SUPPORTING INFORMATION

A New Facile Synthesis of 3-Amidoindole Derivatives and Their Evaluation as Potential GSK-3β Inhibitors

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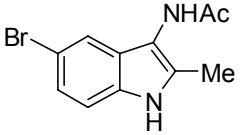
General Information

All reactions were carried out under argon atmosphere. Reactions were monitored by TLC analysis (pre-coated silica gel plates with fluorescent indicator UV_{254}, 0.2 mm) and visualized with 254 nm UV light or iodine. Chemicals were purchased from Aldrich, Fluka, Acros, AlfaAsar, Strem and unless otherwise noted were used without further purification. All compounds were characterized by ^{1}H NMR, ^{13}C NMR, GC-MS, HRMS and IR spectroscopy. ^{1}H spectra were recorded on Bruker AV 300 and AV 400 spectrometers. ^{13}C NMR and ^{19}F NMR spectra were recorded at 75.5 MHz and 282 MHz respectively. Chemical shifts are reported **only for major rotamer** (short signals on NMR scans belong to minor rotamer) in ppm relative to the center of solvent resonance. Melting points were determined on a digital SMP3 (Stuart). IR spectra were recorded on FT-IR ALPHA (Bruker) with Platinum-ATR (Bruker). EI (70 eV) mass spectra were recorded on MAT 95XP (Thermo ELECTRON CORPORATION). GC was performed on Agilent 6890 chromatograph with a 30 m HP5 column. HRMS was performed on MAT 95XP (EI) and Agilent 6210 Time-of-Flight LC/MS (ESI). GC-MS was performed on Agilent 5973 chromatograph Mass Selective Detector. All yields reported refer to isolated yields.

General procedure:

In an Ace-pressure tube to a solution of alkyne derivative **2a-d** (1 mmol) and arylhydrazine derivative **1a-k** (1.5 mmol) in 1,2-dimethoxyethane or toluene (3 mL), zinc bromide or zinc chloride (3 mmol) was added under argon atmosphere. The pressure tube was fitted with a Teflon cap and heated at 110 °C for 20 h (TLC control). After removal of the solvent, the crude product was purified by column chromatography and recrystallized using heptane with ethyl acetate, acetone or dichloromethane.

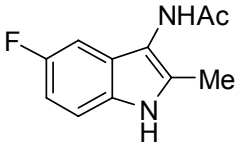
<u>*N*-(5-Bromo-2-methyl-1*H*-indol-3-yl)acetamide (3) from arylhydrazine 1a and alkyne 2a</u>



Yield: 208 mg (**78%**); white crystals; **Mp** 232 °C (from CH_2Cl_2/heptane); $\mathbf{R_f}$ = 0.4 (solvent ethyl acetate/ethanol 20:1); **^{1}H NMR** (300 MHz, DMSO-d_6): δ = 2.05 (s, 3H), 2.08 (s, 3H), 7.09 (dd, 1H, *J* = 3.9, 8.5 Hz), 7.20 (d, 1H, *J* = 8.5 Hz), 7.41 (d, 1H, *J* = 1.9 Hz), 9.23 (s, 1H), 11.08 (s, 1H); **^{13}C NMR** (DMSO-d_6): δ = 11.2, 22.7, 110.0, 110.9, 112.6, 119.7, 122.5, 126.5, 131.1, 132.2, 168.5; **GC-MS** (EI, 70 eV): *m/z* (%) 266 (66) [M^+], 268 (64.7) [M^+]; **HRMS** (EI): Calc for $C_{11}H_{11}BrN_2O$: 266.00493 and 268.00288; found:

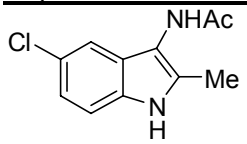
266.00472 and 268.00224; **FTIR** (ATR, cm^{-1}): 3246, 3215, 3191, 3061, 2920, 2732, 1629, 1540, 1423, 1287, 792, 702, 687, 669.

***N*-(5-Fluoro-2-methyl-1*H*-indol-3-yl)acetamide (4) from arylhydrazine 1b and alkyne 2a**



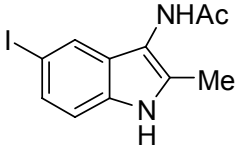
Yield: 149 mg (**72%**); white crystals; **Mp** 180-181 °C (from acetone/heptane); $\mathbf{R_f}$ = 0.37 (solvent ethyl acetate/heptane 5:1); **^{1}H NMR** (300 MHz, DMSO-d_6): δ = 2.07 (s, 3H), 2.27 (s, 3H), 6.82 (m, 1H), 6.98 (dd, 1H, *J* = 2.45, 9.97 Hz), 7.22 (dd, 1H, *J* = 4.41, 8.74 Hz), 9.21 (s, 1H), 10.95 (s, 1H); **^{13}C NMR** (DMSO-d_6): δ = 11.3, 22.7, 102.2 (d, *J* = 23.86 Hz), 107.9 (d, *J* = 25.91 Hz), 110.7 (d, *J* = 4.42 Hz), 111.5 (d, *J* = 9.69 Hz), 125.1 (d, *J* = 10.09 Hz), 130.1, 131.7, 156.7 (d, *J* = 230.92 Hz), 168.5; **GC-MS** (EI, 70 eV): *m/z* (%) 206 (52) [M^+]; **^{19}F NMR** (DMSO-d_6): δ = -125.1; **HRMS** (EI): Calc for $C_{11}H_{11}ON_2F$: 206.08499; found: 206.084715; **FTIR** (ATR, cm^{-1}): 3241, 3055, 2981, 1926, 1626, 1582, 1532, 1489, 1447, 1430, 1372, 1304, 1190, 1130, 1107, 963, 843, 791, 758, 740, 703, 669.

***N*-(5-Chloro-2-methyl-1*H*-indol-3-yl)acetamide (5) from arylhydrazine 1c and alkyne 2a**



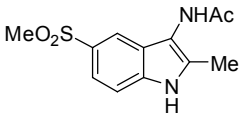
Yield: 198 mg (**89%**); white crystals; **Mp** 213 °C (from acetone/heptane); $\mathbf{R_f}$ = 0.29 (solvent ethyl acetate/heptane 4:1); **^{1}H NMR** (300 MHz, DMSO-d_6): δ = 2.05 (s, 3H), 2.23 (s, 3H), 6.98 (dd, 1H, *J* = 2.0, 8.5 Hz), 7.24 (d, 1H, *J* = 8.7 Hz), 7.26 (d, 1H, *J* ~ 1.9 Hz), 9.23 (s, 1H), 11.06 (s, 1H); **^{13}C NMR** (DMSO-d_6): δ = 11.2, 22.7, 110.2, 112.1, 116.7, 119.9, 122.9, 125.8, 131.3, 131.9, 168.5; **GC-MS** (EI, 70 eV): *m/z* (%) 222 (59) [M^+]; **HRMS** (EI): Calc for $C_{11}H_{11}ON_2Cl$: 222.05544; found: 222.05529; **FTIR** (ATR, cm^{-1}): 3218, 3190, 3095, 3064, 2982, 2955, 2922, 2766, 2736, 1629, 1566, 1541, 1425, 1289, 1055, 873, 780, 792, 697, 672.

***N*-(5-Iodo-2-methyl-1*H*-indol-3-yl)acetamide (6) from arylhydrazine 1d and alkyne 2a**



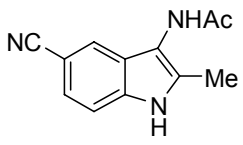
Yield: 220 mg (**70%**); white crystals; **Mp** 231 °C (dec.) (from acetone/heptane); $\mathbf{R_f}$ = 0.33 (solvent ethyl acetate/ethanol 20:1); **^{1}H NMR** (300 MHz, DMSO-d_6): δ = 2.04 (s, 3H), 2.22 (s, 3H), 7.09 (d, 1H, *J* = 8.5 Hz), 7.24 (dd, 1H, *J* = 1.75, 8.5 Hz), 7.59 (d, 1H, *J* = 1.6 Hz), 9.22 (s, 1H), 11.06 (s, 1H); **^{13}C NMR** (DMSO-d_6): δ = 11.3, 22.7, 82.0, 109.6, 113.2, 125.9, 127.4, 128.0, 130.7, 132.6, 168.6; **MS** (EI): *m/z* (%) 314 (100) [M^+]; **HRMS** (EI): Calc for $C_{11}H_{11}ON_2I$: 313.99106; found: 313.99116; **FTIR** (ATR, cm^{-1}): 3244, 3219, 3085, 3056, 2980, 2916, 2726, 1627, 1566, 1539, 1473, 1420, 1285, 1241, 1010, 799, 793, 749, 698, 677, 665.

***N*-(2-Methyl-5-(methylsulfonyl)-1*H*-indol-3-yl)acetamide (7) from arylhydrazine 1e and alkyne 2a**



Yield: 237 mg (**89%**); yellow crystals; **Mp** from 230 °C (dec.) (from acetone/heptane); $\mathbf{R_f}$ = 0.45 (solvent ethyl acetate/ethanol 10:1); **^{1}H NMR** (300 MHz, DMSO-d_6): δ = 2.08 (s, 3H), 2.27 (s, 3H), 3.12 (s, 3H), 7.45 (d, 1H, *J* = 8.52 Hz), 7.53 (dd, 1H, *J* = 1.75, 8.52 Hz), 7.88 (d, 1H, *J* = 1.56 Hz), 9.41 (s, 1H), 11.48 (s, 1H); **^{13}C NMR** (DMSO-d_6): δ = 11.5, 22.8, 44.6, 111.3, 111.8, 117.7, 118.7, 124.1, 130.8, 132.5, 135.6, 168.6; **GC-MS** (EI): *m/z* (%) 266 (42) [M^+]; **HRMS** (EI): Calc for $C_{12}H_{14}O_3N_2S$: 266.07196; found: 266.07217; **FTIR** (ATR, cm^{-1}): 3353, 3291, 3073, 3016, 2991, 2918, 1645, 1594, 1511, 1303, 1280, 1158, 1133, 1119, 1059, 958, 806, 763.

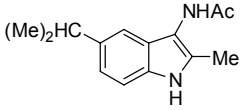
***N*-(5-Cyano-2-methyl-1*H*-indol-3-yl)acetamide (8) from arylhydrazine 1f and alkyne 2a**



Yield: 171 mg (**80%**); white crystals; **Mp** 272 °C (from acetone/heptane); $\mathbf{R_f}$ = 0.43 (solvent ethyl acetate/ethanol 10:1); **^{1}H**

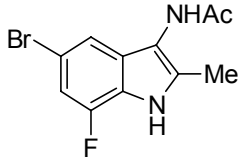
NMR (300 MHz, DMSO-d_6): δ = 2.07 (s, 3H), 2.26 (s, 3H), 7.34 (dd, 1H, *J* = 1.54, 8.39 Hz), 7.40 (dd, 1H, *J* = 0.53, 8.39 Hz), 7.72 (d, 1H, *J* = 0.57 Hz), 9.35 (s, 1H), 11.49 (s, 1H); **^{13}C NMR** (DMSO-d_6): δ = 11.3, 22.7, 100.3, 111.3, 111.9, 120.8, 123.1, 123.2, 124.5, 132.1, 135.3, 168.7; **GC-MS** (EI): *m/z* (%) 213 (54) [M^+]; **HRMS** (EI): Calc for $C_{12}H_{11}ON_3$: 213.08966; found: 213.08999; **FTIR** (ATR, cm^{-1}): 3293, 3236, 3116, 3029, 2920, 2730, 2223, 1628, 1597, 1521, 1476, 1441, 1367, 1310, 1278, 1248, 1197, 1030, 874, 802, 725, 686, 664.

<u>*N*-(5-Isopropyl-2-methyl-1*H*-indol-3-yl)acetamide (9) from arylhydrazine 1g and alkyne 2a</u>



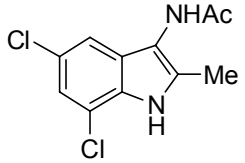
Yield: 216 mg (**94%**); light brown-yellow crystals; **Mp** 171 °C (from acetone/heptane); **R_f** = 0.5 (solvent ethyl acetate/heptane 5:1); **^{1}H NMR** (300 MHz, DMSO-d_6): δ = 1.22 (d, 6H, *J* = 6.92 Hz), 2.05 (s, 3H), 2.20 (s, 3H), 6.89 (dd, 1H, *J* = 1.66, 8.30 Hz), 7.10 (d, 1H, *J* < 0.5 Hz), 7.14 (d, 1H, *J* = 8.30 Hz), 9.15 (s, 1H), 10.68 (s, 1H); **^{13}C NMR** (DMSO-d_6): δ = 11.4, 22.7, 24.7, 33.6, 100.1, 110.4, 113.9, 119.2, 124.9, 129.6, 132.2, 138.3, 168.4; **GC-MS** (EI): *m/z* (%) 230 (83) [M^+]; **HRMS** (EI): Calc for $C_{14}H_{18}ON_2$: 230.14136; found: 230.14183; **FTIR** (ATR, cm^{-1}): 3258, 3066, 2965, 2928, 2889, 2869, 2732, 1630, 1544, 1425, 1285, 1244, 804, 696, 677, 662.

<u>*N*-(5-Bromo-7-fluoro-2-methyl-1*H*-indol-3-yl)acetamide (10) from arylhydrazine 1h and alkyne 2a</u>



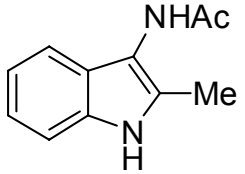
Yield: 188 mg (**66%**); white crystals; **Mp** 228 °C (from acetone/heptane); **R_f** = 0.29 (solvent ethyl acetate/heptane 4:1); **^{1}H NMR** (400 MHz, Acetone-d_6): δ = 2.12 (s, 3H), 2.31 (s, 3H), 6.96 (dd, 1H, *J* = 1.59, 10.56 Hz), 7.34 (dd, 1H, *J* ~ 0.58, 1.63 Hz), 8.55 (s, 1H), 10.57 (s, 1H); **^{13}C NMR** (Acetone-d_6): δ = 11.1, 22.6, 109.2 (d, *J* = 20.6 Hz), 110.6 (d, *J* = 8.7 Hz), 112.1, 117.0 (d, *J* = 3.5 Hz), 121.2 (d, *J* = 12.8 Hz), 130.7, 133.5, 149.1 (d, *J* = 251.2 Hz), 169.0; **^{19}F NMR** (Acetone-d_6): δ = -134.5; **GC-MS** (EI): *m/z* (%) 284 (62) [M^+], 286 (58) [M^+]; **HRMS** (EI): Calc for $C_{11}H_{10}ON_2BrF$: 283.99551; found: 283.99542; **FTIR** (ATR, cm^{-1}): 3255, 3159, 3108, 3063, 2985, 2959, 2924, 2871, 2740, 1629, 1573, 1542, 1460, 1443, 1415, 1361, 1289, 1261, 1215, 886, 860, 818, 737, 701, 686.

<u>*N*-(5,7-Dichloro-2-methyl-1*H*-indol-3-yl)acetamide (11) from arylhydrazine 1i and alkyne 2a</u>



Yield: 198 mg (**77%**); white crystals; **Mp** 205-207 °C (from acetone/heptane); **R_f** = 0.32 (solvent ethyl acetate/heptane 4:1); **^{1}H NMR** (300 MHz, Acetone-d_6): δ = 2.12 (s, 3H), 2.30 (s, 3H), 7.05 (d, 1H, *J* = 1.8 Hz), 7.31 (dd, 1H, *J* = 0.5, 1.8 Hz), 8.61 (s, 1H), 10.42 (s, 1H); **^{13}C NMR** (Acetone-d_6): δ = 11.1, 22.6, 112.3, 116.7 (2C), 120.1, 124.5, 128.1, 130.1, 133.9, 169.2; **GC-MS** (EI): *m/z* (%) 256 (43) [M^+]; **HRMS** (EI): Calc for $C_{11}H_{10}ON_2Cl_2$: 256.01647; found: 256.01652; **FTIR** (ATR, cm^{-1}): 3273, 3154, 3094, 3066, 2958, 2926, 2871, 2778, 1636, 1563, 1539, 1483, 1369, 1288, 1255, 1034, 874, 863, 831, 686.

