Supporting Information

Facile Synthesis of 11-aryl-6H-isoindolo[2,1-a]indol-6-ones *via*Hypervalent Iodine (III)-Promoted Cascade Cyclization

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Content

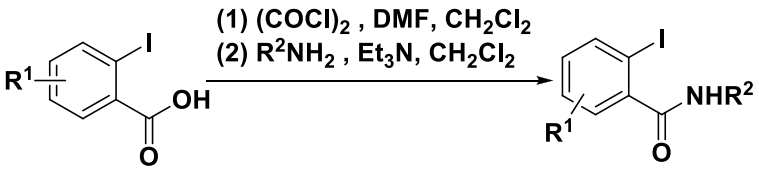
1. General information

All reagents and solvents were purchased from commercial suppliers and used without further purification. Thin layer chromatography (TLC) was performed on silica gel 60 F_{254}coated on aluminium sheet and UV light (254 nm& 365 nm)as well as iodine, adsorbed on silica get were used for visualization of TLC plate. IR spectra of the compounds were recorded on Perkin-Elmer spectrometer using KBr pellets or neat and the infrared frequencies arereported in cm^{-1}. ^{1}H-NMR spectra were recorded on Bruker Advance DPX 300 MHz & 400 MHz spectrometers in $CDCl_3$ or as stated deuterated solvent and ^{13}C-NMR spectra were recorded on 75.4 MHz & 100.6 MHz and DEPT, HSQC, HMBC &^{1}H-^{1}H COSY were also recorded on same NMR instrument. The calibration of the NMR spectra was done by using residual undeuterated solvent as an internal reference.Chemical shifts and coupling constants are reported in parts per million (ppm) relative to residual signal of TMS in deuterated solvents and Hertz, respectively. High resolution mass spectra were acquired on Electro spray ionization massspectrometer in positive ionization mode. Melting points are uncorrected and weredetermined in capillary tubes on a melting point apparatus containing silicon oil.Silica gel 100-200 and 230-400 mesh were used as stationary phase to isolate the compounds.

2. Experimental procedures and compounds characterization

2.1. Synthesis and characterization of 2-iodobenzamides[1]

2-iodo-*N*-phenylbenzamide (S1a)

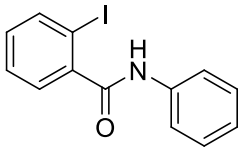


S1a-o

To a solution of 2-iodobenzoic acid (10.1mmol, 1.00 equiv) and oxalyl chloride (20.2mmol) in CH_2Cl_2 50 mL were added the catalytic amount of *N,N'*-dimethylformamide (50 µL). The resulting mixture was then stirred at room temperature continuously till the solid disappeared. The solution was concentrated under reduced pressure and another 50 mL of CH_2Cl_2 was added followed by addition of aniline (11.1mmol) and triethylamine (24.4mmol). The corresponding reaction mixture was stirred at room temperature for 6 h. The reaction mixture was quenched with water and the aqueous phase was extracted with CH_2Cl_2 (3 X 50 mL). The organic phases

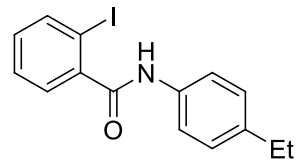
were combined and washed with 10 % HCl (aq.), water, saturated $NaHCO_3$ (aq.), and brine respectively, and dried over anhy. Na_2SO_4. The solvent was removed at reduced pressure and residue was purified by column chromatography on silica gel (100-200 mesh) eluting with hexane/EtOAc (95: 05), afforded white solid product in 90 %. The compound was characterized by comprehensive analysis of ^{1}H NMR and ^{13}C NMR.

***N*-(phenyl)-2-iodobenzamide (S1a)**



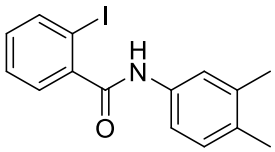
White solid, Yield 90%; FT-IR (KBr): 3436, 2143, 1658, 1601, 1538, 1498, 1440, 1324,1219, 1015, 691, 667 cm^{-1};^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 7.93 (d, *J* = 7.9 Hz, 1H), 7.68 (d, *J* = 7.8 Hz, 3H), 7.55–7.52 (m, 1H), 7.47–7.39 (m, 3H), 7.24–7.15 (m, 2H);^{13}C NMR (75.4 MHz, $CDCl_3$): δ (ppm) 167.3, 142.1, 140.0, 137.5, 131.5, 129.1(2C), 128.5, 128.3, 124.9, 120.1(2C), 92.4;HRMS (ESI): *m/z* calculated for $C_{13}H_{11}INO$ $[M+H]^+$= 323.9879, found $[M+H]^+$= 323.9876.

***N*-(4-ethylphenyl)-2-iodobenzamide (S1b)**



The compound **S1b**was synthesized from commercially available 2-iodobenzoic acid and 4-ethylaniline. The compound was purified by column chromatography on silica gel (100-200 mesh) eluting with hexane/EtOAc (95: 05) and product was afforded as a white solid (91 % yield);FT-IR (KBr): 3418, 3019, 2960, 2400, 1653, 1599, 1516, 1462, 1409, 1328, 1215, 1015, 924, 669 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ 7.88 (d, *J* = 8.0 Hz, 1H), 7.54–7.47 (m, 4H), 7.39 (t, *J* = 7.6 Hz, 1H), 7.19 (d, *J* = 8.4 Hz, 2H), 7.12 (td, *J* = 7.6, 1.6 Hz, 1H), 2.64 (q, *J* = 7.6 Hz, 2H), 1.23 (t, *J* = 7.6 Hz, 3H);^{13}C NMR (75.4 MHz, $CDCl_3$): δ 167.1, 142.2, 142.0, 140.0, 135.1, 131.4, 128.5, 128.4(2C), 128.3, 120.2(2C), 92.4, 28.3, 15.6;HRMS (ESI): *m/z* calculatedfor $C_{15}H_{15}INO$ $[M+H]^+$= 352.0192, found $[M+H]^+$= 352.0188.

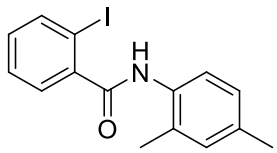
***N*-(3,4-dimethylphenyl)-2-iodobenzamide (S1c)**



The compound **S1c** was synthesized from commercially available 2-iodobenzoic acid and 3,4-dimethylaniline. The compound was purified by column chromatography on silica gel (100-200 mesh) eluting with hexane/EtOAc (95: 05) and product was afforded as a white solid (88 % yield);FT-IR (KBr): 3436, 3417, 3019, 2400, 1671, 1617, 1520, 1449, 1404, 1311, 1215, 1043, 1017, 669cm^{-1};^{1}H

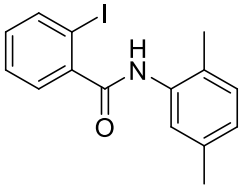
NMR (400 MHz, $CDCl_3$): δ (ppm) 7.89 (d, *J* = 8.0 Hz, 1H), 7.50 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.45–7.39 (m, 3H), 7.34 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.15–7.11 (m, 2H), 2.25 (s, 3H), 2.25 (s, 3H);^{13}C NMR (75.4 MHz, $CDCl_3$): δ (ppm) 167.1, 142.3, 139.9, 137.3, 135.2, 133.3, 131.3, 130.0, 128.5, 128.3, 121.4, 117.6, 92.4, 19.9, 19.2;HRMS (ESI): *m/z* calculated for $C_{15}H_{15}INO$ $[M+H]^+$= 352.0192, found $[M+H]^+$= 352.0189.

N-(2,4-dimethylphenyl)-2-iodobenzamide (S1d)



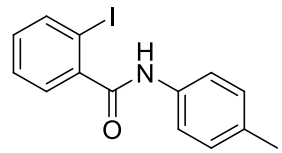
The compound **S1d** was synthesized from commercially available 2-iodobenzoic acid and 2,4-dimethylaniline. The compound was purified by column chromatography on silica gel (100-200 mesh) eluting with hexane/EtOAc (95: 05) and product was afforded as a white solid (90 % yield);FT-IR (KBr): 3418, 3019, 2400, 1646, 1522, 1405, 1215, 929, 669 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.92 (d, *J* = 8.0 Hz, 1H), 7.81 (d, *J* = 8.0Hz, 1H), 7.54 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.44 (t, *J* = 7.6 Hz, 1H), 7.19 (brs, 1H), 7.14 (td, *J* = 7.5, 1.6 Hz, 1H), 7.09–7.05 (m, 2H), 2.324 (s, 3H), 2.320 (s, 3H);^{13}C NMR (100.6MHz, $CDCl_3$ + CD_3OD): δ (ppm) 169.4, 142.3, 139.4, 136.1, 132.6, 131.9, 131.0, 130.7, 127.8, 127.6, 126.6, 125.3, 91.9, 20.2, 17.4; HRMS (ESI): *m/z*calculated for $C_{15}H_{15}INO[M+H]^+$=352.0192, found $[M+H]^+$= 352.0188.

***N*-(2,5-dimethylphenyl)-2-iodobenzamide (S1e)**



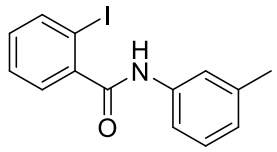
The compound **S1e** was synthesized from commercially available 2-iodobenzoic acid and 2,5-dimethylaniline. The compound was purified by column chromatography on silica gel (100-200 mesh) eluting with hexane/EtOAc (95: 05) and product was afforded as a white solid (90 % yield);FT-IR (KBr): 3431, 3019, 2400, 1636, 1528, 1481, 1446, 1405, 1292, 1043, 928, 669, 626 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.90 (d, *J* = 8.0 Hz, 1H), 7.81 (s, 1H), 7.53–7.51 (m, 1H), 7.44–7.40 (m, 1H), 7.26 (brs, 1H), 7.16–7.12 (m, 1H), 7.10 (d, *J* = 7.6 Hz, 1H), 6.94 (d, *J* = 7.6 Hz, 1H), 2.35 (s, 3H), 2.28 (s, 3H).^{13}C NMR (75.4MHz, $CDCl_3$): δ (ppm) 167.3, 140.0, 136.6, 135.0, 131.4, 130.4(2C), 128.4(2C), 128.3, 126.5, 123.6, 92.3, 21.1, 17.6;HRMS (ESI):*m/z*calculated for $C_{15}H_{15}INO$ $[M+H]^+$= 352.0192, found $[M+H]^+$= 352.0198.

***N*-(*p*-tolyl)-2-iodobenzamide (S1f)**



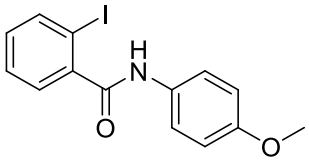
The compound **S1f** was synthesized from commercially available 2-iodobenzoic acid and 4-methylaniline. The compound was purified by column chromatography on silica gel (100-200 mesh) eluting with hexane/EtOAc (96: 04) and product was afforded as a white solid (94 % yield); FT-IR (KBr): 3417, 3019, 2399, 1671, 1517, 1403, 1318, 1215, 1120, 1017, 928, 669 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.91 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.55–7.51 (m, 3H), 7.49 (brs, 1H), 7.43 (dt, *J* = 7.6, 0.8 Hz, 1H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.15 (td, *J* = 7.6, 1.6 Hz, 1H), 2.37 (s, 3H);^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) 167.1, 142.2, 139.9, 135.0, 134.6, 131.4, 129.6 (2C), 128.5, 128.3, 120.2 (2C), 92.4, 20.9;HRMS (ESI): *m/z* calculated for $C_{14}H_{13}INO$ $[M+H]^+$ = 338.0036, found $[M+H]^+$ = 338.0041.

***N*-(m-tolyl)-2-iodobenzamide (S1g)**



The compound **S1g**was synthesized from commercially available 2-iodobenzoic acid and 3-methylaniline. The compound was purified by column chromatography on silica gel (100-200 mesh) eluting with hexane/EtOAc (96: 04) and product was afforded as a white solid (89 % yield);FT-IR (KBr): 3415, 3290, 3018, 1663, 1613, 1537, 1489, 1430, 1312, 1216, 1017, 876, 669 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.90 (d, *J* = 8.0 Hz, 1H), 7.51 (brs 2H), 7.44–7.38 (m, 3H), 7.28–7.24 (m, 2H), 7.14 (t, *J* = 7.2 Hz, 1H), 6.99(d, *J* = 7.2 Hz, 1H), 2.38 (s, 3H);^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) 167.2, 142.1, 140.0, 139.0, 137.5, 131.4, 128.9, 128.5, 128.3, 125.7, 120.7, 117.2, 92.4, 21.5;HRMS (ESI): *m/z* calculated for $C_{14}H_{13}INO$ $[M+H]^+$ = 338.0036, found $[M+H]^+$ = 338.0041.

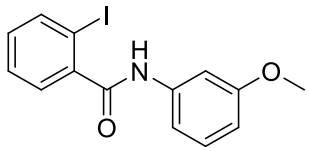
***N*-(4-methoxyphenyl)-2-iodobenzamide (S1h)**



The compound **S1h** was synthesized from commercially available 2-iodobenzoic acid and 4-methoxyaniline. The compound was purified by column chromatography on silica gel (100-200 mesh) eluting with hexane/EtOAc (95: 05) and product was afforded as a white solid (90 % yield); FT-IR (KBr): 3419, 3303, 3019, 2402, 1649, 1514, 1460, 1409, 1216, 1114, 1023, 670 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.90 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.55 (dd, *J* = 6.8, 2.0

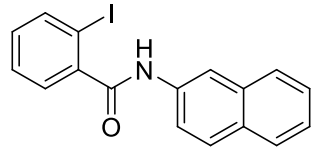
Hz, 2H), 7.51 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.49 (brs, 1H), 7.42 (dt, *J* = 7.6, 0.8 Hz, 1H), 7.14 (td, *J* = 7.6, 1.6 Hz, 1H), 6.92 (d, *J* = 9.2 Hz, 2H), 3.82 (s, 3H);^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) 167.2, 156.8, 142.2, 139.9, 131.3, 130.6, 128.5, 128.3, 122.0 (2C), 114.2 (2C), 92.4, 55.5;HRMS (ESI): *m/z* calculated for $C_{14}H_{13}INO_2$ $[M+H]^+$ = 353.9985, found $[M+H]^+$= 353.9989.

***N*-(3-methoxyphenyl)-2-iodobenzamide (S1i)**



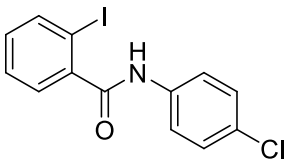
The compound **S1i** was synthesized from commercially available 2-iodobenzoic acid and 3-methoxyaniline. The compound was purified by column chromatography on silica gel (100-200 mesh) eluting with hexane/EtOAc (95: 05) and product was afforded as a white solid (90 % yield); FT-IR (KBr): 3419, 3303, 3019, 2402, 1650, 1514, 1460, 1409, 1216, 1112, 923, 670 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.90 (d, *J* = 7.6 Hz, 1H), 7.51–7.50 (m, 2H), 7.43–7.40 (m, 2H), 7.26–7.24 (m, 1H), 7.16–7.09 (m, 2H), 6.73 (d, *J* = 8.0 Hz, 1H), 3.83 (s, 3H);^{13}C NMR (100.6 MHz, $CDCl_3$ + CD_3OD): δ (ppm) 168.2, 159.9, 142.4, 139.6, 139.0, 131.0, 129.5, 128.1, 128.0, 112.5, 110.4, 105.9, 92.2, 55.2;HRESIMS: *m/z* calculated for $C_{14}H_{13}INO_2$ $[M+H]^+$ = 353.9985, found $[M+H]^+$ = 353.9985.

***N*-(naphthalen-2-yl)-2-iodobenzamide (S1j)**



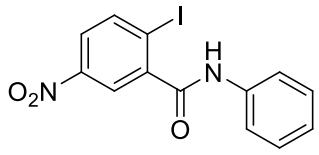
The compound **S1j** was synthesized from commercially available 2-iodobenzoic acid and 2-naphthylamine. The compound was purified by column chromatography on silica gel (100-200 mesh) eluting with hexane/EtOAc (92: 08) and product was afforded as a off white solid (92 % yield);FT-IR (KBr): 3416, 3019, 2399, 1625, 1530, 1497, 1405, 1215, 928, 848, 669 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.35 (d, *J* = 1.2 Hz, 1H), 7.91 (d, *J* = 8.0 Hz, 1H), 7.85–7.80 (m, 3H), 7.76 (s, 1H), 7.58–7.54 (m, 2H), 7.51–7.41 (m, 3H), 7.15 (dt, *J* = 7.6, 1.6 Hz, 1H);^{13}C NMR (75.4 MHz, $CDCl_3$ + CD_3OD): δ (ppm) 168.5, 142.2, 139.4, 135.2, 133.5, 130.8, 130.6, 128.3, 127.8 (2C), 127.4, 127.2, 126.1, 124.8, 119.9, 117.0, 92.4; HRMS (ESI): *m/z* calculated for $C_{17}H_{13}INO$ $[M+H]^+$= 374.0036, found $[M+H]^+$= 374.0038.

***N*-(4-chlorophenyl)-2-iodobenzamide (S1k)**



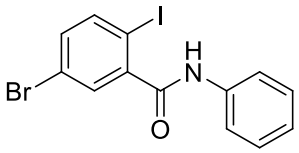
The compound **S1k**was synthesized from commercially available 2-iodobenzoic acid and 4-chloroaniline. The compound was purified by column chromatography on silica gel (100-200 mesh) eluting with hexane/EtOAc (94: 06) and product was afforded as a white solid (84 % yield); FT-IR (KBr): 3414, 3022, 2401, 1622, 1524, 1444, 1319, 1215, 928, 670 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.89 (d, *J* = 7.8 Hz, 1H), 7.76 (brs, 1H), 7.58 (d, *J* = 8.7 Hz, 2H),7.47 (dd, *J* = 7.4, 1.2 Hz, 1H), 7.40 (t, *J* = 7.3 Hz, 1H), 7.33 (d, *J* = 8.7 Hz, 2H), 7.14 (dt, *J* = 7.7, 1.4 Hz, 1H);^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) 167.3, 141.7, 140.0, 136.1, 131.6, 129.9, 129.1 (2C), 128.5, 128.3, 121.4 (2C), 92.3;HRMS (ESI): *m/z* calculated for $C_{13}H_{10}ClINO$ $[M+H]^+$ = 357.9490, found $[M+H]^+$ = 357.9490.

2-iodo-5-nitro-*N*-phenylbenzamide (S1l)



The compound **S1l**was synthesized 2-iodo-5-nitro-benzoic acid[2] and aniline. The compound was purified by column chromatography on silica gel (100-200 mesh) eluting with hexane/acetone (94: 06) and product was afforded as a yellow solid (85% yield);FT-IR (KBr): 3389, 3021, 2401, 1626, 1525, 1410, 1322, 1215, 928, 758 cm^{-1};^{1}H NMR (400 MHz, Acetone-d_6): δ (ppm) 9.79 (s, 1H), 8.35 (d, *J* = 2.6 Hz, 1H), 8.27 (d, *J* = 8.6 Hz, 1H), 8.04 (dd, *J* = 8.6, 2.6 Hz, 1H), 7.80–7.77 (m, 2H), 7.41–7.36 (m, 2H), 7.19–7.14 (m, 1H);^{13}C NMR (100.6 MHz, Acetone-d_6): δ (ppm) 166.5, 148.8, 145.4, 142.2, 139.7, 129.7 (2C), 125.8, 125.2, 123.2, 120.8, 120.7, 102.2; HRMS (ESI): *m/z* calculated for $C_{13}H_{10}IN_2O_3$ $[M+H]^+$ = 368.9731, found $[M+H]^+$ = 368.9732.

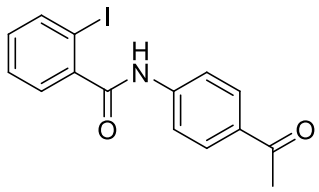
5-bromo-2-iodo-*N*-phenylbenzamide (S1m)



The compound **S1m**was synthesized from 5-bromo-2-iodo-benzoic acid[2] and aniline. The compound was purified by column chromatography on silica gel (100-200 mesh) eluting with hexane/EtOAc (93: 07) and product was afforded as a white solid (80 % yield);FT-IR (KBr): 3410, 3019, 2399, 1630, 1403, 1318, 1215, 1120, 928, 669 cm^{-1};^{1}H NMR (400 MHz, Acetone-d_6): δ (ppm) 9.60 (brs, 1H), 7.88 (d, *J* = 8.4 Hz, 1H), 7.82–7.79 (m, 2H), 7.72 (d, *J* = 2.3 Hz, 1H), 7.43–7.37 (m, 3H), 7.18 (t, *J* = 1.1 Hz, 1H);^{13}C NMR (100.6 MHz, Acetone-d_6): δ (ppm)

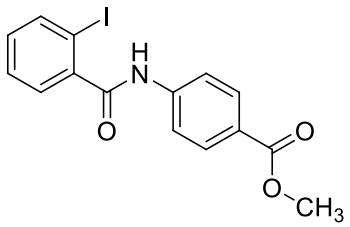
165.8, 145.1, 141.1, 139.0, 133.8, 130.8, 128.7 (2C), 124.1, 121.8, 119.7 (2C), 90.8;HRMS (ESI): *m/z* calculated for $C_{13}H_{10}BrINO$ $[M+H]^+$ = 401.8990, found $[M+H]^+$ = 401.8985.

***N*-(4-acetylphenyl)-2-iodobenzamide (S1n)**



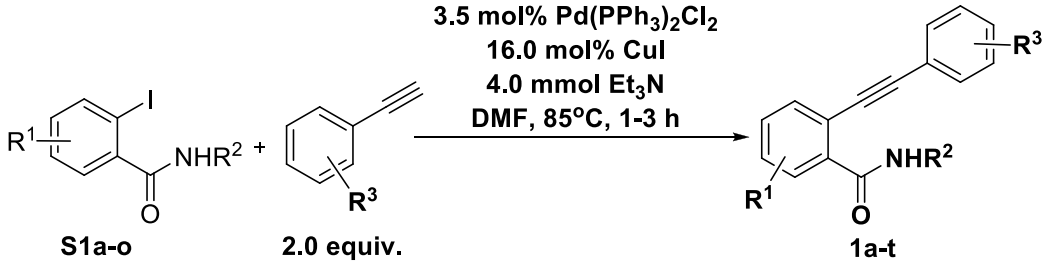
The compound **S1n**was synthesized from commercially available 2-iodobenzoic acid and 4-acetylaniline. The compound was purified by column chromatography on silica gel (100-200 mesh) eluting with hexane/EtOAc (93: 07) and product was afforded as a white solid (70 % yield);FT-IR (KBr): 3375, 3019, 1670, 1539, 1318, 1215, 1120, 765, 669 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.97 (d, *J* = 8.5 Hz, 2H), 7.90 (d,*J* = 8.2 Hz, 2H), 7.75 (d,*J* = 8.2 Hz, 2H), 7.52 (d, *J* = 7.2 Hz, 1H), 7.43 (t, *J* = 7.3 Hz, 1H), 7.16 (dt, *J* = 7.8, 1.2 Hz, 1H), 2.58 (s, 3H);^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) 197.0, 167.4, 141.9, 141.5, 140.1, 133.3, 131.7, 129.7 (2C), 128.5 (2C), 128.3, 119.3, 92.3, 26.4;HRMS (ESI): *m/z* calculated for $C_{15}H_{13}INO_2$ $[M+H]^+$ = 365.9985, found $[M+H]^+$ = 365.9982.

Methyl-4-(2-iodobenzamido)benzoate (S1o)



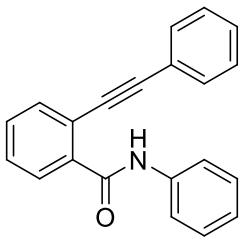
The compound **S1o**was synthesized from commercially available 2-iodo-benzoic acid and methyl-4-aminobenzoate[3]. The compound was purified by column chromatography on silica gel (100-200 mesh) eluting with hexane/EtOAc (90: 10) and product was afforded as a white solid (75 % yield);FT-IR (KBr): 3417, 3019, 1742, 1670, 1403, 1318, 1215, 1017, 928, 669 cm^{-1};^{1}H NMR (400 MHz, CD_3OD + $CDCl_3$): δ (ppm) 7.90 (d, *J* = 8.4 Hz, 2H), 7.78 (d, *J* = 7.8 Hz, 1H), 7.64 (d,*J* = 8.0 Hz, 2H), 7.36–7.28 (m,2H), 7.05–7.01(m, 1H), 3.79 (s, 3H);^{13}C NMR (100.6 MHz, CD_3OD + $CDCl_3$): δ (ppm) 168.4, 166.8, 142.2, 141.8, 139.4, 131.0, 130.4 (2C), 127.8 (2C), 125.3, 119.2 (2C), 92.1, 51.8; HRMS (ESI): *m/z* calculated for $C_{15}H_{13}INO_3$ $[M+H]^+$ = 381.9935, found $[M+H]^+$ = 381.9938.

2.2 General procedure for the synthesis of o-(1-Alkynyl)benzamides[1]



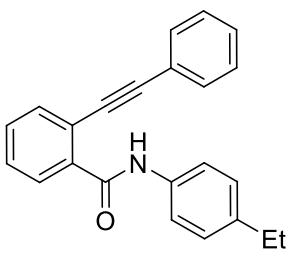
To a solution of *N*-phenyl-2-iodobenzamide (**S1a**) (323 mg, 1 mmol) in DMF (6 mL) were added $Pd(PPh_3)Cl_2$ (24.5 mg, 3.5 mol%), CuI (30.4 mg, 16 mol%) and triethylamine (0.55 mL, 4.0 mmol), consecutively, under inert atmosphere. After 10 min stirring phenylacetylene (0.22 mL, 2.0mmol) was added and the reaction mixture was heated with stirring at 85^{o}C till the disappearance of stating material. The progress of reaction was monitored by TLC. The reaction mixture was cooled down, quenched with saturated aqueous solution of NH_4Cl and extracted with ethyl acetate (3 X 25 mL). The organic layers were combined and washed with brine and dried over anhy. Na_2SO_4. The solvent were removed under vacuum and obtained residue was purified by column chromatography on silica gel (230-400 mesh) eluting with hexane/EtOAc (96: 04) to afford the product **1a** (88% yield).

_N_-phenyl-2- (phenylethynyl)benzamide (1a)



FT-IR (KBr): 3416, 3019, 2400, 1668, 1600, 1537, 1498, 1445, 1322, 1215, 1044, 928, 690,669 cm^{-1};^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) 9.23 (s, 1H), 8.18–8.15 (m, 1H), 7.71–7.68 (m, 3H), 7.53–7.51 (m, 4H), 7.40–7.34 (m, 5H), 7.17 (t, *J* = 7.5 Hz, 1H);^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) 164.4, 137.9, 135.9, 133.5, 131.7(2C), 130.9, 130.3, 129.3, 129.1(3C), 128.6(2C), 124.5, 121.8, 120.0 (2C), 119.5, 96.6, 87.2;HRMS (ESI): *m/z* calculated for $C_{21}H_{16}NO$ $[M+H]^+$ = 298.1226, found $[M+H]^+$ = 298.1234.

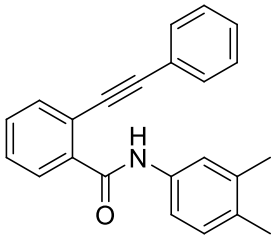
_N_-(_p_-ethylphenyl)-2-(phenylethynyl)benzamide (1b)



The compound **1b** was prepared by using starting materials**S1b** and phenylacetylene as above described general procedure. The compound **1b** was purified by column chromatography on silica gel (230-400

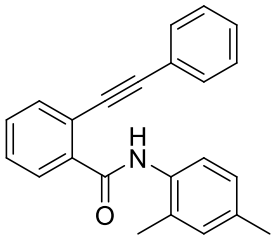
mesh)by eluting with hexane/EtOAc (96: 04) to afford white solid product in 83% yield;FT-IR (KBr): 3413, 3019, 2970, 2930, 2400, 1662, 1599, 1529, 1493, 1409, 1321, 1215, 1125, 1046, 928, 690, 626, 542 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 9.15 (s, 1H), 8.14–8.12 (m, 1H), 7.65–7.63 (m, 1H), 7.56 (d, *J* = 8.4 Hz, 2H), 7.50–7.46 (m, 4H), 7.38–7.33 (m, 3H), 7.15 (d, *J* = 8.0 Hz, 2H), 2.62 (q, *J* = 7.6 Hz, 2H), 1.22 (t, *J* = 7.6 Hz, 3H);^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) 164.2, 140.5, 136.0, 135.6, 133.5, 131.7(2C), 130.8, 130.3 129.2, 129.0, 128.6(2C), 128.4(2C), 121.9, 120.1(2C), 119.5, 96.5, 87.3, 28.3, 15.6;HRMS (ESI): *m/z* calculated for $C_{23}H_{20}NO$ $[M+H]^+$= 326.1539, found $[M+H]^+$= 326.1543.

***N*-(3,4-dimethylphenyl)-2-(phenylethynyl)benzamide (1c)**



The compound **1c** was synthesized by using starting materials **S1c** and phenylacetylene as above described general procedure. The compound **1c** was purified by column chromatography on silica gel (230-400 mesh) by eluting with hexane/EtOAc (96: 04) to afford viscous brown oily product in 80% yield;FT-IR (neat): 3376, 3019, 2401, 1663, 1600, 1531, 1445, 1404, 1316, 1215, 1029, 927, 670 cm^{-1};^1H NMR (400 MHz, $CDCl_3$): δ (ppm)9.14 (s, 1H), 8.15–8.13 (m, 1H), 7.65–7.63 (m, 1H), 7.53–7.46 (m, 4H), 7.41–7.35 (m, 5H), 7.09–7.07 (m, 1H), 2.23(s, 3H), 2.20(s, 3H);^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) 164.1, 137.2, 136.0, 135.7, 133.4, 132.8, 131.7 (2C), 130.8, 130.3, 130.0, 129.3, 129.1, 128.6 (2C), 121.9, 121.3, 119.5, 117.5, 96.5, 87.4, 19.8, 19.2; HRMS (ESI): *m/z*calculated for $C_{23}H_{20}NO$ $[M+H]^+$= 326.1539, found $[M+H]^+$= 326.1546.

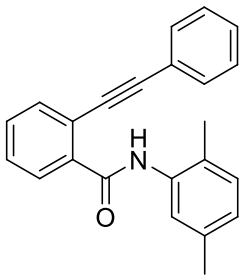
***N*-(2,4-dimethylphenyl)-2-(phenylethynyl)benzamide (1d)**



The compound **1d** was synthesized by using starting materials **S1d** and phenylacetylene as above described general procedure. The compound **1d** was purified by column chromatography on silica gel (230-400 mesh) by eluting with hexane/EtOAc (96: 04) to afford white solid product in 82% yield;FT-IR (KBr): 3407, 3018, 2855, 2402, 1662, 1518, 1459, 1305, 1216, 1037, 927, 670 cm^{-1};^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.80 (s, 1H),8.14–8.12 (m, 1H), 7.83 (d, *J* = 8.0 Hz, 1H), 7.69–7.67 (m, 1H), 7.51–7.49 (m, 2H), 7.45–7.43 (m, 2H), 7.37–7.33 (m, 3H), 7.07 (d, *J* = 8.0 Hz, 1H), 7.02 (s, 1H), 2.32(s, 3H), 2.24(s, 3H);^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) 164.7, 136.3, 135.2, 133.6, 133.2, 131.6 (2C), 131.2, 130.7, 130.2, 130.0,

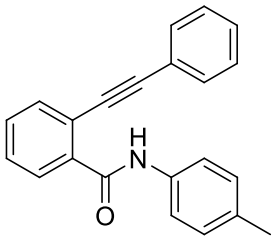
129.1, 129.0, 128.5(2C), 127.3, 123.7, 122.1, 119.6, 96.1, 87.4, 20.9, 17.9;HRMS (ESI): *m/z*calculated for $C_{23}H_{20}NO$ $[M+H]^+$= 326.1539, found $[M+H]^+$= 326.1543.

***N*-(2,5-dimethylphenyl)-2-(phenylethynyl)benzamide (1e)**



The compound **1e** was prepared by using starting materials **S1e** and phenylacetylene as above described general procedure. The compound **1e** was purified by column chromatography on silica gel (230-400 mesh) by eluting with hexane/EtOAc (96: 04) to afford white solid product in 80% yield;FT-IR (KBr): 3417, 3019, 2927, 2400, 1662, 1534, 1492, 1405, 1291, 928, 691, 668, 519 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ (ppm)8.78 (s, 1H), 8.12–8.09 (m, 1H), 7.85 (s, 1H), 7.67–7.65 (m, 1H), 7.50–7.48 (m, 2H), 7.41 (d, *J* = 6.8 Hz, 2H), 7.35–7.31 (m, 3H), 7.06 (d, *J* = 7.6 Hz, 1H), 6.92 (d, *J* = 7.6 Hz, 1H), 2.34(s, 3H), 2.21(s, 3H);^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) 164.8, 136.4, 136.4, 135.6, 133.6, 131.6 (2C), 130.7, 130.3, 130.2, 129.1, 129.0, 128.5(2C), 126.6, 126.2, 124.0, 122.0, 119.6, 96.2, 87.4, 21.1, 17.5;HRMS (ESI): *m/z*calculated for $C_{23}H_{20}NO$ $[M+H]^+$= 326.1539, found $[M+H]^+$= 326.1543.

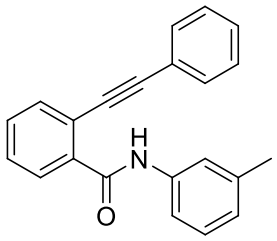
***N*-(*p*-tolyl)-2-(phenylethynyl)benzamide (1f)**



The compound **1f** was prepared by using starting materials **S1f** and phenylacetylene as above described general procedure. The compound **1f** was purified by column chromatography on silica gel (230-400 mesh) by eluting with hexane/EtOAc (96: 04) afforded viscous brown oily product in 82% yield; FT-IR (neat):3415, 3019, 2926, 2398, 1662, 1534, 1491, 1404, 1291, 928, 668 cm^{-1};^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 9.15 (s, 1H), 8.14–8.12 (m, 1H), 7.65–7.63 (m, 1H), 7.54 (d, *J* = 8.4 Hz, 2H), 7.50–7.46 (m, 4H), 7.38–7.34 (m, 3H), 7.13 (d, *J* = 8.4 Hz, 2H), 2.33 (s, 3H);^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) 164.3, 136.0, 135.4, 134.1, 133.5, 131.7 (2C), 130.8, 130.3129.6 (2C), 129.2, 129.0, 128.6 (2C), 121.9, 120.0 (2C), 119.5, 96.5, 87.3, 20.9;HRMS (ESI): *m/z* calculated for$C_{22}H_{18}NO$ $[M+H]^+$=312.1382, found $[M+H]^+$= 312.1386.

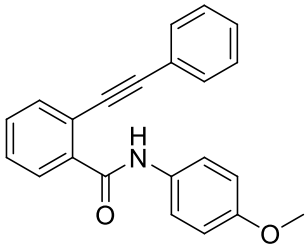
***N*-(*m*-tolyl)-2-(phenylethynyl)benzamide (1g)**

The compound **1g** was prepared by using starting materials **S1g** and phenylacetylene as above described general procedure. The compound **1g** was purified by column chromatography on



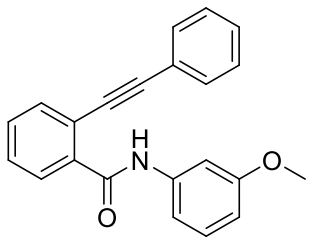
silica gel (230-400 mesh) by eluting with hexane/EtOAc (96: 04) afforded viscous brown oily product in 81% yield; FT-IR (neat):3349, 3027, 2956, 2400, 1725, 1620, 1532, 1381, 1216, 1045, 928cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 9.20 (s, 1H), 8.18–8.16 (m, 1H), 7.69–7.67 (m, 1H), 7.55–7.48 (m, 6H), 7.42–7.36 (m, 3H), 7.24 (t, *J* = 7.6 Hz, 1H), 6.98 (d, *J* = 7.6 Hz, 1H), 2.33 (s, 3H);^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) 164.3, 138.9, 137.8, 136.0, 133.4, 131.7 (2C), 130.8, 130.3, 129.3, 129.1, 128.9, 128.6 (2C), 125.3, 121.9, 120.6, 119.5, 117.1, 96.6, 87.3, 21.4;HRMS (ESI): *m/z* calculated for $C_{22}H_{18}NO$ $[M+H]^+$=312.1382, found $[M+H]^+$= 312.1386.

***N*-(*p*-methoxyphenyl)-2-(phenylethynyl)benzamide (1h)**



The compound **1h** was prepared by using starting materials **S1h** and phenylacetylene as above described general procedure. The compound **1h** was purified by column chromatography on silica gel (230-400 mesh) by eluting with hexane/EtOAc (94: 06) afforded viscous yellow oily product in 75% yield;FT-IR (neat): 3416, 3019, 2400, 1668, 1537, 1498, 1445, 1322, 1215, 1044, 928, 669 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 9.13 (s, 1H), 8.13–8.11 (m, 1H), 7.67–7.65 (m, 1H), 7.59 (d, *J* = 9.0 Hz, 2H), 7.52–7.48 (m, 4H), 7.41–7.35 (m, 3H), 6.89 (d, *J* = 8.9 Hz, 2H), 3.82 (s, 3H);^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) 164.3, 156.5, 136.0, 133.4, 131.6 (2C), 131.1, 130.7, 130.2, 129.2, 129.0, 128.6 (2C), 121.9, 121.7 (2C), 119.5, 114.2 (2C), 96.4, 87.3, 55.5;HRMS (ESI): *m/z* calculated for $C_{22}H_{18}NO_2$ $[M+H]^+$= 328.1332, found $[M+H]^+$= 328.1333.

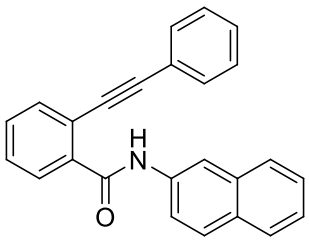
***N*-(*m*-methoxyphenyl)-2-(phenylethynyl)benzamide (1i)**



The compound **1i** was prepared by using starting materials **S1i** and phenylacetylene as above described general procedure. The compound **1i** was purified by column chromatography on silica gel (230-400 mesh) by eluting with hexane/EtOAc (94: 06) afforded viscous yellow oily product in 70% yield;FT-IR (neat): 3416, 3019, 2399, 1665, 1537, 1498, 1445, 1322, 1215, 1044, 928, 669 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 9.23 (s, 1H), 8.15–8.13 (m, 1H), 7.66–7.64 (m, 1H), 7.52–7.48 (m, 4H), 7.41–7.33 (m, 4H), 7.20 (t, *J* = 8.0

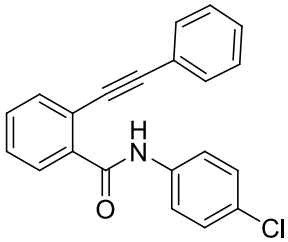
Hz, 1H), 7.13 (d, *J* = 8.0 Hz, 1H), 6.70–6.67 (m, 1H), 3.73 (s, 3H);^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) 164.3, 160.2, 139.1, 135.8, 133.5, 131.7 (2C), 130.9, 130.3, 129.7, 129.3, 129.1, 128.6 (2C), 121.8, 119.5, 112.1, 110.9, 105.2, 96.6, 87.2, 55.2;HRMS (ESI): *m/z* calculated for $C_{22}H_{18}NO_2$ $[M+H]^+$= 328.1332, found $[M+H]^+$= 328.1333.

***N*-(naphthalen-2-yl)-2-(phenylethynyl)benzamide (1j)**



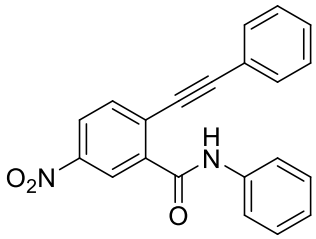
The compound **1j** was prepared by using starting materials **S1j** and phenylacetylene as above described general procedure. The compound **1j** was purified by column chromatography on silica gel (230-400 mesh) by eluting with hexane/EtOAc (94: 06) afforded white solid product in 90% yield;FT-IR (KBr): 3436, 3019, 2400, 1661, 1543, 1503, 1474, 1431, 1358, 1215, 1045, 928, 669 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 9.42 (s, 1H), 8.38 (d, *J* = 1.2 Hz, 1H), 8.20–8.17 (m, 1H), 7.78–7.74 (m, 3H), 7.68–7.57 (m, 1H), 7.56 (dd, *J* = 8.8, 2.0 Hz, 1H), 7.53–7.49 (m, 4H), 7.45–7.32 (m, 5H);^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) 164.6, 135.9, 135.4, 133.9, 133.5, 131.7 (2C), 130.9, 130.8, 130.3, 129.3, 129.1, 128.8, 128.7 (2C), 127.7, 127.6, 126.5, 125.0, 121.8, 120.0, 119.6, 116.9, 96.7, 87.4; HRMS (ESI): *m/z* calculated for $C_{25}H_{18}NO$ $[M+H]^+$= 348.1382, found $[M+H]^+$= 348.1381.

***N*-(4-chlorophenyl)-2-(phenylethynyl)benzamide (1k)**



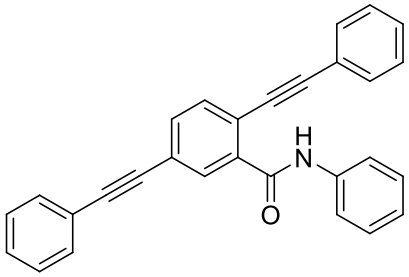
The compound **1k** was prepared by using starting materials **S1k** and phenylacetylene as above described general procedure. The compound **1k** was purified by column chromatography on silica gel (230-400 mesh) by eluting with hexane/EtOAc (93: 07) afforded white solid product in 78% yield;FT-IR (KBr): 3416, 3019, 2399, 1655, 1530, 1497, 1405, 1215, 928, 669 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 9.27 (s, 1H), 8.17–8.14 (m, 1H), 7.69–7.67 (m, 1H), 7.63 (d,*J* = 8.8 Hz, 2H), 7.54–7.50 (m, 4H), 7.45–7.37 (m, 3H), 7.31 (dd, *J* = 6.8, 2.0 Hz, 2H);^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) 164.3, 136.5, 135.5, 133.5, 131.6 (2C), 131.0, 130.3, 129.4, 129.1 (4C), 128.7 (2C), 121.7, 121.1 (2C), 119.5, 96.7, 87.2;HRMS (ESI): *m/z* calculated for $C_{21}H_{15}ClNO$ $[M+H]^+$=332.0836, found $[M+H]^+$= 332.0836.

5-nitro-*N*-phenyl-2-(phenylethynyl)benzamide (1l)



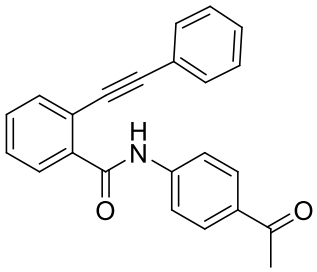
The compound **1l** was prepared by using starting materials **S1l** and phenylacetylene as above described general procedure. The compound **1l** was purified by column chromatography on silica gel (230-400 mesh) by eluting with hexane/EtOAc (92: 08) afforded yellow solid product in 75% yield; FT-IR (KBr): 3853, 3019, 2400, 2345, 1655, 1524, 1404, 1385, 1345, 1104, 929, 626 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 9.10 (s, 1H), 8.99 (d, *J* = 1.8 Hz, 1H), 8.34 (dd, *J* = 8.4, 2.4 Hz, 1H), 7.83 (d, *J* = 8.5 Hz, 1H), 7.68 (d, *J* = 7.8 Hz, 2H), 7.54 (d, *J* = 7.1 Hz, 2H), 7.50–7.46 (m, 1H), 7.43–7.37 (m, 4H), 7.21 (t, *J* = 7.3 Hz, 1H);^{13}C NMR (100.6 MHz, $CDCl_3$ + CD_3OD): δ (ppm) 163.8, 146.6, 138.6, 137.3, 133.7, 131.6 (2C), 129.5, 128.7 (2C), 128.3 (2C), 126.8, 124.7, 124.5, 123.7, 121.0, 120.0 (2C), 99.9, 85.3; HRMS (ESI): *m/z* calculated for $C_{21}H_{15}N_2O_3$ $[M+H]^+$ =343.1077, found $[M+H]^+$ = 343.1077.

***N*-phenyl-2,5-bis(phenylethynyl)benzamide (1m)**



The compound **1m** was prepared by using starting materials **S1m** and phenylacetylene as above described general procedure. The compound **1m** was purified by column chromatography on silica gel (230-400 mesh) by eluting with hexane/EtOAc (96: 04) afforded white solid product in 60% yield;FT-IR (KBr): 3414, 3021, 2399, 1665, 1535, 1497, 1405, 1215, 928, 669 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 9.15 (s, 1H), 8.32 (s, 1H), 7.69 (d, *J* = 7.7 Hz, 2H), 7.65 (d, *J* = 1.3 Hz, 2H), 7.58–7.56 (m, 2H), 7.53–7.51 (m, 2H), 7.42–7.35 (m, 8H), 7.20–7.16 (m, 1H);HRMS (ESI): *m/z* calculated for $C_{29}H_{20}NO$ $[M+H]^+$=398.1539, found $[M+H]^+$= 398.1520.

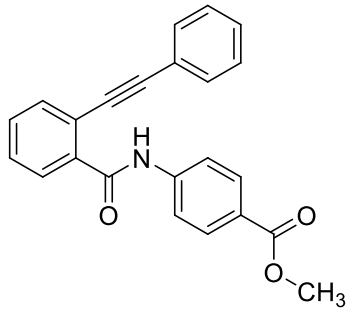
***N*-(3-acetylphenyl)-2-(phenylethynyl)benzamide (1n)**



The compound **1n** was prepared by using starting materials **S1n** and phenylacetylene as above described general procedure. The compound **1n** was purified by column chromatography on silica gel (230-400 mesh) by eluting with hexane/EtOAc (95: 05) afforded white solid product in 77% yield;FT-IR (KBr): 3380, 3019, 2399,

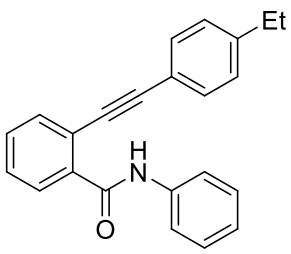
1704,1530, 1497, 1404, 1215, 928, 669 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 9.48 (s, 1H), 8.16–8.14 (m, 1H), 7.94 (d,*J* = 8.6 Hz, 2H), 7.75 (d,*J* = 8.6 Hz, 2H), 7.68–7.66 (m, 1H), 7.53–7.48 (m, 4H), 7.41–7.35(m, 3H) 2.58(s, 3H);^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm)196.9, 164.5, 142.2, 135.2, 133.6, 133.0, 131.6 (2C), 131.3, 130.4, 129.8 (2C), 129.5, 129.2, 128.7 (2C), 121.5, 119.6, 119.1 (2C), 97.0, 87.0, 26.4;HRMS (ESI): *m/z* calculated for $C_{23}H_{18}NO_2$ $[M+H]^+$=340.1332, found $[M+H]^+$= 340.1332.

Methyl 4-(2-(phenylethynyl)benzamido)benzoate (1o)



The compound **1o** was prepared by using starting materials **S1o** and phenylacetylene as above described general procedure. The compound **1o** was purified by column chromatography on silica gel (230-400 mesh) by eluting with hexane/EtOAc (92: 08) afforded white solid product in 85% yield; FT-IR (KBr): 3415, 3020, 1740, 1664, 1403, 1318, 1215, 1017, 928, 669 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 9.43 (s, 1H), 8.16–8.13 (m, 1H), 8.01 (d, *J* = 8.4, 2H), 7.73 (d, *J* = 8.8 Hz, 2H), 7.68–7.65 (m, 1H), 7.52–7.48 (m, 4H), 7.41–7.35 (m, 3H), 3.90 (s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) 166.6, 164.6, 142.1, 135.4, 133.5, 131.6 (2C), 131.2, 130.9 (2C), 130.3, 129.4, 129.1, 128.7 (2C), 125.7, 121.6, 119.6, 119.1 (2C), 96.8, 87.1, 52.0; HRMS (ESI): *m/z* calculated for $C_{23}H_{18}NO_3$ $[M+H]^+$= 356.1281, found $[M+H]^+$= 356.1282.

2-((4-ethylphenyl)ethynyl)-*N*-phenylbenzamide (1p)

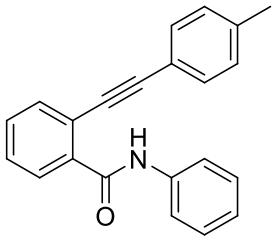


The compound **1p** was prepared by using starting materials **S1a** and *p*-ethylphenylacetylene as above described general procedure. The compound **1p** was purified by column chromatography on silica gel (230-400 mesh) by eluting with hexane/EtOAc (97: 03) afforded white solid product in 80% yield; FT-IR (KBr):3382, 3029, 2958, 2391, 1729, 1629, 1532, 1380, 1318, 1215, 1045, 918 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 9.31 (s, 1H), 8.19–8.17 (m, 1H), 7.70–7.66 (m, 3H), 7.53–7.50 (m, 2H), 7.45 (dd, *J* = 6.4, 1.7 Hz, 2H), 7.38-7.34 (m, 2H), 7.21 (d, *J* = 8.3 Hz, 2H), 7.18-7.14 (m, 1H), 2.70 (q, *J* = 7.6 Hz, 2H), 1.27 (t, *J* = 6.4 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) 164.4, 145.9, 137.9, 135.6, 133.5, 131.7 (2C), 130.9, 130.4, 129.1 (2C), 128.9, 128.2 (2C), 124.2, 120.0 (2C), 119.7, 118.9, 97.0,

86.7, 28.9, 15.2;HRMS (ESI): *m/z* calculated for $C_{23}H_{19}NO$ $[M]^+$ =325.1467, found $[M]^+$ = 325.1466.

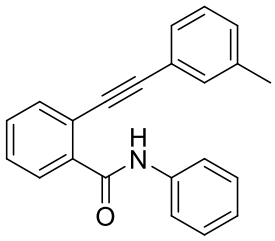
_N_-phenyl-2-(_p_-tolylethynyl)benzamide (1q)

The compound **1q** was prepared by using starting materials **S1a** and *p*-methylphenylacetylene as above described general procedure. The compound **1q** was purified by column chromatography on silica gel (230-400 mesh) by eluting with hexane/EtOAc (96: 03) afforded viscous brown oily



product in 83% yield; FT-IR (neat): 3379, 3027, 2956, 2390, 1729, 1628, 1532, 1381, 1318, 1216, 1045, 928. cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 9.27 (s, 1H), 8.16–8.14 (m, 1H), 7.67–7.63 (m, 3H), 7.51–7.45 (m, 2H), 7.38 (d,*J* = 8.0 Hz, 2H), 7.33 (t, *J* = 7.5 Hz, 2H), 7.17–7.11 (m, 3H), 2.37 (s, 3H);^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) 164.3, 139.7, 138.0, 135.6, 133.4, 131.6 (2C), 130.9, 130.4, 129.4 (2C), 129.0 (2C), 128.9, 124.4, 120.0 (2C), 119.7, 118.7, 97.0, 86.7, 21.5;HRMS (ESI): *m/z* calculated for $C_{22}H_{18}NO$ $[M+H]^+$=312.1383, found $[M+H]^+$= 312.1380.

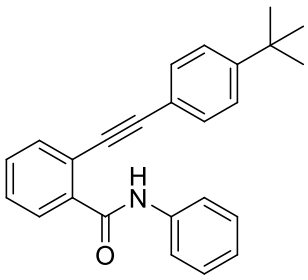
_N_-phenyl-2-(_m_-tolylethynyl)benzamide (1r)



The compound **1r** was prepared by using starting materials **S1a** and *m*-methylphenylacetylene as above described general procedure. The compound **1r** was purified by column chromatography on silica gel (230-400 mesh) by eluting with hexane/EtOAc (96: 03) afforded white solid product in 86% yield; FT-IR (KBr):3349, 3027, 2956, 2400, 1725, 1620, 1532, 1381, 1216, 1045, 928 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 9.20 (s, 1H), 8.15–8.12 (m, 1H), 7.68–7.63 (m, 3H), 7.49–7.47 (m, 2H), 7.35–7.29 (m, 4H), 7.23–7.11 (m, 3H), 2.30 (s, 3H);^{13}C NMR (100.6MHz, $CDCl_3$): δ (ppm) 164.4, 138.4, 138.0, 135.9, 133.4, 132.3, 130.8, 130.3, 130.2, 129.0 (3C), 128.7, 128.5, 124.4, 121.6, 120.0 (2C), 119.7, 96.9, 86.9, 21.1; HRMS (ESI): *m/z* calculated for $C_{22}H_{18}NO$ $[M+H]^+$ =312.1383, found $[M+H]^+$ = 312.1382.

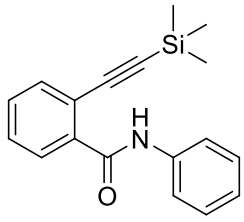
2-((4-_tert_-butylphenyl)ethynyl)-_N_-phenylbenzamide (1s)

The compound **1s** was prepared by using starting materials **S1a** and *p-tert*-butylphenylacetylene as above described general procedure. The compound **1s** was purified by column



chromatography on silica gel (230-400 mesh) by eluting with hexane/EtOAc (96: 04) afforded viscous yellow oily product in 85% yield; IR (neat): 3416, 3020, 2970, 2401, 1625, 1531, 1397, 1218, 928, 669 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 9.32 (s, 1H), 8.19–8.17 (m, 1H), 7.71 (d,*J* = 7.6 Hz, 2H), 7.68–7.66 (m, 1H), 7.51–7.48 (m, 2H), 7.47–7.45 (m, 2H), 7.41–7.35 (m, 4H) 7.19–7.15 (m, 1H), 1.36 (s, 9H);^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) 164.4, 152.8, 138.0, 135.6, 133.5, 131.4 (2C), 130.9, 130.4, 129.1 (2C), 128.9, 125.6 (2C), 124.4, 120.1 (2C), 119.8, 118.7, 97.0, 86.7, 34.9, 31.1 (3C); HRMS (ESI): *m/z* calculated for $C_{25}H_{24}NO$ $[M+H]^+$ =354.1852, found $[M+H]^+$ = 354.1856.

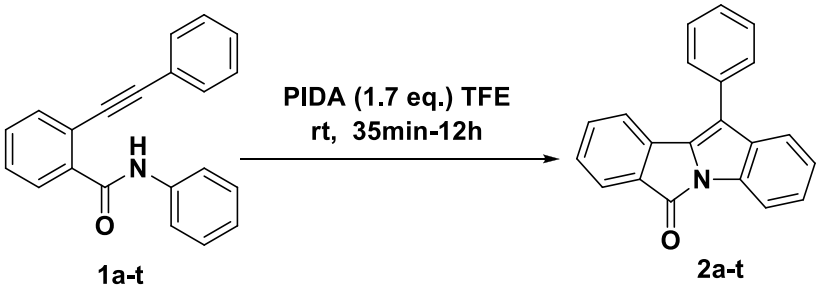
_N_-phenyl-2-((trimethylsilyl)ethynyl)benzamide (1t)



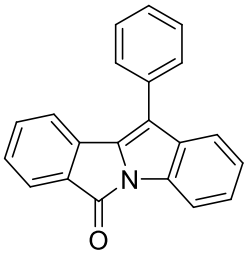
The compound **1t** was prepared by using starting materials **S1a** and trimethylsilylacetylene as above described general procedure. The compound **1t** was purified by column chromatography on silica gel (230-400 mesh) by eluting with hexane/EtOAc (96: 04) afforded viscous yellow oily product in 80% yield; IR (neat): 3440, 3120, 2960, 2401, 1625, 1531, 1397, 1218, 928, 669 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 9.33 (s, 1H), 8.18–8.15 (m, 1H), 7.70–7.68(m, 2H), 7.63–7.61 (m, 1H), 7.53–7.45 (m, 2H), 7.42–7.39 (m, 2H), 7.20–7.16 (m, 1H), 0.26 (s, 9H).^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) 164.0, 137.8, 135.8, 134.0, 130.7, 130.3, 129.3, 128.9 (2C), 124.5, 120.1 (2C), 119.3, 103.0, 102.7, -0.2 (3C); HRMS (ESI): *m/z* calculated for $C_{18}H_{20}NOSi$ $[M+H]^+$ =294.1309, found $[M+H]^+$ = 294.1312.

2.3 General procedure for the synthesis of 11-aryl-6H-isoindolo[2,1-a]indol-6-ones

To a stirred solution of **1a** (100 mg, 0.34mmol, 1.0 eq.) in trifluoroethanol (1.5 mL) was added phenyliodidediacetate (PIDA) (184 mg, 0.57 mmol, 1.7 eq.) in a oven dried round bottom flask at room temperature. The resultant solution was stirred and the progress of reaction was monitored by TLC analysis by visualizing starting material in short wavelength (254 nm) UV-light and product in long wavelength (365 nm) UV-light. The solid product was filtered off and washed with HPLC grade hexane and methanol.

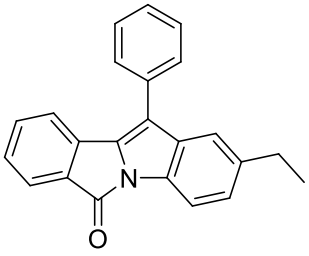


11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2a)[4]



Yellow solid; TLC R_f 0.6 Hexane/EtOAc (98: 02); Yield89%; m.p.= 221–222 °C; FT-IR (KBr): 3436, 3021, 2401, 1721, 1636, 1446, 1386, 1215, 1031, 757, 669 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.95 (d, *J* = 8.0 Hz, 1H), 7.76 (d, *J* = 7.2 Hz, 1H), 7.69 (d, *J* = 7.2 Hz, 2H), 7.57–7.52 (m, 4H), 7.47–7.44 (m, 1H), 7.39 (t, *J* = 7.2 Hz, 1H), 7.31 (q, *J* = 8.0 Hz, 2H), 7.17 (t, *J* = 7.2 Hz, 1H); ^{13}C NMR (75.4 MHz, $CDCl_3$): δ (ppm) 162.5, 134.6, 134.1, 133.9, 133.8, 133.7, 133.6, 132.2, 129.0(2C), 128.9(2C), 128.7, 128.3, 126.8, 125.3, 124.0, 121.2, 121.2, 120.5, 113.3;HRMS (ESI): *m/z* calculated for $C_{21}H_{14}NO$ $[M+H]^+$= 296.1069, found $[M+H]^+$= 296.1064.

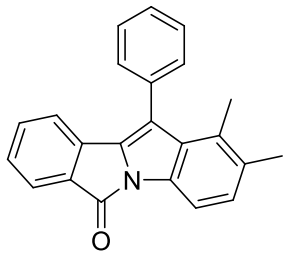
2-ethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2b)



The compound (**2b**) was prepared by using **1b** as a starting material under the same reaction conditions and procedure as stated above. The product was afforded as yellow solidin 70% yield; TLC R_f0.5 Hexane/EtOAc (98: 02); m.p.= 185–187 °C; FT-IR (KBr): 3433, 3019,

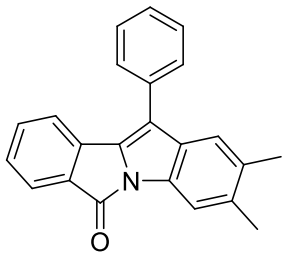
1721, 1625, 1467, 1447, 1399, 1361, 1215, 1138, 1093, 701, 669 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.84 (d, *J* = 8.0 Hz, 1H), 7.74 (d, *J* = 7.2 Hz, 1H), 7.68 (d, *J* = 6.8 Hz, 2H), 7.57–7.52 (m, 3H), 7.45 (t, *J* = 7.6 Hz, 1H), 7.38–7.33 (m, 2H), 7.29–7.25 (m, 1H), 7.16 (d, *J* = 7.6 Hz, 1H), 2.67 (q, *J* = 7.6 Hz, 2H), 1.24 (t, *J* = 7.6 Hz, 3H);^{13}C NMR (75.4 MHz, $CDCl_3$): δ (ppm) 162.4, 140.3, 134.6, 134.3, 134.1, 133.9, 133.4, 132.3, 132.0, 129.0(3C), 128.6, 128.2, 128.3, 126.8, 125.2, 121.0, 120.5, 120.1, 113.2, 29.0, 16.1;HRMS (ESI):*m/z* calculated for $C_{23}H_{18}NO$ $[M+H]^+$= 324.1382, found $[M+H]^+$= 324.1382.

1,2-dimethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2c)



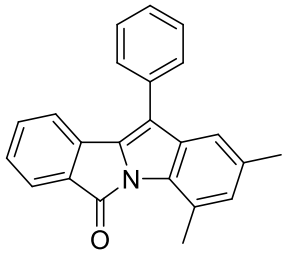
The compound (**2c**) was prepared under the same reaction conditions and procedure as abovestated, by using **1c** as a starting material to afford the product,as yellow solid. The mixture of compound (**2c**) and compound (**2c′**), the regioisomer of **2c**was purified by column chromatography on silica gel (230-400 mesh)and hexane: ethyl acetate (99.5: 0.5) as eluting solvent.Yield 67%; m.p.= 192–194 °C;FT-IR (KBr): 3434, 3019, 1731, 1622, 1467, 1495, 1215, 1127, 752, 699, 669 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.77–7.73 (m, 2H), 7.54–7.50 (m, 5H), 7.30–7.29 (m, 1H), 7.27 (d,*J* = 1.2 Hz, 1H), 7.15 (d, *J* = 8.0 Hz, 1H), 7.02–6.99 (m, 1H), 2.29 (s, 3H), 2.02 (s, 3H);^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) 162.5, 135.2, 134.6, 134.2, 133.8, 133.3, 132.8, 132.6, 132.3, 131.4, 129.9 (2C), 128.9, 128.7, 128.4 (2C), 128.3, 128.1, 125.1, 120.8, 110.6, 19.8, 15.7; HRMS (ESI): *m/z* calculated for $C_{23}H_{18}NO$ $[M+H]^+$= 324.1382, found $[M+H]^+$= 324.1385.

2,3-dimethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2c′)



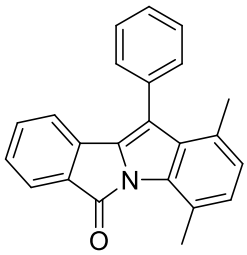
Yellow solid; yield 24%; m.p. = 163–165°C; FT-IR (KBr): 3436, 3020, 1734, 1620, 1465, 1495, 1215, 1127, 752, 699, 669 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.79–7.78 (m, 2H), 7.73 (d,*J* = 1.3 Hz, 1H), 7.71 (s, 1H), 7.60–7.56 (m, 3H), 7.50–7.46 (m, 1H), 7.40 (dt,*J* = 7.5, 1.1 Hz, 1H), 7.33–7.29 (m, 2H), 2.39 (s, 3H), 2.32 (s, 3H);^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) 162.5, 136.2, 134.8, 133.9, 133.5, 133.4, 132.7, 132.5, 132.4, 132.0, 128.9 (4C), 128.4, 128.2, 125.2, 121.6, 120.8, 120.6, 114.3, 20.3, 20.1;HRMS (ESI): *m/z* calculated for $C_{23}H_{18}NO$ $[M+H]^+$ = 324.1382, found $[M+H]^+$ = 324.1385.

2,4-dimethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2d)



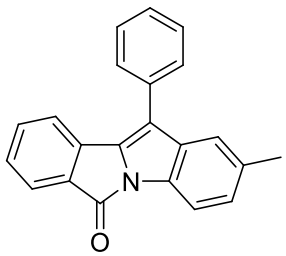
The compound (**2d**) was prepared by using **1d** as a starting material under the same reaction conditions and procedure, as yellow solid product in 45% yield;R_f0.5 Hexane/EtOAc (98: 02); m.p. = 148–149 °C; FT-IR (KBr): 3437, 3019, 2926, 2854, 2399, 1731, 1664, 1522, 1467, 1403, 1215, 1093, 1027, 924, 668 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.74 (d, *J* = 7.2 Hz, 1H), 7.65 (d, *J* = 7.2 Hz, 2H), 7.55 (t, *J* = 7.2 Hz, 2H), 7.45 (d, *J* = 7.2 Hz, 2H), 7.37 (t, *J* = 7.2 Hz, 1H), 7.29 (t, *J* = 7.2 Hz, 1H), 7.08 (s, 1H), 6.92 (s, 1H), 2.89 (s, 3H), 2.33 (s, 3H);^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) 162.1, 135.6, 135.2, 134.2, 133.9, 133.6, 133.4, 132.5, 132.3, 130.5, 129.2 (2C), 128.9 (2C), 128.5, 128.2, 125.2, 124.7, 120.6 (2C) 118.3, 21.2, 21.1;HRMS (ESI): *m/z*calculated for $C_{23}H_{18}NO$ $[M + H]^+$= 324.1382, found $[M + H]^+$=324.1389.

1,4-dimethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2e)



The compound (**2e**) was prepared by using **1e** as a starting material under the same reaction conditions and procedure, as yellow solid product in 75% yield;m.p. = 152–154 °C; FT-IR (KBr): 3434, 3021, 1731, 1625, 1402, 1338, 1215, 1137, 899, 669 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.74 (d, *J* = 6.4 Hz, 1H), 7.51 (brs 5H), 7.31–7.25 (m, 2H), 6.98 (d, *J* = 7.6 Hz, 1H), 6.91 (d, *J* = 7.6 Hz, 1H), 6.81 (d, *J* = 7.6 Hz, 1H), 2.91 (s, 3H), 2.02 (s, 3H);^{13}C NMR (75.4 MHz, $CDCl_3$): δ (ppm) 162.3, 136.3, 134.4, 134.2, 134.0, 133.4, 133.4, 133.1, 129.9(2C), 129.9, 129.1, 128.3 (2C), 128.3, 128.1, 126.4, 125.2, 122.6, 121.0, 120.5, 21.2, 19.6; HRMS (ESI): *m/z*calculated for $C_{23}H_{18}NO$ $[M+H]^+$= 324.1382, found $[M+H]^+$= 324.1384.

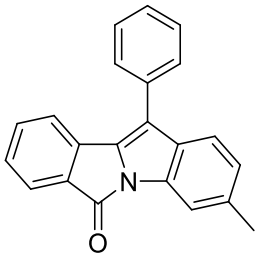
2-methyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2f)



The compound (**2f**) was prepared by using **1f** as a starting material under the same reaction conditions and procedure, as yellow crystalline solid product in 71% yield;m.p. = 176–177 °C;FT-IR (KBr): 3434, 3019, 1730, 1621, 1410, 1335, 1215, 1130, 669 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.82 (d, *J* = 8.4 Hz, 1H), 7.75 (d, *J* = 7.2 Hz, 1H), 7.68 (d, *J* = 7.2 Hz, 2H), 7.55 (t, *J* = 7.2 Hz, 3H), 7.46 (t, *J* = 7.2 Hz, 1H), 7.38 (t, *J* = 7.2 Hz, 1H),

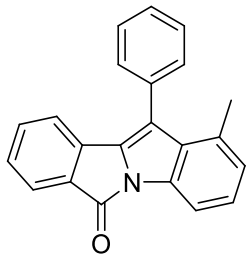
7.31 (brs, 1H), 7.28 (d, *J* = 7.6 Hz, 1H), 7.13 (d, *J* = 8.0 Hz, 1H), 2.38 (s, 3H);^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) 162.4, 134.6, 134.3, 134.1, 133.9, 133.7, 133.4, 132.3, 131.9, 129.0 (4C), 128.6, 128.2, 127.9, 125.2, 121.3, 121.0, 120.4, 113.1, 21.5;HRMS (ESI): *m/z* calculated for $C_{22}H_{16}NO$ $[M+H]^+$= 310.1226, found $[M+H]^+$= 310.1225.

3-methyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2g)



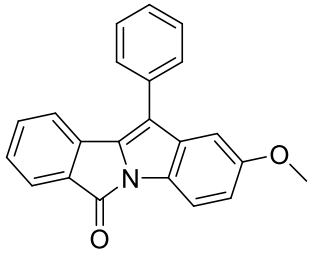
The compound (**2g**) was prepared under the same reaction conditions and procedure as above stated, by using **1g** as a starting material to afford the product, as yellow solid. The mixture of compound (**2g**) and compound (**2g′**), the regioisomer of **2g**was purified by column chromatography on silica gel (230-400 mesh) and hexane: ethyl acetate (99.4: 0.6) as eluting solvent. Yield 64%;m.p. = 181–183 °C; FT-IR (KBr): 3432, 3018, 1725, 1620, 1410, 1332, 1213, 1130, 669 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.83 (t, *J* = 0.7 Hz, 1H), 7.81 (dt, *J* = 7.5, 0.8 Hz, 1H), 7.73–7.71 (m, 2H), 7.61–7.55 (m, 3H), 7.50–7.45 (m, 1H), 7.44–7.40 (m, 2H), 7.35–7.31 (m, 1H), 7.04–7.02 (m,1H), 2.49 (s, 3H);^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) 162.6, 137.4, 134.8, 134.1, 133.8, 133.5, 132.3, 131.6, 129.0 (2C), 128.9 (2C), 128.5, 128.2, 125.3 (2C), 121.0, 120.9, 120.8, 120.7, 113.9, 21.7;HRMS (ESI): *m/z* calculated for $C_{22}H_{16}NO$ $[M+H]^+$=310.1226, found $[M+H]^+$= 310.1225.

1-methyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2g′)



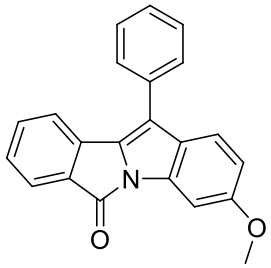
Yield 24%;m.p. = 150–152 °C; FT-IR (KBr): 3434, 3019, 1724, 1621, 1410, 1335, 1214, 1130, 669 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.85 (d, *J* = 7.9 Hz, 1H), 7.77 (dd,*J* = 6.6, 1.4 Hz, 1H), 7.57–7.49 (m, 5H), 7.35–7.30 (m, 2H), 7.23 (t,*J* = 7.6 Hz, 1H), 7.06 (dd,*J* = 6.5, 0.7 Hz, 1H), 6.92 (d, *J* = 7.4Hz, 1H), 2.12 (s, 3H);^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) 162.6, 135.0, 134.6, 133.7 (2C), 133.4, 133.1, 132.5, 132.4, 129.9 (2C), 128.5, 128.3 (2C), 128.1, 126.6, 126.1, 125.2, 121.1, 121.0, 111.2, 19.9;HRMS (ESI): *m/z* calculated for $C_{22}H_{16}NO$ $[M+H]^+$=310.1226, found $[M+H]^+$= 310.1225.

2-methoxy-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2h)



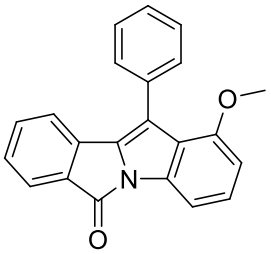
The compound (**2h**) was prepared by using **1h** as a starting material under the same reaction conditions and procedure as yellow solid product in 60% yield;TLC R_f 0.6 Hexane/EtOAc (97: 03); m.p.= 193–195 °C; FT-IR (KBr): 3434, 3019, 1735, 1620, 1467, 1495, 1215, 1127, 669 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.87 (d, *J* = 8.6 Hz, 1H), 7.78 (d, *J* = 7.3 Hz, 1H), 7.71 (d, *J* = 7.0 Hz, 2H), 7.60–7.55 (m, 3H), 7.49 (t, *J* = 7.4 Hz, 1H), 7.41 (t, *J* = 7.4 Hz, 1H), 7.33 (d, *J* = 7.6 Hz, 1H), 7.05 (d, *J* = 2.2 Hz, 1H), 6.95 (dd, *J* = 8.6, 2.4 Hz, 1H), 3.85 (s, 3H);^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm)162.2, 157.0, 135.1, 135.0, 134.6, 133.9, 133.4, 132.2, 129.0 (2C), 128.9 (2C), 128.7, 128.4, 128.3, 125.2, 121.0, 120.3, 114.3, 114.0, 105.1, 55.8; HRMS (ESI): *m/z* calculated for $C_{22}H_{16}NO_2$ $[M+H]^+$ = 326.1176, found $[M+H]^+$ = 326.1182.

3-methoxy-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2i)



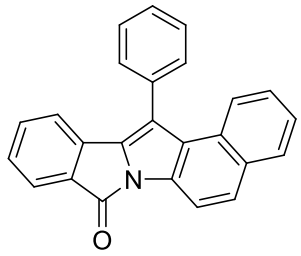
The compound (**2i**) was prepared under the same reaction conditions and procedure as above stated, by using **1i** as a starting material to afford the product, as yellow solid. The mixture of compound (**2i**) and compound (**2i′**), the regioisomer of **2i** was purified by column chromatography on silica gel (230-400 mesh) and hexane: ethyl acetate (99: 01) as eluting solvent. Yield 70%;m.p. = 189–191°C; FT-IR (KBr): 3434, 3019, 1731, 1622, 1467, 1495, 1215, 1127, 752, 699, 669 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.79 (td, *J* = 7.6, 0.8 Hz, 1H), 7.73–7.70 (m, 2H), 7.59–7.55 (m, 3H), 7.53 (d, *J* = 2.4Hz, 1H), 7.50–7.45 (m, 1H), 7.44–7.40 (m, 2H), 7.31 (dd, *J* = 7.6, 1.2 Hz, 1H), 6.80 (dd, *J* = 8.8, 2.8 Hz, 1H), 3.93 (s, 3H);^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) 162.7, 159.9, 134.9, 134.9, 133.6, 133.4, 132.8, 132.3, 129.0 (2C), 128.8 (2C), 128.2, 128.1, 127.3, 125.3, 121.9, 120.9, 120.7, 112.7, 97.9, 55.8;HRMS (ESI): *m/z* calculated for $C_{22}H_{16}NO_2$ $[M+H]^+$= 326.1175, found $[M+H]^+$= 326.1176.

