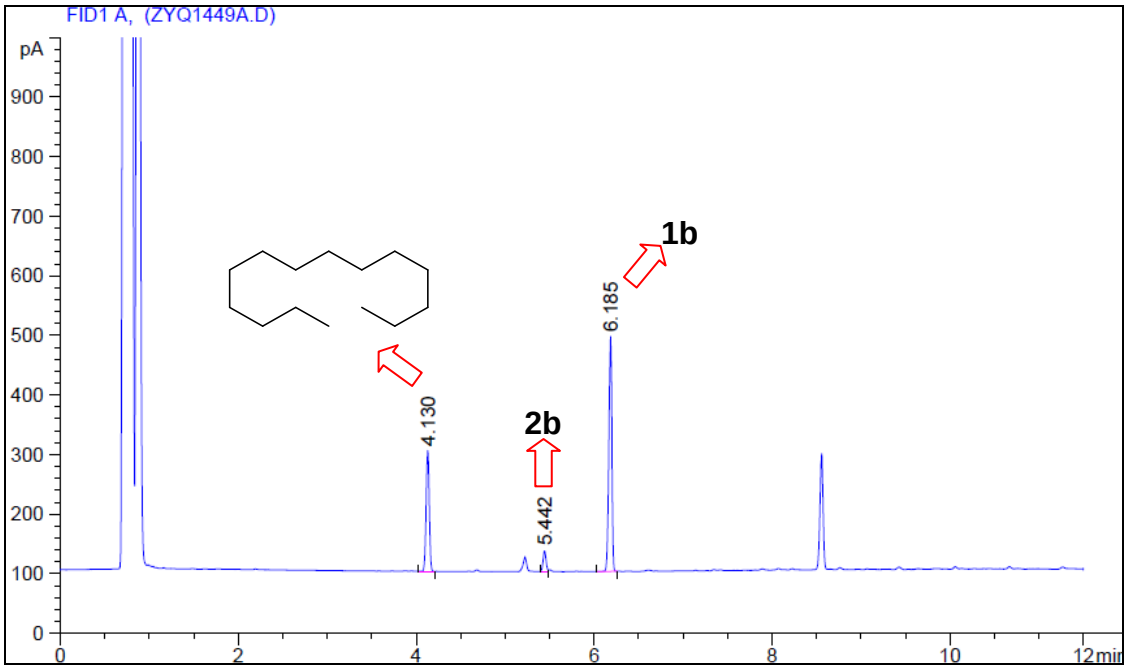


Figure (d). The linear relationship over the concentration range from 0.5 to 10 mM.

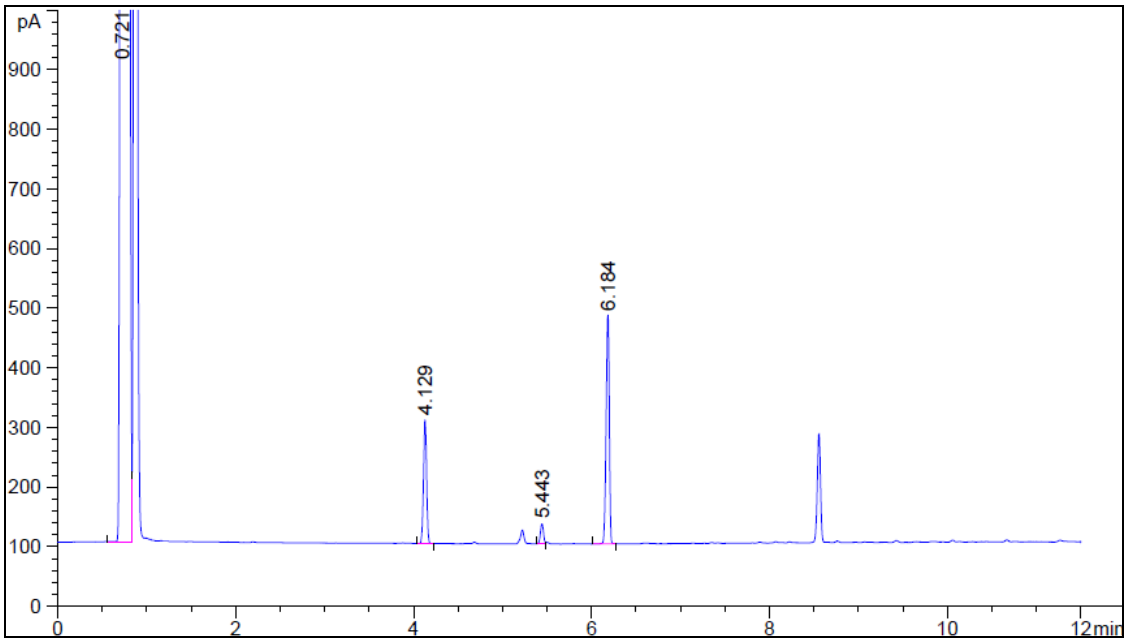
3.2 On-off Swithching of the Light





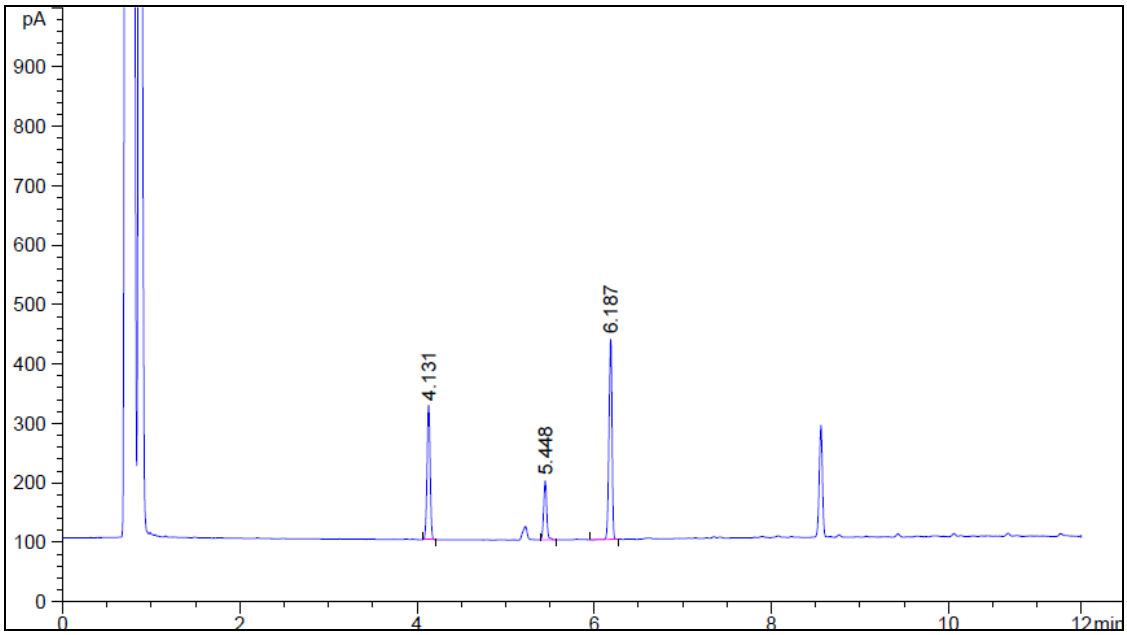
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	4.130	VP	0.0386	503.10623	201.75529	32.87610
2	5.442	BV	0.0379	82.38215	34.46562	5.38336
3	6.185	PP	0.0371	944.82153	392.89935	61.74054
Totals :				1530.30991	629.12027	

Figure 1. 20 min GC sample.



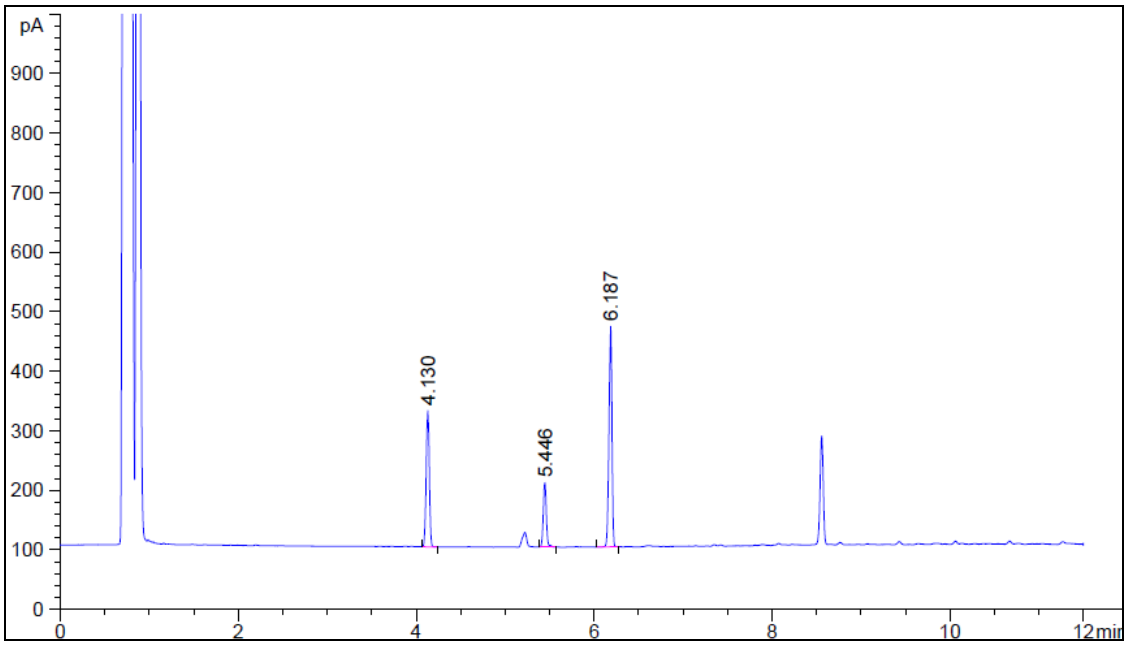
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	0.721	BV S	0.0396	4.22759e6	1.66390e6	99.96375
2	4.129	VB	0.0380	506.23782	206.98761	0.01197
3	5.443	BV	0.0387	82.31999	33.42239	0.00195
4	6.184	PB	0.0368	944.49457	382.18906	0.02233
Totals :				4.22912e6	1.66452e6	

Figure 2. 30 min GC sample.



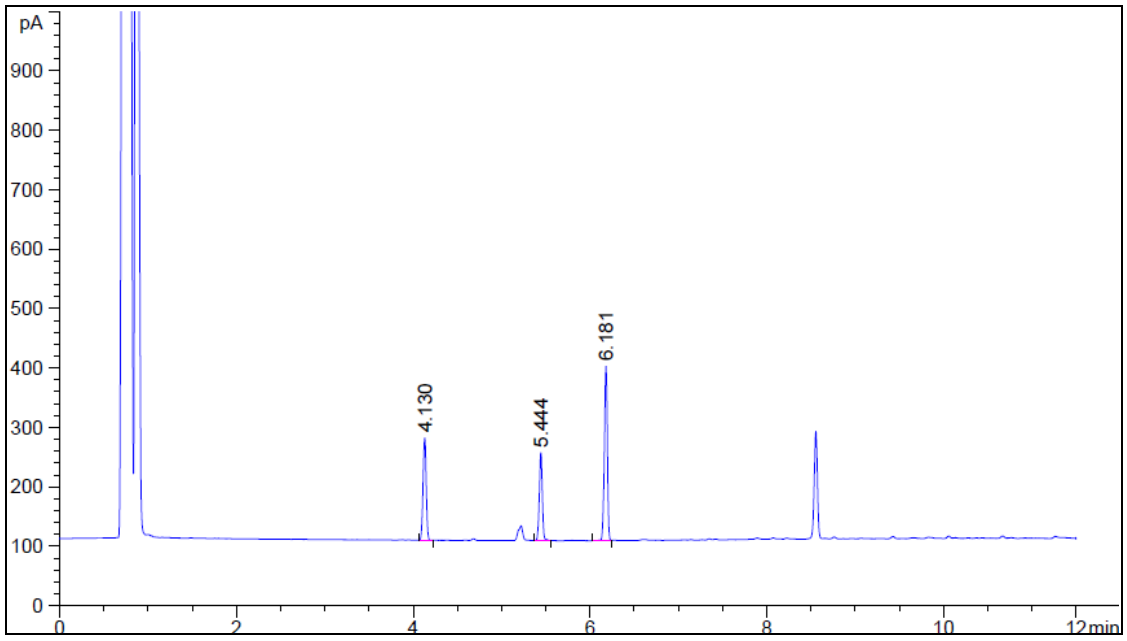
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	4.131	BV	0.0395	551.65881	225.46715	34.56099
2	5.448	BB	0.0379	238.14543	99.52656	14.91962
3	6.187	VB	0.0359	806.38513	336.70319	50.51939
Totals :				1596.18938	661.69689	

Figure 3. 50 min GC sample.



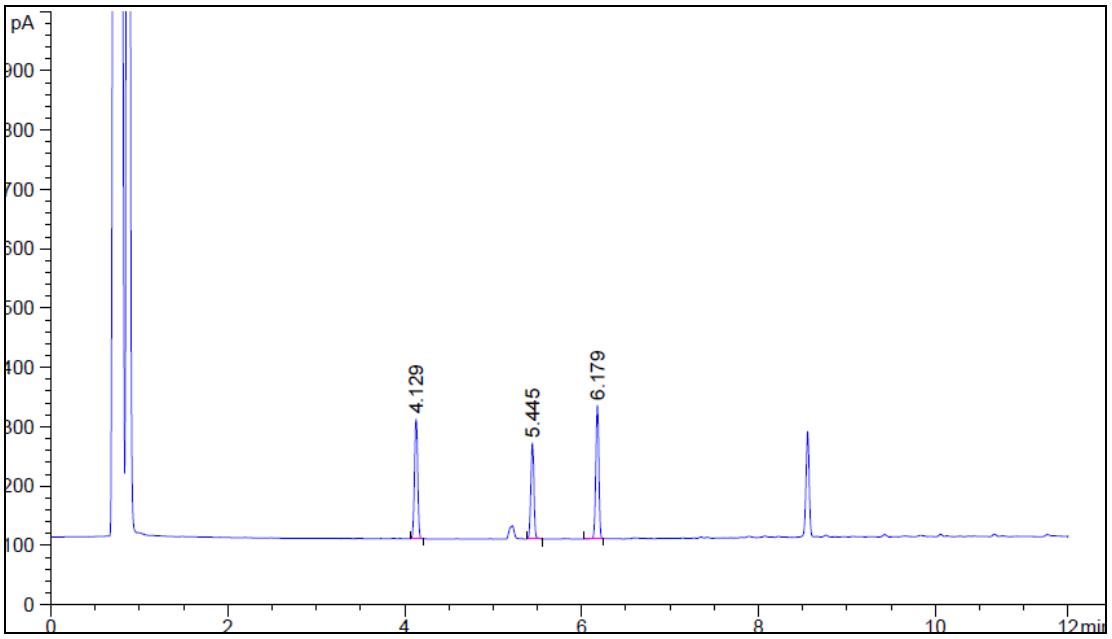
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	4.130	BB	0.0388	564.40796	228.49707	33.09811
2	5.446	BB	0.0390	262.46249	107.38840	15.39137
3	6.187	PB	0.0362	878.38684	370.45303	51.51052
Totals :				1705.25729	706.33851	

Figure 4. 60 min GC sample.



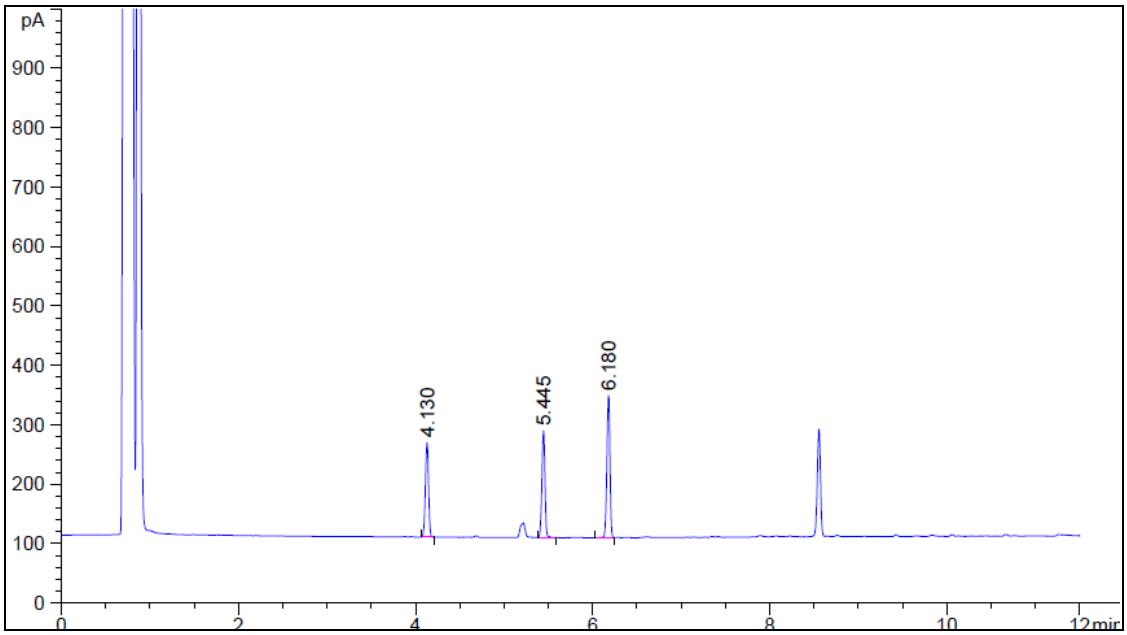
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	4.130	BB	0.0395	427.06665	172.00421	29.16521
2	5.444	VB	0.0365	346.95169	147.29591	23.69400
3	6.181	BV	0.0365	690.28345	293.28397	47.14079
Totals :				1464.30179	612.58409	

Figure 5. 80 min GC sample.



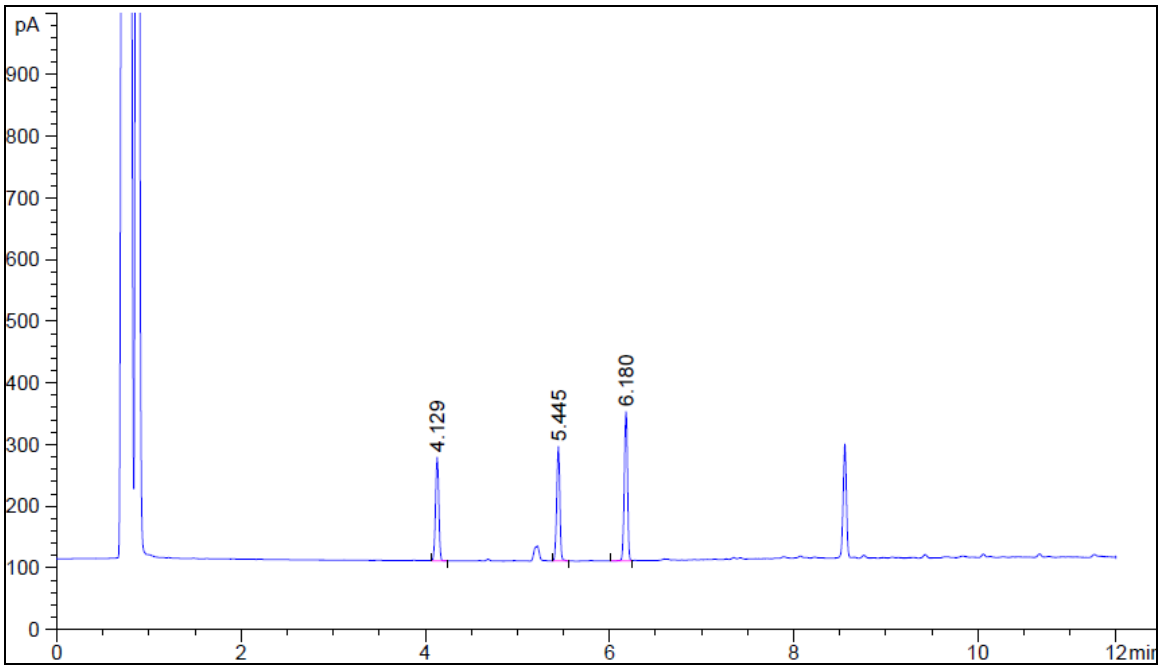
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	4.129	BB	0.0399	507.32230	201.50584	35.18671
2	5.445	BB	0.0382	390.76566	161.66202	27.10261
3	6.179	BV	0.0372	543.71283	224.73750	37.71068
Totals :				1441.80078	587.90536	

Figure 6. 90 min GC sample.



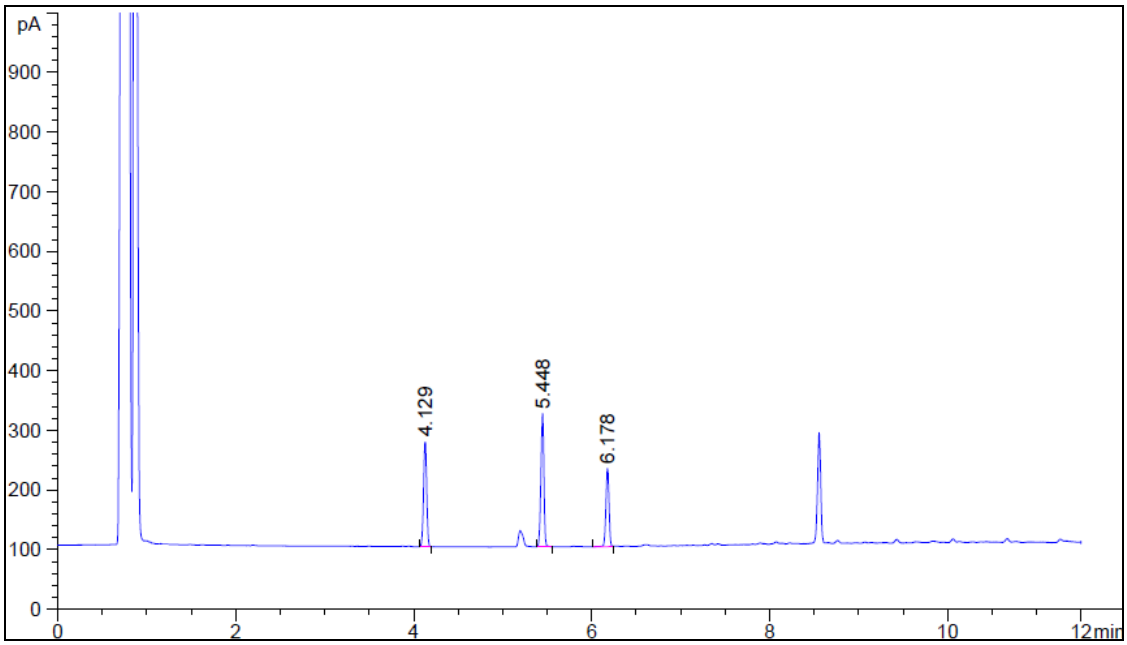
Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	4.130	BP	0.0389	394.11688	158.93971	28.17978
2	5.445	BB	0.0374	429.46033	179.44032	30.70687
3	6.180	BV	0.0376	575.00336	239.08827	41.11335
Totals :				1398.58057	577.46831	

Figure 7. 110 min GC sample.



Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	4.129	BB	0.0392	411.72397	167.65854	28.68003
2	5.445	VB	0.0371	438.65488	185.49800	30.55599
3	6.180	PV	0.0373	585.19836	241.61235	40.76398
Totals :				1435.57721	594.76889	

Figure 8. 120 min GC sample.



Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	4.129	BV	0.0389	435.47351	175.58044	34.15459
2	5.448	BB	0.0370	524.21204	222.60492	41.11444
3	6.178	PV	0.0381	315.32162	130.75710	24.73097
Totals :				1275.00717	528.94246	

Figure 9. 160 min GC sample.

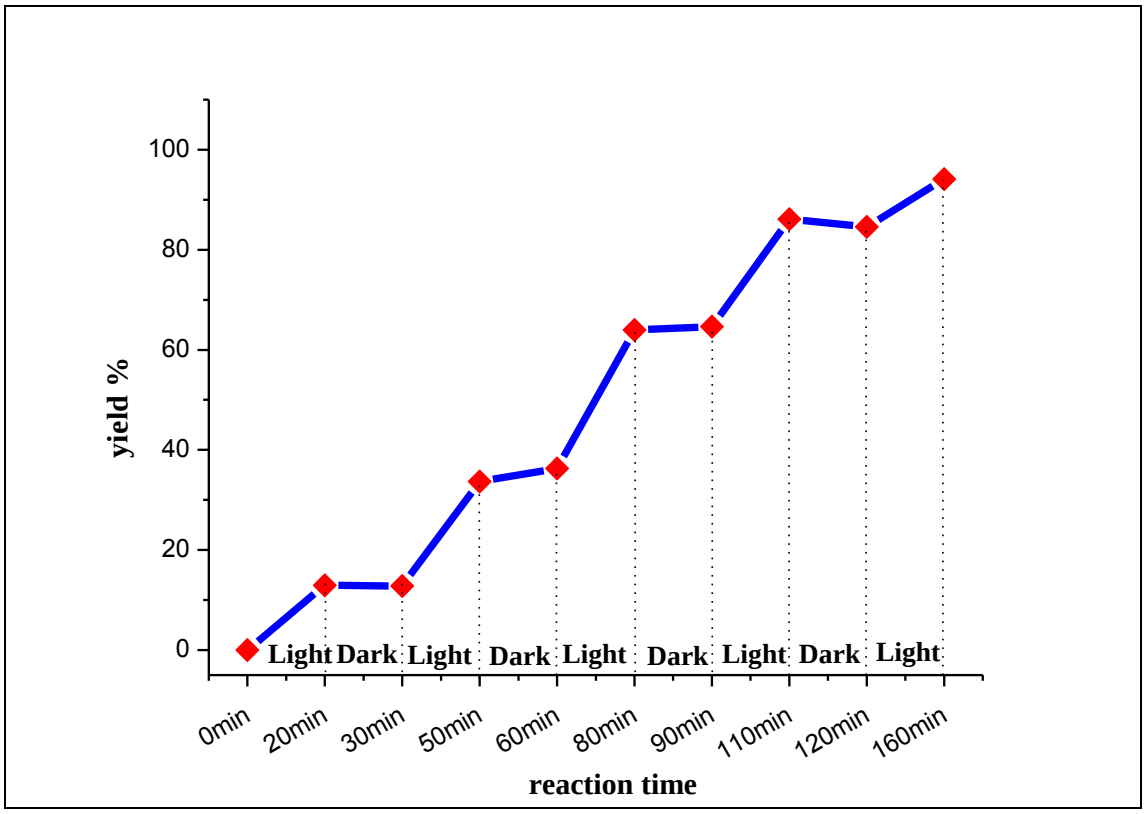
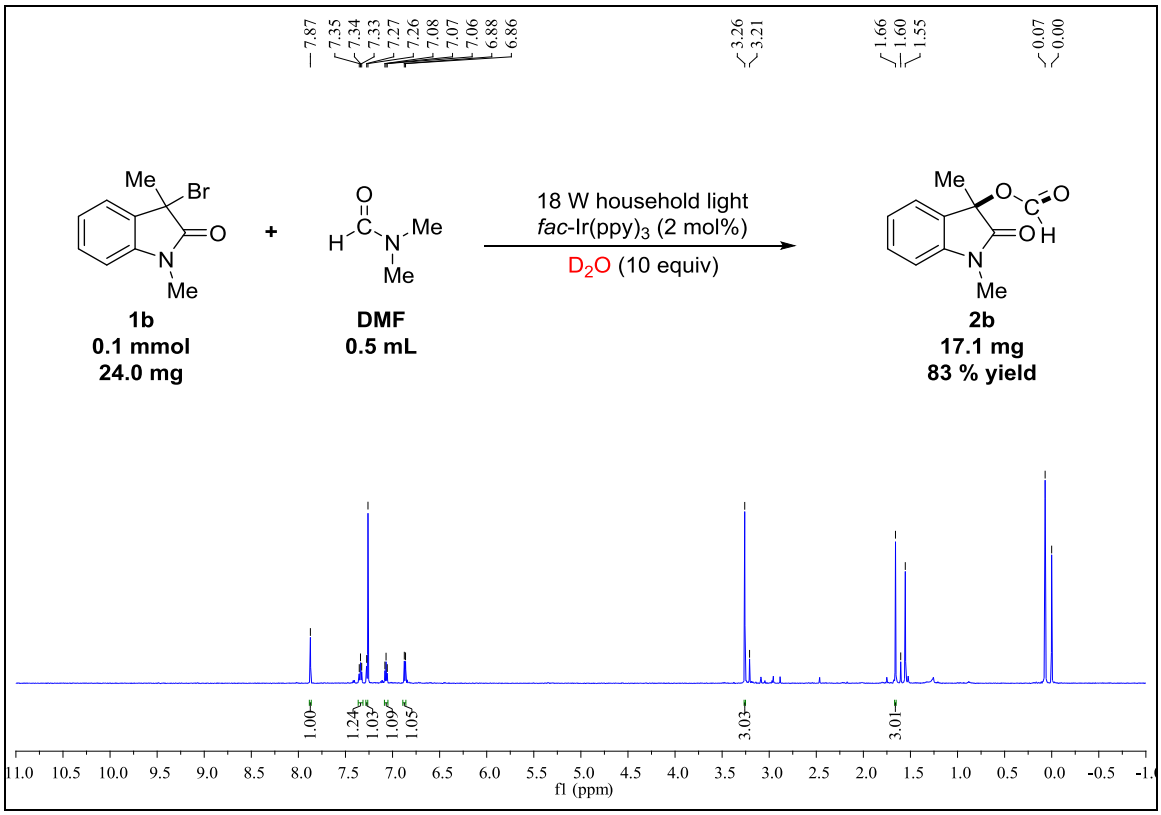
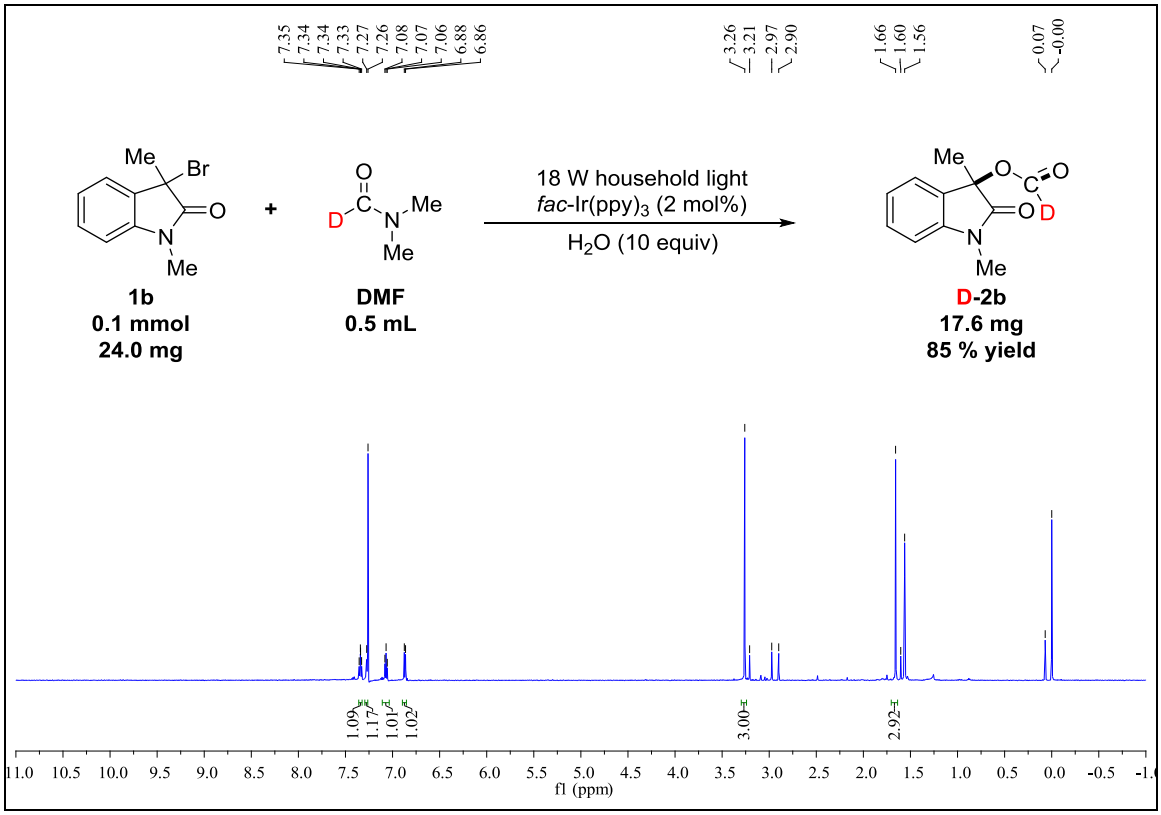


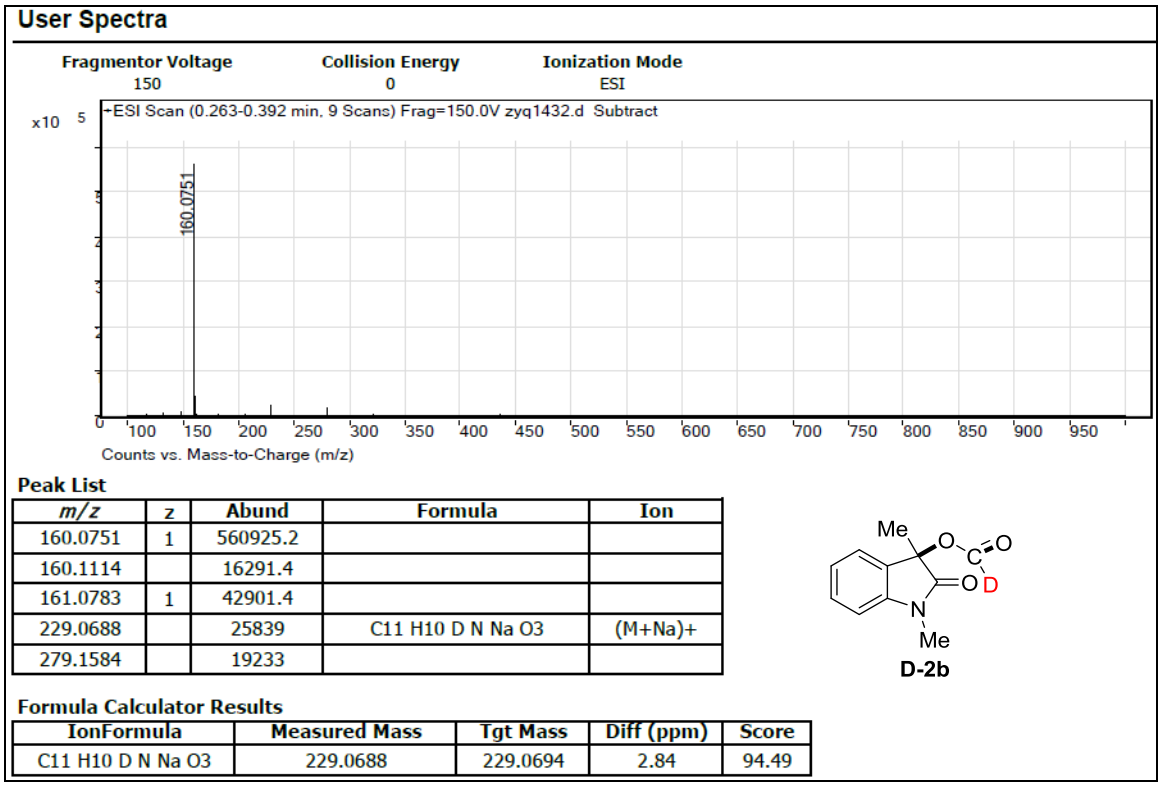
Figure 10. Time profile of visible light induced assembly of **1b**, DMF and water.

3.3 Labeling Experiments and MS Analyses

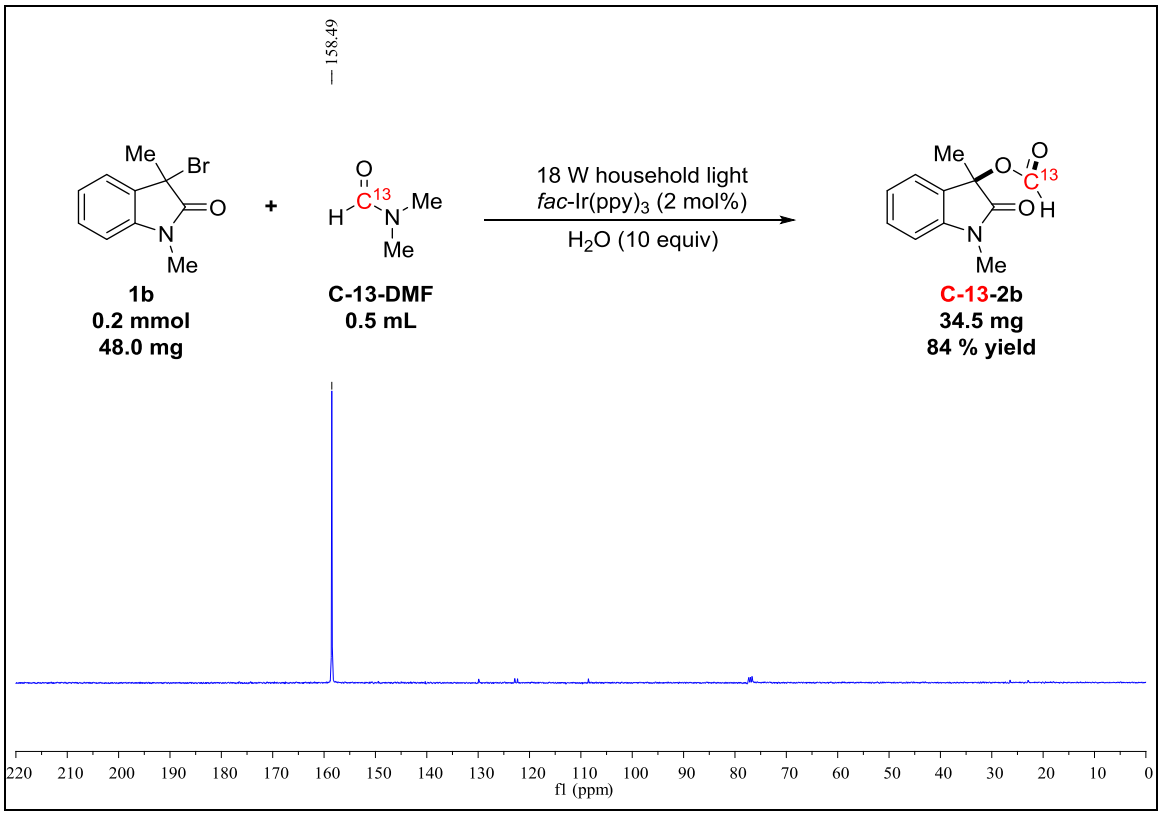
3.3.1 D-Labeling Experiments and MS Analyses


7.87
7.35
7.34
7.33
7.27
7.26
7.08
7.07
7.06
6.88
6.86
3.26
3.21
1.66
1.60
1.55
0.07
0.00
Me
Br
O
N
Me
+
O
H
C
N
Me
Me
18 W household light
fac-Ir(ppy)3 (2 mol%)
D2O (10 equiv)
Me
O
C
O
O H
N
Me
1b
0.1 mmol
24.0 mg
DMF
0.5 mL
2b
17.1 mg
83 % yield
1.00
1.24
1.03
1.09
1.05
3.03
3.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


7.35
7.34
7.34
7.33
7.27
7.26
7.08
7.07
7.06
6.88
6.86
3.26
3.21
2.97
2.90
1.66
1.60
1.56
0.07
-0.00
Me
Br
O
N
Me
+
D
O
C
N
Me
Me
18 W household light
fac-Ir(ppy)3 (2 mol%)
H2O (10 equiv)
Me
O
C
O
O D
N
Me
1b
0.1 mmol
24.0 mg
DMF
0.5 mL
D-2b
17.6 mg
85 % yield
1.09
1.17
1.01
1.02
3.00
2.92
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

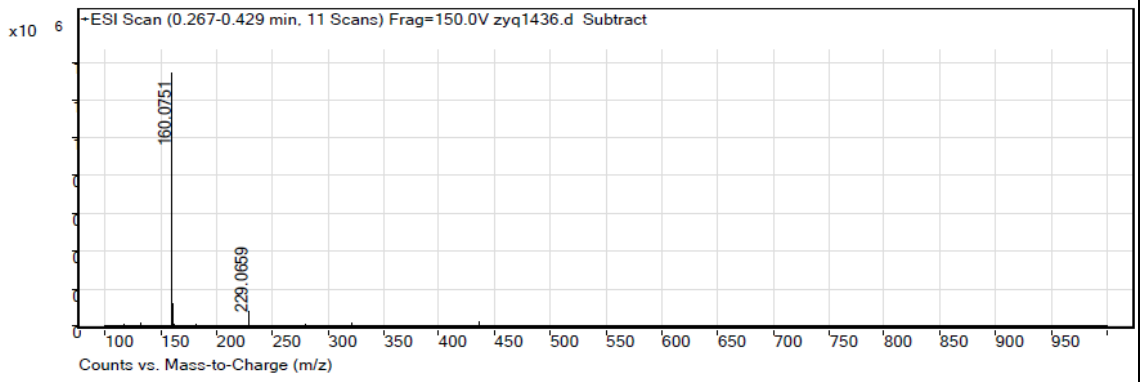


3.3.2 C-13-Labeling Experiments and MS Analyses



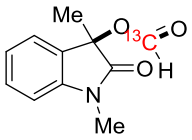
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



Peak List

m/z	z	Abund
160.0751	1	1340464.7
161.0783	1	120282.4
229.0659		73426

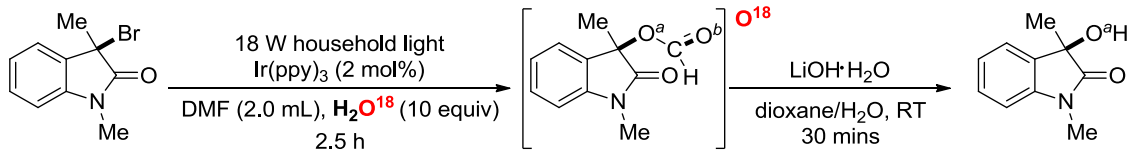


C-13-2b

Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C10 [13C] H11 N Na O3	229.0659	229.0665	2.97	92.09

3.3.3 O-18-Labeling Experiments and MS Analyses



1b, 0.4 mmol

O-18-2b
81% yield

4
85% yield

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
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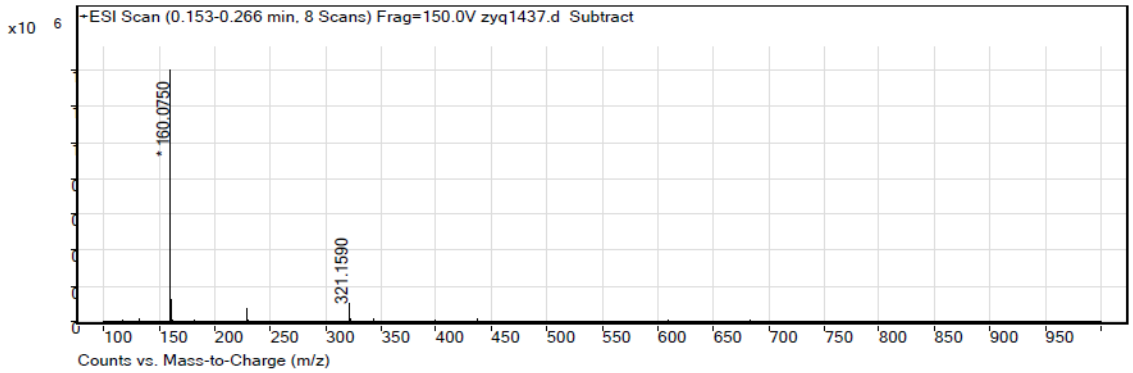
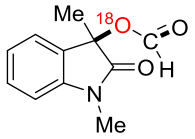