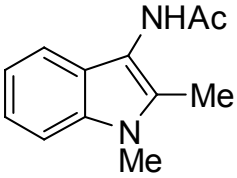
<u>*N*-(2-Methyl-1*H*-indol-3-yl)acetamide (12)</u> [27] **<u>from arylhydrazine 1j and alkyne 2a</u>**



Yield: 172 mg (**91%**); white crystals; **Mp** 113-115 °C (from acetone/heptane) (lit. 156-157°C); **R_f** = 0.2 (solvent ethyl acetate/heptane 4:1); **^{1}H NMR** (300 MHz, DMSO-d_6): δ = 2.04 (s, 3H), 2.22 (s, 3H), 6.92 (ddd, 1H), 6.99 (ddd, 1H), 7.23 (dd, 1H, *J* ~ 8.3 Hz), 7.25 (dd, 1H, *J* ~ 8.4 Hz), 9.17 (s, 1H), 10.82 (s, 1H); **^{13}C NMR** (DMSO-d_6): δ = 11.3, 22.7, 110.3, 110.6, 117.3, 118.3, 120.2, 124.9, 129.5, 133.6, 168.5; **GC-MS** (EI): *m/z* (%) 188 (52) [M^+]; **HRMS** (EI): Calc for $C_{11}H_{12}ON_2$: 188.09441; found: 188.094323; **FTIR** (ATR,

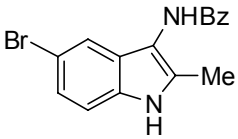
cm^{-1}): 3255, 3226, 3197, 3113, 3081, 3059, 2920, 2885, 1625, 1540, 1427, 1312, 1293, 1245, 1169, 1010, 740, 694, 668.

<u>*N*-(1,2-Dimethyl-1*H*-indol-3-yl)acetamide (13) from arylhydrazine 1k and alkyne 2a</u>



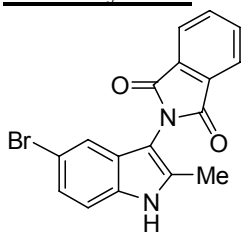
Yield: 111 mg (**55%**); white crystals; **Mp** 185 °C (from acetone/heptane); $\mathbf{R_f}$ = 0.26 (solvent ethyl acetate/heptane 4:1); **^{1}H NMR** (300 MHz, DMSO-d$_6$): δ = 2.05 (s, 3H), 2.22 (s, 3H), 3.64 (s, 3H), 6.95 (m, 1H), 7.06 (m, 1H), 7.27 (d, 1H, *J* = 7.7 Hz), 7.36 (d, 1H, *J* = 8.2 Hz), 9.20 (s, 1H); **^{13}C NMR** (DMSO-d$_6$): δ = 9.9, 22.7, 29.4, 109.0, 110.1, 117.4, 118.5, 120.3, 124.1, 131.3, 134.6, 168.7; **GC-MS** (EI): *m/z* (%) 202 (52) [M$^+$]; **HRMS** (EI): Calc for $C_{12}H_{14}ON_2$: 202.11006; found: 202.10981; **FTIR** (ATR, cm^{-1}): 3230, 3112, 3032, 2914, 2833, 1649, 1525, 1472, 1370, 1334, 1284, 1196, 1010, 733.

<u>*N*-(5-Bromo-2-methyl-1*H*-indol-3-yl)benzamide (14) from arylhydrazine 1a and alkyne 2b</u>



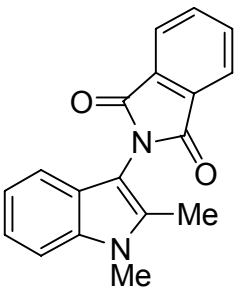
Yield: 244 mg (**74%**); white crystals; **Mp** 230 °C (from acetone/heptane); $\mathbf{R_f}$ = 0.48 (solvent ethyl acetate/heptane 2:1); **^{1}H NMR** (300 MHz, DMSO-d$_6$): δ = 2.30 (s, 3H), 7.13 (dd, 1H, *J* = 1.7, 8.5 Hz), 7.26 (d, 1H, *J* = 8.5 Hz), 7.45 (s, 1H), 7.54 (m, 3H), 8.04 (d, 2H, *J* = 7.9 Hz), 9.81 (s, 1H), 11.20 (s, 1H); **^{13}C NMR** (DMSO-d$_6$): δ = 11.4, 109.9, 111.1, 112.7, 119.8, 122.6, 126.7, 127.7 (2C), 128.4 (2C), 131.4, 132.0, 132.3, 134.5, 165.6; **GC-MS** (EI, 70 eV): *m/z* (%) 328 (87) [M$^+$], 330 (85) [M$^+$]; **HRMS** (EI): Calc for $C_{16}H_{13}BrN_2O$: 328.02058 and 330.01853; found: 328.02040 and 330.01848; **FTIR** (ATR, cm^{-1}): 3429, 3306, 3056, 2965, 2924, 2868, 2710, 1614, 1506, 1469, 1295, 1274, 1243, 1177, 1116, 1066, 794, 718, 690.

<u>2-(5-Bromo-2-methyl-1*H*-indol-3-yl)isoindoline-1,3-dione (15) from arylhydrazine 1a and alkyne 2c</u>



Yield: 238 mg (**67%**); white crystals; **Mp** 249 °C (from acetone/heptane); $\mathbf{R_f}$ = 0.41 (solvent ethyl acetate/heptane 1:1); **^{1}H NMR** (300 MHz, Acetone-d$_6$): δ = 2.35 (s, 3H), 7.20 (dd, 1H, *J* = 1.9, 8.6 Hz), 7.34 (dd, 1H, *J* = 0.5, 8.6 Hz), 7.56 (d, 1H, *J* = 1.9 Hz), 7.90 (m, 2H), 7.95 (m, 2H), 10.66 (s, 1H); **^{13}C NMR** (Acetone-d$_6$): δ = 11.1, 104.9, 113.0, 113.3, 113.4, 120.5, 123.7 (2C), 124.3, 127.5, 127.6, 133.1, 133.7, 134.8 (2C), 135.5, 167.8; **GC-MS** (EI, 70 eV): *m/z* (%) 354 (100) [M$^+$], 356 (97) [M$^+$]; **HRMS** (EI): Calc for $C_{17}H_{11}BrN_2O_2$: 353.99984 and 355.99780; found: 353.99964 and 355.99701; **FTIR** (ATR, cm^{-1}): 3381, 3105, 3047, 3029, 2920, 1716, 1468, 1376, 1307, 1084, 1046, 881, 856, 802, 793, 714.

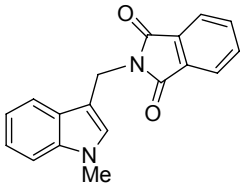
<u>2-(1,2-Dimethyl-1*H*-indol-3-yl)isoindoline-1,3-dione (16a) from arylhydrazine 1k and alkyne 2c</u>



Yield: 151 mg (**52%**); yellow crystals; **Mp** 236 °C (from acetone/heptane); $\mathbf{R_f}$ = 0.5 (solvent ethyl acetate/heptane 1:1); **^{1}H NMR** (300 MHz, Acetone-d$_6$): δ = 2.32 (s, 3H), 3.79 (s, 3H), 7.01 (ddd, 1H, *J* ~ 1.0, 7.2, 8.1 Hz), 7.15 (ddd, 1H, *J* ~ 1.3, 7.1, 8.3 Hz), 7.31 (d, 1H, *J* ~ 7.9 Hz), 7.43 (d, 1H, *J* ~ 8.2 Hz), 7.92 (m, 2H), 7.96 (m, 2H); **^{13}C NMR** (Acetone-d$_6$): δ = 9.8, 29.8, 103.7, 108.1, 109.8, 117.8, 120.1, 121.6, 123.8 (2C), 125.2, 133.0 (2C), 134.9 (2C), 136.2, 168.0 (2C); **GC-MS** (EI, 70 eV): *m/z* (%) 290 (100) [M$^+$]; **HRMS** (EI): Calc for $C_{18}H_{14}N_2O_2$: 290.10498; found: 290.10502; **FTIR** (ATR, cm^{-1}): 3474, 3101, 3044,

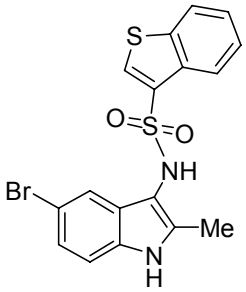
3026, 2951, 2914, 2851, 1717, 1702, 1467, 1391, 1307, 1109, 1086, 879, 747, 715, 686, 644, 527.

2-((1-Methyl-1*H*-indol-3-yl)methyl)isoindoline-1,3-dione (16b) from arylhydrazine 1k and alkyne 2c



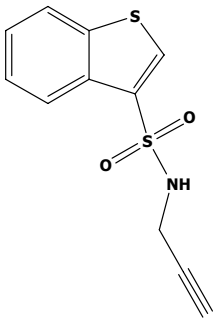
Yield: 55 mg **(19%)**; white crystals; **Mp** 180-181 °C (from acetone/heptane); $\mathbf{R_f}$ = 0.6 (solvent ethyl acetate/heptane 1:1); **^{1}H NMR** (400 MHz, DMSO -d_6): δ = 3.72 (s, 3H), 4.86 (s, 2H), 7.03 (ddd, 1H, *J* ~ 0.9, 7.2, 8.0 Hz), 7.13 (ddd, 1H, *J* ~ 1.3, 7.0, 8.1 Hz), 7.35 (s, 1H), 7.37 (ddd, 1H, *J* ~ 9.1 Hz), 7.67 (ddd, 1H, *J* ~ 8.1 Hz), 7.80 (m, 3H), 7.84 (m, 2H); **^{13}C NMR** (DMSO-d_6): δ = 32.3, 32.4, 108.9, 109.8, 118.6, 119.0, 121.4, 123.1 (2C), 126.3, 129.4, 131.5 (2C), 134.5 (2C), 136.5, 167.7 (2C); **GC-MS** (EI, 70 eV): *m/z* (%) 290 (100) [M^+]; **HRMS** (EI): Calc for $C_{18}H_{14}N_2O_2$: 290.10498; found: 290.10525; **FTIR** (ATR, cm^{-1}): 3453, 3101, 3058, 3028, 2938, 2883, 2833, 1706, 1464, 1422, 1392, 1325, 1305, 1099, 1064, 939, 750, 723, 710, 616, 524, 515, 428.

***N*-(5-Bromo-2-methyl-1*H*-indol-3-yl)benzo[b]thiophene-3-sulfonamide (17) from arylhydrazine 1a and alkyne 2d**



Yield: 215 mg **(51%)**; light yellow crystals; **Mp** 77-80 °C (from acetone/heptane); $\mathbf{R_f}$ = 0.47 (solvent ethyl acetate/heptane 1:1); **^{1}H NMR** (400 MHz, Acetone-d_6): δ = 2.06 (s, 3H), 2.99 (bs, 1H), 6.75 (d, 1H, *J* = 1.9 Hz), 6.99 (dd, 1H, *J* = 2.0, 8.6 Hz), 7.14 (d, 1H, *J* = 8.5 Hz), 7.47 (m, 2H), 8.03 (s, 1H), 8.05 (m, 1H), 8.21 (m, 1H), 10.44 (s, 1H); **^{13}C NMR** (Acetone-d_6): δ = 10.4, 108.5, 112.7, 112.9, 120.0, 123.5, 123.8, 124.0, 125.8, 126.0, 128.5, 128.8, 133.1, 134.9, 135.3, 136.4, 141.0; **HRMS neg.** (**ESI**): Calc for $C_{17}H_{13}N_2O_2BrS_2$: 418.95291 and 420.95085; found: 418.95311 and 420.95108; **HRMS pos.** (**ESI**): Calc for $C_{17}H_{13}N_2O_2BrS_2Na$: 442.9494 and 444.94735; found: 442.94926 and 444.94721; **FTIR** (ATR, cm^{-1}): 3322, 3260, 3102, 3062, 2922, 2853, 1582, 1455, 1424, 1311, 1284, 1142, 976, 865, 796, 755, 731, 707, 678.

N-(Prop-2-ynyl)benzo[b]thiophene-3-sulfonamide (2d)

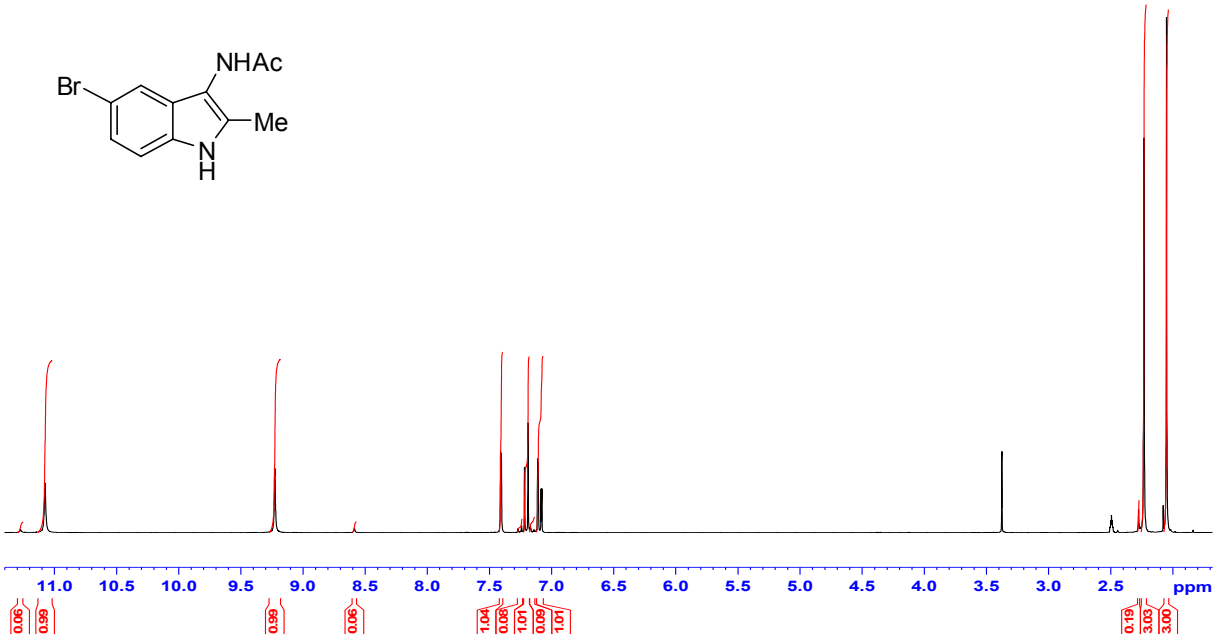


To the solution of propargylamine (165 mg, 3 mmol) in CH_2Cl_2 (3 ml) and triethylamine (3 ml) was added benzo[b]thiophene-3-sulfonyl chloride (465.4 mg, 2 mmol) at 0°C under an argon atmosphere. After 30 min the reaction mixture was warmed to room temperature and stirring was continued for 2 h. After the reaction was complete (TLC control), the solvent was removed in vacuum and the solid rest was recrystallized.