1-methoxy-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2i′)



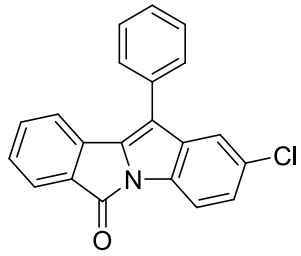
The compound (**2i′**) is the regioisomer of compound (**2i**) which were isolated by column chromatography on silica gel (230-400 mesh) by eluting with hexane/EtOAc (99:01) in very slight (**2i′/2i** = 13.6/1) impurity of compound (**2i**) in 11% yield as yellowsolid;m.p. = 157–159 °C, FT-IR (KBr): 3434, 3019, 1730, 1622, 1467, 1495, 1215, 1127, 752, 699, 669 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.78 (d, *J* = 7.4 Hz, 1H), 7.68 (dd, *J* = 8.2, 1.5 Hz, 2H), 7.64 (d, *J* = 7.9 Hz, 1H), 7.51–7.44 (m, 3H), 7.39–7.35 (m, 2H), 7.31–7.27 (m, 2H), 6.66 (d, *J* = 8.1 Hz, 1H), 3.75 (s, 3H);^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) 162.8, 155.1, 135.1, 133.6, 133.5, 133.4, 133.0, 130.1 (2C), 129.0, 128.3, 128.1, 127.8, 127.6 (2C), 125.3, 122.2, 120.9, 120.8, 106.6, 105.7, 55.2; HRMS (ESI): *m/z* calculated for $C_{22}H_{16}NO_2$ $[M+H]^+$= 326.1175, found $[M+H]^+$= 326.1176.

13-phenyl-8H-benzo[e]isoindolo[2,1-a]indol-8-one (2j)



The compound (**2j**) was prepared by using **1j** as a starting material under the same reaction conditions and procedure, as yellow solid product in 86%yield; TLC R_f 0.6 Hexane/EtOAc (97: 03); m.p. = 209–210 °C; FT-IR (KBr): 3431, 3021, 1732, 1621, 1526, 1400, 1215, 758, 670 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.12 (d, *J* = 8.8 Hz, 1H), 7.85–7.83 (m 1H), 7.76–7.71 (m, 3H), 7.67–7.64 (m, 2H), 7.59–7.54 (m, 3H), 7.37–7.26 (m, 3H), 7.23–7.20 (m, 1H), 7.04 (d, *J* = 7.6 Hz, 1H);^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) 163.1, 135.3, 134.4, 133.8 (2C), 133.1, 131.4, 131.1, 129.8 (2C), 129.1, 128.8 (2C), 128.7, 128.4, 128.1, 127.9, 127.2, 126.3, 125.4, 124.4, 123.1, 121.6, 120.5, 113.2;HRMS (ESI): *m/z* calculated for $C_{25}H_{16}NO$ $[M+H]^+$= 346.1226, found $[M+H]^+$= 346.1226.

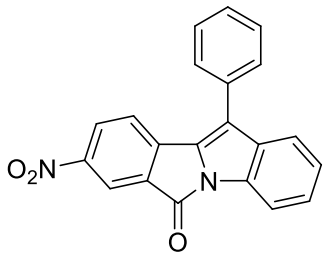
2-chloro-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2k)



The compound (**2k**) was prepared by using **1k** as a starting material under the same condition and procedure as yellow solid product in 81% yield;TLC R_f 0.6 Hxane/EtOAc (96: 04); m.p. = 193–194°C;FT-IR (KBr): 3409, 3021, 2401, 1726, 1622, 1524, 1444, 1319, 1215, 928, 670 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.87 (d, *J* = 8.4 Hz,

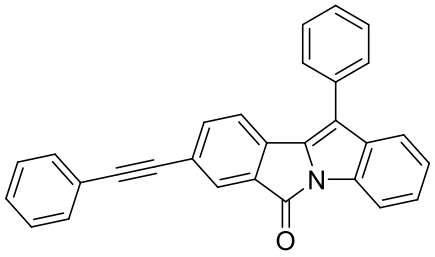
1H), 7.78 (d,*J* = 7.4 Hz, 1H), 7.68–7.65 (m, 2H), 7.58–7.54 (m, 3H), 7.49 (dd, *J* = 8.1, 1.8 Hz, 2H), 7.42 (td, *J* = 7.5, 1.0 Hz, 1H), 7.34 (td,*J* = 7.5, 0.8 Hz, 1H), 7.28 (dd, *J* = 8.4, 1.9 Hz, 1H);^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) 162.2, 135.2, 135.1, 134.3, 133.7, 133.5, 131.9, 131.5, 129.6, 129.1 (3C), 128.8 (2C), 128.5, 126.7, 125.4, 121.3, 120.9, 119.5, 114.2;HRMS (ESI): *m/z* calculated for $C_{21}H_{13}ClNO$ $[M+H]^+$= 330.0680, found $[M+H]^+$ = 330.0675.

8-nitro-11-phenyl-6H-isoindolo[2,1-a]indol-6-one (2l)



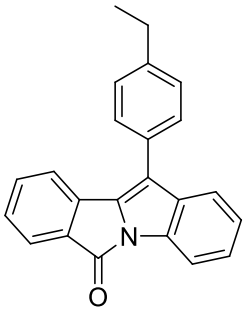
The compound (**2l**) was prepared by using **1l** as a starting material under the same condition and procedure as orange yellow colored solid product in 78% yield;TLC R_f 0.5 Hexane/EtOAc (94: 06); m.p. = 246–248°C; FT-IR (KBr): 3434, 3019, 2340, 1724, 1655, 1524, 1404, 1345, 1215, 1104, 929 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.60 (d, *J* = 1.8 Hz, 1H), 8.31 (dd, *J* = 8.4, 2.0 Hz, 1H), 8.01 (d, *J* = 8.0 Hz, 1H), 7.73–7.69 (m, 3H), 7.64–7.60 (m, 3H), 7.56 (t, *J* = 7.2 Hz, 1H), 7.43 (t, *J* = 7.7 Hz, 1H), 7.27 (t, *J* = 7.6 Hz, 1H);^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) 160.1, 147.8, 139.5, 134.7, 134.2, 133.6, 132.0, 131.2, 129.3 (2C), 129.1, 128.9 (3C), 128.2, 124.9, 124.5, 122.1, 121.3, 120.8, 113.9;HRMS (ESI): *m/z* calculated for $C_{21}H_{13}N_2O_3$ $[M+H]^+$= 341.0921, found $[M+H]^+$= 341.0912.

11-phenyl-8-(phenylethynyl)-6H-isoindolo[2,1-a]indol-6-one (2m)



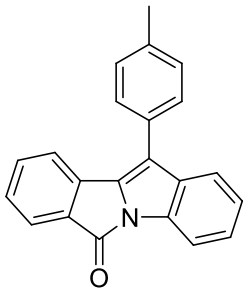
The compound (**2m**) was prepared by using **1m** as a starting material under the same condition and procedure as yellow solid product in 80% yield; TLC R_f 0.6, Hexane/EtOAc (96: 04); mp= 194–195°C; FT-IR (KBr): 3434, 3019, 2401, 2350, 1722, 1622, 1467, 1355, 1215, 1127, 752, 699, 669 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.99 (d, *J* = 7.9 Hz, 1H), 7.95 (s, 1H), 7.73 (d, *J* = 7.0 Hz, 2H), 7.62–7.55 (m, 7H), 7.51 (t, *J* = 7.3 Hz, 1H), 7.40–7.38 (m, 4H), 7.22 (t, *J* = 7.8 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) 161.7, 136.5, 134.0, 133.9, 133.8, 133.7 (2C), 132.0, 131.7 (2C), 129.1 (2C), 128.9 (2C), 128.7, 128.5, 128.4 (2C), 128.3, 127.1, 124.2, 123.9, 122.7, 121.3, 121.2, 121.0, 113.5, 91.7, 88.4;HRMS (ESI): *m/z* calculated for $C_{29}H_{18}NO$ $[M+H]^+$= 396.1383, found $[M+H]^+$= 396.1376.

11-(4-ethylphenyl)-6H-isoindolo[2,1-a]indol-6-one (2p)



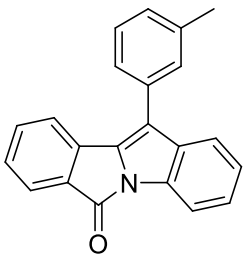
The compound (**2p**) was prepared by using **1p** as a starting material under the same condition and procedure as yellow crystalline solid product in 61% yield;TLC R_f 0.7 (hexane/EtOAc 98:02);m.p. = 140–142°C; FT-IR (KBr): 3433, 3019, 1721, 1625, 1467, 1447, 1399, 1361, 1215, 1138, 1093, 669 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.99 (d, *J* = 7.9 Hz, 1H), 7.81 (d, *J* = 7.4 Hz, 1H), 7.66–7.63 (m, 3H), 7.58 (d, *J* = 7.8 Hz, 1H), 7.45 (dd, *J* = 7.5, 1.0 Hz, 1H), 7.41 (d,*J* = 8.0 Hz, 2H), 7.38–7.36 (m, 1H), 7.31 (dd, *J* = 7.4, 0.9 Hz, 1H), 7.23–7.18 (m, 1H), 2.79 (q, *J* = 7.6 Hz, 2H), 1.36 (t, *J* = 7.6 Hz, 3H);^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) 162.5, 144.5, 134.7, 134.1, 133.9, 133.8 (2C), 133.5, 129.4, 128.9 (2C), 128.6, 128.5 (2C), 126.7, 125.3, 123.9, 121.3, 121.2, 120.7, 113.5, 28.7, 15.4;HRMS (ESI): *m/z* calculated for $C_{23}H_{18}NO$ $[M+H]^+$ = 324.1382, found $[M+H]^+$ = 324.1388.

11-(*p*-tolyl)-6H-isoindolo[2,1-a]indol-6-one (2q)



The compound (**2q**) was prepared by using **1q** as a starting material under the same condition and procedure as yellow crystalline solid product in 65% yield;TLC R_f0.6 Hexane/EtOAc (98: 02);m.p. = 169–170°C; FT-IR (KBr): 3433, 3019, 1721, 1625, 1467, 1447, 1399, 1361, 1215, 1138, 1093, 669 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.98 (d, *J* = 7.9 Hz, 1H), 7.80 (d, *J* = 7.4 Hz, 1H), 7.63–7.61 (m, 3H), 7.56 (d,*J* = 7.8 Hz, 1H), 7.45–7.43 (m, 1H), 7.43-7.31 (m, 4H), 7.20 (t, *J* = 7.8 Hz, 1H), 2.49 (s, 3H);^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) 162.5, 138.2, 134.7, 134.1, 133.9, 133.8 (2C), 133.5, 129.7 (2C), 129.1, 128.8 (2C), 128.6, 126.7, 125.3, 123.9, 121.3, 121.2, 120.6, 113.5, 21.4; HRMS (ESI): *m/z* calculated for $C_{22}H_{16}NO$ $[M+H]^+$ = 310.1226, found $[M+H]^+$ = 310.1225.

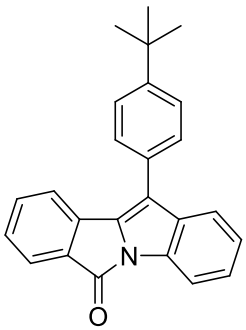
11-(*m*-tolyl)-6H-isoindolo[2,1-a]indol-6-one (2r)



The compound (**2r**) was prepared by using **1r** as a starting material under the same condition and procedure as yellow crystalline solid product in 77% yield;TLC R_f0.6 Hexane/EtOAc (98: 02);m.p. = 217–219°C; FT-IR (KBr): 3433, 3019, 1721, 1625, 1467, 1447, 1399, 1361, 1215, 1138, 1093, 669 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.96 (d, *J* = 8.0 Hz, 1H),

7.78 (d, *J* = 7.4 Hz, 1H), 7.59–7.53 (m, 2H), 7.52–7.49 (m, 2H), 7.45 (d, *J* = 7.4 Hz, 1H), 7.43–7.39 (m, 1H), 7.35–7.31 (m, 2H), 7.29–7.27 (m,1H), 7.20–7.16 (m, 1H), 2.47 (s, 3H);^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) 162.5, 138.7, 134.7, 134.1, 134.0, 133.8, 133.7, 133.6, 132.1, 129.5, 129.1, 128.9, 128.7, 126.7, 126.0, 125.3, 124.0, 121.3, 121.2, 120.7, 113.5, 21.5;HRMS (ESI): *m/z* calculatedfor $C_{22}H_{16}NO$ $[M+H]^+$ = 310.1226, found $[M+H]^+$ = 310.1222.

11-(4-tert-butylphenyl)-6H-isoindolo[2,1-a]indol-6-one (2s)

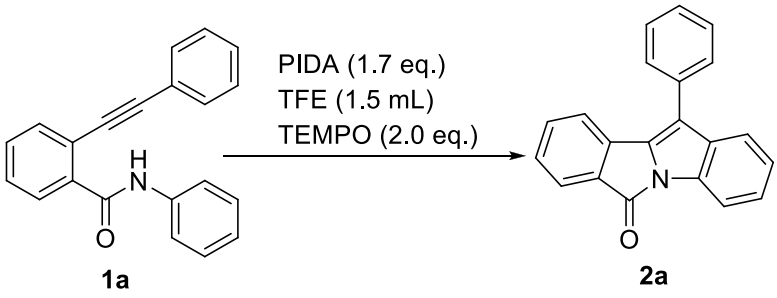


The compound (**2s**) was prepared by using **1s** as a starting material under the same condition and procedure as yellow crystalline solid product in 59% yield;TLC R_f 0.6, Hexane/EtOAc (98; 02); m.p. = 172–175°C; FT-IR (KBr): 3433, 3019, 1721, 1625, 1467, 1447, 1399, 1361, 1215, 1138, 1093, 669 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.99 (d, *J* = 7.5 Hz, 1H), 7.80 (d, *J* = 6.9 Hz, 1H), 7.67–7.59 (m, 6H), 7.46–7.43 (m, 1H), 7.34 (d, *J* = 6.9 Hz, 2H), 7.22–7.19 (m, 1H), 1.45 (s, 9H);^{13}C NMR (100.6 MHz, $CDCl_3$): δ (ppm) 162.5, 151.4, 134.7, 134.1, 133.9, 133.8 (2C), 133.5, 129.1, 128.6 (3C), 126.7, 125.9 (2C), 125.3, 123.9, 121.4, 121.3, 120.6, 113.4, 34.8, 31.3 (3C); HRMS (ESI): *m/z* calculated for $C_{25}H_{22}NO$ $[M+H]^+$ = 352.1696, found $[M+H]^+$ = 352.1696.

3. Procedure for control experiments.

(A) ***Experiment with TEMPO:***

To a stirred solution of **1a** (100 mg, 0.34 mmol, 1.0 eq.) and TEMPO (2.0 eq.) in trifluoroethanol (TFE) (1.5 mL) was added phenyliodidediacetate (PIDA) (184 mg, 0.57 mmol, 1.7 eq.) in an oven dried round bottom flask at room temperature. The resultant solution was stirred and the progress of reaction was monitored by TLC analysis. After the completion of reaction, the reaction mixture was evaporated under vacuum at 45°C and extracted with dichloromethane (30 mL X 3). The organic layers were combined and dried over anhydrous Na_2SO_4 followed by the filtration and then condensed.The obtained solid product was washed with HPLC grade hexane and then methanol. The obtained solid product was characterized as compound **2a** with the yield 85%.



(B) Experiment with 2,6-di-tert-butyl-4-methylphenol (BHT):

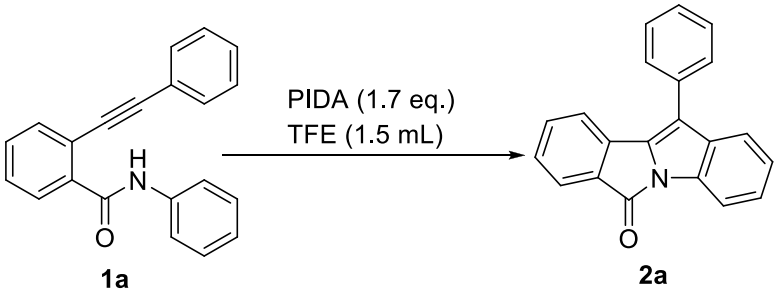
To a stirred solution of **1a** (100 mg, 0.34 mmol, 1.0 eq.) and 2,6-di-*tert*-butyl-4-methylphenol (BHT) (2.0 eq.) in trifluoroethanol (TFE) (1.5 mL) was added phenyliodidediacetate (PIDA) (184 mg, 0.57 mmol, 1.7 eq.) in an oven dried round bottom flask at room temperature. The resultant solution was stirred and the progress of reaction was monitored by TLC analysis. After the completion of reaction, the reaction mixture was evaporated under vacuum at 45°C and extracted with dichloromethane (30 mL X 3). The organic layers were combined and dried over anhydrous Na_2SO_4 followed by the filtration and then condensed. The obtained solid product was washed with HPLC grade hexane and then methanol. The obtained solid product was characterized as compound **2a** with the yield 82%.

(C) Experiment with 1,1-Diphenylethylene (DPE):

To a stirred solution of **1a** (100 mg, 0.34 mmol, 1.0 eq.) and 1,1-diphenylethylene (DPE) (2.0 eq.) in trifluoroethanol (TFE) (1.5 mL) was added phenyliodidediacetate (PIDA) (184 mg, 0.57 mmol, 1.7 eq.) in an oven dried round bottom flask at room temperature. The resultant solution was stirred and the progress of reaction was monitored by TLC analysis. After the completion of reaction, the reaction mixture was evaporated under vacuum at 45°C and extracted with dichloromethane (30 mL X 3). The organic layers were combined and dried over anhydrous Na_2SO_4 followed by the filtration and then condensed. The obtained solid product was washed

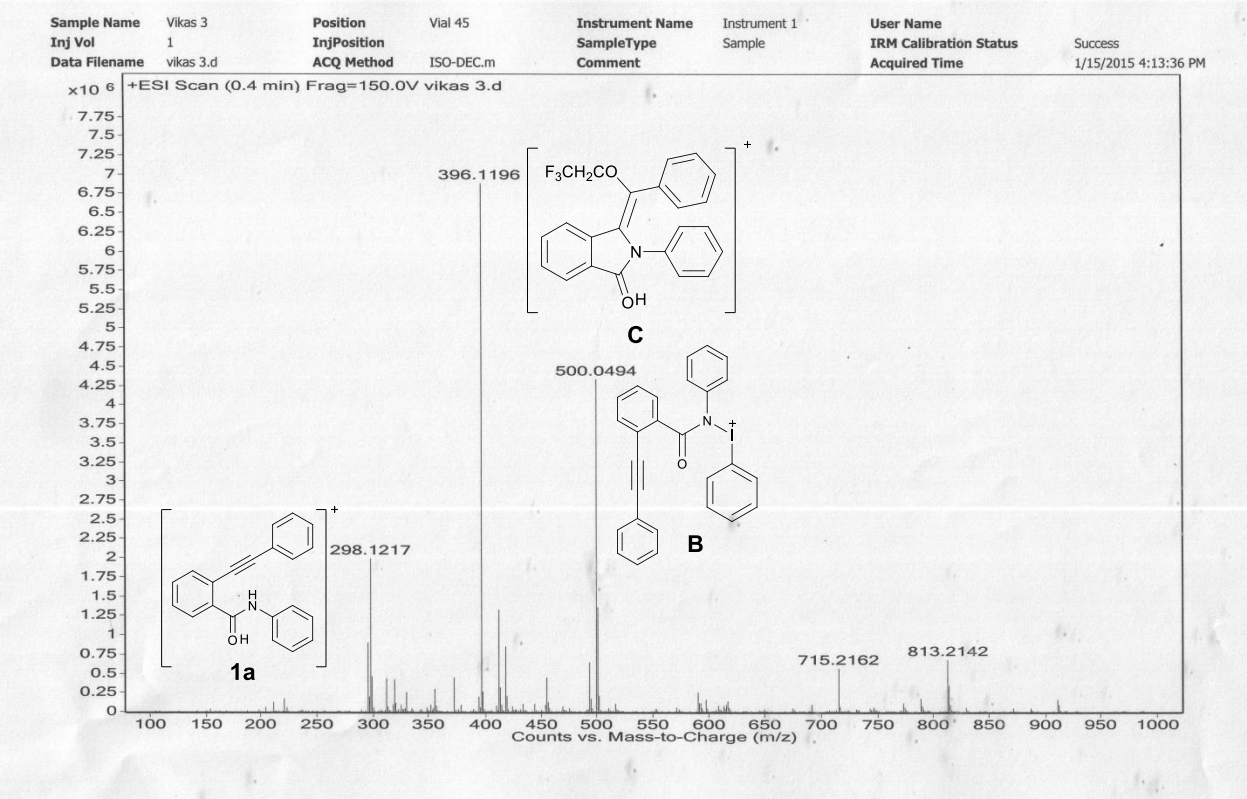
with HPLC grade hexane and then methanol. The obtained solid product was characterized as compound **2a** with the yield 86%.

4. Discussion of Proposed Mechanism by Time Dependent Mass Spectra (ESI-MS):

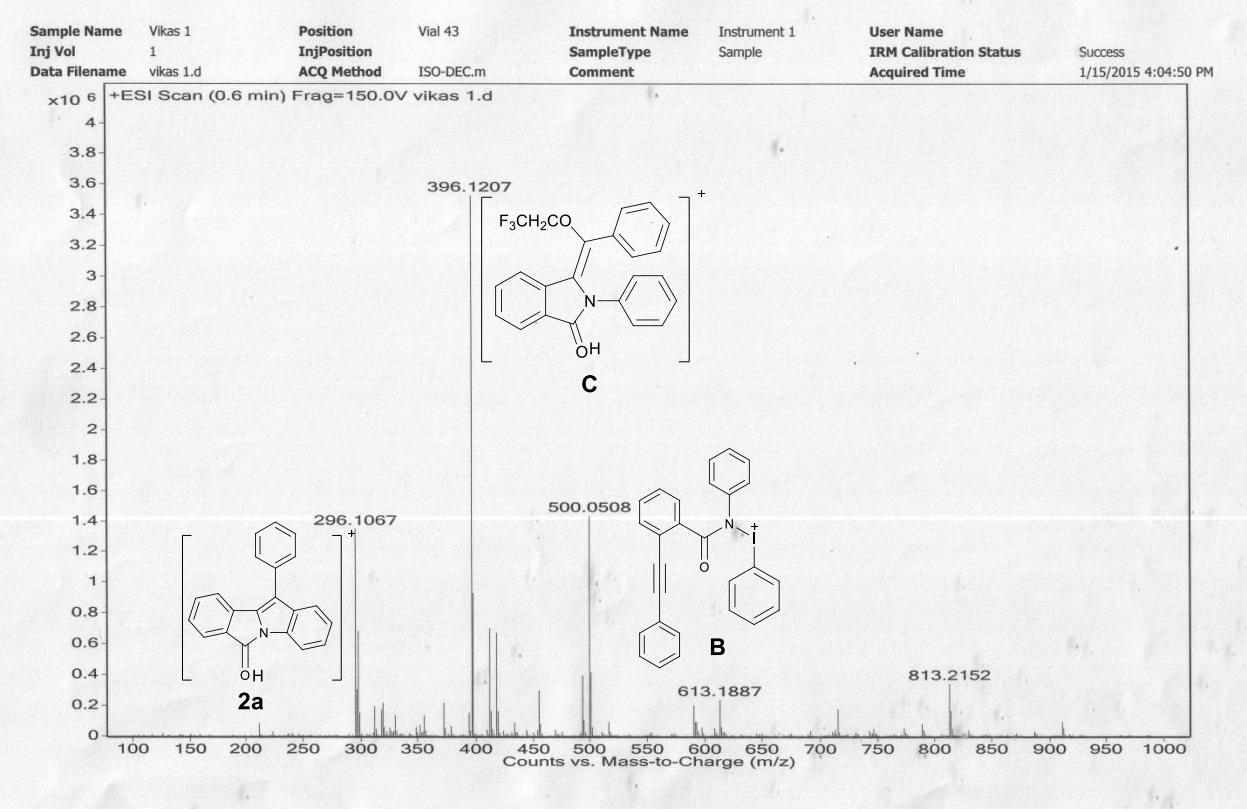


The mechanism and role of solvent were investigated by mass spectra (ESI-MS) of reaction mixture. The mass spectra was recorded after 3 and 10 min of addition of hypervalent iodine reagent, showed peaks at 500.0494 $[C_{27}H_{19}INO_2]^+$, 396.1196 $[C_{23}H_{17}F_3NO_2]^+$ and 298.1217 $[C_{21}H_{16}NO_2]^+$, and peaks at 500.0508 $[C_{27}H_{19}INO_2]^+$, 396.1207 $[C_{23}H_{17}F_3NO_2]^+$ and 296.1067 $[C_{21}H_{14}NO_2]^+$ respectively. In both mass spectra there were peaks at 500.05 and 396.1207 indicated that the formation of intermediates, nitrenium ion **B** and carbonium ion **C**, which was stabilized by iodine and solvent (TFE), respectively.

ESI-MS Spectrum of Reaction Mixture after 3 min of Addition of Hypervalent Iodine Reagent



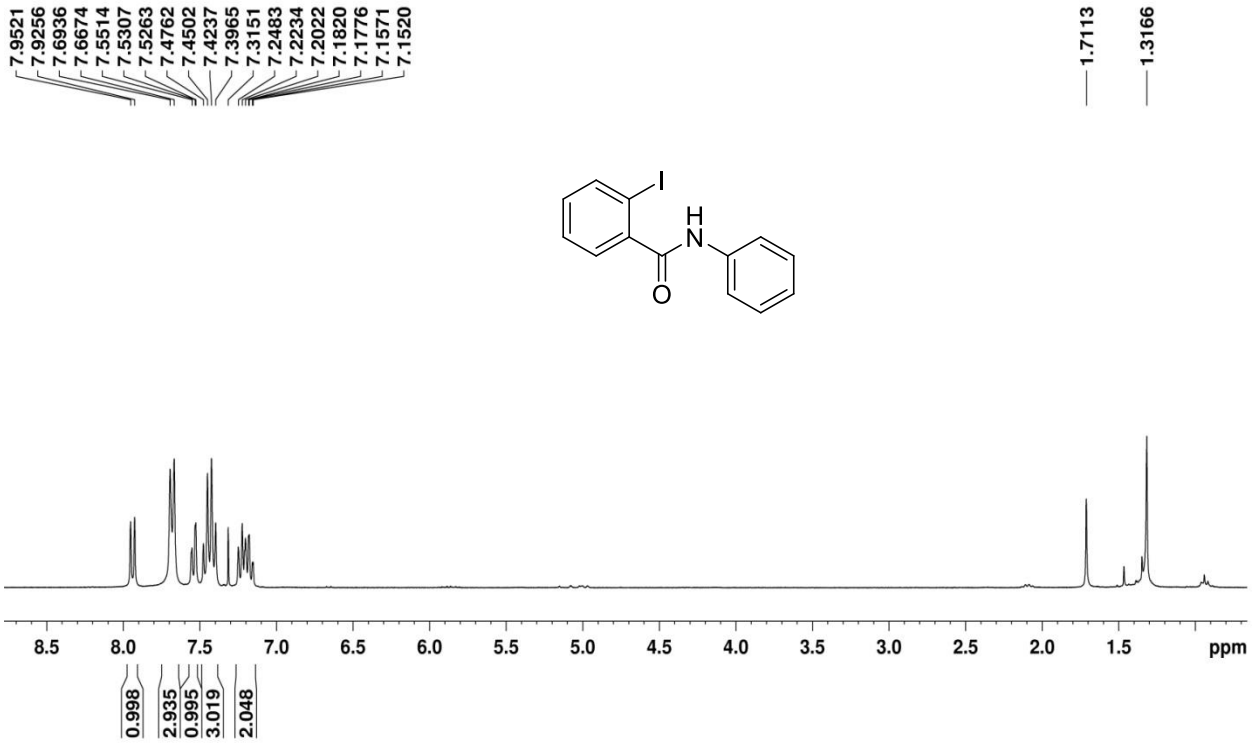
ESI-MS Spectrum of Reaction Mixture after 10 min of Addition of Hypervalent Iodine Reagent



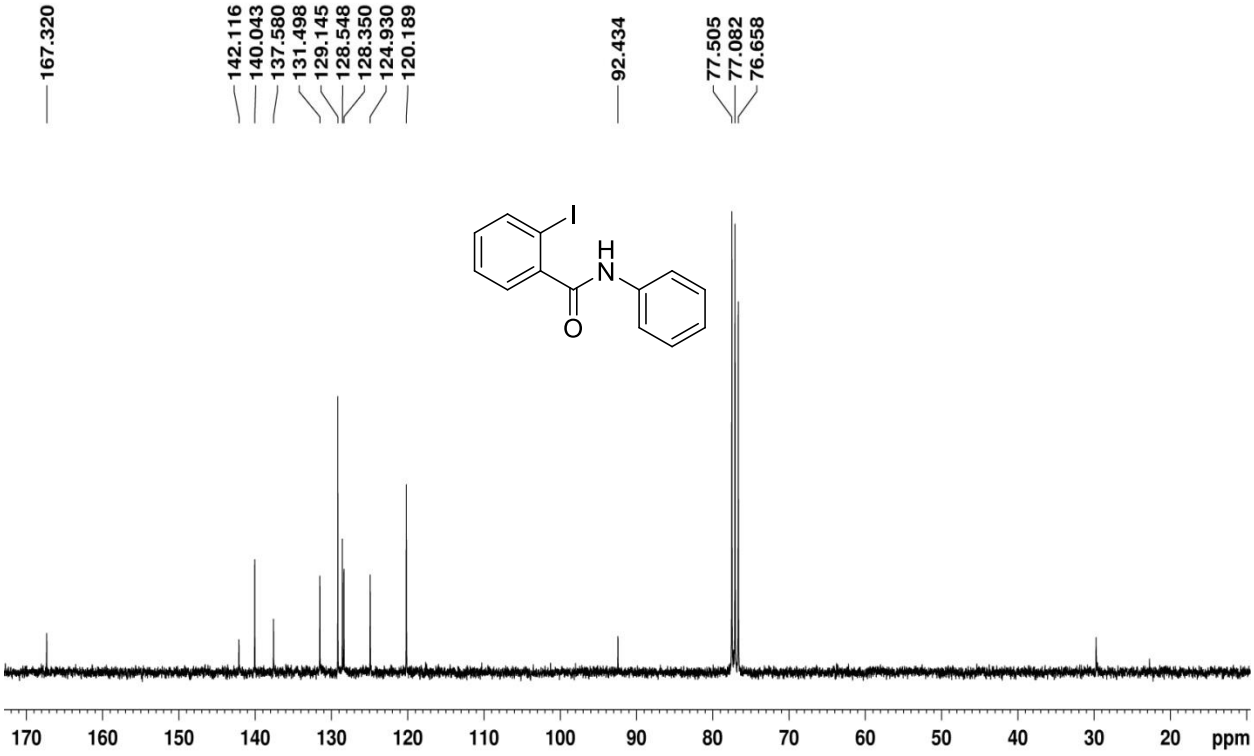
5. References:

1. Yao, B.; Jaccoud, C.; Wang, Q.; Zhu, J. *Chem. Eur. J.* **2012,** *18*, 5864–5868.
2. Escamilla, I. V.; Hernandez, A. A.; Ramos, L. F. R.; Castillo, O. R. S.; Mata, F. A.; Vallejo, G. Z. *Tetrahedron Lett.* **2011,** *52*, 3726–3728.
3. Sheikha, G. A.; Khalaf, R. A.; Melhem, A.;Albadawi, G. *Molecules* **2010,** *15*, 5721-5733.
4. Huang, Q.; Campo, M. A.; Yao, T.; Tian, Q.; Larock, R. C. *J. Org. Chem.* **2004,** *69*, 8251–8257.

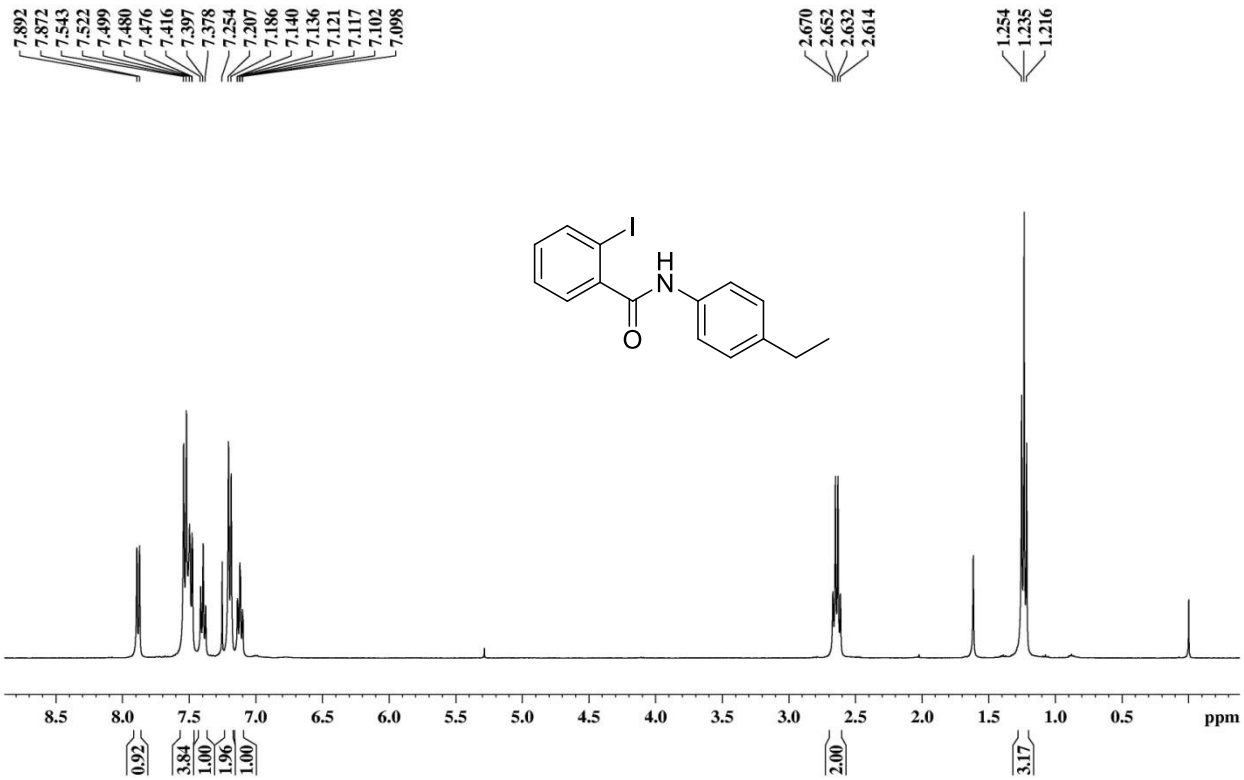
^{1}H NMR Spectrum of*N-(phenyl)-2-iodobenzamide* (S1a) (300 MHz, $CDCl_3$)



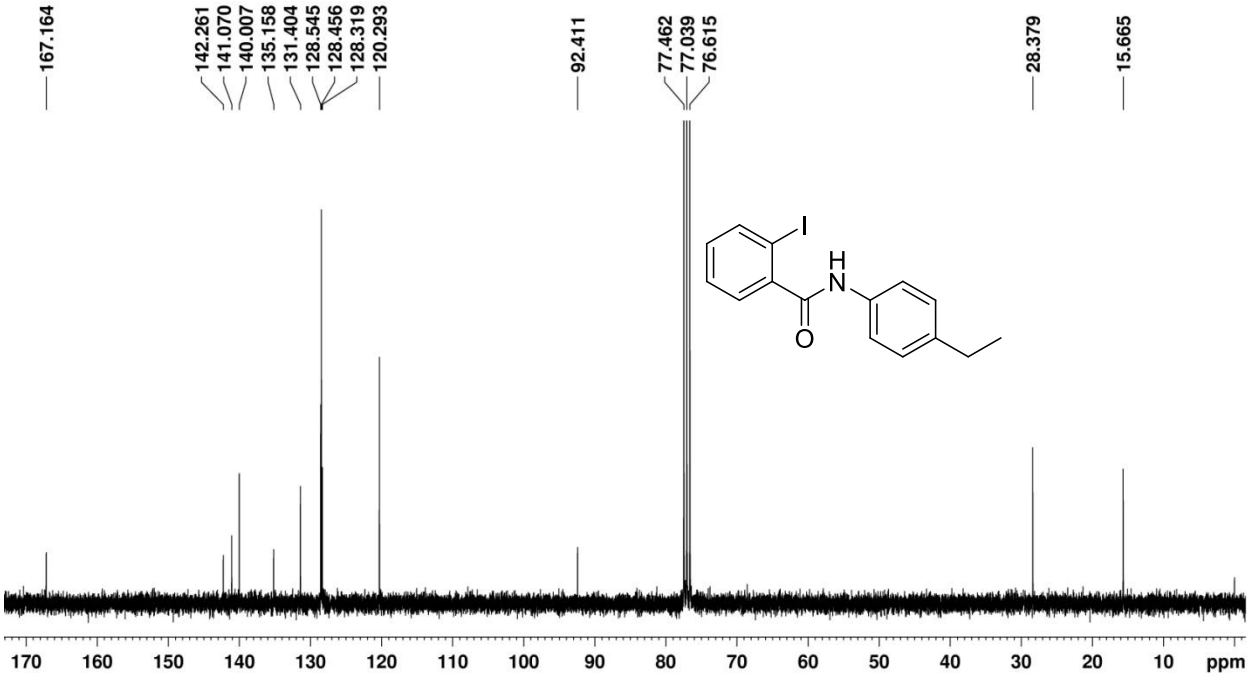
^{13}C NMR Spectrum of*N-(phenyl)-2-iodobenzamide* (S1a) (75 MHz, $CDCl_3$)



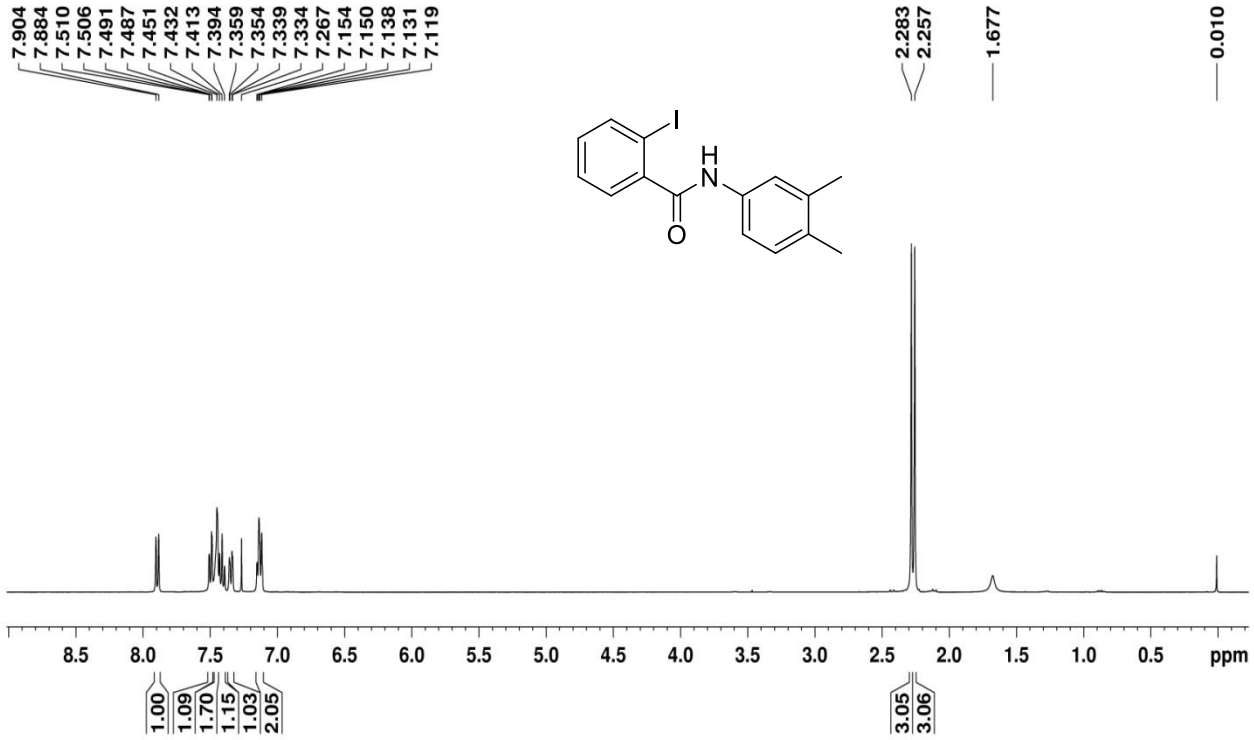
^{1}H NMR Spectrum of*N-(4-ethylphenyl)-2-iodobenzamide* (S1b)(400 MHz, $CDCl_3$)



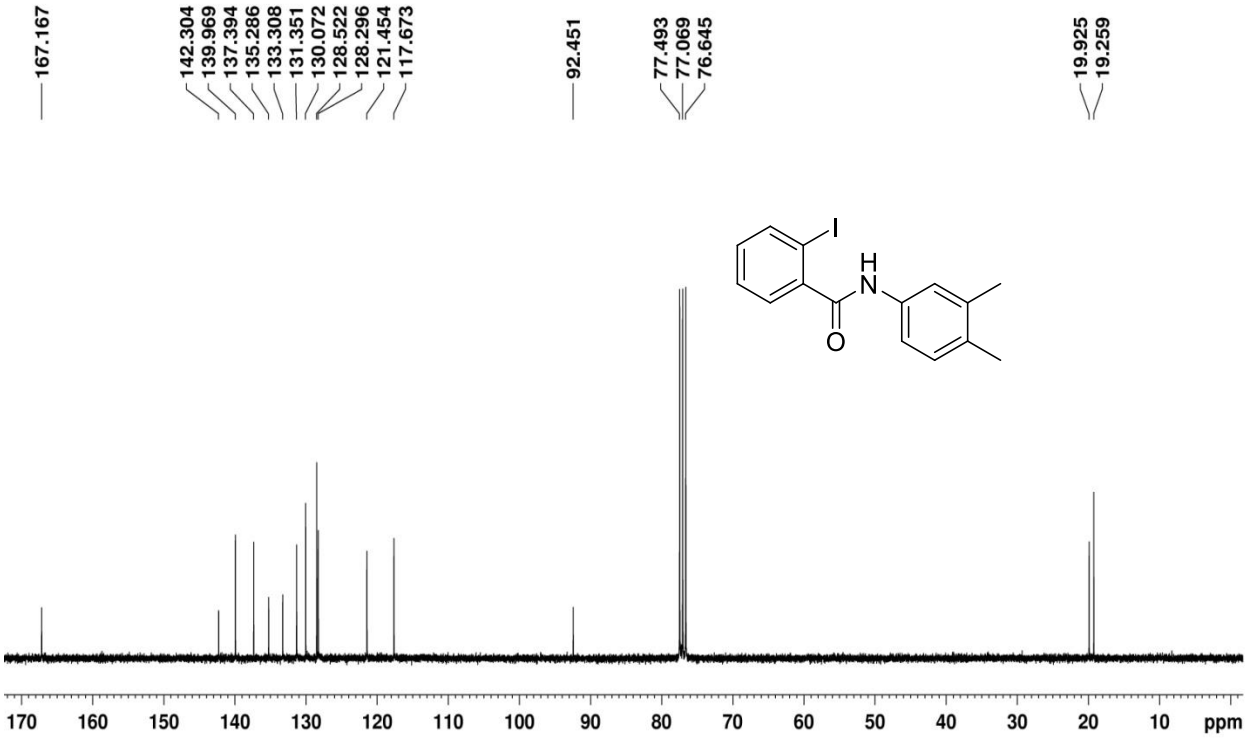
^{13}C NMR Spectrum of*N-(4-ethylphenyl)-2-iodobenzamide* (S1b) (75 MHz, $CDCl_3$)



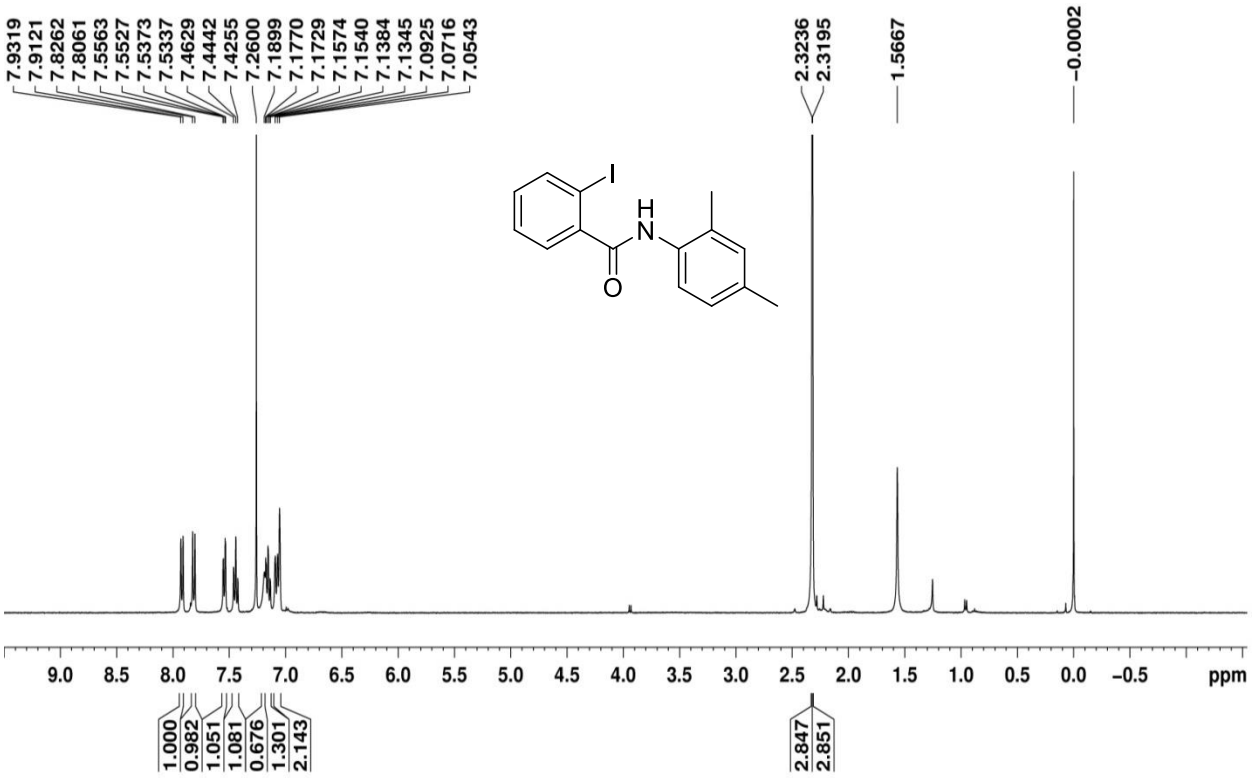
^{1}H NMR Spectrum of*N-(3,4-dimethylphenyl)-2-iodobenzamide* (S1c) (400 MHz, $CDCl_3$)



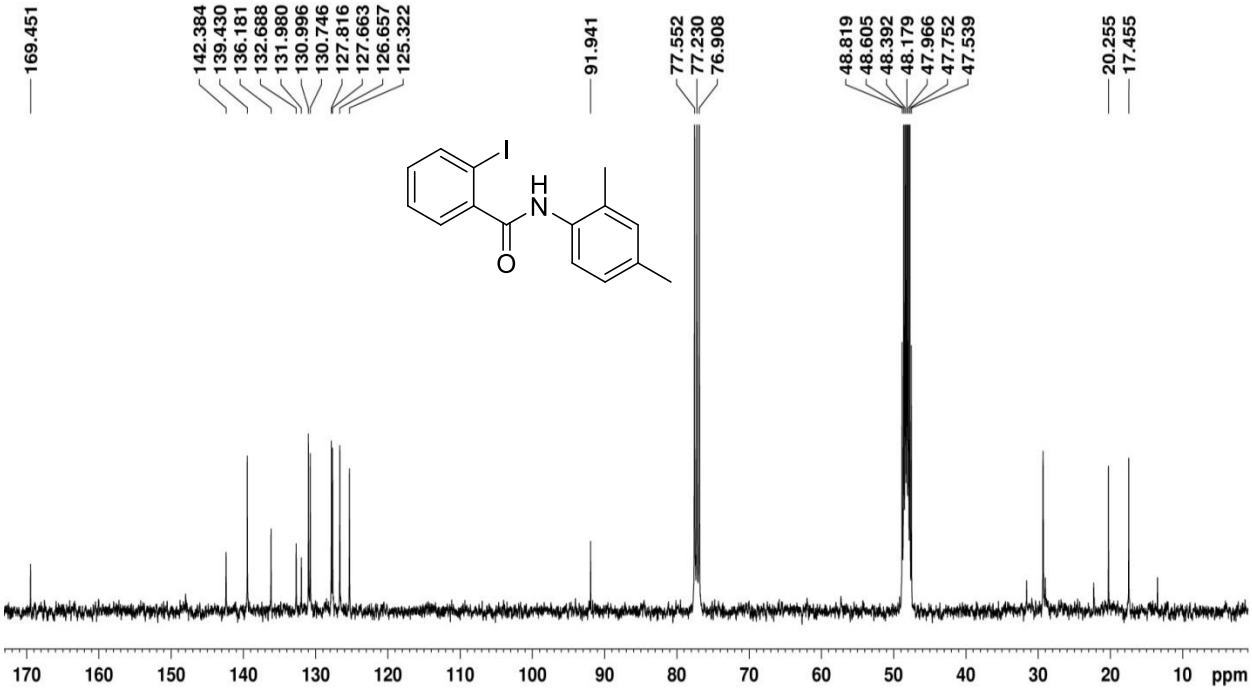
^{13}C NMR Spectrum of*N-(3,4-dimethylphenyl)-2-iodobenzamide* (S1c) (75 MHz, $CDCl_3$)



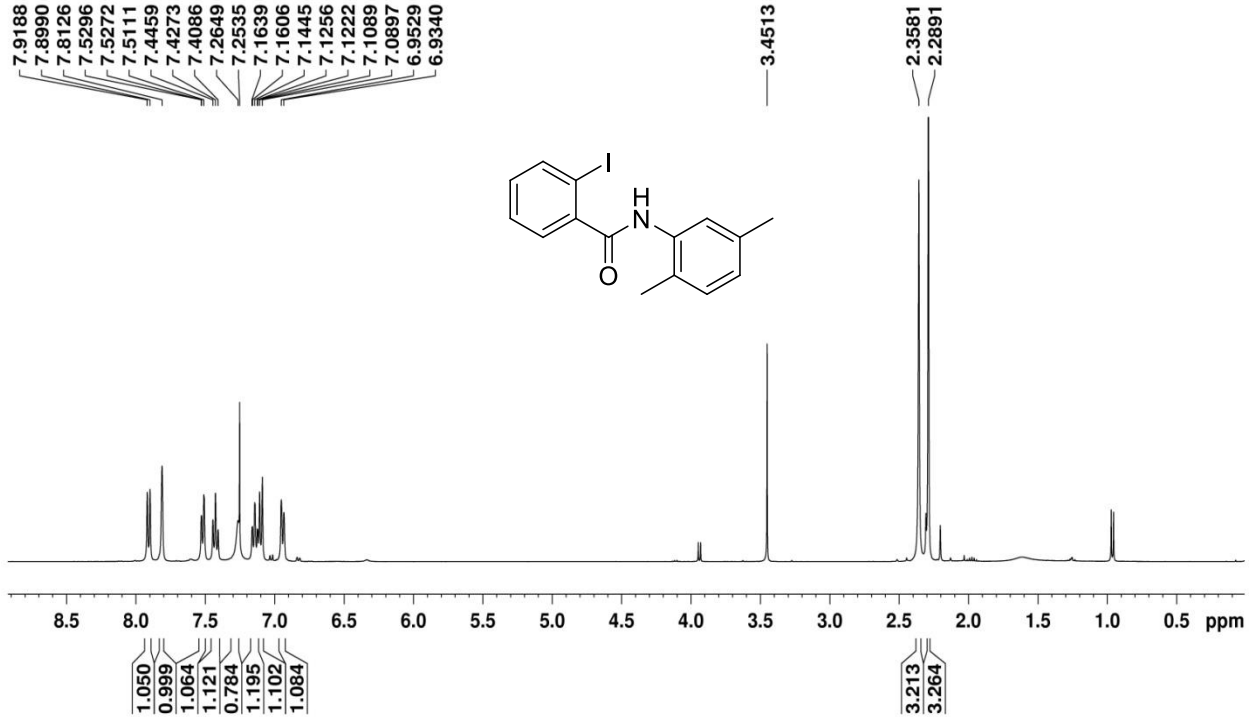
^{1}H NMR Spectrum of*N-(2,4-dimethylphenyl)-2-iodobenzamide* (S1d) (400 MHz, $CDCl_3$)



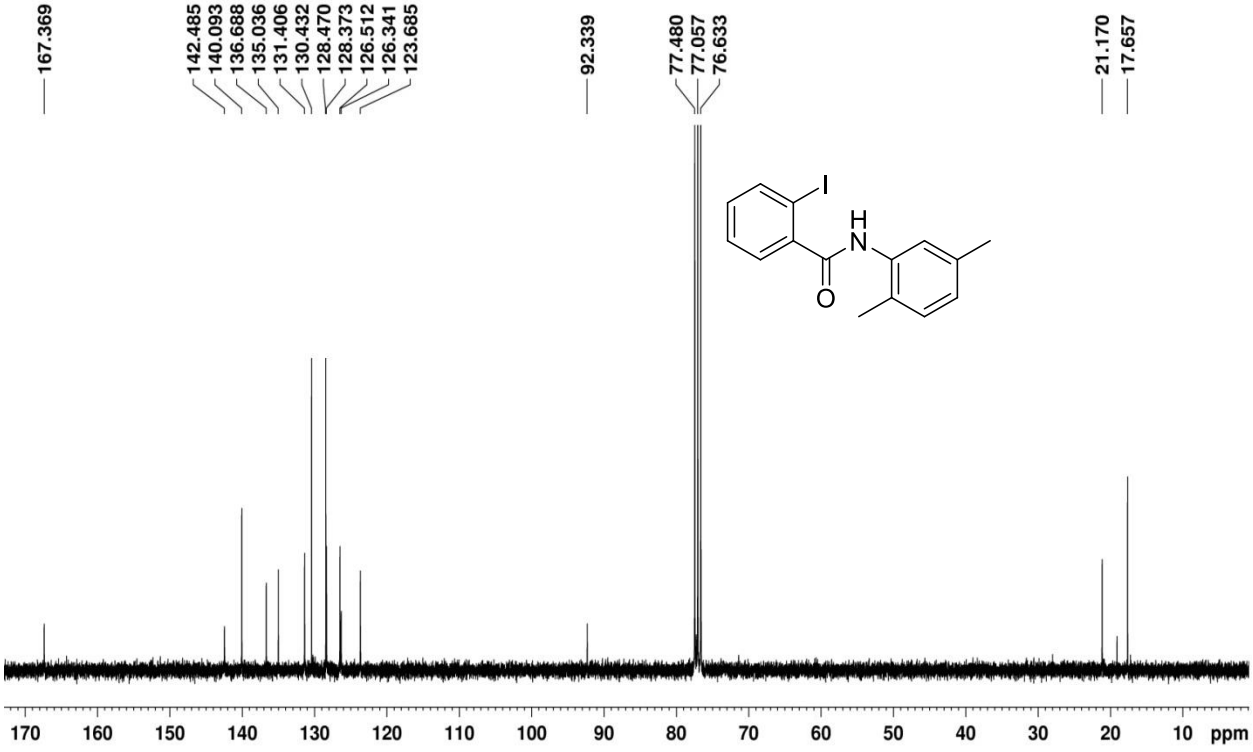
^{13}C NMR Spectrum of *N-(2,4-dimethylphenyl)-2-iodobenzamide* (S1d) (100 MHz, $CDCl_3$ + CD_3OD)



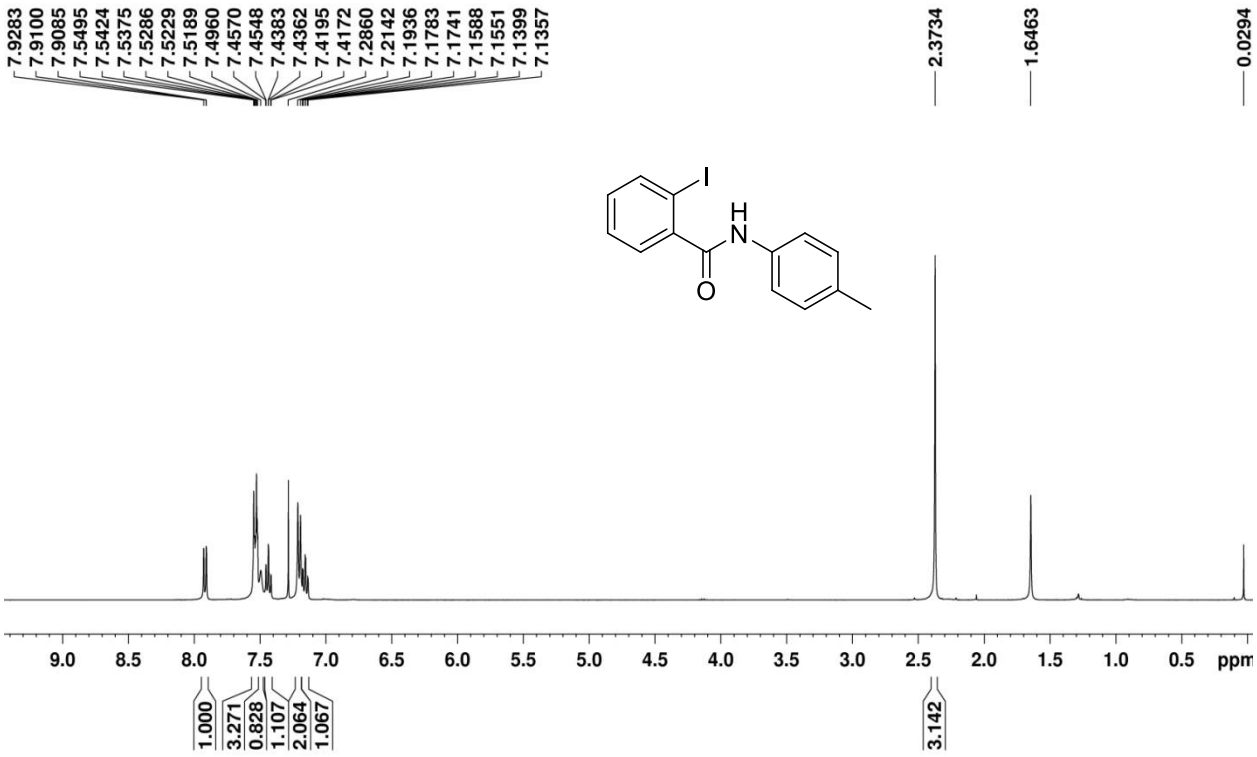
^{1}H NMR Spectrum of *N-(2,5-dimethylphenyl)-2-iodobenzamide* (S1e) (400 MHz, $CDCl_3$)



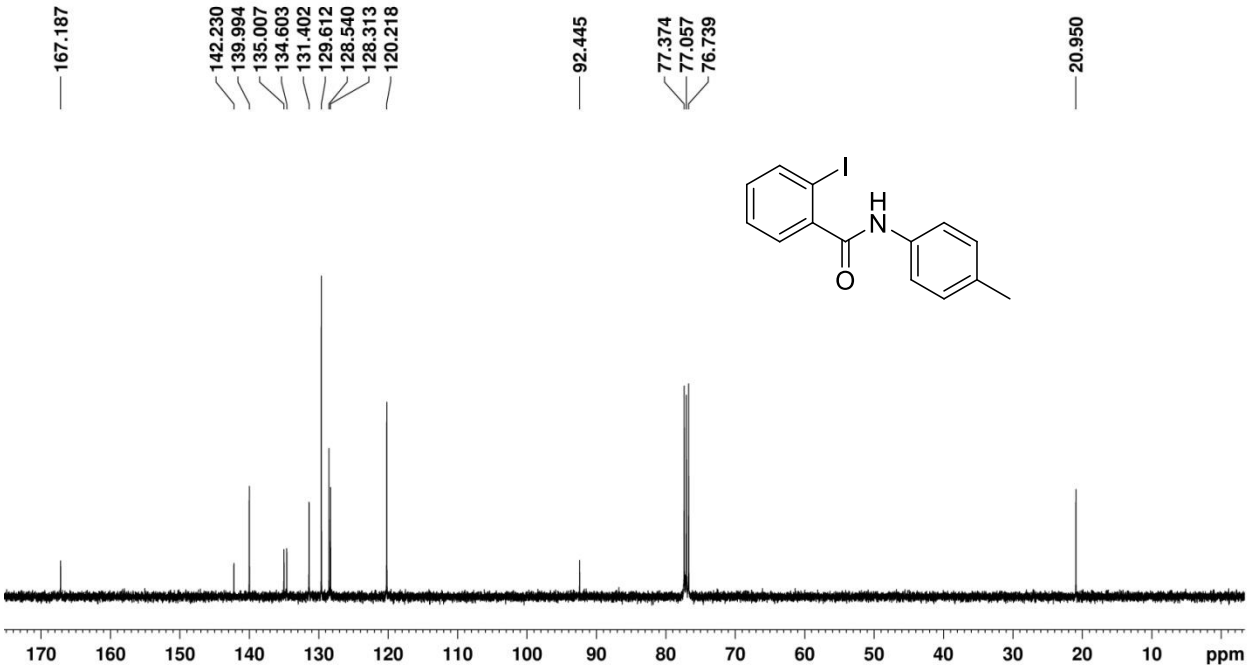
^{13}C NMR Spectrum of *N-(2,5-dimethylphenyl)-2-iodobenzamide* (S1e) (75 MHz, $CDCl_3$)



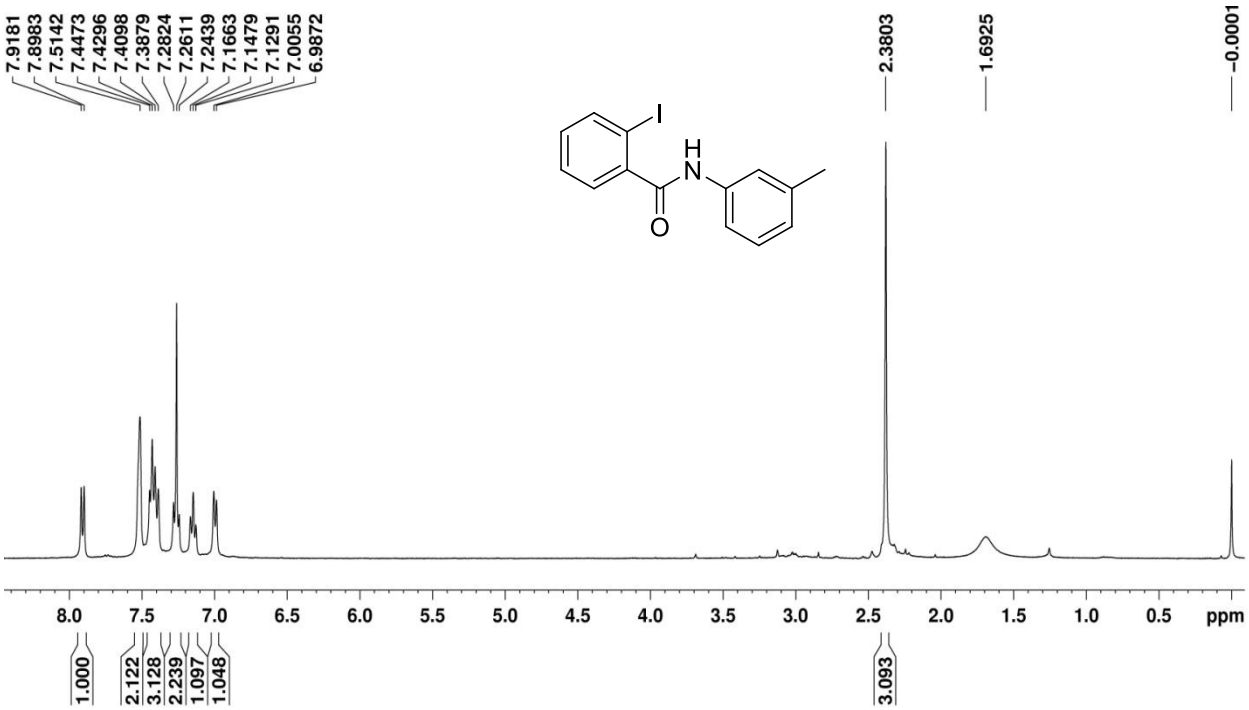
^{1}H NMR Spectrum of *N-(4-methylphenyl)-2-iodobenzamide* (S1f) (400 MHz, $CDCl_3$)



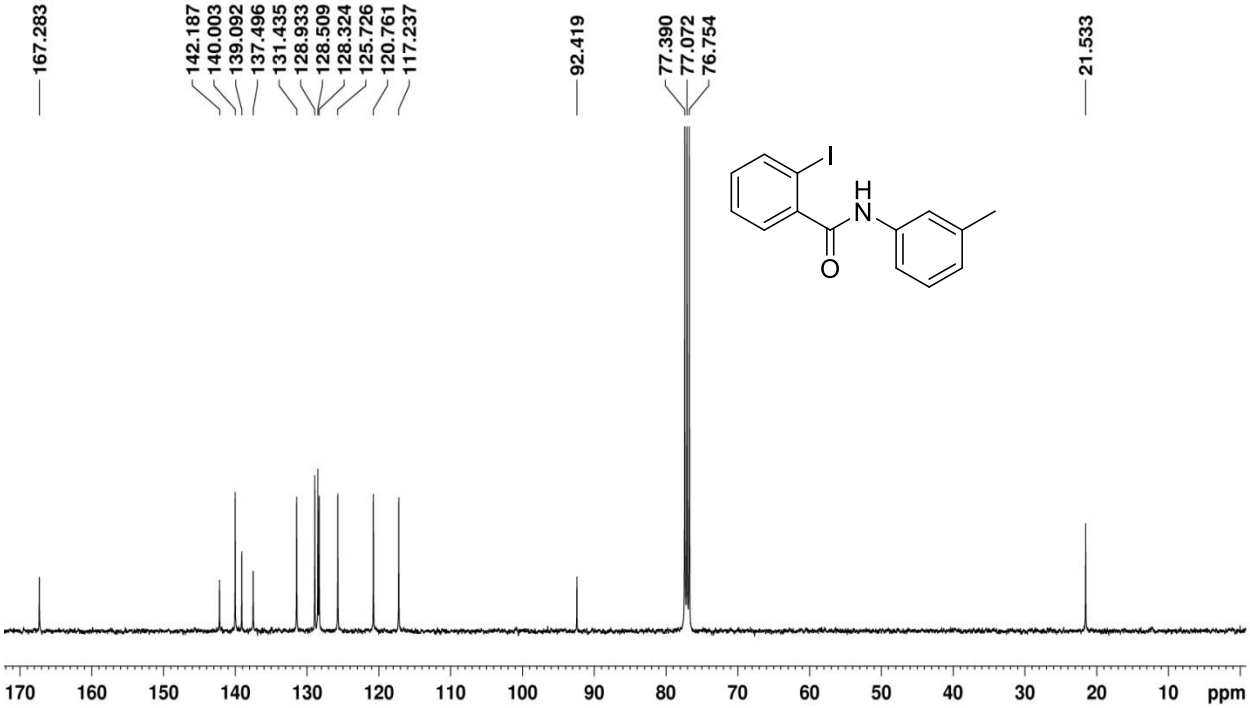
^{13}C NMR Spectrum of*N-(4-methylphenyl)-2-iodobenzamide* (S1f) (100 MHz, $CDCl_3$)



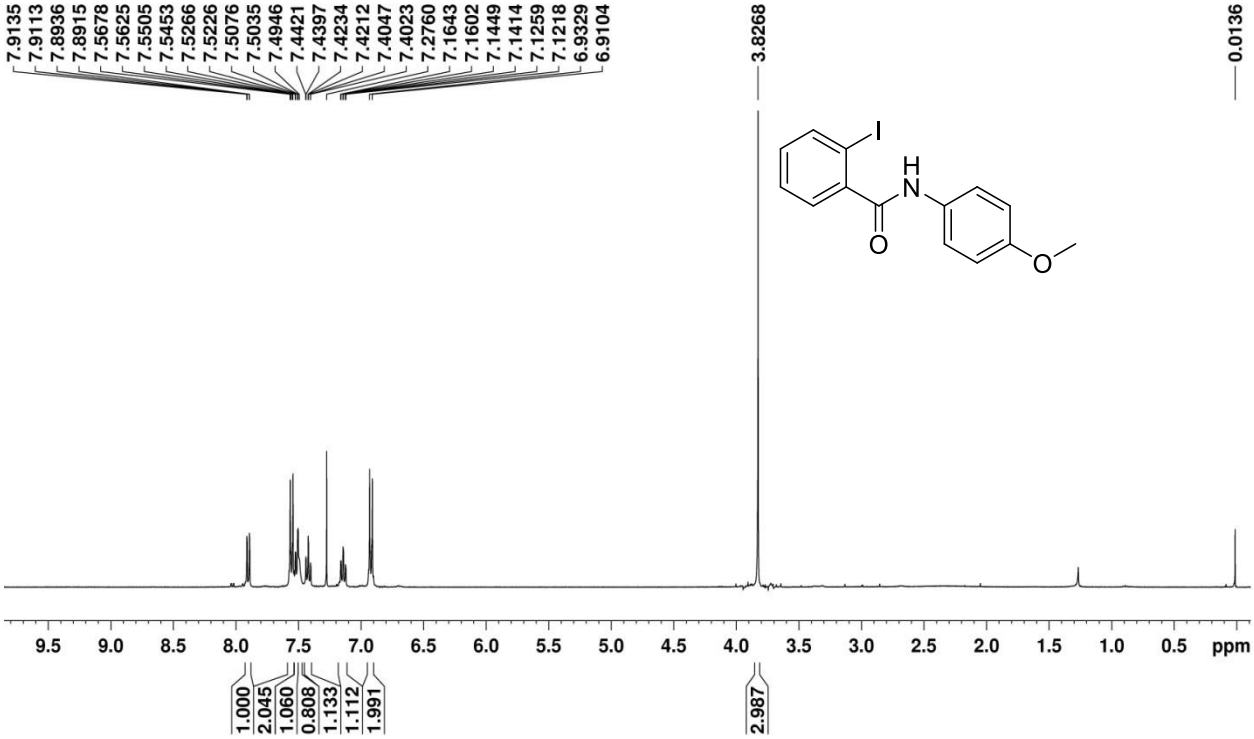
^{1}H NMR Spectrum of*N-(3-methylphenyl)-2-iodobenzamide* (S1g) (400 MHz, $CDCl_3$)



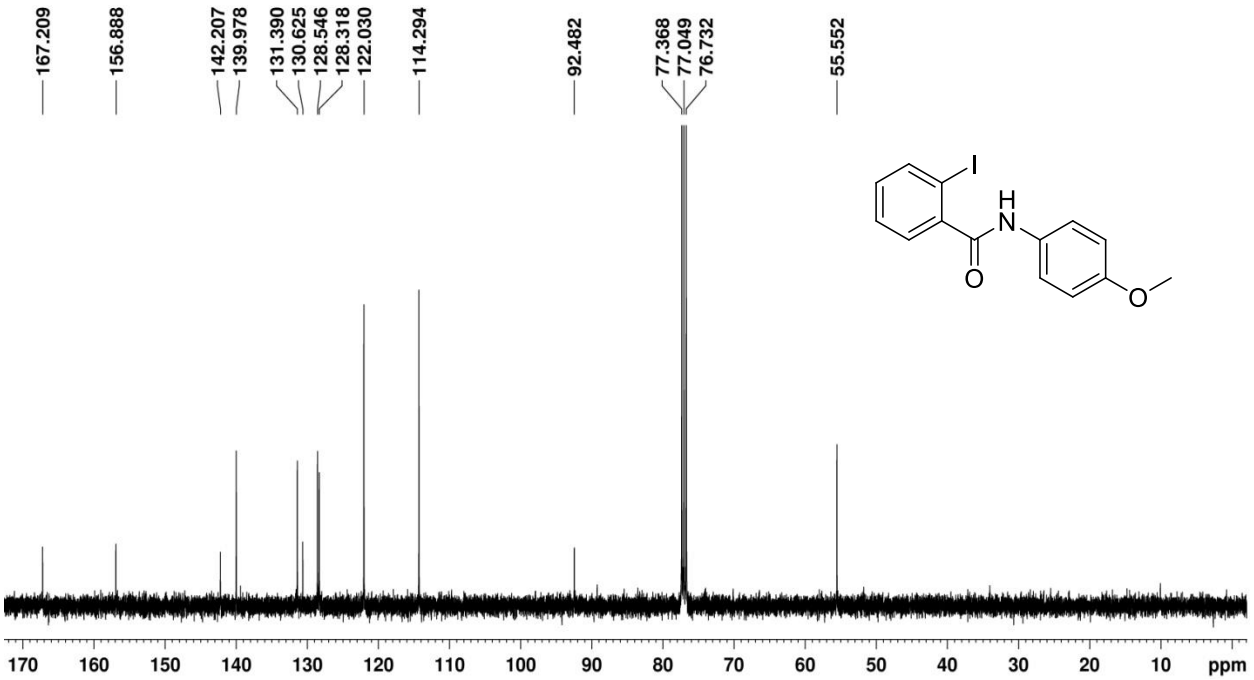
^{13}C NMR Spectrum of*N-(3-methylphenyl)-2-iodobenzamide* (S1g) (100 MHz, $CDCl_3$)