Peak List

m/z	z	Abund
160.075	1	1400172.2
161.0783	1	126337.5
321.159		100731.3



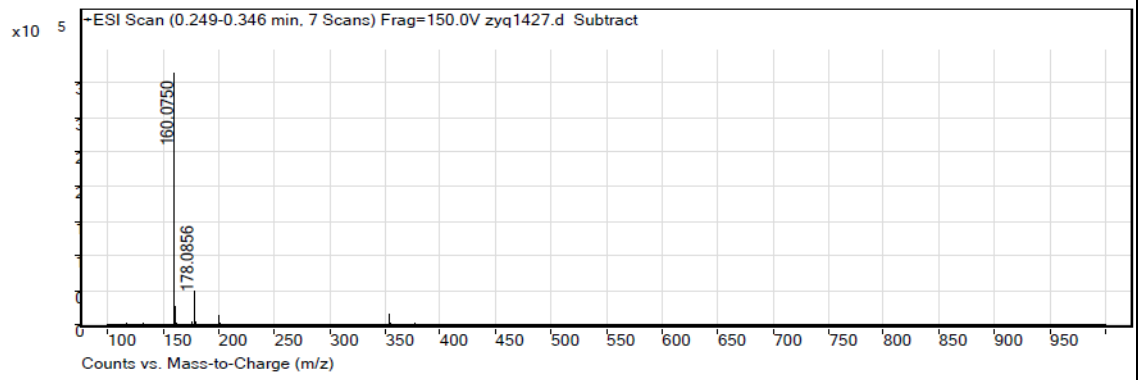
Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C11 H11 N Na O2 [18O]	230.0667	230.0674	3.06	91.95

O-18-2b

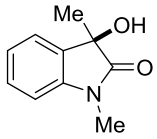
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
160.075	1	362704.7		
161.0783	1	25786.9		
178.0856		48248.9	C10 H12 N O2	(M+H)+

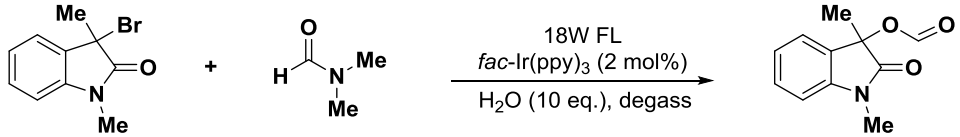


Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C10 H12 N O2	178.0856	178.0863	3.69	92.97

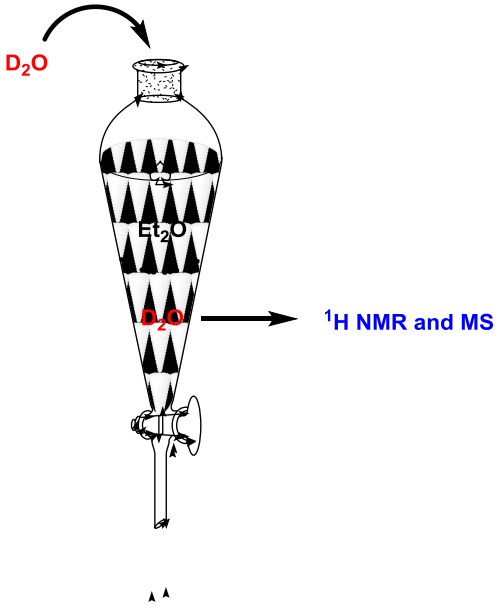
4

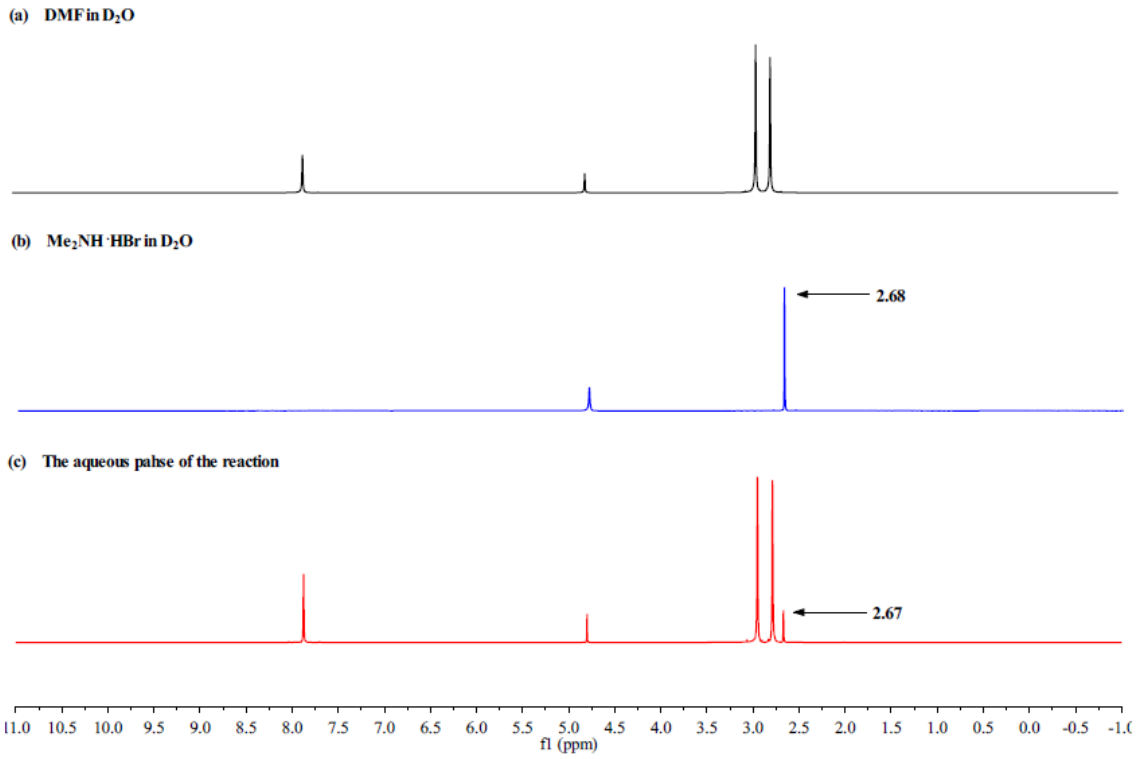
3.4 Possible Byproduct Study

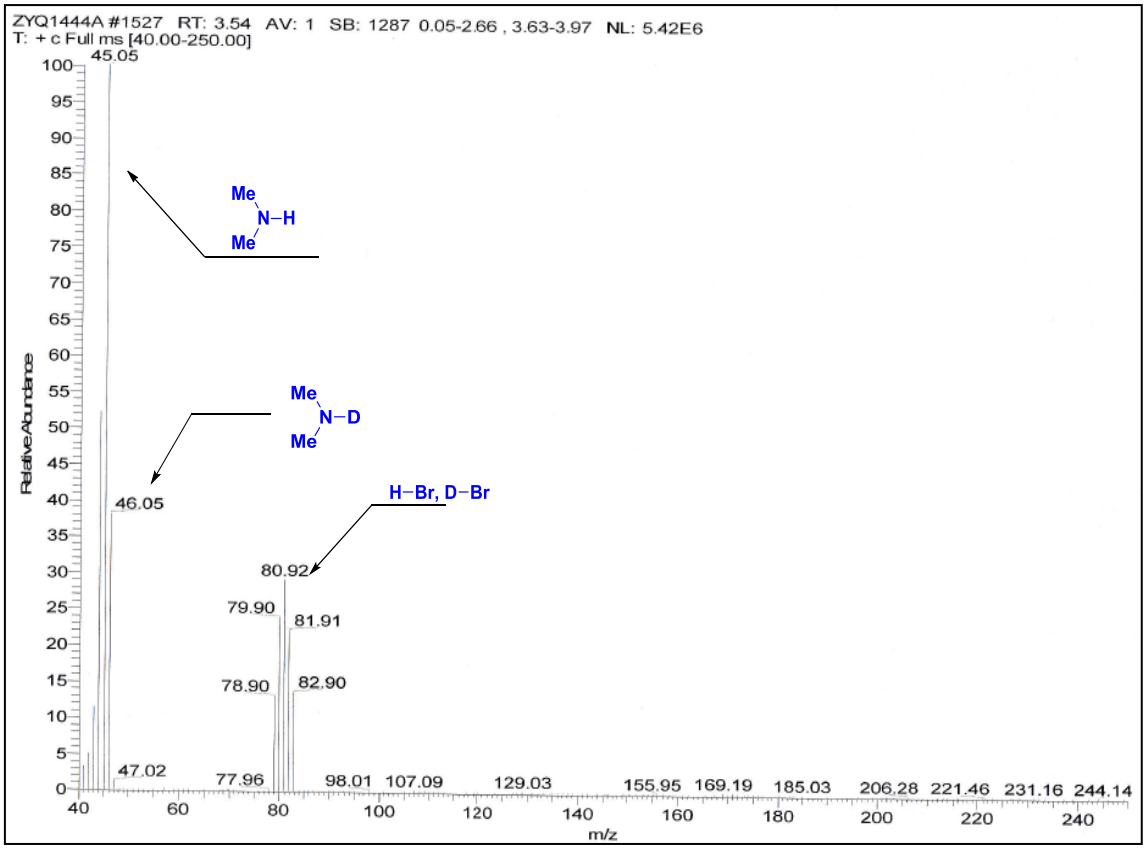


A
0.2 mmol
48.0 mg

Solvent
1.0 mL

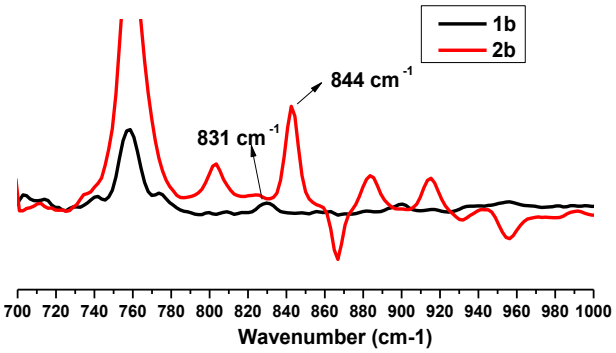






3.5 In Situ IR Experiment

3.5.1 IR spectra of 1b and 2b



3.5.2 General ReactIR Experimental Details

For the ReactIR kinetic experiments, the reaction spectra were recorded using an IC 15 from Mettler-Toledo AutoChem. Data manipulation was carried out using the iC IR software, version 4.2.

The reaction was carried out as follows: a three necked reaction vessel was fitted with a magnetic stirring bar. The IR probe was inserted through an adapter into the middle neck; the other two necks were capped by septa for injections and a nitrogen line. Following evacuation under vacuum and flushing with nitrogen for three times, the three necked vessel was charged with 3,5-dibromo-1,3-dimethylindolin-2-one **1a** (0.40 mmol, 1.0 equiv.), tris-(2-phenylpyridinato-C2,*N*)iridium(III) (*fac*-Ir(ppy)$_3$) (0.008 mmol, 0.02 equiv.), water (4.0 mmol, 10.0 equiv.), and DMF (1.0 mL). After switching on the light source, the data collection was started.

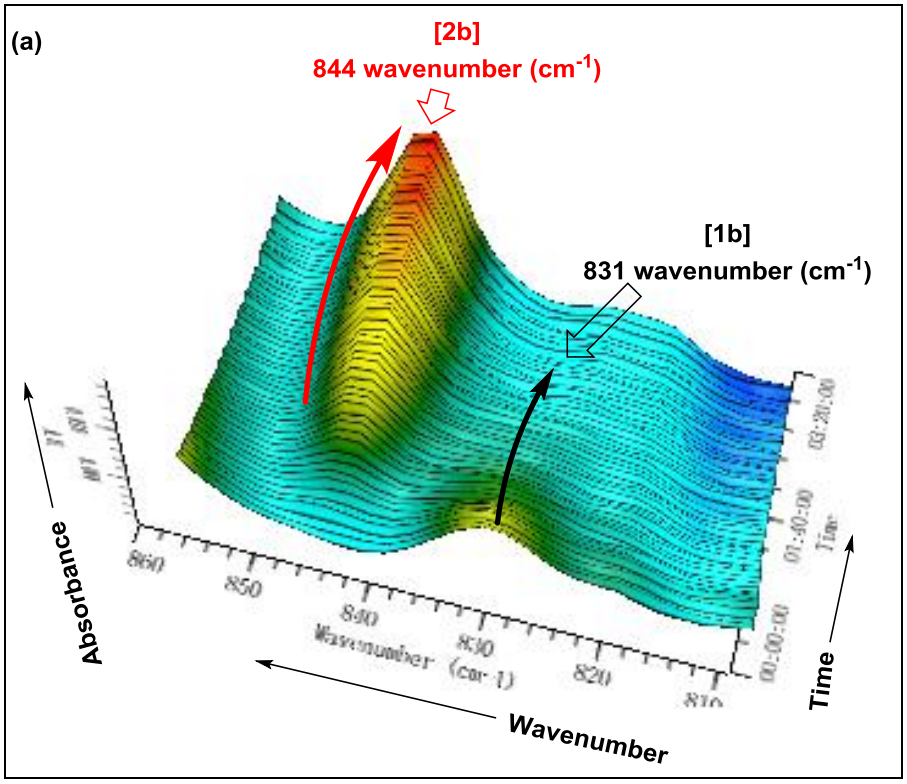


Figure (a). Overall three-dimensional Fourier transform IR (3D-FTIR) profile of the three-component reaction.

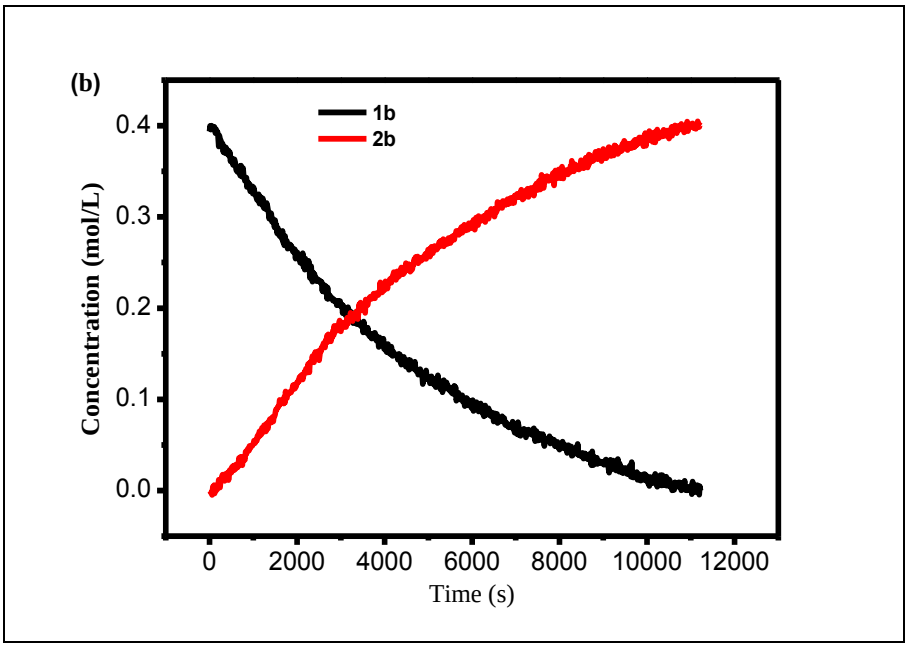
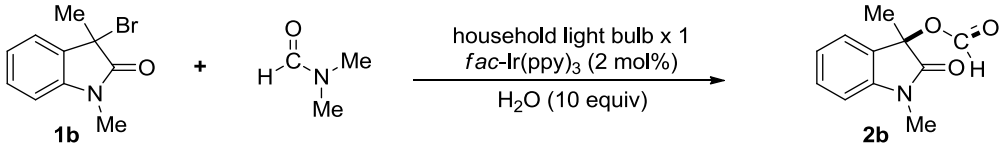
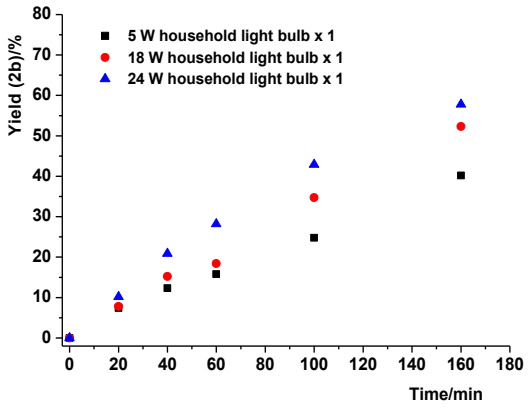


Figure (b). Kinetic profile for the three-component reaction.

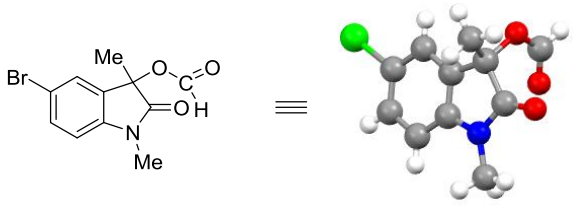
3.6 The Influence of Light Intensity



All reactions were carried out with one household light bulb (5 W, 18 W or 24 W), 3-bromo-1,3-dimethylindolin-2-one **1b** (0.40 mmol, 1.0 equiv.), tris-(2-phenylpyridinato-C2,*N*)iridium(III) (*fac*-Ir(ppy)$_3$) (0.008 mmol, 0.02 equiv.), water (4.0 mmol, 10.0 equiv.), and DMF (2.0 mL). The yields were determined by GC using n-tetradecane as an internal standard.



4. X-Ray Structures of Compound 2a



2a ≡ **X-Ray crystal structure**

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: t

```
Bond precision:  C-C = 0.0038 A          Wavelength=0.71073

Cell:              a=12.936(3)      b=12.022(2)      c=14.578(3)
                   alpha=90         beta=90          gamma=90
Temperature:       298 K

                 Calculated                Reported
Volume           2267.1(8)                 2267.1(8)
Space group      P b c a                   Pbca
Hall group       -P 2ac 2ab                ?
Moiety formula   C11 H10 Br N O3           ?
Sum formula      C11 H10 Br N O3           C11 H10 Br N O3
Mr               284.10                    284.11
Dx,g cm-3        1.665                     0.000
Z                8                         8
Mu (mm-1)        3.617                     3.617
F000             1136.0                    1136.0
F000'            1134.26
h,k,lmax         15,14,17                  15,14,17
Nref             2218                      2209
Tmin,Tmax        0.654,0.696               0.671,0.714
Tmin'            0.641

Correction method= NONE

Data completeness= 0.996          Theta(max)= 25.990

R(reflections)= 0.0346( 1812)     wR2(reflections)= 0.1224( 2209)

S = 1.053                 Npar= 147
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

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ABSTY03_ALERT_1_C  The _exptl_absorpt_correction_type has been given as none.
           However values have been given for Tmin and Tmax. Remove
           these if an absorption correction has not been applied.
  From the CIF: _exptl_absorpt_correction_T_min   0.671
  From the CIF: _exptl_absorpt_correction_T_max   0.714
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Alert level G

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PLAT093_ALERT_1_G No su's on H-positions, refinement reported as .       mixed
PLAT793_ALERT_4_G The Model has Chirality at C8      (Verify) ....          S
```

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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   1 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   3 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   0 ALERT type 2 Indicator that the structure model may be wrong or deficient
   0 ALERT type 3 Indicator that the structure quality may be low
   1 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

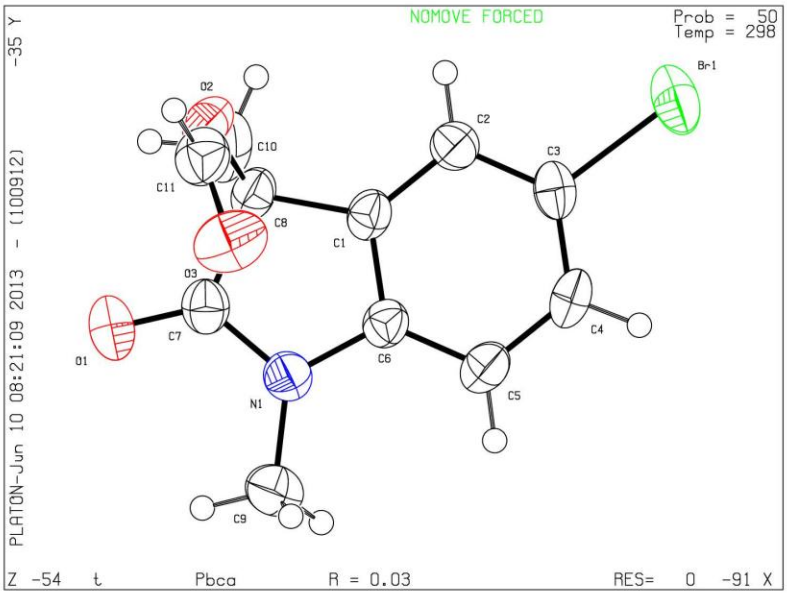
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

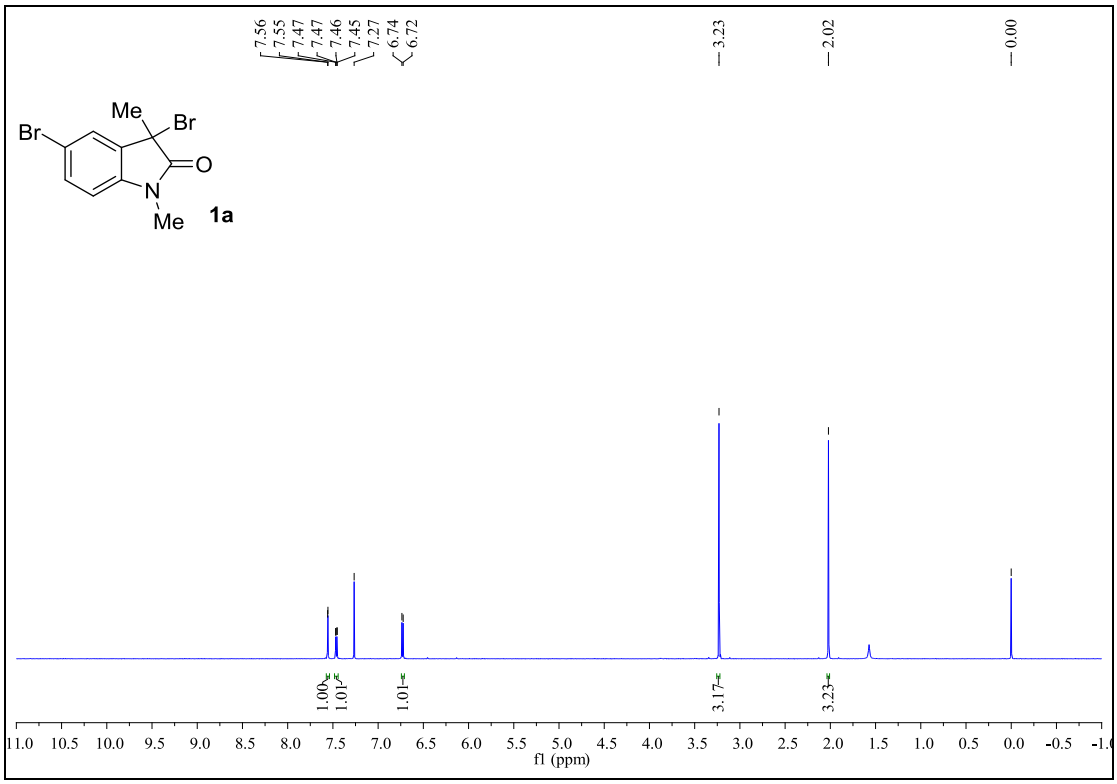
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

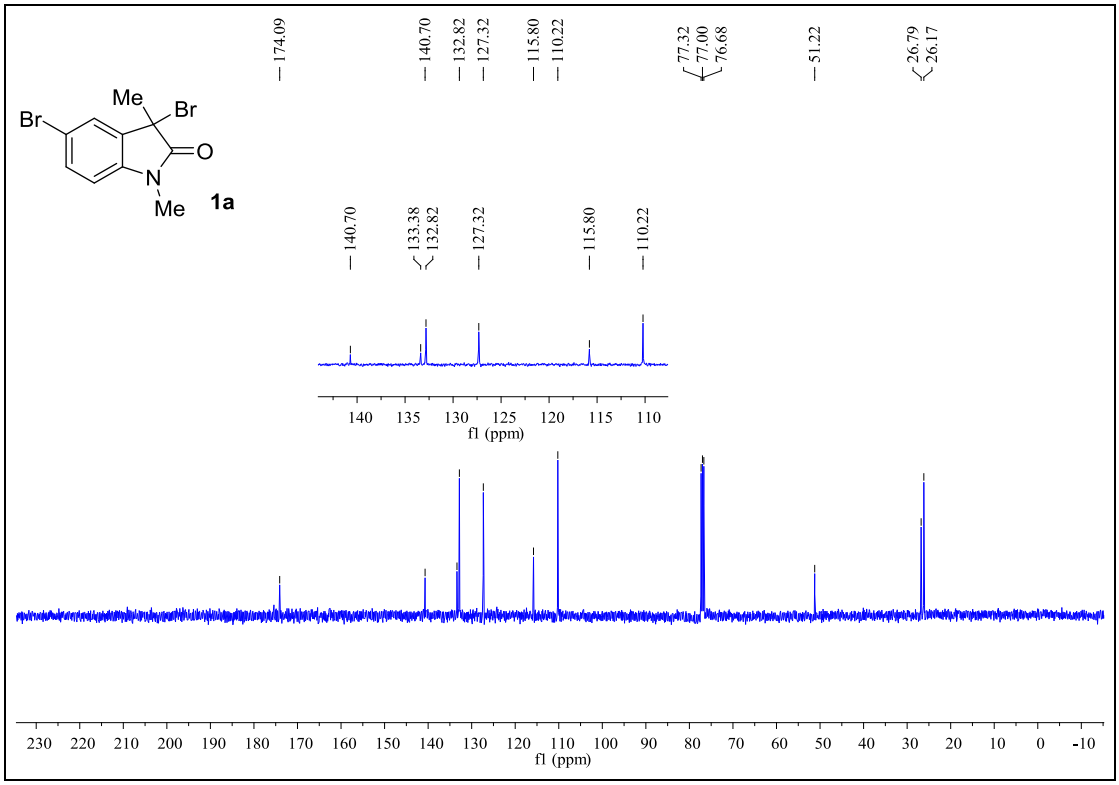
PLATON version of 01/06/2013; check.def file version of 24/05/2013