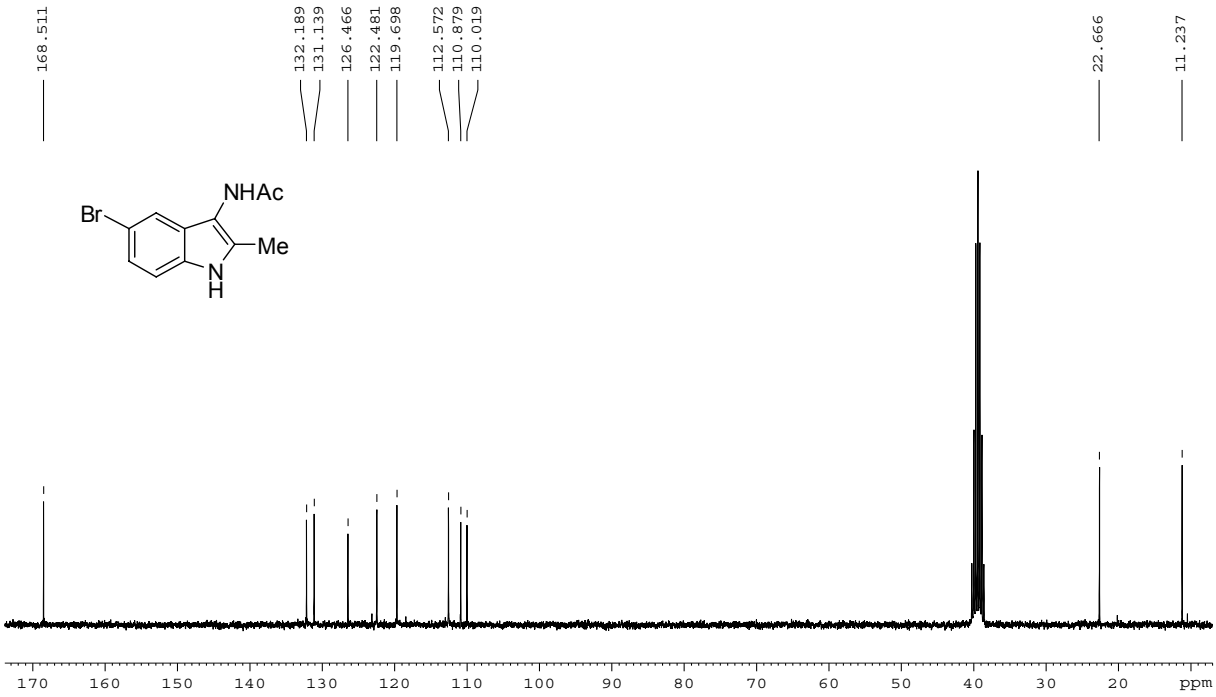
Yield: 452 mg **(90%)**; white crystals; **Mp** 95 °C (from CH_2Cl_2/heptane); $\mathbf{R_f}$ = 0.46 (solvent ethyl acetate/heptane 1:1); **^{1}H NMR** (300 MHz, $CDCl_3$): δ = 1.94 (t, 1H, *J* = 2.5 Hz), 3.86 (dd, 1H, *J* = 2.5, 6.2 Hz), 5.10 (t, 1H, *J* = 5.9 Hz), 7.48 (m, 2H), 7.90 (m, 1H), 8.19 (m, 1H), 8.29 (s, 1H); **^{13}C NMR** ($CDCl_3$): δ = 32.8, 72.7, 77.7, 122.9 (2C), 125.7, 125.8, 132.8, 133.6, 135.3, 140.3; **GC-MS** (EI, 70 eV): *m/z* (%) 251 (53) [M^+]; **HRMS** (EI): Calc for $C_{11}H_9NO_2S_2$: 251.00692; found: 251.00715; **FTIR** (ATR, cm^{-1}): 3360, 3103, 3060, 2968, 1421, 1329, 1319, 1149, 1140, 1053, 973, 851, 812, 749, 720, 709.

***N*-(5-Bromo-2-methyl-1*H*-indol-3-yl)acetamide (3)**

^{1}H NMR

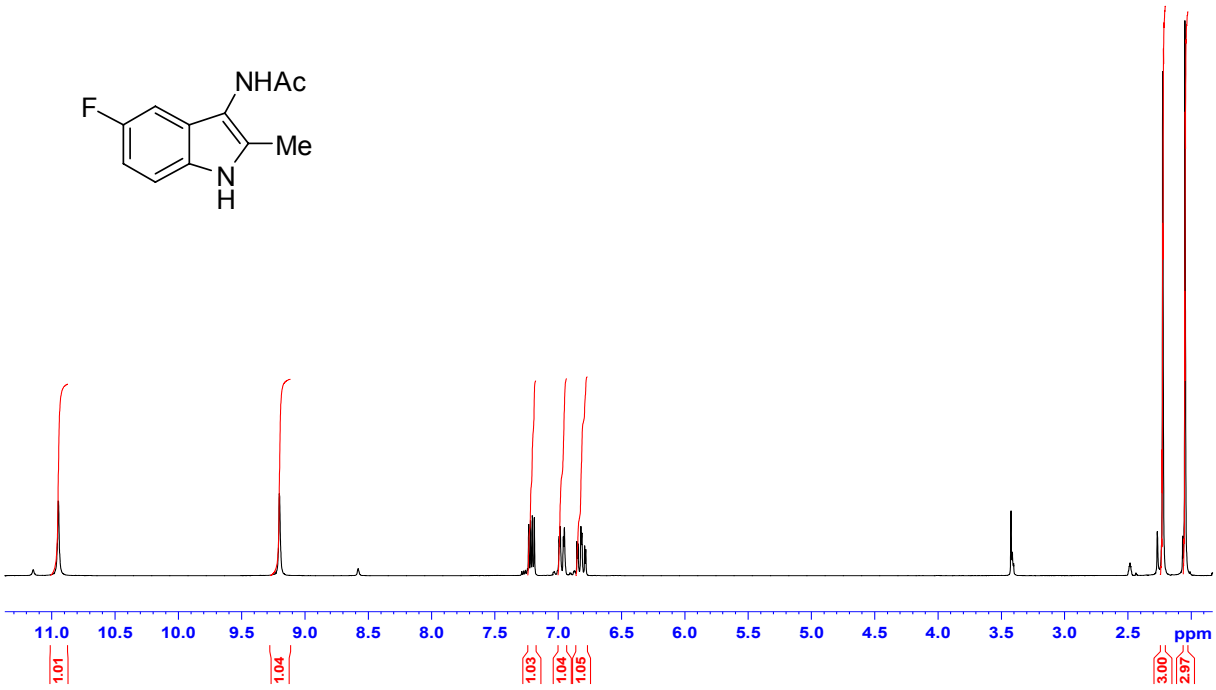


^{13}C NMR

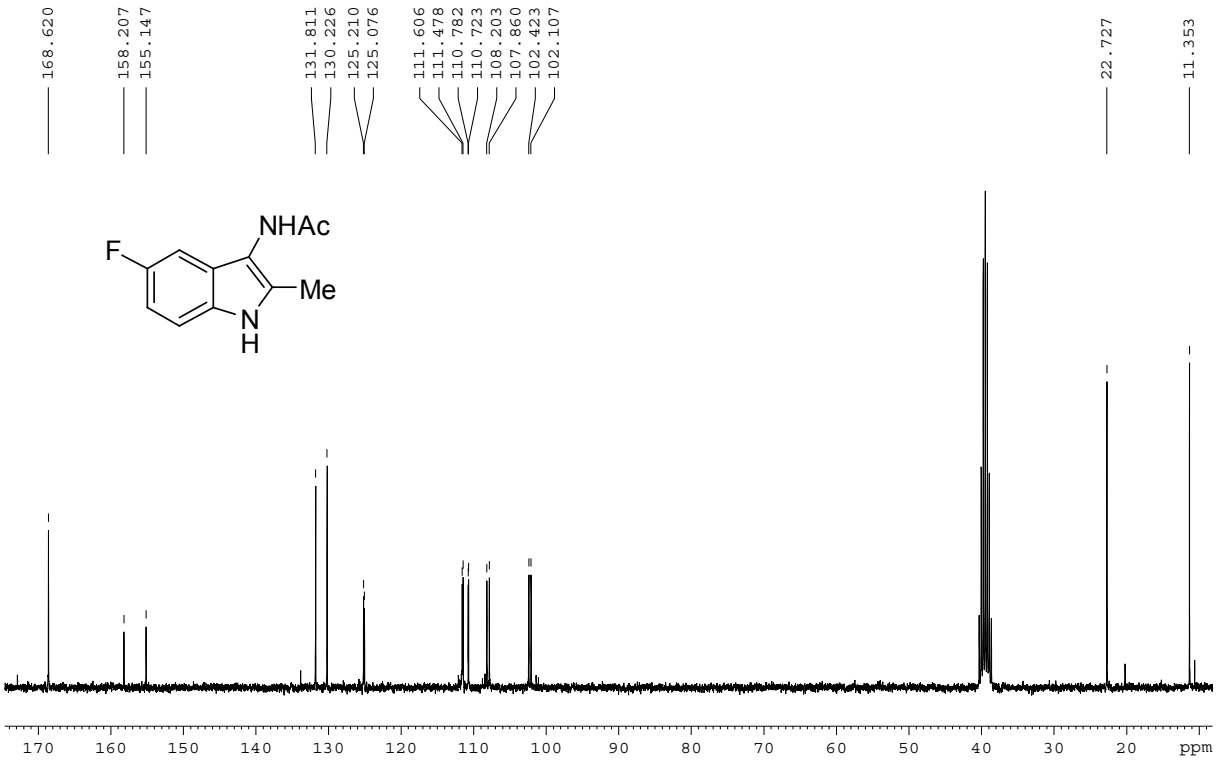


N-(5-Fluoro-2-methyl-1*H*-indol-3-yl)acetamide (4)