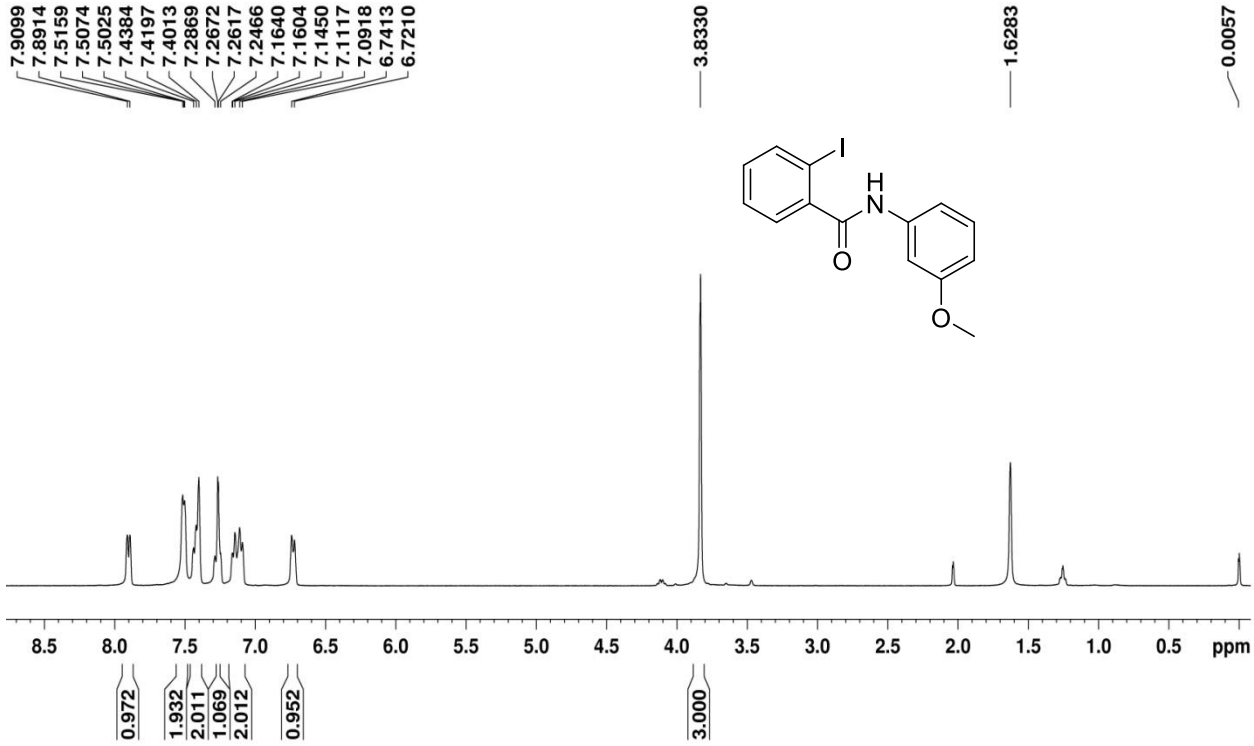
^{1}H NMR Spectrum of*N-(4-methoxyphenyl)-2-iodobenzamide* (S1h)(400 MHz, $CDCl_3$)



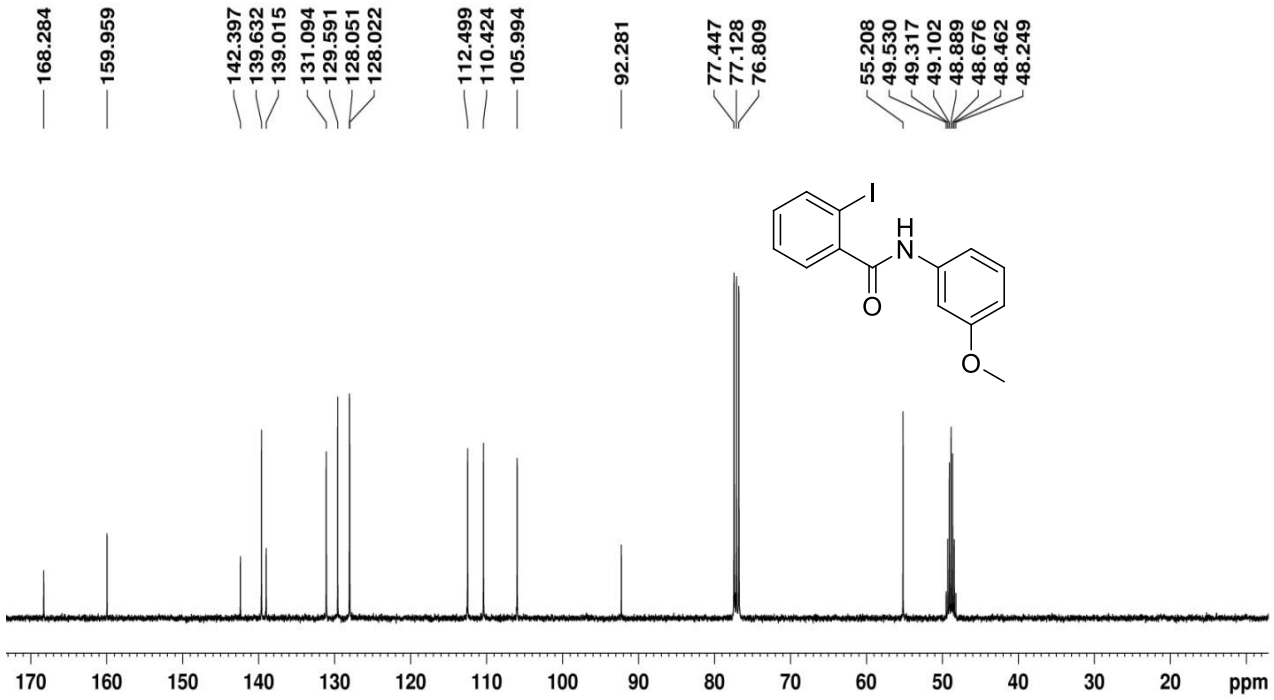
^{13}C NMR Spectrum of*N-(4-methoxyphenyl)-2-iodobenzamide* (S1h)(100 MHz, $CDCl_3$)



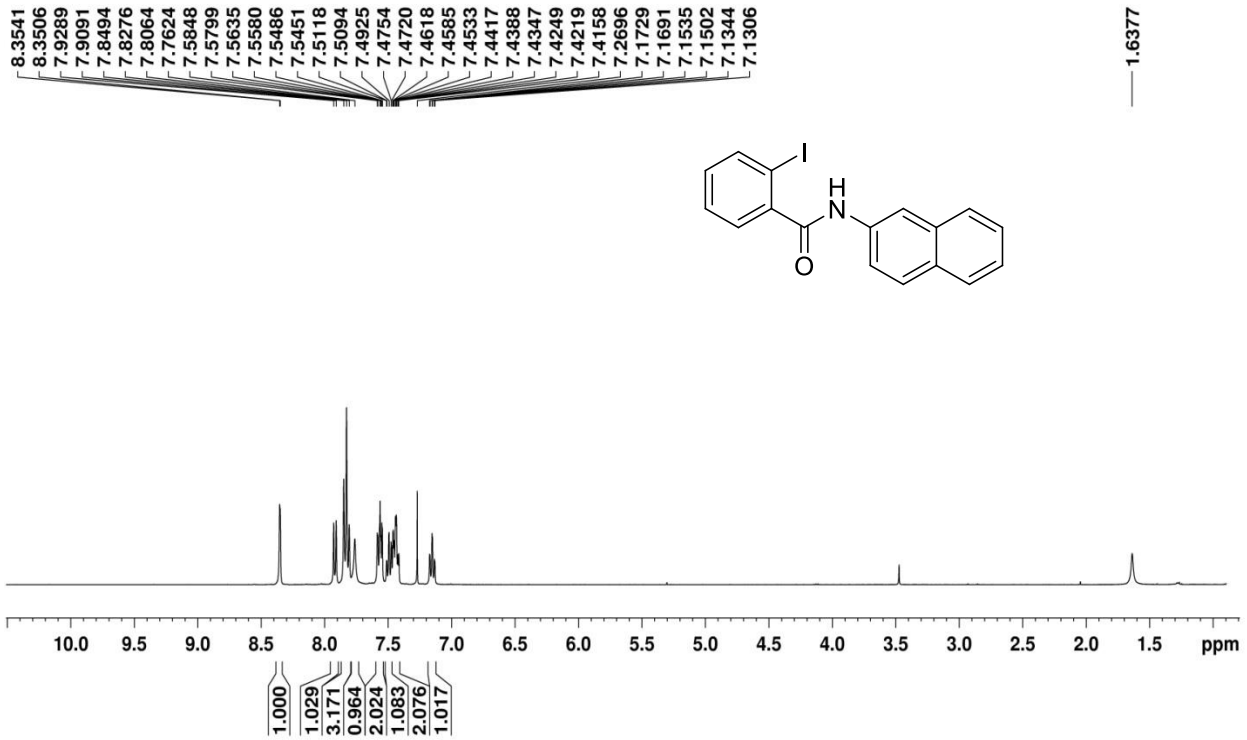
^{1}H NMR Spectrum of*N-(3-methoxyphenyl)-2-iodobenzamide* (S1i) (400 MHz, $CDCl_3$)



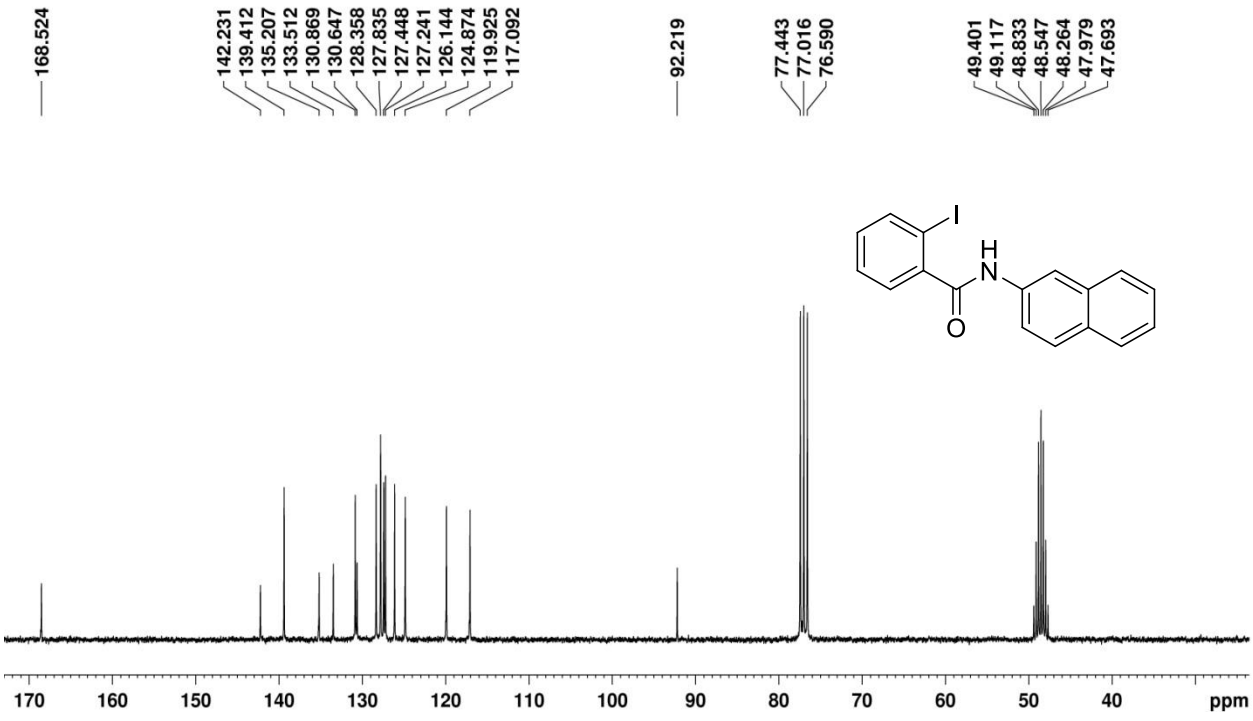
^{13}C NMR Spectrum of*N-(3-methoxyphenyl)-2-iodobenzamide* (S1i) (100 MHz, $CDCl_3$ + CD_3OD)



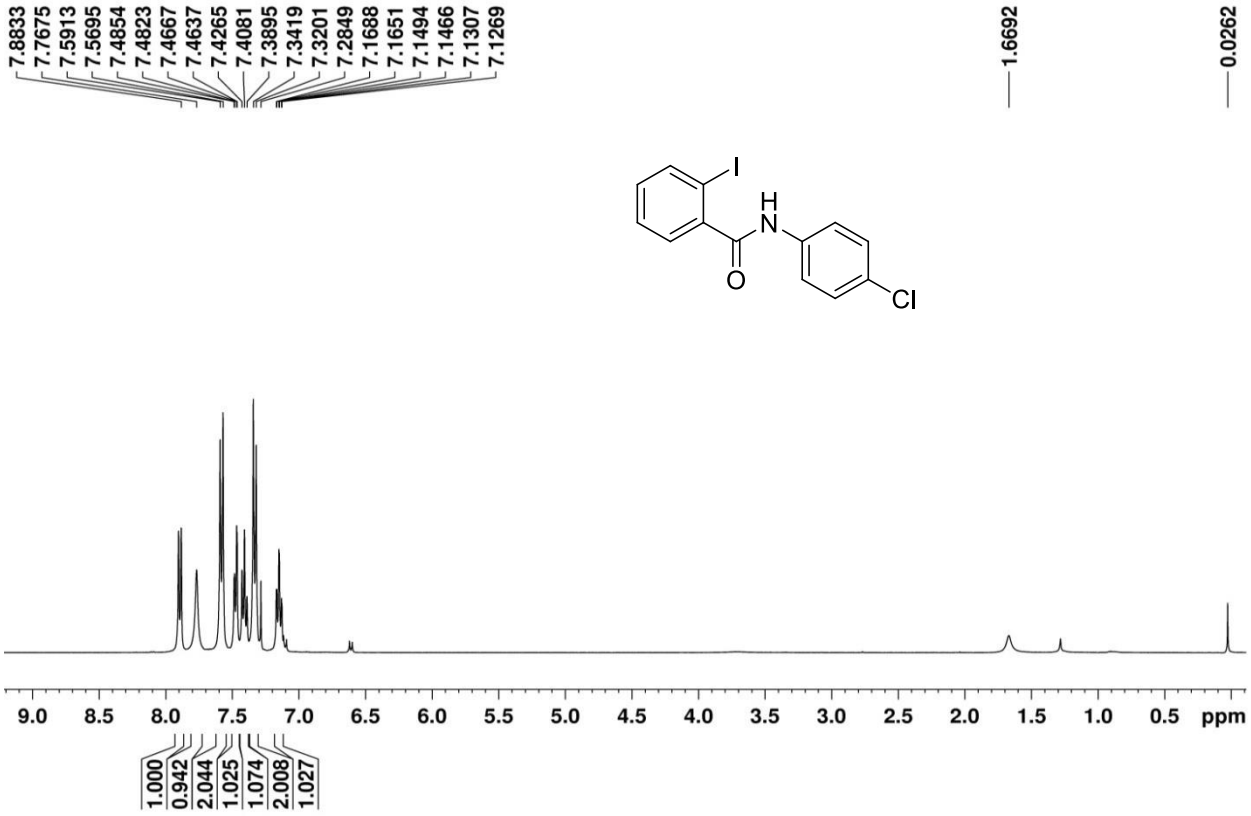
^{1}H NMR Spectrum of*N-(naphthalen-2-yl)-2-iodobenzamide* (S1j) (400 MHz, $CDCl_3$)



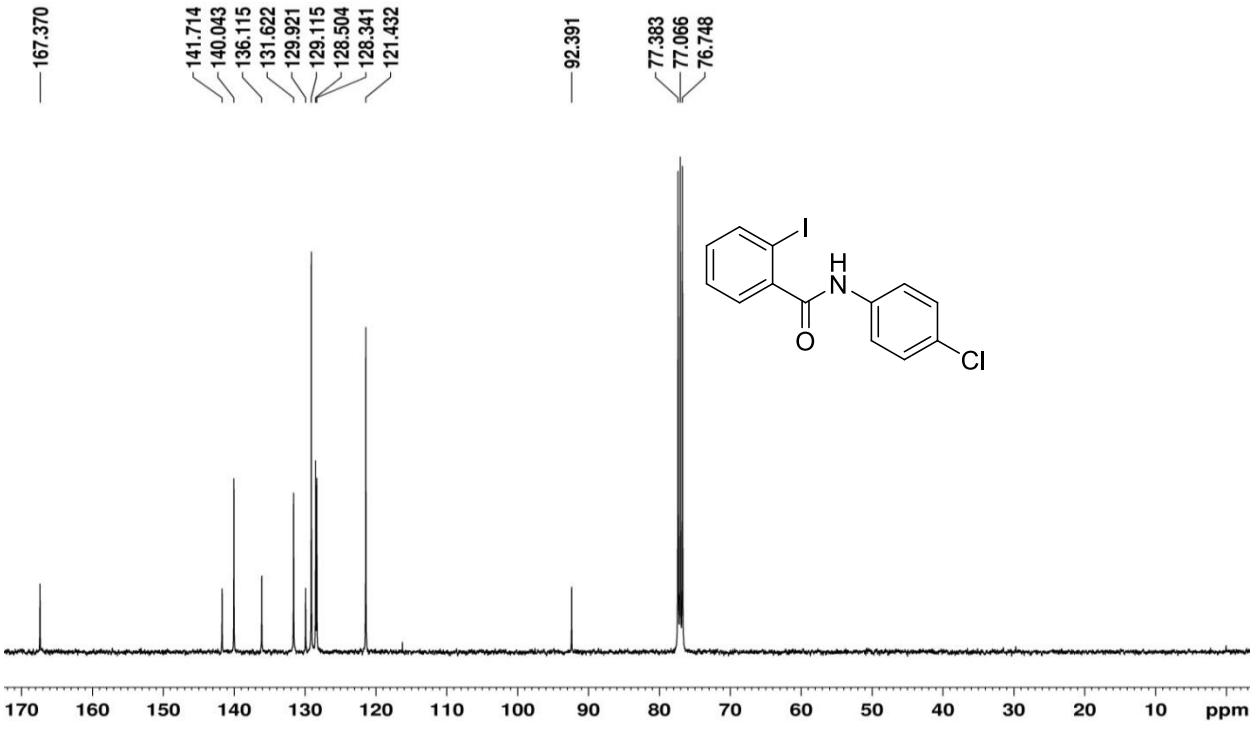
^{13}C NMR Spectrum of *N-(naphthalen-2-yl)-2-iodobenzamide* (S1j) (75 MHz, $CDCl_3$ + CD_3OD)



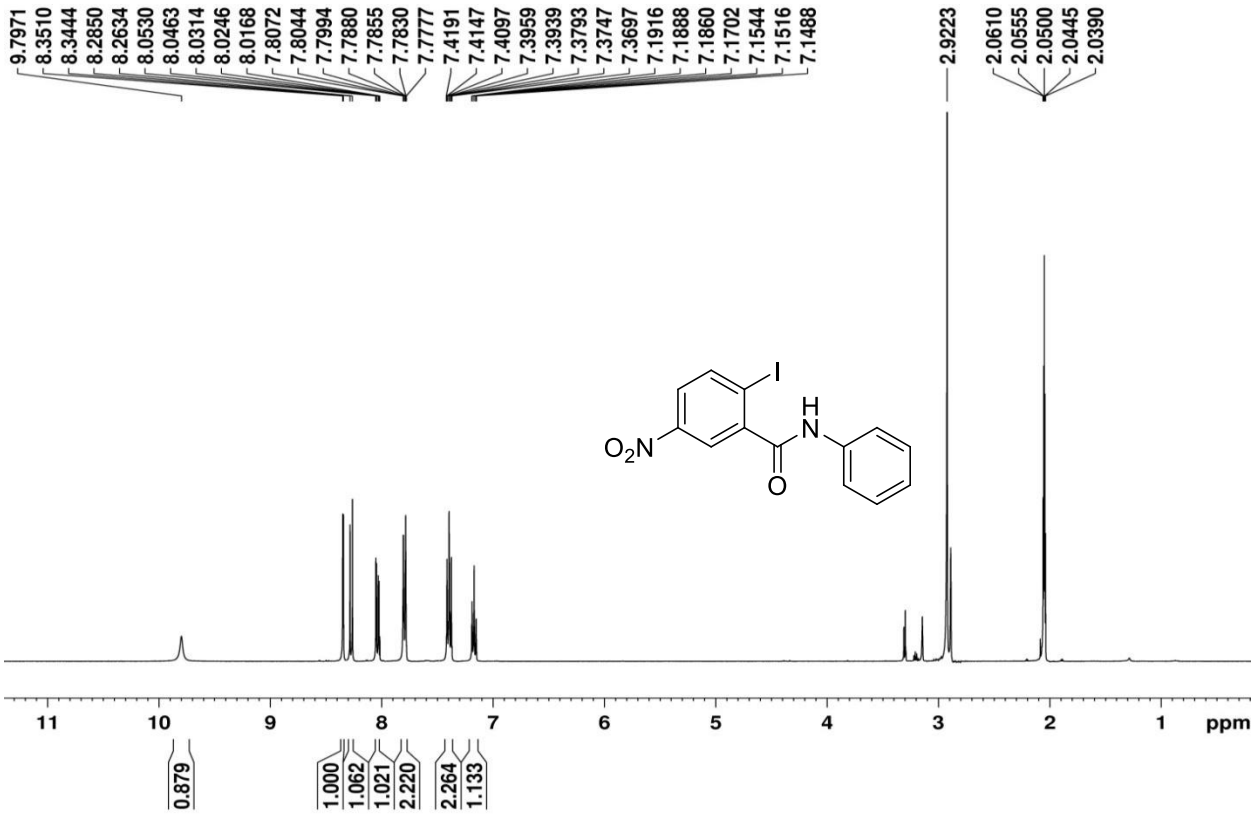
^{1}H NMR Spectrum of*N-(4-chlorophenyl)-2-iodobenzamide* (S1k)(400 MHz, $CDCl_3$)



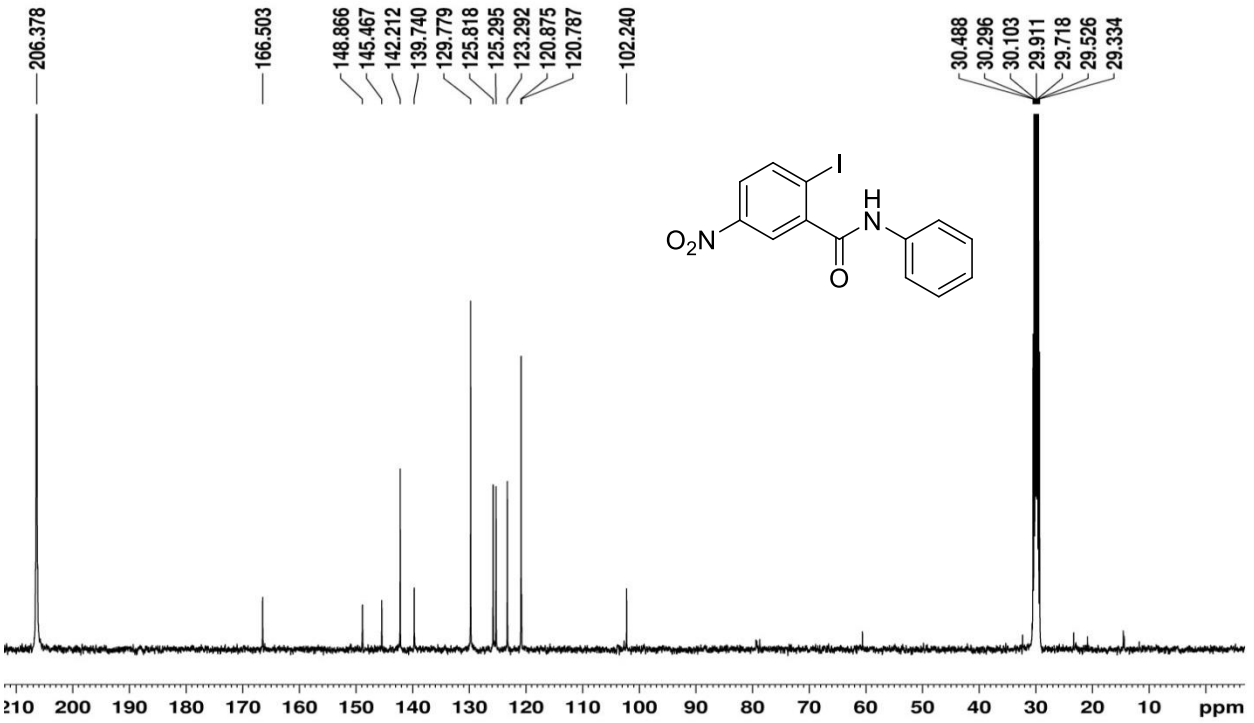
^{13}C NMR Spectrum of*N-(4-chlorophenyl)-2-iodobenzamide* (S1k) (100 MHz, $CDCl_3$)



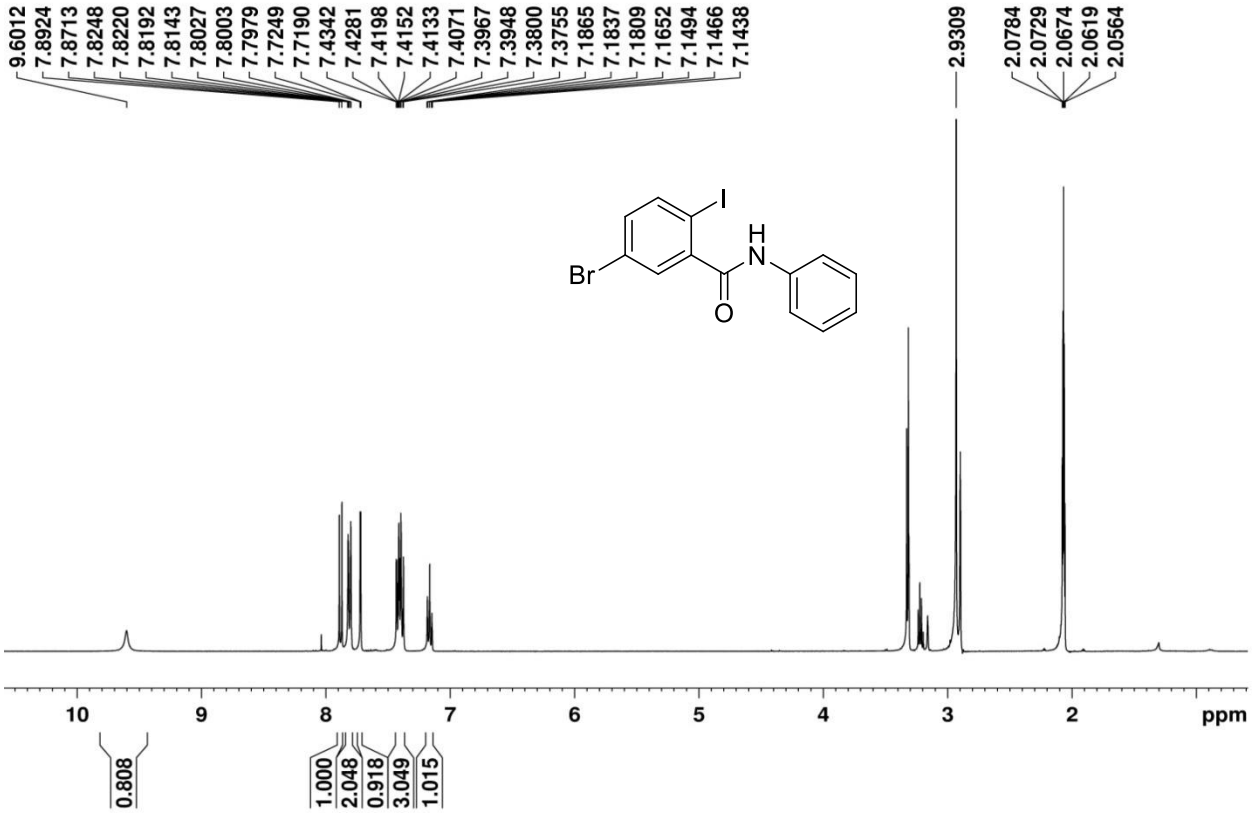
^{1}H NMR Spectrum of*2-iodo-5-nitro-N-phenylbenzamide* (S1l) (400 MHz, Acetone-d_6)



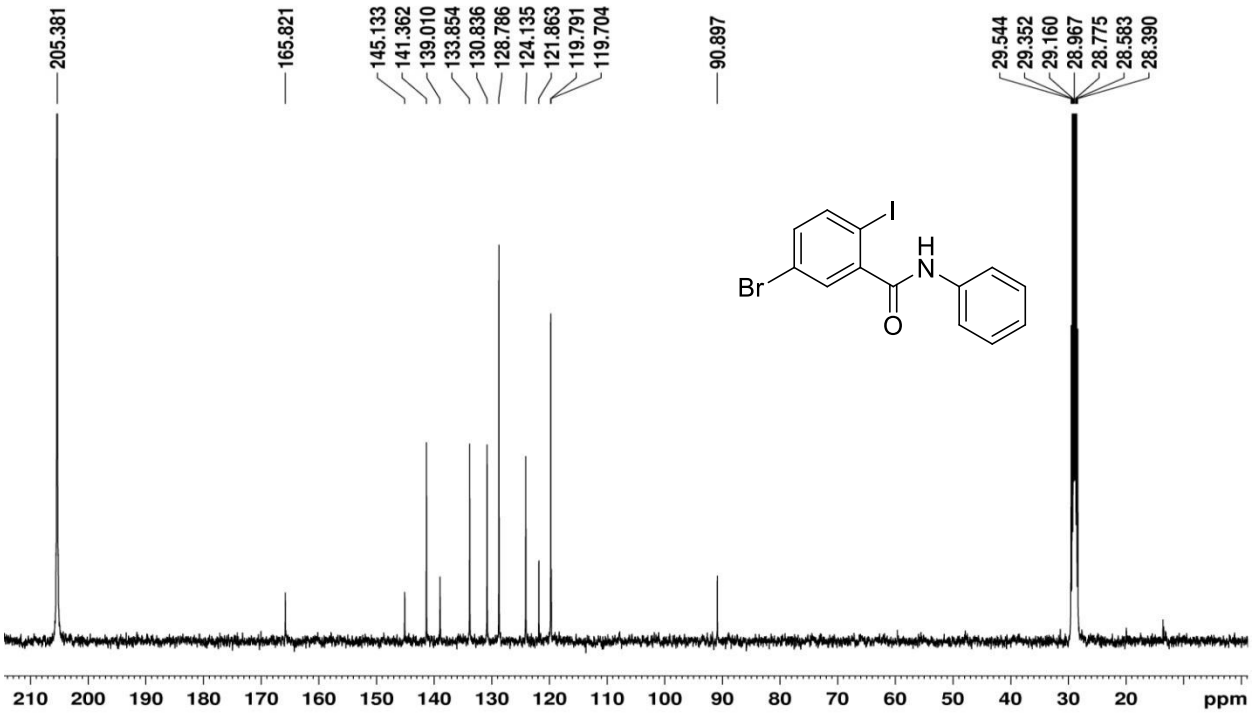
^{13}C NMR Spectrum of*2-iodo-5-nitro-N-phenylbenzamide* (S1l) (100 MHz, Acetone-d_6)



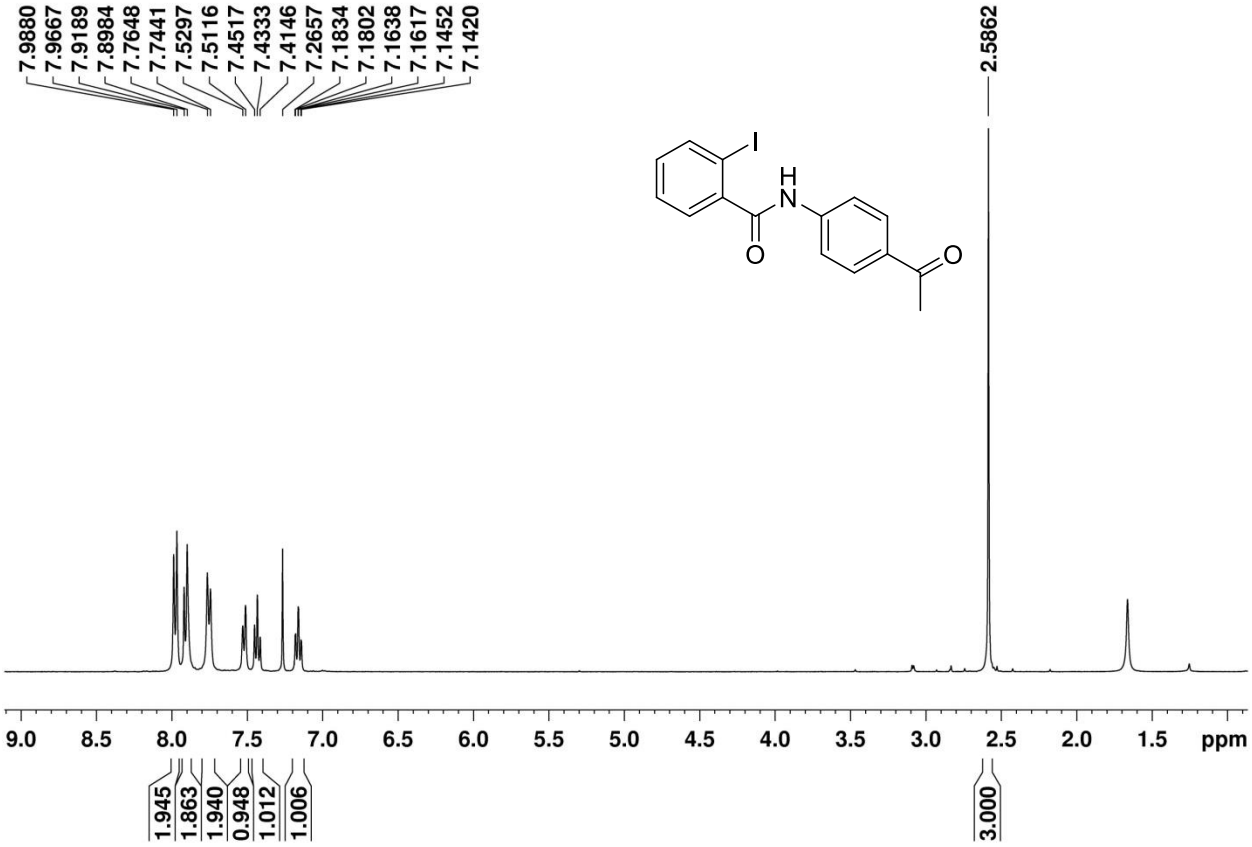
^{1}H NMR Spectrum of*5-bromo-2-iodo-N-phenylbenzamide* (S1m) (400 MHz, Acetone-d_6)



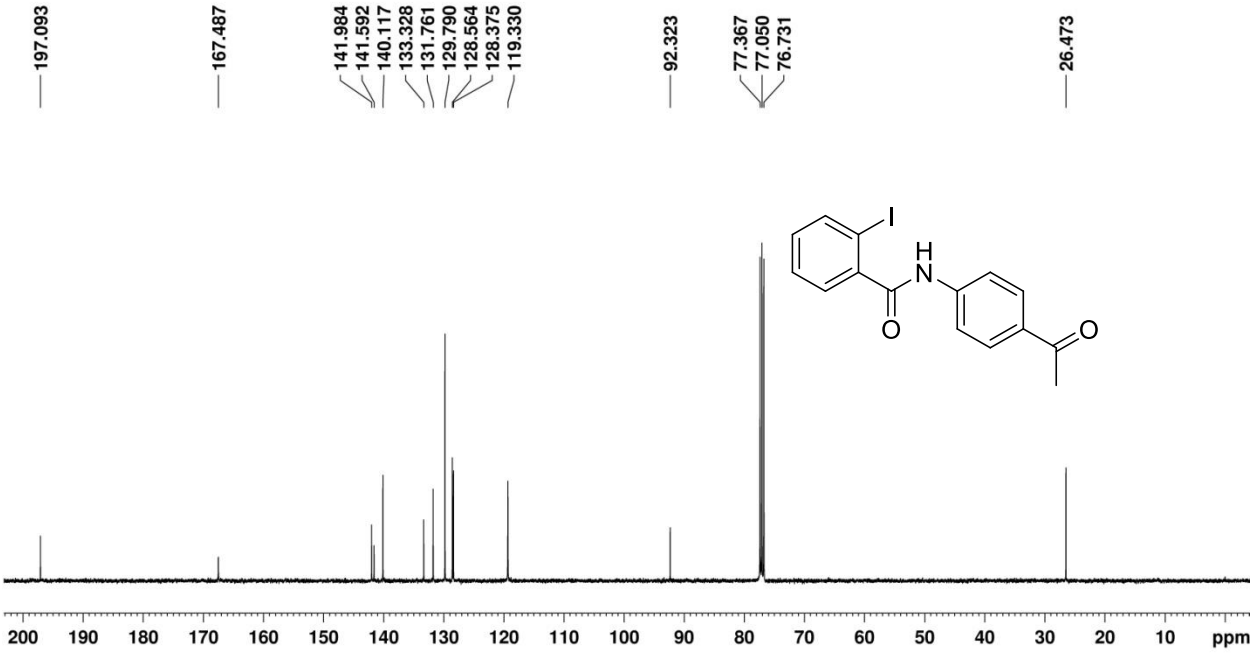
^{13}C NMR Spectrum of*5-bromo-2-iodo-N-phenylbenzamide* (S1m) (100 MHz, Acetone-d_6)



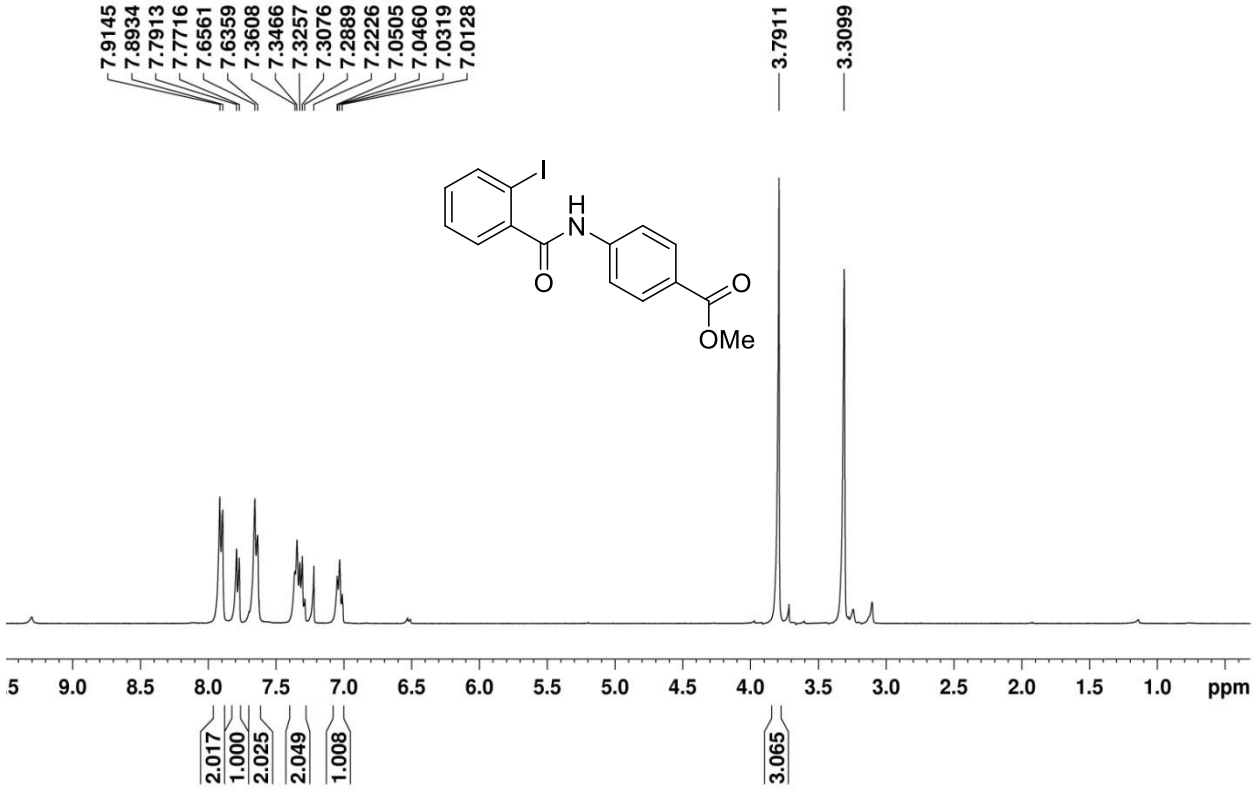
^{1}H NMR Spectrum of*N-(4-acetylphenyl)-2-iodobenzamide* (S1n) (400 MHz, $CDCl_3$)



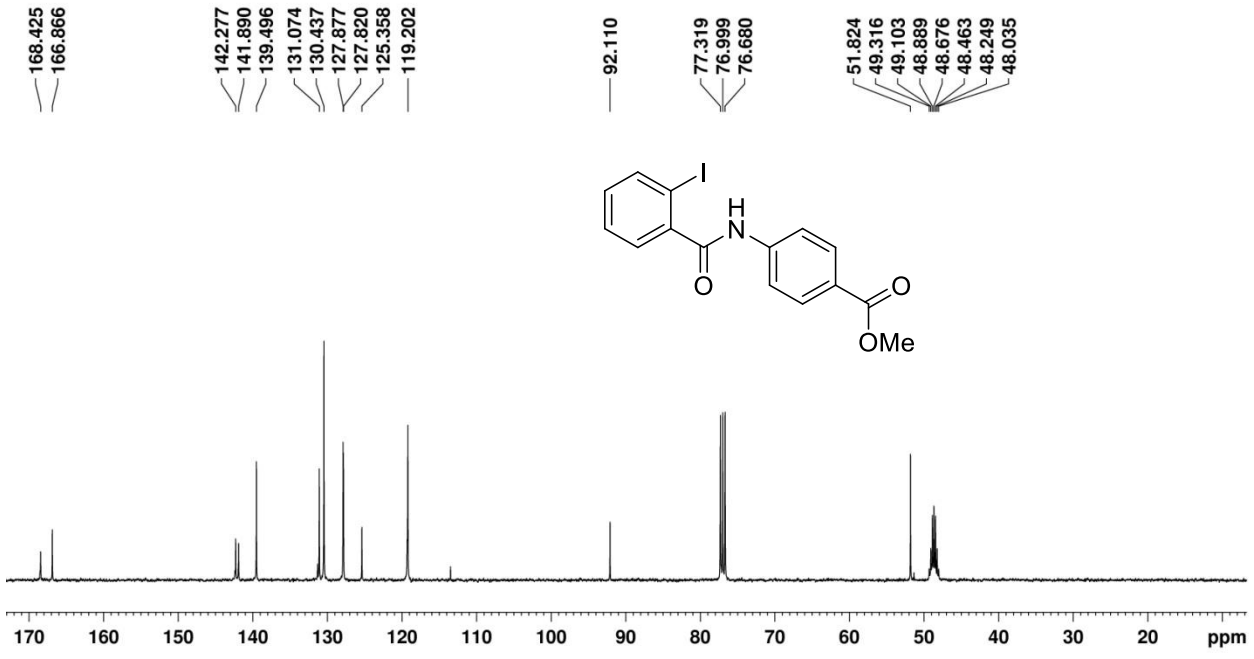
^{13}C NMR Spectrum of*N-(4-acetylphenyl)-2-iodobenzamide* (S1n) (100 MHz, $CDCl_3$)



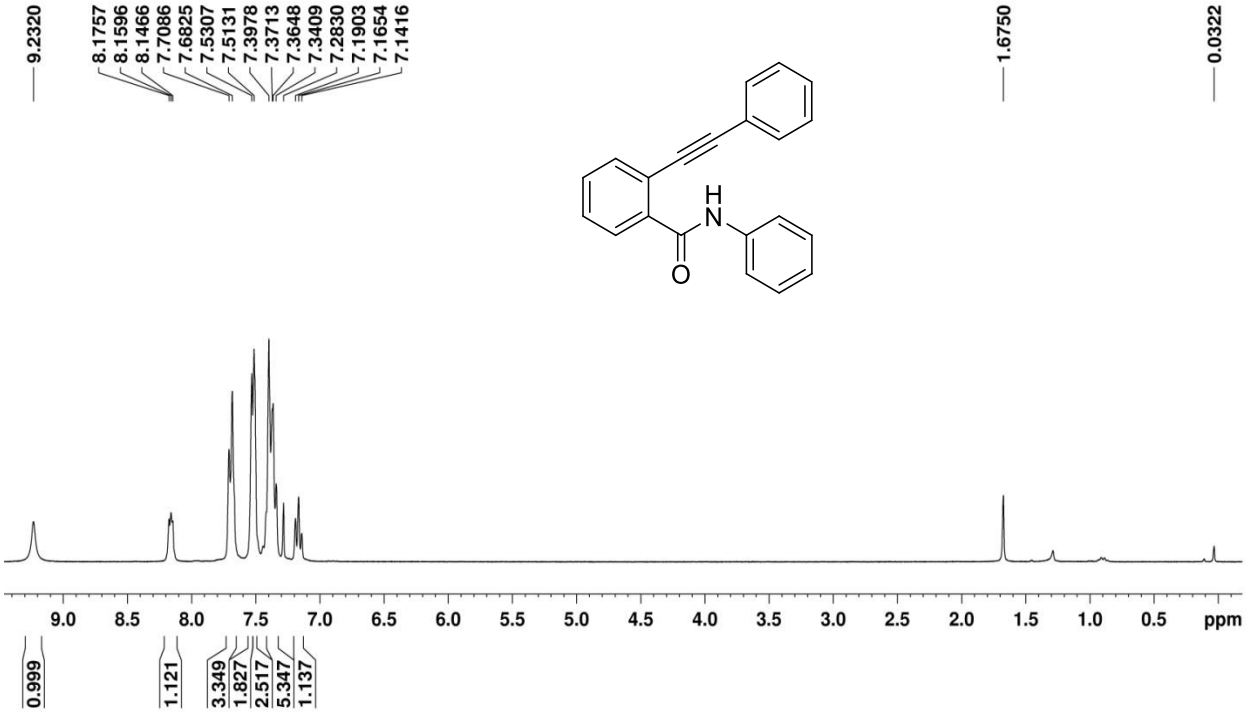
^{1}H NMR Spectrum of *methyl 4-(2-iodobenzamido)benzoate*(S1o) (400 MHz, CD_3OD + $CDCl_3$)



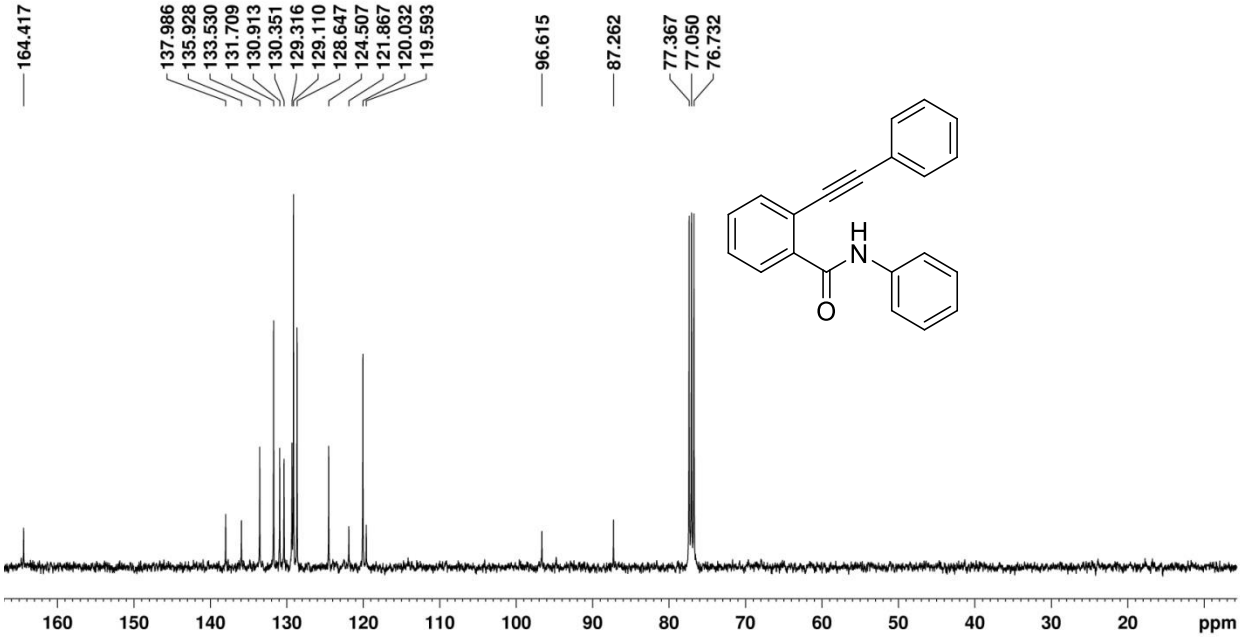
^{13}C NMR Spectrum of *methyl 4-(2-iodobenzamido)benzoate*(S1o) (100 MHz, CD_3OD + $CDCl_3$)



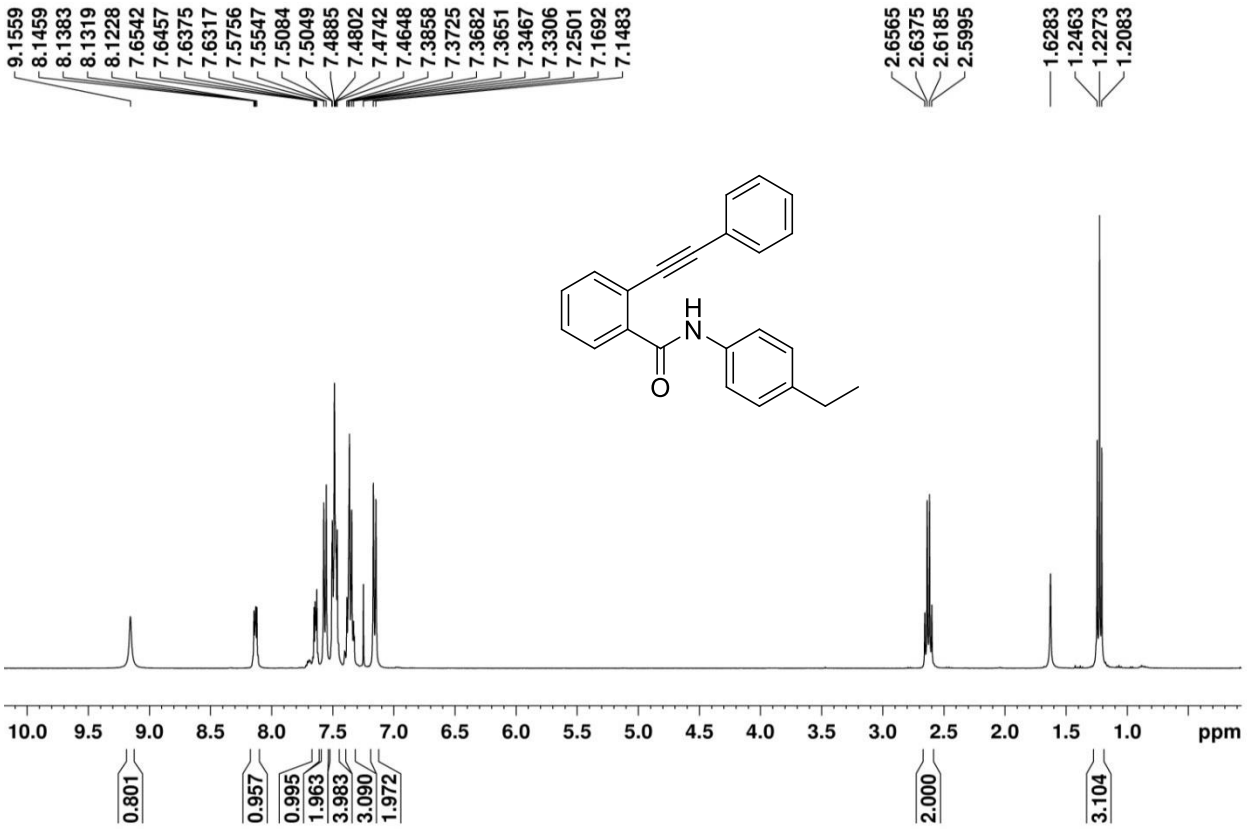
^{1}H NMR Spectrum of*N-phenyl-2-(phenylethynyl)benzamide*(1a) (300 MHz, $CDCl_3$)



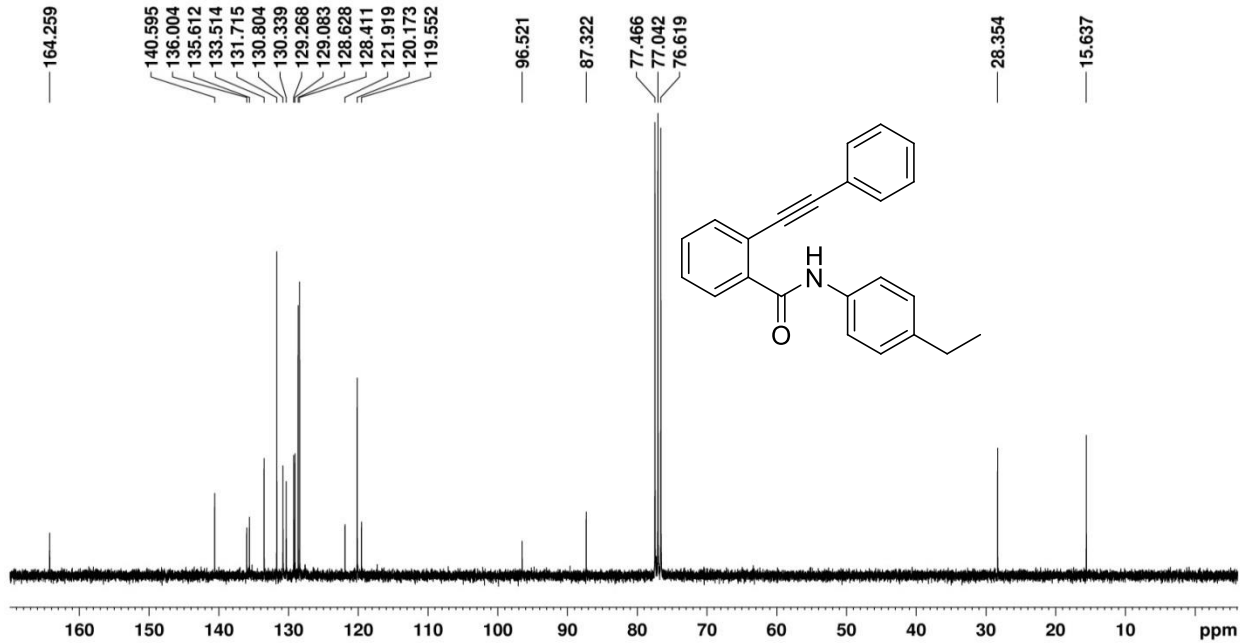
^{13}C NMR Spectrum of*N-phenyl-2-(phenylethynyl)benzamide*(1a) (100 MHz, $CDCl_3$)



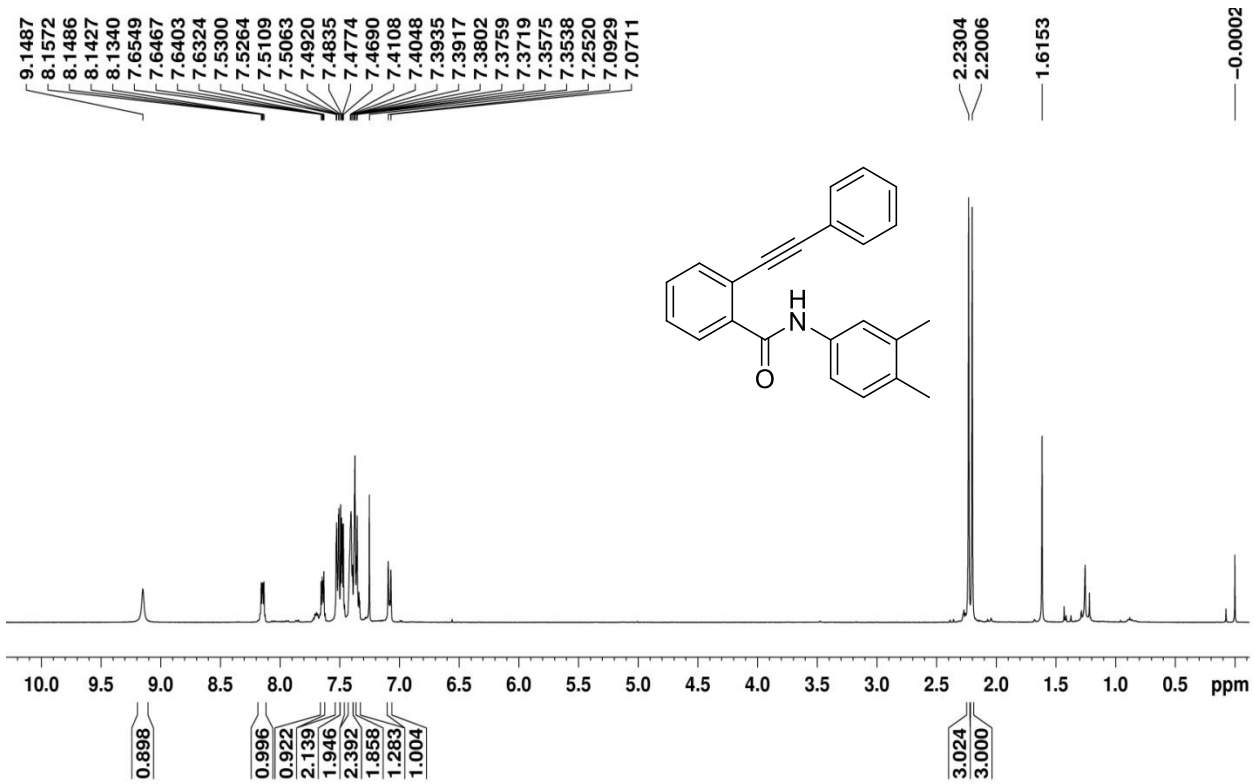
^{1}H NMR Spectrum of*N-(4-ethylphenyl)-2-(phenylethynyl)benzamide*(1b) (400 MHz, $CDCl_3$)



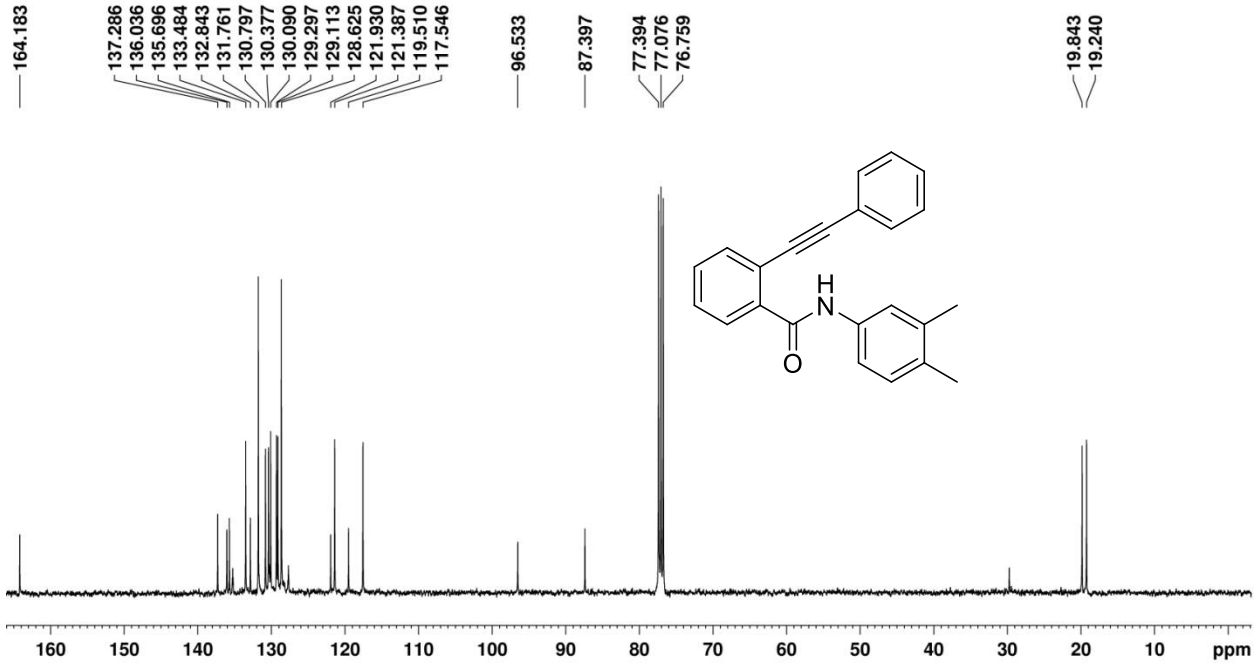
^{13}C NMR Spectrum of*N-(4-ethylphenyl)-2-(phenylethynyl)benzamide*(1b) (100 MHz, $CDCl_3$)



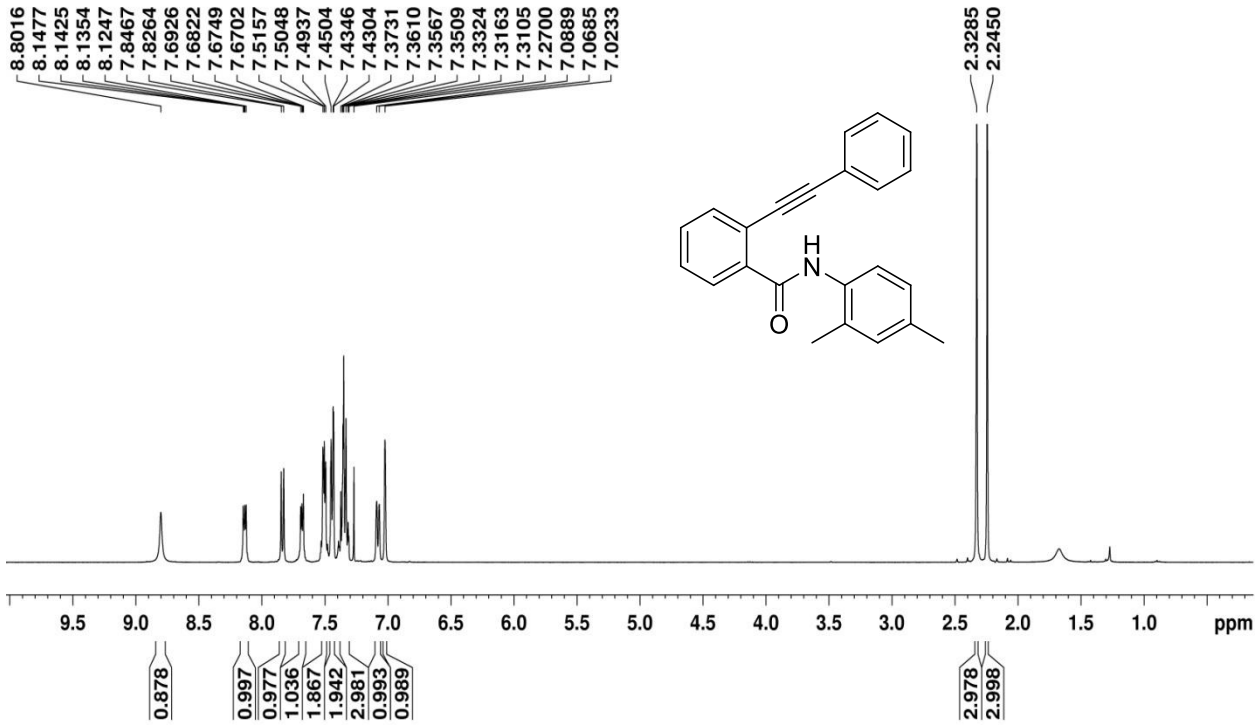
^{1}H NMR Spectrum of*N-(3,4-dimethylphenyl)-2-(phenylethynyl)benzamide*(1c) (400 MHz, $CDCl_3$)



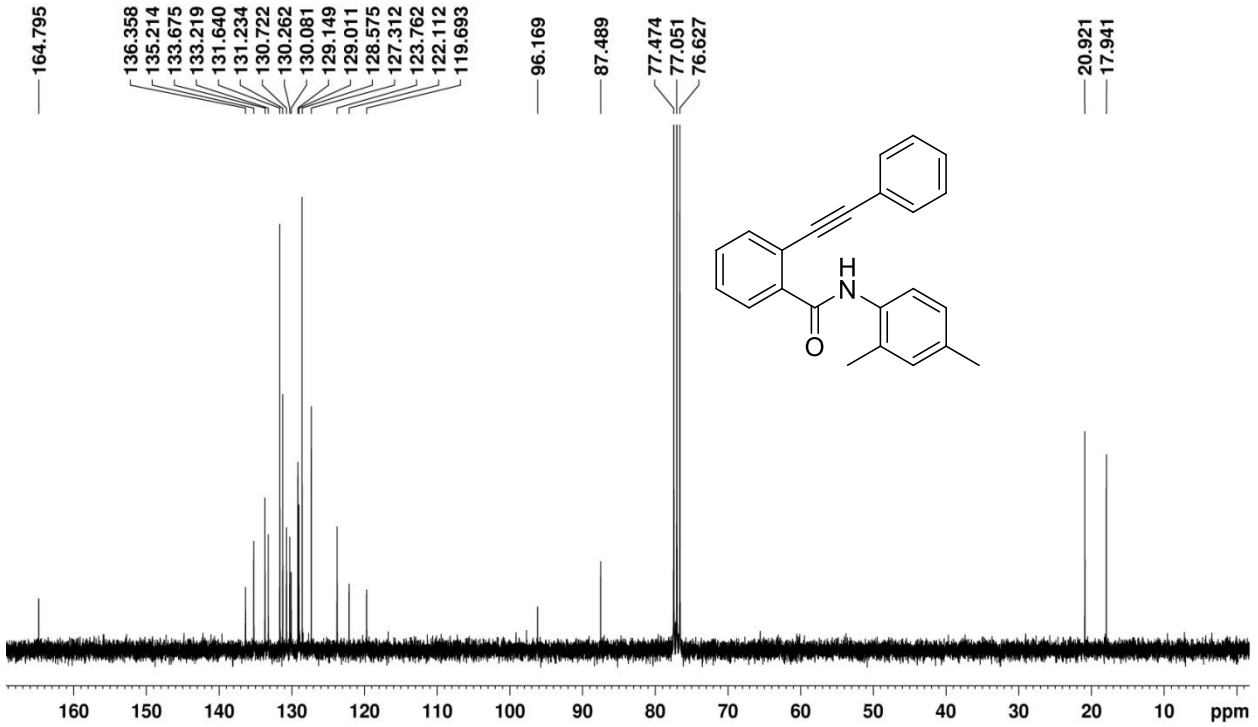
^{13}C NMR Spectrum of *N-(3,4-dimethylphenyl)-2-(phenylethynyl)benzamide*(1c) (100 MHz, $CDCl_3$)



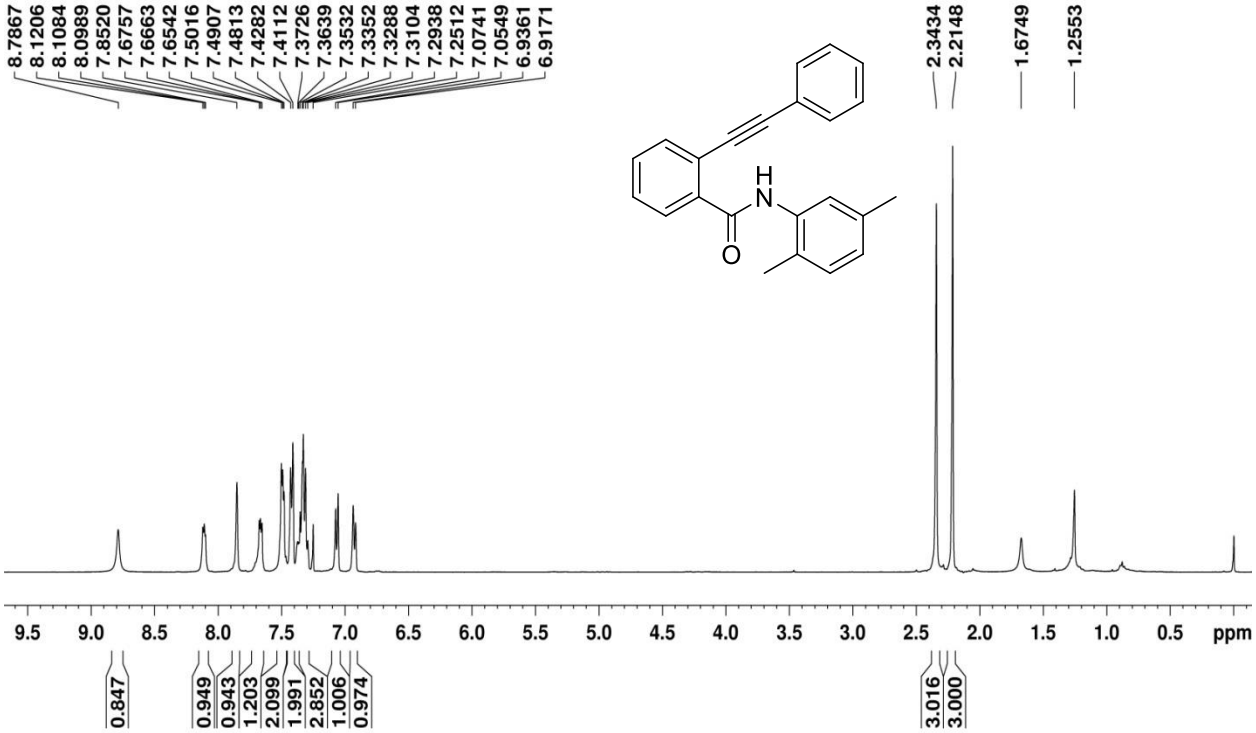
^{1}H NMR Spectrum of*N-(2,4-dimethylphenyl)-2-(phenylethynyl)benzamide*(1d) (400 MHz, $CDCl_3$)



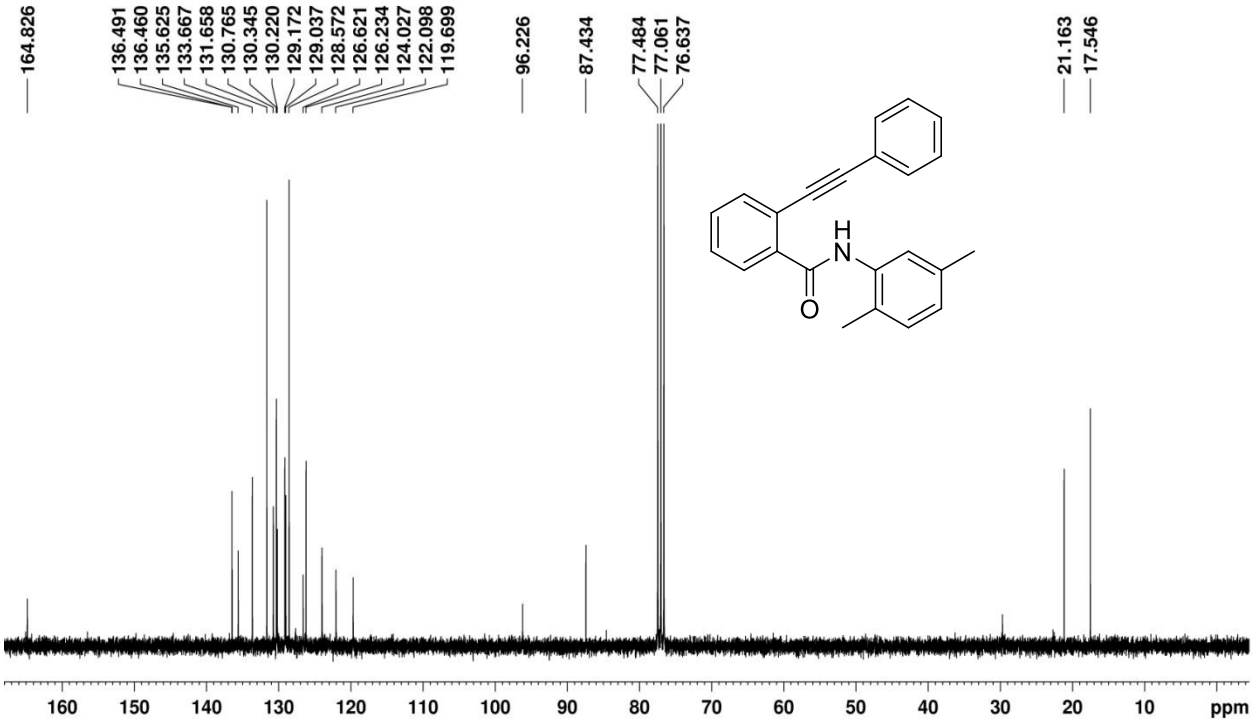
^{13}C NMR Spectrum of*N-(2,4-dimethylphenyl)-2-(phenylethynyl)benzamide*(1d) (100 MHz, $CDCl_3$)