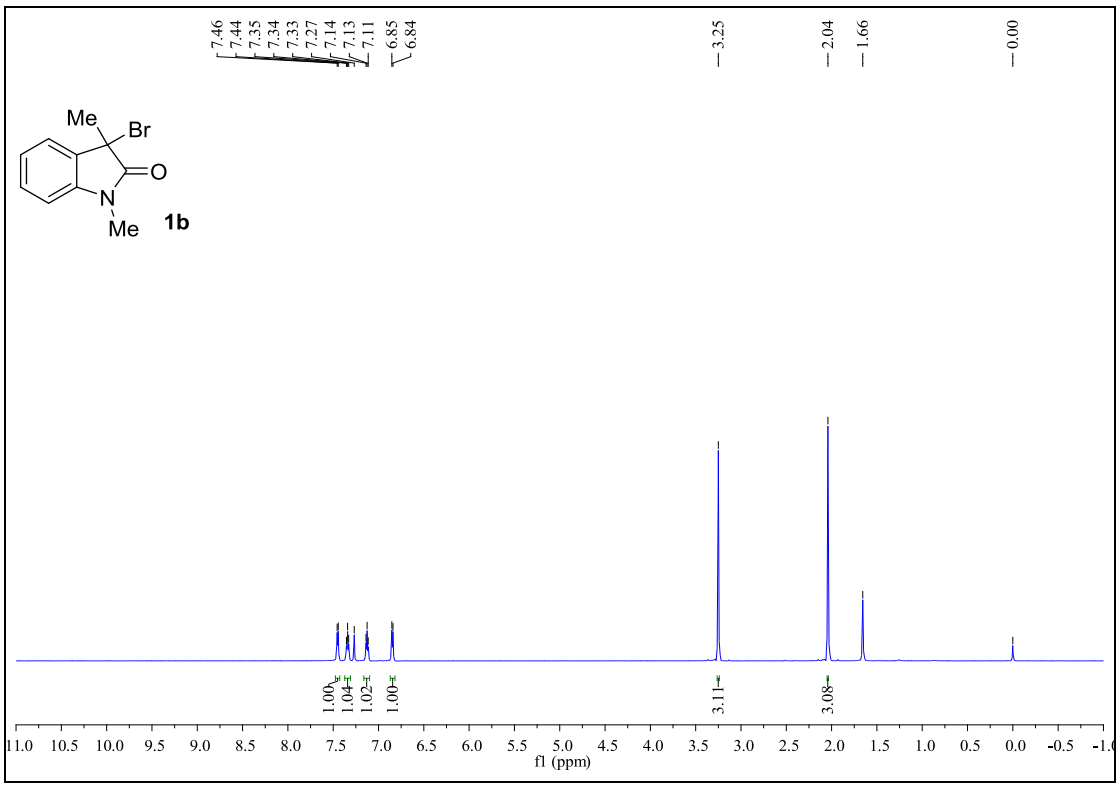
Datablock t - ellipsoid plot



5. Copies of NMR, MS and Elemental Analysis Data



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1.66
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O
N
Me
1b
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1.02
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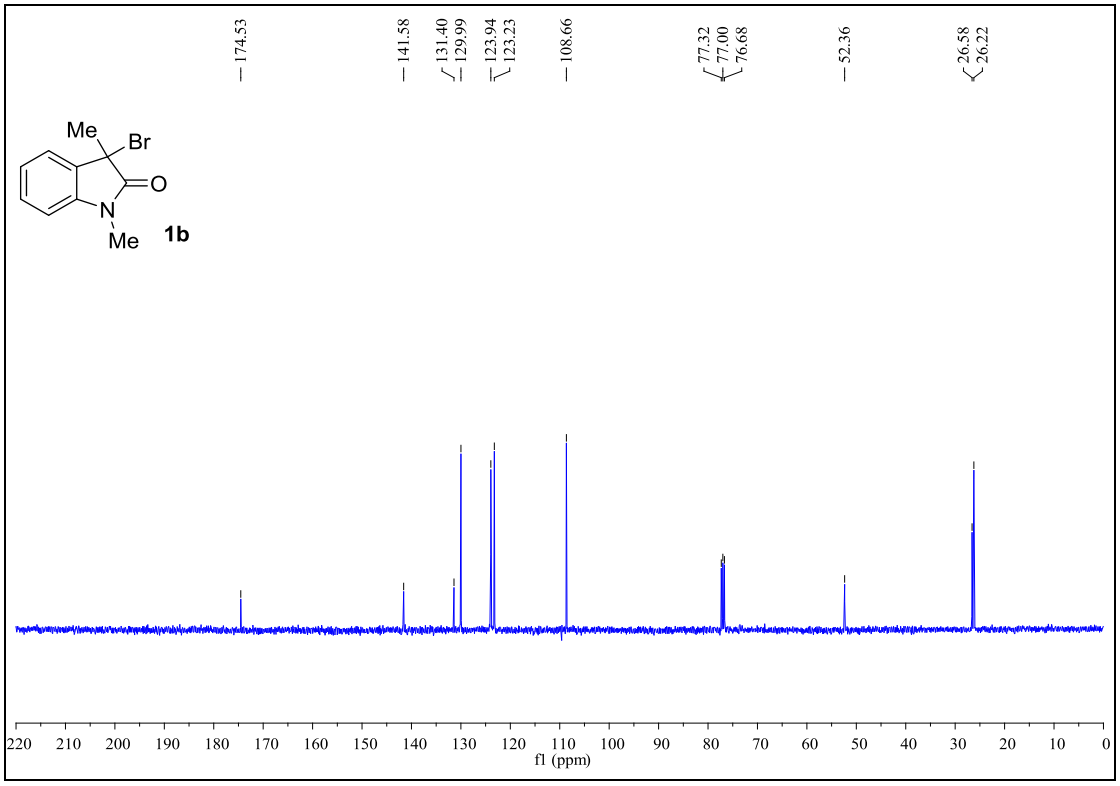
3.08
fl (ppm)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Br
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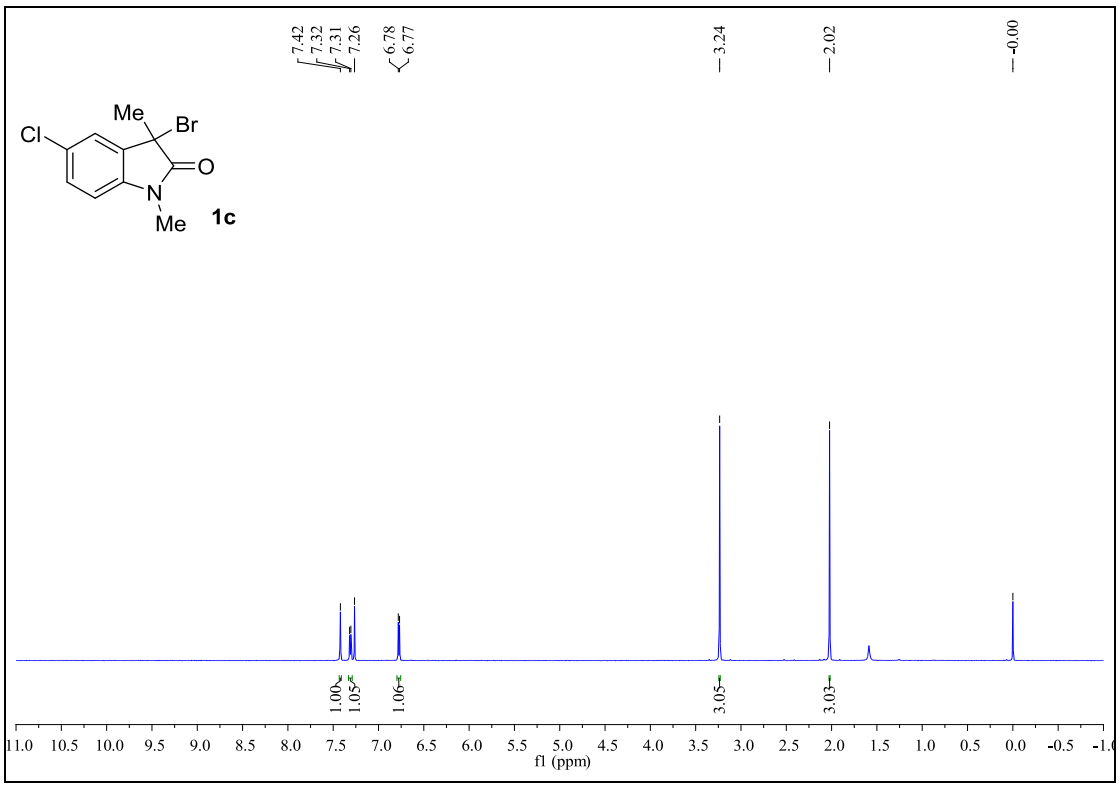
1b
fl (ppm)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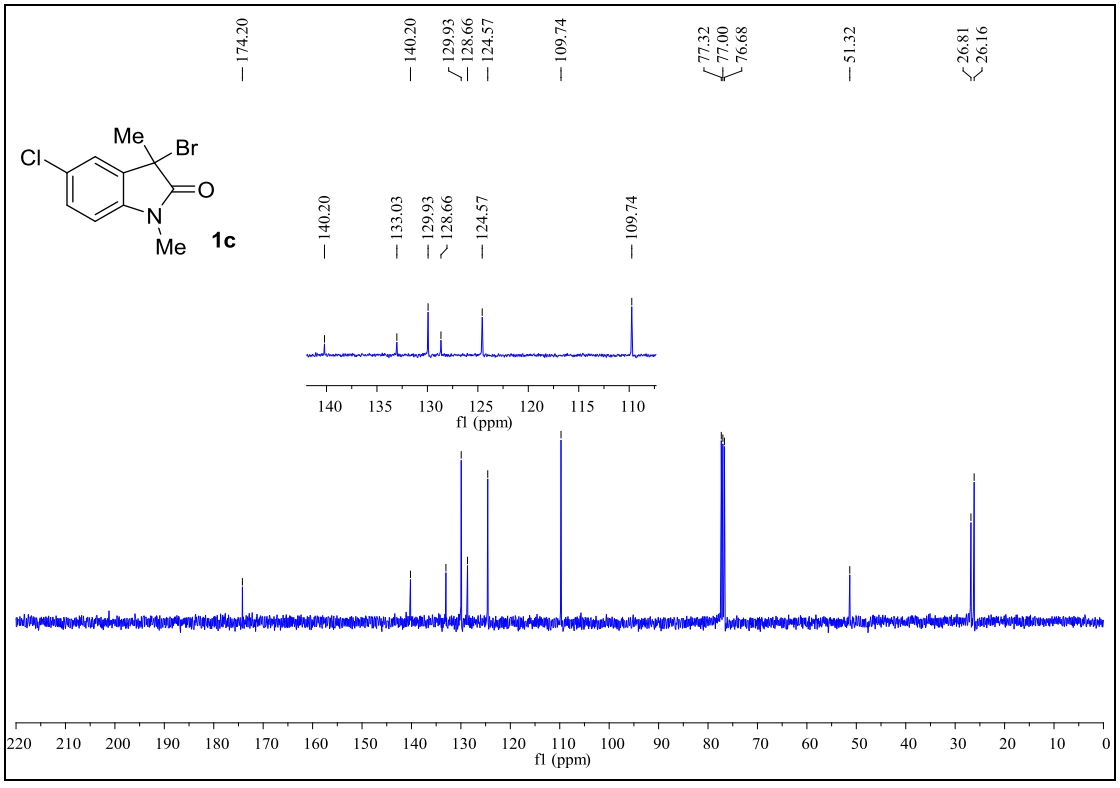
fl (ppm)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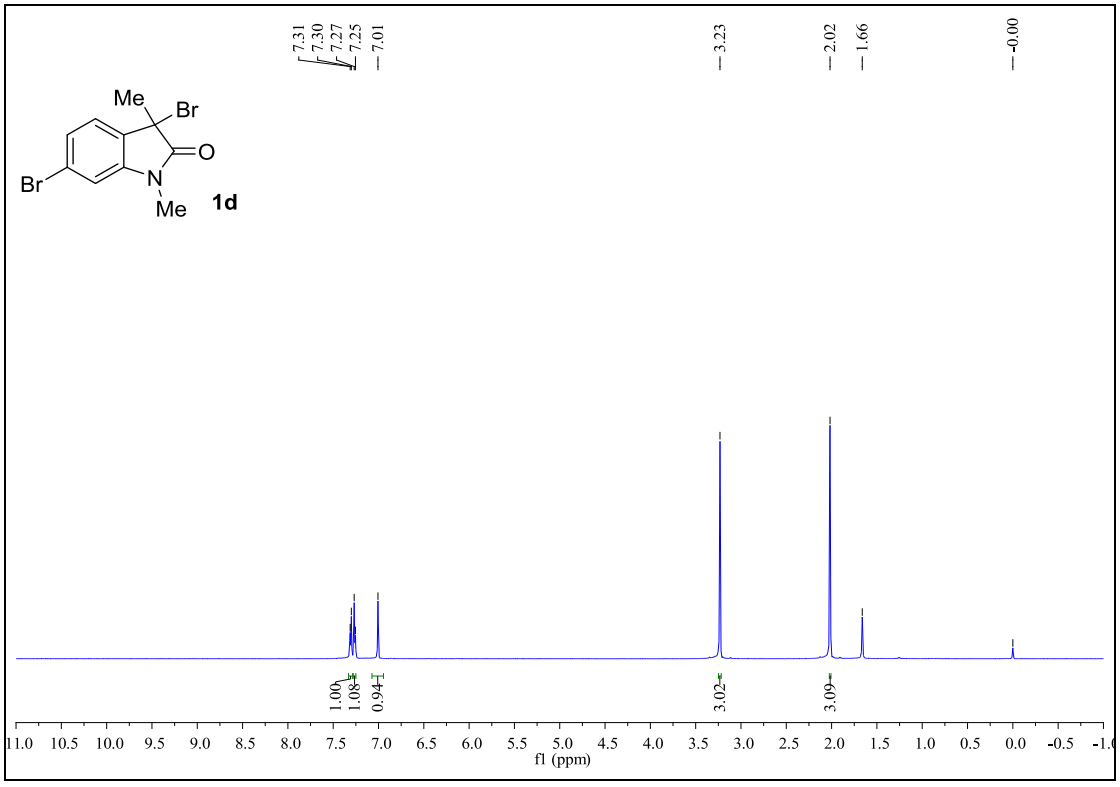
fl (ppm)
fl (ppm)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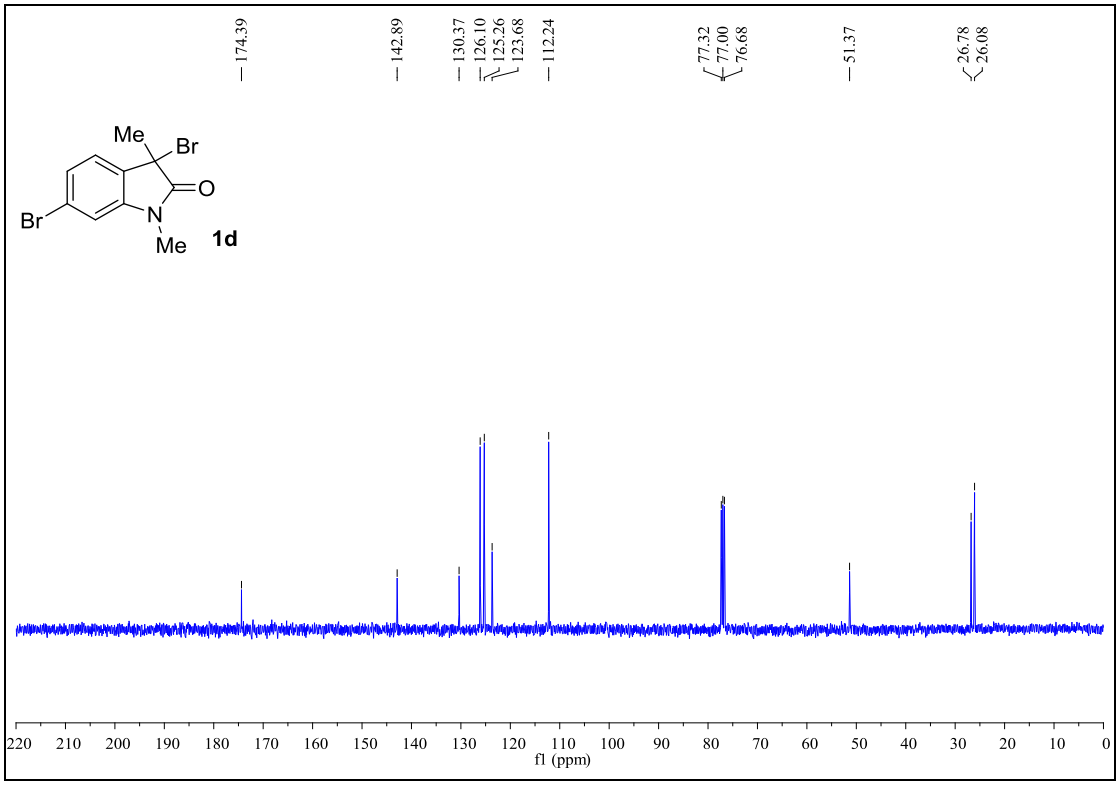
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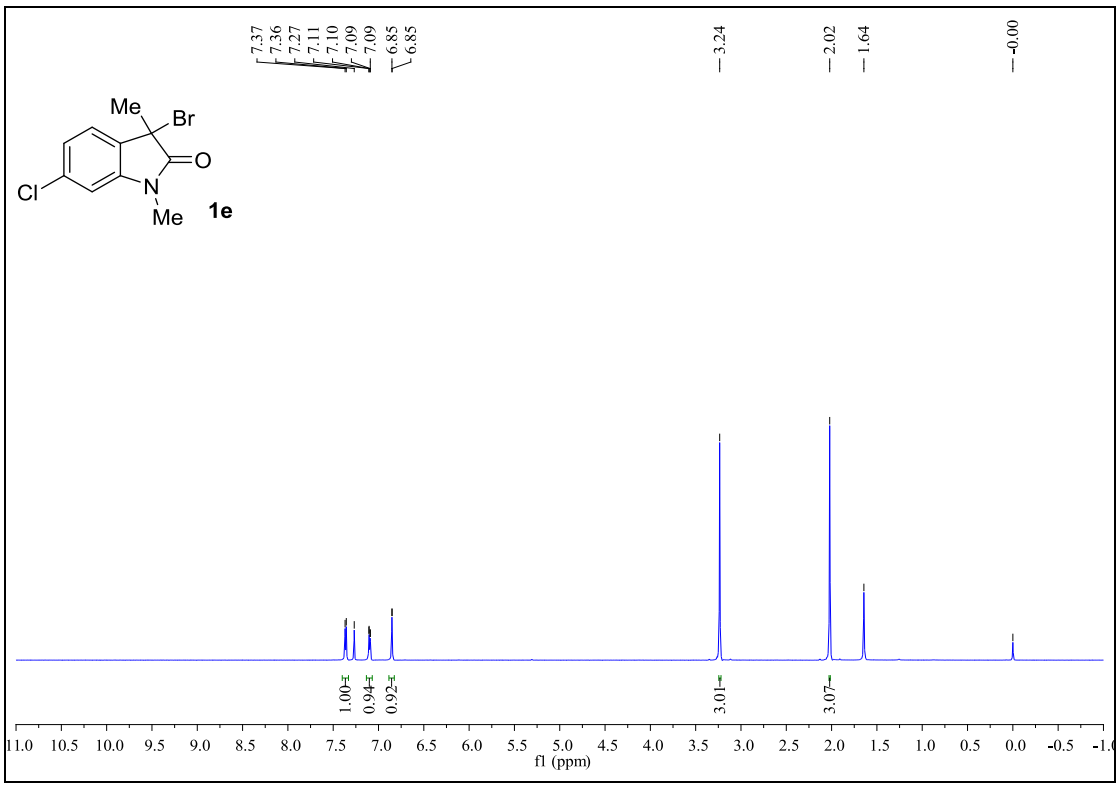
fl (ppm)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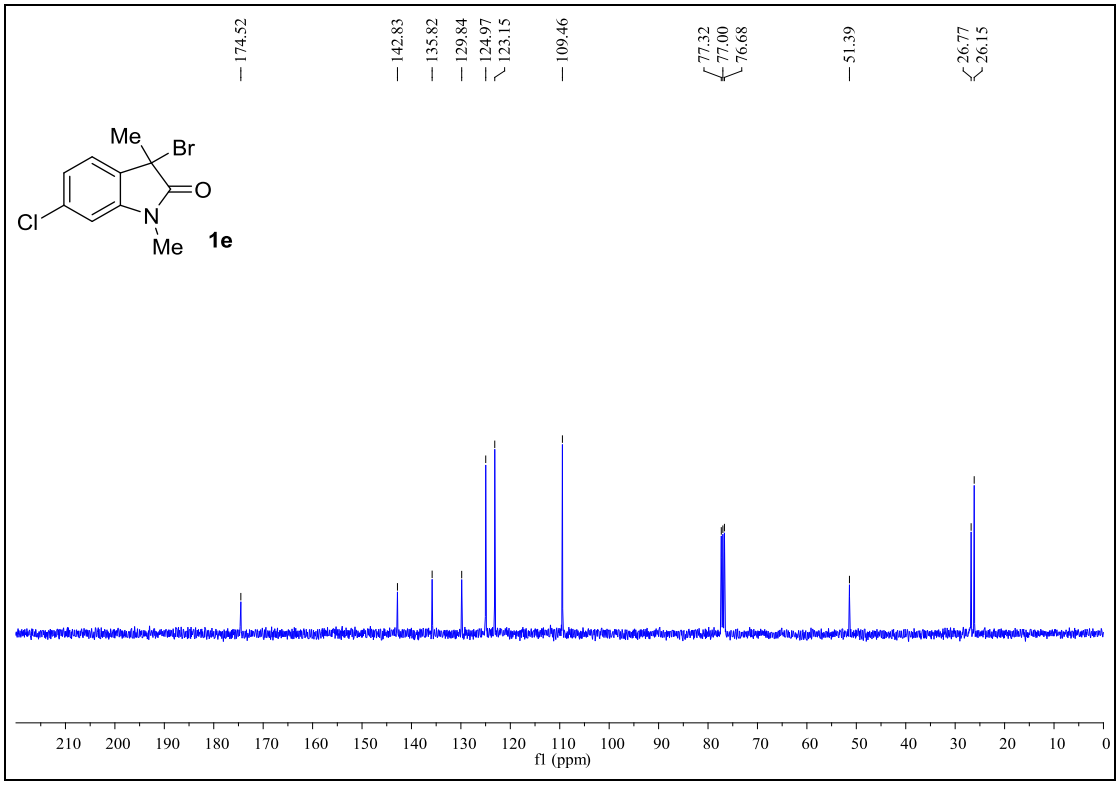
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Cl
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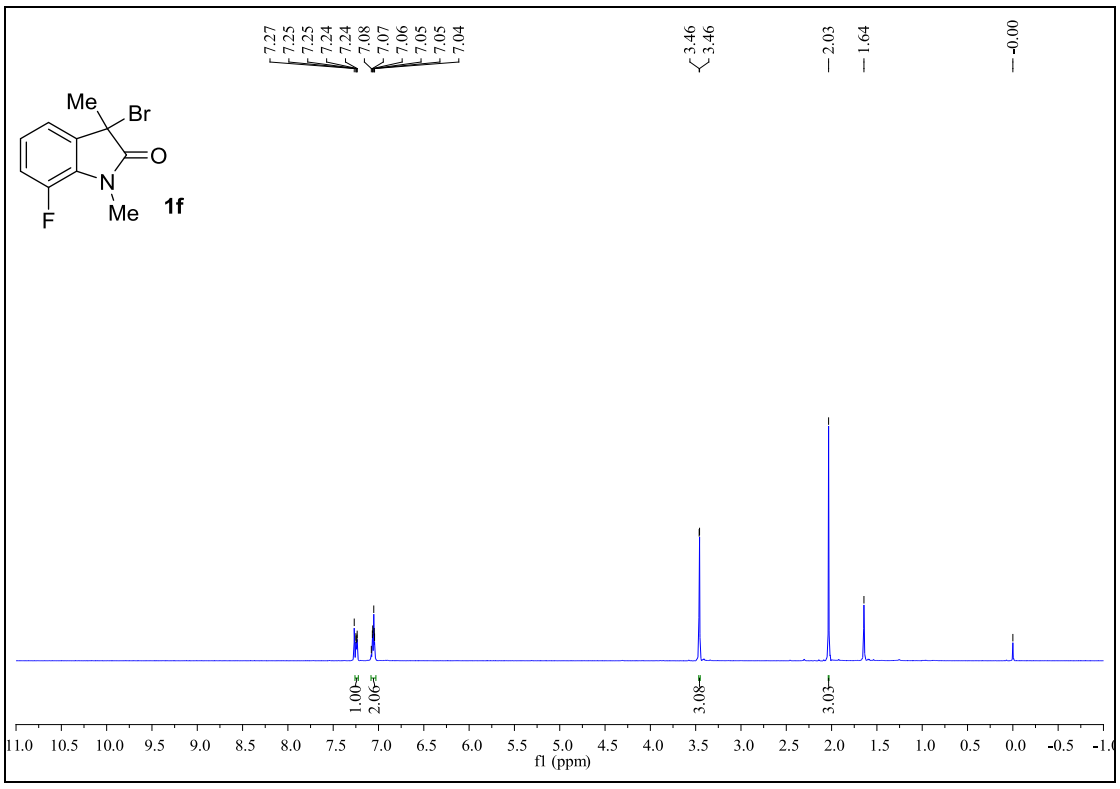
f1 (ppm)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F
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2.06
3.08
3.03
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
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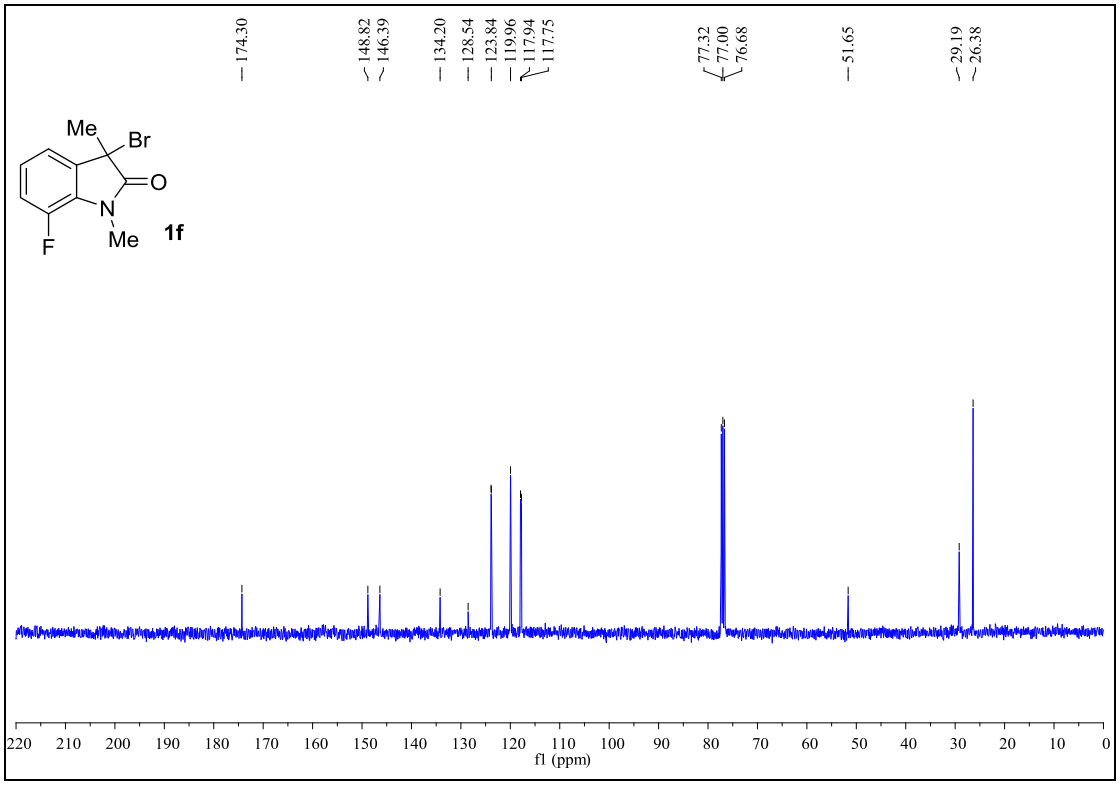
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29.19
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F
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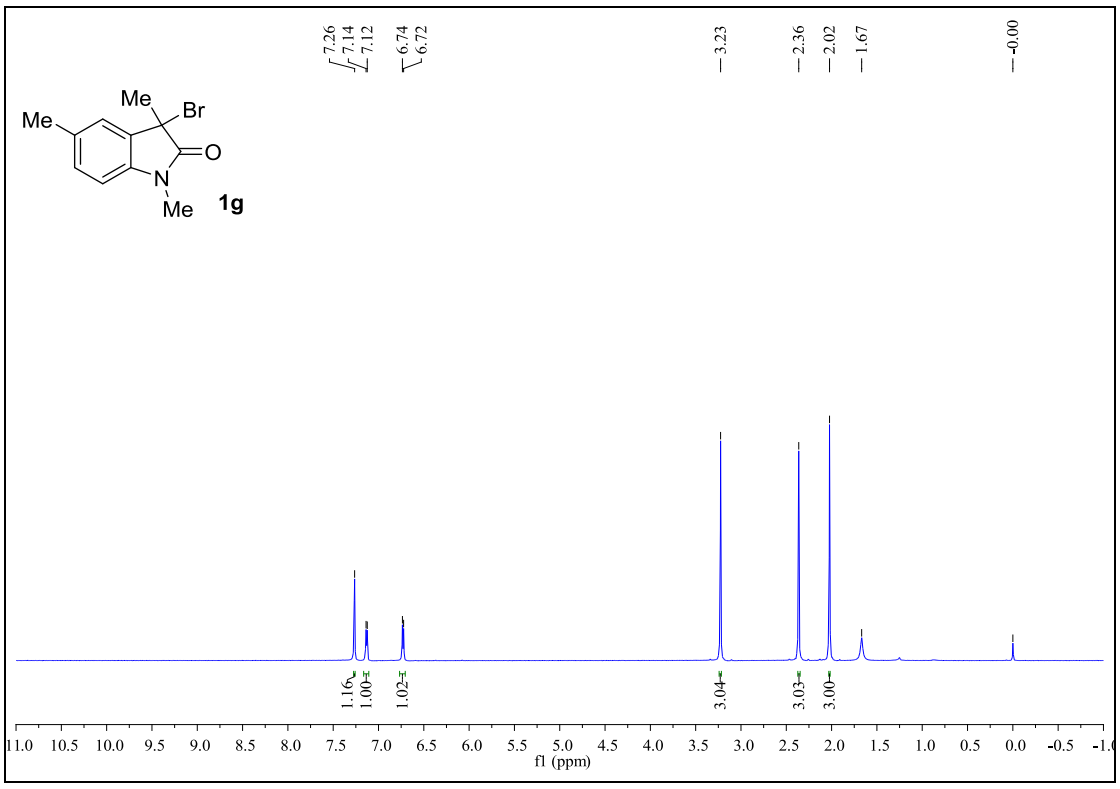
f1 (ppm)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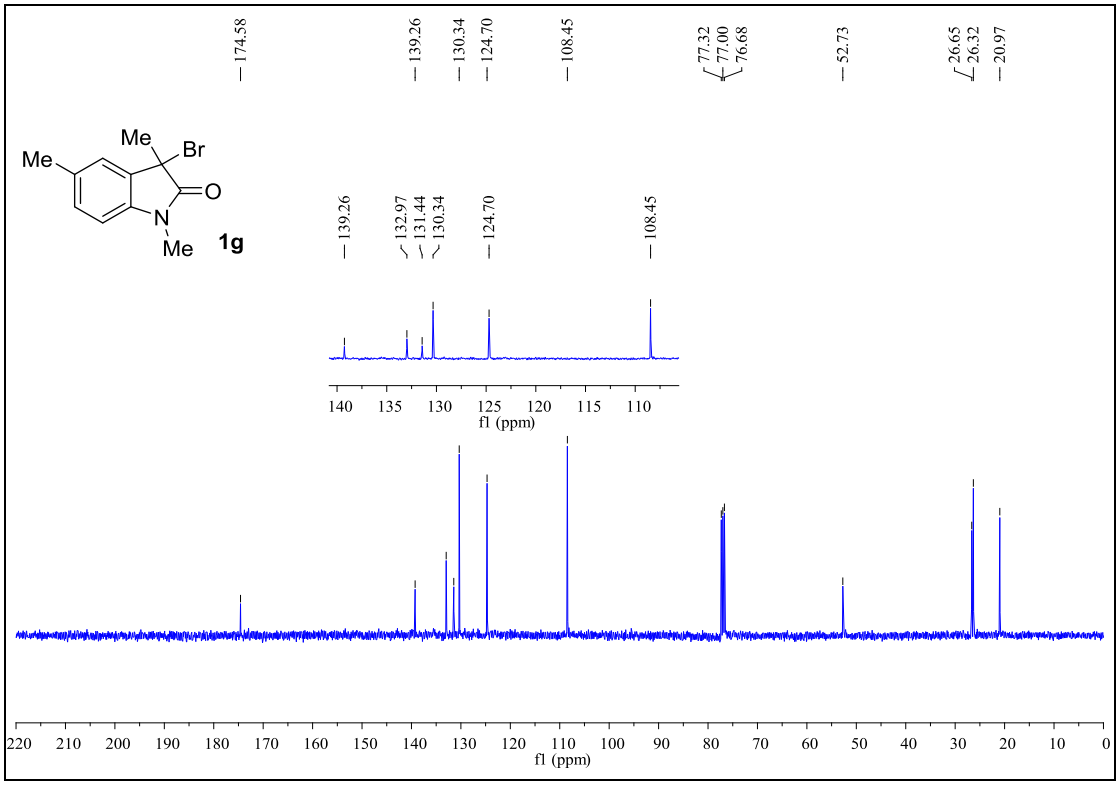
Me
1g
1.16
1.00
1.02
3.04
3.03
3.00
fl (ppm)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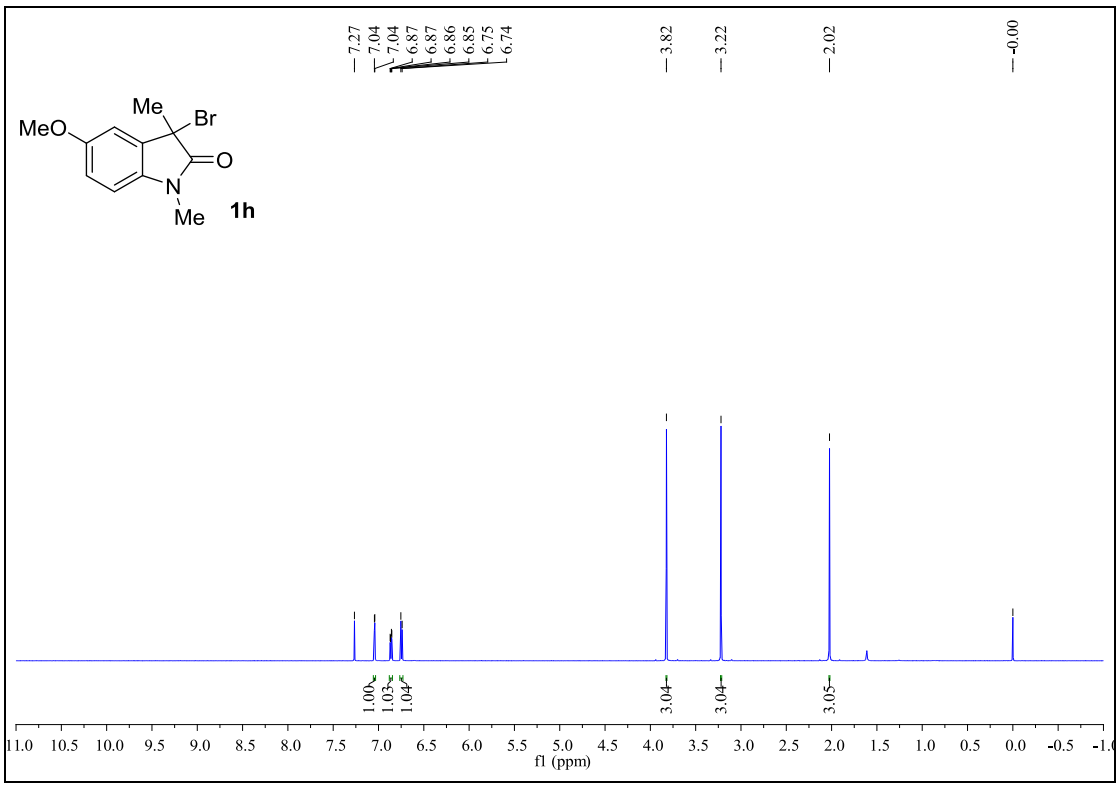
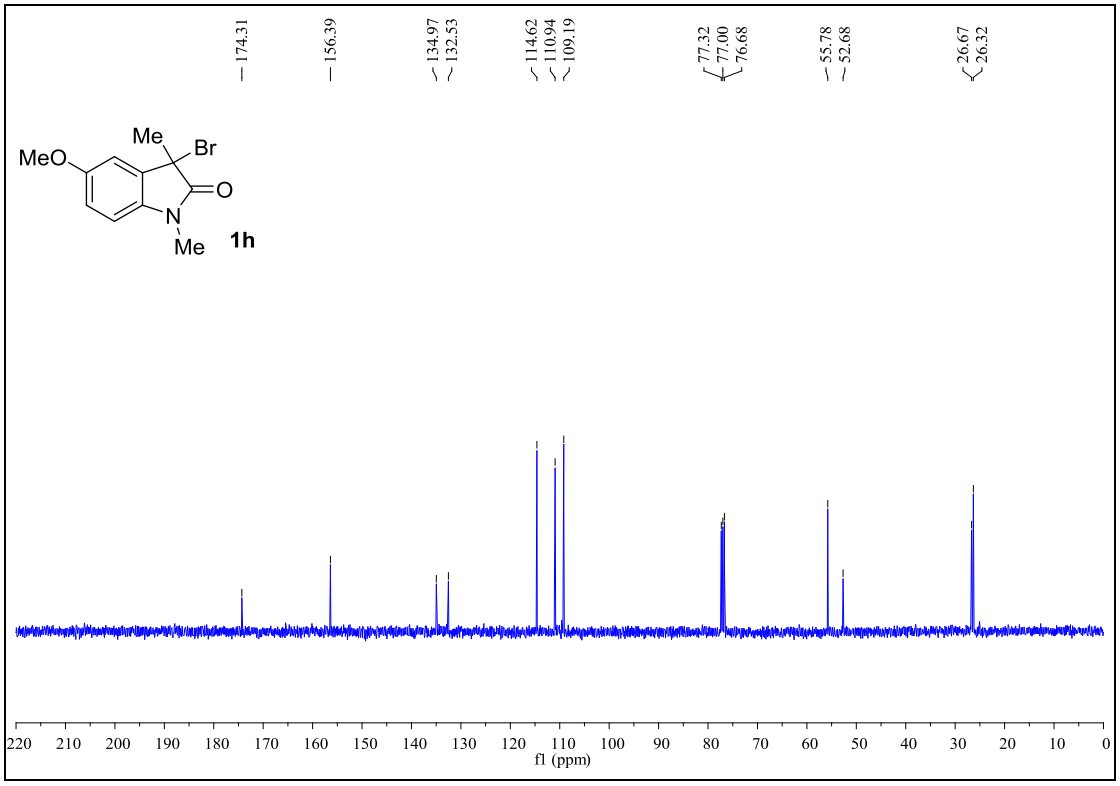
139.26
130.34
124.70
108.45
77.32
77.00
76.68
52.73
26.65
26.32
20.97
Me
Br
Me
O
N
Me
1g
139.26
132.97
131.44
130.34
124.70
108.45
fl (ppm)
fl (ppm)


7.27
7.04
7.04
6.87
6.87
6.86
6.85
6.75
6.74
3.82
3.22
2.02
0.00
Me
Br
MeO
O
N
Me
1h
1.00
1.03
1.04
3.04
3.04
3.05
fl (ppm)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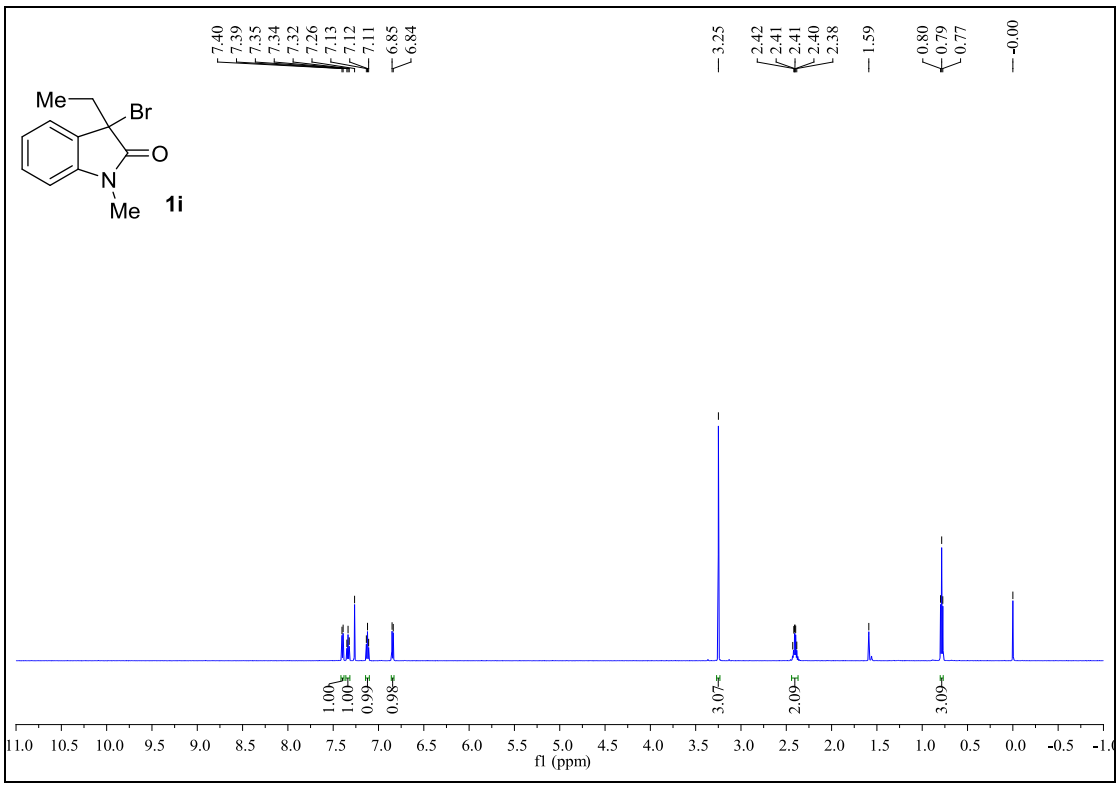
156.39
134.97
132.53
114.62
110.94
109.19
77.32
77.00
76.68
55.78
52.68
26.67
26.32
Me
Br
MeO
O
N
Me
1h
fl (ppm)


7.40
7.39
7.35
7.34
7.32
7.26
7.13
7.12
7.11
6.85
6.84
3.25
2.42
2.41
2.41
2.40
2.38
1.59
0.80
0.79
0.77
0.00
Me
Br
O
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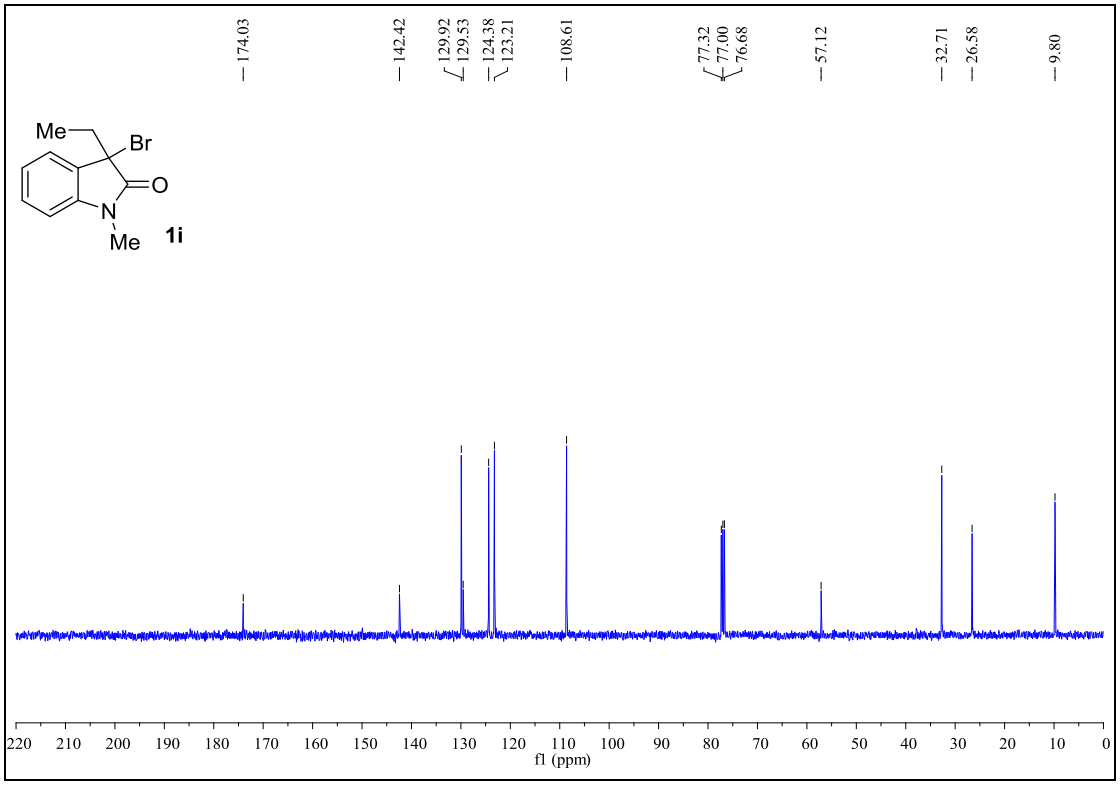
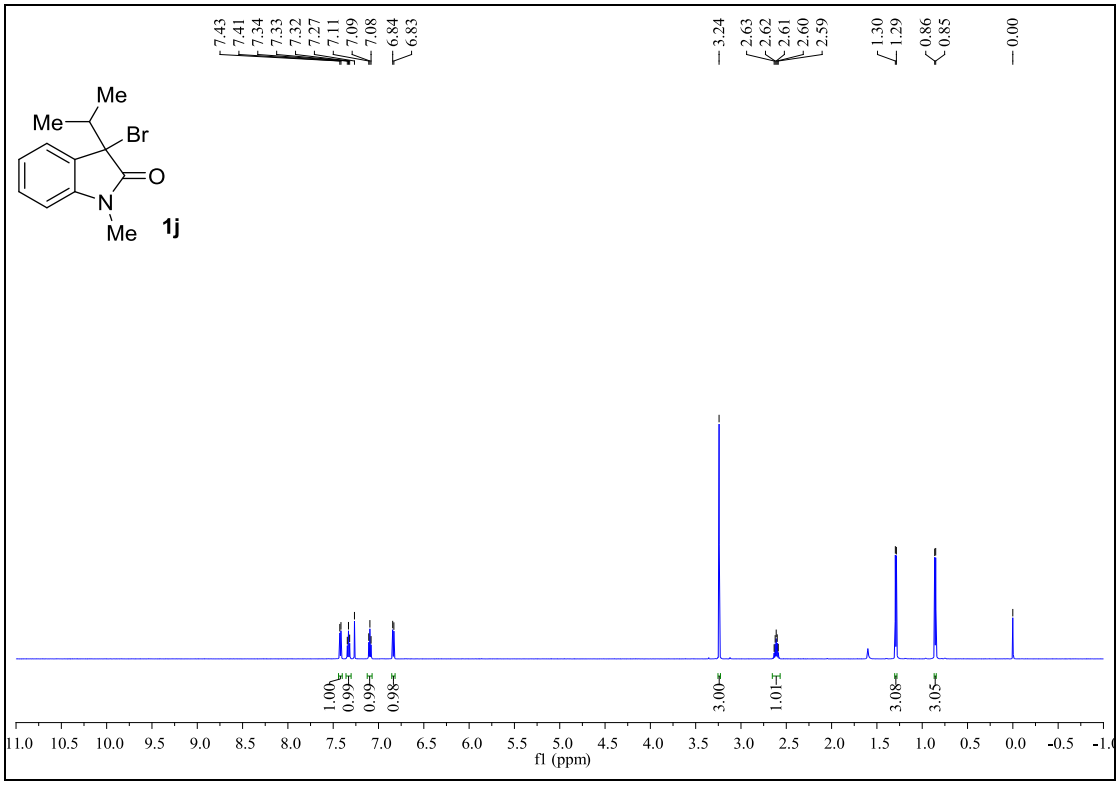
Me
1i
1.00
1.00
0.99
0.98
3.07
2.09
3.09
fl (ppm)


174.03
142.42
129.92
129.53
124.38
123.21
108.61
77.32
77.00
76.68
57.12
32.71
26.58
9.80
Me
Br
O
N
Me
1i
fl (ppm)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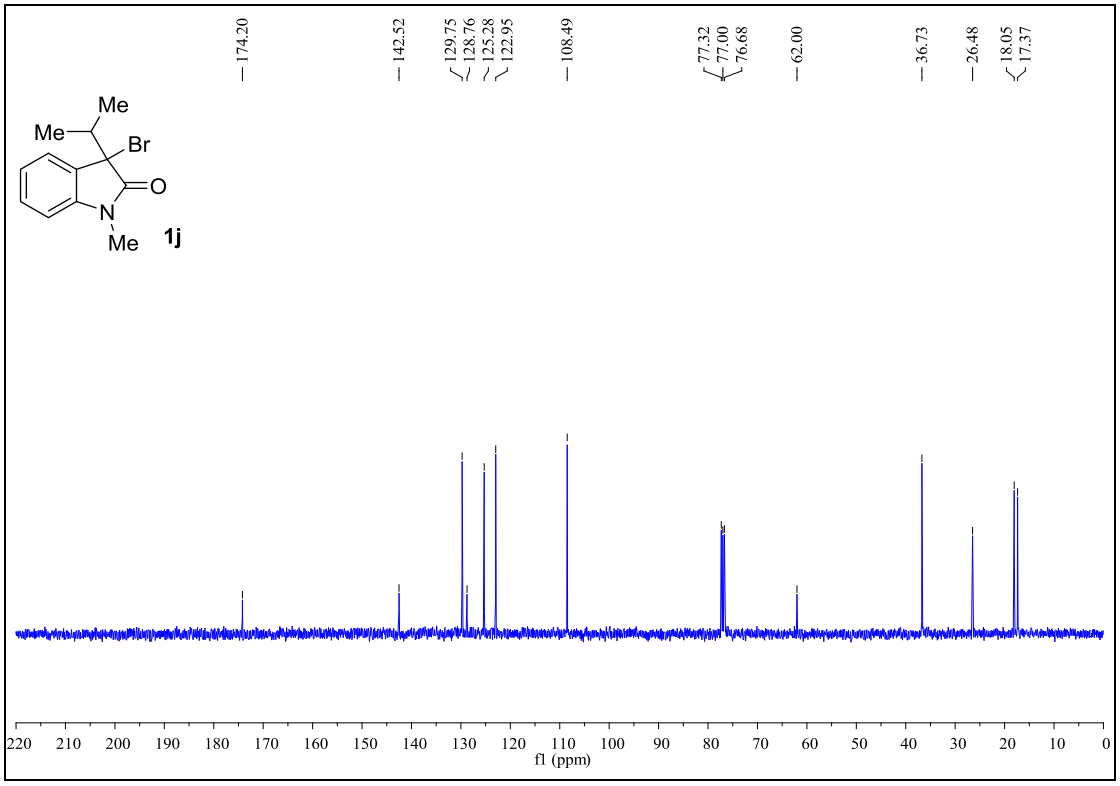
7.41
7.34
7.33
7.32
7.27
7.11
7.09
7.08
6.84
6.83
3.24
2.63
2.62
2.61
2.60
2.59
1.30
1.29
0.86
0.85
0.00
Me
Me
Br
O
N
Me
1j
1.00
0.99
0.99
0.98
3.00
1.01
3.08
3.05
fl (ppm)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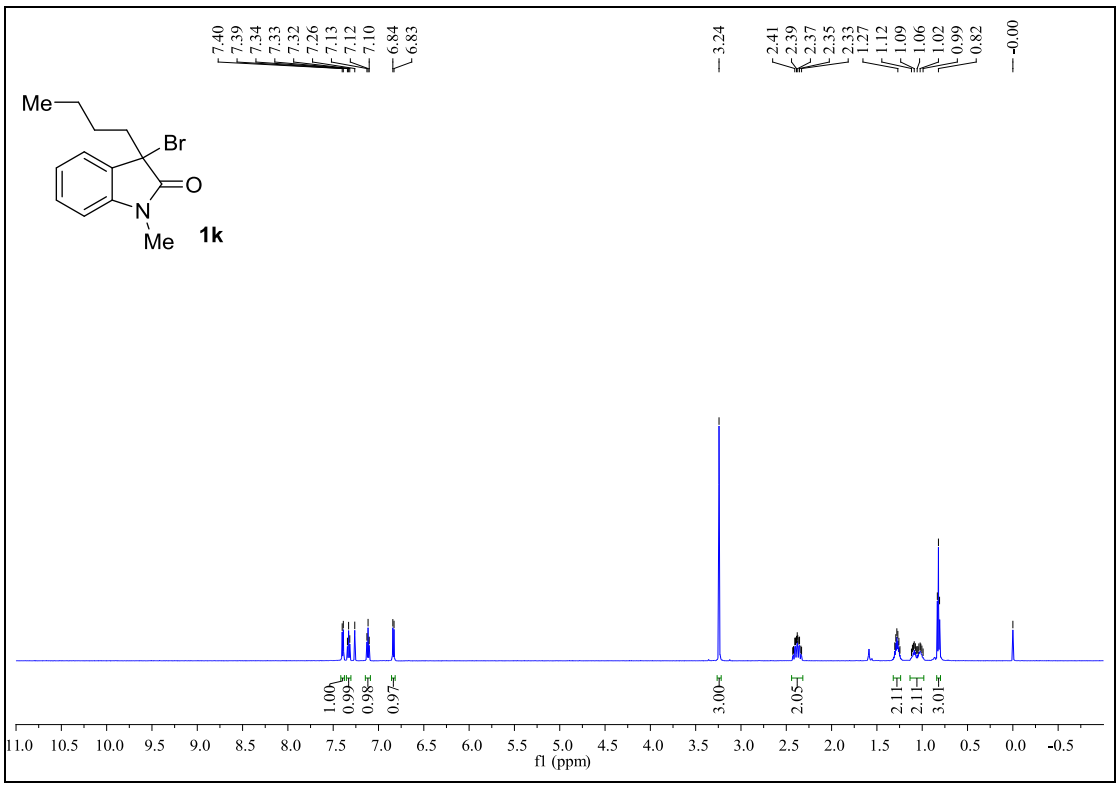
142.52
129.75
128.76
125.28
122.95
108.49
77.32
77.00
76.68
62.00
36.73
26.48
18.05
17.37
Me
Me
Br
O
N
Me
1j
fl (ppm)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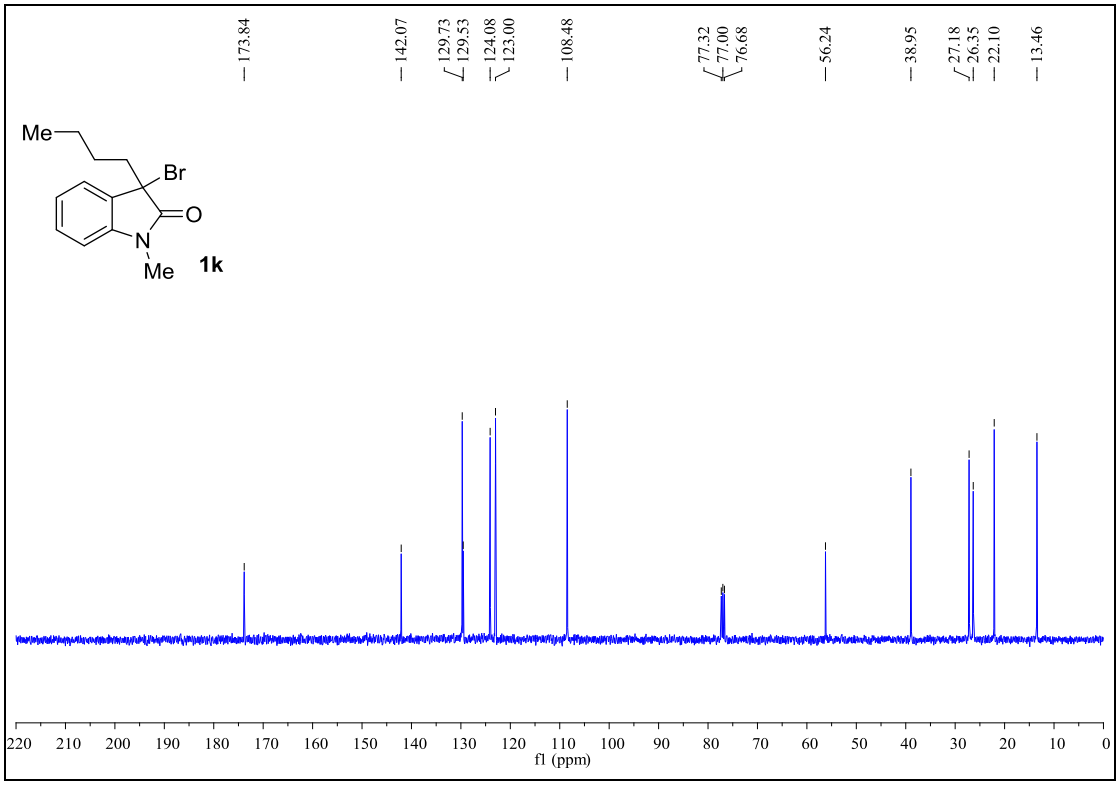
7.39
7.34
7.33
7.32
7.26
7.13
7.12
7.10
6.84
6.83
3.24
2.41
2.39
2.37
2.35
2.33
1.27
1.12
1.09
1.06
1.02
0.99
0.82
0.00
Me
Br
O
N
Me
1k
1.00
0.99
0.98
0.97
3.00
2.05
2.11
2.11
3.01
fl (ppm)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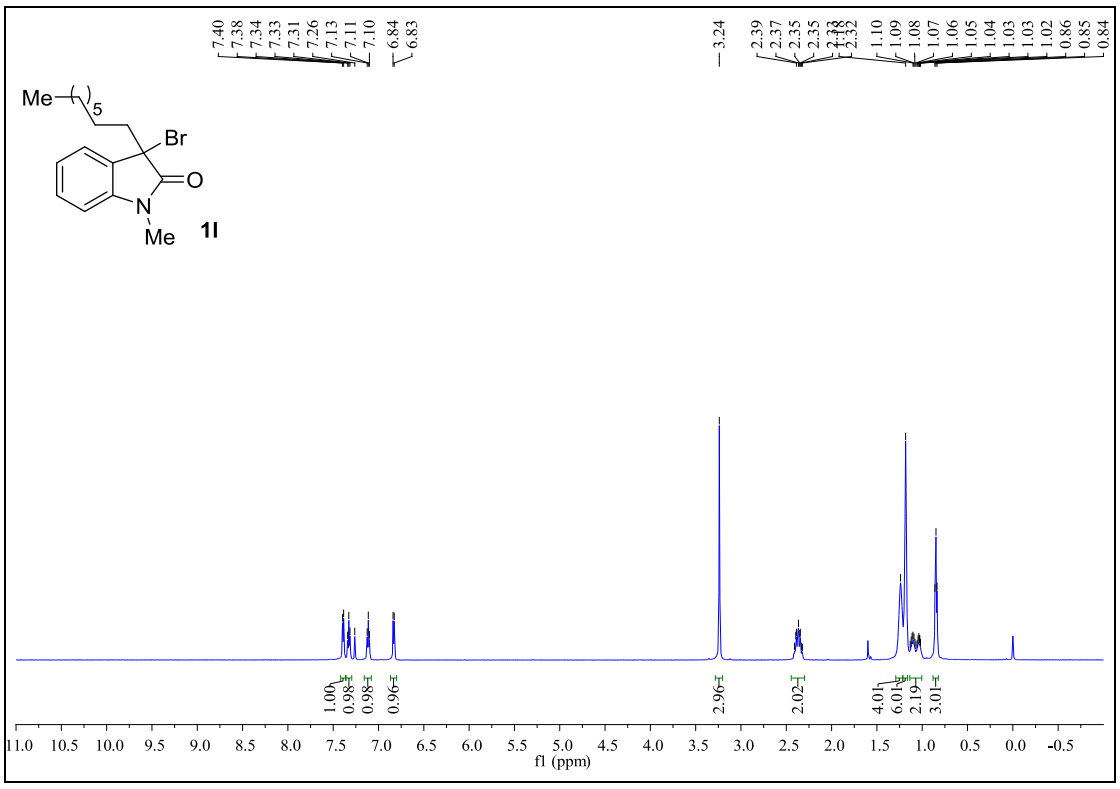
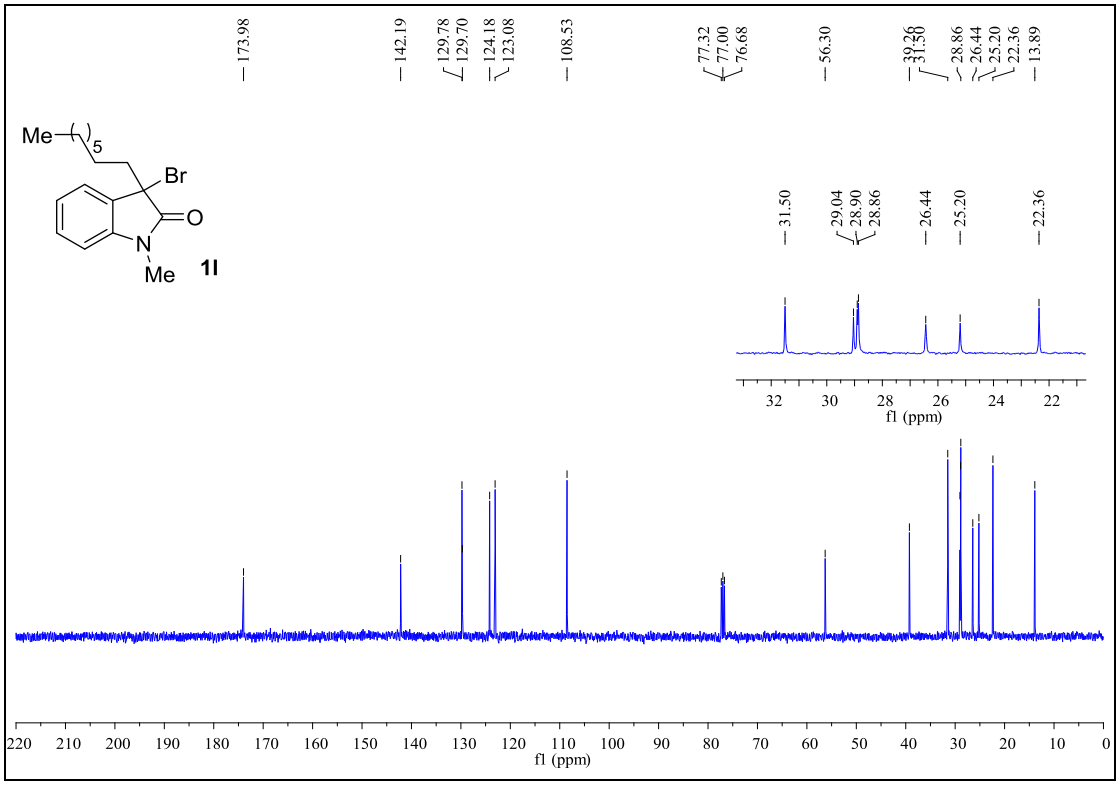
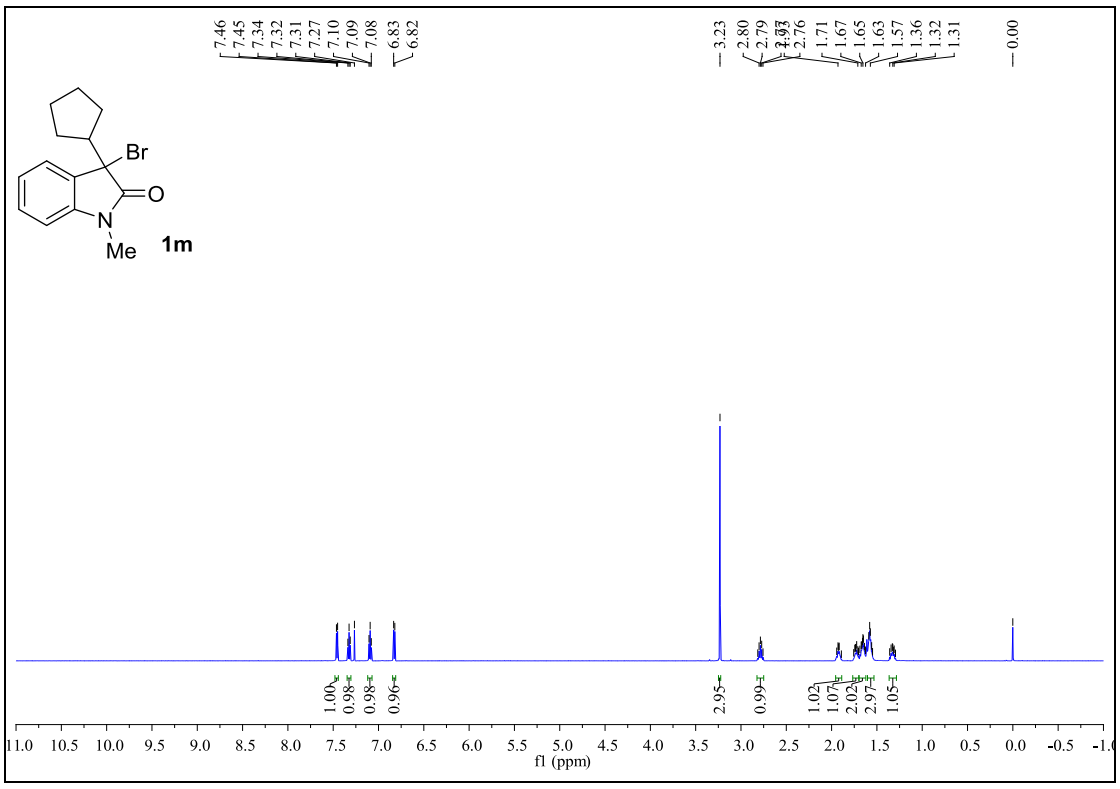
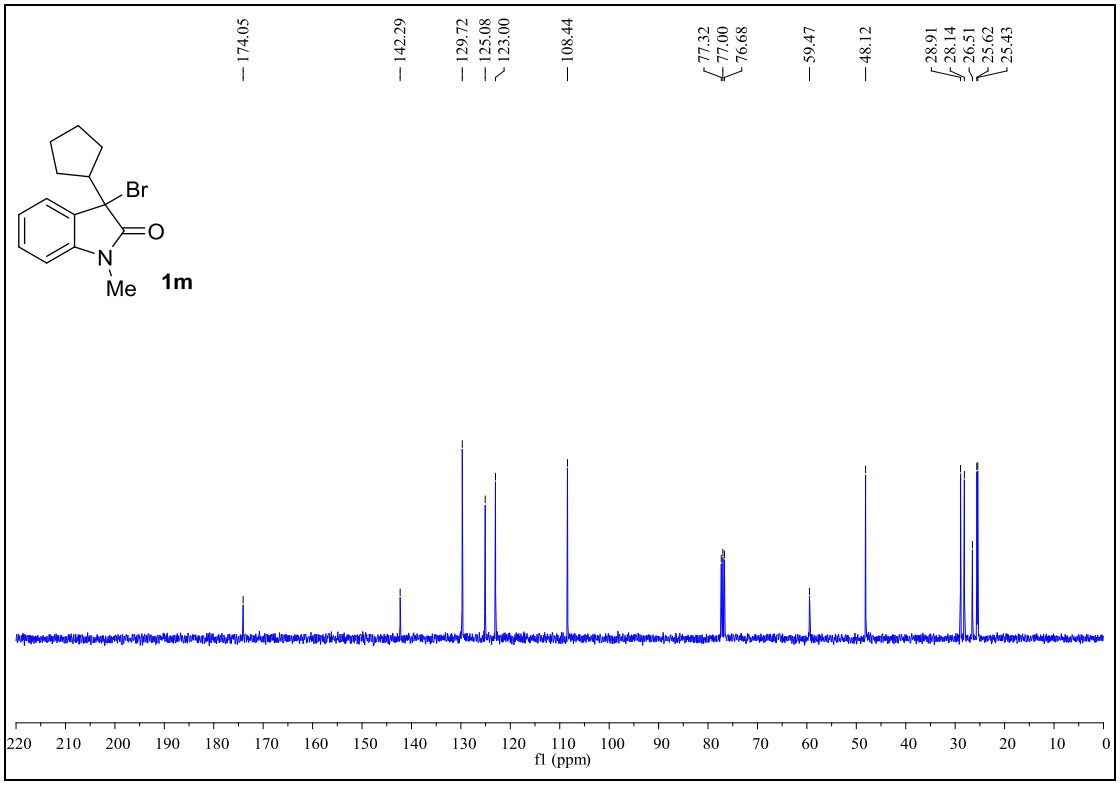
142.07
129.73
129.53
124.08
123.00
108.48
77.32
77.00
76.68
56.24
38.95
27.18
26.35
22.10
13.46
Me
Br
O
N
Me
1k
fl (ppm)