^{1}H NMR

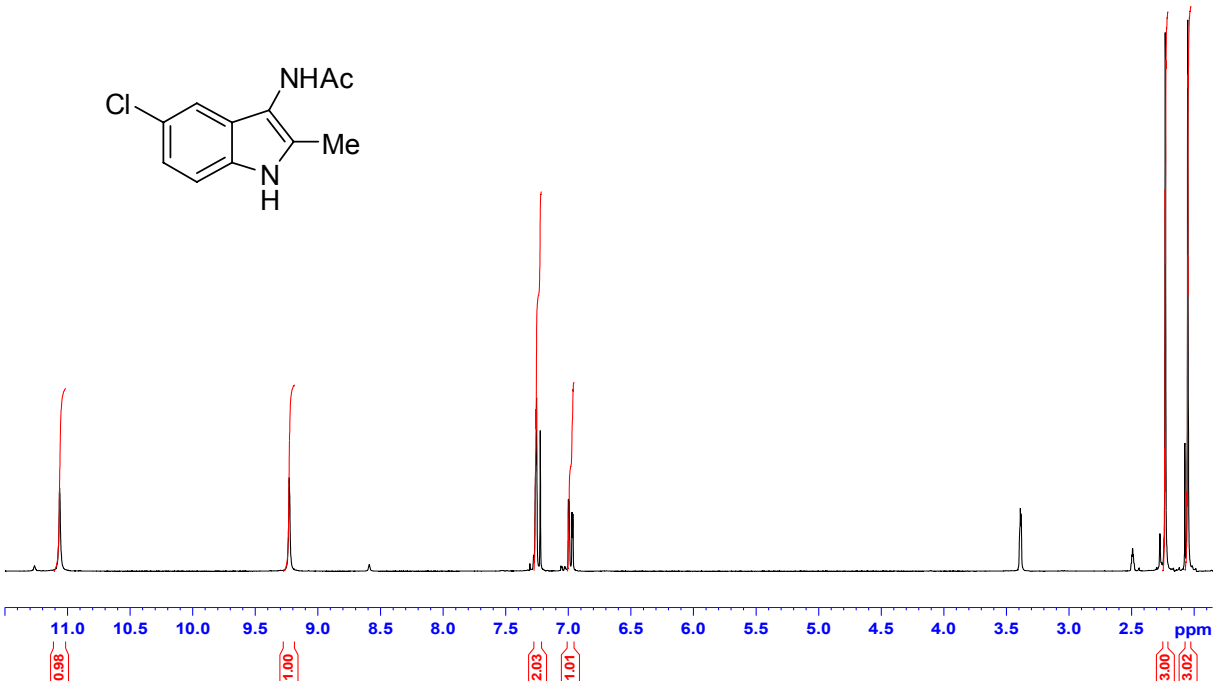


^{13}C NMR

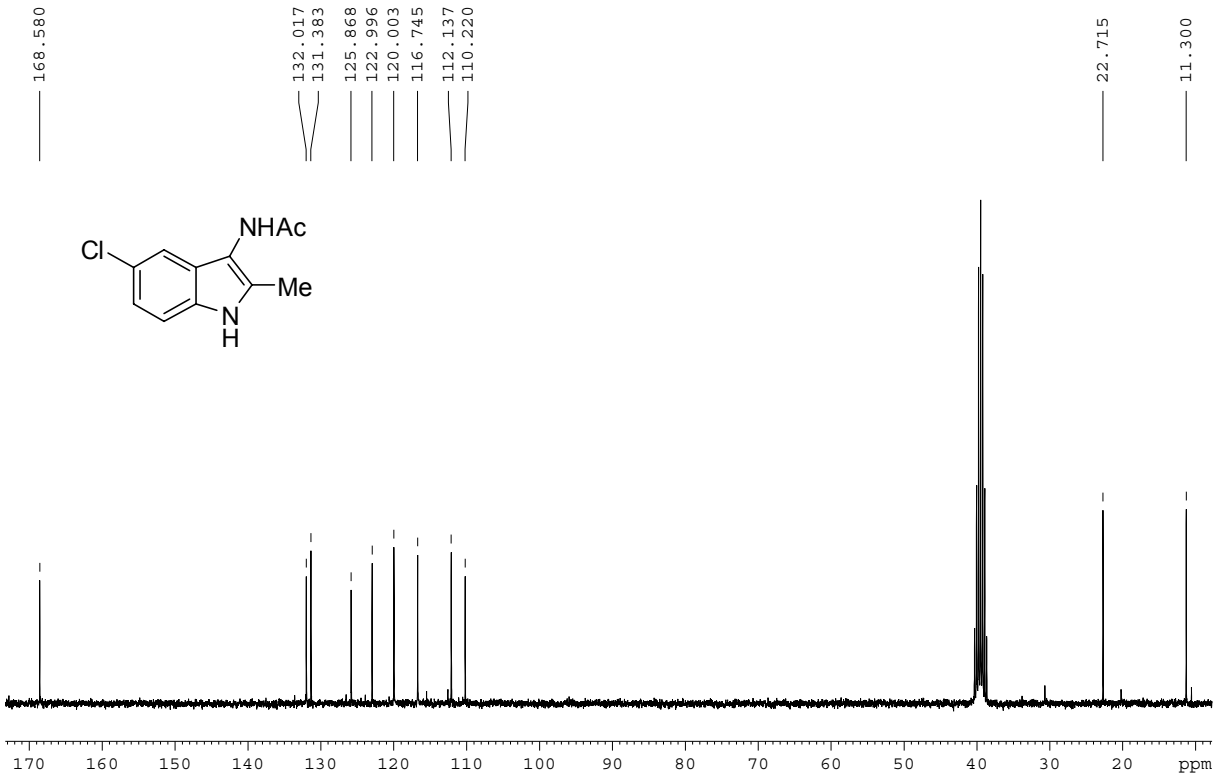


***N*-(5-Chloro-2-methyl-1*H*-indol-3-yl)acetamide (5)**

^{1}H NMR

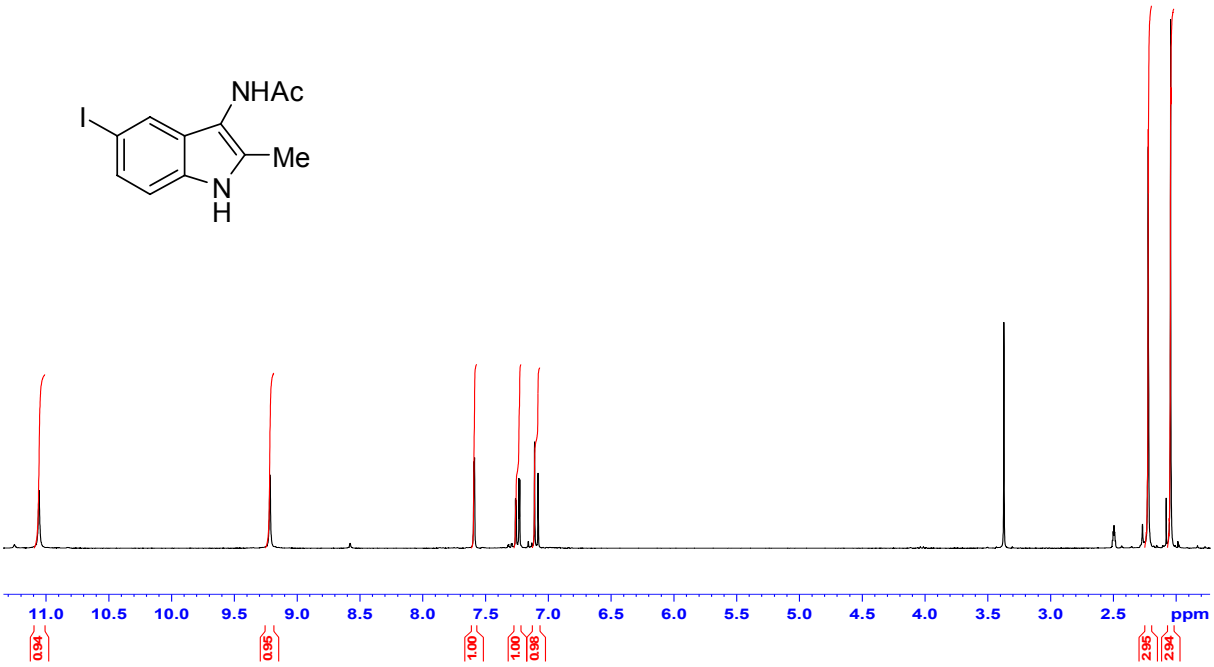


^{13}C NMR

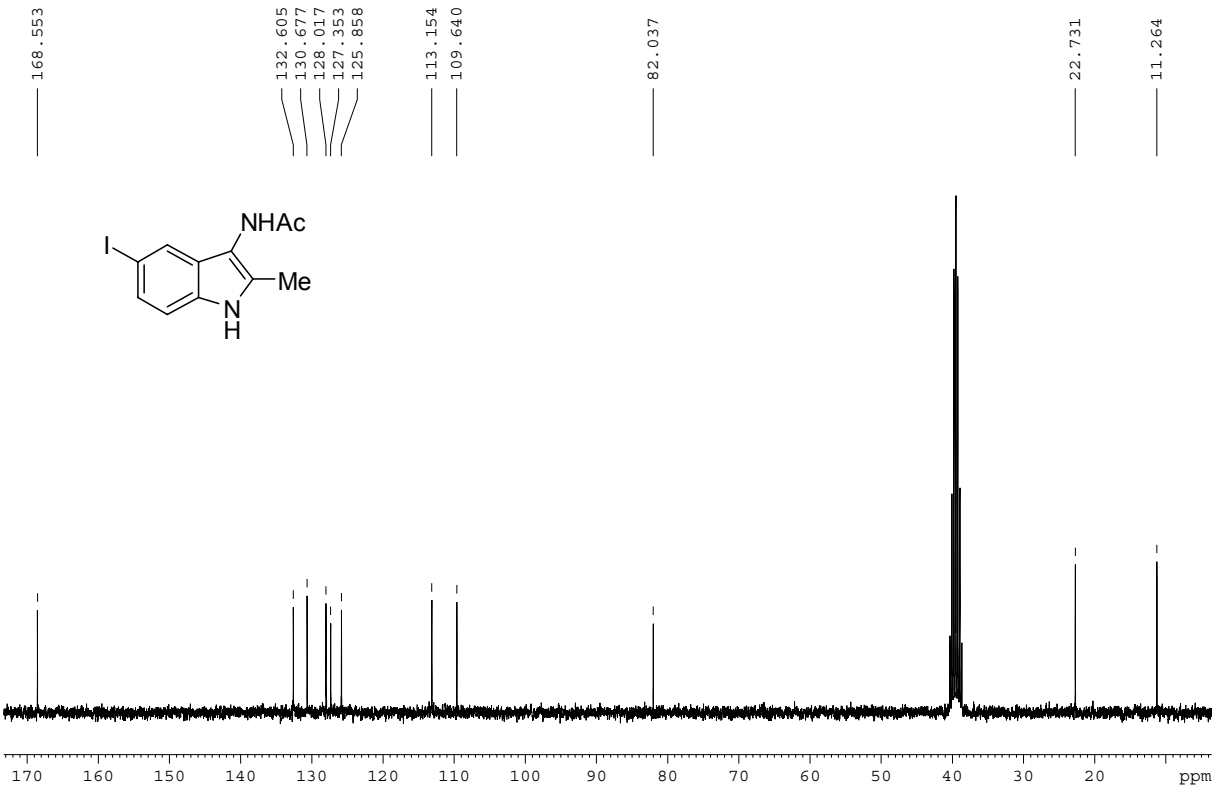


***N*-(5-Iodo-2-methyl-1*H*-indol-3-yl)acetamide (6)**

^{1}H NMR

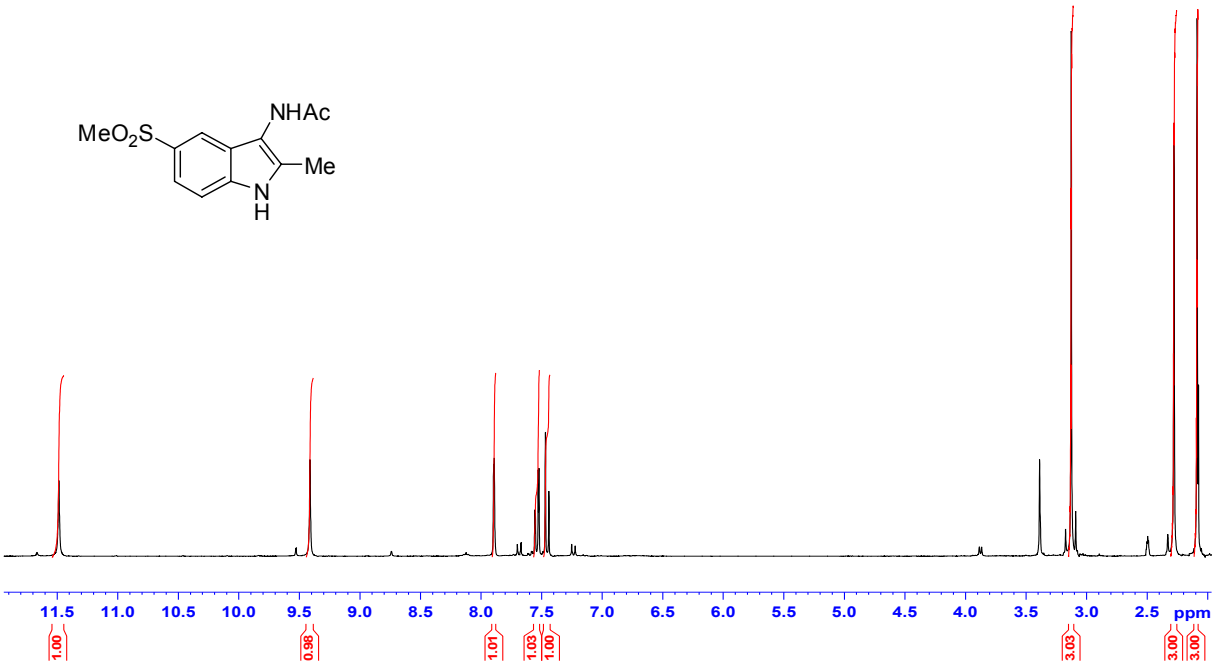


^{13}C NMR

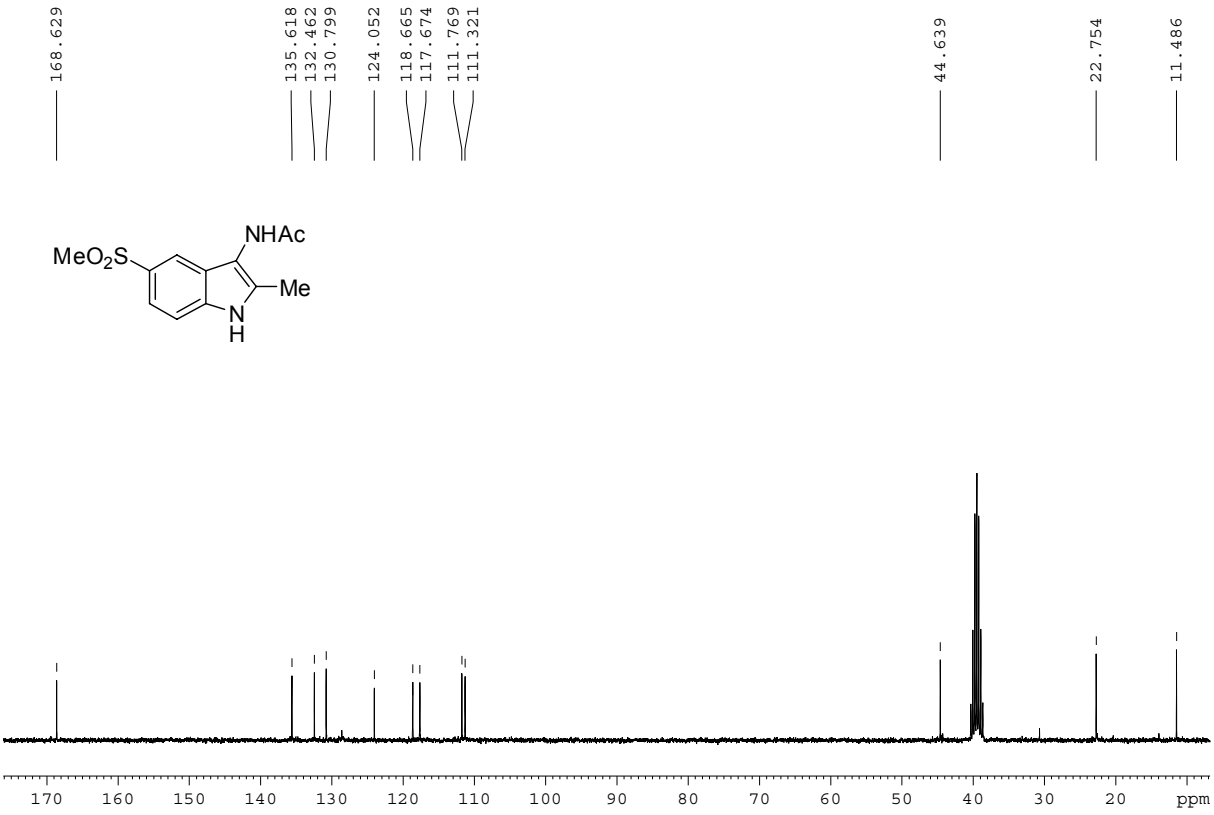


N-(2-Methyl-5-(methylsulfonyl)-1*H*-indol-3-yl)acetamide (7)

^{1}H NMR

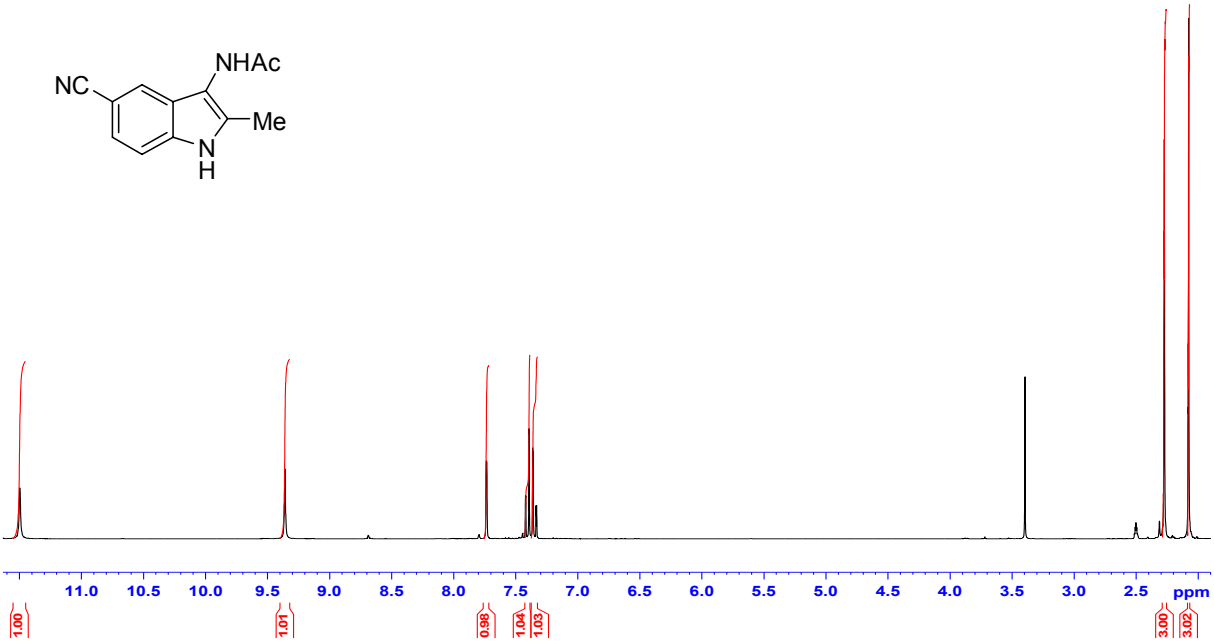


^{13}C NMR

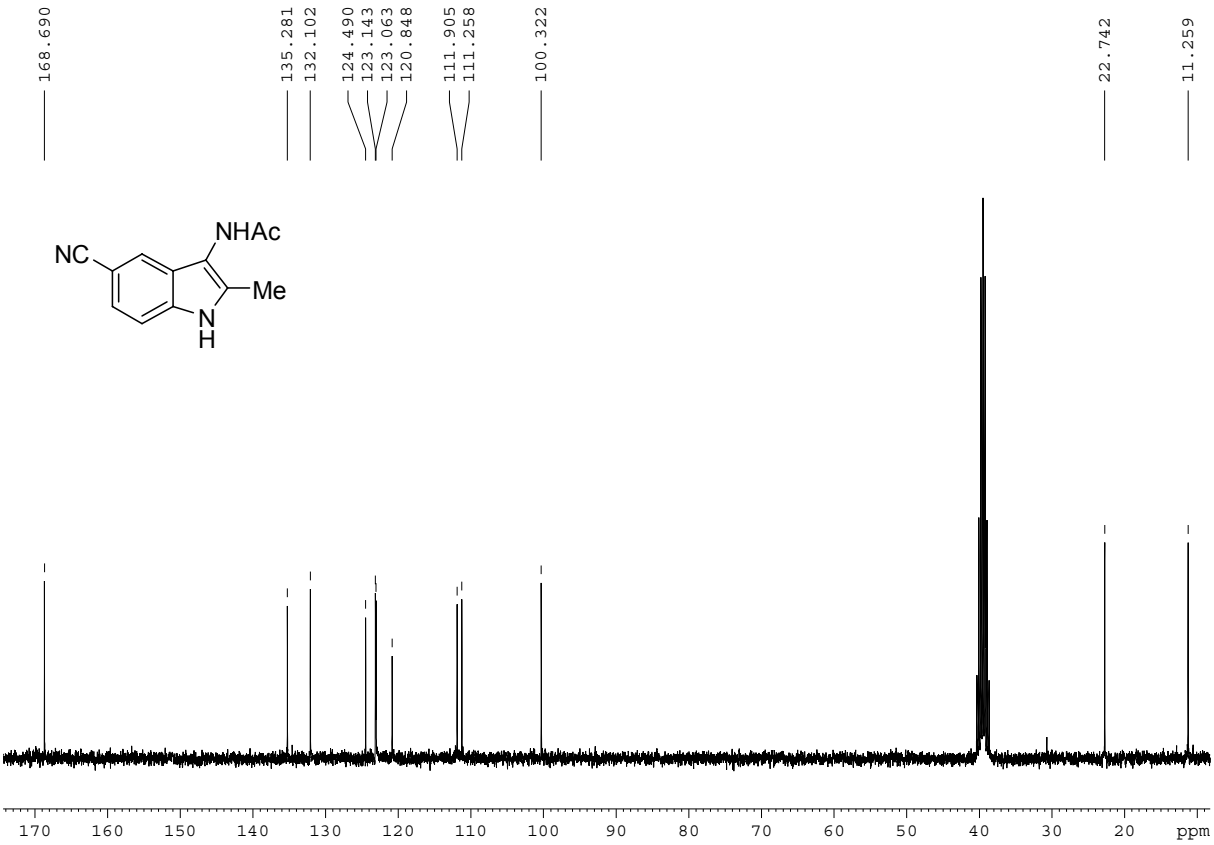


N-(5-Cyano-2-methyl-1*H*-indol-3-yl)acetamide (8)