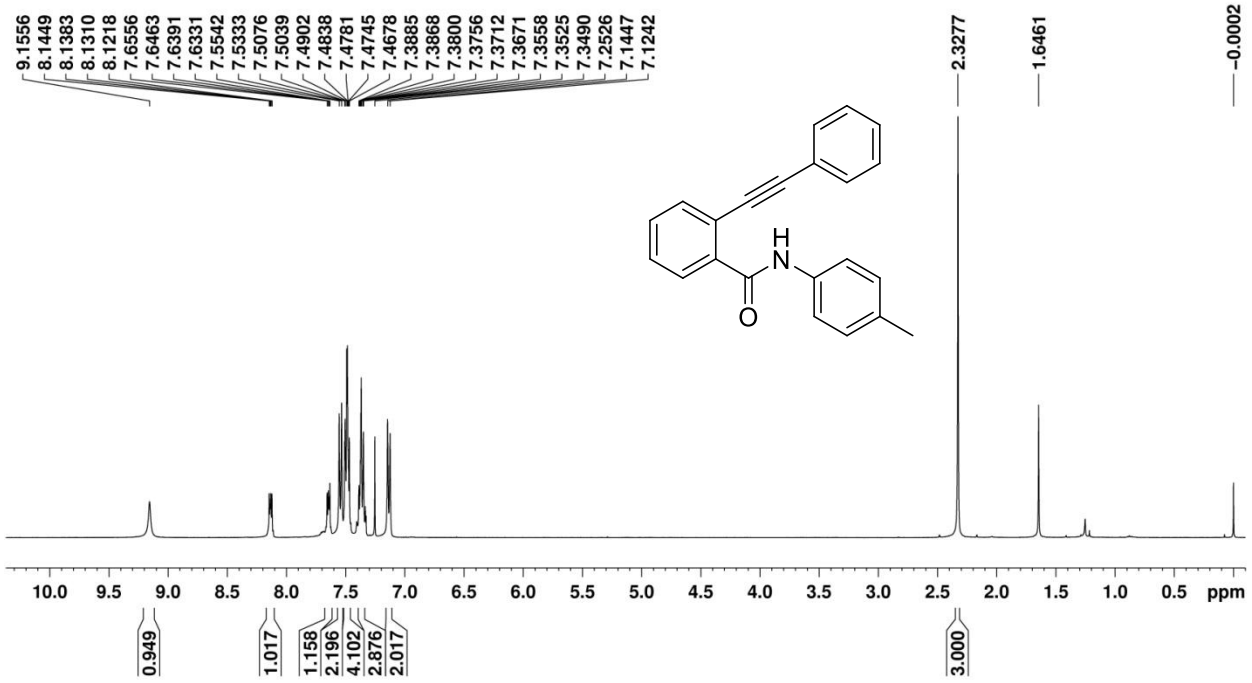
^{1}H NMR Spectrum of *N-(2,5-dimethylphenyl)-2-(phenylethynyl)benzamide*(1e) (400 MHz, $CDCl_3$)



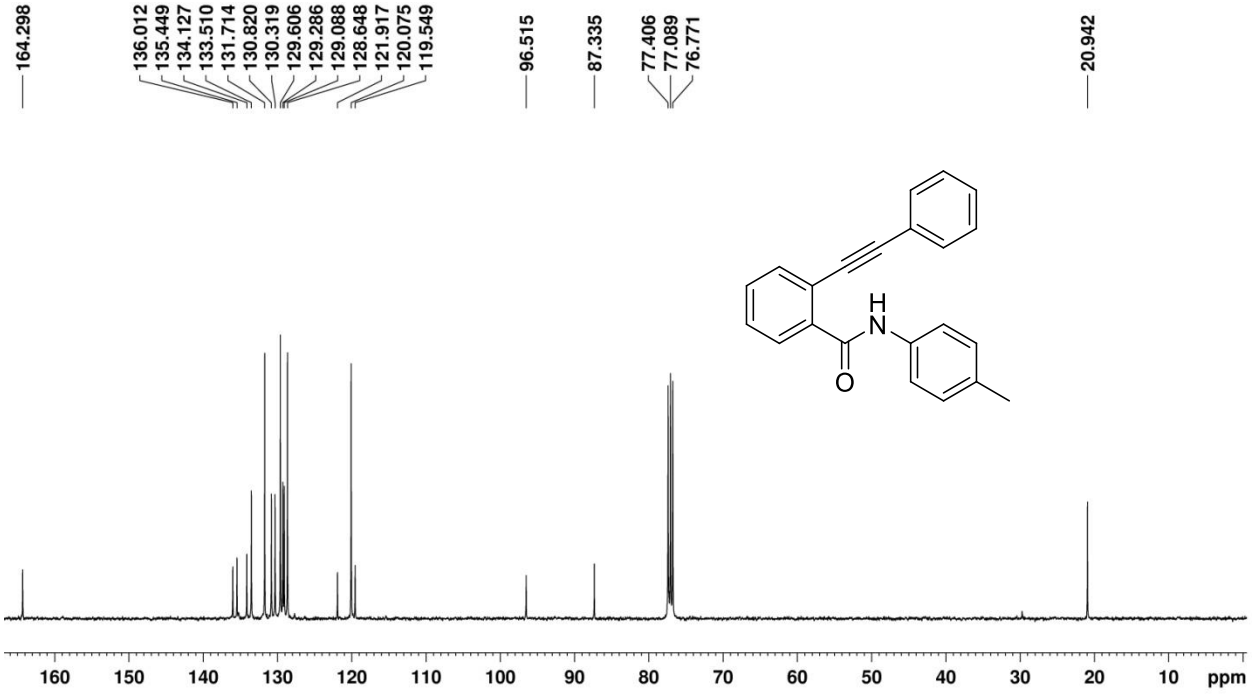
^{13}C NMR Spectrum of *N-(2,5-dimethylphenyl)-2-(phenylethynyl)benzamide*(1e) (100 MHz, $CDCl_3$)



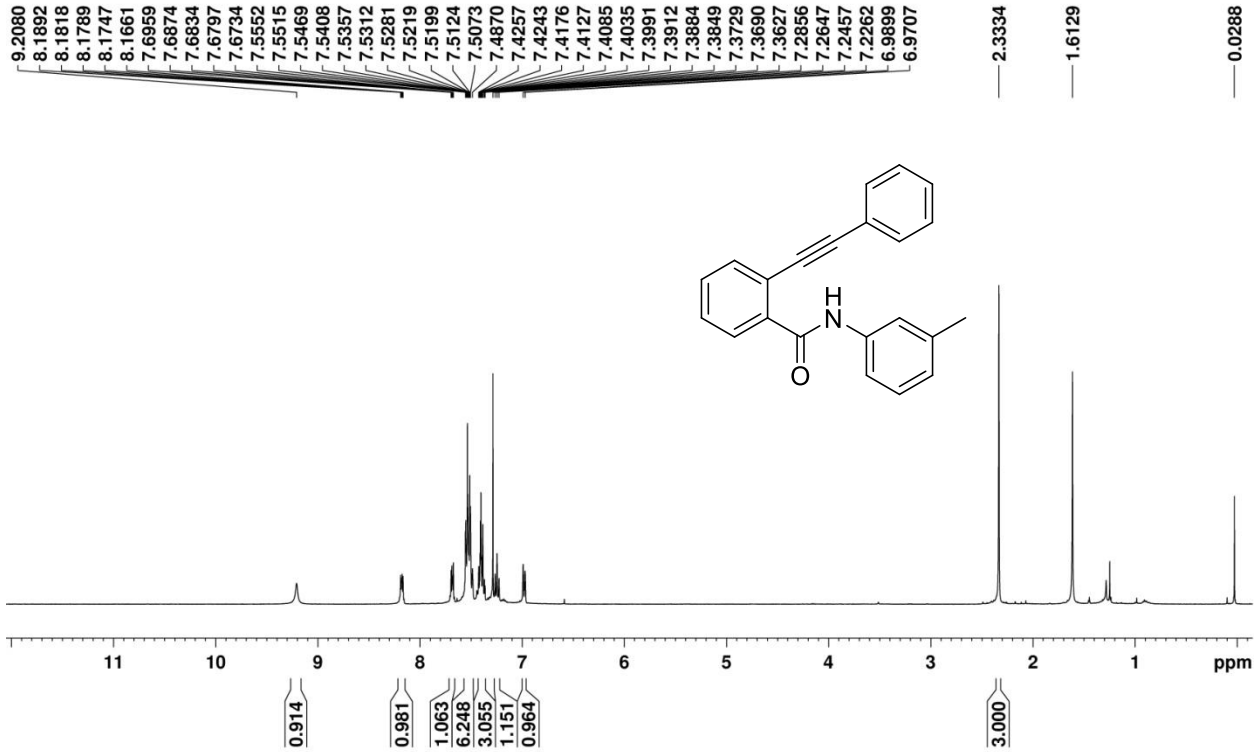
^{1}H NMR Spectrum of *N-(4-methylphenyl)-2-(phenylethynyl)benzamide*(1f) (400 MHz, $CDCl_3$)



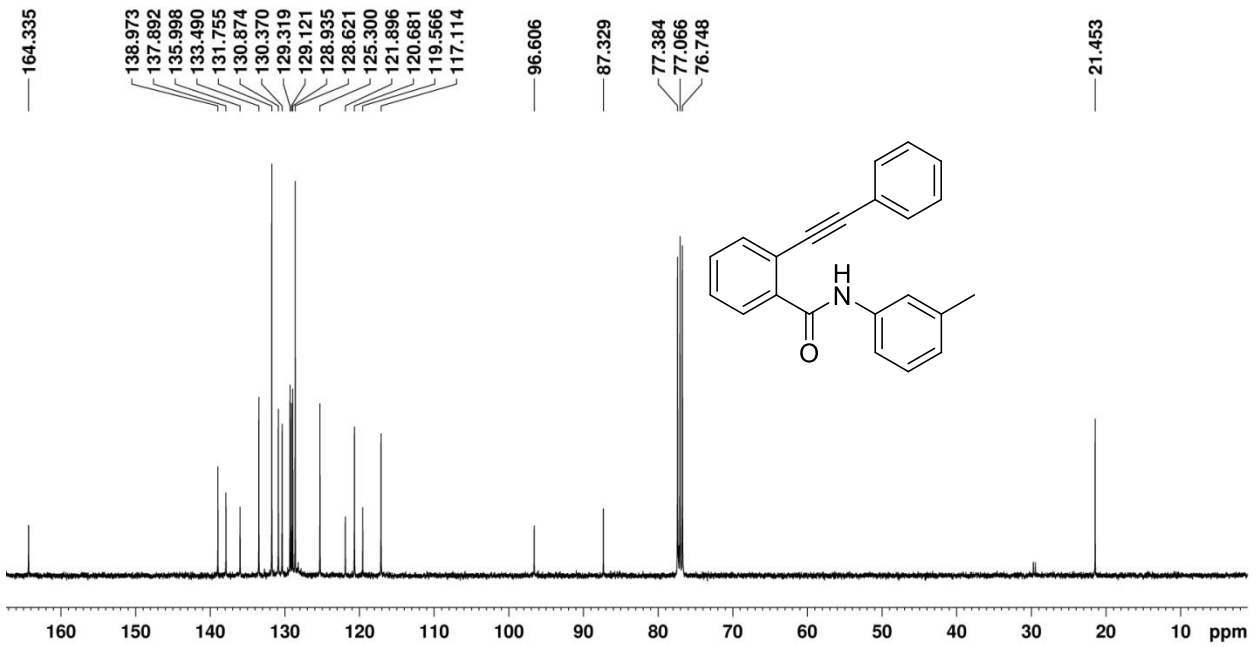
^{13}C NMR Spectrum of *N-(4-methylphenyl)-2-(phenylethynyl)benzamide*(1f) (100 MHz, $CDCl_3$)



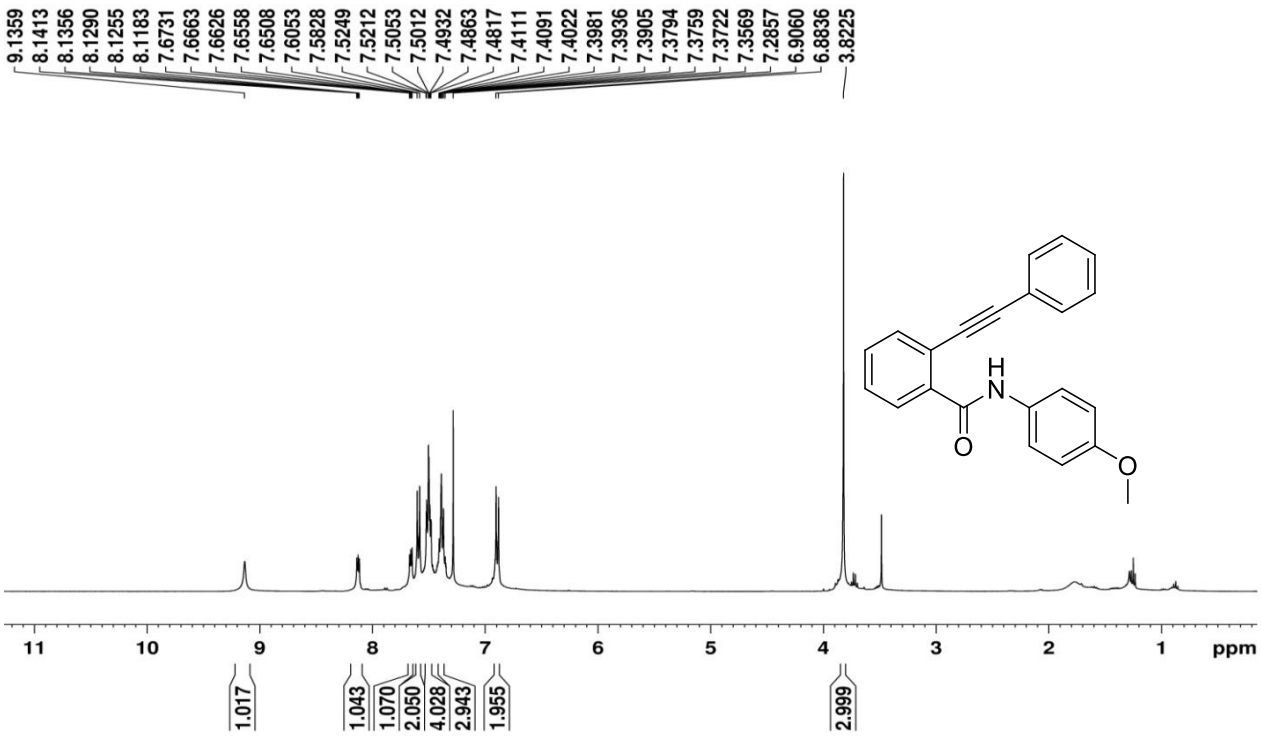
^{1}H NMR Spectrum of *N-(3-methylphenyl)-2-(phenylethynyl)benzamide*(1g) (400 MHz, $CDCl_3$)



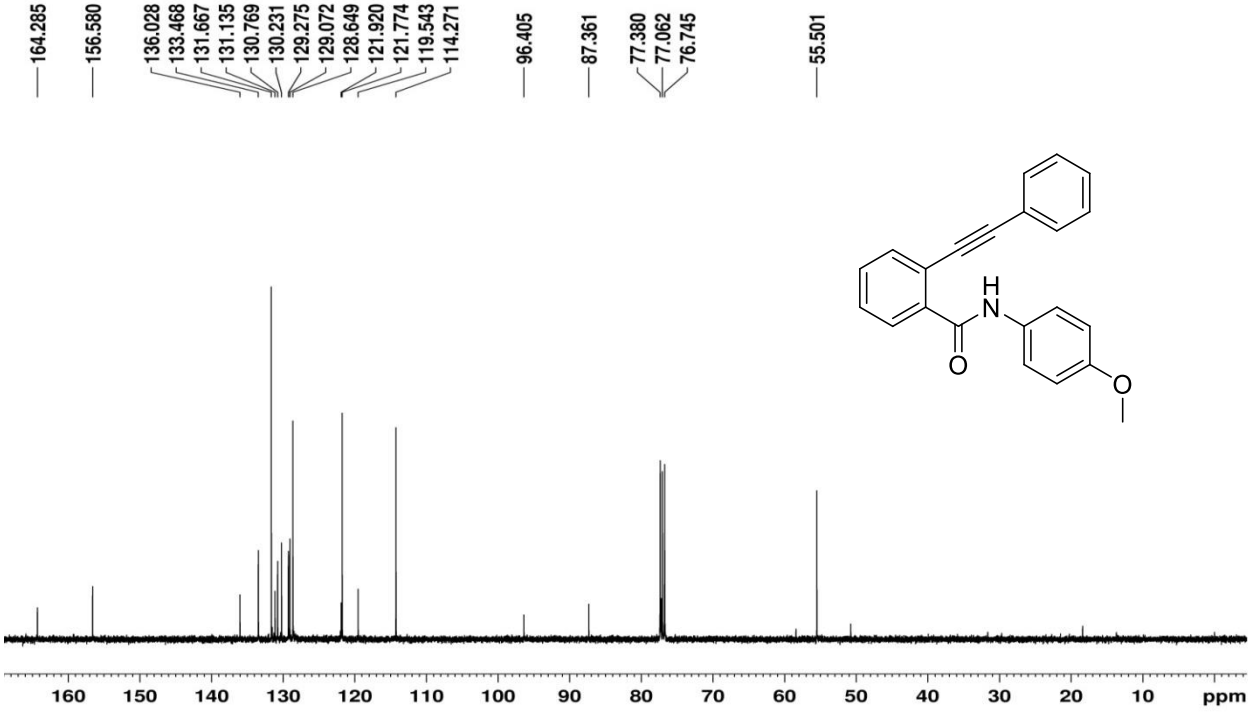
^{13}C NMR Spectrum of *N-(3-methylphenyl)-2-(phenylethynyl)benzamide*(1g) (100 MHz, $CDCl_3$)



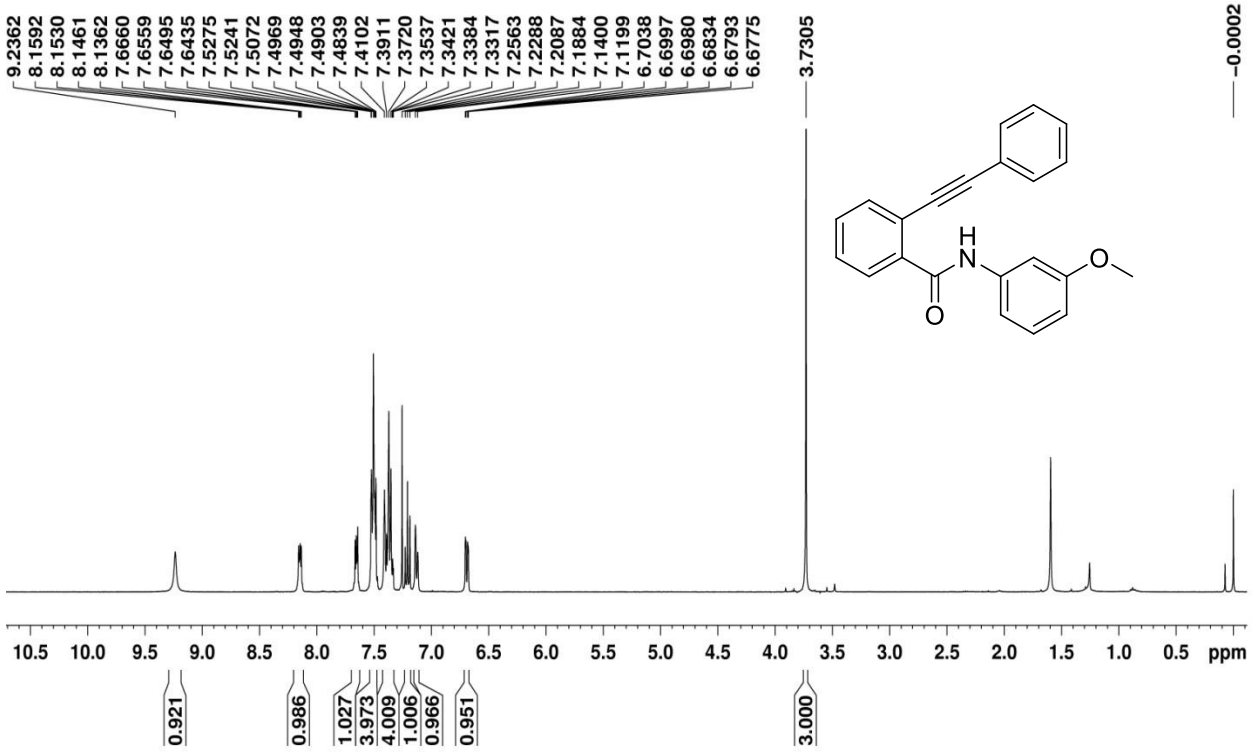
^{1}H NMR Spectrum of *N-(4-methoxyphenyl)-2-(phenylethynyl)benzamide*(1h) (400 MHz, $CDCl_3$)



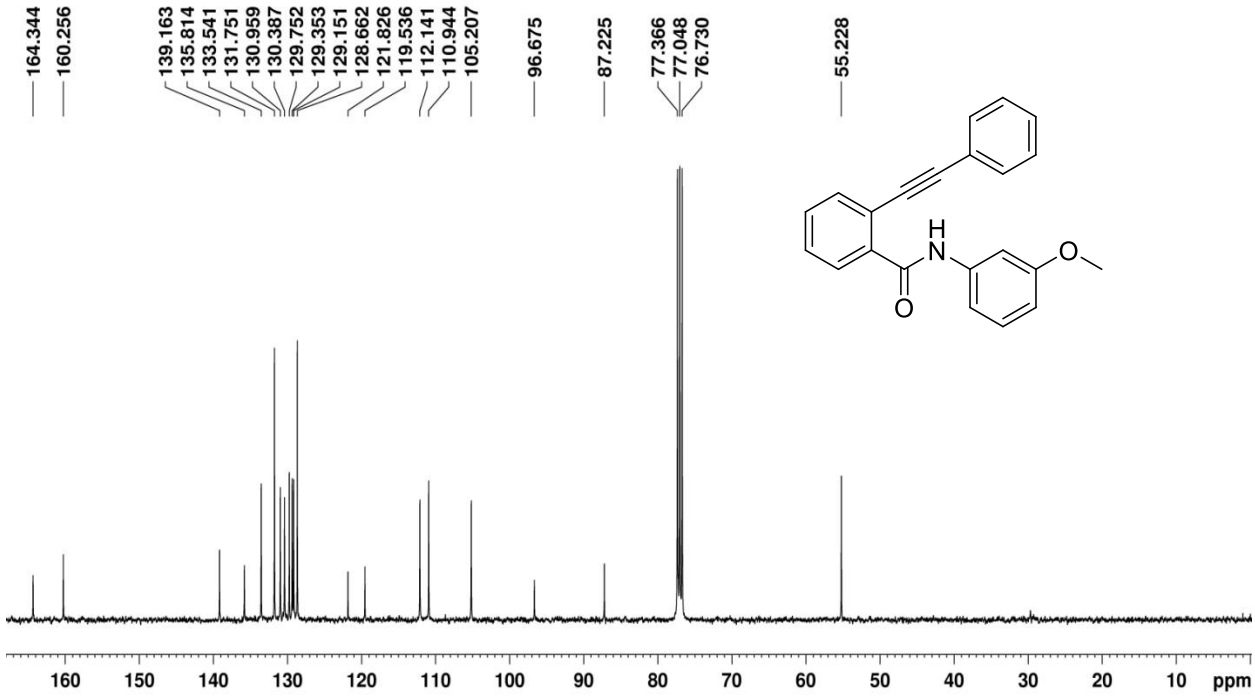
^{13}C NMR Spectrum of *N-(4-methoxyphenyl)-2-(phenylethynyl)benzamide*(1h) (100 MHz, $CDCl_3$)



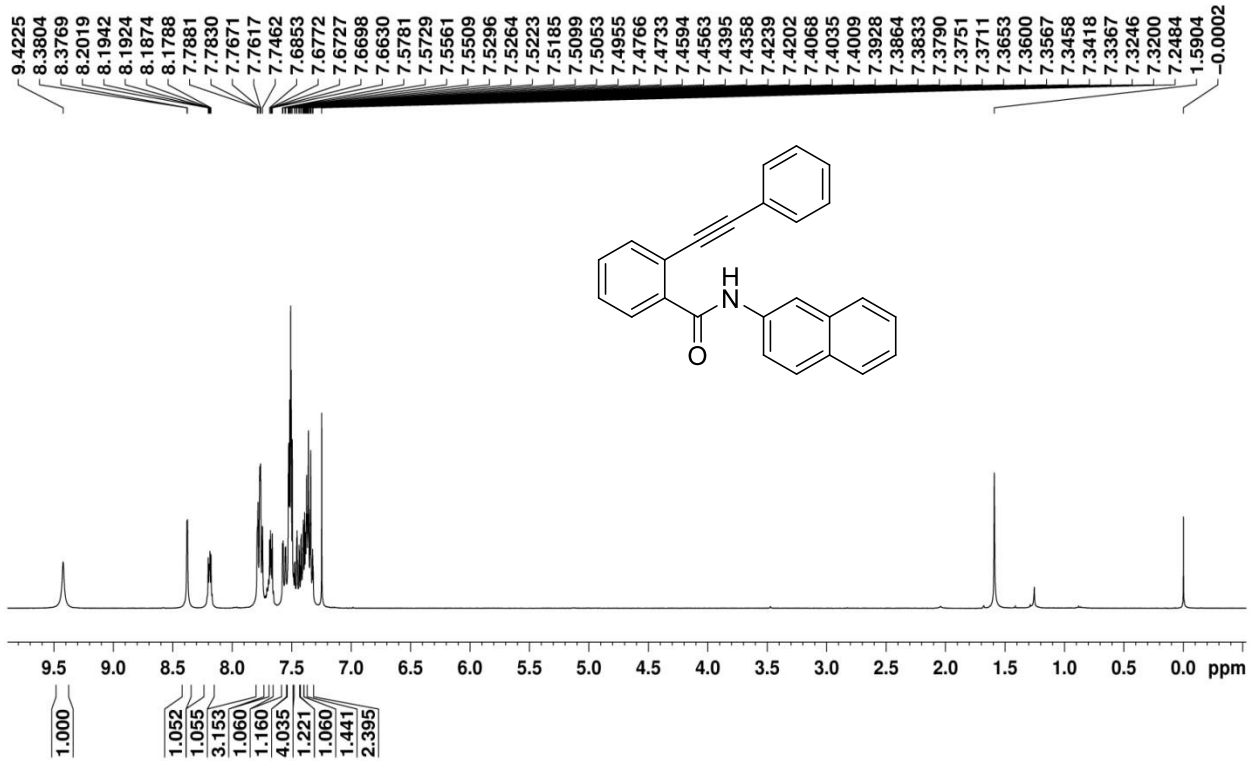
^{1}H NMR Spectrum of *N-(3-methoxyphenyl)-2-(phenylethynyl)benzamide*(1i) (400 MHz, $CDCl_3$)



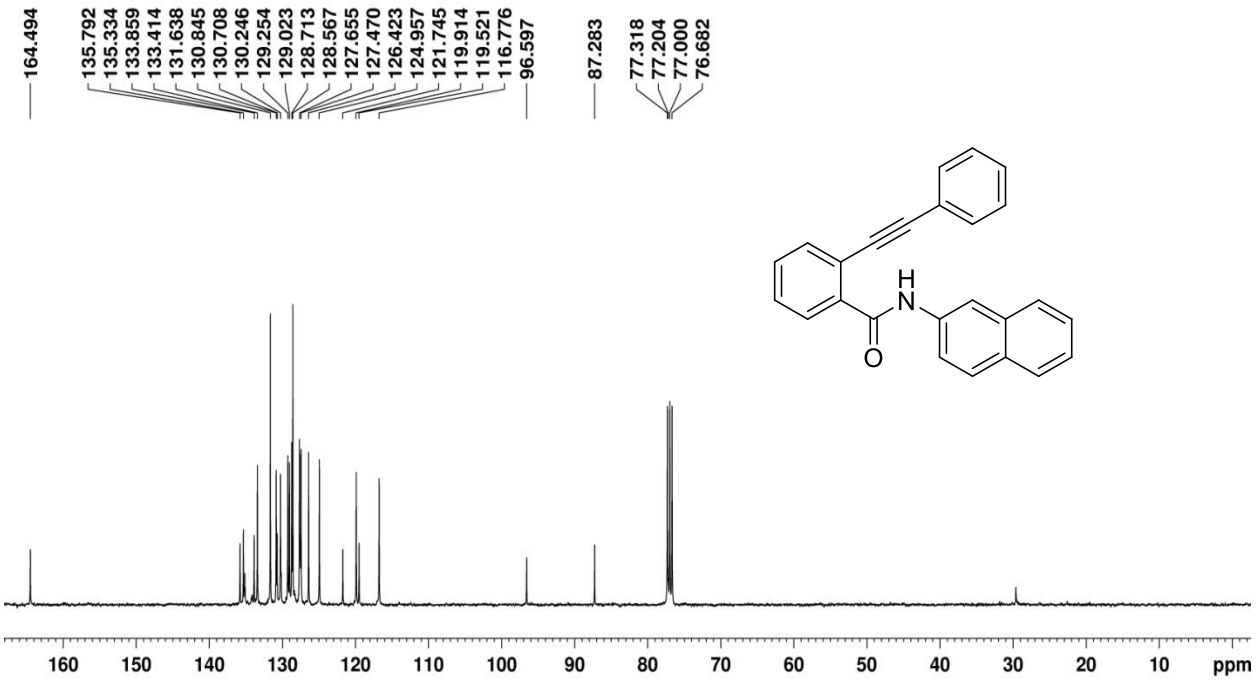
^{13}C NMR Spectrum of *N-(3-methoxyphenyl)-2-(phenylethynyl)benzamide*(1i) (100 MHz, $CDCl_3$)



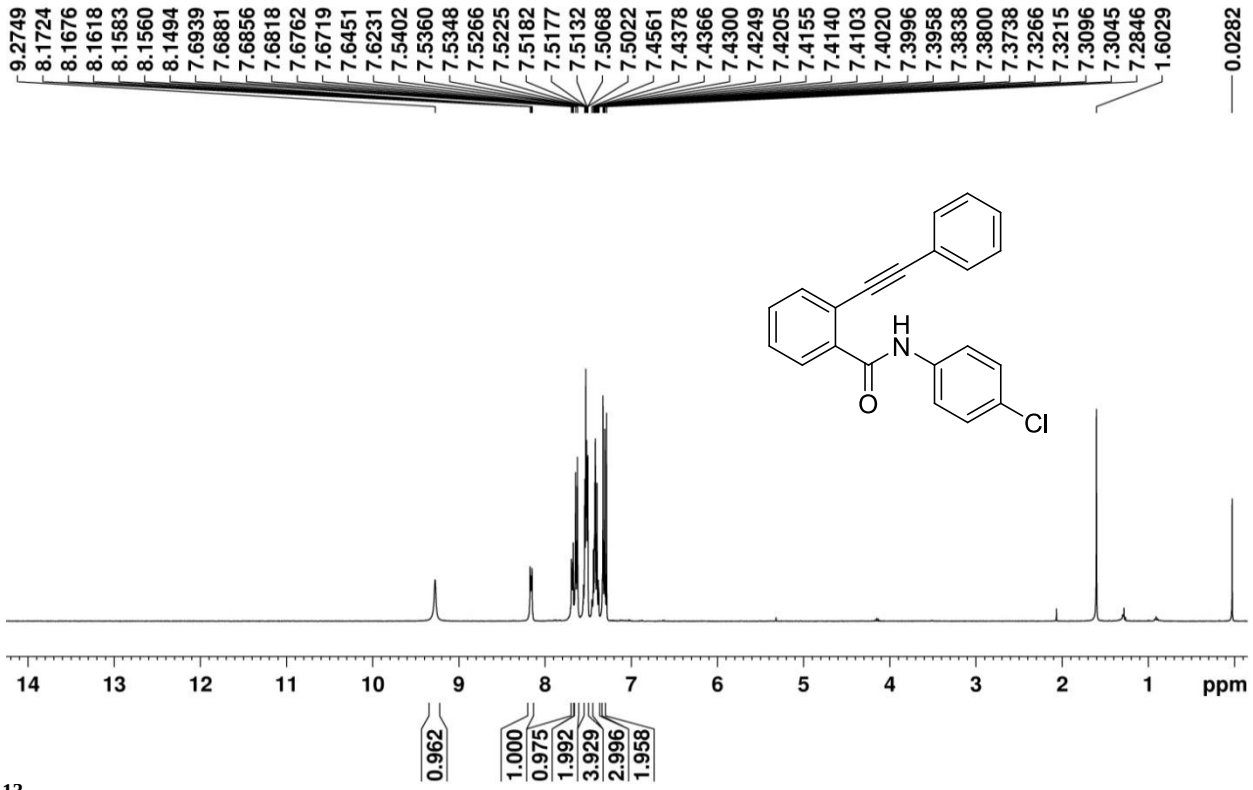
^{1}H NMR Spectrum of *N-(naphthalen-2-yl)-2-(phenylethynyl)benzamide*(1j) (400 MHz, $CDCl_3$)



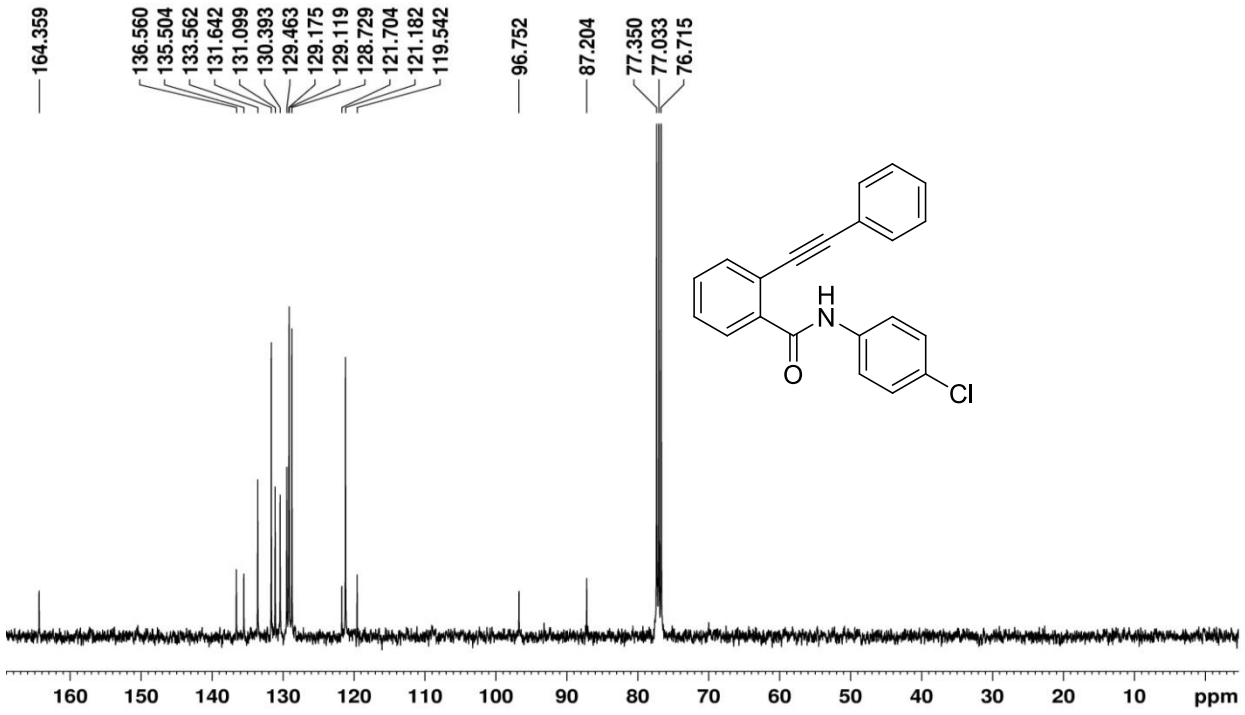
^{13}C NMR Spectrum of *N-(naphthalen-2-yl)-2-(phenylethynyl)benzamide*(1j) (100 MHz, $CDCl_3$)



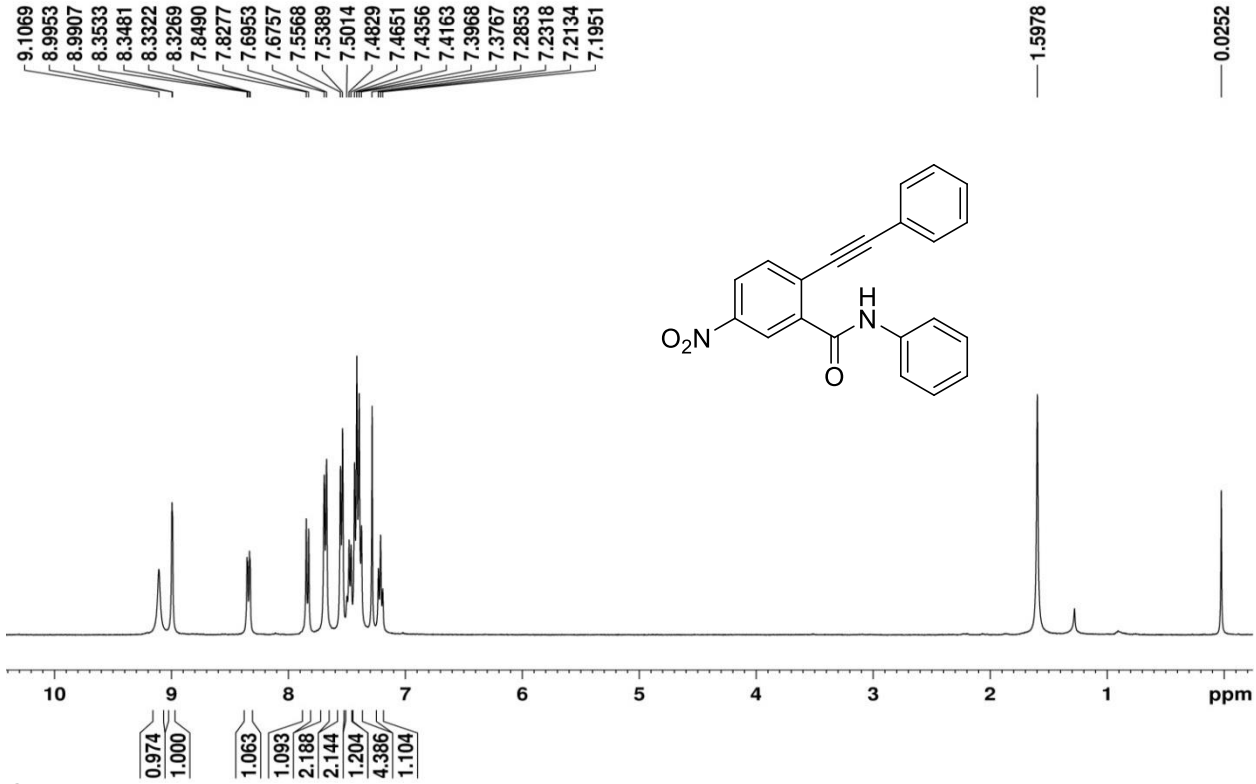
^{1}H NMR Spectrum of *N-(4-chlorophenyl)-2-(phenylethynyl)benzamide*(1k) (400 MHz, $CDCl_3$)



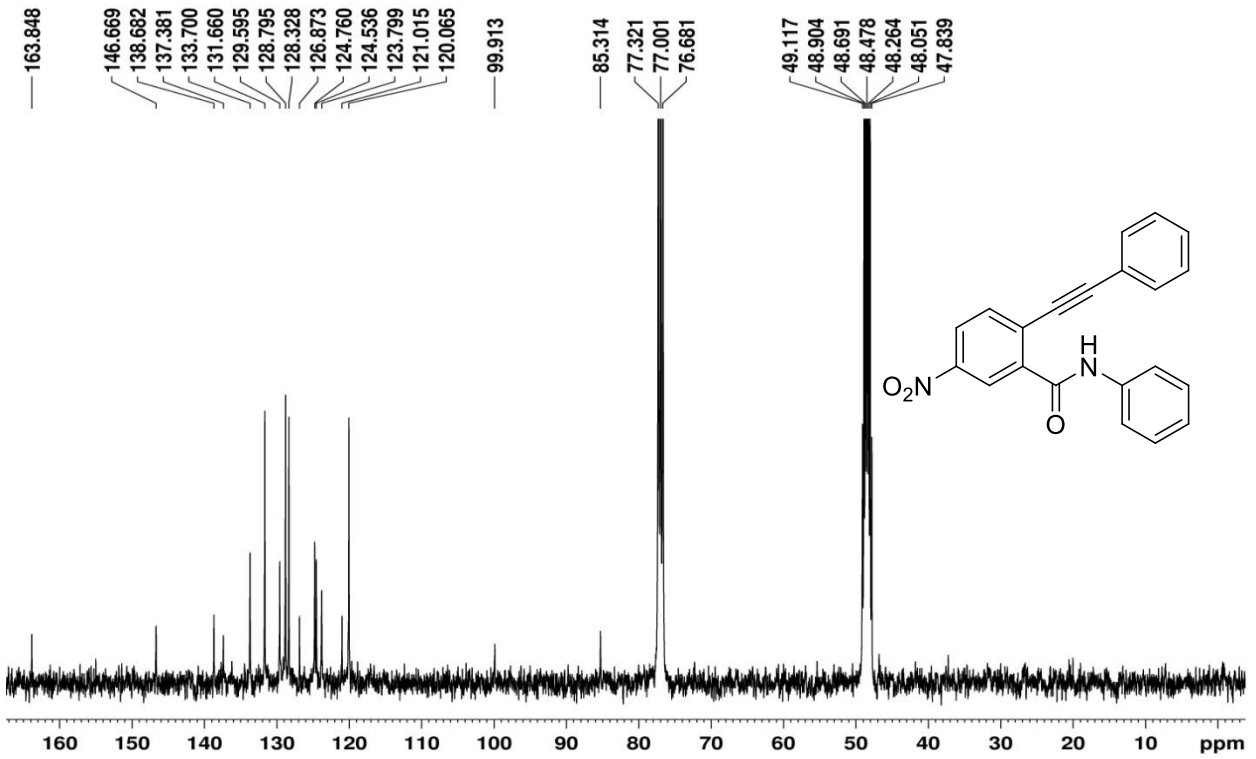
^{13}C NMR Spectrum of *N-(4-chlorophenyl)-2-(phenylethynyl)benzamide*(1k) (100 MHz, $CDCl_3$)



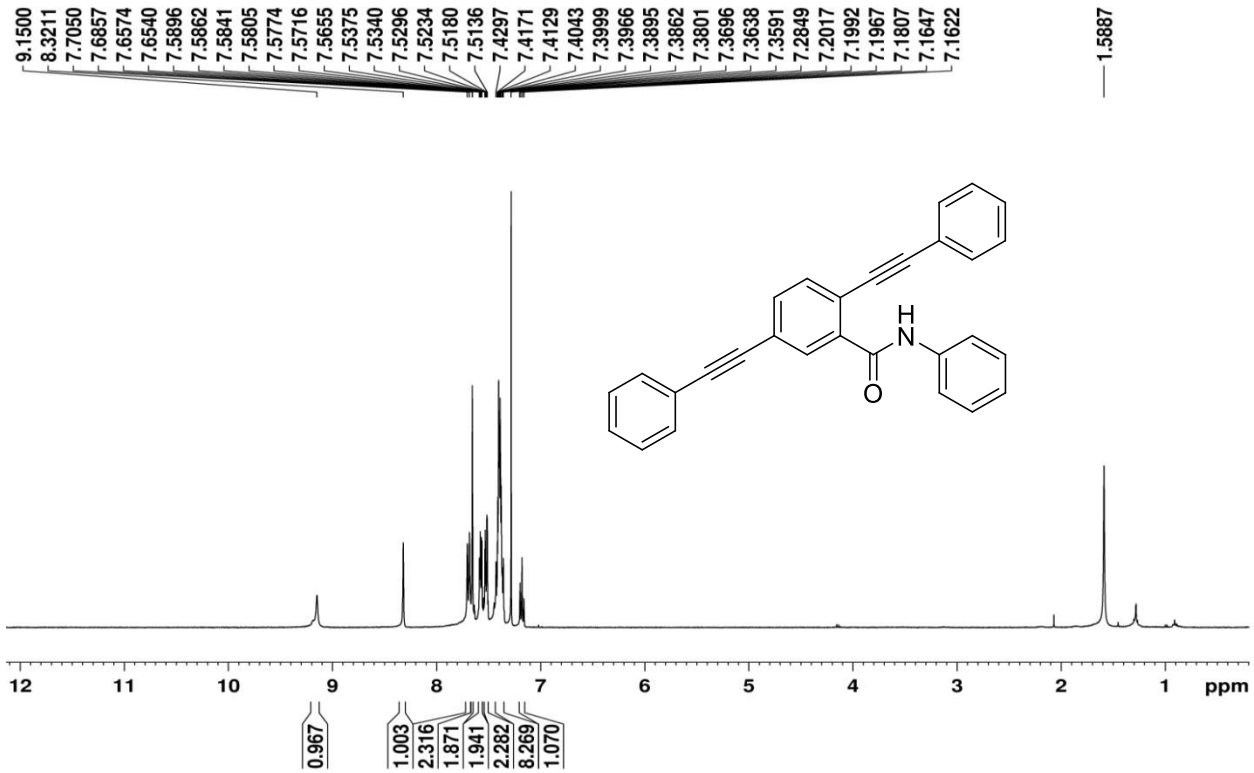
^{1}H NMR Spectrum of *5-nitro-N-phenyl-2-(phenylethynyl)benzamide*(1l) (400 MHz, $CDCl_3$)



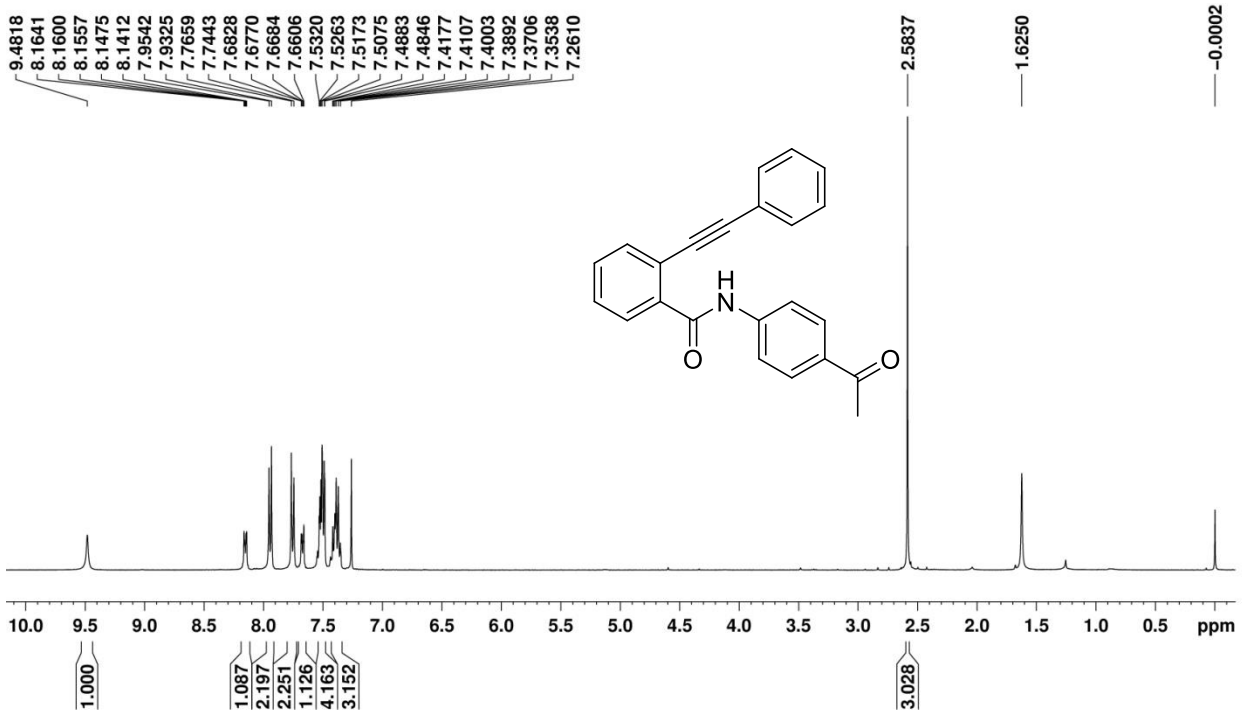
^{13}C NMR Spectrum of *5-nitro-N-phenyl-2-(phenylethynyl)benzamide*(1l) (100 MHz, $CDCl_3$ + CD_3OD)



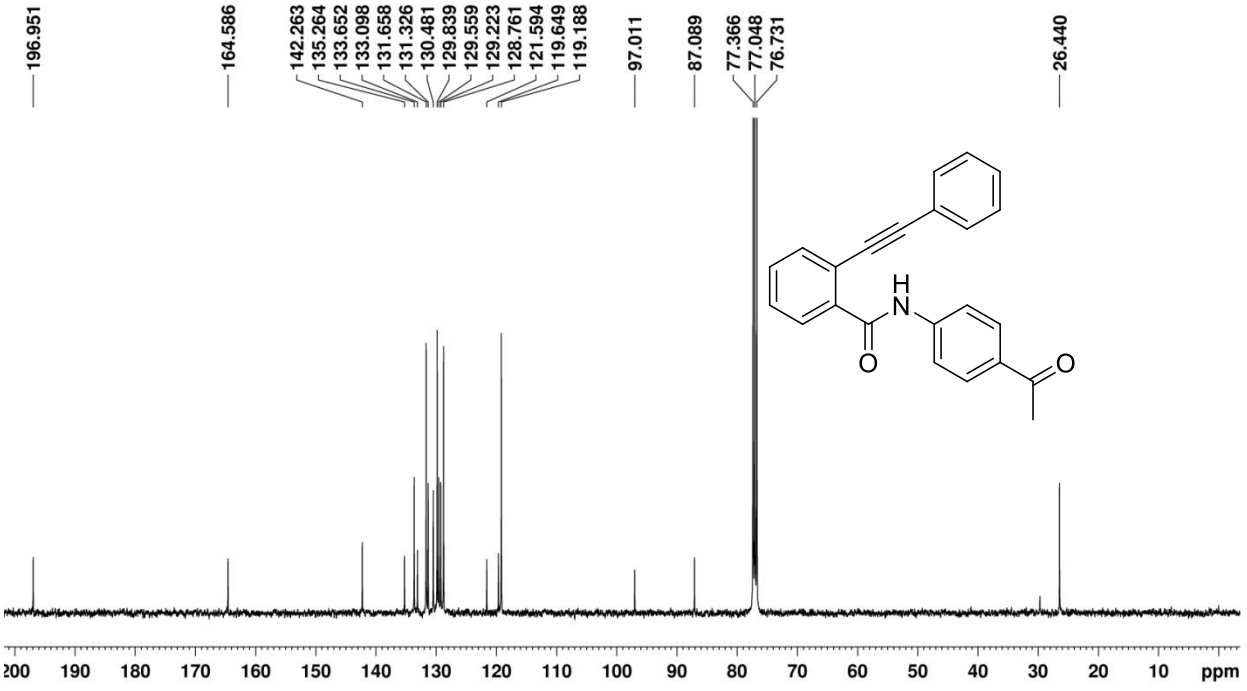
^{1}H NMR Spectrum of *5-bromo-N-phenyl-2-(phenylethynyl)benzamide*(1m) (400 MHz, $CDCl_3$)



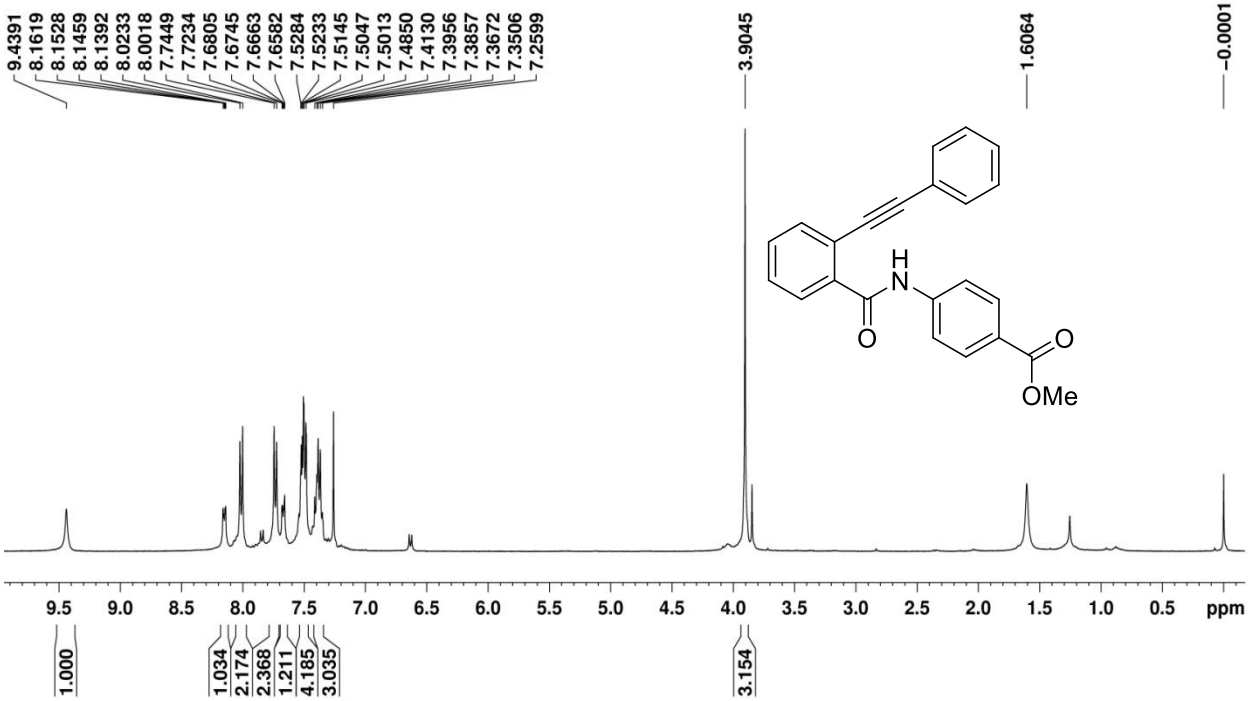
^{1}H NMR Spectrum of *N-(4-acetylphenyl)-2-(phenylethynyl)benzamide*(1n) (400 MHz, $CDCl_3$)



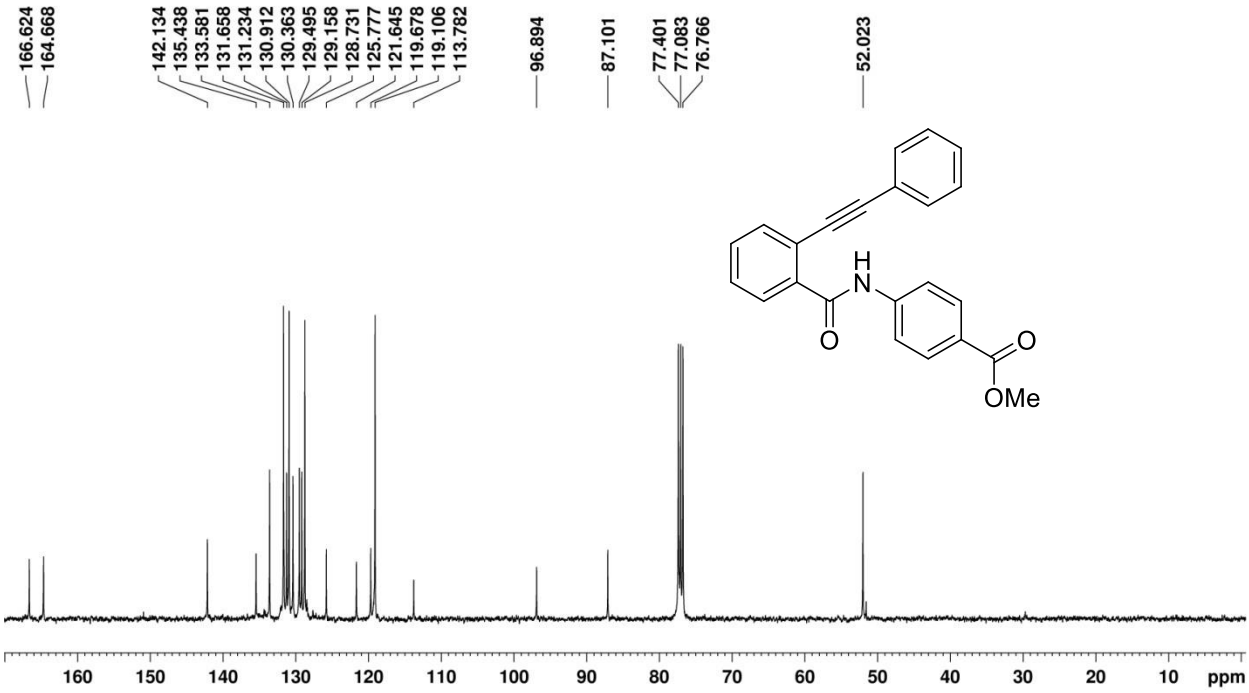
^{13}C NMR Spectrum of *N-(4-acetylphenyl)-2-(phenylethynyl)benzamide*(1n) (100 MHz, $CDCl_3$)



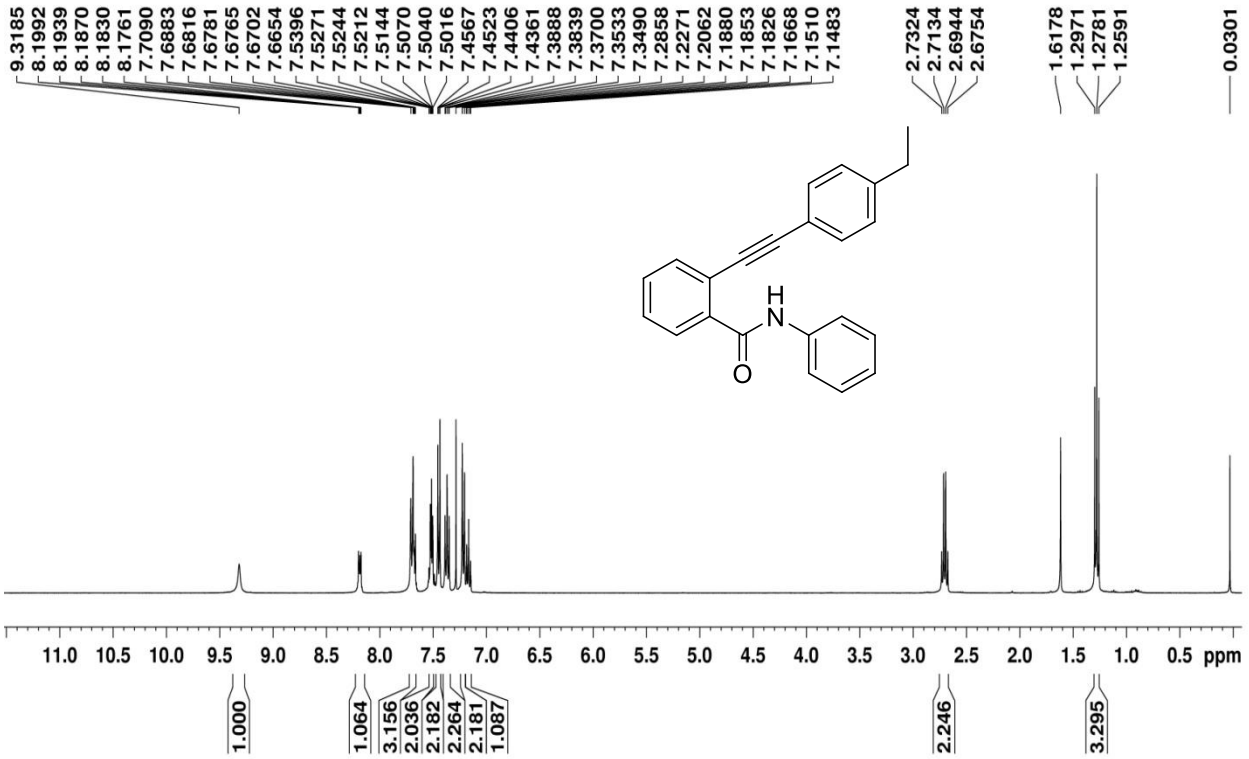
^{1}H NMR Spectrum of *methyl 4-(2-(phenylethynyl)benzamido)benzoate*(1o) (400 MHz, $CDCl_3$)



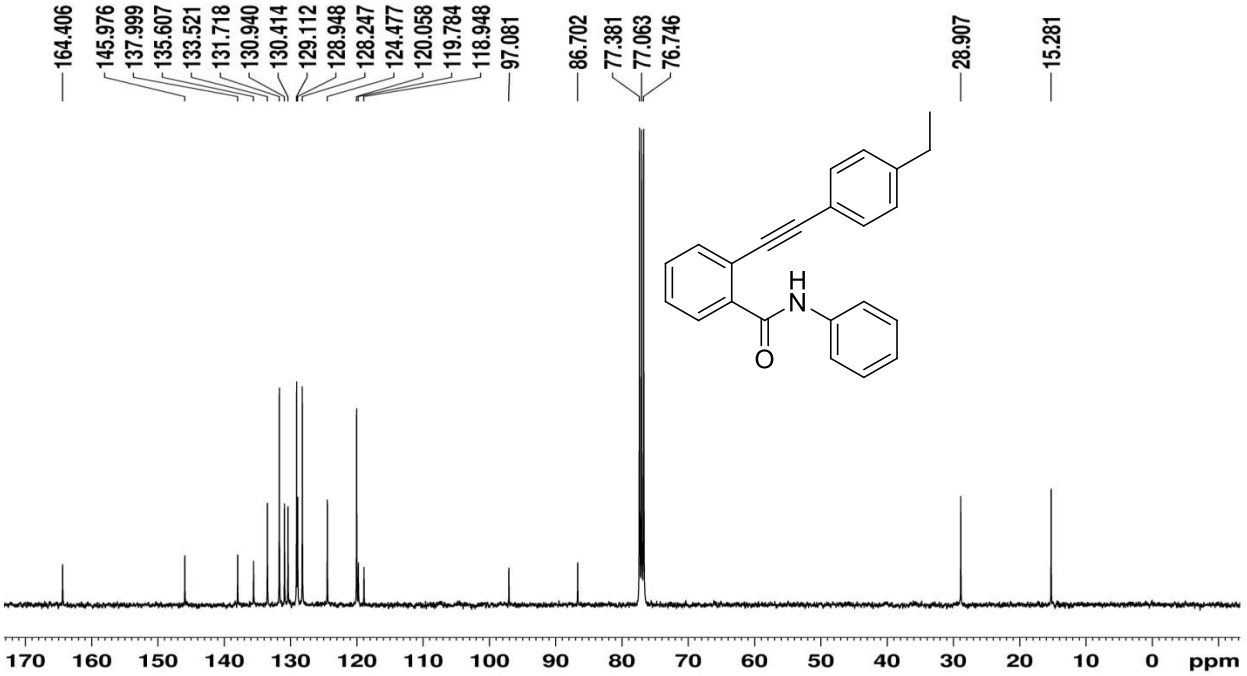
^{13}C NMR Spectrum of *methyl 4-(2-(phenylethynyl)benzamido)benzoate*(1o) (100 MHz, $CDCl_3$)



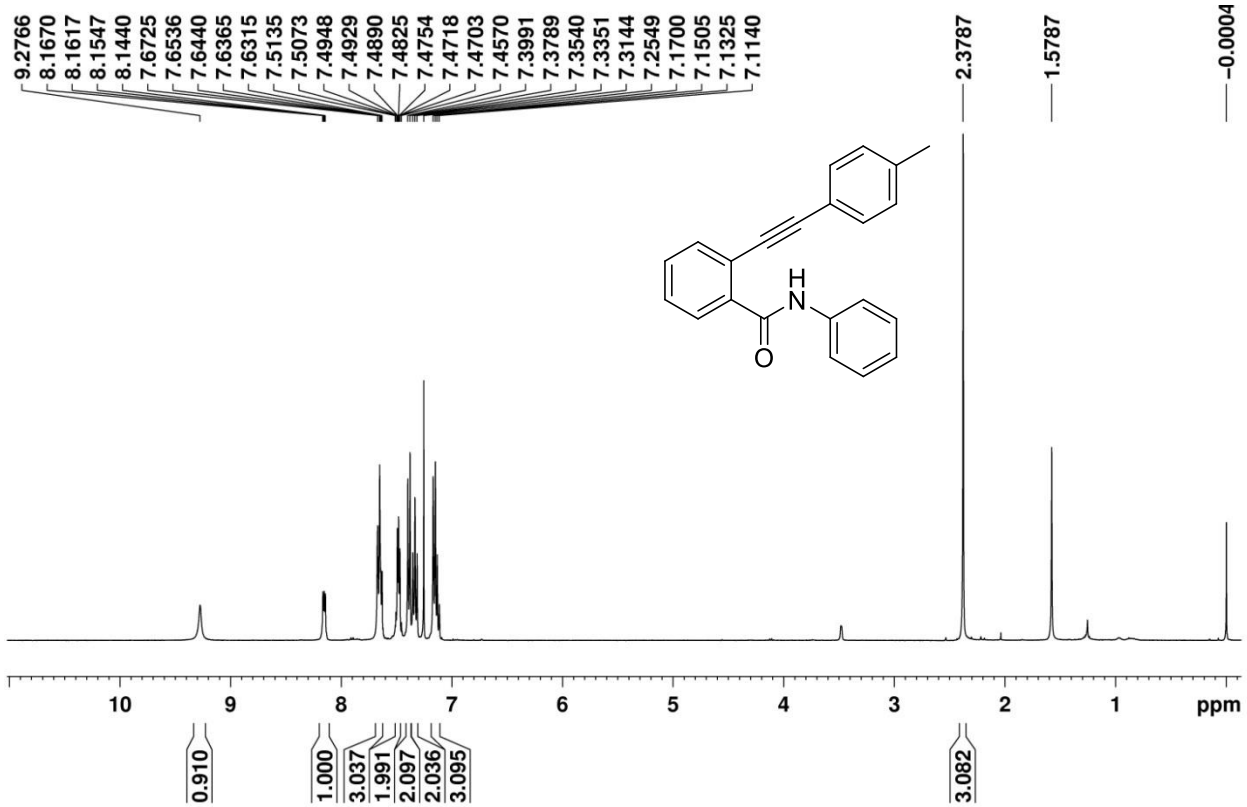
^{1}H NMR Spectrum of *2-((4-ethylphenyl)ethynyl)-N-phenylbenzamide*(1p) (400 MHz, $CDCl_3$)



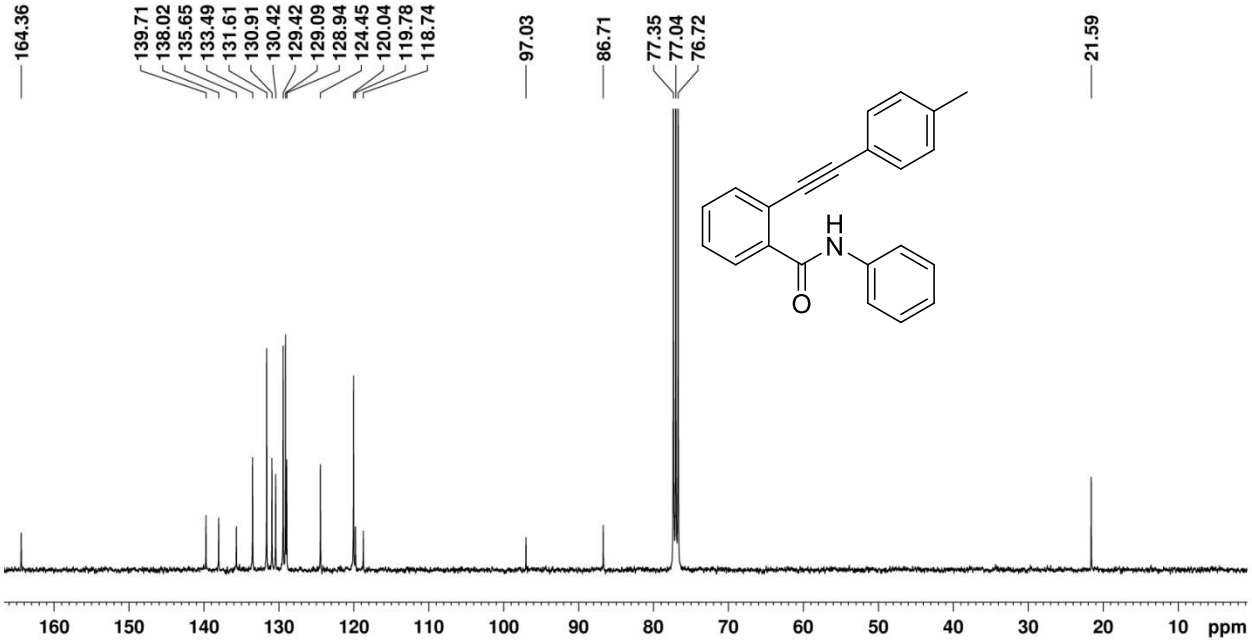
^{13}C NMR Spectrum of *2-((4-ethylphenyl)ethynyl)-N-phenylbenzamide*(1p) (100 MHz, $CDCl_3$)



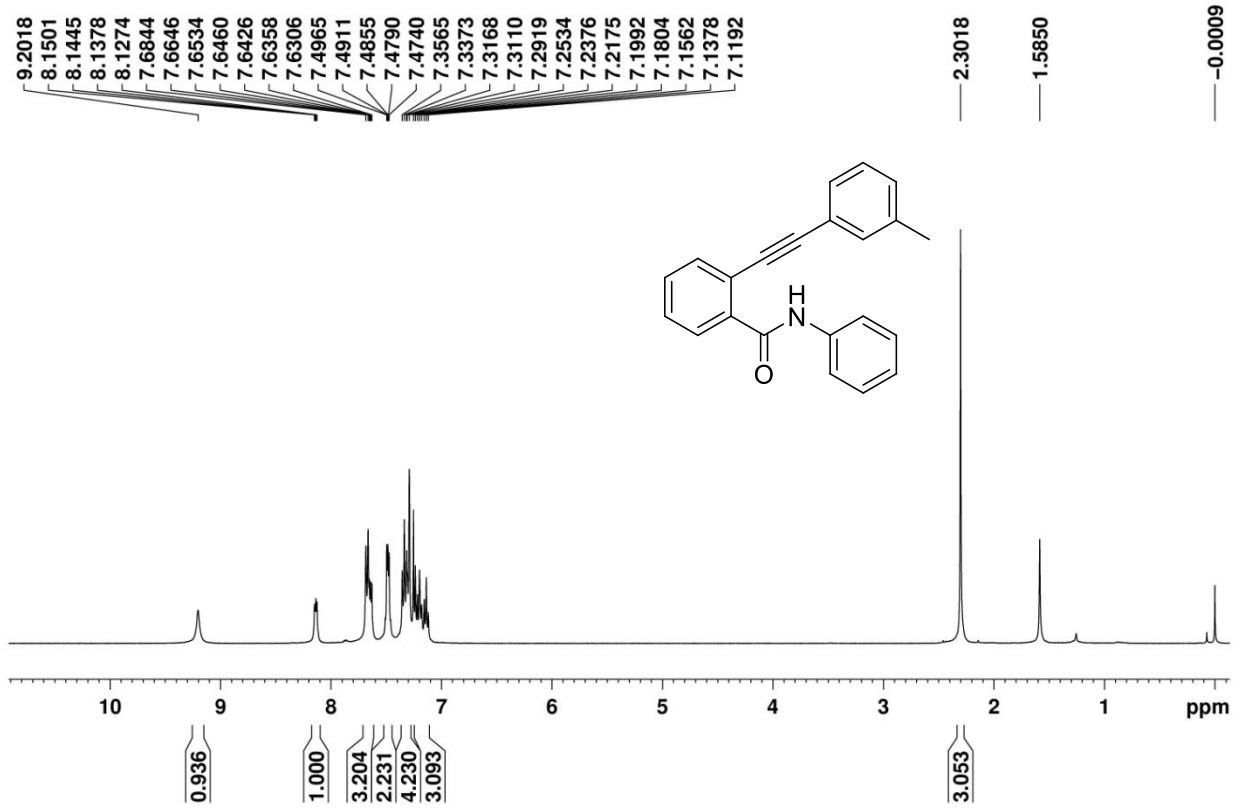
^{1}H NMR Spectrum of *N-phenyl-2-(p-tolylethynyl)benzamide*(1q) (400 MHz, $CDCl_3$)