7.40
7.38
7.34
7.33
7.31
7.26
7.13
7.11
7.10
6.84
6.83
3.24
2.39
2.37
2.35
2.35
2.32
1.10
1.09
1.08
1.07
1.06
1.05
1.04
1.03
1.03
1.02
0.86
0.85
0.84
Me
5
Br
O
N
Me
1l
1.00
0.98
0.98
0.96
2.96
2.02
4.01
6.01
2.19
3.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


173.98
142.19
129.78
129.70
124.18
123.08
108.53
77.32
77.00
76.68
56.30
39.26
31.50
28.86
26.44
25.20
22.36
13.89
Me
5
Br
O
N
Me
1l
31.50
29.04
28.90
28.86
26.44
25.20
22.36
32 30 28 26 24 22
f1 (ppm)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.46
7.45
7.34
7.32
7.31
7.27
7.10
7.09
7.08
6.83
6.82
3.23
2.80
2.79
2.76
1.71
1.67
1.65
1.63
1.57
1.36
1.32
1.31
0.00
Br
O
N
Me
1m
1.00
0.98
0.98
0.96
2.95
0.99
1.02
1.07
2.02
2.97
1.05
fl (ppm)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123.00
108.44
77.32
77.00
76.68
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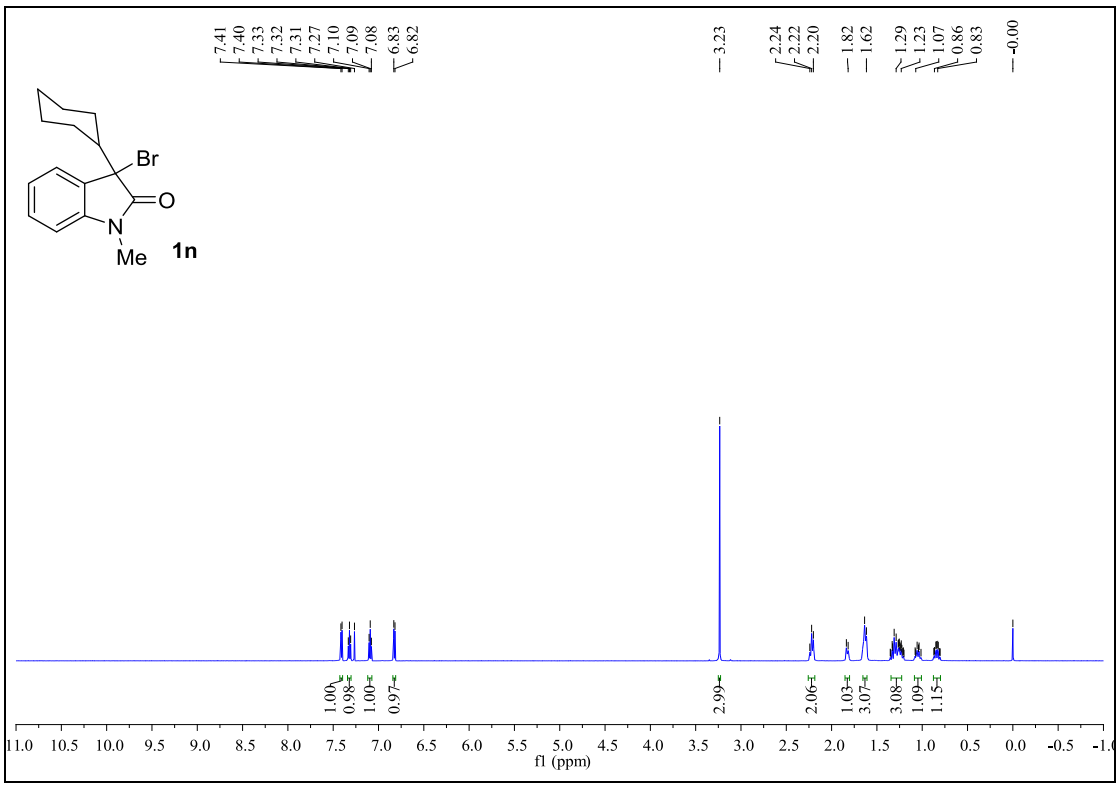
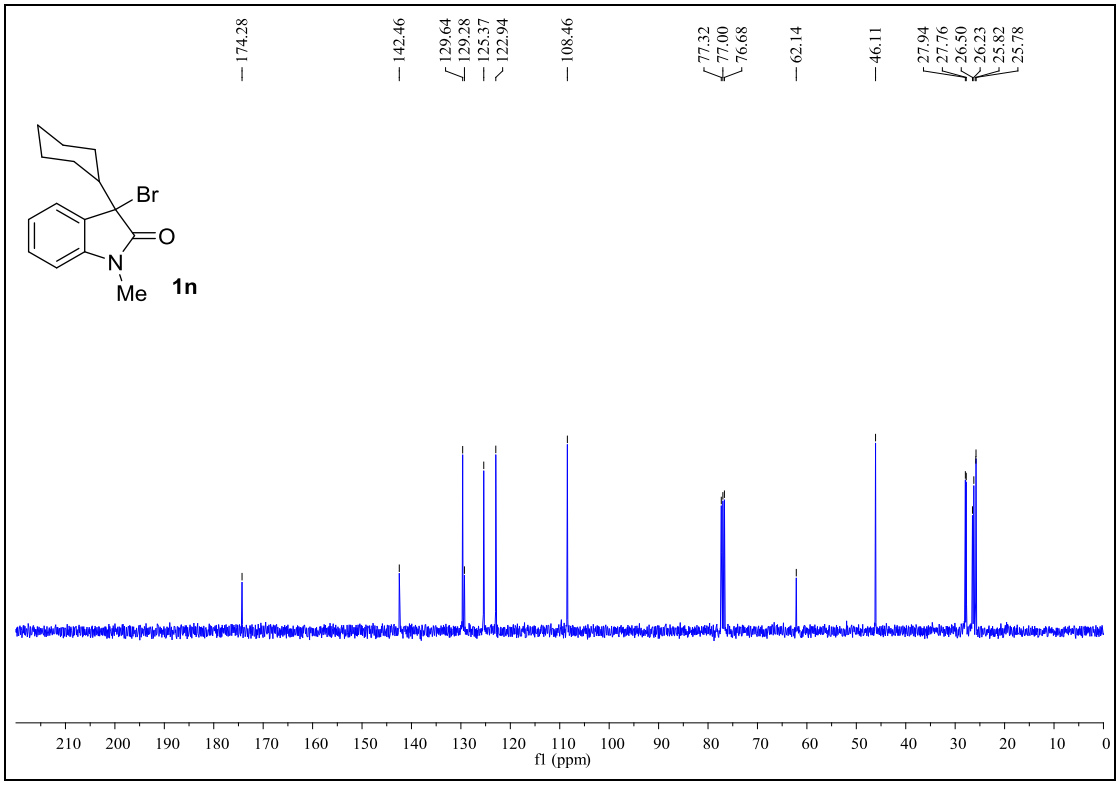
28.91
28.14
26.51
25.62
25.43
Br
O
N
Me
1m
fl (ppm)


7.41
7.40
7.33
7.32
7.31
7.27
7.10
7.09
7.08
6.83
6.82
3.23
2.24
2.22
2.20
1.82
1.62
1.29
1.23
1.07
0.86
0.83
0.00
Br
O
N
Me
1n
1.00
0.98
1.00
0.97
2.99
2.06
1.03
3.07
3.08
1.09
1.15
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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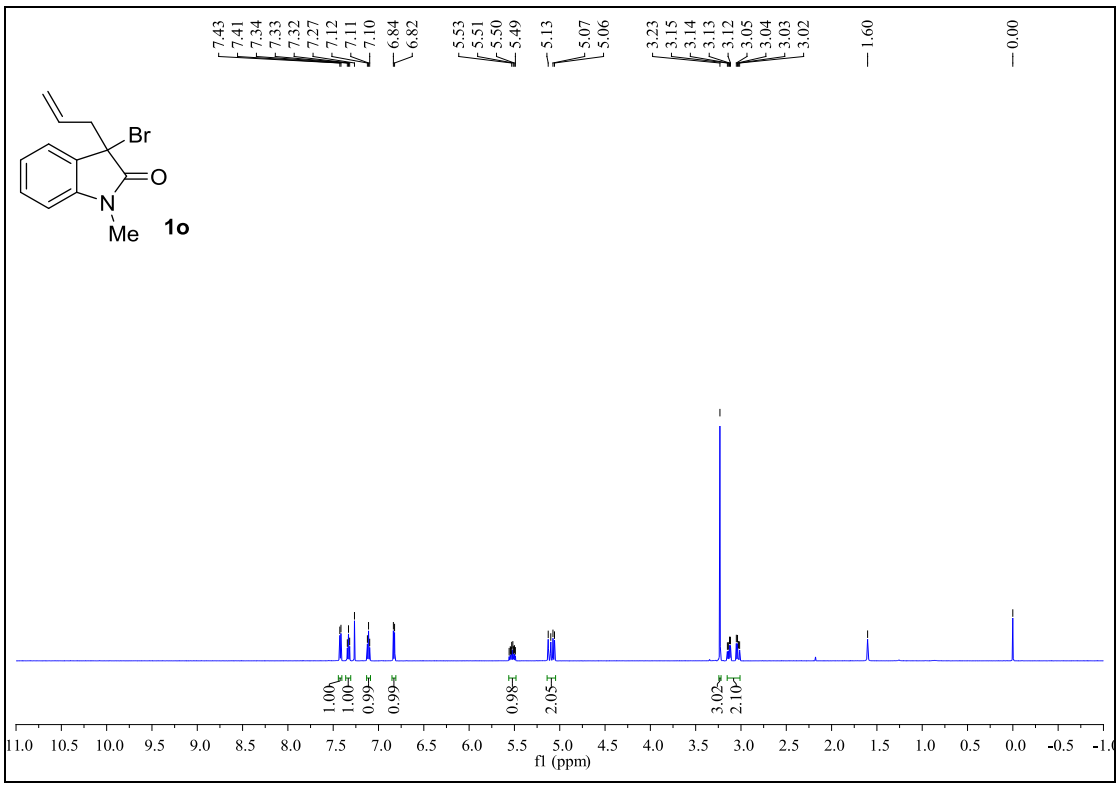
129.64
129.28
125.37
122.94
108.46
77.32
77.00
76.68
62.14
46.11
27.94
27.76
26.50
26.23
25.82
25.78
Br
O
N
Me
1n
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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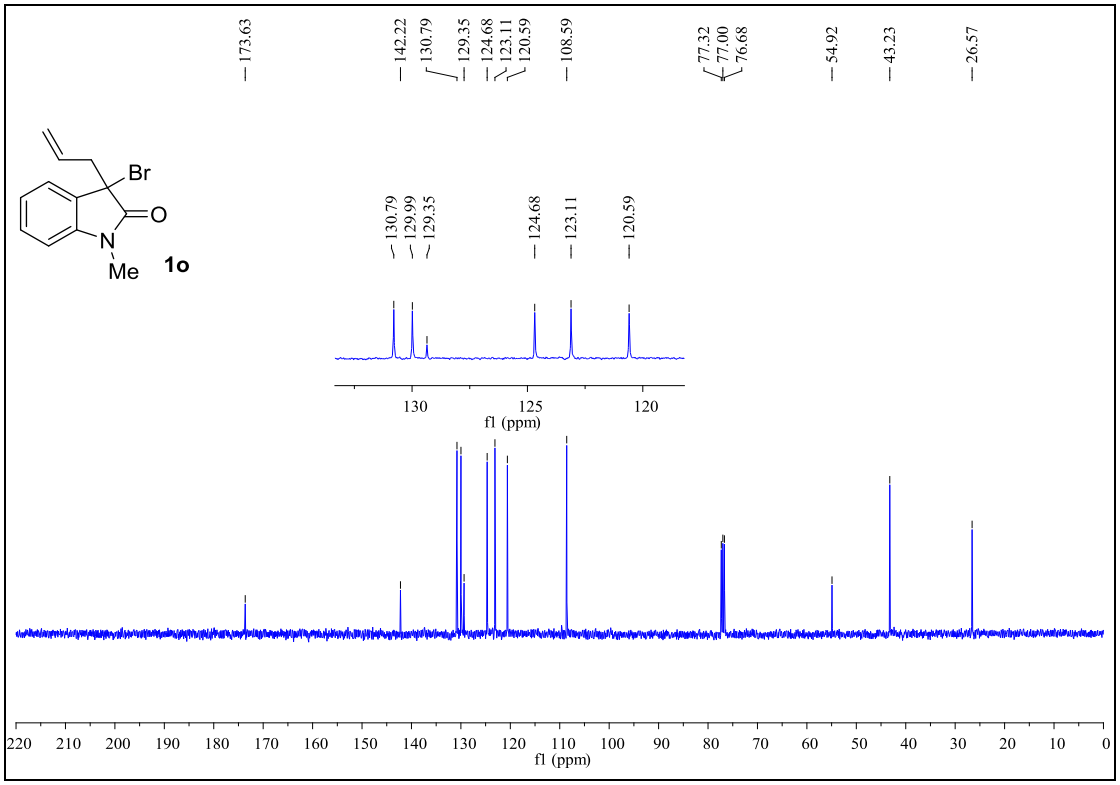
7.41
7.34
7.33
7.32
7.27
7.12
7.11
7.10
6.84
6.82
5.53
5.51
5.50
5.49
5.13
5.07
5.06
3.23
3.15
3.14
3.13
3.12
3.05
3.04
3.03
3.02
1.60
0.00
Br
O
N
Me
1o
1.00
1.00
0.99
0.99
0.98
2.05
3.02
2.10
fl (ppm)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123.11
120.59
108.59
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77.00
76.68
54.92
43.23
26.57
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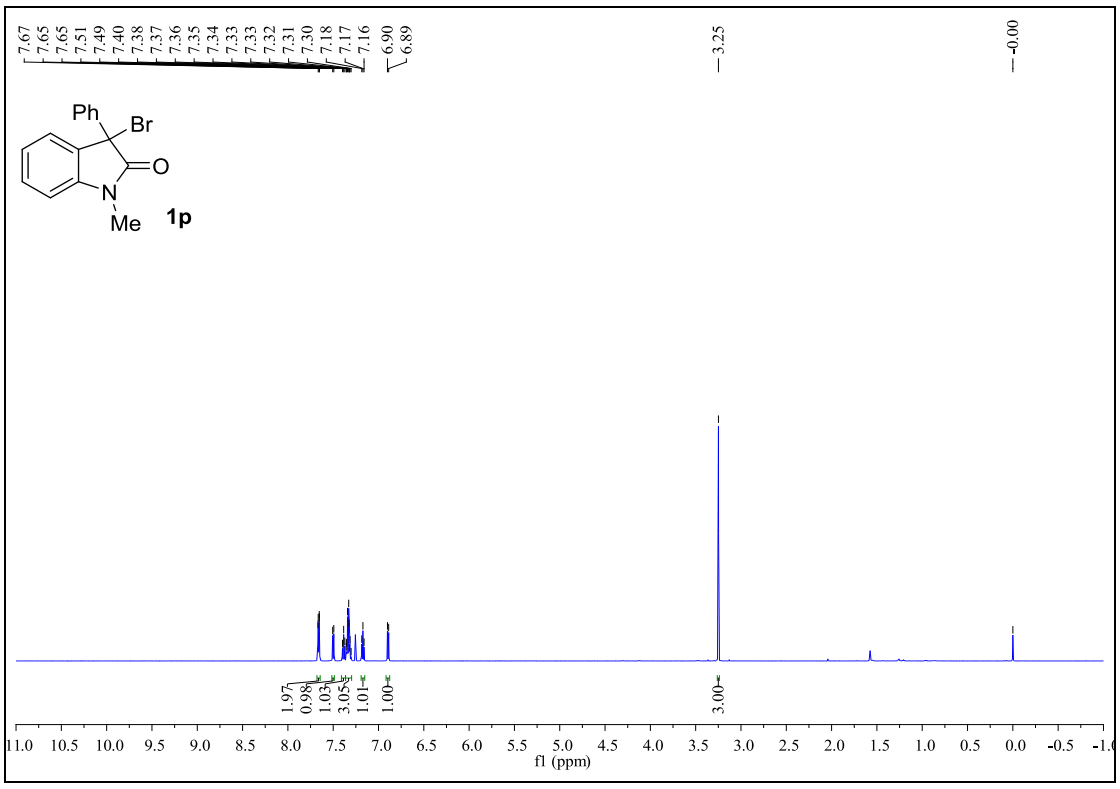
Me
1o
130.79
129.99
129.35
124.68
123.11
120.59
fl (ppm)
fl (ppm)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7.38
7.37
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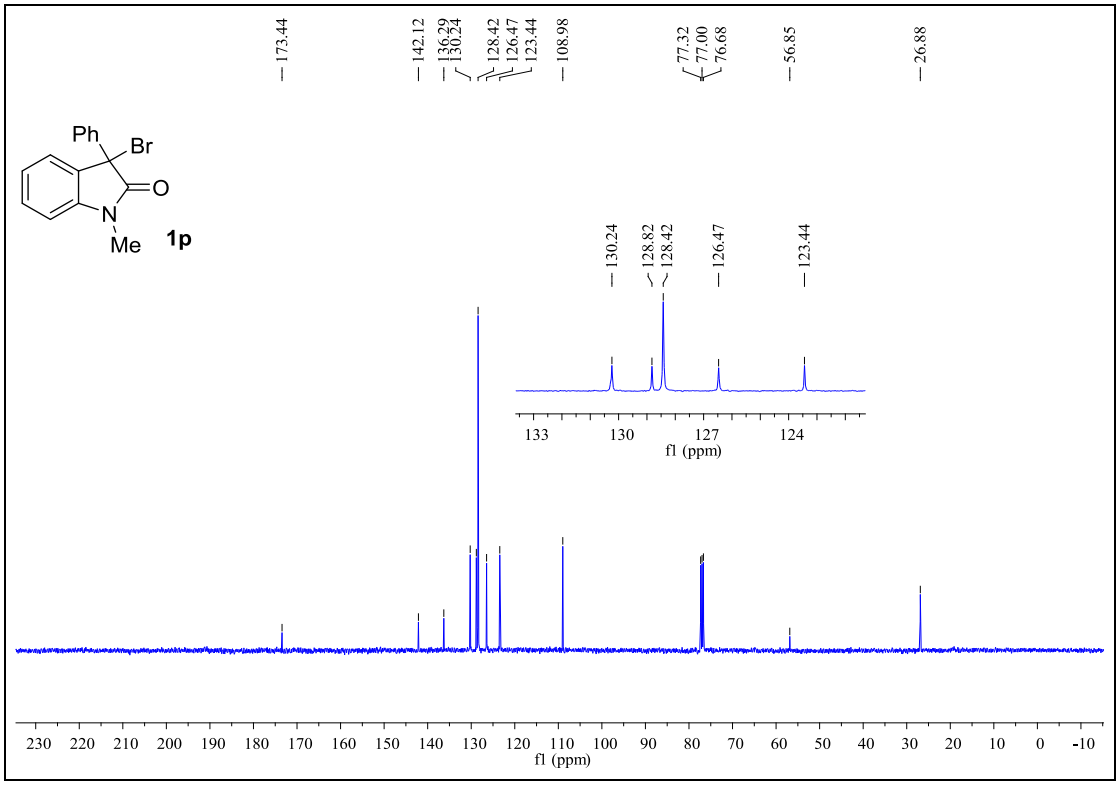
7.35
7.34
7.33
7.33
7.32
7.31
7.30
7.18
7.17
7.16
6.90
6.89
3.25
0.00
Ph
Br
O
N
Me
1p
1.97
0.98
1.03
3.05
1.01
1.00
3.00
fl (ppm)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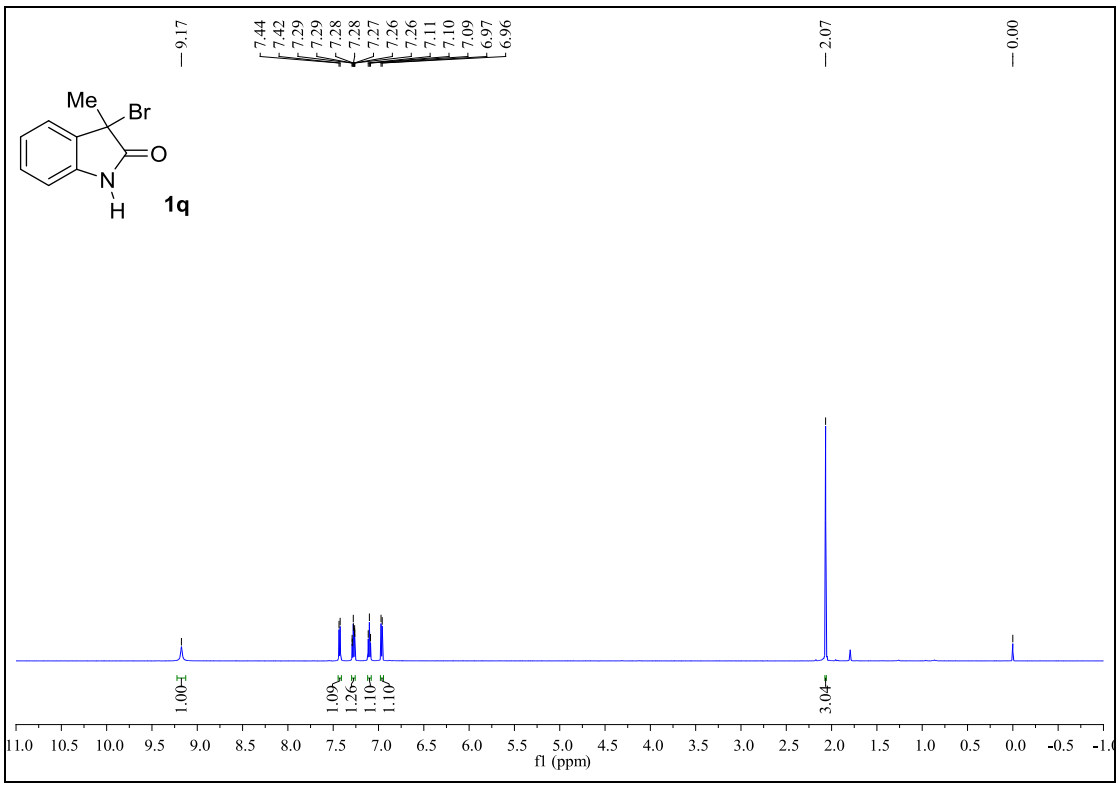
126.47
123.44
108.98
77.32
77.00
76.68
56.85
26.88
Ph
Br
O
N
Me
1p
130.24
128.82
128.42
126.47
123.44
133
130
127
124
fl (ppm)
fl (ppm)


9.17
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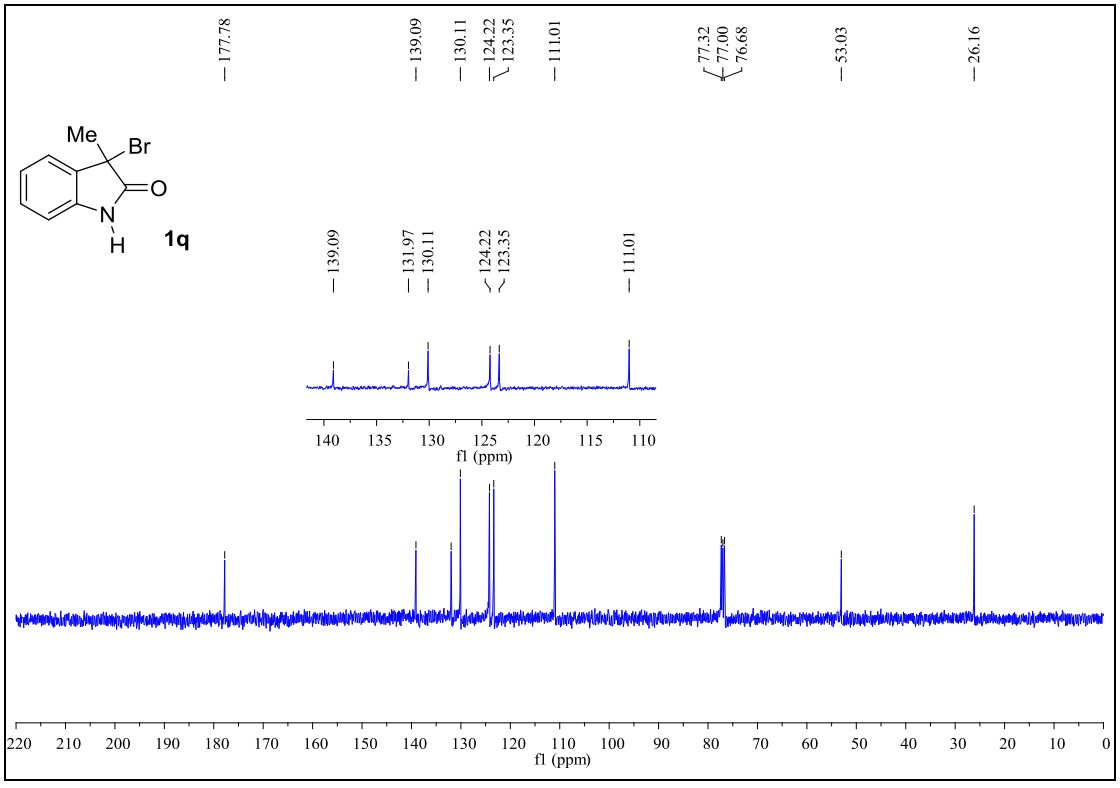
7.42
7.29
7.29
7.28
7.28
7.27
7.26
7.26
7.11
7.10
7.09
6.97
6.96
2.07
0.00
Me
Br
O
N
H
1q
1.00
1.09
1.26
1.10
1.10
3.04
f1 (ppm)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123.35
111.01
77.32
77.00
76.68
53.03
26.16
Me
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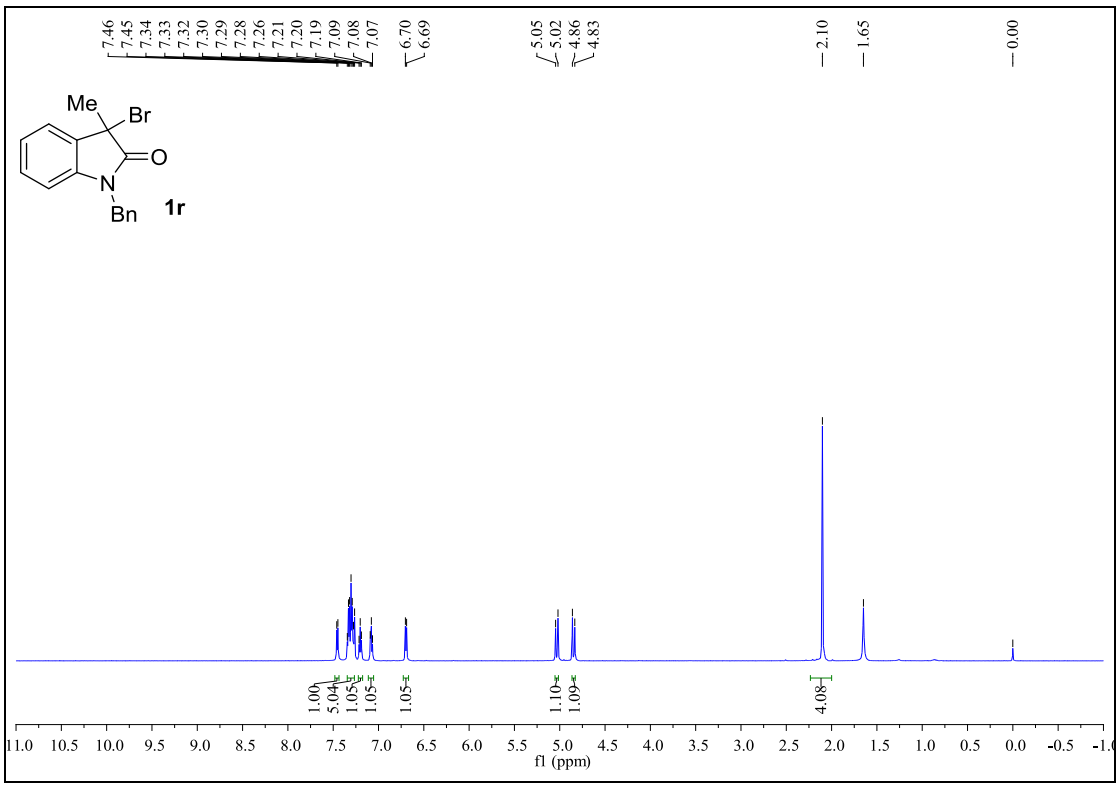
O
N
H
1q
139.09
131.97
130.11
124.22
123.35
111.01
f1 (ppm)
f1 (ppm)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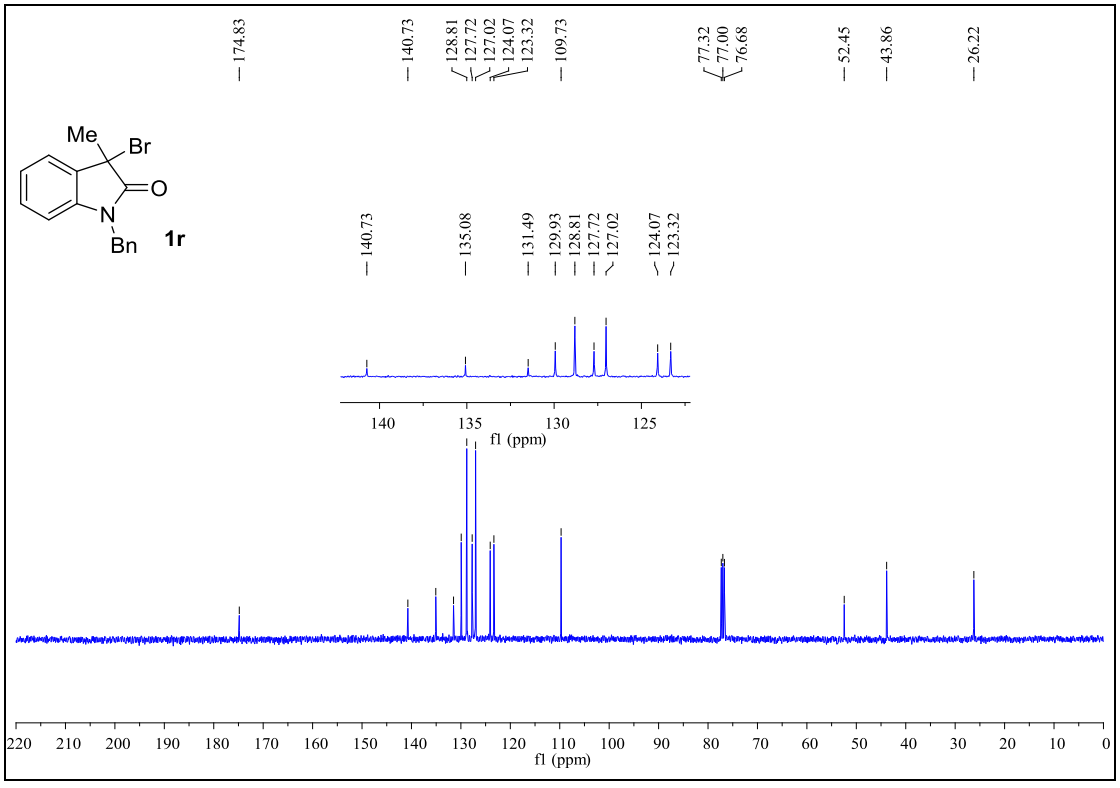
7.33
7.32
7.30
7.29
7.28
7.26
7.21
7.20
7.19
7.09
7.08
7.07
6.70
6.69
5.05
5.02
4.86
4.83
2.10
1.65
0.00
Me
Br
O
N
Bn
1r
1.00
5.04
1.05
1.05
1.05
1.10
1.09
4.08
fl (ppm)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127.72
127.02
124.07
123.32
109.73
77.32
77.00
76.68
52.45
43.86
26.22
Me
Br
O
N
Bn
1r
140.73
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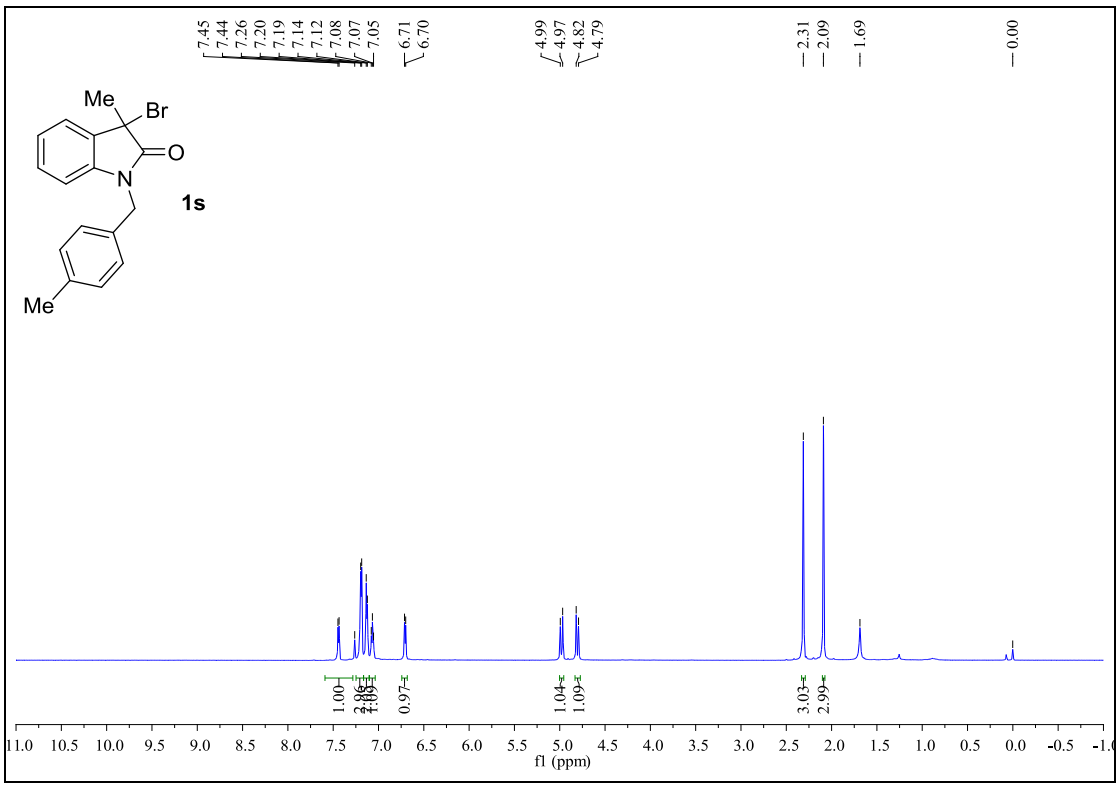
131.49
129.93
128.81
127.72
127.02
124.07
123.32
fl (ppm)
fl (ppm)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7.19
7.14
7.12
7.08
7.07
7.05
6.71
6.70
4.99
4.97
4.82
4.79
2.31
2.09
1.69
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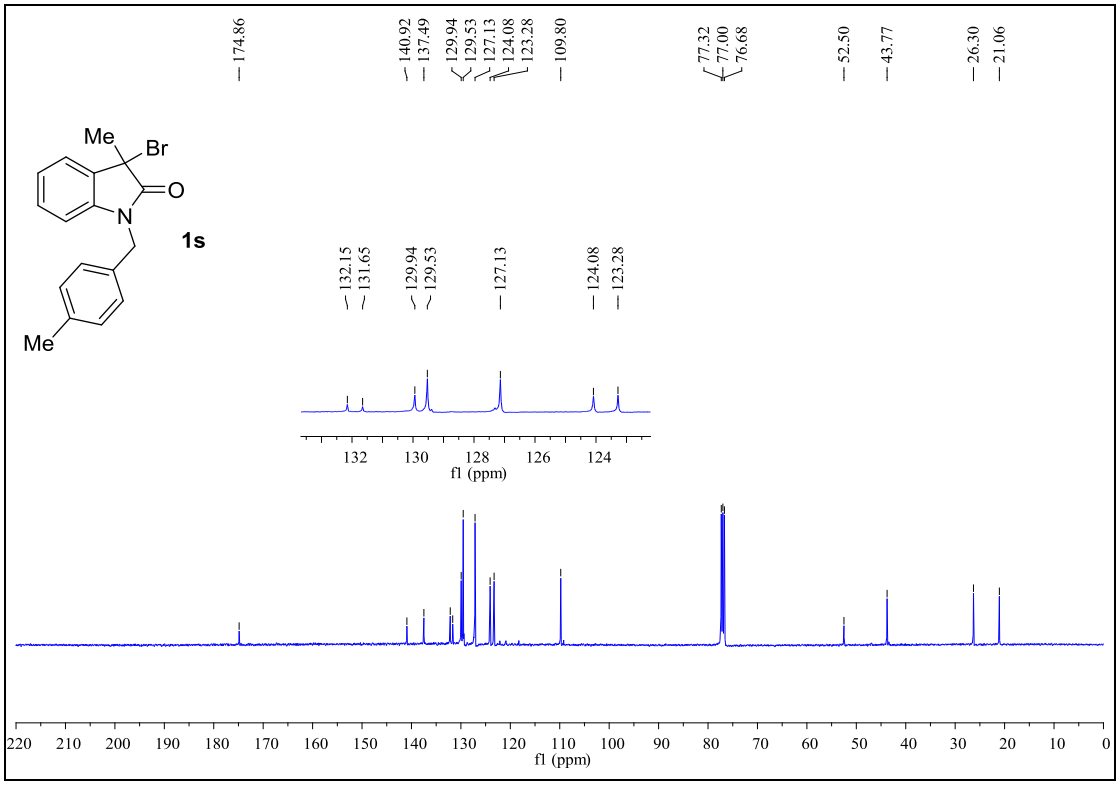
Me
Br
O
N
1s
Me
1.00
0.97
1.04
1.09
3.03
2.99
f1 (ppm)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127.13
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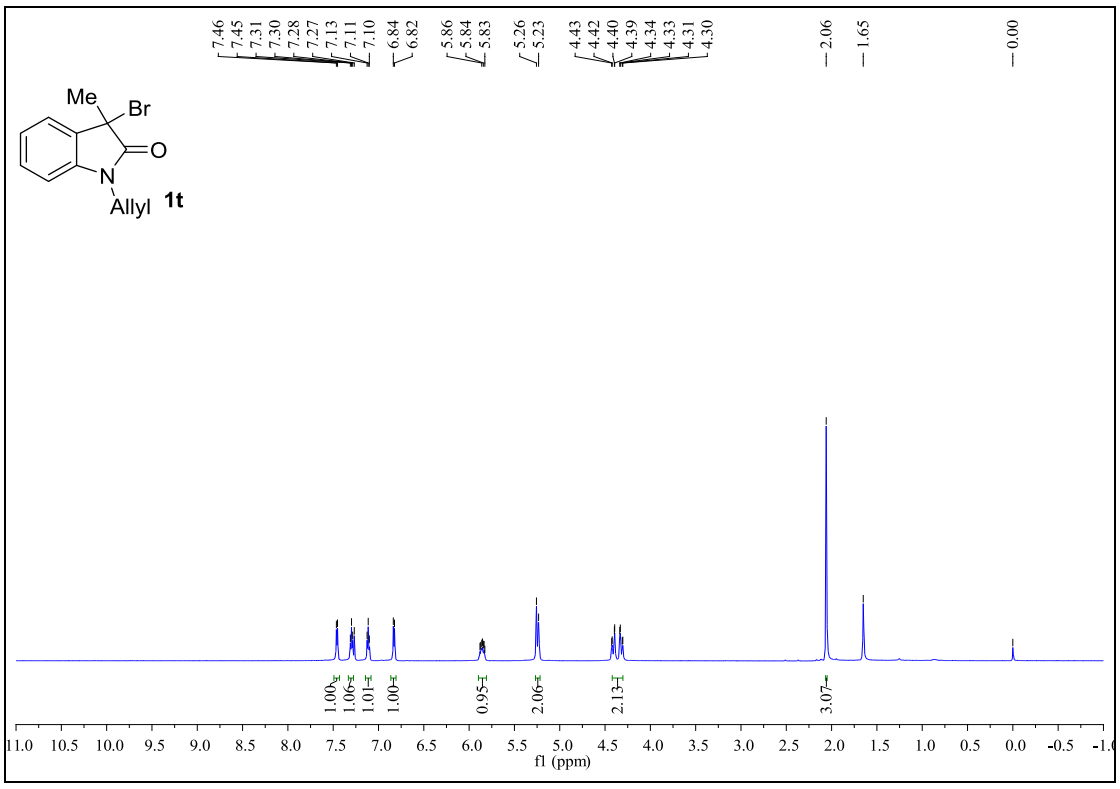
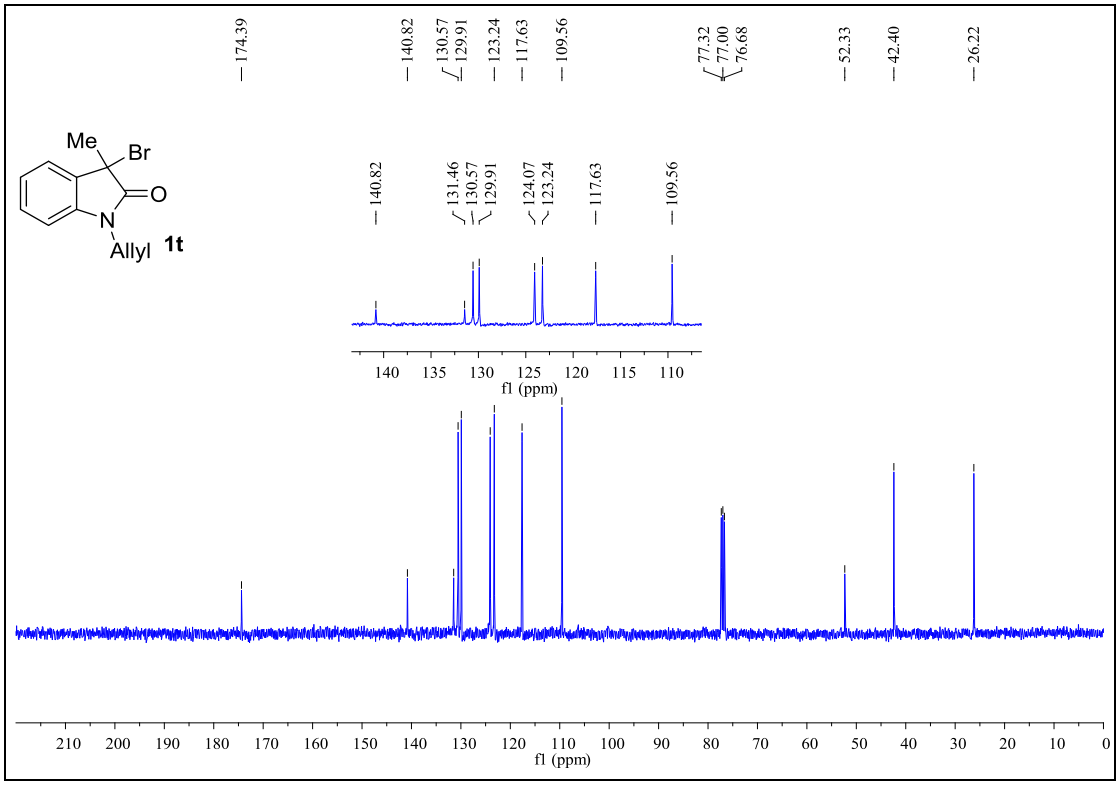
77.32
77.00
76.68
52.50
43.77
26.30
21.06
Me
Br
O
N
1s
Me
132.15
131.65
129.94
129.53
127.13
124.08
123.28
f1 (ppm)
f1 (ppm)