^{1}H NMR

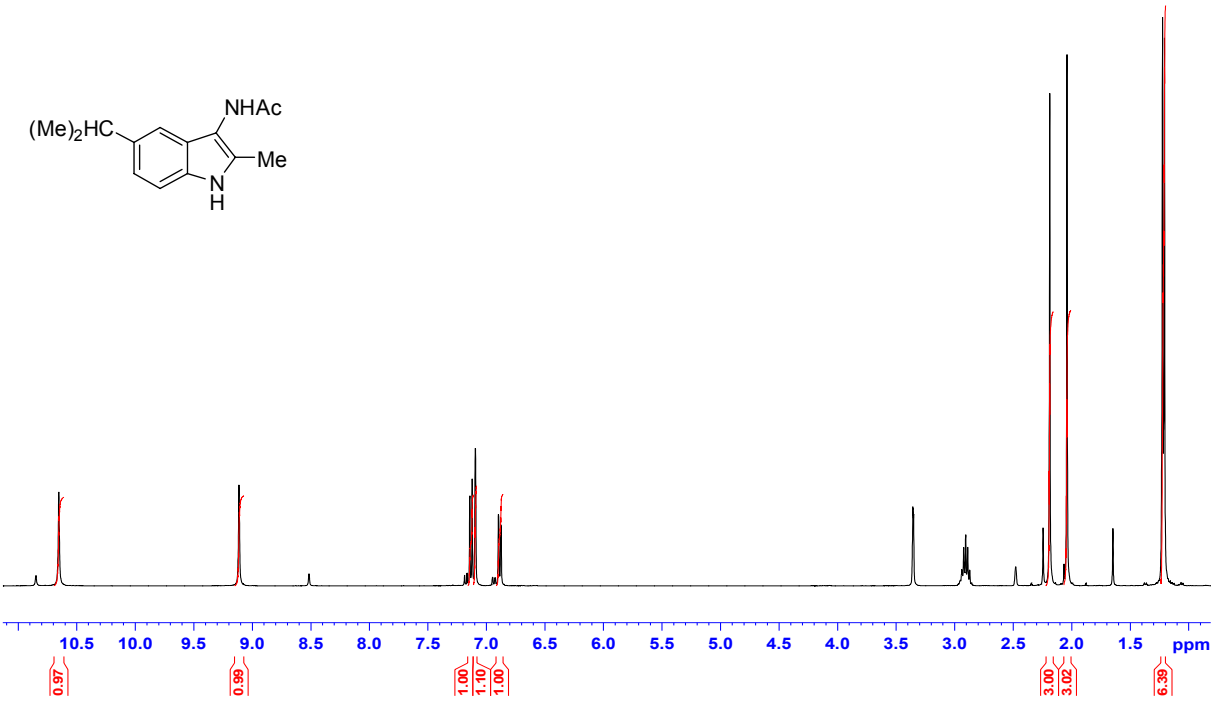


^{13}C NMR

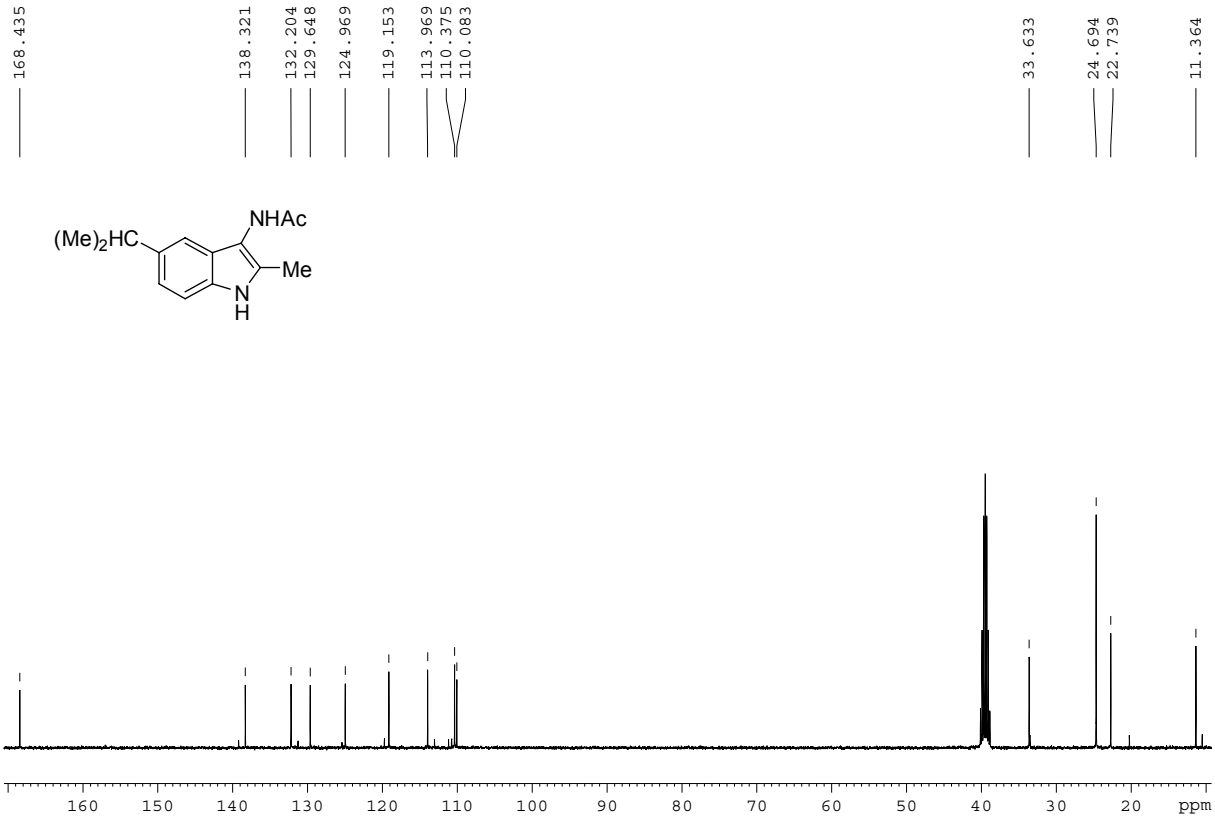


N-(5-Isopropyl-2-methyl-1*H*-indol-3-yl)acetamide (9)

^{1}H NMR

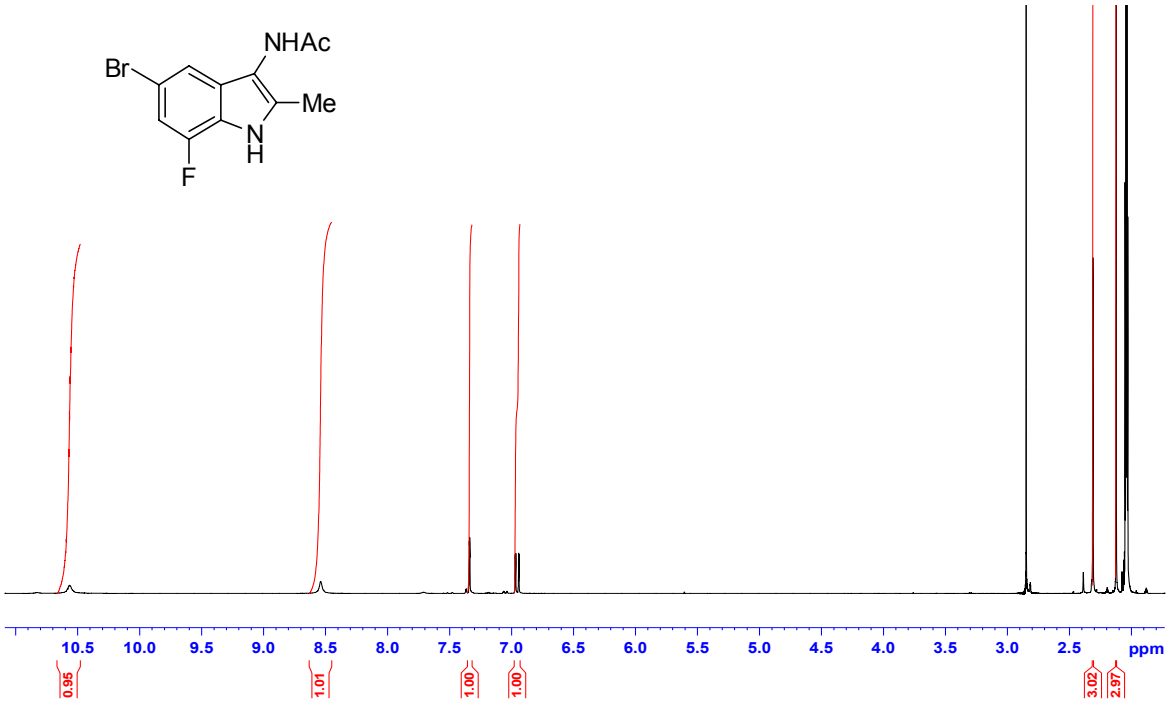


^{13}C NMR

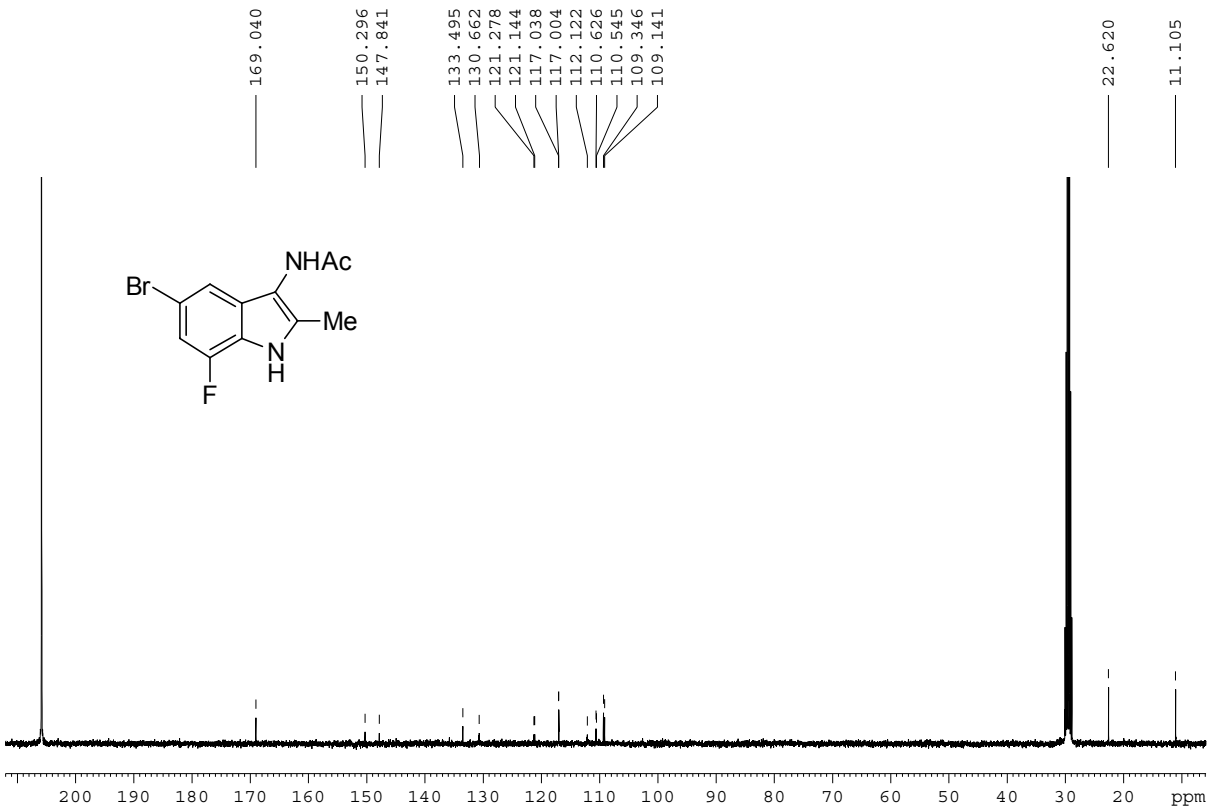


N-(5-Bromo-7-fluoro-2-methyl-1*H*-indol-3-yl)acetamide (10)