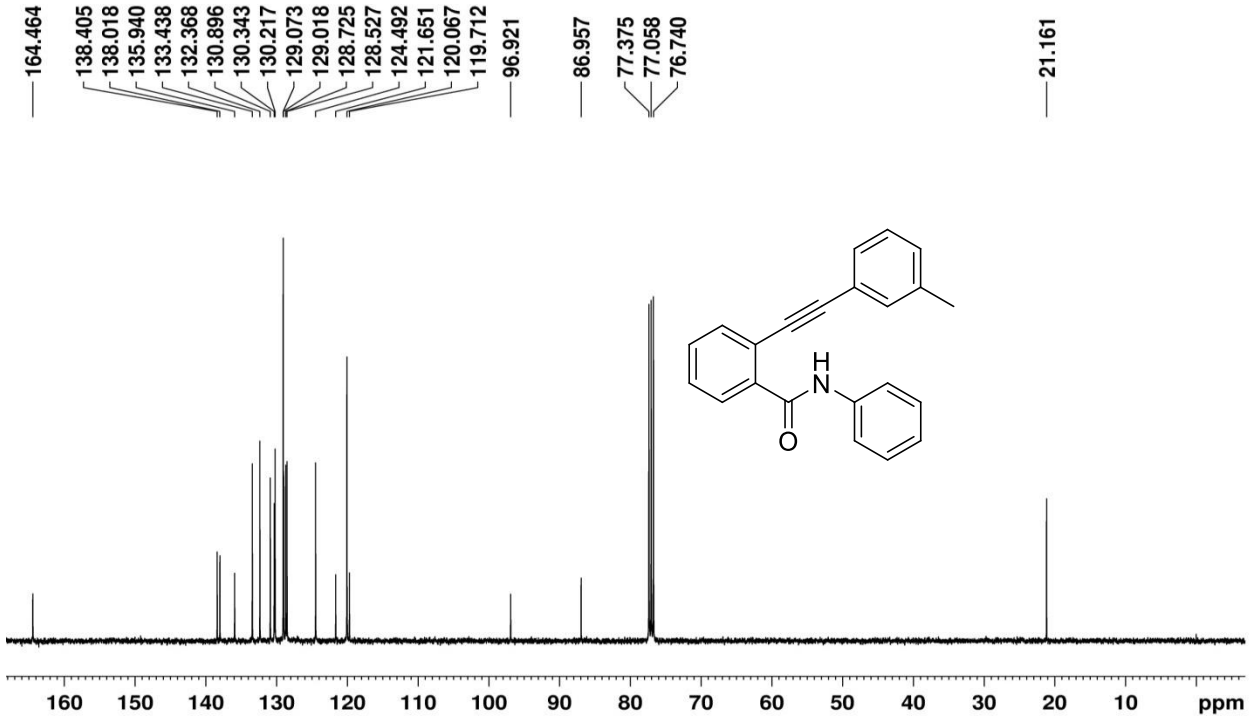
^{13}C NMR Spectrum of *N-phenyl-2-(p-tolylethynyl)benzamide*(1q) (100 MHz, $CDCl_3$)



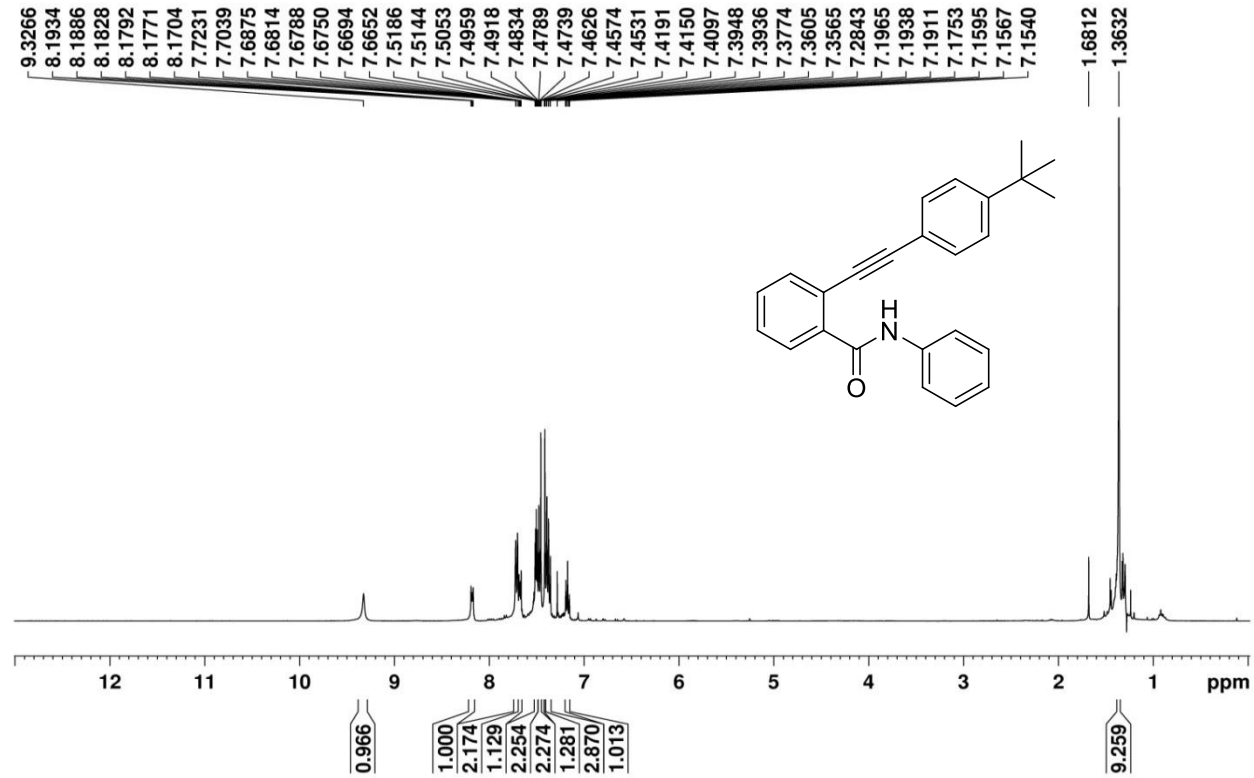
^{1}H NMR Spectrum of *N-phenyl-2-(m-tolylethynyl)benzamide*(1r) (400 MHz, $CDCl_3$)



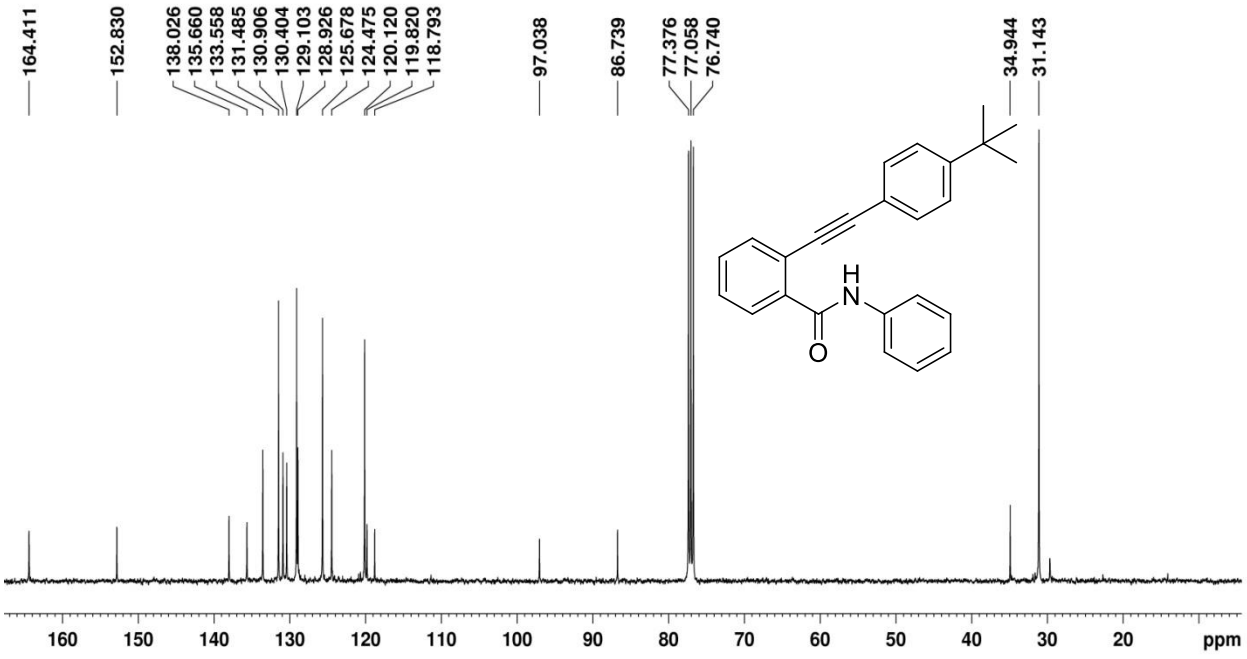
^{13}C NMR Spectrum of *N-phenyl-2-(m-tolylethynyl)benzamide*(1r) (100 MHz, $CDCl_3$)



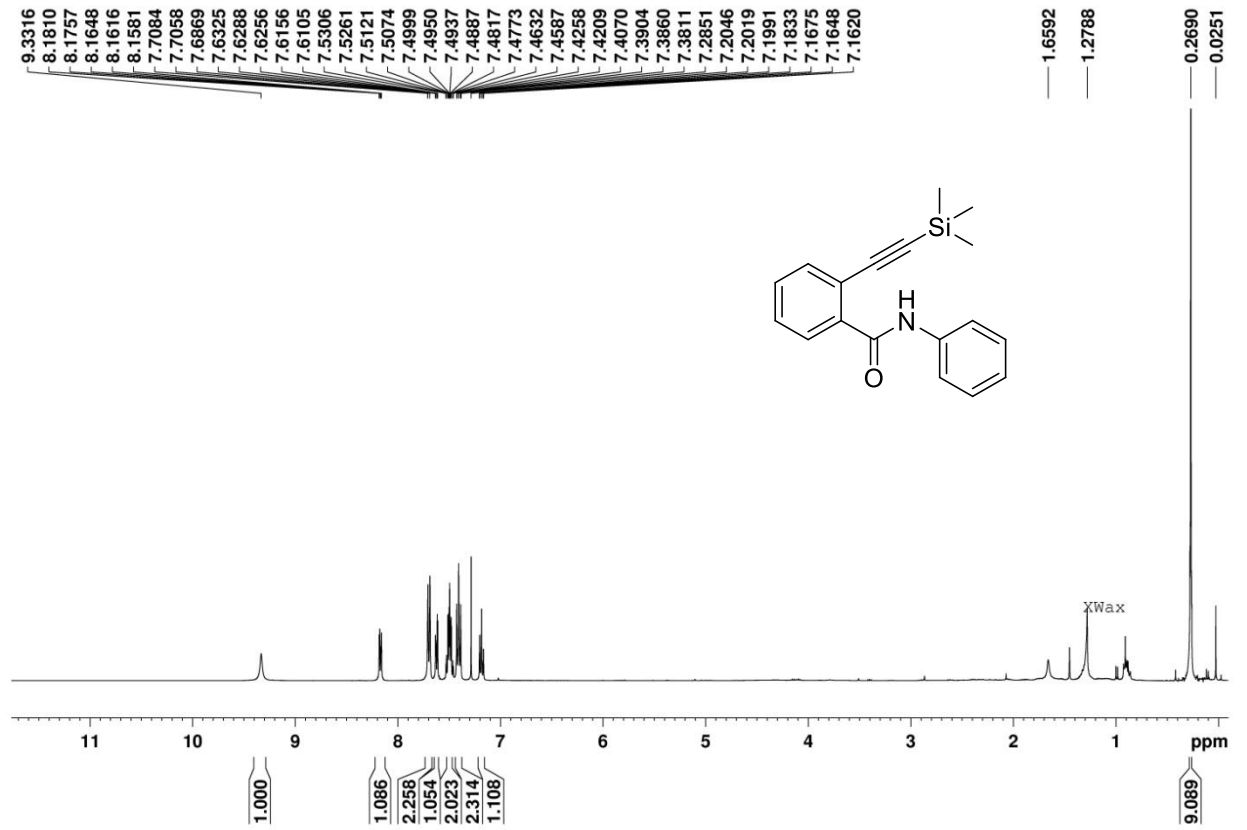
^{1}H NMR Spectrum of *2-((4-tert-butylphenyl)ethynyl)-N-phenylbenzamide*(1s) (400 MHz, $CDCl_3$)



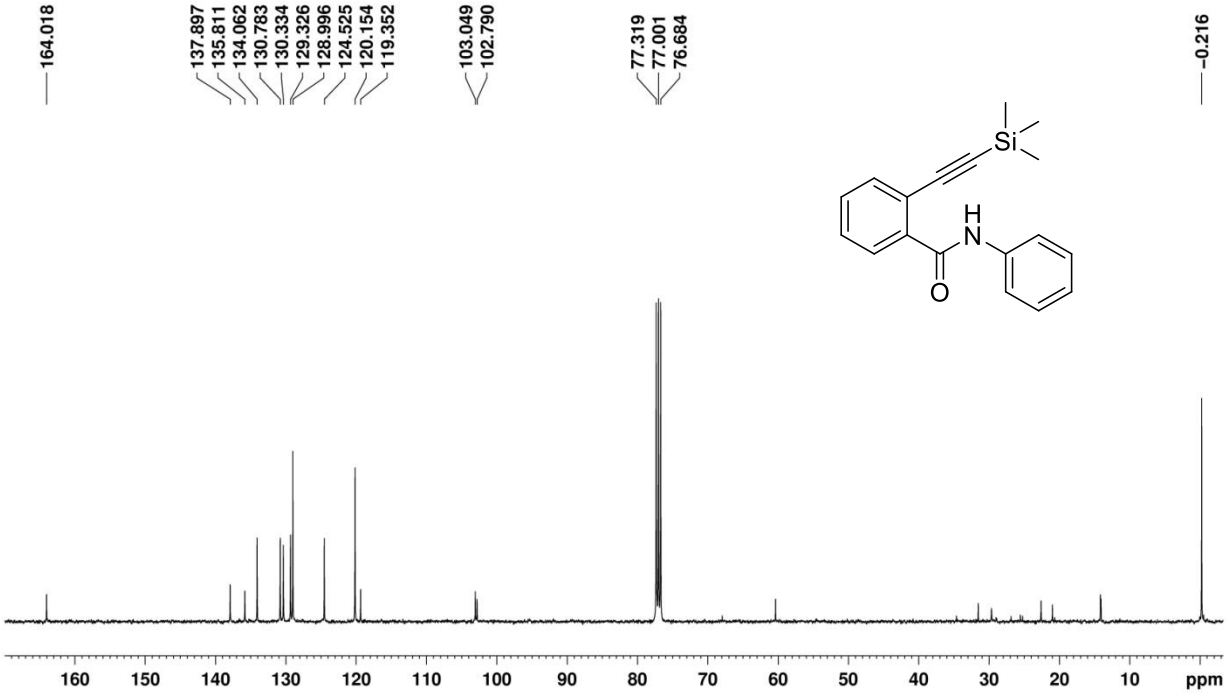
^{13}C NMR Spectrum of *2-((4-tert-butylphenyl)ethynyl)-N-phenylbenzamide*(1s) (100 MHz, $CDCl_3$)



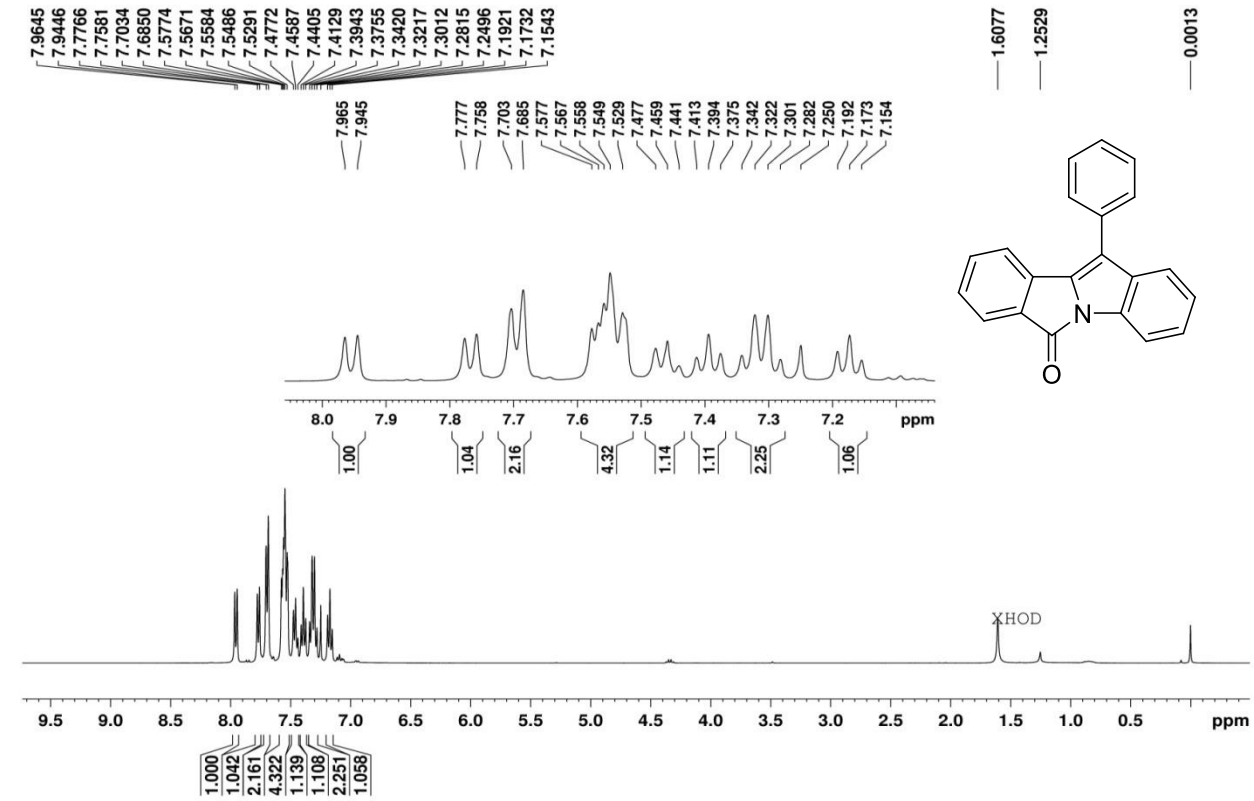
^{1}H NMR Spectrum of *N-phenyl-2-((trimethylsilyl)ethynyl)benzamide*(1t) (400 MHz, $CDCl_3$)



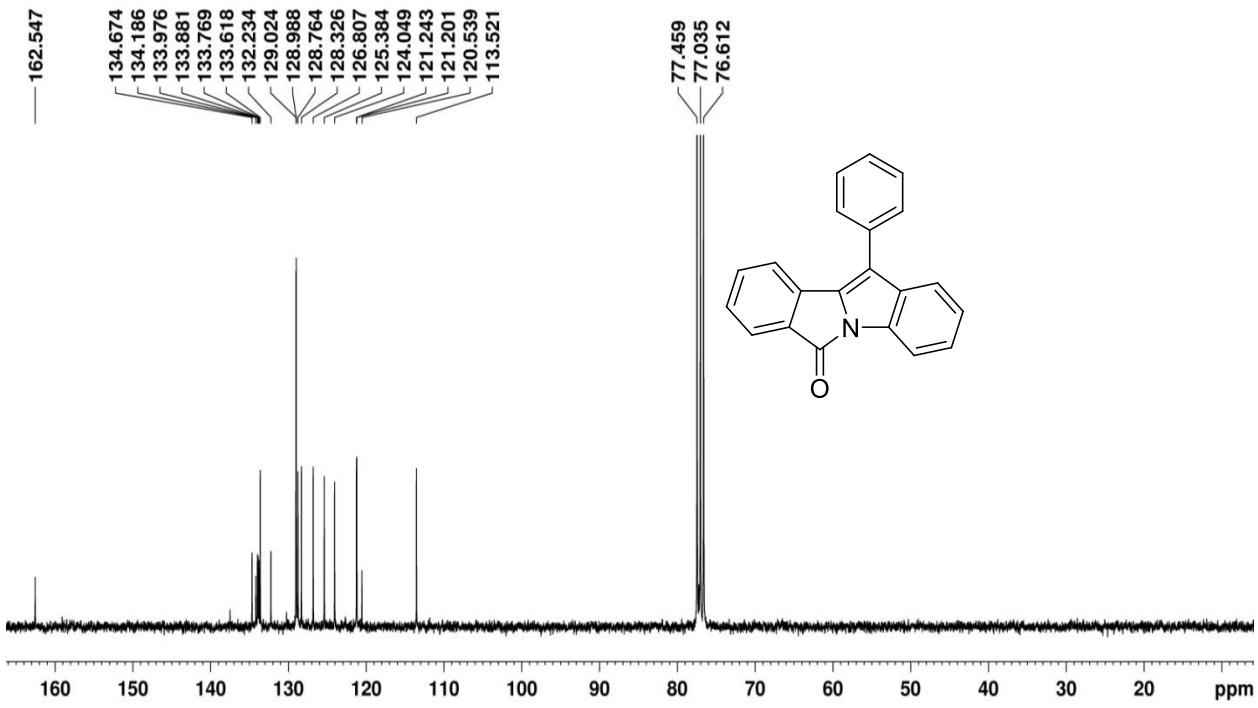
^{13}C NMR Spectrum of *N-phenyl-2-((trimethylsilyl)ethynyl)benzamide*(1t) (100 MHz, $CDCl_3$)



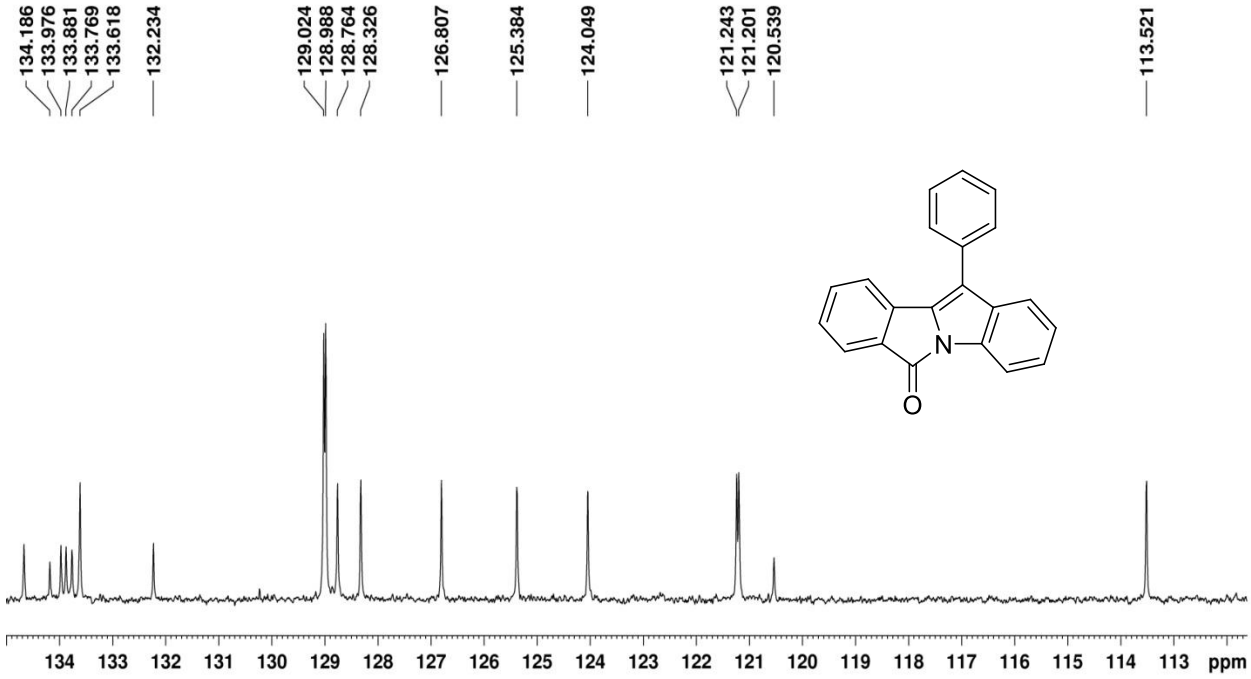
^{1}H NMR Spectrum of *11-phenyl-6H-isoindolo[2,1-a]indol-6-one* (2a) (400 MHz, $CDCl_3$)



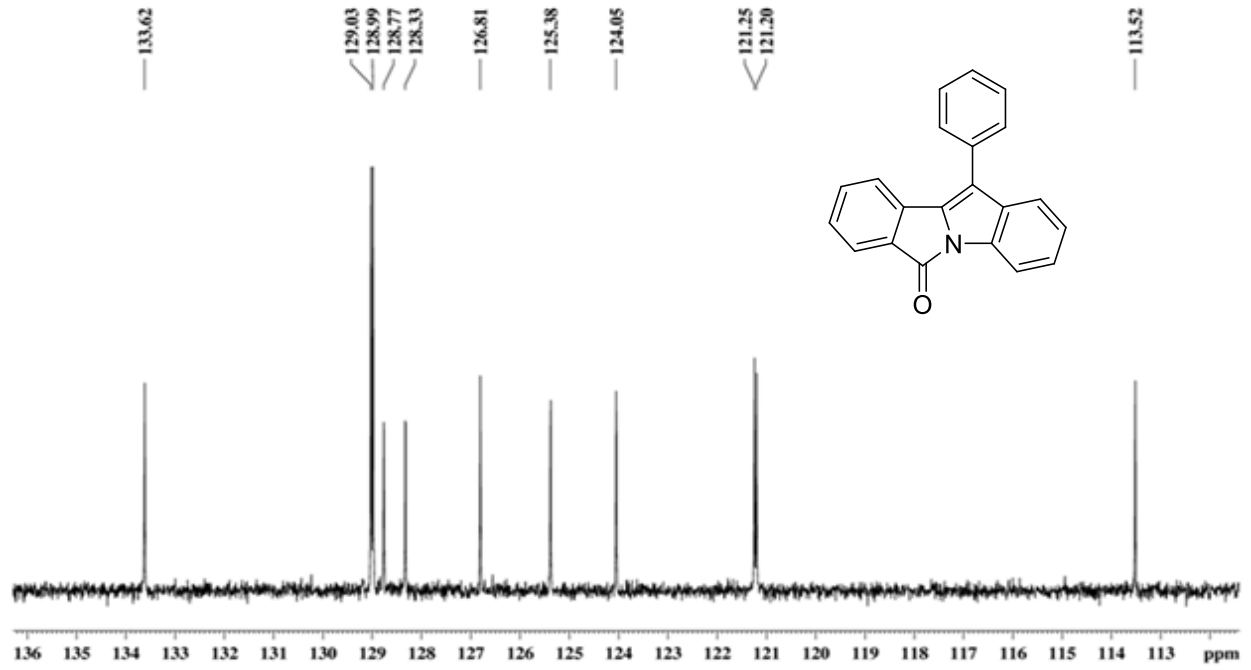
^{13}C NMR Spectrum of *11-phenyl-6H-isoindolo[2,1-a]indol-6-one* (2a) (75 MHz, $CDCl_3$)



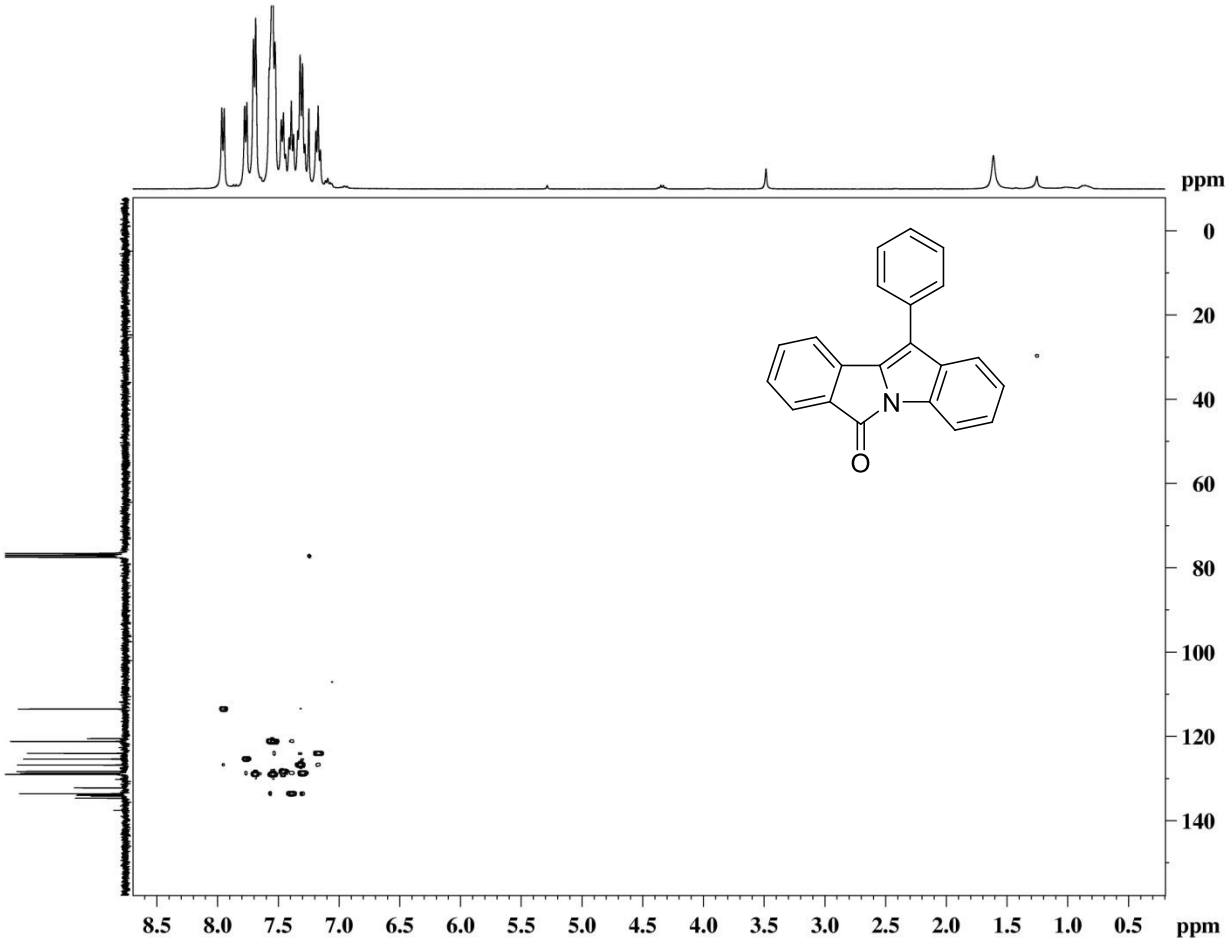
^{13}C NMR Spectrum (expansion) of *11-phenyl-6H-isoindolo[2,1-a]indol-6-one* (2a) (75 MHz, $CDCl_3$)



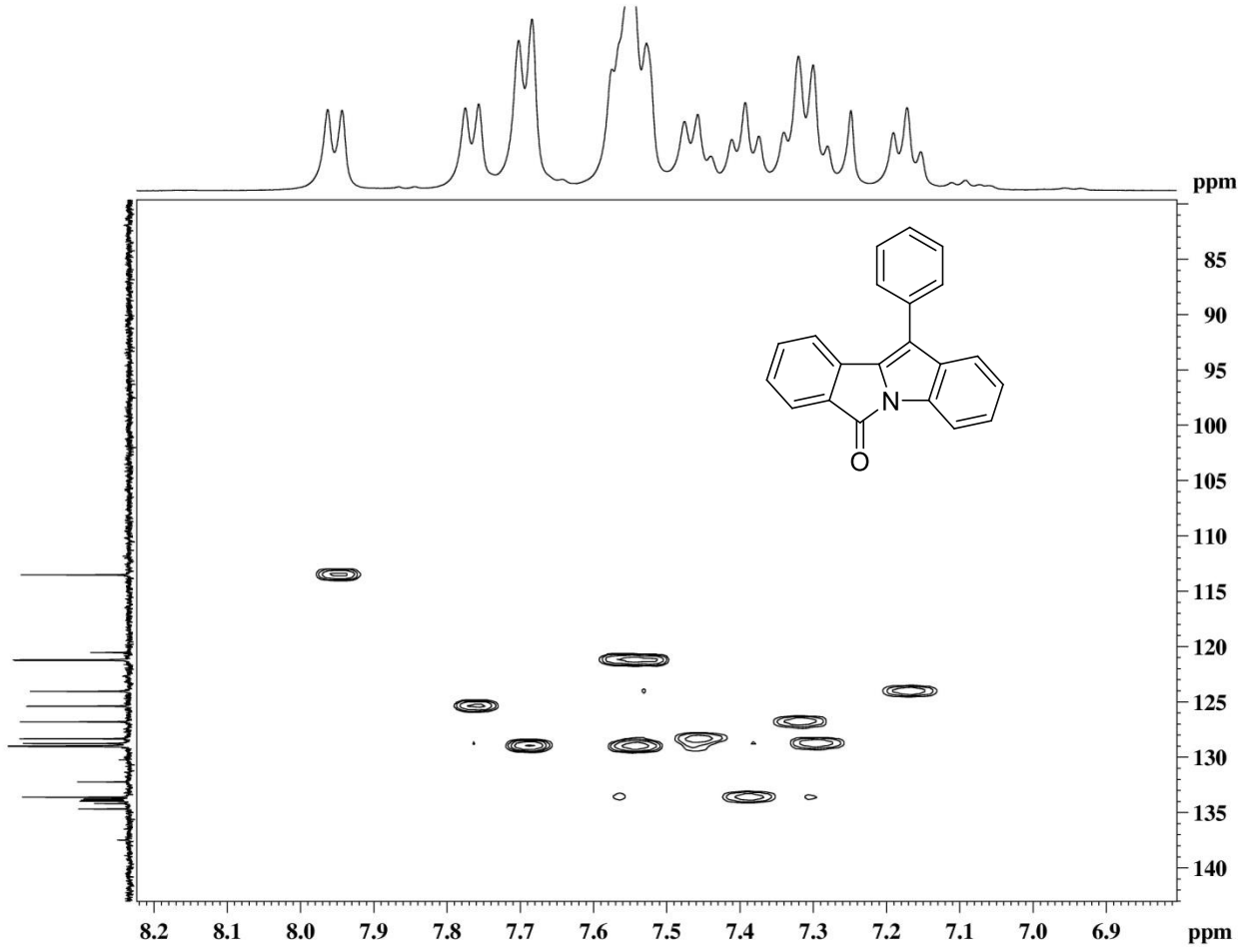
DEPT 135 NMR Spectrum of *11-phenyl-6H-isoindolo[2,1-a]indol-6-one* (2a)



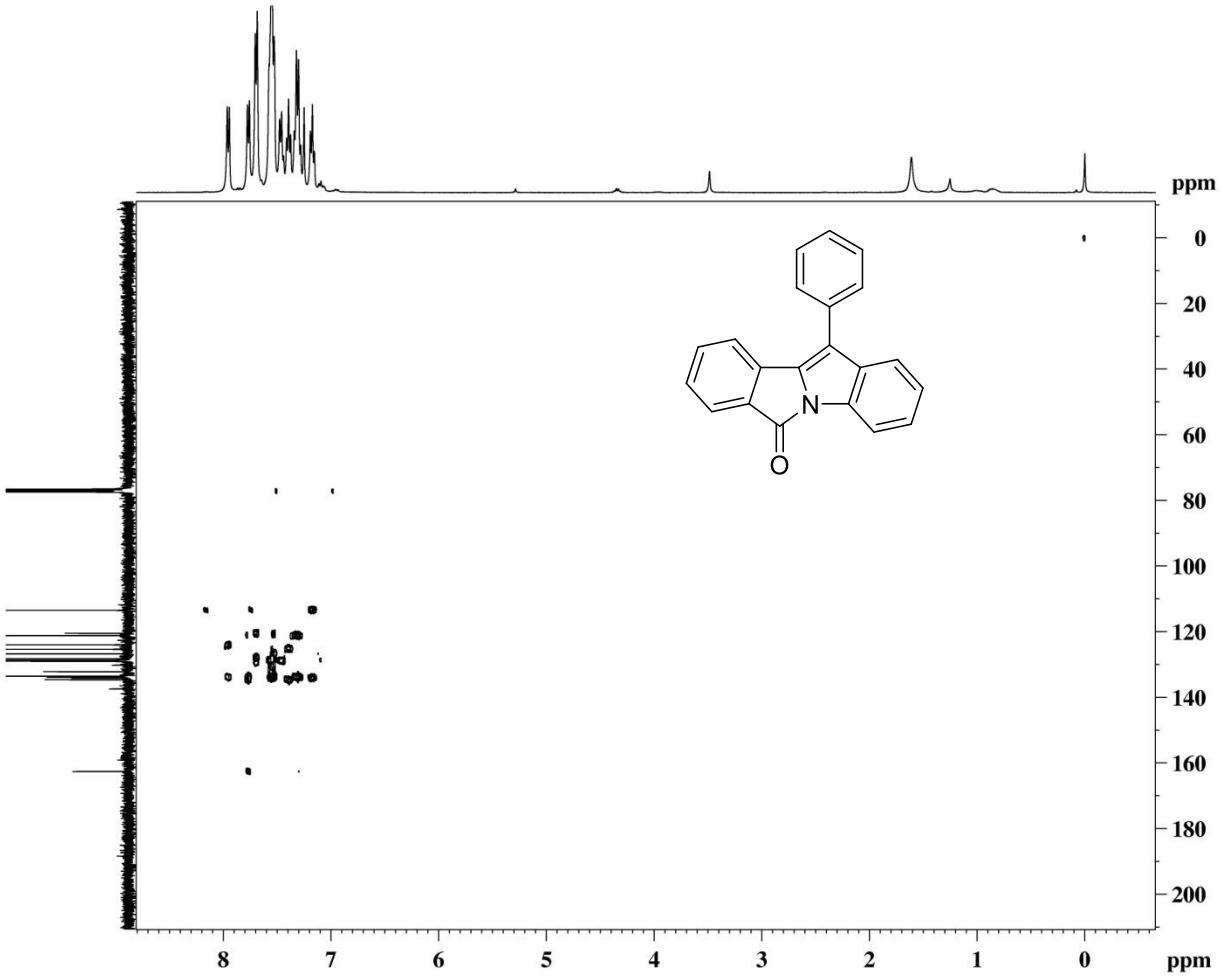
HSQC Spectrum of *11-phenyl-6H-isoindolo[2,1-a]indol-6-one* (2a)



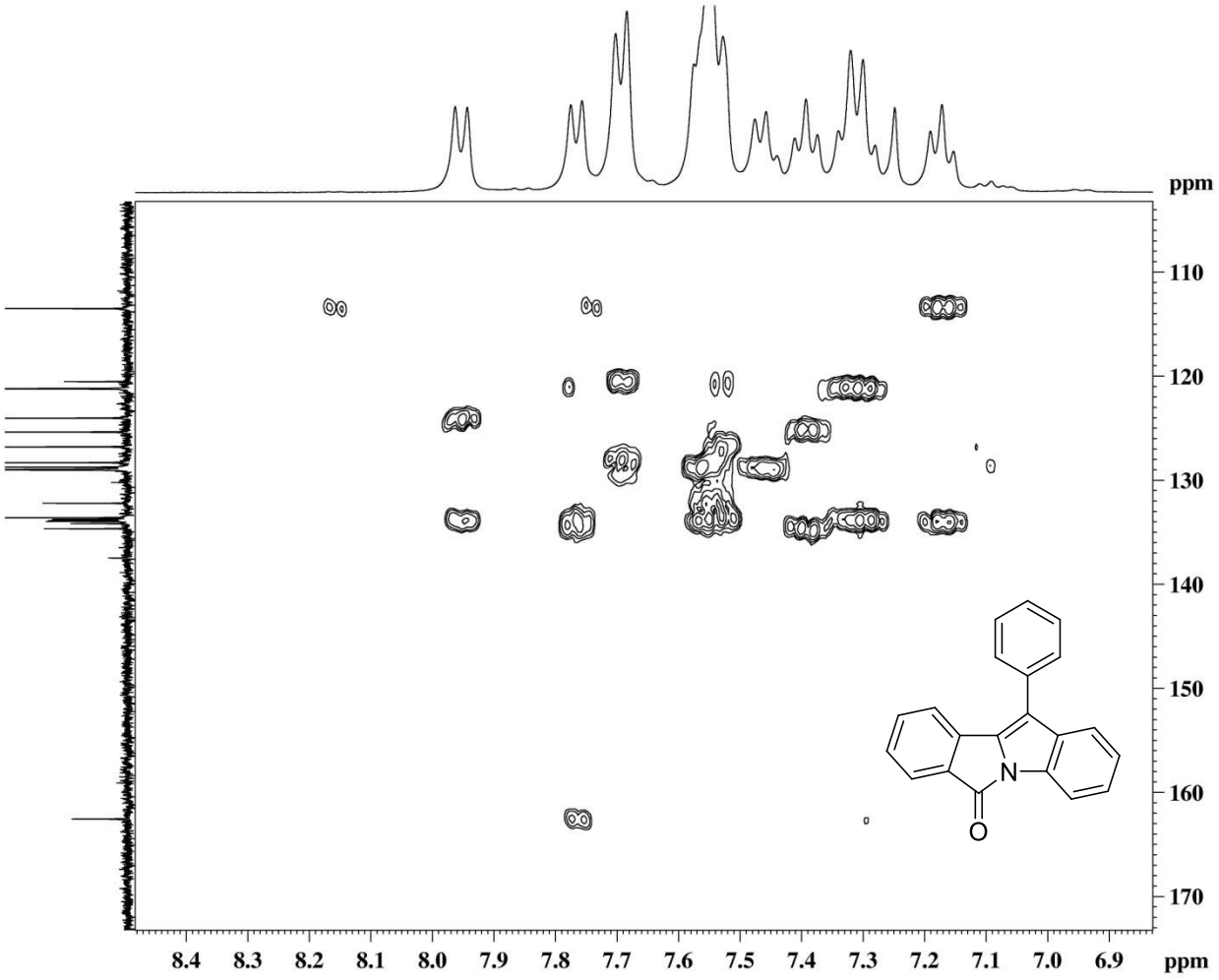
HSQC Spectrum (expansion) of*11-phenyl-6H-isoindolo[2,1-a]indol-6-one* (2a)



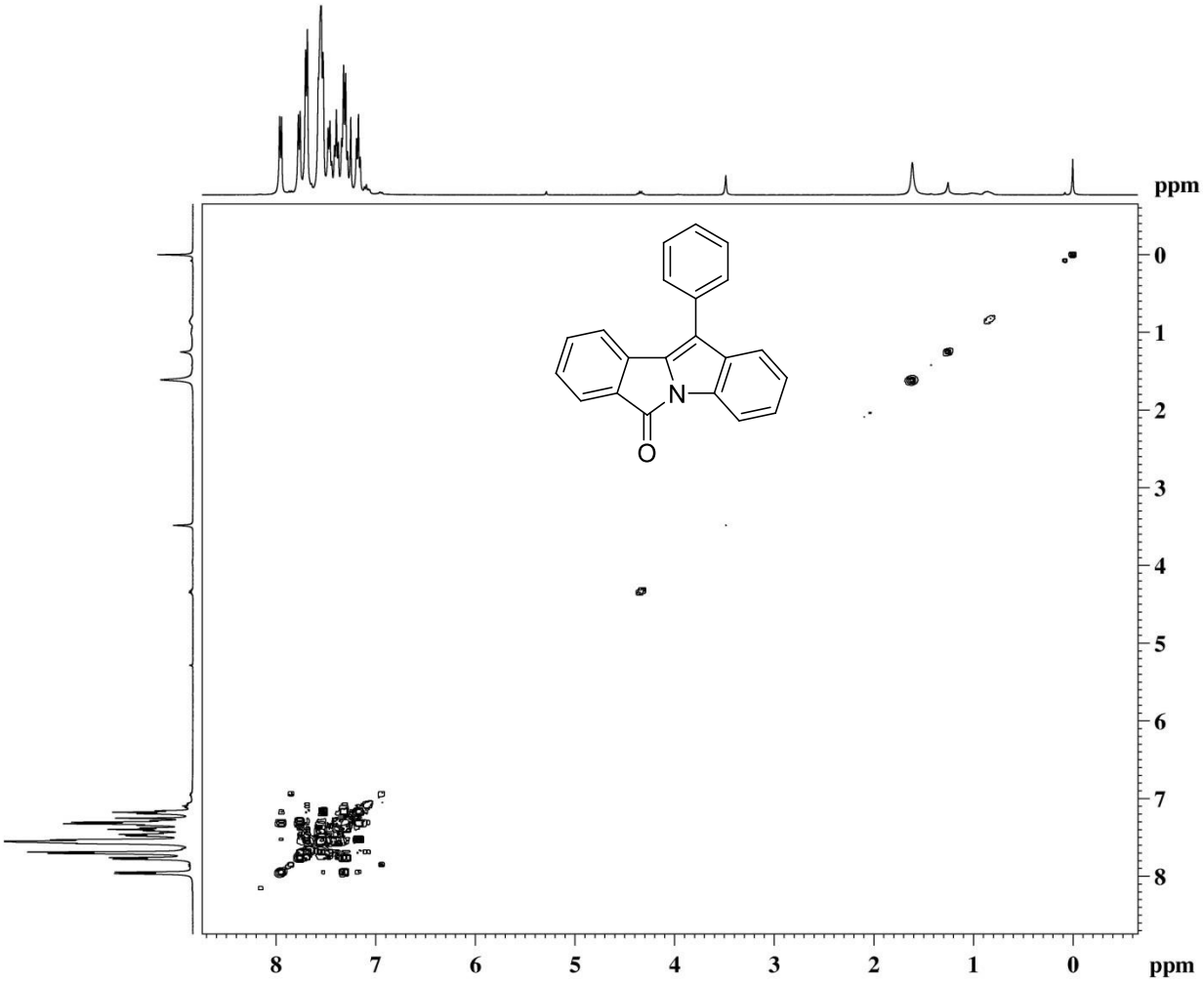
HMBC Spectrum of *11-phenyl-6H-isoindolo[2,1-a]indol-6-one* (2a)



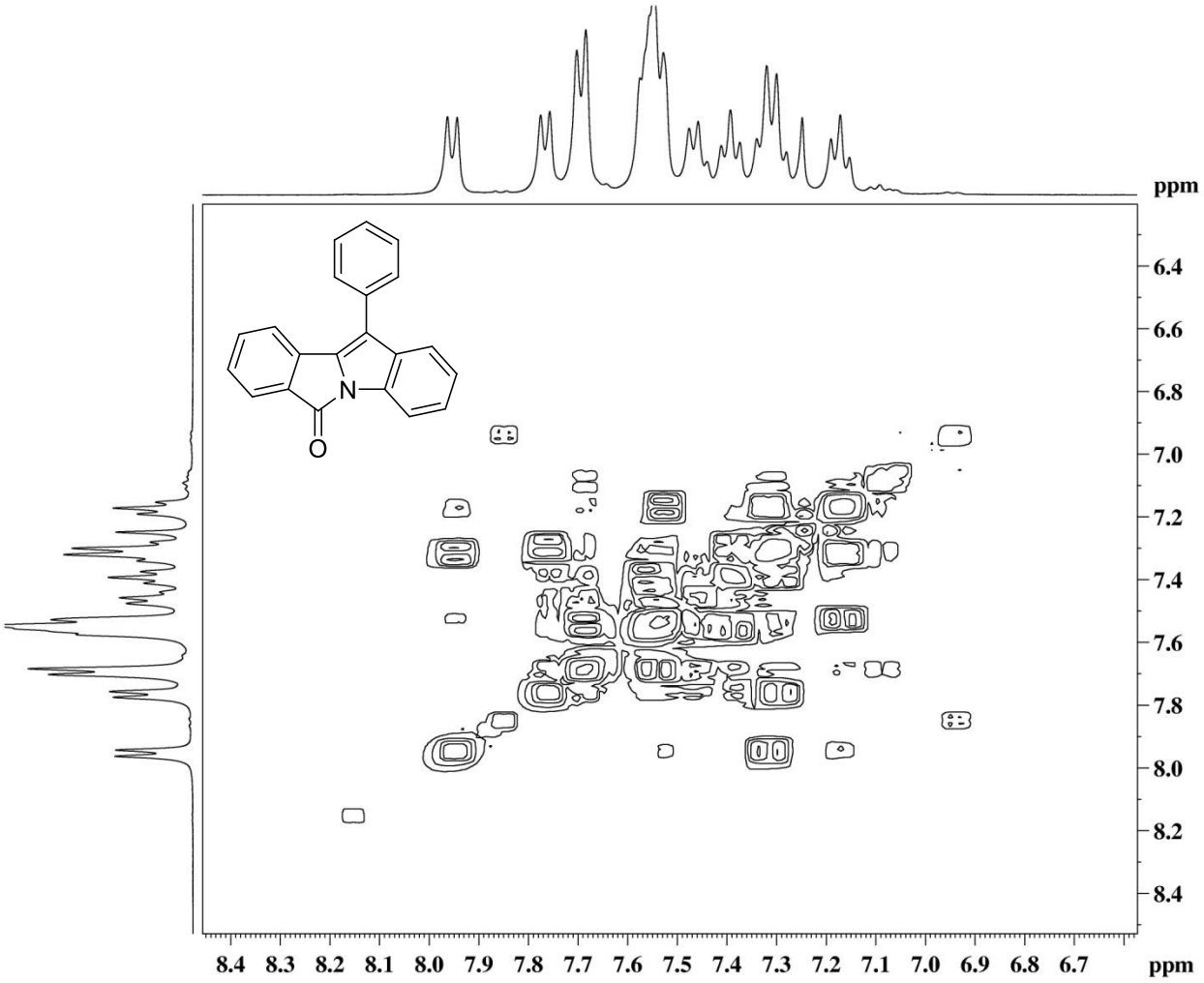
HMBC Spectrum (expansion) of *11-phenyl-6H-isoindolo[2,1-a]indol-6-one* (2a)



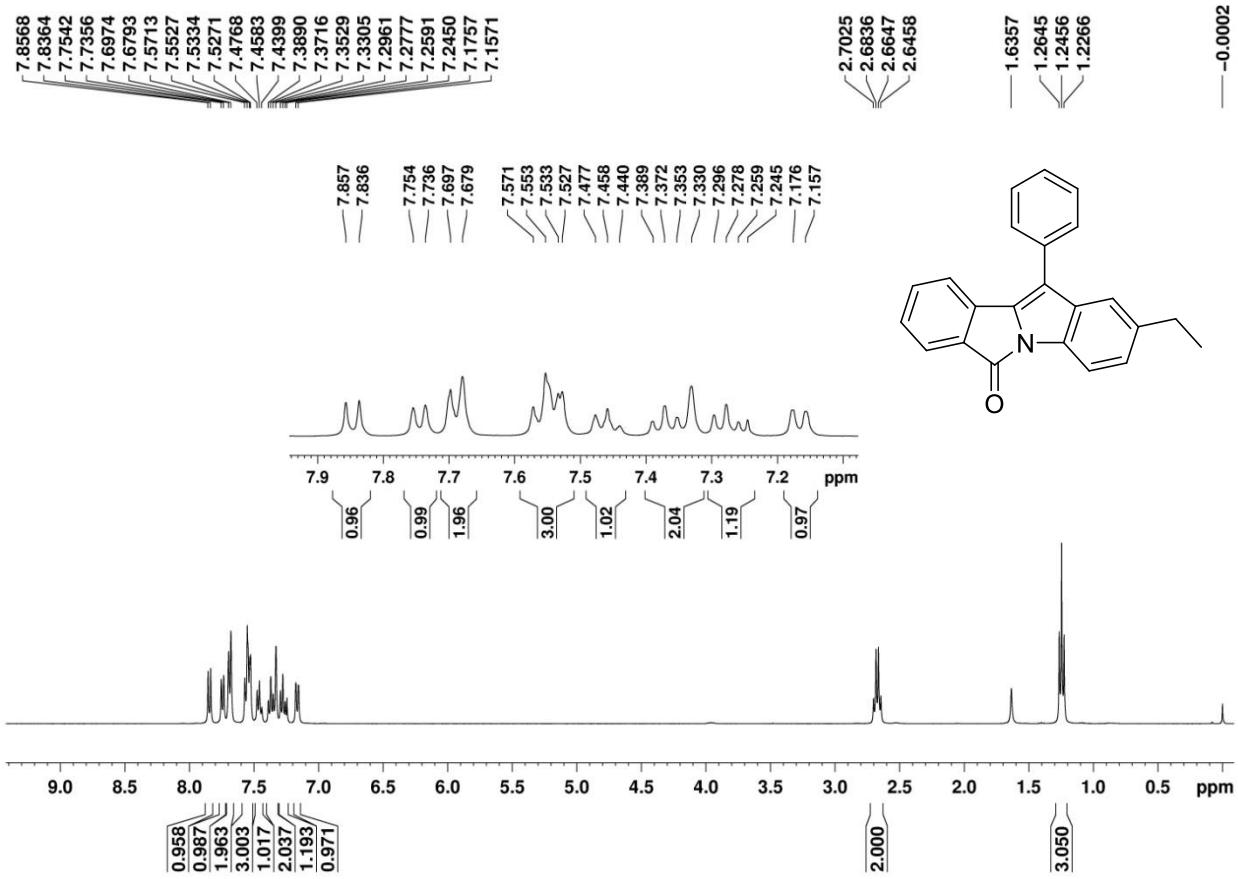
^{1}H-^{1}H COSY Spectrum of *11-phenyl-6H-isoindolo[2,1-a]indol-6-one*(2a)



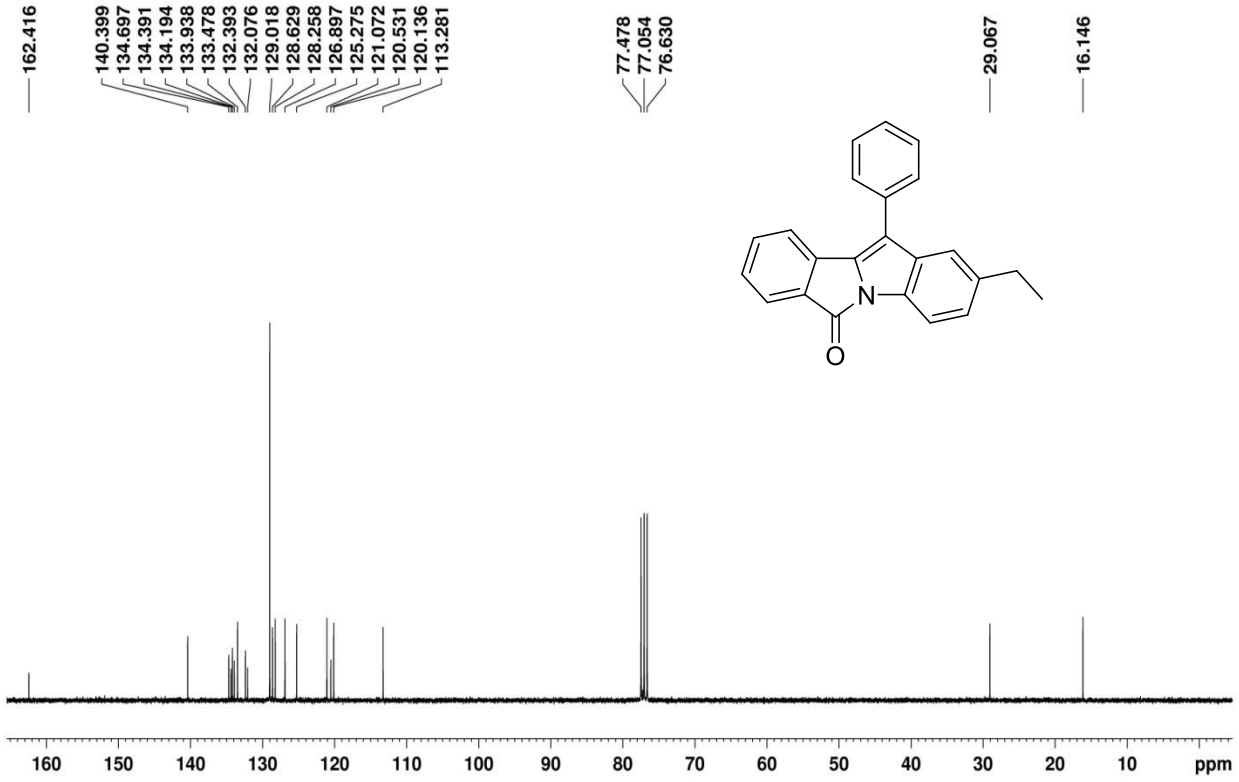
^{1}H-^{1}H COSY Spectrum (expansion) of *11-phenyl-6H-isoindolo[2,1-a]indol-6-one* (2a)



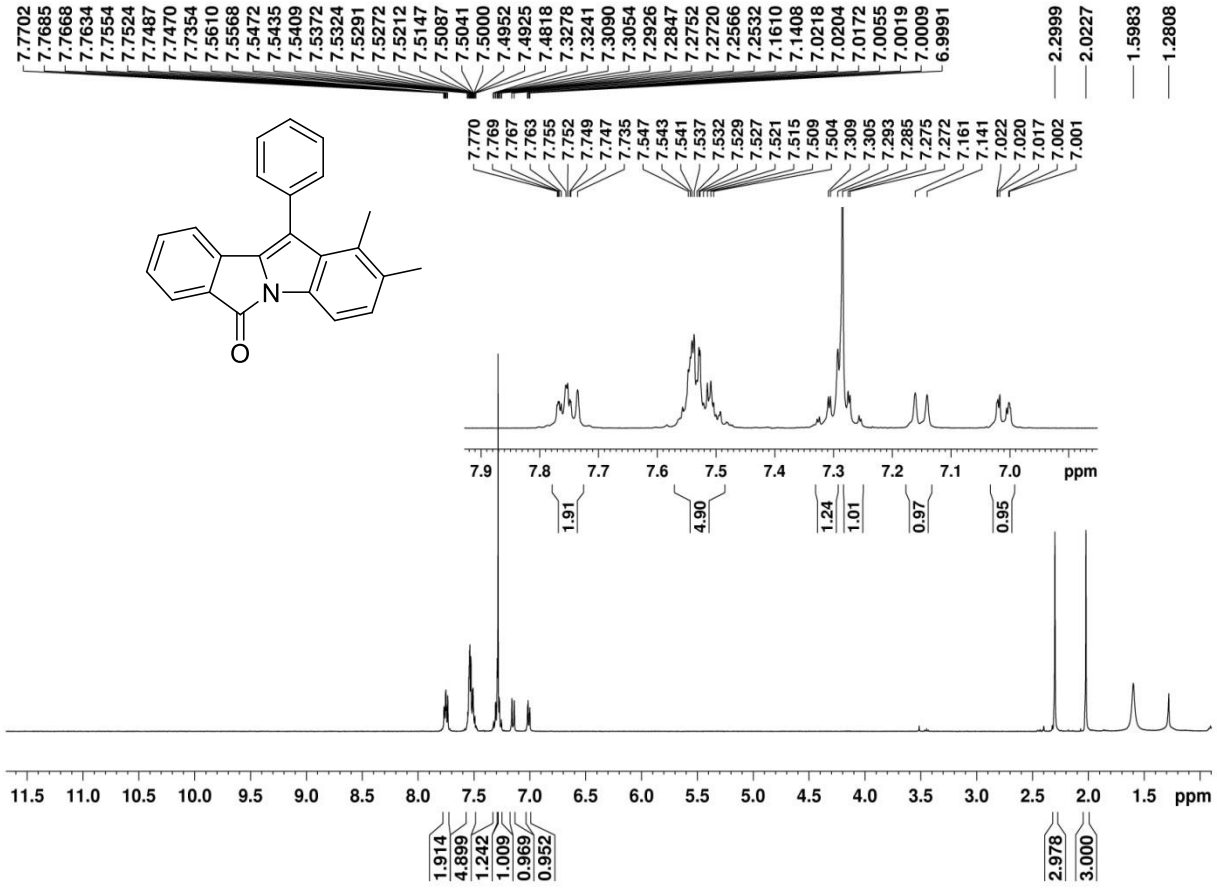
^{1}H NMR Spectrum of *2-ethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one* (2b) (400 MHz, $CDCl_3$)



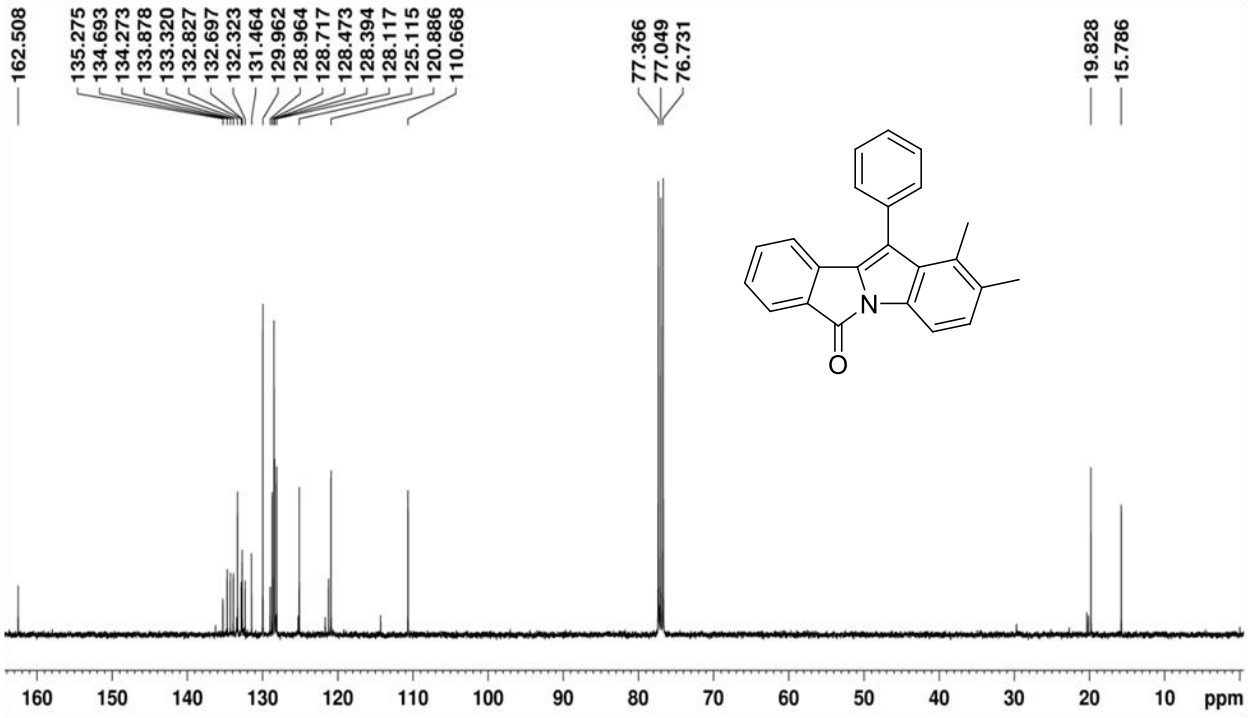
^{13}C NMR Spectrum of *2-ethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one* (2b) (75 MHz, $CDCl_3$)



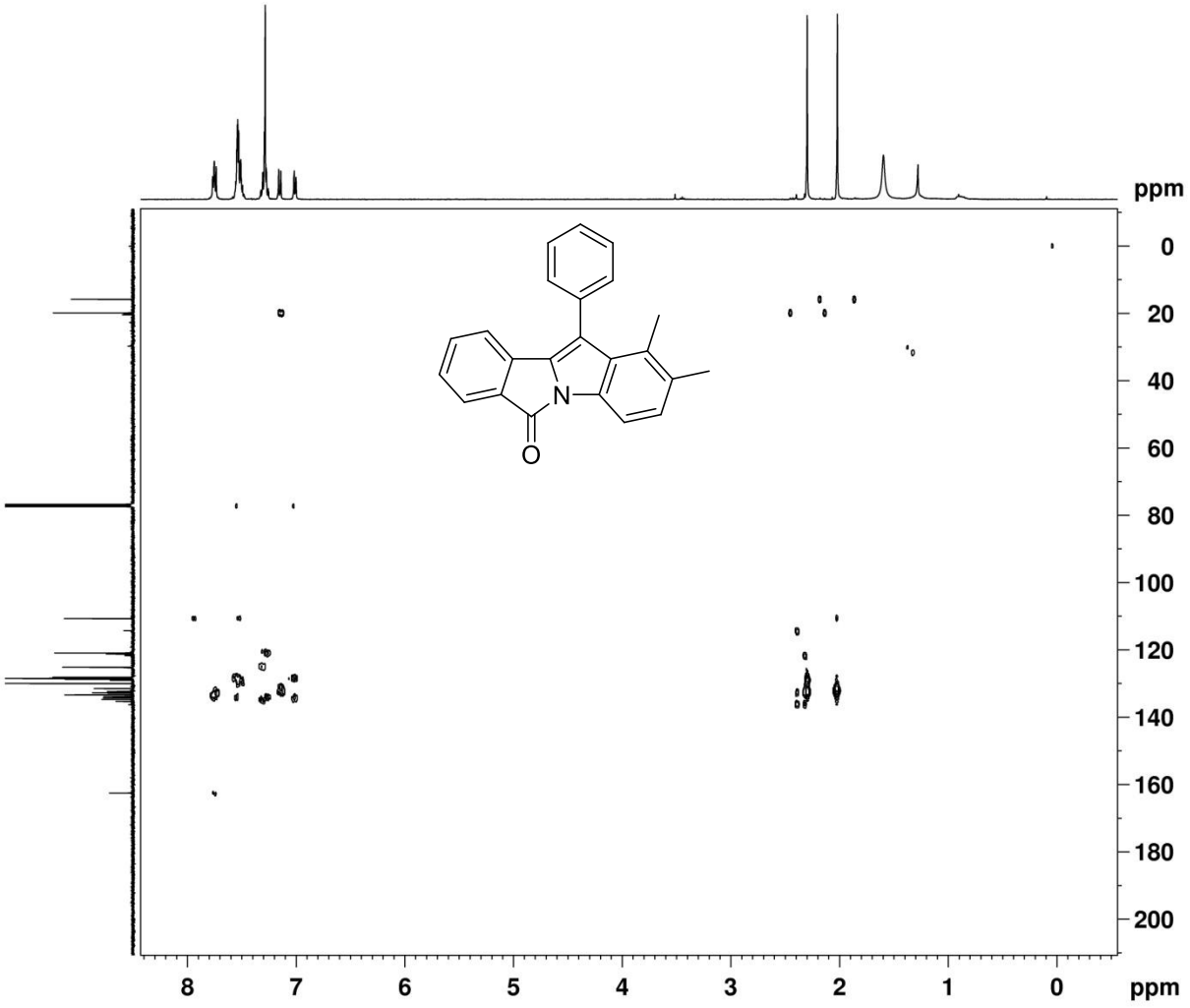
^{1}H NMR Spectrum of *1,2-dimethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one*(2c) (400 MHz, $CDCl_3$)



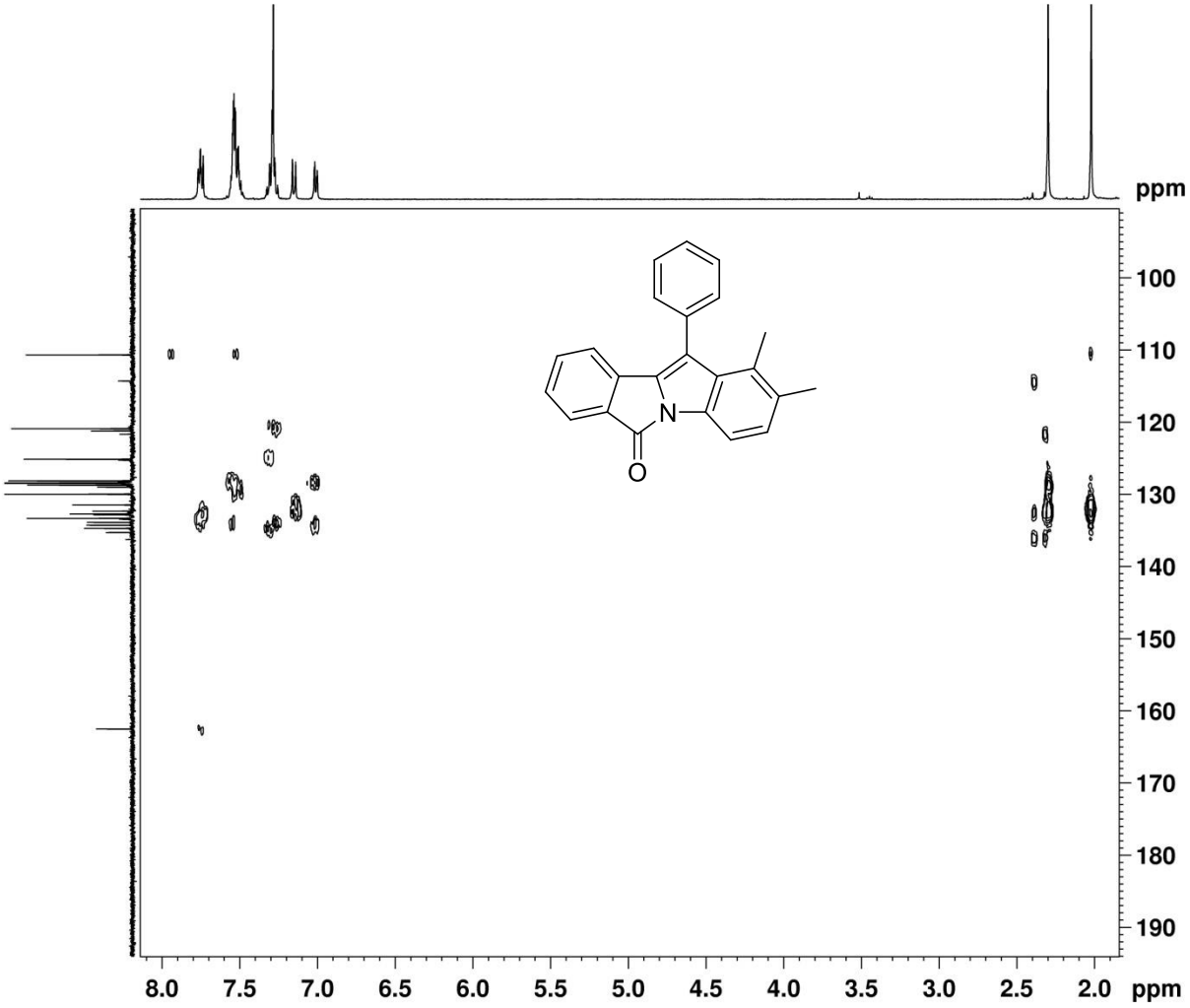
^{13}C NMR Spectrum of *1,2-dimethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one* (2c) (100 MHz, $CDCl_3$)



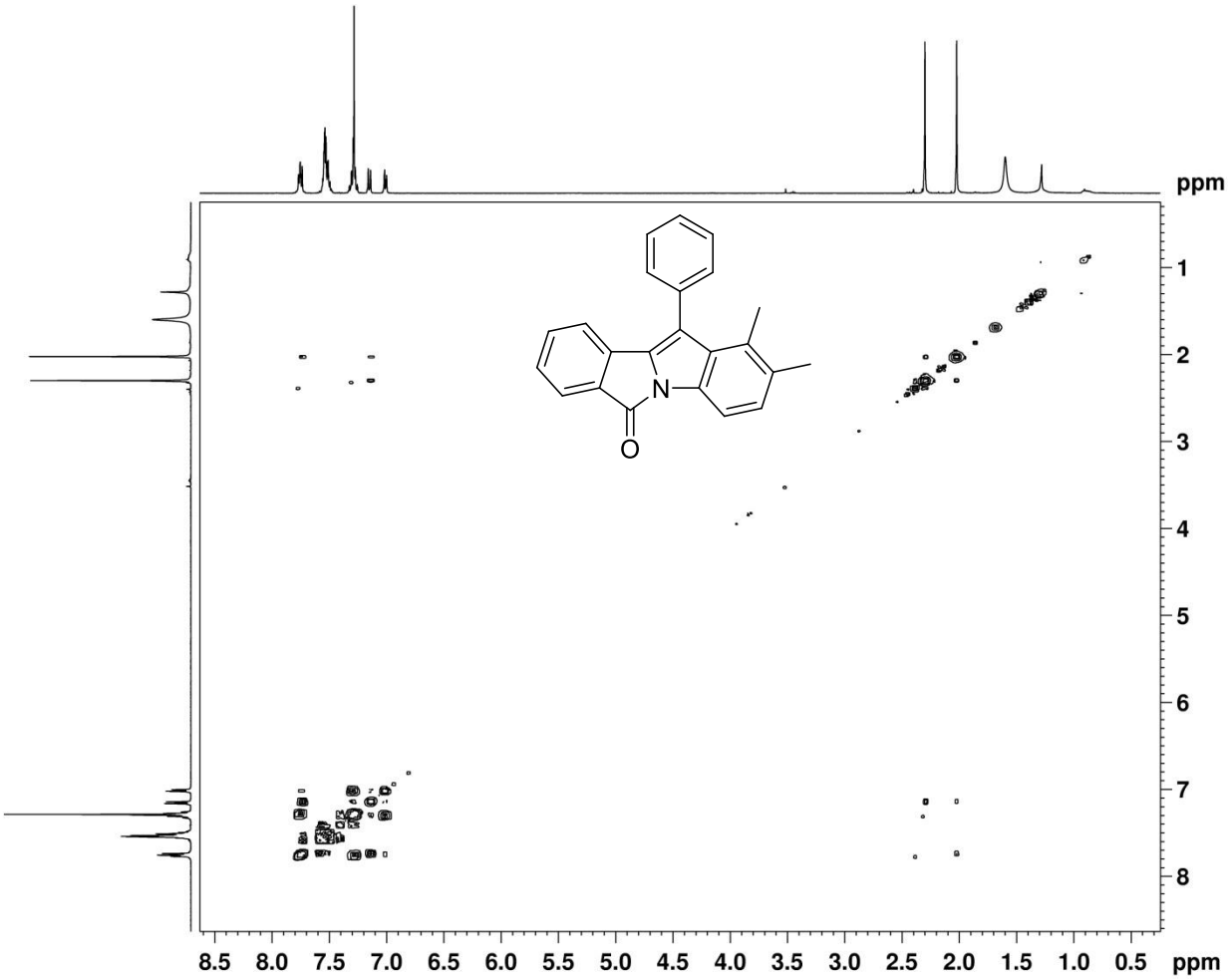
HMBC Spectrum of *1,2-dimethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one* (2c)