7.46
7.45
7.31
7.30
7.28
7.27
7.13
7.11
7.10
6.84
6.82
5.86
5.84
5.83
5.26
5.23
4.43
4.42
4.40
4.39
4.34
4.33
4.31
4.30
2.06
1.65
0.00
Me
Br
O
N
Allyl
1t
1.00
1.06
1.01
1.00
0.95
2.06
2.13
3.07
f1 (ppm)


174.39
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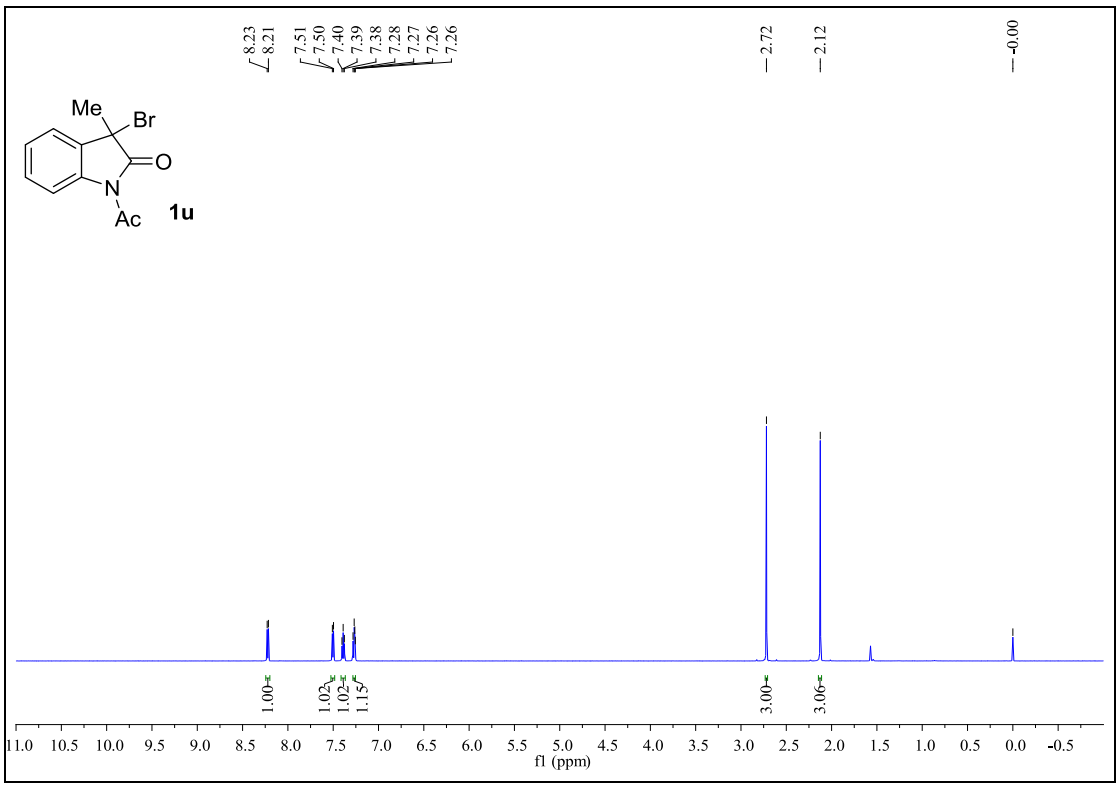
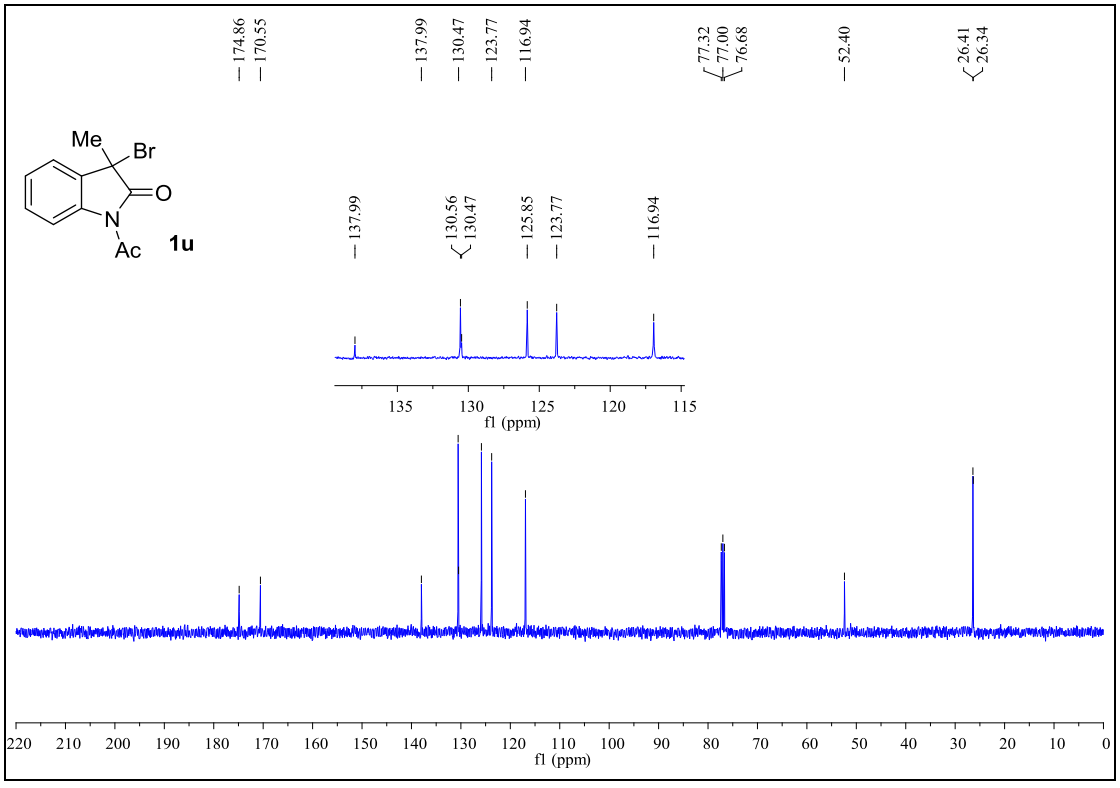
129.91
123.24
117.63
109.56
77.32
77.00
76.68
52.33
42.40
26.22
Me
Br
O
N
Allyl
1t
140.82
131.46
130.57
129.91
124.07
123.24
117.63
109.56
f1 (ppm)
f1 (ppm)


8.23
8.21
7.51
7.50
7.40
7.39
7.38
7.28
7.27
7.26
7.26
2.72
2.12
0.00
Me
Br
O
N
Ac
1u
1.00
1.02
1.02
1.15
3.00
3.06
fl (ppm)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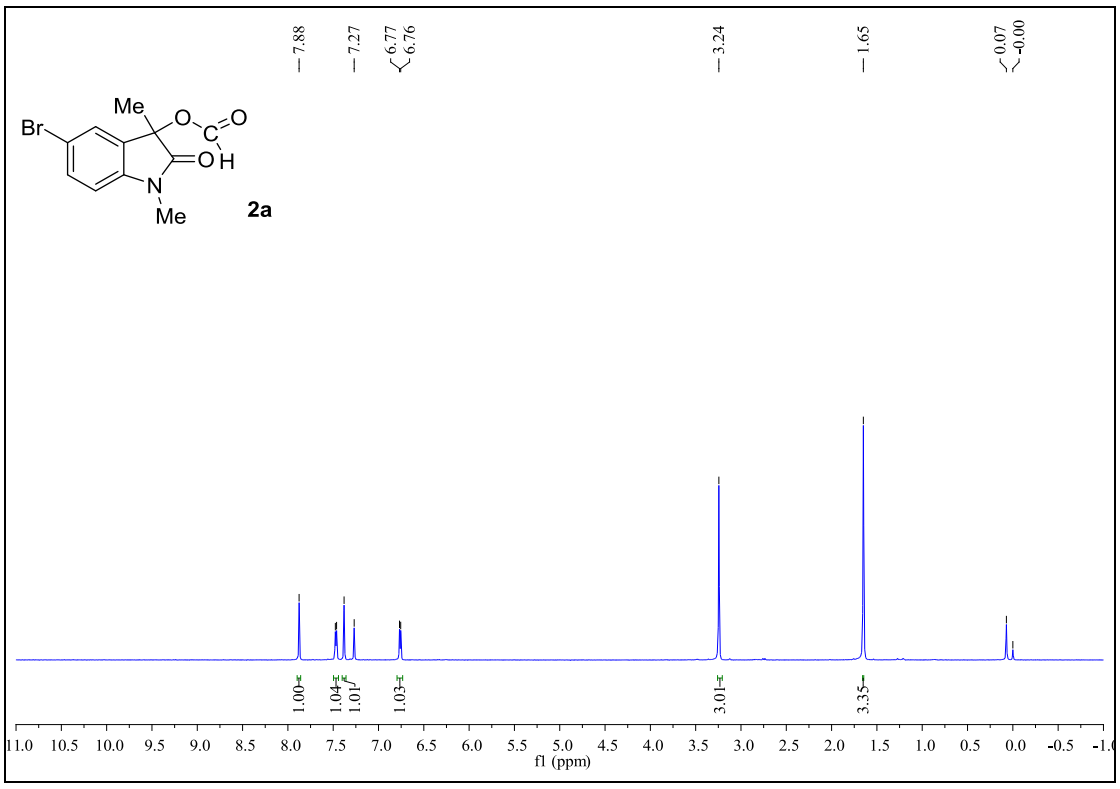
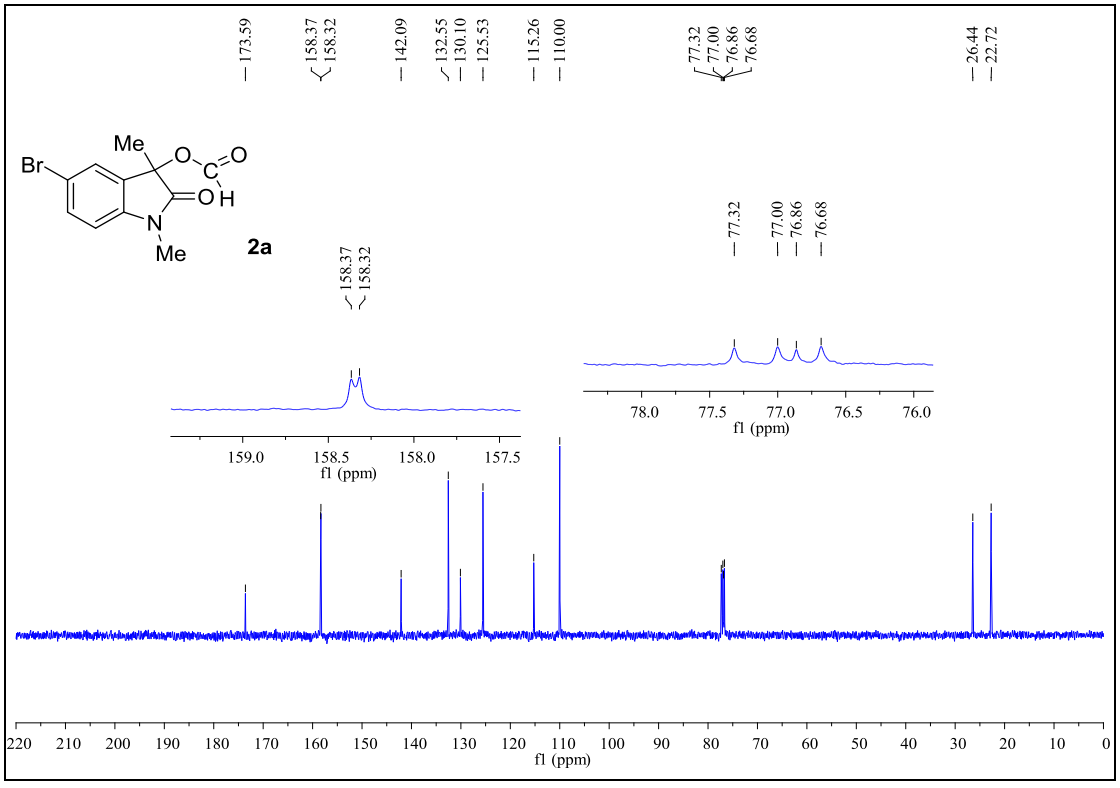
116.94
77.32
77.00
76.68
52.40
26.41
26.34
Me
Br
O
N
Ac
1u
137.99
130.56
130.47
125.85
123.77
116.94
fl (ppm)
fl (ppm)


7.88
7.27
6.77
6.76
3.24
1.65
0.07
-0.00
Me
Br
O
C
O
O H
N
Me
2a
1.00
1.04
1.01
1.03
3.01
3.35
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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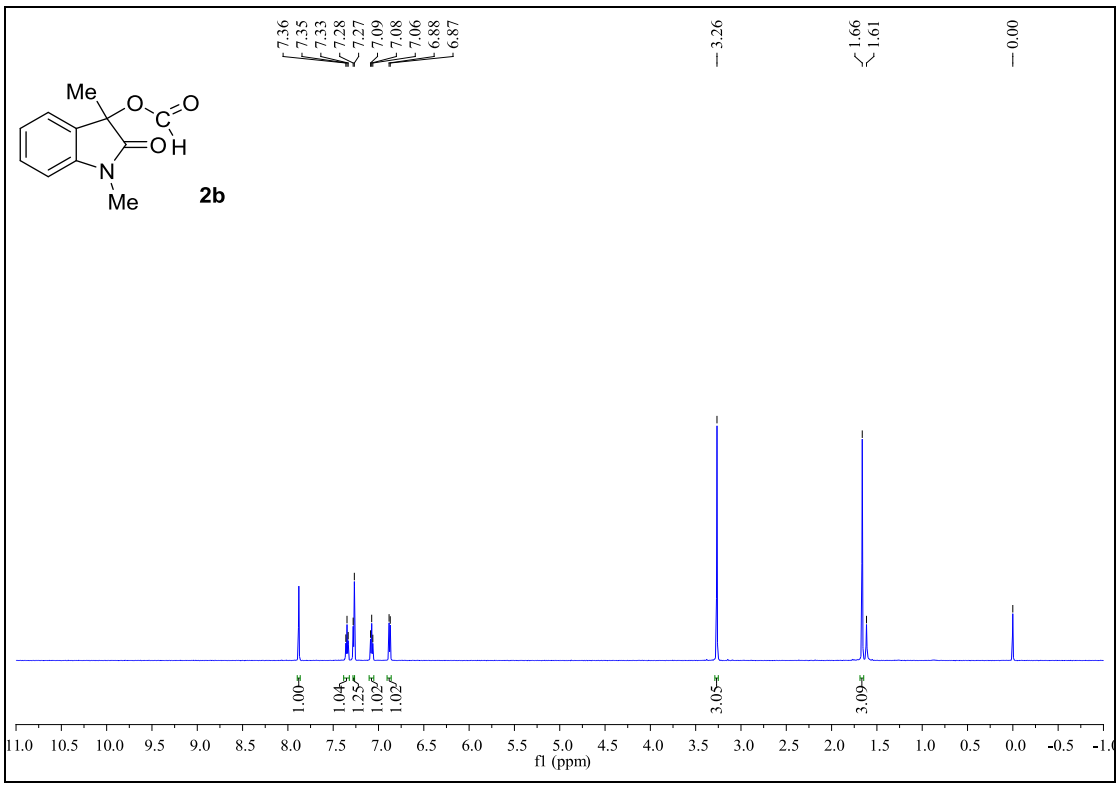
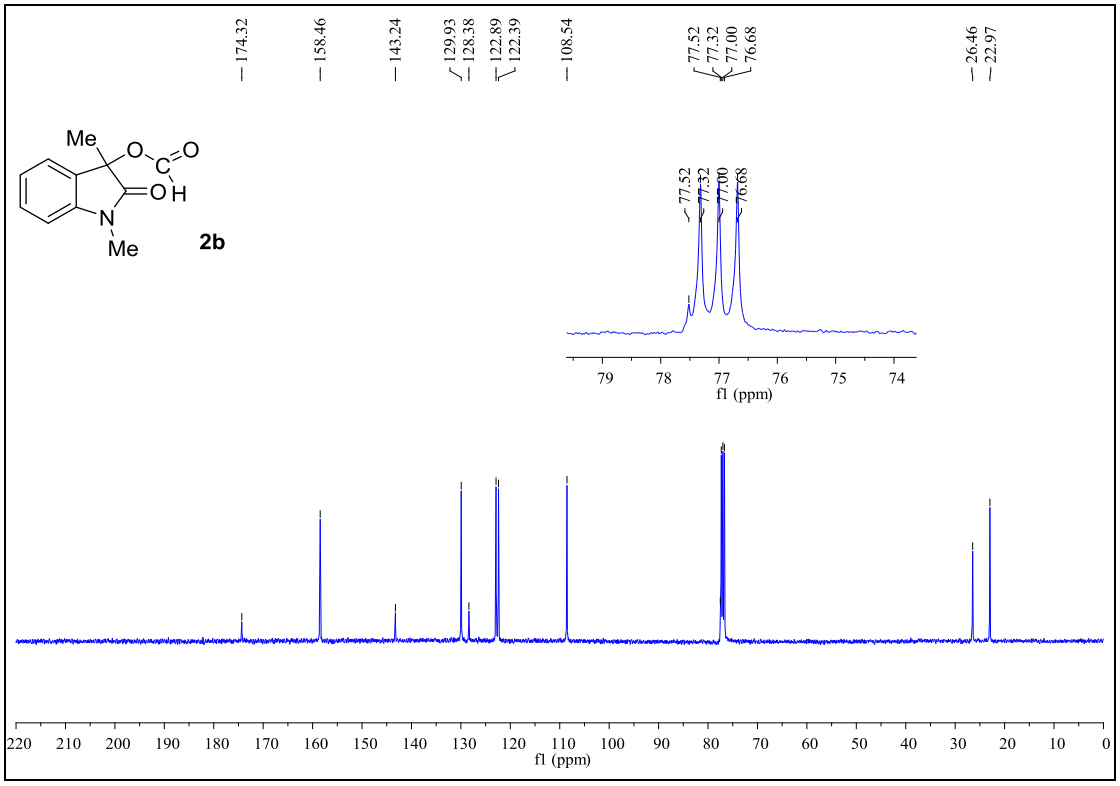
158.37
158.32
142.09
132.55
130.10
125.53
115.26
110.00
77.32
77.00
76.86
76.68
26.44
22.72
Me
Br
O
C
O
O H
N
Me
2a
158.37
158.32
77.32
77.00
76.86
76.68
159.0 158.5 158.0 157.5
f1 (ppm)
78.0 77.5 77.0 76.5 76.0
f1 (ppm)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.36
7.35
7.33
7.28
7.27
7.09
7.08
7.06
6.88
6.87
3.26
1.66
1.61
0.00
Me
O
C
O
O H
N
Me
2b
1.00
1.04
1.25
1.02
1.02
3.05
3.09
fl (ppm)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158.46
143.24
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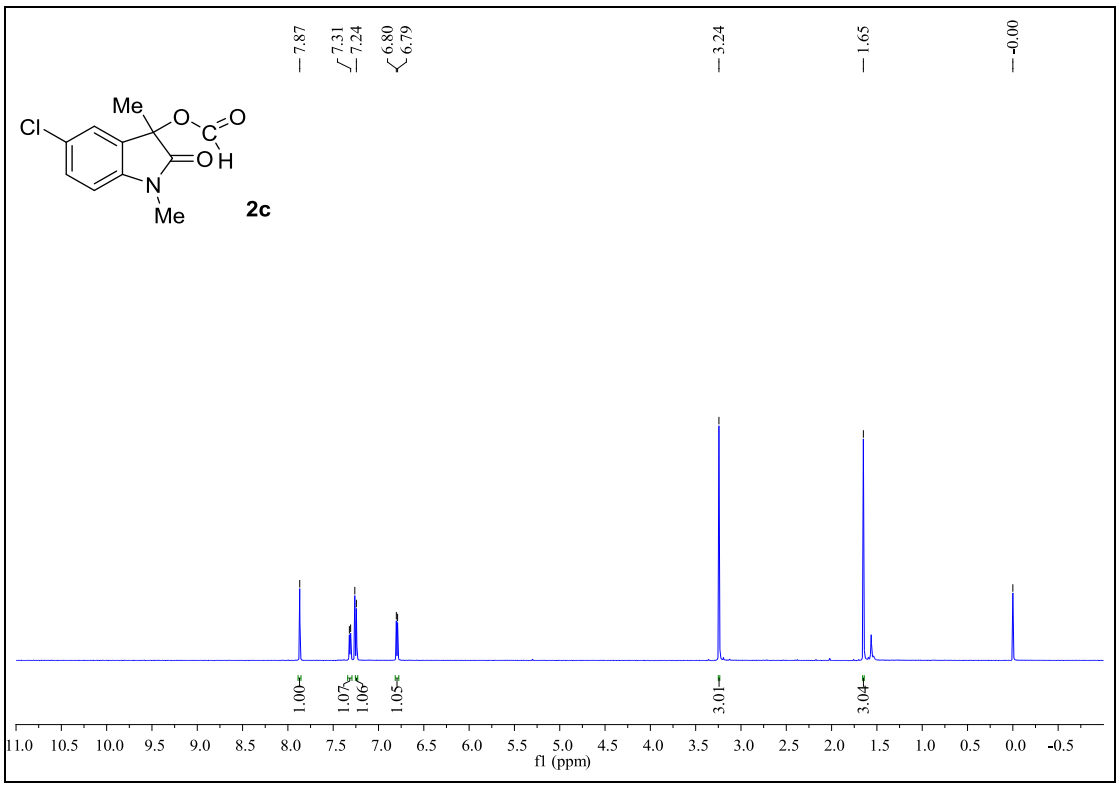
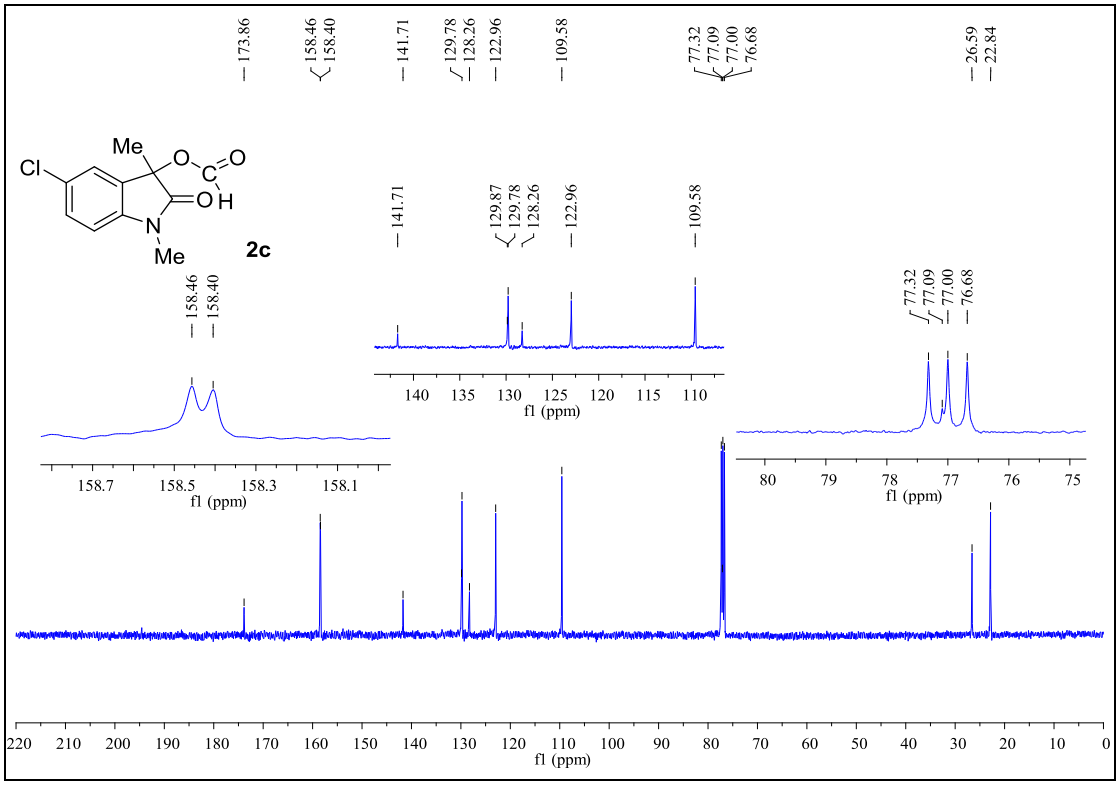
128.38
122.89
122.39
108.54
77.52
77.32
77.00
76.68
26.46
22.97
Me
O
C
O
O H
N
Me
2b
fl (ppm)
fl (ppm)


7.87
7.31
7.24
6.80
6.79
3.24
1.65
0.00
Me
Cl
O
C
O
O H
N
Me
2c
1.00
1.07
1.06
1.05
3.01
3.04
fl (ppm)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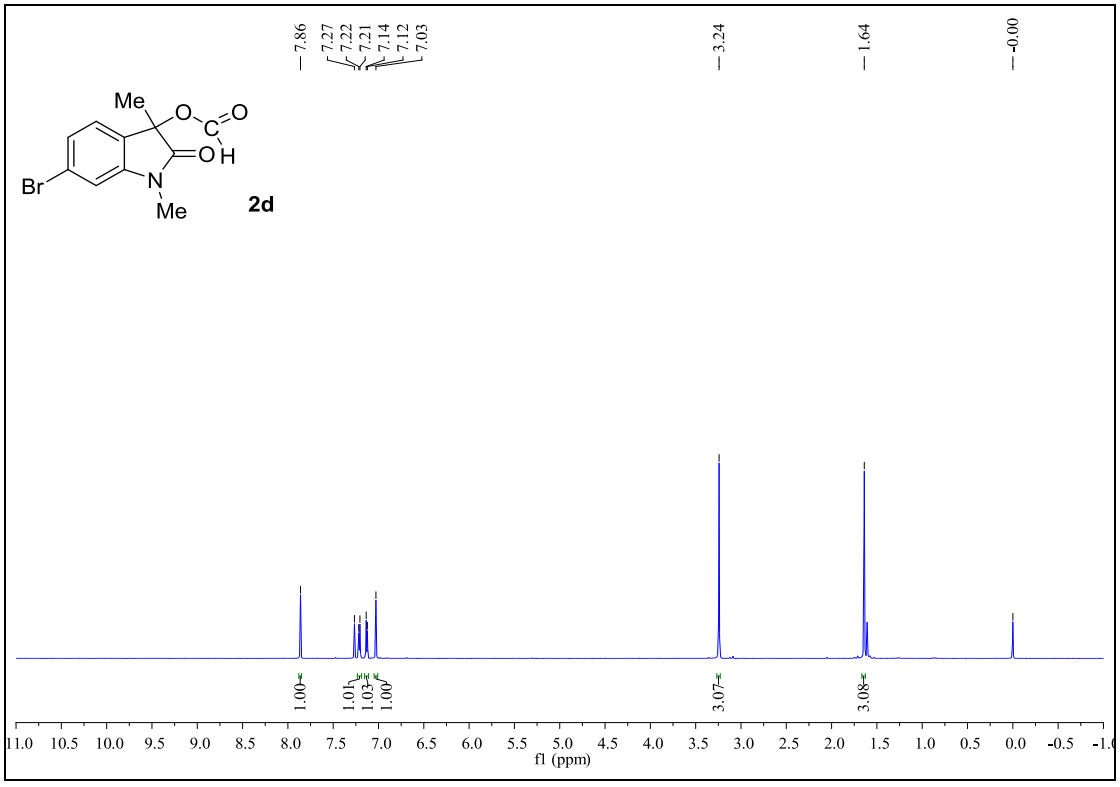
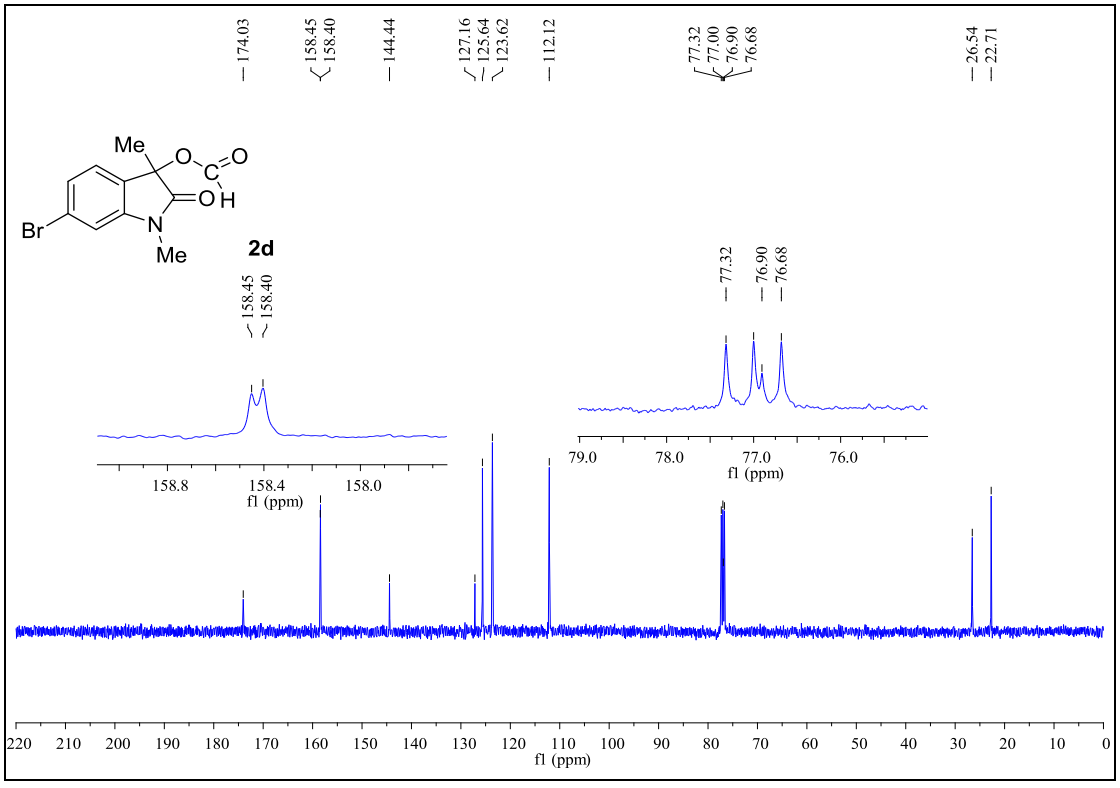
158.46
158.40
141.71
129.78
128.26
122.96
109.58
77.32
77.09
77.00
76.68
26.59
22.84
Me
Cl
O
C
O
O H
N
Me
2c
fl (ppm)


7.86
7.27
7.22
7.21
7.14
7.12
7.03
3.24
1.64
0.00
Me
O
C
O
O H
Br
N
Me
2d
1.00
1.01
1.03
1.00
3.07
3.08
fl (ppm)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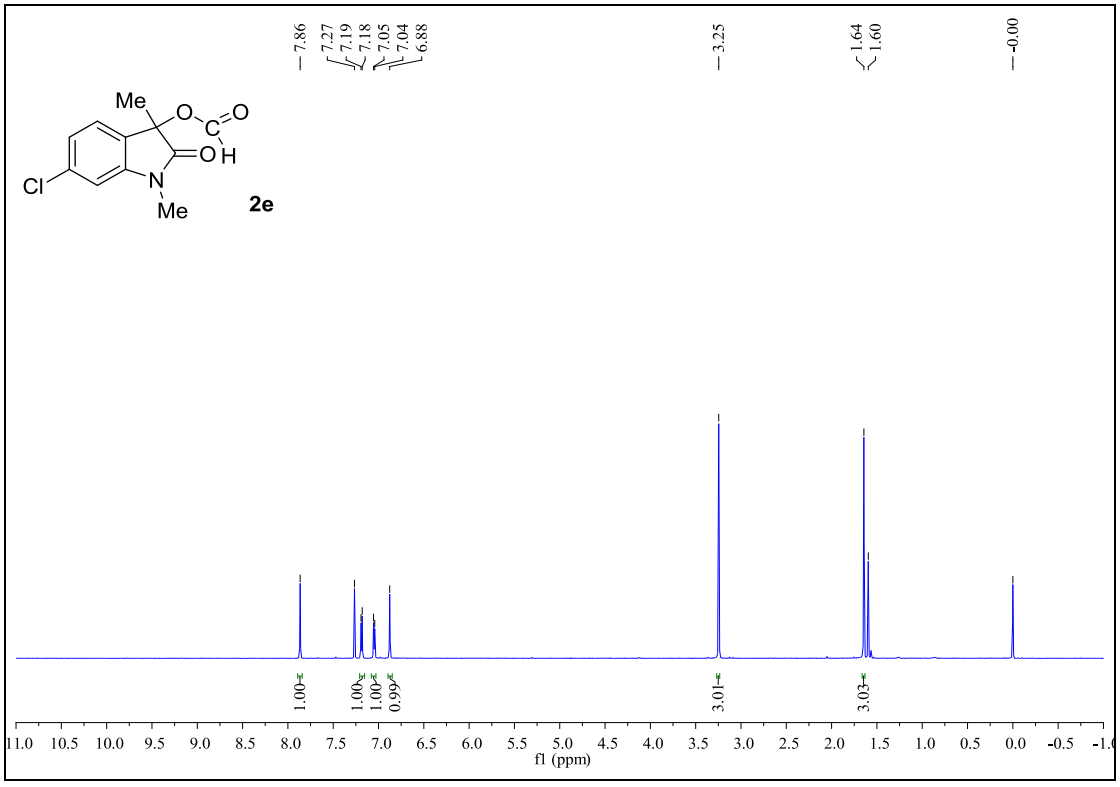
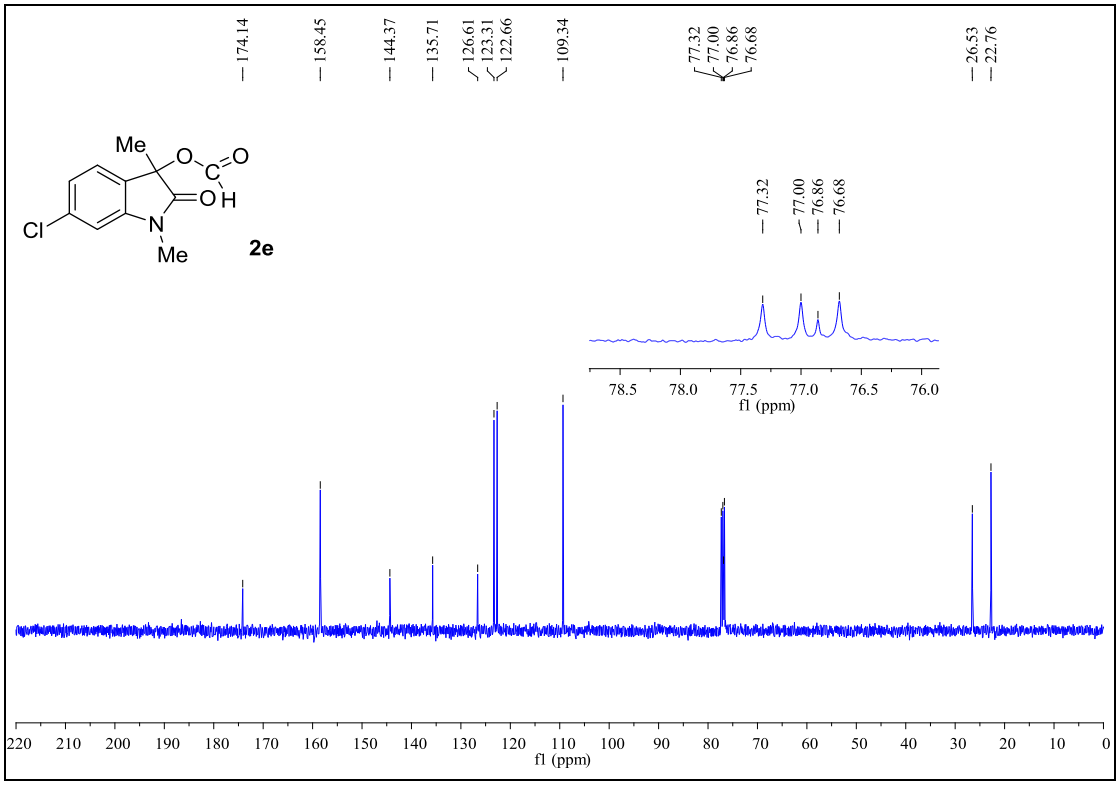
158.45
158.40
144.44
127.16
125.64
123.62
112.12
77.32
77.00
76.90
76.68
26.54
22.71
Me
O
C
O
O H
Br
N
Me
2d
158.45
158.40
77.32
76.90
76.68
158.8
158.4
158.0
79.0
78.0
77.0
76.0
fl (ppm)
fl (ppm)