^{1}H NMR

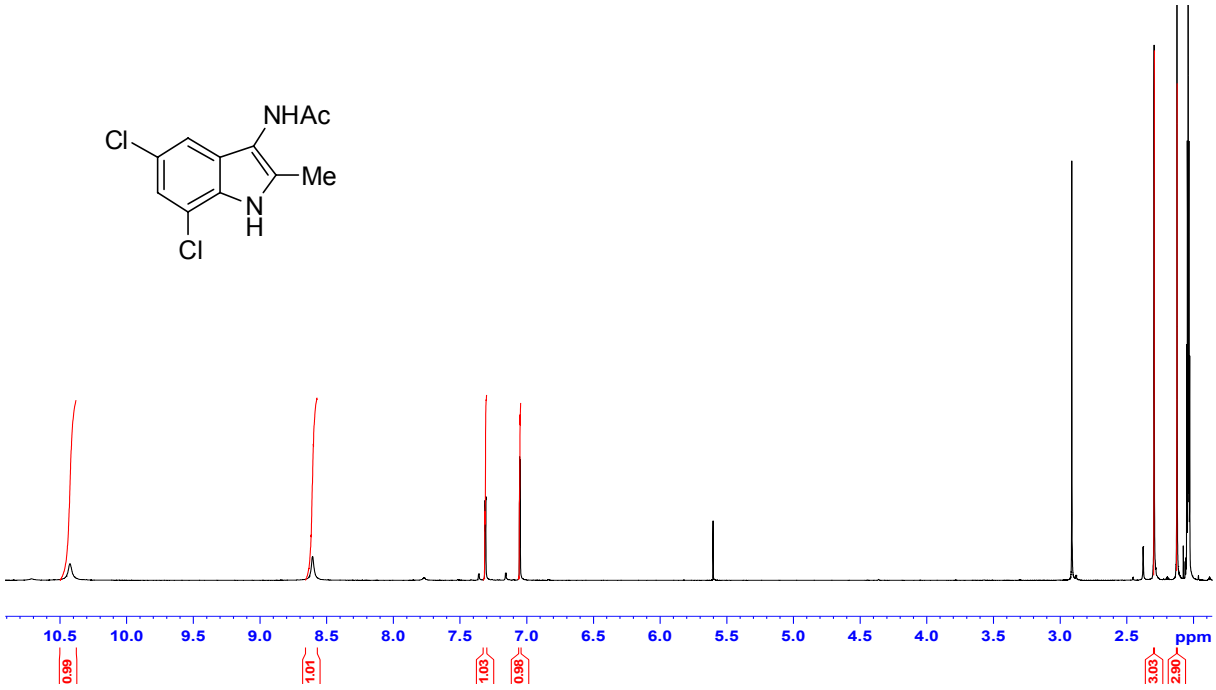


^{13}C NMR

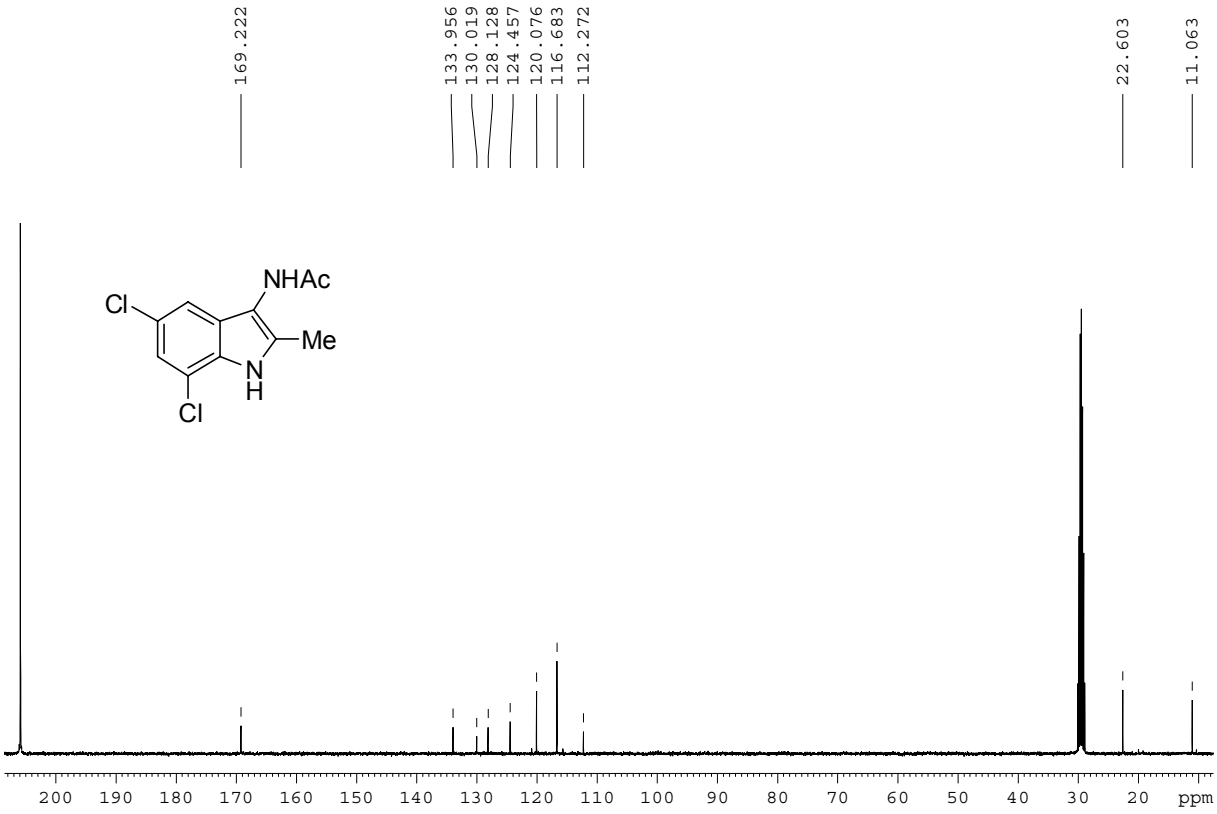


N-(5,7-Dichloro-2-methyl-1*H*-indol-3-yl)acetamide (11)