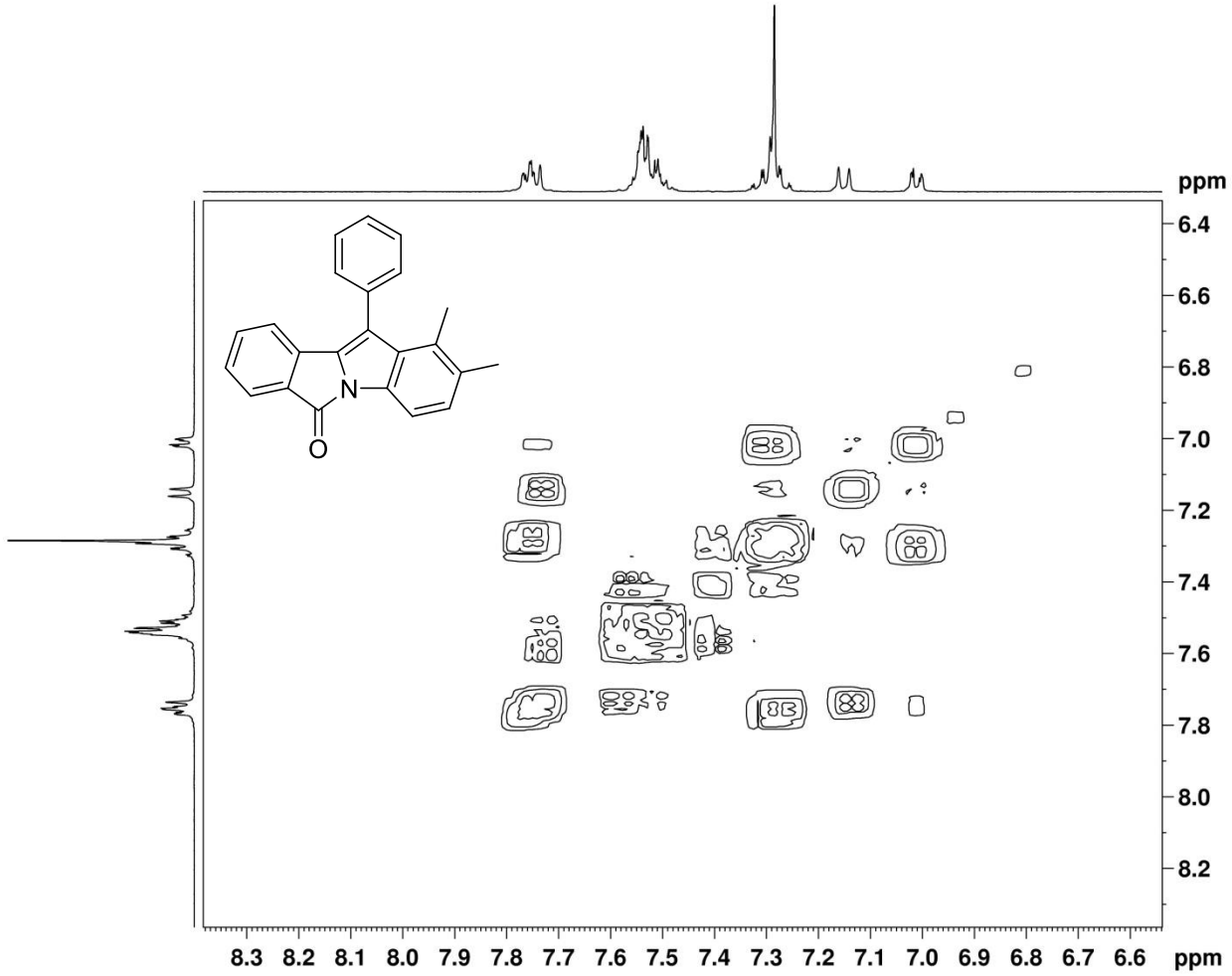
HMBC Spectrum (expansion) of *1,2-dimethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one* (2c)



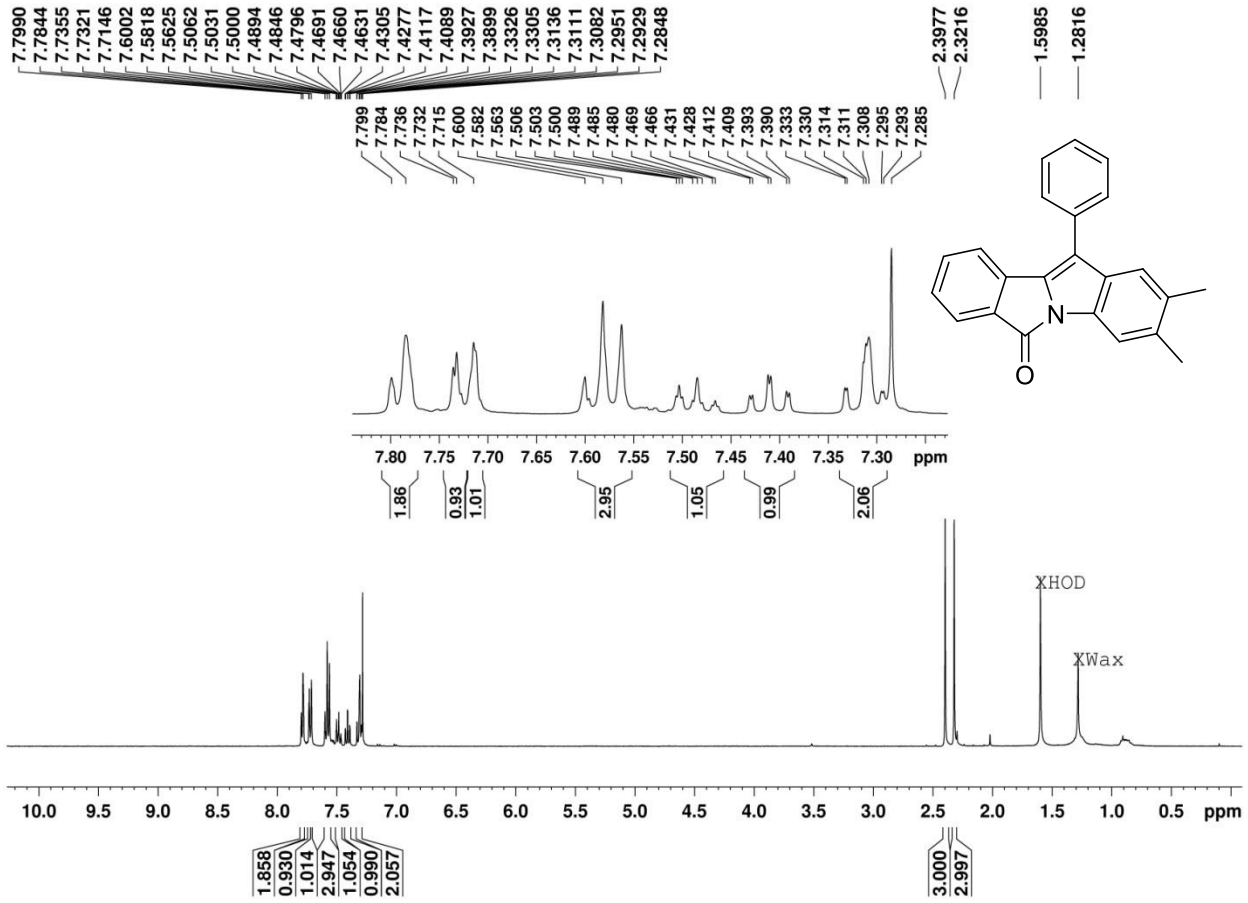
^{1}H-^{1}H COSY Spectrumof *1,2-dimethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one* (2c)



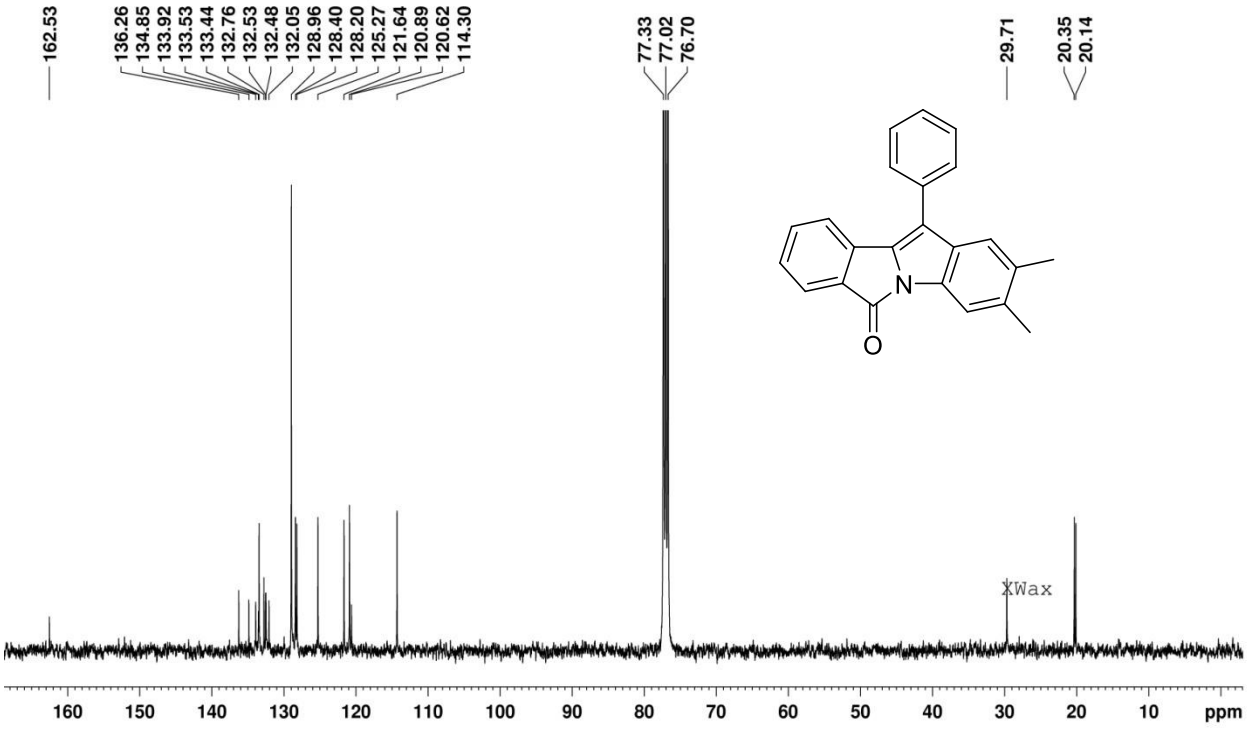
^{1}H-^{1}H COSY Spectrum (expansion) of *1,2-dimethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one* (2c)



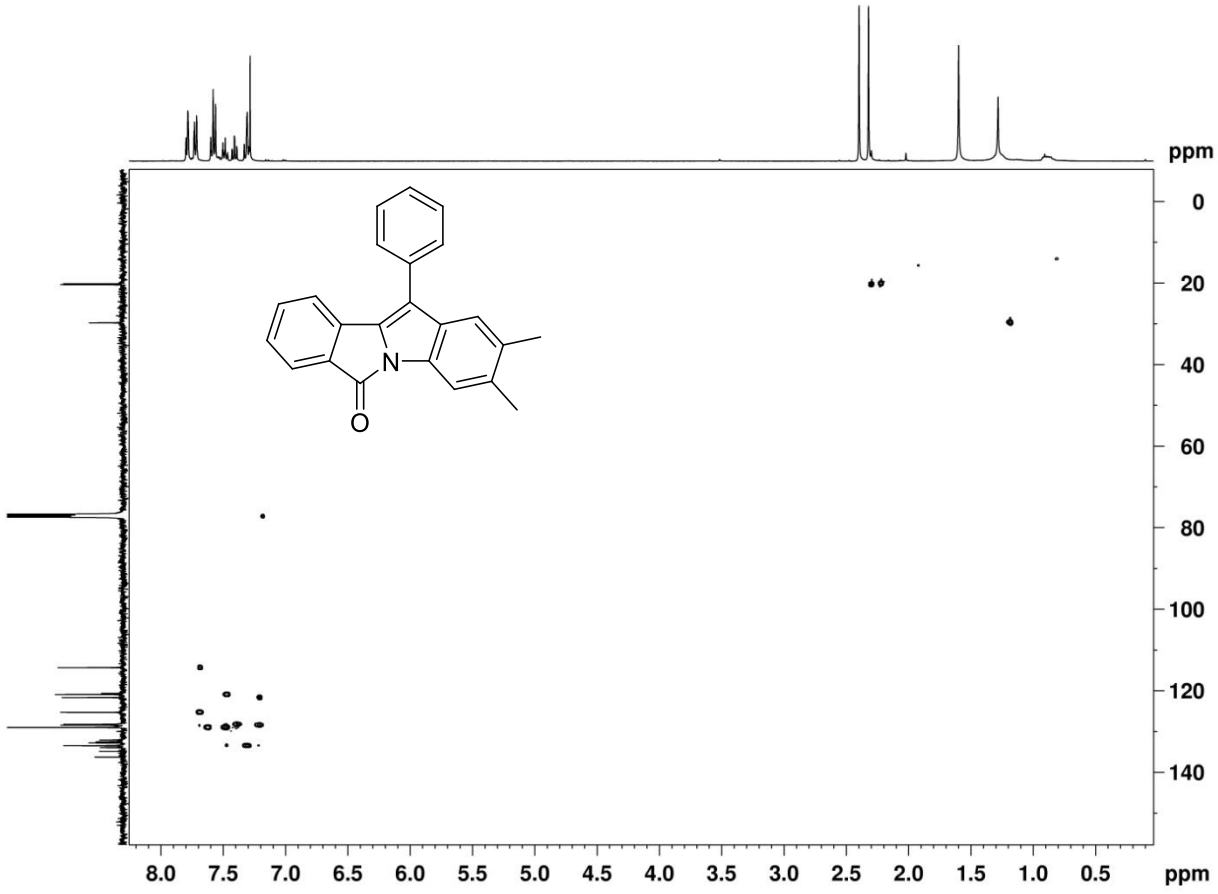
^{1}H NMR Spectrum of *2,3-dimethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one*(2c′) (400 MHz, $CDCl_3$)



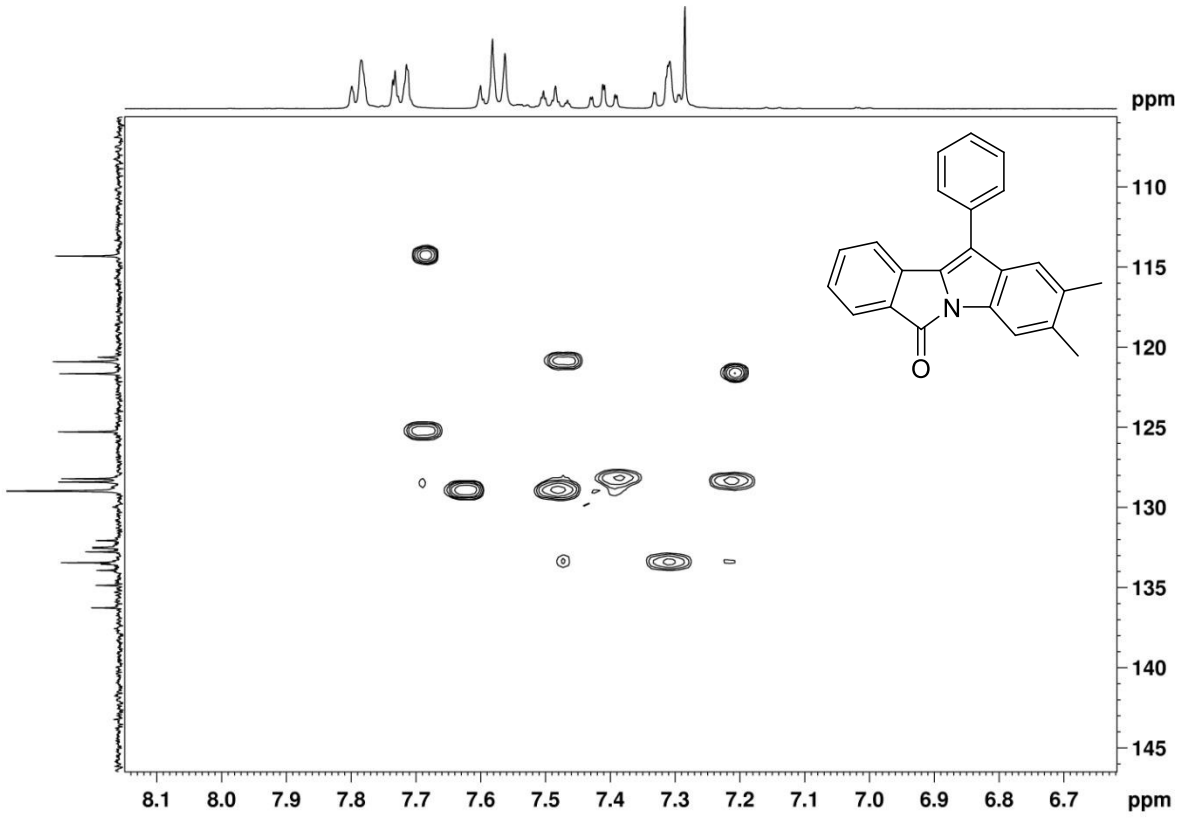
^{13}C NMR Spectrum of *2,3-dimethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one*(2c′) (100 MHz, $CDCl_3$)



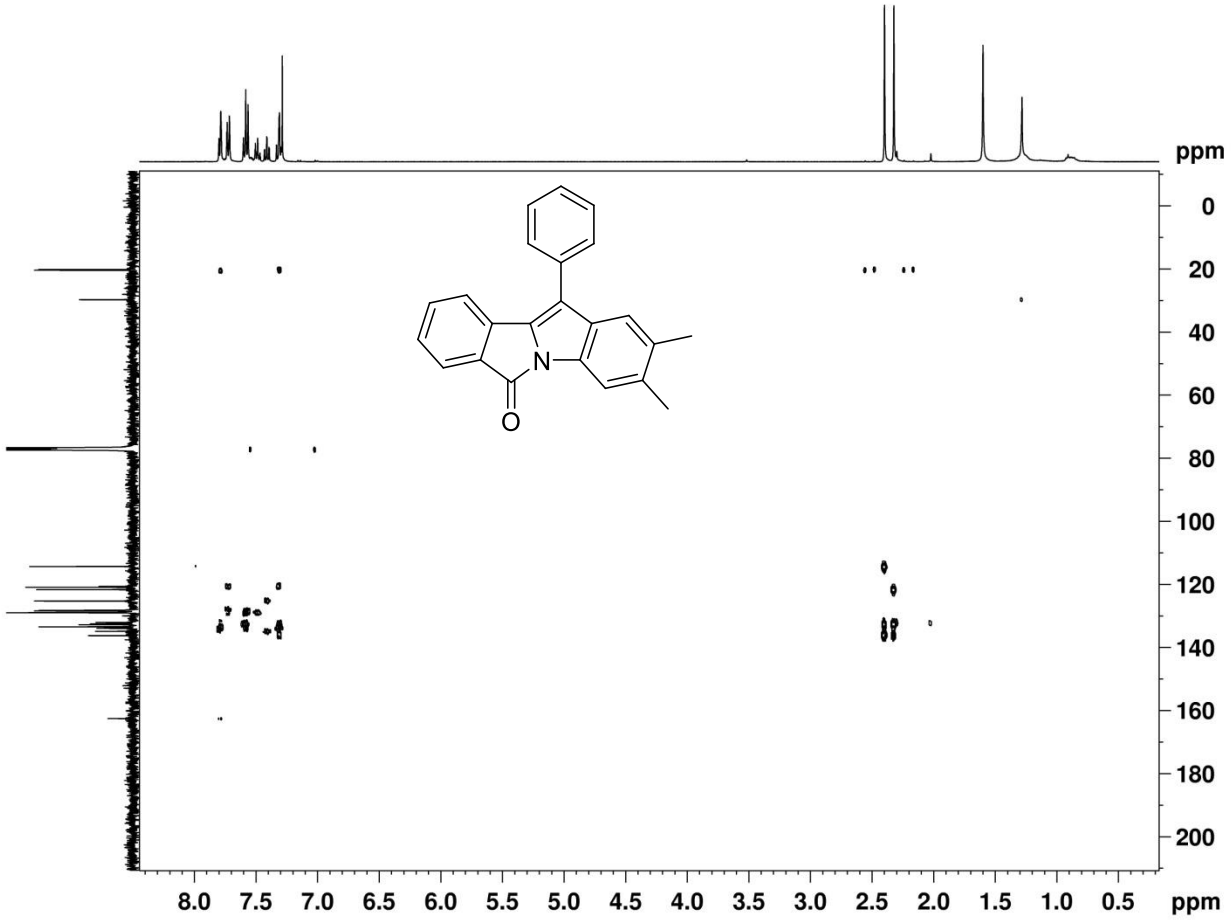
HSQC Spectrum of *2,3-dimethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one*(2c′)



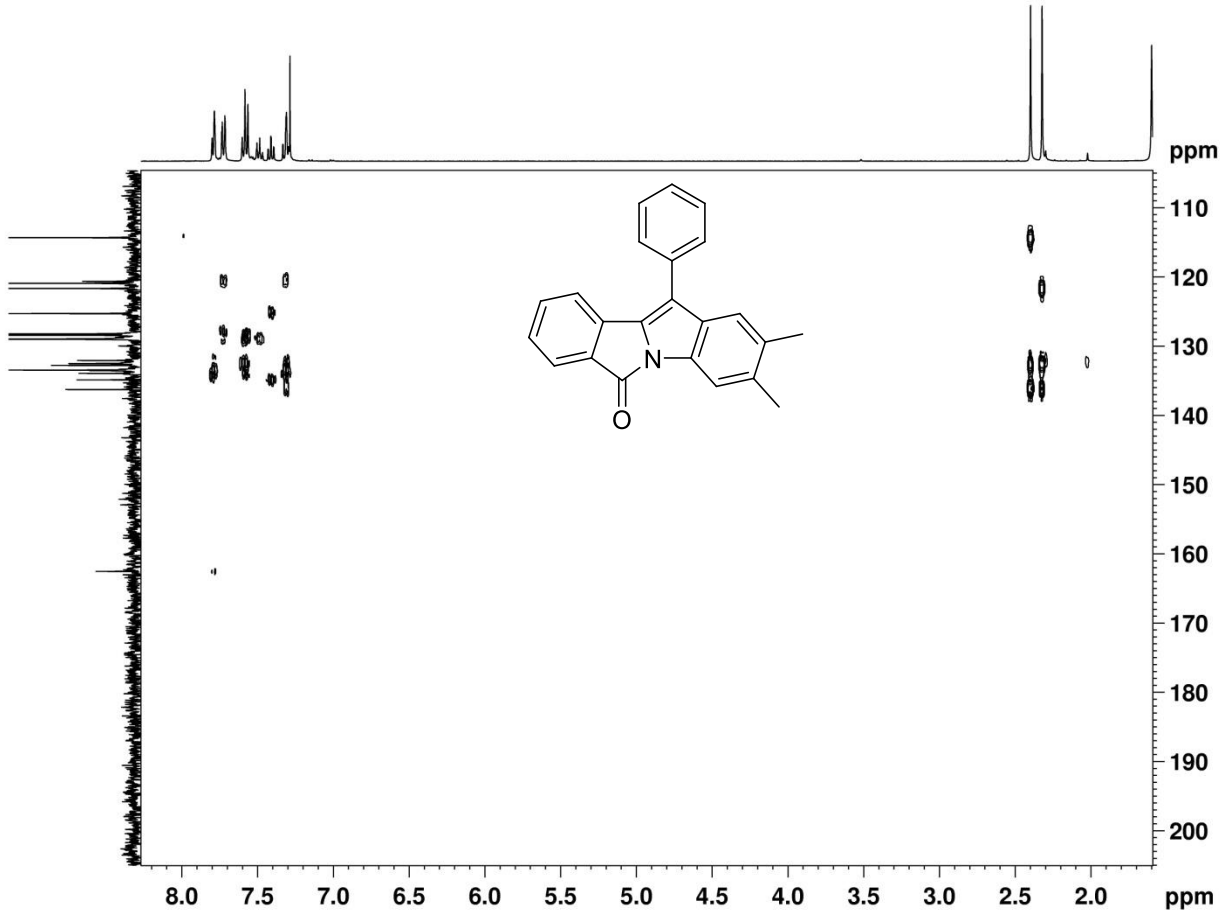
HSQC Spectrum (expansion) of *2,3-dimethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one*(2c′)



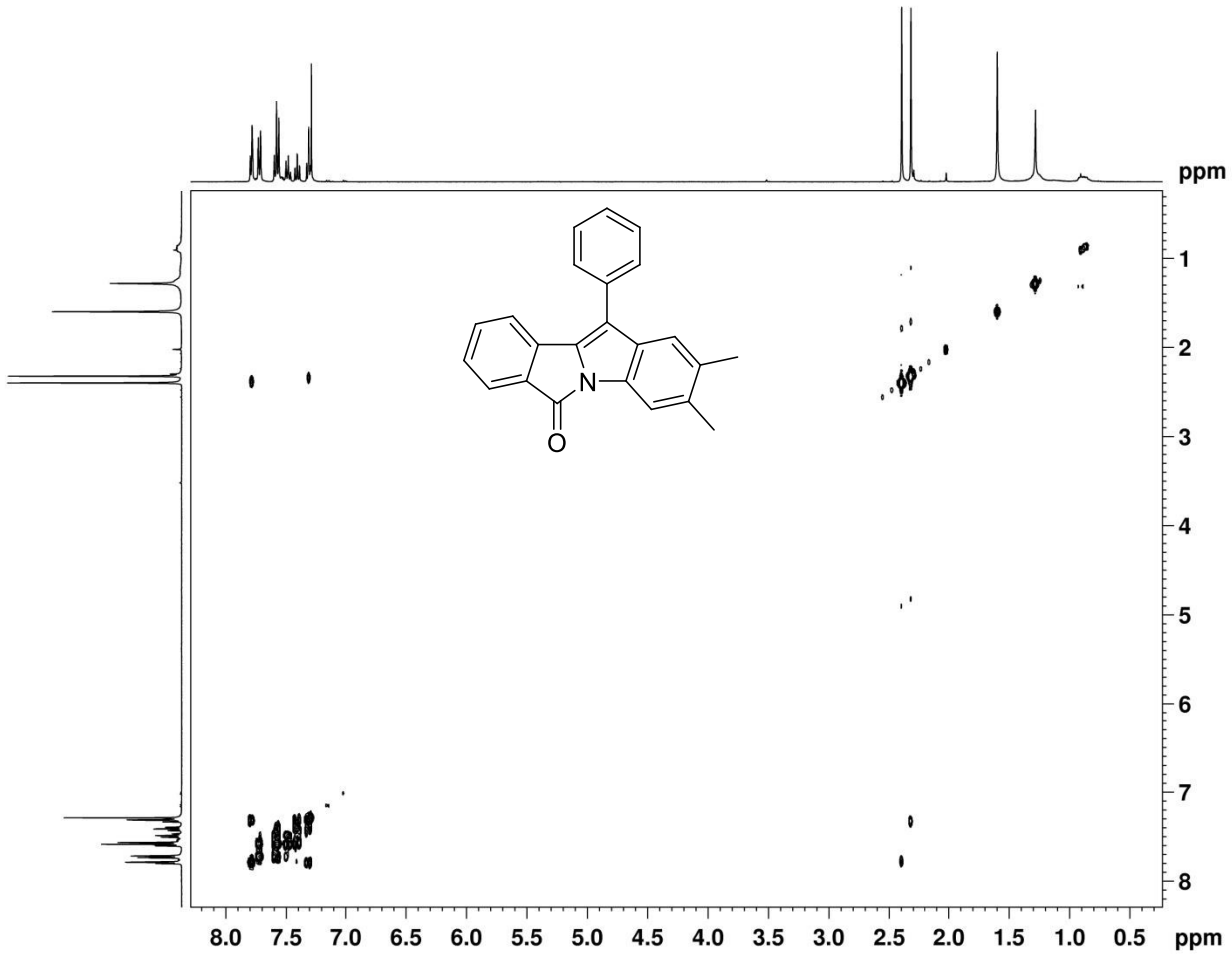
HMBC Spectrum of *2,3-dimethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one*(2c′)



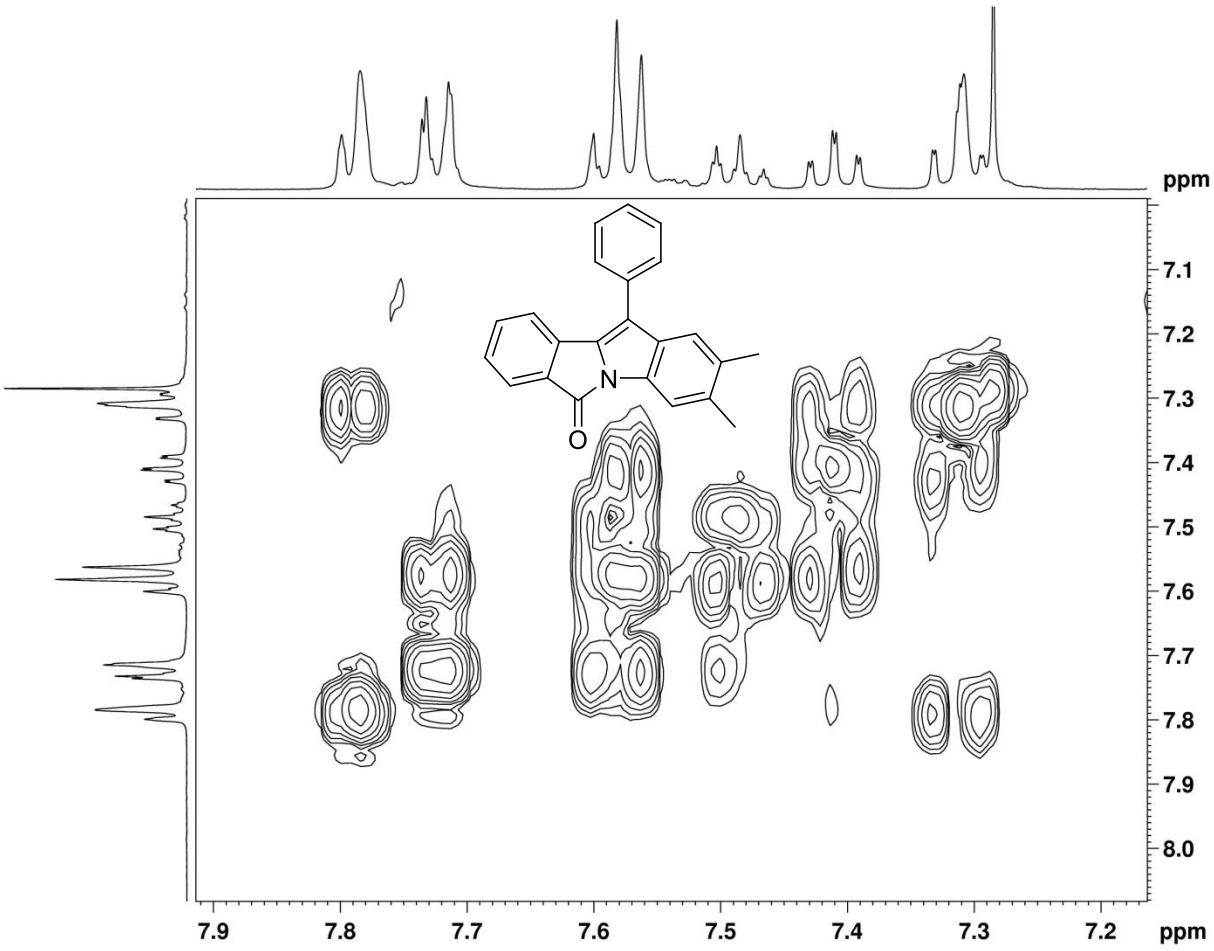
HMBC Spectrum(expansion) of *2,3-dimethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one*(2c′)



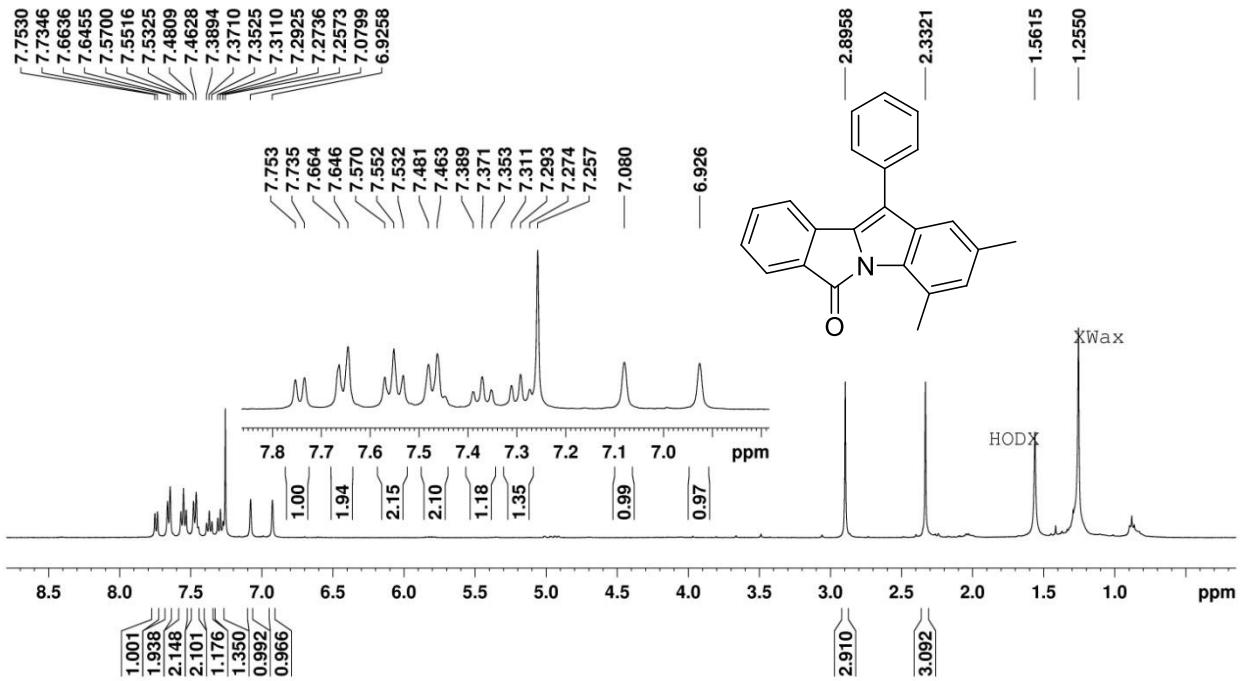
^{1}H-^{1}H COSY Spectrum of *2,3-dimethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one*(2c′)



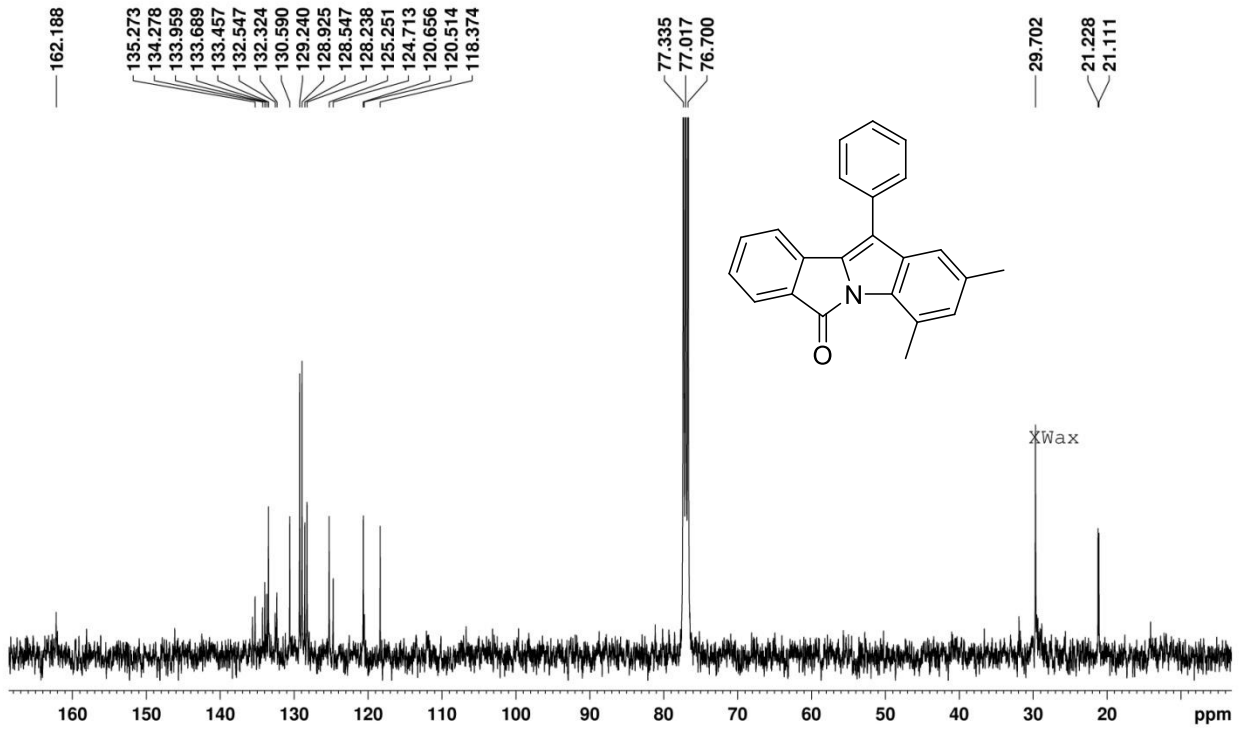
^{1}H-^{1}H COSY Spectrum (expansion) of *2,3-dimethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one*(2c′)



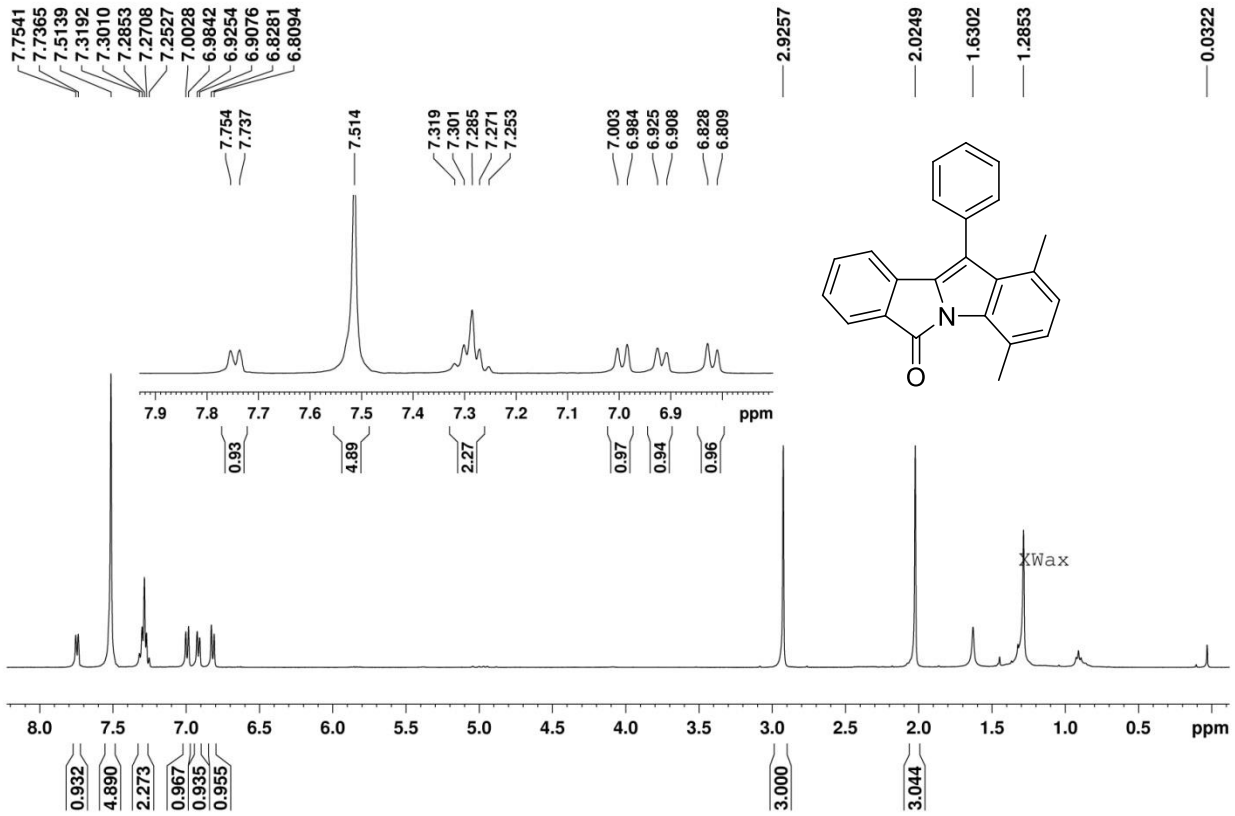
^{1}H NMR Spectrum of *2,4-dimethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one*(2d) (400 MHz, $CDCl_3$)



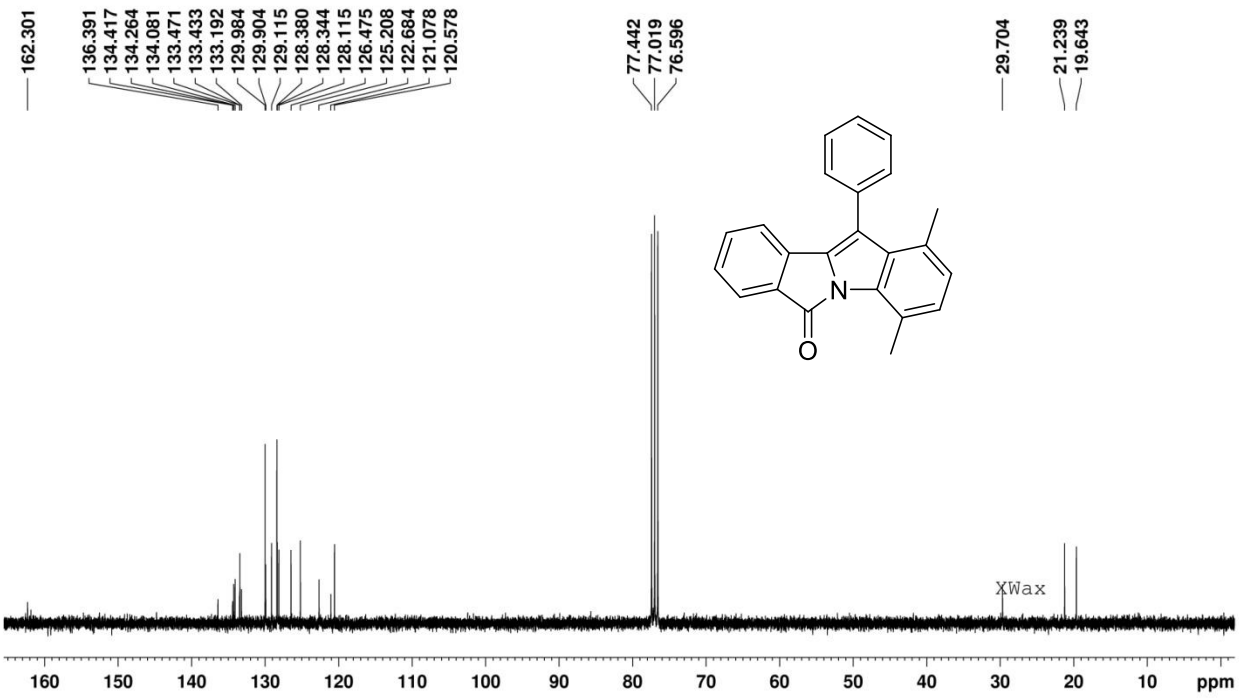
^{13}C NMR Spectrum of *2,4-dimethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one* (2d) (100 MHz, $CDCl_3$)



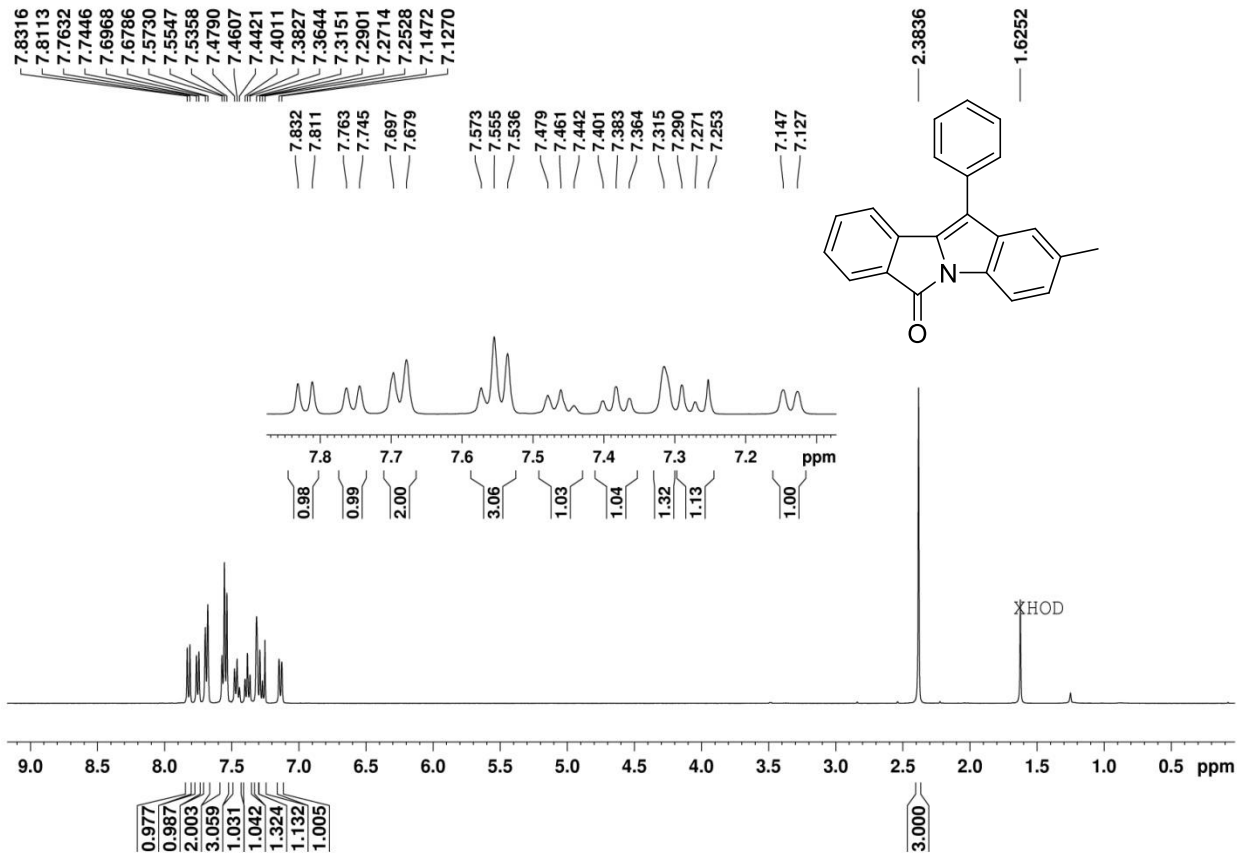
^{1}H NMR Spectrum of *1,4-dimethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one* (2e) (400 MHz, $CDCl_3$)



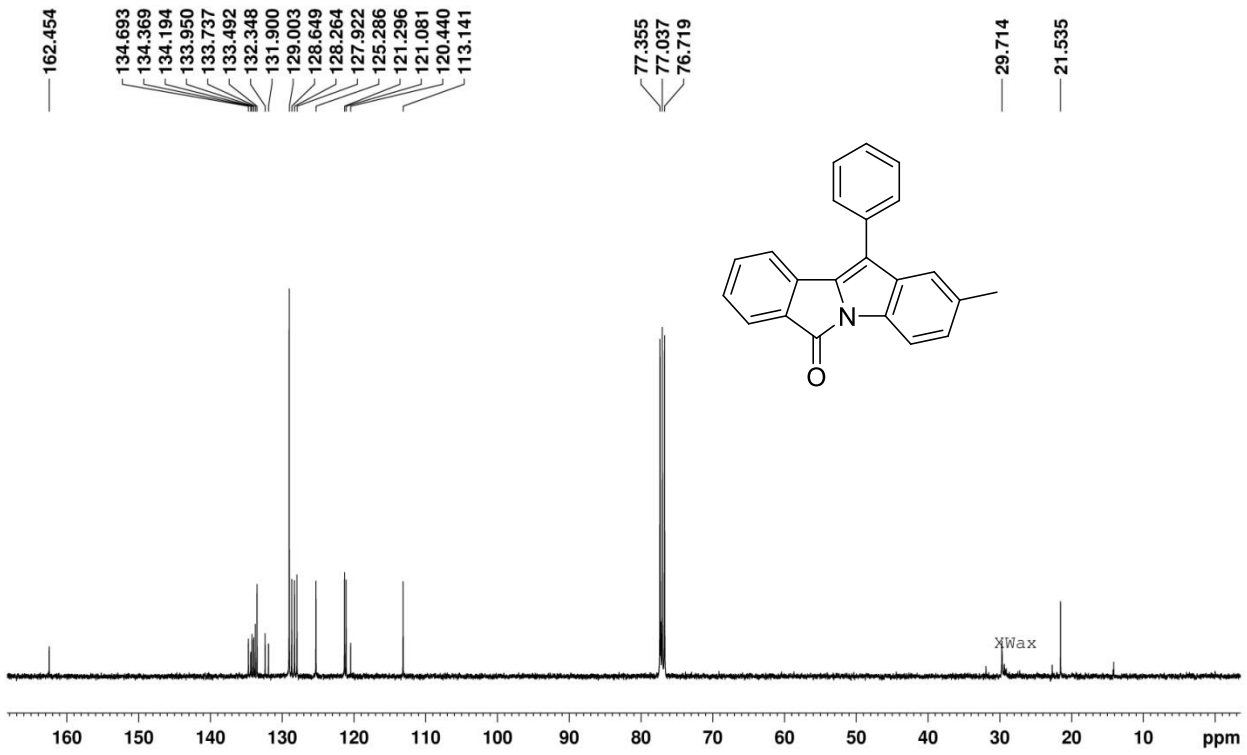
^{13}C NMR Spectrum of *1,4-dimethyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one* (2e) (75 MHz, $CDCl_3$)



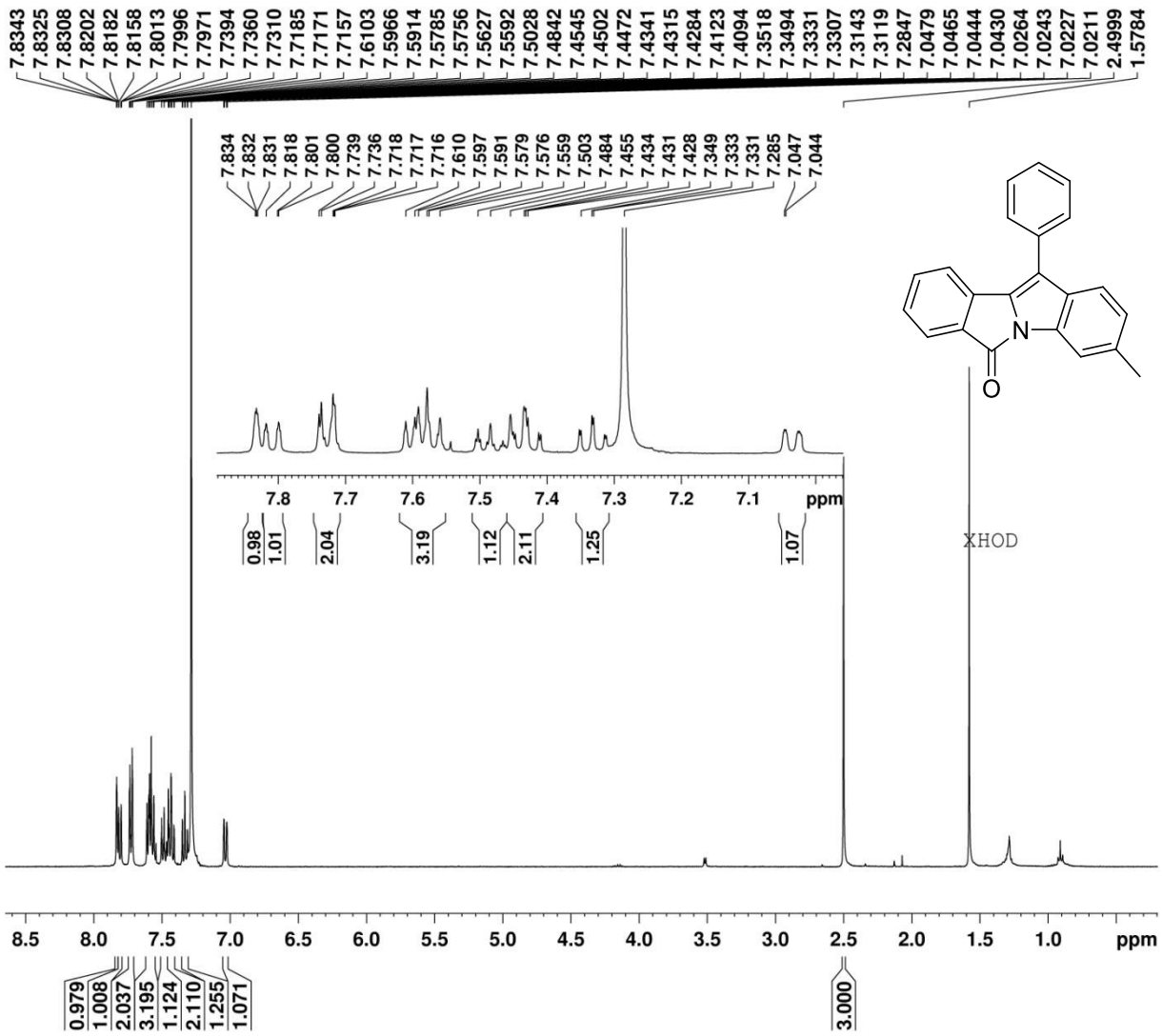
^{1}H NMR Spectrum of *2-methyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one* (2f) (400 MHz, $CDCl_3$)



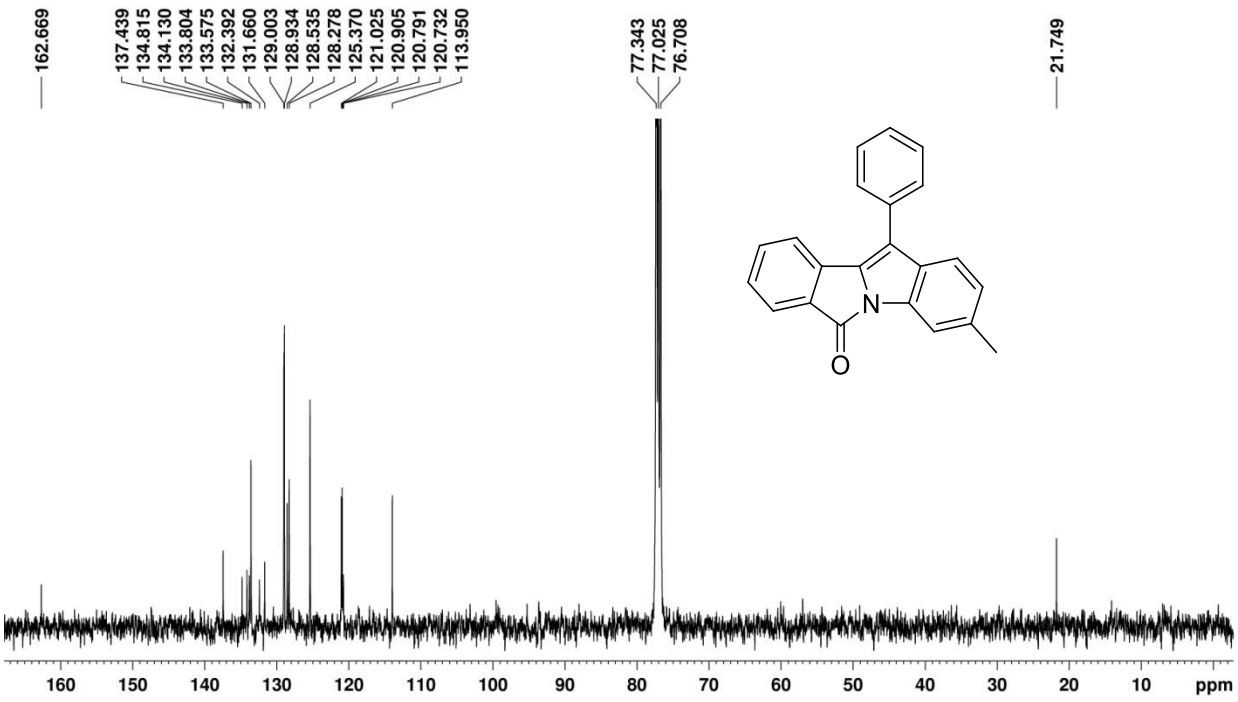
^{13}C NMR Spectrum of *2-methyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one* (2f) (100 MHz, $CDCl_3$)



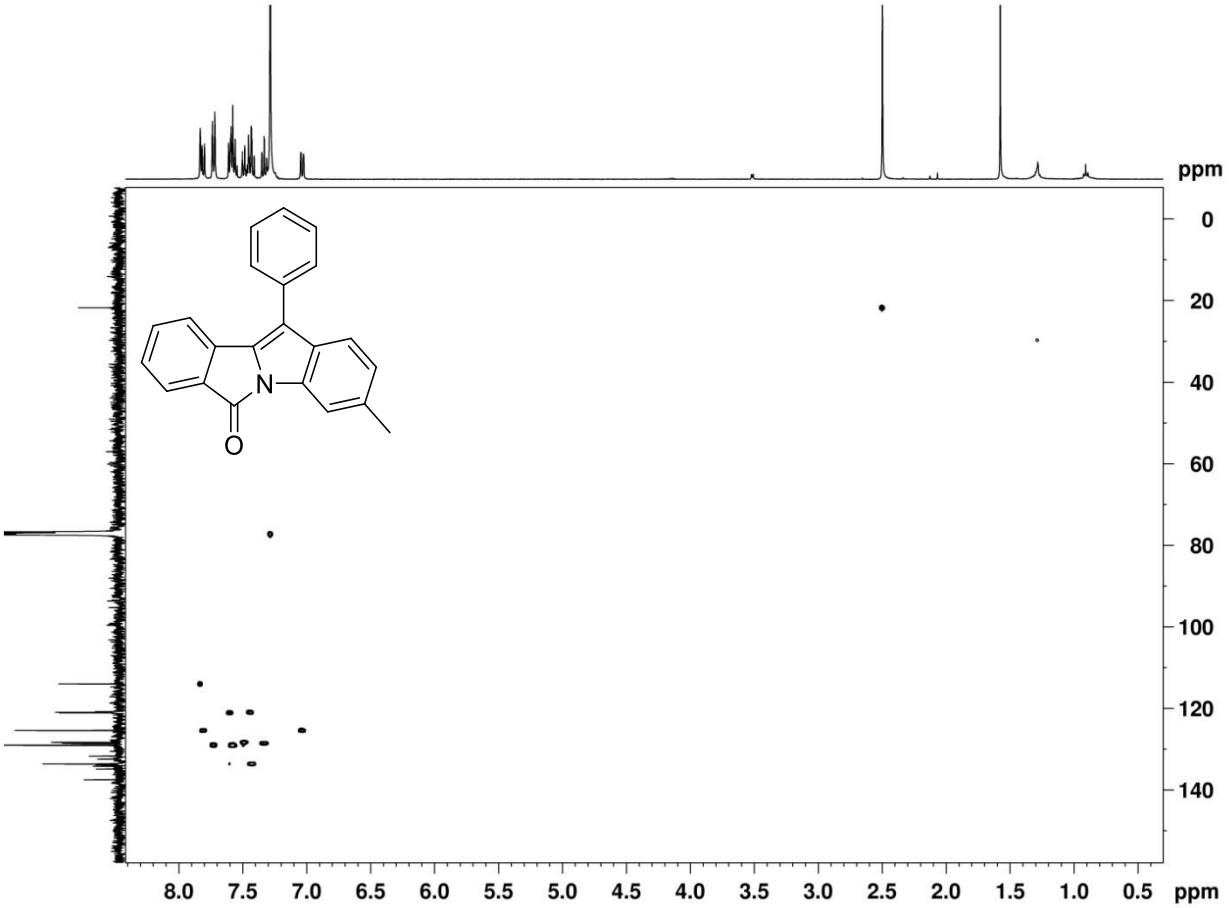
^{1}H NMR Spectrum of *3-methyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one*(2g) (400 MHz, $CDCl_3$)



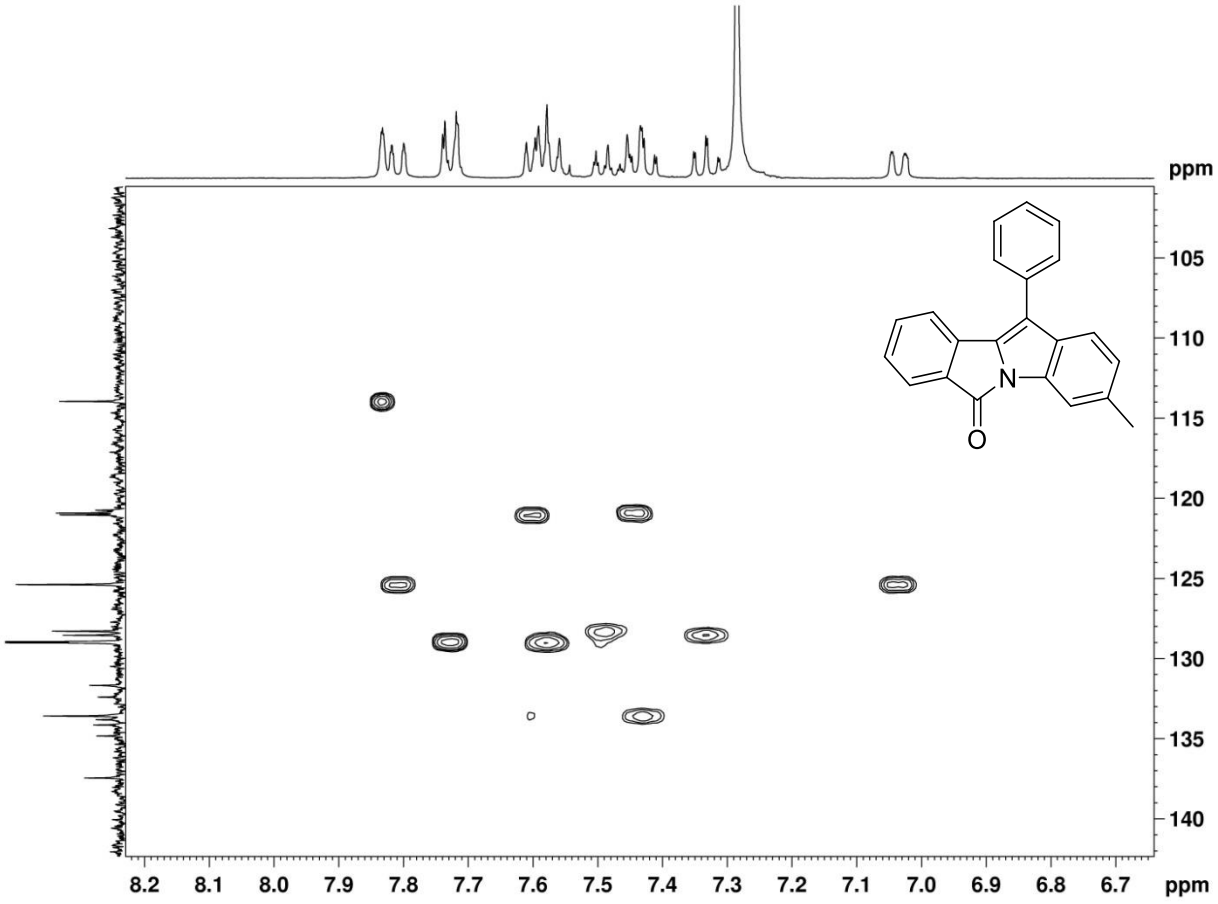
^{13}C NMR Spectrum of *3-methyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one* (2g) (100 MHz, $CDCl_3$)



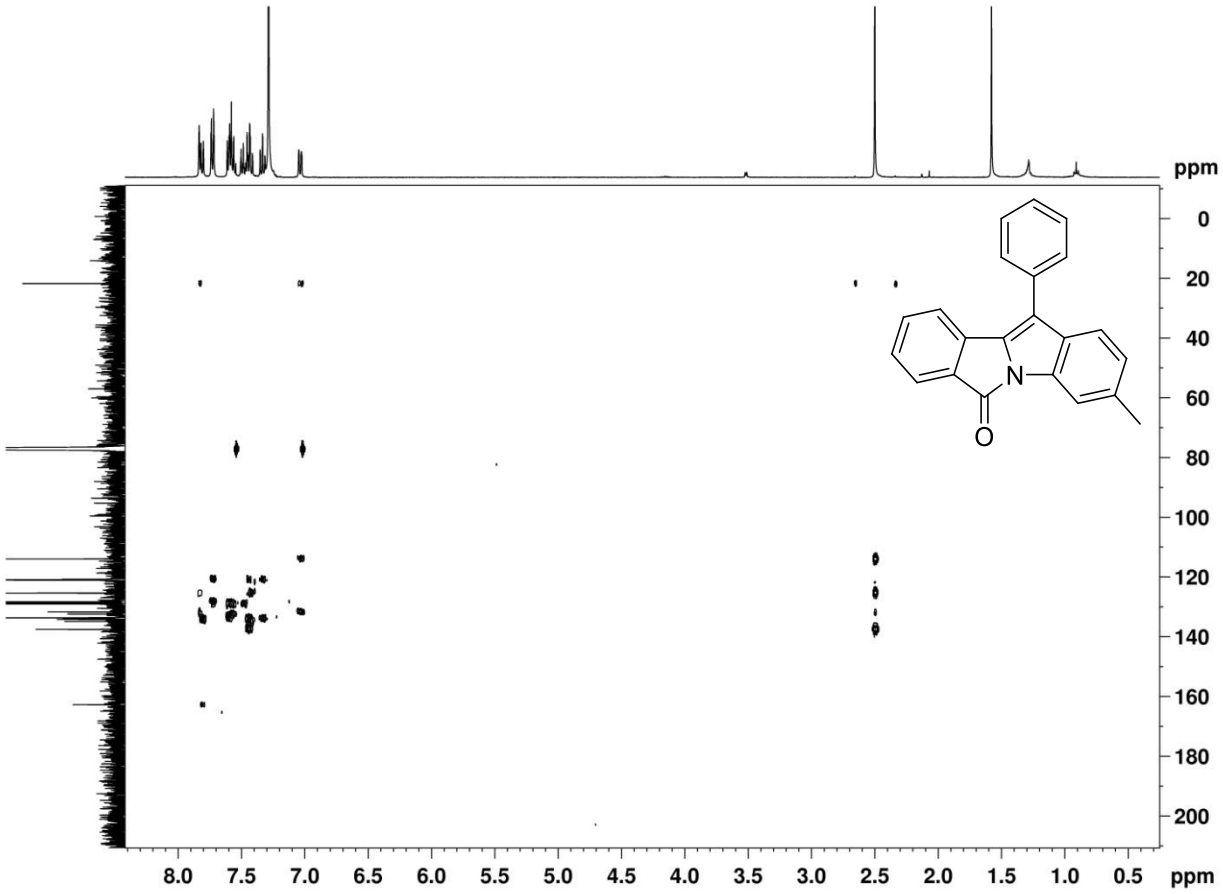
HSQC Spectrum of *3-methyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one*(2g)



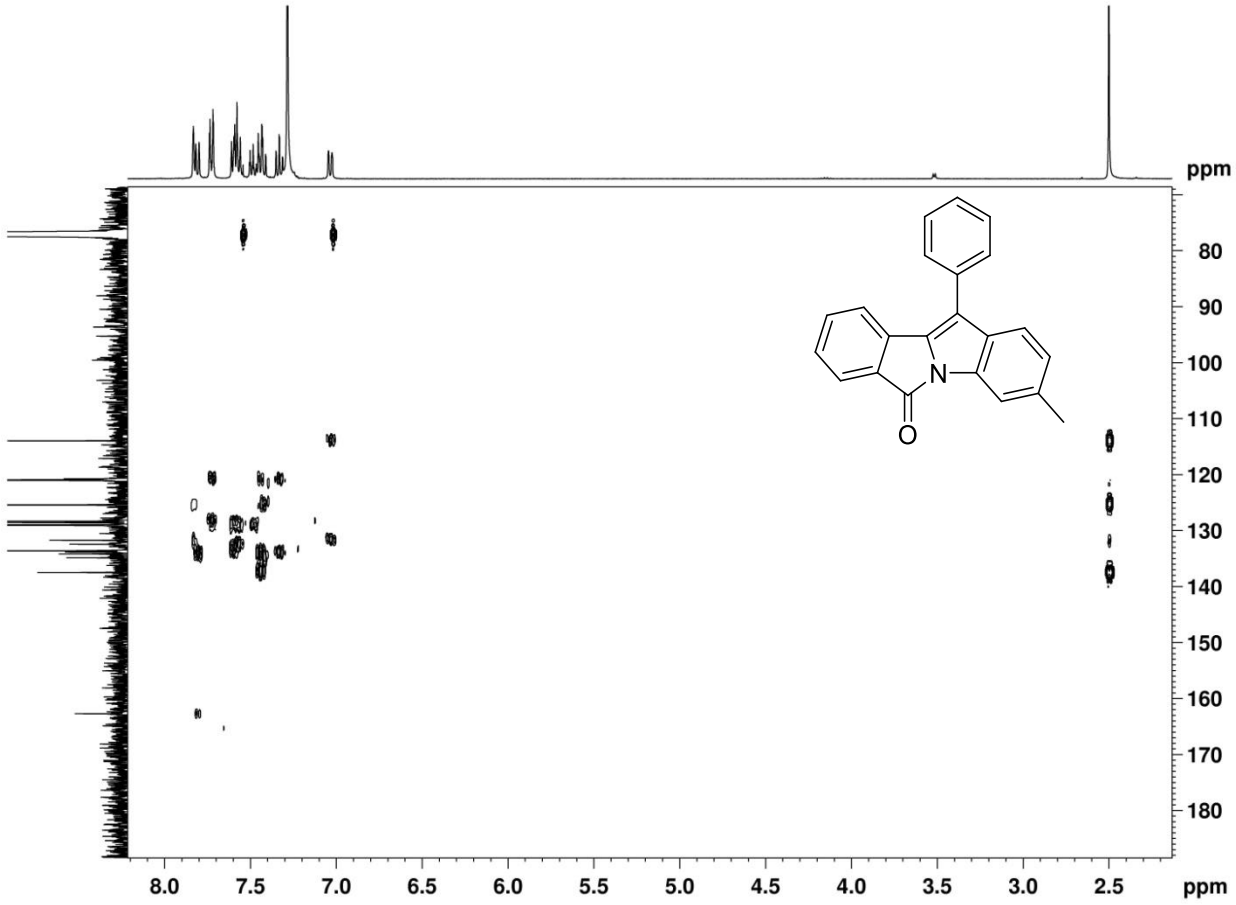
HSQC Spectrum (expansion) of *3-methyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one*(2g)



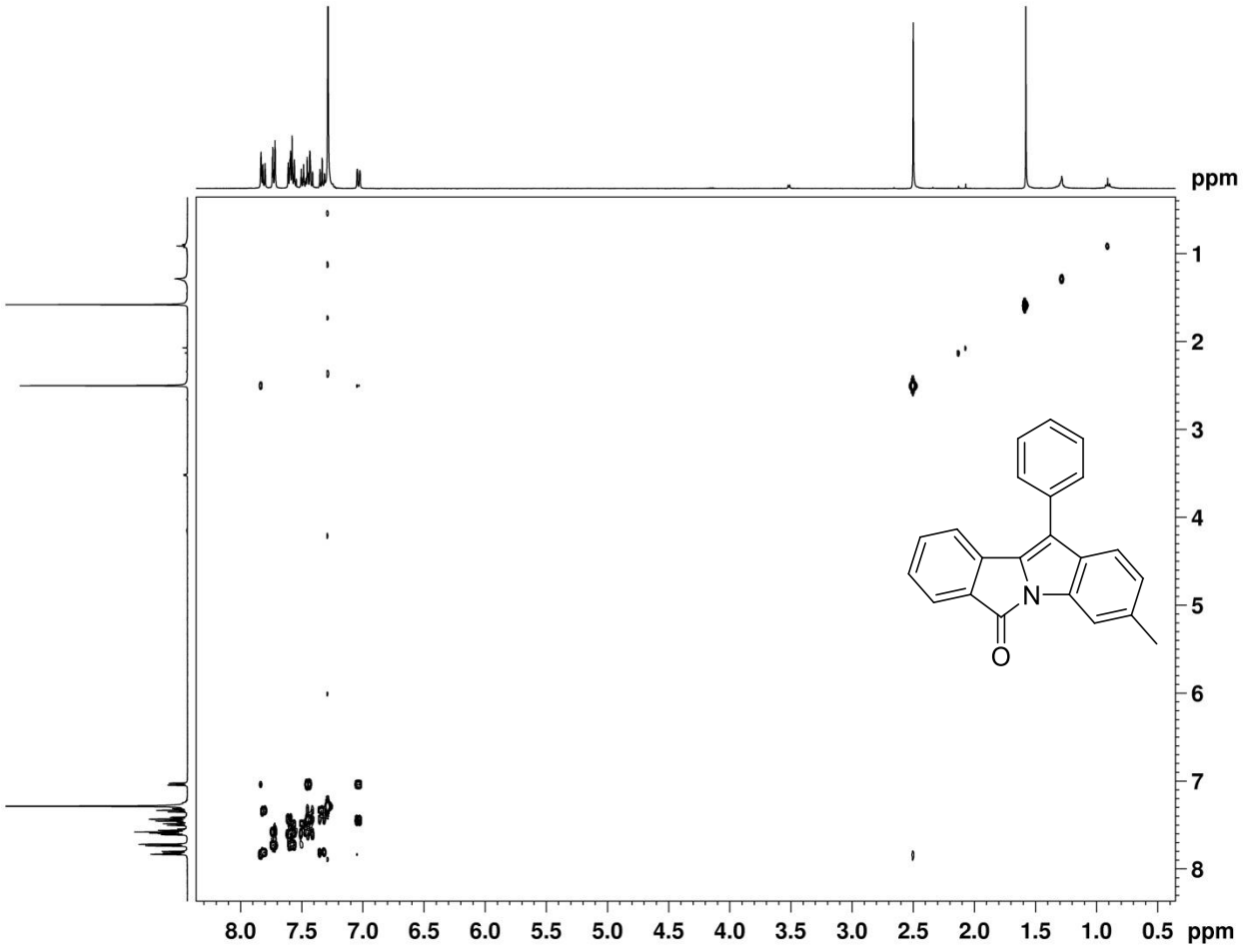
HMBC Spectrum of *3-methyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one*(2g)