7.86
7.27
7.19
7.18
7.05
7.04
6.88
3.25
1.64
1.60
0.00
Me
O
C
O
O H
Cl
N
Me
2e
1.00
1.00
1.00
0.99
3.01
3.03
fl (ppm)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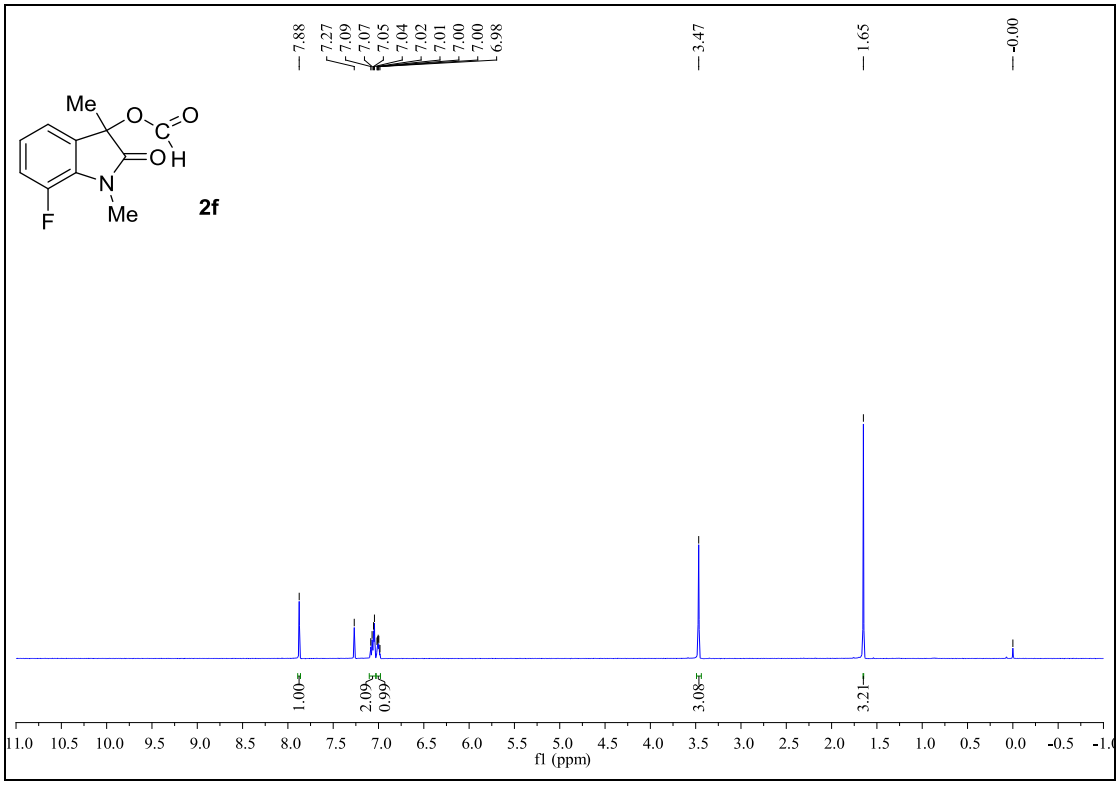
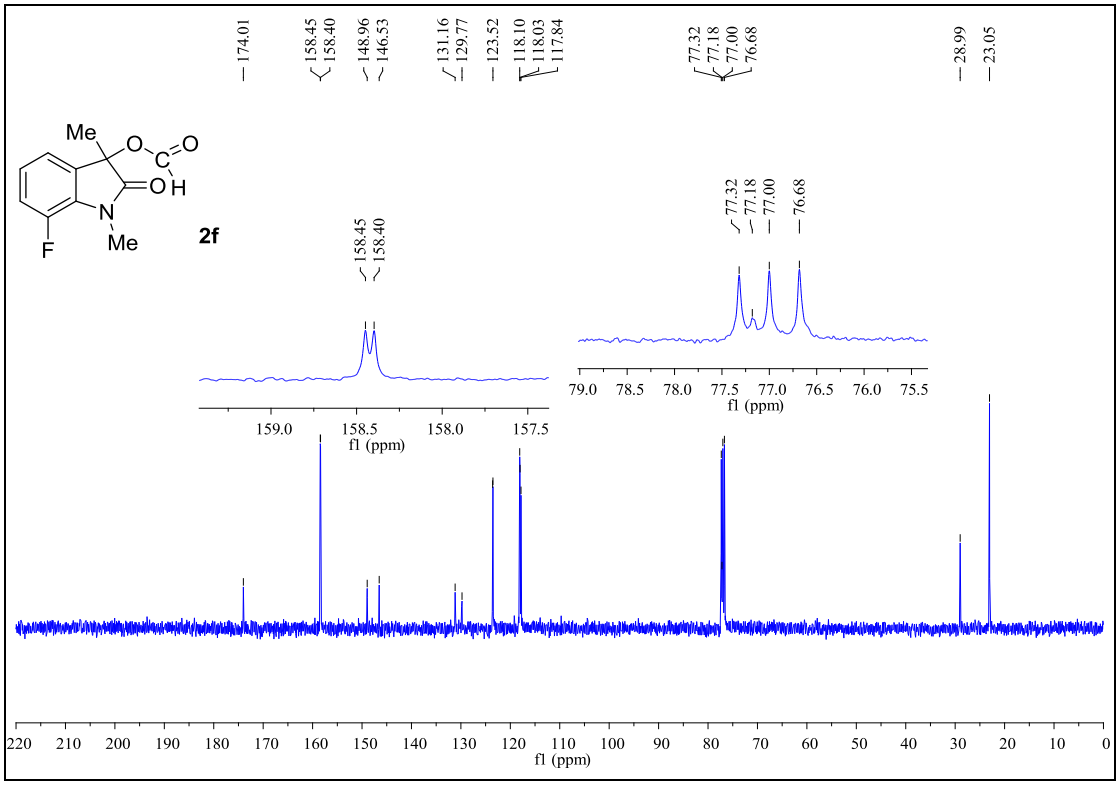
158.45
144.37
135.71
126.61
123.31
122.66
109.34
77.32
77.00
76.86
76.68
26.53
22.76
Me
O
C
O
O H
Cl
N
Me
2e
fl (ppm)
fl (ppm)


7.88
7.27
7.09
7.07
7.05
7.04
7.02
7.01
7.00
7.00
6.98
3.47
1.65
0.00
Me
O
C
O
O H
N
Me
F
2f
1.00
2.09
0.99
3.08
3.21
fl (ppm)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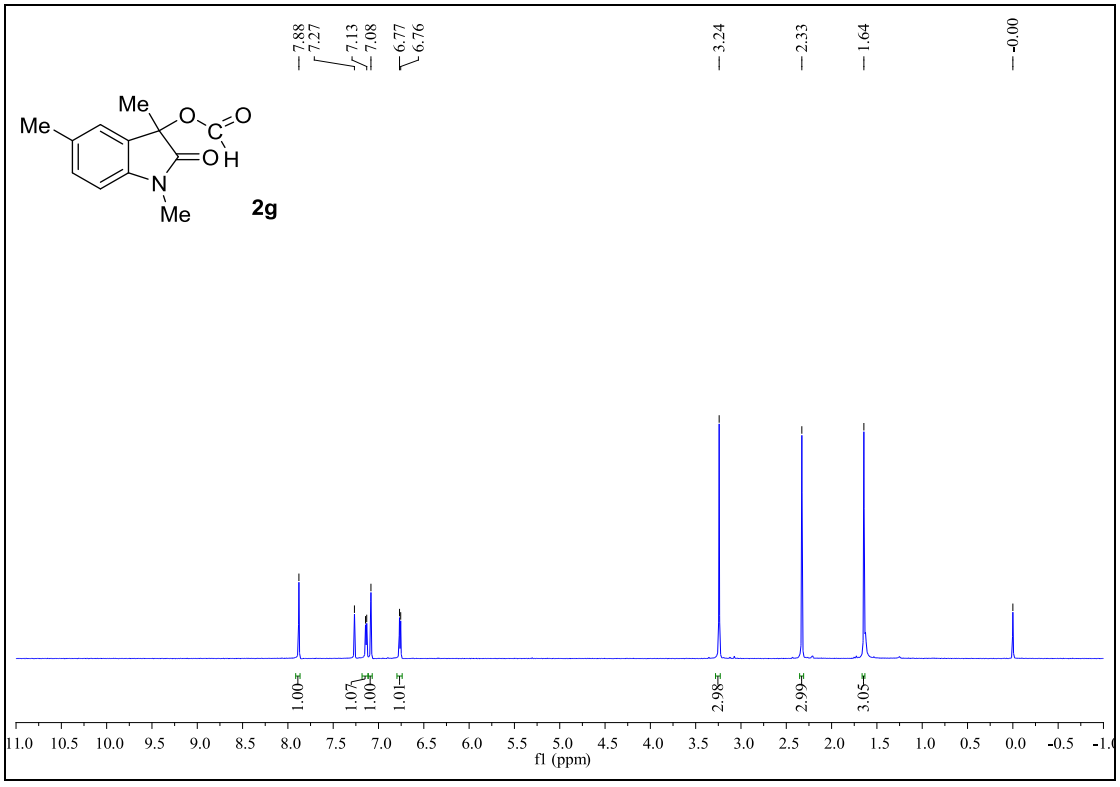
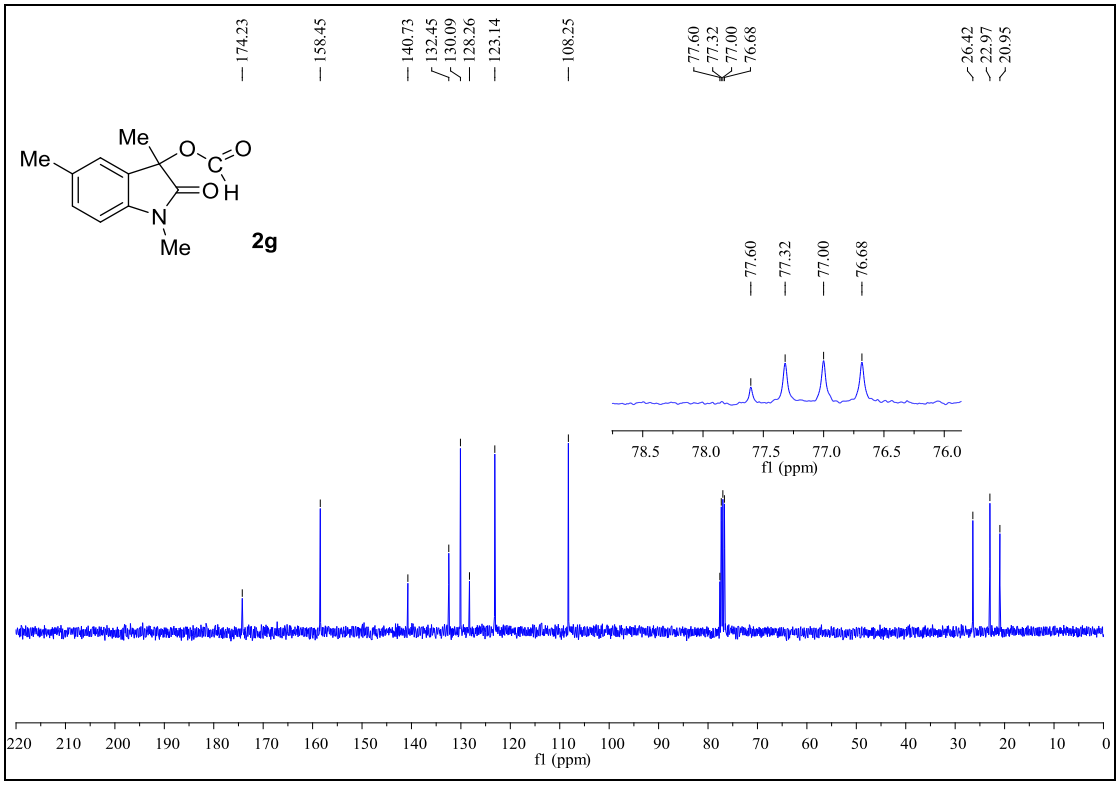
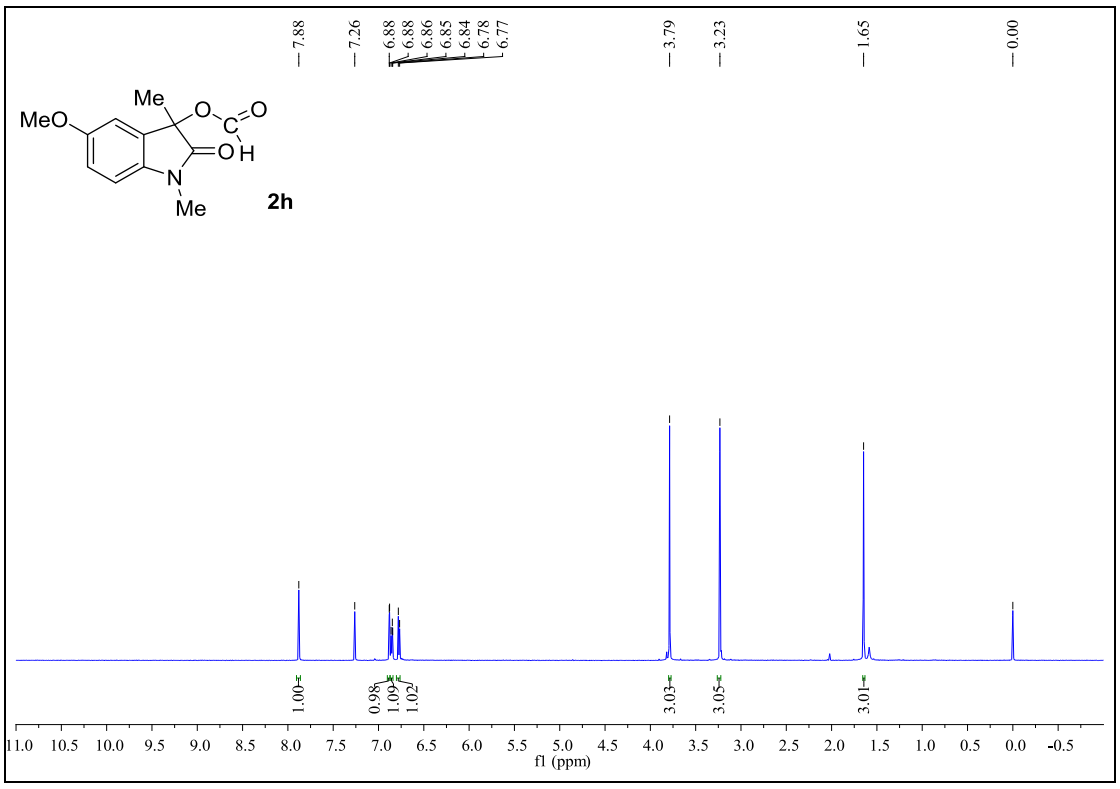
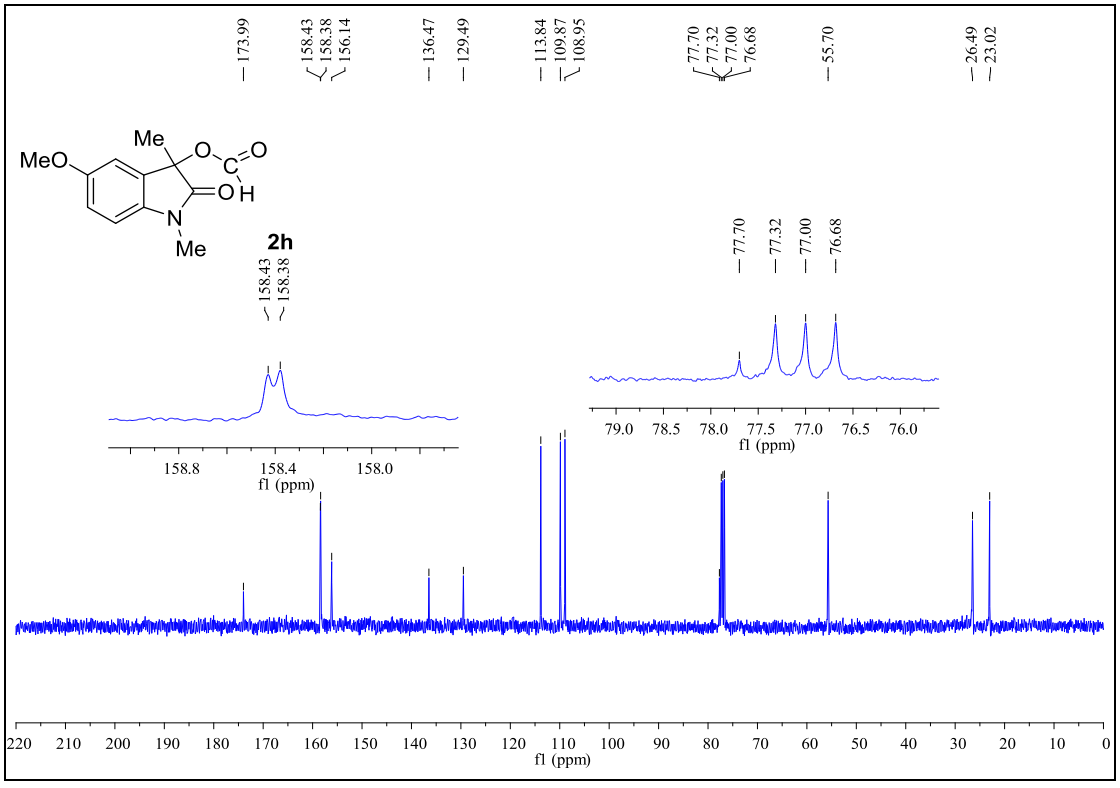
158.45
158.40
148.96
146.53
131.16
129.77
123.52
118.10
118.03
117.84
77.32
77.18
77.00
76.68
28.99
23.05
Me
O
C
O
O H
N
Me
F
2f
158.45
158.40
77.32
77.18
77.00
76.68
fl (ppm)
fl (ppm)
fl (ppm)


7.88
7.27
7.13
7.08
6.77
6.76
3.24
2.33
1.64
0.00
Me
Me
O
C
O
O H
N
Me
2g
1.00
1.07
1.00
1.01
2.98
2.99
3.05
fl (ppm)


174.23
158.45
140.73
132.45
130.09
128.26
123.14
108.25
77.60
77.32
77.00
76.68
26.42
22.97
20.95
Me
Me
O
C
O
O H
N
Me
2g
fl (ppm)
fl (ppm)


7.88
7.26
6.88
6.88
6.86
6.85
6.84
6.78
6.77
3.79
3.23
1.65
0.00
Me
MeO
O
C
O
O H
N
Me
2h
1.00
0.98
1.09
1.02
3.03
3.05
3.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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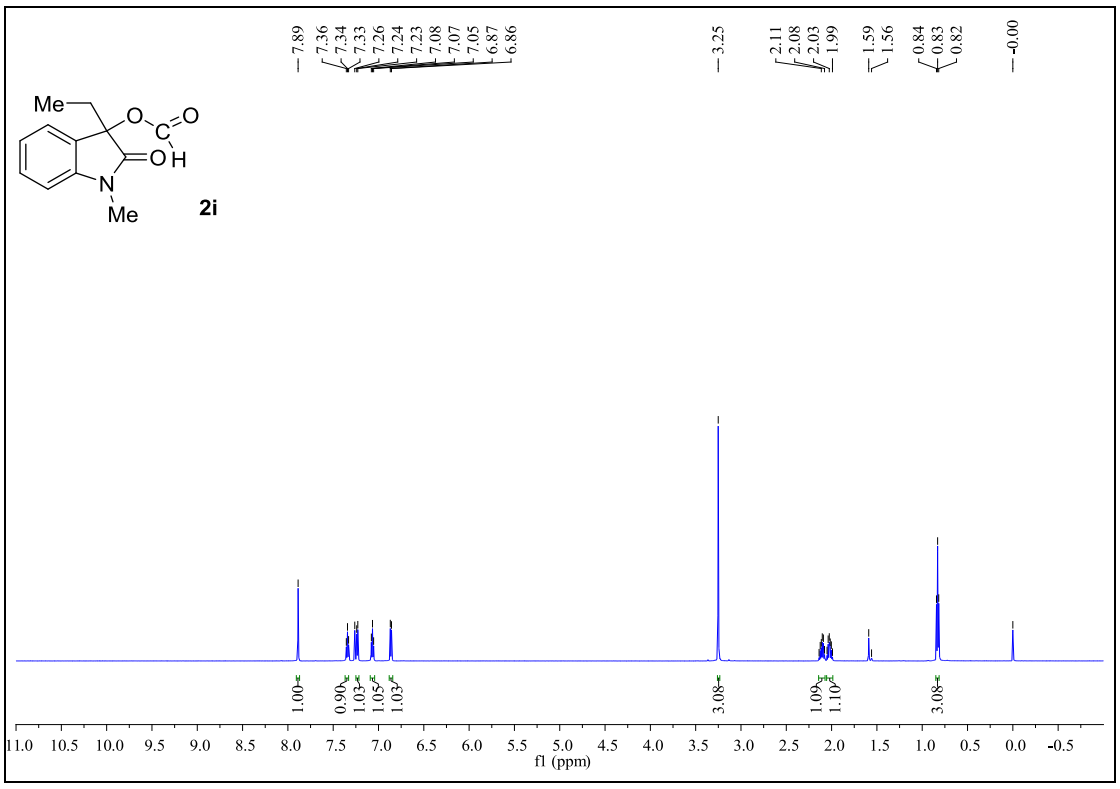
158.43
158.38
156.14
136.47
129.49
113.84
109.87
108.95
77.70
77.32
77.00
76.68
55.70
26.49
23.02
Me
MeO
O
C
O
O H
N
Me
2h
158.43
158.38
158.8 158.4 158.0
f1 (ppm)
77.70
77.32
77.00
76.68
79.0 78.5 78.0 77.5 77.0 76.5 76.0
f1 (ppm)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.36
7.34
7.33
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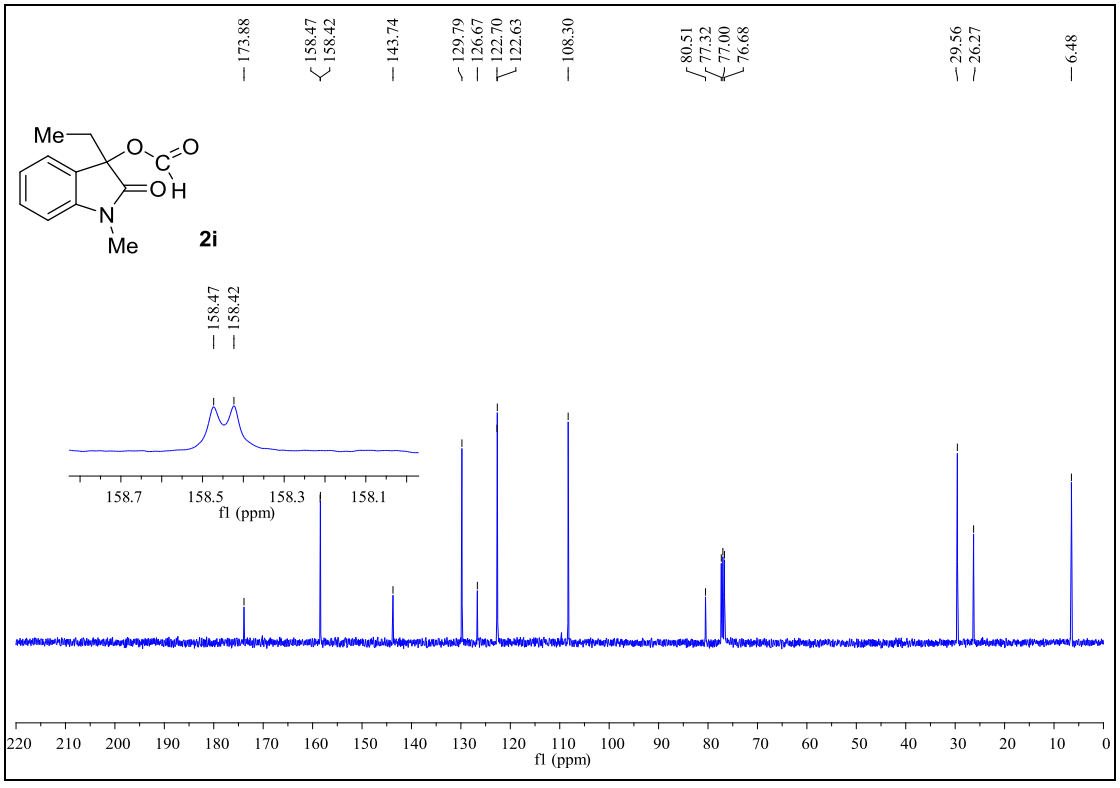
7.24
7.23
7.08
7.07
7.05
6.87
6.86
3.25
2.11
2.08
2.03
1.99
1.59
1.56
0.84
0.83
0.82
0.00
Me
O
C
O
O H
N
Me
2i
1.00
0.90
1.03
1.05
1.03
3.08
1.09
1.10
3.08
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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129.79
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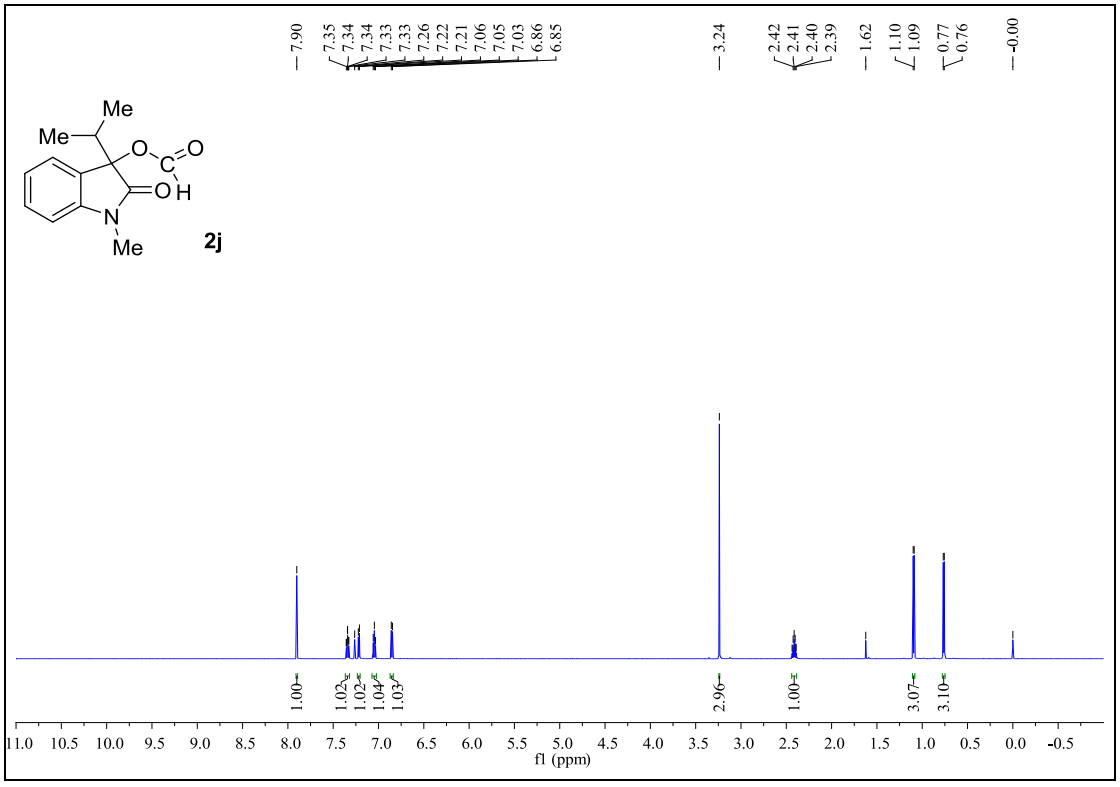
122.70
122.63
108.30
80.51
77.32
77.00
76.68
29.56
26.27
6.48
Me
O
C
O
O H
N
Me
2i
158.47
158.42
158.7 158.5 158.3 158.1
f1 (ppm)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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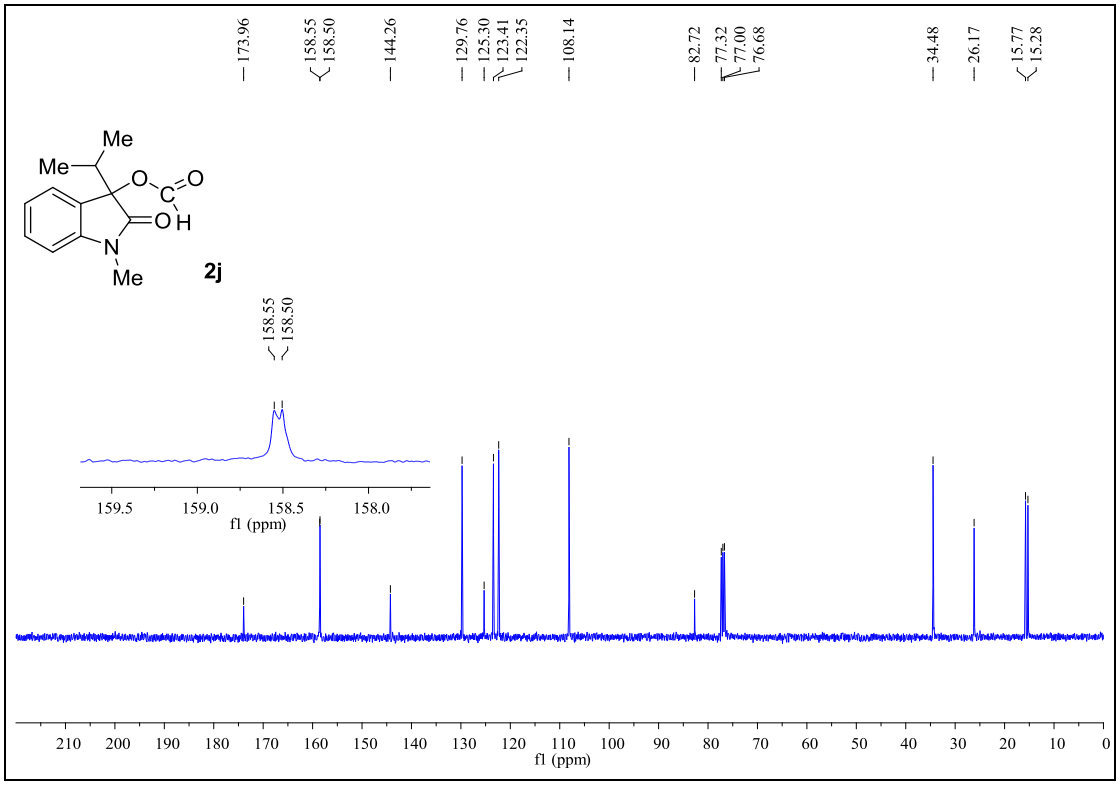
7.34
7.34
7.33
7.33
7.26
7.22
7.21
7.06
7.05
7.03
6.86
6.85
3.24
2.42
2.41
2.40
2.39
1.62
1.10
1.09
0.77
0.76
0.00
Me
Me
O
C
O
O H
N
Me
2j
1.00
1.02
1.02
1.04
1.03
2.96
1.00
3.07
3.10
fl (ppm)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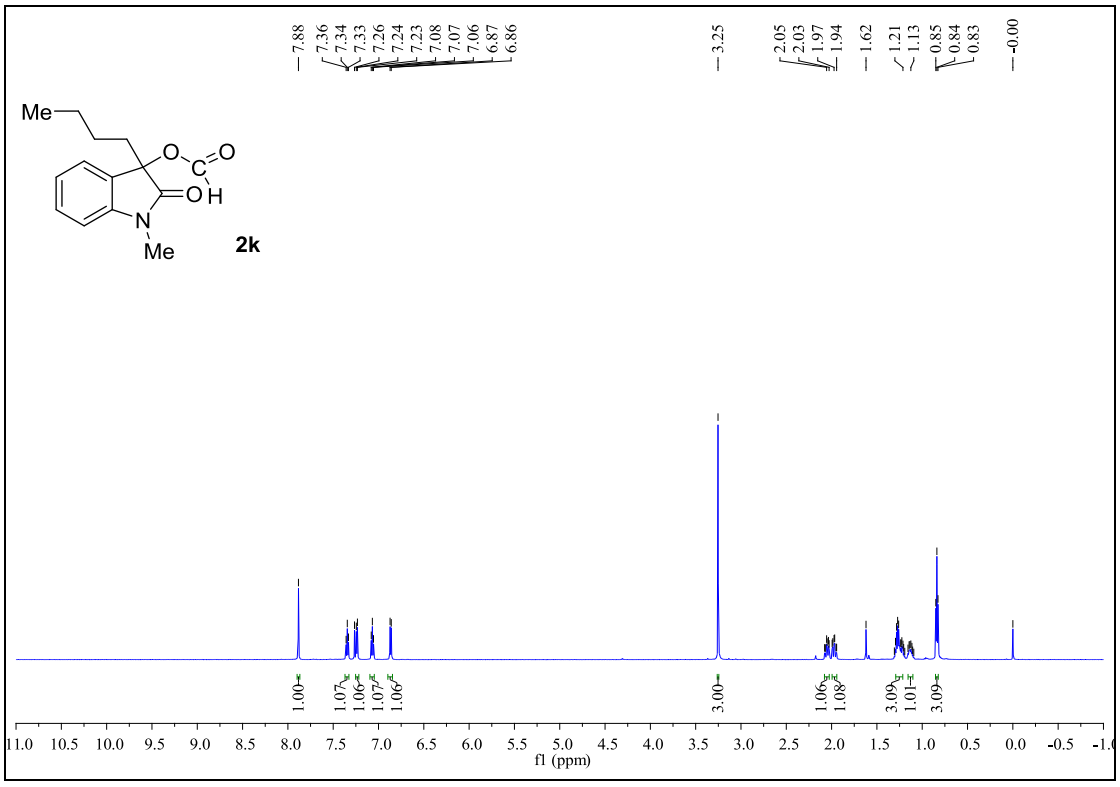
129.76
125.30
123.41
122.35
108.14
82.72
77.32
77.00
76.68
34.48
26.17
15.77
15.28
Me
Me
O
C
O
O H
N
Me
2j
158.55
158.50
159.5
159.0
158.5
158.0
fl (ppm)
fl (ppm)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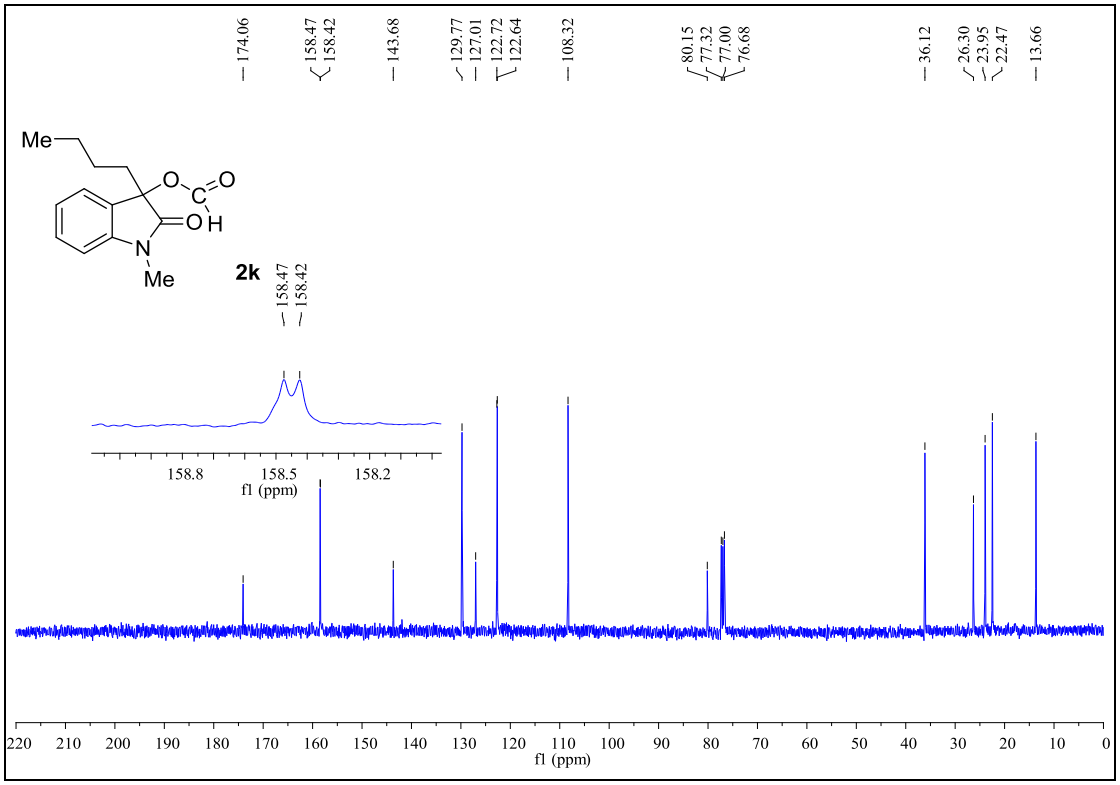
7.34
7.33
7.26
7.24
7.23
7.08
7.07
7.06
6.87
6.86
3.25
2.05
2.03
1.97
1.94
1.62
1.21
1.13
0.85
0.84
0.83
-0.00
Me
O
C
O
O H
N
Me
2k
1.00
1.07
1.06
1.07
1.06
3.00
1.06
1.08
3.09
1.01
3.09
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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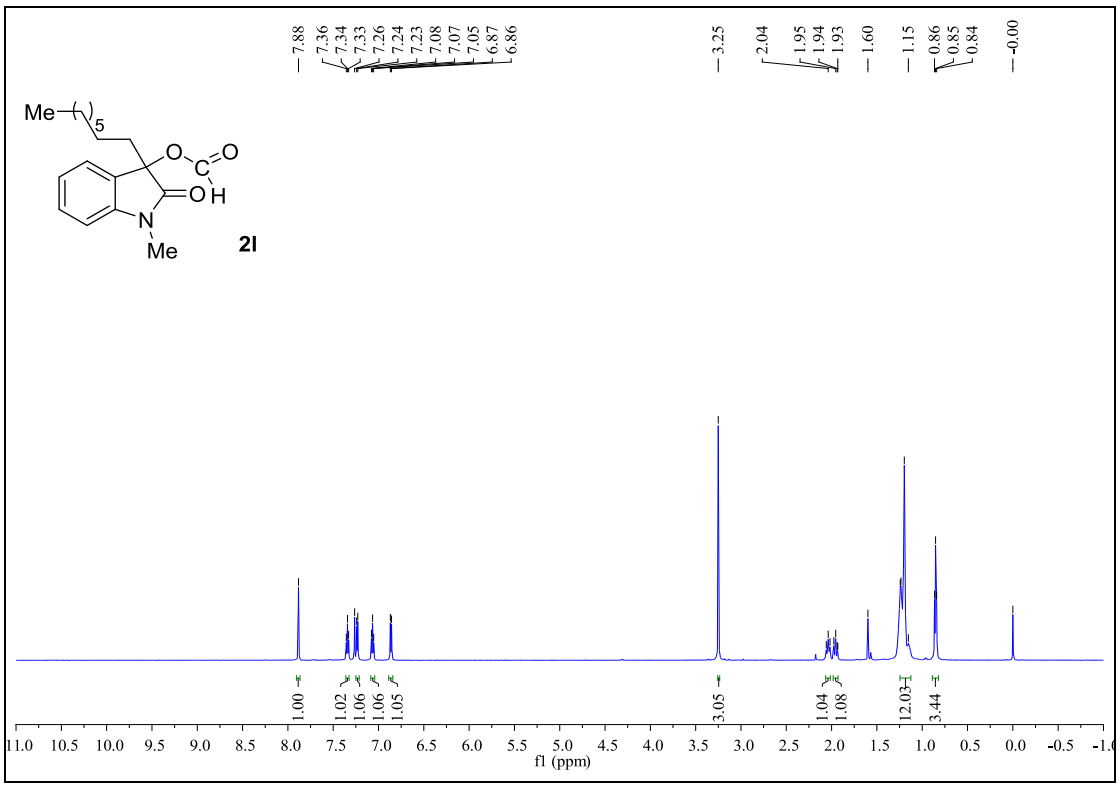
127.01
122.72
122.64
108.32
80.15
77.32
77.00
76.68
36.12
26.30
23.95
22.47
13.66
Me
O
C
O
O H
N
Me
2k
158.47
158.42
158.8 158.5 158.2
f1 (ppm)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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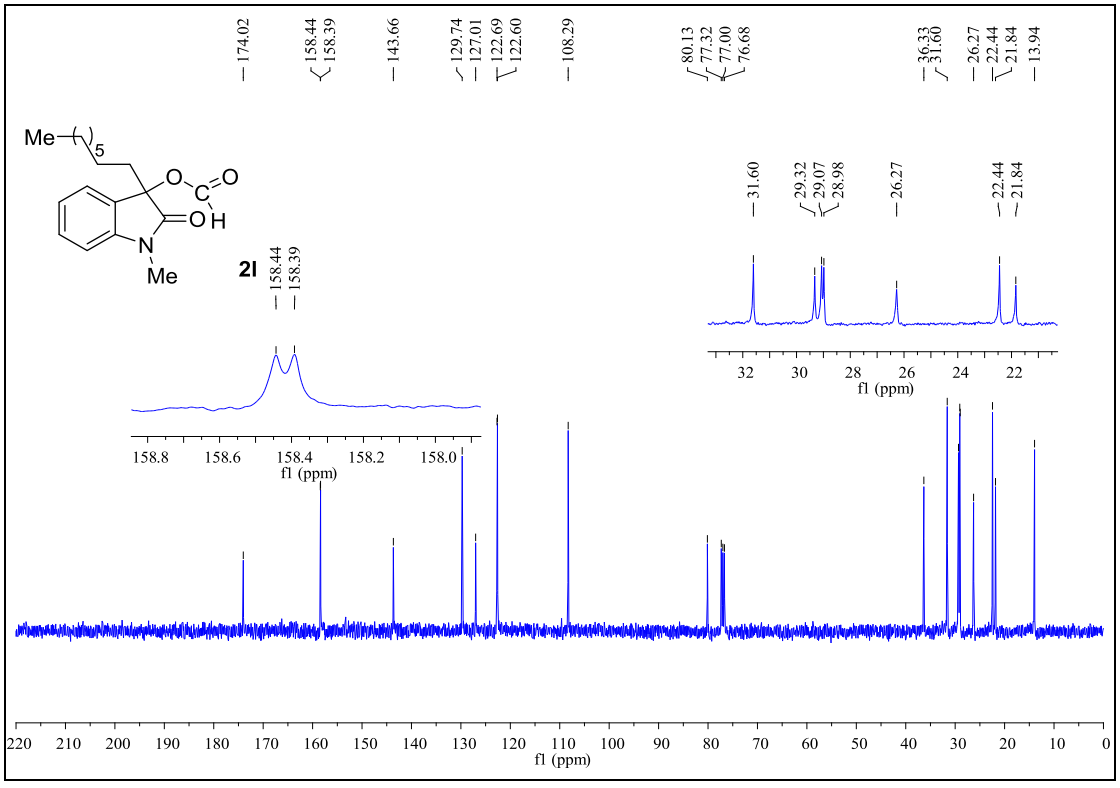
7.36
7.34
7.33
7.26
7.24
7.23
7.08
7.07
7.05
6.87
6.86
3.25
2.04
1.95
1.94
1.93
1.60
1.15
0.86
0.85
0.84
0.00
Me
5
O
C
O
O H
N
Me
2l
1.00
1.02
1.06
1.06
1.05
3.05
1.04
1.08
12.03
3.44
f1 (ppm)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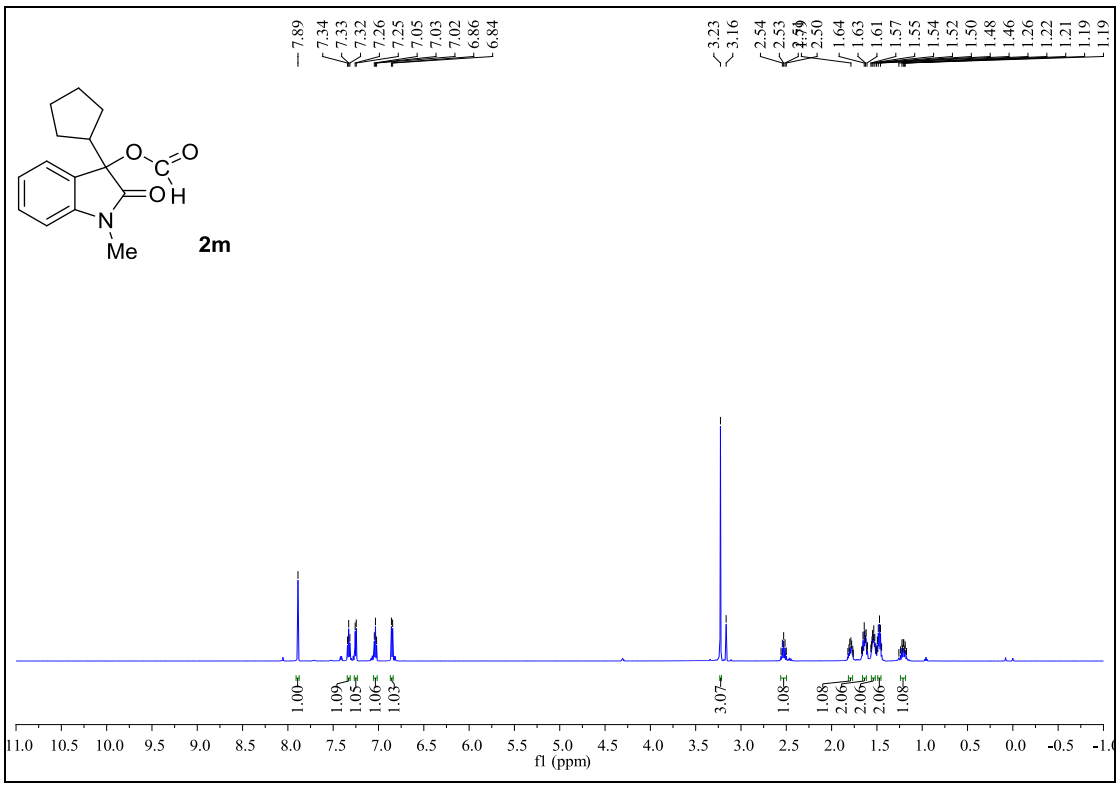
127.01
122.69
122.60
108.29
80.13
77.32
77.00
76.68
36.33
31.60
26.27
22.44
21.84
13.94
Me
5
O
C
O
O H
N
Me
2l
158.44
158.39
158.8
158.6
158.4
158.2
158.0
f1 (ppm)
31.60
29.32
29.07
28.98
26.27
22.44
21.84
32
30
28
26
24
22
f1 (ppm)
f1 (ppm)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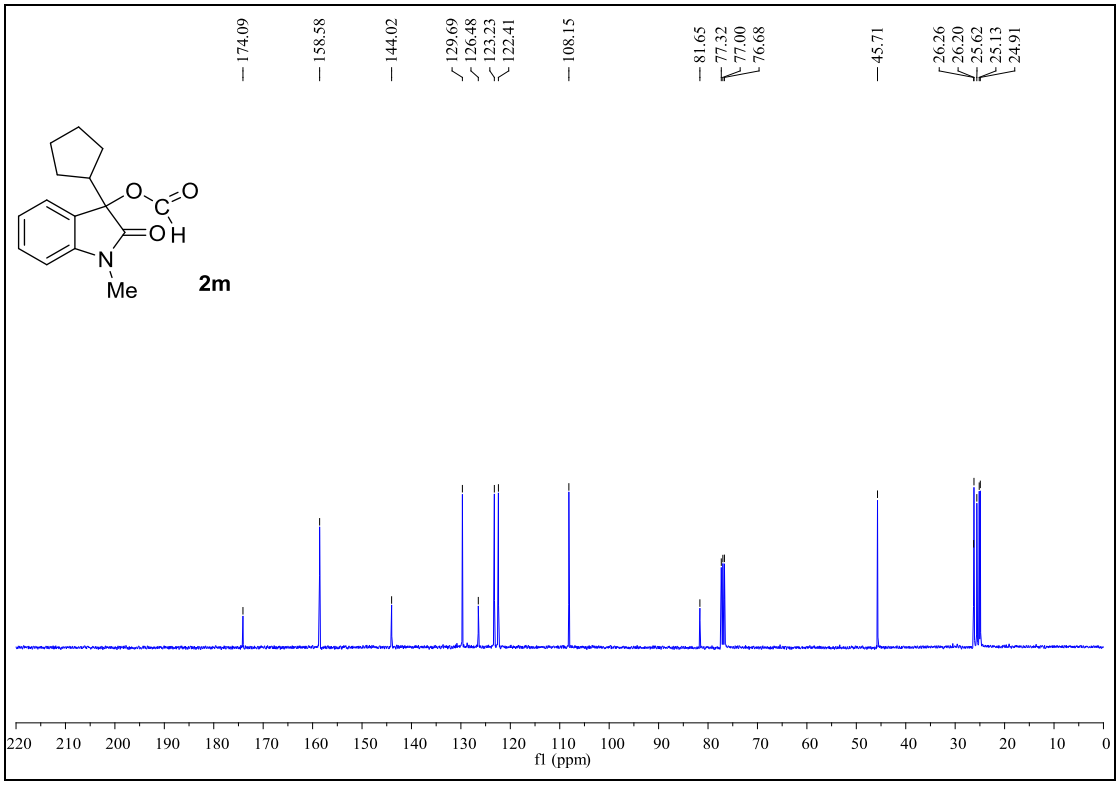
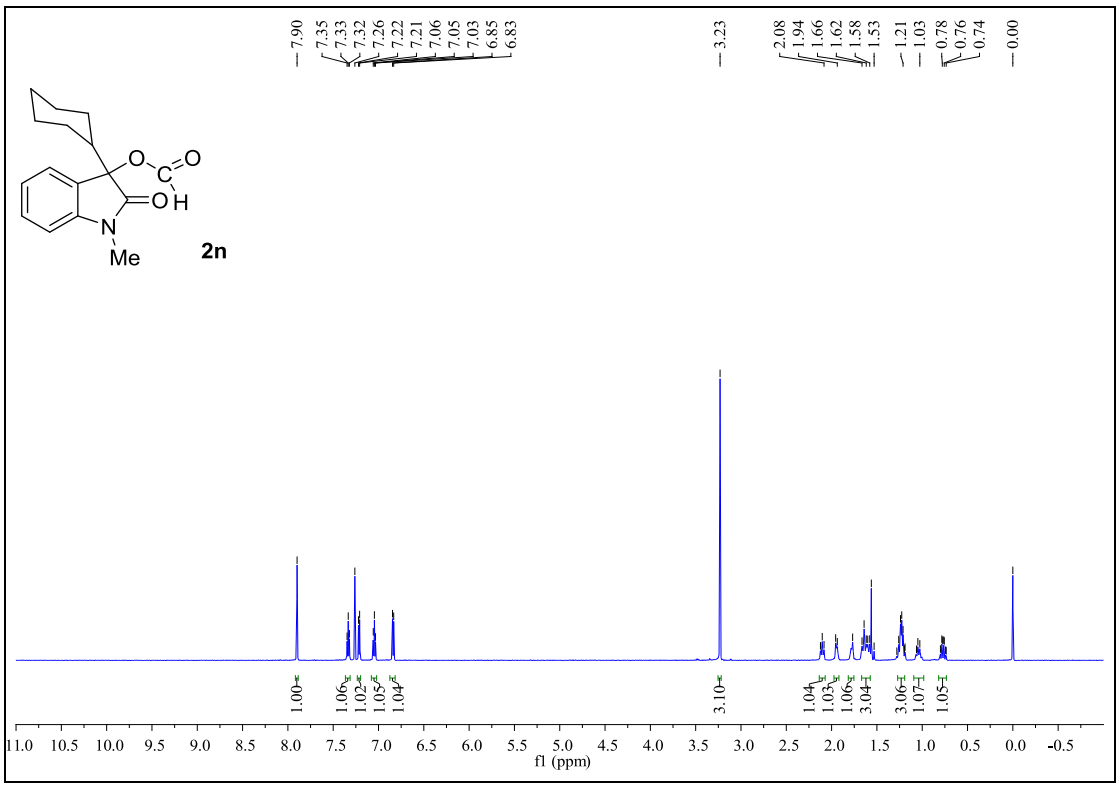
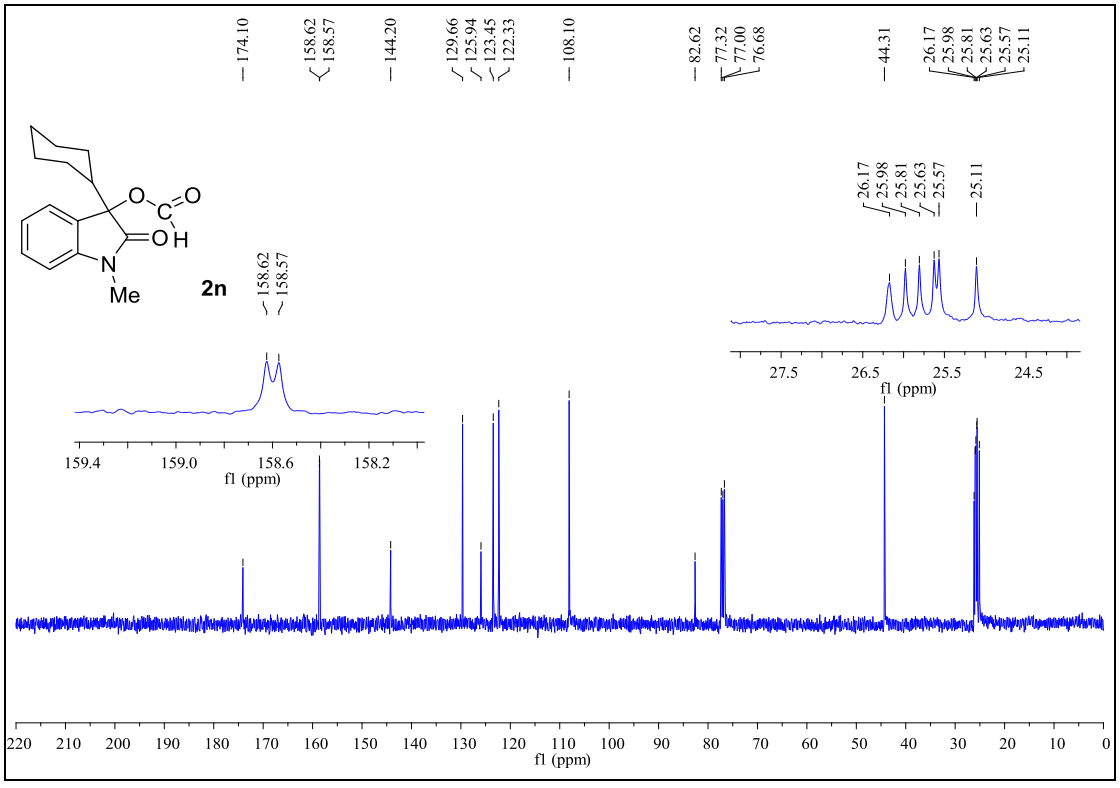
7.33
7.32
7.26
7.25
7.05
7.03
7.02
6.86
6.84
3.23
3.16
2.54
2.53
2.50
1.64
1.63
1.61
1.57
1.55
1.54
1.52
1.50
1.48
1.46
1.26
1.22
1.21
1.19
1.19
O
C
O
O H
N
Me
2m
1.00
1.09
1.05
1.06
1.03
3.07
1.08
1.08
2.06
2.06
2.06
1.08
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