^{1}H NMR

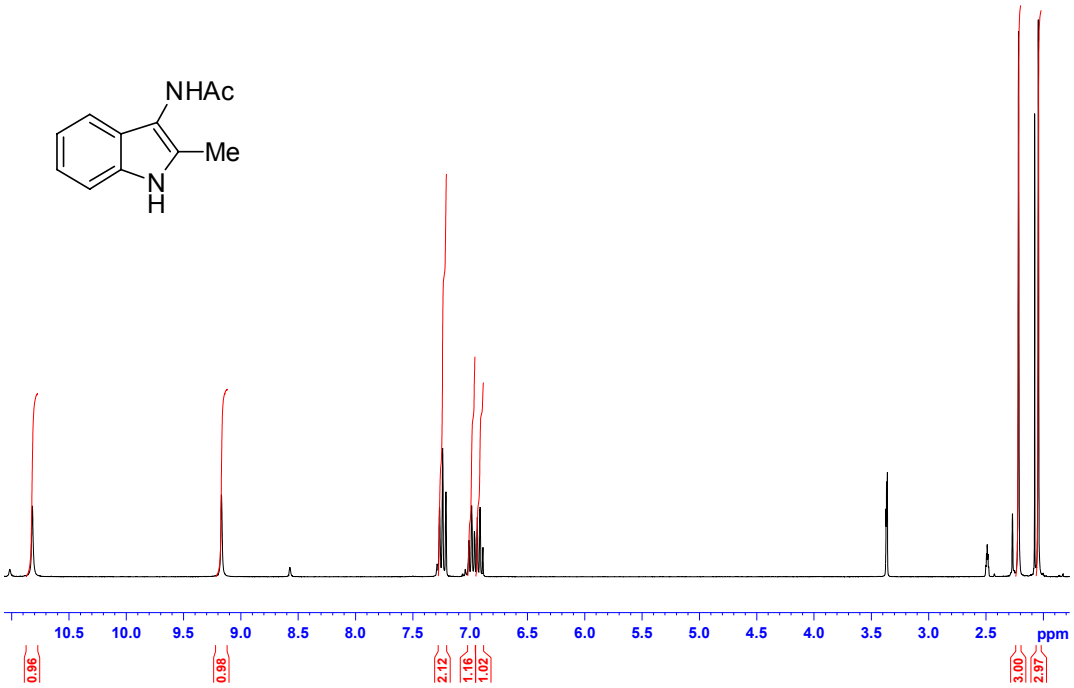


^{13}C NMR

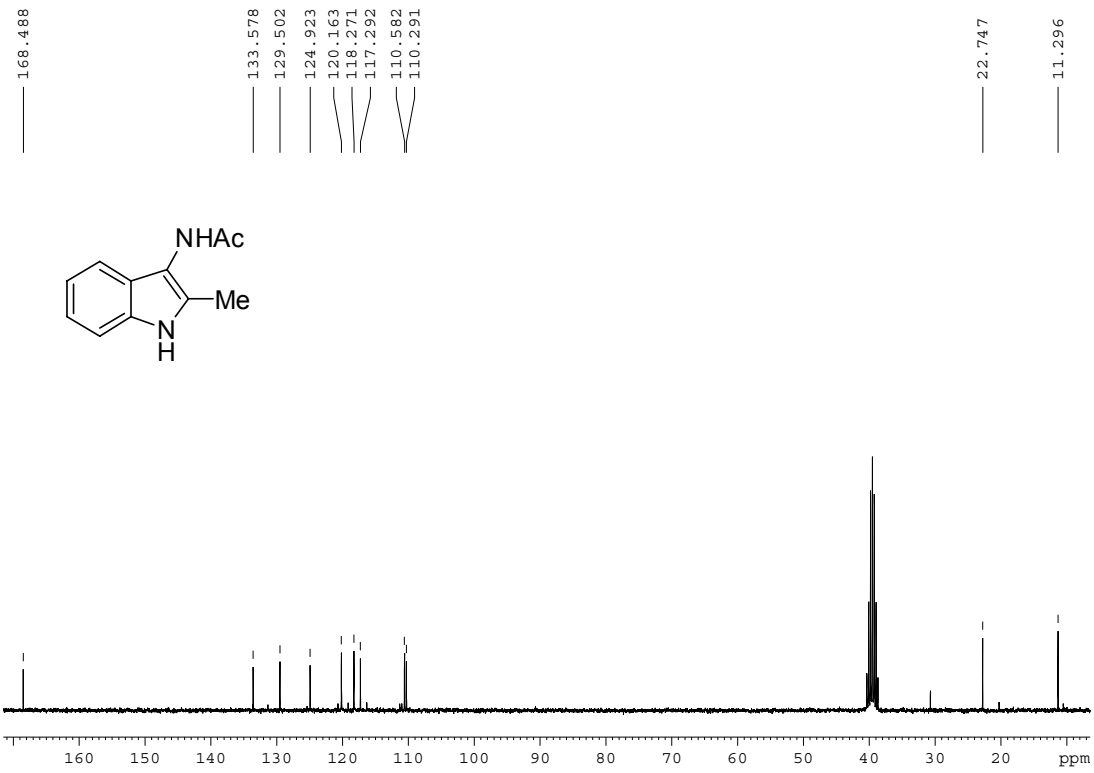


***N*-(2-Methyl-1*H*-indol-3-yl)acetamide (12)**

^{1}H NMR

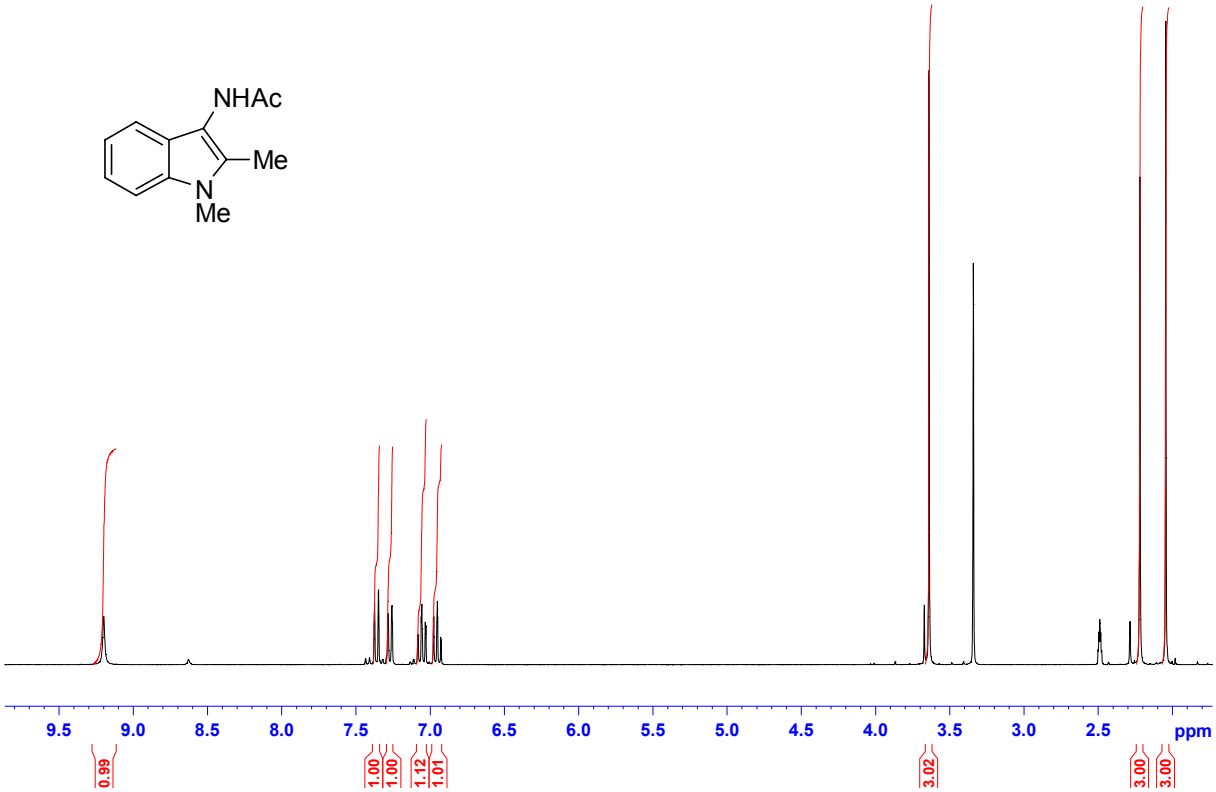


^{13}C NMR

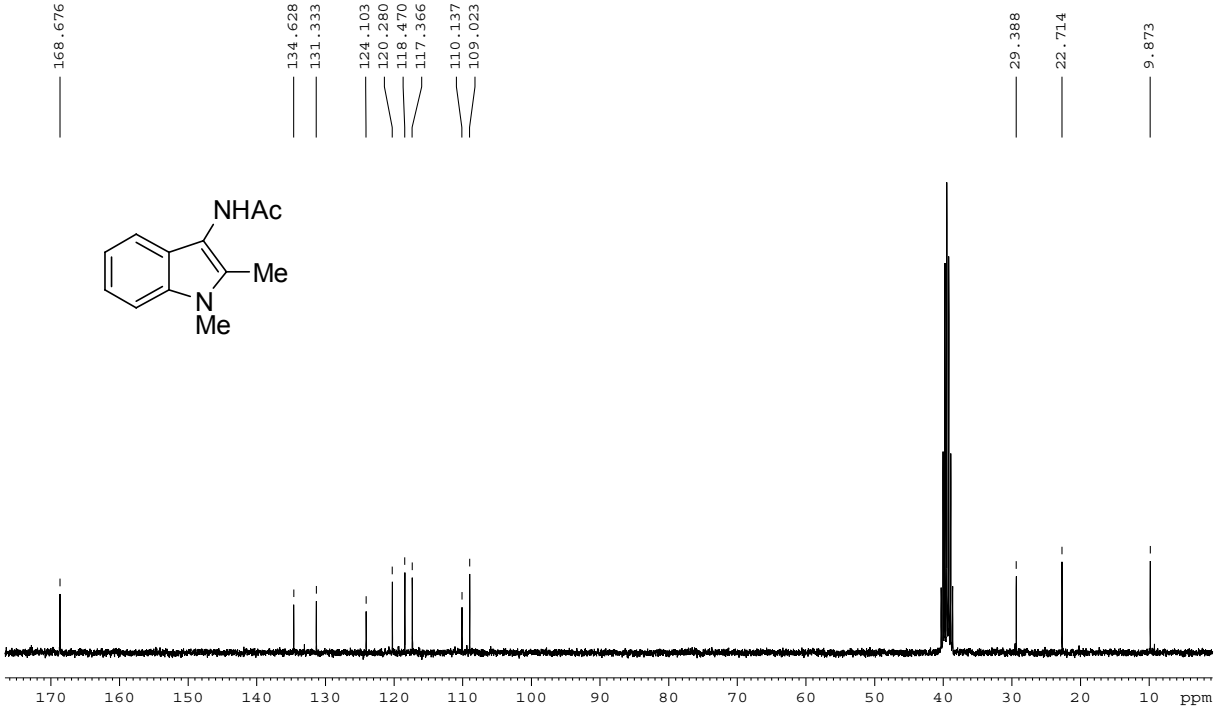


***N*-(1,2-Dimethyl-1*H*-indol-3-yl)acetamide (13)**

^{1}H NMR

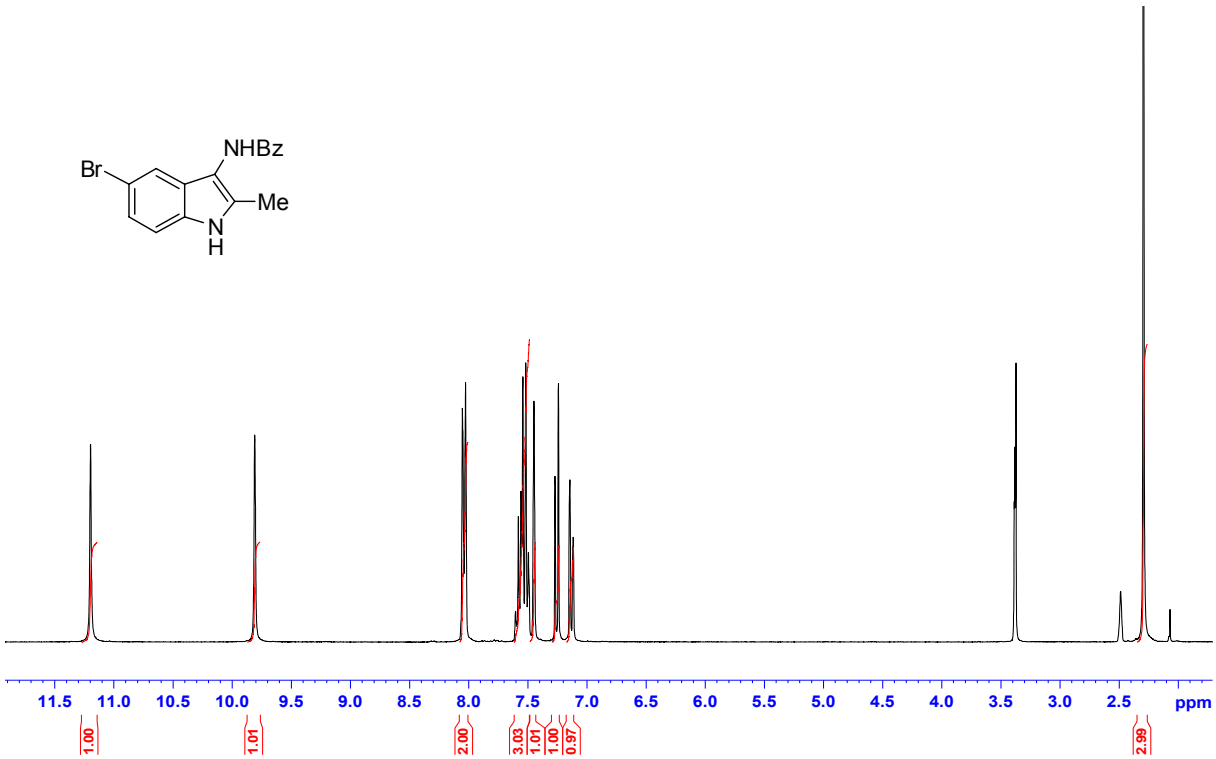


^{13}C NMR

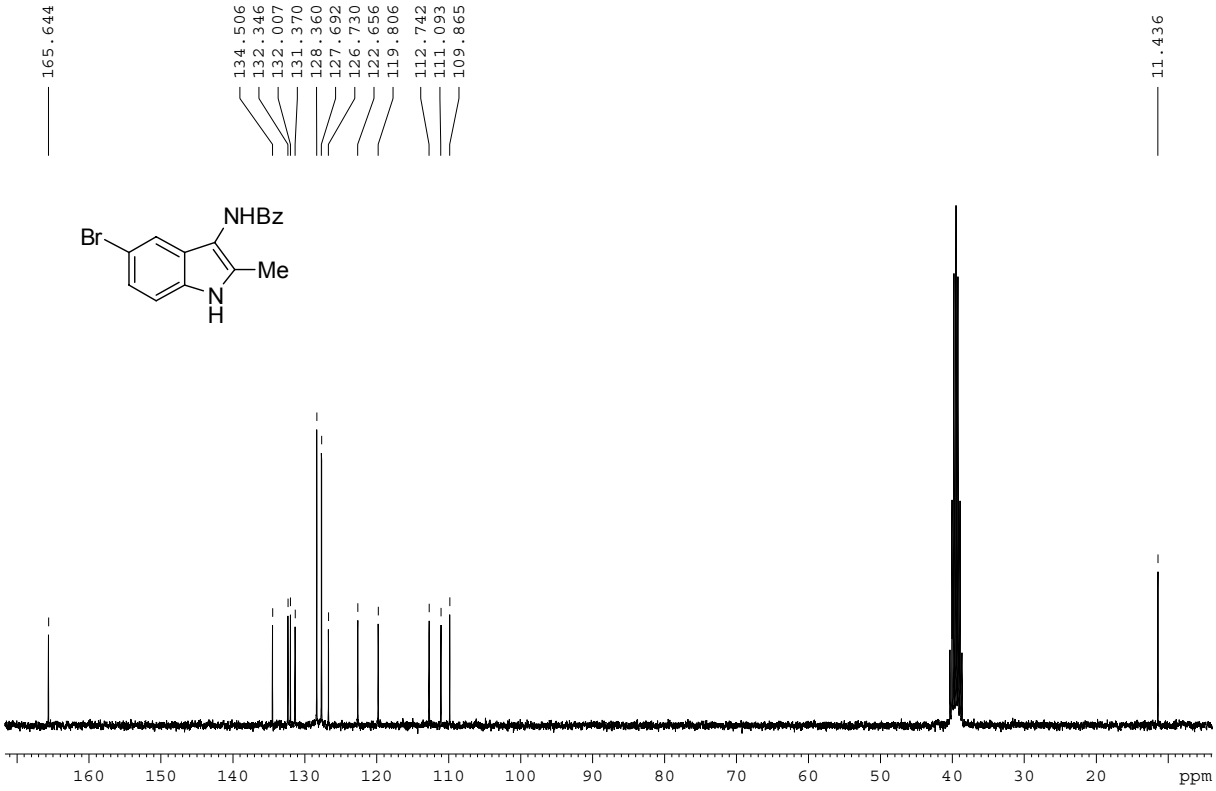


***N*-(5-Bromo-2-methyl-1*H*-indol-3-yl)benzamide (14)**

^{1}H NMR

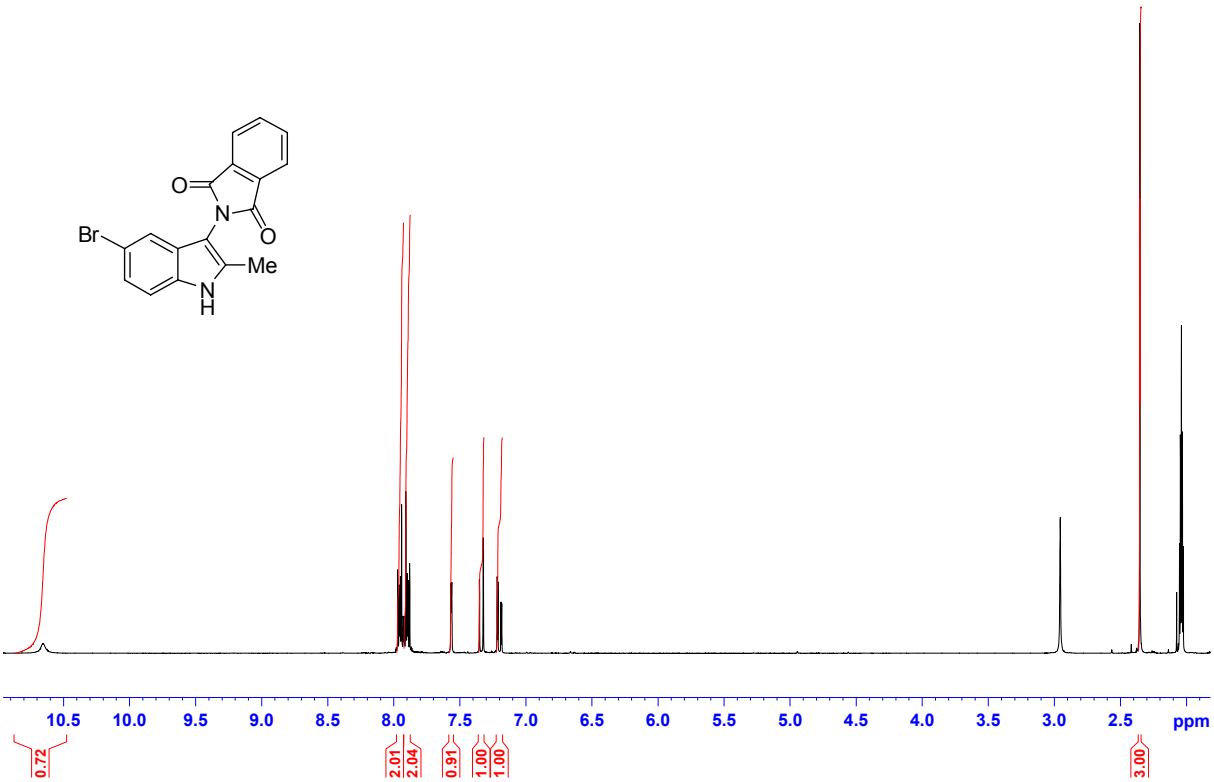


^{13}C NMR

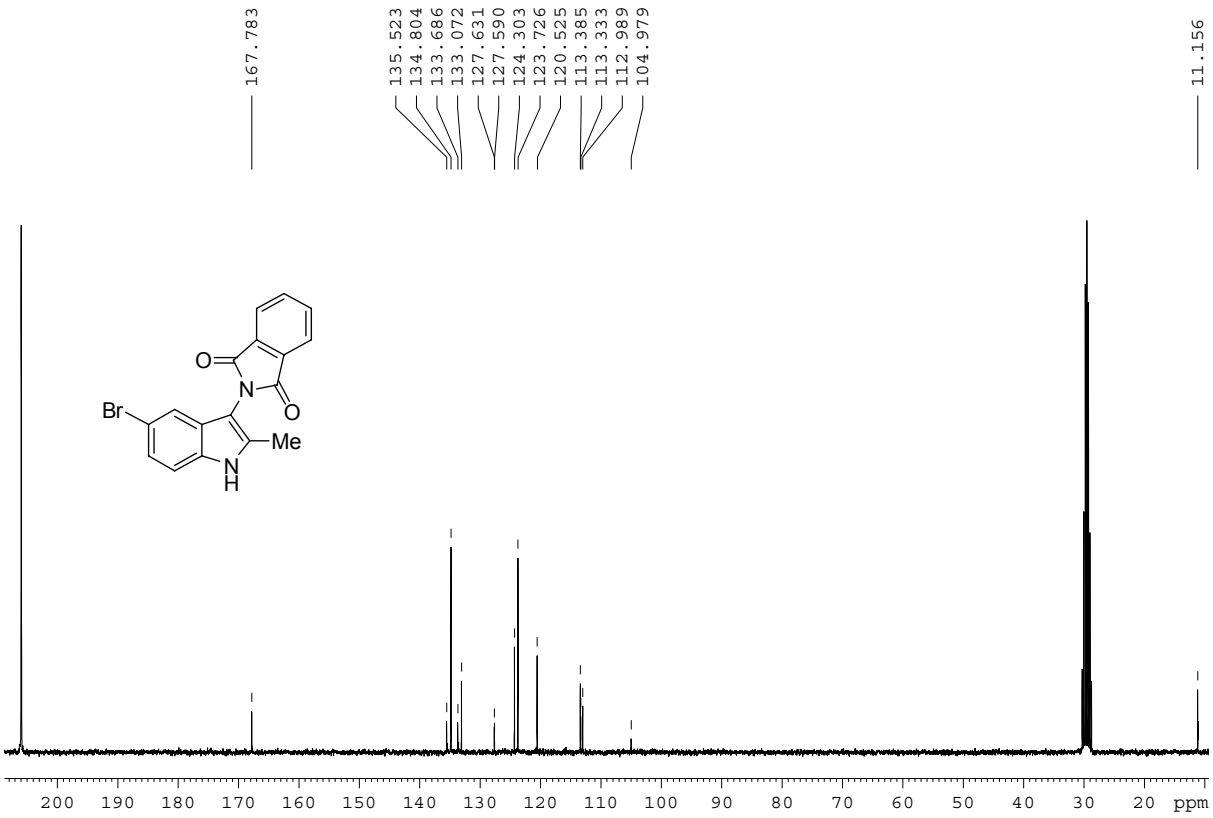


2-(5-Bromo-2-methyl-1*H*-indol-3-yl)isoindoline-1,3-dione (15)

^{1}H NMR

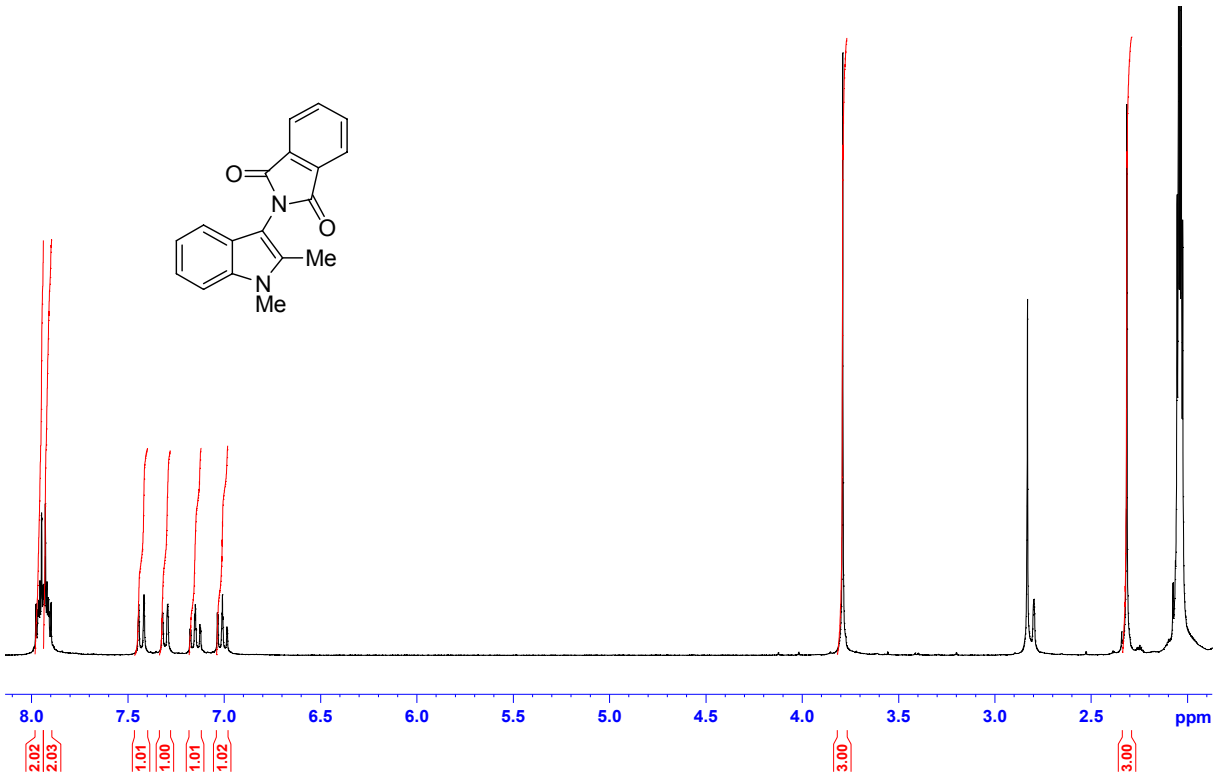


^{13}C NMR

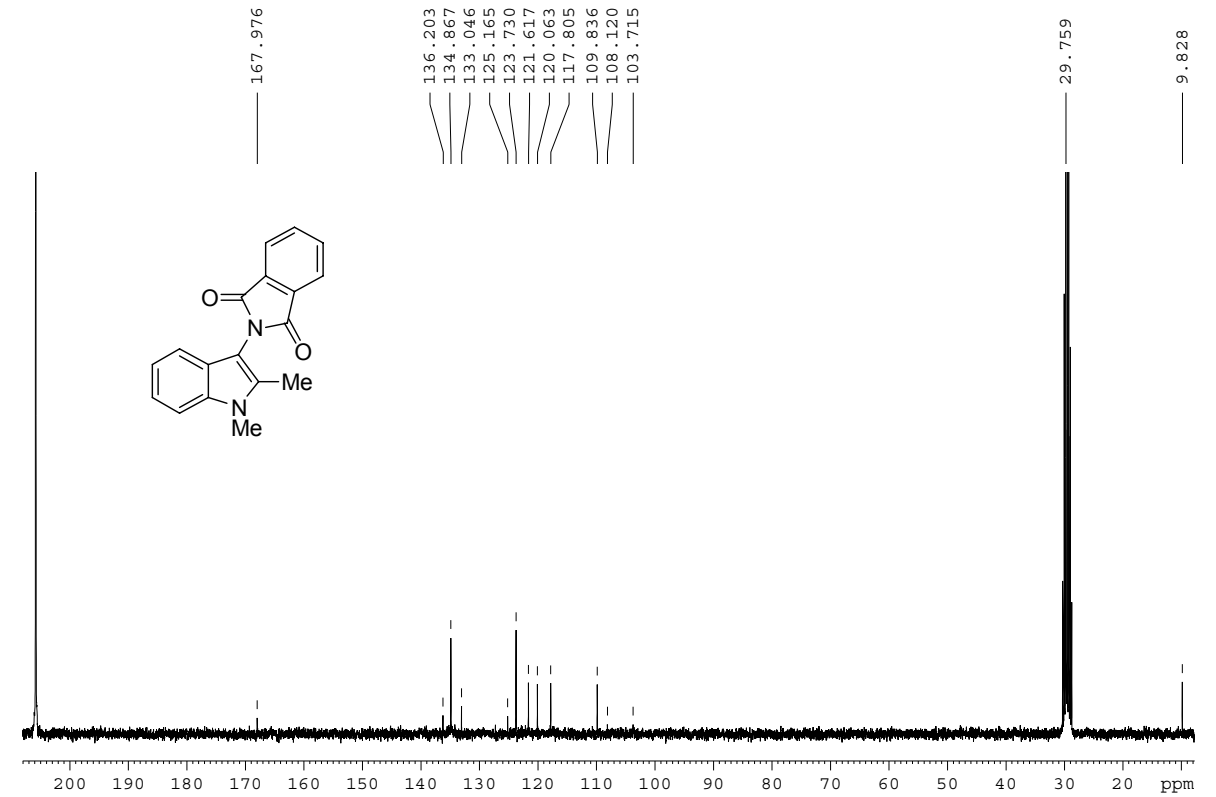


2-(1,2-Dimethyl-1*H*-indol-3-yl)isoindoline-1,3-dione (16a)