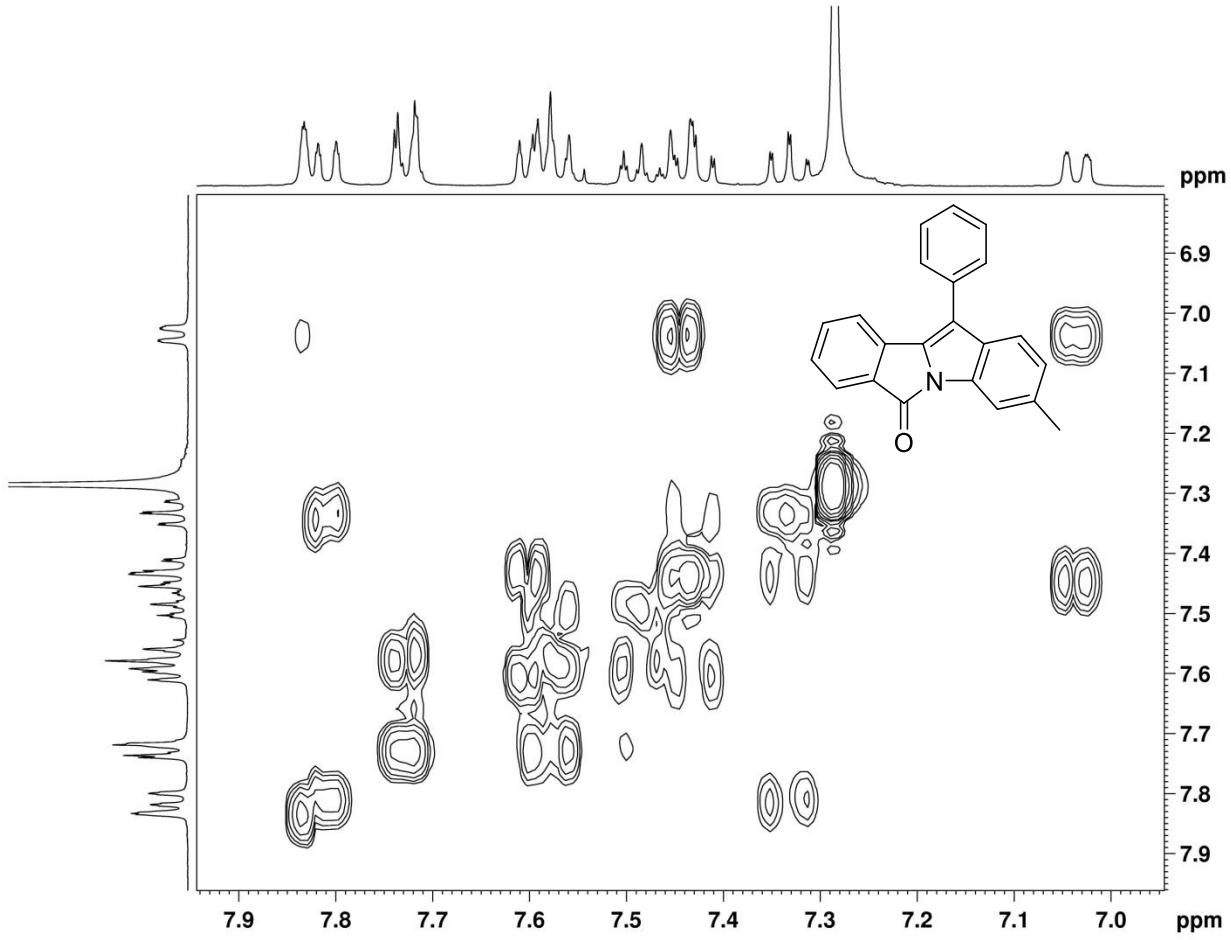
HMBC Spectrum (expansion) of *3-methyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one*(2g)



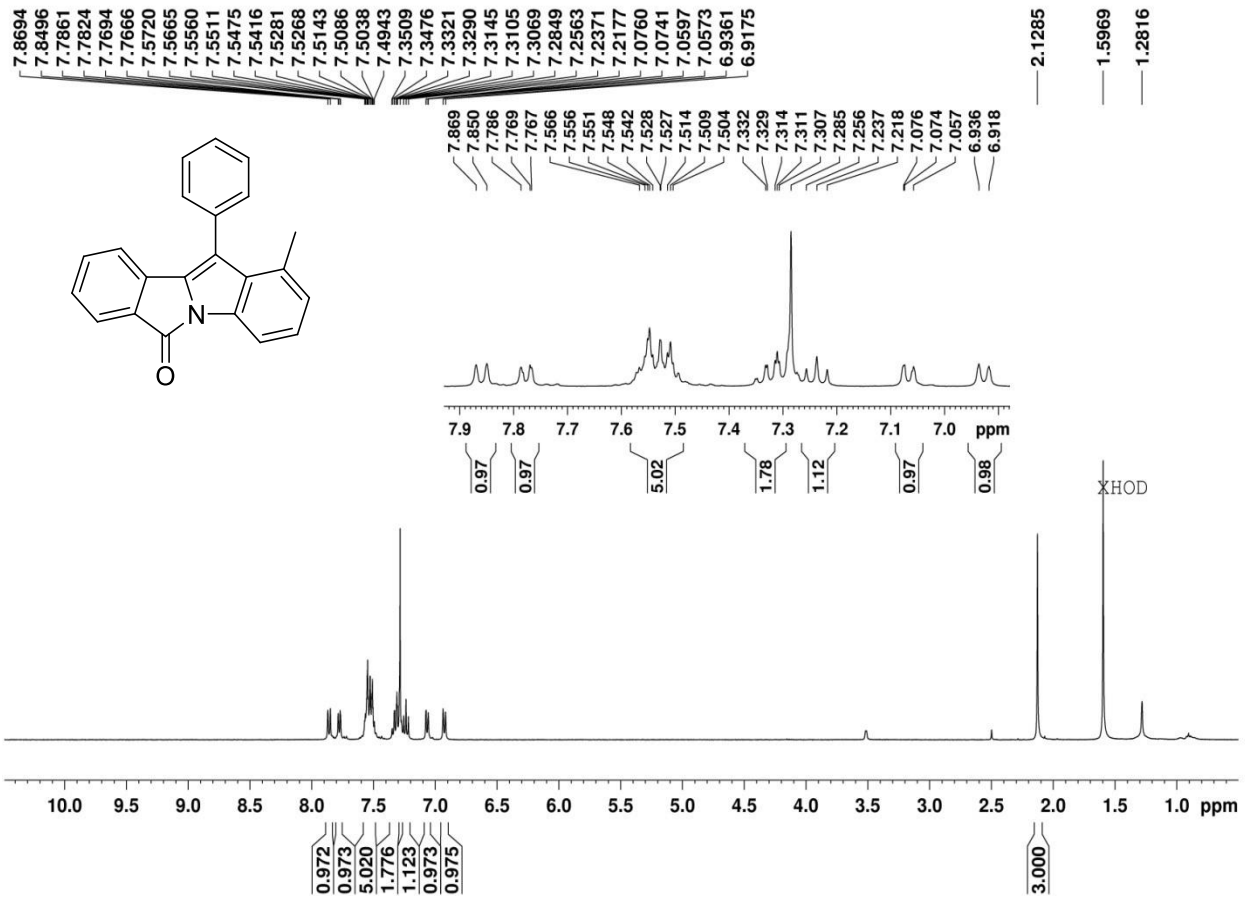
^{1}H-^{1}H COSY Spectrum of *3-methyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one*(2g)



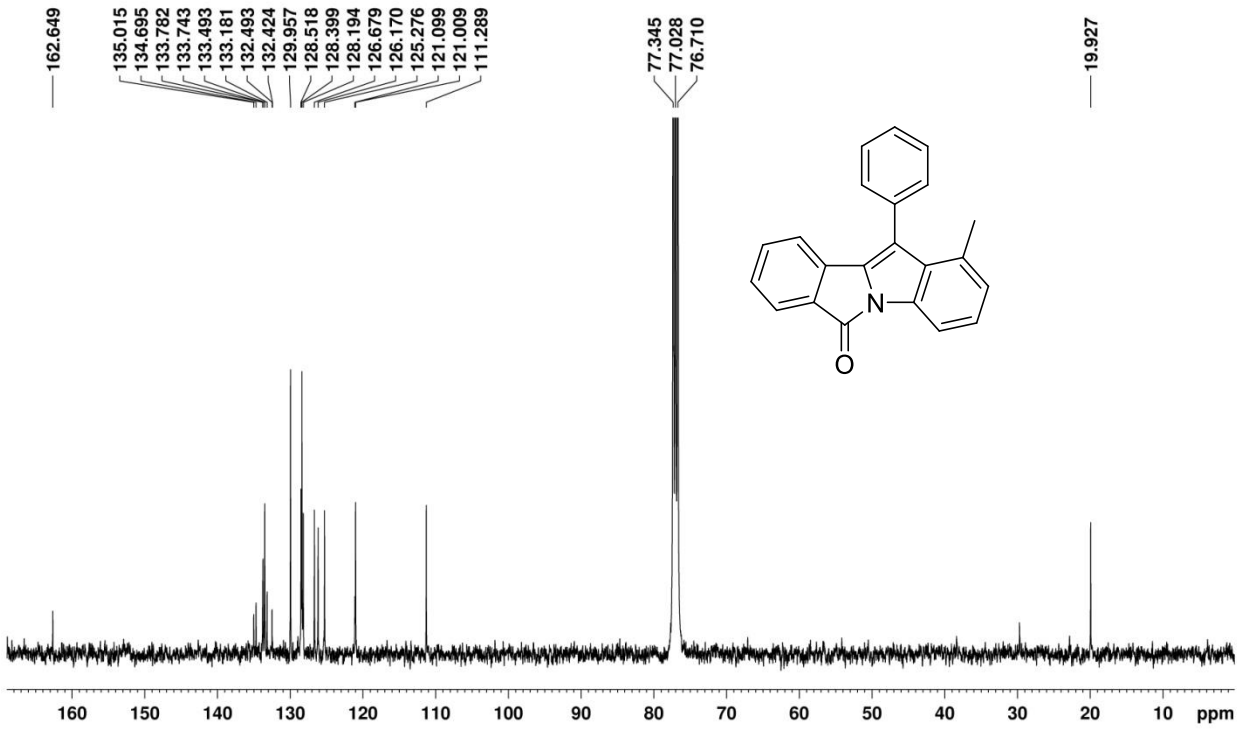
^{1}H-^{1}H COSY Spectrum (expansion) of *3-methyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one*(2g)



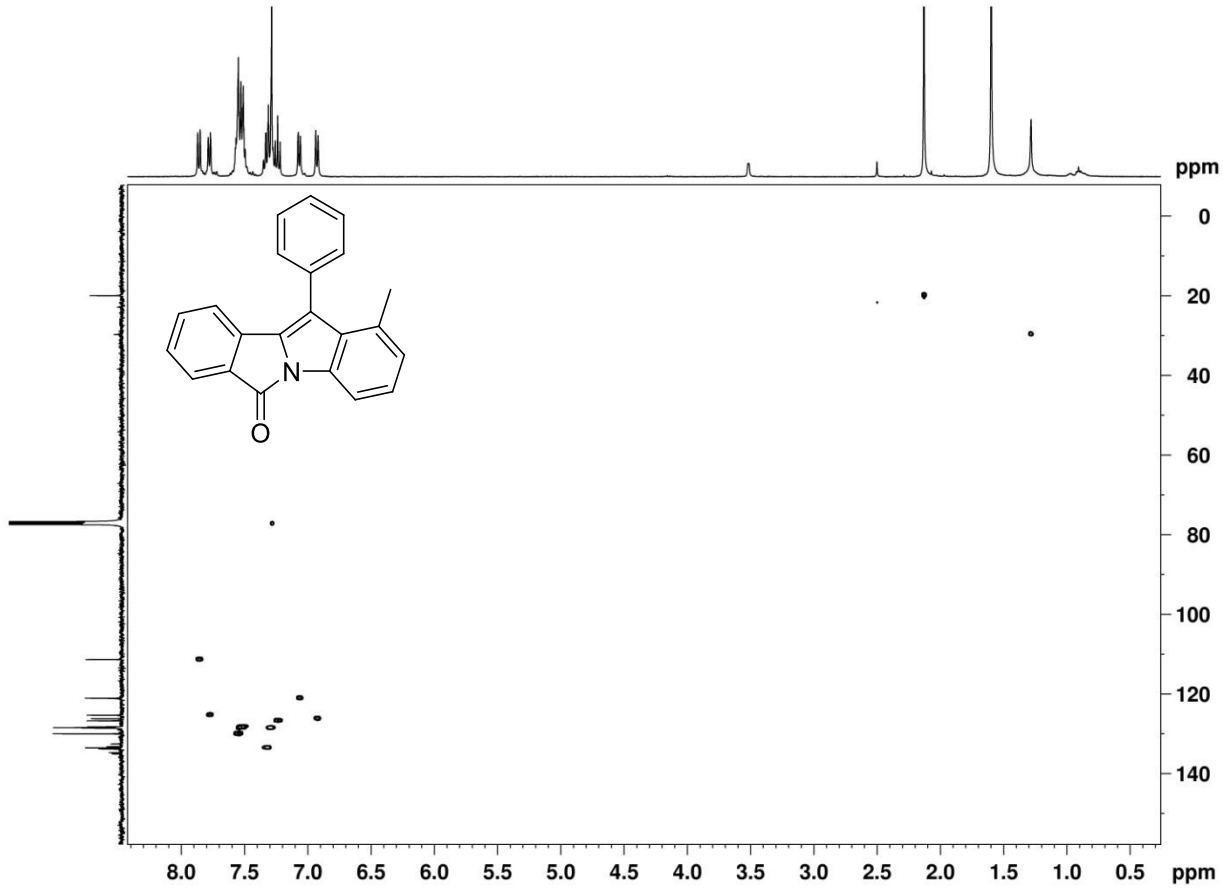
^{1}H NMR Spectrum of *1-methyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one*(2g′) (400 MHz, $CDCl_3$)



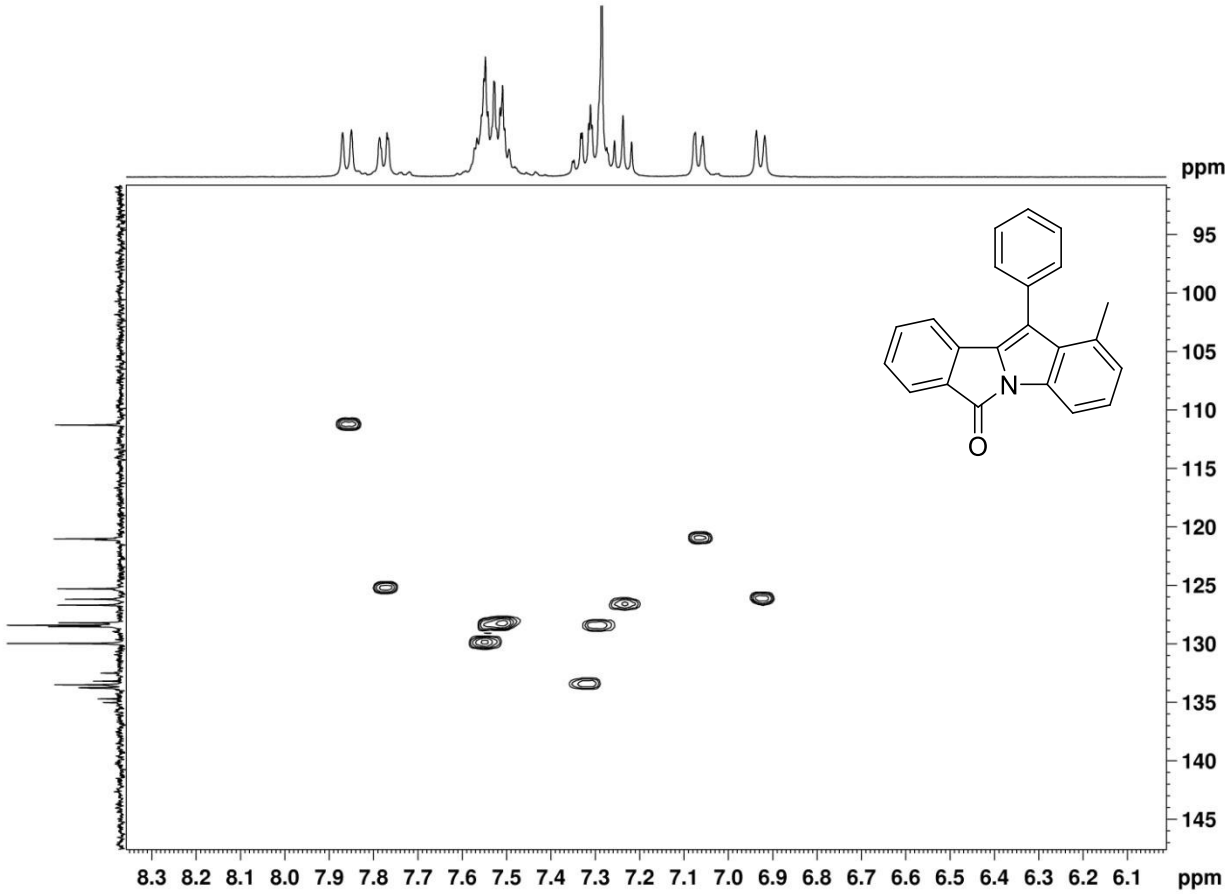
^{13}C NMR Spectrum of *1-methyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one*(2g′) (100 MHz, $CDCl_3$)



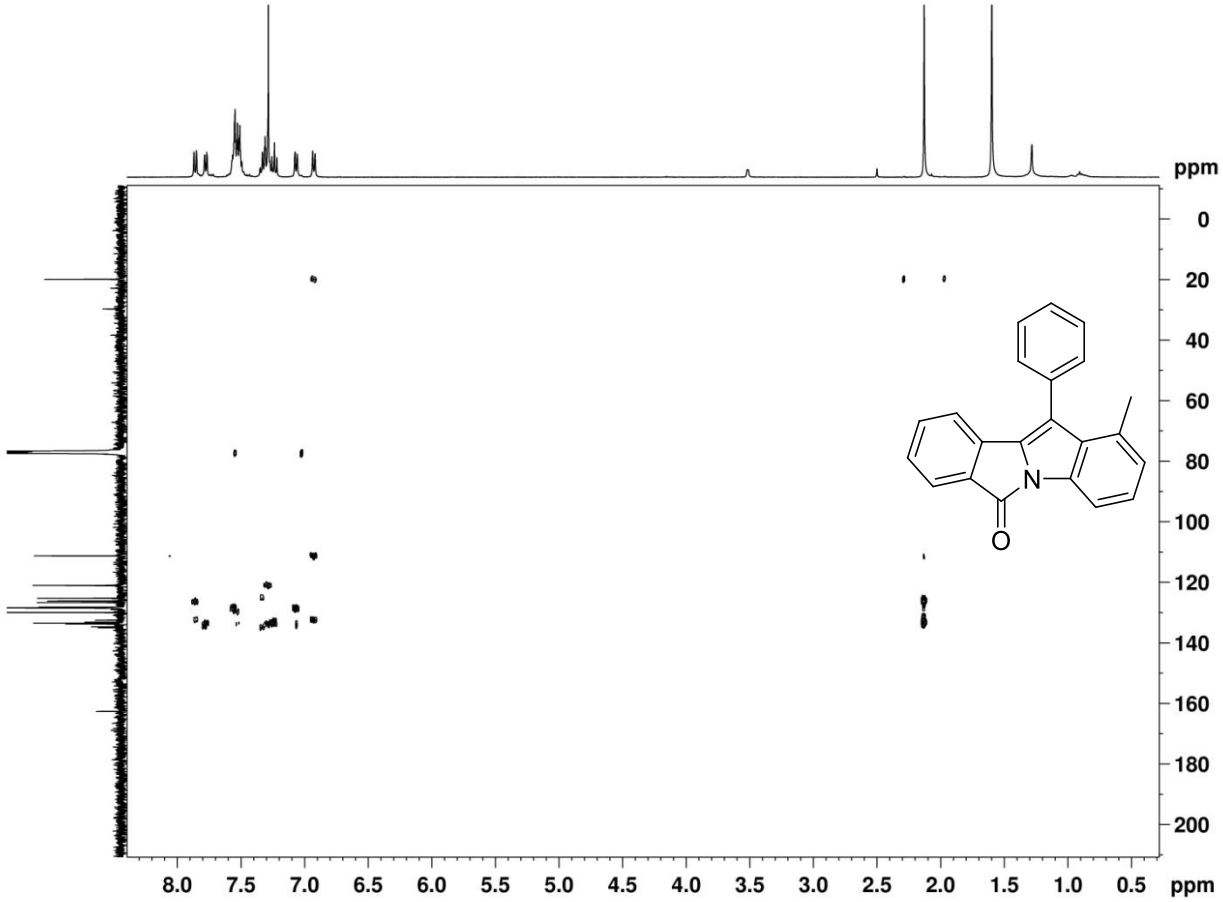
HSQC Spectrum of *1-methyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one*(2g′)



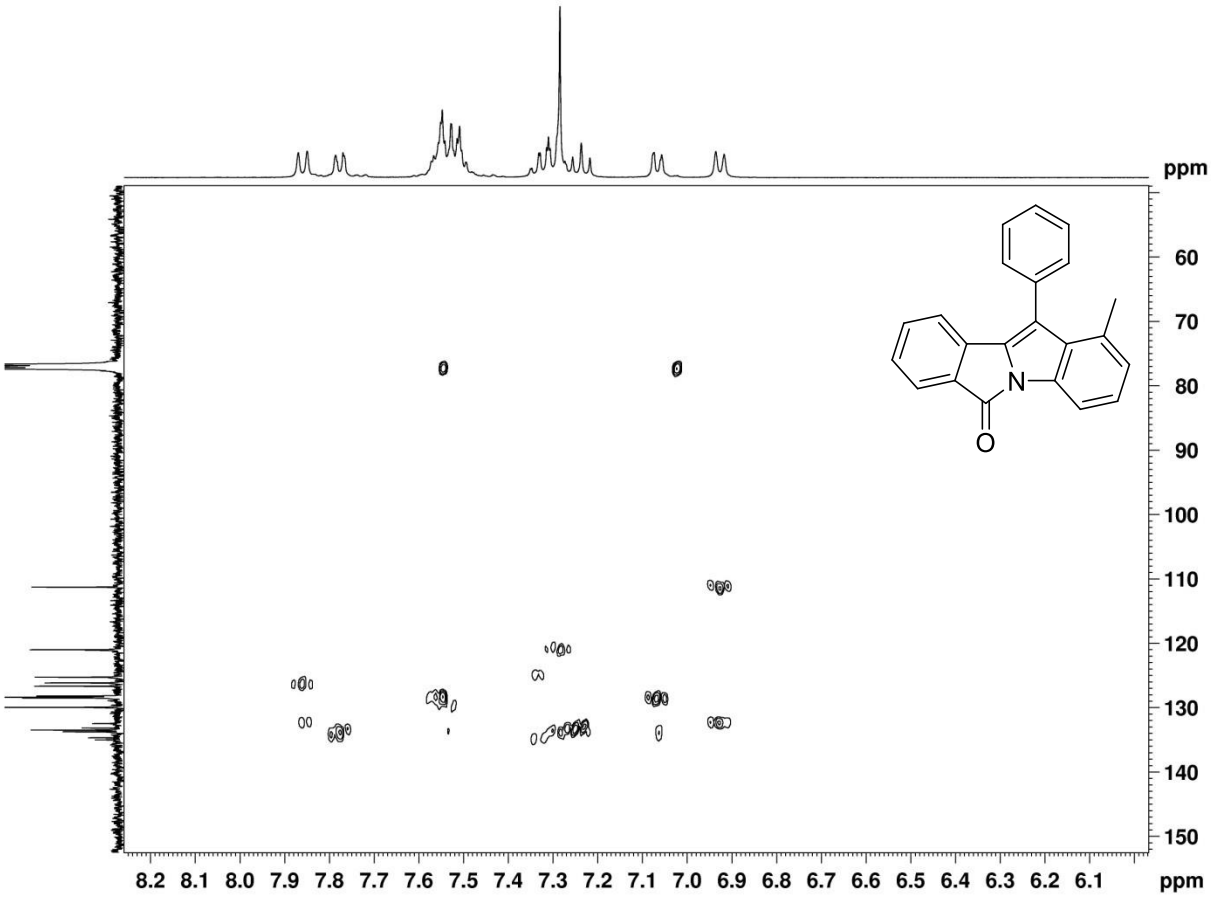
HSQC Spectrum (expansion) of *1-methyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one*(2g′)



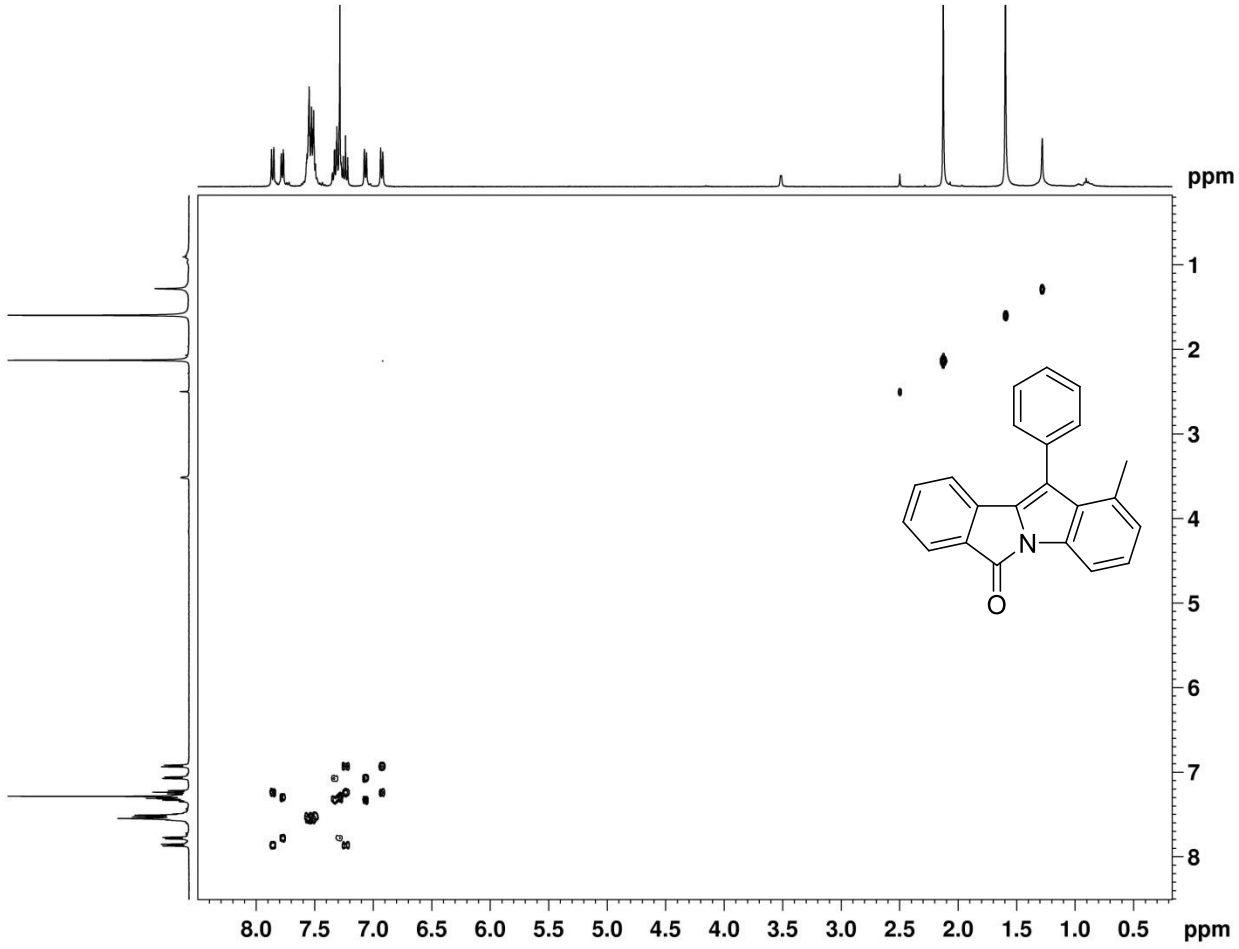
HMBC Spectrum of *1-methyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one*(2g′)



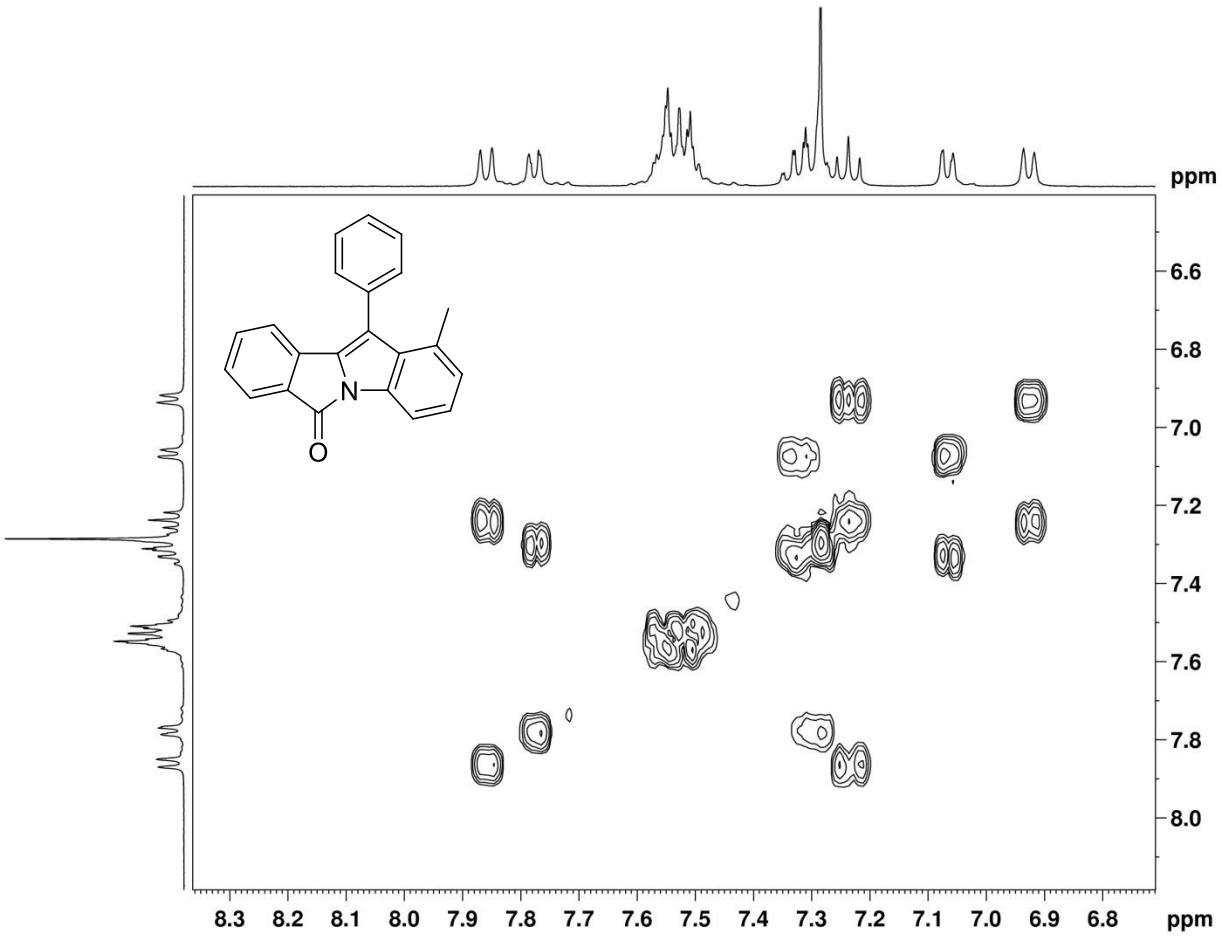
HMBC Spectrum (expansion) of *1-methyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one*(2g′)



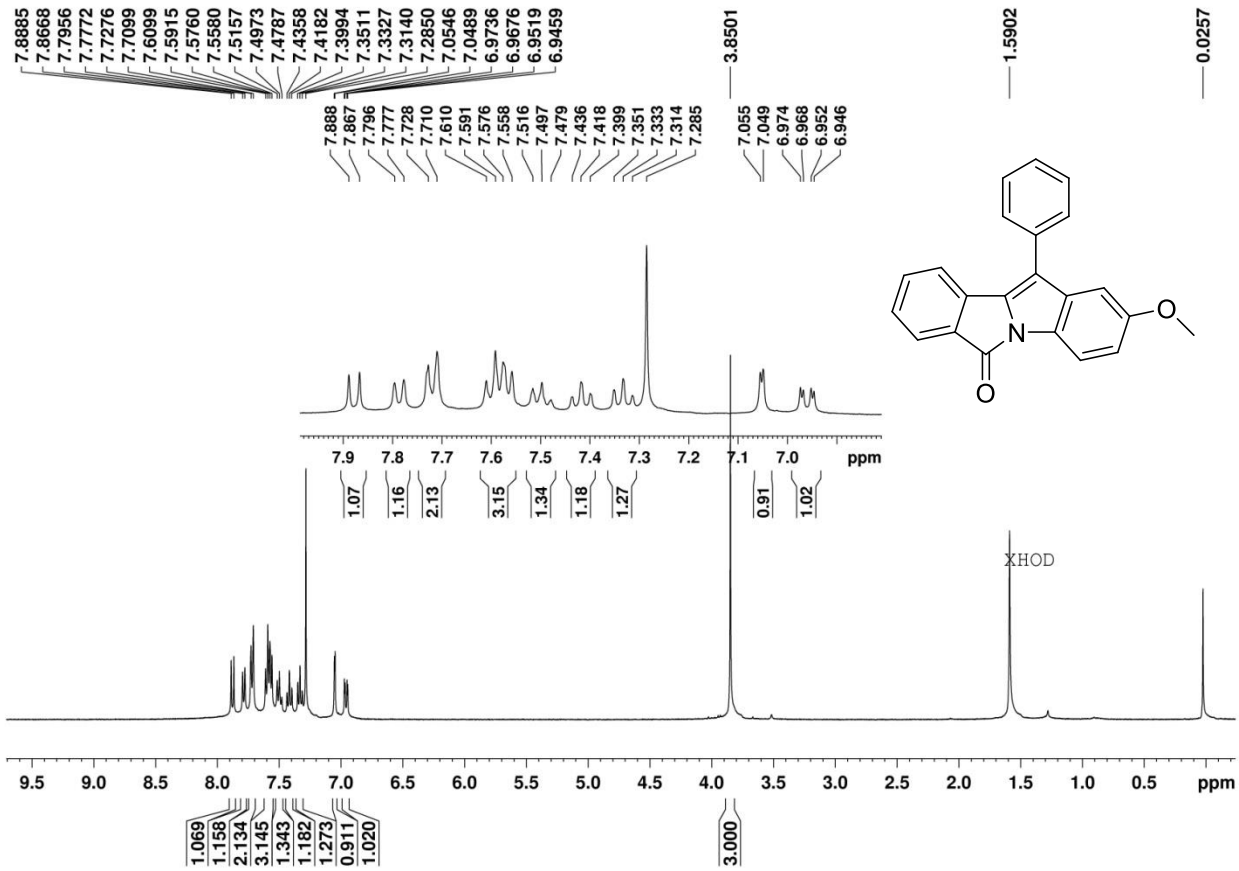
^{1}H-^{1}H COSY Spectrumof *1-methyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one*(2g′)



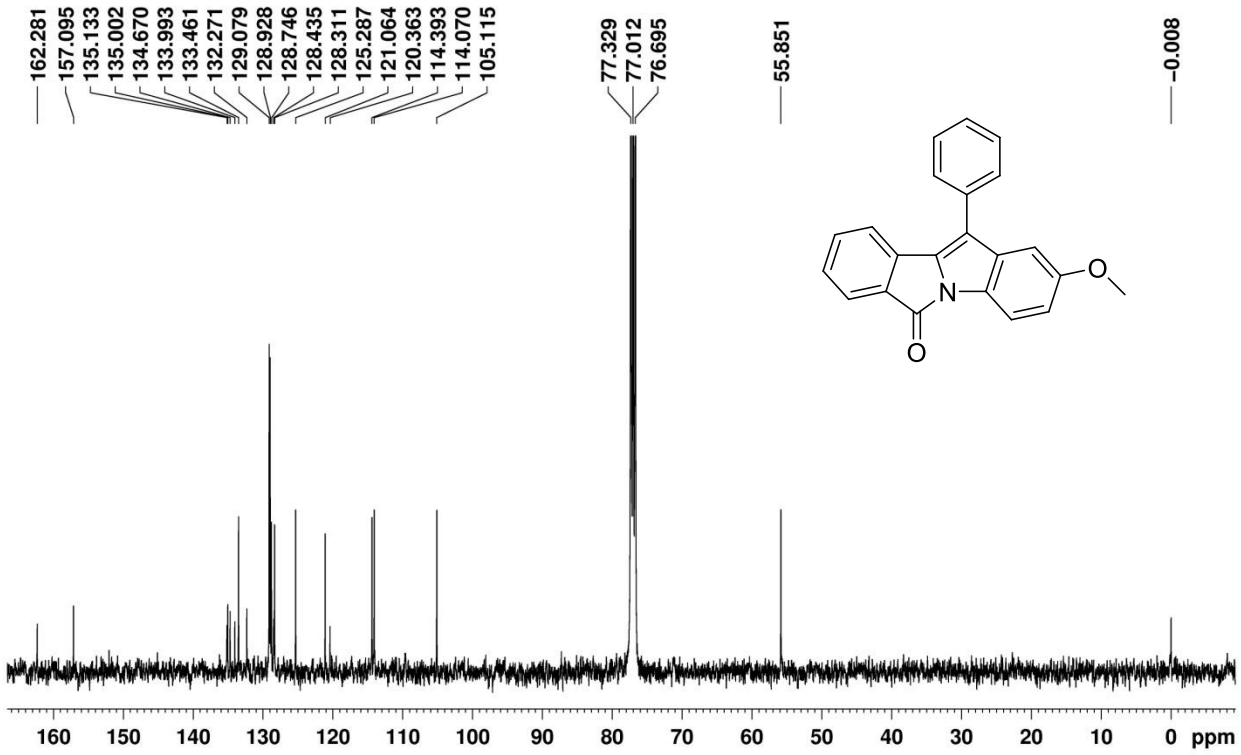
^{1}H-^{1}H COSYSpectrum (expansion) of *1-methyl-11-phenyl-6H-isoindolo[2,1-a]indol-6-one*(2g′)



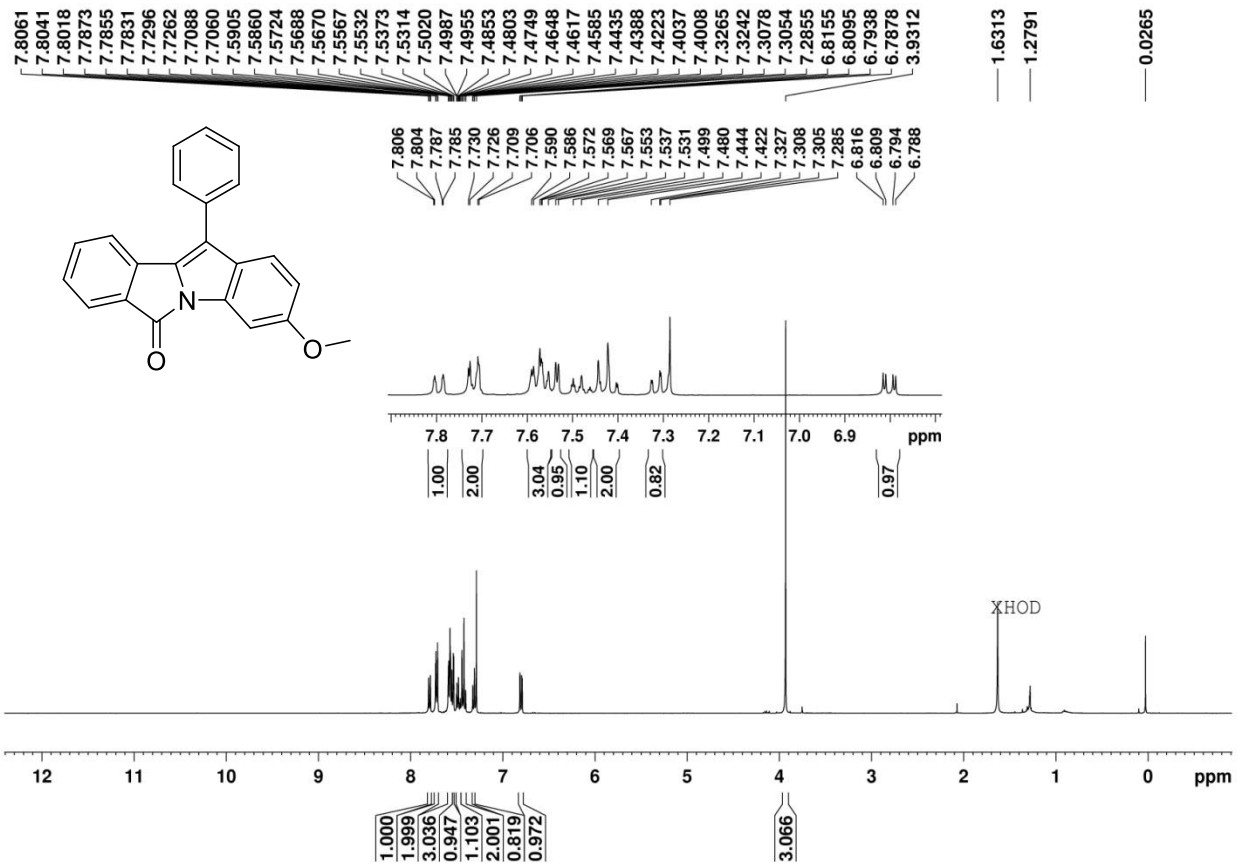
^{1}H NMR Spectrum of *2-methoxy-11-phenyl-6H-isoindolo[2,1-a]indol-6-one* (2h) (400 MHz, $CDCl_3$)



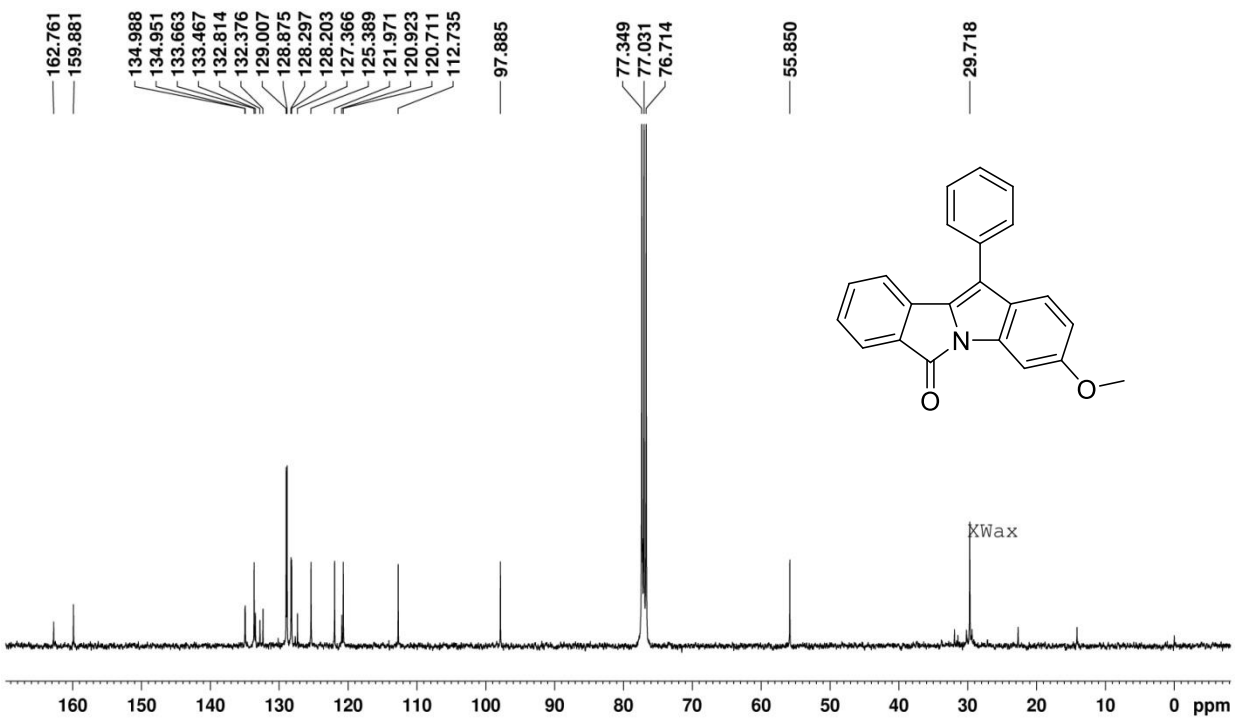
^{13}C NMR Spectrum of *2-methoxy-11-phenyl-6H-isoindolo[2,1-a]indol-6-one* (2h) (100 MHz, $CDCl_3$)



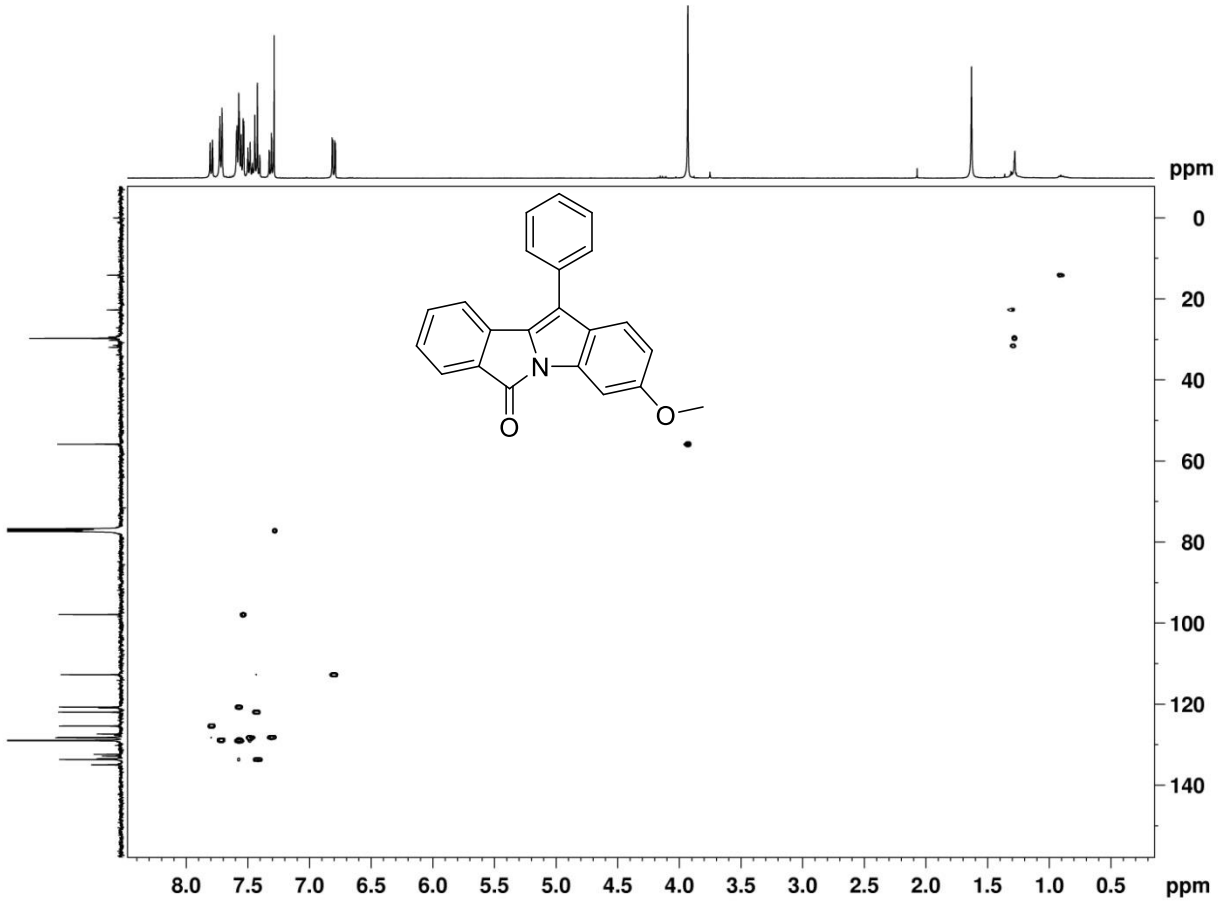
^{1}H NMR Spectrum of *3-methoxy-11-phenyl-6H-isoindolo[2,1-a]indol-6-one* (2i) (400 MHz, $CDCl_3$)



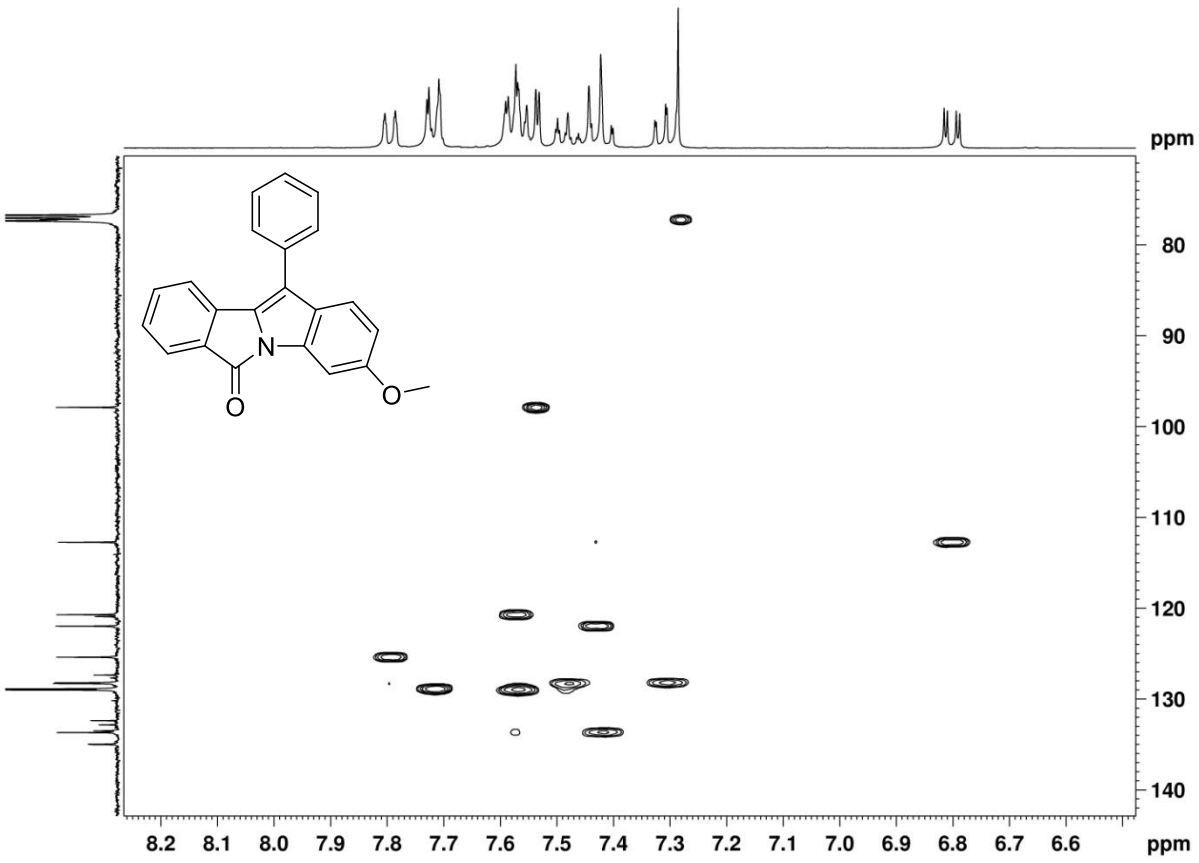
^{13}C NMR Spectrum of *3-methoxy-11-phenyl-6H-isoindolo[2,1-a]indol-6-one*(2i) (100 MHz, $CDCl_3$)



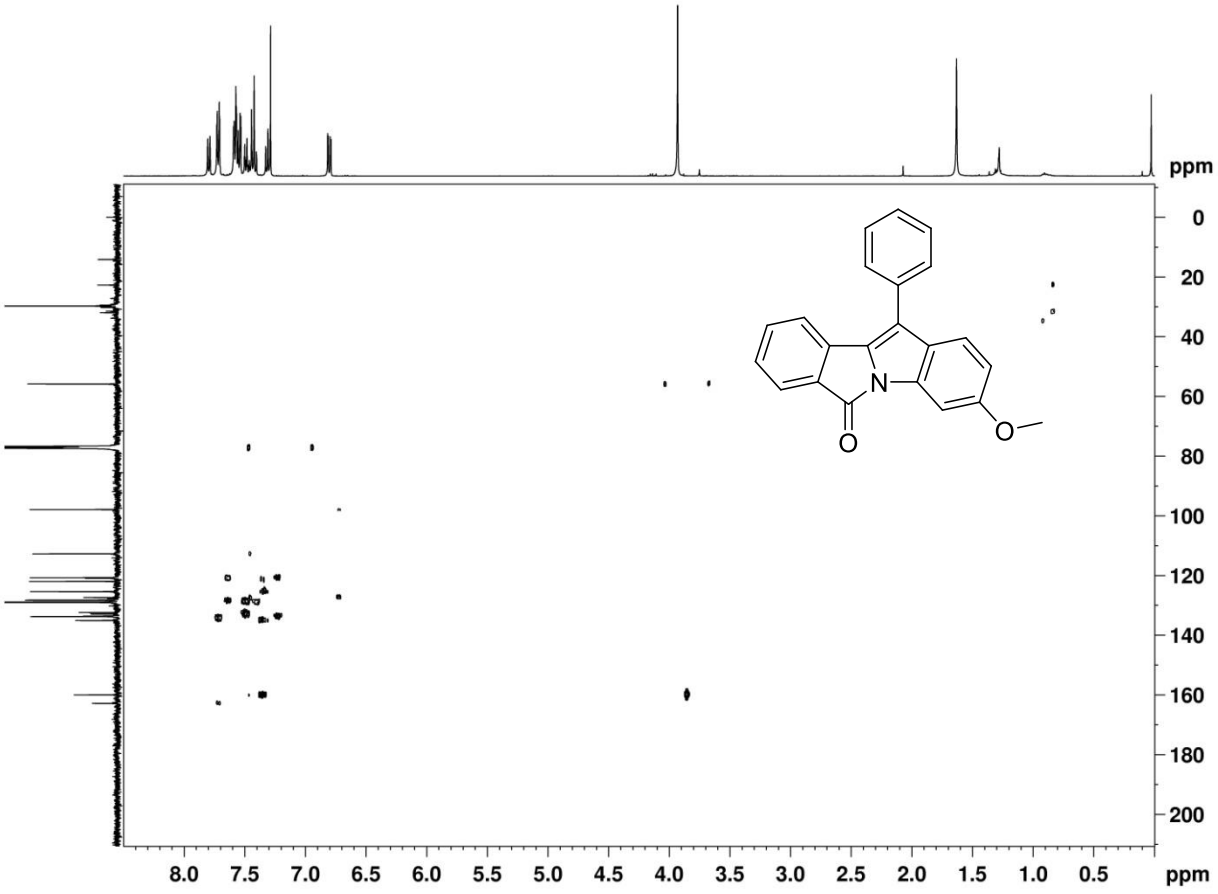
HSQC Spectrum of *3-methoxy-11-phenyl-6H-isoindolo[2,1-a]indol-6-one*(2i)



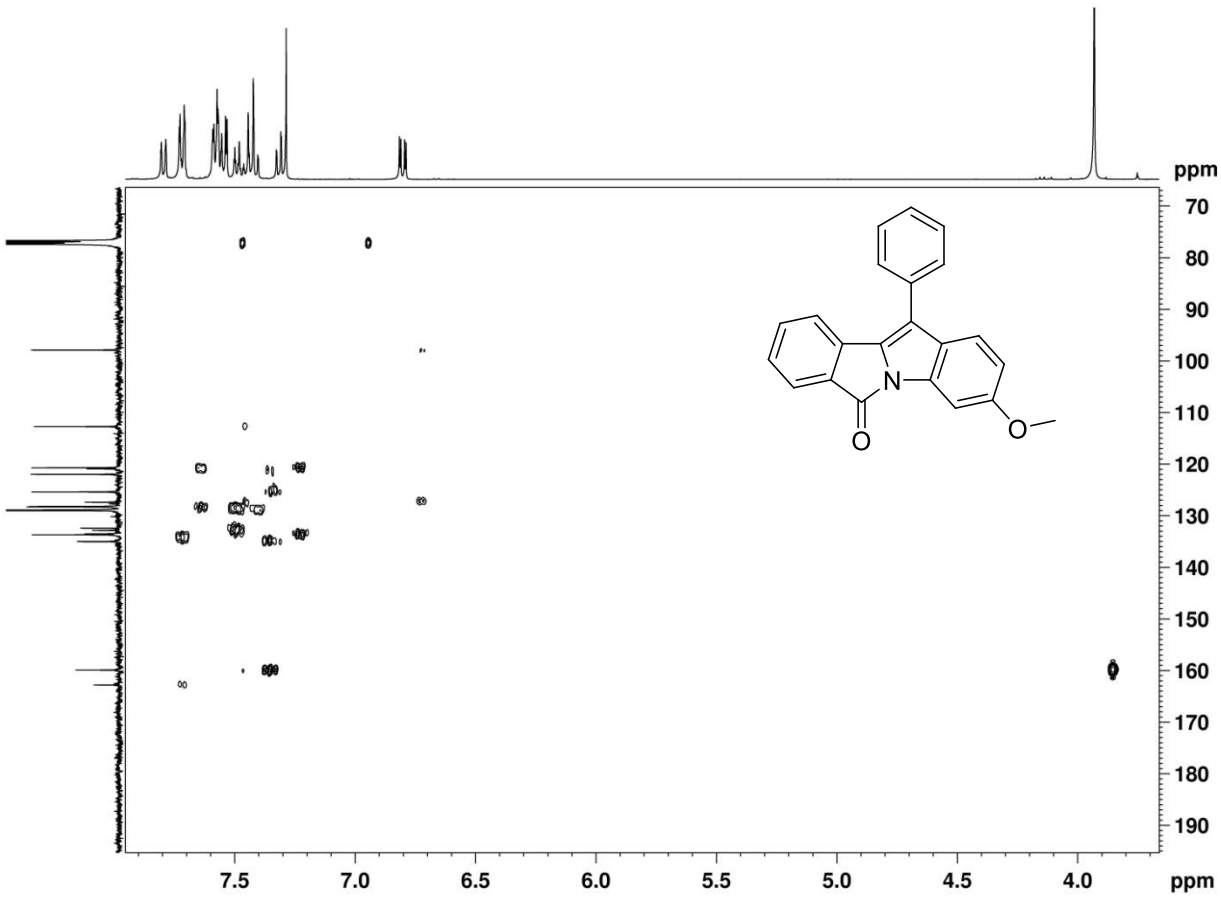
HSQC Spectrum (expansion) of *3-methoxy-11-phenyl-6H-isoindolo[2,1-a]indol-6-one*(2i)



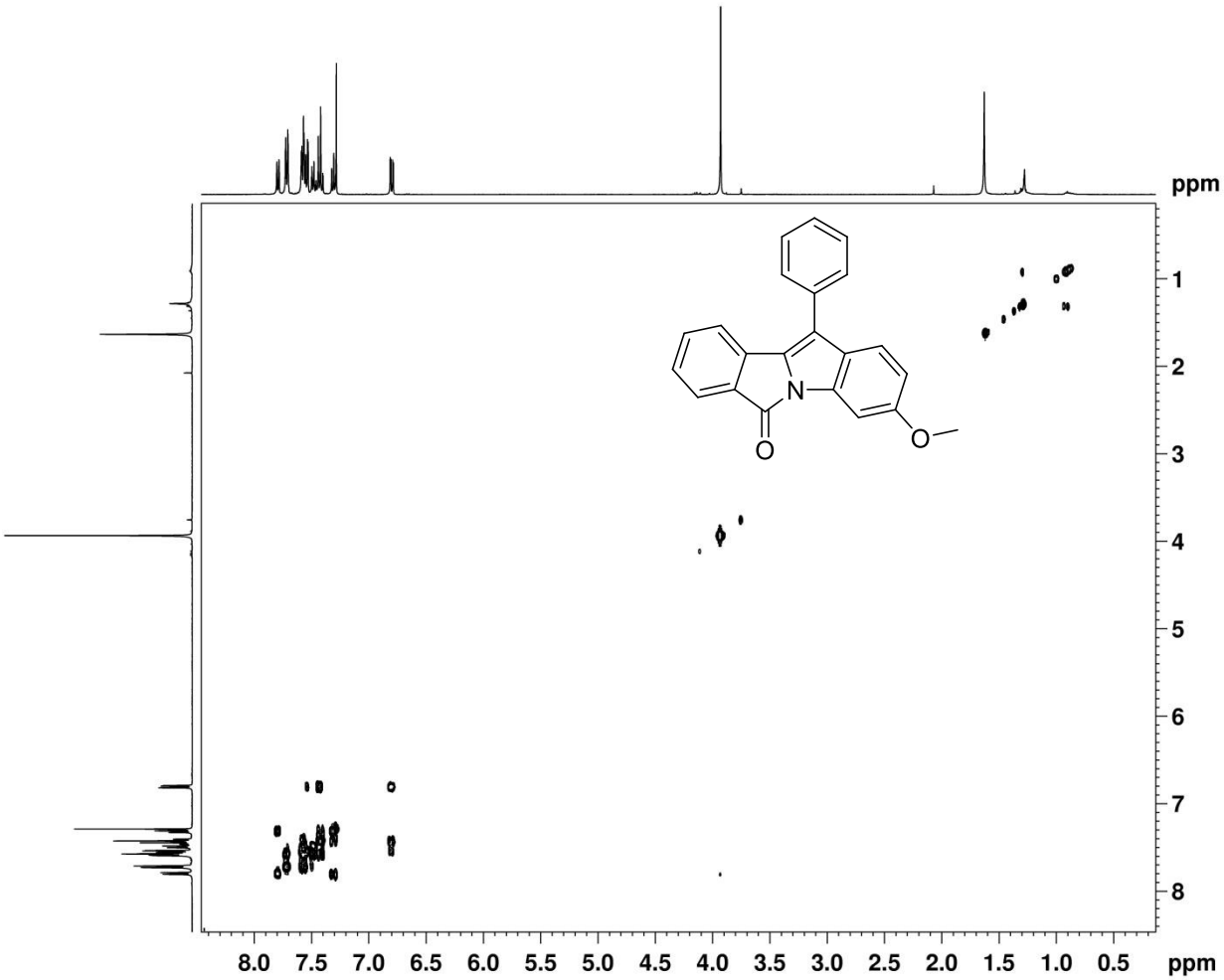
HMBC Spectrum of *3-methoxy-11-phenyl-6H-isoindolo[2,1-a]indol-6-one*(2i)



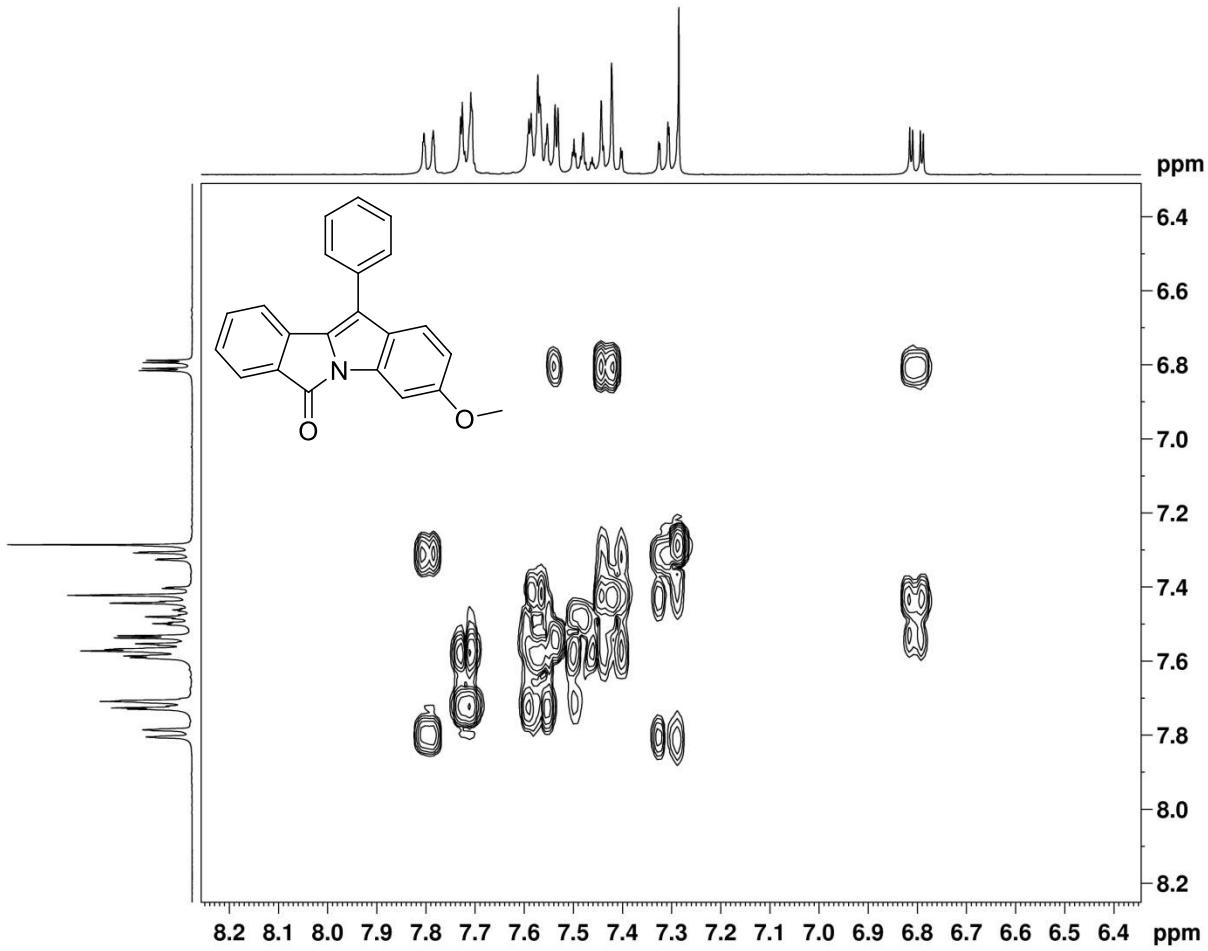
HMBC Spectrum (expansion) of *3-methoxy-11-phenyl-6H-isoindolo[2,1-a]indol-6-one*(2i)



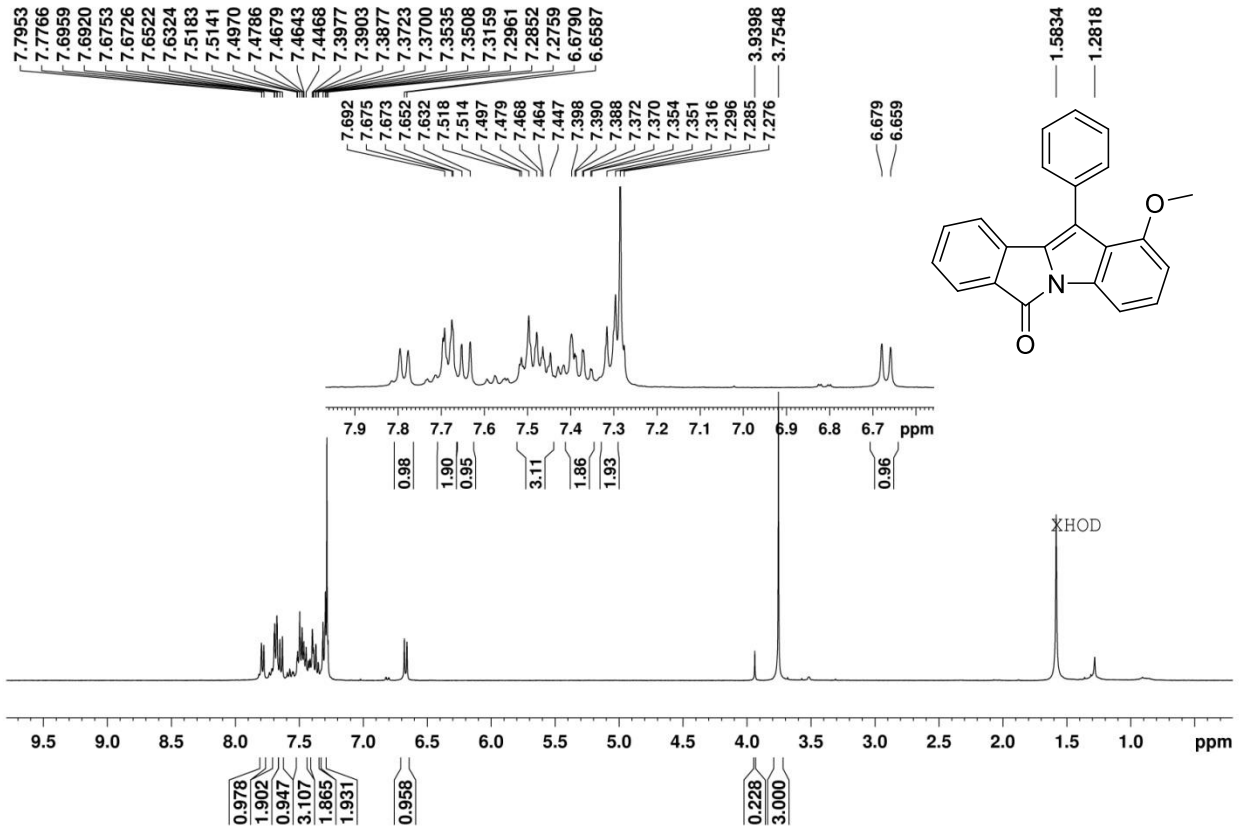
^{1}H-^{1}H COSYSpectrumof *3-methoxy-11-phenyl-6H-isoindolo[2,1-a]indol-6-one*(2i)



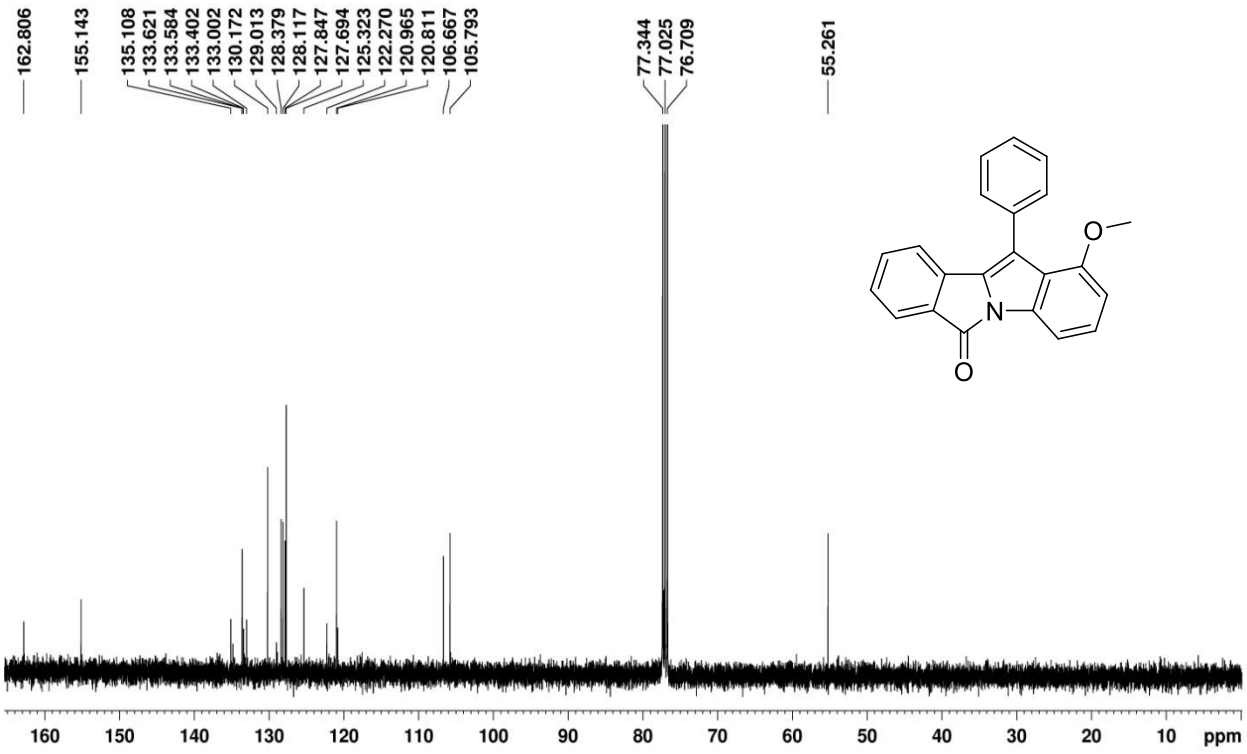
^{1}H-^{1}H COSYSpectrum (expansion) of *3-methoxy-11-phenyl-6H-isoindolo[2,1-a]indol-6-one*(2i)