174.09
158.58
144.02
129.69
126.48
123.23
122.41
108.15
81.65
77.32
77.00
76.68
45.71
26.26
26.20
25.62
25.13
24.91
O
C
O
O H
N
Me
2m
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.90
7.35
7.33
7.32
7.26
7.22
7.21
7.06
7.05
7.03
6.85
6.83
3.23
2.08
1.94
1.66
1.62
1.58
1.53
1.21
1.03
0.78
0.76
0.74
0.00
O
C
O
O H
N
Me
2n
1.00
1.06
1.02
1.05
1.04
3.10
1.04
1.03
1.06
3.04
3.06
1.07
1.05
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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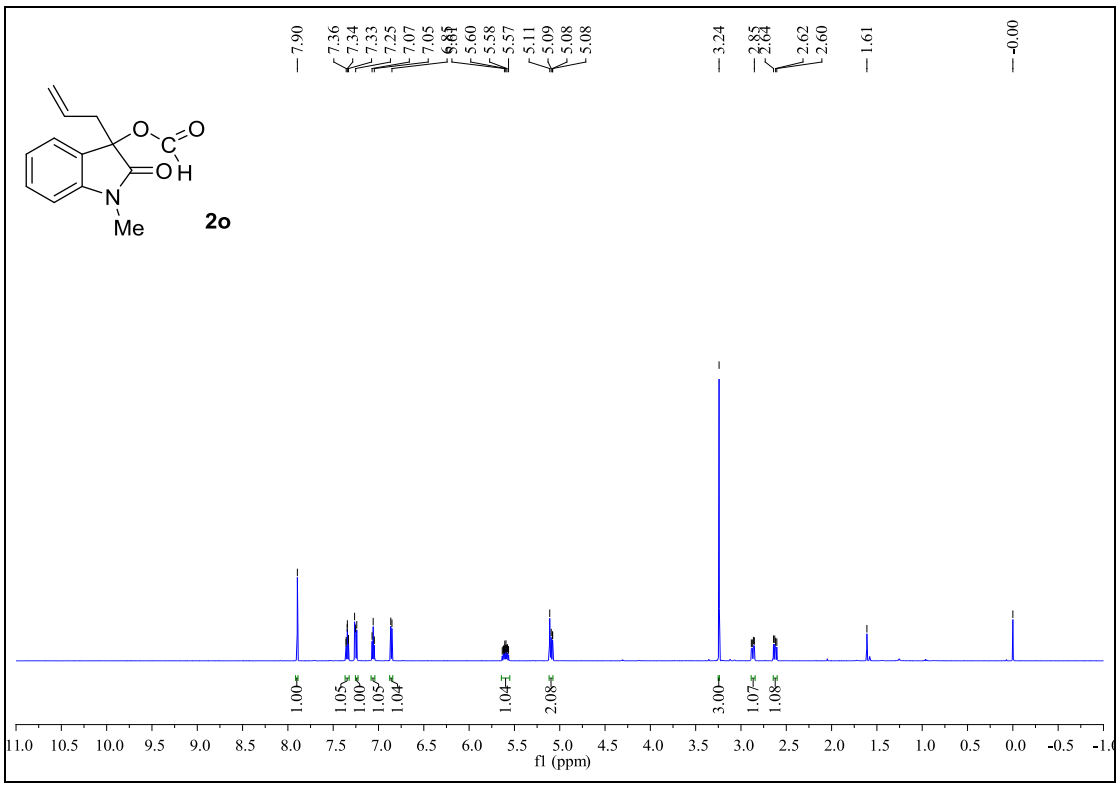
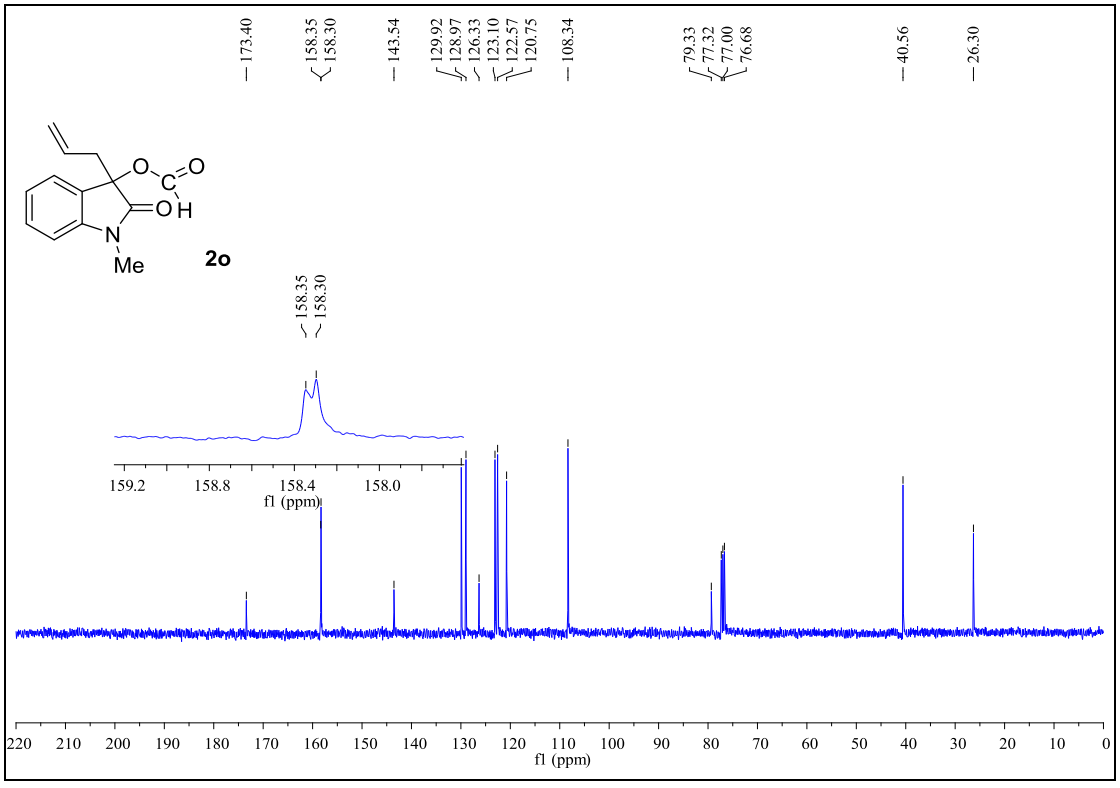
158.62
158.57
144.20
129.66
125.94
123.45
122.33
108.10
82.62
77.32
77.00
76.68
44.31
26.17
25.98
25.81
25.63
25.57
25.11
O
C
O
O H
N
Me
2n
158.62
158.57
159.4 159.0 158.6 158.2
f1 (ppm)
26.17
25.98
25.81
25.63
25.57
25.11
27.5 26.5 25.5 24.5
f1 (ppm)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.90
7.36
7.34
7.33
7.25
7.07
7.05
6.81
5.60
5.58
5.57
5.11
5.09
5.08
5.08
3.24
2.85
2.84
2.62
2.60
1.61
0.00
O
C
O
O H
N
Me
2o
1.00
1.05
1.00
1.05
1.04
1.04
2.08
3.00
1.07
1.08
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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158.30
143.54
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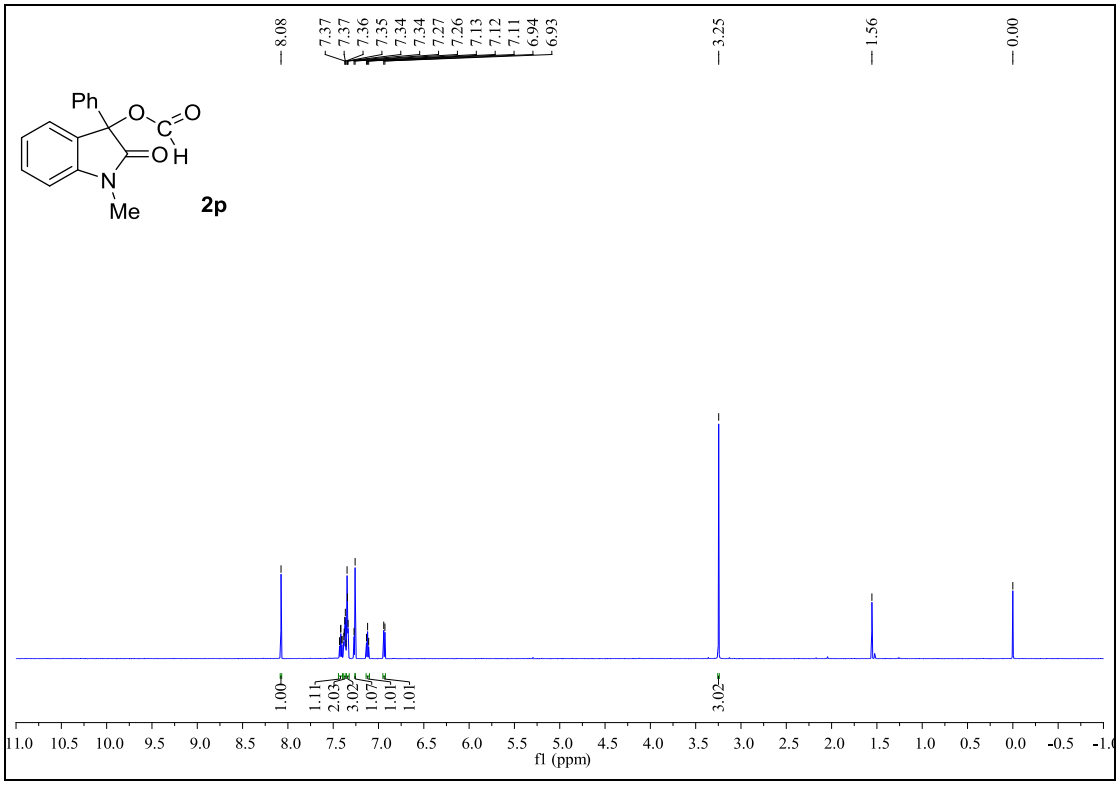
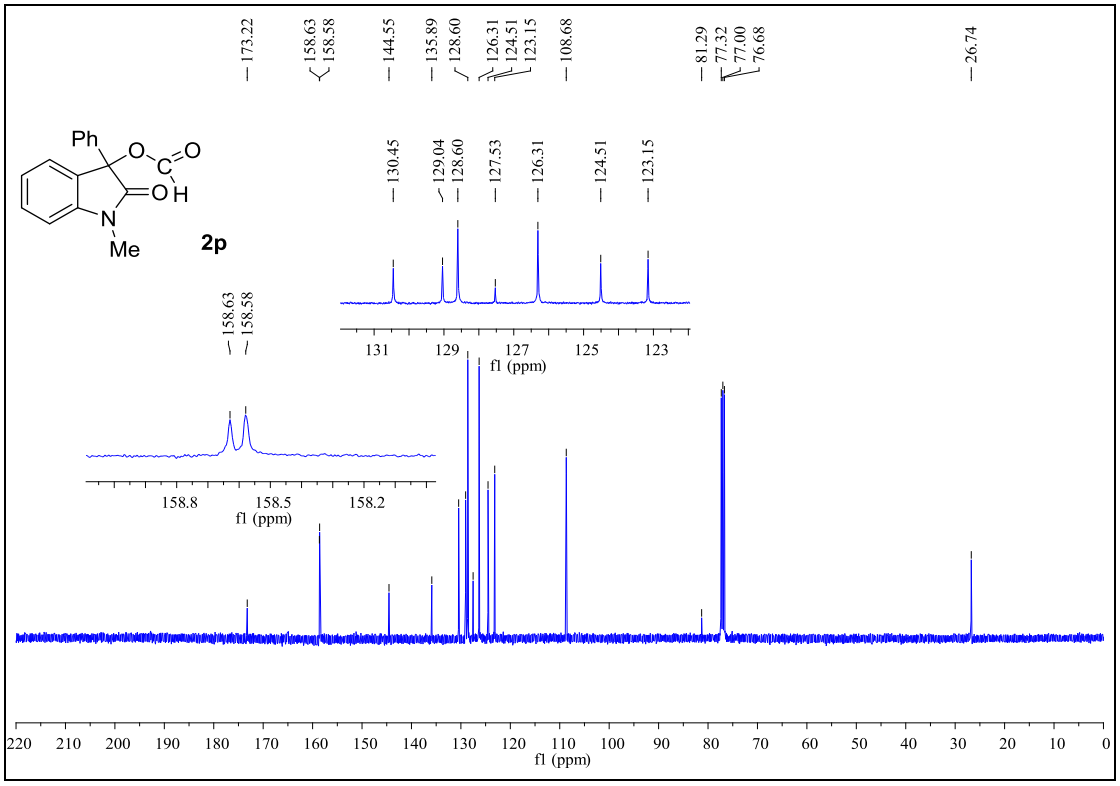
128.97
126.33
123.10
122.57
120.75
108.34
79.33
77.32
77.00
76.68
40.56
26.30
O
C
O
O H
N
Me
2o
158.35
158.30
159.2 158.8 158.4 158.0
f1 (ppm)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.08
7.37
7.37
7.36
7.35
7.34
7.34
7.27
7.26
7.13
7.12
7.11
6.94
6.93
3.25
1.56
0.00
Ph
O
C
O
O H
N
Me
2p
1.00
1.11
2.03
3.02
1.07
1.01
1.01
3.02
fl (ppm)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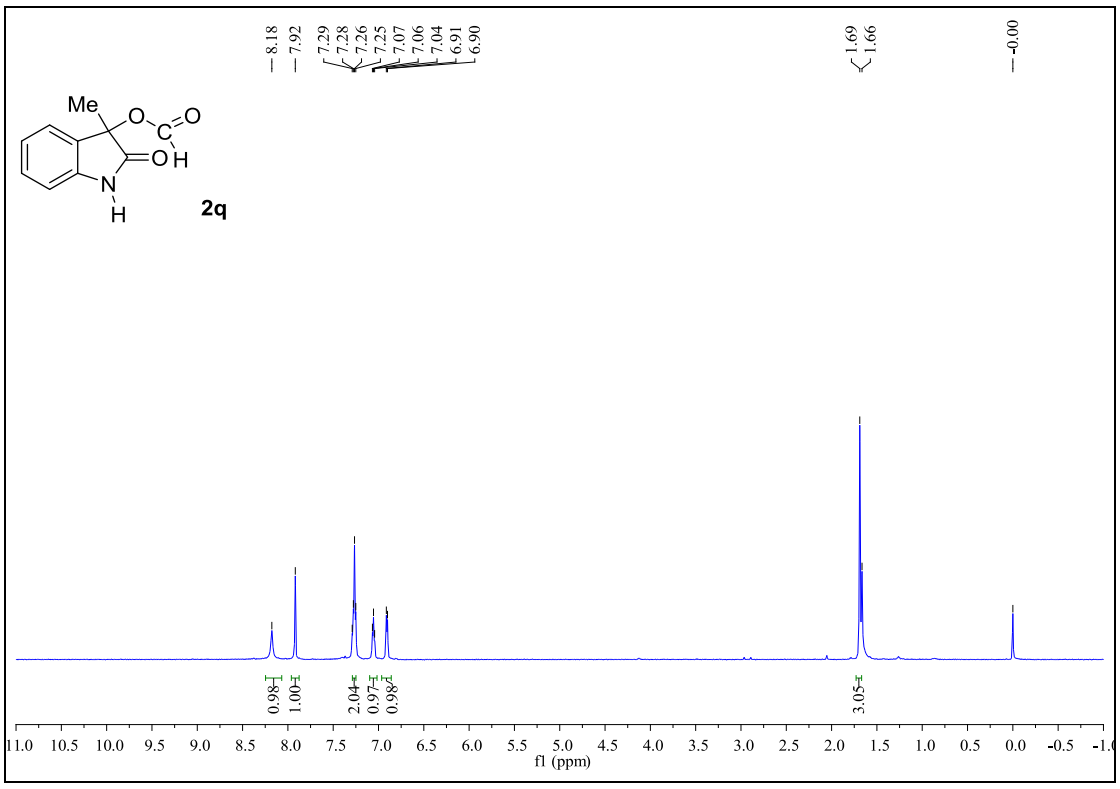
158.58
144.55
135.89
128.60
126.31
124.51
123.15
108.68
81.29
77.32
77.00
76.68
26.74
Ph
O
C
O
O H
N
Me
2p
130.45
129.04
128.60
127.53
126.31
124.51
123.15
158.63
158.58
131
129
127
125
123
fl (ppm)
158.8
158.5
158.2
fl (ppm)
fl (ppm)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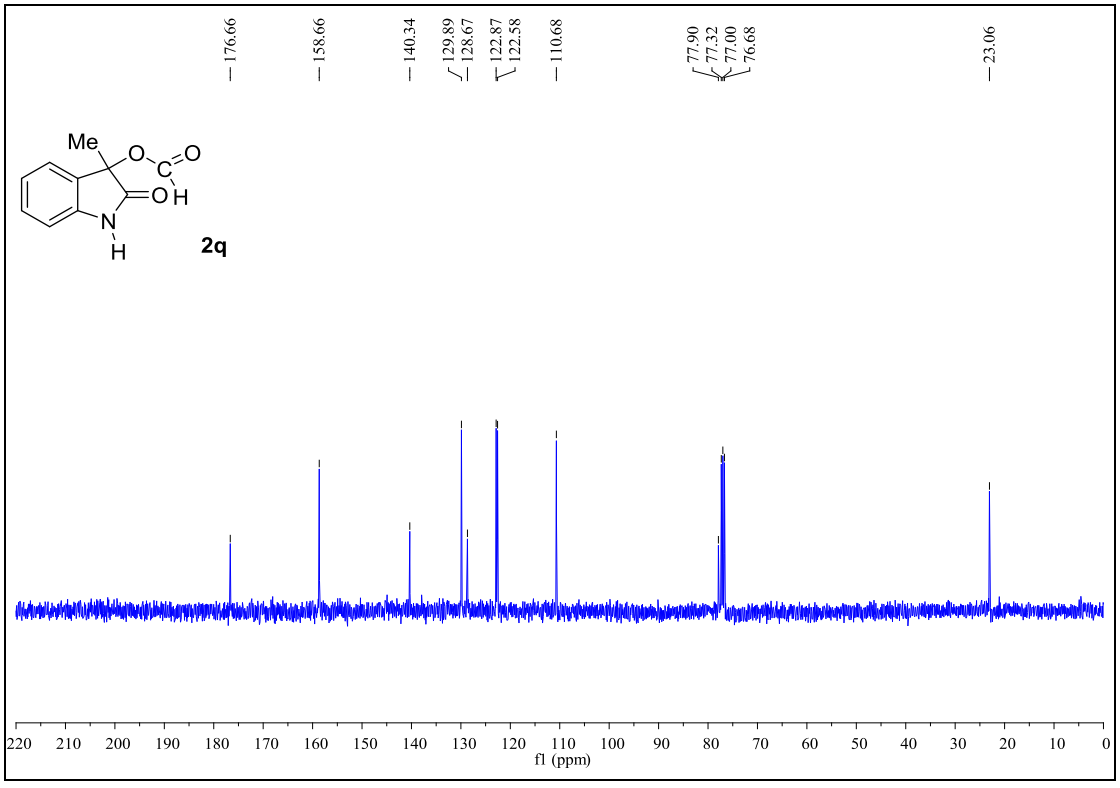
7.92
7.29
7.28
7.26
7.25
7.07
7.06
7.04
6.91
6.90
1.69
1.66
0.00
Me
O
C
O
O H
N
H
2q
0.98
1.00
2.04
0.97
0.98
3.05
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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140.34
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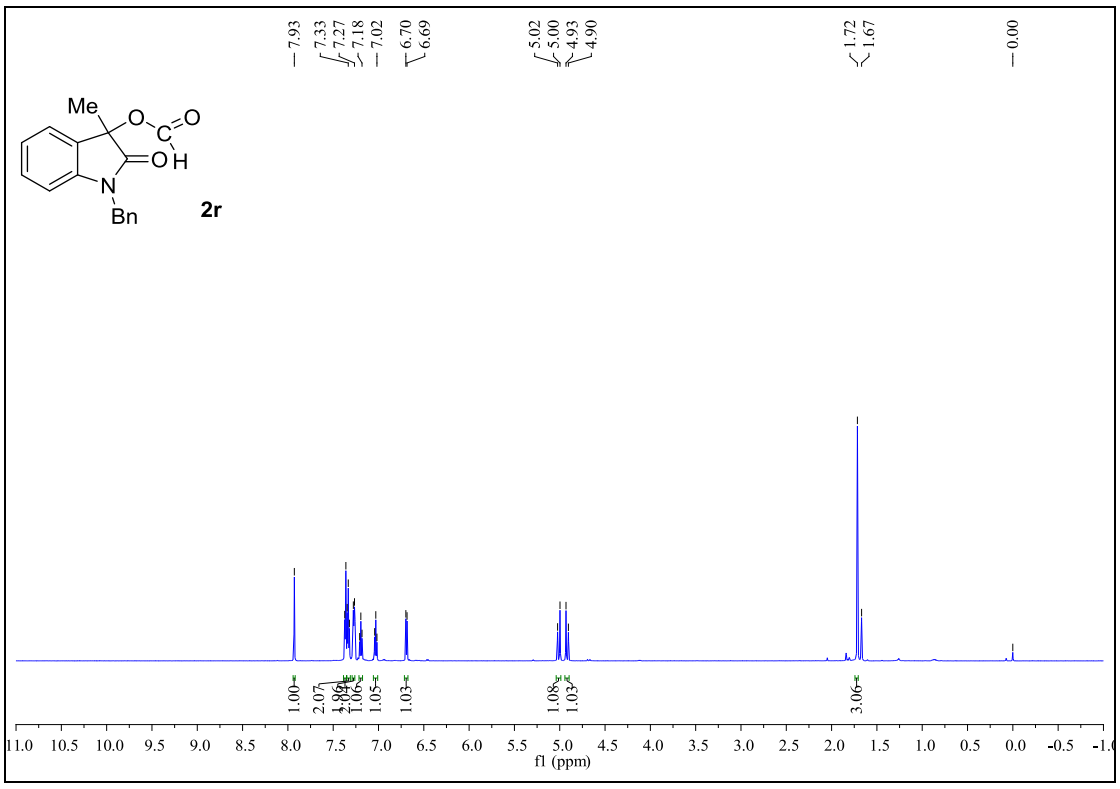
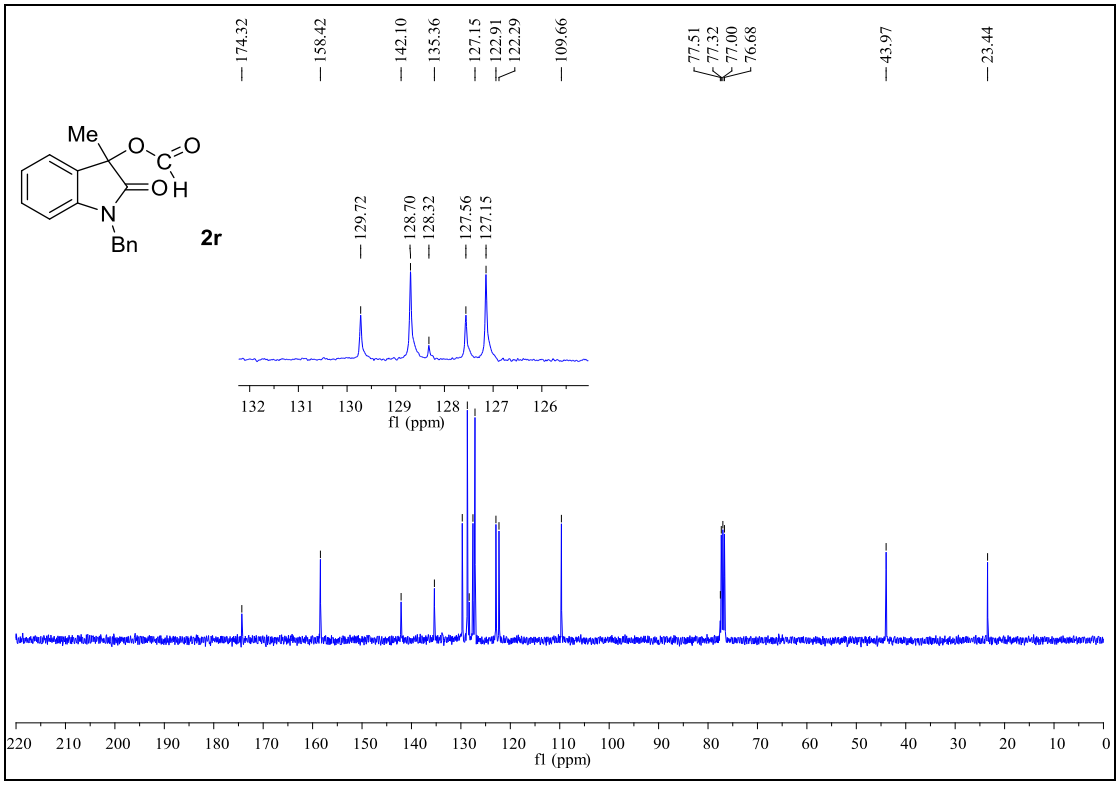
128.67
122.87
122.58
110.68
77.90
77.32
77.00
76.68
23.06
Me
O
C
O
O H
N
H
2q
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.93
7.33
7.27
7.18
7.02
6.70
6.69
5.02
5.00
4.93
4.90
1.72
1.67
0.00
Me
O
C
O
O H
N
Bn
2r
1.00
2.07
1.06
1.05
1.03
1.08
1.03
3.06
fl (ppm)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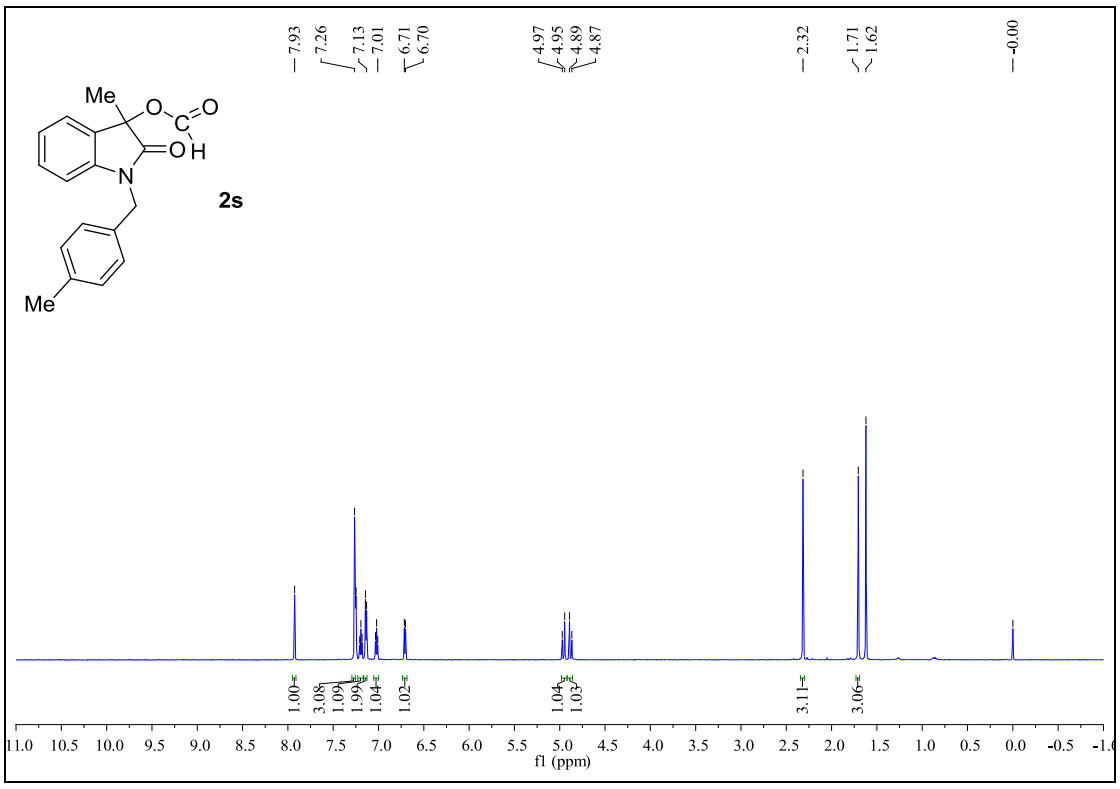
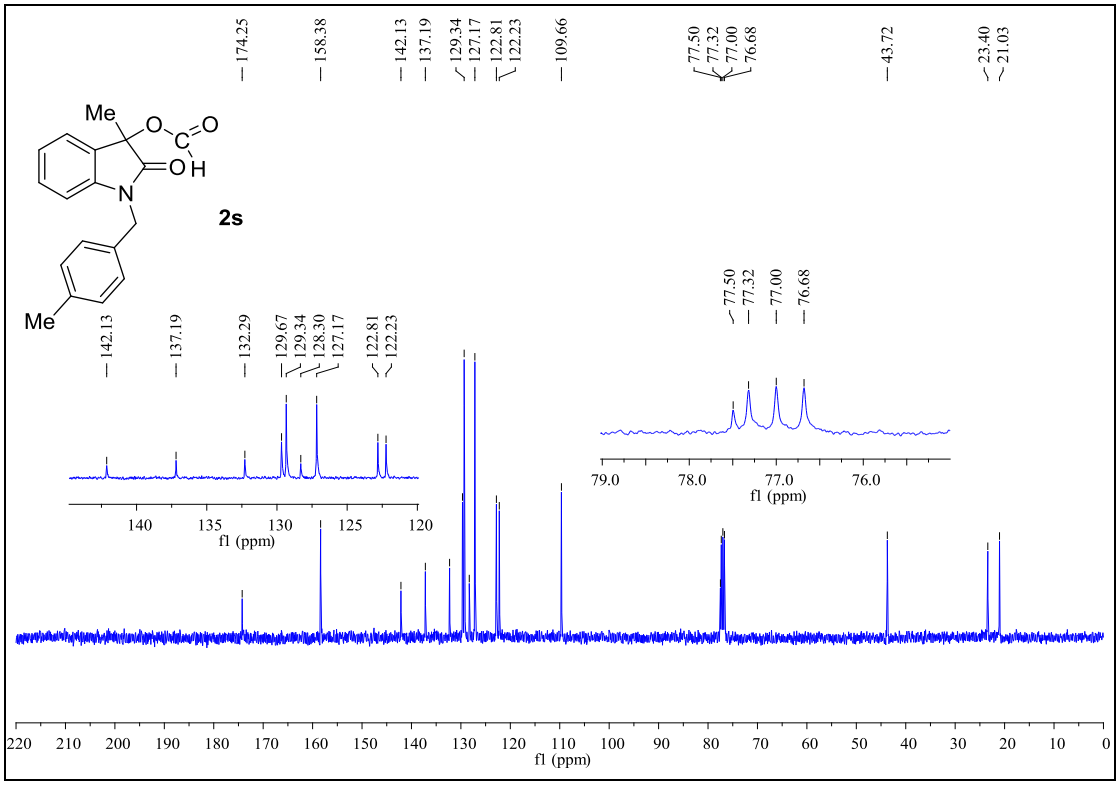
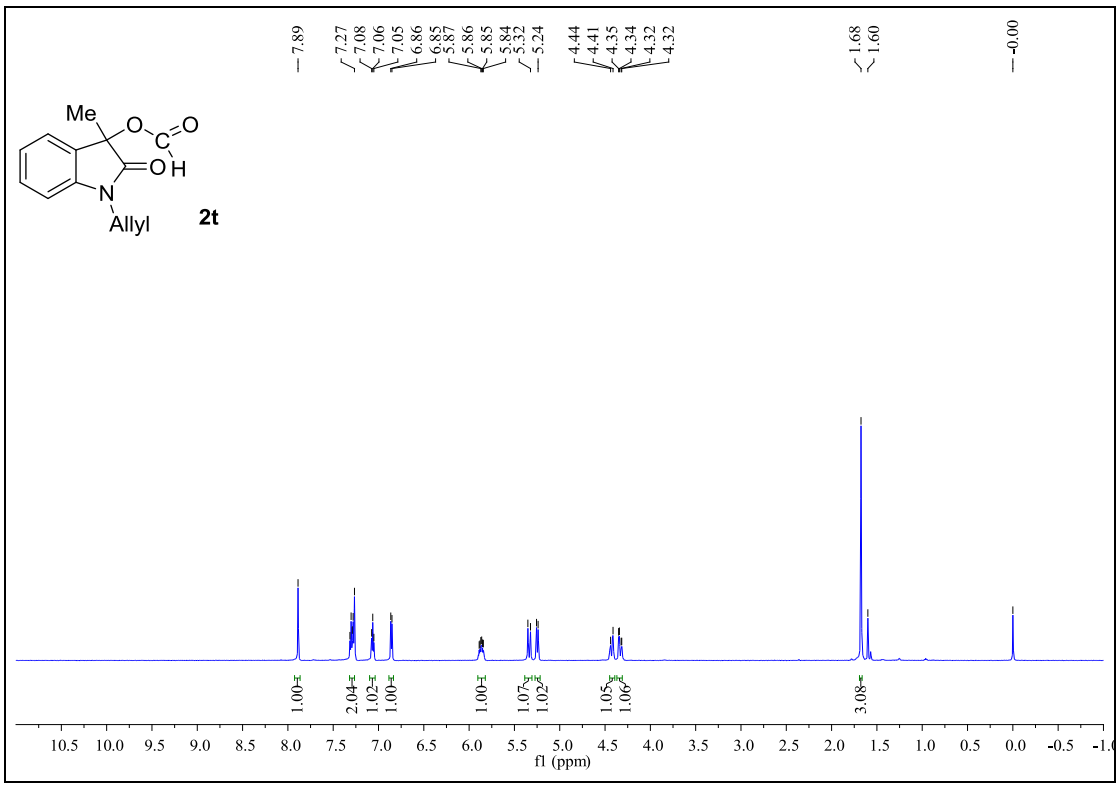
158.42
142.10
135.36
127.15
122.91
122.29
109.66
77.51
77.32
77.00
76.68
43.97
23.44
129.72
128.70
128.32
127.56
127.15
Me
O
C
O
O H
N
Bn
2r
fl (ppm)
fl (ppm)