^{1}H NMR

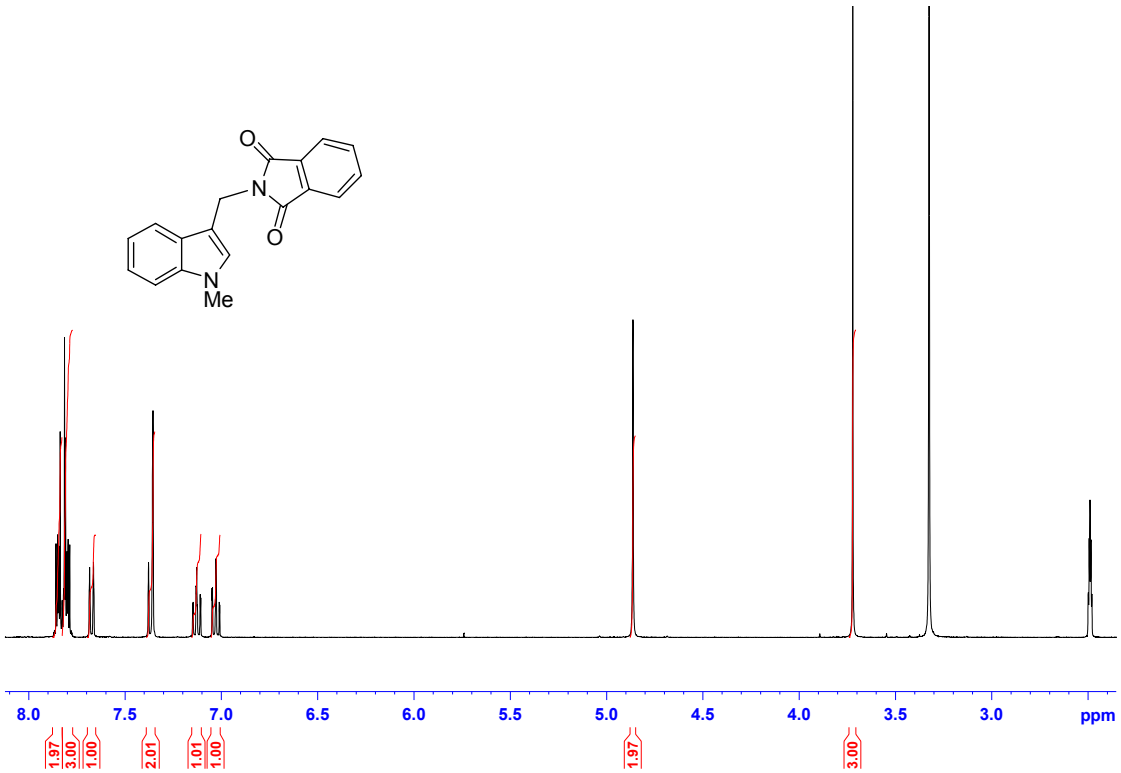


^{13}C NMR

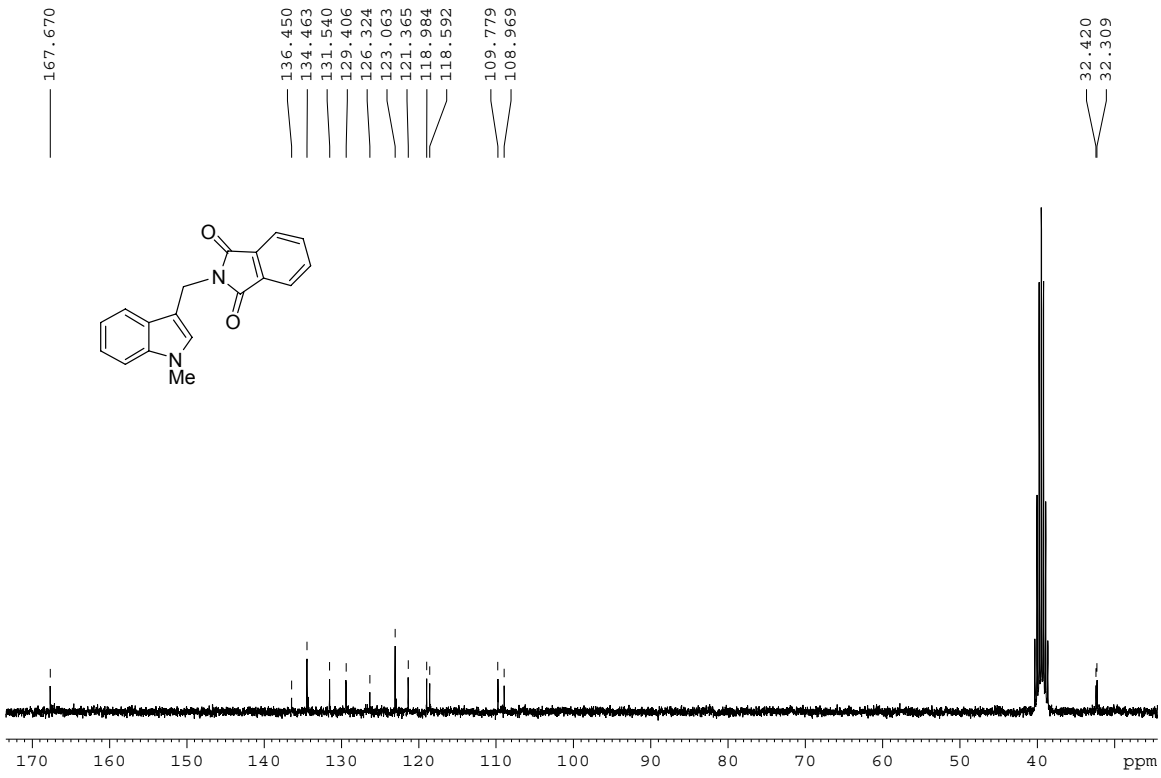


2-((1-Methyl-1*H*-indol-3-yl)methyl)isoindoline-1,3-dione (16b)

^{1}H NMR

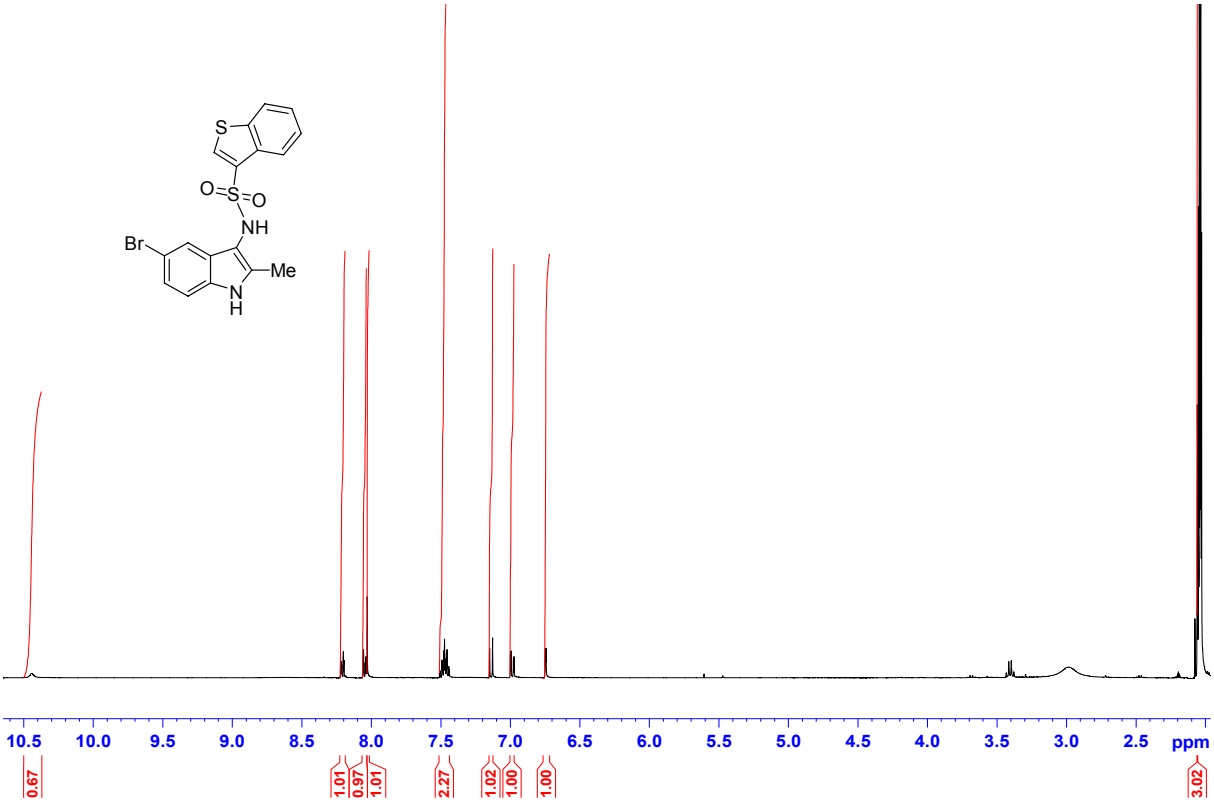


^{13}C NMR

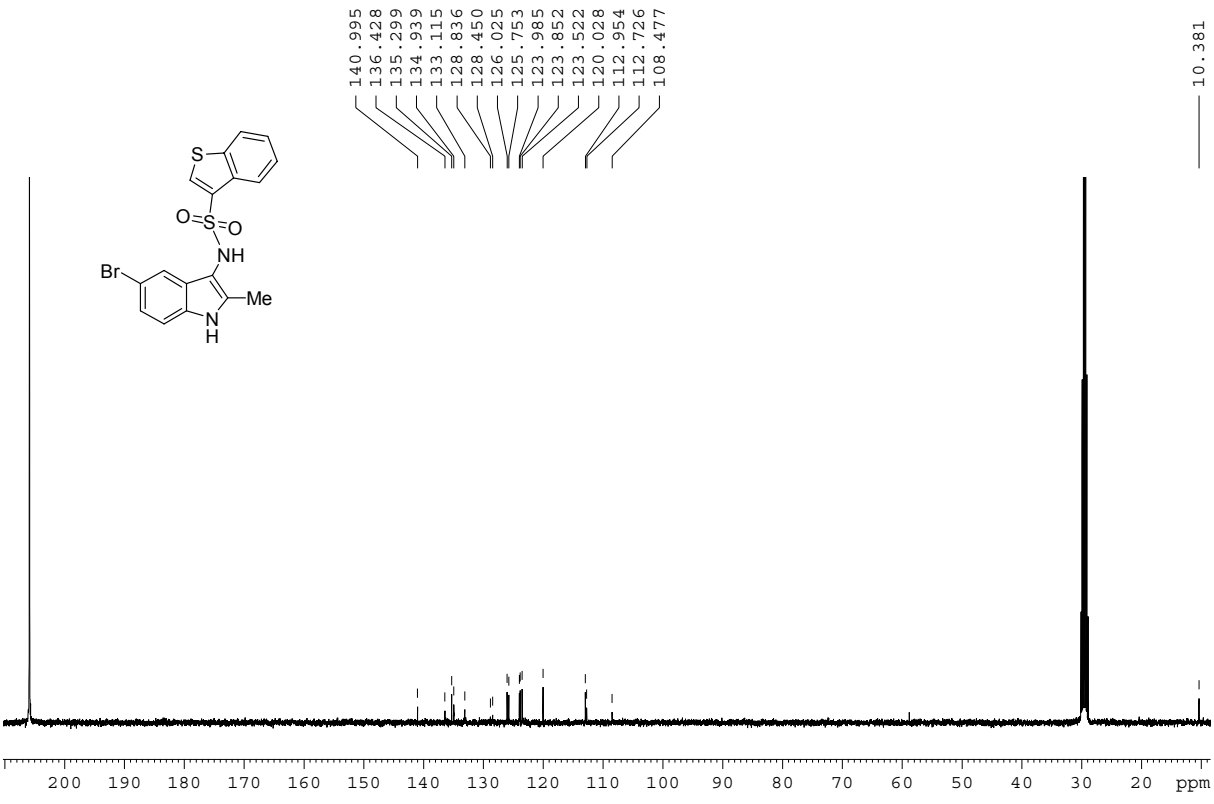


***N*-(5-Bromo-2-methyl-1*H*-indol-3-yl)benzo[b]thiophene-3-sulfonamide (17)**

^{1}H NMR

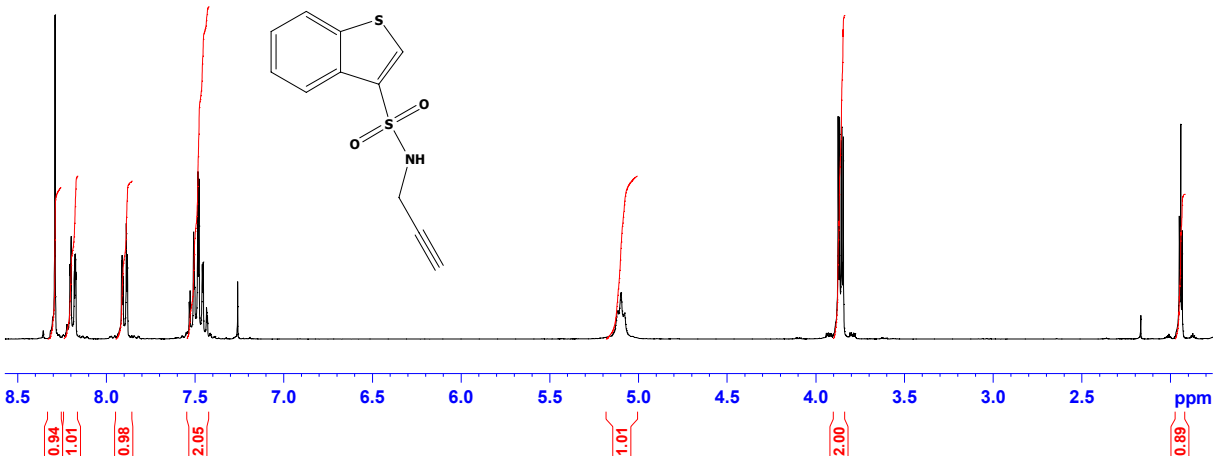


^{13}C NMR



N-(Prop-2-ynyl)benzo[b]thiophene-3-sulfonamide (2d)

^{1}H NMR



^{13}C NMR