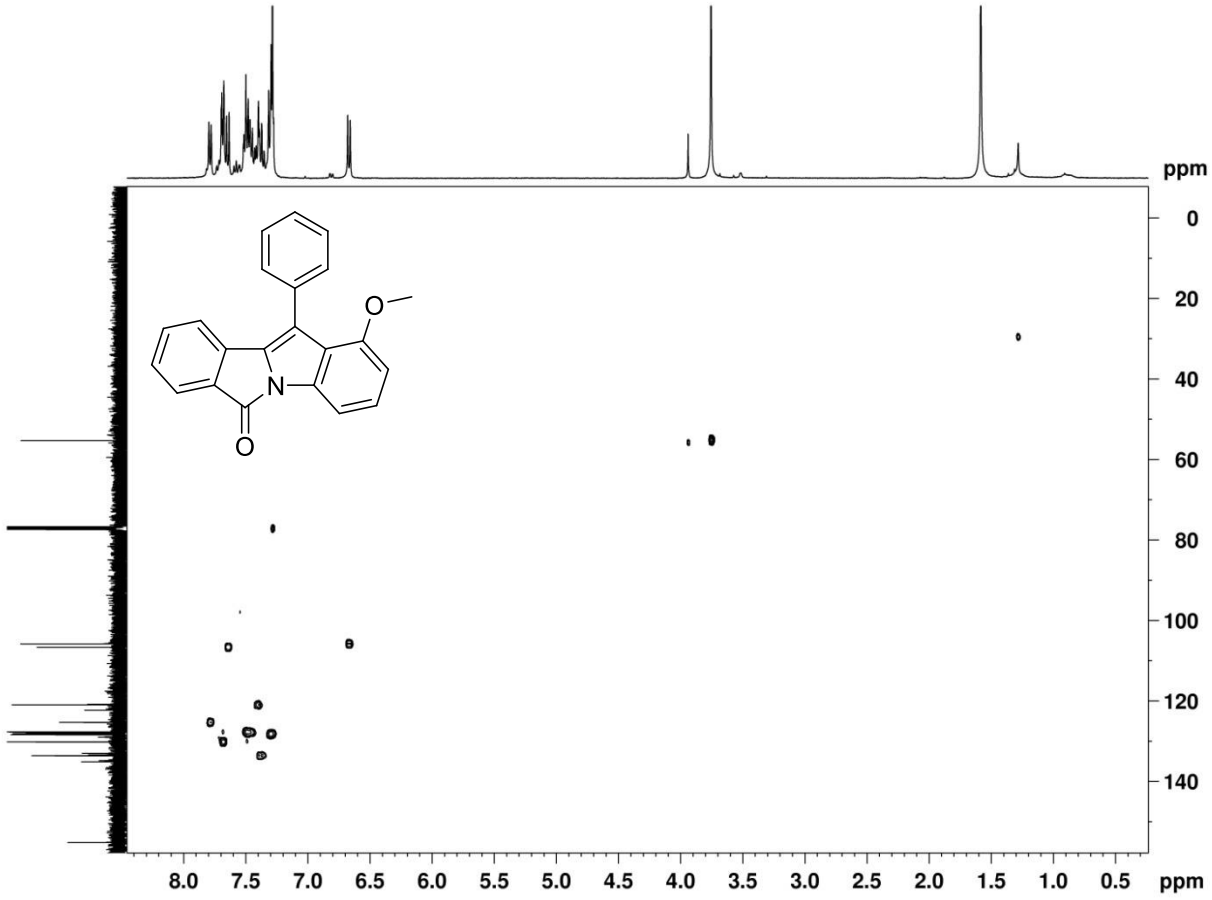
^{1}H NMR Spectrum of *1-methoxy-11-phenyl-6H-isoindolo[2,1-a]indol-6-one* (2i′) (400 MHz, $CDCl_3$)



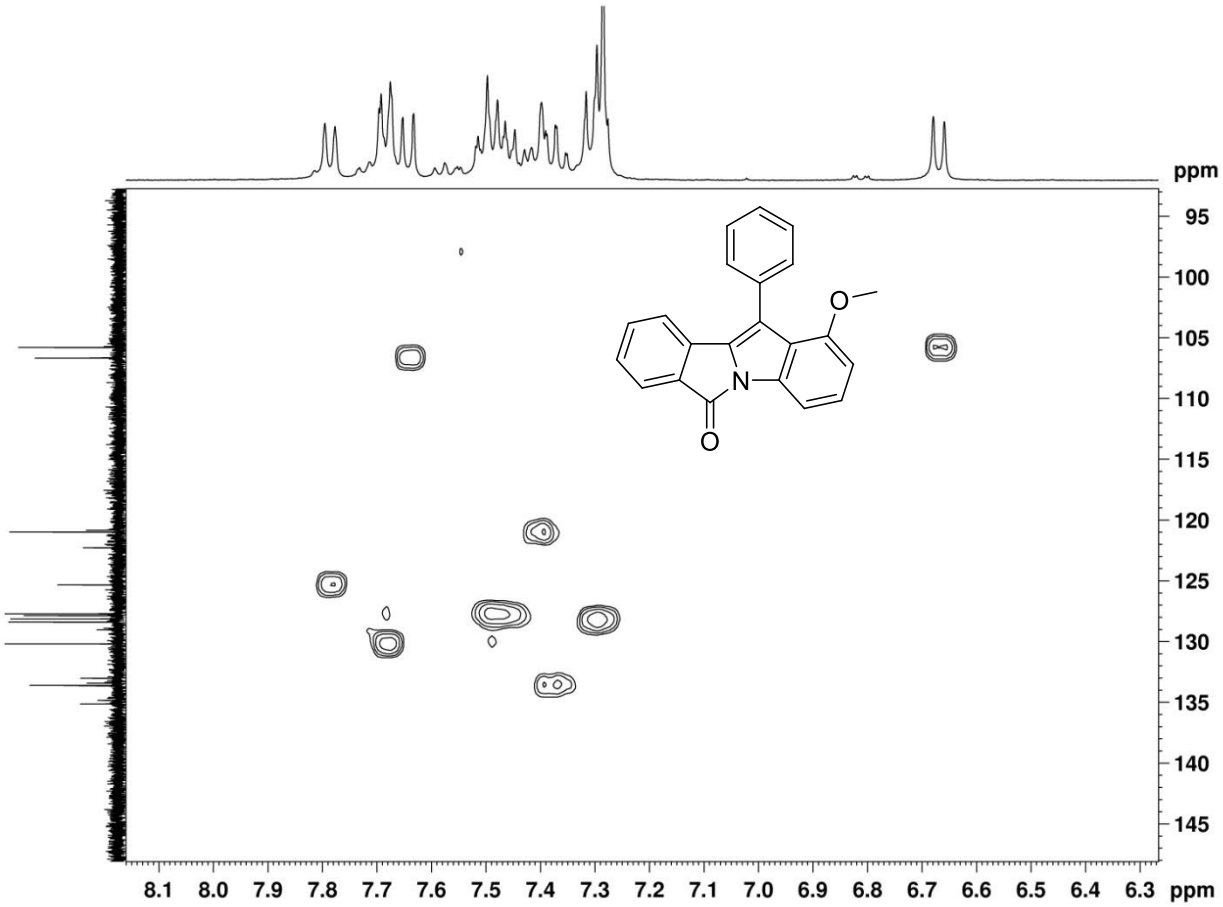
^{13}C NMR Spectrum of *1-methoxy-11-phenyl-6H-isoindolo[2,1-a]indol-6-one* (2i') (100 MHz, $CDCl_3$)



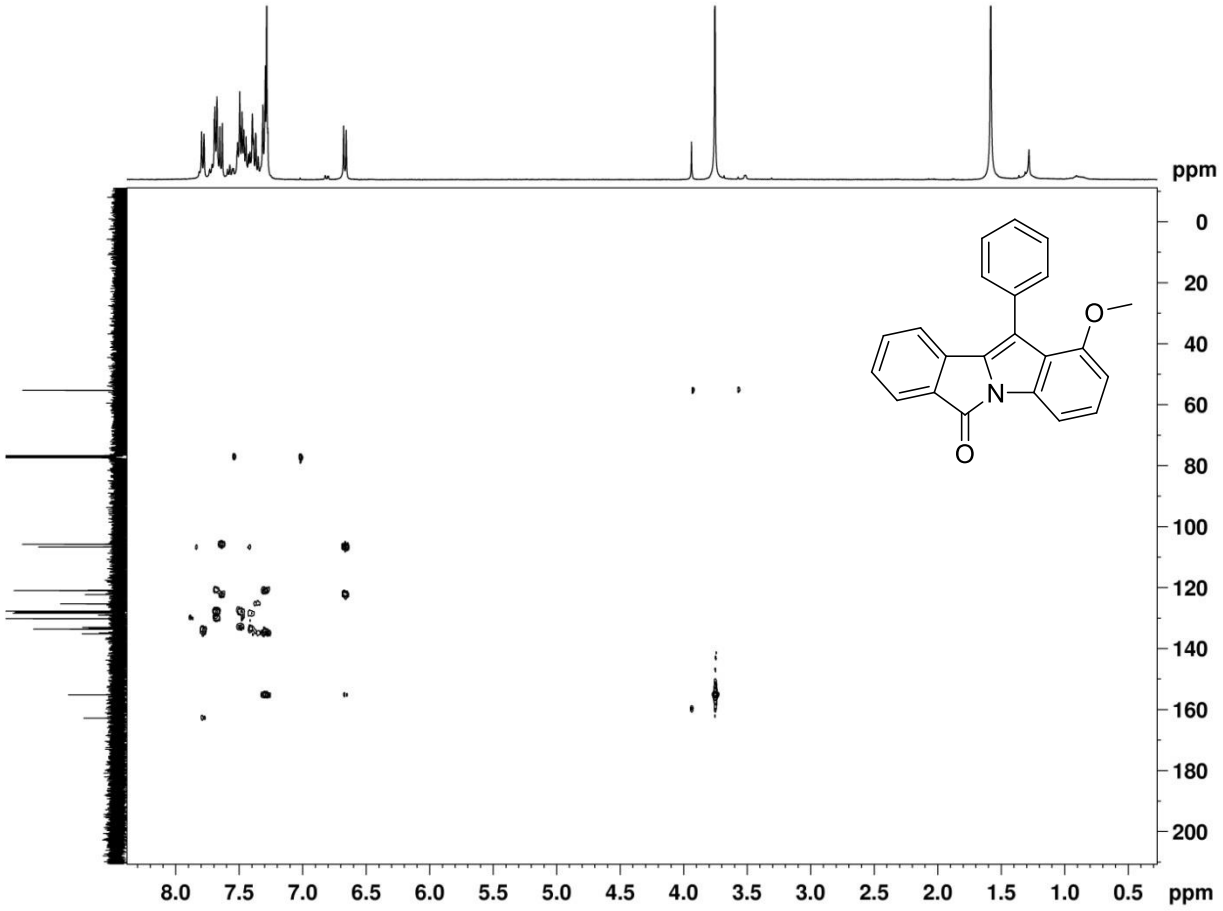
HSQC Spectrum of *1-methoxy-11-phenyl-6H-isoindolo[2,1-a]indol-6-one* (2i′)



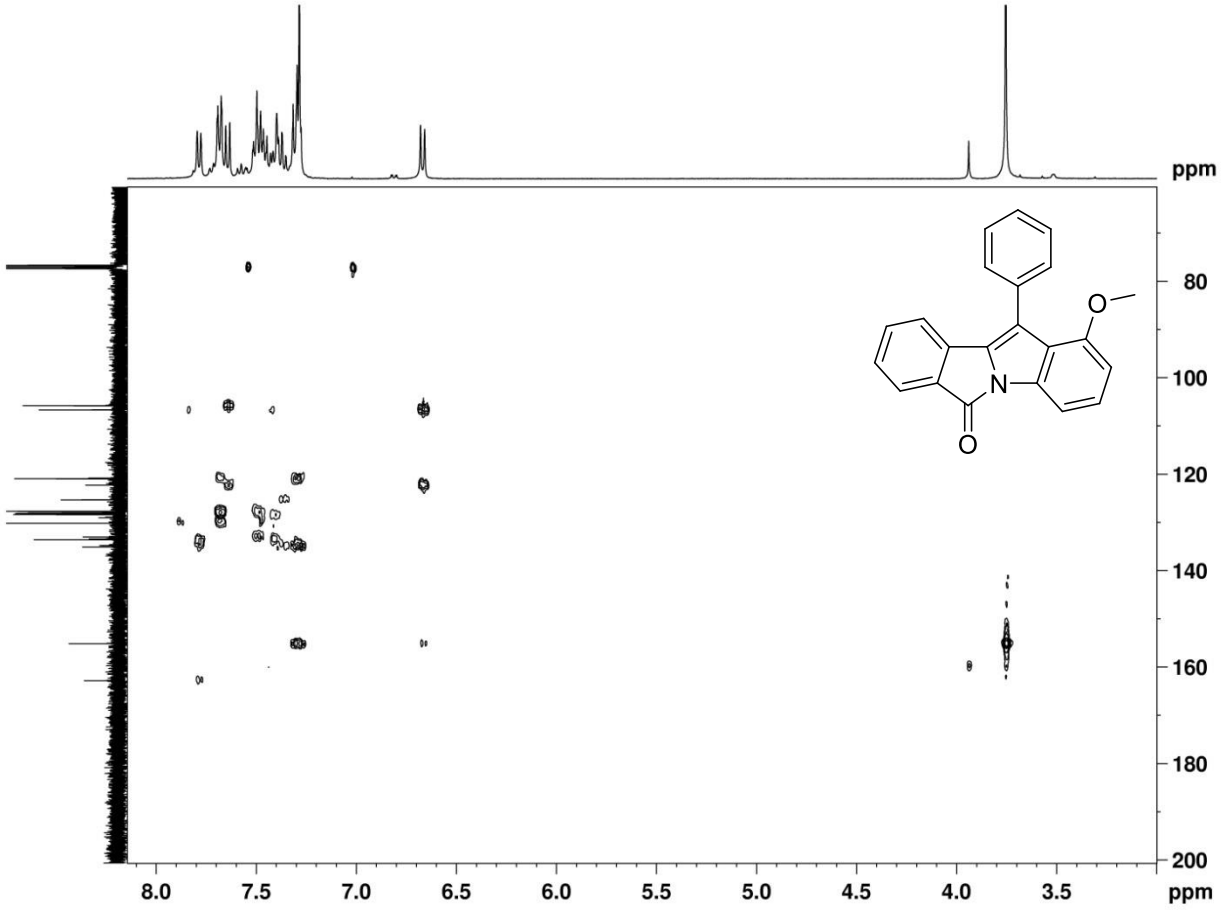
HSQC Spectrum (expansion) of *1-methoxy-11-phenyl-6H-isoindolo[2,1-a]indol-6-one* (2i′)



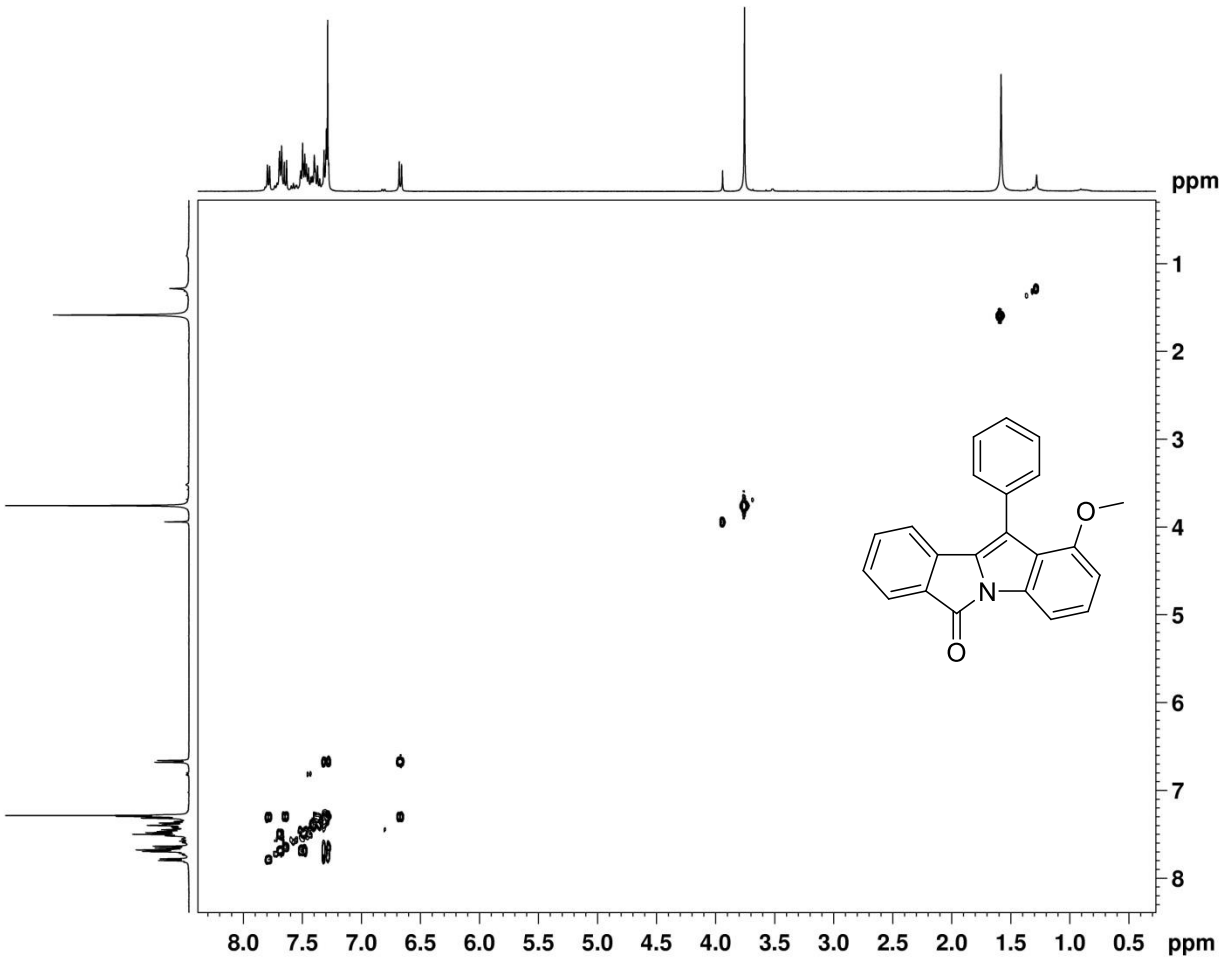
HMBC Spectrum of *1-methoxy-11-phenyl-6H-isoindolo[2,1-a]indol-6-one* (2i')



HMBC Spectrum (expansion) of *1-methoxy-11-phenyl-6H-isoindolo[2,1-a]indol-6-one* (2i′)



^{1}H-^{1}H COSY NMR Spectrum of *1-methoxy-11-phenyl-6H-isoindolo[2,1-a]indol-6-one* (2i′)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4
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6
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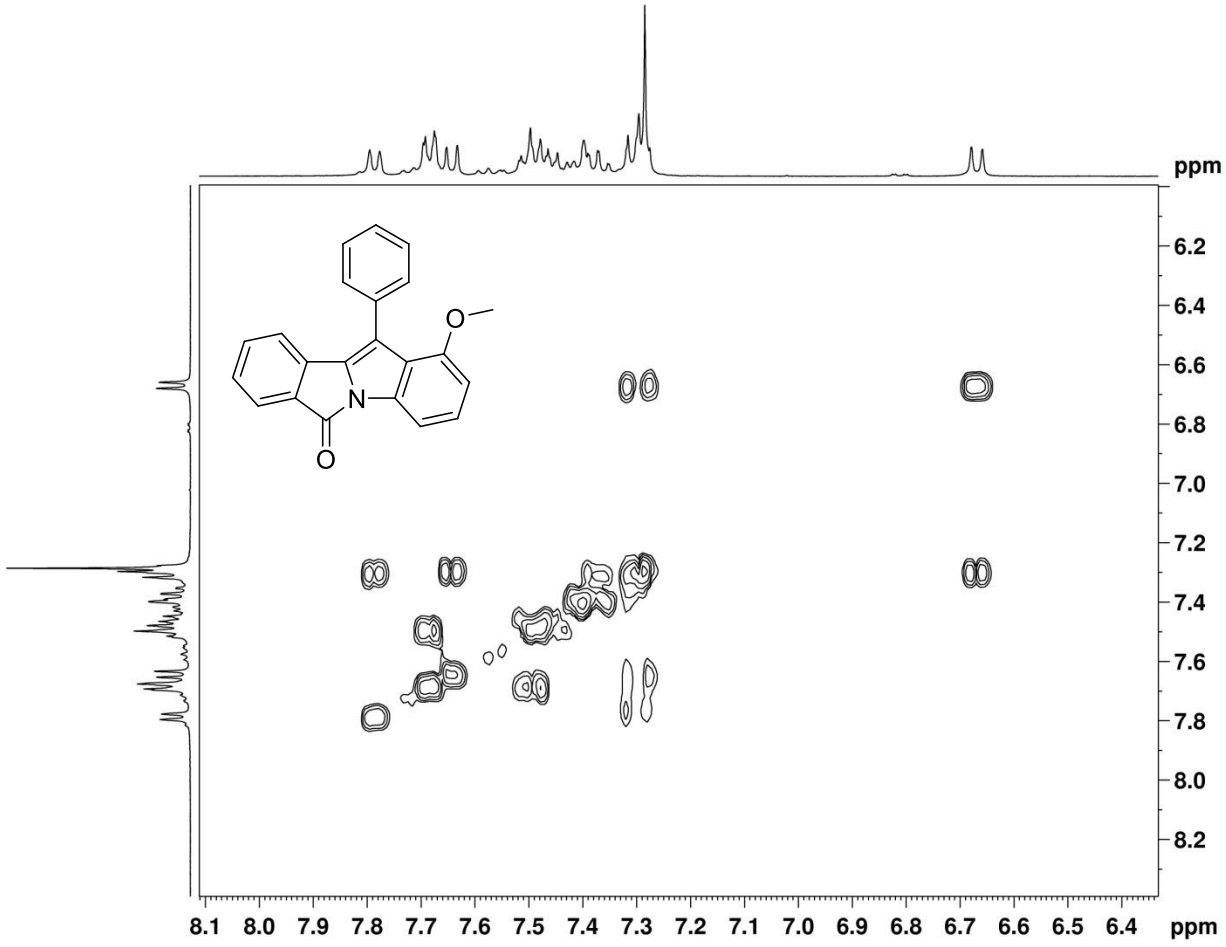
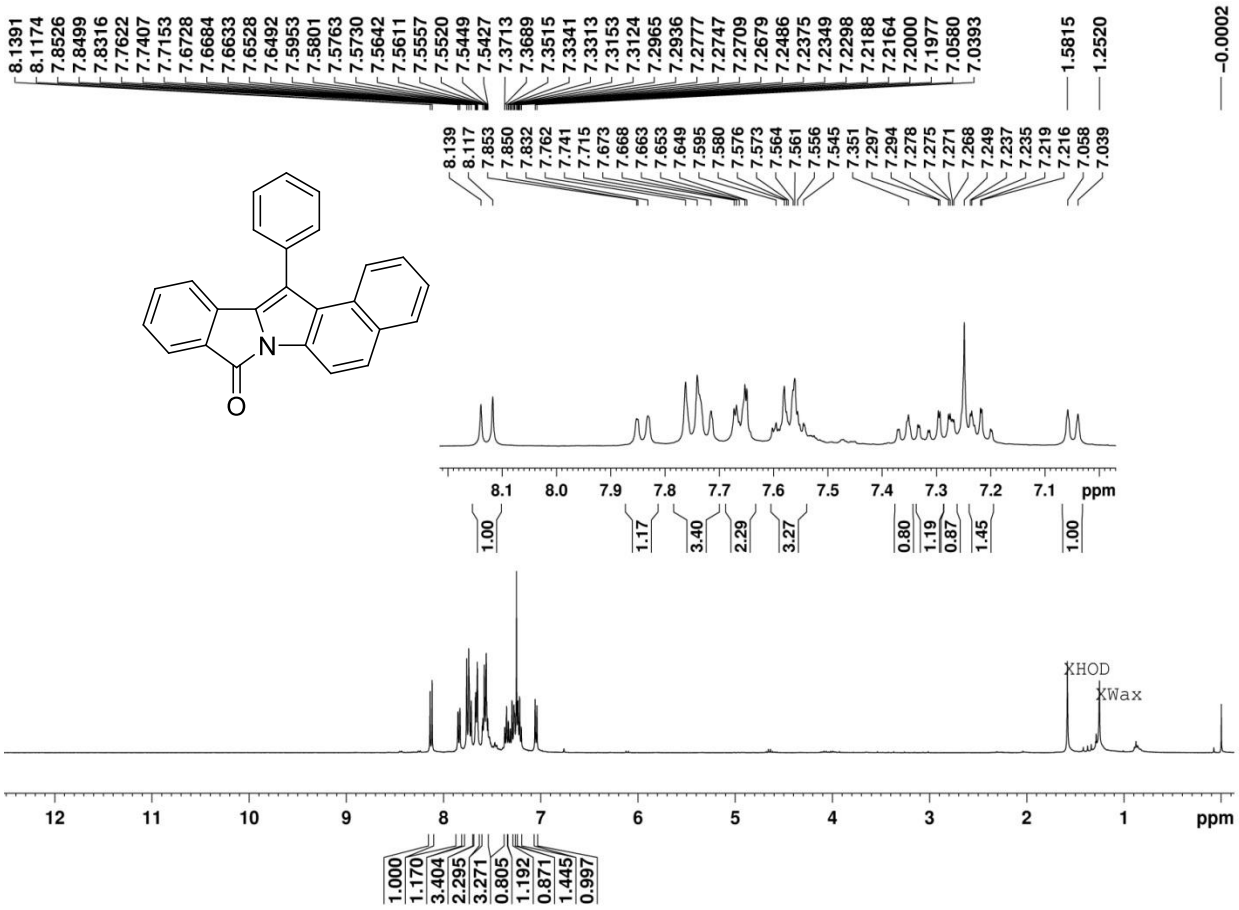
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
O
N
O

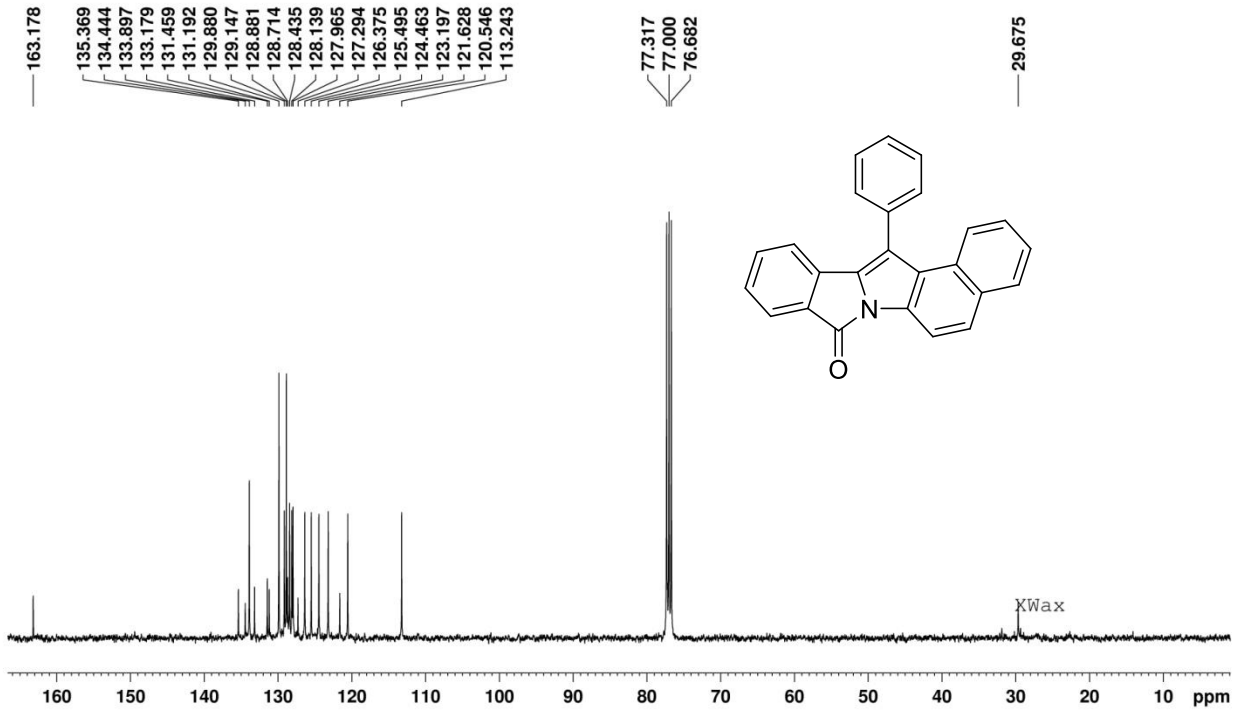
^{1}H-^{1}H COSY Spectrum (expansion) of *1-methoxy-11-phenyl-6H-isoindolo[2,1-a]indol-6-one* (2i′)



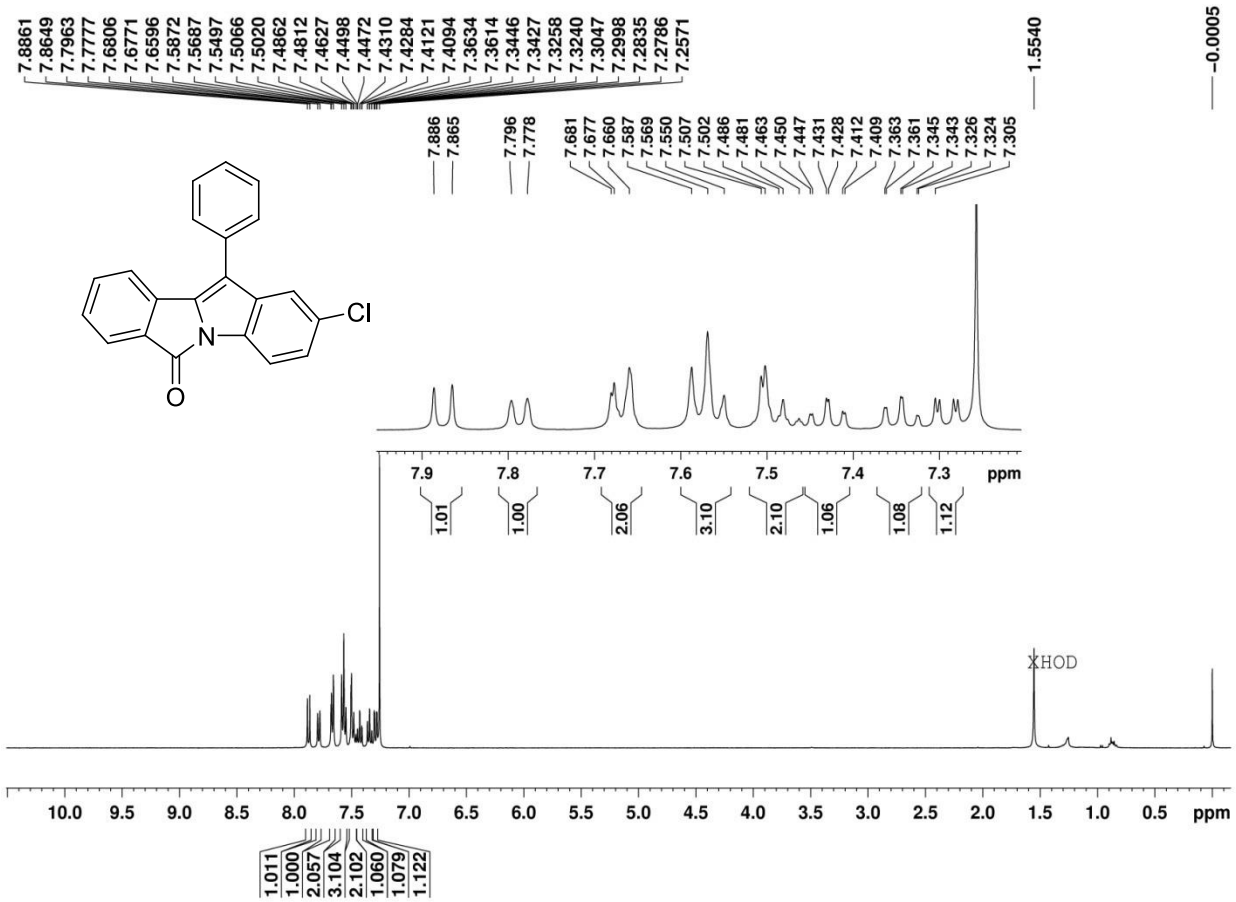
^{1}H NMR Spectrum of *13-phenyl-8H-benzo[e]isoindolo[2,1-a]indol-8-one* (2j) (400 MHz, $CDCl_3$)



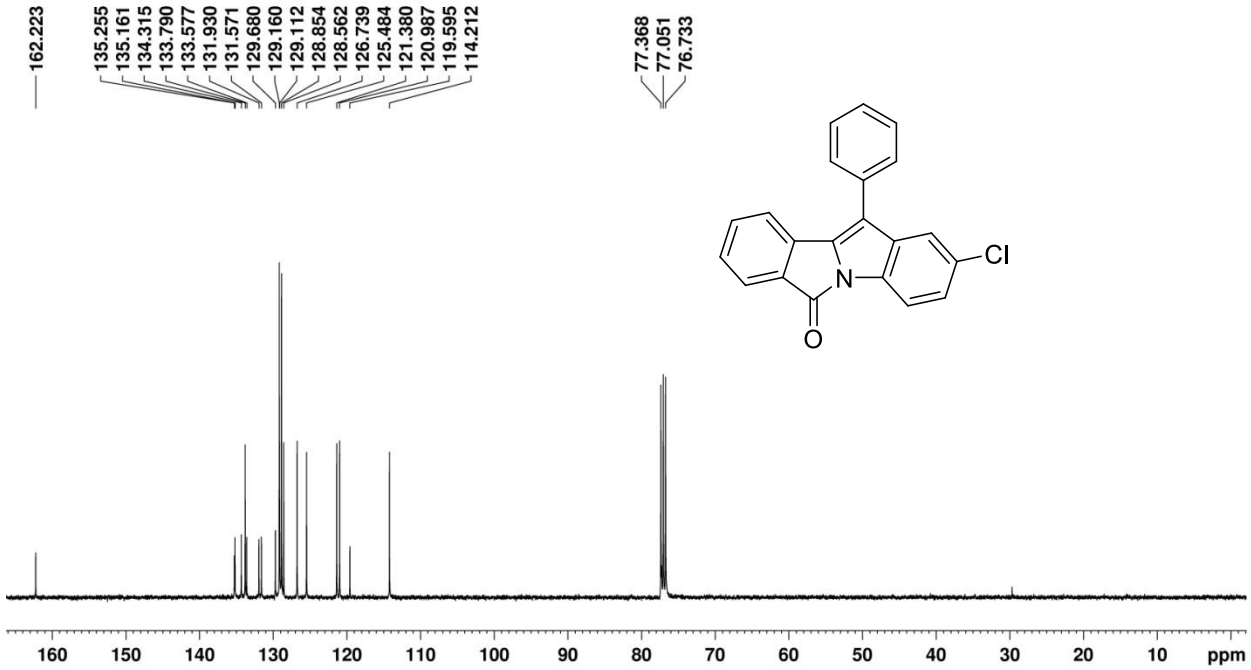
^{13}C NMR Spectrum of *13-phenyl-8H-benzo[e]isoindolo[2,1-a]indol-8-one* (2j) (100 MHz, $CDCl_3$)



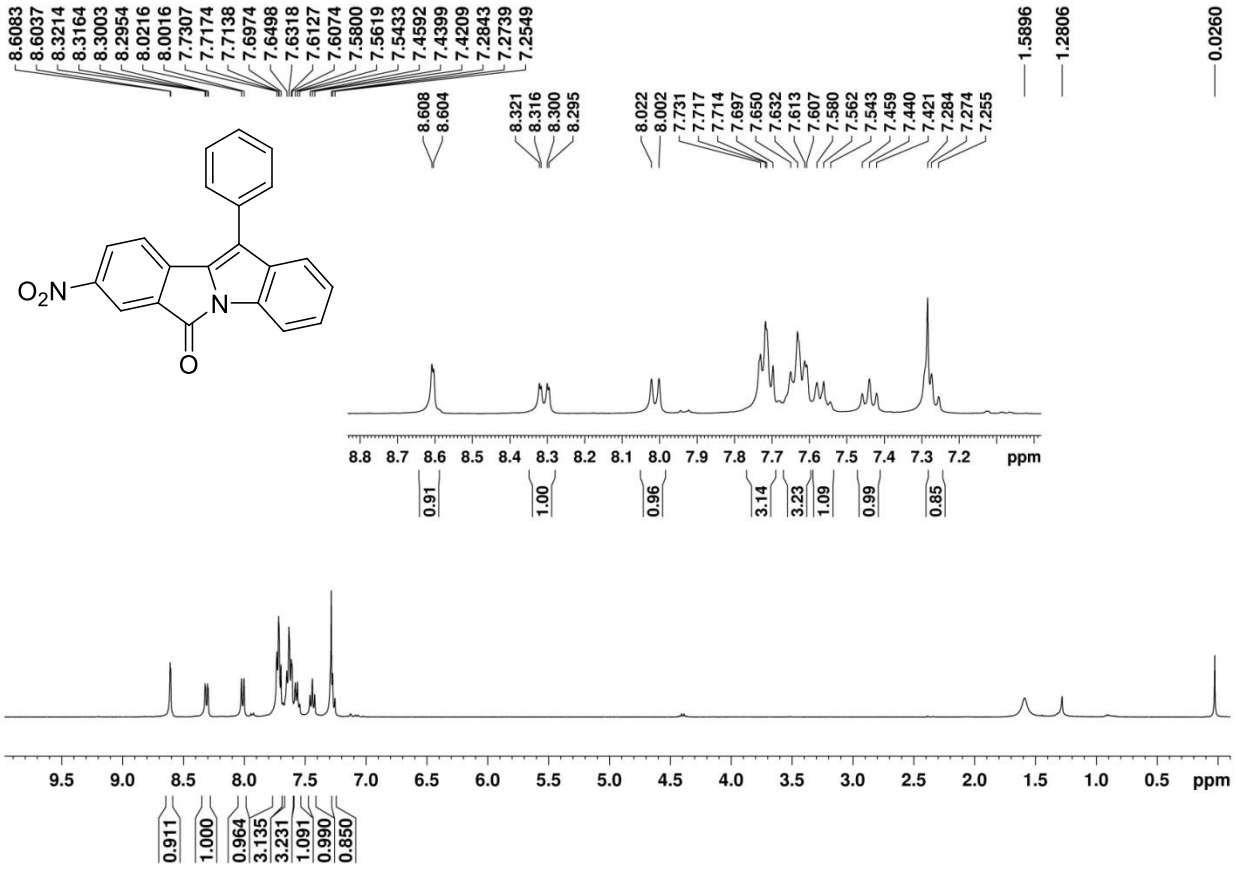
^{1}H NMR Spectrum of *2-chloro-11-phenyl-6H-isoindolo[2,1-a]indol-6-one* (2k) (400 MHz, $CDCl_3$)



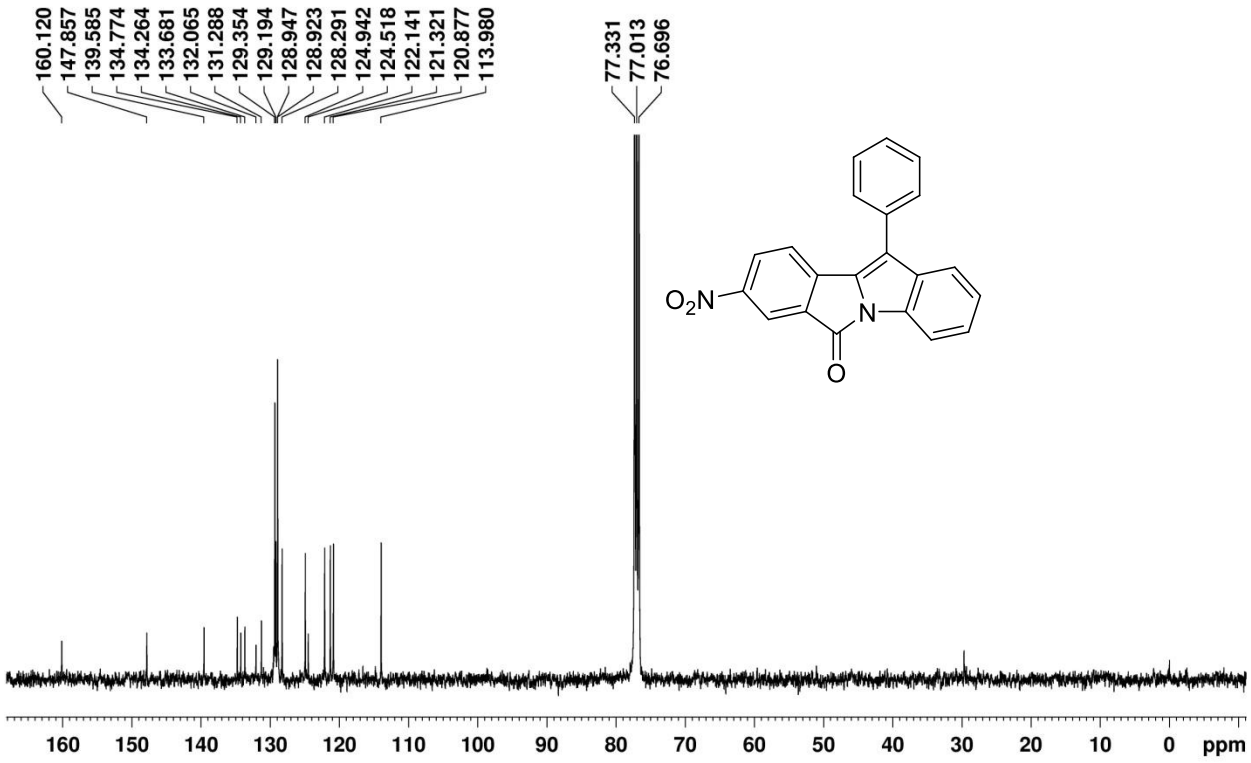
^{13}C NMR Spectrum of *2-chloro-11-phenyl-6H-isoindolo[2,1-a]indol-6-one* (2k) (100 MHz, $CDCl_3$)



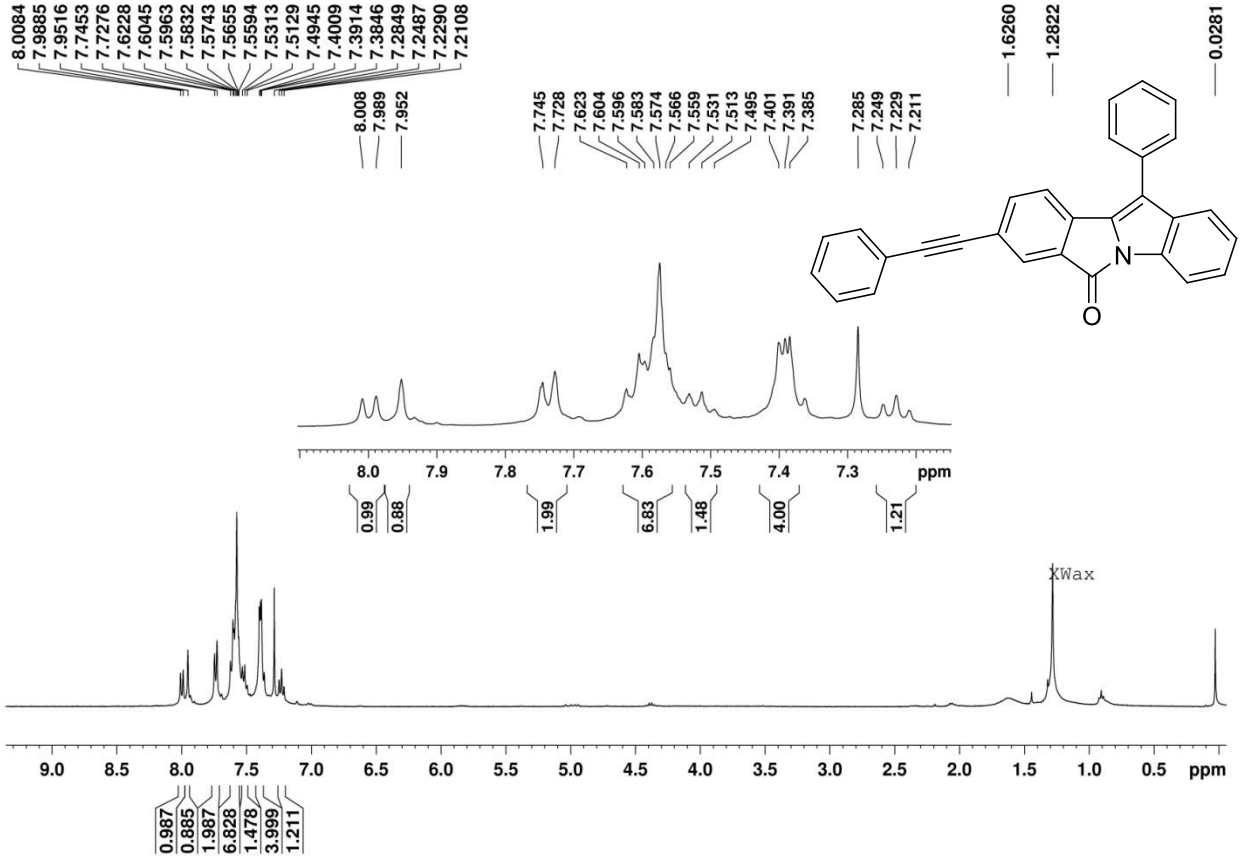
^{1}H NMR Spectrum of *8-nitro-11-phenyl-6H-isoindolo[2,1-a]indol-6-one* (2l) (400 MHz, $CDCl_3$)



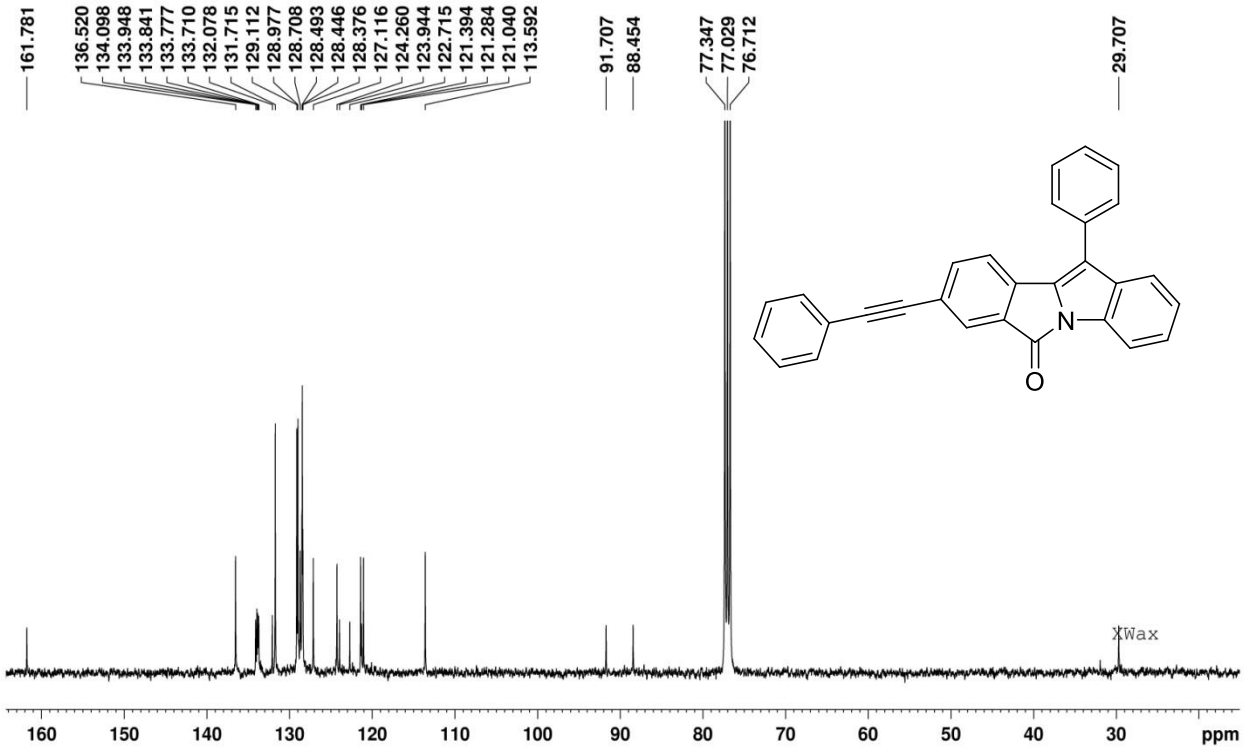
^{13}C NMR Spectrum of *8-nitro-11-phenyl-6H-isoindolo[2,1-a]indol-6-one* (2l) (100 MHz, $CDCl_3$)



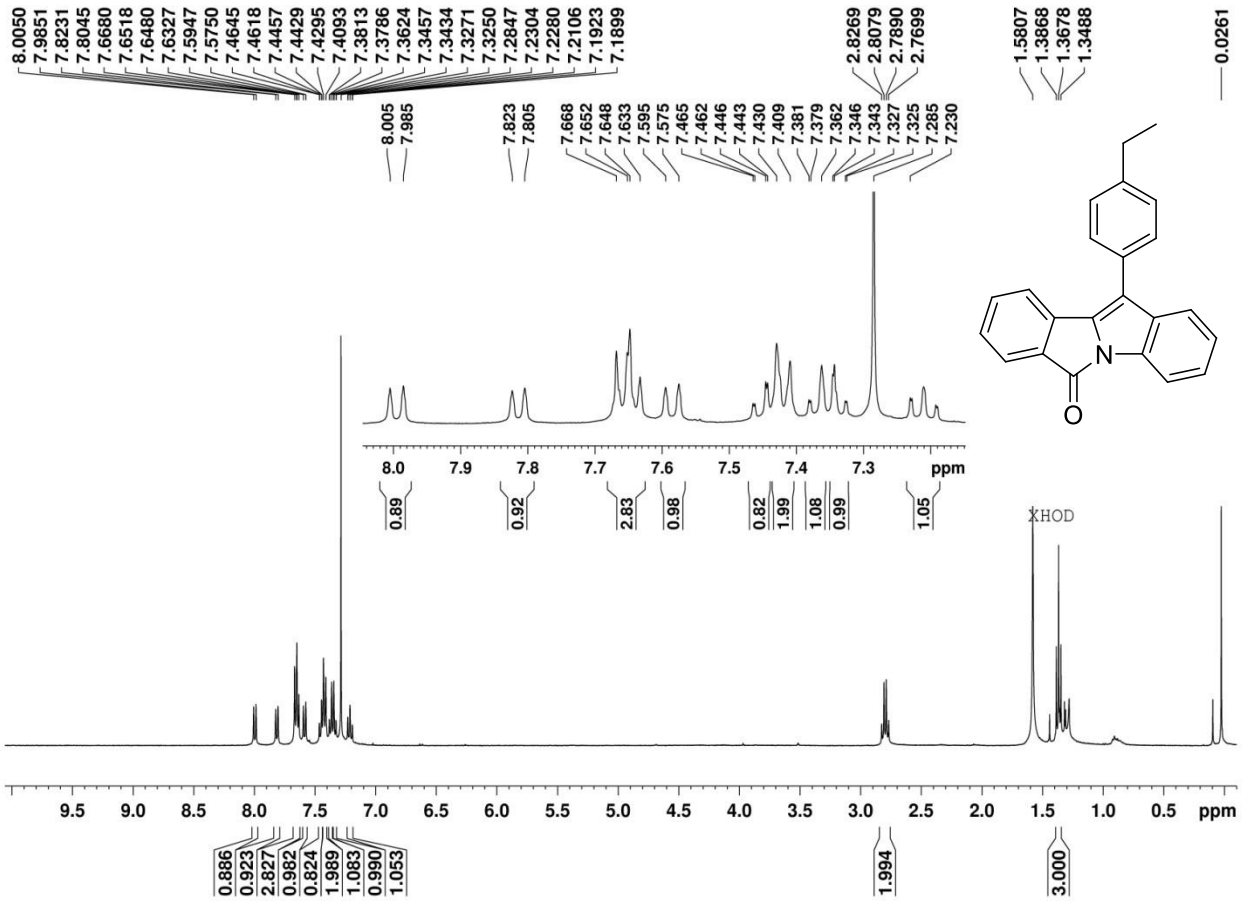
^{1}H NMR Spectrum of *11-phenyl-8-(phenylethynyl)-6H-isoindolo[2,1-a]indol-6-one* (2m) (400 MHz, $CDCl_3$)



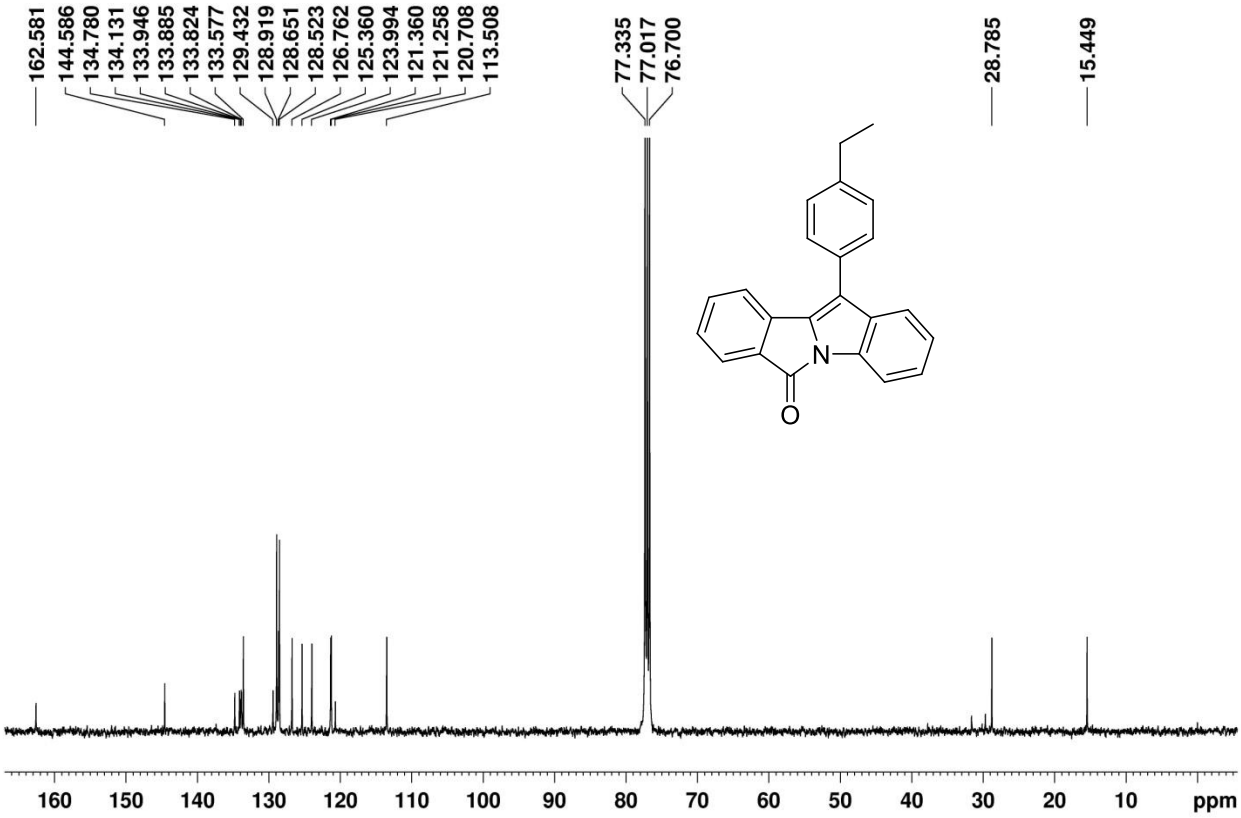
^{13}C NMR Spectrum of *11-phenyl-8-(phenylethynyl)-6H-isoindolo[2,1-a]indol-6-one* (2m) (100 MHz, $CDCl_3$)



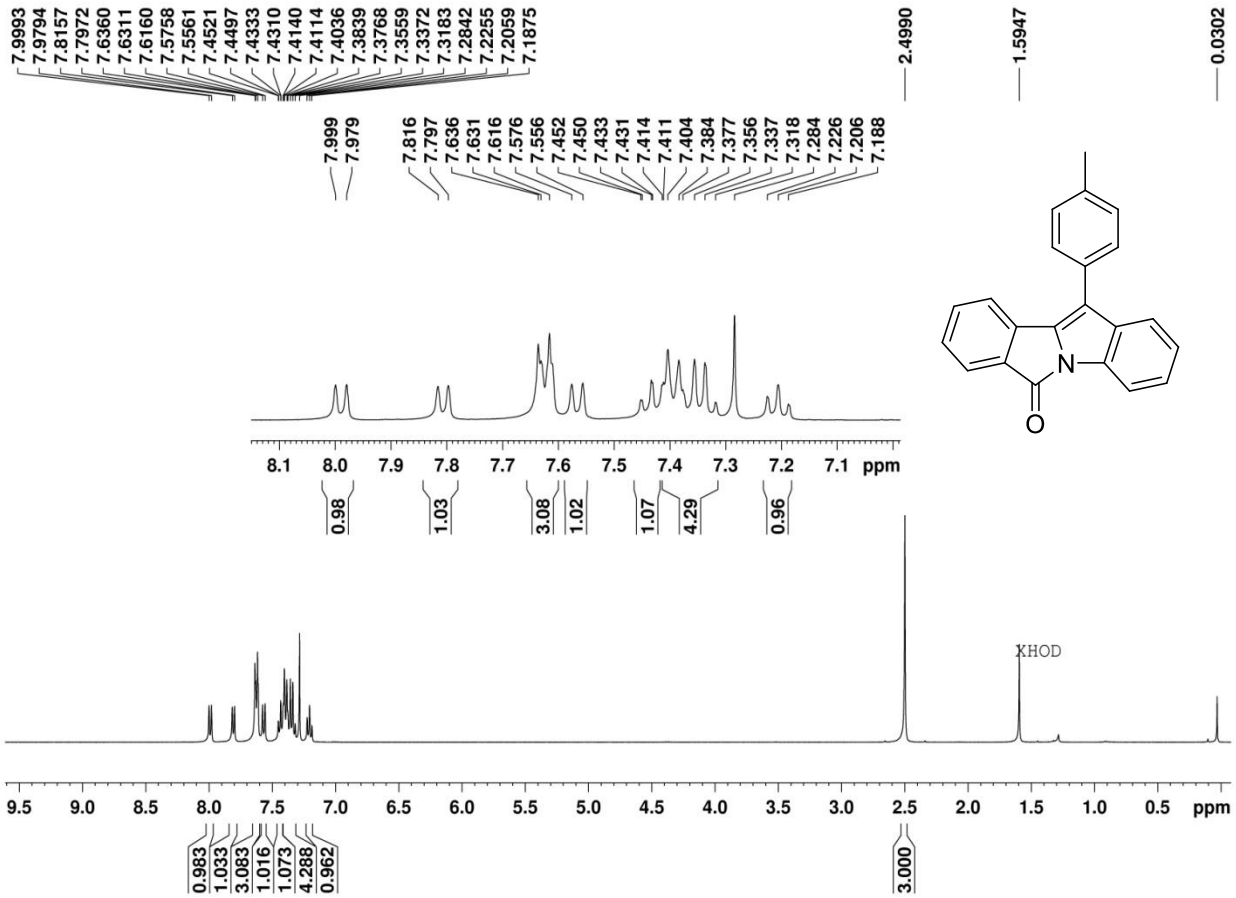
^{1}H NMR Spectrum of *11-(4-ethylphenyl)-6H-isoindolo[2,1-a]indol-6-one* (2p) (400 MHz, $CDCl_3$)



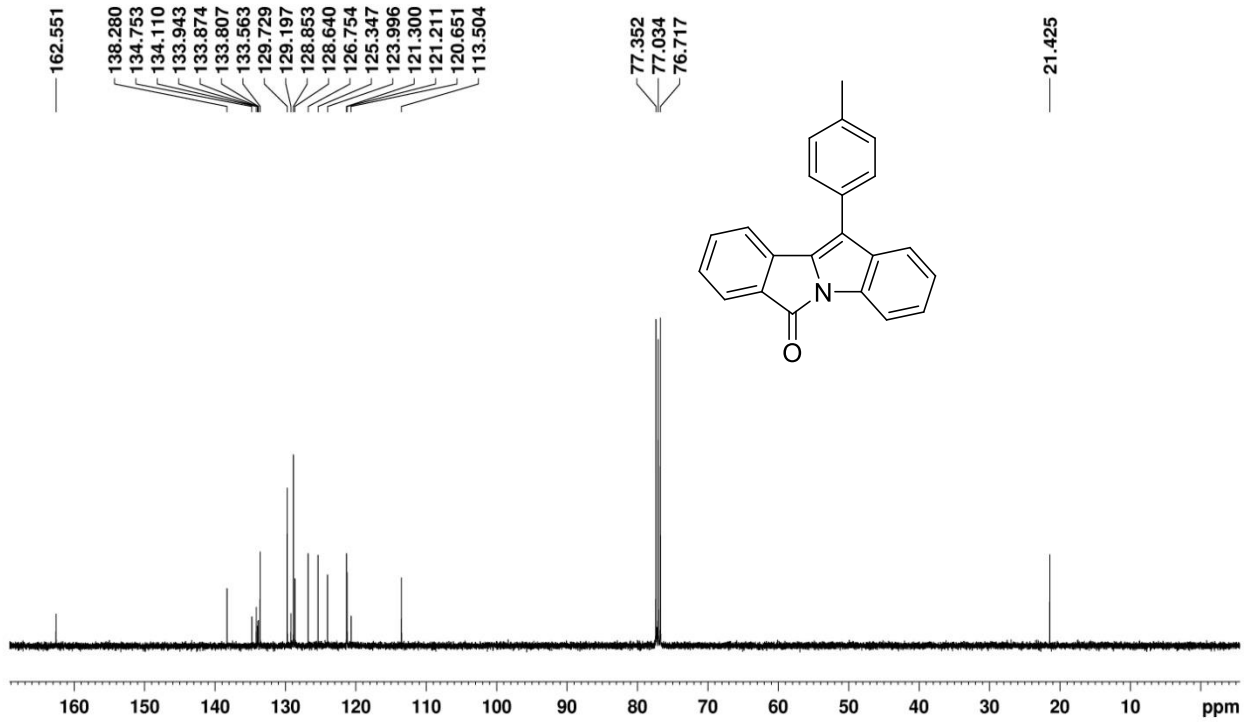
^{13}C NMR Spectrum of *11-(4-ethylphenyl)-6H-isoindolo[2,1-a]indol-6-one* (2p) (100 MHz, $CDCl_3$)



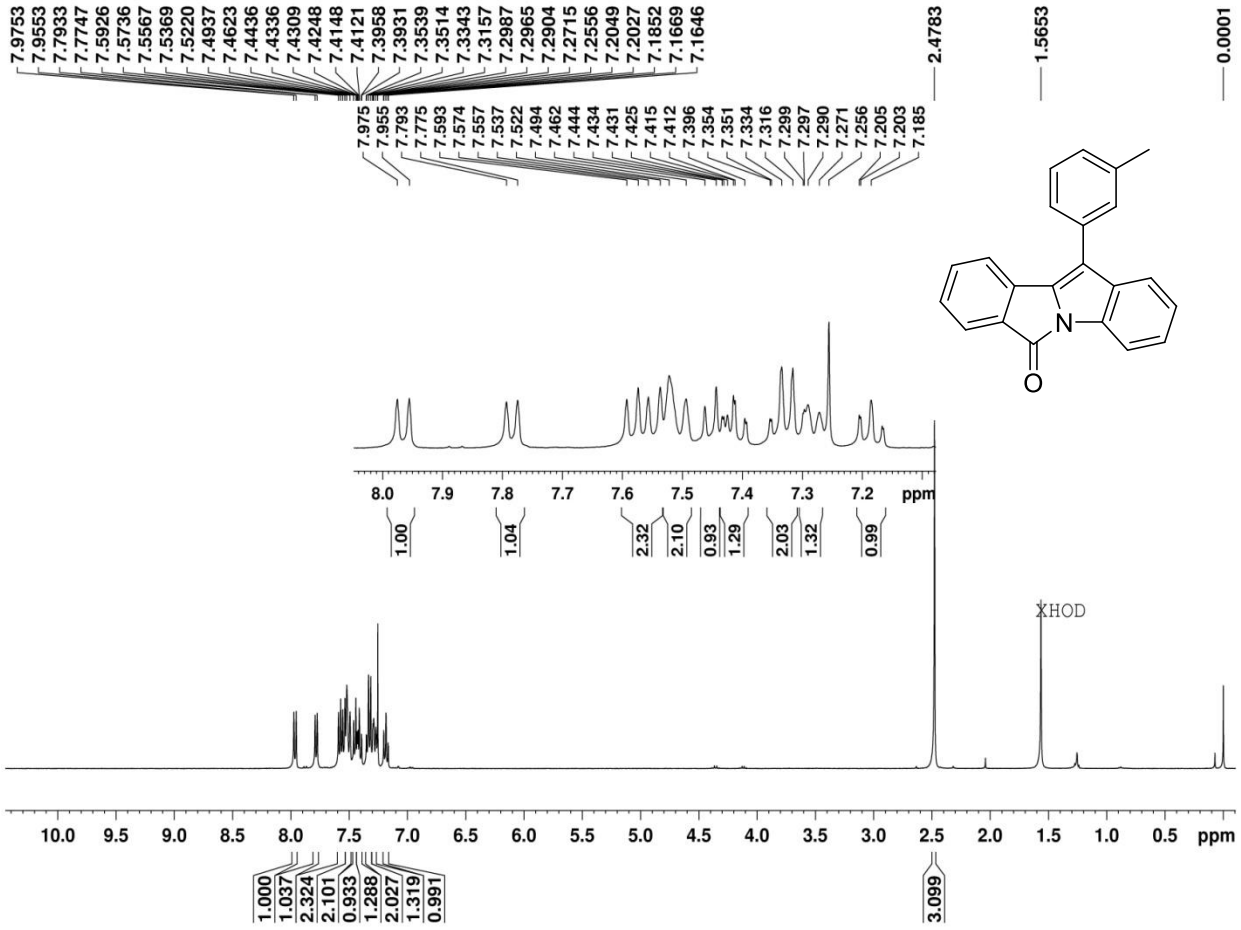
^{1}H NMR Spectrum of *11-p-tolyl-6H-isoindolo[2,1-a]indol-6-one* (2q) (400 MHz, $CDCl_3$)



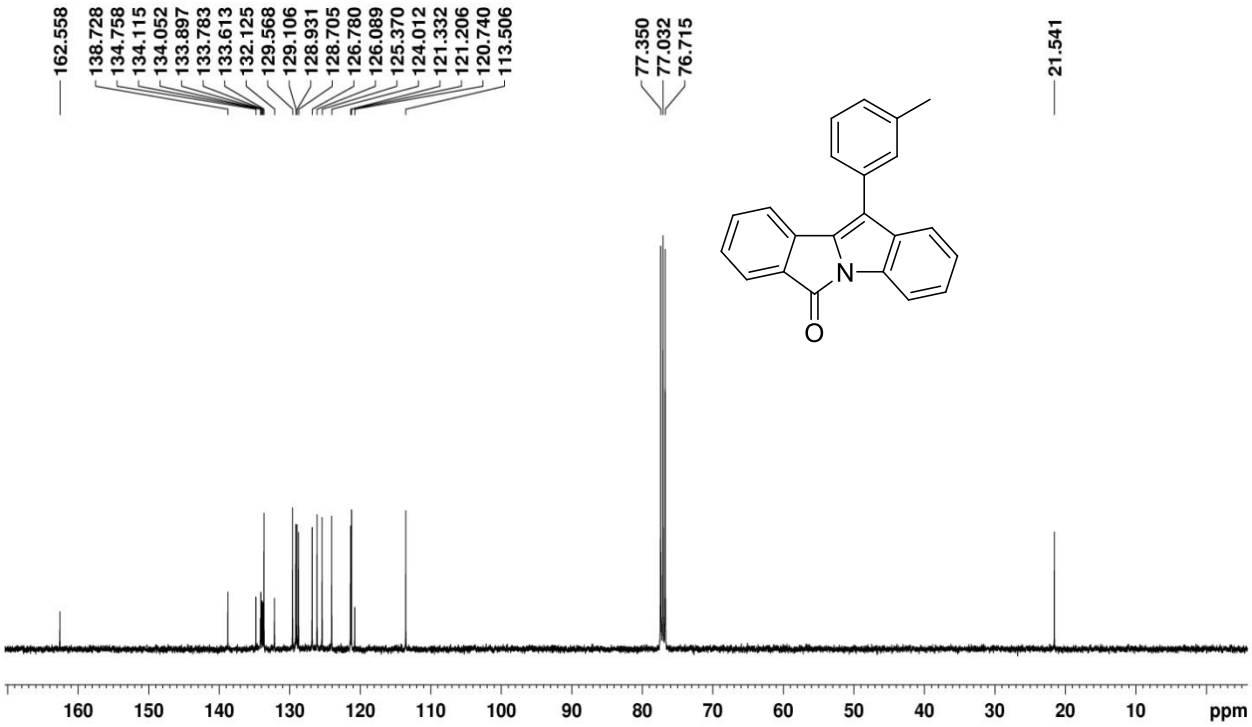
^{13}C NMR Spectrum of *11-p-tolyl-6H-isoindolo[2,1-a]indol-6-one* (2q) (100 MHz, $CDCl_3$)



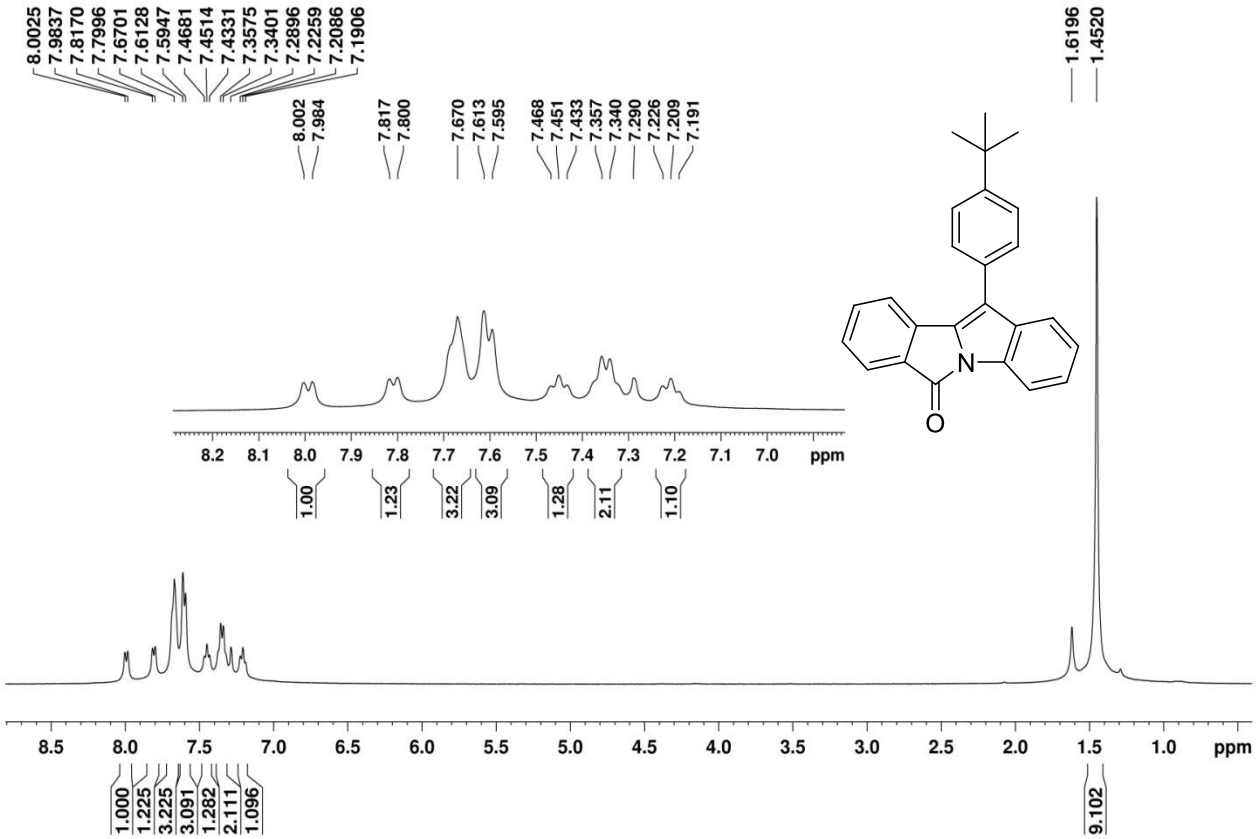
^{1}H NMR Spectrum of *11-m-tolyl-6H-isoindolo[2,1-a]indol-6-one* (2r) (400 MHz, $CDCl_3$)



^{13}C NMR Spectrum of *11-m-tolyl-6H-isoindolo[2,1-a]indol-6-one* (2r) (100 MHz, $CDCl_3$)



^{1}H NMR Spectrum of *11-(4-tert-butylphenyl)-6H-isoindolo[2,1-a]indol-6-one*(2s) (400 MHz, $CDCl_3$)



^{13}C NMR Spectrum of *11-(4-tert-butylphenyl)-6H-isoindolo[2,1-a]indol-6-one*(2s) (100 MHz, $CDCl_3$)