2s
Me
O
C
O
O H
N
Me
7.93
7.26
7.13
7.01
6.71
6.70
4.97
4.95
4.89
4.87
2.32
1.71
1.62
0.00
1.00
3.08
1.09
1.99
1.04
1.02
1.04
1.03
3.11
3.06
fl (ppm)


2s
174.25
158.38
142.13
137.19
129.34
127.17
122.81
122.23
109.66
77.50
77.32
77.00
76.68
43.72
23.40
21.03
132.29
129.67
128.30
fl (ppm)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7.27
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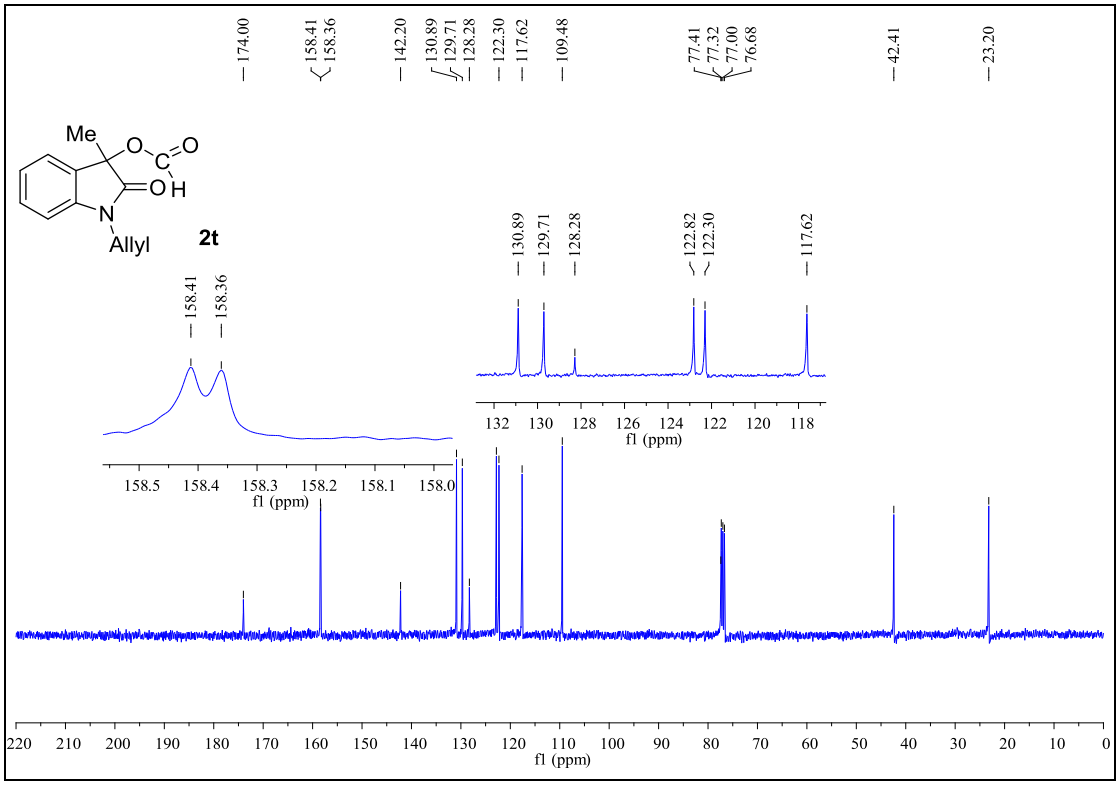
7.06
7.05
6.86
6.85
5.87
5.86
5.85
5.84
5.32
5.24
4.44
4.41
4.35
4.34
4.32
4.32
1.68
1.60
0.00
Me
O
C
O
O H
N
Allyl
2t
1.00
2.04
1.02
1.00
1.00
1.07
1.02
1.05
1.06
3.08
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


174.00
158.41
158.36
142.20
130.89
129.71
128.28
122.30
117.62
109.48
77.41
77.32
77.00
76.68
42.41
23.20
Me
O
C
O
O H
N
Allyl
2t
158.41
158.36
158.5 158.4 158.3 158.2 158.1 158.0
f1 (ppm)
130.89
129.71
128.28
122.82
122.30
117.62
132 130 128 126 124 122 120 118
f1 (ppm)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

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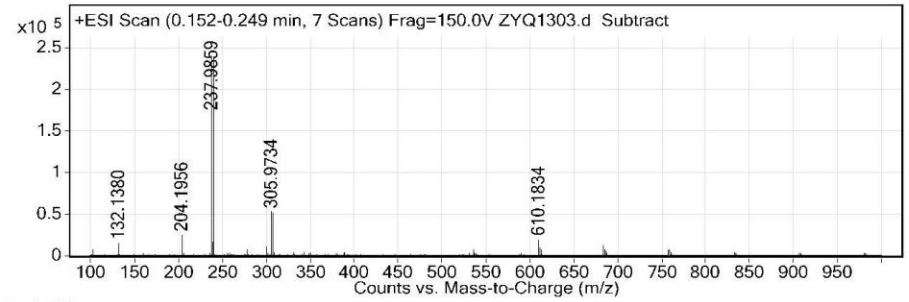
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report

Data Filename ZYQ1303.d
Sample Name ZYQ1303
User Name
Acquired Time 2013-4-16 2:05:36 PM
Instrument
Agilent Technologies 6224 TOF LC/MS

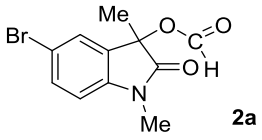
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
132.138		14934.1		
204.1956		25373.5		
237.9859	1	251587.3		
238.989	1	16686.4		
239.9839	1	243525.2		
240.987	1	15843.2		
305.9734		53641.3	C11 H10 Br N Na O3	(M+Na)+
307.9714		52513.8		
610.1834		19609.3		



2a

Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C11 H10 Br N Na O3	305.9734	305.9736	0.96	95.19

--- End Of Report ---

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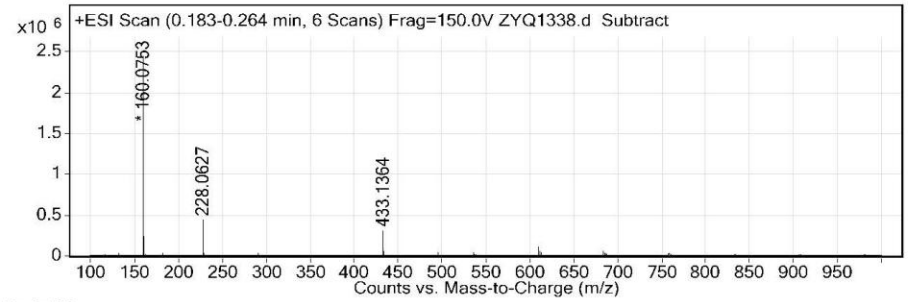
Chinese Academy of Sciences
ESI High Resolution MS Date Report

Data Filename	ZYQ1338.d
Sample Name	ZYQ1338
User Name	
Acquired Time	2013-4-9 2:54:31 PM
Instrument	

Agilent Technologies 6224 TOF LC/MS

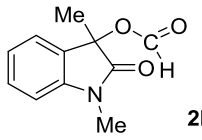
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
160.0753	1	2536041.1		
161.0785	1	244427.3		
228.0627		438809.4	C11 H11 N Na O3	(M+Na)+
433.1364		319486		



2b

Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C11 H11 N Na O3	228.0627	228.0631	2.11	92.56
C14 H9 N2 Na	228.0627	228.0658	15.18	56.67

--- End Of Report ---

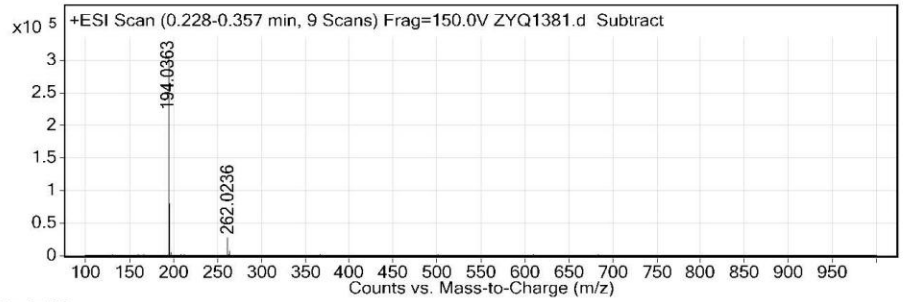
State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report

Data Filename	ZYQ1381.d
Sample Name	ZYQ1381
User Name	
Acquired Time	2013-4-16 2:03:46 PM
Instrument	

Agilent Technologies 6224 TOF LC/MS

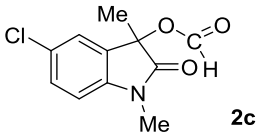
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
194.0363	1	305621.1		
195.0396	1	22319.7		
196.0336	1	81285.9		
262.0236		27276.9	C11 H10 Cl N Na O3	(M+Na)+



2c

Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C11 H10 Cl N Na O3	262.0236	262.0241	2.09	91.47

--- End Of Report ---

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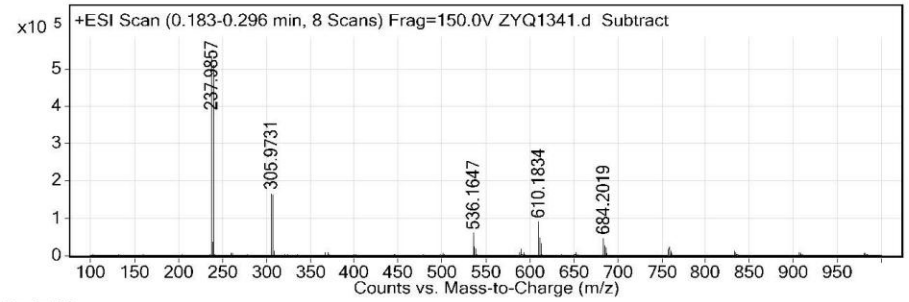
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report

Data Filename	ZYQ1341.d
Sample Name	ZYQ1341
User Name	
Acquired Time	2013-4-9 3:01:32 PM
Instrument	

Agilent Technologies 6224 TOF LC/MS

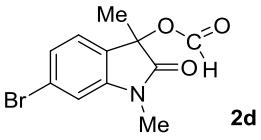
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
237.9857	1	541352.1		
238.989	1	37808.7		
239.9837	1	530042.9		
240.9869	1	36930.9		
305.9731		167489.2	C11 H10 Br N Na O3	(M+Na)+
307.9712		164414.3		
536.1647		60545.7		
610.1834	1	91862.8		
611.1841	1	46774.9		
684.2019		46008.9		



2d

Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C11 H10 Br N Na O3	305.9731	305.9736	1.74	93.02

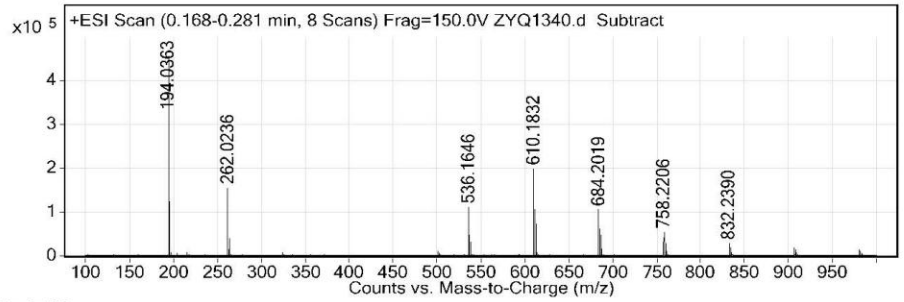
--- End Of Report ---

State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report

Data Filename ZYQ1340.d
Sample Name ZYQ1340
User Name
Acquired Time 2013-4-9 2:52:10 PM
Instrument
Agilent Technologies 6224 TOF LC/MS

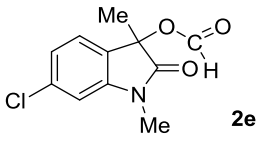
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
194.0363	1	464382		
196.0334	1	122401.4		
262.0236		154923.9	C11 H10 Cl N Na O3	(M+Na)+
536.1646	1	113831.3		
610.1832	1	202584		
611.184	1	104332.8		
612.1821	1	72500		
684.2019	1	104796.9		
685.2027	1	61203.3		
758.2206	1	53764.7		



2e

Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C11 H10 Cl N Na O3	262.0236	262.0241	2.16	89.5
C14 H8 Cl N2 Na	262.0236	262.0268	13.37	59.58

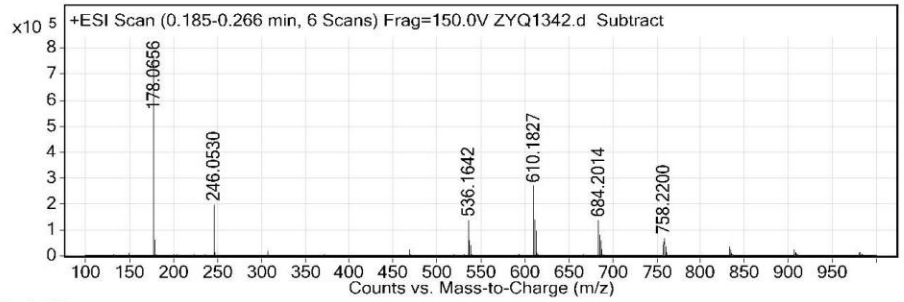
--- End Of Report ---

State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report

Data Filename ZYQ1342.d
Sample Name ZYQ1342
User Name
Acquired Time 2013-4-9 2:49:52 PM
Instrument
Agilent Technologies 6224 TOF LC/MS

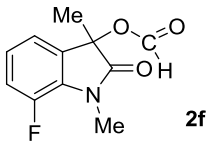
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
178.0656	1	768505.2		
246.053		200041.7	C11 H10 F N Na O3	(M+Na)+
536.1642	1	141232.6		
537.165	1	60280.4		
610.1827	1	270629		
611.1835	1	139464.3		
612.1817	1	97317.9		
684.2014	1	134036.4		
685.2021	1	78437		
758.22	1	67183.5		



2f

Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C11 H10 F N Na O3	246.053	246.0537	3.05	78.6
C14 H9 N Na O2	246.053	246.0525	-2.08	71.97

--- End Of Report ---

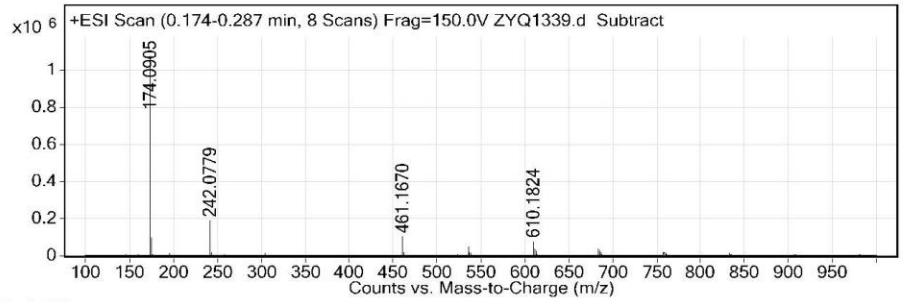
State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report

Data Filename	ZYQ1339.d
Sample Name	ZYQ1339
User Name	
Acquired Time	2013-4-9 3:03:54 PM
Instrument	

Agilent Technologies 6224 TOF LC/MS

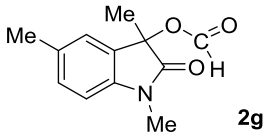
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
174.0905	1	1093434.5		
175.0939	1	100367.2		
242.0779		187387	C12 H13 N Na O3	(M+Na)+
461.167		102770.5		
610.1824		75749.1		



2g

Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C12 H13 N Na O3	242.0779	242.0788	3.9	89.26

--- End Of Report ---

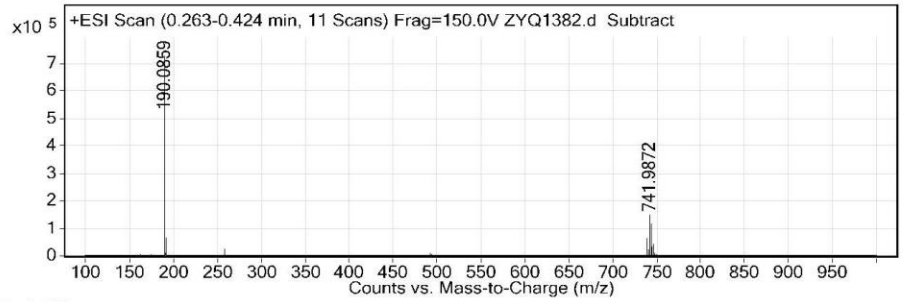
State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report

Data Filename	ZYQ1382.d
Sample Name	ZYQ1382
User Name	
Acquired Time	2013-4-16 2:07:22 PM
Instrument	

Agilent Technologies 6224 TOF LC/MS

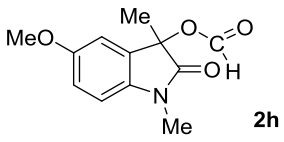
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



Peak List

m/z	z	Abund
190.0859	1	723518.2
191.0892	1	65413.6
739.9899		60900.6
741.9872	1	145769.9
742.9903	1	43997.3
743.9848	1	115271.8
745.9827		41366



2h

Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C12 H13 N Na O4	258.0732	258.0737	2.03	94.12

--- End Of Report ---

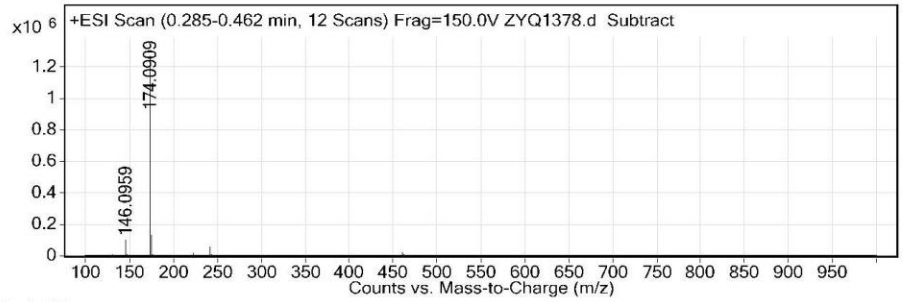
State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report

Data Filename	ZYQ1378.d
Sample Name	ZYQ1378
User Name	
Acquired Time	2013-4-16 1:56:36 PM
Instrument	

Agilent Technologies 6224 TOF LC/MS

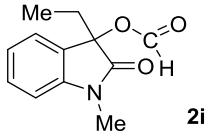
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



Peak List

m/z	z	Abund
146.0959		103167.2
174.0909	1	1337749.2
175.0942	1	128718.7



2i

Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C12 H13 N Na O3	242.0784	242.0788	1.78	93.66

--- End Of Report ---

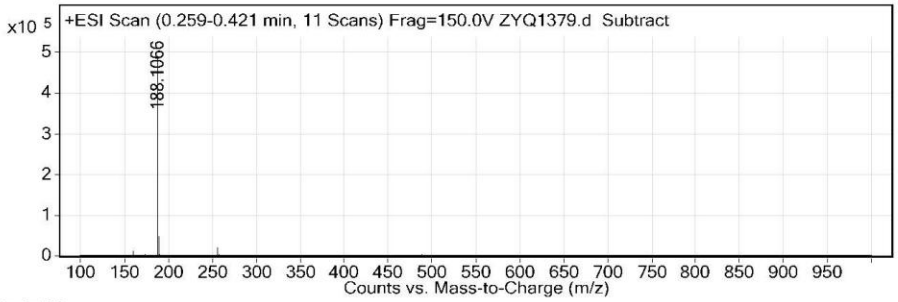
State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report

Data Filename	ZYQ1379.d
Sample Name	ZYQ1379
User Name	
Acquired Time	2013-4-16 2:01:59 PM
Instrument	

Agilent Technologies 6224 TOF LC/MS

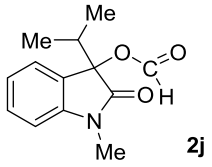
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



Peak List

m/z	z	Abund
188.1066	1	491972
189.1099	1	46923.4



2j

Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C13 H15 N Na O3	256.094	256.0944	1.91	95.09

--- End Of Report ---

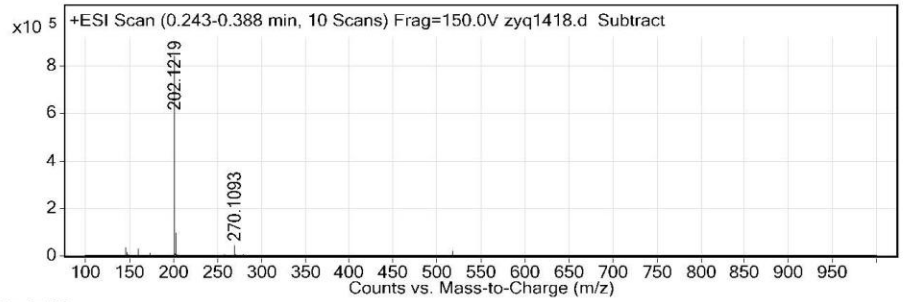
State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report

Data Filename	zyq1418.d
Sample Name	zyq1418
User Name	
Acquired Time	2013-4-17 4:25:50 PM
Instrument	

Agilent Technologies 6224 TOF LC/MS

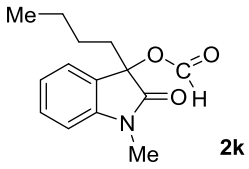
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
202.1219	1	863931.1		
203.1252	1	96697.6		
270.1093		44732.5	C14 H17 N Na O3	(M+Na)+



2k

Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C14 H17 N Na O3	270.1093	270.1101	3.17	90.22

--- End Of Report ---

State Key Laboratory of Organometallic Chemistry
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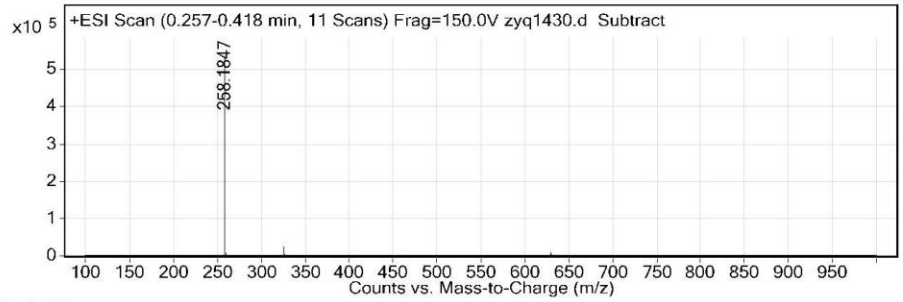
Chinese Academy of Sciences
ESI High Resolution MS Date Report

Data Filename	zyq1430.d
Sample Name	zyq1430
User Name	
Acquired Time	2013-4-17 4:18:30 PM
Instrument	

Agilent Technologies 6224 TOF LC/MS

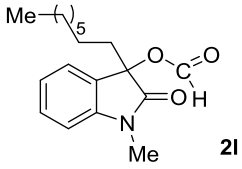
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



Peak List

m/z	z	Abund
258.1847	1	534731.4
259.188	1	78307.2



2l

Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C18 H25 N Na O3	326.1721	326.1727	1.84	90.71

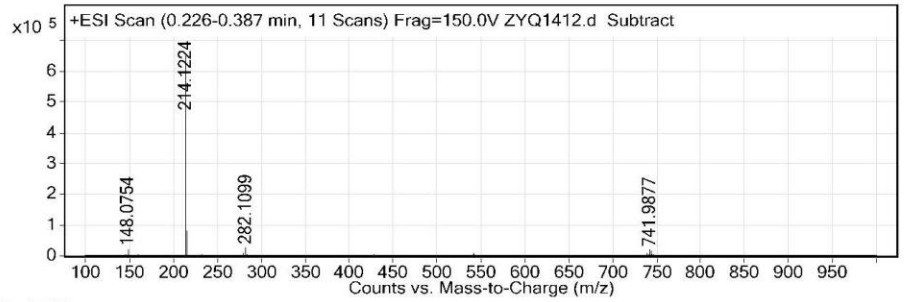
--- End Of Report ---

State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report

Data Filename ZYQ1412.d
Sample Name ZYQ1412
User Name
Acquired Time 2013-4-16 2:10:58 PM
Instrument
Agilent Technologies 6224 TOF LC/MS

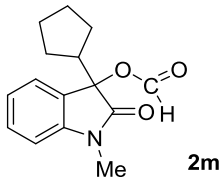
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
148.0754		18998.4		
214.1224	1	679773.9		
214.1966		13178.7		
214.2595		16527.9		
215.1257	1	82233.8		
282.1099		26109.8	C15 H17 N Na O3	(M+Na)+
741.9877		16490.5		
743.9851		13015.9		



2m

Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C15 H17 N Na O3	282.1099	282.1101	0.77	93.72

--- End Of Report ---

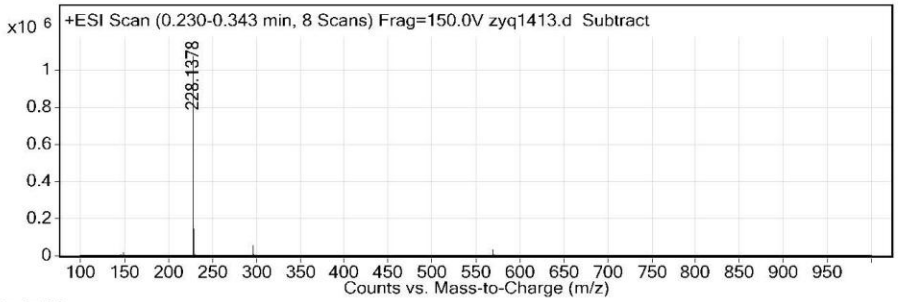
State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report

Data Filename	zyq1413.d
Sample Name	zyq1413
User Name	
Acquired Time	2013-4-17 4:20:22 PM
Instrument	

Agilent Technologies 6224 TOF LC/MS

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI

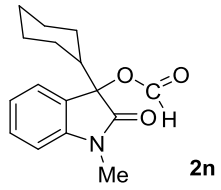


Peak List

m/z	z	Abund
228.1378	1	1078101
229.1411	1	150864.3

Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C16 H19 N Na O3	296.1251	296.1257	2.34	90.01



2n

--- End Of Report ---

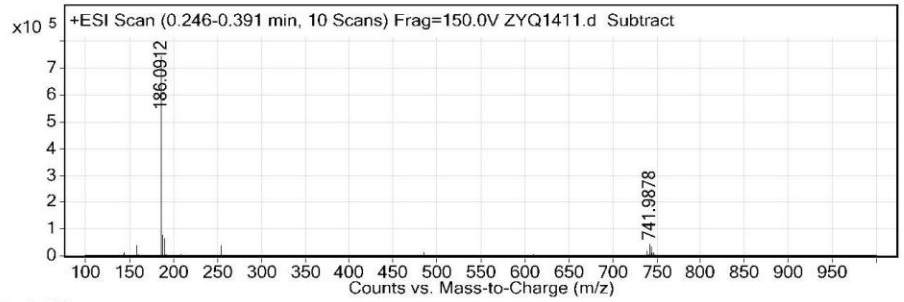
State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report

Data Filename	ZYQ1411.d
Sample Name	ZYQ1411
User Name	
Acquired Time	2013-4-16 2:09:08 PM
Instrument	

Agilent Technologies 6224 TOF LC/MS

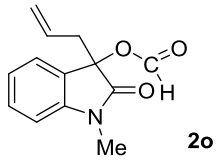
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



Peak List

m/z	z	Abund
186.0912	1	778440.1
187.0945	1	76848.2
190.0861		61158.4
741.9878		43955.1



2o

Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C13 H13 N Na O3	254.0787	254.0788	0.49	94.64

--- End Of Report ---

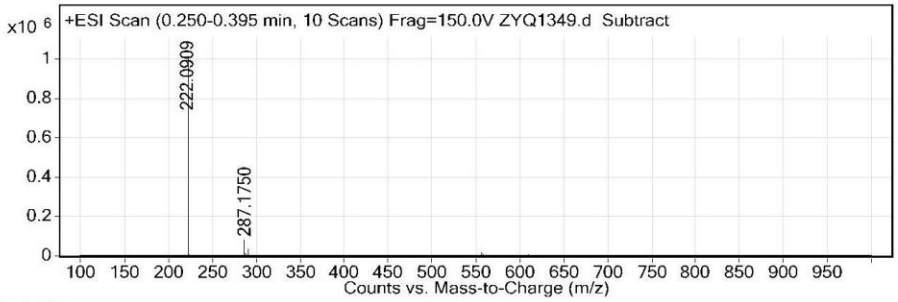
State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report

Data Filename	ZYQ1349.d
Sample Name	ZYQ1349
User Name	
Acquired Time	2013-4-16 1:54:49 PM
Instrument	

Agilent Technologies 6224 TOF LC/MS

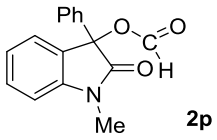
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



Peak List

m/z	z	Abund
222.0909	1	1049667.8
223.0942	1	141370
287.175		78343.3



2p

Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C16 H13 N Na O3	290.0783	290.0788	1.7	92.61

--- End Of Report ---

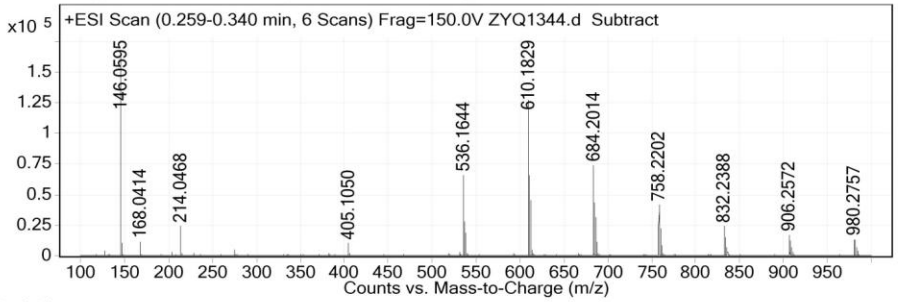
State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report

Data Filename	ZYQ1344.d
Sample Name	ZYQ1344
User Name	
Acquired Time	2013-4-9 2:47:35 PM

Instrument
Agilent Technologies 6224 TOF LC/MS

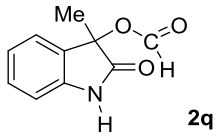
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



Peak List

m/z	z	Abund
146.0594	1	113937.1
536.1644	1	44391.3
537.1651	1	18711.9
610.1828	1	83656.5
611.1836	1	42715.2
612.1818	1	29562.5
684.2014	1	48531.9
685.2026	1	28575
686.2005	1	20961.9
758.2201	1	27512.2



2q

Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C10 H9 N Na O3	214.0467	214.0475	3.74	83.09

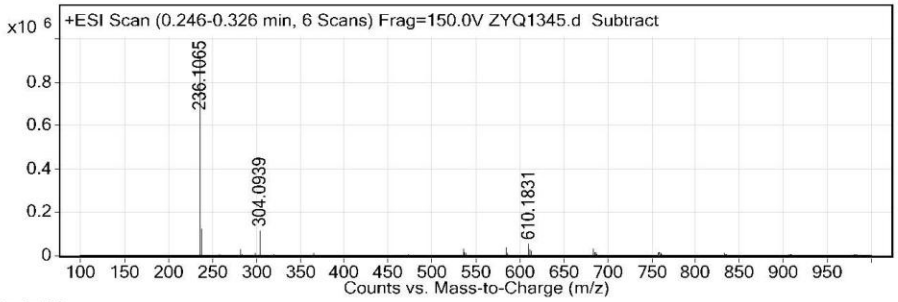
--- End Of Report ---

State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report

Data Filename ZYQ1345.d
Sample Name ZYQ1345
User Name
Acquired Time 2013-4-9 2:56:52 PM
Instrument
Agilent Technologies 6224 TOF LC/MS

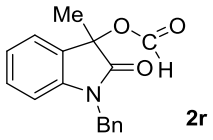
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
236.1065	1	925210.6		
237.1098	1	128977.9		
304.0939		116340.5	C17 H15 N Na O3	(M+Na)+
610.1831		54960.7		



2r

Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C17 H15 N Na O3	304.0939	304.0944	1.84	89.63
C20 H13 N2 Na	304.0939	304.0971	11.38	58.16

--- End Of Report ---

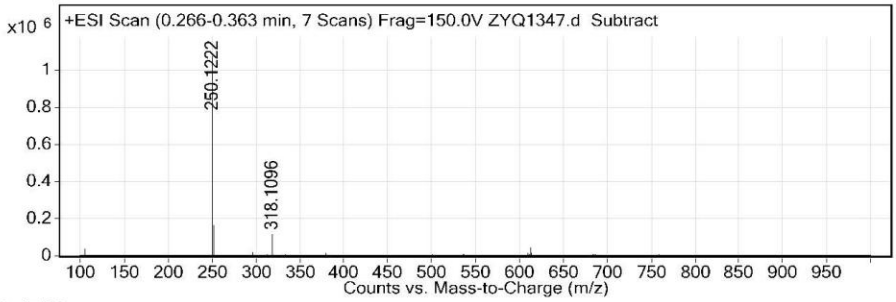
State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report

Data Filename	ZYQ1347.d
Sample Name	ZYQ1347
User Name	
Acquired Time	2013-4-9 3:23:54 PM
Instrument	

Agilent Technologies 6224 TOF LC/MS

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI

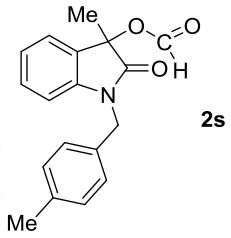


Peak List

m/z	z	Abund	Formula	Ion
250.1222	1	704845.5		
251.1255	1	105724.3		
318.1096		73391.8	C18 H17 N Na O3	(M+Na)+

Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C18 H17 N Na O3	318.1096	318.1101	1.63	89.63



2s

--- End Of Report ---

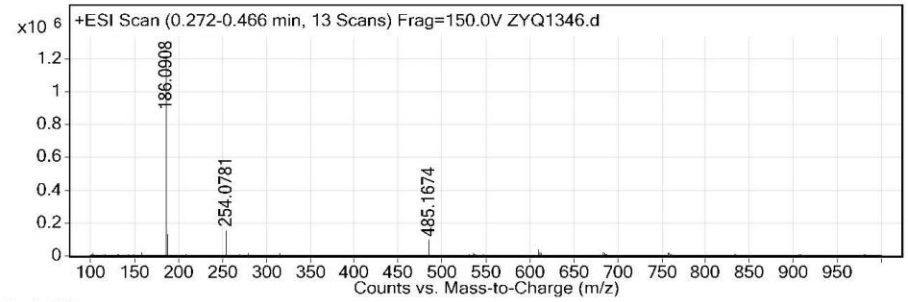
State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report

Data Filename	ZYQ1346.d
Sample Name	ZYQ1346
User Name	
Acquired Time	2013-4-9 2:45:18 PM
Instrument	

Agilent Technologies 6224 TOF LC/MS

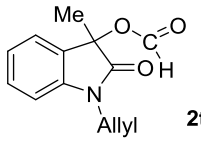
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
186.0907	1	1087445.3		
187.094	1	110862		
254.0781		136273.4	C13 H13 N Na O3	(M+Na)+
485.1675		61007.3		



2t

Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C13 H13 N Na O3	254.0781	254.0788	2.72	78.34

--- End Of Report ---

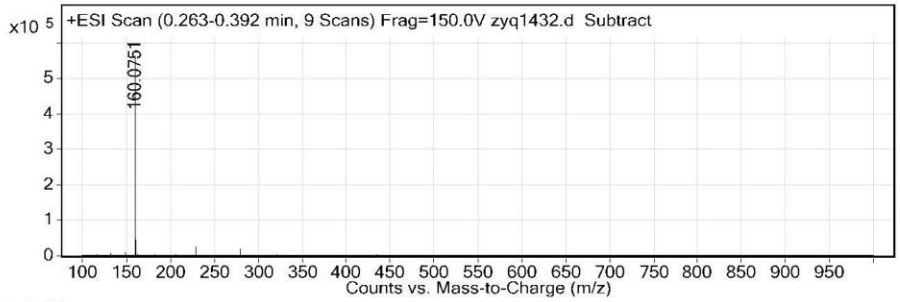
State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report

Data Filename	zyq1432.d
Sample Name	zyq1432
User Name	
Acquired Time	2013-4-17 4:16:44 PM
Instrument	

Agilent Technologies 6224 TOF LC/MS

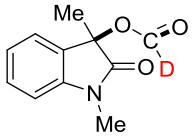
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
160.0751	1	560925.2		
160.1114		16291.4		
161.0783	1	42901.4		
229.0688		25839	C11 H10 D N Na O3	(M+Na)+
279.1584		19233		



D-2b

Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C11 H10 D N Na O3	229.0688	229.0694	2.84	94.49

--- End Of Report ---

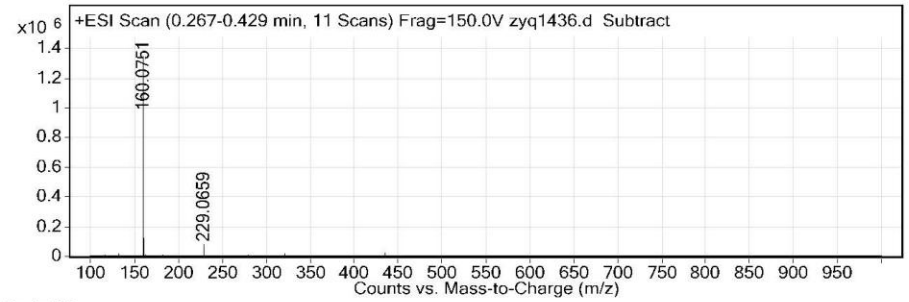
State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report

Data Filename	zyq1436.d
Sample Name	zyq1436
User Name	
Acquired Time	2013-4-17 4:22:11 PM

Instrument
Agilent Technologies 6224 TOF LC/MS

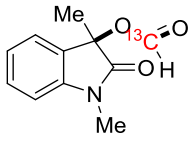
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



Peak List

m/z	z	Abund
160.0751	1	1340464.7
161.0783	1	120282.4
229.0659		73426



C-13-2b

Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C10 [13C] H11 N Na O3	229.0659	229.0665	2.97	92.09

--- End Of Report ---

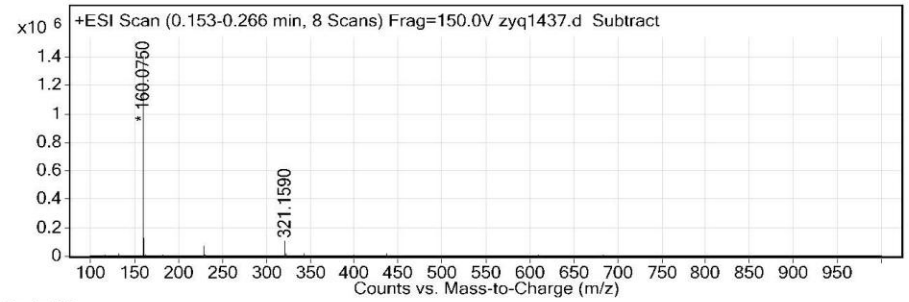
State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report

Data Filename	zyq1437.d
Sample Name	zyq1437
User Name	
Acquired Time	2013-4-17 4:27:36 PM

Instrument
Agilent Technologies 6224 TOF LC/MS

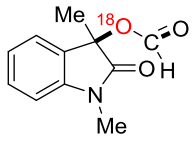
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



Peak List

m/z	z	Abund
160.075	1	1400172.2
161.0783	1	126337.5
321.159		100731.3



O-18-2b

Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C11 H11 N Na O2 [18O]	230.0667	230.0674	3.06	91.95

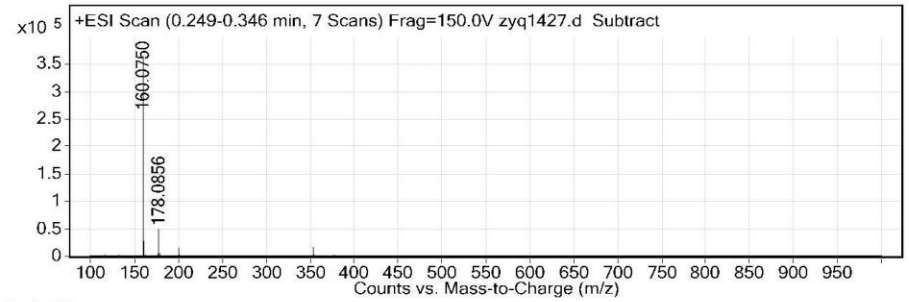
--- End Of Report ---

State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report

Data Filename zyq1427.d
Sample Name zyq1427
User Name
Acquired Time 2013-4-17 4:24:01 PM
Instrument
Agilent Technologies 6224 TOF LC/MS

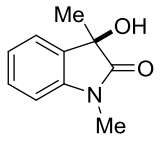
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
160.075	1	362704.7		
161.0783	1	25786.9		
178.0856		48248.9	C10 H12 N O2	(M+H)+



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Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C10 H12 N O2	178.0856	178.0863	3.69	92.97

--- End Of Report ---